The identification and characterization of breast cancer associated lipid(s) found in hair

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2014

Submitted in partial fulfillment of the requirements for the degree of
Doctor of Philosophy in Advanced Medicine

Table of contents

1. Introduction 29

1.1. The extent of the breast cancer problem 1

1.1.1. Incidence by age 1

1.2. Normal breast structure 1

1.3. Development of the disease 4

1.3.1. Theories on the pathogenesis of breast cancer 5

1.3.2. Staging and survival rates 6

1.4. Detection and diagnosis 6

1.4.1. Current recommended screening 6

1.4.1.1. Mammography 7

1.4.1.2. Ultrasound 8

1.4.1.3. Magnetic Resonance Imaging (MRI) 8

1.5. Assessment of current gold standard, mammography: 8

1.6. The importance of early detection 11

1.7. A better screening test is necessary 12

1.8. Biomarkers for breast cancer 13

1.8.1. Proteins 13

1.8.2. MicroRNA (miRNA) 14

1.8.3. Lipids 15

1.9. Alternative diagnostic technologies 19

1.9.1. Saliva 19

1.9.2. Breath 20

1.9.3. Urine 21

1.9.4. Hair 21

1.10. Hair: Composition and structure 22

1.11. X-ray diffraction of hair 24

1.11.1. Rings and X-ray diffraction patterns 25

1.12. Hair testing as a screening tool for breast cancer 26

1.12.1. Association between breast cancer and the X-ray diffraction pattern of hairs 26

1.13. Clinical Studies on the breast cancer and the X-ray diffraction of hair 27

1.13.1. Corino and French 27

1.13.2. Fer2k trial 28

1.13.3. Sensitivity of mammography when combined with a hair test 28

1.14. Molecular mechanism underlying the altered X-ray diffraction pattern of hair in patients with breast cancer 29

1.15. Evidence that the "ring" feature in XRD pattern of hair is lipid-based 31

1.16. Fundamentals of lipidomics 32

1.17. Hypothesis on how breast cancer-associated lipids are incorporated into hair 38

1.18. Implications 38

1.19. Aims 38

2. Preliminary data 39

2.1. Introduction 40

2.2. Aims 42

2.3. Methods 42

2.3.1. X-ray diffraction of hair 42

2.3.1.1. Samples 42

2.3.1.2. Synchrotron X-ray diffraction 42

2.3.1.3. Image analysis 43

2.3.1.4. Addition of fatty acids to hair 43

2.3.1.5. Chemical enhancement of lipids in hairs and solvent extraction of hairs 44

2.3.2. Lipid profiling of hair 44

2.3.2.1. Samples 44

2.3.2.2. Extraction of lipid from hair 45

2.3.2.3. Liquid Chromatography Mass Spectrometry (LCMS) analysis of hair 45

2.3.2.4. Data processing for all LCMS data 46

2.3.1. Lipid nomenclature 46

2.4. Results 47

2.4.1. Addition of fatty acids to hair 47

2.4.2. Chemical enhancement of lipids in hairs and solvent extraction of hairs 48

2.4.3. Extraction of lipid from hair 49

2.5. Discussion 51

3. Lipid extraction from cell culture supernatant 55

3.1. Introduction 56

3.2. Aims 57

3.3. Methods 58

3.3.1. Lipid profiling of cell culture 58

3.3.1.1. Samples 58

3.3.1.2. Cell culture 58
3.3.1.3. Extraction of lipid from cell culture 59
3.3.1.4. Liquid Chromatography Mass Spectrometry (LCMS) analysis of cell culture supernatant 59
3.3.1.5. Data processing for all LCMS data 60
3.3.1. Lipid nomenclature 60
3.4. Results 61
3.5. Discussion 68

4. Lipid extraction from hair fibre 71
4.1. Introduction 72
4.2. Aims 72
4.3. Methods 73
4.3.1. Lipid profiling of hair 73
4.3.1.1. Samples 73
4.3.1.2. Extraction of lipid from hair 73
4.3.1.3. Liquid Chromatography Mass Spectrometry analysis of hair samples 74
4.3.1.4. Data processing for all LCMS data 74
4.3.2. Lipid nomenclature 76
4.4. Results 77
4.5. Discussion 102

5. Lipid extraction from serum 105
5.1. Introduction 106
5.2. Aims 106
5.3. Methods 107
5.3.1. Lipid profiling of serum samples 107
5.3.1.1. Samples 107
5.3.1.2. Extraction of lipid from serum 107
5.3.1.3. Preparation of pooled biological quality control (PBQC) samples 108
5.3.1.4. Liquid Chromatography Mass Spectrometry (LCMS) analysis of serum 108
5.3.1.5. Data processing for all LCMS data 108
5.3.2. Lipid nomenclature 108
5.4. Results 109
5.5. Discussion 142

6. Conclusion 145

7. Reference 163

8. Appendix.....187

8.1. From Chapter 2.....188

8.2. From chapter 3.....193

8.2.1. Raw peak area data.....194

8.2.2. Normalised peak area data.....196

8.3. From Chapter 4.....198

8.3.1. Raw peak area data.....198

8.3.2. Normalised to the mean data matrix.....212

8.3.3. Heteroscadascity plots for hair samples.....225

8.3.4. Two sided t-test.....227

8.3.1. Weight of hair samples.....232

8.3.1. Principle component analysis for hair samples including pooled biological quality controls 233

8.3.2. Lipids from along the hair fibre.....234

8.3.3. Optimization of the method of extraction of lipids from hair.....235

8.4. From Chapter 5.....239

8.4.1. Raw peak area data.....239

8.4.1. Normalised to the mean data matrix.....275

8.4.2. Heteroscadascity plots for serum samples.....315

8.4.3. Two sided t-test.....317

8.4.4. Principle component analysis for serum samples including pooled biological quality controls 325

8.5. From Chapter 4 and 5.....326

8.5.1. Clinical data.....326

8.6. From all chapters.....333

8.6.1. LCMS technical data (ion scans and chromatograms of standards).....333

8.7. Ethics approval letter.....339

Table of figures and tables

Figure 1.1: Schematic diagram of the human female breast (adapted/modified from (Hindle, 1999, Pandya, 2011). 3

Table 1.1: Theories on the pathogenesis of breast cancer 5

Table 1.2: The categories into which breast cancers are staged and the respective five-year survival rate (American Cancer Society, 2013). 6

Figure 1.2: schematic representation of a phospholipid specie structure, adapted from (Kelly, 2011). .16

Table 1.3: Common phospholipids and their structure, where X is the headgroup of the phospholipid as represented in figure xxx (Kelly, 2011). 17

Figure 1.3: The structure of other membrane phospholipid species (Merrill, 2008, Liscum, 2008).....17

Figure 1.4: schematic representation of lipid orgnaisation on the cellular membrane,adapted from (Alberts, 2002). 18

Figure 1.5: Schematic diagram of the structure of human scalp hair (adapted/ modified from (Villa, 2013, Wei, 2006). Keratin is a coiled alpha helix polypeptide chain (Tilstone, 2006). A single hair is composed of three alpha helices twisted together to form a protofibril. Protofibrils are packed around each other to form a highly organised structure called microfibril/ intermediate filament. Microfibrils embedded in a high sulfur protein matrix become a macrofibril, which makes up a cortical cell set in an extracellular matrix of the cortex of the hair fibre. 23

Figure 1.6: X-ray diffraction patterns of human scalp hair from (Trounova, 2002) (A, B); Sample 1275, Advanced Photon Source, Chicago (own image) (C). 30

Figure 1.7: X-ray diffraction pattern of human scalp hair from Bertrand *et al*'s 2003 paper (Bertrand, 2003). 31

Figure 1.8: Approaches to metabolomics (adapted from (Loizides-Mangold, 2013)). 34

Figure 1.9: schematic representation of mass spectrometer, adapted from Ashcroft, 2014 (Ashcroft, 2014). 35

Figure 1.10: Schematic diagram of a triple quadrupole mass spectrometer with multiple analysers adapted from Ashcroft, 2014 (Ashcroft, 2014). 36

Figure 2.1: XRD patterns of hair from a healthy woman (left) and from a woman with breast cancer (right). The arrow indicates the altered feature in the breast cancer patient's hair, referred to as the "ring". These patterns were taken on the SAXS beamline at the Australian Synchrotron. This pattern is consistent with those reported by Corino *et al* in 2009, who demonstrated that the feature was present in greater than 60% of patients with breast cancer (Corino, 2009). 40

Figure 2.3: Addition of fatty acids to hair (n=6). In the first experiment, hair that did not have a " "ring" " (confirmed by XRD) (before) was soaked in olive oil for 10 minutes, wiped dry, and then re-exposed to X-rays. A clear "breast cancer-like ring" was seen post-oil application (after, arrow indicates breast cancer-associated feature). 47

Figure 2.4: Solvent extraction of hairs. Hairs from breast cancer patients, with XRD alterations (left), were treated with chloroform/methanol, a solvent solution known to extract lipids. The intensity

of the "ring" was diminished (right) and the other (keratin-associated) features in the patterns were not affected. Arrow indicates location of the breast cancer-associated feature. 48
Figure 2.5: Lead nitrate treatment of hair. When hairs, which produce the "ring" in XRD, were soaked in lead nitrate solution, the intensity of the rings was enhanced and reflected in another circular feature around the original one. Lead nitrate has been shown to bind to lipids in hair and reflect the diffraction pattern (Bertrand, 2003). Arrow indicates location of the breast cancer-associated feature. 49
Figure 2.6: Average concentration of specific phosphatidylcholine (PC) species in hair samples collected from patients with breast cancer and controls, where an asterix indicates significantly different levels of specific phospholipids (n=8). 50
Refer to Chapter 2: Methods, page 46. 60
Figure 3.3: Concentration of specific phosphatidylinositol (PI) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations. 61
Figure 3.4: Concentration of specific cholesterol ester (CE) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations. 62
Figure 3.5: Concentration of specific ceramide (Cer) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations. 62
Figure 3.6: Concentration of specific phosphatidylethanolamine (PE) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations. 63
Figure 3.7: Concentration of specific lyso-phosphatidylcholine (LPC) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations. 63
Figure 3.8: Concentration of specific sphingomyelin (SM) species in cell culture supernatant samples collected from tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations. 64
Figure 3.9: Concentration of specific lyso-phosphatidylglycerol (LPG) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations. 64
Figure 3.10: Concentration of specific phosphatidylglycerol (PG) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations. 65
Figure 3.11: Concentration of specific phosphatidylcholine (PC) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations. 66

Figure 3.12: Concentration of specific phosphatidylcholine (PC) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations. 67
Refer to Chapter 2: Methods, page 46. 76
Figure 4.3: Principle component analysis of all 40 hair samples for cholesterol ester where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20). 77
Figure 4.4: Principle component analysis of all 40 hair samples for ceramide where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20). 77
Figure 4.5: Principle component analysis of all 40 hair samples for phosphatidic acid where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20). 78
Figure 4.6: Principle component analysis of all 40 hair samples for phosphatidylcholine and lyso phosphatidylcholine where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20). 78
Figure 4.7: Principle component analysis of all 40 hair samples for phosphatidylethanolamine where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20). 79
Figure 4.8: Principle component analysis of all 40 hair samples for phosphatidylglycerol where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20). 79
Figure 4.9: Principle component analysis of all 40 hair samples for phosphatidylinositol where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20). 80
Figure 4.10: Principle component analysis of all 40 hair samples for sphingomyelin where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20). 80
Figure 4.11: Average of log transformed and normalised peak area of cholesterol ester in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. 81
Figure 4.12: Average of log transformed and normalised peak area of ceramide in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. 82
Figure 4.13: Average of log transformed and normalised peak area of phosphatidic acid in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. PA- 1 to 7 and 9 are unknown PA species, which require further studies to identify their structure. 83

Figure 4.14: Average of log transformed and normalised peak area of lyso phosphatidylcholine in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. 84
Figure 4.15: Average of log transformed and normalised peak area of phosphatidylcholine in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. 85
Figure 4.16: Average of log transformed and normalised peak area of phosphatidylcholine in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. 86
Figure 4.17: Average of log transformed and normalised peak area of phosphatidylcholine in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. 87
Figure 4.18: Average of log transformed and normalised peak area of phosphatidylethanolamine in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. 88
Figure 4.19: Average of log transformed and normalised peak area of phosphatidylglycerol in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. 89
Figure 4.20: Average of log transformed and normalised peak area of phosphatidylinositol in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. PI- 1 to 2 are unknown PI species, which require further studies to identify their structure. 90
Figure 4.21: Average of log transformed and normalised peak area of sphingomyelin in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. 91
Figure 4.22: Principle component analysis of all 20 patient serum samples for tumour size. S (purple) - less than 10cm; M (blue) - between 10cm and 29cm; L (red) - 30cm and greater ; U (green) – Unknown, N/A. No separation or trends can be seen between the patients (n=20). 93
Figure 4.23: Principle component analysis of all 20 patient serum samples for patient age. 0 (blue) - patient under 50 years old ; 1 (green) - patient over 50 and under 60 years old ; 2 (purple) - patient over 60 and under 70 years old ; 3 (red) - patient over 70 years old. No separation or trends can be seen between the patients (n=20). 94
Figure 4.24: Principle component analysis of all 20 patient serum samples for tumour grade. PG1 (green) - grade 1; PG2 (red) - grade 2; PG3 (purple) - grade 3; PGNA (blue) - N/A. No separation or trends can be seen between the patients (n=20). 95
Figure 4.25: Principle component analysis of all 20 patient serum samples for tumour type. PDC (green) - ductal carcinoma in situ (localised); PO (blue) - other type of breast cancer ; PID (red) - invasive ductal carcinoma. No separation or trends can be seen between the patients (n=20). 96
Figure 4.26: Principle component analysis of all 20 patient serum samples for hair length of participants. CS (red)- control, short hair, CL (blue)-control, long hair, PS (purple)- patient,

short hair, PL (green)- patient, long hair, PNA (yellow)- N/A. Short hair was considered 8cm long or less and long hair was considered greater than 8cm long. No separation or trends can be seen between the patients (n=20). 97
Figure 4.27, A-H : Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. LPC 18:1, B. PI 38:4, C. PC Cer 18:0/ 24:1, D. SM 34:1, E. CE 18:2, F. PG 32:0, G. PC 38:5, H. PE 38:1. Figures A-F are examples of ideal, clean peaks and Figures G-H are examples of noisy, unclear peaks. 98
Figure 4.27, A-H : Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. LPC 18:1, B. PI 38:4, C. PC Cer 18:0/ 24:1, D. SM 34:1, E. CE 18:2, F. PG 32:0, G. PC 38:5, H. PE 38:1. Figures A-F are examples of ideal, clean peaks and Figures G-H are examples of noisy, unclear peaks. 99
Figure 4.27, A-H : Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. LPC 18:1, B. PI 38:4, C. PC Cer 18:0/ 24:1, D. SM 34:1, E. CE 18:2, F. PG 32:0, G. PC 38:5, H. PE 38:1. Figures A-F are examples of ideal, clean peaks and Figures G-H are examples of noisy, unclear peaks. 100
Figure 4.27, A-H : Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. LPC 18:1, B. PI 38:4, C. PC Cer 18:0/ 24:1, D. SM 34:1, E. CE 18:2, F. PG 32:0, G. PC 38:5, H. PE 38:1. Figures A-F are examples of ideal, clean peaks and Figures G-H are examples of noisy, unclear peaks. 101
Figure 4.28: Protocol used to extract lipids from hair for the initial 40 samples. This method proved to be difficult with uneven homogenization of hair samples and burst vials.....102
Table 4.1: List of variables, which were compared to optimise the method of extraction of lipids from hair. 103
Figure 4.29: optimised protocol used to extract lipids from hair for the final 40 samples. This method allowed even homogenization of hair samples and did not cause the vials to burst.....103
Refer to Chapter 2: Methods, page 46. 108
Figure 5.3: Principle component analysis of all 80 serum samples for cholesterol ester where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40). 109
Figure 5.4: Principle component analysis of all 80 serum samples for ceramide where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40). 110
Figure 5.5: Principle component analysis of all 80 serum samples for phosphatidic acid and lyso-phosphatidic acid where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40).....110

Figure 5.6: Principle component analysis of all 80 serum samples for phosphatidylcholine and lyso-phosphatidylcholine where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40). 111
Figure 5.7: Principle component analysis of all 80 serum samples for phosphatidylethanolamine and lyso- phosphatidylethanolamine where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40). ... 111
Figure 5.8: Principle component analysis of all 80 serum samples for phosphatidylglycerol and lyso-phosphatidylglycerol where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40). 112
Figure 5.9: Principle component analysis of all 80 serum samples for phosphatidylinositol where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40). 112
Figure 5.10: Principle component analysis of all 80 serum samples for phosphatidylserine where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40). 113
Figure 5.11: Principle component analysis of all 80 serum samples for sphingomyelin where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40). 113
Figure 5.12: Average of log transformed and normalised peak area of cholesterol ester in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 115
Figure 5.13: Average of log transformed and normalised peak area of ceramide in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 116
Figure 5.14: Average of log transformed and normalised peak area of phosphatidic acid and lyso phosphatidic acid in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 117
Figure 5.15: Average of log transformed and normalised peak area of lyso phosphatidylcholine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 118
Figure 5.16: Average of log transformed and normalised peak area of phosphatidylcholine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 119
Figure 5.17: Average of log transformed and normalised peak area of phosphatidylcholine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 120
Figure 5.18: Average of log transformed and normalised peak area of phosphatidylcholine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 121

Figure 5.19: Average of log transformed and normalised peak area of phosphatidylethanolamine and lyso phosphatidylethanolamine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 122
Figure 5.20: Average of log transformed and normalised peak area of phosphatidylglycerol and lyso phosphatidylglycerol in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 123
Figure 5.21: Average of log transformed and normalised peak area of phosphatidylinositol in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 124
Figure 5.22: Average of log transformed and normalised peak area of phosphatidylserine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 125
Figure 5.23: Average of log transformed and normalised peak area of sphingomyelin in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation. 126
Figure 5.24: Principle component analysis of all 40 patient serum samples for tumour size. S (red)- less than 10cm; M (green)- between 10cm and 30cm; L (purple) - 30cm and greater ; U (blue) – Unknown, N/A. No separation or trends can be seen amongst the patients (n=40). 127
Figure 5.25: Principle component analysis of all 40 patient serum samples for patient age. 0 (purple) - patient under 50 years old ; 1 (green) - patient over 50 and under 60 years old ; 2 (blue) - patient over 60 and under 70 years old ; 3 (red) - patient over 70 years old. No separation or trends can be seen amongst the patients (n=40). 128
Figure 5.26: Principle component analysis of all 40 patient serum samples for tumour grade. PG1 (green) - grade 1; PG2 (purple) - grade 2; PG3 (blue) - grade 3; PGNA (red) - N/A. No separation or trends can be seen amongst the patients (n=40).....129
Figure 5.27: Principle component analysis of all 40 patient serum samples for tumour type. PDC (green) - ductal carcinoma in situ (localised); PO (red) - other type of breast cancer ; PID (blue) - invasive ductal carcinoma. No separation or trends can be seen amongst the patients (n=40). ..130
Figure 5.28, A-C: Normalised peak areas for each individual in this study were graphed for select phospholipids (A. PC 38:5, B. PE 38:4, C. PI 38:4) to determine if there were any differences that may have been skewed by averaging the groups. Controls (n=40) are seen in white and patients (n=40) are seen in black. 131
Figure 5.28, A-C: Normalised peak areas for each individual in this study were graphed for select phospholipids (A. PC 38:5, B. PE 38:4, C. PI 38:4) to determine if there were any differences that may have been skewed by averaging the groups. Controls (n=40) are seen in white and patients (n=40) are seen in black. 132
Figure 5.29, A-C: Raw peak areas for each individual in this study were graphed for select phospholipids (A. PC 38:5, B. PE 38:4, C. PI 38:4) to determine if there were any differences that may have been skewed by averaging the groups. Controls (n=40) are seen in white and patients (n=40) are seen in black. 133

Figure 5.29, A-C: Raw peak areas for each individual in this study were graphed for select phospholipids (A. PC 38:5, B. PE 38:4, C. PI 38:4) to determine if there were any differences that may have been skewed by averaging the groups. Controls (n=40) are seen in white and patients (n=40) are seen in black. 134
Figure 5.30, A-J: Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. PI 38:4, B. LPC 18:1, C. PC 38:5, D. SM 34:1, E. PG 20:0, F. PE 38:1, G. LPA 20:1, H. SM 34:2, I. CE 20:0, J. PS 34:0. Figures A-F are examples of ideal, clean peaks and Figures G-J are examples of noisy, unclear peaks. 135
Figure 5.30, A-J: Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. PI 38:4, B. LPC 18:1, C. PC 38:5, D. SM 34:1, E. PG 20:0, F. PE 38:1, G. LPA 20:1, H. SM 34:2, I. CE 20:0, J. PS 34:0. Figures A-F are examples of ideal, clean peaks and Figures G-J are examples of noisy, unclear peaks. 136
Figure 5.30, A-J: Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. PI 38:4, B. LPC 18:1, C. PC 38:5, D. SM 34:1, E. PG 20:0, F. PE 38:1, G. LPA 20:1, H. SM 34:2, I. CE 20:0, J. PS 34:0. Figures A-F are examples of ideal, clean peaks and Figures G-J are examples of noisy, unclear peaks. 137
Figure 5.30, A-J: Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. PI 38:4, B. LPC 18:1, C. PC 38:5, D. SM 34:1, E. PG 20:0, F. PE 38:1, G. LPA 20:1, H. SM 34:2, I. CE 20:0, J. PS 34:0. Figures A-F are examples of ideal, clean peaks and Figures G-J are examples of noisy, unclear peaks. 138
Figure 5.30, A-J: Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. PI 38:4, B. LPC 18:1, C. PC 38:5, D. SM 34:1, E. PG 20:0, F. PE 38:1, G. LPA 20:1, H. SM 34:2, I. CE 20:0, J. PS 34:0. Figures A-F are examples of ideal, clean peaks and Figures G-J are examples of noisy, unclear peaks. 139
Table 5.1: Significantly changing lipid species between breast cancer free control samples (n=40) and patients with breast cancer (n=40) using a two-sided t-test (t statistic shown). Those species with an adjusted p-value lower than 0.05 and a fold change great than 2 were considered significantly different (p-value shown) between the two groups (control and patient). 140
Figure 6.1: Schematic diagram of the hypothesis of this study. 146
a. X-ray of the breast (circle around tumour) (http://radiographics.rsna.org); 146

b. Blood vessels (http://www.telegraph.co.uk/health); 146
c. The hair follicle (http://www.spencerclinic.co.uk); 146
d. The hair fibre (http://animaldiversity.ummz.umich.edu); 146
e. X-ray diffraction pattern of a human scalp hair taken from a patient with breast cancer (own image). 146
Table 6.1: Phospholipid species, which were significantly elevated in the cell culture supernatant study (Chapter 3). 154
Table 8.1: All images showing solvent extraction (n=15). Arrow indicates approximate region where breast cancer-associated feature is typically located. 188
Table 8.2: All images showing lead nitrate treatment (n=15). Arrow indicates approximate region where breast cancer-associated feature is typically located.....190
Table 8.3: Concentration (nM/mg) of phosphatidylcholine lipids species extracted from hair. 192
Table 8.4: Basic data for cell lines used in the cell culture supernatant study 193
Table 8.5: Raw peak area matrix for the supernatant from a tumorigenic and non- tumorigenic cell line for all lipid species 194
Table 8.6: Raw peak area matrix for the supernatant from a tumorigenic and non- tumorigenic cell line for all lipid species 195
Table 8.7: Normalised peak area matrix for the supernatant from a tumorigenic and non- tumorigenic cell line for all lipid species.....196
Table 8.8: Normalised peak area matrix for the supernatant from a tumorigenic and non- tumorigenic cell line for all lipid species.....197
Table 8.9: Raw peak area data matrix for cholesterol ester for hair samples taken from breast cancer free controls.....198
Table 8.10: Raw peak area data matrix for cholesterol ester for hair samples taken from patients with breast cancer.....199
Table 8.11: Raw peak area data matrix for ceramide for hair samples taken from breast cancer free controls.....199
Table 8.12: Raw peak area data matrix for ceramide for hair samples taken from patients with breast cancer. 200
Table 8.13: Raw peak area data matrix for phosphatidic acid for hair samples taken from breast cancer free controls.....201
Table 8.14: Raw peak area data matrix for phosphatidic acid for hair samples taken from patients with breast cancer.....201
Table 8.15: Raw peak area data matrix for lyso-phosphatidylcholine for hair samples taken from breast cancer free controls. 202
Table 8.16: Raw peak area data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls. 202
Table 8.17: Raw peak area data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls. 203

Table 8.18: Raw peak area data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls. 203
Table 8.19: Raw peak area data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls. 204
Table 8.20: Raw peak area data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls. 204
Table 8.21: Raw peak area data matrix for lyso-phosphatidylcholine for hair samples taken from patients with breast cancer. 205
Table 8.22: Raw peak area data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer. 205
Table 8.23: Raw peak area data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer. 206
Table 8.24: Raw peak area data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer. 206
Table 8.25: Raw peak area data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer. 207
Table 8.26: Raw peak area data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer. 207
Table 8.27: Raw peak area data matrix for phosphatidylethanolamine for hair samples taken from breast cancer free controls. 208
Table 8.28: Raw peak area data matrix for phosphatidylethanolamine for hair samples taken from patients with breast cancer. 208
Table 8.29: Raw peak area data matrix for phosphatidylglycerol for hair samples taken from breast cancer free controls. 209
Table 8.30: Raw peak area data matrix for phosphatidylglycerol for hair samples taken from patients with breast cancer. 209
Table 8.31: Raw peak area data matrix for phosphatidylinositol for hair samples taken from breast cancer free controls. 210
Table 8.32: Raw peak area data matrix for phosphatidylinositol for hair samples taken from patients with breast cancer. 210
Table 8.33: Raw peak area data matrix for sphingomyelin for hair samples taken from breast cancer free controls. 211
Table 8.34: Raw peak area data matrix for sphingomyelin for hair samples taken from patients with breast cancer. 211
Table 8.35: Normalised data matrix for cholesterol ester for hair samples taken from breast cancer free controls. 212
Table 8.36: Normalised data matrix for cholesterol ester for hair samples taken from patients with breast cancer. 212
Table 8.37: Normalised data matrix for ceramide for hair samples taken from breast cancer free controls. 213

Table 8.38: Normalised data matrix for ceramide for hair samples taken from patients with breast cancer. 213
Table 8.39: Normalised data matrix for phosphatidic acid for hair samples taken from breast cancer free controls.....214
Table 8.40: Normalised data matrix for phosphatidic acid for hair samples taken from patients with breast cancer.....214
Table 8.41: Normalised data matrix for lyso phosphatidylcholine for hair samples taken from breast cancer free controls. 215
Table 8.42: Normalised data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.....215
Table 8.43: Normalised data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.....216
Table 8.44: Normalised data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.....216
Table 8.45: Normalised data matrix for phosphatidylcholine for hair samples taken from breast cancer controls.....217
Table 8.46: Normalised data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.....217
Table 8.47: Normalised data matrix for lyso phosphatidylcholine for hair samples taken from patients with breast cancer.....218
Table 8.48: Normalised data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.....218
Table 8.49: Normalised data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.....219
Table 8.50: Normalised data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.....219
Table 8.51: Normalised data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.....220
Table 8.52: Normalised data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.....220
Table 8.53: Normalised data matrix for phosphatidylethanolamine for hair samples taken from breast cancer free controls. 221
Table 8.54: Normalised data matrix for phosphatidylethanolamine for hair samples taken from patients with breast cancer.....221
Table 8.55: Normalised data matrix for phosphatidylglycerol for hair samples taken from breast cancer free controls.....222
Table 8.56: Normalised data matrix for phosphatidylglycerol for hair samples taken from patients with breast cancer.....222
Table 8.57: Normalised data matrix for phosphatidylinositol for hair samples taken from breast cancer free controls.....223

Table 8.58: Normalised data matrix for phosphatidylinositol for hair samples taken from patients with breast cancer. 223
Table 8.59: Normalised data matrix for sphingomyelin for hair samples taken from breast cancer free controls. 224
Table 8.60: Normalised data matrix for sphingomyelin for hair samples taken from patients with breast cancer. 224
Figure 8.1: Heteroscadascity plot of the average of the control hair samples for all lipid species before log transformation 225
Figure 8.2: Heteroscadascity plot of the average of the control hair samples for all lipid species after log transformation 225
Figure 8.3: Heteroscadascity plot of the average of the patient hair samples for all lipid species before log transformation 226
Figure 8.4: Heteroscadascity plot of the average of the patient hair samples for all lipid species after log transformation 226
Table 8.61: Data generated from a two sided t-test comparing control hair samples to the breast cancer patient hair samples. Those species with an adjusted p-value < 0.05 and fold change > 2 were considered significantly different (in red with pink fill) between the two groups. 227
Table 8.62: Weight (mg) of each hair sample for LCMS analysis. Hair was cut from as close to the scalp as possible and then cut finely, washed in acetone, dried and weighed to 30mg (or as close as possible). 232
Figure 8.5: PCA with the PBQC's, which are clustering (in green), compared to the controls samples in red and the patient's samples in blue. This indicates that the data is robust. 233
Figure 8.6 (A-C): Analysis of the levels of LPC (A), PC (B) and SM (C) along the hair fibre where shoulder length hair from three individuals was split equally into three sections and profiled for lipids (scalp, centre, end). The average of the three participants was graphed for each section and results showed variation in the amount of lipids between the three sections. 234
Figure 8.7: Average (of four replicates) for each sample shaken for 5, 15 and 30 minutes. The highest amount of lipid was obtained from shaking for 5 minutes. 235
Figure 8.8: The various weights of samples (7mg, 15mg, 30mg) were compared for three solvent amounts, 0ul (A), 750ul (B) and 1500ul (C) to determine the ideal weight of a sample. This was an average of four replicates for each weight. The optimal sample weight, for which the highest amount of lipid was extracted, was found to be 30mg of hair. 236
Figure 8.8: The different amounts of solvent (0ul, 750ul, 1500ul) were compared for three sample weights, 7mg of hair (A), 15mg of hair (B) and 30mg of hair (C), to determine the ideal amount of solvent required to homogenise the hair but also extract the maximum amount of lipid. This was an average of four replicates for each solvent amount. The optimal sample amount of solvent, for which the highest amount of lipid was extracted, was found to be 0ul during homogenization. 237
Figure 8.9: To determine the ideal number of cycles in the cryomill (3 or 9) to fully homogenise the hair sample and for maximum lipid extraction the number of cycles were compared for the

optimal amount of hair (30mg) in 0ul, 750ul and 1500ul of solvent (A) and also for the optimal amount of solvent (0ul) for 7mg, 15mg and 30mg of hair (B). This was an average of four replicates for each solvent amount and hair amount. The optimal number of cycles, for which the highest amount of lipid was extracted, was found to be 3 cycles for full homogenization of the hair. 238
Table 8.63: Raw peak area data matrix for cholesterol ester for serum samples taken from breast cancer free controls. 239
Table 8.64: Raw peak area data matrix for cholesterol ester for serum samples taken from breast cancer free controls. 240
Table 8.65: Raw peak area data matrix for cholesterol ester for serum samples taken from patients with breast cancer. 241
Table 8.66: Raw peak area data matrix for cholesterol ester for serum samples taken from patients with breast cancer. 242
Table 8.67: Raw peak area data matrix for ceramide for serum samples taken from breast cancer free controls. 243
Table 8.68: Raw peak area data matrix for ceramide for serum samples taken from breast cancer free controls. 244
Table 8.69: Raw peak area data matrix for ceramide for serum samples taken from patients with breast cancer. 245
Table 8.70: Raw peak area data matrix for ceramide for serum samples taken from patients with breast cancer. 246
Table 8.71: Raw peak area data matrix for phosphatidic acid and lyso-phosphatidic acid for serum samples taken from breast cancer free controls. 247
Table 8.72: Raw peak area data matrix for phosphatidic acid and lyso-phosphatidic acid for serum samples taken from breast cancer free controls. 248
Table 8.73: Raw peak area data matrix for phosphatidic acid and lyso-phosphatidic acid for serum samples taken from patients with breast cancer. 249
Table 8.74: Raw peak area data matrix for phosphatidic acid and lyso-phosphatidic acid for serum samples taken from patients with breast cancer. 250
Table 8.75: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls. 251
Table 8.76: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls. 252
Table 8.77: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls. 253
Table 8.78: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls. 254
Table 8.79: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls. 255

Table 8.80: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls. 256
Table 8.81: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer. 257
Table 8.82: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer. 258
Table 8.83: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer. 259
Table 8.84: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer. 260
Table 8.85: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer. 261
Table 8.86: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer. 262
Table 8.87: Raw peak area data matrix for phosphatidylethanolamine and lyso-phosphatidylethanolamine for serum samples taken from breast cancer free controls. 263
Table 8.88: Raw peak area data matrix for phosphatidylethanolamine and lyso-phosphatidylethanolamine for serum samples taken from breast cancer free controls. 264
Table 8.89: Raw peak area data matrix for phosphatidylethanolamine and lyso-phosphatidylethanolamine for serum samples taken from patients with breast cancer. 265
Table 8.90: Raw peak area data matrix for phosphatidylethanolamine and lyso-phosphatidylethanolamine for serum samples taken from patients with breast cancer. 266
Table 8.91: Raw peak area data matrix for phosphatidylglycerol and lyso-phosphatidylglycerol for serum samples taken from breast cancer free controls. 267
Table 8.92: Raw peak area data matrix for phosphatidylglycerol and lyso-phosphatidylglycerol for serum samples taken from patients with breast cancer. 268
Table 8.93: Raw peak area data matrix for phosphatidylinositol for serum samples taken from breast cancer free controls. 269
Table 8.94: Raw peak area data matrix for phosphatidylinositol for serum samples taken from patients with breast cancer. 270
Table 8.95: Raw peak area data matrix for phosphatidylserine for serum samples taken from breast cancer free controls. 271
Table 8.96: Raw peak area data matrix for phosphatidylserine for serum samples taken from patients with breast cancer. 272
Table 8.97: Raw peak area data matrix for sphingomyelin for serum samples taken from breast cancer free controls. 273
Table 8.98: Raw peak area data matrix for sphingomyelin for serum samples taken from patients with breast cancer. 274
Table 8.99: Normalised data matrix for cholesterol ester for serum samples taken from breast cancer free controls. 275

Table 8.100: Normalised data matrix for cholesterol ester for serum samples taken from breast cancer free controls. 276
Table 8.101: Normalised data matrix for cholesterol ester for serum samples taken from patients with breast cancer. 277
Table 8.102: Normalised data matrix for cholesterol ester for serum samples taken from patients with breast cancer. 278
Table 8.103: Normalised data matrix for ceramide for serum samples taken from breast cancer free controls. 279
Table 8.104: Normalised data matrix for ceramide for serum samples taken from breast cancer free controls. 280
Table 8.105: Normalised data matrix for ceramide for serum samples taken from patients with breast cancer. 281
Table 8.106: Normalised data matrix for ceramide for serum samples taken from patients with breast cancer. 282
Table 8.107: Normalised data matrix for phosphatidic acid and lyso phosphatidic acid for serum samples taken from breast cancer free controls. 283
Table 8.108: Normalised data matrix for phosphatidic acid and lyso phosphatidic acid for serum samples taken from breast cancer free controls. 284
Table 8.109: Normalised data matrix for phosphatidic acid and lyso phosphatidic acid for serum samples taken from patients with breast cancer. 285
Table 8.110: Normalised data matrix for phosphatidic acid and lyso phosphatidic acid for serum samples taken from patients with breast cancer. 286
Table 8.111: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls. 287
Table 8.112: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls. 288
Table 8.113: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls. 289
Table 8.114: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls. 290
Table 8.115: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer controls. 291
Table 8.116: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls. 292
Table 8.117: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls. 293
Table 8.118: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls. 294
Table 8.119: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer. 295

Table 8.120: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer. 296
Table 8.121: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer. 297
Table 8.122: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer. 298
Table 8.123: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer. 299
Table 8.124: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer. 300
Table 8.125: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer. 301
Table 8.126: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer. 302
Table 8.127: Normalised data matrix for phosphatidylethanolamine and lyso phosphatidylethanolamine for serum samples taken from breast cancer free controls. 303
Table 8.128: Normalised data matrix for phosphatidylethanolamine and lyso phosphatidylethanolamine for serum samples taken from breast cancer free controls. 304
Table 8.129: Normalised data matrix for phosphatidylethanolamine and lyso phosphatidylethanolamine for serum samples taken from patients with breast cancer. 305
Table 8.130: Normalised data matrix for phosphatidylethanolamine and lyso phosphatidylethanolamine for serum samples taken from patients with breast cancer. 306
Table 8.131: Normalised data matrix for phosphatidylglycerol and lyso phosphatidylglycerol for serum samples taken from breast cancer free controls. 307
Table 8.132: Normalised data matrix for phosphatidylglycerol and lyso phosphatidylglycerol for serum samples taken from patients with breast cancer. 308
Table 8.133: Normalised data matrix for phosphatidylinositol for serum samples taken from breast cancer free controls. 309
Table 8.134: Normalised data matrix for phosphatidylinositol for serum samples taken from patients with breast cancer. 310
Table 8.135: Normalised data matrix for phosphatidylserine for serum samples taken from breast cancer free controls. 311
Table 8.136: Normalised data matrix for phosphatidylserine for serum samples taken from patients with breast cancer. 312
Table 8.137: Normalised data matrix for sphingomyelin for serum samples taken from breast cancer free controls. 313
Table 8.138: Normalised data matrix for sphingomyelin for serum samples taken from patients with breast cancer. 314
Figure 8.10: Heteroscadascity plot of the average of the control serum samples for all lipid species before log transformation 315

Figure 8.11: Heteroscadascity plot of the average of the control serum samples for all lipid species after log transformation 315
Figure 8.12: Heteroscadascity plot of the average of the patient serum samples for all lipid species before log transformation 316
Figure 8.13: Heteroscadascity plot of the average of the patient serum samples for all lipid species after log transformation 316
Table 8.139: Data generated from a two-sided t-test comparing control serum samples to the breast cancer patient serum samples. Those species with an adjusted p-value < 0.05 and fold change > 2 were considered significantly different (in red) between the two groups. 317
Figure 8.14: PCA with the PBQC's, which are clustering (in green), compared to the controls samples in red and the patient's samples in blue. This indicates that the data is robust. 325
Table 8.140: Clinical data for the 40 healthy control individuals who participated in the studies, which extracted lipid from, scalp hair and serum. 326
Table 8.141: Clinical data, for the 40 individuals with breast cancer, who participated in the studies, which extracted lipid from, scalp hair and serum. 328
Table 8.142: Electrospray ionisation mode and ion scans for LCMS used in this study 333
Figure 8.15: Chromatogram of PC(34:1) standard (MRM 760.5 > 184.1 , RT = 6.84 min) 334
Figure 8.16: Chromatogram of SM(34:1) standard (MRM 703.5 > 184.1 , RT = 6.14 min) 334
Figure 8.17: Chromatogram of LPC(17:0) standard (MRM 510.5 > 184.1 , RT = 4.00 min) 335
Figure 8.18: Chromatogram of PG(34:0) standard (MRM 768.7 > 579.6 , RT = 6.9 min) 335
Figure 8.19: Chromatogram of Cer(d18:1\17:0) standard (MRM 552.5 > 264 , RT = 7.4 min) 336
Figure 8.20: Chromatogram of PE(34:0) standard (MRM 720.5 > 579.6 , RT = 7.27 min) 337
Figure 8.21: Chromatogram of PA(24:0) standard (MRM 534.5 > 153 , RT = 6.3 min) 337
Figure 8.22: Chromatogram of PI(36:2) standard (MRM 861.7 > 241 , RT = 6.77 min) 337
Figure 8.23: Chromatogram of PS(34:0) standard (MRM 762.7 > 675.7 , RT = 6.87 min) 338

Abbreviations

BCL 2	B-cell lymphoma 2
BRCA	Breast cancer
CA	Cancer antigen
CE	Cholesterol ester
CEA	Carcinoembryonic antigen
Cer	Ceramide
DCIS	Ductal carcinoma in situ
DMEM	Dulbecco's modified eagle medium
DNA	Deoxyribonucleic acid
EDTA	Ethylenediaminetetraacetic acid
ESI -MS	Electrospray ionisation-mass spectrometry
FT-IR	Fourier transform infrared
FT-ICR	Fourier transform ion cyclotron resonance
FTIR-ATR	Fourier transform infrared attenuated total reflection
GCMS	Gas chromatography mass spectrometry
HCA	Hierarchical cluster analysis
HER-2	Human Epidermal Growth Factor Receptor 2
HPLC	High pressure liquid chromatography
IS	Internal standard
LCMS	Liquid chromatography mass spectrometry
LPC	Lyso-phosphatidylcholine
LPE	Lyso- phosphatidylethanolamine
LPG	Lyso- Phosphatidylglycerol
MALDI	Matrix associated laser desorption ionisation
miRNA	Micro ribonucleic acid
MRI	Magnetic resonance imaging
MRM	Multiple reaction monitoring
MRS	Magnetic resonance spectroscopy
MSMS	Tandem mass spectrometry
MUC 1	Mucin 1, cell surface associated

N2	Nitrogen
P-ACCA	Phosphorylated acetyl-CoA carboxylase alpha
PA	Phosphatidic acid
PBQC	Pooled biological quality control
PC	Phosphatidylcholine
PCA	Principle component analysis
PCho	Phosphocholine
PE	Phosphatidylethanolamine
PG	Phosphatidylglycerol
PI	Phosphatidylinositol
PLC	Phospholipase C
PLD	Phospholipase D
PS	Phosphatidylserine
QTOF	Quadrupole time of flight
RPMI	Roswell Park Memorial Institute
SAXS	Small angle X-ray scattering
SAXS-WAXS	Small angle X-ray scattering- Wide angle X-ray scattering
SM	Sphingomyelin
TDLU	Terminal duct lobular unit
UV	Ultra violet
VOC	Volatile organic compound
WAXS	Wide angle X-ray scattering
XRD	X-ray diffraction

Abstract

The key to surviving breast cancer is early detection, and so a more accurate screening test for women of all ages, which can detect the cancer at a cellular level, would be a significant advancement in preventing the disease. A correlation between the presence of breast cancer and a change in the synchrotron generated X-ray diffraction (XRD) pattern of hair from afflicted individuals has been reported in several studies by various groups and has shown to detect approximately 75% of breast cancer patients in blinded studies. To date, however, the molecular mechanism(s) leading to this alteration are largely unknown. This study determined that the alteration observed in an XRD pattern of hair from cancer patients is due to changes in breast-cancer associated lipid(s), in particular phospholipid species. Liquid chromatography mass spectrometry identified and quantified lipids from biological samples including a breast cancer cell line and a control cell lines, and from hair and serum (from the same individual) from patients with breast cancer and controls. Significant differences were discovered between the two cell lines in the levels of some phosphatidylinositol, ceramide, phosphatidylethanolamine and phosphatidylcholine species, however, we were unable to find consistent differences in the serum and hair lipid profiles of women with or without breast cancer.

The changes observed in the cell culture supernatant study suggests that there may be lipid changes that are localised to the area of the tumour and not extendable to hair or serum unless a more specific method of extraction is devised. Further characterization of these phospholipids associated with breast cancer using more refined methodology could still be used to develop a novel sensitive and specific diagnostic screening test for breast cancer using serum.

Declaration

I certify that this work contains no material which has been accepted for the award of any other degree or diploma in any university or other tertiary institution in my name and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text. In addition, I certify that no part of this work will, in the future, be used in a submission in my name, for any other degree or diploma in any university or other tertiary institution without the prior approval of the Macquarie University and where applicable, any partner institution responsible for the joint award of this degree.

Work in the thesis is based on joint research or publications:

- All sample preparation was carried out by Dharmica Mistry and Dr. Thusitha Rupasinghe
- All Liquid Chromatography Mass Spectrometry was carried out at Metabolomics Australia (Bio21 Molecular Science & Biotechnology Institute, 30 Flemington Road, The University of Melbourne, Parkville, VIC 3010 Australia) by Dr. Thusitha Rupasinghe and under the guidance of Professor Malcolm McConville and Dr. Dedreia Tull, Node leader
- All data analysis was carried out by Dharmica Mistry, Dr. Thusitha Rupasinghe and Dr. Amsha Nahid

Ethics approval for the collection of 80 hair and 80 serum samples was obtained through the Macquarie University Human Research Ethics Committee. Ethics approval was granted on the 2nd of May 2011 for the project titled: "The identification and characterization of breast cancer-associated lipid (s) in hair and blood and their use in the development of a diagnostic test for breast cancer." The ethics committee reference number is 5201100091. The personnel authorised to conduct this research were Professor Mark Connor- Chief Investigator/Supervisor and Ms. Dharmica Mistry- Co-Investigator.

Acknowledgements

A major research project like this is never the work of anyone alone. The contributions of many different people, in their different ways, have made this possible.

Firstly, I would like to thank Macquarie University for giving me the opportunity to be a PhD student in the Faculty of Human Sciences at the Australian School of Advanced Medicine.

Secondly, My mentors. To my primary supervisor, Professor Mark Connor, I thank you for being the coolest supervisor around town. Your honest advice, ongoing support and amazing baking skills have made this a most wonderful experience for me. Thank you for always making the time to have a chat and for giving me the direction I most definitely needed. To Dr. Peter French, thank you for believing that I would be an ideal candidate for a PhD, and for ever giving me the chance to embark on this journey. Right from the very beginning you have been there for the real highs and the downright lows! You have always pushed me to keep going when the going got tough, and although your schedule was always fully booked, you always made the time for a discussion over coffee or lunch to ensure I could see the positive side of a PhD life! Thank you for your tire-less support, sincere advice and never-ending encouragement. To both of my supervisors, your guidance and advice throughout this project, as well as your pain-staking efforts in proof reading the drafts, are greatly appreciated.

I would like to extend my appreciation to SBC Research, in particular, Ron Phillips and Jayne Shaw, for their full support, both financially and also in their encouragement for me to undertake the project. Without SBC Research, this project wouldn't have existed.

I express my gratitude to the team under Professor Malcolm McConville at Metabolomics Australia in Melbourne. To Dr. Dedreia Tull, thank you for always taking the time for deep, lengthy discussions about the project and for helping me to understand the lipid world! I am deeply grateful to Dr. Thusitha Rupasinghe for her non-stop, around the clock assistance with this project over the years. You really are a gem and I have greatly benefited from having you as my mentor throughout this project. No matter the time, no matter the place, you have always assisted me in

understanding the lipidomics, from the laboratory to the office, so thank you. To Dr. Amsha Nahid, my deepest thanks for your tireless efforts in helping me to understand the statistics through countless emails and phone calls! Your assistance and extremely hard work do not go unappreciated. To the Metabolomics Australia team, thank you for making me feel a part of the family, for always having a coffee ready for me and the endless invitations to potluck lunches!

I would like to offer my special thanks to Dr. Andrew Spillane and Dr. Kylie Snook, from the Poche Centre, and the Sydney Breast Clinic and their nurses, for their support and participation in this project and for assisting me in recruiting participants for the studies. Of course, this project would not have been possible without the participation of the subjects, so many thanks to those who participated.

To the Connor Laboratory (my dear labrats), what a mixed bunch from around the world we are. Thank you so very much for making the environment surrounding my PhD a mad, funny and food-filled one! You were the smiling faces at my data club talks, the hysterical laughter at karaoke and the ever-supportive friends in the laboratory. May we always be that way!

My deepest appreciation goes to my amazing parents, Haridutt and Hasu Mistry, for their lifetime support, unconditional love and their greatest belief in me always. Thank you for sacrificing so much for me so that I could have such a successful and happy life. Without you I would not be who I am, or had the opportunity to achieve all I have, and I hope I have done you nothing but proud. To my brother Neel, thank you always and forever, for your love, understanding and your constant question of "when will you finish your PhD?" You are the aggressive motivator that I truly do need and your optimistic view on life continually inspires me to be better.

Finally, the person whose title has changed the most over the course of my PhD: my boyfriend turned fiancé turned husband, Sarat Chavali…What a crazy ride it has been! Thank you for always having faith in me and my abilities, for helping me get back upon my feet when I was down and out, and for being the radiant glow of positivity in my life. You are my strength and my willpower and my absolute partner in life.

This PhD experience has been an interesting and most rewarding one and I have not only learnt so much throughout this journey, but also met many people who have impacted my life along the way. Thank you all so very much.

1. Introduction

1.1. The extent of the breast cancer problem

The most common type of cancer among women is breast cancer, with over 1.3 million women worldwide diagnosed with the disease annually (DeSantis, 2011) and of these women, 35% will lose their lives to the disease (Jemal, 2011). In Australia, the chance of developing metastatic breast cancer during a woman's lifetime is approximately 1 in 8 (12%) (Australian Institute of Health and Welfare & Cancer Australia, 2012).

1.1.1. Incidence by age

Breast cancer occurs in women of all ages, although, as a woman ages, her risk of developing breast cancer increases. Women between the ages of 20 and 29 account for only 0.3% of breast cancer cases. Around 20% of breast tumours are found in women aged younger than 50, and 40% in women aged 65 years and older (Siegel, 2012). About 80% of women with breast cancer are over age 50 at the time of diagnosis.

Each woman's individual breast cancer risk depends upon several factors, including family history, genetics, age of menarche, and other factors that have not yet been identified (Feuer, 1999).

1.2. Normal breast structure

The mature female breast (see Figure 1.1) is composed of glands, ducts (passages for milk), connective tissue and fat. From the nipple a branching system of major and minor ducts leads into the breast tissue, ending in lobules (which make up larger units called lobes), which are the milk-producing glands (Pandya, 2011). The lobules make up larger units called lobes, and each breast is composed of 6-8 lobes. The final branching of ducts connected to the lobule is called the terminal duct lobular unit (TDLU). The architecture of the TDLU, which radiates from the nipple, allows the ducts and lobes to expand in all directions during puberty, pregnancy and lactation (Pandya, 2011).

Once the breast develops as a bud, composed of cuboidal epithelial cells *in utero*, it does not develop again until puberty. Just before puberty the hormonally-responsive fibrous stroma, which will surround ducts and lobes, begin to form (Sternlicht, 2006) and the cuboidal epithelial cells differentiate into myoepithelial cells, columnar luminal secretory cells, and cuboidal basal cells bounded by a basement membrane (Ramakrishnan, 2002). After puberty the pigmentation of the nipple increases and the dense fibrous stroma is dispersed by fat, causing the breast to enlarge. This is also when the ducts and lobules develop and branch out into the tissue (Hens, 2005).

The amount of glandular (lobular) tissue in the breast is sensitive to the activity of changing hormones and fluctuates with the menstrual cycle (Kopans, 2007). During the proliferative phase of the menstrual cycle, when estrogen, luteinising hormone and follicle stimulating hormone levels are highest, the lobules are small, mitoses are infrequent and specialised stroma is condensed. It is the inverse in the secretory phase of the cycle, when progesterone is at its peak, lobules are larger, there is more mitotic activity and stromal edema (breast fullness) and the cytoplasm of the luminal secretory cell is vacuolated (Rosen, 2009). The shape of the myoepithelium cell is dependent upon the level of the hormones, estrogen and progesterone (Birkenfeld, 1994). During menstruation when hormone levels are higher the cells retain a tall shape with an abundant cytoplasm. When hormonal levels are lower, the cells have a cuboidal configuration and a sparse cytoplasm (Ramakrishnan, 2002).

The upper outer section of the breast is mostly composed of glandular tissue, which makes the breast more dense and is predominant in the breasts of younger women (Tortora, 2001). The ducts and lobes are surrounded by fat and fibrous stroma that vary from individual to individual and make up the majority of the breast (Pandya, 2011). The stroma also contains fibroblasts, blood cells and lymphocytes. The nipple and subareola is composed of smooth muscle tissue in dense fibrous stroma and stratified squamous epithelium with increased melanin pigment. Both the nipple and areola have sebaceous glands (Birkenfeld, 1994).

During pregnancy the levels of progesterone and estrogen increase and changes in the breast result. There is the proliferation of the TDLU and a decrease in the amount of surrounding stroma, and fat droplets accumulate in the cytoplasm of the columnar luminal secretory cells (Merviel, 1996). The myoepithelial cells are highly sensitive to the hormone oxytocin (released postpartum) and on release of the hormone the cells contract expelling the milk into the ducts (Mcneilly, 1983). Milk is squeezed from the

ducts and pushed towards the larger lactiferous ducts that are joined to the nipple (Beth Israel Health Care System, 2012) by a smooth muscle contractile protein, which is found in the myoepithelial cells (Ramakrishnan, 2002). There are also changes in the hormone prolactin, which stimulates alveolar epithelium to produce and secrete casein, alpha-lactalbumin and lipids. When prolactin levels decrease, milk production stops (Macias, 2012).

The postmenopausal breast shows a reduction in the amount of ducts and lobules and relatively increased adipose tissue and connective stroma (Macias, 2012). Both the epithelial and myoepithelial cells are smaller. With age, a woman's breast contains more fat and they lose their support and density, making them easier to examine by mammography (Tortora, 2001).

The breast also drains into the lymphatic system, specifically into the axillary lymph nodes (under the arm), which act as filters between breast and venous circulation (Kopans, 2007).

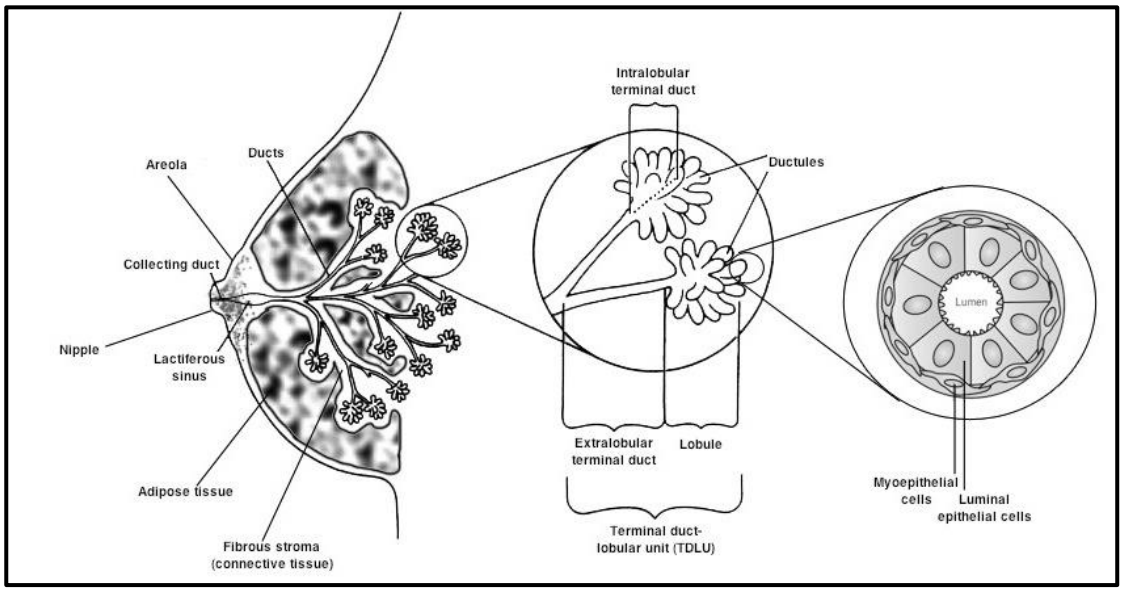


Figure 1.1: Schematic diagram of the human female breast (adapted/modified from (Hindle, 1999, Pandya, 2011).

1.3. Development of the disease

A breast tumour forms from breast cells. A malignant tumour is described as an assemblage of cancer cells that may spread to surrounding tissues or other organs in the body. Breast cancer is mostly a disease of females but 1 in 1100 males may develop the disease (Ottini, 2010). There are several theories on the aetiology of breast cancer but there is no definite known cause of the disease (American Cancer Society, 2005).

Breast cancer is considered a heterogeneous disease (Curtis, 2012) with some breast cancers evolving into metastatic carcinomas while others remain localised or benign for years (Ricks, 2005).

1.3.1. Theories on the pathogenesis of breast cancer

Table 1.1: Theories on the pathogenesis of breast cancer

Halsted Theory- spread from one source	- Breast cancer arises in one location of the breast and, if left untreated, spreads through the lymphatic system first to nearby lymph nodes and subsequently to other organs in the body (Hollingsworth, 2005). - "Contiguous" development of metastases (Hollingsworth, 2005). - Supports the view of mass screening to prevent mortality (Hollingsworth, 2005).
Alternative Theory- systemic disease	- Any distant metastases of any significance have already occurred by the time a breast tumour is detected (Fisher, 1977, Fisher, 2002). - Favours the view that there is little value in terms of reduction of mortality by introducing population screening (Smith, 2003).
Spectrum Theory- combination of theories	- Breast cancer is a spectrum of biologies such that many, but not all, breast cancers are vulnerable to early detection, supporting efforts to improve mammography as well as other diagnostic measures (Hollingsworth, 2005). - Breast cancers might be of two types (Hellman, 1994): o One group who *have "indolent and clinically unimportant cancers,"* o Second group who have *"a localised cancer that, if left to grow, will become disseminated and result in the patient's death."*
Genetic basis- Cancers which develop from genetic mutations	The genes BRCA1 and BRCA2: - Mostly account for hereditary susceptibility to breast cancer which make up 5-10% of breast cancers (Bradbury, 2007, De Gre`ve, 2008, Hall, 1990, Miki, 1994b, Wooster, 1994, Wooster, 1995). - A women carrying a mutation of BRCA has between a 60-85% risk of developing breast cancer throughout her life (Hall, 1990, Meindl, 2002, New York Breast Cancer Study Collaborative Group, 2001, Szabo, 1995).

1.3.2. Staging and survival rates

The procedure used to evaluate the extent of breast cancer, based on size and location, is called staging. Staging information assists in establishing the optimal treatment regime. The five-year survival rate demonstrates that the earlier the cancer is detected the greater the chance of survival is for the patient (American Cancer Society, 2005).

Table 1.2: The categories into which breast cancers are staged and the respective five-year survival rate (American Cancer Society, 2013).

Stage	Tumour size and location	Five year survival rate
0	Contained within ductal system – very early	93%
I	< 2 cm	88%
IIA	2 – 5 cm	81%
IIB	2 – 5 cm + spread to axillary lymph nodes	74%
IIIA	>5 cm + spread to axillary lymph nodes	67%
IIIB	> 5 cm + spread to chest lymph nodes	41%
IIIC	Spread to other areas of the breast such as chest wall, skin, lymph nodes (10> axillary lymph nodes, nodes below collarbone and breastbone)	49%
IV	Metastatic- spread to other organs of the body	15%

1.4. Detection and diagnosis

1.4.1. Current recommended screening

Currently, mammography and ultrasound are used to screen for breast cancer, and tissue biopsies are used for a more precise diagnosis (Michell, 2001). Breast self examination has been recommended for younger women to detect breast lumps (Hackshaw, 1996). The limitation of these methods is that they rely on imaging for detection, which means in practice that the tumour has to be of a minimum size (at least 5-10mm), by which time it may have metastasised. Furthermore, interpretation of the image in both technologies is a subjective process and relies on the operators and clinicians.

Therefore, breast cancer may require multiple screenings using one or both of these methods before a confident diagnosis of possible breast cancer can be confirmed. In addition, regular exposure to ionising radiation from X-rays (required for mammography screening) can increase the chance of breast cancer development (Pijpe, 2012).

1.4.1.1. Mammography

Mammography is the X-ray of the breasts and is recommended for use to screen women 40 and over (American Cancer Society, 2005). Breasts are clamped and flattened between two plates and exposed to low levels of ionising radiation. The image is captured on either radiographic film or digitally. The resulting image is analysed for areas of density, which may indicate masses in the breast. These may be cysts, calcifications or tumours (American Cancer Society, 2005). Mammography can be less effective for younger women as their breasts are denser and the identification of masses is less obvious in breast imaging (Elwood, 1993, Yankaskas, 2010). Since most breast cancers occur in older women, this is not considered a major problem, but for young women who have a genetic risk factor for breast cancer the relative lack of effectiveness of mammograms is a serious concern because breast cancer often develops at a younger age in these women (Bastiaannet, 2010) and is often more aggressive than in older women (Anders, 2009, Foxcroft, 2004, Fredholm, 2009). High breast density accounts for 40% of the population, primarily in women under the age of 40 (Boyd, 2007). As breast density is an issue for breast imaging, mammographic sensitivity in dense breasts has been reported to be 30-48%, which means that potentially more than half of the possible breast cancers are being overlooked (Hooley, 2012, Mandelson, 2000).

It is recognised that mammography is imperfect at diagnosing breast cancer, however it is the current "gold standard" and the most commonly used and most cost effective screening modality for breast cancer detection (Ferrini, 1996).

1.4.1.2. Ultrasound

This method of diagnosis uses an image that is generated using reflection from the sound waves transmitted into the body (American Cancer Society, 2005). It is a commonly used tool and is able to target specific areas of the breast, especially useful if a suspicious area has first been identified by mammography (Leucht, 1992). Although it is useful, it is subject to the ability of the operator carrying out the examination as they determine the path of the equipment over the breast (Sohn, 1999). Some studies have reported that ultrasound has double the accuracy when detecting small tumours in women with denser breasts compared to mammography (Benson, 2004, Devolli-Disha, 2009, Gokhale, 2009, Lehman, 2012, Zhi, 2007).

1.4.1.3. Magnetic Resonance Imaging (MRI)

MRI uses radio waves transmitted into and out of tissue in a specific pattern. MRI is a very expensive, highly specialised tool for breast examination, which is not widely available (Weinstein, 2010). As high breast density can cause some breast cancers to be missed using mammography, some studies are now suggesting MRI in addition to mammograms for screening in this situation because they have been found to be more than twice as sensitive as mammograms (Khatri, 2001, Kriege, 2004, Kuhl, 2005, Weinstein, 2010).

1.5. Assessment of current gold standard, mammography:

Breast cancer is one of the few malignancies where mass screening, through the use of mammography, has been validated as reducing mortality (Andersson, 1988, Feig, 2002, Shapiro, 1971). A 52% reduction in breast cancer mortality was observed in Australia as a result of women participating in a national breast screening program (Nickson, 2012) and a metanalysis by the same group, using worldwide studies, found the reduction in mortality rate due to screening participation was 49% (Allgood, 2008, Fielder, 2004, Gabe, 2007, Miltenburg, 1998, Otto, 2012, Palli, 1989, Puliti, 2008, Roder, 2008, van Schoor, 2011). However, the benefit of screening only applies to women who comply with guidelines. In Australia, these guidelines are annual

appointments for those at risk of the disease and biennial appointments for those women over the age of 50 (Taylor, 2004). Around 45% of women in Australia (Australian Institute of Health and Welfare, 2011) do not comply with guidelines and multiple reasons have been identified for the lack of higher compliance, including fear of radiation exposure, cost, pain due to breast compression and fear of negative outcomes (Aro, 2001, Feldstein, 2011).

There are additional limitations in using mammography as a screening modality, including that women under the age of 40 are not advised to undergo mammograms unless risk factors are present (Australian Institute of Health and Welfare & Cancer Australia, 2012). Thus, the 6.5% of women worldwide who will develop breast cancer, prior to the age of 40, are excluded from mammographic screening (Hankey, 1994).

Mammography is considered the "gold standard" for breast cancer screening so it is important to ascertain how many clinically detectable and treatable cancers it misses. There is a widespread assertion that mammography can find "*90% of breast cancers in women who have no symptoms of the disease"* (Park, 2007a), however, the origin of these statistics is not always quoted (Hollingsworth, 2005). Published studies on population screening using mammography range widely from 39% to 92% (the higher figure being in women aged between 70-74) with the majority of sensitivity results falling in the 60-66% range (Honjo, 2007, Shen, 2001). In reality the sensitivity of mammography screening rarely reaches 90%.

The reliance on anatomic contrasts is a crucial limitation of mammography as the cancer may be overlooked if it does not stand out from the high background that may be present (Houssami, 2002, Houssami, 2003). Even if the quality of the image is improved through technological advances it still does not appear to significantly improve the accuracy of diagnosis, which is dependent on visual contrast methods (Hollingsworth, 2005).

Another limitation of the use of mammography is that the interpretation of the resulting images by a radiologist is highly subjective, requiring a "double read" in many cases. Using mammography in conjunction with MRI or ultrasound allows researchers to ascertain the true sensitivity of this technology which can be as low as

60% (Honjo, 2007, Saslow, 2007, Shen, 2001), but utilising such combinations, on a larger scale, as a screening test is expensive and is currently limited to those individuals with a high risk (Weinstein, 2010).

A number of randomised trials involving 600,000 women worldwide (Bleyer, 2012, DeAngelis, 2010, Esserman, 2009, Kolata, 2009, McNeil, 2010, Raffe, 2011, The Canadian Task Force for Preventive Health Care, 2011, US Preventive Services Task Force, 2009) have found that the benefits of mammography mass screening outweigh its shortcomings and that although not perfect, it is still reducing mortality rates. Despite these limitations, it has been established that screening with mammography on a larger scale leads to a reduction in mortality and this validates early detection as a method of saving lives of those affected with the disease (Duffy, 2001, Duffy, 2002, Health Council of the Netherlands, 2002, International Agency for Research on Cancer, 2002, Miller, 1993, Nass, 2001, Nyström, 2002, Smith, 2003, Tabár, 2002, Tabár, 2003, US Preventive Services Task Force, 2002, US Preventive Services Task Force, 2002b, Weir, 2003). Breast cancer screening assumes that such screening will reduce the incidence of advanced (metastatic) breast cancer through early detection, therefore, the success of a screening technology is dependent upon its accuracy (Mushlin, 1998). However, mammography requires the tumour to be of a detectable size, by which time it may have metastasised (Bleyer, 2012). This makes early detection using mammography possible but not consistently accurate. In addition, the reduction in mortality rates must be assessed against the risks of the technology (Jørgensen, 2010). Although mammography has helped reduce mortality rates, it can also result in false positives (Bleyer, 2012, Duffy, 2005, Duffy, 2010). Currently there is no method of detection that can determine if a tumour is localised or invasive, so every case is treated as prospectively life-threatening. The number of false positives is an increasing concern in mammographic breast screening as it leads to the detection of tumours which may never have been discovered in the woman's lifetime (such as those which are slow growing and localised like ductal carcinoma in situ, DCIS), turning these women into cancer patients unnecessarily subjected to toxic treatment and life long psychological distress (Bleyer, 2012, Jørgensen, 2013, Vainio, 2002).

The need to develop an improved screening test is therefore not only based on the need to increase sensitivity and specificity of detection of all current cancers and abnormalities, it is also about the need to have a test that provides biological information about the tumour, and discriminate between those tumours that pose a threat to life and those that do not.

An ideal screening test for breast cancer would therefore reliably detect cancers before they have metastasised, when they are benign rather than malignant. This is not achievable by current breast screening using mammography. A biological marker that is present in malignant cancer patients, at a high enough level to be detectable, at an early stage of the development of malignancy for it to be used in conjunction with treatment to prevent mortality and avoid unnecessary surgery is imperative for the development of a highly effective screening test.

1.6. The importance of early detection

Although the overall incidence of breast cancer has been increasing for more than two decades, there has been almost a 30% reduction in mortality beginning in 1990 (Kopans, 2009). The two factors that have attributed to improved mortality rates are, (Berry, 2005) early detection (primarily by mammography screening), combined with more effective and increased application of anti-hormonal drugs and chemotherapy. This has been basis for developing improved methods for the early detection of various forms of breast cancer, prior to it metastasising, in order to maximise treatment outcomes (Ruffin, 2000). Breast cancer is one of the cancers where early detection can significantly improve survival rates using current therapies (de Waard, 1984, Weissberg, 1982). This is further confirmed by the many patients for whom diagnosis of breast cancer is made too late. It is estimated that 40% of breast cancer patients have regional (stage II-III) or distant (stage IV) spread of their disease at the time of diagnosis (Jemal, 2008) and this has changed little in the past 20 years despite the introduction of screening mammography in many countries for women in the target age group of 50-69 years old. If breast cancer could be reliably detected prior to metastisising, there would be a significant reduction of individual mortality in the community (Etzioni, 2003).

1.7. A better screening test is necessary

Simply stated, "if a tool, such as mammography, with only 40 to 70% sensitivity can reduce breast cancer mortality, then not only is early detection valid, but it is also a more powerful approach than ever imagined" (Hollingsworth, 2005). The impact of a technology that has 80% sensitivity or more and that has the potential to find 30-60% of currently undetectable cancers (Kuhl, 2007) would have the potential to achieve an enormous reduction in breast cancer mortality.

A screening test should satisfy several criteria in order to reach the guidelines of public health and to reduce the morbidity and mortality of the diseased or symptomatic population. The criterion are (Galen, 1982):

1. High precision and accuracy
2. High sensitivity and specificity
3. Useful for medical decision making
4. High predictive value
5. Favourable cost/benefit ratio
6. High throughput

Additionally, a screening test should be able to detect the disease at an early enough stage to allow for effective treatment (Knottneurus, 2002, Sackett, 2002). Attaining all of these requirements, while achievable in theory, is still highly challenging considering today's current breast cancer screening technologies.

High throughput of samples to rapidly detect breast cancer in its early stages would be ideal in a screening test. Although pathology tests are regularly used in clinical environments (Burtis, 2006), there is currently no technology that is available to rapidly screen a sample for any non-specific abnormality in breast cancer. If available, such a technology would revolutionise the practice of screening for the disease, as the accuracy of the detection would be limited only by the sensitivity of the device.

Advances in mammography technology have not led to increased accuracy, as ultimately it is a subjective test based on interpretation by an operator of an image. However, despite its relatively modest sensitivity, it has been recognised as effective at reducing mortality from breast cancer (Baker, 1982, Baker, 1985, Collette, 1984, Shapiro, 1982, Tabar, 1985, Verbeek, 1984). This realization highlights the potential ability to save more lives if a more accurate screening test for breast cancer is available. If the accuracy of mammography is limited by the fact that it relies on image interpretation, the basis for a more accurate breast cancer test needs to be re-defined. A biological marker, the measurement of which is objective, provides the direction required to develop a screening test for breast cancer that can realize this potential.

1.8. Biomarkers for breast cancer

Current screening tests for breast cancer (essentially imaging methods) are looking to identify suspicious masses in the breast, rather than biological change at a cellular level (Kuhl, 2005). Breast cancer, like all cancers is an alteration of a biological system, so a rational basis for detection of the disease is to identify surrogate markers of the biological change before an advanced cancer develops. Ideally, if a highly reliable marker of the biological change (one which is specific and sensitive) could be found, then treatment could be administered prior to the cancer forming an advanced mass.

1.8.1. Proteins

The most commonly analysed molecules, for cancer biomarkers, are proteins that are associated with malignant transformation (Brooks, 2008). Protein biomarkers, such as mammoglobin (Bernstein, 2005), kallikrein 14 (Borgoño, 2003), osteopontin (Rodrigues and H., 2007), and mutant p53 protein (Balogh, 2006), have long been of interest to those researchers identifying a biomarker for the disease. The most successful marker to date is Human Epidermal Growth Factor Receptor 2 (HER2) in serum (Quaranta, 2006, Slamon, 2001) which has proved more useful for monitoring the disease progression and the effect of treatment on the patient (Imoto, 2007) than

for screening for the presence of cancer. HER2 overexpression is used to identify those women with an aggressive form of breast cancer and a low level of survival (Press, 1993, Ravdin, 1995, Seshadri, 1993, Slamon, 1987), therefore, as a result of identifying these patients, the best course of treatment can then be determined (Imoto, 2007). Attempts have been made to identify other protein biomarkers for breast cancer. Some glycoproteins (encoded by the MUC1 gene which is expressed in epithelial cells) such as Cancer Antigen (CA) 15-3 and CA 27-29 tend to be elevated in serum of some patients (Keshaviah, 2007) and have been used to monitor those patients with distant metastatic breast cancer under treatment when imaging is not effective (Duffy, 2006). However, they are not highly recommended for screening because they have such low sensitivity and specificity in early stage disease (Molina, 2005). Another glycoprotein, carcinoembyonic antigen (CEA), is also used as an indicator, however it is more sensitive for colon cancer. It is therefore not specific to breast cancer, but may indicate the presence of a carcinoma (Vizcarra, 1996).

1.8.2. MicroRNA (miRNA)

These small non-coding RNA molecules have been recognised to have significant roles in biological processes such as differentiation and proliferation and as global regulators of gene expression (Kent, 2006). Breast cancer is a multifaceted disease, which is associated with familial genetic expression (Foulkes, 2008). Breast cancer tissue, when compared to control tissue, has been shown to exhibit deregulated miRNA expression, suggesting up- or down-regulation of some specific miRNA may function as a tumour suppressor gene or oncogene (Iorio, 2005). Over 100 miRNAs have been identified in breast tumour tissue (Blenkiron, 2007) and some have been associated with estrogen and progesterone receptor levels, HER2 levels and tumour stage (Mattie, 2006, Smith, 2008, Yan, 2008).

In addition to tissue studies, increased levels of specific miRNAs in the serum of patients with breast cancer has been found to distinguish between those women with the disease and controls (Heneghan, 2010, Roth, 2010) and the levels of these miRNAs have been shown to decrease in breast cancer patients postoperatively (Heneghan, 2010, Roth, 2010). However, it is not known whether the circulating miRNA originate from the tumour itself or circulating cells (Mostert, 2011). MiRNA

has been shown to be of potential value for both prognosis and diagnosis (Kosaka, 2010, Krell, 2012, Tricoli, 2007) for breast cancer, however, the lack of understanding around the processes by which its expression is deregulated make it difficult to determine endogenous controls for normalisation (Kosaka, 2010, Shi, 2009).

1.8.3. Lipids

Lipids are a carboxylic acid composed of a carboxyl group and hydrocarbon chain with a polar hydrophilic end and a non-polar hydrophobic end (Fahy, 2005). Lipids may be saturated or unsaturated and are insoluble in water and able to be extracted using organic solvents and are routinely quantified using mass spectrometry platforms (Christie, 2010). Lipids are known to play a multitude of roles in cellular biology. They make up at least 50% of the cellular membrane, serving as structural molecules (Yeung, 2007), and are influential in the signaling pathways within cells through their interaction with transmembrane proteins (Hannun, 2008, van Meer, 2008, Wymann, 2008). Lipids are of increasing interest in cell biology research as they can shed light on metabolic processes occurring within the cell and the consequences of small changes at a cellular level.

Lipids can be classified into eight classes based on their structure: fatty acyls, glycerolipids, glycerophospholipids, sphingolipids, sterol lipids, prenol lipids, saccharolipids, and polyketides (Fahy, 2005). Of these, the three main classes that make up cellular membranes are the glycerophospholipids, sphingolipids and sterol lipids (Dowhan, 1997). Glycerophospholipids, which also commonly referred to as phospholipids, have roles in cellular signaling as second messengers or precursors for the initiation of second messengers (Vance, 1996). Phospholipids are a class of lipids that consist of two fatty acyl molecules esterified at the *sn*-1 and *sn*-2 positions of glycerol, and contain a head group linked by a phosphate residue at the *sn*-3 position (Kelly, 2011). They are composed hydrophobic fatty acyl chains and a hydrophilic head group, which defines what type of phospholipid it is (Figure 1.2)

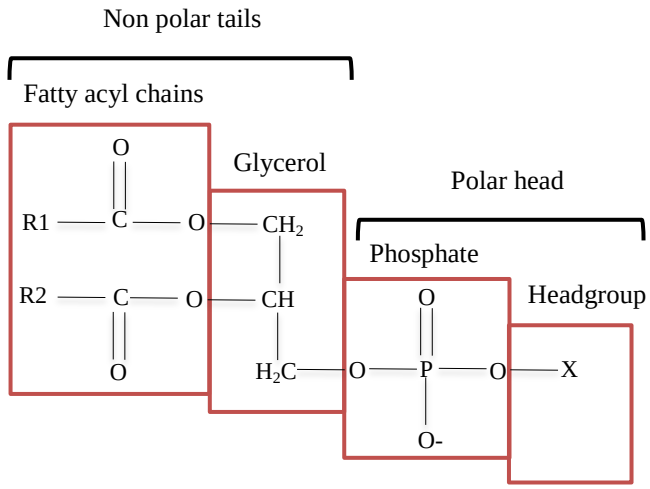
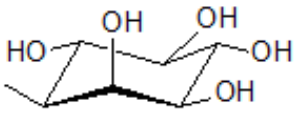


Figure 1.2: schematic representation of a phospholipid specie structure, adapted from (Kelly, 2011).

There are six classes of phospholipids characterised by their head group: phosphatidic acid (PA), phosphatidylserine (PS), phosphatidylglycerol (PG), phosphatidylcholine (PC), phosphatidylethanolamine (PE), and phosphatidylinositol (PI) (Table 1.3) (Christie, 2010). Lysospecies exist having only one FA or fatty alcohol moiety attached to the glycerol phosphate backbone and occur as intermediates in phospholipid biosynthesis, as well as functioniong as second messengers (Fahy, 2005). Biological membranes are primarily composed of these lipids and thus they have essential roles in structuring the cell membrane, storing energy as well as being involved in cell signaling through molecules such as arachidonic acid, phosphatidate, diacylglycerol and inositol trisphosphate (Vance, 1996, Wu, 2010).

Table 1.3: Common phospholipids and their structure, where X is the headgroup of the phospholipid as represented in figure xxx (Kelly, 2011).

Glycerophospholipids (PL)	X	
Glycerophosphatidic acid/ (PA)	Acid	—H
Glycerophosphocholine/ (PC)	Choline	$—CH_2-CH_2-\overset{+}{N}(CH_3)_3$
Glycerophosphoethanolamine/ (PE)	Ethanolamine	$—CH_2-CH_2-\overset{+}{N}H_3$
Glycerophosphoinositol/ (PI)	Inositol	
Glycerophosphoglycerol / (PG)	Glycerol	$—CH_2-CH(OH)-CH_2OH$
Glycerophosphoserine / (PS)	Serine	$—CH_2-CH(\overset{+}{N}H_3)-COO^-$

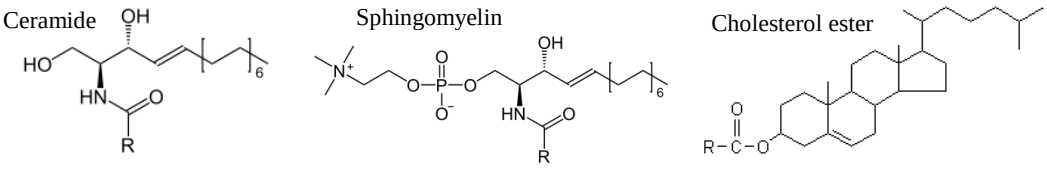


Figure 1.3: The structure of other membrane phospholipid species (Merrill, 2008, Liscum, 2008).

In a cell membrane the phospholipids are orientated so that they create a hydrophobic wall around the cell by directing their hydrophilic head groups towards the internal and external surfaces and their hydrophobic tails point towards each other (Figure 1.4) (Dowhan, 1997).

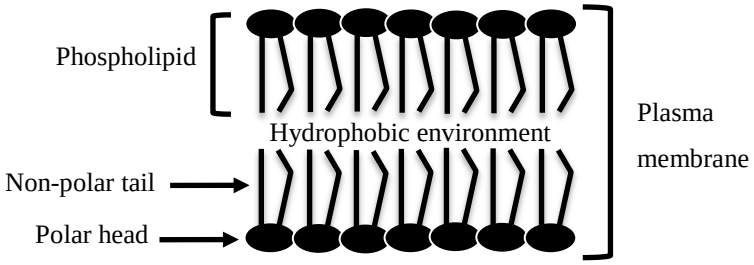


Figure 1.4: schematic representation of lipid orgnaisation on the cellular membrane,adapted from (Alberts, 2002).

A few studies have demonstrated an association between breast cancer and the presence of lipids in serum. Alexopoulos *et al* reported that breast cancer patients have increased serum total cholesterol, free cholesterol, low-density lipoprotein cholesterol, and triglycerides in comparison to non-cancer patients (Alexopoulos *et al*., 1987). In a more recent paper (Hammad, 2009) it was reported that there was a significant difference in serum phospholipid content between stage-IV breast cancer patients and disease-free individuals. The most significant differences in lipid profiles among disease-free and cancer subjects were attributed to three phosphocholine (PCho) species and to three fatty acid species, which were not identified. The phosphocholine lipids that displayed a statistically significant change as a consequence of cancer progression were found to contain an oxidised fatty acid moiety. They added a note of caution regarding specificity: "*The perturbed lipids reported here originate from common lipoprotein components. For example, glycerophosphocholines are the most abundant glycerophospholipids in mammalian cells and account for more than 30% of the total lipid content. Therefore, it is expected that they are severely affected by any organ malfunction*…". Serum lipids elevated in breast cancer may be affected by treatment for the cancer, in that they have been reported to decrease significantly after treatment (Ray, 2001).

While the majority of studies indicate that elevated levels of phosphatidylcholine (PC) and phosphatidylethanolamine (PE) are observed in tumour cells and tissue (Ackerstaff, 2003), two new studies, by the same group, one in human cells and one in murine cells, reported different results to previous studies. The studies found that the total amount of PC was actually decreased in metastatic breast cancer cells and lyso phosphatidylcholine (LPC) was elevated. They also found that metastatic breast cancer cells exhibited altered PE profiles associated with proliferation and malignant progression and that a "*switch from unsaturated to saturated fatty acids in phosphatidylinositol (PI) was observed in cancer cells as compared with non-tumourigenic cells*" (Dória, 2012, Dória, 2013).

Such inconsistent results establish the need for an extensive study that profiles the specific phospholipids associated with breast cancer. The heterogeneity of breast cancer makes it challenging to find universal changes associated with the disease (Ellis, 1991). It may be likely that each breast cancer variant could have a different phospholipid, attributed to specific species of phospholipids, rather than just an overall phospholipid change (Hilvo, 2011).

1.9. Alternative diagnostic technologies

In addition to searching for effective biomarkers to detect the presence of the disease, a number of alternative approaches utilising different technologies and/or different biological samples have been explored.

1.9.1. Saliva

Proteins released from the salivary gland have been demonstrated to be possible markers for breast cancer (Paige, 2007). Using isotope labeling combined with liquid chromatography mass spectrometry (LCMS), it was reported that by-products of oncogenic expression accumulate in the saliva and result in proteins (CA 15-3, Her-2) which are differentially expressed in those patients with breast cancer, compared to the saliva from healthy controls (Bigler, 2002, Brooks, 2008, Navarro, 1997, Streckfus, 2000, Streckfus, 2000(b), Zhang, 2010). In addition, it has been reported

that some salivary proteins may be indicative of ductal carcinoma *in situ* (DCIS) (Streckfus, 2008). The mechanism by which these changes in salivary proteins occur has not been clarified and is not specific to breast cancer, with reports of some of these salivary proteins also associated with melanoma, lung cancer (Gao, 2009) and oral cancer (Hu, 2008, Li, 2004). Further studies are needed to ascertain the specificity of these protein changes for breast cancer in large studies (Castagnola, 2011).

1.9.2. Breath

Another potential screening technology is the breath biomarker test for breast cancer, which profiles the volatile organic compounds (VOCs) found in the breath of patients. Deep exhalations are analysed using gas chromatography mass spectrometry (GCMS) (Lee, 2009, Mangler, 2012, Patterson, 2011, Phillips, 2003). One study found that this method of detection had 72% sensitivity and 64% specificity for breast cancer (Patterson, 2011). Another study found that the breath test could differentiate between individuals with breast cancer and controls with a sensitivity of 94.1% and specificity of 73.8% (Phillips, 2003). These researchers suggested that oxidative stress is markedly increased in breast cancer and that this increase influences the level of volatile organic compounds in breath *"due to lipid peroxidation of fatty acids in the membrane*". However, different studies have found varying VOCs with little or no consistency. For example, Phillips *et al* found eight VOCs had 94.1% sensitivity and 73.8% specificity for breast cancer (Nonane; Tridecane 5-methyl; Undecane 3-methyl; Pentadecane 6–methyl; Propane 2-methyl; Nonadecane 3-methyl; Dodecane 4-methyl; Octane 2-methyl) (Phillips, 2003) but in another study in 2006 by the same group (Phillips, 2006), found 5 VOCs (2-propanol; 2,3-dihydro-1-phenyl-4 (1-H)-quinazolinone; 1-phenyl-ethanone; heptanal; isopropyl myristate) which were 93.8% sensitive and 84.6% specific for breast cancer. Other studies found phenylethylketone and hexadecane (Song, 2010) and hydrogen peroxide (Stolarek, 2010) to be the VOCs specific for breast cancer. In addition, there are limitations to this method of detection, including a lack of knowledge of the source of VOCs, a lack of mechanism for the observed changes, and the uncertainty as to the best way to standardise the sampling of an exhalation (Li, 2013). The other issue is that this method of biomarker detection

has also been highly associated with lung cancer (Mazzone, 2012, Song, 2010 (b), Wang, 2012, Westhoff, 2009) and colon cancer (Altomare, 2013, Matuchansky, 2013); therefore, the specificity for breast cancer of this technique must first be established.

1.9.3. Urine

Recent mass spectrometry studies discovered that there was more PC and PE in the urine of breast cancer patients pre-surgery, when compared in the same patient, post-surgery. There was a correlation between the species of interest found in urine and those in the literature reported to be found in breast tumour tissue. The group goes on to recommended phospholipid profiling of body fluids, such as urine and blood, to identify lipid biomarkers associated with breast cancer and its progression but suggest further studies must be carried out to define the lipids involved (Kim, 2009, Min, 2010).

1.9.4. Hair

There is a recognised association between a person's overall health and the condition of their hair and nails (Hinds, 2008). Aberrations in hair and nails can result from alterations in nutrient supply, inflammation, toxins, heavy metals, physical damage and systemic disease through mechanisms yet to be fully understood (Hinds, 2008). Thus, the examination of hair and nails may provide important diagnostic clues to the patient's state of health, as an alternative to more traditional biological samples such as serum. It has been demonstrated that molecules such as estrogen receptor alpha, progesterone receptors, BCL-2 and HER-2 that are up-regulated in breast tumours are also up-regulated in skin from the same patient. On the basis of these results they proposed that the influence of discrete breast cancers is systemically expressed and leads to changes in skin and hair (Lawson, 2007). In support of this, James *et al* demonstrated the ability to detect first diabetes (James, 1997), and then breast cancer (James, 1999) from X-ray diffraction (XRD) of human hair and reported that this method of detection could be used to detect cancer at a very early stage. These

changes were seen in all samples of scalp and pubic hair taken from women diagnosed with breast cancer.

The above technologies demonstrate an intriguing possibility: that a mass-screening test for a range of abnormalities based on a biological sample remote from the site of disease is potentially feasible. We will examine hair in more detail, as it has been intensively studied and provides the potential of a durable and robust biological sample allowing for easy collection and transport.

1.10. Hair: Composition and structure

Hair is composed of dead cells filled with alpha-keratin, a structural protein that is also found in skin and nails of mammals (Wei, 2006). The hair fibre is divided into three distinct parts: the cuticle, cortex and medulla (Figure 1.5). The cuticle protects the cortex and is made up of dead cells produced from the hair follicle (Patil, 2010). They are arranged in 5- 10 overlapping layers to form a barrier and each cell is made up of the epicuticle, the a-layer, the exocuticle and the endocuticle, followed by the cell membrane complex (polysaccharides and lipids) which act as an adhesive (Feughelman, 1997). The cortex is composed of spindle-shaped cortical cells, and provides strength, as well as the colour and texture to the hair fibre (Randebrook, 1964). It also contains the cell membrane complex, which binds the cuticle layer to the cortex layer (Wei, 2006).

Cortical cells contain macrofibrils, which are highly organised protein-based structures (Figure 1.5) (Wolfram, 2003). In some cases, usually in thicker hair fibres, a medullary canal may be present in the centre of the fibre. The medulla is generally amorphous in appearance, and it can contain foreign debris and excreted products from the body (Patil, 2010).

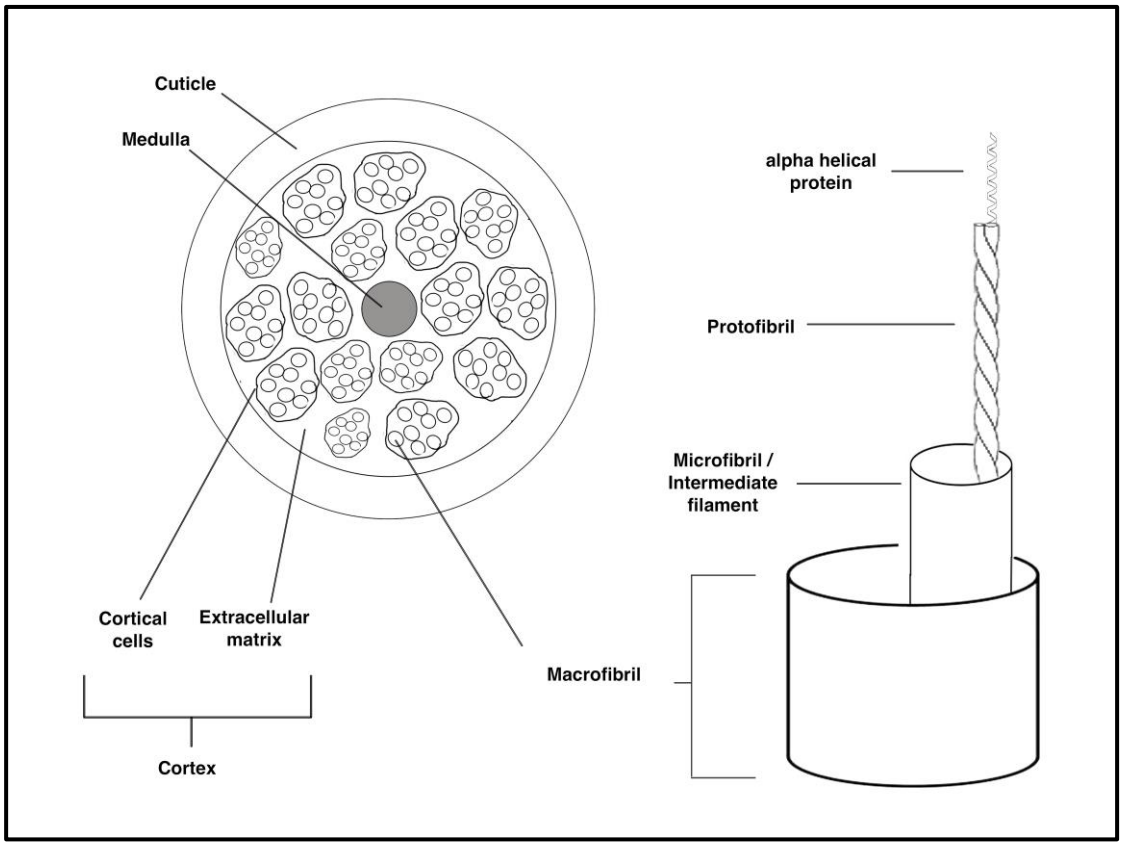


Figure 1.5: Schematic diagram of the structure of human scalp hair (adapted/ modified from (Villa, 2013, Wei, 2006). Keratin is a coiled alpha helix polypeptide chain (Tilstone, 2006). A single hair is composed of three alpha helices twisted together to form a protofibril. Protofibrils are packed around each other to form a highly organised structure called microfibril/ intermediate filament. Microfibrils embedded in a high sulfur protein matrix become a macrofibril, which makes up a cortical cell set in an extracellular matrix of the cortex of the hair fibre.

The hair root is enclosed within the follicle below the skin's surface and contains nerve and blood vessels, as well as, specialised mesenchymal cells, which form the dermal papilla (Krause, 2006). These cells are fed by the bloodstream, and contain sex hormone receptors (which regulate hair growth) (Matsuzaki, 1998). Cells of the hair shaft are pushed up from the hair follicle towards the surface of the skin as they differentiate, fill up with hard keratin fibres and eventually die, forming the inert structural hair fibre, which protrudes out of the follicle (Patil, 2010). Thus the end of the fibre closest to the follicle contains the most recently produced keratin filaments

and is most likely to represent the current state of the individual's health. Two sheaths surround the follicle, the inner and outer root sheaths, the former ends below the sebaceous gland and the latter continue all the way up the shaft (Krause, 2006). Below the gland and around the outer root sheath is the erector pili muscle, which causes the hair to stand erect. The sebaceous gland produces sebum, a natural oil, which can cover the scalp surface and the hair (Hashimoto, 1988). While sebaceous lipids may serve to lubricate and waterproof, they are not membrane-forming lipids (Wertz, 1988).

Hair follicles can run through the normal cycles of growth entirely independently of neighbouring follicles, which means each hair fibre can grow at different rates. The three main phases of growth are: anagen, catagen and telogen (Patil, 2010). Anagen is the active growth phase where hair is produced. It is the longest phase and 90% of hairs at any time are in this state. Catagen is a controlled regression of the hair follicle (breaking away from the dermal papilla) and telogen is when the follicle is in a resting state (Kligman, 1959).

The structure of the fibre allows hair to slowly absorb and retain penetrating materials from its external environment in addition to internal metabolites(Coderch, 2007). These metabolites can also be extracted from the fibre for further analysis, making hair a useful tool for biological monitoring of toxic metals and the detection of trace elements in forensic and medical investigations(Kintz, 1992). Hair is a useful tissue for diagnostic purposes and for mass screening, because as a sample it is non-invasive and easy to collect and store (Attar, 1990). It can be useful as it can signify the "time-weighted average-exposure" values of metabolites rather than body fluids, which represent levels of metabolites at specific times (Attar, 1990, Bertrand, 2003).

1.11. X-ray diffraction of hair

The structural arrangement of keratin intermediate filaments in the hair fibre can be determined using X-ray diffraction. It was intensively studied in the first half of the twentieth century (Popescu, 2007). Astbury and co-workers (Astbury, 1931, Astbury, 1933) used X-rays to demonstrate that hair contained a crystalline phase. Interpreting these results Pauling *et al* proposed the alpha-helical secondary structure of hair

structure to account for the X-ray diffraction patterns (Pauling, 1951). Recent X-ray investigations illustrated that along the first 1400 mm, the alpha-helices arrangement form a crystalline phase but in the root, they develop an amorphous structure (Rafik, 2006).

Low angle X-ray diffraction analysis of hair is a well-accepted technique (Corey, 1936). Whilst X-rays from any source can theoretically be used for such studies of hair, X-rays generated in a synchrotron are ideally suited for such analysis, as they are of very high intensity and thus the time taken for collection of data is significantly shorter. The disadvantage of having to use synchrotron-generated X-rays is that synchrotrons are very large particle accelerators, and there are only a limited number of them in the world (Willmott, 2011). Studies using low-angle synchrotron X-ray diffraction of hair have yielded a description of the fibrillar structure of alpha-keratin. Such studies have shown that during keratinisation in the follicle, two alpha keratin molecules are wound together very tightly to form a double helix. Two of these double helices are then wound together to form a tetramer and then eight of these tetramers wind together as a staggered array to form the slow helix of the intermediate filament. As the hair grows, these alpha-keratin intermediate filaments align in fibrils along the hair (Kreplak, 2002, Rafik, 2004).

1.11.1. Rings and X-ray diffraction patterns

The first published report of the use of X-ray analysis of hair structure for diagnosis of disease was that for insulin-dependent diabetes (James, 1997). In this study, exposure of single hairs to synchrotron X-ray radiation was reported to reveal clear and consistent changes in the molecular structure of alpha-keratin. The nature of the changes suggested that the change was endogenous, occurring via the modification of extracellular matrix materials during the aggregation of the intermediate filaments in the follicle.

1.12. Hair testing as a screening tool for breast cancer

1.12.1. Association between breast cancer and the X-ray diffraction pattern of hairs

In 1999, James and colleagues reported differences in the small angle X-ray scatter (SAXS) patterns of hair from individuals with breast cancer compared to healthy subjects (James, 1999). The SAXS patterns of hair from cancer patients contained a "ring" of comparatively low intensity, which was superimposed on the normal α-keratin pattern obtained from healthy control subjects. Subsequent papers from the same group reported SAXS analysis results of blinded human samples, which were consistent with the initial publication (James, 2005a, Meyer, 2001). The later paper reported on the results of 503 blinded hair sample analyses and demonstrated a sensitivity of 100% and a specificity of 86% (by comparison to mammography) for breast cancer (James, 2005a). Pre-clinical data supporting the finding was presented using an animal model of breast cancer. To correlate the observed change with the presence of breast cancer, whiskers removed from nude mice prior to, and 8 weeks post subcutaneous implantation of a human breast adenocarcinoma cell line were analysed using SAXS. The post-implantation whiskers showed the presence of a "ring" in the SAXS pattern, similar to that seen for human subjects affected by breast cancer, but the study did not however examine potential candidate factors (James, 2005a), nor were appropriate controls used, being whiskers from age-matched non-tumour-bearing mice.

All samples from subjects diagnosed with breast cancer were positive by the James study, however there were several samples, which were adjudged positive by the James test but negative by mammography. The researchers did not follow up the reason for, and the significance of, these inconsistencies.

Several groups independent of James attempted to replicate the original findings and were unsuccessful (Aksirov, 2001, Amenitsc, 1999, Briki, 1999, Chu, 1999, Howell, 2000, Laaziri, 2002, Schroer, 1999). James responded that in most cases other groups failed to confirm her findings because of technical issues such as the method of sample collection, the physical state of the hair, the positioning of the fibre in the

beam and the method of image analysis and the interpretation of data (James, 2001a, James, 2003a, James, 1999, James, 2003b, James, 2003c). These statements would indicate that the use of hair as a diagnostic screening test for breast cancer may be more complex than James' original papers implied, and also suffers from the same limitation as mammography, which is the need to interpret an image.

1.13. Clinical Studies on the breast cancer and the X-ray diffraction of hair

1.13.1. Corino and French

In 2008, the first replication of the finding independent of the original author was reported (Corino, 2008). In the study, thirty-nine hair samples (scalp and/or pubic) were examined. Nineteen hair samples were collected from women presenting at a radiology clinic, fourteen positive controls (samples from women known to be diagnosed with breast cancer) and six samples from women assumed negative by mammography, were analysed. Synchrotron SAXS experiments were carried out on two beamlines, which had been previously used for studies on detection of cancer by hair X-ray diffraction. Diffraction images were analysed using two different image-processing programs. They reported a sensitivity of 86% and a specificity of 81%. The degree of this correlation was lower than previously reported (James, 2005a, James, 1999) but they indicated that there was an association between the appearance of a circular feature, or "ring" at a q spacing of $0.132 \pm 0.002 Å^{-1}$ and the presence of breast cancer. The "ring" correlating to the presence of breast cancer was identified in 13 of the 14 positive controls at the defined spacing. The results presented in the study confirmed the existence of a correlation between an altered X-ray diffraction pattern of hair and the presence of breast cancer.

The authors excluded some hairs from the study because they were classified as "indeterminate" due to the presence of abnormal features, which were likely due to damage. As a result, the overall specificity (80%) and sensitivity (71%) were both less than 100%, as reported by James *et al* (James, 1999). It was commented that more samples were needed to more accurately define the accuracy of the test.

1.13.2. Fer2k trial

A 2000 patient trial using the hairs from women attending radiology clinics was completed in July 2008. Hairs from patients were exposed to a small angle X-ray and the resulting diffraction patterns were analysed. This was a blinded study and the presence/ absence of cancer was predicted from the visual examination of X-ray diffractions patterns (Corino, 2009). The sensitivity (64%) and specificity (77.6%) of the technique was significantly lower than that originally claimed by James *et al* (James, 1999). Analysis of the results indicated that this method of detection had a greater sensitivity (74%) for women under 70 years of age, and the greatest accuracy (almost 80%) for women under 40. When used in conjunction with biopsy, this method of detection was able to positively predict the presence of breast cancer 47% of the time with a false positive rate of 19% (Corino, 2009).

1.13.3. Sensitivity of mammography when combined with a hair test

A comparison of the performance of using hair to detect breast cancers alone with mammogram alone in confirmed cases was also instructive. Of 36 confirmed breast cancers, using hair as a detection method alone detected 23 (sensitivity 64%); mammography alone detected 22 (sensitivity 61%); and the two combined detected 33 cancers (sensitivity 85%) (Corino, 2009). This suggests that the two methods of screening may detect different cancers from each other, thus identifying more cancers together, than each alone.

Overall the data from the Fer2k trial was suggestive that X-ray diffraction of hair may have a place in breast cancer detection for some groups of women, however the biological mechanism remained unknown. This, and the need for a synchrotron, are significant limitations in the widespread adoption of the technology, as are the relatively low accuracy levels achieved.

1.14. Molecular mechanism underlying the altered X-ray diffraction pattern of hair in patients with breast cancer

Although little progress until now had been made in determining a mechanism for the effect, a number of hypotheses concerning the origin of the "ring" present in X-ray diffraction patterns of hair from individuals with breast cancer have been suggested. James and her colleagues were unable to define a molecular mechanism by which diseases such as cancer and diabetes are able to affect the structure of hair, but indulged in some speculation. One theory was that the "ring" is a result of a variation in the structure of the cell membrane of the fibre as it is assembled in the follicle (James, 1999). It has also been proposed that an "additional component" could theoretically bind to the alpha-keratin fibres forming in the intermediate filaments or to other structural elements such as the lipid bilayers (James, 1999).
Vazina *et al* stated that the proposed cancer "ring" reflection was due to the interaction of calcium with proteoglycans of the extracellular matrix in the hair fibre and reflected the periodicity of the polysaccharide chain attached to the protein core (Vazina, 2005).

A paper from Trounova *et al*, 2002, also indicated that the 4.5nm "ring" was due to calcification of the hair (Trounova, 2002). However, comparing the hair XRD image in (Figure 1.6, A) from that paper with other images from similar studies, there is a significant lack of alpha-keratin features present in the pattern (no meridional arcs or reflections), just one or two heavy features. Furthermore, the "rings" shown in the paper are thick, solid (Figure 1.6, B) and run into or obscure the equatorial spots, which are present in good X-ray diffraction patterns of hair (Figure 1.6, C).

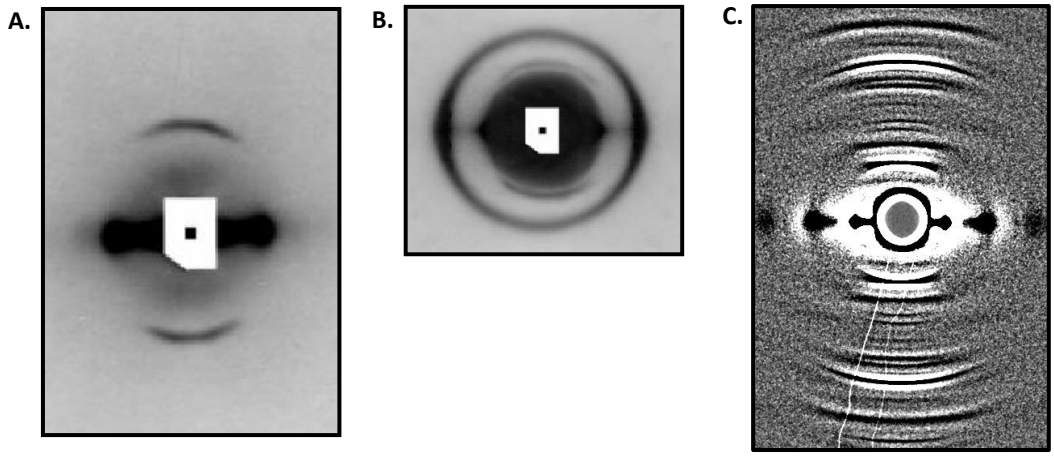


Figure 1.6: X-ray diffraction patterns of human scalp hair from (Trounova, 2002) (A, B); Sample 1275, Advanced Photon Source, Chicago (own image) (C).

Another possibility is that the "ring" is due to an alteration in proteoglycans in hair. It has been reported that there are significant changes in proteoglycans in malignant breast cancer cells. Rykova *et al* showed that proteoglycan composition drastically changes after malignant transformation. They reported that normal tissue contains heparan sulfate proteoglycan and dermatan sulfate proteoglycan, while tumour tissue contains normal levels of chondroitin sulfate proteoglycan fraction, while the dermatan sulfate proteoglycan fraction decreases or in some cases completely disappears after malignant transformation (Rykova, 2007). However, how this change in breast cancer might affect the composition of hair is unknown.

In 2003, Bertrand *et al* stated that the "ring" described by James in the diffraction pattern of hair from breast cancer patients (Figure 1.7) was in fact simply due to lipids in hair (Bertrand, 2003). They described lipid rings as follows: "*Part of lipids appears in an organised state and leads to fine rings in the hair diffraction pattern. A 4.5-nm ring and observable higher harmonics are reported to correspond to the lamellar periodicity of structured lipid bilayers… Two reflections around 0.41 and 0.37 nm are related to interatomic distances within these layers. Such organised lipids have been observed in skin stratum corneum. Hair lamellar lipids would be present as lipid granules, or ''lipid crystals'' and not lipid layers of cell membranes. Neither the composition nor the origin of these lipids has been elucidated so far*." The rings shown in their paper are similar to those of Trounova *et al* (Trounova, 2002).

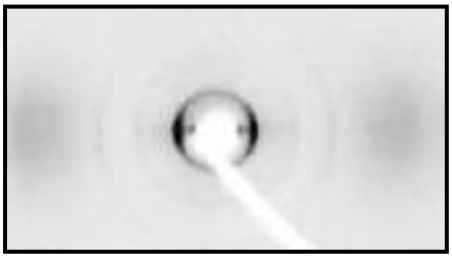


Figure 1.7: X-ray diffraction pattern of human scalp hair from Bertrand *et al*'s 2003 paper (Bertrand, 2003).

Whilst the evidence presented by Bertrand *et al* was unconvincing, given the equality of the images, there is in fact other good evidence that the "ring" is lipid-based (Bertrand, 2003).

1.15. Evidence that the "ring" feature in XRD pattern of hair is lipid-based

The fact that the XRD feature associated with breast cancer is circular gives some clues as to its chemical nature. A circular feature (a "broad halo") in an X-ray diffraction pattern can be produced by an amorphous material such as oils (Clark, 1927). There are a variety of lipids found naturally occurring in human hair. Exogenous lipids, which coat the hair, are predominantly those secreted by the sebaceous gland and consist mostly of cholesterol esters and free fatty acids (Coderch, 2007). Endogenous lipids, including phospholipids, cholesterol, ceramides, cholesterol sulphate and other free fatty acids, are synthesised in the hair matrix cells (Coderch, 2007). These internal lipids, found in the cell membranes, stabilise the hair matrix cell complex and function as a barrier to external materials and environmental damage (Grubauer, 1989, Hilterhaus-Bong, 1989, Körner, 1995, Swarzeneruber, 1989). Some studies suggest that hair lipids may also have a role in fluidising cell membranes, cell diffusion, cell cohesion and mechanical strength (Braida, 1994, Philippe, 1995, Sideris, 1990).

In 2005, a study of hairs from cancer and normal subjects by Fourier transform infrared attenuated total reflection (FTIR-ATR) provided independent validation of the underlying hypothesis that hair from individuals with breast cancer exhibits a

structural abnormality (Lyman, 2005). When the FTIR-ATR spectra of hairs from subjects with cancer were compared with the spectra of hairs from non-cancer subjects, differences in the amide I region [1750-1450 cm^{-1}] and the C-H overtone region [1500-1300 cm^{-1}] were observed. Interpretation of the spectra of these regions led the researchers to conclude that there was a modification of the hair fibre growth as a result of the presence of a developing cancer. The changes in the amide I region were indicative of an increase in beta-sheet disorder content compared to alpha-helical structures. The changes in the C-H overtone region were suggestive of an increase in lipid content. When unknown samples were analysed by reference to these two regions of the resulting spectra, the researchers were able to correctly identify all of the cancer patients.

As stated above, Lyman and Murray-Wijelath noted that part of the alteration in FT-IR spectroscopic profiles of hair from breast cancer patients was due to increased lipid content (Lyman, 2005), supporting the proposition by Bertrand *et al* that the circular features present in X-ray diffraction patterns were lipid-based (Bertrand, 2003).
Thus, the most likely explanation for the presence of the "ring" is an incorporation of lipid into the fibre.

1.16. Fundamentals of lipidomics

The field of lipidomics is an ever-expanding sector of metabolomics, which uses a variety of platforms to answer biological questions. Although it known that lipids have structural roles and are heavily involved in energy storage, the fundamentality of their roles in cellular signaling and regulation processes are now emerging (Hannun, 2008, van Meer, 2008, Wymann, 2008). Lipid structure largely determines their biological property and thus their role in the cell; therefore, any fluctuations in their profiles may lead to various pathophysiological conditions (Fahy, 2005).

Lipid extraction from biological samples requires the use of solvent. Membrane-bound lipids need polar solvents (ethanol, methanol) to disrupt the hydrogen bonds and for the lipids to be released, where as, other lipids can be extracted using non-polar solvents such as chloroform or diethyl ether (Han, 2003). There are many

methods of extraction but the most commonly used is the Folch method which was further adapted to create the Bligh and Dyer method which allowed lipid extraction to take place in a single vial. Both methods involve the homogenisation of the sample and the addition of chloroform and methanol for the extraction of lipids and the discarding of the upper phase once the solvents are mixed with the sample and centrifuged (Bligh, 1959, Folch, 1957). To understand how lipids function in health and disease, lipids must first be identified and quantified. There are many platforms to do this but to profile human samples for their lipid metabolome is highly challenging due because of the diversity and complexities of lipids (Fernie, 2004). There are likely to be tens of thousands of possible lipid species in the cellular lipidome and so there are multiple approaches to profiling of lipids from biological samples.

The two main approaches are untargeted and targeted analysis; An untargeted analysis is an unbiased approached which is based upon a question, whereas a targeted analysis has a predetermined set of lipids as a focus to demonstrate a proof of concept (Figure 1.8) (Tan, 2009a, Tan, 2009b). The untargeted approach profiles broadly to identify and filter out lipids of interest, as opposed to a targeted approach, which identifies predefined lipids using a particular technique. As the parameters are already predefined, a targeted approach can be much more straightforward because the method validation period can be short and the lipids are quantified in the sample matrix (Loizides-Mangold, 2013).

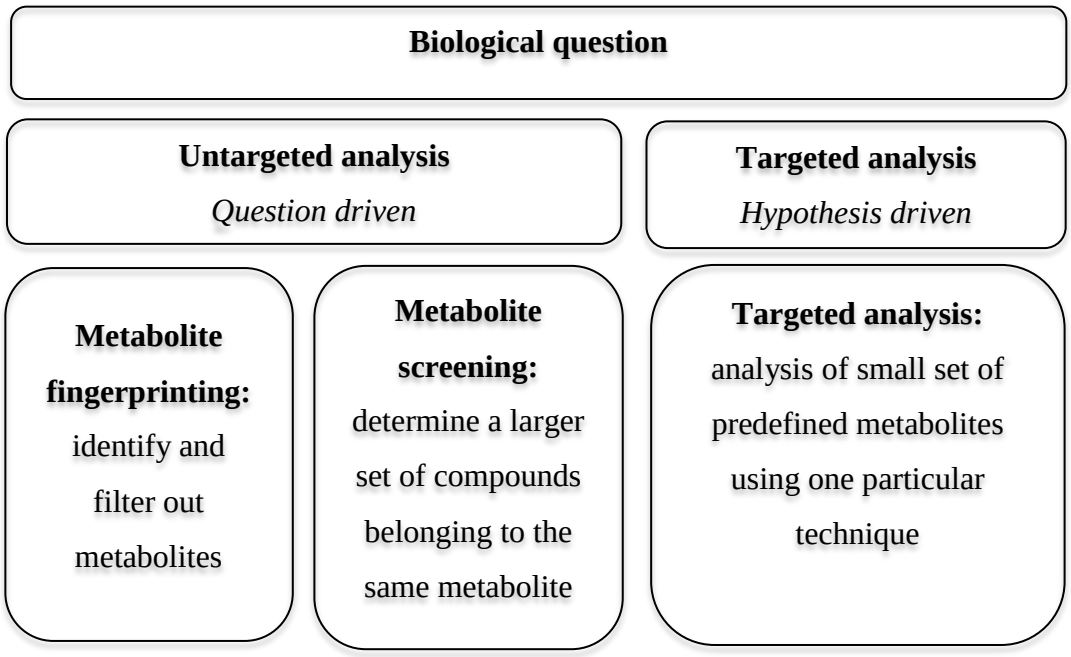


Figure 1.8: Approaches to metabolomics (adapted from (Loizides-Mangold, 2013)).

Lipidomic studies primarily utilise analysis by mass spectrometry, as this is the technique that allows the most sensitive and selective identification and quantification of a variety of lipids (Ryhage, 1960). As there are so many possible lipid structures that may be found in a sample, lipidomics analysis aims to define as many lipids as possible as it is not yet feasible to detect and quantify the entire cellular lipidome (Wenk, 2005). Different lipid classes have particular fragmentation patterns and ionisation competencies and this makes establishing a standardised methodology for all lipids very difficult. Therefore, there is no definitive mass spectrometry approach to detect all biological lipids species and multiple techniques and platforms are utilised in lipidomic studies (Li, 2011).

Mass spectrometry measures the molecular mass of a sample using three functional components: an ionisation source, an analyser and a detector (Figure 1.9) (Ashcroft, 2014). The sample is injected into the ionisation source where molecules of the sample are ionised making them easier to manipulate than neutral molecules (Scott, 2014). The ions then enter the highly vacuumed region of the spectrometer, the analyser and detector. This vacuum ensures that the ions travel through the instrument without an interference from air molecules. The analyser separates the ions according to their mass to charge ratio (m/z) and they are identified on the detector as a signal

on an attached computer. The m/z ratios along with the relative abundance present the sample as an m/z spectrum and allow qualitative and quantitative detection.

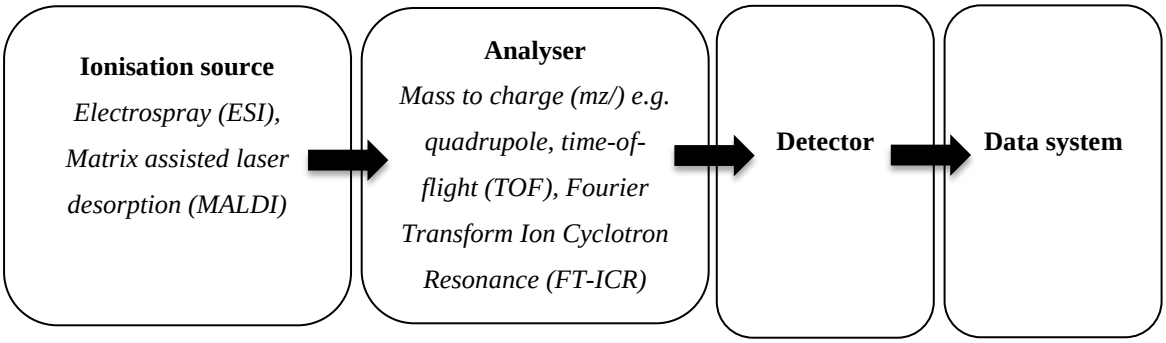


Figure 1.9: schematic representation of mass spectrometer, adapted from Ashcroft, 2014 (Ashcroft, 2014).

The two most commonly used methods of introducing the sample to the ionisation source are electrospray ionisation (ESI) and matrix associated laser desorption ionisation (MALDI) (Hunt, 1998). These methods form aerosol particles from a liquid sample and then into bare ions. ESI uses a very fine capillary to expel the liquid as an aerosol mist (Han, 2003). MALDI involves co-crystallising the sample with a UV-absorbing matrix, which absorbs laser radiation resulting in vaporisation of the analyte (Fuchs, 2010). Both techniques are soft ionisation methods which keep the molecular ions intact, but ESI allows the formation of multiply charged molecular ions, whereas MALDI leads to the formation of singly charged molecular ions (Hunt, 1998). Samples can be directly introduced into the ionisation source or can go through chromatography, such as liquid, gas or capillary electrophoresis, on its way to the ionisation source, which allows the sample components to enter the instrument sequentially for separable and specific analysis and more accurate identification of the species (Park, 2007b). Although this step can be omitted it does allow for a more comprehensive resolution of species from complex sample and consistent quantification because the chromatogram is represented by a distinctive retention time and specific m/z.

The analyser is required to separate the ions after ionisation. There are a variety of mass analysers, which differ in their m/z ranges and their ability to achieve certain resolution that can be used including quadrupole, time-of-flight (TOF) and Fourier Transform Ion Cyclotron Resonance (FT-ICR) (Scott, 2014). Some mass spectrometers have multiple analysers, which fragment the sample inside the instrument and can therefore give further information about the structure of the lipids within a sample. They are called tandem mass spectrometers and the most commonly used are the triple quadrupole and the quadrupole time-of-flight (Scott, 1988). The detector amplifies and records the ion current as a signal, which is transmitted to the data system as a mass spectrum (peak). The number of lipids, their class and relative abundance are then generated when the m/z values are plotted against their intensities. The plot of the retention time against the m/z can quickly and thoroughly examine the changes between groups in a study (Schwudke, 2007).

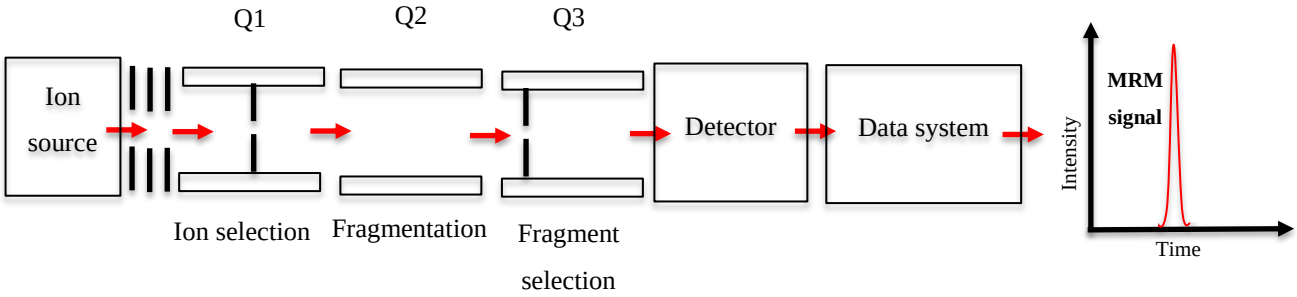


Figure 1.10: Schematic diagram of a triple quadrupole mass spectrometer with multiple analysers adapted from Ashcroft, 2014 (Ashcroft, 2014).

In a triple quad such as the one used in this study the first analyser (Q1) separates ionized fragments according to their mass and pass into the second analyser (Q2) where they are further fragmented using collision ionisation. The new fragments then move to the third analyser (Q3) where the fragments are isolated into individual masses and identified by the detector as a spectrum (Schwudke, 2007). This allows selection of specific fragments from the first analyser to be chosen for further analysis by the next two analysers resulting in resolution of selective lipids from complex samples. Ion scans can only be acquired one at a time and so the analysis is repeated to profile all the different lipid classes in a study (Scott, 1988).

Using liquid chromatography coupled with mass spectrometry (LCMS) to identify novel biomarkers in complex biological samples can be time consuming and can require a targeted approach, which is focused on a few metabolite species. This is achieved using precursor scans which target a specific class of lipids by focusing on certain fragments and neutral loss ion scans which identifies those lipids that lose the same fragment upon collision in a triple quad mass spectrometer (Ashcroft, 2014).

Raw data from the mass spectrometer is processed using commercial software, which contains information about the masses identified from the precursor scans and subsequent analysis. This data is then matched against an internal lipid library containing potential lipid species identification. Although it is very useful, it can be limiting due to the lack of comprehensive lipidomic data available (Yetukuri, 2007, Hartler, 2012).

1.17. Hypothesis on how breast cancer-associated lipids are incorporated into hair

The theory underlying this thesis is that in breast cancer there is an increase in phospholipids in the hair fibres of afflicted individuals, which is also reflecting an alteration in their serum lipid profile.

1.18. Implications

If this hypothesis is correct then the lipids incorporated into the hair fibre can be detected directly in serum and therefore used as a biomarker for the disease. This thesis aims to elucidate the composition and alteration of breast cancer associated lipids in hair and serum.

1.19. Aims

1. To identify the lipid(s) in hair fibres that are associated with breast cancer
2. Compare the identified lipid(s) in the hair from the same patient with breast cancer and relative controls.
3. To assess the potential of the identified lipid(s) as specific biomarkers for breast cancer *in vitro* and clinically.

2. Preliminary data

2.1. Introduction

In 1999 a correlation between the presence of breast cancer and an observed change in the X-ray diffraction (XRD) pattern of hair from afflicted individuals was reported (James, 1999). Using synchrotron-generated X-rays, the diffraction patterns of hair samples collected from women diagnosed with breast cancer all exhibited a circular feature specific to the pathological state. This observed change presented as a new circular feature (in a specific region of 4.6 Angstroms) superimposed on the normal X-ray diffraction pattern of hair (Figure 2.1).

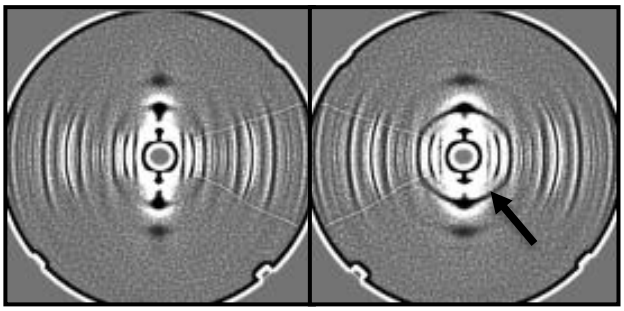


Figure 2.1: XRD patterns of hair from a healthy woman (left) and from a woman with breast cancer (right). The arrow indicates the altered feature in the breast cancer patient's hair, referred to as the "ring". These patterns were taken on the SAXS beamline at the Australian Synchrotron. This pattern is consistent with those reported by Corino *et al* in 2009, who demonstrated that the feature was present in greater than 60% of patients with breast cancer (Corino, 2009).

Of the samples taken from patients not suspected of having breast cancer, 86% of the diffraction patterns were normal. Further studies by James *et al* in 2005, using a xenograft model of breast cancer in nude mice, indicated that the diffraction change specific to breast cancer was observed in hair or whiskers in early stages of tumour development. The data illustrated that the change occurred within days of cell implantation and provided support for the potential that this technique could be used as an early diagnostic test for the presence of breast cancer (James, 2005b). Other groups, independent of the original discoverer, reported their inability to reproduce similar results to those obtained in the initial study (Briki, 1999, Laaziri, 2002). Some

subsequent studies by other groups however, confirmed an association between the XRD hair pattern alteration and the presence of breast cancer, although the initial reported accuracy was not attained (Corino, 2008, Corino, 2009). The authors agreed, with other independent groups, that that the analysis and interpretation of the data is complex and requires strict adherence to the methodology to ensure accurate reproduction (James, 2003a, James, 2001b, James, 2003b, James, 2003c).

The biological mechanisms leading to the "ring" phenomenon have not been identified. Speculations on the origin of the "ring" have included that it is derived from calcium-associated soap residues (Bertrand, 2003, Trounova, 2002) in the hair fibre, or from the interaction of hair tissue and calcium with proteoglycans, which cause a structural transformation of the extracellular matrix in the cortex of the hair fibre (Vazina, 2005).

Two groups have proposed that the "ring" shown by the James group was lipid in nature. In 2003, Bertrand *et al* simply referred to the breast cancer-associated feature shown by James and colleagues as "*hair lipid diffraction rings*" (Bertrand, 2003). A study of hairs from cancer and normal subjects by fourier transform infrared attenuated total reflection provided independent validation of the underlying hypothesis that hair from individuals with breast cancer exhibits a structural abnormality. Interpretation of the spectra of these regions led the researchers to conclude that there was a modification of the hair fibre growth as a result of the presence of a developing cancer. The changes in one of the regions of interest were suggestive of an increase in lipid content (Lyman, 2005). The fact that the XRD feature associated with breast cancer is a "ring" gives some clues as to its chemical nature; a circular feature (a "broad halo") in an XRD pattern can be produced by an amorphous material such as oils (Clark, 1927). Thus, a possible explanation for the presence of the "ring" in the XRD patterns seen in the hair from breast cancer patients is an incorporation of lipid into the fibre.

2.2. Aims

In this study we conducted a range of experiments to determine if the feature, seen in the X-ray diffraction pattern on hair in breast cancer patients, was related to lipids, and if so, what is the nature of the lipids.

2.3. Methods

2.3.1. X-ray diffraction of hair

2.3.1.1. Samples

Donated human hair samples were cut close to the scalp from a total of 18 individuals whose breast cancer status was determined by mammography. Women were excluded if their scalp hair had been dyed or chemically treated.

2.3.1.2. Synchrotron X-ray diffraction

X-ray diffraction assessment required the analysis of individual hair fibres from each subject, which were loaded onto specially designed sample holders. Synchrotron X-ray diffraction experiments were carried out as described in previous publications (Corino, 2008) on the Small Angle X-ray Scattering - Wide Angle X-ray Scattering (SAXS-WAXS) beam line at the Australian Synchrotron, Melbourne. A MAR165 detector was used online to aid in the alignment of the sample and also for data collection.

2.3.1.3. Image analysis

Image analysis was performed according to that described previously (Corino, 2008). Diffraction patterns were analysed using FIT2D (www.esrf.fr/computing/scientific/FIT2D) and Saxs15ID software programs. Both programs offer the data processing and smoothing routines that are required to perform the data reduction and subsequent analysis. Background correction was carried out without compromising any of the features present in the original pattern using FIT2D. One-dimensional data was extracted from each XRD pattern and presented in the form of a graph alongside the corrected image. Samples were determined as either "positive for breast cancer" or "negative for breast cancer" by examination of the resulting XRD patterns by two trained analysts who were not provided with the clinical status of the patient. A negative call was one where the circular feature was not present in the pattern but the underlying keratin reflections were. A positive call was one where the circular feature was present at a q space of 1.32 +/- □0.02 angstroms along with the underlying keratin reflections. A standard set of hairs was used (hairs from patients confirmed to have breast cancer and confirmed to be free of breast cancer) to calibrate the assay. The pathology results (following biopsy) were forwarded to an auditor. The diffraction analyses were separately forwarded to the independent auditor, who de-coded the results, matched the imaging and pathology results with the XRD data, and communicated the results to the investigators.

2.3.1.4. Addition of fatty acids to hair

In order to attempt to recreate the feature seen in the XRD pattern of hair using lipids, hair fibres from subjects confirmed to be free of breast cancer were initially checked by SAXS to confirm the absence of the circular feature associated with breast cancer. Each fibre was removed from the holder and soaked in olive oil for 10 minutes, then patted dry with tissue paper and re-exposed to the SAXS beam for another 20 seconds. The resulting image was analysed for the presence or absence of a breast cancer-associated feature.

2.3.1.5. Chemical enhancement of lipids in hairs and solvent extraction of hairs

Two hair fibres from each patient with breast cancer were soaked in 5ml of 100% acetone for 5 minutes to remove external lipids. They were then washed in 5ml of water for 5 minutes. This was repeated three more times. They were patted dry with tissue paper, mounted in the sample holder and exposed to the SAXS beam for 20 seconds. The resulting image was analysed. For each sample with the circular breast cancer-associated feature, the two fibres were treated differently:

- One hair fibre from each patient was soaked in 4ml chloroform: methanol (1:2) for 2 hours.
- The other hair fibre from each patient was soaked in 4ml acetone for 5 minutes, wiped dry and exposed to the SAXS beam for 20 seconds, and then soaked in 4ml of unbuffered 0.1M/L of lead nitrate for 3.5 hours.

All fibres were then washed in 10ml of water for 5 minutes. This was repeated three times. Hairs were wiped dry and exposed to the SAXS beam for 20 seconds. The resulting image was analysed for the presence/absence of a breast cancer-associated feature.

2.3.2. Lipid profiling of hair

2.3.2.1. Samples

Seven hair samples from breast cancer patients were pooled according to their cancer stage (P1-P3) and five healthy un-pooled controls (H1-H5) were chosen for lipid extraction. Replicates were taken from each sample.

2.3.2.2. Extraction of lipid from hair

The protocol used for lipid extraction from samples is a monophasic extraction, modified from the Bligh and Dyer protocol (Bligh, 1959).

Hair samples were cut very finely using surgical grade scissors and placed into a glass vial. Samples were then washed in acetone for five minutes to remove exterior fatty acids. 30mg of air-dried sample were weighed into cryomill tubes and 1000 µL of extraction solution (methanol, chloroform, water (2:1:0.6)) was added into each tube. Samples were spiked with 10µL of 100µM internal standard (Cholesterol ester (18:0) d) to 10µM final concentration. Hair was ground using a cryomill (Precellys) with 1.4 mm ceramic beads at 6800 rpm for three times 30 second with 45 second between intervals and the samples were centrifuged for 10 minutes at 10000 rpm. Supernatant (500 µL) was transferred into Eppendorf tubes and dried in a speed-vac. Samples were resuspended in 100µl of n-butanol and methanol (v/v 1:1), centrifuged for 10 min at 1 0000 rpm and 50 µL of supernatant transferred to high pressure liquid chromatography (HPLC) vials for further analysis.

2.3.2.3. Liquid Chromatography Mass Spectrometry (LCMS) analysis of hair

Lipids were separated by injecting 5µL aliquots onto a 50 mm × 2.1 mm × 2.7 µm Ascentis Express RP-Amide column (Supelco) using an Agilent LC 1200. Briefly, sample elution was performed at 0.2 mL/min over a gradient of 50% water (v/v)/methanol 20% (v/v)/tetrahydrofuran 20% (v/v) to water/methanol/ tetrahydrofuran (5:20:75, v/v/v). Lipids were analysed by electrospray ionisation-mass spectrometry (ESI-MS) using an Agilent Triple Quad 6460. The mass spectrometer was set up to specifically identify phosphatidylcholines. The capillary voltage used was 4000 V, fragment or voltage 140 – 380 V, and collision energy 15–60 V. The collision gas throughout was nitrogen at a rate of 7 L/ min. LCMS data was processed using an Agilent MassHunter quantitative software.

2.3.2.4. Data processing for all LCMS data

Mass spectra data was collected from Agilent QQQ 6460 mass spectrometer in positive mode and negative mode. The MRM data was processed using Agilent MassHunter software to generate the peak area values for each lipid species. All the masses that were present in blanks were deleted. Data was normalised to the median and weight of samples. Replicates were averaged. Samples in each lipid species were averaged and graphed as bar charts with standard deviation error bars.

2.3.1. Lipid nomenclature

Lipids in this study were putatively identified using Agilent MassHunter software, which labels lipids based on their mass. In this study lipids are labeled with the head group and presented as the total number of carbons in the fatty acid chains (R1+R2) and the total number of double bonds in the fatty acid chains (n1+n2). So phospholipids will be represented as PL(R1 + R2 : n1 + n2) (Fahy, 2005). There are a number of variations and combinations that the lipids can form in the biological environment and although many have a confirmed identity in plasma (Quehenberger, 2010, Meikle, 2011), there are still many unknown species that may be present but have not been reported in the literature. Putatively assigned lipids require further analysis by tandem mass spectrometry in order to validate their structure and therefore their identity.

2.4. Results

2.4.1. Addition of fatty acids to hair

XRD of hair before and after soaking in olive oil showed that a circular feature similar to the previously reported breast cancer-associated feature could be induced and suggested that the feature was lipid in nature (Figure 2.2). There was some variability in the strength of the olive oil-induced feature. This variability could be attributed to the differential uptake of oil into the hair fibre due to the individual variability in structural features such as in the arrangement of the cuticle and intermediate filaments of the fibres. Cuticles that are more tightly packed are less likely to absorb as much external lipid as those cuticles that are more loosely packed.

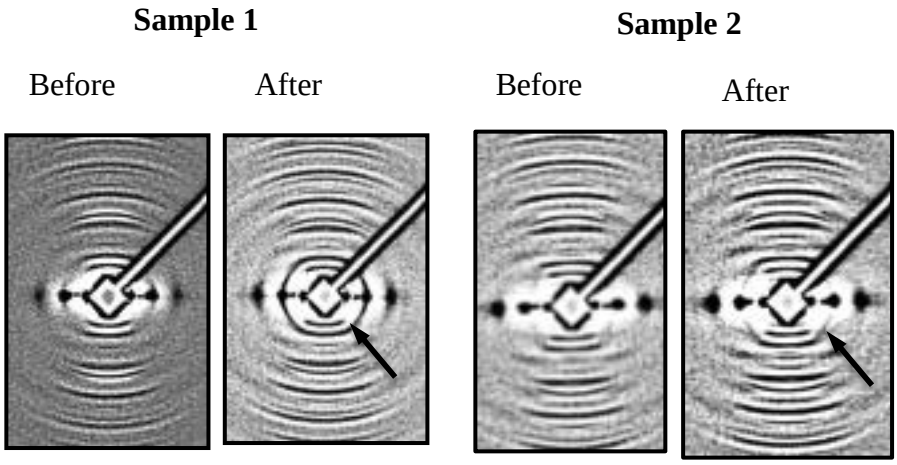


Figure 2.3: Addition of fatty acids to hair (n=6). In the first experiment, hair that did not have a " "ring" " (confirmed by XRD) (before) was soaked in olive oil for 10 minutes, wiped dry, and then re-exposed to X-rays. A clear "breast cancer-like ring" was seen post-oil application (after, arrow indicates breast cancer-associated feature).

2.4.2. Chemical enhancement of lipids in hairs and solvent extraction of hairs

Chloroform and methanol solutions are used routinely to extract lipids from biological samples (Seppanen-Laakso, 2009). When hair fibres, which initially exhibited the feature, were soaked in chloroform: methanol (1:2), the intensity of the feature diminished in XRD analysis compared to pre-exposure to the solvent solution. No other component of the pattern was similarly diminished, indicating that the molecular nature of the feature was susceptible to solvent extraction (Figure 2.3). Out of the 15 samples (and replicates) this "extraction" occurred in 9 of the samples.

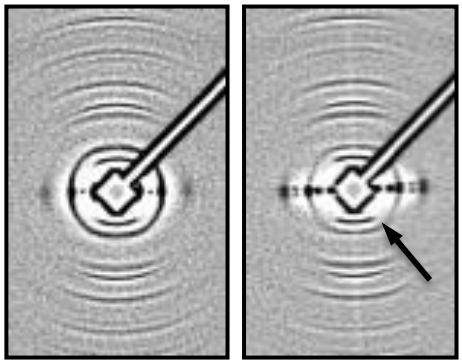


Figure 2.4: Solvent extraction of hairs. Hairs from breast cancer patients, with XRD alterations (left), were treated with chloroform/methanol, a solvent solution known to extract lipids. The intensity of the "ring" was diminished (right) and the other (keratin-associated) features in the patterns were not affected. Arrow indicates location of the breast cancer-associated feature.

Lead has been shown to enhance the intensity of lipid-derived features (corresponding to the "ring" that we see in our data) in the XRD pattern of hair (Bertrand, 2003). This is thought to be due to the binding of lead ions to free fatty acids. Lead nitrate-treated hairs show an enhancement of the intensity of the "ring" and an additional reflection of the "ring" in 5 out of the 15 samples (Figure 2.4). Again, in both experiments, the variation in chemical absorption could be attributed to the structural differences between hairs from different individuals.

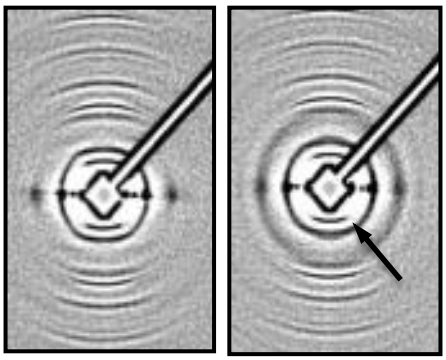


Figure 2.5: Lead nitrate treatment of hair. When hairs, which produce the "ring" in XRD, were soaked in lead nitrate solution, the intensity of the rings was enhanced and reflected in another circular feature around the original one. Lead nitrate has been shown to bind to lipids in hair and reflect the diffraction pattern (Bertrand, 2003). Arrow indicates location of the breast cancer-associated feature.

2.4.3. Extraction of lipid from hair

When samples of hair from breast cancer patients and controls were extracted and then analysed for phosphatidylcholine lipid species, using liquid chromatography mass spectrometry (LCMS), the profiles showed that overall, the level of particular species of phosphatidylcholine were higher in the hair of breast cancer patients than in controls (Figure 2.5). Some of the lipids found to be significantly different were PC18: 6 (p= 0.0023), PC30:0 (p=0.0314), PC 32:0 (p=0.0417), PC 32:6 (p=0.0064) and PC 23:4 (p=0.0333), which showed the most, marked change in breast cancer compared to hair from healthy controls.

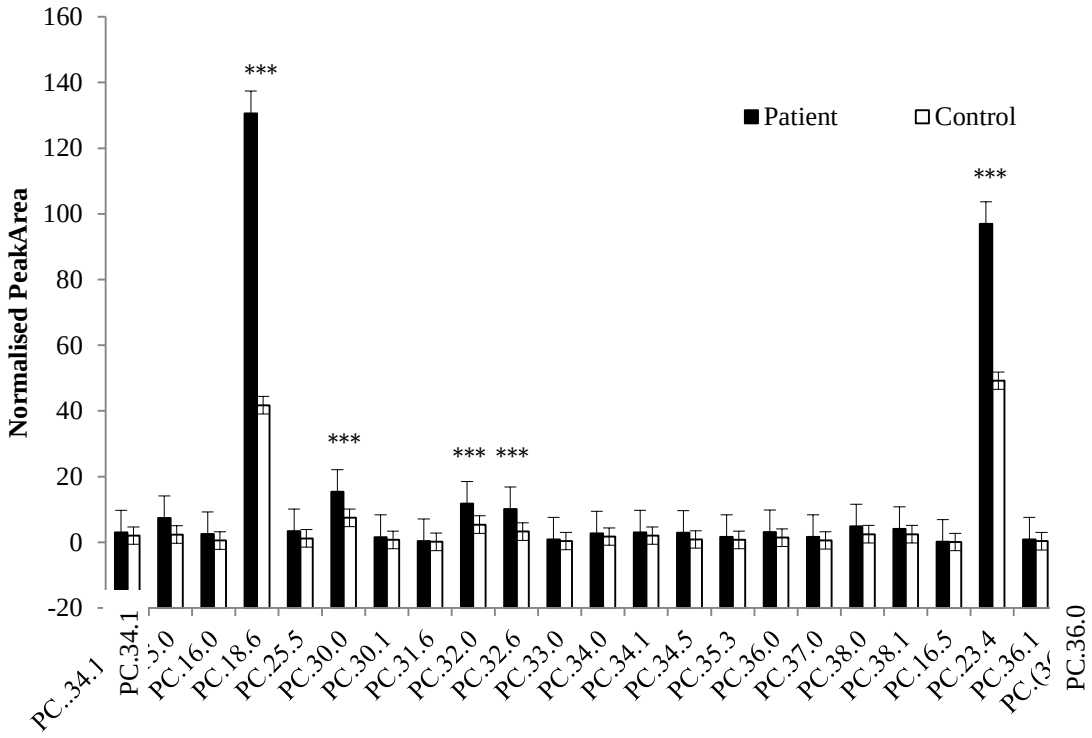


Figure 2.6: Average concentration of specific phosphatidylcholine (PC) species in hair samples collected from patients with breast cancer and controls, where an asterix indicates significantly different levels of specific phospholipids (n=8).

2.5. Discussion

This is the first study to report that breast cancer-associated changes seen in XRD analysis of hair samples are of lipid origin, in particular phospholipids.

To demonstrate that a similar feature to that reported for XRD analysis of hair from breast cancer patients could be added to hair samples *ex vivo,* olive oil was applied to hair samples that did not demonstrate the breast cancer "ring", and subsequently the presence of a "ring" in those samples was reported. Olive oil was used because it is the vegetable oil that is most similar to human fatty acids (Robbins, 2002). Interestingly, olive oil contains significant amounts of phospholipids, including phosphatidylinositol (PI) (Hatzakis, 2008). We were able to remove the "ring" from a majority of samples using a range of organic solvents known to solubilise lipids. The XRD intensity of the "ring" was also enhanced in several of the breast cancer positive samples using a chemical known to bind to lipids. Not every sample reacted the same to the treatments, and this was likely due to the variation in the ability of the solvents and chemicals to penetrate the hair fibre, which could be attributed to the individual differences in the cuticle density packing.

In attempting to characterise the lipid(s) associated with breast cancer, mass spectrometry was used on hair samples that had been extensively extracted using a cryomill, to overcome the individual extractability variation. This showed that there is significantly more phosphatidylcholine present in the hairs of breast cancer patients when compared to controls. It could be that the tumour in the breast produces and releases phospholipids, probably from the tumour cell membrane, which enter the circulation and are incorporated into the matrix of the hair fibre resulting in an alteration in the pattern represented by a circular feature when the hair is subjected to XRD.

There are several lines of evidence which support this proposal and suggest that lipogenesis is closely linked to tumourigenesis. BRCA1 (breast cancer susceptibility gene 1) was the first susceptibility gene linked to breast and ovarian cancer (Miki, 1994a). It is frequently lost in breast cancer. In 1999, James also reported that women who tested positive for a mutation of the BRCA1 gene also showed the alteration in their hair XRD pattern (James, 1999). A study by Moreau *et al* demonstrated that

BRCA1 negatively regulates lipogenesis through binding to the phosphorylated and inactive form of acetyl coenzyme A carboxylase (P-ACCA) (Moreau, 2006). Thus there is a link between loss of BRCA1 and increased lipogenesis.

A number of other groups have also suggested that lipogenesis is closely linked to tumourigenesis in breast cancer. Chajes *et al* examined lipids in breast cancer tissues in comparison to normal tissue from the same patients and found that mechanisms specifically related to malignant transformation and tumour progression influence the membrane fatty acid profile of breast carcinoma (Chajes, 1995). A mouse study showed similar effects. Only mammary tumour tissues showed a drastic increase in the total phospholipid content ($p<0.0001$) associated with a significant upregulation of phosphatidylethanolamine (PE), phosphatidylcholine (PC), and sphingomyelin (SM) ($p<0.05$) (Monteggia, 2000). Breast cancer has been associated with increased levels of PC in several studies which have suggested it can serve as a biomarker of breast cancer reflecting upregulation of specific choline transporters and choline kinase genes (Eliyahu, 2007). The level of PC in human breast cancer cells has been reported to be 10-fold higher than in normal mammary epithelial cells (Katz-Brull, 2002).

In addition to being upregulated in breast cancer tissues and in cultured breast cancer cell membranes, it has been reported that lipids are also elevated in serum. In 1971 Feldman and Carter reported the association between serum lipids and breast cancer (Feldman, 1971). More recently, Alexopoulos *et al* found that there was a significant difference in serum phospholipid content between stage-IV breast cancer patients and disease-free individuals. The most significant differences in lipid profiles among disease-free and cancer subjects were attributed to three phosphocholine (PCho) species (precursors to PC) and to three unidentified fatty acid species (Alexopoulos *et al*., 1987). Serum lipids elevated in breast cancer decrease significantly after treatment (Ray, 2001), in a parallel fashion to the reported disappearance of the "ring" following mastectomy and chemotherapy (Corino, 2008). There are no reports, which have looked at whether elevated levels of phosphocholine in serum are also seen in hair from the same patient.

The results presented in this study are from a very small sample size designed as a pilot study to establish the nature of the circular breast cancer-associated XRD feature and formulate an idea of the likely lipids involved. The data suggests that phosphatidylcholine, and in particular sub-species thereof, is the most likely candidate, however, the possible association of other phospholipid molecules needs to be investigated and an understanding of the relationship between lipid shedding and the cancer process needs to be elucidated in a larger sample size. Furthermore, it is possible that hair from patients with other cancers may also exhibit incorporation of cancer-associated phospholipids. Therefore in future studies on breast cancer it would be necessary to rule out the presence of other cancers in the patients from which the hair samples have been collected. This data illustrates that the breast cancer-associated feature, seen in the XRD pattern of hair, is phospholipid in nature.

3. Lipid extraction from cell culture supernatant

3.1. Introduction

Some of the first reports of elevated levels of phospholipids were reported in the serum of patients with breast cancer when compared to controls (Feldman and Carter, 1971); (Bani, 1986). A more recent study, which used electrospray ionization mass spectrometry, reported that there was a two-fold increase in phosphatidylcholine in the serum of patients with breast cancer when compared to controls (Hammad, 2009). There is considerable evidence that some phospholipids (PC, PE) and their precursors (PCho, phosphoethanolamine (PEth)) are elevated in breast cancer cell lines and tissue with some studies suggesting the source of these serum lipids is likely to be the breast tumour itself, as some species of phospholipids have been found to accumulate in the breast cancer cells (Aboagye, 1999, Chajes, 1995, Eliyahu, 2007, Hilvo, 2011, Katz-Brull, 1996, Katz-Brull, 2002, Monteggia, 2000, Podo, 1999, Singer 1995, Ting, 1996, Tse, 2007).

Lipogenesis was shown to be associated with breast cancer tissue when compared to surrounding healthy tissue due to the increased levels of lipids in the cell membrane of the tumour tissue. Whether this influence was causative or associative was not clear but the authors suggested that it was to promote tumour progression (Chajes, 1995). An increase in total phospholipids was found using magnetic resonance spectroscopy (MRS) in tumour tissue when compared to the control tissue (Hilvo, 2011, Monteggia, 2000). These elevations were significant for three species of phospholipids, phosphatidylethanolamine (PE), phosphatidylcholine (PC), and sphingomyelin (SM) (Hilvo, 2011). Another study on breast and tumour tissue found that the distribution of individual phospholipid species varied and was "*not uniform, reflecting micro environment differences*" due to the integration of tumour tissue into healthy breast tissue (Smith, 1991). The same group also found that the level of PC was 28% higher in high-grade tumour tissue when compared to low-grade tumour tissue, but that PE was not associated with tumour grade (Smith, 1993). Choline metabolism has also been shown to be up-regulated in breast cancer cells (Aboagye, 1999). Singer *et al* used magnetic resonance spectroscopy (MRS) to measure key metabolite levels and fluxes through enzymes regulating phospholipid and mitochondrial metabolism in normal human mammary epithelial cells (HMEC) and

compared these values to those found in a progression series of breast cancer cell lines of varying metastatic potential established from a single patient. They found a 16-19-fold increase in phosphocholine (PCho), a precursor of PC, content in two primary breast cancer cell lines and a 27-fold increase in PCho content in a metastatic breast cancer cell line compared with normal breast epithelial cells (Singer 1995).

3.2. Aims

Preliminary studies (Chapter 2) have demonstrated that phospholipids have also been identified in the hair of patients with breast cancer and the hypothesis being investigated in this project is that these phospholipids reach the hair from the tumour via the bloodstream. Cell culture is a contained environment, which allows the analysis of those metabolites specifically associated with the tumour cells. It is therefore likely that the potential lipids of interest (i.e. those associated with breast cancer cells) will be present in the cell culture supernatant. This theory was tested in cell culture models of breast cancer and we expected to see increased phospholipids in supernatant from breast cancers cells compared to normal epithelial mammary cells. This chapter outlines a study, which examined the species of lipids, and their relative levels in the cell culture supernatant of a cell line derived from a patient with breast cancer and a cell line derived from an individual free of the disease. These cell lines were selected as one is established from a highly invasive breast cancer and the other from a healthy control.

3.3. Methods

3.3.1. Lipid profiling of cell culture

3.3.1.1. Samples

Cell lines purchased from America Type Culture Collection (USA). MDA-MB-231 (Caucasian female, 51 years old) is a metastatic breast cell line cell line. MCF-10-A (Caucasian female, 36 years old) is a non-tumourigenic breast cell line. In addition, serum free RPMI media and DMEM media were also used as controls in this study.

3.3.1.2. Cell culture

MDA-MB-231 were cultured using RPMI media (Invitrogen) supplemented with 8% Foetal Bovine Serum and 2% L-glutamine. MCF-10-A cells were cultured in DMEM media (Invitrogen) with 10% Foetal Bovine Serum, 1% L-glutamine, 0.125% Humulin, 1% Hydrocortison, 0.1% Cholera Toxin and 20 ng/ml Epidermal Growth Factor. The medium was replaced every 2 days and once the cells reached approximately 80% confluence, the cells were removed using trypsin (0.05% EDTA, 0.25% trypsin; Sigma) and reseeded. Cells were passaged using above media until 50% confluent, after which cells were passaged and grown in serum free media (media as above without Fetal Bovine Serum). The supernatant was collected after 2 days. Supernatant was centrifuged for 5 minutes at 1500 rpm and the supernatant was stored in glass vials at -80˚C until use. Cells in flasks were counted using trypan blue. (MDA-MB-231: 2.68 x 10^8 / 50ml, 0.052/ml ; MCF-10-A: 3.20 x 10^8 / 75ml, 0.043/ml). There were two replicates for each cell line.

3.3.1.3. Extraction of lipid from cell culture

The protocol used for lipid extraction from samples is a monophasic extraction, modified from the Bligh and Dyer protocol (Bligh, 1959).

Samples were thawed to room temperature and 1000 µL of cell culture supernatant was added to 1000 µL of extraction solution (methanol, chloroform, water (2:1:0.6)) into a 2.0ml Eppendorf tube. Samples were spiked with 10ul of 100 µM internal standard (Cholesterol ester (18:0) d) to 10µM final concentration. Then 10 µL of 100 µM of CE (d8) and 10 µL of 100 µM of Arachidonic (d4) acid were added. The samples were vortexed for 5 minutes and shaken at 37˚C for 45 minutes. All vials were centrifuged at 10,000g for 5 minutes and the supernatant was transferred to a clean tube. The supernatant was dried in a speed-vac and resuspended in 200ul of n-butanol and methanol (v/v 1:1), centrifuged for 10 min at 10000 rpm and 50 µL of supernatant transferred to high-pressure liquid chromatography (HPLC) vials for further analysis.

3.3.1.4. Liquid Chromatography Mass Spectrometry (LCMS) analysis of cell culture supernatant

Lipids were separated by injecting 5µL aliquots of the prepared sample onto a 50 mm × 2.1 mm × 2.7 µm Ascentis Express RP-Amide column (Supelco) using an Agilent LC 1200. Lipid samples were eluted at 0.2 $mLmin^{-1}$ over a 5 min gradient of water/methanol/tetrahydrofuran (50:20:30, v/v/v) to water/methanol/tetrahydrofuran (5:20:75, v/v/v), with the final buffer held for 3 min. Lipids were analysed by electrospray ionisation-mass spectrometry (ESI-MS) using an Agilent Triple Quad 6460. The mass spectrometer in the positive mode was set to scan in precursor ion mode to identify phosphatidylcholines (precursors of m/*z* 184.1), sphingomyelins (precursors of m/*z* 184.1), ceramides (precursors of m/*z* 264.6), cholesterol esters precursors of (m/*z* 369.4), phosphatidylglycerols (precursors of m/*z* 189) and in the negative mode phosphatidylinositol's (precursors of m/*z* 241). The mass spectrometer was set to scan in neutral loss mode to identify phosphatidylethanolamines (loss of m/*z* 141 in the positive ion mode) and phosphatidylserines (loss of m/*z* 87 in the negative ion mode). Multiple reaction monitoring (MRM) scans were used to quantify

the identified lipids with the capillary voltage, fragmentor voltage, and collision energy were 4000 V, 140 – 380 V, and 15–60 V, respectively. In all cases, the collision gas was nitrogen at 7 $Lmin^{-1}$. LCMS data was processed using an Agilent MassHunter quantitative software.

3.3.1.5. Data processing for all LCMS data

Mass spectra data was collected from Agilent QQQ 6460 mass spectrometer in positive mode and negative mode. Refer to Appendix 8.6.1 for ESI mode, ion scan mode and chromatograms of the standards. Refer to Appendix 8.2.1. for raw data. The MRM data was processed using Agilent MassHunter software to generate the peak area values for each lipid species. All the masses that were present in blanks were deleted. Data was normalised using the cell count as follows: MDA-MB-231: 2.68 x 10^8 / 50ml = 5360000 /ml and MCF-10-A: 3.20 x 10^8 / 75ml = 4266666 /ml. Therefore: 5360000/4266666 = 1.26, normalization factor. All MDA-MB-231 peak area values were divided by 1.26 so that the amount of phospholipids was relative. There were two technical replicates for each cell line, which were averaged and graphed as bar charts with standard deviation error bars for each sample for each of the lipid species.

3.3.1. Lipid nomenclature

Refer to Chapter 2: Methods, page 46.

3.4. Results

Although a small sample set was used in this study, some large differences were seen between the phospholipid compositions of the cell culture supernatants. Figures 3.1-3.10 are bar graphs comparing the control and patient cell culture supernatant for each phospholipid type and each specie within that type. Specific species with a significant difference were seen in all phospholipid types except sphingomyelin (SM). Some species, CE (21:0), Cer dl (18:1/15:2) and PC (43:3) were significantly higher in the control cell culture supernatant compared to the tumourigenic cell culture supernatant. Such changes suggest that there are altered phospholipid levels in the cell culture supernatant of breast cancer cells when compared to controls.

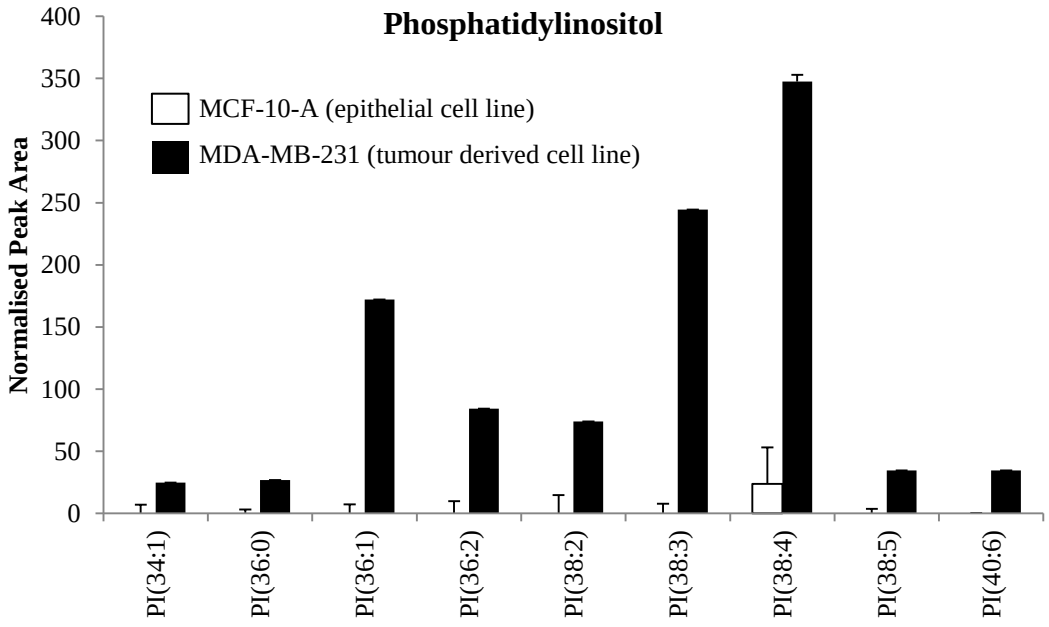


Figure 3.3: Concentration of specific phosphatidylinositol (PI) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations.

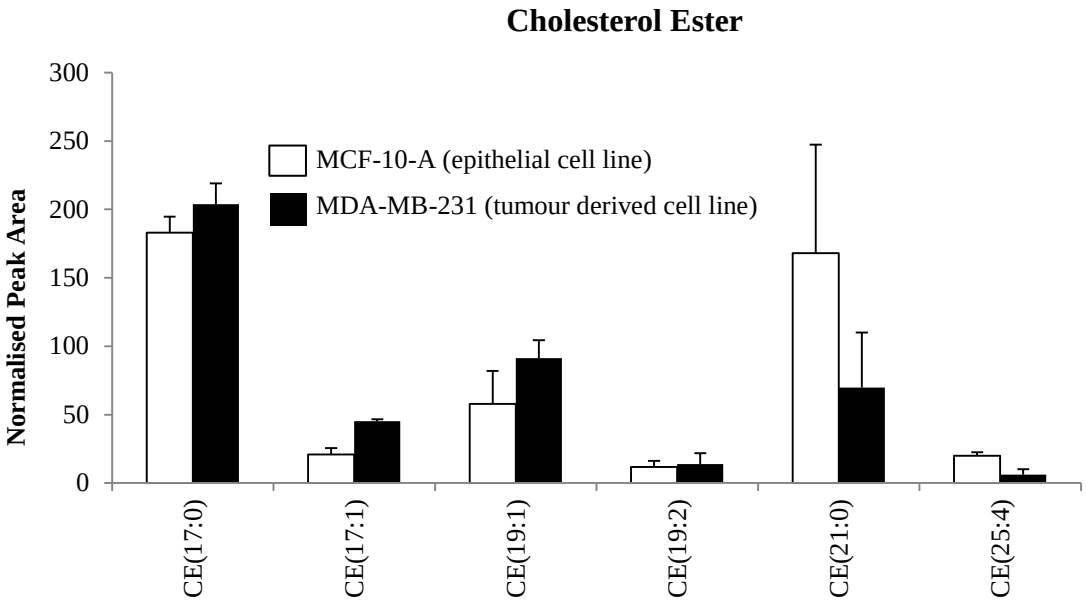


Figure 3.4: Concentration of specific cholesterol ester (CE) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations.

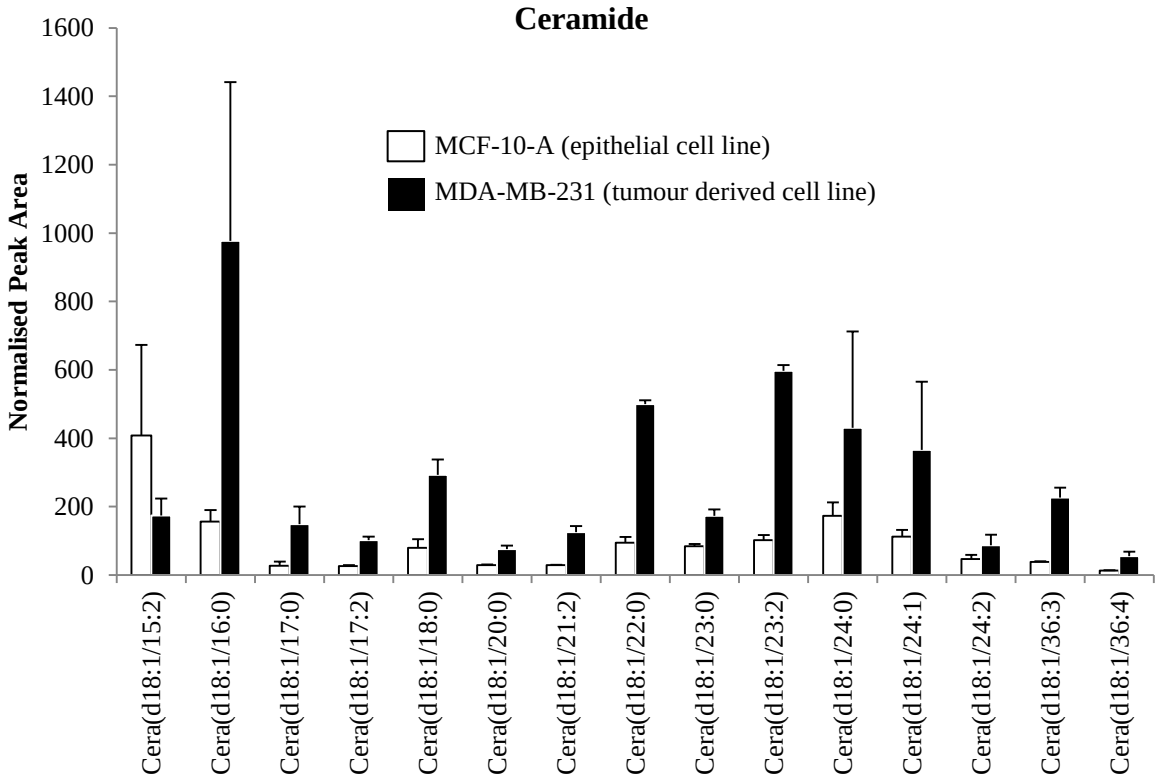


Figure 3.5: Concentration of specific ceramide (Cer) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations.

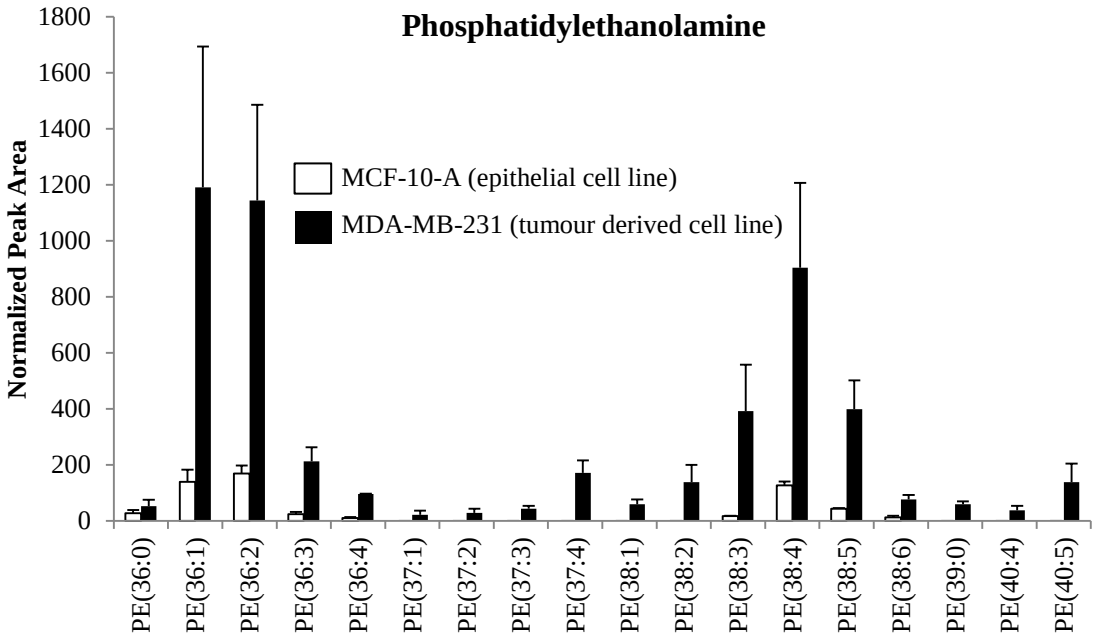


Figure 3.6: Concentration of specific phosphatidylethanolamine (PE) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations.

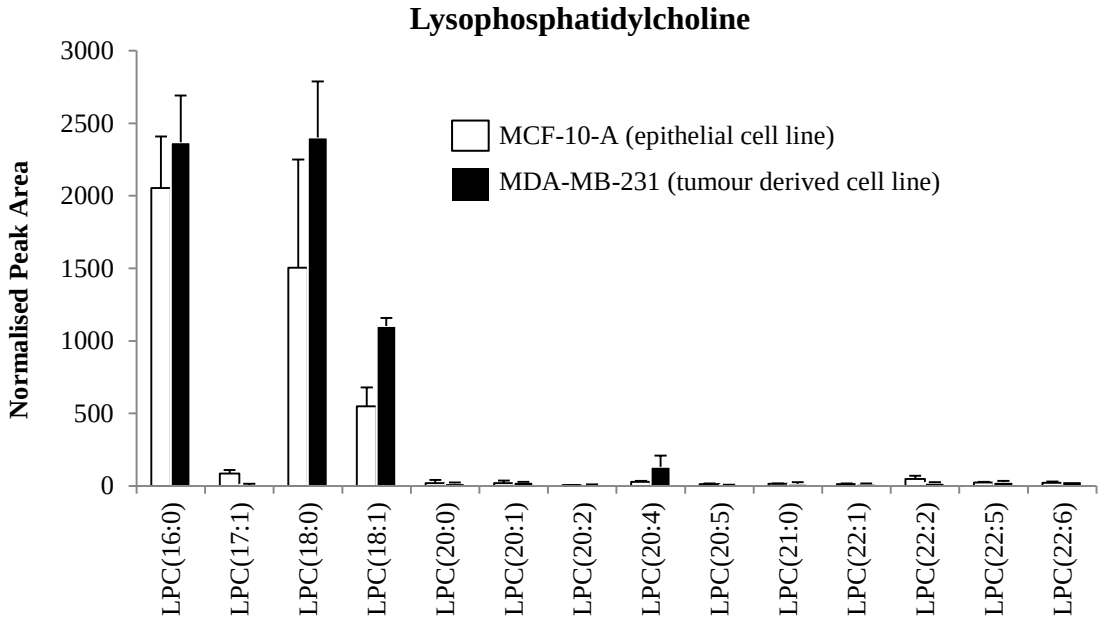


Figure 3.7: Concentration of specific lyso-phosphatidylcholine (LPC) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations.

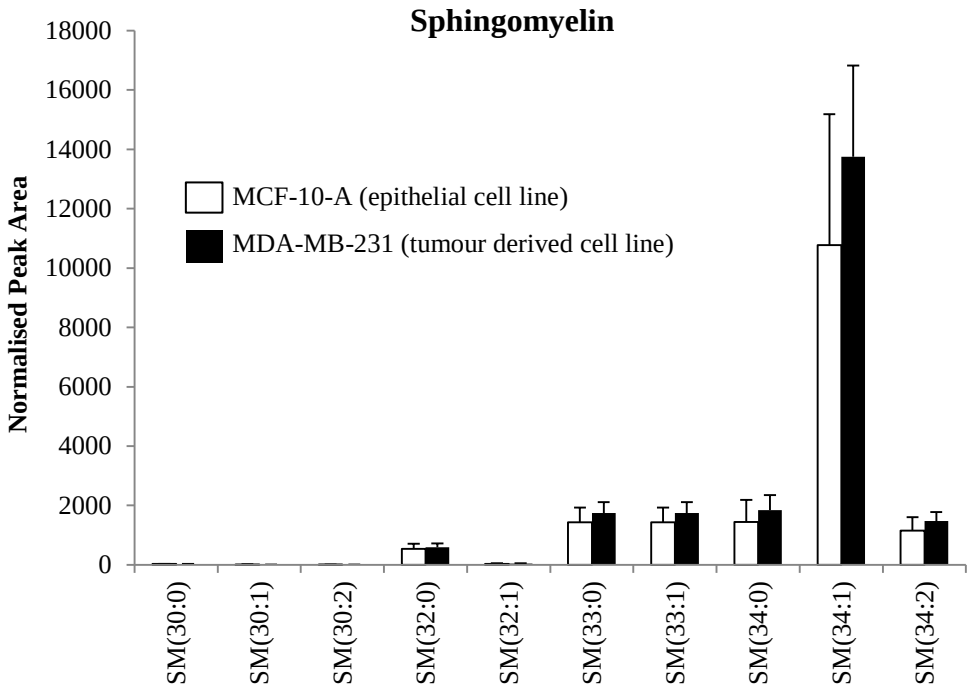


Figure 3.8: Concentration of specific sphingomyelin (SM) species in cell culture supernatant samples collected from tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations.

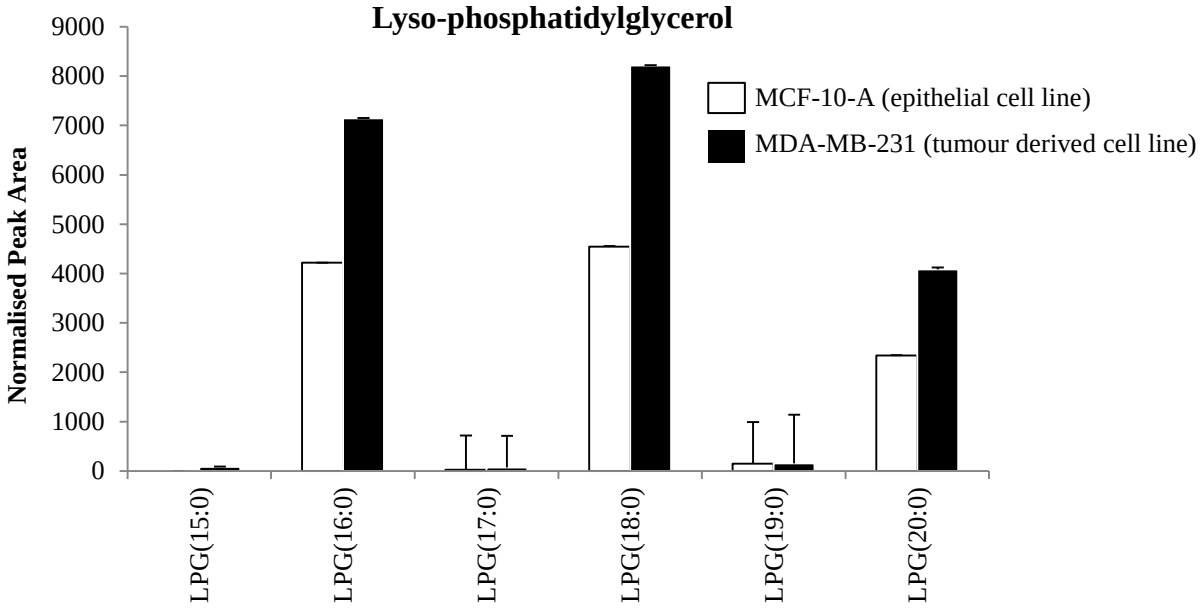


Figure 3.9: Concentration of specific lyso-phosphatidylglycerol (LPG) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations.

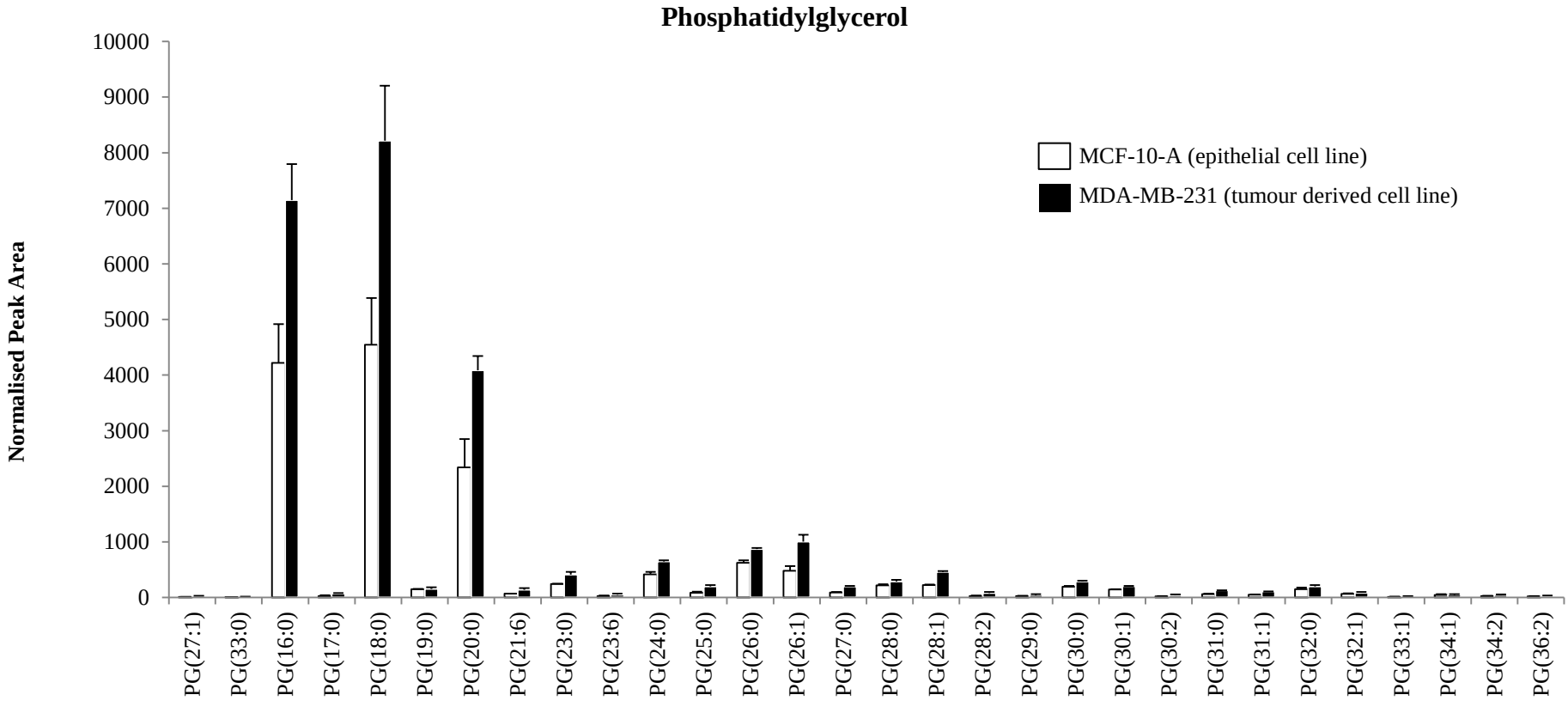


Figure 3.10: Concentration of specific phosphatidylglycerol (PG) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations.

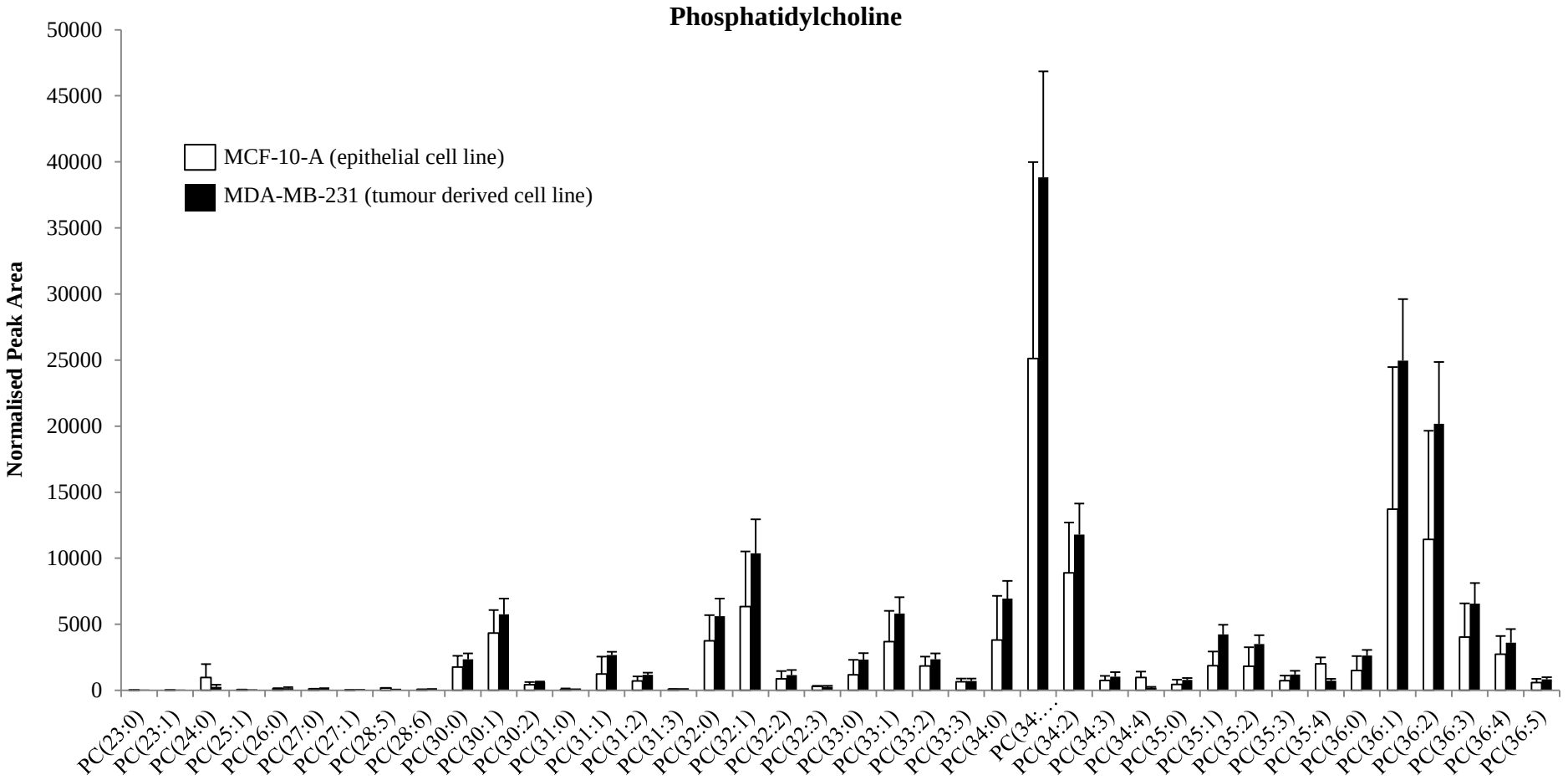


Figure 3.11: Concentration of specific phosphatidylcholine (PC) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations.

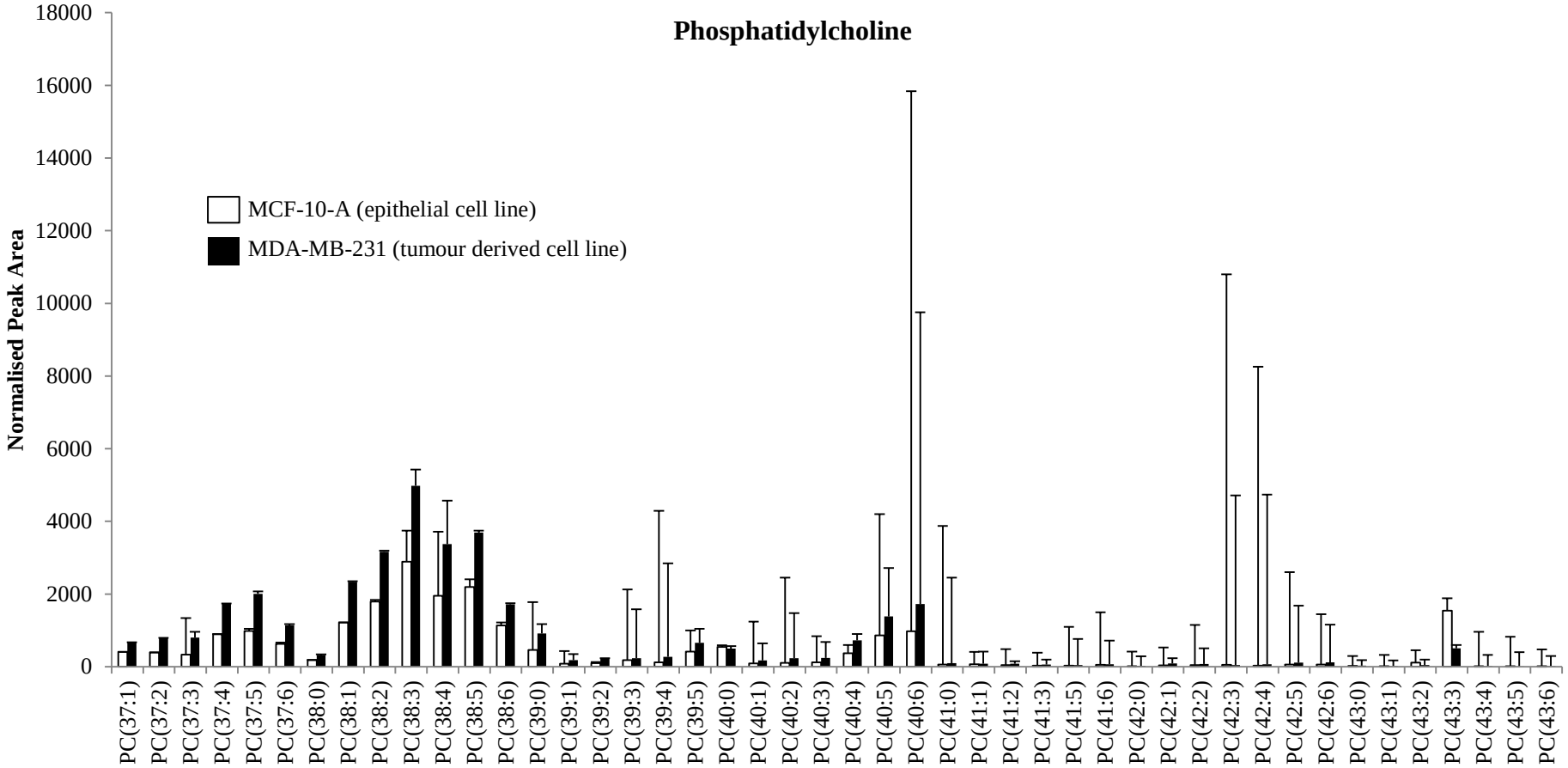


Figure 3.12: Concentration of specific phosphatidylcholine (PC) species in cell culture supernatant samples collected from a tumour derived cell line and an epithelial cell line, where the average was taken from two different determinations.

3.5. Discussion

This study identified phospholipids, which are elevated in the cell culture supernatant of breast cancer cells compared to control cells. There are series of reports in which the association between breast cancer and lipids has been discussed and so we have aimed to distinguish those species and to characterise the profile of lipids found in the cell culture supernatant of breast cancer cells.

It was found that there were specific phospholipid species, which were increased significantly in breast cell culture supernatant compared to controls. Three species were significantly elevated in the control supernatant when compared to the tumourigenic supernatant. The identification of these lipids in the supernatant gives a guide to those lipids species that could be expected to be elevated in serum or hair from women with breast cancer.

There are several studies that demonstrate that breast cancer cells have an altered phospholipid profile, in particular phosphatidylcholine profile and suggest the possible mechanisms for these alterations.

The expression of the enzyme choline kinase is significantly higher in breast cancer cells when compared to normal mammary epithelial cells (Glunde, 2004, Ramirez de Molina, 2002), and there is some evidence that phospholipase D (PLD), or phospholipase C (PLC) may also have an increased expression in breast cancer cells. (Glunde, 2004, Noh, 2000). This is supported by a study, which found similar trends in choline kinase but also found that the rate of choline transport into the cell was also greatly elevated in breast cancer cells. This report went on to suggest that phosphocholine has potential as a biomarker for breast cancer (Eliyahu, 2007).

Magnetic resonance spectroscopy (MRS) studies of breast cancer cells came to the same conclusion (Aboagye, 1999, Singer 1995, Ting, 1996), with one study reporting a 27-fold increase in phosphocholine content in a metastatic breast cancer cell line compared with normal breast epithelial cells. The authors proposed that the elevation in phosphocholine was due to either an increase in the rate of phosphocholine synthesis or a reduction in the utilisation of phosphocholine in the breast cancers cells (Singer 1995). Either theory could be plausible in creating elevated levels of lipids in breast cancer cells, which promote tumour progression though membrane fluidity. In

addition to increased choline transport, other MRS studies have demonstrated that the phosphorylation of choline to phosphocholine was 10-fold higher in breast cancer cells than in controls (Katz-Brull, 1996, Katz-Brull, 2002). Choline metabolism has also been proposed as a method of monitoring breast cancer patients in response to treatment (Kenny, 2010). Another study suggested that there is an early transformation in the form of a glycerophosphocholine to phosphocholine "switch" which occurs in malignant cell lines, where breast tumour cells exhibit more choline containing metabolites due to elevated levels of phosphocholine (Ackerstaff, 2003). Furthermore, twice the amount of phosphoethanolamine has been found in breast tumour cells when compared to controls (Daly, 1987).

Similarly, our study found that there was an elevation in more than one type of phospholipid found in the supernatant of breast cancer cell lines. We hypothesise that the invasive tumour in the breast produces and releases specific lipids into the blood stream, from its membrane, and these lipids could be possible biomarkers for the disease. In order for phospholipids to enter the bloodstream and reach the hair fibre, to produce the irregular XRD pattern, they must be shed from the tumour microenvironment into the bloodstream. The mechanism by which the breast cancer associated lipids reach the supernatant could be by direct shedding or excretion, from the tumour, into the medium (Hellstrom, 2006, Ladisch, 1987) or as a result of extracellular vesicles, such as exosomes or microvesicles, which are released into the media (Caby, 2005, Dorai, 2009).

This study provides a rationale for looking for these candidate lipids in the plasma and hair of patients with breast cancer and to identify a set of potential biomarkers for the disease and to better understand the mechanisms by which this elevation are occurring due to malignant transformation.

4. Lipid extraction from hair fibre

4.1. Introduction

A number of alternative approaches have been studied as potential technologies for detecting the breast cancer. These unconventional methods are intriguing, in that they utilise different biological samples as a source for screening, and in some cases, this is based on a single sample remote from the site of the disease. This project was established on the principle that there is an association between breast cancer and the XRD pattern from the hair of individuals with the disease. Early XRD studies proposed that the XRD of hair could be a non-invasive method of screening for breast cancer because there is an extra feature present in the XRD pattern of women with the disease when compared to healthy women (Corino, 2008, Corino, 2009, James, 1999). The preliminary data from this project (Chapter 2) demonstrates that the feature associated with the disease is due to the presence of lipids, in particular, phosphatidylcholine in the hair. There may also be other phospholipid species, which are increased in hair samples from breast cancer patients, compared to disease-free controls, as demonstrated in the cell culture supernatant study (Chapter 3).

4.2. Aims

Repeating the preliminary experiment (Chapter 2) in a larger sample, and comparing the data to the cell culture supernatant data (Chapter 3), will allow further identification and confirmation of those lipid species which are associated with the disease. In the previous hair study (Chapter 2), the fibres were first soaked in acetone to remove external lipids, this implies that these breast cancer associated lipids are internally bound and exhibit a systemic change. The hypothesis being studied in this project asserts that the lipids in the hair fibre are derived from the tumour, and if this is proved then this could form the basis of a non-invasive diagnostic test for breast cancer. This study concerned the extraction of lipids from hair of patients, with and without the disease, to determine those lipids, which have an association with breast cancer.

4.3. Methods

4.3.1. Lipid profiling of hair

4.3.1.1. Samples

Hair samples were collected from the Sydney Breast Clinic (Sydney, NSW Australia) and the Poche Centre (North Sydney, NSW Australia) under ethics governed by Macquarie University Human Ethics Committee (reference 5201100091). Clinical data was also collected for each individual for data analysis. There were 80 samples in this study (same individuals from which the serum was taken, Chapter 4), 40 confirmed free of breast cancer (controls) and 40 confirmed to have breast cancer (patients).

4.3.1.2. Extraction of lipid from hair

The protocol used for lipid extraction from samples is a monophasic extraction, modified from the Bligh and Dyer protocol (Bligh, 1959).

Hair samples were cut into 3mm pieces using surgical grade scissors, placed into a glass vial, and washed in in acetone for 5 minutes to remove exterior fatty acids. Samples were air dried over night. 30mg of hair sample was weighed* into a cryomill tube (Precellys) containing 1.4 mm ceramic beads and ground in the cryomill at 6100 rpm for three 45-second cycles with 45 second intervals between each cycle. 1000 µL of extraction solution (methanol, chloroform, water (2:1:0.6)) was added to each tube and spiked with 10µl of 100µM internal standard (Cholesterol ester (18:0) d8) to 10µM final concentration). A single 45-second cycle at 6100 rpm in the cryomill was run to complete uniform homogenisation of the samples. Samples were shaken at 1100 rpm for 15 minutes at 20°C and centrifuged for 10 minutes at 10,000 rpm at 0°C. The supernatant was transferred to a new Eppendorf tube (2ml). Steps 5, 7 and 8 were repeated for the second extraction from the tissue and both supernatant extractions were combined. Samples were dried under liquid nitrogen at 30˚C, resuspended in 100µL of butanol/methanol (1:1) with 10mM ammonium formate and

shaken at 30°C for 30 minutes. Samples were centrifuged at 100 rpm for 10 minutes at room temperature and the supernatant was transferred to high-pressure liquid chromatography (HPLC) vials.
*See appendix for sample weights (Table 8.58).

4.3.1.3. Liquid Chromatography Mass Spectrometry analysis of hair samples

Lipids were separated by injecting 5µL aliquots onto a 50 mm × 2.1 mm × 2.7 µm Ascentis Express RP-Amide column (Supelco) using an Agilent LC 1200 Rapid Resolution System Liquid Chromatography. Lipid samples were eluted at 0.2 mL min^{-1} over a 5 min gradient of water/methanol/tetrahydrofuran (50:20:30, v/v/v) to water/methanol/tetrahydrofuran (5:20:75, v/v/v), with the final buffer held for 3 min. Lipids were analysed by electrospray ionisation-mass spectrometry (ESI-MS) using an Agilent Triple Quad 6460. The mass spectrometer in the positive mode was set to scan in precursor ion mode to identify phosphatidylcholines (precursors of m/*z* 184.1), sphingomyelins (precursors of m/*z* 184.1), ceramides (precursors of m/*z* 264.6), cholesterol esters precursors of (m/*z* 369.4), phosphatidylglycerols (precursors of m/*z* 189) and in the negative mode phosphatidylinositol's (precursors of m/*z* 241). The mass spectrometer was set to scan in neutral loss mode to identify phosphatidylethanolamines (loss of m/*z* 141 in the positive ion mode) and phosphatidylserines (loss of m/*z* 87 in the negative ion mode). Multiple reaction monitoring (MRM) scans were used to quantify the identified lipids with the capillary voltage, fragmentor voltage, and collision energy were 4000 V, 140 – 380 V, and 15–60 V, respectively. In all cases, the collision gas was nitrogen at 7 $Lmin^{-1}$. LCMS data was processed using Agilent MassHunter quantitative software.

4.3.1.4. Data processing for all LCMS data

Mass spectra data was collected from Agilent QQQ 6460 mass spectrometer in positive mode and negative mode. The MRM data was processed using Agilent MassHunter software to generate the peak area values for each lipid species. Refer to Appendix 8.6.1 for ESI mode, ion scan mode and chromatograms of the standards.

All the masses that were present in blanks were deleted. If the given peak area value for a given species was absent in greater than 60% of the samples then the remaining data was not considered any further. The hair data had 1.5% missing values. Refer to Appendix 8.3.1 for raw data. Due to large differences in the relative abundance of the lipid species when the data was compared within itself, the raw matrices were log transformed to bring the variance to a similar level and allowed comparability (Appendix 8.3.3.). Log transformation is routinely used in statistical analysis when the standard deviation is proportional to the mean of the data (Roessner, 2011). Data was transformed to natural logarithm before normalisation in order to make it comparable. Once data was log transformed, each data point was normalised by subtraction of this value from the mean of the total lipids. This results in negative values, which appear to be inaccurate but have been treated correctly in order to compare the data. Statistical Analysis (multivariate analysis) was carried out using a Principle component analysis (PCA), which was used to look for trends in the data. PCA is an unsupervised data transformation technique used to approximate multidimensional data sets using a lower number of dimensions (Jolliffe, 2002). A data set is transformed to a new set of variables such that the maximum overall variation is put onto orthogonal axes called principal components (PCs). PC's are linear combinations of the original variables. The first PC (PC1) defines the axis of maximal variation through the multidimensional data while the second PC (PC2) defines the axis of maximal variation perpendicular to PC1. A PCA reveals separations between groups when the variability between groups is sufficiently greater than within the groups. Samples in each lipid species were averaged and graphed as bar charts with standard deviation error bars. T-tests were conducted to determine significant differences between patient and control serum samples. It should be noted that the probability value was adjusted to account for multiple comparisons using the R package limma (Smyth, 2004). The p-value was obtained from the t-statistic after adjustment for multiple testing. The adjusted p-value is one where the error rate is controlled for multiple comparisons so that the level of significance has the same threshold across all parameters being examined (Hochberg, 1990). In this study, the adjustment method "False Discovery Rate" (FDR) was used within R, where the error rate is controlled by multiplying the p-value by the number of comparisons (parameters) (Benjamini, 1995). FDR is the proportion of findings that are false among all findings, so, the proportion of incorrect rejections (false positives) among

all rejections of the null hypothesis (Benjamini, 2001, Yekutieli, 1999). This requires a stronger level of evidence to be observed in order for an individual comparison to be deemed "significant", so as to compensate for the multiple comparisons. Phospholipids were considered significantly different if the adjusted p value was <0.05 and the fold change was > 2.

4.3.2. Lipid nomenclature

Refer to Chapter 2: Methods, page 46.

4.4. *Results*

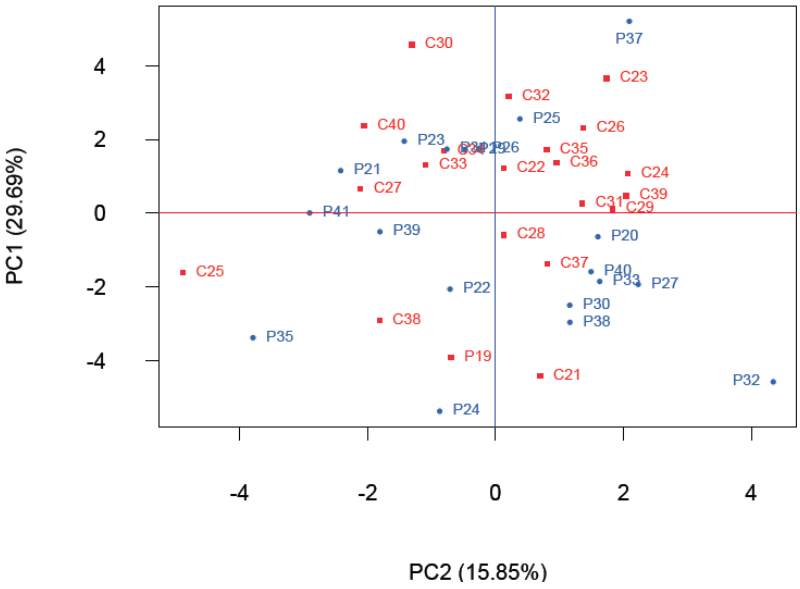


Figure 4.3: Principle component analysis of all 40 hair samples for cholesterol ester where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20).

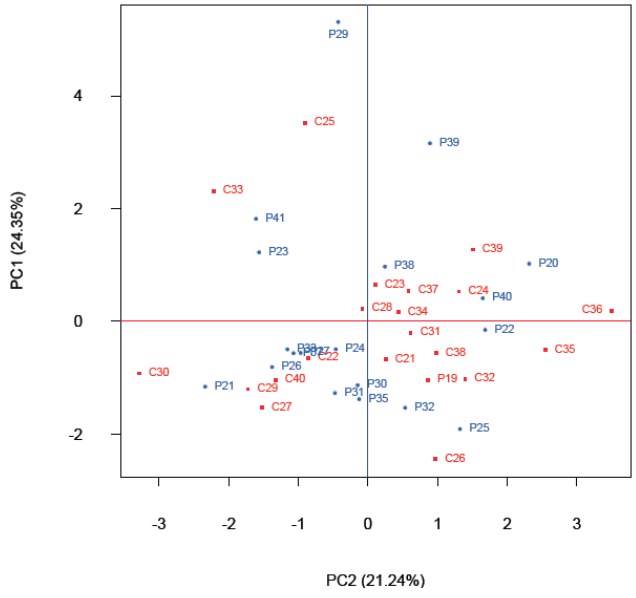


Figure 4.4: Principle component analysis of all 40 hair samples for ceramide where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20).

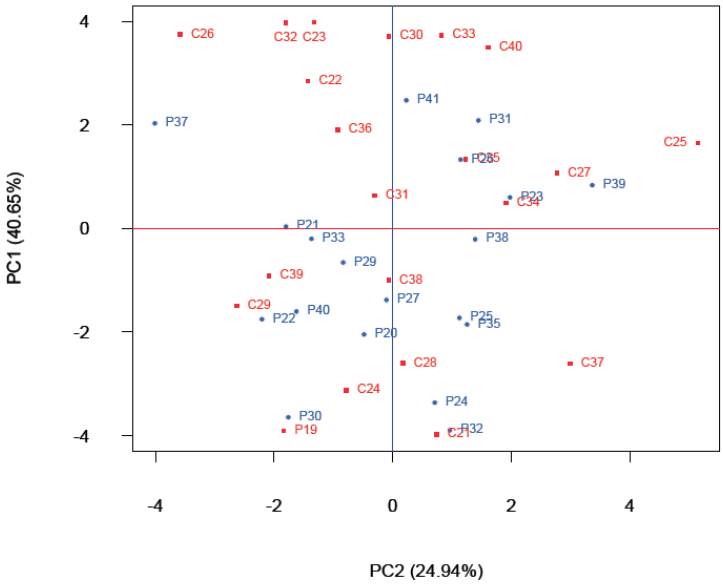


Figure 4.5: Principle component analysis of all 40 hair samples for phosphatidic acid where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20).

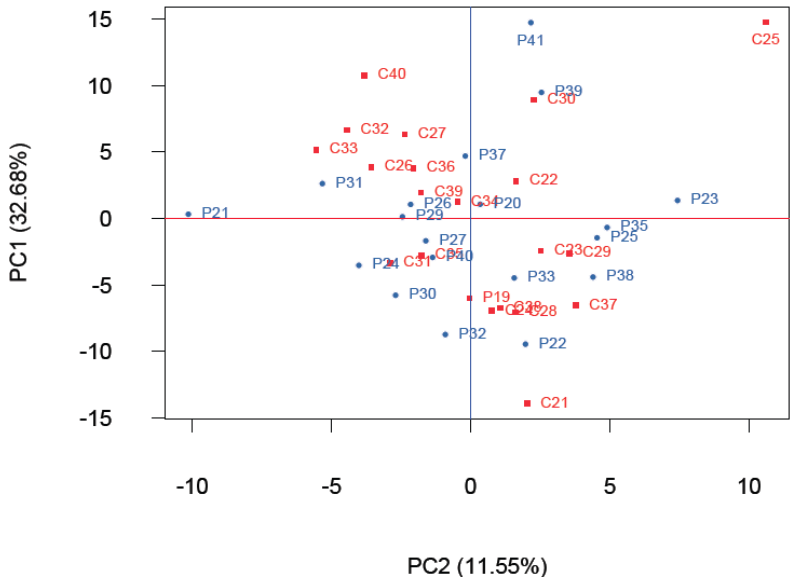


Figure 4.6: Principle component analysis of all 40 hair samples for phosphatidylcholine and lyso phosphatidylcholine where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20).

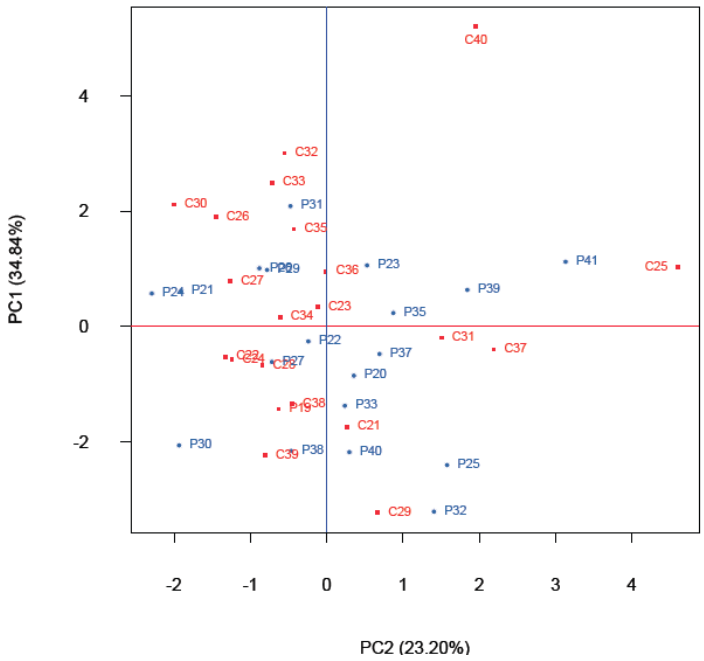


Figure 4.7: Principle component analysis of all 40 hair samples for phosphatidylethanolamine where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20).

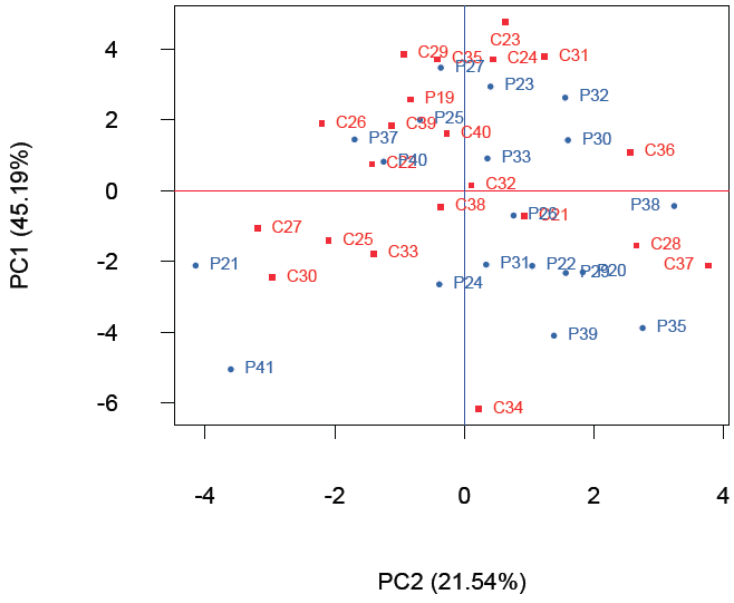


Figure 4.8: Principle component analysis of all 40 hair samples for phosphatidylglycerol where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20).

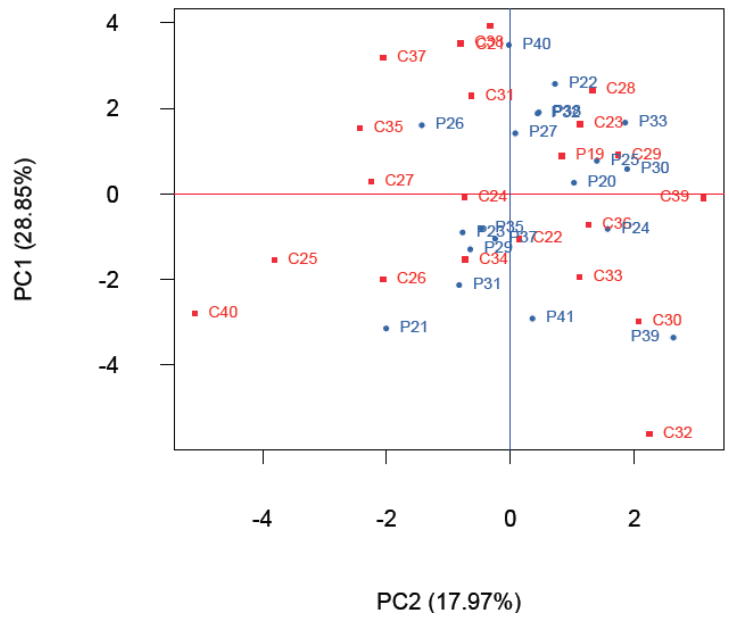


Figure 4.9: Principle component analysis of all 40 hair samples for phosphatidylinositol where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20).

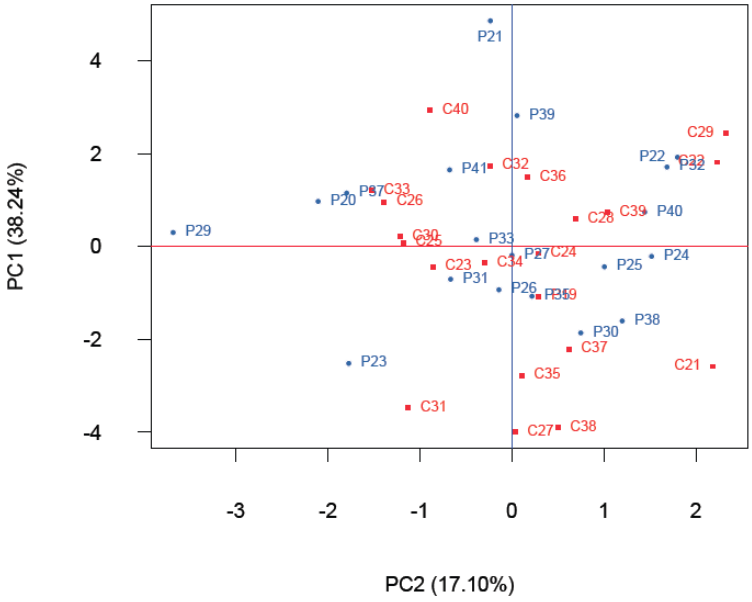


Figure 4.10: Principle component analysis of all 40 hair samples for sphingomyelin where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=20) and controls (n=20).

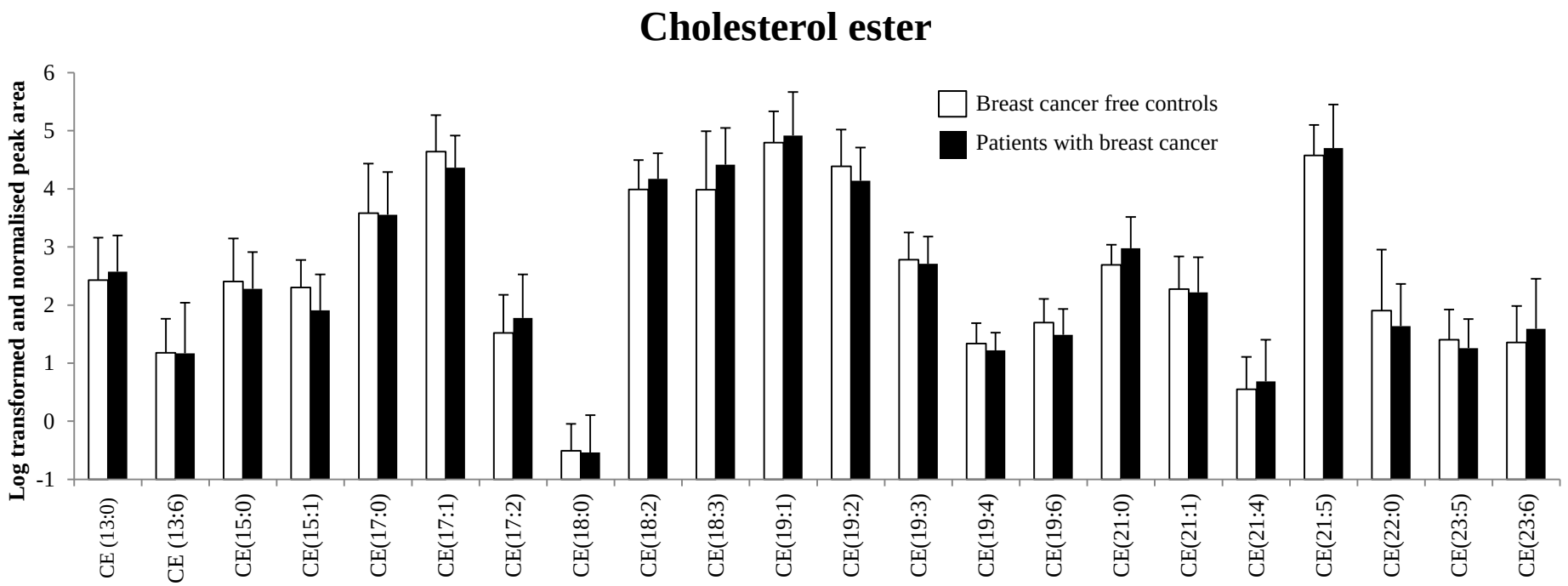


Figure 4.11: Average of log transformed and normalised peak area of cholesterol ester in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation.

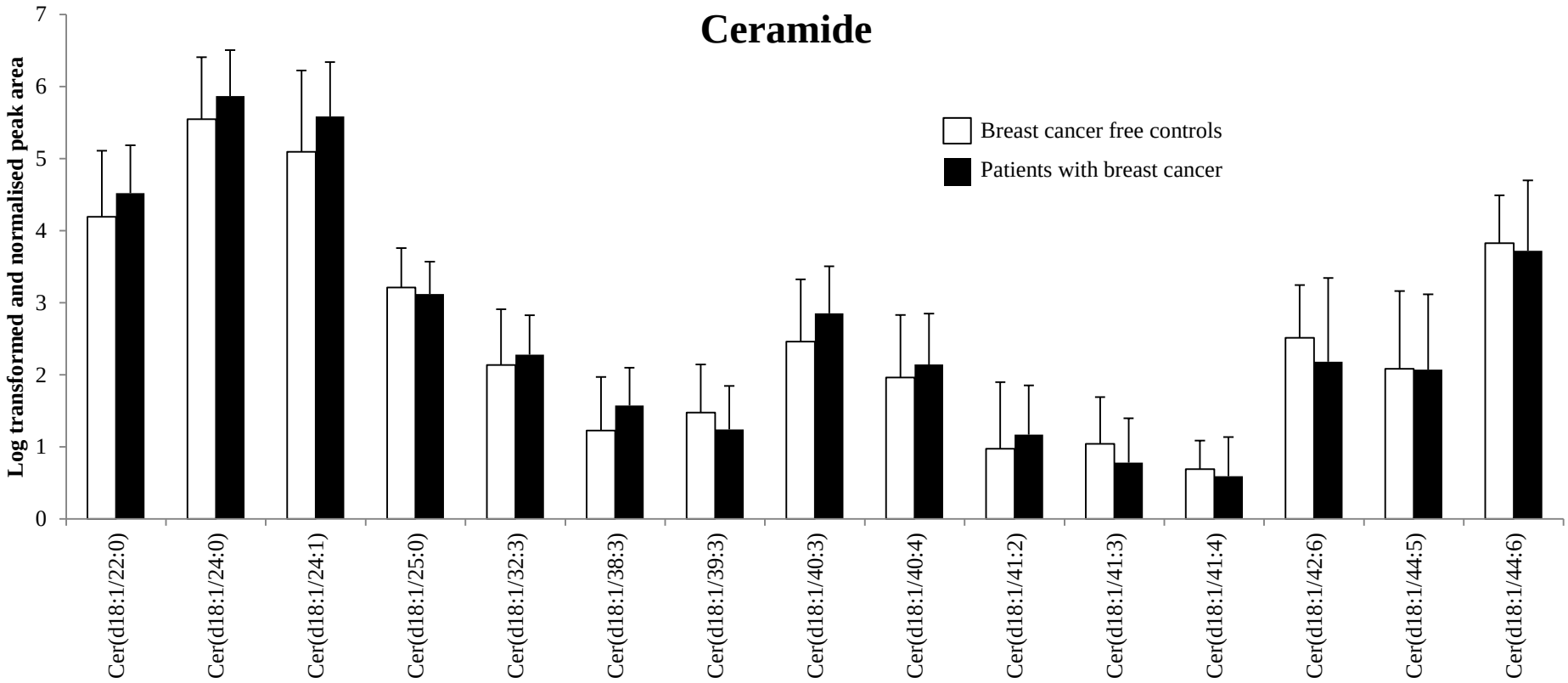


Figure 4.12: Average of log transformed and normalised peak area of ceramide in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation.

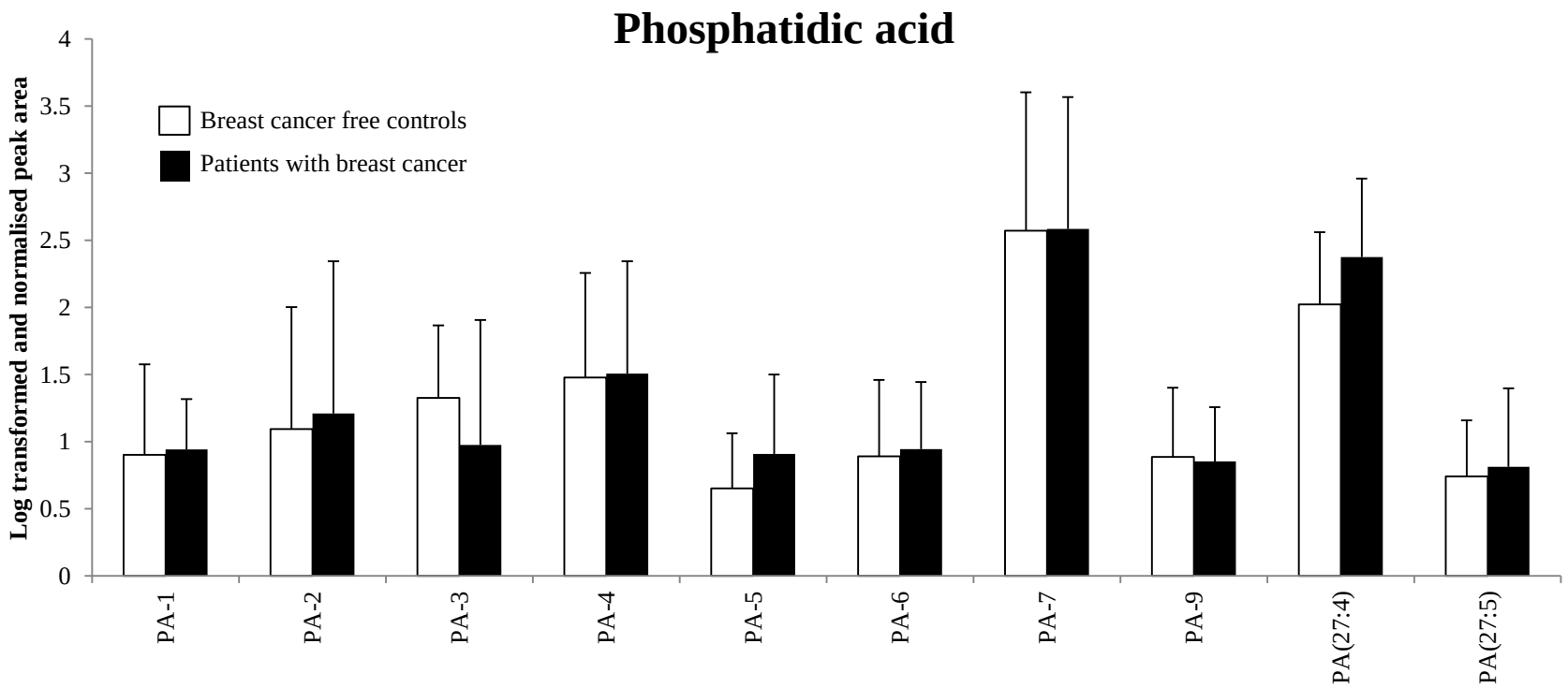


Figure 4.13: Average of log transformed and normalised peak area of phosphatidic acid in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. PA- 1 to 7 and 9 are unknown PA species, which require further studies to identify their structure.

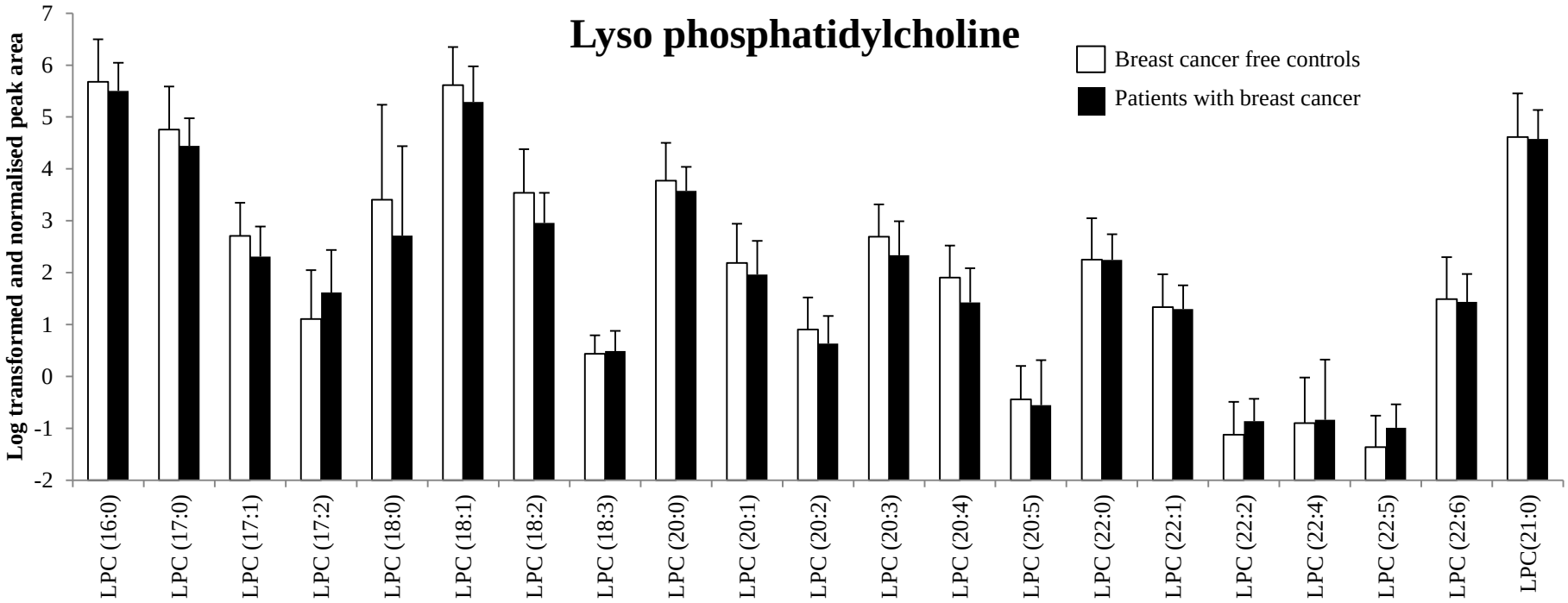


Figure 4.14: Average of log transformed and normalised peak area of lyso phosphatidylcholine in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation.

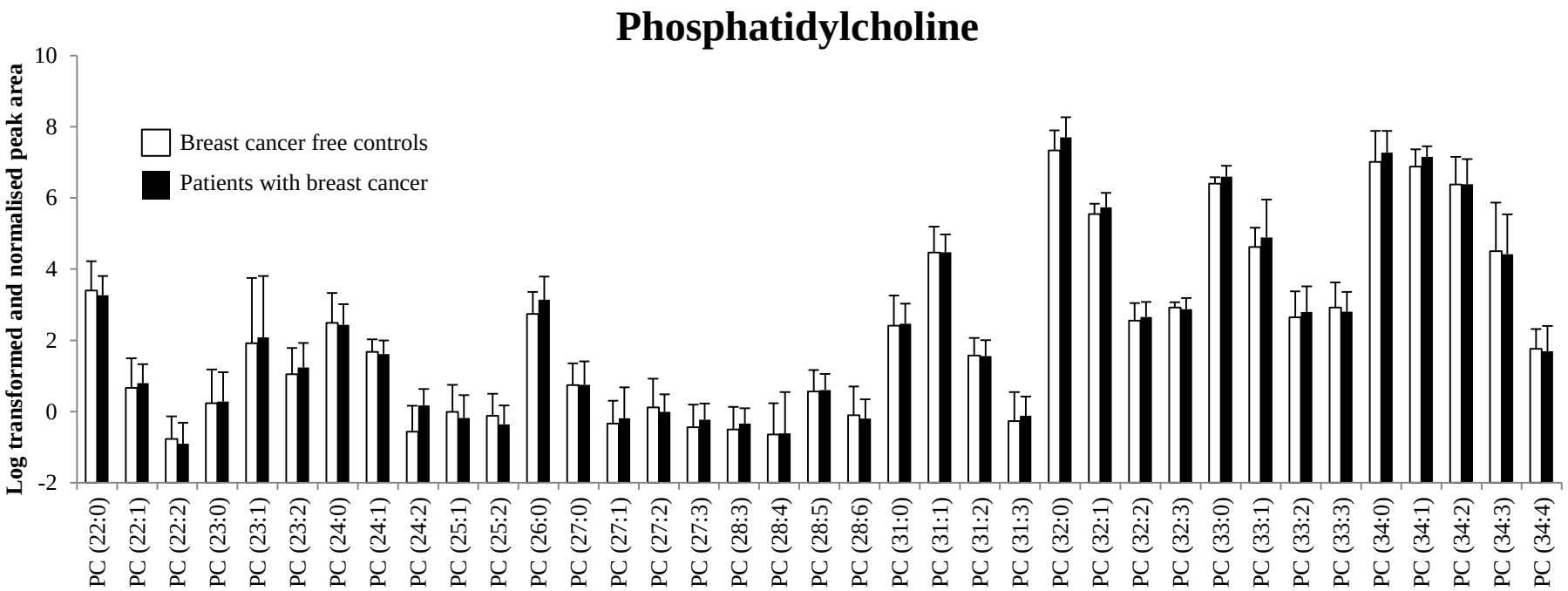


Figure 4.15: Average of log transformed and normalised peak area of phosphatidylcholine in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation.

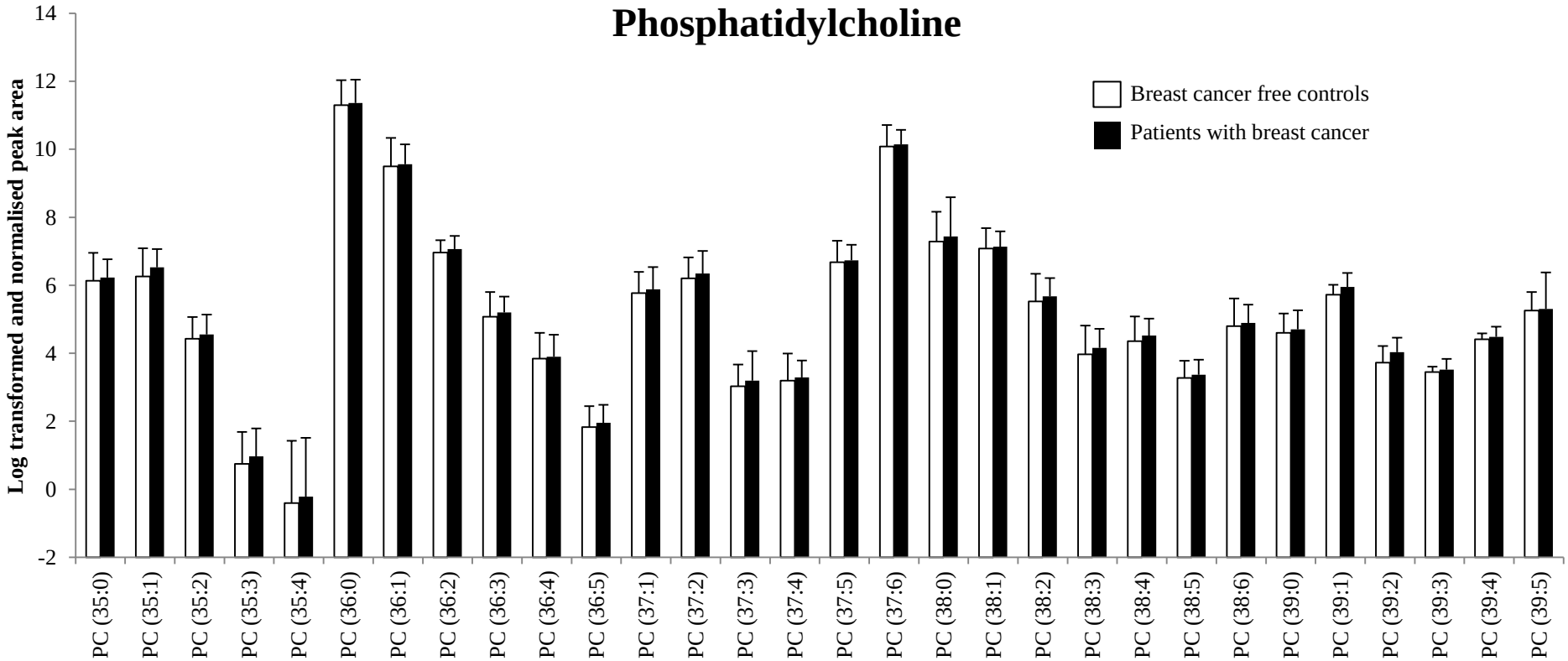


Figure 4.16: Average of log transformed and normalised peak area of phosphatidylcholine in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation.

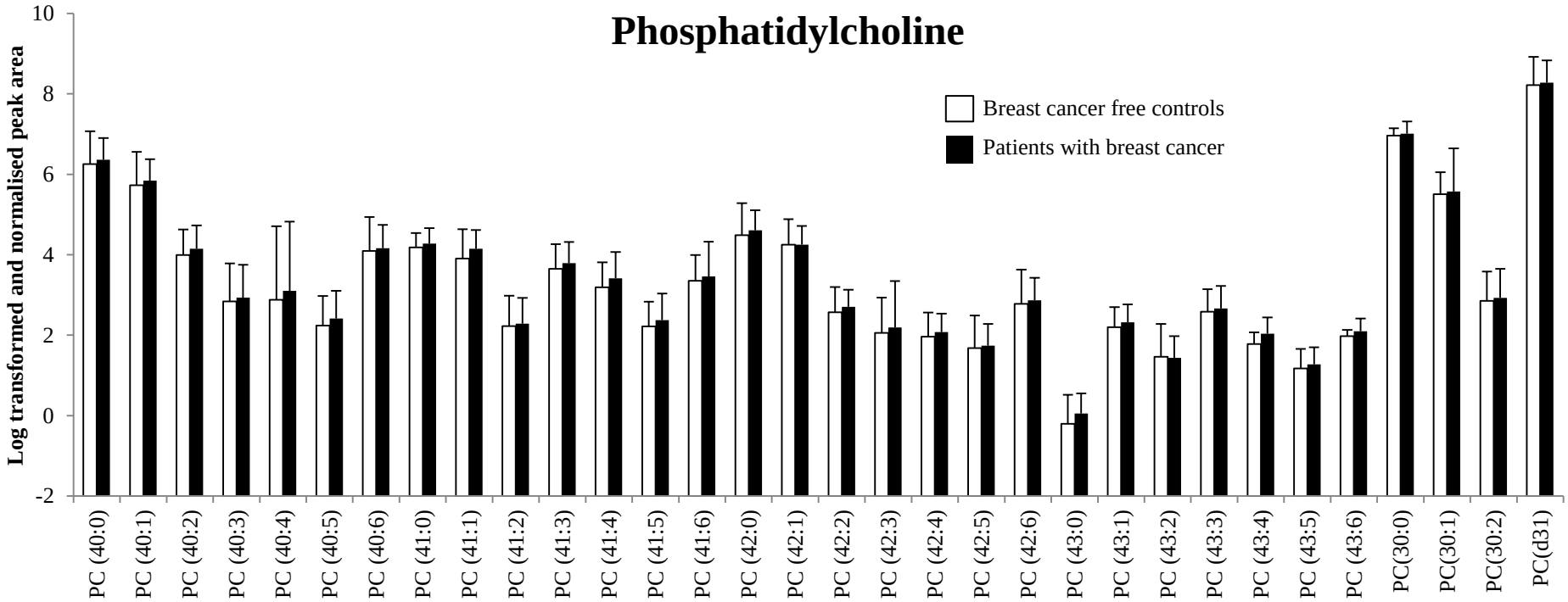


Figure 4.17: Average of log transformed and normalised peak area of phosphatidylcholine in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation.

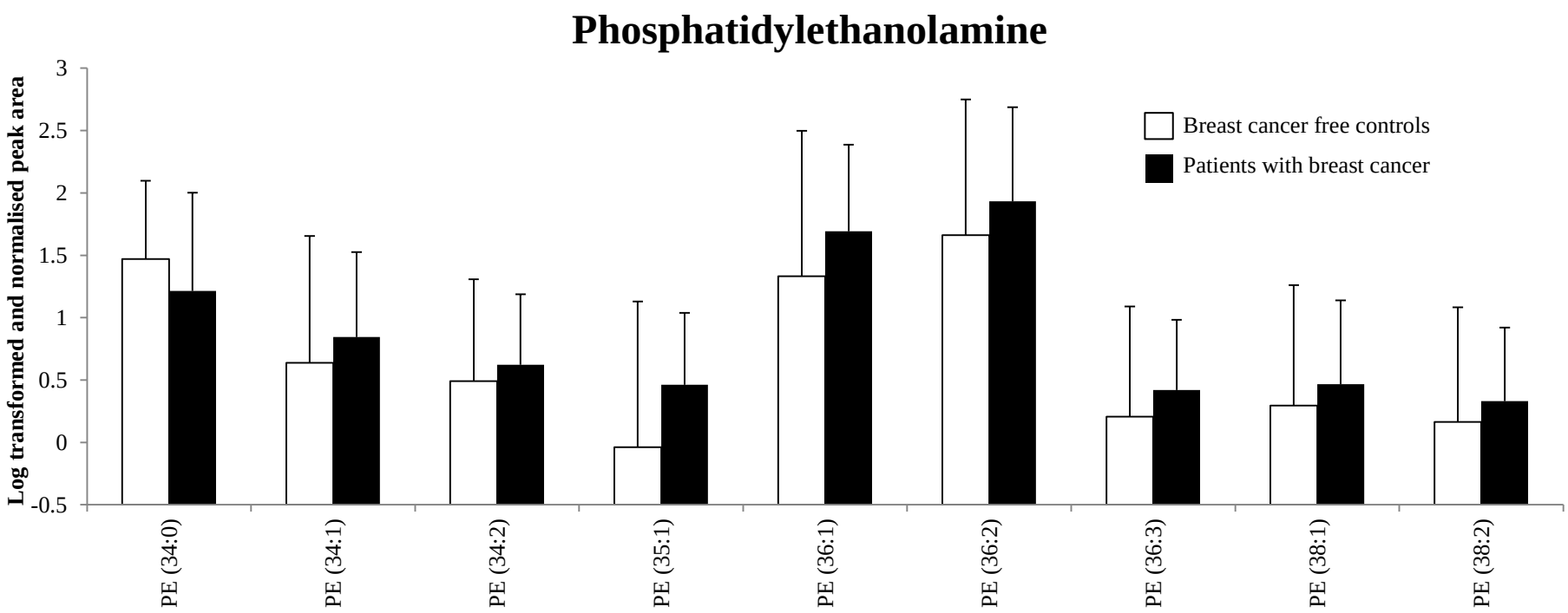


Figure 4.18: Average of log transformed and normalised peak area of phosphatidylethanolamine in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation.

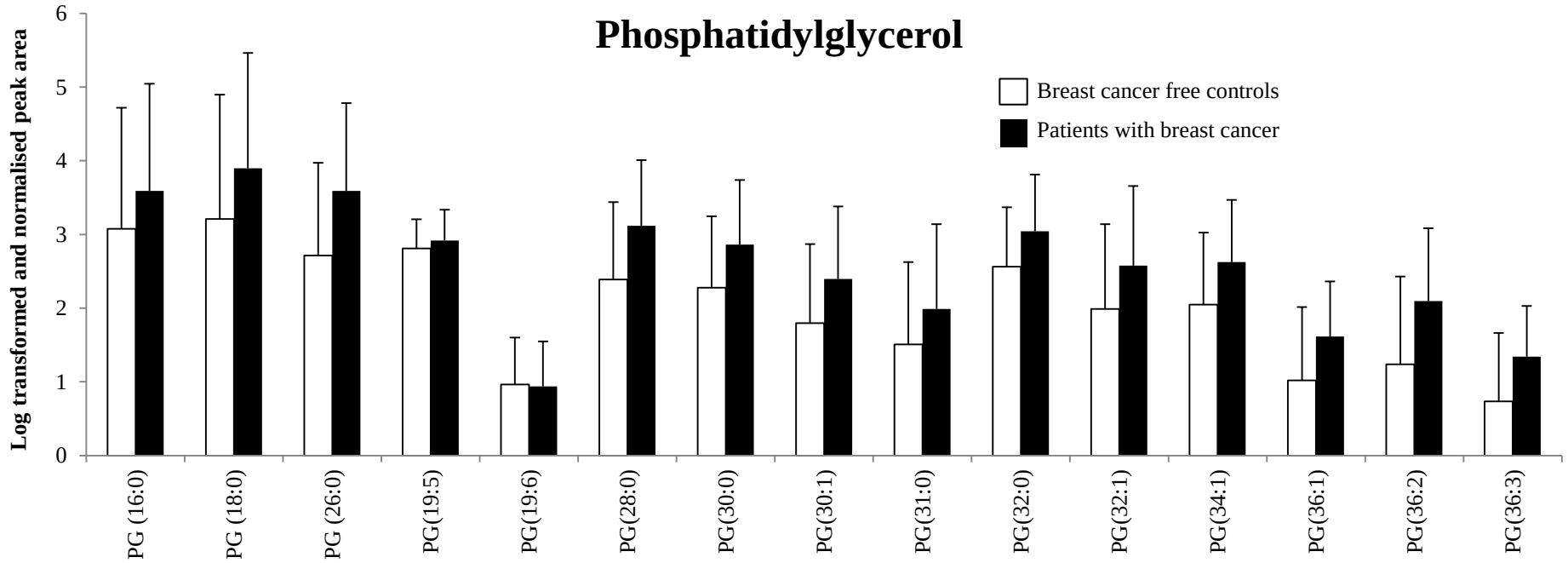


Figure 4.19: Average of log transformed and normalised peak area of phosphatidylglycerol in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation.

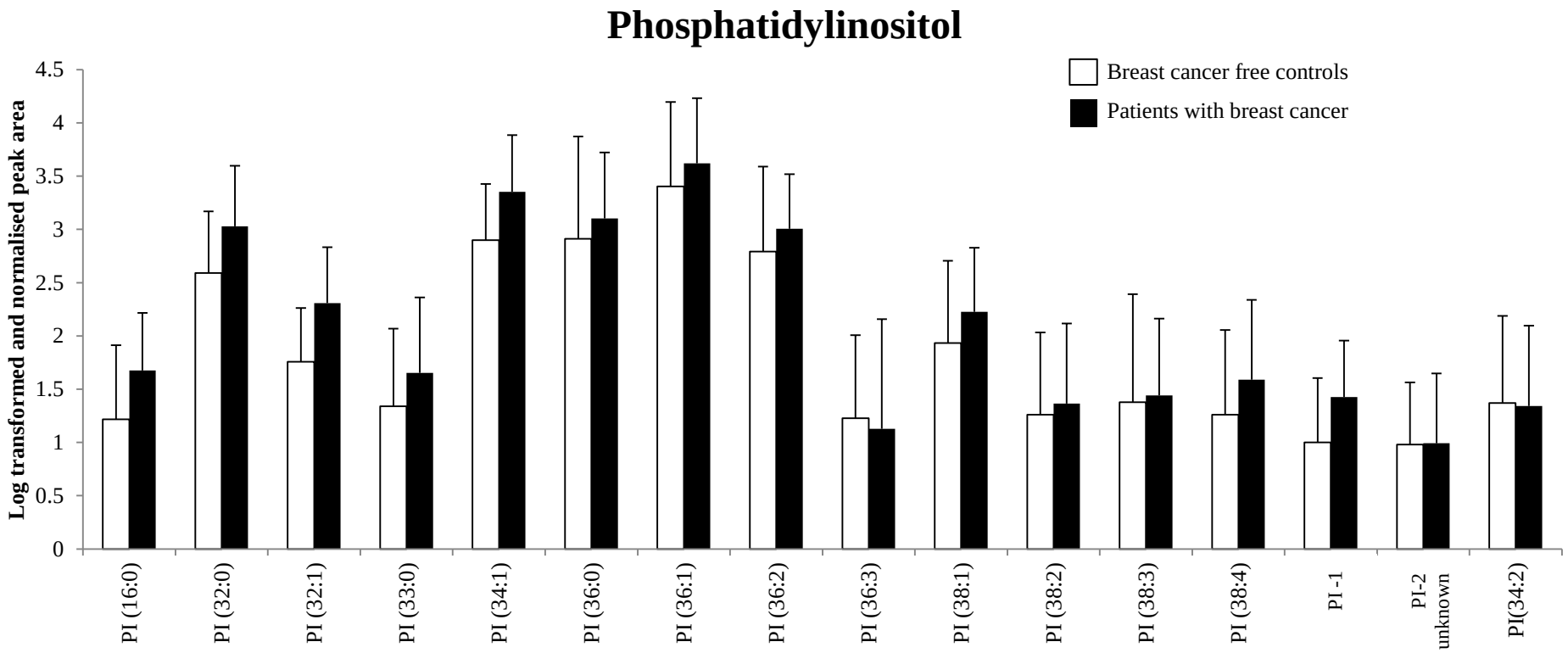


Figure 4.20: Average of log transformed and normalised peak area of phosphatidylinositol in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation. PI- 1 to 2 are unknown PI species, which require further studies to identify their structure.

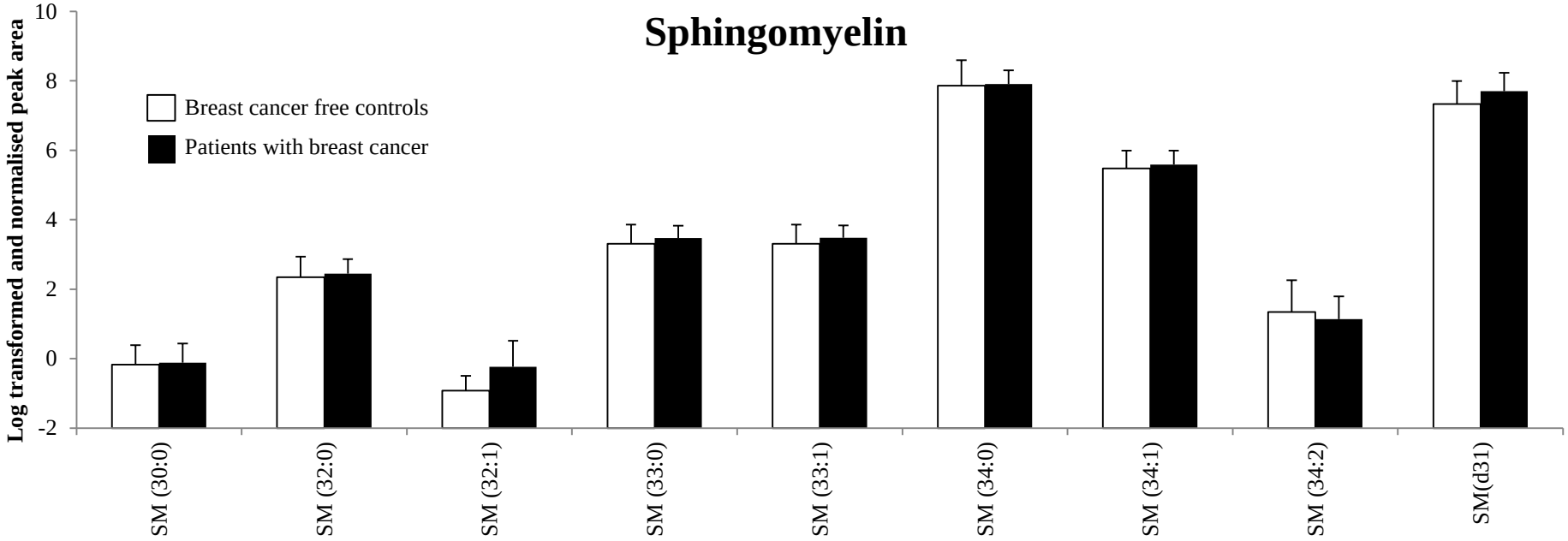


Figure 4.21: Average of log transformed and normalised peak area of sphingomyelin in the hair samples from breast cancer free controls (white, n=20) and patients with breast cancer (black, n=20). Error bars are the standard deviation.

Due to technical issues outlined in the discussion, there were only 40 samples in this study, 20 hair samples from breast cancer free individuals and 20 hair samples from patients with breast cancer.

Differences between the 40 samples, in terms of their phospholipid profile, were examined using a PCA, which indicates the differences through clustering and separation (Figures 4.3 – 4.10). The data for this study did not show any trends between lipid profiles of the hair from breast cancer patients compared to healthy controls. The data was considered robust, as regardless of how the samples were graphed, the pooled biological quality control's (PBQC) still sat in a tight cluster demonstrating consistency (see Appendix, Figure 8.5). Individual variability could explain the lack of clustering between the samples and the distribution of the samples across the PCA.
Normalised averages of the breast cancer free controls and patients with breast cancer were graphed in this study to explore any differences that were accountable to the specific phospholipid species (Figures 4.11- 4.21).

Another PCA was generated which plotted the two groups of samples based on their overall lipid profiles for all phospholipids in this study. The samples were then labeled according to the patients' clinical data (Figures 4.22-4.26). Five of the same PCA's were labeled with the size of the tumour, the age of the patient as the time of examination, the type of breast cancer that the patient had, the grade of this breast tumour and the length of the patients' hair. There was no clear clustering between samples based on these criteria. There appears to be some separation by tumour grade (Figure 4.24), but it is not a tight clustering and as the sample size is still small, individual variability may be affecting the results.

When a two-sided t-test was carried out (Appendix, Table 8.57) there were no significantly different species between the control and patient hair samples.

Figure 4.27 shows the raw ion chromatograms, collected from multiple reaction monitoring (MRM) scans, using liquid chromatography triple quad mass spectrometer. These chromatograms are shown for four random samples, two breast cancer free controls and two patients with breast cancer. Examples of the quality of the data and the peaks that were analysed in this study can be seen with some noisy and unclear chromatograms (Figure 4.27 A-F) compared to the ideal clean smooth chromatograms (Figure 4.27 G-H). Lipid species were selected as they were found to increase in a study by Hilvo *et al* (Hilvo, 2011) or elevated in the cell culture study from Chapter 3. Unclear peaks were included in the study but caution was taken when they indicated to be significantly changed.

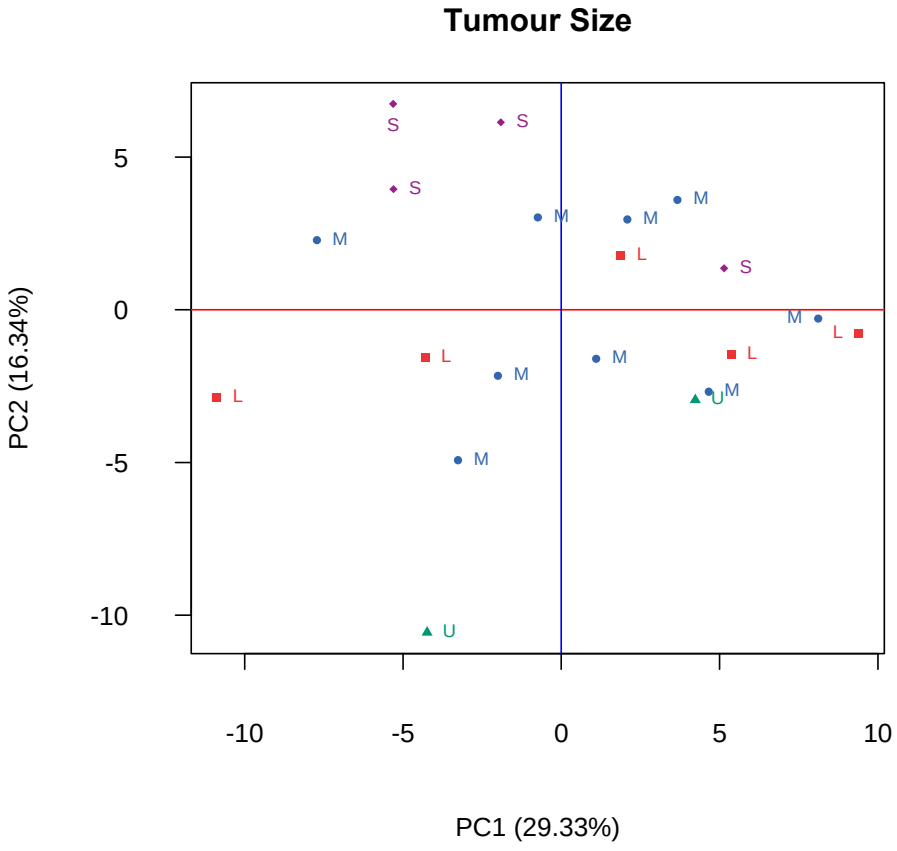


Figure 4.22: Principle component analysis of all 20 patient serum samples for tumour size. S (purple) - less than 10cm; M (blue) - between 10cm and 29cm; L (red) - 30cm and greater ; U (green) – Unknown, N/A. No separation or trends can be seen between the patients (n=20).

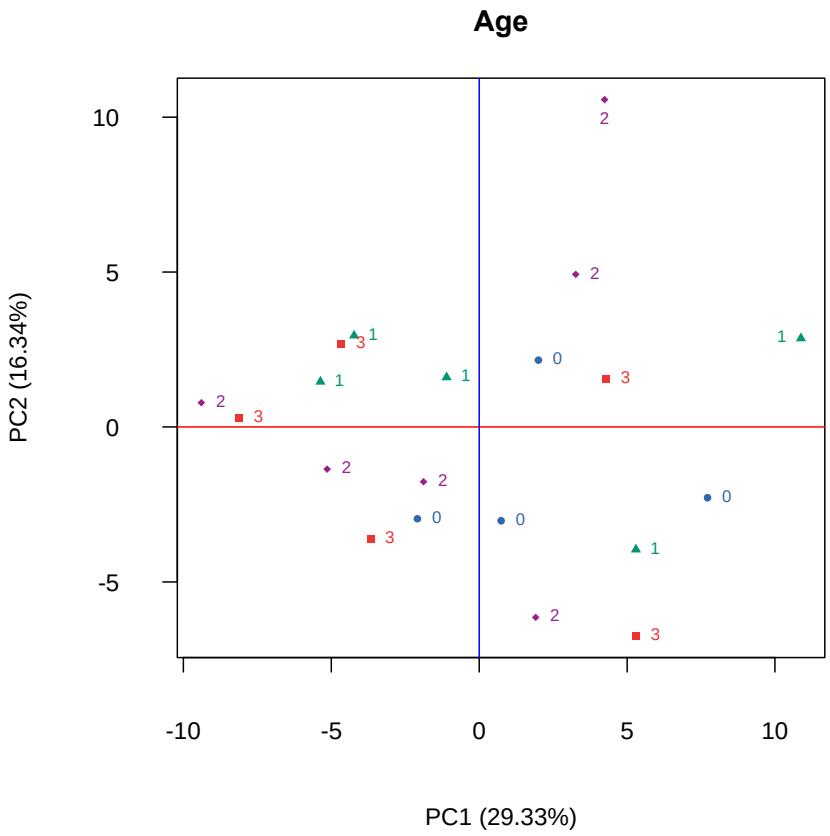


Figure 4.23: Principle component analysis of all 20 patient serum samples for patient age. 0 (blue) - patient under 50 years old ; 1 (green) - patient over 50 and under 60 years old ; 2 (purple) - patient over 60 and under 70 years old ; 3 (red) - patient over 70 years old. No separation or trends can be seen between the patients (n=20).

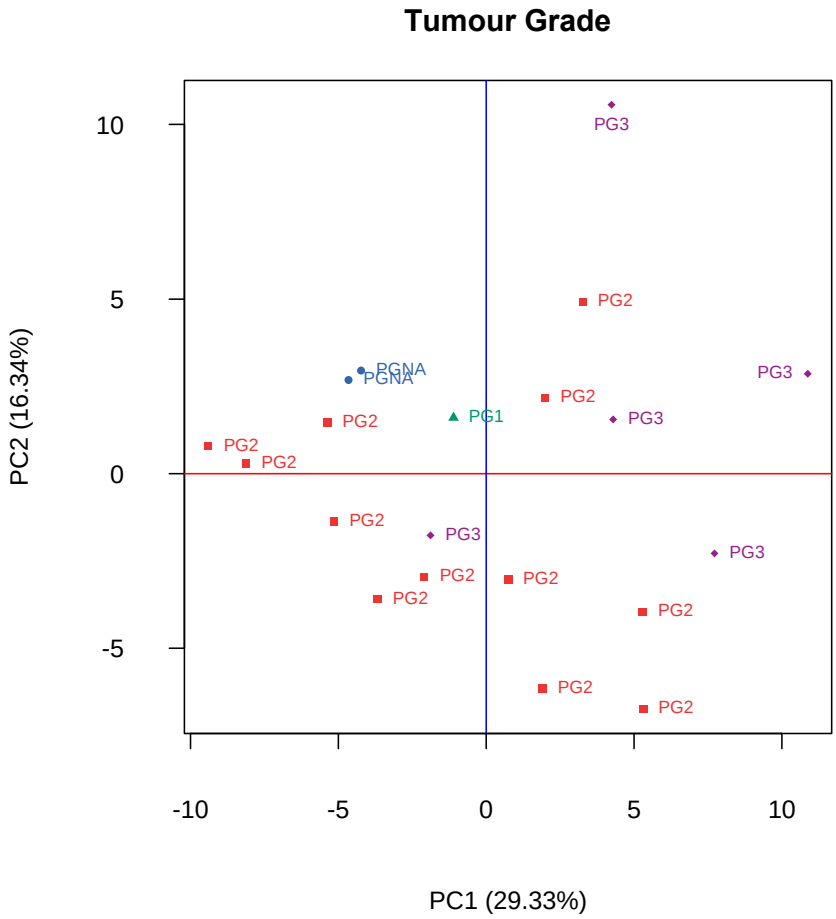


Figure 4.24: Principle component analysis of all 20 patient serum samples for tumour grade. PG1 (green) - grade 1; PG2 (red) - grade 2; PG3 (purple) - grade 3; PGNA (blue) - N/A. No separation or trends can be seen between the patients (n=20).

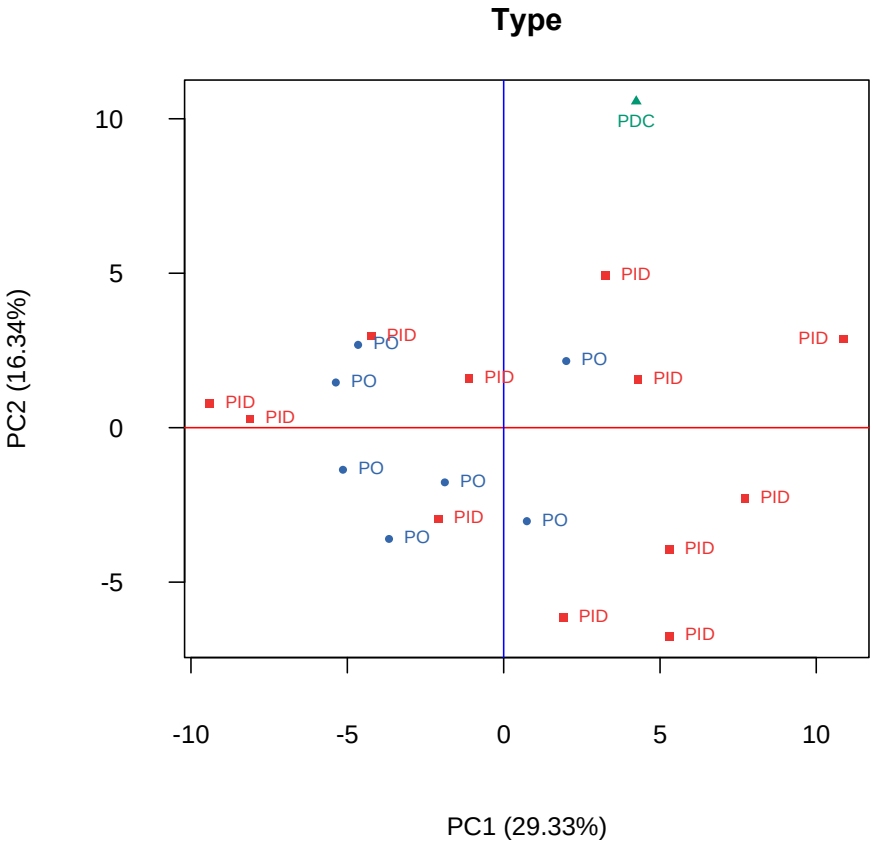


Figure 4.25: Principle component analysis of all 20 patient serum samples for tumour type. PDC (green) - ductal carcinoma in situ (localised); PO (blue) - other type of breast cancer ; PID (red) - invasive ductal carcinoma. No separation or trends can be seen between the patients (n=20).

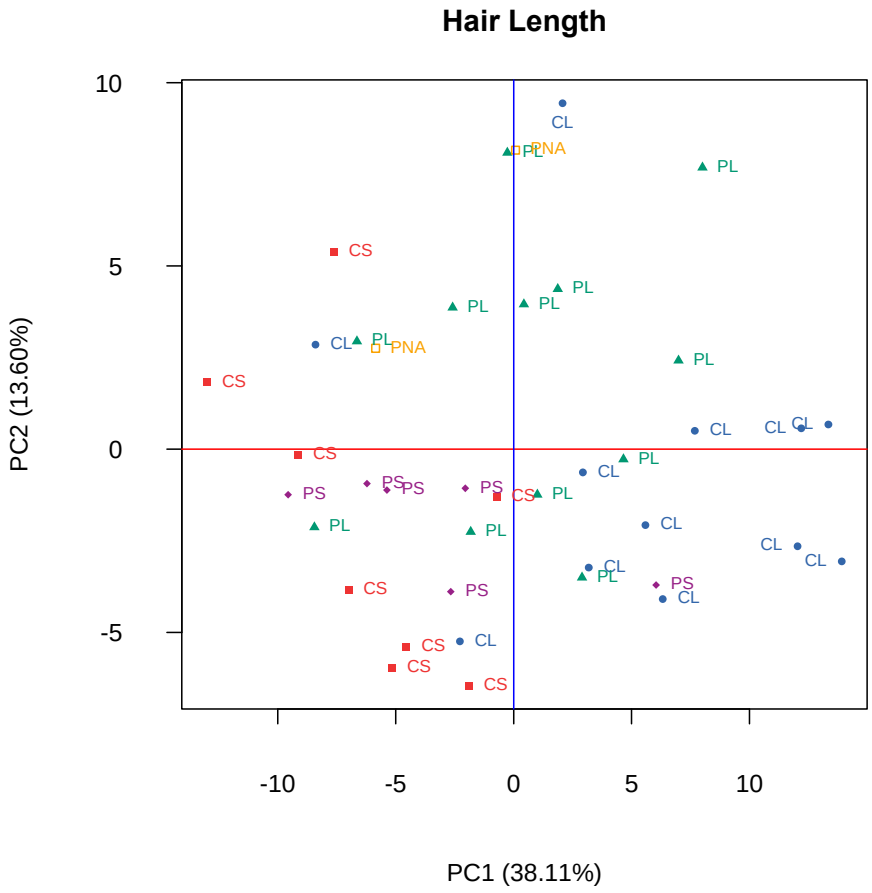


Figure 4.26: Principle component analysis of all 20 patient serum samples for hair length of participants. CS (red)- control, short hair, CL (blue)-control, long hair, PS (purple)- patient, short hair, PL (green)- patient, long hair, PNA (yellow)- N/A. Short hair was considered 8cm long or less and long hair was considered greater than 8cm long. No separation or trends can be seen between the patients (n=20).

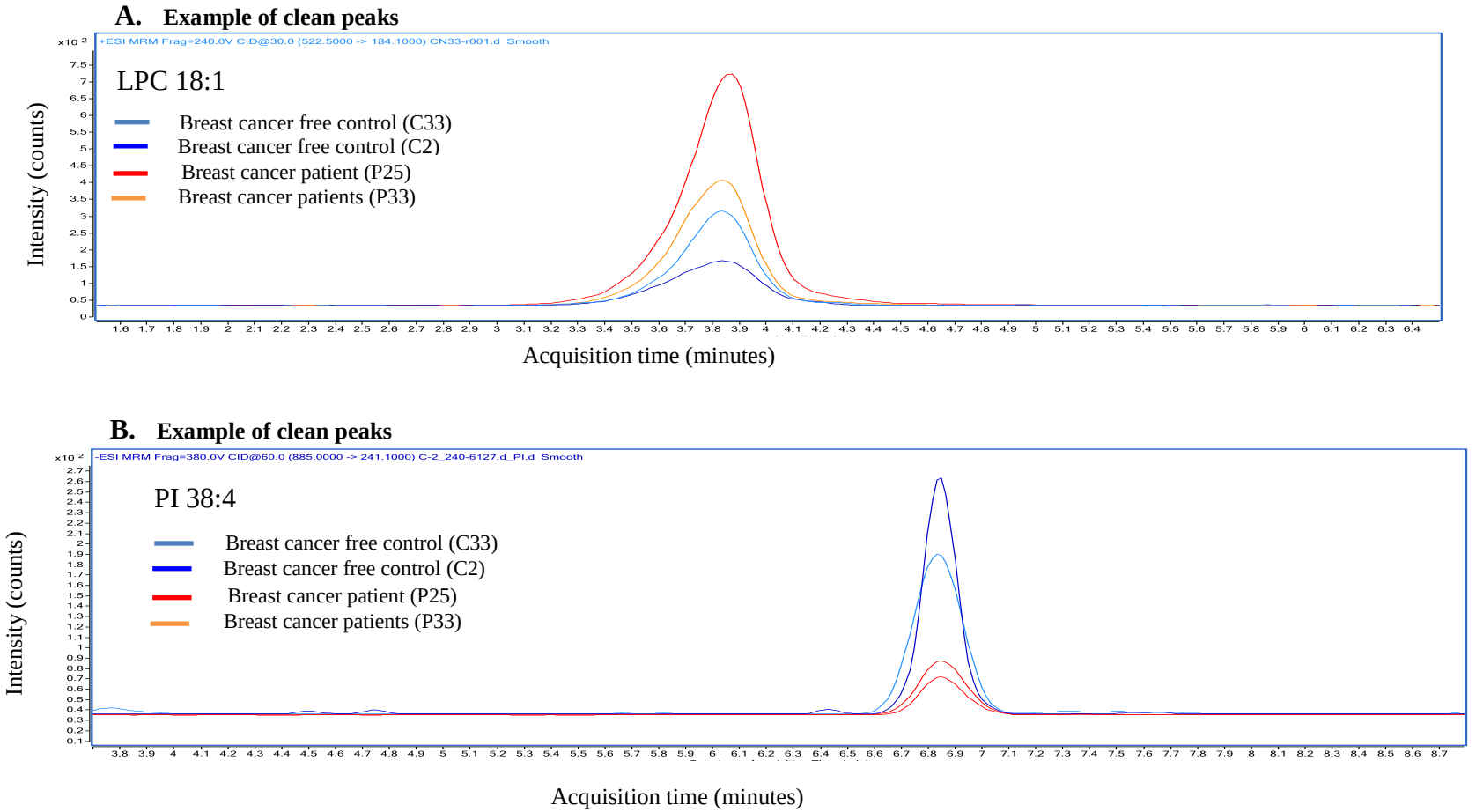
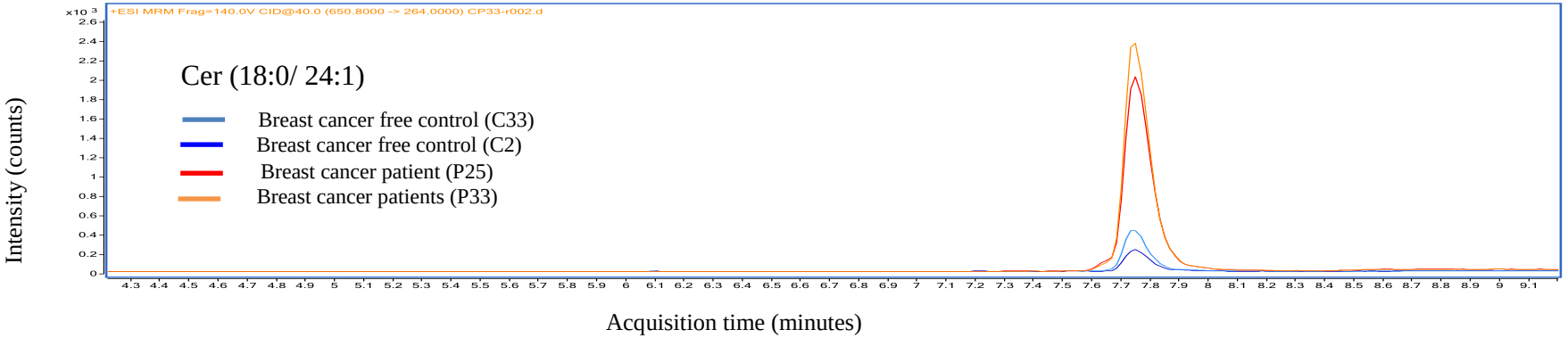


Figure 4.27, A-H : Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. LPC 18:1**, B.** PI 38:4**, C.** PC Cer 18:0/ 24:1**, D.** SM 34:1**, E.** CE 18:2**, F.** PG 32:0**, G.** PC 38:5**, H.** PE 38:1**. Figures A-F are examples of ideal, clean peaks and Figures G-H are examples of noisy, unclear peaks.**

C. Example of clean peaks



D. Example of clean peaks

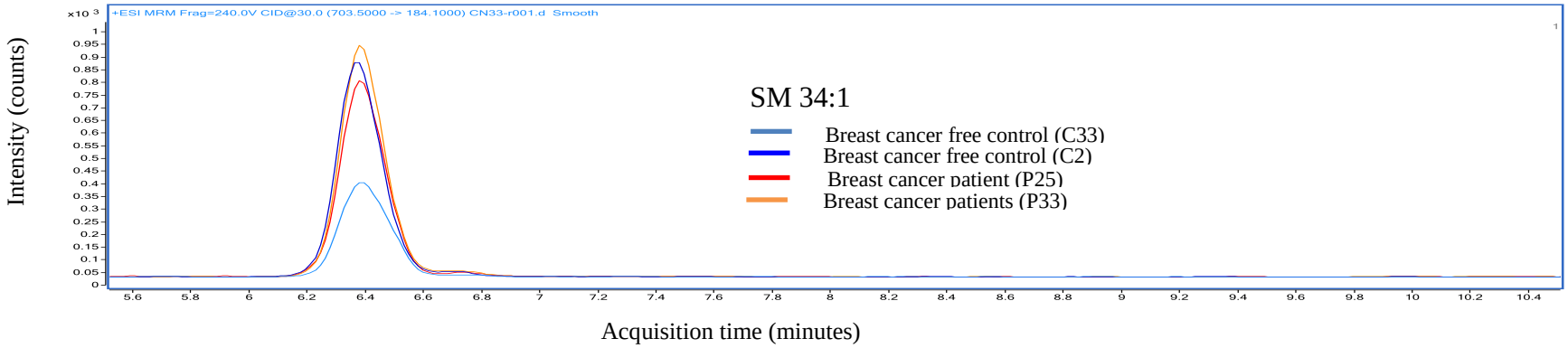
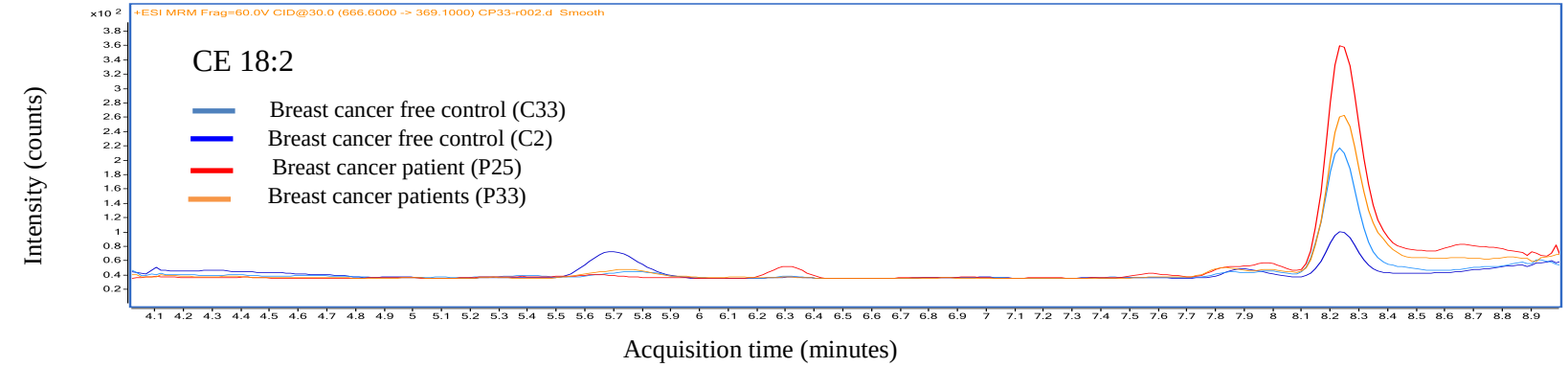


Figure 4.27, A-H : Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. LPC 18:1**, B.** PI 38:4**, C.** PC Cer 18:0/ 24:1**, D.** SM 34:1**, E.** CE 18:2**, F.** PG 32:0**, G.** PC 38:5**, H.** PE 38:1**. Figures A-F are examples of ideal, clean peaks and Figures G-H are examples of noisy, unclear peaks.**

E. Example of clean peaks



F. Example of clean peaks

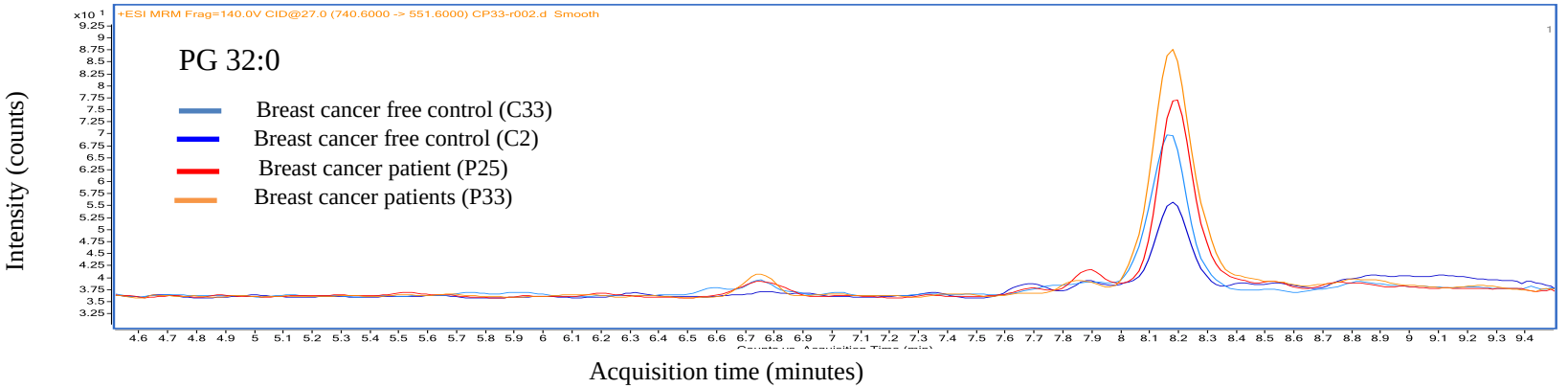


Figure 4.27, A-H : Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. LPC 18:1**, B.** PI 38:4**, C.** PC Cer 18:0/ 24:1**, D.** SM 34:1**, E.** CE 18:2**, F.** PG 32:0**, G.** PC 38:5**, H.** PE 38:1**. Figures A-F are examples of ideal, clean peaks and Figures G-H are examples of noisy, unclear peaks.**

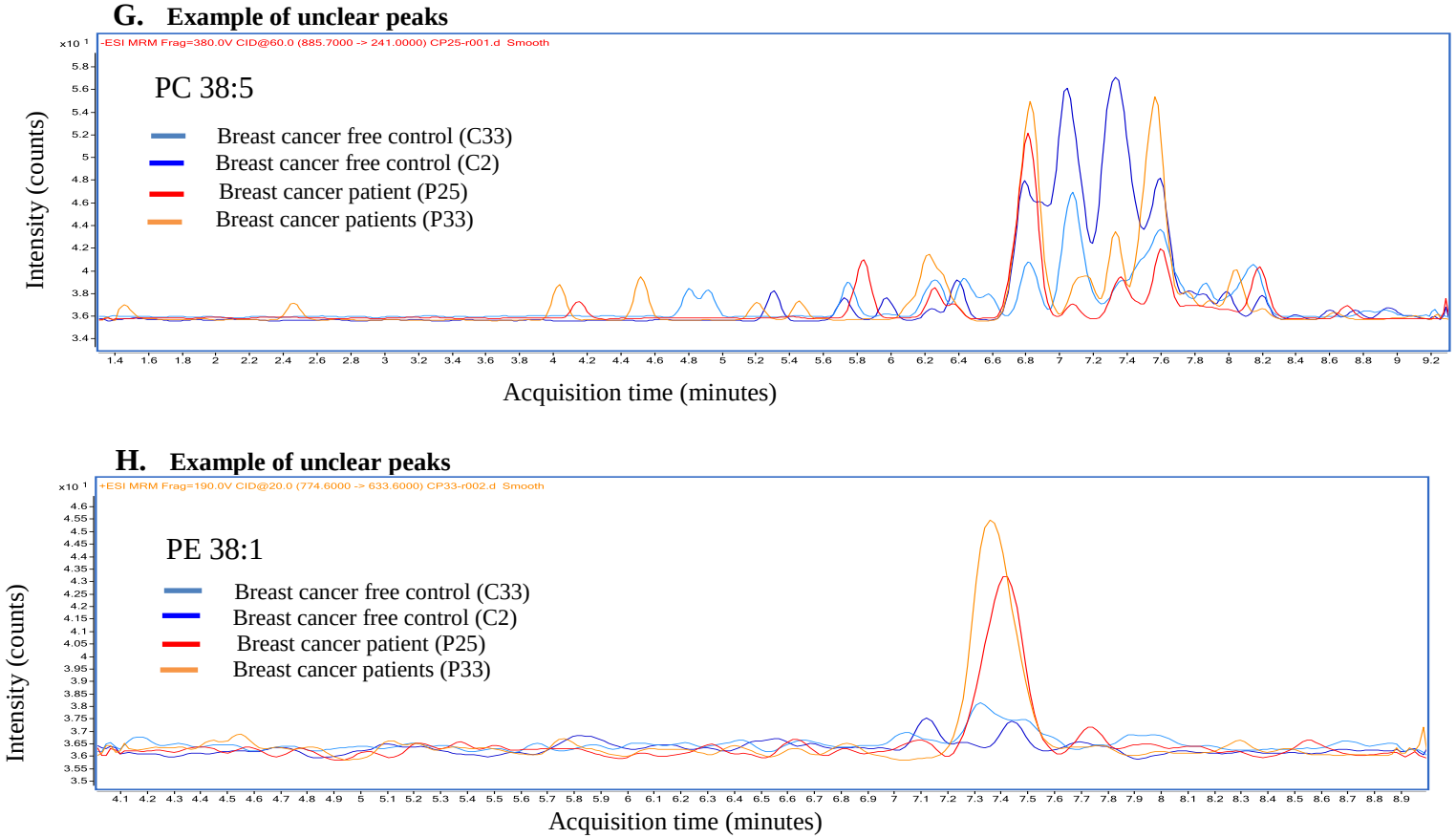


Figure 4.27, A-H : Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. LPC 18:1**, B.** PI 38:4**, C.** PC Cer 18:0/ 24:1**, D.** SM 34:1**, E.** CE 18:2**, F.** PG 32:0**, G.** PC 38:5**, H.** PE 38:1**. Figures A-F are examples of ideal, clean peaks and Figures G-H are examples of noisy, unclear peaks.**

4.5. Discussion

This data is the first study to use LCMS to analyse scalp hair for lipids associated with breast cancer. Data from this study indicates that there was not a difference between the lipids found in hair of patients with breast cancer and healthy controls. Although the preliminary study (Chapter 2) indicated that hair may be a source for lipids that are specific to breast cancer, which could be identified using LCMS, there are many reasons why the larger study did not reproduce the results of the pilot study.

Initially, 80 hair samples were collected and split into two groups: initial 40 samples with 20 control samples and 20 breast cancer patients samples and the final 40 samples, with 20 control samples and 20 breast cancer patients samples. Extraction of lipids from the initial 40 samples proved highly difficult with major inconsistencies in the homogenisation of the hair fibres and loss of samples due to vials bursting during cryomill cycles (bursting after 3 rounds in the cryomill, out of 6 cycles required). Optimization of the methodology was carried out before the final 40 samples were processed and analysed (Appendix, Figures 8.7- 8.9). The protocol, which was used for the initial 40 samples, can be seen in Figure 4.28, was modified from Bligh and Dyer is a monophasic lipid extraction protocol (Bligh, 1959).

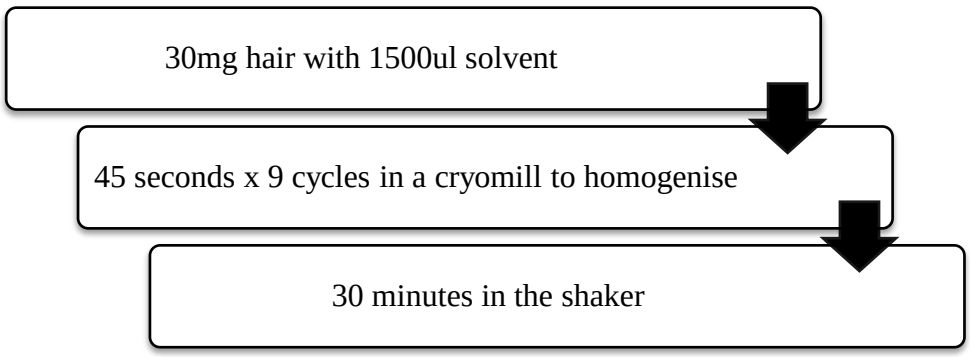


Figure 4.28: Protocol used to extract lipids from hair for the initial 40 samples. This method proved to be difficult with uneven homogenization of hair samples and burst vials.

Optimization experiments, which were carried out as a consequence of these difficulties, assessed a set of key variables (Table 5.1 and also see Appendix, Figures 8.7- 8.9).

Table 4.1: List of variables, which were compared to optimise the method of extraction of lipids from hair.

Amount of hair	7mg	15mg	30mg
Amount of solvent during homogenization of hair	0ul	750ul	1500ul
Number of cycles in the cryomill	3 cycles	6 cycles	9 cycles
Time in shaker	5 minutes	15 minutes	30 minutes

Following optimization experiments, the improved protocol was developed and this method yielded even homogenization of all hair samples with less cryomill cycles than previously required without causing the vials to burst (Figure 4.29). It would appear that the vials might have previously burst due to a manufacture default.

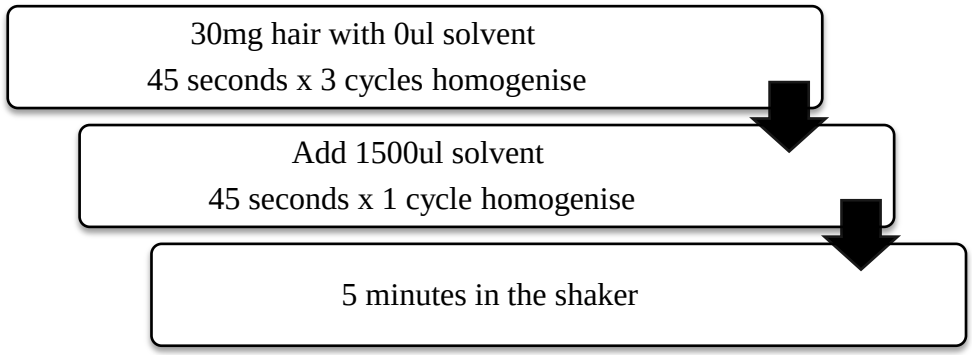


Figure 4.29: optimised protocol used to extract lipids from hair for the final 40 samples. This method allowed even homogenization of hair samples and did not cause the vials to burst.

Another source of variability that was discovered, after the processing of the 80 samples, was in a small study (Appendix, Figure 8.6, A-C), using the same methods, analysing the levels of PC, LPC and SM along the hair fibre was carried out. Shoulder length hair from three individuals was split equally into three sections and profiled for lipids (scalp, middle, end). Results showed variation in the amount of lipids between the three sections and for LPC, PC and SM the scalp and middle section contained the highest level of lipid compared to the end of the hairs. Women with shorter hair require more of their full-length hair to reach the 30mg required for this extraction compared to women with longer hair. As a result, they would have a lipid profile with more lipids in their hair, as the hair collected is closer to the scalp. This indicates that sample collection would be hard to define, as women have different lengths of hair, and specifying how much hair and how far from the scalp it is to be collected for analysis, can be difficult to standardise.

Although extraction of lipids from hair is achievable, reproducibility and consistency in results were difficult obtain due to the variables previously described. Even though the method of extraction of lipid from hair was further optimised, it was concluded that there are other variables, which may still affect the uniform extraction of lipids from hair. These include the:

- Temperature at which extraction is carried out as there may be degradation of lipids during homogenisation due to friction and heat
- The length of hair taken from an individual, as this can determine the amount of lipids extracted

While hair has been suggested as non-invasive sources for detecting lipid biomarkers (Corino, 2009), it does have limitations as a potential sample type. A better alternative is blood, which is readily collected, easily available and commonly used in pathology and diagnostics to screen for diseases such as Alzheimer's disease (Hye, 2006), cardiovascular disease (Wang, 2006) and ovarian cancer (Gorelik, 2005). Serum lipids are a more practical resource for diagnostic screening, compared to metabolites in the breast tumour (Kreunin, 2007), as they do not require a biopsy, which can be painful for the patient and can be impractical on a large scale.

5. Lipid extraction from serum

5.1. Introduction

There have been a small number of publications, which have demonstrated an association between breast cancer, and the presence of lipids in serum. As far back as 1971, Feldman and Carter identified the association between serum lipids and breast cancer (Feldman, 1971). In 1986, Bani *et al* found that "*serum lipids, phospholipids, triglycerides, cholesterol and free fatty acids were all higher in blood obtained from breast cancer patients prior to surgery"* (Bani, 1986). Such an apparent overall alteration highlights the need to understand this change and what may be happening on a cellular level. More recent studies have reported increases in phospholipid content, in particular phosphatidylcholine, in the serum of breast cancer patients when compared to controls. One study found that the most significant difference in serum phospholipid content, between stage-IV breast cancer patients and disease-free controls was due to three unidentified phospholipid species and three unidentified fatty acid species (Hammad, 2009). The concentration of serum lipids has been shown to be affected following treatment of the disease as Ray *et al* found that those lipids that were elevated in breast cancer decreased after treatment (Ray, 2001b).

5.2. Aims

Since these lipid biomarkers are present in the cell culture supernatant of breast cancer cells then it is likely that they will enter the bloodstream as a result of being in contact with the tumour microenvironment. As blood is routinely screened for other diseases, serum samples have been profiled for these breast cancer associated phospholipids from individuals with the disease and those without.

5.3. Methods

5.3.1. Lipid profiling of serum samples

5.3.1.1. Samples

Serum samples were collected from the Sydney Breast Clinic (Sydney, NSW Australia) and the Poche Centre (North Sydney, NSW Australia) under ethics governed by Macquarie University Human Ethics Committee (reference 5201100091). Clinical data was also collected for each individual for data analysis. There were 80 samples (5ml) in this study, 40 confirmed free of breast cancer (controls) and 40 confirmed to have breast cancer (patients).

5.3.1.2. Extraction of lipid from serum

The protocol used for lipid extraction from samples is a monophasic extraction, modified from the Bligh and Dyer protocol (Bligh, 1959).

50μL of serum was placed into a 1.5 ml Eppendorf tube. 1000μL of chilled methanol: chloroform (2:1) was added to the serum, along with 2.5μM/mL deuterated - PE (internal standard). The Eppendorf was vortexed vigorously for 5 minutes and shaken for 30 minutes at 37ºC. Samples were centrifuged at 100 rpm and 0°C for 10 minutes and the supernatant was transferred into a new Eppendorf tube (2 ml) tube. Steps 2, 3 and 4 were repeated for the second extraction from the protein precipitate. Both supernatant extractions were combined into one Eppendorf and dried under liquid nitrogen at 30˚C. Samples were resuspended in 100μL of butanol/methanol (1:1) with 10mM ammonium formate and shaken at 30°C for 30 minutes. Samples were centrifuged at 100 rpm for 10 minutes at room temperature and the supernatant was transferred to high pressure liquid chromatography (HPLC) vials.

5.3.1.3. Preparation of pooled biological quality control (PBQC) samples

20ul aliquots from each sample were combined to create the PBQC. From this PBQC, a 50 uL aliquot was placed into a 1.5 ml Eppendorf tube, (20 µL x80 samples = 1600 µL, 1600µl/ 50µl = 32 PBQCs). These PBQC samples were then processed the same way as the other serum samples, according to the protocol above.

5.3.1.4. Liquid Chromatography Mass Spectrometry (LCMS) analysis of serum

Refer to Chapter 4: Methods, page 58.

5.3.1.5. Data processing for all LCMS data

Refer to Chapter 4: Methods, page 58-59. Refer to Appendix 8.6.1 for ESI mode, ion scan mode and chromatograms of the standards.
Note: The serum data had 0.15% missing values.
Refer to Appendix 8.1.1. for raw data. Due to large differences in the relative abundance of the lipid species when the data was compared within itself, the raw matrices were log transformed to bring the variance to a similar level and allowed comparability.(Appendix 8.1.2.). Log transformation is routinely used in statistical analysis when the standard deviation is proportional to the mean of the data (Roessner, 2011). Data was transformed to natural logarithm before normalisation in order to make it comparable. Once data was log transformed, each data point was normalised by subtraction of this value from the mean of the total lipids. This results in negative values, which appear to be inaccurate but have been treated correctly in order to compare the data.

5.3.2. Lipid nomenclature

Refer to Chapter 2: Methods, page 46.

5.4. Results

A PCA was used to give a visual interpretation of any significant differences that existed between the samples in this study (Figures 5.3- 5.11). The PCA's for all 80 samples for each lipid type did not illustrate any separation, clustering or trends in the data that would indicate a significant difference between the two groups (controls free of breast cancer and patients with breast cancer). The pooled biological quality control's (PBQC) however, do sit tightly in a cluster, indicating that the data is robust (see Appendix, Table 8.14).

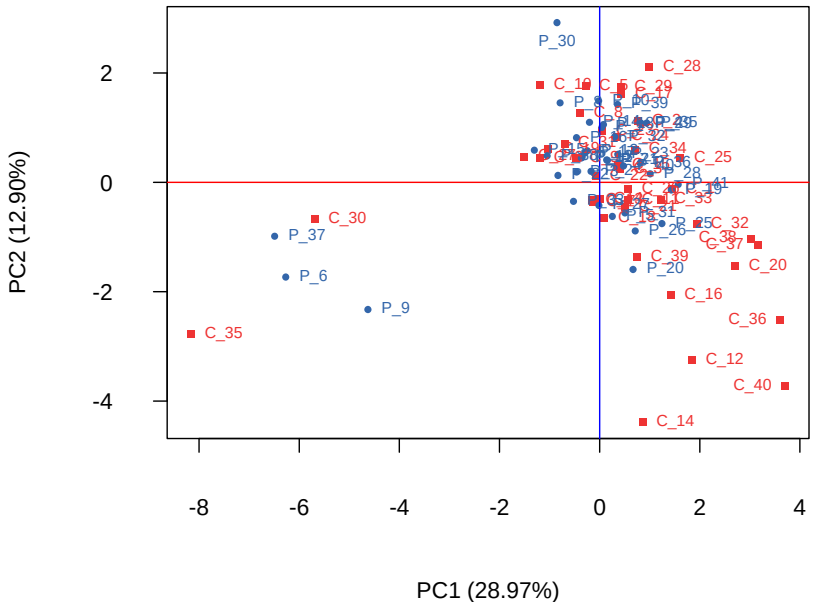


Figure 5.3: Principle component analysis of all 80 serum samples for cholesterol ester where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40).

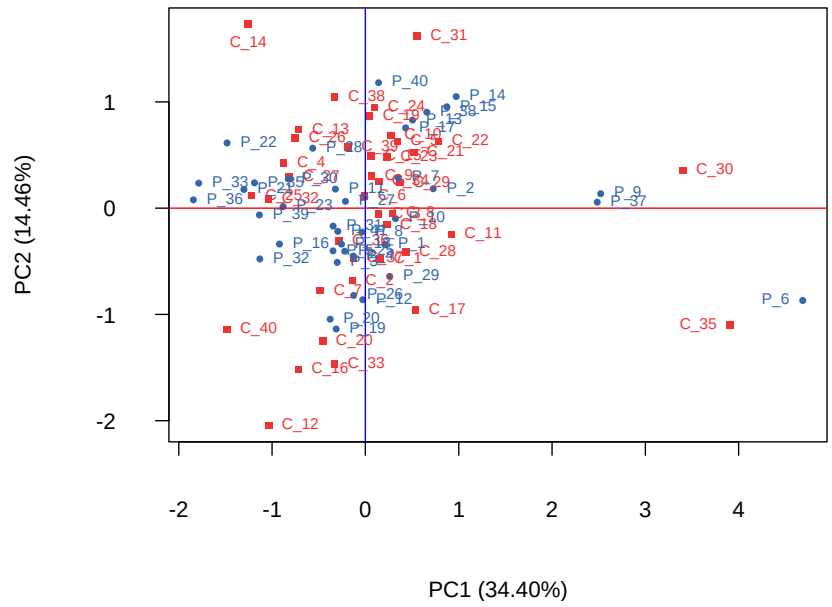


Figure 5.4: Principle component analysis of all 80 serum samples for ceramide where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40).

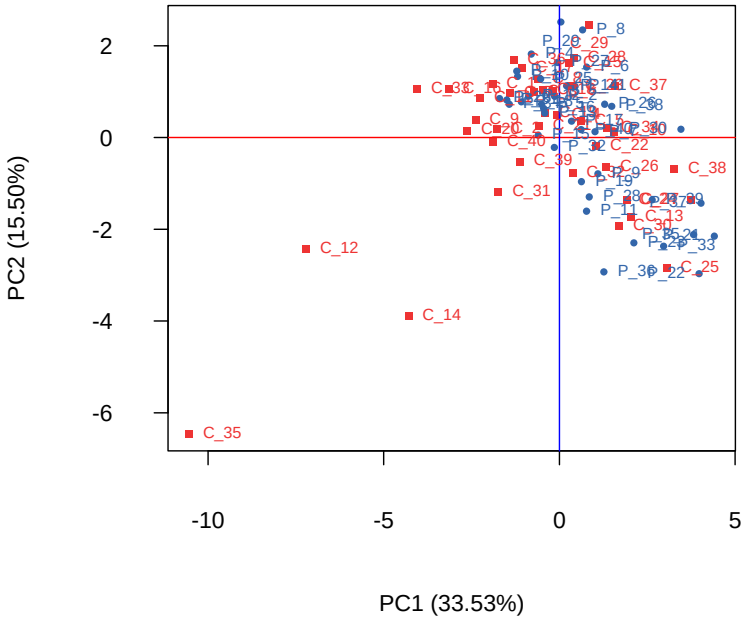


Figure 5.5: Principle component analysis of all 80 serum samples for phosphatidic acid and lyso-phosphatidic acid where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40).

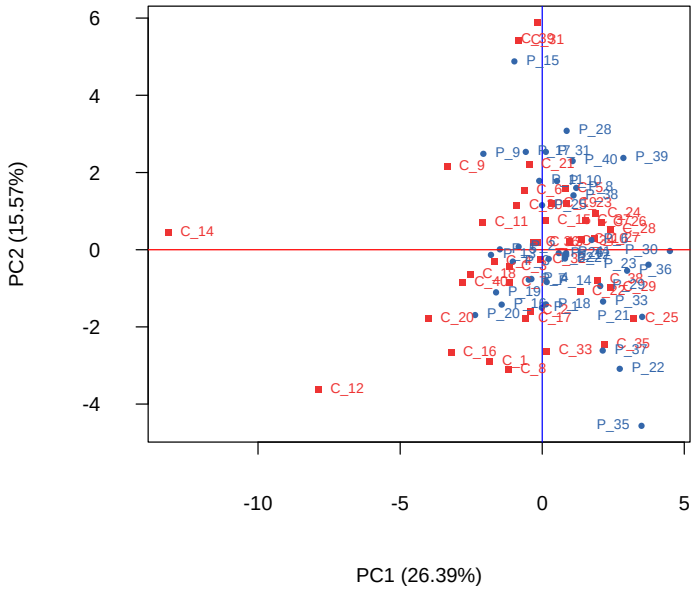


Figure 5.6: Principle component analysis of all 80 serum samples for phosphatidylcholine and lyso- phosphatidylcholine where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40).

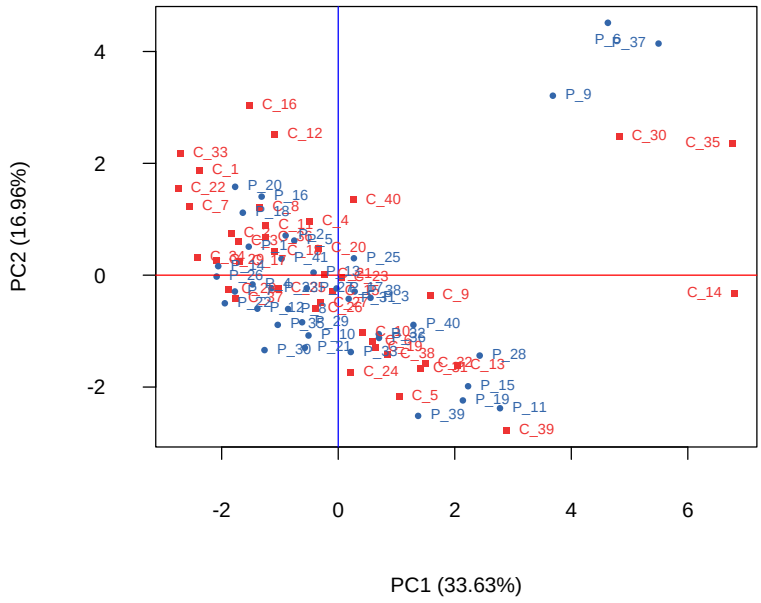


Figure 5.7: Principle component analysis of all 80 serum samples for phosphatidylethanolamine and lyso- phosphatidylethanolamine where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40).

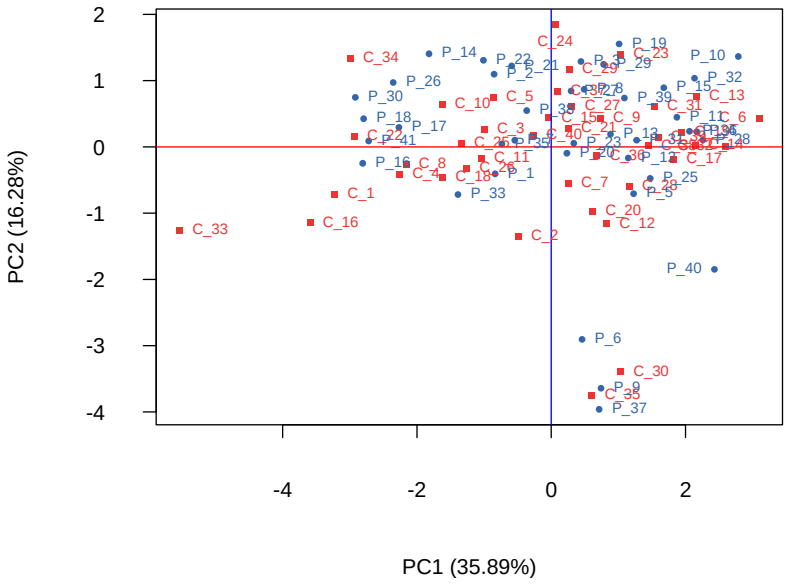


Figure 5.8: Principle component analysis of all 80 serum samples for phosphatidylglycerol and lyso- phosphatidylglycerol where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40).

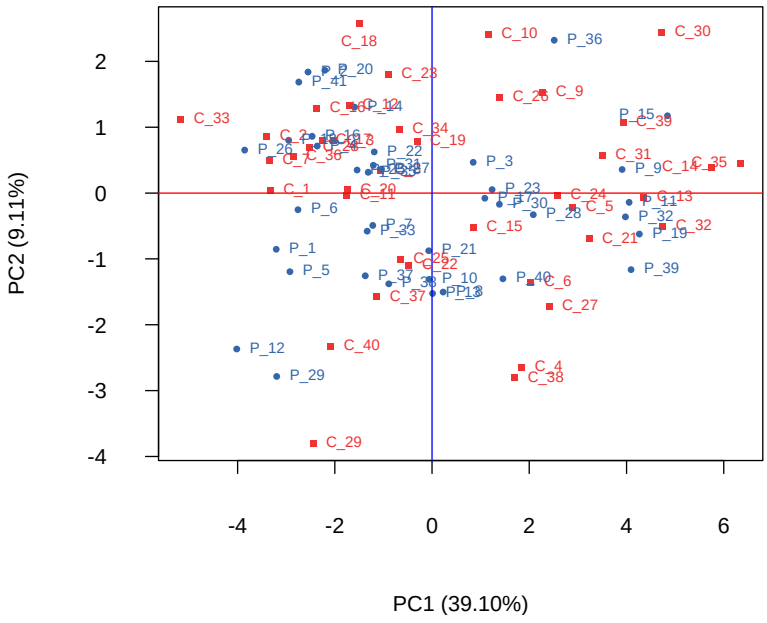


Figure 5.9: Principle component analysis of all 80 serum samples for phosphatidylinositol where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40).

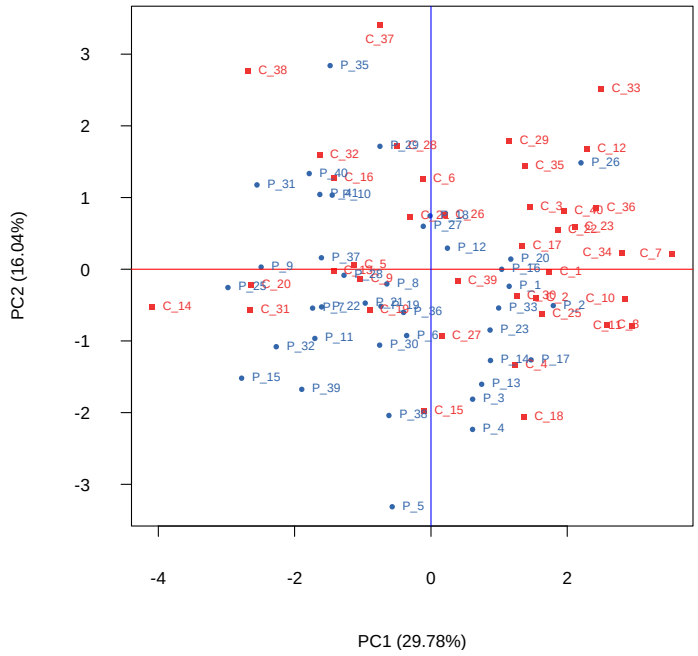


Figure 5.10: Principle component analysis of all 80 serum samples for phosphatidylserine where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40).

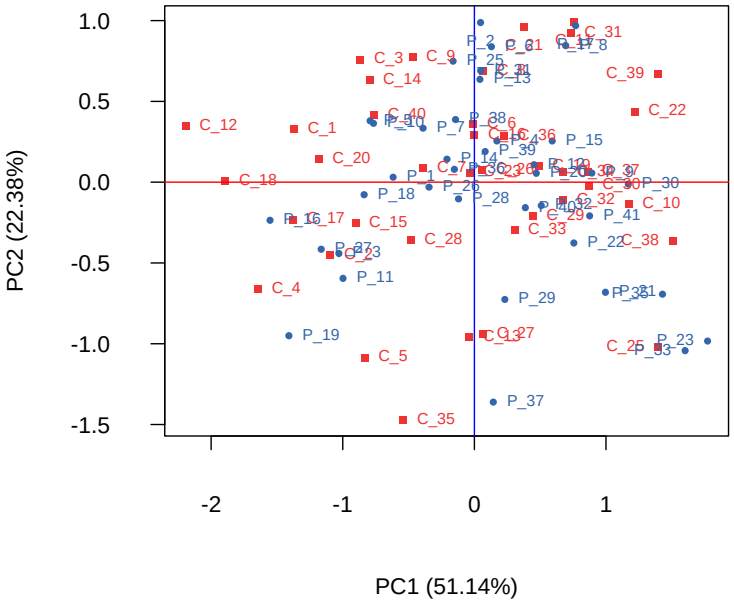


Figure 5.11: Principle component analysis of all 80 serum samples for sphingomyelin where control samples are red and breast cancer patients are blue. No separation or trends can be seen between the patients (n=40) and controls (n=40).

The average of the normalised peak area for the control and patient samples was then graphed for each lipid species to illustrate where the differences between the two groups could be accounted (Figures 5.12 -5.23). The spread of the samples across all the PCA's is diverse with some overall clustering and some pushed out towards the sides or just a random dispersal of samples. This indicates a high level of variability amongst the 80 participants and this is likely due to individual variability from person to person.

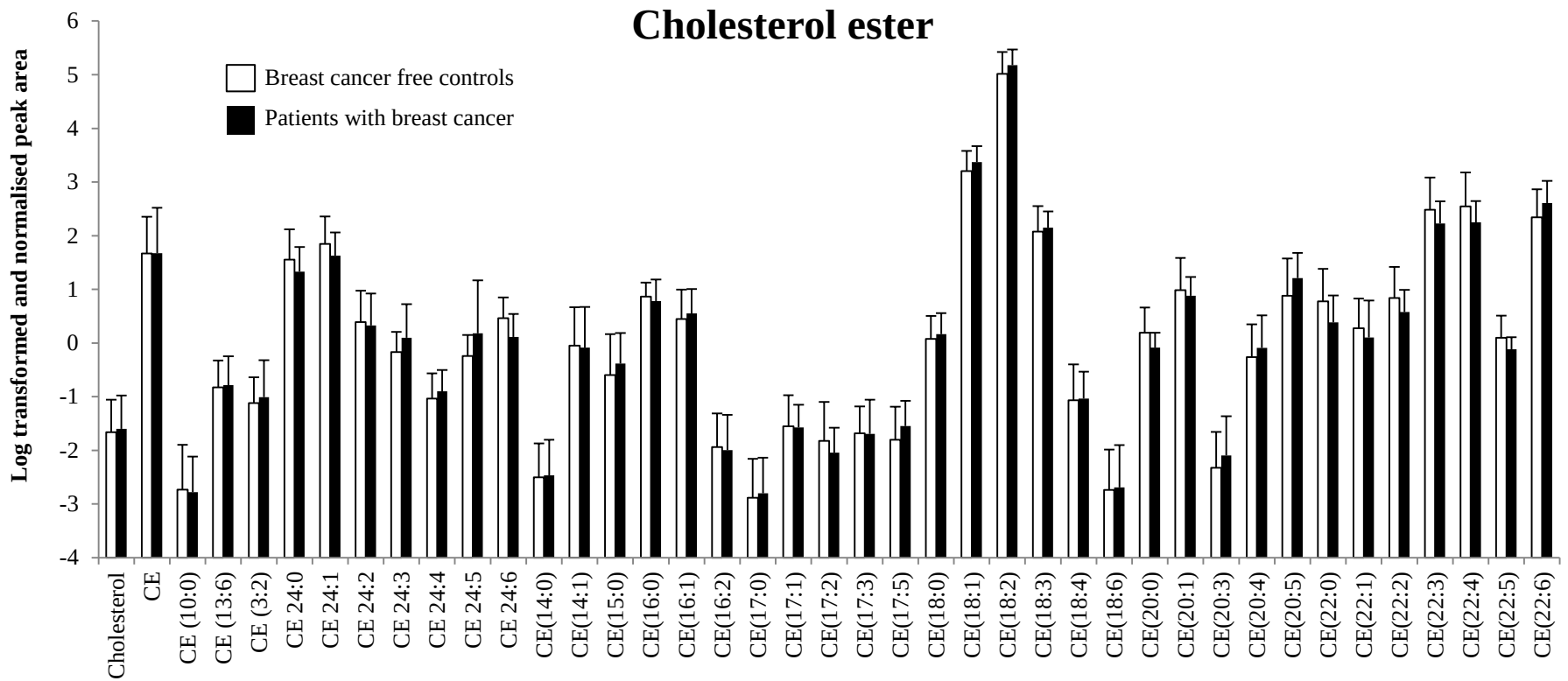


Figure 5.12: Average of log transformed and normalised peak area of cholesterol ester in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

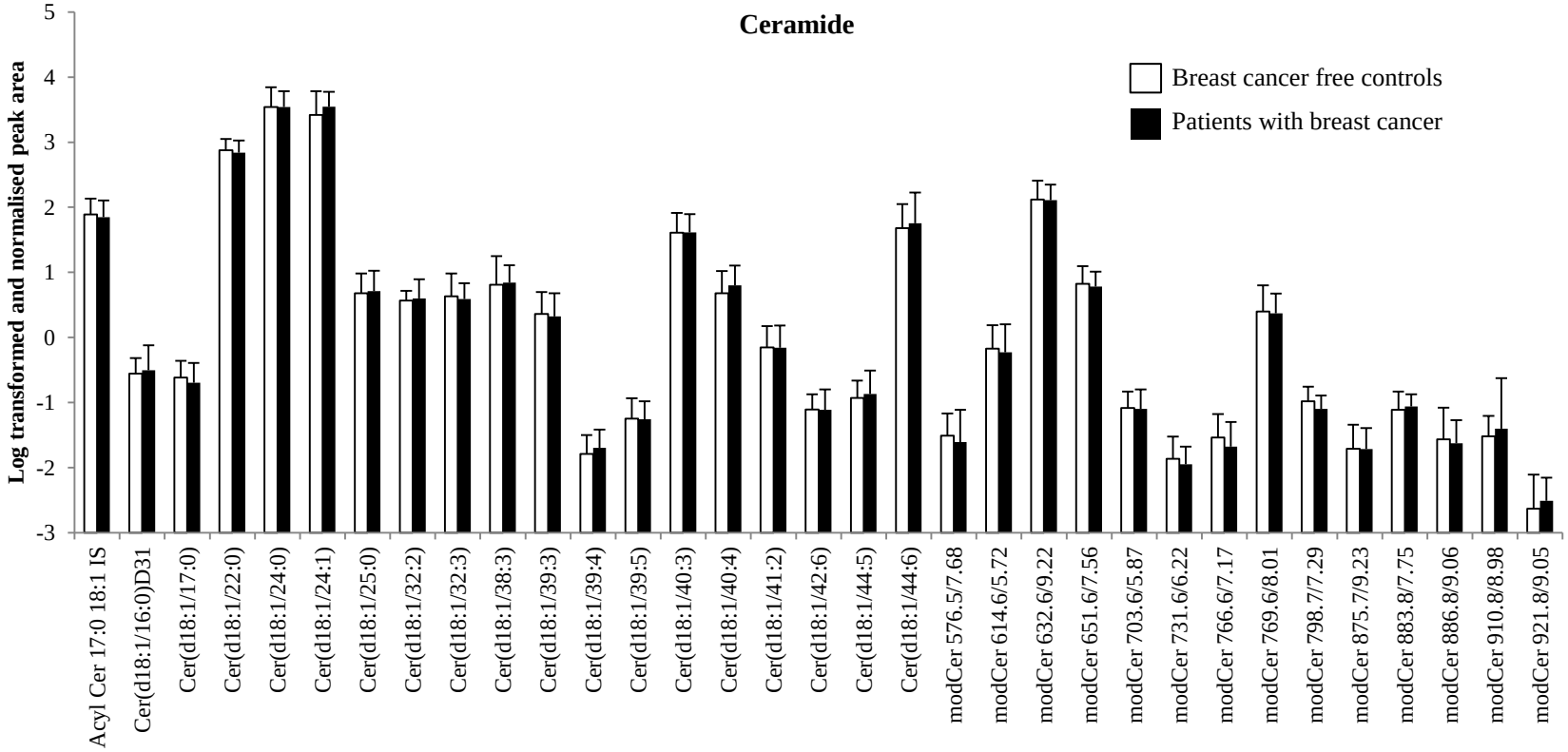


Figure 5.13: Average of log transformed and normalised peak area of ceramide in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

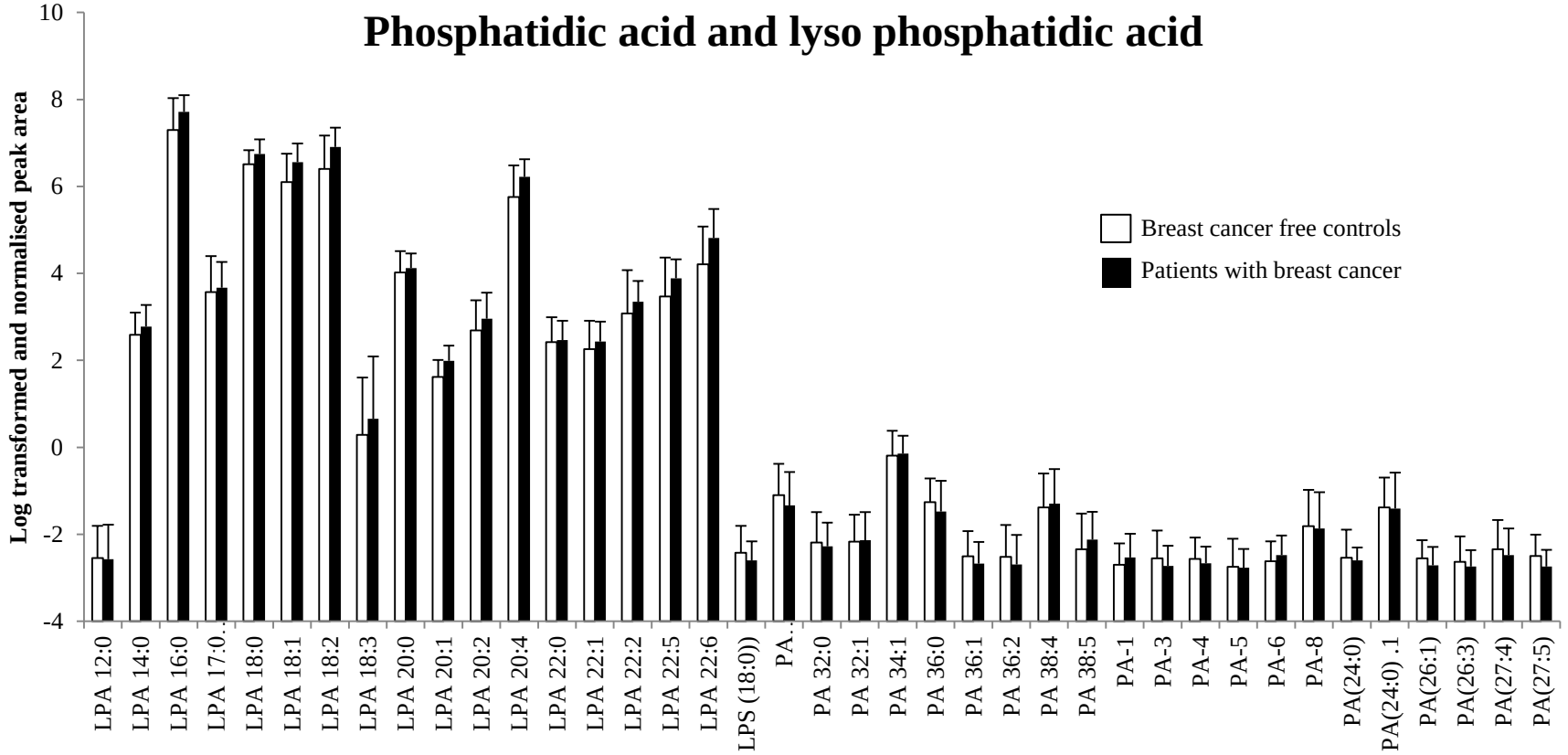


Figure 5.14: Average of log transformed and normalised peak area of phosphatidic acid and lyso phosphatidic acid in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

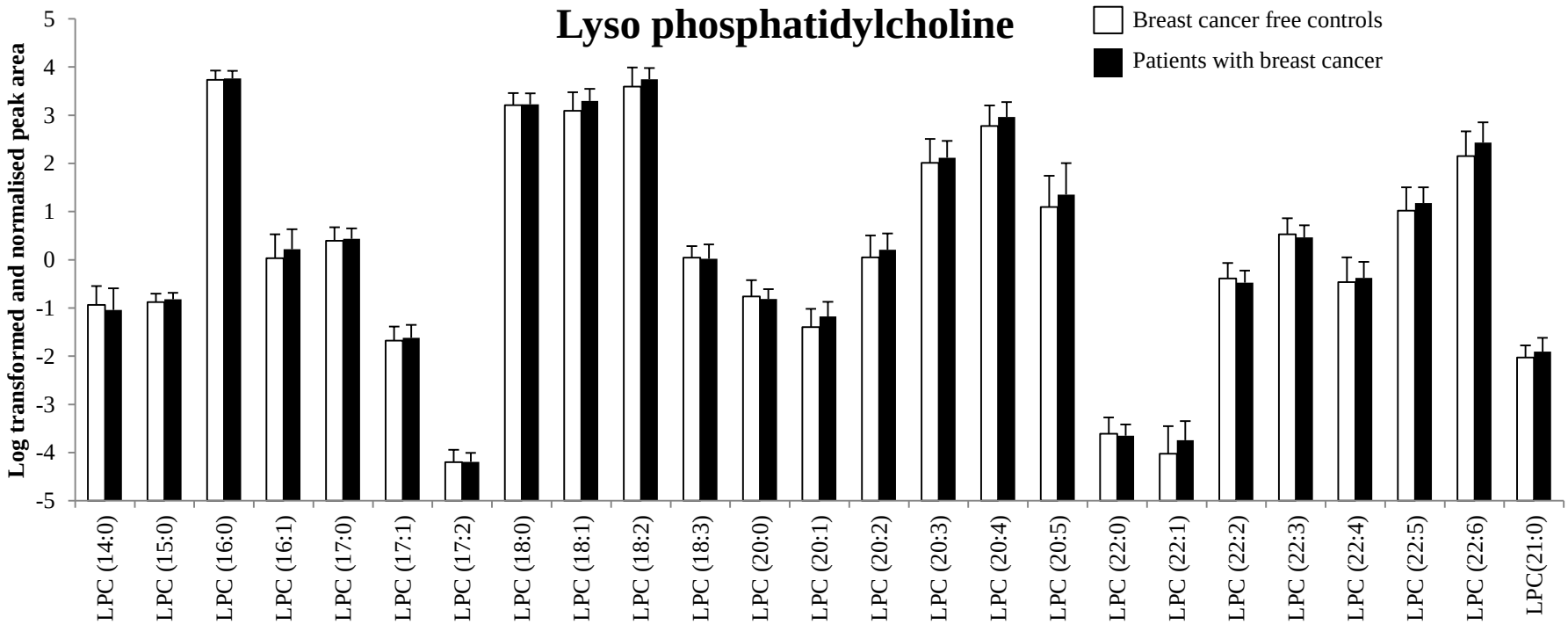


Figure 5.15: Average of log transformed and normalised peak area of lyso phosphatidylcholine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

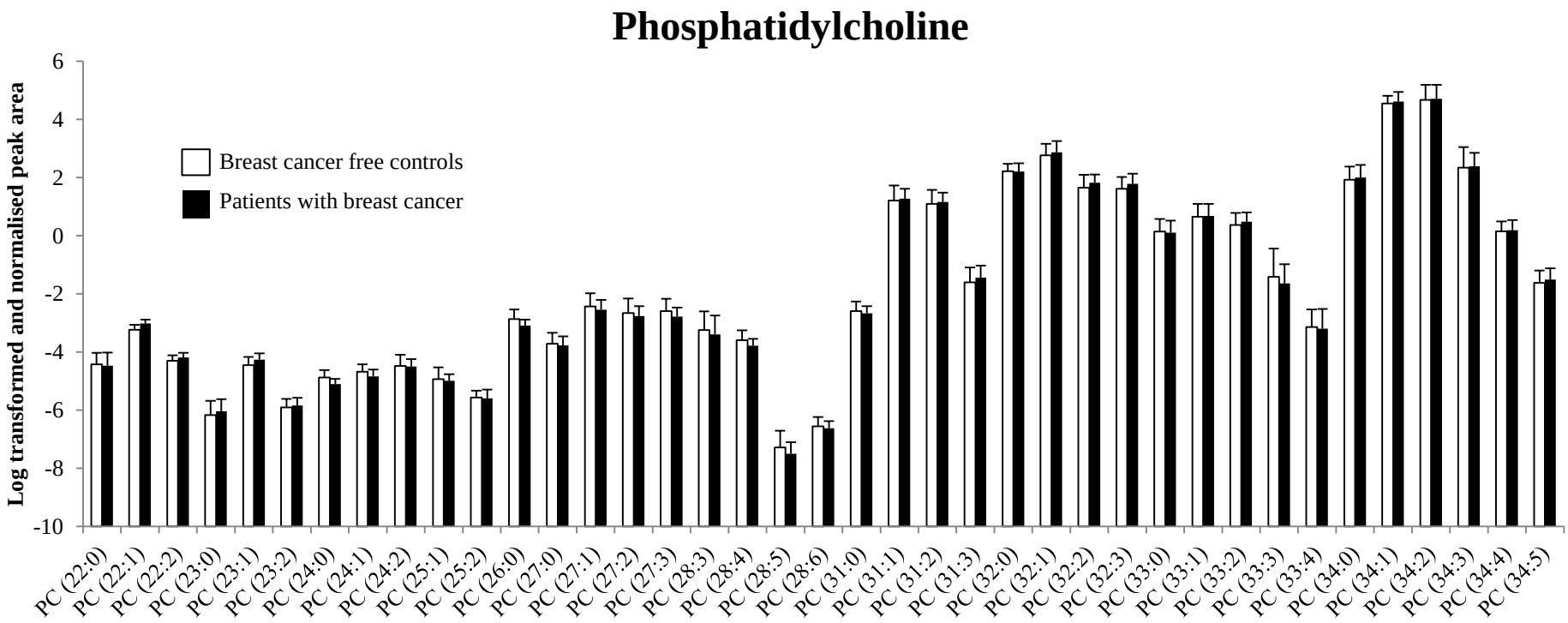


Figure 5.16: Average of log transformed and normalised peak area of phosphatidylcholine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

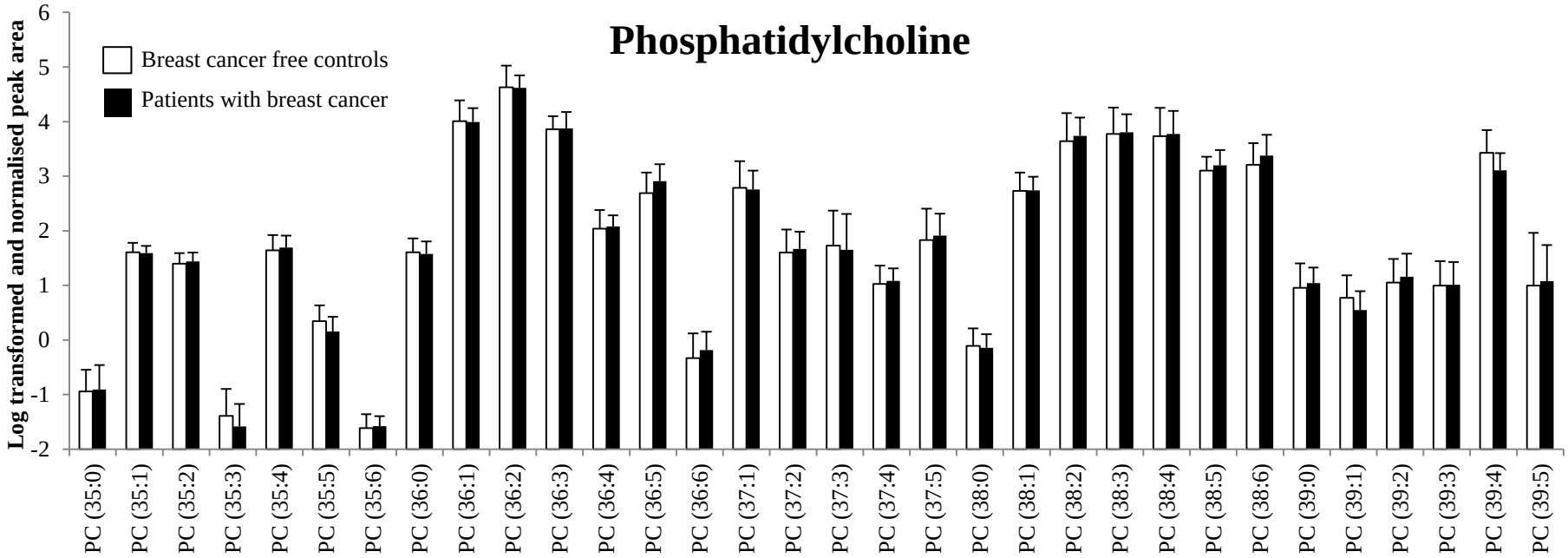


Figure 5.17: Average of log transformed and normalised peak area of phosphatidylcholine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

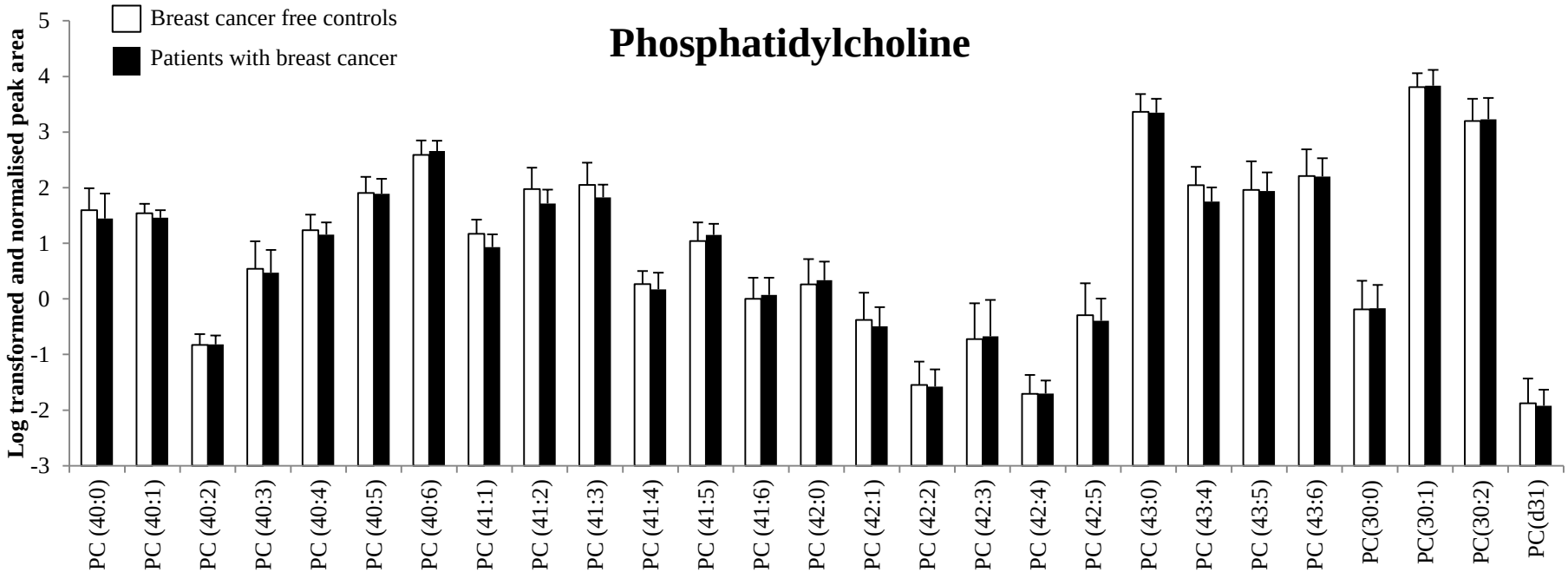


Figure 5.18: Average of log transformed and normalised peak area of phosphatidylcholine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

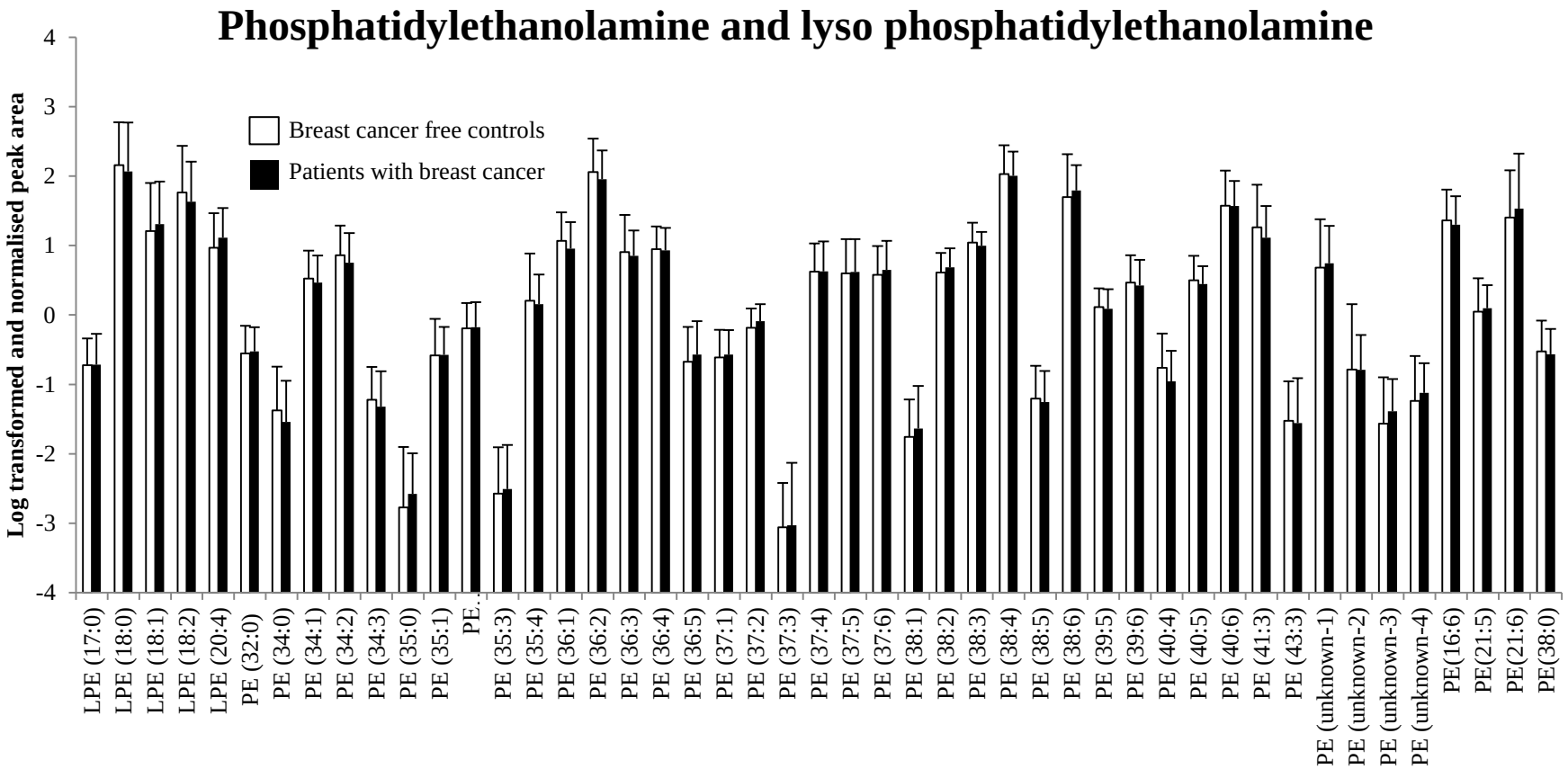


Figure 5.19: Average of log transformed and normalised peak area of phosphatidylethanolamine and lyso phosphatidylethanolamine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

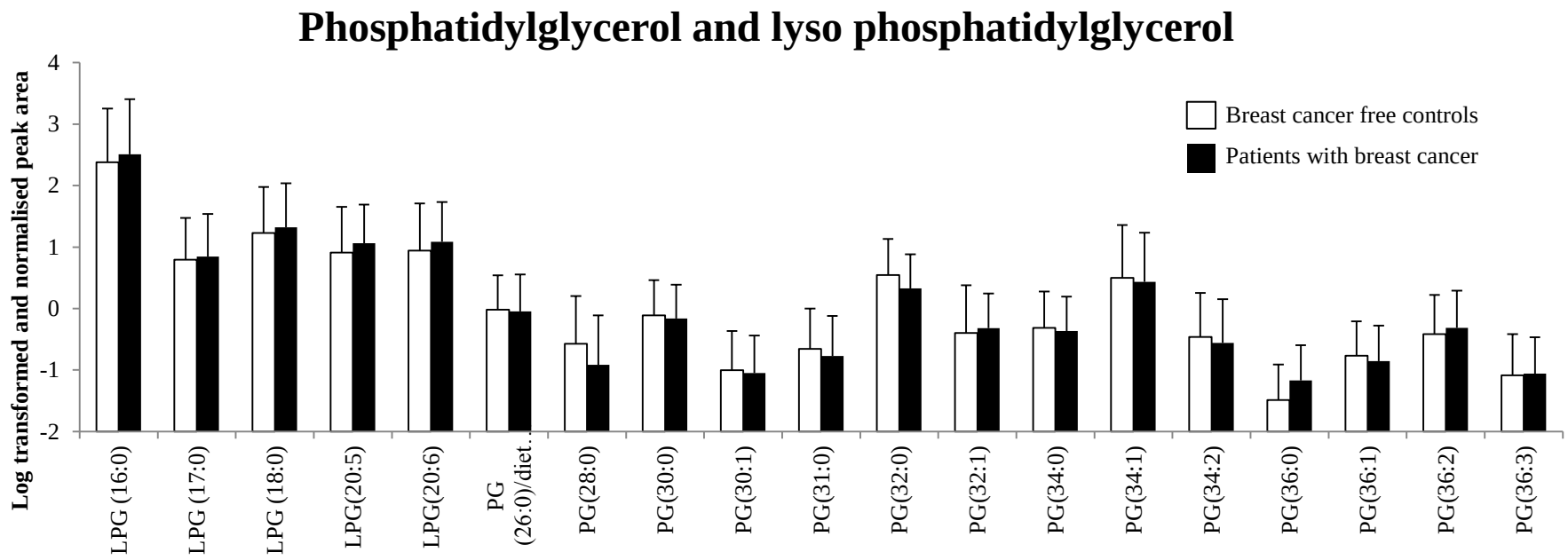


Figure 5.20: Average of log transformed and normalised peak area of phosphatidylglycerol and lyso phosphatidylglycerol in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

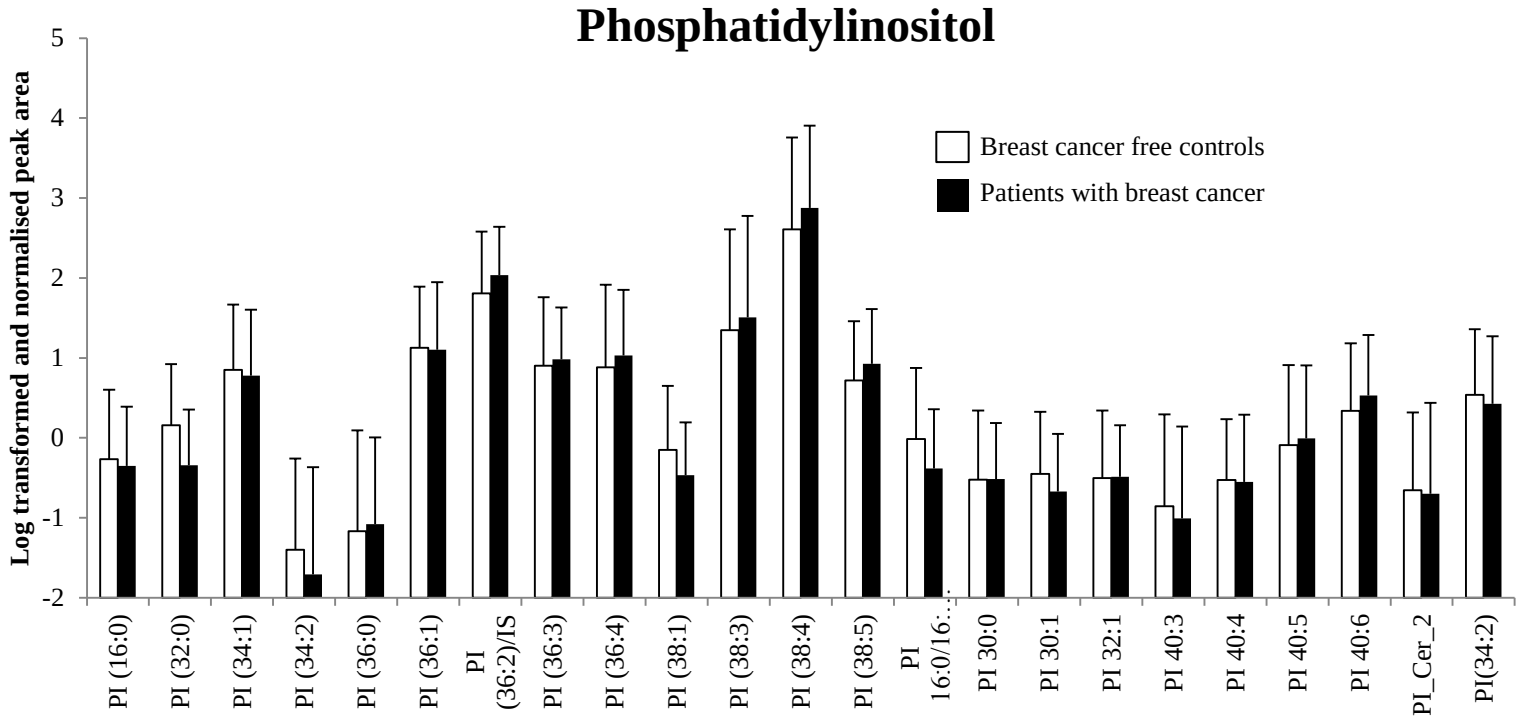


Figure 5.21: Average of log transformed and normalised peak area of phosphatidylinositol in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

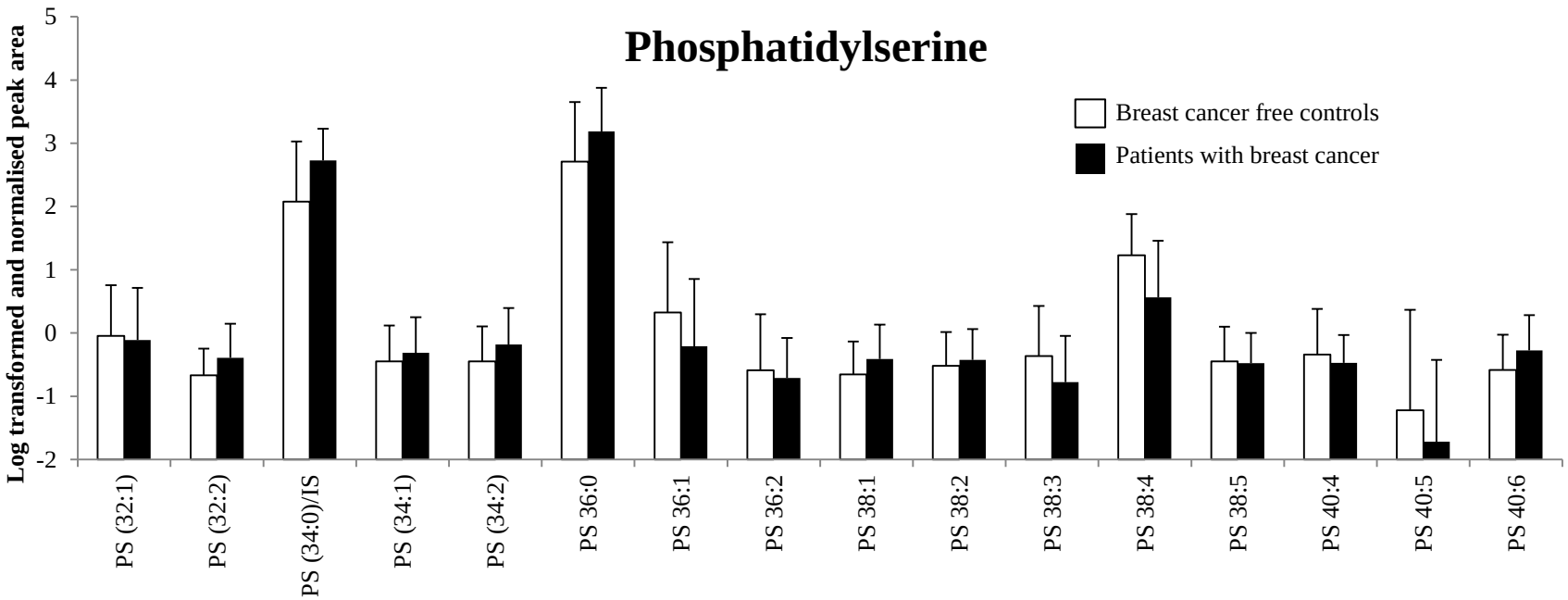


Figure 5.22: Average of log transformed and normalised peak area of phosphatidylserine in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

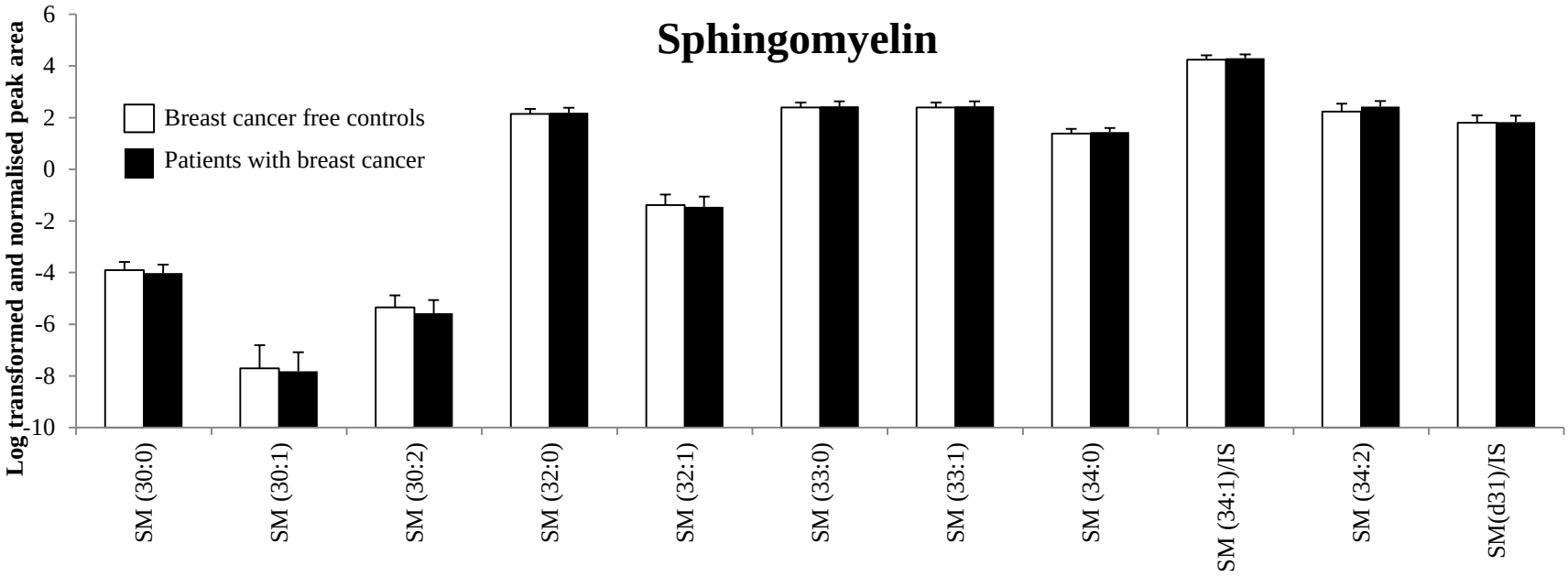


Figure 5.23: Average of log transformed and normalised peak area of sphingomyelin in the serum samples from breast cancer free controls (white, n=40) and patients with breast cancer (black, n=40). Error bars are the standard deviation.

An unsupervised PCA was carried out to explore any groupings that may have been occurring amongst the samples due to the patients' clinical data (Figures 5.24 to 5.27). This data included: the size of the tumour, the age of the patient as the time of examination, the type of breast cancer that the patient had and the grade of this breast tumour. A PCA was performed and the samples were then labeled according to the different patient criteria. There was no major separation between samples based on the clinical data.

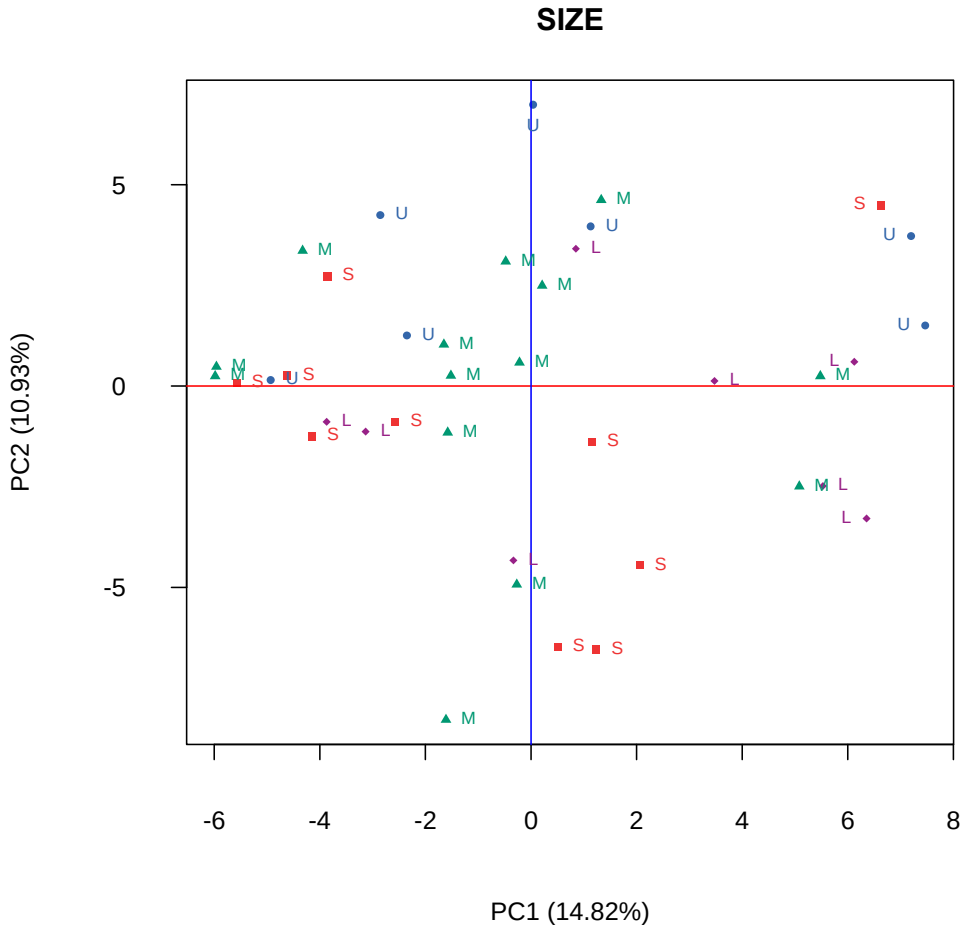


Figure 5.24: Principle component analysis of all 40 patient serum samples for tumour size. S (red)- less than 10cm; M (green)- between 10cm and 30cm; L (purple) - 30cm and greater ; U (blue) –Unknown, N/A. No separation or trends can be seen amongst the patients (n=40).

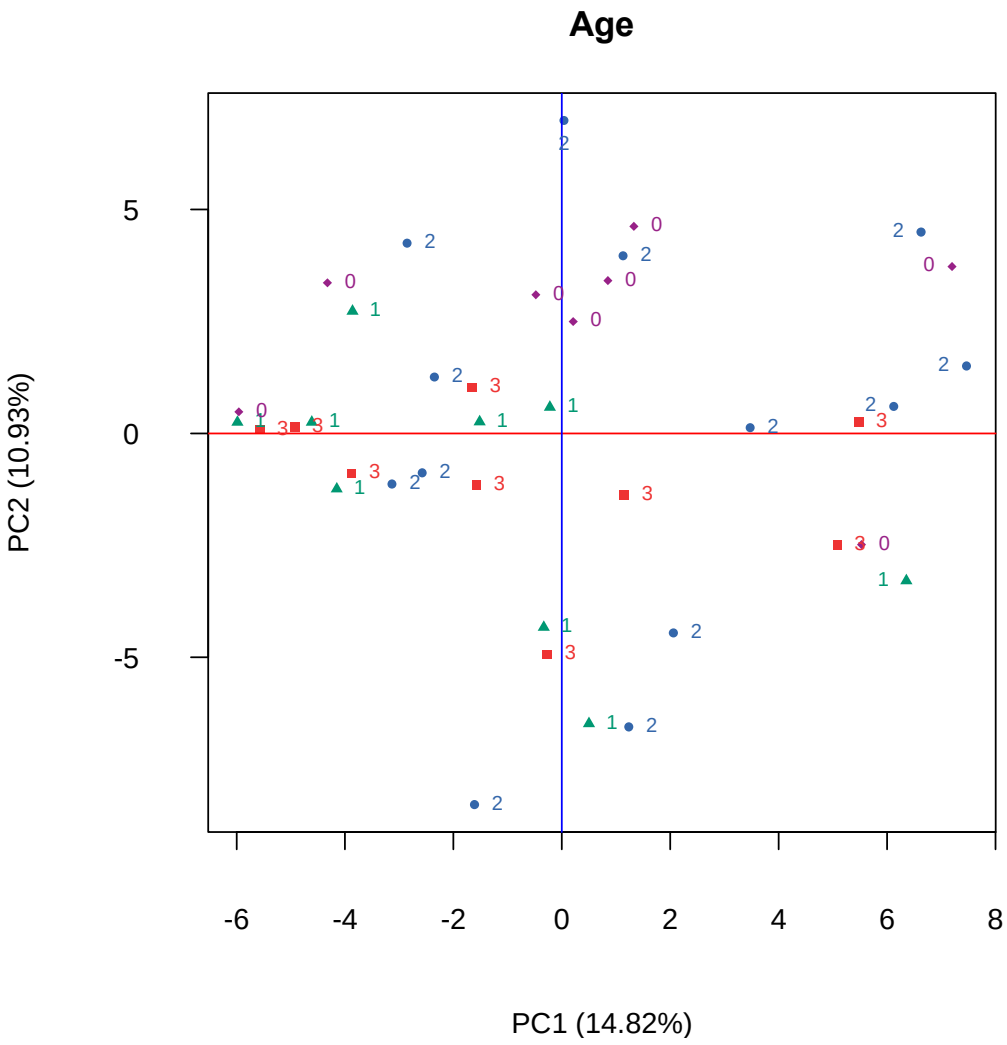


Figure 5.25: Principle component analysis of all 40 patient serum samples for patient age. 0 (purple) - patient under 50 years old ; 1 (green) - patient over 50 and under 60 years old ; 2 (blue) - patient over 60 and under 70 years old ; 3 (red) - patient over 70 years old. No separation or trends can be seen amongst the patients (n=40).

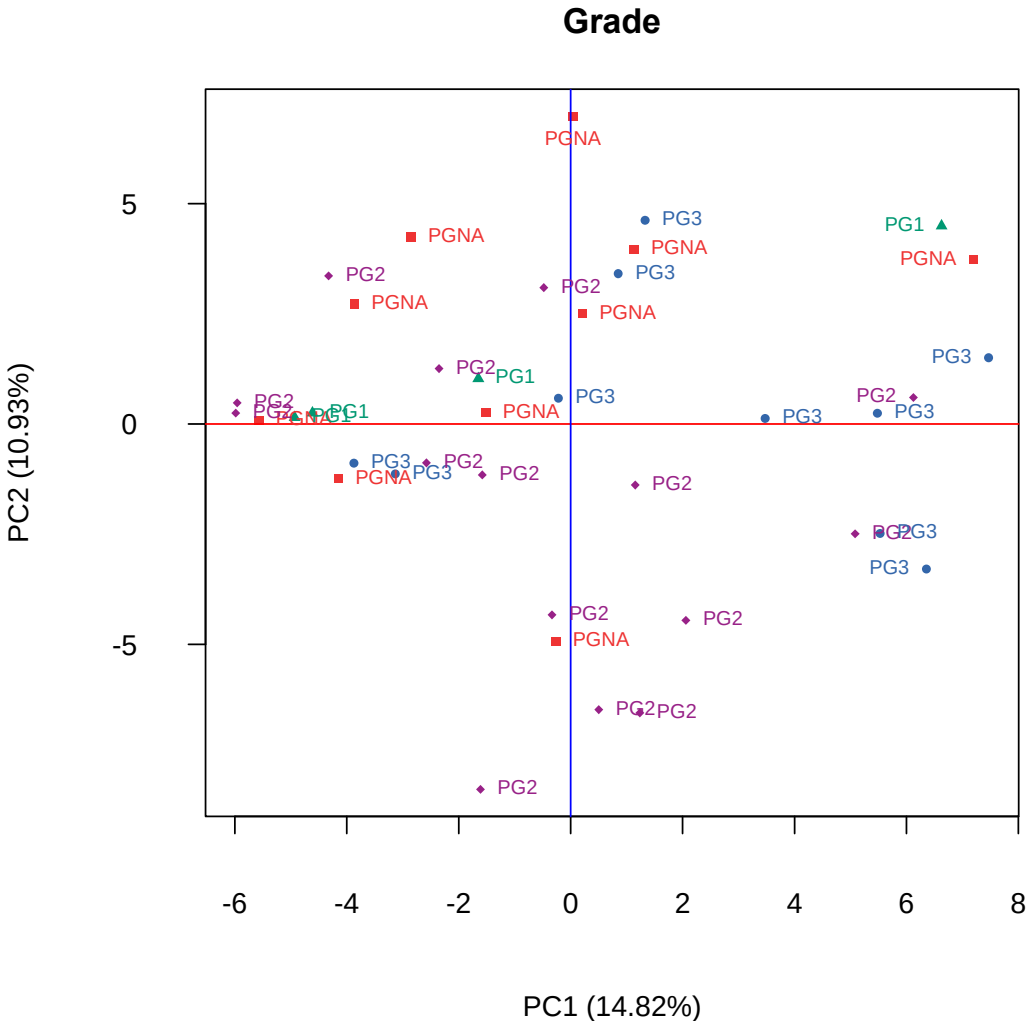


Figure 5.26: Principle component analysis of all 40 patient serum samples for tumour grade. PG1 (green) - grade 1; PG2 (purple) - grade 2; PG3 (blue) - grade 3; PGNA (red) - N/A. No separation or trends can be seen amongst the patients (n=40).

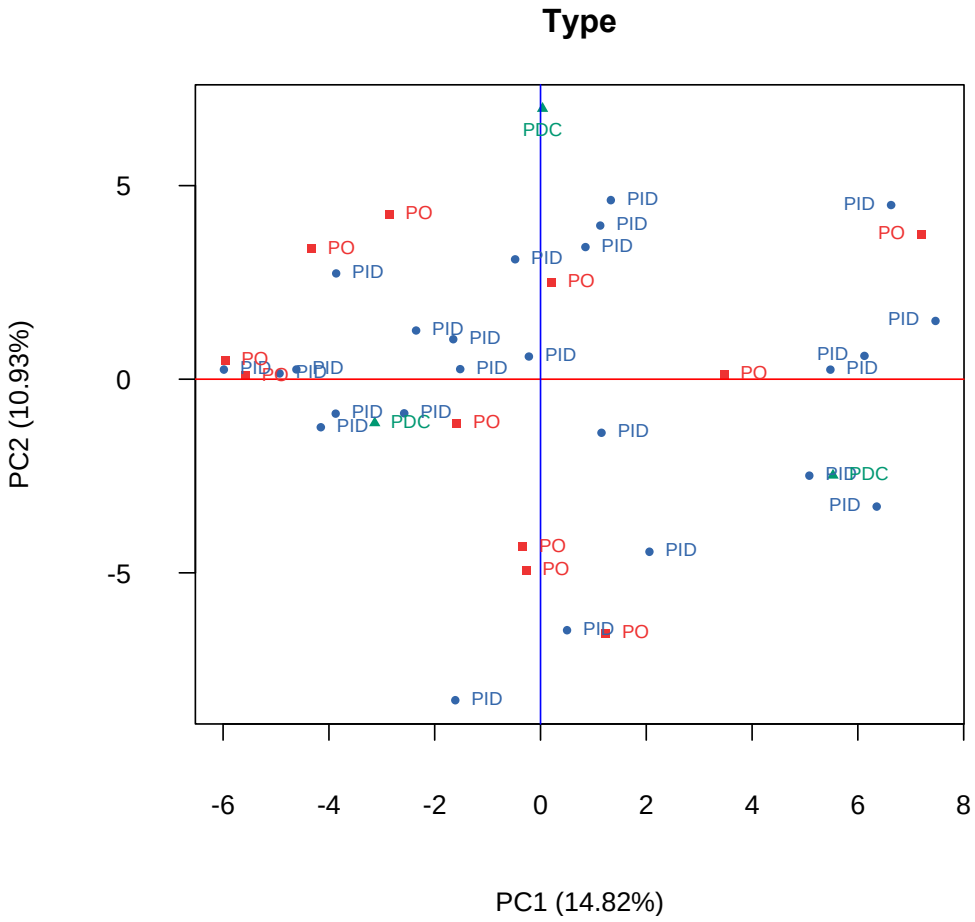


Figure 5.27: Principle component analysis of all 40 patient serum samples for tumour type. PDC (green) - ductal carcinoma in situ (localised); PO (red) - other type of breast cancer ; PID (blue) - invasive ductal carcinoma. No separation or trends can be seen amongst the patients (n=40).

Individual control and patient samples were graphed for specific phospholipid species to look for any subtle differences that may have been over shadowed by averaging the peak areas. Three phospholipids were chosen because they were found to be elevated, in tumour tissue, in a study by Hilvo *et al* (Hilvo, 2011) and also elevated in the cell culture study from Chapter 3 (Figures 3.1, 3.4, 3.10). These phospholipids were PC (38:5), PI (38:4) and PE (38:4) and for each of the 80 individuals in this study, these species were graphed using normalised data and also using raw data for comparison (Figures 5.28 and 5.29). As the normalised data has been transformed it was relatively uniform across all samples. Raw data, however, showed variability among the samples with some much higher than others but the overall trend was similar for both groups (control and patient).

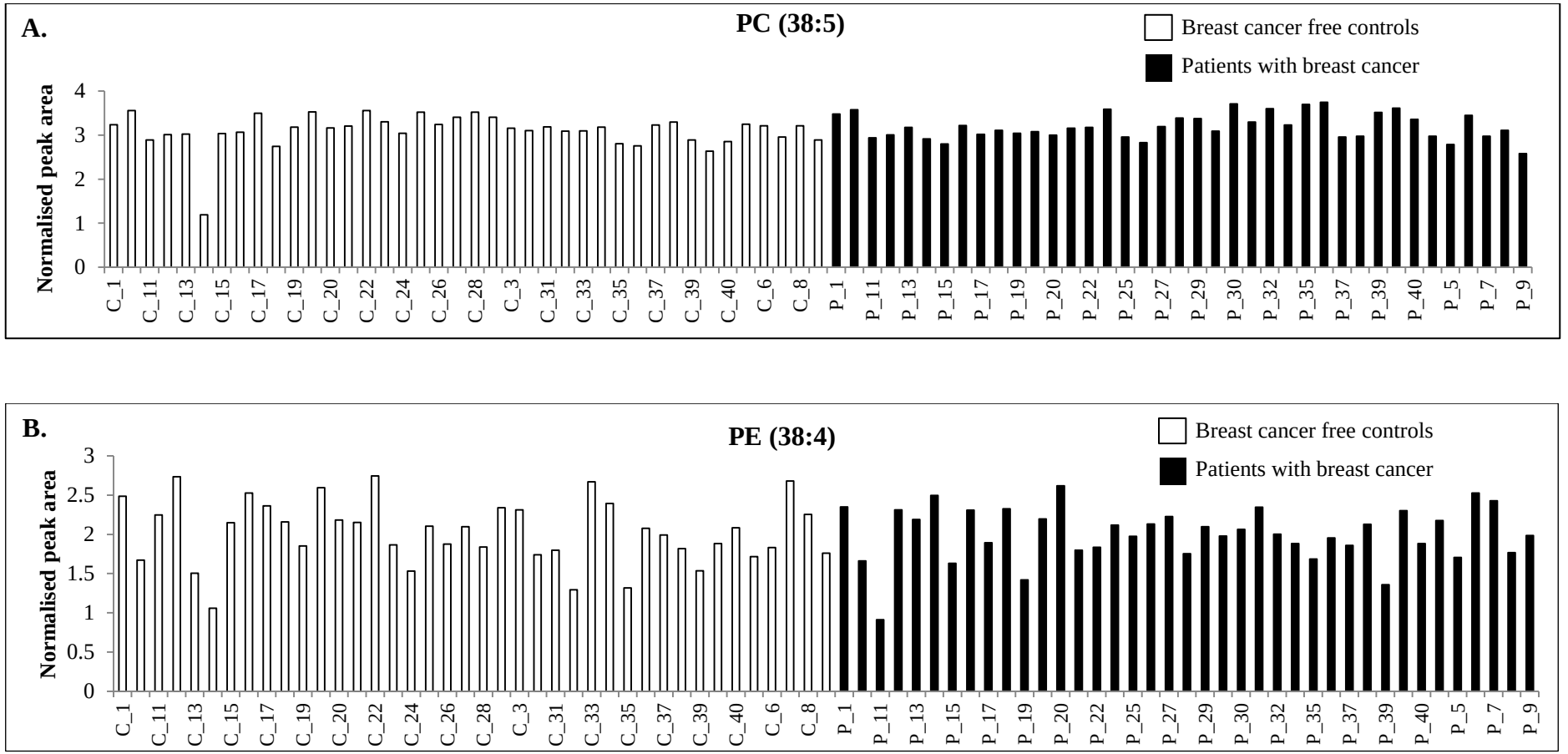


Figure 5.28, A-C: Normalised peak areas for each individual in this study were graphed for select phospholipids (A. PC 38:5, B. PE 38:4, C. PI 38:4) to determine if there were any differences that may have been skewed by averaging the groups. Controls (n=40) are seen in white and patients (n=40) are seen in black.

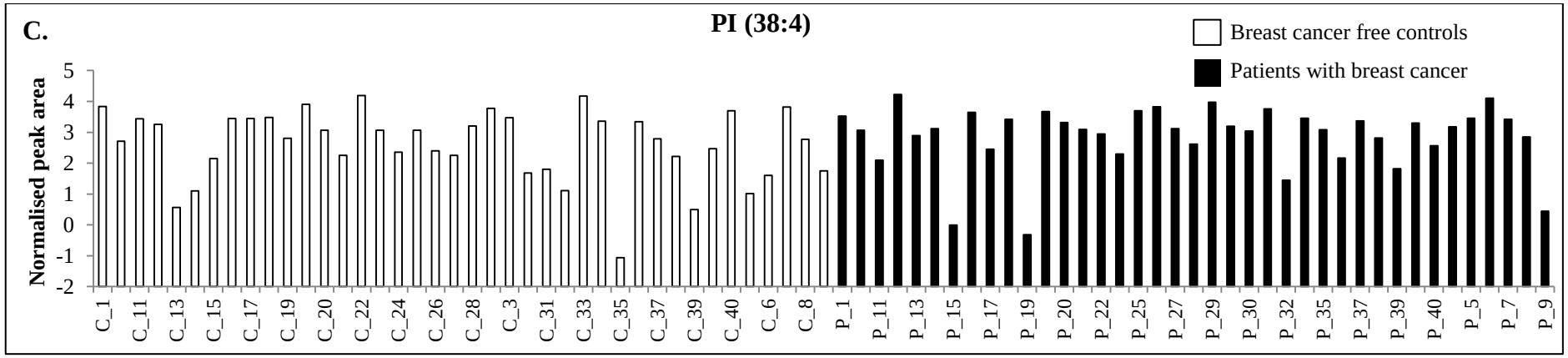
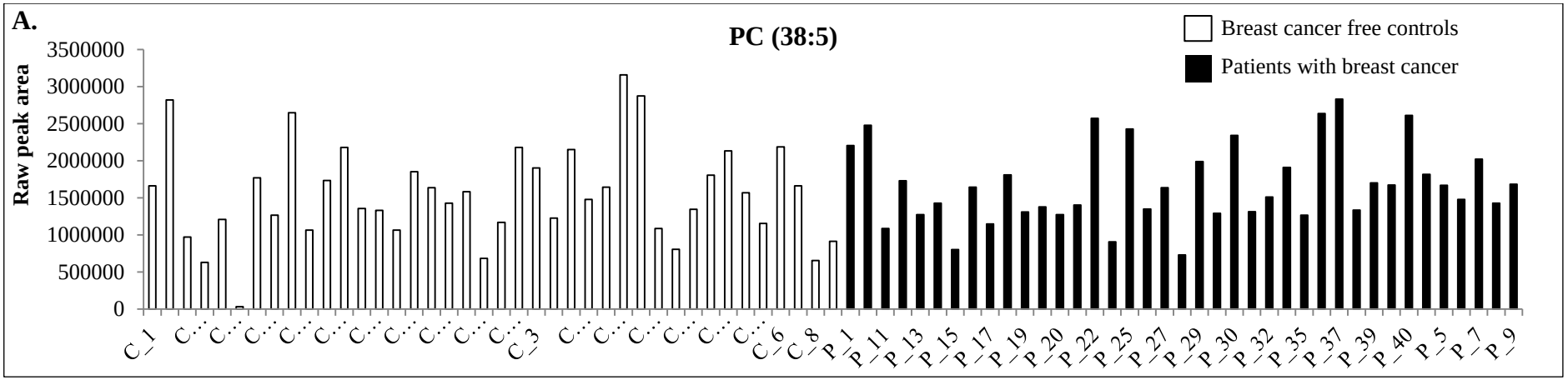


Figure 5.28, A-C: Normalised peak areas for each individual in this study were graphed for select phospholipids (A. PC 38:5, B. PE 38:4, C. PI 38:4) to determine if there were any differences that may have been skewed by averaging the groups. Controls (n=40) are seen in white and patients (n=40) are seen in black.



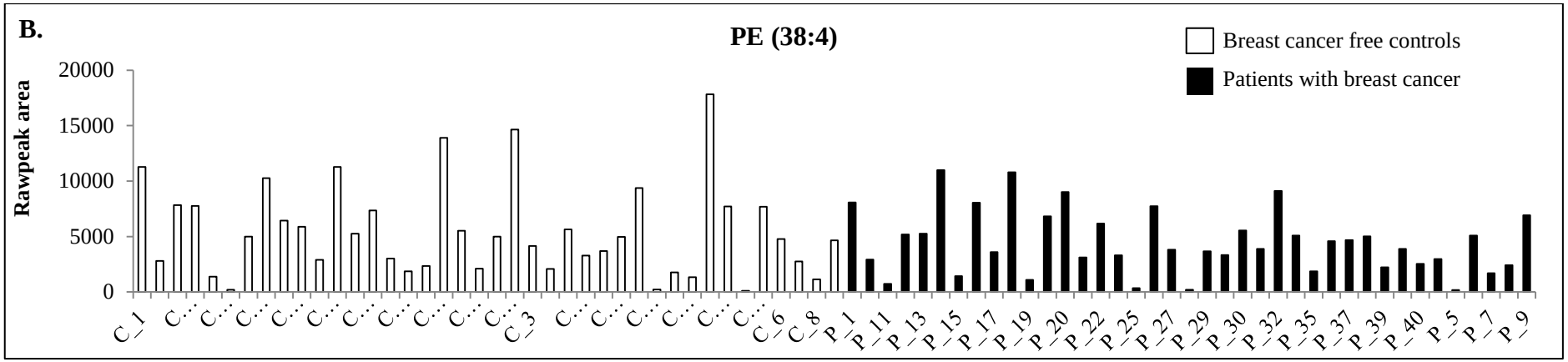


Figure 5.29, A-C: Raw peak areas for each individual in this study were graphed for select phospholipids (A. PC 38:5, B. PE 38:4, C. PI 38:4) to determine if there were any differences that may have been skewed by averaging the groups. Controls (n=40) are seen in white and patients (n=40) are seen in black.

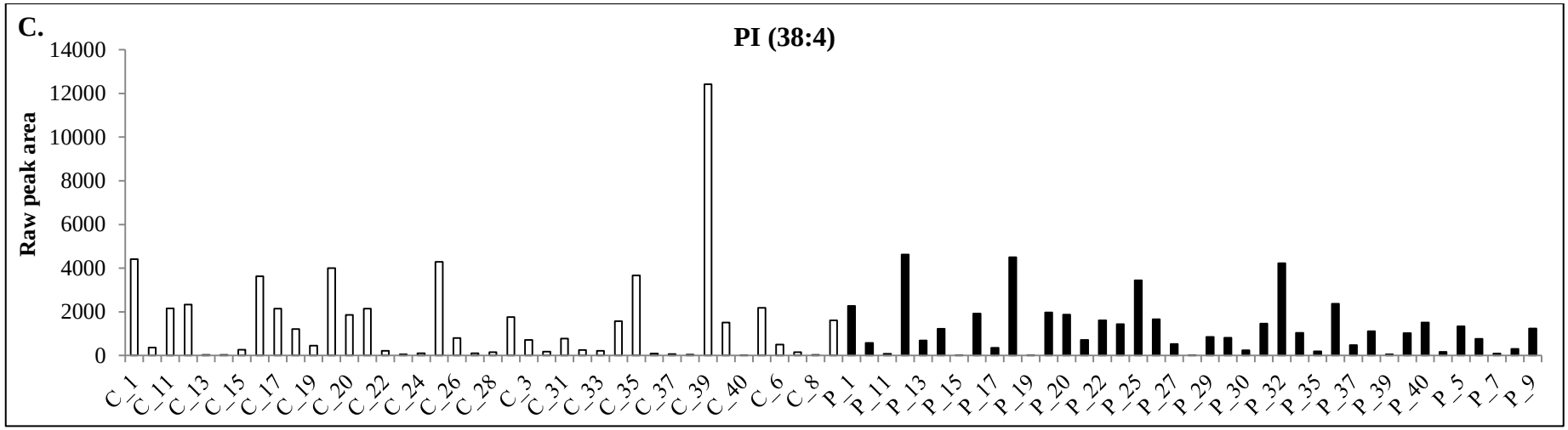


Figure 5.29, A-C: Raw peak areas for each individual in this study were graphed for select phospholipids (A. PC 38:5, B. PE 38:4, C. PI 38:4) to determine if there were any differences that may have been skewed by averaging the groups. Controls (n=40) are seen in white and patients (n=40) are seen in black.

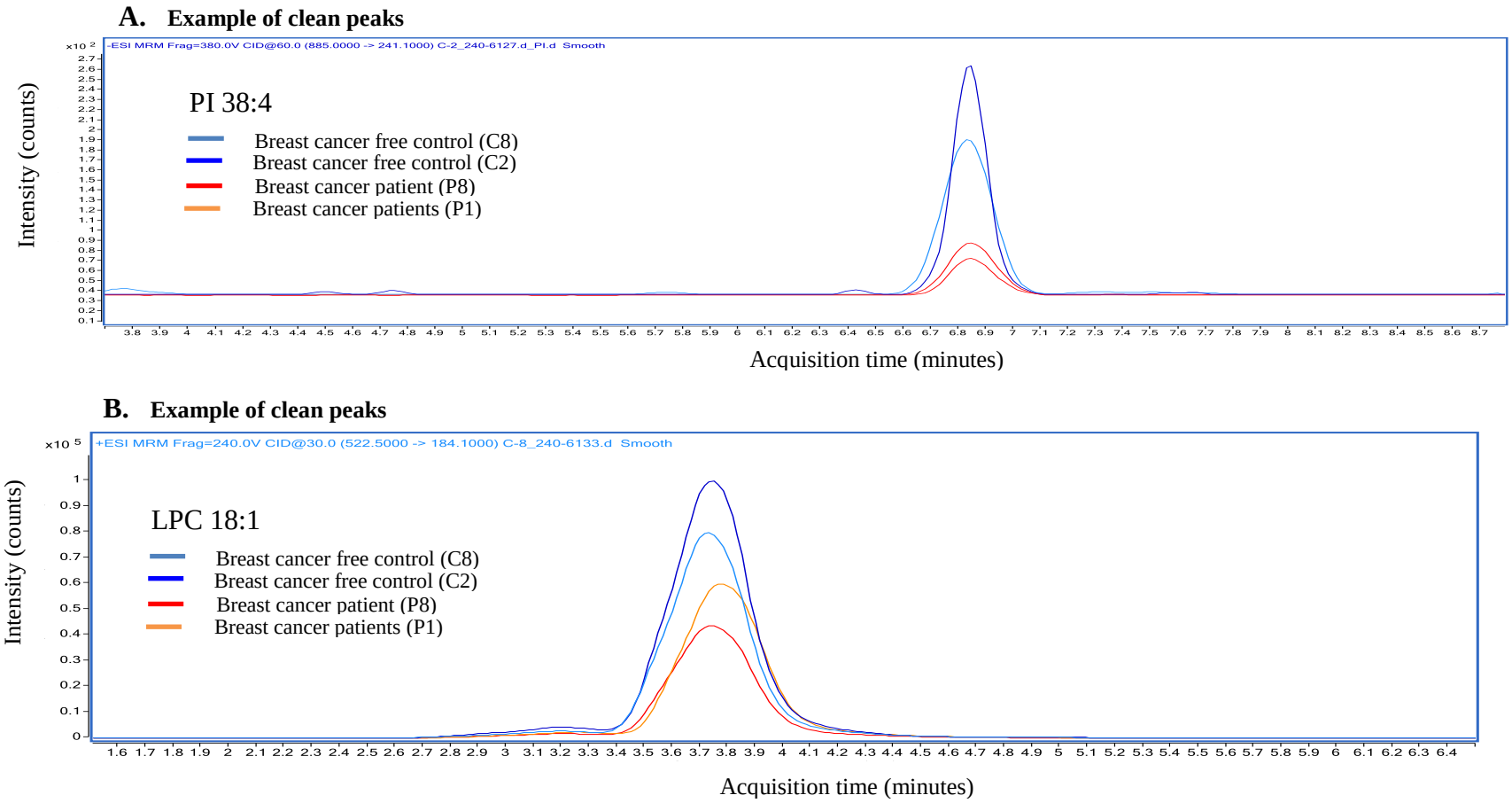
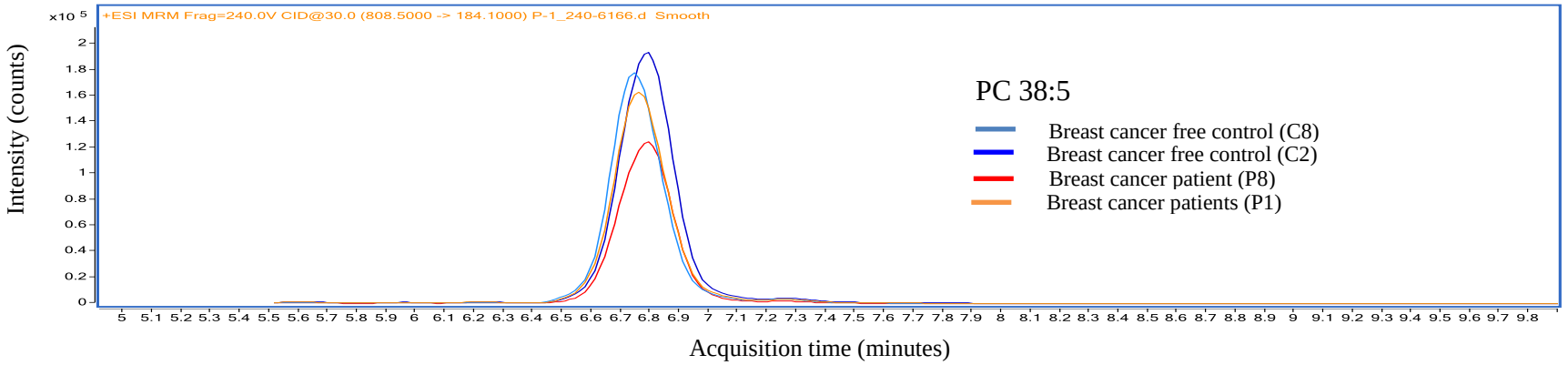


Figure 5.30, A-J: Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. PI 38:4**, B.** LPC 18:1**, C.** PC 38:5**, D.** SM 34:1**, E.** PG 20:0**, F.** PE 38:1**, G.** LPA 20:1**, H.** SM 34:2**, I.** CE 20:0**, J.** PS 34:0**. Figures A-F are examples of ideal, clean peaks and Figures G-J are examples of noisy, unclear peaks.**

C. Example of clean peaks



D. Example of clean peaks

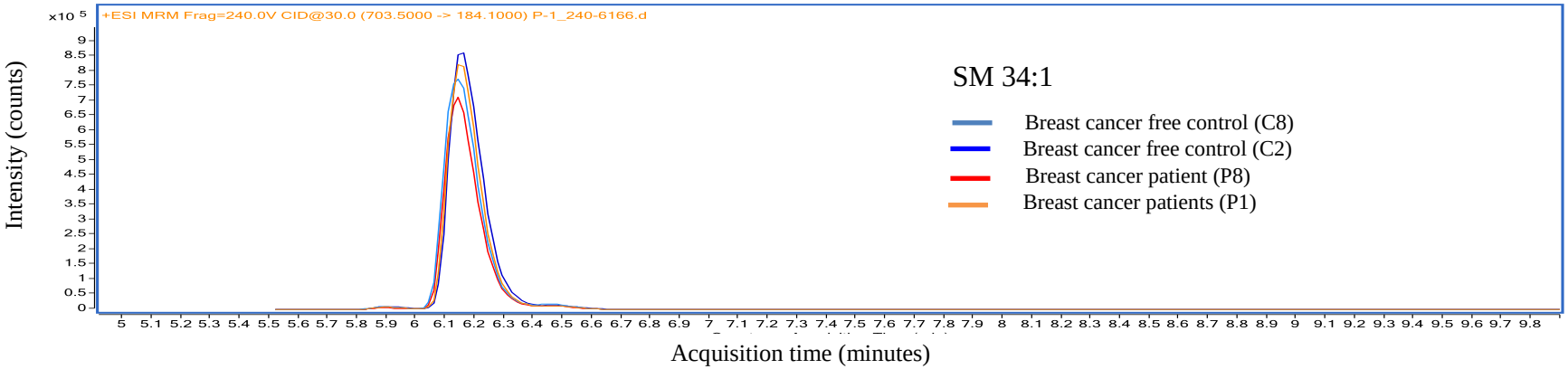


Figure 5.30, A-J: Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. PI 38:4**, B.** LPC 18:1**, C.** PC 38:5**, D.** SM 34:1**, E.** PG 20:0**, F.** PE 38:1**, G.** LPA 20:1**, H.** SM 34:2**, I.** CE 20:0**, J.** PS 34:0**. Figures A-F are examples of ideal, clean peaks and Figures G-J are examples of noisy, unclear peaks.**

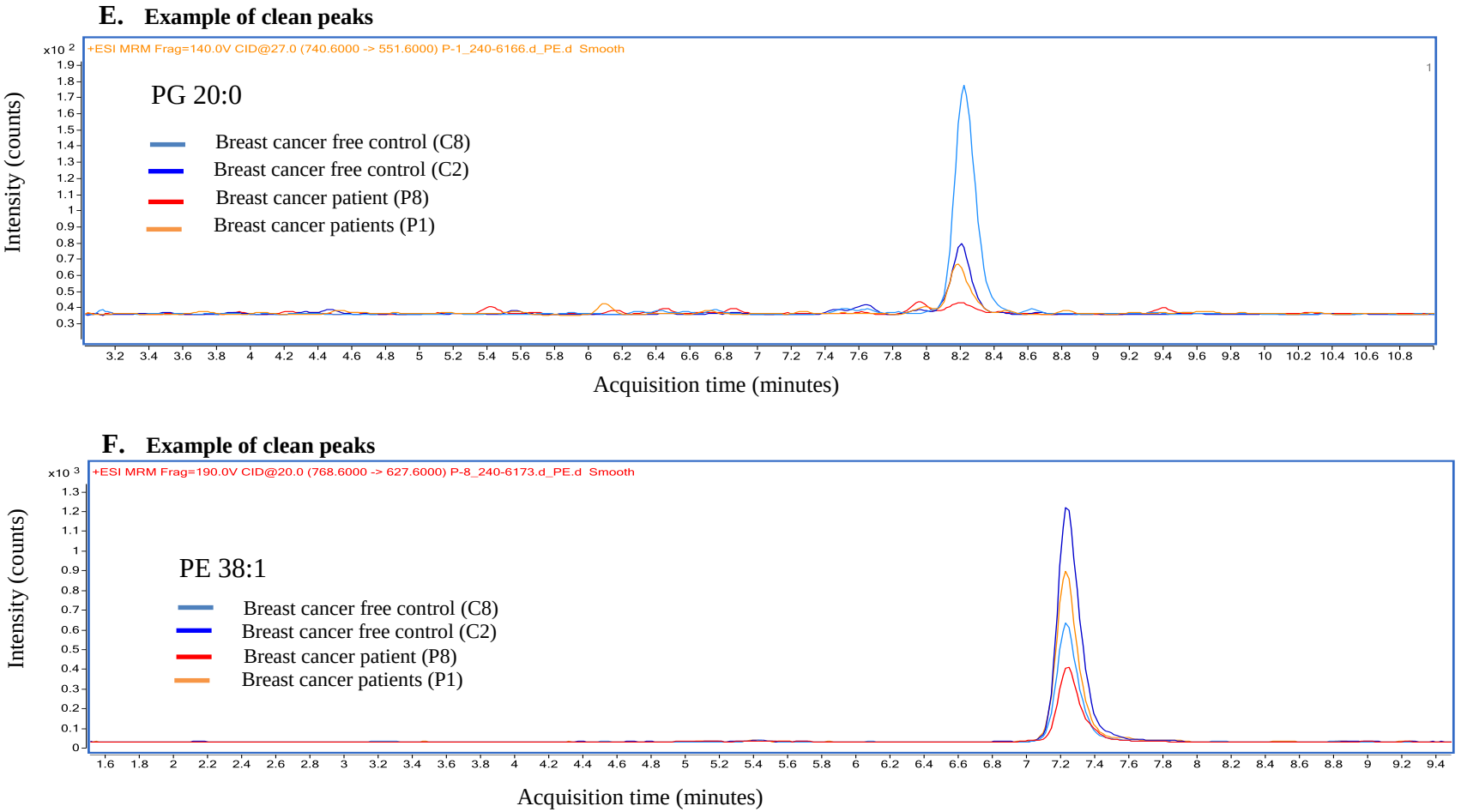
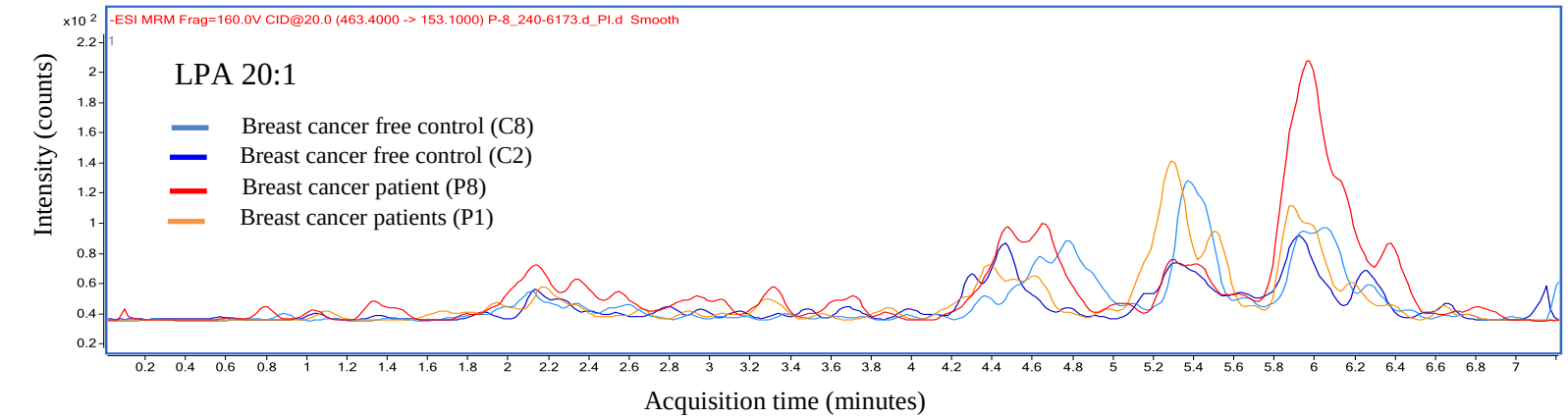


Figure 5.30, A-J: Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. PI 38:4**, B.** LPC 18:1**, C.** PC 38:5**, D.** SM 34:1**, E.** PG 20:0**, F.** PE 38:1**, G.** LPA 20:1**, H.** SM 34:2**, I.** CE 20:0**, J.** PS 34:0**. Figures A-F are examples of ideal, clean peaks and Figures G-J are examples of noisy, unclear peaks.**

G. Example of unclear peaks



H. Example of unclear peaks

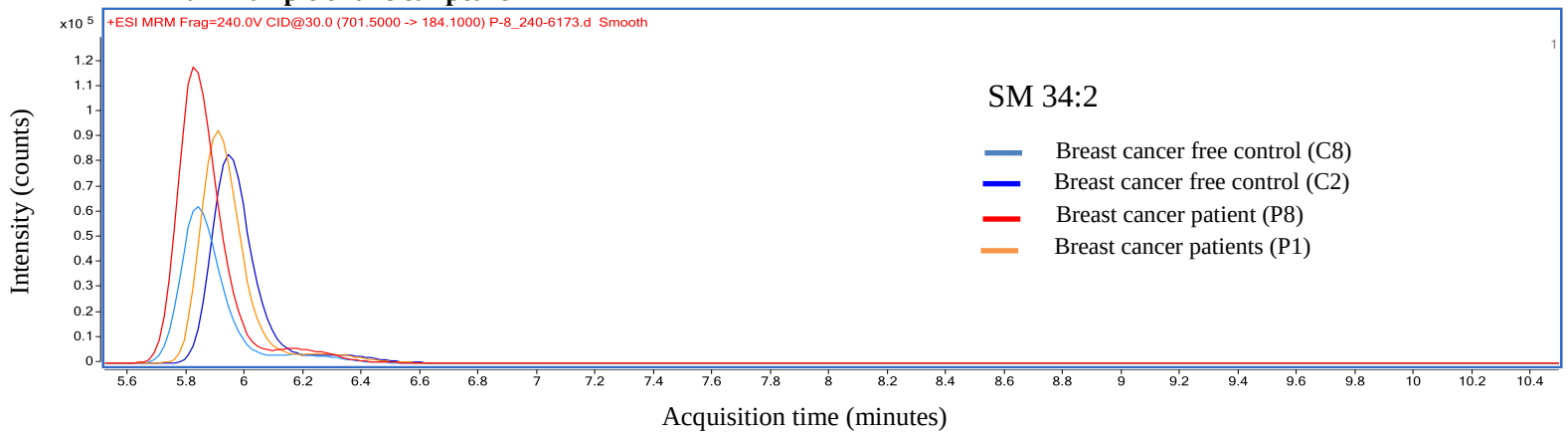
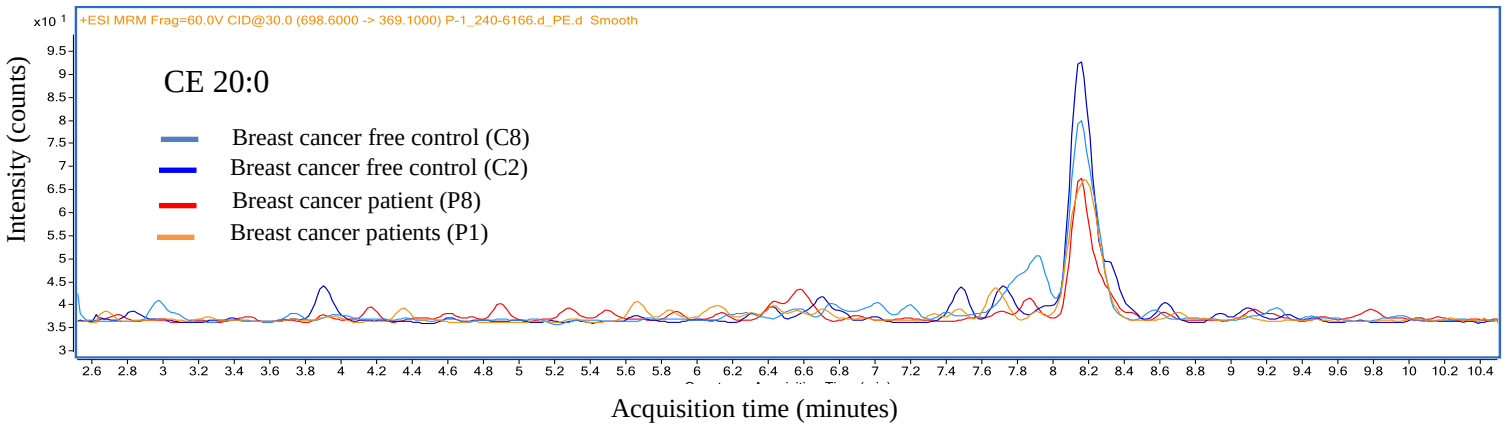


Figure 5.30, A-J: Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. PI 38:4**, B.** LPC 18:1**, C.** PC 38:5**, D.** SM 34:1**, E.** PG 20:0**, F.** PE 38:1**, G.** LPA 20:1**, H.** SM 34:2**, I.** CE 20:0**, J.** PS 34:0**. Figures A-F are examples of ideal, clean peaks and Figures G-J are examples of noisy, unclear peaks.**

I. Example of unclear peaks



J. Example of unclear peaks

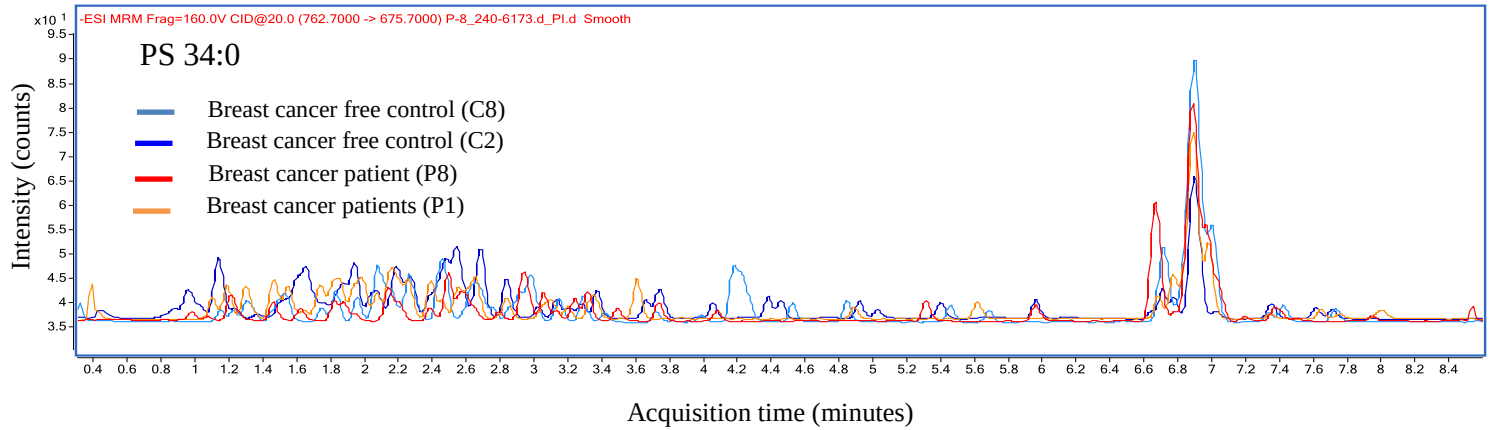


Figure 5.30, A-J: Raw ion chromatograms collected from multiple reaction monitoring (MRM) scans using liquid chromatography triple quad mass spectrometer for two breast cancer free controls and two patients with breast cancer for selected phospholipids: A. PI 38:4**, B.** LPC 18:1**, C.** PC 38:5**, D.** SM 34:1**, E.** PG 20:0**, F.** PE 38:1**, G.** LPA 20:1**, H.** SM 34:2**, I.** CE 20:0**, J.** PS 34:0**. Figures A-F are examples of ideal, clean peaks and Figures G-J are examples of noisy, unclear peaks.**

Table 5.1: Significantly changing lipid species between breast cancer free control samples (n=40) and patients with breast cancer (n=40) using a two-sided t-test (t statistic shown). Those species with an adjusted p-value lower than 0.05 and a fold change great than 2 were considered significantly different (p-value shown) between the two groups (control and patient).

Phospholipid specie	Fold change	Log Fold Change	T statistic	P value	Adjusted P value	Higher in
CE 24:6	0.70370891	-0.351390489	-3.70003191	0.000374439	0.015351981	Control
CE 20:0	0.757399933	-0.277863852	-3.046498515	0.00305333	0.041728844	Control
CE 22:0	0.678062936	-0.388515169	-3.127608624	0.00238762	0.041728844	Control
LPA 16:0	1.516585084	0.416461152	3.16657589	0.002135912	0.013883427	Patient
LPA 18:0	1.267253668	0.236852093	2.921082886	0.004456149	0.024827114	Patient
LPA 18:1	1.579582498	0.45716057	3.668364806	0.000422705	0.005860726	Patient
LPA 18:2	1.654539264	0.50352258	3.612216267	0.000510492	0.005860726	Patient
LPA 20:1	1.452496331	0.373283684	4.21879628	6.07E-05	0.002366202	Patient
LPA 20:4	1.589937344	0.463694609	3.495461759	0.000751375	0.005860726	Patient
LPA 22:5	1.521002475	0.41936964	2.672597418	0.009006554	0.043906949	Patient
LPA 22:6	1.831144806	0.604941348	3.553740387	0.000620151	0.005860726	Patient
PC 39:4	0.725774622	-0.320515751	-3.511235529	0.000728511	0.040056477	Control
PS 32:2	1.318937556	0.276826531	2.463245955	0.015814951	0.046223865	Patient
PS 34:0/ IS	1.913213581	0.648784331	3.826880408	0.000249215	0.001993718	Patient
PS 36:0	1.61244412	0.477751115	2.604754564	0.010875734	0.046223865	Patient
PS 38:3	0.662812565	-0.411263037	-2.42775047	0.017333949	0.046223865	Control
PS 38:4	0.512964887	-0.667547883	-3.849830076	0.000230195	0.001993718	Control
PS 40:6	1.36502046	0.311169418	2.44278734	0.016675231	0.046223865	Patient
SM 34:2	1.221713797	0.200254625	3.365428571	0.001177186	0.014126235	Patient

Although the bar graphs did not show any valid differences between the breast cancer free serum samples and the serum samples of those patients with breast cancer, there were some statistically significant species found when the data was analysed using a two-sided t-test. (Table 5.1). These species had adjusted p-values less than 0.05 but the fold changes were very low. Looking back at the raw peaks in Agilent Mass Hunter software, it may have been due to noise as the raw peaks for these species were not acquired at the same time and/or were not smooth peaks. This is illustrated in Figure 5.30 where the raw ion chromatograms, collected from multiple reaction monitoring (MRM) scans, using liquid chromatography triple quad mass spectrometer, are shown for four samples which were selected at random (two breast cancer free controls and two patients with breast cancer). Examples of smooth, clean traces are shown in Figure 5.30 (A-F) for those species, which were found to be elevated in the study by Hilvo *et al* (Hilvo, 2011), or elevated in the cell culture study

from Chapter 3. Samples, which were found to be significantly different, were examined manually and found to have poorly defined peaks (Table 5.1). Examples of these poorly defined or multiple peak traces are shown in Figure 5.30 (G-J) for those samples. Upon individual examination of the chromatograms of all species determined to be statistically significant, it was found that the traces were poorly defined and in some cases there were multiple peaks. This could be due to the lipid species being of low abundance in the sample or less than optimal sensitivity of the mass spectrometer on these runs. This suggests that apparent variations in the abundance of these species arise from noise or contamination. It may be possible that lipid changes are still present but are more subtle and for detection the study needs to be a more sensitive, targeted one.

5.5. Discussion

In the previous study there was evidence of differences in the lipid profiles of the supernatant from a breast cancer cell line when compared to a control cell line. This study aimed to draw those species, which were significantly different, together, to better understand the overall phospholipid profile in the serum of women with breast cancer. This experiment characterised the subspecies of phospholipids that appear in serum in patients with breast cancer with particular focus on phospholipids because of a range of scattered reports implicating a role for these lipids.

There were no significant differences identified in the serum of patients with breast cancer and breast cancer free controls in this study, and this could be attributed to other lipids, such a dietary and medical, which are overshadowing the concentration of these phospholipids in the blood. In such a small study, with these variables in the blood, which differ greatly from individual to individual, a larger sample size with more types of the same breast cancers would need to be used to further characterise these lipids.

As the role of lipids in disease is fast becoming of interest, the use of these molecules as biomarkers is one of great significance. Although there is a strong indication that phospholipids, in particular PC and PE, could be potential biomarkers for breast cancer, the mechanisms behind their role are not well established.

Some studies suggest that the increased levels of PC in breast tumours have been attributed to the overexpression of related enzymes such as choline kinase and phospholipase C in breast cancer cells (Glunde, 2004, Podo, 1999) but it has also been proposed that this elevation is due high rates of transport of precursors (choline and ethanolamine) into the cell (Katz-Brull, 2001). The high rates of precursor metabolites in the cell could result in the overexpression of these enzymes. This increase in the activity of enzymes, specific to PC and PE, may create excess pools of these phospholipids in a tumour or actively proliferating cells (Podo, 1999). A similar theory is that enzymes such as sphingomylinases release PC directly into the aqueous environment, as a result of their active sites being positioned towards the extracellular environment when in cells, causing an overabundance of PC in the interstitial fluid and therefore plasma (Hofmann, 1998). Furthermore, a cell culture study from 1995

proposed the elevation of PC in breast tumour cells, compared to control cells, was due to either the increased synthesis of PC or the reduction in exploitation of PC within the cell (Singer 1995). If the different propositions are true then the elevation in phospholipids in tumour tissue, serum and cell culture supernatant, could also be a result of both increased synthesis of phospholipids and a decrease in the utilization of these phospholipids in tumour cells and as a result there is a accumulation of lipids in the cells.

Currently available markers detect the cancer at late stages and the key to surviving the disease is early detection, therefore, there is a need for a more reliable diagnostic screening test for breast cancer. If there are metabolic changes that take place as soon as a tumour is formed, the ideal diagnostic marker would be one that could identify this specific molecular change as soon as it begins to take place. Most biomarkers studies have tried to find one specific marker for breast cancer, but due to the heterogeneity of the disease, a single marker, thus far, has low accuracy and has not proved successful (Gara, 2008). If combining more than one diagnostic tool increases the accuracy of screening for breast cancer, multiparameter biomarkers would be a more sensitive and specific approach to detecting the disease in the future (Fernandis, 2009).

6. Conclusion

The underlying hypothesis that this study sought to test was that invasive breast cancer cells (Figure 6.1a) continuously shed lipids into the blood stream (Figure 6.1b), and are transported throughout the body in serum, including to the active hair follicles (Figure 6.1c), where they are taken up and incorporated into the developing hair fibre (Figure 6.1d), thereby altering its composition. As evidence for this hypothesis, hair fibres from breast cancer patients exhibit a circular feature when subjected to small angle X-ray diffraction using synchrotron-generated X-rays (Corino, 2009) (Figure 6.1e). Typically, circular features in X-ray diffraction of biological material are produced by lipids.

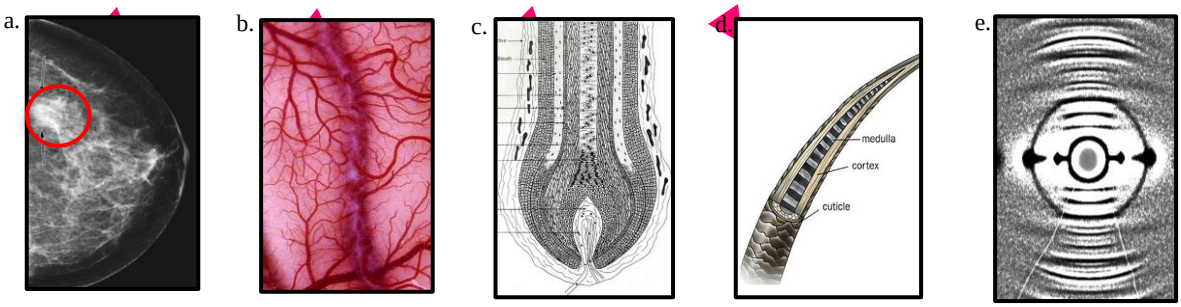


Figure 6.1: Schematic diagram of the hypothesis of this study.
a. X-ray of the breast (circle around tumour) (http://radiographics.rsna.org)**;**
b. Blood vessels (http://www.telegraph.co.uk/health)**;**
c. The hair follicle (http://www.spencerclinic.co.uk)**;**
d. The hair fibre (http://animaldiversity.ummz.umich.edu)**;**
e. X-ray diffraction pattern of a human scalp hair taken from a patient with breast cancer (own image)**.**

However, the circular feature that appears in the XRD pattern of hair from individuals with breast cancer could be caused by lipids derived from anywhere in the body and not just breast cancer-associated lipids, therefore this observation may not necessarily support the major hypothesis. It could be that the lipids arise secondary to the cancer and come from somewhere other than the breast but are caused by the presence of the cancer. This may also account for the high number of false positives (22%) reported in the studies on the XRD pattern of hair and breast cancer. Therefore this study was established to test the hypothesis and to determine if there are a number of lipids that may act as specific biomarkers in serum for the presence of invasive breast cancer.

Lipids have a variety of roles in cellular biology. At least half of the cell membrane is composed of lipids, which act as structural molecules, but they also have important roles in intracellular signaling pathways (Hannun, 2008, van Meer, 2008, Wymann, 2008). Lipids are also heavily involved in carrier-mediated transport, they regulate the composition of several membrane-bound enzymes, ligand binding to receptors, phagocytosis, endocytosis and cell growth (Spector, 1985).

Membrane fluidity is also directly affected by the changes in the lipid environment since lipid signaling regulates the behaviour of fundamental membrane proteins (Vereb, 2003) as well as cell polarization (Escriba, 2008). Many of the functional responses are likely to be caused directly by membrane lipid structural changes, which affect either bulk lipid fluidity or specific lipid domains (Spector, 1985). Phosphatidylcholine, phosphatidylethanolamine and sphingomyelin are the most dominant phospholipids in the majority of biological membranes, comprising up to 80% of the membrane (Fajardo, 2011).

De novo fatty acid synthesis is frequently upregulated in cancer cells, even in the early stages of cancer progression. This "reprogramming" of lipid metabolism is thought to be associated with the proliferation, membrane fluidity, and apoptosis of cancer cells by affecting membrane lipid remodeling. Recent studies have demonstrated the accumulation of several phospholipids in breast cancer tissues (Kawashima et al, 2013).

The structure of the phospholipids themselves has been shown to vary between tissue from healthy breast and malignant tissue. Azordegan *et al*, examined the interface tissue (breast tumour adjacent) and suggested there was a "*transitional change in the levels of palmitic acid from normal to malignant tissue, where there was more palmitic acid in the phosphatidylcholine and lyso-phosphatidylcholine in the cancer tissue"*. In addition to palmitic acid, this same trend was observed for arachidonic acid and oleic acid (Azordegan, 2013). Another interesting observation was in regards to the overall lipid content, the interface tissue contained 85% more total lipid than the tumour tissue and around 40% more total lipid than the healthy tissue. The healthy tissue contained 75% more total lipid than the tumour tissue, and therefore tumour tissue had less total lipid than both healthy and interface tissue samples. The authors proposed that this change in lipid content influenced the function of the tissues and that the higher lipid content found in the interface tissue acted as a protective layer

from malignant tissue. They went on to suggest that as lipids have regulatory roles on the cell membrane, the decreased lipid content in cancer tissue promoted cell death and was a "*protective measure for the removal of abnormal cells*" (Azordegan, 2013). This also suggests that different areas of the tumour exhibit different lipid elevations and that the site from which the tissue is selected may influence the measured lipid levels of the tissue and this study found that there are increased lipids in the growing edge of the tumour. This may also relate to increased membrane fluidity assisting invasiveness of the tumour.

Given the fundamental roles that lipids play in cellular regulation, a change in lipid composition could have a role in the carcinogenic process. The role of alterations in lipid synthesis in tumorigenesis is increasingly being reported by a number of studies (Fernandis, 2009, Ramirez de Molina, 2002, Rysman, 2010), and it is likely that a detailed understanding of the changes of lipid composition and concentration associated with carcinogenesis will lead to improved diagnostic and therapeutic options.

The data from this study did not demonstrate differences in lipid composition between serum and hair from patients with breast cancer and healthy controls. Potential explanations for this include:

- The hypothesis is incorrect,
- High individual variability is obscuring real differences
- Lack of sensitivity of the analytical methodology resulting in potential subtle changes being masked by dietary and environmental lipids in the blood or hair sample.

The hypothesis of this study was that there is an increase in phospholipids in the hair fibres of individuals with breast cancer, which is also reflected in their serum. This hypothesis was supported by some earlier preliminary reports in the literature, particularly around phosphocholine elevation in tumour tissue and serum of patients with breast cancer. A number of studies using X-ray diffraction analysis of hair fibres from patients with breast cancer showed the presence of a circular feature that is a typical of a lipid component of the material.

Preliminary data (Chapter 2) suggested there were lipids in hair, which are detectable in the hair fibre as circular features in X-ray diffraction studies and were correlated with the presence of breast cancer (LCMS studies). This study demonstrated that solvents, which removed lipids, also removed the circular XRD feature from hair fibres from breast cancer patients, and enhancement of the XRD feature could be achieved using a chemical that binds to lipids. This is strong evidence that there is an additional lipid-based component in hair fibres in breast cancer patients. It could only be present in the fibre after deposition from the circulation. This was a very small data set which encouraged further studies to be carried out using cell culture supernatant, hair and serum.

Data from the cell culture study (Chapter 3) indicated that there were lipid families that were elevated in the supernatant of the tumorigenic breast cell line when compared to a non-malignant mammary epithelial cell line. This indicative result was only from two cell lines, therefore further studies need to be carried out to confirm the validity of this result. The data suggested that these elevated lipids were being shed from the cell into the cell culture media, which appeared to support the first part of the hypothesis.

This study aimed to identify these lipids in hair (Chapter 4), as this was previously demonstrated (Chapter 2) and had the potential to provide the basis for a non-invasive screening test for breast cancer. If those specific lipids being shed from the breast tumour could be identified in hair from patients with the disease, then the role of these lipids as biomarkers for breast cancer could be validated. The hair lipid profiles were not found to be statistically significantly different between those patients with breast cancer and healthy controls (Chapter 4), and similarly, the serum lipids profiles from the same set of individuals did not exhibit any significant biological changes (Chapter 5). This is consistent as there were no significantly changing lipids found in the serum of patients with the disease, so likely, these changes had not altered the composition of the hair via systemic uptake. It could be that there is a localised change in which altered lipids contribute to the invasiveness of the tumour cells, as hypothesized by Kawashima, 2013, (Kawashima, 2013) but are not consistently shed into the serum in sufficient concentration to effect a detectable (by the methodology employed in this project) alteration in hair fibre composition.

The cell culture data (Chapter 3) and the literature on the association between elevated phospholipids and breast cancer provide evidence of significant changes between the two groups, but it could be that the methodology used in this project was not sensitive enough or was too selective for phospholipids and as a result did not address the full lipid profile in the serum. Although these species were identified in cell culture supernatant, the result required more replicates and cell lines so that a t-test could be carried out.

Phospholipids were selected as the focus for analysis in this study based upon an extensive literature review. For this reason, there are many lipid families that we did not explore such as cholesterol, triglycerides and diglycerides, which may also be of interest and appear to be involved in a range of biological processes (Alexopoulos et al., 1987, Owiredu, 2009, Shah, 2008). It could be that different lipid profiles change due to the type of breast cancer a patient may have. This means that there needs to be lipid identification studies in a variety of breast cancer types.

It may be that phospholipids are not elevated at all in hair or serum as a result of breast cancer and that lipid changes in hair were in fact due to other medical conditions or external factors such as high cholesterol, hair products used over an excessive period of time, which have been stubbornly absorbed into the fibre. If the hypothesis is not true for hair, then it is less likely to be elevated in the serum either. The changes seen in cell culture supernatant may reflect tumor tissue changes that do not extend beyond the tumor microenvironment.

Serum lipids consist of a mixture of endogenous and dietary lipids, the latter varying on a daily basis. Furthermore, breast cancer is in fact a multitude of diseases, and therefore to be able to discern a consistent pattern of phospholipid species across different breast cancer types above the noise of dietary lipids was quite a challenge. Therefore this study was unable to confirm the hypothesis in relation to the serum phospholipids using this methodology in this sample set.

There is however sufficient interesting data to expand the approach and there are other methods that may be useful to further explore the underlying hypothesis. Low abundant lipid species require highly sensitive methods of identification. Extracellular vesicles (EV), containing cellular proteins and lipids, are produced by the outward budding and release of vesicles into the extracellular environment.

(Muralidharan-Chari, 2010, Thery, 2011). One type of these EV's is of endosomal origin, called exosomes. Exosomes are released into the extracellular environment when an endocytic invagination forms a multivesicular body, which fuses with the plasma membrane (Booth, 2006, Muralidharan-Chari, 2010, Thery, 2011, Wendler, 2013). Another type of EV is derived from the plasma membrane, called microvesicles, which are directly pinched off the plasma membrane towards the extracellular environment (Booth, 2006, Muralidharan-Chari, 2010, Thery, 2011, Wendler, 2013). These extracellular vesicles have been postulated to have a role in intercellular communication as transport vehicles of proteins, lipids and RNA (Raposo, 2013) and also appear to be involved in tumour progression (Muralidharan-Chari, 2010). They have been suggested to facilitate malignancy, invasiveness and the evasion of the immune response (Cocucci, 2009, Dolo, 1999, Graves, 2004, Muralidharan-Chari, 2009).

The cellular origin of these extracellular vesicles determines their make up, but they are distinct from their parent cell (Muralidharan-Chari, 2009), and once they are released into the extracellular environment, they may be involved in transfer of molecules between cells and also enable the deposit or removal of molecules at distal sites (Muralidharan-Chari, 2010). As a result, they have been identified in blood and urine, which makes them a candidate as markers for identifying intracellular changes (Hugel, 2005, Ratajczak, 2006).

Therefore, the lipid composition of these exosomes or microvesicles, originating from tumour cells, may exhibit molecular changes, which reflect specific cellular alterations and could be potential markers for breast cancer. One of the major issues that cannot be controlled for is individual variability, which causes the data to be inconsistent and for any potential subtle changes to be masked by dietary and environmental lipids in the blood or hair sample. EV's could overcome this issue by providing a highly specific sample that reflects only the cells themselves and any chronic changes but not other transient lipids, such as dietary lipids. In addition, participants who have fasted for 12 hours prior to sample collection would assist in eliminating the affect of these transient lipids. Some of the graphs from the hair and serum study did show differences, between patients with breast cancer and healthy controls, however they were not significant differences. It may be that precise extraction of exosomes or microvesicles, using ultracentrifugation, from serum will uncover any subtle differences between patients with the disease and controls. If

repeated, this method of analysis may be of interest in identifying the subtle changes that may be taking place in the body of a patient with breast cancer.

Ironically, hair is one way of focusing on these endogenous lipids, however the variables of hair length, hair treatments and difficulty in achieving consistent extraction from different hair types ultimately make this source unsuitable for a routine screening sample and difficult to standardise. A finding from the study was that the lipid composition of hair changes along the length of the fibre. Although it may seem obvious, it is interesting that many published hair studies do not take this into account when carrying out quantitative experiments. In the literature, many studies include the entire hair fibre rather than standardizing to the region that has the most lipid. As such, an 'average" lipid content is derived, that may merely reflect variable lengths of hair rather than actual lipid content. Accounting for this variable should become common practice in performing such studies.

There were substantial changes in specific lipid species in the cell culture supernatant between the two cell lines (Table 6.1). Whilst the majority of species were elevated in breast cancer cell media, some were higher in the non-tumorigenic cell media too. The role of these lipids in the biological system is important in understanding the potential mechanisms behind these changes.

PC is the most abundant phospholipid on the cell membrane comprising of 50% of the phospholipids, followed by PE, which makes up around 30% of the total phospholipid content. PC is found positioned on the outer layer of the cell membrane and integral to structural support of the cell where as PE is found on the inner layer and assists in the stable incorporation of proteins into the membrane (Vance, 1996). As PC is able to form lipid bilayers, it provides structural integrity to the cell membrane and therefore influences membrane fluidity (Arouri, 2013). The hydrolysis of PC by phospholipase A2 produces LPC (Cole, 2012). Both PC and LPC have roles in cell signaling through the production of diacylglycerols when hydrolysed by phospholipase C or D in the nucleus (Kent, 2005). PC is also the precursor of SM, PA and PS. LPC can also diffuse into membranes and therefore affect membrane proteins and their regulation (Arouri, 2013). PE tends to form non-bilayer structures, which are key in vesicle formation, and membrane budding and can allow negatively charged molecules access to the cytosolic surface to assist in protein function (Christie, 2010). PS makes up 10% of the total phospholipid content on the cell membrane and it is found on the

inner layer. An essential signaling process of PS is when it is externalized to the outer layer and stimulates the phagocytosis of apoptic cells (Leventis, 2010). PS has also been reported to assist in interactions between proteins and their membrane bound receptors through its anionic serine head group as well as stimulating protein kinase C which has roles in regulation of cell proliferation, differentiation and apoptosis (Buckland, 2000). PS is synthesised from PC and PE through head group exchanges (Leventis, 2010). PI makes up 1% of the total phospholipid content, are also found in the inner layer of the cell membrane and are the principal source of diacylglycerols, which regulate protein kinase C activity, when hydrolyzed by the enzyme phospholipase C, whose activity is stimulated by protein receptors and calcium ions (Boss, 2012). The diacylglycerols generated are less saturated than those generated from PC and are therefore more active (Gardocki, 2005). Phosphorylated phopsphotidylinositols are called phosphoinositides and have the ability to bind to membrane proteins via their polar head group and generate downstream signaling effects (Sasaki, 2009). Therefore, they can regulate many different membrane proteins. PG makes up 2% of the total phospholipid cell membrane and is found in amniotic fluid and used to monitor fetal maturity (Telezhkin, 2012). Sphingolipids can be divided into several classes, and those on the cellular membrane are ceramides (Cer) and sphingomyelin (SM) (figure xxx), which mediate interactions with extracellular matrix proteins and receptors, and are used by pathogens to attach and enter cells (Aureli, 2011, Vance, 1996). They also have roles as second messengers in signal transduction cascades (Futerman, 2004). Ceramide itself is a signaling substance that can be released from sphingomyelin in response to extracellular and intracellular stimuli. In general, it mediates cell differentiation andapoptosis (Hannun, 2001).

The most common sterol lipid in the cellular lipidome is cholesterol and its derivatives. In this study we have profiled cholesterol ester (CE), which is involved in regulating cell membrane permeability (Haines, 2001) but also have roles in tissue development (Eaton, 2006).

Table 6.1: Phospholipid species, which were significantly elevated in the cell culture supernatant study (Chapter 3).

Lipid species	Cell line specie is elevated in	Lipid species	Cell line specie is elevated in	Lipid species	Cell line specie is elevated in
PI(34:1)	Tumorigenic	PE(36:1)	Tumorigenic	PG(25:0)	Tumorigenic
PI(36:0)	Tumorigenic	PE(36:2)	Tumorigenic	PG(26:0)	Tumorigenic
PI(36:1)	Tumorigenic	PE(36:3)	Tumorigenic	PG(26:1)	Tumorigenic
PI(36:2)	Tumorigenic	PE(36:4)	Tumorigenic	PG(27:0)	Tumorigenic
PI(38:2)	Tumorigenic	PE(37:1)	Tumorigenic	PG(28:0)	Tumorigenic
PI(38:3)	Tumorigenic	PE(37:2)	Tumorigenic	PG(28:1)	Tumorigenic
PI(38:4)	Tumorigenic	PE(37:3)	Tumorigenic	PG(30:0)	Tumorigenic
PI(38:5)	Tumorigenic	PE(37:4)	Tumorigenic	PG(30:1)	Tumorigenic
PI(40:6)	Tumorigenic	PE(38:1)	Tumorigenic	PG(32:0)	Tumorigenic
CE(17:0)	Tumorigenic	PE(38:2)	Tumorigenic	PC(24:0)	Non-tumorigenic
CE(17:1)	Tumorigenic	PE(38:3)	Tumorigenic	PC(34:4)	Non-tumorigenic
CE(19:1)	Tumorigenic	PE(38:4)	Tumorigenic	PC(35:1)	Tumorigenic
CE(21:0)	Non-tumorigenic	PE(38:5)	Tumorigenic	PC(35:2)	Tumorigenic
CE(25:4)	Non-tumorigenic	PE(38:6)	Tumorigenic	PC(35:4)	Non-tumorigenic
Cera(d18:1/15:2)	Non-tumorigenic	PE(39:0)	Tumorigenic	PC(36:0)	Tumorigenic
Cera(d18:1/16:0)	Tumorigenic	PE(40:4)	Tumorigenic	PC(36:1)	Tumorigenic
Cera(d18:1/17:0)	Tumorigenic	PE(40:5)	Tumorigenic	PC(36:2)	Tumorigenic
Cera(d18:1/17:2)	Tumorigenic	LPC(17:1)	Non-tumorigenic	PC(37:1)	Tumorigenic
Cera(d18:1/18:0)	Tumorigenic	LPC(18:0)	Tumorigenic	PC(37:2)	Tumorigenic
Cera(d18:1/20:0)	Tumorigenic	LPC(18:1)	Tumorigenic	PC(37:4)	Tumorigenic
Cera(d18:1/21:2)	Tumorigenic	LPC(20:4)	Tumorigenic	PC(37:5)	Tumorigenic
Cera(d18:1/22:0)	Tumorigenic	LPC(22:2)	Non-tumorigenic	PC(37:6)	Tumorigenic
Cera(d18:1/23:0)	Tumorigenic	LPG(16:0)	Tumorigenic	PC(38:0)	Tumorigenic
Cera(d18:1/23:2)	Tumorigenic	LPG(18:0)	Tumorigenic	PC(38:1)	Tumorigenic
Cera(d18:1/24:0)	Tumorigenic	LPG(20:0)	Tumorigenic	PC(38:2)	Tumorigenic
Cera(d18:1/24:1)	Tumorigenic	PG(16:0)	Tumorigenic	PC(38:3)	Tumorigenic
Cera(d18:1/24:2)	Tumorigenic	PG(18:0)	Tumorigenic	PC(38:5)	Tumorigenic
Cera(d18:1/36:3)	Tumorigenic	PG(20:0)	Tumorigenic	PC(38:6)	Tumorigenic
Cera(d18:1/36:4)	Tumorigenic	PG(23:0)	Tumorigenic	PC(43:3)	Non-tumorigenic
PE(36:0)	Tumorigenic	PG(24:0)	Tumorigenic		

As breast cancer is considered a heterogeneous disease, it may be that the breast tumour microenvironment is influenced by the type of breast cancer a patient has, thereby affecting the progression of the disease and its metastasis. These influential factors could be the oxygenation status and the recruitment of inflammatory cells (Marusyk, 2012).

Serum is a human sample so it is therefore a very "noisy" sample due to all the individual variability, including from dietary as well as cellular sources. In this study, the lipids, which were significantly elevated in the cell culture supernatant, were abundant lipid species found in the literature in serum (Quehenberger, 2010, Meikle, 2011). This would suggest that the breast cancer would have to produce a very high amount of these lipid biomarkers in order for them to be detectable. Therefore, results from this study would indicate that if tumours did contribute to higher serum lipid levels, the tumours would have to be bigger than those produced in the patients from this study in order to be detectable by their effects on serum lipids. This implies that the approach is not ideal for early detection but may provide biological information about the tumour. This was a focus study based on the literature and X-ray diffraction studies, which required easily accessible sample types. Therefore, breast and breast tumour tissues, such as those studied extensively in the literature, were not readily available but serum was. Even then, hair and blood samples from confirmed breast cancer patients who were undergoing treatment for their disease at the time of sample collection were time consuming and difficult to procure. In addition, clinical data varies from clinic to clinic and between the clinicians so there were also inconsistences in the amount and type of data collected from the clinics that participated in this study. This made standardising the categorisation of the patients difficult.

Lipidomics is an ever-evolving area and is not as standardised in its methodologies and classifications. There are thousands of lipid species and combinations in the cellular system and many unidentified species. The lipidomic field is still very varied in the platforms used and the degree of information that can be translated from the mass spectrometry data set and data analysis remains reliant on customised software solutions. There were also technical complexities, which may have contributed to the unsuccessful identification of specific phospholipid alterations associated with breast cancer. In this study the hair and serum samples were collected from the blood of patients with breast cancer and healthy controls and cell culture supernatant was taken from a growing tumorigenic cell line and a non-tumorigenic cell line. Lipids were extracted using a monophasic chloroform methanol extraction with an added internal standard.

A potential issue that could influence the ability of the technology to differentiate

changes between cancer samples and controls is the reproducibility of the methods. To control for this, replicates were run. The relative standard deviation of the replicates shows reproducibility but the methodology itself may not be ideal due to challenges associated with the non-standardised nature of lipidomics and the different types of breast cancer samples, which were analysed. To further investigate the reproducibility of the lipid analysis methodology for sample preparation as well as LCMS analysis, pooled biological quality controls (PBQC) samples were prepared along with samples and analysed by LCMS between every ten samples. The results for PBQCs indicate the mass spectrometry data collection was internally highly consistent and this implies that this component of this methodology was reliable and would not contribute to the lack of reproducibility of the results. Sample preparation was carried out dependably using calibrated equipment. There were no spillages or errors, aside from the first set of forty hair samples, which were excluded from this study. Therefore, It is not highly likely that the LCMS methodology may have contributed to any inability to distinguish between samples or to the results of this study. LCMS is still not as sensitive as some other mass spectrometry platforms and perhaps more platforms need to be considered such as QTOF and MSMS for distinguishability between these samples. (Ryhage, 1960).

This study only used one internal standard for all lipid classes due to the way in which the project unfolded. Initially this was a PC targeted study and so PC internal standards were added to plasma and hair samples, which were processed and then later re-run for other lipid classes. Samples were too scarce to be re-prepared and re-processed and so there was only one internal standard across all samples for all lipid classes.

Statistical analysis was used to correct for this through exploration of the raw data sets to establish whether normalising to the internal standard or the median of the total lipid content changed the results. Firstly, the internal standard was plotted against the sum, average and median of total lipids and the weight of hair samples or cells per ml was plotted against sum, average and median of total lipids to determine any trends in data. The plots showed that there was no difference in the data trends between all the different methods modeled and for that reason the data was not normalised to the internal standard for any of the sample types. In addition to these raw data trends, it was decided that the median of total lipids was the ideal way to normalise the data because it allowed the data to be compared across the board because lipids from hair

would need to be analysed per mg of hair, the cell media data would need to be to cells per ml and serum data would be per □l. The different sample types were difficult to compare due to the different types of sample matrices, therefore, a relative abundance approach was used rather than absolute quantification to attempt to overcome this issue. The extracted lipid content in hair is dependent on the type of hair and was difficult to normalise to the weight and so it was more accurate to normalise to the median of the total lipid content. Similarly, the lipid content in cell culture supernatant could be not related to the cell number due to the different sizes of the two cell types and different growth rate, therefore, the data from the cell culture supernatant was normalised to the median of total lipid content too. Based on the experimental design which incorporated three different sample types, normalisng to the median of the total lipids extracted allowed direct comparison across all three sample types. The recovery was tracked as a percentage to total lipid content in each sample type, which allowed any significant changes in lipid content in between patients and control to be determined independently of the type of sample matrix.

Data was treated for missing values as outlined in the methodology of each chapter and then transformed to the log scale for univariate analysis to remove heteroscedasticity, linearise the data and allow lipid profiles to be comparable. This data was plotted as bar graphs with standard deviation error bars as the averages of the replicates for two groups. One challenge with this method of analysis is that it creates negative values due to the log transformation. The values are true despite being represented as negative areas. The univariate analysis carried out in this data analysis was a t-test, which was used to obtain a ranking of significantly changing lipid species. This was followed by multivariate analysis, which looked at multiple variables simultaneously to obtain an overview of the entire data set. This was represented by the PCA plots. It should be noted that regardless of all of these issues, the data set is considered robust and consistent as the pooled quality controls were grouping when the samples were plotted in a PCA.

The lipid species were identified according to the triple quad precursor and neutral loss scan techniques based on the head group of each lipid class (Appendix 8.6.1). The appropriate MRM transition for each identified lipid species was then created and the m/z signal collected. The lipids could be species present in the sample but could

also potentially be from impurities or contaminants in the sample or chromatography column. In addition, the presence of lysophospholipids and phosphatidic acid can indicate a possible degradation before extraction (Meikle, 2011). Further steps may need to be taken as precaution to minimise rapid degradation of the lipids extracted. The data was reviewed and thoroughly analysed using solvent blanks and any inappropriately identified lipid species were removed. The lipid species in this study were presented with a putative identification and were compared to those in the literature (Meikle, 2011, Quehenberger, 2010). Further structural identification by tandem mass spectrometry (MSMS), of any of the lipids species detected in this study, would be required to validate their classification.

As there is not a fully identified biological lipidome, the lipidomic databases are ever changing and not very well defined and there is no standardised method of data analysis (Hartler, 2012). The current hurdle in this field is data analysis because much of the raw lipid mass spectrometry data requires high levels of processing to be able to identify and quantify hundreds of species in an analytical run (Köfeler, 2012). Once the spectrum is detected, the lipids are putatively identified by matching the analytical information (mass, retention time) against a lipid library from commercial software, in this case Agilent MassHunter software. Certain software applications have different lipid libraries and are intended for certain instruments which makes data processing methods variable from brand to brand. There is also the lengthy step of manually reviewing the peak selection for every lipid species, for every sample analysed, to ensure a correct and accurate peak has been assigned. Any peaks that were considered to be noise were deleted before analysis but due to the noisy nature of the serum data, a small amount of peaks were still not ideal and were included in the analysis. The lipid data was revalidated based on retention time and peak shape, then unclear peaks were identified and removed before the statistical analysis. The noisy data was useful in looking for data above the noise to avoid over interpretation of the data. It has been presented here solely in order to assist in data interpretation.

Many of these assignments do not correspond with the literature on biological lipids (Meikle, 2011, Quehenberger, 2010), however, this study was concerned with using mass spectrometry to screen samples for patterns in lipid profiles (artifactual or biological) in order to confirm the presence of breast cancer. Therefore, because the lipid species putatively identified in serum and hair were not significantly changing

no further analysis was carried out. If significantly changing lipids species were identified in the samples then tandem mass spectrometry would have been used to define their structure and fully identify these biomarkers.

The removal of lipid species not previously identified in serum or hair would not have changed the outcome, as no species were changing significantly. It is likely that not all biological lipid species have been identified to date, and that some of the lipids, which may seem inaccurate, but identified in this study might be genuine. It was however, beyond the scope of this study to make this determination.

A targeted and focused approach was used to identify biomarkers using the literature as a basis for targeting phospholipid species, which have well known fragmentation patterns (Meikle, 2011, Quehenberger, 2010). MRM mode, as used in this study, allows fast and accurate quantification of entire lipid classes in a single chromatographic run on a triple quad mass spectrometer. This is due to the selectivity of the retention time in combination with known ion pairs from precursor scanning which increases the sensitivity of the study. Using a targeted approach provided the project with a specific set of molecules to identify and so certain fragments were targeted using precursor ion and neutral loss scans on the mass spectrometer. Precursor scanning analyses from the same classes and neutral loss scanning analyses of lipids that lost the same fragment on collision in triple quad (second analyser on the mass spectrometer) were performed. These methods allow more thorough analysis of lipid that have similar structures and the ability to distinguish subtle but significantly changing lipids through the reduction of baseline noise (Loizides-Mangold, 2013). Using precursor and neutral ion scanning provides the ability to uncover unexpected species within the lipid classes that the study focused on. It is also fast to develop and once developed, quite reproducible allowing the analysis of many lipids in the same experiment because of high-throughput (Loizides-Mangold, 2013). There are however limitations to the number of targeted species and this means many species are not profiled.

It may be that untargeted lipidomics is better suited to investigating the question of whether lipids in the circulation can be used to determine the presence of breast cancer, as it has a much broader scope and is an unbiased approach. From all the detected lipids, further analysis of those of interest could uncover significantly changing lipids and ones, which were not included in this study. Although ideal for

identifying unexpected metabolites, the challenge with this approach is that due to such a complex resulting data set, this method is the least sensitive approach.

In the case of both hair and serum samples it appears that the sample size was too small to take into account individual variability, other dietary or environmental lipids and the heterogeneity of breast cancer. For instance, it has been reported that the fatty acid composition of serum lipid esters (including phospholipids) mirrors dietary fatty acid intakes over the previous few weeks and also reflects endogenous fatty acid metabolism (Warensjö, 2006). There is also evidence that a Mediterranean type diet can result in a higher serum concentration of n-3 fatty acids, which alters the composition of phospholipids (Ambring, 2006). To determine whether the non-significant results in the serum data were due to a lack of statistical power, a power analysis was conducted on the basis of the mean of the two independent sample groups, using a power of .80 (Champely, 2012). This analysis demonstrated that sample size would have to be 3,122,536 in order for a significant result ($p< 0.05$) to be achieved. Conversely, starting with a sample size of 40 (as used in this study) the power statistic for the p-value is only 0.03. Therefore, it is unlikely that the negative findings in this study can be attributed to a modest sample size and even if many more samples are collected, the data will still show very similar results, which suggests that hair and serum are probably not useful types of samples for biomarker discovery for breast cancer.

Whilst one conclusion from this study is that there might be no difference in lipid composition in serum between breast cancer patients and healthy women, there were some non-significant differences detected that, given the limitations of the methodology and the clinical and dietary variability, would justify a follow-up study.
The cell culture supernatant data implies that there is a biological change involving lipids that is associated with breast cancer. In addition there are indications in the literature that would justify further research on this question. If the study is repeated, it is clear that there must be more participants with better-defined tumours to give a higher statistical power. Furthermore it would be essential to focus on exosome or microvesicle fractions in serum to avoid contamination of the cellular-derived lipids with dietary lipids. If the changes are localised, as the data suggests, then further studies to fully identify the lipids of interest should be carried out using the breast

tumour tissue and the surrounding healthy tissue to validate these changing lipids before targeted analysis in serum. An additional key variable that must be taken into account accordingly, is the issue of the heterogeneity of breast cancer. It may be that different subspecies of lipids are altered in the various types of breast cancers. Future targeted studies, with more sensitive methods would need to use more carefully processed samples (to enrich for microvesicles) as a source for identifying these possible biomarkers.

The need for a set of biomarkers to detect invasive breast cancer at an early stage justifies further study in this area. This project identifies the potential that serum lipids has to provide the basis of such a test, and has increased the understanding of the complex factors required for the development of an appropriate assay.

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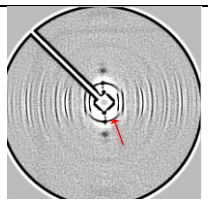
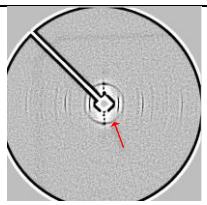
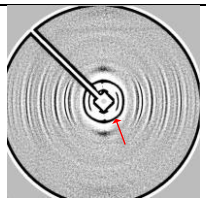
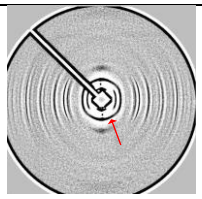
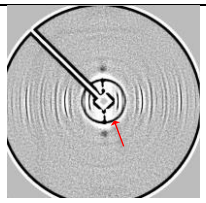
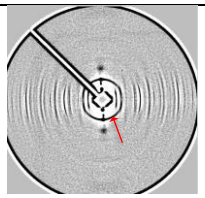
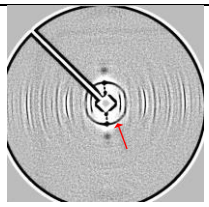
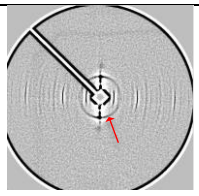
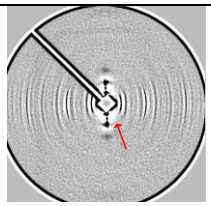
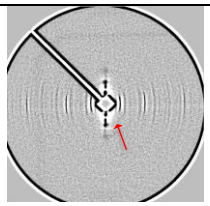
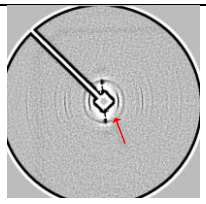
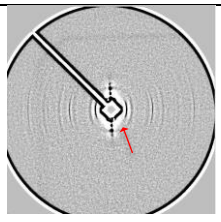
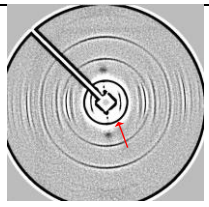
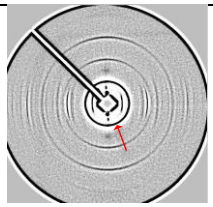
ZHANG, L., XIAO, H, KARLAN, S, ZHOU, H, GROSS, J, ELASHOFF, D, AKIN, D, YAN, X, CHIA, D, KARLAN, B, WONG, DT 2010. Discovery and preclinical validation of salivary transcriptomic and proteomic biomarkers for the non-invasive detection of breast cancer. *PLoS One,* 5**,** e15573.

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8. Appendix

8.1. From Chapter 2

Table 8.1: All images showing solvent extraction (n=15). Arrow indicates approximate region where breast cancer-associated feature is typically located.

Sample	Before	Solvent Extraction
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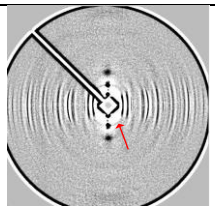
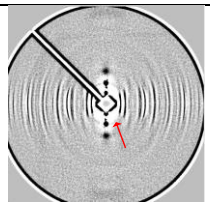
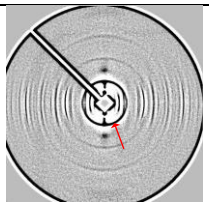
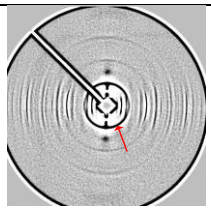
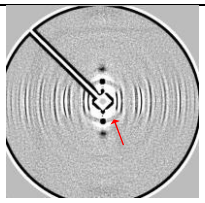
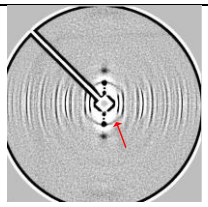
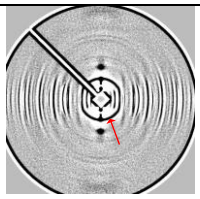
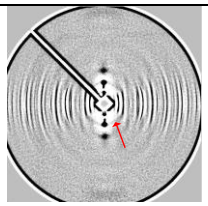
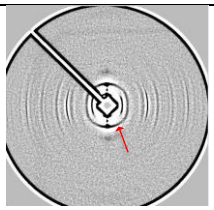
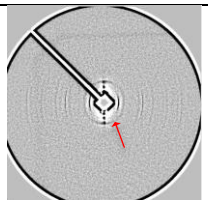
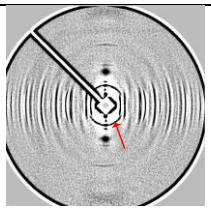
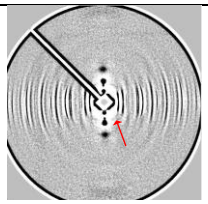
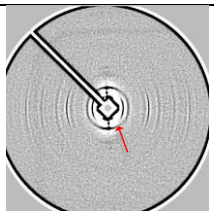
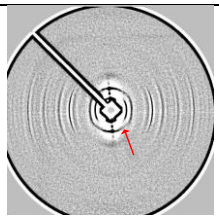
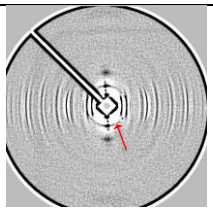
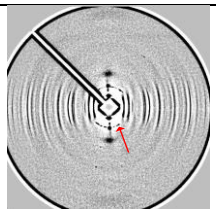
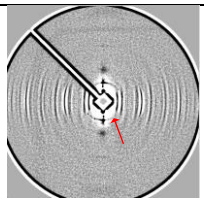
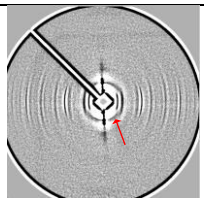
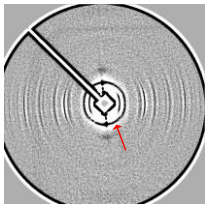
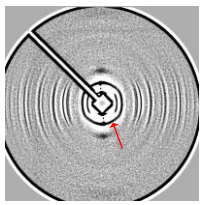
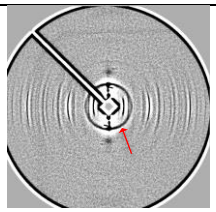
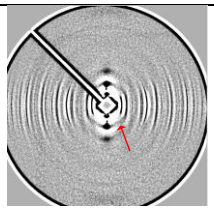
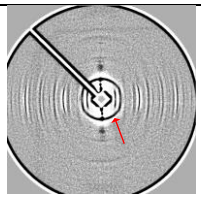
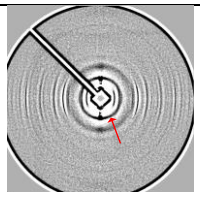
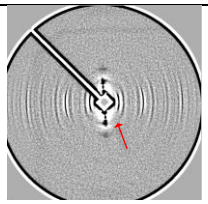
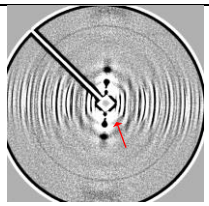
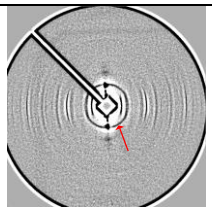
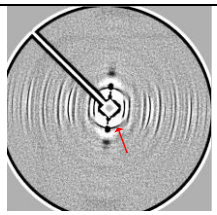
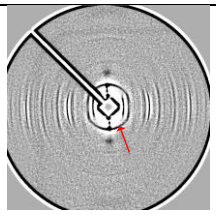
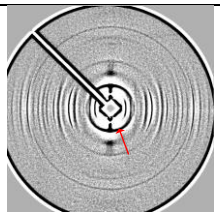
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Table 8.2: All images showing lead nitrate treatment (n=15). Arrow indicates approximate region where breast cancer-associated feature is typically located.

Sample	Before	After Lead Nitrate Treatment
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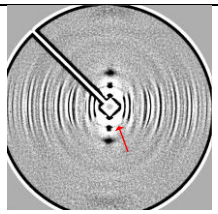
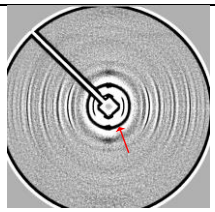
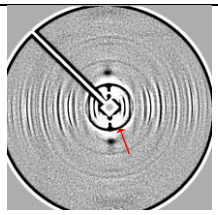
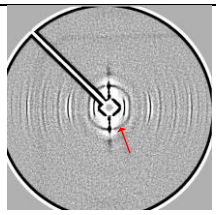
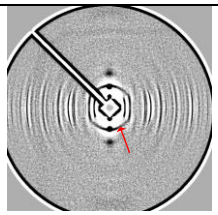
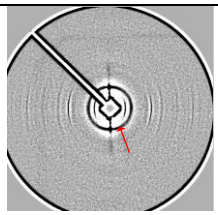
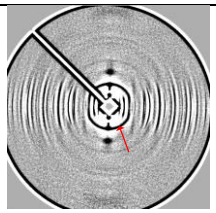
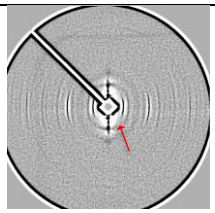
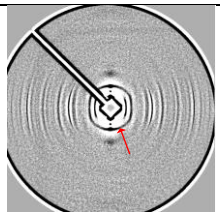
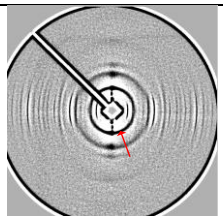
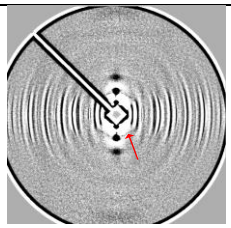
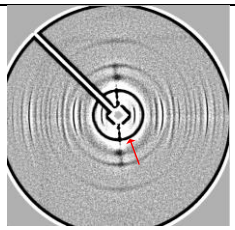
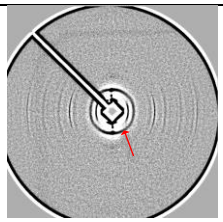
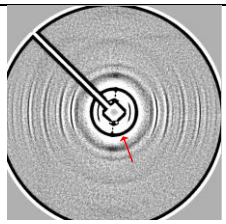
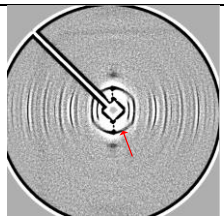
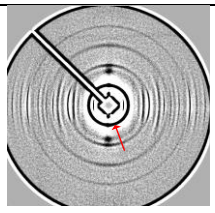
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Table 8.3: Concentration (nM/mg) of phosphatidylcholine lipids species extracted from hair.

Concentration (nM/mg)

Sample	D-PC 34.1	PC.15.0	PC.16.0	PC.18.6	PC.25.5	PC.30.0	PC.30.1	PC.31.6	PC.32.0	PC.32.6	PC.33.0	PC.34.0
S2	3.42	6.46	2.38	160.00	4.54	14.44	1.32	0.30	9.01	11.80	1.06	2.45
S2B	2.55	5.57	2.12	122.27	3.00	12.87	1.85	0.21	9.85	7.24	0.62	1.60
SP	2.95	10.14	2.94	109.62	2.71	18.77	1.62	0.58	16.51	11.23	0.85	4.08
C1	1.95	3.36	0.25	63.17	1.42	12.45	1.41	0.27	6.06	5.23	0.33	1.92
C2	4.89	4.99	1.51	62.17	2.01	10.80	1.27	0.29	7.11	5.93	0.95	2.75
C3	2.22	2.03	0.71	47.29	1.46	3.10	0.08	0.00	2.41	1.60	0.20	0.67
C4	0.94	0.86	0.21	23.06	0.64	7.48	0.80	0.11	9.08	2.48	0.41	2.65
C5	0.19	0.57	0.05	13.02	0.41	3.41	0.19	0.03	2.34	1.14	0.09	0.74

Concentration (nM/mg)

Sample	PC.34.1	PC.34.5	PC.35.3	PC.36.0	PC.37.0	PC.38.0	PC.38.1	PC.16.5	PC.23.4	PC.36.1	PC.36.0
S2	3.42	4.55	2.03	3.54	1.80	6.70	5.45	0.35	130.49	1.12	1.00
S2B	2.55	1.90	1.25	1.89	1.30	3.49	3.76	0.29	89.97	0.77	0.77
SP	2.95	2.23	1.67	3.82	1.75	4.35	3.11	0.00	70.29	0.83	0.84
C1	1.95	1.03	1.35	1.43	0.26	3.14	3.30	0.15	74.19	0.38	0.34
C2	4.89	1.22	0.86	2.87	1.66	4.50	4.67	0.25	64.31	0.66	0.73
C3	2.22	0.78	0.64	1.34	0.73	2.22	1.61	0.02	44.01	0.26	0.35
C4	0.94	0.76	0.55	1.06	0.30	1.55	2.18	0.07	34.36	0.43	0.28
C5	0.19	0.50	0.23	0.35	0.01	0.97	0.55	0.00	29.16	0.08	0.00

8.2. From chapter 3

Table 8.4: Basic data for cell lines used in the cell culture supernatant study

Cell line	Age	Gender	Ethnicity	Disease	Cell count
MDA-MB-231	51	Female	Caucasian	Breast adenocarcinoma tumourigenic	2.68 x 10^8 / 50ml, 0.052/ml
MCF-10-A	36	Female	Caucasian	Breast fibrocystic not tumourigenic	3.20 x 10^8 / 75ml, 0.043/ml

8.2.1. Raw peak area data

Table 8.5: Raw peak area matrix for the supernatant from a tumorigenic and non- tumorigenic cell line for all lipid species

Sample	PI(34:1)	PI(36:0)	PI(36:1)	PI(36:2)	PI(38:2)	PI(38:3)	PI(38:4)	PI(38:5)	PI(40:6)	LPG(15:0)	LPG(16:0)	LPG(17:0)	LPG(18:0)	LPG(19:0)	LPG(20:0)	PG(27:1)	PG(33:0)	PG(16:0)	PG(17:0)	PG(18:0)
MCF 1a	0	0	0	0	0	0	20.28155	0	0	0	4747.70803	40.197025	5065.51278	172.7373	2600.01558	13.514575	5.08965	4747.70803	40.197025	5065.51278
MCF 1b	0	0	0	0	0	0	19.29515	0	0	0	4673.77903	31.461525	5216.41278	133.1095	2802.16958	7.700475	5.08965	4673.77903	31.461525	5216.41278
MCF 2a	0	0	0	0	0	0	24.39455	0	0	0	3800.74283	21.223425	4047.71948	143.3935	2362.37208	7.700475	4.42965	3800.74283	21.223425	4047.71948
MCF 2b	0	0	0	0	0	0	30.67855	0	0	0	3652.12573	9.412525	3845.04058	143.4495	1590.51218	10.211075	9.10785	3652.12573	9.412525	3845.04058
MDA 1a	31.8471	37.5418	226.2181	113.1807	103.3455	287.3641	461.2791	39.389	39.439	96.481525	7553.89923	91.6433	8097.53168	175.473125	4482.0667	38.8705	19.57775	7553.89923	91.6433	8097.53168
MDA 1b	42.6312	35.6604	219.0231	116.062	108.4841	313.0675	464.1568	41.4419	48.0476	154.784925	9258.08013	68.1444	10796.1439	149.806825	5330.3135	39.3243	5.17355	9258.08013	68.1444	10796.1439
MDA 2a	22.8477	28.383	218.4247	91.561	79.2232	314.2602	414.833	48.6596	47.5454	83.346025	9552.06923	95.2782	11198.095	220.960625	5363.9684	28.605	17.28935	9552.06923	95.2782	11198.095
MDA 2b	26.9414	33.6413	200.9225	102.9992	80.5596	313.8587	405.6342	44.9251	38.3764	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Sample	**PG(19:0)**	**PG(20:0)**	**PG(21:6)**	**PG(23:0)**	**PG(23:6)**	**PG(24:0)**	**PG(25:0)**	**PG(26:0)**	**PG(26:1)**	**PG(27:0)**	**PG(28:0)**	**PG(28:1)**	**PG(28:2)**	**PG(29:0)**	**PG(30:0)**	**PG(30:1)**	**PG(30:2)**	**PG(31:0)**	**PG(31:1)**	**PG(32:0)**
MCF 1a	172.7373	2600.01558	66.187025	203.256075	29.1105	386.259475	77.44185	506.6195	543.493225	108.731525	189.407725	223.841325	44.965075	14.95165	133.6371	122.069425	4.7721	61.9421	54.27585	125.104275
MCF 1b	133.1095	2802.16958	75.921425	291.137575	16.4391	383.302075	73.32355	680.8356	535.372825	86.302325	273.068325	238.361625	20.161175	26.36755	239.2822	170.771925	41.3918	70.1329	39.23775	216.636475
MCF 2a	143.3935	2362.37208	71.223725	226.011175	36.9916	397.413975	103.56485	681.8081	481.995925	98.182225	223.828325	257.514125	34.405275	30.67675	226.9911	127.563425	21.6502	65.603	43.37945	128.967875
MCF 2b	143.4495	1590.51218	72.185125	243.821975	27.7913	501.980375	92.73275	630.0797	371.310425	63.715825	191.102625	166.927525	8.567175	28.89445	183.8941	148.303625	16.0919	40.8218	68.25675	125.615075
MDA 1a	175.473125	4482.0667	150.2984	600.384775	90.963225	885.046425	200.0138	1250.65278	905.535375	211.6432	512.897075	548.328025	58.367875	55.83575	472.72485	287.978825	75.578	164.589	125.8144	243.963725
MDA 1b	149.806825	5330.3135	142.362	515.285975	71.104825	778.253625	254.1757	976.908375	1406.54228	274.6227	264.289875	580.021825	115.558175	37.82725	278.61675	235.161025	52.9011	157.4425	155.0849	297.509225
MDA 2a	220.960625	5363.9684	199.7946	470.122175	42.766625	802.645725	273.0261	1080.33028	1373.26318	259.7808	331.459475	589.296625	120.130075	73.25355	342.25015	247.649925	34.5802	162.7355	139.4911	222.313225
MDA 2b	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Sample	**PG(32:1)**	**PG(33:1)**	**PG(34:1)**	**PG(34:2)**	**PG(36:2)**	**CE(17:0)**	**CE(17:1)**	**CE(19:1)**	**CE(19:2)**	**CE(21:0)**	**CE(25:4)**	**Cera(d18:1/15:2**	**Cera(d18:1/16:0**	**Cera(d18:1/17:0)/(**	**Cera(d18:1/17:2**	**Cera(d18:1/18:0**	**Cera(d18:1/20:0**	**Cera(d18:1/21:2**	**Cera(d18:1/22:0**	**Cera(d18:1/23:0**
MCF 1a	32.797	6.383075	27.315925	21.10495	26.66705	174.462575	24.2856	71.82075	12.1755	99.596775	10.670025	NA	169.0107	45.838825	21.168075	95.10975	26.14245	37.4586	119.8327	71.1687
MCF 1b	78.9722	23.043775	36.763125	36.72635	19.83265	207.953675	NA	77.90235	17.6073	124.573075	25.581525	595.55685	190.5253	24.951525	26.141275	99.73975	33.82265	22.0372	92.991	89.0424
MCF 2a	66.2029	12.018775	75.241525	23.60785	20.66435	183.655175	14.1392	31.70475	3.2165	175.498475	27.909225	349.54205	128.8424	19.730325	26.267075	53.95525	27.82815	39.4816	65.0452	80.5741
MCF 2b	73.7786	4.750475	34.073225	17.98955	16.04065	165.797875	21.2404	50.27595	14.043	272.815375	15.688725	90.79505	134.7168	18.208925	30.060175	67.67915	27.22975	16.5964	100.9265	96.6888
MDA 1a	162.063825	31.4492	78.791675	73.751075	46.38155	269.495925	80.9403	141.870825	22.3003	158.612925	5.691625	168.8141	1749.74165	223.1326	141.02265	444.80285	94.193825	191.1088	640.43695	234.148525
MDA 1b	73.733625	27.4446	38.466375	59.248875	34.72515	215.606825	35.2848	110.714625	26.7885	88.247325	3.180225	178.2241	1530.00265	241.4051	133.26545	371.07745	75.972325	155.4064	635.25125	234.893425
MDA 2a	96.359525	31.8574	72.360775	45.699075	19.56575	269.495625	55.4507	102.958525	10.0559	51.721125	11.305925	191.7954	318.72585	112.4435	108.36025	326.41425	87.755525	152.7789	597.30475	191.364825
MDA 2b	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	333.9306	1312.96805	171.2586	128.50075	330.49845	121.397525	131.5966	639.86445	210.953825
Sample	**Cera(d18:1/23:2**	**Cera(d18:1/24:0**	**Cera(d18:1/24:1**	**Cera(d18:1/24:2**	**Cera(d18:1/36:3**	**Cera(d18:1/36:4**	**PE(36:0)**	**PE(36:1)**	**PE(36:2)**	**PE(36:3)**	**PE(36:4)**	**PE(37:1)**	**PE(37:2)**	**PE(37:3)**	**PE(37:4)**	**PE(38:1)**	**PE(38:2)**	**PE(38:3)**	**PE(38:4)**	**PE(38:5)**
MCF 1a	98.652575	206.537	140.85345	48.7653	36.4851	13.2976	20.4217	166.7841	212.627	31.745125	3.1446	0	0	0	0	0	0	17.7394	131.205	45.1038
MCF 1b	126.589975	195.3919	112.02345	61.6206	42.0628	NA	50.0864	172.7753	166.1469	27.930625	11.1011	0	0	0	0	0	0	18.3564	142.0092	45.2905
MCF 2a	101.511875	130.2307	92.54865	45.0971	38.2207	13.2183	21.7047	99.207	150.865	13.598125	10.4584	0	0	0	0	0	0	10.3725	129.447	32.9401
MCF 2b	82.509075	160.8635	103.45235	32.4416	35.8241	13.85	15.6791	116.4666	147.657	22.662525	14.5883	0	0	0	0	0	0	21.6689	103.7074	49.8171
MDA 1a	859.037725	682.381625	587.774125	131.685475	330.1628	68.1088	92.7305	1950.4137	1739.48638	316.5128	100.1346	39.7607	21.6263	52.6946	263.7801	88.9452	261.3421	628.7735	1389.2828	598.9177
MDA 1b	670.509025	900.557825	685.770825	141.615375	290.9964	92.9191	78.5529	1936.4614	1742.44688	307.1141	139.369	40.0271	75.8898	73.5999	246.8307	90.3866	195.3247	650.7291	1419.6198	585.6701
MDA 2a	670.915125	276.163125	241.339525	75.467975	269.9141	44.8946	21.2927	625.3731	763.168775	157.3699	110.7581	6.1802	19.8205	28.2776	116.2576	61.8869	40.9251	220.5463	483.4781	314.2935
MDA 2b	799.021925	303.782825	324.351225	89.449475	247.1674	68.7834	71.4571	1474.3678	1506.18848	284.9697	132.219	19.5296	26.1431	61.893	235.4069	59.0889	196.0431	469.4245	1250.2358	505.9327
Sample	**PE(38:6)**	**PE(39:0)**	**PE(40:4)**	**PE(40:5)**	**LPC(16:0)**	**LPC(17:0)**	**LPC(17:1)**	**LPC(18:0)**	**LPC(18:1)**	**LPC(20:0)**	**LPC(20:1)**	**LPC(20:2)**	**LPC(20:4)**	**LPC(20:5)**	**LPC(21:0)**	**LPC(22:1)**	**LPC(22:2)**	**LPC(22:5)**	**LPC(22:6)**	**PC(23:0)**
MCF 1a	12.265775	0	0	0	1796.46505	935564.421	112.991225	920.76055	784.792025	2.683875	6.889725	3.352525	15.354575	24.201425	8.55775	10.340475	63.01695	31.268825	13.969375	3.891875
MCF 1b	4.597775	0	0	0	1806.24895	924824.484	92.443225	1033.35635	126.176425	2.135075	4.277225	8.583325	49.021075	6.452425	15.91885	10.748575	63.08205	12.268425	41.958175	13.722875
MCF 2a	16.433975	0	0	0	1348.35025	958224.472	114.186525	630.93145	138.601525	NA	7.323825	2.977925	1.122875	14.199925	5.80695	13.704475	47.91345	15.657625	10.536375	2.332875
MCF 2b	NA	0	0	0	3262.9764	1199744.49	18.5099	3433.48208	1143.90488	34.704075	55.042875	5.829775	44.946575	2.26495	25.02715	18.1586	13.668475	38.164125	16.159425	4.40175
MDA 1a	101.355	90.1365	51.5561	226.8901	3262.9764	1199744.49	18.5099	3433.48208	1143.90488	34.704075	55.042875	5.829775	44.946575	2.26495	25.02715	18.1586	13.668475	38.164125	16.159425	4.40175
MDA 1b	117.7877	77.0406	70.8888	237.305	NA	1146291.37	13.7729	3288.23778	1532.60508	22.332675	17.038675	19.133175	145.905275	9.93435	32.74855	24.5656	34.645375	21.221125	35.022325	5.79425
MDA 2a	59.1853	42.6929	25.8288	53.9861	2690.1259	1044314.58	NA	2836.76498	1483.58348	26.861375	57.500575	12.223775	349.610675	7.91045	13.21445	16.5795	8.246175	66.815425	94.510025	18.79835
MDA 2b	104.053	86.0667	38.3012	175.083	2687.8157	997550.977	4.9206	2509.20498	1383.50848	8.969575	13.349475	14.869875	117.914075	12.69895	1.50235	15.1913	52.354775	14.827925	18.143425	2.46925

Table 8.6: Raw peak area matrix for the supernatant from a tumorigenic and non- tumorigenic cell line for all lipid species

Sample	PC(23:1)	PC(24:0)	PC(25:1)	PC(26:0)	PC(27:0)	PC(27:1)	PC(28:5)	PC(28:6)	PC(30:0)	PC(30:1)	PC(30:2)	PC(31:0)	PC(31:1)	PC(31:2)	PC(31:3)	PC(32:0)	PC(32:1)	PC(32:2)	PC(32:3)	PC(33:0)
MCF 1a	6.5936	1716.8113	15.500675	73.929575	96.89835	25.15015	191.154125	3.70975	1170.12248	3117.01693	246.12745	12.68505	316.33585	537.96245	31.41595	2420.5938	3368.82573	408.592	249.548825	360.606675
MCF 1b	5.0736	1657.6044	61.881275	NA	52.50385	7.21685	190.838025	NA	1133.94598	3054.98363	294.71495	3.76135	282.22755	383.94875	80.69165	2329.2253	3394.47303	507.3596	279.367425	345.469175
MCF 2a	2.602	380.8713	62.722175	14.011375	51.55165	13.74395	287.817725	NA	1146.06228	2853.57203	261.93665	NA	583.97235	304.57075	33.57525	2252.7167	3061.67513	410.0936	259.891925	346.087175
MCF 2b	4.302775	134.613775	35.736675	291.25635	189.5398	35.145975	93.6593	64.67485	3581.5832	8291.39298	882.015325	120.445375	3737.45465	1595.2326	149.26225	8009.82983	15508.5913	2159.29433	404.28925	3611.91438
MDA 1a	4.302775	134.613775	35.736675	291.25635	189.5398	35.145975	93.6593	64.67485	3581.5832	8291.39298	882.015325	120.445375	3737.45465	1595.2326	149.26225	8009.82983	15508.5913	2159.29433	404.28925	3611.91438
MDA 1b	0.475075	258.821375	11.316075	262.74495	169.1179	49.580875	33.6904	69.68735	3104.9204	8307.51848	769.169725	46.604175	3430.31595	1661.0176	108.23145	8465.31483	15136.2621	1413.07793	396.51335	3091.99958
MDA 2a	1.173975	632.238075	13.551275	290.94745	136.4263	9.909875	20.9133	110.83115	2534.7464	6104.53308	738.927225	44.098975	3507.79245	1382.3745	89.75375	5892.83783	10823.5489	1283.90543	287.64715	2585.79048
MDA 2b	20.071775	319.819475	43.650375	15.31105	95.4809	31.322375	61.1955	NA	2576.2991	6241.06508	725.379925	26.153775	2757.29065	1292.1564	136.88075	5813.74403	10674.8107	934.900025	272.31595	2445.12248
Sample	**PC(33:1)**	**PC(33:2)**	**PC(33:3)**	**PC(34:0)**	**PC(34:1)/IS**	**PC(34:2)**	**PC(34:3)**	**PC(34:4)**	**PC(35:0)**	**PC(35:1)**	**PC(35:2)**	**PC(35:3)**	**PC(35:4)**	**PC(36:0)**	**PC(36:1)**	**PC(36:2)**	**PC(36:3)**	**PC(36:4)**	**PC(36:5)**	**PC(37:1)**
MCF 1a	2084.5956	1322.0862	460.9526	1904.80113	14846.7231	6066.4744	475.31425	1250.9153	161.798875	1145.79378	1050.01448	473.002625	2475.746	686.033475	6276.00678	5602.58898	2285.23128	1792.46498	409.0063	185.761175
MCF 1b	1965.893	1333.1416	526.0024	984.891325	14384.0409	6340.7297	531.38975	1314.3324	246.337675	1074.79898	560.922875	404.586525	2216.3351	755.649575	5965.53018	5592.35158	2190.18858	1717.67868	400.6678	185.852575
MCF 2a	1893.4382	1326.9845	486.3834	1798.67233	13631.844	5526.6987	377.36735	1046.5522	200.844575	702.073275	415.597575	308.634825	2210.2589	550.721675	6146.94768	5401.25668	1930.68878	1824.13238	233.2771	234.428375
MCF 2b	8782.3423	3358.0995	1143.93855	10529.8207	57642.4378	17654.1453	1593.30348	276.164125	1203.0708	4550.21525	5267.73948	1698.26065	1100.05705	4007.0767	36496.5449	29064.8659	9753.4308	5605.19815	1337.8152	1012.11905
MDA 1a	8782.3423	3358.0995	1143.93855	10529.8207	57642.4378	17654.1453	1593.30348	276.164125	1203.0708	4550.21525	5267.73948	1698.26065	1100.05705	4007.0767	36496.5449	29064.8659	9753.4308	5605.19815	1337.8152	1012.11905
MDA 1b	8012.1734	3343.8702	970.01415	9285.35343	54186.0631	16135.1326	1600.56308	357.614525	1034.1174	7377.56035	4713.48588	1798.58965	1002.58265	3376.3882	34498.36	29923.7815	9513.2322	5269.16915	1038.0967	959.05365
MDA 2a	6279.8317	2640.305	900.40195	7930.17593	43124.327	13145.5449	1035.29868	197.675925	909.0254	5751.32335	3803.32498	1193.39735	911.12725	3178.0415	28686.0583	21901.5107	6877.0993	3784.29715	1036.3898	770.44635
MDA 2b	6109.7785	2507.7825	592.28195	7148.67503	40160.0527	12265.8966	972.751675	192.322825	845.0627	3598.23515	3857.89548	1362.06005	687.27595	2662.1038	25708.3103	20507.2773	6808.5192	3421.10885	812.2636	643.38455
Sample	**PC(37:2)**	**PC(37:3)**	**PC(37:4)**	**PC(37:5)**	**PC(37:6)**	**PC(38:0)**	**PC(38:1)**	**PC(38:2)**	**PC(38:3)**	**PC(38:4)**	**PC(38:5)**	**PC(38:6)**	**PC(39:0)**	**PC(39:1)**	**PC(39:2)**	**PC(39:3)**	**PC(39:4)**	**PC(39:5)**	**PC(40:0)**	**PC(40:1)**
MCF 1a	130.778725	62.4777	239.7207	475.852725	277.8177	43.241875	456.2076	861.594225	1410.78933	963.769925	1090.77925	691.03405	132.1326	36.2724	42.972	115.447375	28.220325	175.313475	518.4921	27.30105
MCF 1b	173.765025	116.6859	211.1315	355.315225	326.341	140.983975	423.9446	811.476325	1260.10683	956.746925	1120.26745	679.03355	220.394	60.5477	58.7659	31.778875	60.372225	126.173375	483.0669	35.66635
MCF 2a	150.789125	170.785	217.1148	305.687825	303.9829	77.381175	429.2986	672.332425	1349.05033	1008.50493	1111.58245	585.53465	181.7006	37.5145	21.7184	107.426775	47.634525	250.939475	517.3775	24.18615
MCF 2b	1103.64628	970.49635	2915.75985	2810.09013	1611.0926	472.01	3563.72478	4833.64383	7527.08848	4888.94823	5440.86063	2594.47235	1318.0094	199.65175	280.24205	456.021875	332.028275	1097.3211	661.373225	278.50235
MDA 1a	1103.64628	970.49635	2915.75985	2810.09013	1611.0926	472.01	3563.72478	4833.64383	7527.08848	4888.94823	5440.86063	2594.47235	1318.0094	199.65175	280.24205	456.021875	332.028275	1097.3211	661.373225	278.50235
MDA 1b	1143.31968	880.42755	1993.15435	2920.21173	1758.6662	435.2964	3112.92758	4840.80163	7162.42778	4898.41603	5266.52943	2408.35185	1357.2066	230.14255	283.76355	242.783675	409.208475	962.2072	537.808825	176.57835
MDA 2a	840.404875	1149.49905	2082.19845	2295.97173	1216.4685	374.7949	2726.77068	3202.22663	5286.13698	3675.35013	4051.39923	1923.72355	1072.4293	340.00935	380.37045	355.801175	305.974675	622.1726	608.366825	213.50255
MDA 2b	879.151575	1020.69025	1724.27965	2041.34843	1145.5938	353.4514	2350.24918	3028.50303	5052.56878	3478.11203	3783.71653	1718.11685	864.4025	144.10915	196.98355	129.830375	320.294175	637.9849	714.346925	196.85595
Sample	**PC(40:2)**	**PC(40:3)**	**PC(40:4)**	**PC(40:5)**	**PC(40:6)**	**PC(41:0)**	**PC(41:1)**	**PC(41:2)**	**PC(41:3)**	**PC(41:5)**	**PC(41:6)**	**PC(42:0)**	**PC(42:1)**	**PC(42:2)**	**PC(42:3)**	**PC(42:4)**	**PC(42:5)**	**PC(42:6)**	**PC(43:0)**	**PC(43:1)**
MCF 1a	19.681375	17.059775	152.34925	460.61835	492.60835	25.575	27.8804	14.4685	7.78085	27.996475	43.030775	3.07095	11.602925	24.21	46.04175	13.5245	30.975375	10.1256	11.6077	8.589175
MCF 1b	20.300275	55.086275	111.98645	511.37345	532.51925	44.8618	6.1321	23.8201	11.47885	24.504075	28.887375	10.62865	4.281325	10.6081	46.83565	10.1208	8.519375	19.0485	11.3851	11.840175
MCF 2a	62.205275	55.808575	197.87175	386.86925	306.29345	48.9786	NA	14.4147	1.28505	25.561275	25.299075	16.49165	11.507125	24.7909	46.17195	3.4529	7.496275	9.5467	8.7632	39.658075
MCF 2b	321.589025	350.6757	1021.7374	2083.08013	2567.2239	131.050625	124.400225	114.7026	106.053125	33.06115	125.038325	39.637	124.2024	121.188075	61.726825	89.973825	181.901475	196.29025	68.2869	5.915325
MDA 1a	321.589025	350.6757	1021.7374	2083.08013	2567.2239	131.050625	124.400225	114.7026	106.053125	33.06115	125.038325	39.637	124.2024	121.188075	61.726825	89.973825	181.901475	196.29025	68.2869	5.915325
MDA 1b	302.937625	341.7723	1061.0008	1941.75703	2330.0448	144.971525	62.240525	61.8607	43.778825	44.19485	119.919125	36.8583	129.9632	97.255275	59.801525	90.176025	162.139575	195.33845	40.0487	13.963925
MDA 2a	265.046125	278.4275	715.4179	1567.97003	1894.0821	134.864525	142.332025	105.4142	73.708025	91.15395	47.801725	9.4489	95.9478	68.062375	57.415725	83.867825	121.228075	112.41345	30.8775	22.399025
MDA 2b	301.795825	252.1082	840.9875	1372.97683	1859.7294	74.410125	69.583525	119.3951	80.753725	40.98985	29.767025	20.6364	111.1397	81.349775	51.167725	74.979525	96.552575	109.01495	7.5736	25.266725
Sample	**PC(43:2)**	**PC(43:3)**	**PC(43:4)**	**PC(43:5)**	**PC(43:6)**	**SM(30:0)**	**SM(30:1)**	**SM(30:2)**	**SM(32:0)**	**SM(32:1)**	**SM(33:0)**	**SM(33:1)**	**SM(34:0)**	**SM(34:1)**	**SM(34:2)**					
MCF 1a	166.7526	1770.55135	11.7545	33.876375	20.568125	32.5522	5.63355	7.47935	414.530125	10.073	1230.14225	1230.14225	935.2678	7617.1629	850.43655					
MCF 1b	191.4711	1905.63945	15.1273	25.963675	15.660725	32.0552	13.94035	6.72555	414.534325	39.6896	951.87645	951.87645	875.8144	7674.3558	796.64465					
MCF 2a	67.5766	1838.30085	6.4753	7.441775	8.240725	29.3347	14.32255	2.59725	416.896525	46.2923	1018.21115	1018.21115	1016.8171	7273.7522	759.39135					
MCF 2b	35.683075	663.928425	20.70395	6.417075	6.980525	35.0771	17.60525	13.293125	907.93275	45.714475	2550.1244	2550.1244	2927.07925	20502.5757	2191.29883					
MDA 1a	35.683075	663.928425	20.70395	6.417075	6.980525	35.0771	17.60525	13.293125	907.93275	45.714475	2550.1244	2550.1244	2927.07925	20502.5757	2191.29883					
MDA 1b	88.113575	633.204725	15.59865	5.740175	19.857425	18.1053	8.92645	11.175225	802.28375	78.466875	2488.882	2488.882	2606.66985	19504.1263	2062.17993					
MDA 2a	69.584275	648.900225	17.60825	11.348375	17.347925	24.1155	8.56345	5.469125	644.39165	48.473075	1886.7867	1886.7867	1967.43235	14961.2159	1592.20803					
MDA 2b	42.836875	613.362125	5.81335	21.093775	14.614725	47.3943	26.49395	7.127025	633.58015	60.791275	1867.1455	1867.1455	1777.90495	14136.1964	1588.02423					

8.2.2. Normalised peak area data

Table 8.7: Normalised peak area matrix for the supernatant from a tumorigenic and non- tumorigenic cell line for all lipid species

Sample	PI(34:1)	PI(36:0)	PI(36:1)	PI(36:2)	PI(38:2)	PI(38:3)	PI(38:4)	PI(38:5)	PI(40:6)	LPG(15:0)	LPG(16:0)	LPG(17:0)	LPG(18:0)	LPG(19:0)	LPG(20:0)	PG(27:1)	PG(33:0)	PG(16:0)	PG(17:0)	PG(18:0)
MCF 1a	0	0	0	0	0	0	20.28155	0	0	0	4747.70803	40.197025	5065.51278	172.7373	2600.01558	13.514575	5.08965	4747.70803	40.197025	5065.51278
MCF 1b	0	0	0	0	0	0	19.29515	0	0	0	4673.77903	31.461525	5216.41278	133.1095	2802.16958	7.700475	5.08965	4673.77903	31.461525	5216.41278
MCF 2a	0	0	0	0	0	0	24.39455	0	0	0	3800.74283	21.223425	4047.71948	143.3935	2362.37208	7.700475	4.42965	3800.74283	21.223425	4047.71948
MCF 2b	0	0	0	0	0	0	30.67855	0	0	0	3652.12573	9.412525	3845.04058	143.4495	1590.51218	10.211075	9.10785	3652.12573	9.412525	3845.04058
MDA 1a	31.8471	37.5418	226.2181	113.1807	103.3455	287.3641	461.2791	39.389	39.439	96.481525	7553.89923	91.6433	8097.53168	175.473125	4482.0667	38.8705	19.57775	7553.89923	91.6433	8097.53168
MDA 1b	42.6312	35.6604	219.0231	116.062	108.4841	313.0675	464.1568	41.4419	48.0476	154.784925	9258.08013	68.1444	10796.1439	149.806825	5330.3135	39.3243	5.17355	9258.08013	68.1444	10796.1439
MDA 2a	22.8477	28.383	218.4247	91.561	79.2232	314.2602	414.833	48.6596	47.5454	83.346025	9552.06923	95.2782	11198.095	220.960625	5363.9684	28.605	17.28935	9552.06923	95.2782	11198.095
MDA 2b	26.9414	33.6413	200.9225	102.9992	80.5596	313.8587	405.6342	44.9251	38.3764	0	0	0	0	0	0	0	0	0	0	0
Sample	**PG(19:0)**	**PG(20:0)**	**PG(21:6)**	**PG(23:0)**	**PG(23:6)**	**PG(24:0)**	**PG(25:0)**	**PG(26:0)**	**PG(26:1)**	**PG(27:0)**	**PG(28:0)**	**PG(28:1)**	**PG(28:2)**	**PG(29:0)**	**PG(30:0)**	**PG(30:1)**	**PG(30:2)**	**PG(31:0)**	**PG(31:1)**	**PG(32:0)**
MCF 1a	172.7373	2600.01558	66.187025	203.256075	29.1105	386.259475	77.44185	506.6195	543.493225	108.731525	189.407725	223.841325	44.965075	14.95165	133.6371	122.069425	4.7721	61.9421	54.27585	125.104275
MCF 1b	133.1095	2802.16958	75.921425	291.137575	16.4391	383.302075	73.32355	680.8356	535.372825	86.302325	273.068325	238.361625	20.161175	26.36755	239.2822	170.771925	41.3918	70.1329	39.23775	216.636475
MCF 2a	143.3935	2362.37208	71.223725	226.011175	36.9916	397.413975	103.56485	681.8081	481.995925	98.182225	223.828325	257.514125	34.405275	30.67675	226.9911	127.563425	21.6502	65.603	43.37945	128.967875
MCF 2b	143.4495	1590.51218	72.185125	243.821975	27.7913	501.980375	92.73275	630.0797	371.310425	63.715825	191.102625	166.927525	8.567175	28.89445	183.8941	148.303625	16.0919	40.8218	68.25675	125.615075
MDA 1a	175.473125	4482.0667	150.2984	600.384775	90.963225	885.046425	200.0138	1250.65278	905.535375	211.6432	512.897075	548.328025	58.367875	55.83575	472.72485	287.978825	75.578	164.589	125.8144	243.963725
MDA 1b	149.806825	5330.3135	142.362	515.285975	71.104825	778.253625	254.1757	976.908375	1406.54228	274.6227	264.289875	580.021825	115.558175	37.82725	278.61675	235.161025	52.9011	157.4425	155.0849	297.509225
MDA 2a	220.960625	5363.9684	199.7946	470.122175	42.766625	802.645725	273.0261	1080.33028	1373.26318	259.7808	331.459475	589.296625	120.130075	73.25355	342.25015	247.649925	34.5802	162.7355	139.4911	222.313225
MDA 2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sample	**PG(32:1)**	**PG(33:1)**	**PG(34:1)**	**PG(34:2)**	**PG(36:2)**	**CE(17:0)**	**CE(17:1)**	**CE(19:1)**	**CE(19:2)**	**CE(21:0)**	**CE(25:4)**	**Cera(d18:1/15:2**	**Cera(d18:1/16:0**	**Cera(d18:1/17:0)/(**	**Cera(d18:1/17:2**	**Cera(d18:1/18:0**	**Cera(d18:1/20:0**	**Cera(d18:1/21:2**	**Cera(d18:1/22:0**	**Cera(d18:1/23:0**
MCF 1a	32.797	6.383075	27.315925	21.10495	26.66705	174.462575	24.2856	71.82075	12.1755	99.596775	10.670025	0	169.0107	45.838825	21.168075	95.10975	26.14245	37.4586	119.8327	71.1687
MCF 1b	78.9722	23.043775	36.763125	36.72635	19.83265	207.953675	0	77.90235	17.6073	124.573075	25.581525	595.55685	190.5253	24.951525	26.141275	99.73975	33.82265	22.0372	92.991	89.0424
MCF 2a	66.2029	12.018775	75.241525	23.60785	20.66435	183.655175	14.1392	31.70475	3.2165	175.498475	27.909225	349.54205	128.8424	19.730325	26.267075	53.95525	27.82815	39.4816	65.0452	80.5741
MCF 2b	73.7786	4.750475	34.073225	17.98955	16.04065	165.797875	21.2404	50.27595	14.043	272.815375	15.688725	90.79505	134.7168	18.208925	30.060175	67.67915	27.22975	16.5964	100.9265	96.6888
MDA 1a	162.063825	31.4492	78.791675	73.751075	46.38155	269.495925	80.9403	141.870825	22.3003	158.612925	5.691625	168.8141	1749.74165	223.1326	141.02265	444.80285	94.193825	191.1088	640.43695	234.148525
MDA 1b	73.733625	27.4446	38.466375	59.248875	34.72515	215.606825	35.2848	110.714625	26.7885	88.247325	3.180225	178.2241	1530.00265	241.4051	133.26545	371.07745	75.972325	155.4064	635.25125	234.893425
MDA 2a	96.359525	31.8574	72.360775	45.699075	19.56575	269.495625	55.4507	102.958525	10.0559	51.721125	11.305925	191.7954	318.72585	112.4435	108.36025	326.41425	87.755525	152.7789	597.30475	191.364825
MDA 2b	0	0	0	0	0	0	0	0	0	0	0	333.9306	1312.96805	171.2586	128.50075	330.49845	121.397525	131.5966	639.86445	210.953825
Sample	**Cera(d18:1/23:2**	**Cera(d18:1/24:0**	**Cera(d18:1/24:1**	**Cera(d18:1/24:2**	**Cera(d18:1/36:3**	**Cera(d18:1/36:4**	**PE(36:0)**	**PE(36:1)**	**PE(36:2)**	**PE(36:3)**	**PE(36:4)**	**PE(37:1)**	**PE(37:2)**	**PE(37:3)**	**PE(37:4)**	**PE(38:1)**	**PE(38:2)**	**PE(38:3)**	**PE(38:4)**	**PE(38:5)**
MCF 1a	98.652575	206.537	140.85345	48.7653	36.4851	13.2976	20.4217	166.7841	212.627	31.745125	3.1446	0	0	0	0	0	0	17.7394	131.205	45.1038
MCF 1b	126.589975	195.3919	112.02345	61.6206	42.0628	0	50.0864	172.7753	166.1469	27.930625	11.1011	0	0	0	0	0	0	18.3564	142.0092	45.2905
MCF 2a	101.511875	130.2307	92.54865	45.0971	38.2207	13.2183	21.7047	99.207	150.865	13.598125	10.4584	0	0	0	0	0	0	10.3725	129.447	32.9401
MCF 2b	82.509075	160.8635	103.45235	32.4416	35.8241	13.85	15.6791	116.4666	147.657	22.662525	14.5883	0	0	0	0	0	0	21.6689	103.7074	49.8171
MDA 1a	859.037725	682.381625	587.774125	131.685475	330.1628	68.1088	92.7305	1950.4137	1739.48638	316.5128	100.1346	39.7607	21.6263	52.6946	263.7801	88.9452	261.3421	628.7735	1389.2828	598.9177
MDA 1b	670.509025	900.557825	685.770825	141.615375	290.9964	92.9191	78.5529	1936.4614	1742.44688	307.1141	139.369	40.0271	75.8898	73.5999	246.8307	90.3866	195.3247	650.7291	1419.6198	585.6701
MDA 2a	670.915125	276.163125	241.339525	75.467975	269.9141	44.8946	21.2927	625.3731	763.168775	157.3699	110.7581	6.1802	19.8205	28.2776	116.2576	61.8869	40.9251	220.5463	483.4781	314.2935
MDA 2b	799.021925	303.782825	324.351225	89.449475	247.1674	68.7834	71.4571	1474.3678	1506.18848	284.9697	132.219	19.5296	26.1431	61.893	235.4069	59.0889	196.0431	469.4245	1250.2358	505.9327
Sample	**PE(38:6)**	**PE(39:0)**	**PE(40:4)**	**PE(40:5)**	**LPC(16:0)**	**LPC(17:0)**	**LPC(17:1)**	**LPC(18:0)**	**LPC(18:1)**	**LPC(20:0)**	**LPC(20:1)**	**LPC(20:2)**	**LPC(20:4)**	**LPC(20:5)**	**LPC(21:0)**	**LPC(22:1)**	**LPC(22:2)**	**LPC(22:5)**	**LPC(22:6)**	**PC(23:0)**
MCF 1a	12.265775	0	0	0	1796.46505	935564.421	112.991225	920.76055	784.792025	2.683875	6.889725	3.352525	15.354575	24.201425	8.55775	10.340475	63.01695	31.268825	13.969375	3.891875
MCF 1b	4.597775	0	0	0	1806.24895	924824.484	92.443225	1033.35635	126.176425	2.135075	4.277225	8.583325	49.021075	6.452425	15.91885	10.748575	63.08205	12.268425	41.958175	13.722875
MCF 2a	16.433975	0	0	0	1348.35025	958224.472	114.186525	630.93145	138.601525	0	7.323825	2.977925	1.122875	14.199925	5.80695	13.704475	47.91345	15.657625	10.536375	2.332875
MCF 2b	0	0	0	0	3262.9764	1199744.49	18.5099	3433.48208	1143.90488	34.704075	55.042875	5.829775	44.946575	2.26495	25.02715	18.1586	13.668475	38.164125	16.159425	4.40175
MDA 1a	101.355	90.1365	51.5561	226.8901	3262.9764	1199744.49	18.5099	3433.48208	1143.90488	34.704075	55.042875	5.829775	44.946575	2.26495	25.02715	18.1586	13.668475	38.164125	16.159425	4.40175
MDA 1b	117.7877	77.0406	70.8888	237.305	0	1146291.37	13.7729	3288.23778	1532.60508	22.332675	17.038675	19.133175	145.905275	9.93435	32.74855	24.5656	34.645375	21.221125	35.022325	5.79425
MDA 2a	59.1853	42.6929	25.8288	53.9861	2690.1259	1044314.58	0	2836.76498	1483.58348	26.861375	57.500575	12.223775	349.610675	7.91045	13.21445	16.5795	8.246175	66.815425	94.510025	18.79835
MDA 2b	104.053	86.0667	38.3012	175.083	2687.8157	997550.977	4.9206	2509.20498	1383.50848	8.969575	13.349475	14.869875	117.914075	12.69895	1.50235	15.1913	52.354775	14.827925	18.143425	2.46925

Table 8.8: Normalised peak area matrix for the supernatant from a tumorigenic and non- tumorigenic cell line for all lipid species

Sample	PC(23:1)	PC(24:0)	PC(25:1)	PC(26:0)	PC(27:0)	PC(27:1)	PC(28:5)	PC(28:6)	PC(30:0)	PC(30:1)	PC(30:2)	PC(31:0)	PC(31:1)	PC(31:2)	PC(31:3)	PC(32:0)	PC(32:1)	PC(32:2)	PC(32:3)	PC(33:0)
MCF 1a	6.5936	1716.8113	15.500675	73.929575	96.89835	25.15015	191.154125	3.70975	1170.12248	3117.01693	246.12745	12.68505	316.33585	537.96245	31.41595	2420.5938	3368.82573	408.592	249.548825	360.606675
MCF 1b	5.0736	1657.6044	61.881275	0	52.50385	7.21685	190.838025	0	1133.94598	3054.98363	294.71495	3.76135	282.22755	383.94875	80.69165	2329.2253	3394.47303	507.3596	279.367425	345.469175
MCF 2a	2.602	380.8713	62.722175	14.011375	51.55165	13.74395	287.817725	0	1146.06228	2853.57203	261.93665	0	583.97235	304.57075	33.57525	2252.7167	3061.67513	410.0936	259.891925	346.087175
MCF 2b	4.302775	134.613775	35.736675	291.25635	189.5398	35.145975	93.6593	64.67485	3581.5832	8291.39298	882.015325	120.445375	3737.45465	1595.2326	149.26225	8009.82983	15508.5913	2159.29433	404.28925	3611.91438
MDA 1a	4.302775	134.613775	35.736675	291.25635	189.5398	35.145975	93.6593	64.67485	3581.5832	8291.39298	882.015325	120.445375	3737.45465	1595.2326	149.26225	8009.82983	15508.5913	2159.29433	404.28925	3611.91438
MDA 1b	0.475075	258.821375	11.316075	262.74495	169.1179	49.580875	33.6904	69.68735	3104.9204	8307.51848	769.169725	46.604175	3430.31595	1661.0176	108.23145	8465.31483	15136.2621	1413.07793	396.51335	3091.99958
MDA 2a	1.173975	632.238075	13.551275	290.94745	136.4263	9.909875	20.9133	110.83115	2534.7464	6104.53308	738.927225	44.098975	3507.79245	1382.3745	89.75375	5892.83783	10823.5489	1283.90543	287.64715	2585.79048
MDA 2b	20.071775	319.819475	43.650375	15.31105	95.4809	31.322375	61.1955	0	2576.2991	6241.06508	725.379925	26.153775	2757.29065	1292.1564	136.88075	5813.74403	10674.8107	934.900025	272.31595	2445.12248
Sample	**PC(33:1)**	**PC(33:2)**	**PC(33:3)**	**PC(34:0)**	**PC(34:1)/IS**	**PC(34:2)**	**PC(34:3)**	**PC(34:4)**	**PC(35:0)**	**PC(35:1)**	**PC(35:2)**	**PC(35:3)**	**PC(35:4)**	**PC(36:0)**	**PC(36:1)**	**PC(36:2)**	**PC(36:3)**	**PC(36:4)**	**PC(36:5)**	**PC(37:1)**
MCF 1a	2084.5956	1322.0862	460.9526	1904.80113	14846.7231	6066.4744	475.31425	1250.9153	161.798875	1145.79378	1050.01448	473.002625	2475.746	686.033475	6276.00678	5602.58898	2285.23128	1792.46498	409.0063	185.761175
MCF 1b	1965.893	1333.1416	526.0024	984.891325	14384.0409	6340.7297	531.38975	1314.3324	246.337675	1074.79898	560.922875	404.586525	2216.3351	755.649575	5965.53018	5592.35158	2190.18858	1717.67868	400.6678	185.852575
MCF 2a	1893.4382	1326.9845	486.3834	1798.67233	13631.844	5526.6987	377.36735	1046.5522	200.844575	702.073275	415.597575	308.634825	2210.2589	550.721675	6146.94768	5401.25668	1930.68878	1824.13238	233.2771	234.428375
MCF 2b	8782.3423	3358.0995	1143.93855	10529.8207	57642.4378	17654.1453	1593.30348	276.164125	1203.0708	4550.21525	5267.73948	1698.26065	1100.05705	4007.0767	36496.5449	29064.8659	9753.4308	5605.19815	1337.8152	1012.11905
MDA 1a	8782.3423	3358.0995	1143.93855	10529.8207	57642.4378	17654.1453	1593.30348	276.164125	1203.0708	4550.21525	5267.73948	1698.26065	1100.05705	4007.0767	36496.5449	29064.8659	9753.4308	5605.19815	1337.8152	1012.11905
MDA 1b	8012.1734	3343.8702	970.01415	9285.35343	54186.0631	16135.1326	1600.56308	357.614525	1034.1174	7377.56035	4713.48588	1798.58965	1002.58265	3376.3882	34498.36	29923.7815	9513.2322	5269.16915	1038.0967	959.05365
MDA 2a	6279.8317	2640.305	900.40195	7930.17593	43124.327	13145.5449	1035.29868	197.675925	909.0254	5751.32335	3803.32498	1193.39735	911.12725	3178.0415	28686.0583	21901.5107	6877.0993	3784.29715	1036.3898	770.44635
MDA 2b	6109.7785	2507.7825	592.28195	7148.67503	40160.0527	12265.8966	972.751675	192.322825	845.0627	3598.23515	3857.89548	1362.06005	687.27595	2662.1038	25708.3103	20507.2773	6808.5192	3421.10885	812.2636	643.38455
Sample	**PC(37:2)**	**PC(37:3)**	**PC(37:4)**	**PC(37:5)**	**PC(37:6)**	**PC(38:0)**	**PC(38:1)**	**PC(38:2)**	**PC(38:3)**	**PC(38:4)**	**PC(38:5)**	**PC(38:6)**	**PC(39:0)**	**PC(39:1)**	**PC(39:2)**	**PC(39:3)**	**PC(39:4)**	**PC(39:5)**	**PC(40:0)**	**PC(40:1)**
MCF 1a	130.778725	62.4777	239.7207	475.852725	277.8177	43.241875	456.2076	861.594225	1410.78933	963.769925	1090.77925	691.03405	132.1326	36.2724	42.972	115.447375	28.220325	175.313475	518.4921	27.30105
MCF 1b	173.765025	116.6859	211.1315	355.315225	326.341	140.983975	423.9446	811.476325	1260.10683	956.746925	1120.26745	679.03355	220.394	60.5477	58.7659	31.778875	60.372225	126.173375	483.0669	35.66635
MCF 2a	150.789125	170.785	217.1148	305.687825	303.9829	77.381175	429.2986	672.332425	1349.05033	1008.50493	1111.58245	585.53465	181.7006	37.5145	21.7184	107.426775	47.634525	250.939475	517.3775	24.18615
MCF 2b	1103.64628	970.49635	2915.75985	2810.09013	1611.0926	472.01	3563.72478	4833.64383	7527.08848	4888.94823	5440.86063	2594.47235	1318.0094	199.65175	280.24205	456.021875	332.028275	1097.3211	661.373225	278.50235
MDA 1a	1103.64628	970.49635	2915.75985	2810.09013	1611.0926	472.01	3563.72478	4833.64383	7527.08848	4888.94823	5440.86063	2594.47235	1318.0094	199.65175	280.24205	456.021875	332.028275	1097.3211	661.373225	278.50235
MDA 1b	1143.31968	880.42755	1993.15435	2920.21173	1758.6662	435.2964	3112.92758	4840.80163	7162.42778	4898.41603	5266.52943	2408.35185	1357.2066	230.14255	283.76355	242.783675	409.208475	962.2072	537.808825	176.57835
MDA 2a	840.404875	1149.49905	2082.19845	2295.97173	1216.4685	374.7949	2726.77068	3202.22663	5286.13698	3675.35013	4051.39923	1923.72355	1072.4293	340.00935	380.37045	355.801175	305.974675	622.1726	608.366825	213.50255
MDA 2b	879.151575	1020.69025	1724.27965	2041.34843	1145.5938	353.4514	2350.24918	3028.50303	5052.56878	3478.11203	3783.71653	1718.11685	864.4025	144.10915	196.98355	129.830375	320.294175	637.9849	714.346925	196.85595
Sample	**PC(40:2)**	**PC(40:3)**	**PC(40:4)**	**PC(40:5)**	**PC(40:6)**	**PC(41:0)**	**PC(41:1)**	**PC(41:2)**	**PC(41:3)**	**PC(41:5)**	**PC(41:6)**	**PC(42:0)**	**PC(42:1)**	**PC(42:2)**	**PC(42:3)**	**PC(42:4)**	**PC(42:5)**	**PC(42:6)**	**PC(43:0)**	**PC(43:1)**
MCF 1a	19.681375	17.059775	152.34925	460.61835	492.60835	25.575	27.8804	14.4685	7.78085	27.996475	43.030775	3.07095	11.602925	24.21	46.04175	13.5245	30.975375	10.1256	11.6077	8.589175
MCF 1b	20.300275	55.086275	111.98645	511.37345	532.51925	44.8618	6.1321	23.8201	11.47885	24.504075	28.887375	10.62865	4.281325	10.6081	46.83565	10.1208	8.519375	19.0485	11.3851	11.840175
MCF 2a	62.205275	55.808575	197.87175	386.86925	306.29345	48.9786	0	14.4147	1.28505	25.561275	25.299075	16.49165	11.507125	24.7909	46.17195	3.4529	7.496275	9.5467	8.7632	39.658075
MCF 2b	321.589025	350.6757	1021.7374	2083.08013	2567.2239	131.050625	124.400225	114.7026	106.053125	33.06115	125.038325	39.637	124.2024	121.188075	61.726825	89.973825	181.901475	196.29025	68.2869	5.915325
MDA 1a	321.589025	350.6757	1021.7374	2083.08013	2567.2239	131.050625	124.400225	114.7026	106.053125	33.06115	125.038325	39.637	124.2024	121.188075	61.726825	89.973825	181.901475	196.29025	68.2869	5.915325
MDA 1b	302.937625	341.7723	1061.0008	1941.75703	2330.0448	144.971525	62.240525	61.8607	43.778825	44.19485	119.919125	36.8583	129.9632	97.255275	59.801525	90.176025	162.139575	195.33845	40.0487	13.963925
MDA 2a	265.046125	278.4275	715.4179	1567.97003	1894.0821	134.864525	142.332025	105.4142	73.708025	91.15395	47.801725	9.4489	95.9478	68.062375	57.415725	83.867825	121.228075	112.41345	30.8775	22.399025
MDA 2b	301.795825	252.1082	840.9875	1372.97683	1859.7294	74.410125	69.583525	119.3951	80.753725	40.98985	29.767025	20.6364	111.1397	81.349775	51.167725	74.979525	96.552575	109.01495	7.5736	25.266725
Sample	**PC(43:2)**	**PC(43:3)**	**PC(43:4)**	**PC(43:5)**	**PC(43:6)**	**SM(30:0)**	**SM(30:1)**	**SM(30:2)**	**SM(32:0)**	**SM(32:1)**	**SM(33:0)**	**SM(33:1)**	**SM(34:0)**	**SM(34:1)**	**SM(34:2)**					
MCF 1a	166.7526	1770.55135	11.7545	33.876375	20.568125	32.5522	5.63355	7.47935	414.530125	10.073	1230.14225	1230.14225	935.2678	7617.1629	850.43655					
MCF 1b	191.4711	1905.63945	15.1273	25.963675	15.660725	32.0552	13.94035	6.72555	414.534325	39.6896	951.87645	951.87645	875.8144	7674.3558	796.64465					
MCF 2a	67.5766	1838.30085	6.4753	7.441775	8.240725	29.3347	14.32255	2.59725	416.896525	46.2923	1018.21115	1018.21115	1016.8171	7273.7522	759.39135					
MCF 2b	35.683075	663.928425	20.70395	6.417075	6.980525	35.0771	17.60525	13.293125	907.93275	45.714475	2550.1244	2550.1244	2927.07925	20502.5757	2191.29883					
MDA 1a	35.683075	663.928425	20.70395	6.417075	6.980525	35.0771	17.60525	13.293125	907.93275	45.714475	2550.1244	2550.1244	2927.07925	20502.5757	2191.29883					
MDA 1b	88.113575	633.204725	15.59865	5.740175	19.857425	18.1053	8.92645	11.175225	802.28375	78.466875	2488.882	2488.882	2606.66985	19504.1263	2062.17993					
MDA 2a	69.584275	648.900225	17.60825	11.348375	17.347925	24.1155	8.56345	5.469125	644.39165	48.473075	1886.7867	1886.7867	1967.43235	14961.2159	1592.20803					
MDA 2b	42.836875	613.362125	5.81335	21.093775	14.614725	47.3943	26.49395	7.127025	633.58015	60.791275	1867.1455	1867.1455	1777.90495	14136.1964	1588.02423					

8.3. From Chapter 4

8.3.1. Raw peak area data

Table 8.9: Raw peak area data matrix for cholesterol ester for hair samples taken from breast cancer free controls.

	CE	CE(13:6)	CE(15:0)	CE(15:1)	CE(17:0)	CE(17:1)	CE(17:2)	CE(18:0)	CE(18:2)	CE(18:3)	CE(19:1)	CE(19:2)	CE(19:3)	CE(19:4)	CE(19:6)	CE(21:0)	CE(21:1)	CE(21:4)	CE(21:5)	CE(22:0)	CE(23:5)	CE(23:6)
C21	257.0421	74.8519	137.718	119.1618	722.4785	1301.2529	98.1475	38.0860249	2794.1527	4676.6202	6958.666	1125.6219	249.6718	84.8437	79.5585	346.4927	105.6817	86.5931	5751.9319	229.4829	73.2139	231.2659
C22	215.8046	137.0342	331.4373	285.6379	1416.2775	3509.3076	135.4615	18.320137	1454.9079	1436.5769	2634.1355	2700.7725	492.8207	146.6245	143.6404	467.747	633.4115	45.8362	2186.9142	7426.7029	66.1474	70.5345
C23	197.7216	96.2905	721.8072	338.4917	3778.3059	6508.607	121.2076	60.4811348	1546.2671	1962.3963	1786.7135	4928.4721	631.6252	128.1413	200.3625	498.0012	416.2649	23.4994	1623.8878	163.7891	131.9273	133.6908
C24	430.2671	38.4803	544.1625	407.4344	1882.153	5084.9552	301.2796	16.5254165	1787.3206	2511.5886	3947.3358	3093.1373	793.1078	112.1579	226.5397	455.6222	251.7028	63.0955	3226.8156	206.1384	69.9239	222.4406
C25	144.753	91.6534	51.6958	118.3357	121.7009	904.3873	81.6588	19.3767189	572.5244	177.1742	4715.4595	548.0723	238.3474	76.1919	130.5764	401.3366	296.6295	63.5228	3526.5232	274.4699	104.7804	53.9421
C26	199.2161	43.9369	525.5039	474.5933	1579.8861	4970.0824	44.1344	15.178179	1421.002	1536.9905	4151.194	2736.9084	852.6772	120.2761	175.722	428.5491	311.2926	69.1456	3164.3854	109.1014	119.3429	115.6971
C27	167.9828	152.6128	384.9252	374.1354	1356.8652	3508.5394	115.0772	8.04435948	2188.9129	680.673	5516.9738	1754.2372	511.2974	208.38	278.8193	866.0156	329.4001	106.0888	4617.8347	174.7121	270.6681	153.5056
C28	615.3619	350.1026	342.0748	198.3519	843.8313	1540.9223	242.6858	23.8167592	3414.3909	5904.4915	2580.2735	5934.077	451.472	130.8806	137.4229	516.6062	323.3887	41.096	1795.3764	76.8649	132.2406	358.7013
C29	329.0725	57.5106	521.127	368.031	1875.1512	4233.66	255.9988	9.04003255	2159.3719	3355.0778	5612.7437	3425.2867	669.6686	109.052	146.3236	455.3482	498.8119	85.9962	4641.6273	242.5603	131.7053	154.5255
C30	249.4323	113.8829	321.5883	386.5567	1234.3512	3751.5324	26.0082	18.7884902	465.4855	178.0724	2129.8125	2010.215	242.2418	71.2005	151.4956	374.4057	313.6591	25.0201	1591.3692	124.1588	165.4826	25.4035
C31	301.1716	155.2541	755.0965	518.9592	2318.7711	5455.2462	173.1646	15.9289973	1647.2162	2562.9323	13729.3002	4933.5453	858.9662	178.2419	235.3247	529.7471	373.5867	173.5014	10921.9455	513.4047	121.306	161.9275
C32	1918.5849	167.3864	495.6938	388.5917	1513.9823	4428.1098	108.1618	18.2590157	927.2812	908.0766	3295.6372	3172.1862	550.1501	103.5469	204.7683	379.2145	84.9077	38.9075	2315.8224	72.1578	100.9562	70.7227
C33	801.0234	105.6201	142.6089	411.9617	498.5049	2725.9412	98.6561	17.1927473	1346.7405	1043.1321	2959.4281	1664.2425	481.221	91.182	156.0429	470.6745	196.907	26.6828	2476.6436	150.9398	49.8577	47.2242
C34	235.6597	72.3661	177.0823	288.3356	569.4028	2367.5526	141.7882	23.2497774	1367.9897	1839.4173	1503.9844	1978.1069	703.8229	102.5245	219.1262	339.6793	380.405	35.1688	1341.897	760.9463	93.347	67.3529
C35	242.2933	113.4358	562.344	503.0272	1643.4873	6276.0126	235.6261	31.0677675	1949.565	3150.1191	3401.7728	3952.002	751.6048	146.1271	167.7672	544.7925	360.9013	73.9633	2929.1039	123.8436	224.1081	127.5938
C36	907.9365	107.5125	703.2469	391.9225	2453.59	6280.8675	195.2177	15.3402309	3087.6492	4517.9295	4711.9402	6548.7304	758.1125	200.1911	196.9606	748.7818	344.1939	82.0152	3614.0293	110.165	297.8217	172.1369
C37	182.1196	26.8501	180.8938	148.751	381.7859	1310.9786	261.5027	10.5812913	1480.7364	2249.3912	1759.1916	1219.1063	205.3209	66.9471	51.6694	169.8546	491.5719	25.5415	1530.1682	81.2	69.0379	160.367
C38	297.7431	134.2905	137.3809	184.3801	315.1338	1321.4917	177.5448	18.3306012	2424.287	3848.039	6628.9995	1473.5342	337.2746	101.4297	204.6216	420.2669	458.9457	80.9166	4899.1989	250.0052	151.9881	152.7143
C39	257.669	85.9868	586.0921	355.605	1775.945	3300.5069	365.8022	18.2912845	2117.5579	3161.097	3575.3835	2717.5775	405.6905	72.8425	146.475	377.8619	368.5223	24.8622	2872.2732	166.5327	102.5313	195.3027
C40	1220.2168	160.4352	478.967	288.0656	1537.3242	3544.781	86.9625	11.2482532	1864.1141	414.0464	2889.3127	1525.4104	435.9343	171.302	241.0435	545.4815	81.2743	46.7995	2412.8878	90.5205	328.4826	86.2932

Table 8.10: Raw peak area data matrix for cholesterol ester for hair samples taken from patients with breast cancer.

	CE	CE(13:6)	CE(15:0)	CE(15:1)	CE(17:0)	CE(17:1)	CE(17:2)	CE(18:0)	CE(18:2)	CE(18:3)	CE(19:1)	CE(19:2)	CE(19:3)	CE(19:4)	CE(19:6)	CE(21:0)	CE(21:1)	CE(21:4)	CE(21:5)	CE(22:0)	CE(23:5)	CE(23:6)
P19	300.3408	80.6257	176.8086	128.6699	1601.2214	1948.6452	415.005	44.8268842	3614.3298	5415.7397	6736.9989	1771.6007	706.4376	146.5886	94.1163	2243.7647	596.8317	91.1072	5347.9134	255.1369	172.8136	661.4366
P20	629.4321	48.2313	427.8242	296.0816	1068.5414	3603.1236	172.33	9.9552508	1289.959	1926.8945	7181.0076	2155.4398	344.5362	56.9895	112.76	380.5028	251.0019	116.8599	5548.0505	186.1032	100.5324	65.8269
P21	146.1884	146.4286	264.1932	242.0897	486.1578	2403.7143	107.7707	37.1585422	1414.5495	993.8785	2290.8028	1372.8165	383.1421	105.4025	187.3581	726.3151	136.849	40.6225	1731.3569	70.1428	228.6398	72.6484
P22	222.8439	46.9379	125.2591	173.0923	426.1094	1072.404	176.9963	14.4770157	2096.6859	2895.4161	2406.0644	911.2075	355.1422	75.3428	138.3327	386.1046	264.1791	47.3956	2123.3449	87.9368	79.2244	214.0802
P23	633.7265	183.9819	317.9366	216.4312	1065.1795	1833.9403	259.0713	14.9614646	943.7548	958.1437	1339.6273	1763.5682	286.5276	79.8944	174.1181	462.2277	187.2766	27.4781	1073.2849	544.0545	144.0271	53.3903
P24	198.0685	83.938	85.0096	36.5182	757.2195	675.1651	153.7806	20.0469164	3025.7808	4804.9733	4904.7647	875.9643	270.2881	75.4742	69.4592	526.8068	230.5246	81.4625	4027.1791	82.2864	117.2805	224.2255
P25	220.5334	244.4121	749.7459	357.3746	2375.1428	3859.9836	260.0083	9.2176822	2040.9708	2611.171	2338.1661	2802.5474	684.2371	124.6282	187.779	633.5702	443.3463	26.0489	1798.283	131.3532	145.9736	101.3037
P26	443.7938	76.5987	291.2199	126.2766	975.699	2345.2524	129.9119	27.4522775	1464.1916	2232.8281	2955.4373	6897.5195	1116.9536	170.9049	97.1217	514.1772	299.953	57.2157	2253.8222	91.5972	148.8119	32.2869
P27	298.5606	73.9625	483.4954	263.7012	2289.4512	3140.1596	248.9136	10.3705651	2861.9346	4675.1629	8043.2625	3077.4299	405.7114	103.6374	122.1437	505.6825	487.5718	103.9861	6191.9231	267.5322	102.6005	297.0865
P29	539.1203	551.1659	538.0596	241.6728	1637.8509	2711.6588	92.4865	18.4601067	1670.3168	2015.0073	2368.4376	2250.3397	433.1318	103.8964	176.2686	501.0417	279.4707	30.2718	1938.7439	59.9768	159.5628	163.3213
P30	264.0752	113.5724	352.8917	188.8217	2306.9345	2497.4085	445.8624	24.6531242	4193.5965	6795.826	5497.3379	2919.1769	809.0649	122.782	97.2231	1426.295	309.1223	66.147	4105.7787	152.5958	159.7514	817.3574
P31	1230.6264	89.6804	261.5493	226.0714	897.5081	3137.3256	74.154	12.3610658	1175.659	1084.8095	2562.2495	1615.6299	390.4895	82.4233	203.2821	580.4521	147.8288	25.6076	2114.7712	56.67	86.9355	93.4015
P32	330.1352	17.188	436.8612	217.7531	1126.2419	2271.4096	41.6698	29.1308967	2603.8562	4688.3229	13591.1273	1725.4256	283.4634	68.3118	53.5001	356.4153	61.9964	190.5703	11656.8654	510.6709	42.9131	475.8308
P33	1209.1226	98.6421	398.1174	216.5804	2082.9983	2791.7974	213.6809	45.227352	2673.6646	4066.8691	7289.8247	2182.8894	365.8245	100.405	142.5758	494.1037	374.4042	103.1069	5703.7472	204.9056	37.0771	86.4863
P35	364.4684	368.0522	84.2235	77.2074	163.8662	776.0348	137.1464	5.06054928	1262.154	1581.0499	4127.9392	679.2234	209.6844	151.2314	94.3711	325.1728	187.7108	73.1503	3409.2467	134.9198	70.19	155.6878
P37	198.039	43.3397	553.1832	493.6154	2231.7846	5290.2617	47.1572	10.1889771	1431.2421	1627.8652	704.7263	3106.3986	709.1615	95.7593	173.936	463.1791	426.5292	12.6008	592.1871	130.4988	55.0493	122.4259
P38	505.4743	25.9629	244.9621	154.4597	1429.5763	2355.1208	178.2785	9.05573248	2624.638	3726.1439	9871.021	1357.5516	384.7368	106.0651	127.8695	393.7662	218.3292	113.4717	8043.8459	332.0015	95.5745	117.1538
P39	790.4089	45.7626	142.2823	151.9092	301.9498	1909.0231	227.0749	24.420315	975.1473	920.0099	2931.0401	816.8901	292.2437	73.2973	105.8313	357.1332	187.8137	34.7011	2313.8519	51.4043	92.8912	59.3503
P40	228.5056	133.2663	497.4597	339.0749	1524.8824	4561.1102	289.5453	34.3149942	2633.019	4015.8546	7126.1969	3021.356	752.1538	113.5495	131.3615	1015.4509	343.324	151.7674	6107.1397	250.9653	83.9173	372.6144
P41	284.1408	127.3775	157.5559	216.4355	303.8169	1448.0545	366.6147	4.9410572	950.3805	733.5189	3187.2716	917.603	295.2778	62.9565	179.5459	587.7581	442.2438	29.0802	2702.717	117.4753	87.7998	42.4806

Table 8.11: Raw peak area data matrix for ceramide for hair samples taken from breast cancer free controls.

	Cer(d18:1/22:0)	Cer(d18:1/24:0)	Cer(d18:1/24:1)	Cer(d18:1/25:0)	Cer(d18:1/32:3)	Cer(d18:1/38:3)	Cer(d18:1/39:3)	Cer(d18:1/40:3)	Cer(d18:1/40:4)	Cer(d18:1/41:2)	Cer(d18:1/41:3)	Cer(d18:1/41:4)	Cer(d18:1/42:6)	Cer(d18:1/44:5)	Cer(d18:1/44:6)
C21	5858.6366	26284.2027	21113.4597	1266.6011	963.8077	319.931	94.9373	1213.0086	977.1918	234.3133	46.5936	32.4672	346.1069	242.4089	1668.2448
C22	1400.13	5750.9044	2567.7554	935.5095	100.1635	57.8125	103.7214	108.8166	71.1923	17.6799	59.8174	46.8058	286.0855	66.5917	1523.5189
C23	2815.8917	10371.6142	6332.5257	1172.4181	163.8766	53.6149	263.9595	293.5062	94.9387	55.0318	154.0013	81.6503	1250.3559	2689.6656	3751.6889
C24	4687.7865	15524.1851	15690.7871	881.1773	358.7286	225.7232	95.9092	750.9844	446.6341	301.8278	54.2958	44.1321	187.1744	113.432	826.3881
C25	281.1168	1457.7605	373.3214	331.3483	387.4089	87.332	88.5654	243.1216	438.9556	35.8166	56.2401	27.552	171.163	241.8508	817.5556
C26	2177.2357	8274.1942	4123.9355	745.958	118.7011	37.2753	308.7417	126.1078	55.1112	41.2115	205.4335	124.1034	110.6051	135.1607	596.375
C27	865.8118	3252.9343	2031.8884	319.5264	317.3258	126.4179	88.5845	237.7465	295.2685	36.9265	80.4416	58.4444	240.4152	200.2172	1122.2562
C28	5761.9205	19629.1372	19797.0137	912.9981	429.4806	225.5863	87.6784	1035.6926	571.2244	124.5047	63.362	51.2076	799.5452	86.1065	1834.4124
C29	3840.577	11880.4187	10059.9012	634.9402	124.3672	119.5288	73.9976	426.4536	142.2475	144.2343	54.749	55.8603	123.3248	286.9151	527.5015
C30	542.8931	2203.5674	730.9406	588.9843	88.7831	45.5494	118.476	96.7147	76.5358	70.4848	78.6942	58.9706	163.1882	123.8029	676.5117
C31	3183.2175	13220.6928	7799.9262	1252.952	545.7396	190.925	420.188	699.6011	262.1967	383.1329	261.9896	95.361	332.1817	121.6379	1783.2037
C32	1171.0627	5078.3075	2914.0478	730.99	69.1097	39.9058	218.6704	156.6192	58.9231	33.1026	125.292	65.2401	436.5718	88.2391	1250.7173
C33	592.3085	2669.1142	1336.3795	422.8134	151.5522	32.4059	132.8344	133.1767	98.3472	45.8305	92.8899	59.2102	379.1991	207.6263	787.8076
C34	1710.894	7198.9495	5823.8924	668.727	474.7383	160.5082	104.413	417.9736	282.057	56.0575	77.2402	58.7678	695.6963	284.3543	2214.9704
C35	3478.377	13745.2645	8992.5722	1587.3089	667.3349	211.3915	394.0131	934.7541	618.186	59.2739	249.8524	112.739	841.3988	110.9523	4954.8353
C36	5113.1445	18427.2759	12473.9529	1786.2876	399.3767	105.7698	319.7328	580.9954	293.6574	141.6512	255.3083	99.2593	1391.6827	309.4393	3459.3526
C37	2772.3441	9966.6381	9757.9461	553.0235	716.3939	269.587	31.7954	912.2118	569.4738	212.1368	34.2002	66.6656	846.04	403.8872	3507.8252
C38	4785.9401	17952.2953	10724.1068	1340.6548	490.5153	208.4625	135.0512	802.3318	432.436	312.4666	91.736	60.1112	527.6514	1224.4292	2084.2917
C39	3364.8627	12506.0705	11033.5267	752.511	151.8303	106.2589	64.1334	524.35	208.2334	77.2278	47.7538	64.851	211.3053	2952.6242	490.4716
C40	479.3776	1617.9093	1186.412	213.2789	89.1669	28.1128	120.4729	77.1246	80.0394	15.7801	30.7018	32.1413	363.5593	144.8312	981.4646

Table 8.12: Raw peak area data matrix for ceramide for hair samples taken from patients with breast cancer.

	Cer(d18:1/22:0)	Cer(d18:1/24:0)	Cer(d18:1/24:1)	Cer(d18:1/25:0)	Cer(d18:1/32:3)	Cer(d18:1/38:3)	Cer(d18:1/39:3)	Cer(d18:1/40:3)	Cer(d18:1/40:4)	Cer(d18:1/41:2)	Cer(d18:1/41:3)	Cer(d18:1/41:4)	Cer(d18:1/42:6)	Cer(d18:1/44:5)	Cer(d18:1/44:6)
P19	7411.4152	28288.3278	22826.4621	1212.6095	394.5337	272.5788	108.7107	1165.4833	365.6139	277.2954	19.9592	75.3053	237.2863	178.6653	878.0551
P20	3676.0814	13147.9805	10550.5131	693.8378	264.0245	174.8468	71.0706	664.4183	372.2818	293.5565	64.2868	83.9815	263.7908	81.4726	1218.5977
P21	1131.9425	4501.9876	3439.0657	350.8156	127.2673	71.4163	84.6435	164.7189	64.5102	51.0592	50.9264	44.656	45.8085	74.9059	211.6207
P22	2454.0535	9017.2073	7065.2126	496.2285	170.4492	115.9314	70.6846	347.517	118.3647	106.8901	40.7782	50.9523	52.2073	245.611	290.5892
P23	1840.7046	6664.8529	5921.3536	644.7718	406.2187	144.4736	138.5502	442.195	271.4591	49.6803	93.2246	40.8135	687.235	123.3671	3191.956
P24	4732.6208	18464.0109	14694.4997	748.07	481.2511	239.1546	85.2966	1009.3481	492.8546	205.8107	32.378	36.6334	392.0822	139.4872	2407.5377
P25	4030.4083	13867.3283	13887.9868	580.7276	357.8607	224.6485	125.2141	811.9179	499.116	197.3836	70.7169	56.4054	804.6569	118.7568	3001.919
P26	2985.6649	11248.2364	9997.0446	682.4523	451.1056	120.1666	259.3247	541.1217	339.8681	99.1556	184.1664	72.5258	968.2985	500.6304	3838.4678
P27	7192.2167	25666.1814	24839.0114	1333.3468	449.7285	272.3104	132.5534	1127.0193	613.7635	70.1333	94.9265	93.275	1289.5475	104.6623	3472.5742
P29	1033.9513	4209.8631	2926.6123	368.7979	94.308	77.7687	19.122	264.4031	112.0219	47.6738	48.7799	36.5686	71.1626	933.4408	296.0219
P30	5904.4379	24824.3751	18003.6475	1200.7689	367.0318	294.1552	86.6108	1175.8313	344.6106	114.5686	41.9164	53.7593	50.2869	208.1664	1524.2481
P31	922.4842	3789.3332	2440.1656	381.8249	200.7308	92.873	149.3239	217.9157	148.7455	61.7259	81.1301	56.468	352.5794	513.5953	1271.3535
P32	4552.8897	19246.5015	15724.7021	709.2635	517.6644	228.2043	82.0196	1122.8217	631.5793	178.2333	33.6157	24.0532	443.0619	122.2494	1751.9878
P33	4084.8913	15415.5788	12351.0527	889.0861	214.2975	98.7518	102.8895	468.8925	171.3795	82.9676	92.2905	50.8413	634.8686	92.2825	1820.391
P35	1774.7065	6904.3202	4840.4399	368.3911	335.7033	151.7658	48.2038	494.3644	207.9504	87.6819	35.7367	20.4298	139.5673	5276.8596	841.1683
P37	1742.9166	6863.9514	4372.9877	803.204	113.9406	37.2332	155.6554	149.7675	57.6935	17.4371	118.941	54.5097	31.3781	173.8542	223.1868
P38	4152.7539	13339.3377	12901.88	645.3186	641.1761	168.5741	131.9932	695.7339	464.8721	123.4008	76.035	191.3363	979.7521	117.5908	4188.7866
P39	1100.4537	4629.1138	2088.3586	472.2649	428.127	115.2464	136.3754	486.8971	258.3956	57.2573	59.3275	32.4108	706.4829	228.6442	2985.1645
P40	3866.7254	14606.3874	9446.8259	795.7212	206.6992	168.857	89.7243	724.5909	221.8667	115.1627	83.1337	41.842	186.7091	1039.7445	593.8187
P41	717.4921	3195.9397	1759.5442	581.7666	146.4099	66.7313	128.3407	119.7459	184.4826	47.7377	96.0674	55.0738	133.5101	148.0564	528.2348

Table 8.13: Raw peak area data matrix for phosphatidic acid for hair samples taken from breast cancer free controls.

	PA-1	PA-2	PA-3	PA-4	PA-5	PA-6	PA-7	PA-9	PA(27:4)	PA(27:5)
C21	58.964	67.7757	103.3582	46.8907	55.9604	40.5934	303.5808	87.3458	211.0858	40.3974
C22	73.3717	47.1461	76.2728	162.8145	56.3697	49.903	247.6316	93.397	286.0294	63.4709
C23	13.7739	26.2419	137.0375	256.1002	57.071	66.493	245.958	75.2164	120.7417	28.7498
C24	174.4108	205.1689	295.0034	157.9509	54.3508	89.1007	1072.8978	71.2455	217.5858	60.4357
C25	71.4021	845.6658	71.9843	291.2897	124.4608	123.0168	180.1775	23.2947	106.6222	60.4102
C26	49.0841	50.9642	237.1948	41.2685	36.5958	65.527	261.2302	157.7114	304.3751	71.0275
C27	206.465	63.9324	85.8474	108.9835	48.5813	90.6228	80.923	56.9281	215.1373	112.7652
C28	84.8732	99.9526	276.5627	222.2048	69.2226	71.8679	328.3016	123.4027	165.753	48.4752
C29	115.659	47.5231	130.5744	122.2305	48.6757	60.5423	103.9798	89.4288	98.8186	97.8543
C30	173.7929	53.4686	39.0128	227.2176	42.6814	22.5488	97.2699	108.9875	168.9365	102.0865
C31	27.1348	36.2419	95.2022	56.9112	58.0584	48.5444	778.8422	57.4043	146.1444	67.646
C32	130.8987	49.0993	89.2288	98.1289	97.1212	170.9687	1424.0087	99.0304	668.841	56.4791
C33	69.7367	281.5192	70.8696	841.3537	151.4408	98.6686	205.0895	110.9669	159.809	69.2734
C34	159.2396	156.1965	125.736	213.3829	41.7592	80.0198	366.102	36.8949	472.5043	82.3004
C35	51.5894	43.7363	187.7678	41.2489	34.3948	42.3341	1862.9017	30.8458	337.8506	63.9365
C36	54.3811	344.1058	200.0519	56.9505	73.0185	281.8401	1361.6742	76.3607	540.9756	40.1383
C37	52.0623	40.113	93.6527	211.5943	54.5537	78.9636	1050.3236	56.4537	161.1019	50.7939
C38	82.9229	106.038	77.026	93.718	37.6792	49.0134	978.4331	86.7601	429.8294	64.5733
C39	103.1254	193.0472	56.0808	130.7288	65.1353	109.4102	1526.3456	49.8096	282.2743	33.1644
C40	40.6163	101.4345	164.3741	166.333	46.3573	71.2634	96.5167	129.0991	170.0772	157.7784

Table 8.14: Raw peak area data matrix for phosphatidic acid for hair samples taken from patients with breast cancer.

	PA-1	PA-2	PA-3	PA-4	PA-5	PA-6	PA-7	PA-9	PA(27:4)	PA(27:5)
P19	100.2566	71.1659	79.3161	54.9722	58.9074	91.3088	597.6637	102.6171	280.9846	43.4184
P20	54.1683	248.8944	91.4713	207.3805	49.694	119.9714	1385.7051	50.7529	798.3757	46.6633
P21	80.5047	77.401	6.555	155.9466	48.0996	63.1752	203.2213	108.1783	438.5439	122.0705
P22	94.8606	55.6891	172.6902	105.0432	54.7365	86.6142	1467.7883	55.4589	286.0329	53.1689
P23	49.4844	69.5993	9.85	166.3767	53.4456	36.9489	229.1149	28.3433	208.1556	42.5018
P24	38.312	50.784	26.3489	65.9033	56.8071	52.4734	164.199	48.1414	365.2902	44.4053
P25	69.7899	52.4739	246.2921	118.0078	52.77	244.302	140.0439	90.7479	645.4316	50.8346
P26	107.1907	49.5676	91.7873	112.11	115.705	78.3239	121.6912	74.3066	352.3578	77.1783
P27	NA	124.7612	104.1873	113.0197	123.855	119.1788	180.4333	101.0278	355.1801	127.1269
P29	NA	2122.3709	184.4705	966.1029	339.6119	62.1849	1066.2062	45.2722	446.6131	70.6261
P30	87.915	36.1984	87.6593	86.2754	91.4363	59.9494	204.4009	95.8682	628.3076	34.5854
P31	144.7384	70.2635	82.3138	107.6726	56.6973	86.1982	263.3798	69.1803	405.0755	110.6985
P32	35.6183	42.4846	120.8176	75.141	74.9781	116.3186	220.4681	73.5384	657.1216	92.6883
P33	71.4459	35.6216	70.5575	229.5398	67.8463	56.7006	450.6548	73.1697	302.0273	134.7772
P35	67.1718	40.0392	82.7556	67.6678	39.2732	37.4961	416.35	68.7637	295.5733	100.4327
P37	66.7167	45.0931	81.9209	47.707	48.3366	41.6378	178.0806	46.957	65.064	77.3607
P38	77.8752	1100.226	53.4386	69.3608	47.553	66.1249	158.4499	68.8765	271.65	41.7103
P39	114.0024	360.1378	207.0376	363.3872	92.8	45.5266	2107.3062	61.0377	160.5224	30.7792
P40	69.9496	108.8663	100.8891	113.5044	57.4552	101.9863	932.8435	NA	299.9678	30.4676
P41	60.4165	72.9061	88.4981	357.163	126.0381	74.6094	936.3808	72.6886	53.9775	115.1474

Table 8.15: Raw peak area data matrix for lyso-phosphatidylcholine for hair samples taken from breast cancer free controls.

	LPC(16:0)	LPC(17:0)	LPC(17:1)	LPC(17:2)	LPC(18:0)	LPC(18:1)	LPC(18:2)	LPC(18:3)	LPC(20:0)	LPC(20:1)	LPC(20:2)	LPC(20:3)	LPC(20:4)	LPC(20:5)	LPC(22:0)	LPC(22:1)	LPC(22:2)	LPC(22:4)	LPC(22:5)	LPC(22:6)	LPC(21:0)
C21	11702.9271	2455.56047	346.020697	54.7580445	189.954104	4668.62592	3539.97232	51.013085	1242.6028	315.60312	41.6909625	348.904785	211.154393	10.0457097	347.731138	134.174702	20.5876939	16.8803394	13.2413742	184.781807	4101.91647
C22	5756.77861	1906.42341	243.415951	35.3635681	1938.30632	4767.53385	480.051661	38.4218568	1191.49025	331.692903	53.6910306	360.109445	256.542072	28.931177	219.151995	120.227907	1.96268994	NA	4.01489456	133.850989	2913.30115
C23	29621.2065	12115.1546	1247.02925	NA	18981.5281	25948.9193	2152.67067	34.7529672	1899.00569	338.386245	208.534632	1206.48865	515.46546	26.2718883	502.464507	123.83514	5.81911743	NA	7.82058738	183.964046	5210.37097
C24	12954.6678	5389.14364	745.887197	295.834529	389.939188	8816.85734	1508.24668	47.915765	1633.36399	262.818398	96.0933715	742.941824	243.004688	38.5372939	550.944971	148.280869	8.73329041	15.8281112	9.433444	250.704406	5245.20755
C25	3605.14245	819.069611	198.761253	NA	140.974346	3251.49595	472.582813	34.7739226	542.265701	90.7421298	47.0335218	137.45017	90.4072234	26.9342275	101.010542	51.6505543	7.05801489	2.47144647	9.73183561	35.532202	778.77765
C26	4658.42975	2497.14442	313.060323	NA	243.865854	4371.63307	442.915413	59.7929841	617.957075	106.21226	36.4767265	349.581238	139.287474	24.7970253	79.5824481	43.9453312	13.7254196	12.4705798	19.0904336	40.4086647	1096.66935
C27	7836.49046	3575.76766	326.87139	49.7636069	197.541734	7395.74357	3799.62093	68.1534588	1465.99512	134.797261	40.1505595	272.127296	144.963989	54.4942429	377.269288	106.119755	NA	36.2709177	7.39874309	162.654911	3469.21867
C28	57113.8969	29194.7309	2056.04087	670.452933	43009.7811	45059.5578	2053.48248	53.3243199	10974.2897	1989.05027	226.409603	1186.76894	340.192307	11.0200614	1720.41698	646.62557	NA	19.5335646	11.4167072	990.174724	25121.6391
C29	34060.8675	9579.12431	687.028413	37.5497575	3924.36218	18550.2914	1331.20714	27.2037948	2644.93608	849.757001	133.761352	686.799918	310.878214	6.02719739	594.124766	210.100181	8.91292178	10.6725679	15.0366803	309.700519	6996.95828
C30	3857.74841	1860.56576	288.495106	55.8274131	1260.07458	4478.5822	563.492988	50.6398742	562.809936	97.8877808	60.3976373	200.070764	108.761698	40.9215257	128.389491	43.4285079	NA	3.46279881	4.20503304	44.4902479	807.856189
C31	13086.1785	7140.97015	722.0578	63.6390291	179.966359	13125.4174	1081.11242	55.6377307	2626.94828	541.11192	151.938656	695.107533	498.113403	39.6143629	455.538623	229.356035	NA	49.7824521	7.7093915	253.512208	5813.20449
C32	4941.04647	3243.10723	458.491863	33.3798525	37783.4275	25382.1455	856.199817	31.3800115	1861.41476	332.04508	47.9228678	297.573722	198.659877	12.2420464	567.175498	90.9024903	13.6039742	1.6229502	NA	87.2268467	2346.31841
C33	3687.2922	2436.71929	757.369391	617.793931	2665.00096	5521.41962	311.035035	39.0456797	1593.26291	234.646835	39.9334092	276.201931	82.7362436	17.4537617	353.008392	113.017155	8.87559496	7.06436722	6.34762299	191.453732	4002.78303
C34	5032.33897	1986.55285	226.22744	NA	947.720632	5505.06074	588.217292	79.3552494	509.492876	295.206993	68.9834427	556.901815	143.840103	12.7120573	121.367313	72.1007153	5.92367222	5.70402962	2.537315	59.1902318	1328.22838
C35	9733.46172	4242.89201	448.247868	46.2947625	444.163495	8991.11723	1243.14123	39.1001596	1685.8562	239.642223	139.128601	825.949573	439.836608	22.4235654	530.938493	182.925261	17.5748928	31.797237	10.0681702	172.66909	4370.53807
C36	4273.61115	1960.46399	239.19752	54.6163876	758.170382	5654.67918	838.911696	117.169702	841.311058	251.353496	56.757243	265.503243	113.568551	17.7188418	75.8499158	77.5545925	2.97788654	12.6157441	7.55670465	60.3007937	1546.21703
C37	11577.8123	2842.09292	419.900068	34.9208185	229.213367	8436.01231	6538.14154	27.4933795	1069.48176	182.833743	52.3334912	604.626609	274.103597	5.68488223	253.930229	90.8240426	17.5381308	11.1174898	NA	132.559991	3111.98049
C38	20835.8139	6120.66391	747.57778	65.480414	750.041347	13989.1949	1667.43936	62.7342297	2192.5732	585.974928	126.521221	843.095895	555.886389	14.34896	463.819106	210.84598	8.31069417	14.6710312	1.83480225	275.662365	6491.15734
C39	8350.41709	3800.82992	550.851021	219.120391	358.071281	5921.73772	597.797366	32.0708693	802.544894	194.077626	141.173414	621.272509	143.990594	16.2195094	158.747432	123.310284	11.2955647	30.841382	6.31709301	117.830067	2594.11091
C40	2994.68546	1156.35313	186.526551	45.7895104	104.36263	3028.3559	275.646184	50.4786932	592.281784	115.126031	32.5057301	170.689671	72.514876	35.4743489	191.563406	60.5659204	33.7339568	14.8088208	16.1873038	77.4656245	1207.45817

Table 8.16: Raw peak area data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.

	PC(22:0)	PC(22:1)	PC(22:2)	PC(23:0)	PC(23:1)	PC(23:2)	PC(24:0)	PC(24:1)	PC(24:2)	PC(25:1)	PC(25:2)	PC(26:0)	PC(27:0)	PC(27:1)	PC(27:2)	PC(27:3)	PC(28:3)	PC(28:4)	PC(28:5)	PC(28:6)	PC(31:0)	PC(31:1)	PC(31:2)
C21	1653.19163	53.3426579	9.93633118	38.9663765	141.59992	118.8668	356.087361	134.873733	10.9955794	32.6439095	23.084134	1281.3082	83.4403194	20.3176779	85.5314377	9.90543007	36.6602096	11.5361706	57.7360457	23.722183	261.76039	6147.49321	282.287441
C22	596.828767	69.8333057	28.2255456	22.2665296	166.008359	117.17495	458.196151	160.373453	8.26736398	16.5439638	13.437138	361.340734	65.9656393	15.5950842	6.95205843	21.3075106	NA	20.5204207	87.5010208	19.0389963	287.416446	1841.47296	177.523134
C23	1270.99557	44.0575553	NA	14.1622479	203.508225	111.735476	388.422647	155.657586	28.1075896	40.6693934	22.512795	438.388872	45.1310829	12.2693992	16.302658	17.3846362	29.5629996	10.9311664	48.9784313	21.0478078	356.400866	2293.85973	180.778997
C24	1616.79804	44.656969	14.9838817	35.4831966	243.594893	84.160123	352.287265	176.873034	8.47795738	75.8535539	32.5511807	802.002409	104.205171	12.100636	12.8993615	16.1636547	8.62059571	2.4997312	97.3101653	38.7648527	636.203848	3427.78643	258.126759
C25	272.842009	24.4775127	13.411925	11.3785341	137.753472	43.5486351	383.295177	178.262288	6.99390223	16.2777019	NA	62.5276611	29.9308135	11.6443863	37.1334855	NA	36.7982721	20.9883995	40.2070696	26.7398787	296.88581	2392.48162	86.1718751
C26	589.876632	51.2354469	48.3049826	23.7182449	201.526074	134.856004	420.853318	198.280006	NA	30.6077672	15.5504159	419.8275	42.3683739	16.6004553	6.80553282	14.0659975	5.44028902	4.88061321	106.164915	24.9312748	433.382157	1850.14276	46.2593112
C27	820.89415	68.7741195	1.122557	57.8957642	329.661575	24.7703887	353.134723	202.089537	57.0273247	52.8960698	16.9615384	262.32469	130.273519	48.8522958	13.9165281	13.8570397	NA	31.8170344	50.1927208	33.8187941	585.080553	3619.59992	303.274952
C28	4352.52205	123.247082	6.67535945	43.4390874	399.534718	172.84704	375.822152	133.079048	42.0414155	47.7263817	51.7582024	1467.47596	114.724065	22.0983549	12.8408083	29.2316727	NA	2.79310829	54.5218443	27.5113928	310.889157	3188.32384	115.427117
C29	1735.92343	84.3148459	22.7989726	52.751479	227.236065	103.415949	403.730499	189.57777	8.87227731	23.8185047	20.0541601	1027.23613	97.5494158	7.37171784	15.5757553	11.7358288	NA	38.3116177	84.2091039	25.7853362	256.408526	3179.63838	128.008623
C30	379.85997	24.5862973	13.4068796	22.1776229	146.382366	56.0676495	341.638168	205.922024	15.6787135	7.77944757	33.2915483	80.4608073	34.8425539	9.78177972	NA	20.9971092	16.0423382	8.92608617	19.3527818	23.6946632	292.268634	1399.48396	68.4718906
C31	1408.80284	146.069013	NA	38.50395	256.978763	61.4665499	376.874072	145.105571	NA	50.5050196	111.962143	523.27412	49.2556879	98.0135511	531.703009	9.14986729	7.68382821	70.4117457	178.131131	36.7078115	633.702916	6409.55087	282.749746
C32	1182.30062	53.1583135	8.68647768	68.9815089	159.205642	53.2342474	241.388213	132.477372	NA	NA	10.9779443	175.055972	21.4878762	44.0087139	26.2835194	34.4879788	9.17609292	12.4822024	29.3857944	11.867951	172.828182	603.313271	49.5752838
C33	1168.6784	65.5656982	8.06906655	102.636976	200.552157	76.1147233	370.594015	133.091625	NA	3.6121756	NA	199.440486	39.9992441	13.9017861	23.6412574	32.1250778	15.5017027	8.22892706	18.6361439	9.17776888	328.369098	1690.60468	111.90732
C34	303.852434	35.6118779	11.7089441	33.4193041	163.291411	58.584735	345.36644	161.267691	22.1455899	25.6056873	7.73717334	840.797522	60.3291416	21.9244401	38.93489	35.4317241	NA	NA	33.0518823	40.5795398	372.957346	3596.04169	188.436837
C35	1356.50391	60.0427593	21.2735623	40.1275158	222.032816	81.8222527	347.932837	186.940114	12.6122381	43.1690396	23.9293263	874.055564	73.6635787	25.1420755	8.13127608	9.36985455	25.7424898	24.3065137	37.3090263	22.1504801	347.425196	4471.6384	164.380116
C36	485.399129	91.6664444	7.7102303	67.0655491	245.4066	107.314278	291.180357	169.079753	13.230597	27.863528	21.6814307	1107.28023	78.9913198	30.6429773	119.481602	23.2870676	12.4117826	39.4823148	77.6295437	54.189234	162.552486	1313.51972	143.914116
C37	1429.51475	49.9550637	15.7154714	77.2708459	234.663093	124.371644	386.191326	141.338002	36.3052825	91.6835511	40.707035	671.771325	70.1925259	45.337836	106.532884	19.8135067	NA	19.2210795	38.7923444	11.3477017	401.200513	4455.17363	236.040992
C38	1782.99427	128.185372	16.5554056	35.8040032	269.573992	172.209877	380.538101	144.644332	18.4903595	30.8380502	NA	813.891845	67.3983568	11.9888196	9.76515157	83.3157903	16.9694585	27.8848759	145.558733	30.978609	673.027145	7175.83164	421.948802
C39	497.709923	68.9512552	27.0388819	31.4989962	213.161681	113.809545	354.314442	184.896067	NA	30.2637845	135.264629	657.091274	95.1817969	125.289589	803.107687	9.24504794	77.6511132	58.3609038	26.6167495	94.4930275	218.751151	2453.66784	156.533731
C40	329.673289	31.3357365	40.9751091	56.7875741	123.204017	85.4539656	397.455619	116.672982	11.4799783	46.6672851	14.5590319	309.799767	93.6395548	9.09572222	43.9685795	23.1518653	10.3055518	9.84646838	44.1103169	50.7454814	257.152168	1061.74926	53.1613158

Table 8.17: Raw peak area data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.

	PC[31:3]	PC[32:0]	PC[32:1]	PC[32:2]	PC[32:3]	PC[33:0]	PC[33:1]	PC[33:2]	PC[33:3]	PC[34:0]	PC[34:1]	PC[34:2]	PC[34:3]	PC[34:4]	PC[35:0]	PC[35:1]	PC[35:2]	PC[35:3]	PC[35:4]	PC[36:0]
C21	31.0745444	140494.065	25633.9907	1298.33787	761.388379	107943.8	19790.8775	1351.90738	674.443536	157005.486	140443.841	28699.4857	3200.04819	586.949063	77835.4263	120952.611	10371.1249	348.341984	23.6022725	2784997.79
C22	27.6801897	50515.0188	6354.26247	353.228379	563.035253	13417.0011	2656.20518	362.852328	735.282221	22463.2958	23057.3954	16737.3357	2812.02334	184.403389	8508.81939	10510.9308	1878.1443	16.9842152	10.9863506	2438216.27
C23	NA	41847.8653	7865.02791	552.091559	709.938492	23545.4968	5294.91745	788.149926	522.74493	36934.2946	53653.2812	15394.2183	2573.03383	134.176964	15452.7488	34827.8528	3378.90227	208.014766	12.8423835	1926012.24
C24	18.4352478	90253.8951	14015.1481	554.852519	569.98869	52348.9452	7094.28941	731.335275	656.503011	93196.7463	58363.9376	25727.2872	3525.19681	235.642963	49351.9912	41713.4284	4366.77266	222.351634	4.17162917	3131508.36
C25	11.9467324	17310.3225	11117.2337	473.261194	383.70878	2739.22129	2307.63105	288.367474	613.251878	6490.11371	21407.2346	16806.8756	2566.82714	182.735309	1331.25461	3240.97187	1653.09307	19.2554063	34.4397847	2501857.7
C26	NA	36170.6661	4032.86041	226.794786	428.547082	13780.9909	1883.10429	269.377242	457.386579	21493.9107	15574.3049	14603.2383	2434.48218	162.517744	5983.3307	9275.80128	1605.48321	9.45090902	10.8062358	2235639.61
C27	23.2669076	44276.0246	8951.40752	605.516432	502.653775	10382.5852	1765.75348	261.347204	759.223839	22158.6932	19133.9487	13812.6265	2167.36528	146.22031	9718.08148	6810.07979	1270.4198	13.3137443	45.6649641	2077022.7
C28	26.0288328	86614.0087	17747.1075	529.637831	905.042732	68828.6566	8812.33974	873.247709	482.096714	105489.536	79942.7199	25799.116	3370.69424	164.702529	51020.2192	73027.5529	5577.08791	242.265671	56.5974558	2379485.24
C29	14.8721841	125363.268	15573.1767	806.41611	906.102803	51369.3827	7404.18741	968.239508	736.56212	83837.6989	89197.0724	29756.9428	4142.54321	265.369016	27007.63	39002.7373	3960.57142	228.416523	8.9009837	3030529.49
C30	11.1057969	14174.242	2106.36726	162.892371	406.579505	8786.32463	798.894969	259.579499	614.654064	13833.0895	9057.2439	12857.555	2057.74196	141.471495	5257.81698	5997.45161	1140.73961	17.2334948	27.6872437	1881791.01
C31	NA	68176.3985	13614.1924	712.271464	801.690179	32985.3645	4940.67447	630.861728	965.249288	60970.3675	44617.8722	24424.0628	3671.42663	232.630553	29831.1335	33061.1789	3023.00423	26.4708252	7.68483388	2623722.21
C32	11.2790074	14595.3445	1601.17993	51.3634075	425.26164	3424.34143	708.315399	79.6895394	107.911293	8126.57139	5770.66133	8784.40632	1338.73099	92.1036315	3013.29665	3278.37797	1075.21907	20.9283953	7.44249854	1824256.79
C33	28.4555584	19608.1287	2019.10993	128.810019	481.861749	9802.47869	1419.89977	195.552799	425.10161	18535.5139	11026.8489	10141.6271	1762.53589	79.6656916	10375.4876	8552.92242	1367.90841	63.1203269	58.1267256	2315214.28
C34	80.3209266	35918.9104	7210.7524	384.177696	273.272408	12178.1382	2163.20293	262.86573	599.769979	25250.7782	20698.9088	12863.1684	1878.28603	131.438554	10548.42	10325.0639	1973.07283	80.1248951	46.5437847	2112173.48
C35	NA	51853.3743	13717.1763	912.048694	443.11805	16112.1024	2690.99686	678.7909	916.724247	35474.6191	39435.8599	17797.0474	3008.24826	151.580627	16042.264	14547.4425	2493.21271	115.501947	NA	2375302.49
C36	15.2358426	42126.1667	5755.81528	265.11656	613.278315	10876.8663	1319.43355	288.711822	555.695429	24506.0642	16655.1746	17242.986	2758.61115	200.186587	11061.936	7394.62061	1863.65819	52.7315521	13.9690511	2828076.7
C37	36.5672302	75929.9938	14534.8545	1160.64888	753.487195	49716.7608	7116.42986	1001.67087	911.554261	88416.259	69248.7904	29373.7005	4410.28742	261.058362	42074.4338	43862.1332	5281.38564	229.147446	51.2875364	2654731.75
C38	53.3634566	86640.4313	17506.4958	1054.28929	830.088355	63440.986	9077.45101	1312.88276	1197.97436	103734.849	88948.2982	30978.0066	4416.78908	259.298583	52587.504	67387.901	5237.87459	375.795929	63.5244185	3081492.38
C39	11.1070163	48114.8883	6726.89527	364.850121	787.950857	18834.987	2971.9067	392.739568	465.814944	33640.5419	25765.4718	21404.0242	3447.67951	188.038221	17014.9727	15096.0639	3490.31938	49.1622969	34.665985	2861271.27
C40	22.0470858	32778.3123	2996.97912	46.3301246	289.183946	4836.99625	840.356252	117.363418	162.065876	10980.0414	7824.23559	9291.30178	1665.41629	95.9008705	3795.29508	2944.34156	1143.75215	24.9505444	5.31513497	2219717.71

Table 8.18: Raw peak area data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.

	PC[36:1]	PC[36:2]	PC[36:3]	PC[36:4]	PC[36:5]	PC[37:1]	PC[37:2]	PC[37:3]	PC[37:4]	PC[37:5]	PC[37:6]	PC[38:0]	PC[38:1]	PC[38:2]	PC[38:3]	PC[38:4]	PC[38:5]	PC[38:6]	PC[39:0]	PC[39:1]	PC[39:2]
C21	526367.8	80590.1815	15908.8984	5299.77862	744.445044	54625.8309	80697.6839	5673.12872	3709.74645	28133.3632	819533.557	146636.105	97032.5799	28716.9602	10066.0266	15207.8624	1336.45869	7470.10808	9060.16374	66503.4241	10287.6193
C22	396364.834	26615.5211	4114.83751	1378.33242	367.14298	6124.24054	9810.60243	509.015257	654.211077	23484.669	718328.825	27347.2912	23338.6069	3977.76614	1641.538	1339.02592	630.721169	2918.31507	1866.42492	5148.82782	690.003474
C23	327072.85	36320.206	5795.04074	1800.34906	467.185854	13198.7371	14308.5121	1732.09585	880.093829	18779.4601	558853.439	43094.4393	33559.3051	7929.04958	3147.7935	5280.67561	848.361065	3779.78003	3704.84569	10800.9261	2065.31235
C24	486335.483	50301.8409	8840.08027	2055.1928	476.057444	28333.2324	48155.6578	1550.30619	1040.083	30768.1005	925888.406	75016.8517	56570.4405	15012.1169	4219.29569	6612.07886	1302.16451	6555.83856	7483.98138	30493.0882	3870.7637
C25	396207.306	24386.2688	3464.09513	700.059374	121.603955	1942.59638	1622.61848	128.075338	392.520037	23862.9063	742721.226	14134.5249	16276.1283	4356.49675	656.969656	634.939172	535.335581	1830.78089	1250.5334	1549.18383	291.105655
C26	354777.386	21179.9008	3389.85708	657.010915	119.281587	4137.80845	9252.91971	447.267428	527.287394	21860.6507	665220.158	32902.3435	17405.2305	2587.97876	835.134511	1194.70603	616.154152	2318.38068	2094.22127	5624.11021	498.894166
C27	332338.391	20804.2367	3083.14167	1996.33048	39.1669164	7521.87347	9394.62394	222.145627	504.208879	20088.4934	620726.204	38620.0493	46146.5622	9285.99067	530.125589	1183.14311	427.614859	2130.88282	2316.91597	5357.31785	589.842551
C28	440424.59	52688.266	8320.1889	2391.15887	975.519294	26752.8184	40647.1821	2541.55053	1422.35201	24610.8955	730691.244	91236.7144	58850.1629	15986.3632	5374.1493	8304.37397	1318.25304	7216.57866	4343.73867	22047.5707	3741.73311
C29	512228.419	56697.4232	8178.52223	2746.93276	814.903239	13458.5769	32189.3419	731.864349	1284.45263	29451.4556	889353.154	68074.401	41101.2538	8117.55135	3850.59357	4100.1469	1259.25949	6656.03505	4265.29482	15206.6989	1422.54721
C30	303908.7	17066.7682	2095.37254	557.425106	23.6445442	3180.64591	4874.45647	221.26967	361.119129	18679.6424	557961.739	13576.983	13964.9289	3288.11382	342.385412	870.192179	578.291669	2915.58146	1438.3898	2097.04515	454.076595
C31	406043.285	39101.026	5333.63919	1910.35598	455.178583	19312.1506	27593.0023	1241.86485	988.344315	25903.2847	764026.854	64818.5151	44059.2609	9907.63529	3375.06153	4485.44923	814.538663	4027.80299	5137.92017	20166.7833	2575.25633
C32	281675.683	15286.0124	2242.40268	356.466814	53.711112	2718.51217	3987.03208	170.078277	451.259312	18199.5568	549882.532	16630.9985	12745.1439	2258.24239	451.635164	506.892336	415.611496	1844.41786	1303.32409	2935.14905	294.13968
C33	373333.391	21550.0566	2604.88943	485.558098	16.4223336	7784.5495	11096.9903	288.768732	410.348422	22537.3448	677727.628	40634.4191	33838.6062	5263.25228	582.577842	1039.07419	686.588863	2895.0429	1987.0937	6670.56841	551.207255
C34	345461.772	24842.449	3125.19726	1237.18015	74.8334917	8896.42235	10706.4925	531.992185	607.283164	21070.812	622479.309	38925.8975	45702.6421	8269.842	1319.70481	1935.75886	719.672073	2517.85231	3323.1811	7700.05721	1112.49394
C35	393972.977	31068.6193	4691.68051	1322.93366	235.602464	11224.7589	21114.3251	882.32353	571.944694	22971.2756	703180.526	63320.4317	54780.5685	12099.9997	1827.66833	3818.6063	954.771454	3451.62545	2723.89865	13282.9108	2769.04156
C36	455717.751	29092.4928	3903.96072	807.954754	100.075257	6179.35379	13108.0605	365.117882	490.66763	27938.0256	837317.628	37109.3429	27019.8737	5297.85775	1057.22101	1388.42208	850.597991	4305.85851	1981.46165	7022.97763	778.18256
C37	458117.112	56888.1469	13951.2554	14808.5518	3754.83184	22566.3097	40838.0097	1608.8989	1064.78465	26295.2914	790305.084	88075.3162	60711.1984	16506.5453	4328.51798	7245.1456	1022.80908	5933.64094	7144.0816	24811.9434	3957.84841
C38	537641.39	57579.468	8193.97025	2674.95256	1011.92819	34181.6442	54463.265	1912.31057	1286.48204	29695.6288	916823.377	116033.768	72595.7909	18338.562	4218.33971	6768.93917	1587.16671	7765.37649	6428.37006	35950.0804	4437.17379
C39	465206.046	31950.9669	5523.64317	1415.89778	124.055691	9083.45404	16202.4268	719.556557	750.526647	28869.8336	852022.146	46217.1055	40483.5546	7852.02803	2057.83484	2524.19202	939.540545	4155.30989	3047.34943	7896.0494	1373.88728
C40	350621.94	18754.884	2540.07968	411.606339	14.6767294	3280.58894	4676.31093	78.3252823	414.848944	21722.5871	655979.161	18683.9409	26449.1928	4167.99855	291.428896	444.193566	432.53098	1620.61677	1494.71693	2681.72825	321.44892

Table 8.19: Raw peak area data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.

	PC(39:3)	PC(39:4)	PC(39:5)	PC(40:0)	PC(40:1)	PC(40:2)	PC(40:3)	PC(40:4)	PC(40:5)	PC(40:6)	PC(41:0)	PC(41:1)	PC(41:2)	PC(41:3)	PC(41:4)	PC(41:5)	PC(41:6)	PC(42:0)	PC(42:1)	PC(42:2)	PC(42:3)	PC(42:4)	PC(42:5)
C21	6505.31264	8572.19508	8541.50874	40612.2314	27882.7226	6885.27732	3016.72596	4011.04545	2071.50117	6150.42809	7400.26263	8958.77547	750.590312	6947.69521	6155.66697	1546.46619	2563.73699	7101.13575	5022.01236	1374.54876	1166.31044	1215.66769	881.26827
C22	578.152178	1896.20325	4341.37398	10558.4861	4585.30212	685.765924	345.661406	438.985284	241.96478	1452.86471	1523.10146	973.815914	451.392831	896.310534	735.039731	227.81942	559.507415	2014.96633	1087.74915	290.105909	143.230325	211.778092	56.0199939
C23	1972.90955	2143.51235	4677.35593	19004.3569	10108.7736	1949.55143	840.180689	1009.06692	367.104513	2070.44907	2163.90369	1566.70288	389.93317	2143.91509	826.428423	397.400804	1200.89603	3537.4119	2499.68353	459.885335	237.117199	177.786269	156.664358
C24	2559.37424	4346.03609	10004.3285	20692.8035	12830.1977	3291.77043	1393.72772	1511.93067	804.399191	3918.12283	4155.79598	4771.06295	628.475137	3442.40672	1462.00071	643.303034	1323.12604	3716.51596	2501.02907	754.26442	500.432837	494.506914	368.290557
C25	189.072393	1348.82177	3811.8205	3525.00937	3002.45523	566.479164	109.552849	158.357113	70.2542311	338.184608	258.009999	226.293066	108.008964	75.9117101	124.115015	57.0008021	190.879311	544.254646	611.546686	113.770372	37.2643503	34.1543987	37.3313654
C26	423.115419	1114.56449	3031.29879	14445.0286	5850.89461	745.23393	223.636244	190.557421	134.406746	1331.19721	2003.79079	1460.03116	264.43309	863.508779	397.702025	141.705547	904.27269	2562.1503	1495.37176	217.059032	170.174729	149.671166	92.5980905
C27	387.571267	1183.29898	3833.98075	14737.6732	9455.64879	1720.35635	325.843784	177.804577	123.969768	1269.77912	1204.49707	897.508221	57.5528763	623.976111	328.155685	155.896465	796.236705	2010.65387	2254.55381	399.536685	95.0067458	111.131953	127.03971
C28	3784.53114	5133.57107	9347.8829	28938.7146	18021.1201	3183.73437	1458.45189	2078.2866	1325.92423	3796.46417	3748.6705	2429.17513	1257.44493	3388.80738	2293.44	1112.86752	1562.50087	4340.08459	3659.02877	637.02472	572.248255	601.749361	486.861014
C29	797.22626	3421.61978	7667.71958	21210.0557	11269.5832	1912.3579	476.367306	951.303969	556.907851	2537.57797	3108.0489	2297.46792	377.928062	1007.5202	1054.98564	462.726647	1195.81917	3928.48694	2137.54198	380.339672	234.551039	355.438918	260.122141
C30	399.094897	1643.10852	4654.24556	5495.97188	3324.3942	641.524482	152.491724	162.654557	158.478292	737.148695	674.69541	427.803117	115.986271	368.53394	252.286003	199.314205	255.740086	1038.13978	843.530234	163.502249	40.4336639	60.6858773	115.51196
C31	2116.95827	3863.969	6316.75851	27791.1273	14876.8728	2726.67064	949.88221	1313.44967	713.478394	2881.063	3863.46486	3128.3976	727.924224	2132.97995	1836.6698	545.799331	1321.61992	6464.16215	3770.148	688.292942	476.589669	333.033817	345.456205
C32	338.52018	1171.7714	3541.99088	7539.68112	3946.62394	576.835615	229.038373	189.294036	99.2057242	836.437987	1024.26957	591.100011	64.8133206	701.192745	520.080363	84.827241	403.387045	1596.82432	1062.23678	159.368556	214.072368	204.496914	64.0062065
C33	567.529603	1922.18893	5594.52927	14068.4307	8868.52148	1377.04126	306.343905	164.859165	76.4115796	1528.05662	1527.28098	855.789915	65.4038802	691.587623	305.919634	133.404789	750.609393	2222.69681	2289.72987	329.873058	189.355799	78.8502454	63.5876794
C34	981.244015	2035.04929	4806.6312	12898.5068	9977.62206	1709.50791	493.005563	448.306777	124.593861	1465.39288	1522.51782	1057.9075	233.017995	1404.18792	569.840941	277.165956	679.223101	2205.43703	2515.78332	312.470781	237.880776	173.550236	148.84633
C35	1418.13171	2961.34424	6600.75459	23959.6308	14273.9482	2576.59005	1126.80851	1086.66409	388.086116	1966.02449	3200.51117	2806.72038	596.40218	2714.64097	1562.89161	273.872362	1227.33597	4236.5038	3479.39056	677.164894	514.129033	553.212132	178.629547
C36	545.820615	3071.30805	8043.98024	13317.8366	7985.78171	1245.25543	343.372481	334.72509	265.931532	1875.90038	1797.59618	1311.27641	136.753302	819.598053	498.921438	217.169929	696.160227	2240.61736	2171.50806	383.203782	223.154064	115.178961	95.6469582
C37	2438.39618	3755.50556	7474.99527	27918.3509	17752.4583	3509.88678	1355.55474	1385.72851	1180.97734	3563.66605	3123.71823	3726.6274	1008.36281	2959.5732	1927.86173	828.386356	1395.11338	3065.2085	3744.59476	840.681457	503.484994	535.493839	393.886179
C38	2980.82574	4606.62539	9134.00378	34518.7901	17318.3305	3342.70493	1526.56272	1853.92733	1074.43884	4162.44951	5266.72054	5056.35816	970.808774	4208.35082	2748.44865	698.958997	1728.68052	6014.19581	3367.87615	759.66466	710.875538	569.17346	337.443656
C39	1303.41794	3157.09347	8628.22522	18969.7066	11137.7389	1843.26917	623.440329	619.427086	144.083558	1917.70885	2527.20722	1578.99761	456.023659	1490.17417	682.576944	129.762832	1151.26587	3271.46825	2384.72417	460.630375	351.376971	220.918002	160.213683
C40	174.240117	1084.37097	3517.64882	7926.53045	5611.56107	816.020824	104.791086	77.9373527	41.3236574	887.833563	735.250705	394.58226	42.0879702	130.258115	74.4432661	80.2874197	513.385231	1241.6652	1242.04378	160.660174	65.0701807	59.1565239	103.00026

Table 8.20: Raw peak area data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.

	PC(42:6)	PC(43:0)	PC(43:1)	PC(43:2)	PC(43:3)	PC(43:4)	PC(43:5)	PC(43:6)	PC(30:0)	PC(30:1)	PC(30:2)	PC(d31)
C21	1382.01834	89.6763706	987.178828	456.303353	1951.14151	1420.03174	686.702964	612.367361	69688.7531	16202.9131	1061.64569	126978.265
C22	376.580648	21.3539514	196.238993	145.957853	233.184263	248.045515	127.821127	183.079595	30108.8844	6202.96518	332.493754	111757.533
C23	628.069978	19.8682117	198.168669	122.047237	497.22784	133.425791	90.0155298	258.079296	39229.9139	8399.03743	569.733077	87191.21
C24	842.518553	32.3460149	652.380851	273.492859	1010.02083	480.985886	258.062675	365.879852	32557.449	8647.74421	684.038075	143058.161
C25	88.6540455	12.7633636	68.0537085	18.4907967	32.0157614	16.2330247	22.9892127	41.3725806	23338.457	7065.7705	663.892175	115544.886
C26	432.892967	18.3264107	210.566233	161.096365	438.223499	153.55985	112.359256	247.935481	19545.7328	4433.92849	300.968218	101345.251
C27	262.327955	17.4788325	176.350894	84.3124441	163.392158	66.5387078	56.9113416	165.059092	67509.2776	15829.9295	1210.90627	95404.4634
C28	934.3221	22.6697625	346.311565	212.998716	1052.72261	498.300398	191.113889	347.36489	26811.7796	5847.80124	525.441924	109026.605
C29	751.88263	13.0353668	304.132869	162.94184	247.691685	348.502405	166.691089	290.48512	35811.9667	6622.90628	385.651184	138865.455
C30	222.60707	12.9278691	110.251969	65.1625376	62.630009	14.0984714	34.4823329	93.1159671	18513.1402	4155.79122	271.328435	87681.4965
C31	846.28528	83.2431257	548.289539	298.321298	963.583865	480.391349	169.414796	416.522758	89373.2632	17508.3497	874.280761	119821.226
C32	298.567088	18.7172467	80.6320487	67.2404903	376.037166	207.310485	24.1910808	146.292492	3599.70739	1357.71412	274.242688	80571.81
C33	412.204481	14.7315317	246.242866	71.9118039	232.620256	53.1328586	15.1251597	168.349606	23957.6934	5398.24938	336.652957	104762.773
C34	328.792792	20.4591114	349.339723	158.002224	410.986366	185.503702	116.2558	155.332234	52852.7107	10770.9307	543.262217	96864.4554
C35	395.814511	27.8644565	414.508748	225.366801	1164.74891	557.170017	117.281621	395.24678	59215.3481	12729.5201	862.101738	110758.127
C36	502.601244	14.4769401	239.60243	126.843339	416.419593	164.78763	86.1748665	168.218914	19801.7674	4477.11573	329.8184	129609.014
C37	890.748102	63.6186885	455.273763	248.665471	1031.85974	505.661928	288.281681	254.027539	59613.2674	12887.8713	912.677632	121473.698
C38	1209.41524	61.4857141	681.350398	88.7214909	1557.84778	664.468646	219.285972	442.411425	91898.7088	20096.4975	1316.60777	141377.959
C39	785.647247	30.5562354	337.699796	458.234426	449.918201	129.091059	62.7356121	219.719687	27532.5071	6122.74493	368.493847	130839.606
C40	219.070315	14.3457933	153.055179	22.0645792	94.5786233	30.517125	59.7145812	128.56754	11156.4974	3461.79498	234.821435	102021.501

Table 8.21: Raw peak area data matrix for lyso-phosphatidylcholine for hair samples taken from patients with breast cancer.

	LPC(16:0)	LPC(17:0)	LPC(17:1)	LPC(17:2)	LPC(18:0)	LPC(18:1)	LPC(18:2)	LPC(18:3)	LPC(20:0)	LPC(20:1)	LPC(20:2)	LPC(20:3)	LPC(20:4)	LPC(20:5)	LPC(22:0)	LPC(22:1)	LPC(22:2)	LPC(22:4)	LPC(22:5)	LPC(22:6)	LPC(21:0)
P19	13433.317	6012.01826	449.984975	NA	278.105901	9263.36501	1385.14987	75.3053305	1948.09949	529.493073	117.541228	611.235587	259.37557	29.129496	598.50189	239.849241	NA	21.4792539	NA	347.445822	8467.30492
P20	4360.57459	1875.2104	288.682466	93.884121	394.191349	4746.049	557.914781	54.9241128	831.309632	223.437489	46.6166238	249.068025	122.358408	27.8933922	157.132554	80.3363453	NA	2.63665796	11.3977398	69.6154048	1594.69297
P21	5520.61137	2523.32783	196.120512	58.2581093	63.6067432	2598.27984	171.660646	33.5696745	797.981176	178.390423	37.0678623	165.347251	50.7545254	28.0683593	268.120951	78.1289108	13.5485101	75.1862388	8.26275916	88.9124749	2658.4132
P22	17575.5957	7356.83894	531.614323	44.4609419	75.9801667	9875.96492	1407.41413	31.500448	2495.12587	259.717128	133.814882	944.166372	401.947439	9.78674358	568.733649	247.705749	17.378668	14.5577498	15.4095293	330.615312	8914.41675
P23	6920.28963	2295.75366	318.96212	104.435216	229.131989	6115.48312	729.402145	51.1519226	694.5323	175.002423	62.5706616	488.40476	201.27166	16.5703513	181.549099	69.9724777	13.9361022	0.87353284	9.10768744	62.038597	1876.94576
P24	5909.57444	1251.88874	192.43985	56.4387082	183.970423	4808.14984	387.289144	44.4586979	997.332308	98.5001671	29.9667831	332.816689	78.0359373	3.98997812	225.547958	140.151235	9.20840177	28.1470352	20.7888901	123.642784	2756.2286
P25	12018.9552	3023.97356	268.396695	NA	491.158971	7804.46679	623.174284	53.0082013	845.014744	383.0842	61.5903236	373.242736	122.148501	17.8449283	203.046032	93.7627487	9.36147729	10.1878448	7.73597373	74.7479632	1859.30372
P26	4087.42846	1644.31847	194.280123	NA	598.675136	3450.19547	423.342903	94.0682365	1100.90376	104.397572	33.8106658	191.063427	87.4940836	30.6490005	439.147285	136.330465	6.61629699	1.02805664	24.0043937	146.29183	2762.61611
P27	7549.42399	2942.22867	326.677394	213.558452	391.057284	6413.32827	537.96499	56.5050409	1028.64915	234.802783	56.8770079	365.210358	146.89783	20.3631081	229.46583	104.141388	46.563368	9.37020852	NA	110.570444	2294.52291
P29	6798.49695	2783.30832	1385.70228	791.925827	93.9026417	4582.70586	766.263727	71.9191263	1053.12474	145.336091	34.6295169	329.496689	108.568274	21.1097209	321.170421	108.478564	16.3006425	61.8121452	8.52603333	213.604154	4569.73123
P30	6071.11516	2464.67769	184.774905	NA	300.980452	4248.23588	420.960597	62.6493635	1554.35358	179.544713	31.5525666	253.676527	88.6239758	5.10500885	557.83308	126.922828	7.27478935	13.3395848	4.25032361	211.805375	4722.6984
P31	5712.19387	2119.53913	218.483329	134.456268	191.377657	3219.04398	355.734588	25.5924599	1090.67492	163.61813	47.9355897	192.840637	157.618583	16.6835842	273.984686	68.8340857	11.8069764	12.8489832	6.17717615	149.422504	3178.42112
P32	6949.87849	2125.04273	272.938704	41.94218	278.804357	5647.93584	611.969688	36.0981827	1654.05793	298.172333	56.3544712	388.205809	130.471137	95.2292943	400.142497	157.55252	14.7044859	9.08461231	15.5110078	164.782446	4353.58087
P33	14862.2338	6049.84754	489.695694	49.5191995	12465.6304	14574.3495	1019.3527	54.383788	1768.46965	704.880104	118.758211	1059.66237	344.95555	14.1137468	323.835509	171.052987	NA	NA	10.1004128	174.868773	4258.33865
P35	15127.3178	2252.66709	311.572081	NA	186.713272	5152.7366	809.027665	36.7234993	1393.24422	179.306103	49.4604249	301.116522	177.839258	12.0598318	396.02994	141.318883	11.0792897	22.2692766	NA	97.2039966	2865.39927
P37	3805.14613	2027.52927	174.798582	NA	3902.76521	4945.24152	310.758433	38.2821205	349.405396	103.815894	38.599748	226.954508	76.1345017	12.0578966	119.360778	44.3329736	11.5226785	18.7741227	10.4457951	86.7127836	1434.59621
P38	15128.6249	4175.48431	383.286817	NA	360.113758	10616.5412	1100.10297	48.1884777	1479.06617	529.481024	121.497657	585.93431	299.345857	2.54940051	274.919981	156.00966	8.67453497	8.47229758	NA	168.728128	3150.09098
P39	3497.97363	775.364387	511.204124	538.263873	1044.07757	4008.96727	602.7034	26.6964807	459.112468	52.3076617	37.5559965	80.8807101	67.1182711	19.0622277	103.64236	48.6089328	7.21271365	41.5440562	7.91550121	40.2300937	825.248524
P40	2804.31687	1562.46419	76.4616229	NA	134.250096	1841.32808	180.648267	53.9649043	907.269001	226.928317	36.7249749	88.595303	25.0874167	31.6097577	428.924826	99.104161	12.9243553	17.8743812	NA	120.277196	2972.12371
P41	4604.56998	1316.40611	166.9101	NA	26403.3758	18698.2467	388.723353	37.8999851	426.668153	161.549041	NA	134.512453	40.9677231	23.6914634	89.2456832	41.4923821	9.79853543	9.65419418	NA	45.7120709	928.552525

Table 8.22: Raw peak area data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.

	PC(22:0)	PC(22:1)	PC(22:2)	PC(23:0)	PC(23:1)	PC(23:2)	PC(24:0)	PC(24:1)	PC(24:2)	PC(25:1)	PC(25:2)	PC(26:0)	PC(27:0)	PC(27:1)	PC(27:2)	PC(27:3)	PC(28:3)	PC(28:4)	PC(28:5)	PC(28:6)	PC(31:0)	PC(31:1)	PC(31:2)
P19	1754.97262	50.6258933	18.1686958	45.6687905	308.604534	140.349725	487.260062	191.991225	NA	28.0425729	16.3790747	1379.00685	72.0255224	8.3060146	7.13669309	22.1893347	NA	10.0271772	59.9230042	11.8665858	620.663775	4093.88284	333.628146
P20	500.109828	51.5074643	14.0995547	38.1445926	178.787496	115.185491	245.602529	194.053894	11.7319592	16.6196699	12.2625502	469.147944	52.8443669	NA	34.458264	NA	13.2093914	12.0172856	94.3145629	11.4769945	417.644101	2078.16754	145.697767
P21	687.374123	43.5400758	25.1158016	16.5652602	194.554701	68.7461841	261.999739	118.803026	14.7937103	82.1030636	126.164885	344.231332	44.9437282	186.585801	1189.73194	NA	19.4306865	139.937457	85.4966982	90.5523177	462.22672	2199.75512	112.461151
P22	2053.17926	79.7855095	10.4279035	21.7023528	231.434802	137.969317	205.164512	106.435836	6.72214152	31.8442544	25.0171604	896.247587	82.7142516	50.8350857	47.6846465	30.513906	16.9455005	2.41870853	32.2021639	33.5278569	329.234625	2940.09155	150.777155
P23	558.264253	58.9750563	20.2872643	30.8668026	163.482526	79.1636036	355.993123	160.927099	20.7287975	22.5088416	12.58804	402.515962	60.339848	8.75380739	18.8367337	11.4051344	12.1138217	15.5961801	10.0088716	10.6770101	411.544704	2023.80014	125.228214
P24	957.820115	65.5407843	10.593675	54.5873641	164.186622	103.382983	344.877908	124.504565	111.884608	22.8761076	28.1377017	1334.8008	100.389084	24.9808616	126.283544	99.7710906	NA	48.3600944	60.4228548	28.8160243	440.188144	3430.21079	56.2648134
P25	848.238519	69.989844	4.61797368	29.9626058	208.476021	105.797385	347.82096	143.158719	65.4200464	20.3366309	23.3059264	741.012202	66.3271562	15.0518745	11.3452226	7.58360465	21.6562997	8.70347719	115.10712	12.1339854	187.17876	2571.08915	171.260447
P26	708.1434	53.5752461	9.39487872	40.1108408	340.891464	107.368548	380.488836	203.970156	53.3867398	23.8552919	26.8364807	992.710444	44.690835	13.3836385	23.0100445	NA	26.7464943	22.1359231	67.855802	18.2478929	416.313238	2965.33631	153.214598
P27	668.935315	125.072312	14.3837742	45.1639839	336.093957	140.005874	363.161395	186.723468	10.8415646	25.0811893	27.733995	1462.75811	102.881982	NA	14.0024756	12.0086619	13.1358623	NA	52.1133118	19.6033711	418.090874	3444.75845	141.223235
P29	1093.95569	59.2338282	6.66775345	77.5350636	181.011934	92.8536218	373.300666	152.324947	107.024824	19.8877305	11.4516183	530.560739	52.4994737	27.6514857	27.6632011	39.3827222	20.821435	14.9303876	60.0273749	21.1052498	393.16545	1589.56205	166.335109
P30	983.842082	76.9482017	NA	48.9347988	240.0497	144.359619	334.737136	114.487287	169.232396	2.27511151	14.7618015	1368.96872	38.5289574	37.4147727	15.9193037	18.9096193	216.126419	9.93689632	59.8769724	7.67380051	378.184148	2620.83244	190.159993
P31	950.029423	NA	5.60047986	58.8468246	174.922081	75.271781	337.467991	98.7361488	21.5256206	43.5961923	34.6238121	350.951786	79.0023283	28.5402603	30.0763364	13.0564963	NA	13.3698998	40.6928407	NA	312.965514	1460.83392	92.5480644
P32	1410.37593	72.5477633	NA	16.0661514	213.32469	31.8355906	395.860358	205.971521	10.7460353	64.3762908	11.2009504	1046.02585	75.3206265	17.9851504	12.1608021	15.5827135	11.0364707	14.6323934	61.2400364	310.976909	258.483499	4676.34063	150.232734
P33	753.303034	198.685022	12.8310831	37.7817179	331.622823	133.139234	318.023521	128.55988	16.9889573	13.9072511	29.1798527	1314.1285	102.280554	NA	28.6069007	11.7979599	17.8691056	7.88637733	88.1197052	35.4039414	515.090729	2749.39929	110.879421
P35	1101.15825	29.7425501	9.24307696	20.5372121	237.527609	68.8641904	240.789676	108.459702	265.527599	20.858739	16.5008892	387.65545	66.304272	NA	38.0506545	55.2016423	NA	21.978753	33.0201888	15.5674821	362.485038	2099.03384	115.8183
P37	403.828523	NA	9.47649534	33.805201	125.305045	99.4232191	422.903359	151.476011	NA	30.6786914	24.0458263	451.214152	44.3129384	15.425424	11.5285565	20.502108	9.45568765	24.2147562	44.4252148	13.4686095	356.557045	2523.78781	222.817024
P38	721.238017	126.242776	12.9709842	62.072523	288.536853	91.7793711	312.302054	140.212723	65.2082654	21.0581879	14.463873	1180.60521	59.4678231	11.5300239	NA	37.0703779	13.9137228	22.6700949	63.2658609	23.5806325	312.62372	3599.11745	102.713696
P39	236.646009	30.8703654	12.2875103	40.754591	246.94558	84.5168472	383.951331	182.965238	61.5061567	25.8500491	16.5734874	183.656904	35.6620754	18.0682968	21.851234	9.53506099	14.7854385	15.2430465	29.6599128	9.62162597	149.003278	1013.53344	76.9978224
P40	930.863109	54.46382	10.7554556	34.3380689	245.750943	131.292539	217.998601	107.891895	7.24611334	29.9140417	13.2743913	894.844649	63.9796733	27.2905259	22.9600852	NA	17.5049088	11.2009631	72.0240491	32.4907074	373.045727	2706.48015	154.108962
P41	148.858923	33.0534207	19.194806	78.0918319	336.853446	110.141004	343.405085	117.542507	20.0589693	22.5874818	9.92965963	172.009674	32.8793776	18.0723003	9.16270949	41.3449227	18.3456927	9.57041809	34.8151844	42.6860901	112.544185	2217.15511	132.873741

Table 8.23: Raw peak area data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.

	PC[31:3]	PC[32:0]	PC[32:1]	PC[32:2]	PC[32:3]	PC[33:0]	PC[33:1]	PC[33:2]	PC[33:3]	PC[34:0]	PC[34:1]	PC[34:2]	PC[34:3]	PC[34:4]	PC[35:0]	PC[35:1]	PC[35:2]	PC[35:3]	PC[35:4]	PC[36:0]
P19	36.307634	143704.885	17311.7626	921.892655	705.438739	43499.9928	6464.54212	797.566665	568.072174	110481.511	73503.7497	26181.4401	3533.37731	221.405805	30266.5425	47937.0385	4360.3454	158.84791	26.0553452	3316760.62
P20	NA	35175.9428	6948.54461	272.332895	412.163645	18311.4786	3907.83099	575.764295	477.777309	28848.796	36316.8209	16156.3468	2395.3905	146.640141	13643.5121	18736.0581	2707.51622	28.8308594	9.24756306	2675026.15
P21	10.1153043	37497.0627	2653.45628	149.147141	231.924235	19074.1835	2181.51576	187.642506	255.127175	23714.3828	16498.5065	7526.78481	1084.87975	85.0718092	11807.4327	9347.28237	1067.57975	27.1817181	23.620319	1238456
P22	40.9660251	129234.524	11852.4014	379.038814	360.906194	45634.6111	6243.03116	743.617536	483.549792	85980.2757	58512.661	16317.0747	1985.25276	160.72984	35246.6751	54114.6022	4400.50498	216.735003	79.7150861	1995226.11
P23	12.4211457	47518.2627	8365.03517	410.287324	361.373617	17529.9043	4058.47515	523.813906	357.514268	31304.5659	39343.8948	15046.3089	1919.74086	81.4756398	10901.929	18059.4393	2680.50759	46.9531928	12.02941	2398361.89
P24	78.7970704	104944.795	12687.4405	440.924152	461.070594	18814.3958	3474.54464	401.37012	374.831795	72700.5322	40870.7889	16182.9771	2050.85547	79.6384991	12957.6141	18134.8387	3185.71579	102.254101	33.0590308	2696029.59
P25	25.2750357	73209.3361	13288.1432	582.92811	720.12264	23708.2129	5911.2202	729.487756	612.307144	44623.6751	57039.7133	23478.8435	3275.85528	252.659018	17174.134	27379.4396	3380.7099	113.239982	29.9437135	2880216.73
P26	30.558773	54859.3076	9210.08585	473.617492	533.837651	14799.6248	2315.86936	360.988709	595.255338	35217.0353	26850.735	13775.4326	2002.12153	111.427541	12101.651	12365.1607	2093.68371	101.859692	10.8281422	2337057.69
P27	20.7854203	62945.1897	12219.0765	535.1513	589.324646	22248.0521	3945.10844	464.857319	535.085378	53831.9563	44423.1363	19119.2462	2958.56812	205.387184	21447.6254	22775.6626	3215.32729	112.117852	24.2371125	3039068.82
P29	18.7729026	43790.6647	4621.04956	309.089336	353.725009	23422.2555	2966.77147	247.041196	389.342815	39925.0261	26493.0707	13946.6708	2012.25426	124.235984	16199.8104	22028.7411	2236.67422	161.418106	28.4681635	2482276.75
P30	62.6235633	150037.789	11668.1766	630.832951	408.616191	36368.0049	4541.02229	362.897787	369.359108	90621.8829	48240.6395	15355.8654	2038.06687	136.412326	33919.9	26338.8177	2801.64504	110.739424	9.22333925	2373921.78
P31	13.9749967	43143.094	4518.28699	154.357637	347.81194	11854.7642	1872.67035	201.923751	208.816503	22584.6449	15642.5437	9485.81822	1331.15186	102.509851	9156.23768	8406.26726	1633.04196	24.9780539	35.8843466	1981597.87
P32	16.6023947	73892.7711	18803.5813	1018.27197	765.88233	42971.0829	6958.78831	987.653679	717.19029	77592.4807	76926.7833	26995.0719	3938.49789	246.932423	34340.3971	52066.5538	5284.21703	232.097604	21.5880187	3018916.65
P33	34.220332	83780.9208	9496.36231	404.31538	974.198104	43398.6951	6994.54488	889.538235	522.844013	83033.4044	67992.6	20559.9634	2917.28152	160.870205	28290.7395	54891.0703	3765.58207	147.447217	15.5973209	2563749.88
P35	121.619202	79482.9872	11223.0924	460.60302	552.144187	29742.2752	6364.80681	807.569537	409.247752	38829.074	66526.8045	21519.0643	2487.83829	201.048758	14946.4144	23750.4544	3652.1572	101.008165	29.1694676	2293621.63
P37	NA	45573.6077	4896.04684	296.919257	672.351734	14026.2635	2377.57384	411.084299	771.222501	19773.4914	14888.3501	17760.1677	3052.65424	236.481261	6122.78002	10824.3986	1979.08344	40.6088673	9.03152426	2483433.15
P38	8.57294666	156102.546	21027.767	619.678314	497.868501	37609.4832	7672.24989	644.80778	425.220609	88516.0717	76017.5338	22849.9151	2585.09566	185.418768	22974.6537	43744.5997	4743.88545	120.674743	26.081942	2754206.98
P39	24.0204204	21972.5657	4656.24638	218.55725	500.875106	8258.51357	2135.45157	316.861802	487.115282	11791.5209	19799.7109	13851.2378	2024.95942	158.100986	4500.64793	6315.49974	1751.34032	32.3548752	45.6168682	2594106.42
P40	4.27032803	78467.8576	9057.96086	437.872737	341.511531	22823.7542	4119.91872	387.25854	554.089415	46101.8062	33169.6999	15775.1282	2402.87524	162.050337	16992.3418	25391.1953	2252.8464	75.5338153	34.9487634	2069272.91
P41	45.5445614	18432.0515	6417.96708	388.14633	1022.0312	2543.0618	1035.60492	376.763286	821.048583	7525.73293	11541.2864	22947.0295	3768.69565	238.028107	1905.03463	2350.587	1628.53309	10.1566591	35.7444328	2692991.79

Table 8.24: Raw peak area data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.

	PC[36:1]	PC[36:2]	PC[36:3]	PC[36:4]	PC[36:5]	PC[37:1]	PC[37:2]	PC[37:3]	PC[37:4]	PC[37:5]	PC[37:6]	PC[38:0]	PC[38:1]	PC[38:2]	PC[38:3]	PC[38:4]	PC[38:5]	PC[38:6]	PC[39:0]	PC[39:1]	PC[39:2]
P19	556563.329	55093.6106	7852.37772	2548.43191	369.600503	20859.0996	41460.0601	1583.50555	1164.4009	32090.1721	969344.298	104151.098	60511.6635	14934.0784	3281.79605	5690.07703	1387.55849	5941.58811	5462.421	31813.9268	4494.34355
P20	439384.376	32155.5556	4970.59149	1413.30903	212.576354	10267.7961	15274.0636	501.977202	655.869117	26123.8776	790901.004	44908.0622	37162.8857	8816.357	1427.39483	2136.35475	852.20549	3951.21495	3442.96706	11167.6098	1485.75656
P21	202013.994	14111.2064	2299.22297	478.280184	134.5628	5831.16193	13822.0123	351.346662	356.700422	12145.041	367709.534	32826.9355	20168.4592	3637.30867	608.225997	853.705794	318.67738	2089.5975	2675.44968	6019.10741	886.71486
P22	355087.122	44257.3899	7248.06518	2158.51429	413.602569	26691.7843	28003.8965	1940.60525	1210.01929	19036.8681	581835.987	52446.0123	46128.3446	14058.3124	4537.88773	8047.47134	854.977057	4243.00044	3949.04143	23434.8455	6240.06387
P23	395269.312	32991.3966	5467.1956	1423.39886	340.287958	8231.605	8476.13532	828.173693	683.96756	22996.9537	715034.847	24131.6383	30153.0404	8300.81903	1875.28999	2698.14515	836.629877	3656.77199	3286.88413	6037.9105	1275.64848
P24	442110.699	35714.2135	5869.46106	1396.68376	148.18923	9547.29017	23144.8892	769.603957	854.646584	26086.9831	799523.264	83474.3346	49106.6327	12017.176	2557.76083	3832.38691	1115.33601	4560.1569	5705.21194	14892.923	1955.43416
P25	479879.532	42291.2909	6768.89029	1935.05734	421.446905	13662.5277	16160.8112	819.225121	921.441559	28002.892	861828.474	41221.2878	39983.9712	11743.1017	2935.36458	3578.34959	1092.66926	4974.6035	3586.4098	12812.7489	1991.46067
P26	381388.603	27815.9995	3783.61723	783.0393	122.3197	8508.7497	13265.5135	505.055437	576.56988	23356.5593	693913.426	47307.9123	44652.4029	9999.27507	1133.0602	2407.23867	793.038521	3257.13847	3844.21869	8049.3322	1254.61236
P27	502149.463	41567.2594	5777.52557	1189.32528	143.440681	15159.3772	22454.9172	897.917687	896.773772	29578.1037	892226.418	78814.7153	64160.6456	15240.8239	2516.53212	4157.94963	1149.30269	6232.11358	6087.75811	13635.8327	1488.48109
P29	407119.532	30212.4135	4230.61926	1202.67531	73.2307555	11816.0483	16713.2402	749.472538	764.1467	24392.124	734008.596	48334.3339	32107.3985	6311.6733	1540.00245	2299.86019	924.486926	3709.94857	3142.73315	11540.0375	1697.06574
P30	398673.344	33833.7434	5461.94288	1734.2322	454.136447	18008.3959	37045.8948	733.64281	774.200631	23577.5094	697314.288	75526.9578	48186.1635	13021.364	2049.00257	3186.98088	786.930923	3928.18872	4261.76773	20498.9679	2201.94685
P31	316748.012	19496.4635	3095.14169	754.218779	30.3545673	5308.58845	9900.52473	322.182166	596.138915	19234.7863	589315.72	37015.9722	25431.0849	4987.92202	867.835959	1107.828	392.849677	2399.57307	1898.10431	6130.43013	899.805504
P32	512655.863	64496.0685	9737.6376	2305.80477	566.251239	26693.7418	44287.5017	1731.72332	1175.07127	29167.5962	891627.012	101676.881	61756.3863	17065.1477	5208.12814	8195.50804	1429.36091	6933.94949	4990.86063	38636.7097	5391.18506
P33	435250.991	44224.24	7323.75199	2251.23994	491.836854	18165.6393	24560.8348	1850.14368	989.328375	25156.6636	759524.365	63489.3945	51839.4347	12551.0993	4143.40701	6457.11301	1218.34275	6696.55052	5106.57406	16255.4748	3129.83403
P35	381109.795	36039.9543	7036.9466	2239.97814	912.458372	8258.91676	15615.1195	874.859366	868.621364	22294.3093	688638.592	32412.3209	22217.1619	5665.18233	2329.26313	2263.61099	709.468377	2279.65978	1887.25825	8694.4245	1656.72864
P37	400848.06	25680.3265	3423.16428	896.241307	55.9118233	4820.4786	10991.8362	401.646112	624.419926	24830.6149	738271.263	29354.6651	18790.9506	3243.06038	880.46788	1110.79604	599.888027	2756.98976	1817.19319	7749.68517	977.806343
P38	469896.301	50427.0698	8838.44656	2239.94528	206.303502	16858.164	20730.6401	1703.99887	1354.10442	27248.6158	820826.259	62724.0304	49375.561	13977.9521	4553.93497	6547.89597	1180.8108	5538.99015	4131.18419	15273.5309	1999.26074
P39	415902.007	25865.1371	4138.47343	1359.43781	134.728483	3033.19589	5629.55362	251.586068	590.325846	25014.5671	772360.145	23057.5595	15909.2027	3010.97044	792.37534	652.933519	599.121314	1946.25736	809.786116	3588.65499	416.546681
P40	344473.898	28303.969	4440.67714	1869.47925	189.935632	12725.3715	15955.8875	871.919284	681.469784	20425.106	614605.313	50459.5866	30754.7958	7048.22295	2020.06933	3225.45456	743.331402	3772.09154	3652.71357	11614.5955	1574.48352
P41	426769.658	23901.3031	3339.13691	752.43325	103.620296	2488.8216	3543.42781	79.9413904	446.044059	27041.319	801608.438	31245.6967	27557.8621	4433.20337	402.609625	523.270439	682.320823	2610.69932	1028.02105	2671.28625	335.782788

Table 8.25: Raw peak area data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.

	PC(39:3)	PC(39:4)	PC(39:5)	PC(40:0)	PC(40:1)	PC(40:2)	PC(40:3)	PC(40:4)	PC(40:5)	PC(40:6)	PC(41:0)	PC(41:1)	PC(41:2)	PC(41:3)	PC(41:4)	PC(41:5)	PC(41:6)	PC(42:0)	PC(42:1)	PC(42:2)	PC(42:3)	PC(42:4)	PC(42:5)
P19	2018.17314	4788.93832	10829.3186	26665.089	16798.643	3639.31941	1126.83477	1451.06076	783.707584	2968.75472	4392.99748	4270.20648	758.215444	3827.25318	2335.01496	555.19295	1661.28658	5407.34962	3102.17821	712.143589	733.149527	635.175398	293.706464
P20	738.002791	2370.29988	6452.40076	13977.5594	9882.30998	1842.80572	499.638573	495.564173	200.483834	1692.44189	1710.18095	1767.00084	140.728057	1057.68276	674.717971	201.294569	869.14062	2374.9335	1978.93861	386.987321	163.786347	245.982148	142.977028
P21	328.074196	726.628222	1996.8874	15987.5057	6082.96541	861.817732	242.104551	221.762682	166.220672	1678.08567	2538.36212	1385.83346	170.405982	702.753604	320.615817	255.749355	924.731031	3348.52367	1361.627	330.005736	230.690088	101.145819	101.633999
P22	3559.11651	4948.53562	6363.532	18227.391	8435.3675	2370.03414	1790.51551	2321.39799	1196.95611	2595.26033	3198.73921	3746.32796	750.170682	4412.87734	3952.74208	965.798437	1039.87721	3596.21971	1916.68875	517.610404	615.330562	690.81401	487.250472
P23	1004.48371	2087.6238	5425.04845	8778.85272	7076.22063	1413.48289	454.539124	644.216484	377.413819	1400.57529	895.832246	771.417603	302.701685	1081.22092	668.012634	336.497875	396.154213	1205.07853	1305.94065	294.542687	205.265175	138.296112	96.2460764
P24	906.192698	2981.30388	6599.50063	26776.7152	16069.8712	2818.0139	571.843917	835.873672	490.296	2455.87044	3602.83283	2968.24962	455.786516	1532.46444	1253.9758	375.804918	1417.02427	4041.77694	3196.00389	662.678634	515.656958	453.250817	239.881293
P25	1450.3826	3453.31287	8516.26995	13765.1597	9874.89228	1768.80841	839.41781	876.152501	248.694789	1898.61029	1837.15661	1923.43341	249.977139	2111.60131	1129.52192	382.593427	699.781963	2271.70796	1917.19902	446.265085	301.102092	316.659499	262.514597
P26	834.689307	2295.50854	5759.69036	17445.1308	12670.8957	2122.83241	470.375974	515.480481	163.743478	1414.24412	1822.43285	1441.55545	153.777206	1197.40564	721.845299	193.385014	958.05764	2671.99894	3098.29263	567.031037	292.867544	238.469329	185.049879
P27	1490.53953	4227.94317	10170.2766	25492.909	18213.587	2795.54922	807.672229	901.148779	461.434925	2680.32324	2804.70409	1970.75582	235.913196	1595.16373	1322.56634	302.428543	1253.84688	3944.83998	3124.48475	601.62923	409.031438	348.99506	279.925208
P29	1024.59996	2307.25217	5314.72647	17229.4051	8767.16756	1366.43347	381.351458	450.454796	285.272781	1786.90016	2075.92258	1759.83724	287.784543	914.317997	805.371681	258.076603	990.919111	3175.83024	1996.41104	287.13056	132.932504	180.578351	97.8490981
P30	1099.67647	3091.58799	7333.81852	18584.6663	9717.82548	2042.03899	642.797913	841.120068	360.216878	2692.33751	3823.41919	3181.57924	485.148476	1812.25338	1188.30884	608.32929	1248.36492	4505.42582	1789.41693	447.45546	428.007519	345.907494	265.826885
P31	420.246663	1577.32429	3731.67616	16975.8131	8095.79207	1277.47824	290.153555	280.556235	220.787595	1318.59708	1697.25144	1219.99891	65.1929248	701.970055	438.769132	124.539803	818.858399	3136.76341	1723.60741	297.493425	119.324944	73.2997531	100.44351
P32	2661.6719	4818.70491	8085.43164	30262.7409	20244.381	4399.90654	1703.76021	2056.86533	971.84728	3978.61742	5746.94688	5885.27162	948.086966	4225.18925	2642.47088	792.989526	1706.02877	6506.01625	4274.55368	1065.41332	1000.75493	707.617307	486.981561
P33	3013.36975	3935.58435	7696.27248	20371.3129	13890.8659	2414.20611	1074.99203	1603.81918	662.31162	2738.49051	2916.18838	2244.8957	724.704501	2499.56522	1602.52581	505.916793	1109.75145	3370.80559	3190.28192	578.685941	295.722116	506.129608	298.02342
P35	577.737497	2005.76669	4619.92584	11310.1861	5697.63445	1428.49854	546.639217	660.286394	385.495932	1593.25378	1508.71976	1684.5071	481.244713	788.637714	824.323271	351.218329	753.016466	1934.88537	968.738926	295.17328	185.926066	205.345849	86.0325663
P37	358.42473	875.974148	2029.11282	10035.0323	5027.00079	1044.1401	197.510833	294.556791	146.64493	1242.71799	1727.85624	1395.48512	254.722749	600.68411	394.103822	205.7498	494.449028	1806.28615	1085.15109	223.753425	124.516741	64.6882918	68.6836342
P38	2219.67407	3915.35716	7944.21284	22705.7187	14238.4235	2423.99991	1320.36788	1727.88726	646.84544	2230.32668	1710.62771	2274.96537	187.88346	2656.94403	1633.91477	331.712606	1093.06924	2726.75842	2953.67716	654.508118	446.837396	647.732283	337.005202
P39	238.119599	1422.128	4146.32922	10065.5672	6068.85491	1043.75901	130.789404	140.208568	141.694651	786.455878	743.411449	633.444982	101.221068	235.104821	188.91359	119.345274	542.174196	1608.98911	1239.43695	242.429182	65.8971118	56.8812666	26.0784616
P40	1929.93888	3177.83323	6234.4681	17561.8798	9246.792	1645.7961	575.444795	778.415369	279.43777	1865.64949	1931.93971	1848.12947	343.505306	1720.91862	1332.39763	453.598249	995.487454	3189.57537	1881.41002	417.338756	219.302558	217.257513	237.360283
P41	204.806891	1957.64343	5674.7941	9961.02568	7724.69838	1039.00565	128.752294	105.611773	53.0445109	769.208643	630.028221	487.304305	103.03412	197.158668	126.925225	67.4309802	519.48196	1603.98845	1471.53545	258.47655	69.6085661	47.4047769	57.196533

Table 8.26: Raw peak area data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.

	PC(42:6)	PC(43:0)	PC(43:1)	PC(43:2)	PC(43:3)	PC(43:4)	PC(43:5)	PC(43:6)	PC(30:0)	PC(30:1)	PC(30:2)	PC(d31)
P19	860.959262	67.2423188	560.934632	296.720603	1464.97652	834.0449	234.648462	467.012865	58149.4545	13459.2492	957.066375	152679.152
P20	372.943732	40.7842555	349.055763	131.896084	509.264091	103.37872	16.9443017	148.919458	20970.1675	5584.78885	462.310147	123178.829
P21	522.982373	56.5321729	327.677142	561.519606	156.719324	52.7885727	44.3536916	244.464413	30215.0382	5876.79392	256.376547	57189.8261
P22	675.378274	32.54038	397.627581	290.587968	1024.65914	987.740241	292.828878	322.617977	42271.124	8631.28454	336.471695	90588.5348
P23	328.39921	2.56366323	140.846203	24.6158211	176.962376	87.0639836	76.334595	106.656528	27762.633	7598.00196	753.6737	111798.906
P24	617.679442	114.521401	480.456685	261.963842	1018.50271	678.856982	156.026166	354.527778	34860.4982	9132.95519	763.827431	126097.648
P25	438.698592	14.9490103	243.334318	117.294814	569.980514	285.78787	67.6813283	263.611048	28407.1259	7991.21793	680.957493	132401.68
P26	348.302877	22.5217743	246.212191	119.238264	422.174641	230.898751	169.606112	196.27165	41675.3803	9619.56911	624.672629	106001.931
P27	700.874464	44.2781734	331.839805	169.26383	489.243467	373.823366	111.980285	366.893803	35379.0367	8693.56068	511.561243	139029.586
P29	438.503425	31.9259598	292.150116	87.9243228	275.201805	139.378154	272.265444	196.859808	22550.3037	4777.44761	338.92444	114250.446
P30	731.365605	99.0272893	404.294092	162.31404	586.939604	464.325528	231.609055	434.759134	39740.7383	12813.0094	1423.11925	107455.186
P31	368.945966	29.8176837	283.539616	78.0979082	186.988318	113.925692	32.3267645	183.183992	15245.1186	4285.04864	375.034627	89612.4629
P32	878.566899	123.600082	774.671449	384.789537	1765.14812	964.809668	354.990011	652.637385	47801.7859	10604.2519	728.667566	137030.198
P33	778.879321	31.9192547	400.178991	170.333495	576.284519	351.612346	119.140179	331.682361	39828.805	8259.45938	545.632708	116634.808
P35	373.857803	18.4300407	216.289416	98.9408134	291.99404	200.221115	184.808628	226.289691	27217.6021	6034.02017	480.809638	103743.7
P37	403.166976	20.350338	265.3879	66.3834899	220.411326	129.642623	94.05562	191.20601	27427.4216	6147.12294	505.422311	115923.244
P38	671.450268	6.91821348	304.149384	188.594463	897.183283	423.284615	141.942385	157.646819	37151.6848	9434.1453	768.884676	127037.155
P39	255.049859	23.8808169	94.9060498	35.45642	64.1764462	44.1967205	49.4590234	109.463485	17574.7606	4569.06981	376.447046	120242.584
P40	545.78687	17.4477338	238.853125	138.04427	568.038257	299.155291	158.959871	210.090356	40623.862	8368.72973	408.425396	94740.0678
P41	345.017061	40.2075838	120.31725	8.36695181	101.632966	24.8047863	11.7231483	95.2623692	30176.4892	6237.18461	366.077939	122251.725

Table 8.27: Raw peak area data matrix for phosphatidylethanolamine for hair samples taken from breast cancer free controls.

	PE(34:0)	PE(34:1)	PE(34:2)	PE(35:1)	PE(36:1)	PE(36:2)	PE(36:3)	PE(38:1)	PE(38:2)
C21	67.2695	192.9973	172.2952	117.3223	476.289	568.7347	134.202	137.6953	128.5944
C22	117.8008	53.7948	37.5228	44.209	127.1725	205.2767	24.792	37.044	48.7858
C23	211.541	72.6656	60.8228	35.4555	190.268	309.0033	66.9867	60.5031	60.6043
C24	221.5617	148.8815	118.2423	123.161	388.3358	463.8901	80.0068	150.1932	111.7965
C25	111.3574	39.9147	32.5355	25.6665	30.4226	94.5501	32.0122	8.5318	6.7376
C26	264.84	36.6018	20.9814	18.3137	54.3174	61.652	18.7389	27.3787	21.8778
C27	74.5054	55.9965	32.9101	14.8687	64.3524	63.1899	22.4559	30.1808	34.2847
C28	172.9104	94.0298	58.4415	82.7214	267.253	260.8823	54.3843	75.1371	52.9366
C29	64.7367	299.1736	109.6455	76.0907	544.1699	763.8944	99.6379	103.7521	79.3766
C30	139.5689	23.9876	17.9481	5.2322	40.5085	42.6961	11.379	29.7895	15.5186
C31	333.8977	128.4726	93.7096	89.4122	257.4097	452.4679	85.1328	50.4009	52.1621
C32	103.6167	9.8313	9.3855	4.0533	13.5989	24.6006	8.9852	5.3348	13.2943
C33	208.1925	14.7489	25.2541	18.77	51.5008	48.9579	14.7152	18.8392	15.6327
C34	109.9686	39.264	37.7396	21.6055	105.4721	110.7453	17.7175	19.7701	30.5749
C35	326.3882	70.1583	52.2833	18.8586	107.124	164.8173	45.0011	66.9018	36.298
C36	60.3189	38.415	68.7232	12.3853	93.6151	127.4857	33.6585	49.6768	36.727
C37	61.9067	115.8842	233.3679	57.063	292.9145	409.1969	130.7238	84.4633	77.4891
C38	222.9312	206.3232	95.3887	126.187	483.3194	702.1468	135.7806	139.4119	118.198
C39	35.4826	81.1386	53.9886	63.8002	205.7984	233.5621	32.417	62.9465	43.4337
C40	224.0188	5.4937	16.2666	2.0897	8.9219	22.7187	9.0099	7.2596	3.987

Table 8.28: Raw peak area data matrix for phosphatidylethanolamine for hair samples taken from patients with breast cancer.

	PE(34:0)	PE(34:1)	PE(34:2)	PE(35:1)	PE(36:1)	PE(36:2)	PE(36:3)	PE(38:1)	PE(38:2)
P19	103.7919	131.0683	88.6985	65.8711	321.4954	398.0467	58.0994	87.4579	77.0409
P20	103.6143	98.556	49.0689	56.6566	142.8205	221.7106	46.5327	38.7432	41.5942
P21	158.4002	56.8584	27.0194	35.4749	77.3713	112.9421	25.952	53.2486	35.9128
P22	139.3892	87.5909	101.8065	73.9463	296.1575	319.6433	76.024	78.9737	81.4389
P23	283.9836	63.9646	58.8812	38.2757	132.6179	232.6144	58.3669	47.0366	41.8957
P24	110.4887	28.0249	21.7697	22.3014	92.6751	68.4669	16.6932	20.8375	37.2036
P25	56.8097	183.3314	102.6311	102.0403	303.2386	539.7743	96.4001	80.8094	53.9006
P26	91.5982	26.4233	30.6535	24.0359	86.9697	93.2486	32.7241	59.0121	22.1403
P27	112.8279	85.897	60.7105	61.8822	225.8716	255.8713	61.3605	70.4532	64.8164
P29	266.5255	47.3277	37.0585	37.6538	116.4553	119.2518	28.1994	31.9059	31.9235
P30	105.9267	161.6208	73.595	103.2484	413.8901	423.4038	56.0224	116.6465	102.5491
P31	143.6828	18.5483	23.4924	20.7661	60.1388	51.4343	26.7107	21.518	20.0881
P32	30.4958	216.9388	137.9596	129.5696	520.8627	705.5172	163.4425	126.5997	85.8032
P33	100.2415	130.2946	88.7782	48.1389	379.4536	513.5614	105.1315	100.6399	76.8154
P35	160.9563	61.4973	52.1361	42.3234	117.5375	171.0315	36.8274	17.9332	41.1477
P37	65.8949	56.1782	36.2782	48.9804	81.0741	125.2537	31.478	23.3215	26.3641
P38	35.2799	97.8344	75.5976	61.6137	230.7609	272.7262	38.2022	72.5343	50.986
P39	46.8973	30.0225	30.2779	13.0096	45.6253	69.3525	25.5729	15.9348	12.2199
P40	19.7606	60.6524	73.6079	53.9538	210.3808	263.0894	46.2829	59.7713	46.4166
P41	240.6536	23.7267	44.8183	23.0068	68.9893	116.3582	14.4324	10.4721	6.1943

Table 8.29: Raw peak area data matrix for phosphatidylglycerol for hair samples taken from breast cancer free controls.

	PG(16:0)	PG(18:0)	PG(26:0)	PG(19:5)	PG(19:6)	PG(28:0)	PG(30:0)	PG(30:1)	PG(31:0)	PG(32:0)	PG(32:1)	PG(34:1)	PG(36:1)	PG(36:2)	PG(36:3)
C21	3521.176	4843.4189	1520.1983	742.8549	57.3302	967.0925	824.0469	577.4947	496.5344	1024.1133	887.6082	646.6461	191.955	309.9888	257.7465
C22	281.4539	309.7396	301.8926	463.8867	81.6937	220.9361	189.8799	86.5882	100.296	334.9791	189.2342	152.4807	49.2538	45.4924	37.9683
C23	186.0151	210.5644	117.406	577.8755	67.2298	75.1523	90.1574	28.3592	34.9462	153.028	48.0646	81.4079	37.8734	36.1818	133.6038
C24	332.4832	349.8383	324.3161	676.6025	237.8262	217.5343	166.0827	99.5813	67.8174	261.3861	115.278	191.9347	93.6961	70.143	155.7277
C25	227.2868	320.9516	311.9721	316.1726	93.7027	239.5737	268.1406	198.7859	137.2708	202.4882	218.0526	150.0327	25.4426	38.2938	8.1887
C26	91.4811	198.9202	189.6698	601.281	52.11	194.366	183.5282	82.9169	76.4708	331.3553	79.209	148.0858	58.2734	46.9428	63.2552
C27	322.1226	102.4031	165.7203	168.3302	48.0211	234.128	252.7272	184.3313	173.8156	309.3145	281.7606	213.5147	43.3812	51.5588	28.5636
C28	13166.2265	17108.6275	1882.64	695.5981	49.5078	985.5765	896.6602	476.2131	411.1523	1196.859	772.7294	912.3913	302.4183	735.5444	124.4204
C29	172.9618	156.2929	148.8558	531.739	153.2843	131.0633	134.2527	65.5737	24.7991	296.309	61.9882	116.5503	53.8811	48.3286	66.8431
C30	509.6798	457.9478	370.1731	392.8832	24.1053	323.3083	488.835	270.856	184.934	606.076	407.2009	432.6548	130.2998	141.4303	23.3718
C31	357.6192	489.187	175.1029	828.4973	105.9187	165.3801	134.9199	86.3696	44.5937	174.7825	76.743	93.7346	42.2804	49.177	132.9486
C32	328.9088	422.5328	329.2432	599.5166	51.5545	178.4304	151.3211	132.3039	54.6625	176.5057	87.1587	109.0559	34.3918	63.2357	20.4407
C33	405.6661	364.401	700.8088	526.8798	39.4475	513.1096	309.3541	336.6438	227.5356	323.9066	344.7014	210.4436	37.9131	78.5994	36.351
C34	20462.7158	31221.5403	14213.5649	368.9112	229.3133	5960.2182	4492.2251	3244.0145	3512.6644	4218.7921	4517.8946	3876.5335	1729.5672	2599.6214	62.8769
C35	229.3388	281.1776	166.78	638.0816	77.2438	120.4827	136.8591	62.4483	56.5665	273.4102	68.0403	101.035	56.9549	32.8258	122.205
C36	1249.945	1988.2266	824.6253	592.3577	110.8638	481.9068	240.0389	201.8484	85.7333	311.7543	139.3215	169.5481	117.697	164.0025	49.6797
C37	34888.1912	25601.9354	2594.505	299.0604	76.4407	1177.4586	869.8455	597.3373	525.5626	1176.3583	1104.5628	1022.8904	364.5422	838.4744	168.202
C38	431.2077	881.4118	2004.1533	620.1608	128.0049	1159.7917	910.4885	560.2786	230.2477	464.0373	451.5911	278.594	87.9269	157.8808	216.4685
C39	343.0744	456.2124	213.5041	659.4689	193.1848	241.4635	265.3287	145.9178	114.514	360.2327	200.3318	233.9808	84.7569	86.4309	75.4009
C40	286.8169	237.7565	89.6848	354.3613	33.3975	77.0503	67.2163	55.4293	88.4909	161.4043	83.562	73.3617	34.7711	33.052	14.5793

Table 8.30: Raw peak area data matrix for phosphatidylglycerol for hair samples taken from patients with breast cancer.

	PG(16:0)	PG(18:0)	PG(26:0)	PG(19:5)	PG(19:6)	PG(28:0)	PG(30:0)	PG(30:1)	PG(31:0)	PG(32:0)	PG(32:1)	PG(34:1)	PG(36:1)	PG(36:2)	PG(36:3)
P19	395.7525	465.9653	358.5672	815.256	84.6976	382.8912	381.3754	146.4764	92.8647	657.9147	194.7448	328.1358	190.512	176.3124	329.6815
P20	6028.7665	8403.5351	1998.1428	685.8085	75.1157	939.0516	637.7317	592.3191	469.1096	790.4726	752.7916	778.9137	203.728	481.8464	68.5195
P21	156.4115	178.0654	331.295	230.2881	25.8727	309.4478	464.9897	244.6808	298.9194	634.3596	496.461	465.188	101.7337	189.9733	55.0879
P22	2963.4523	6293.0272	3400.2784	458.486	25.9829	1960.2836	1305.7519	913.6254	535.7723	944.0611	1001.8843	673.6771	103.9161	257.6654	532.3474
P23	162.2064	319.6921	149.2775	405.3956	57.5887	128.3412	115.9996	55.7375	78.6455	152.1324	111.5175	101.8266	38.0047	58.1909	121.8197
P24	1802.4388	1970.1229	2812.1125	443.1133	82.5473	2044.5561	1216.6898	1004.1409	214.7285	1136.7744	677.0252	669.1508	233.3689	464.236	89.3173
P25	347.6507	407.8868	327.7388	399.2924	181.2579	349.1481	335.3992	157.2869	80.8951	372.7861	211.5139	298.8393	104.3175	123.3284	171.3956
P26	405.2995	446.1832	649.6862	273.5531	65.9263	500.8939	256.24	212.8989	53.8928	240.5835	112.4982	238.1254	71.9299	348.1884	63.4644
P27	189.3605	267.5672	254.2019	850.641	119.4028	232.3757	180.3414	78.7623	66.7567	331.3331	79.0034	147.4999	92.0012	85.9169	108.8634
P29	2944.0533	4419.1882	2643.0903	681.4369	44.4319	1448.7068	708.3337	419.1261	400.2655	798.0575	484.7893	622.5683	316.6637	660.3085	67.2358
P30	786.3847	1119.1572	684.8971	548.6558	72.2454	489.4989	329.346	400.5445	53.6739	286.8092	146.2699	265.1905	147.4688	153.2434	216.9717
P31	1430.6946	2605.9918	1672.8317	531.0709	45.6773	758.3521	500.9403	333.8309	288.2272	636.9317	568.4015	489.8791	189.2215	235.0048	48.5921
P32	2039.1011	1557.5857	527.9579	523.8176	193.867	401.8902	327.6363	157.042	122.9107	583.1225	207.7212	297.1054	214.9759	152.5604	198.938
P33	726.7188	1066.6084	972.7291	653.6932	107.5478	486.7221	374.7605	214.5947	253.8343	593.964	297.8544	303.6217	170.9524	197.2062	168.1611
P35	20688.5589	34257.2269	6628.3406	432.9291	78.3304	2484.8618	1806.1011	979.1409	1006.1726	1714.8061	1540.4811	1512.3285	530.3545	1522.8505	110.3193
P37	153.4057	155.6793	402.6227	556.8541	50.1762	311.0038	188.2394	122.9846	60.6843	336.535	114.4877	90.3779	29.1083	25.26	58.3954
P38	5357.4391	7529.3142	3055.4287	646.9546	90.9723	1039.122	655.4754	525.6285	323.9926	598.4803	623.716	407.5711	128.4735	312.333	255.2348
P39	8314.6111	15637.3603	4314.7989	738.2682	44.8451	1385.0564	1171.2622	841.9747	756.3048	1233.9141	1341.1375	843.2736	196.2982	531.6067	37.1705
P40	348.7357	348.2366	475.539	531.4521	121.0089	354.6532	377.1174	232.9312	138.4638	449.8535	329.8787	325.0489	154.7105	175.4966	107.9805
P41	935.0884	1475.1181	3959.2129	665.9351	100.8634	1599.8342	1977.7878	1226.5939	1758.5058	2185.268	2363.0067	1281.2739	275.0102	592.548	42.0367

Table 8.31: Raw peak area data matrix for phosphatidylinositol for hair samples taken from breast cancer free controls.

	PI(16:0)	PI(32:0)	PI(32:1)	PI(33:0)	PI(34:1)	PI(36:0)	PI(36:1)	PI(36:2)	PI(36:3)	PI(38:1)	PI(38:2)	PI(38:3)	PI(38:4)	PI_Cer_1	PI_Cer_2	PI(34:2)
C21	378.9843	1018.9772	134.9259	100.3677	1343.868	1404.5679	2639.6557	1776.2436	142.3259	386.9251	162.6175	410.2991	320.35	37.9072	70.9522	268.6016
C22	69.2077	277.5527	130.5432	63.1817	490.6493	510.4647	621.9167	210.5544	82.0736	233.3306	96.1691	111.1707	184.3938	76.6471	181.2654	27.1071
C23	86.691	703.0467	80.0106	230.2336	867.6326	1060.021	1538.0016	625.4739	111.1061	214.6043	47.9554	184.8478	115.07	46.7092	160.922	78.1258
C24	178.2112	377.415	196.3385	178.5735	574.9438	662.9161	1206.8524	673.4092	63.7508	265.5191	218.0197	182.6376	125.7323	158.1295	110.5002	144.1373
C25	239.441	107.7164	268.0195	79.164	509.9996	215.1044	713.1095	623.0328	454.9474	213.127	291.3557	249.2713	141.1423	146.24	58.904	226.5232
C26	80.526	364.2364	248.0054	198.781	408.9666	495.8454	783.6836	332.2005	127.1509	260.9472	369.3898	279.0211	117.3943	141.019	114.6311	108.1198
C27	83.0513	549.1304	321.38	629.7662	727.8868	915.8922	1248.6741	1089.325	217.9201	440.6002	113.7492	287.4497	235.8421	70.4513	116.9227	528.2742
C28	169.9976	617.5412	168.9175	64.6216	596.8448	1139.0066	1376.4839	742.7873	47.752	177.3903	62.5539	116.8051	148.7404	43.2725	60.8725	104.8928
C29	76.0412	1045.8539	176.4864	87.302	823.6691	1361.1541	1910.3501	420.8346	75.9029	426.6213	60.5812	157.4253	188.8592	117.1302	135.236	79.3935
C30	142.5888	611.2559	269.4636	69.3229	404.8125	1259.2201	1187.6615	249.6841	283.4684	220.9645	77.1961	44.2211	144.8174	199.7175	252.4253	132.302
C31	80.0755	504.7679	105.7877	142.2005	754.1023	832.4449	1584.6658	992.5278	80.194	307.8937	152.4531	149.224	210.7974	73.2838	98.3732	134.9768
C32	85.8105	210.5119	75.9425	35.5319	121.3914	46.4078	98.5044	68.7669	46.8636	34.2847	20.0959	8.2195	20.6957	158.3485	80.6446	39.9395
C33	71.359	219.2256	172.4932	95.0131	257.0675	677.5124	604.1462	196.4905	83.3623	112.1122	82.9728	21.3583	34.1613	49.3128	85.1665	32.1802
C34	221.5891	372.5788	296.2723	130.8844	580.0445	257.3123	616.6147	474.6002	62.5224	262.3953	150.543	97.1266	45.3843	124.7883	73.6405	147.4277
C35	164.1432	475.3672	353.6815	164.2323	785.2972	832.5115	1513.7845	1305.0823	218.1217	386.6426	275.9268	320.7582	135.8663	48.7509	57.564	238.2551
C36	22.1233	273.532	87.12	24.8109	332.7616	286.8165	325.5891	188.8389	52.055	47.5272	38.1101	40.4116	25.6204	143.7268	25.039	93.453
C37	129.3478	660.694	197.1365	129.6969	1309.6183	1025.5954	2150.5285	1529.2391	122.0155	402.2379	273.2489	375.028	189.9716	39.9559	53.8147	760.0143
C38	50.6197	572.9741	285.2902	170.257	665.2472	1310.011	1988.1995	915.3658	42.7147	323.75	184.6778	207.9755	259.7517	35.4872	43.4878	54.9582
C39	178.9443	261.3904	68.5245	92.21	425.4629	587.9904	692.0985	341.2159	28.5763	38.3551	35.1162	37.4869	38.6559	145.5421	57.4066	73.5551
C40	25.4664	166.2456	299.323	304.8036	429.0948	58.8025	241.6817	318.237	470.9722	390.8375	78.5664	146.4765	54.428	54.9737	33.1335	142.8719

Table 8.32: Raw peak area data matrix for phosphatidylinositol for hair samples taken from patients with breast cancer.

	PI(16:0)	PI(32:0)	PI(32:1)	PI(33:0)	PI(34:1)	PI(36:0)	PI(36:1)	PI(36:2)	PI(36:3)	PI(38:1)	PI(38:2)	PI(38:3)	PI(38:4)	PI_Cer_1	PI_Cer_2	PI(34:2)
P19	196.9747	814.7782	263.0747	198.6543	1285.013	882.6377	1581.7968	678.4466	85.1039	272.4083	173.7729	132.1531	164.3297	89.3561	81.0691	97.9073
P20	207.5056	474.7683	166.4087	89.0705	494.8581	590.7747	982.726	585.0641	39.8014	169.9421	57.1352	105.1354	94.3856	109.3907	95.292	221.5464
P21	189.5724	950.2284	473.4817	634.9701	845.0741	708.0514	1953.5253	643.526	2032.0879	902.1614	289.25	296.2291	203.6641	196.1455	283.5755	180.5177
P22	248.6091	860.724	340.8676	122.088	1466.6067	1083.7728	2114.7075	1193.8828	57.6062	388.4784	106.4798	258.5666	398.3044	150.0197	62.297	146.2092
P23	131.104	293.4767	209.8391	80.6715	424.1858	263.2993	1031.2432	500.0797	102.8557	180.9062	135.6578	115.2402	117.5599	116.5912	128.9588	139.9638
P24	176.1966	281.8172	302.9878	100.0314	635.0273	662.2868	605.6508	221.5654	23.8046	105.2461	70.7374	54.2679	204.4024	106.3546	42.0455	118.4148
P25	40.9727	573.7202	366.7726	135.3471	791.3323	715.2261	961.9495	513.9903	61.3399	200.1748	113.8326	32.4001	138.9987	189.1222	29.8252	23.3146
P26	87.2695	337.1068	178.0272	69.5744	660.024	298.8688	590.5347	701.3628	78.4572	204.2967	117.6634	191.4522	186.0975	51.6301	52.5977	57.4318
P27	275.5561	440.2546	143.9856	112.0902	628.8344	899.7225	1188.3674	626.1239	47.2057	274.3773	82.8886	220.6708	153.4956	146.2801	34.6568	144.6277
P29	144.7143	871.6575	611.6654	317.5704	1615.0547	430.7585	702.836	676.9595	195.2436	514.8286	132.6818	67.5672	207.8784	92.4692	87.1393	428.4628
P30	69.0758	630.6645	799.3848	123.5683	782.1163	782.3189	1144.872	430.5138	24.6835	151.5135	67.4301	86.1879	68.3229	80.6832	47.9688	52.7974
P31	147.173	532.8835	429.0573	268.7753	611.8198	282.6998	461.1259	468.4974	115.7255	276.1117	89.3535	118.1633	72.9133	102.7937	90.9487	161.1743
P32	310.8596	622.7669	223.7494	228.6071	873.3978	1596.6022	1891.5356	1122.1713	36.9814	367.3586	155.8753	199.8906	97.573	140.9204	61.9138	142.762
P33	180.8122	855.5639	91.3909	129.2326	757.0113	1022.6019	1578.1994	547.5837	70.3506	226.0096	71.1725	162.5474	157.6324	126.3182	66.3853	37.9755
P35	291.9548	445.206	341.3223	71.1293	749.8902	576.0887	1090.0001	505.882	87.1058	417.9389	234.8621	175.0771	208.9122	406.1327	57.0403	122.9649
P37	102.4032	296.6418	210.8776	47.377	453.4715	681.3025	751.2901	267.0853	211.7843	344.0878	138.8302	51.4816	77.0598	64.9502	83.542	31.3407
P38	122.2737	1161.7873	429.2996	277.0736	2183.9545	988.0313	1696.8717	944.5908	54.4535	458.3833	147.2657	215.3264	414.2067	87.5816	99.5691	172.5488
P39	160.8739	381.145	330.5861	127.6723	511.2711	181.5987	344.5204	305.4792	98.5237	74.6823	12.4399	33.2917	15.7246	163.501	115.2388	84.7883
P40	131.1711	2086.9649	327.3054	573.0334	3178.0604	2209.716	4540.1721	1808.7333	153.6656	657.5851	295.8984	388.838	432.3217	67.3466	90.1478	265.5175
P41	161.7246	617.5486	235.6389	115.6387	391.0083	339.3985	547.0192	357.5931	164.0512	137.0426	178.3498	82.4978	94.286	171.3675	171.0047	107.5075

Table 8.33: Raw peak area data matrix for sphingomyelin for hair samples taken from breast cancer free controls.

	SM(30:0)	SM(32:0)	SM(32:1)	SM(33:0)	SM(33:1)	SM(34:0)	SM(34:1)	SM(34:2)	SM(d31)
C21	11.3656226	673.940055	12.0974134	1112.56643	1114.83165	167495.806	14812.5241	197.117884	140494.065
C22	23.1471859	184.862493	NA	373.591094	372.146529	75223.147	4320.45069	74.7649416	49375.8612
C23	21.4857323	299.060144	NA	975.683899	975.683899	97009.0662	8338.42335	88.6182709	41828.9051
C24	71.0026411	300.763366	8.16517617	1207.86519	1207.86519	73915.8864	9829.85759	303.593019	90253.8951
C25	65.5627978	462.78165	37.8234695	1088.79979	1088.79979	52891.6112	9322.17657	193.466845	17310.3225
C26	22.76178	194.755678	20.3855554	826.936856	826.936856	49532.1888	4642.66024	84.1253816	36170.6661
C27	27.105001	618.22028	6.43243589	1625.00214	1625.00214	169344.451	16165.8987	309.07283	44995.4477
C28	20.7351556	491.551447	NA	807.846092	807.846092	55638.2652	5695.03219	171.599561	86614.0087
C29	43.2304585	162.946469	8.88834958	490.914152	490.914152	83581.2602	4546.78047	92.041154	125363.268
C30	39.4584127	298.618608	9.18985181	608.788371	608.788371	45297.0818	4046.32932	63.838748	14085.2987
C31	16.2314756	538.701795	8.56617416	2046.5671	2046.5671	219147.809	13110.6784	172.419901	68238.1045
C32	16.085899	144.747999	10.6033133	256.498511	265.256839	9189.65755	2516.25259	52.6850308	14595.3445
C33	13.8456354	127.92018	18.1437857	554.120825	560.964282	59977.1378	4461.96368	40.8284966	19608.1287
C34	NA	439.149179	NA	1025.27761	1025.27761	133424.276	7567.71162	167.93714	35918.9104
C35	23.5830709	632.735902	12.184103	1566.97833	1566.97833	146734.431	10044.9735	349.485001	51853.3743
C36	15.2826621	111.796957	16.6227269	401.499028	406.831538	49856.2395	4717.87953	18.0022812	42126.1667
C37	21.3280128	553.002752	8.17370989	1258.2493	1249.09309	143158.942	11040.3307	220.423669	75929.9938
C38	13.4263068	875.189165	8.17978949	1977.55381	1977.55381	229197.718	17639.5354	611.975518	86640.4313
C39	63.2459596	263.356277	7.6305308	613.382676	613.382676	70423.8767	7229.77694	101.045704	47661.4948
C40	NA	149.498349	17.5783131	398.610444	406.115727	29520.6524	4751.42265	16.0588548	32778.3123

Table 8.34: Raw peak area data matrix for sphingomyelin for hair samples taken from patients with breast cancer.

	SM(30:0)	SM(32:0)	SM(32:1)	SM(33:0)	SM(33:1)	SM(34:0)	SM(34:1)	SM(34:2)	SM(d31)
P19	29.9569964	416.032457	NA	1511.92687	1511.92687	143848.502	12874.7845	155.262981	143704.885
P20	NA	284.703069	19.0849505	823.011945	823.011945	50725.1128	6847.25717	22.3612894	34867.4498
P21	128.514733	145.623734	57.6748866	625.888942	625.888942	76510.7288	4376.44969	56.6984312	37400.0053
P22	NA	400.873507	21.2154036	731.935542	731.935542	103799.171	5049.73176	120.905498	129234.524
P23	10.6255345	406.658759	10.0159581	1487.99429	1487.99429	69445.1761	9908.56374	213.14192	46719.2612
P24	48.7866526	580.007071	15.0644984	946.283984	946.283984	86965.2832	10993.0644	122.239397	104124.55
P25	22.1402815	313.032099	28.4326256	888.989727	888.989727	69279.5527	9919.91755	135.952999	73139.3067
P26	26.6880281	467.011465	20.3671479	1193.39737	1193.39737	102699.509	8319.02272	140.397418	54469.3891
P27	19.9434971	317.180865	NA	998.094848	998.094848	86960.5964	8434.38897	92.0046478	62945.1897
P29	27.6596387	232.489055	14.2008501	1439.88765	1439.88765	57225.9475	4776.33589	46.666153	43790.6647
P30	13.714917	821.253076	111.896329	2165.38506	2165.38506	98924.976	19234.6408	461.311316	150037.789
P31	15.8040062	295.316407	14.6211968	796.83353	796.83353	37235.4485	5800.27378	81.4203327	43143.094
P32	23.4785001	466.80664	104.975321	839.813628	839.813628	108485.089	9219.19128	165.233937	73892.7711
P33	NA	302.557269	13.4961508	1022.13494	1022.13494	94107.8863	8453.92064	63.1356368	83780.9208
P35	14.6233414	332.798385	7.99887474	813.053188	813.053188	65012.2734	6514.79566	70.3552673	79482.9872
P37	25.608665	207.799759	21.5483937	936.104896	930.727331	68265.3965	5780.39143	43.9128019	45573.6077
P38	26.1383741	528.649013	7.63722178	1016.31073	1016.31073	88368.3247	10576.3652	68.9402986	156102.546
P39	35.6233502	187.368146	NA	451.891604	451.891604	44005.6563	5049.48854	74.6099719	21972.5657
P40	20.2018089	310.582544	NA	747.253019	747.253019	103647.52	5943.73609	110.55647	78110.6693
P41	19.5346054	198.557486	15.8236208	434.612198	478.088991	73831.9587	5803.87581	29.4491958	19191.4449

8.3.2. Normalised to the mean data matrix

Table 8.35: Normalised data matrix for cholesterol ester for hair samples taken from breast cancer free controls.

	CE	CE(13:6)	CE(15:0)	CE(15:1)	CE(17:0)	CE(17:1)	CE(17:2)	CE(18:0)	CE(18:2)	CE(18:3)	CE(19:1)	CE(19:2)	CE(19:3)	CE(19:4)	CE(19:6)	CE(21:0)	CE(21:1)	CE(21:4)	CE(21:5)	CE(22:0)	CE(23:5)	CE(23:6)
C21	2.1184837	0.88475531	1.49445193	1.34972605	3.15193148	3.74032666	1.15571527	0.20909123	4.50452801	5.01957476	5.41698688	3.59533478	2.08939107	1.01005456	0.94573642	2.41710557	1.22967556	1.03046395	5.22653488	2.00507233	0.86262911	2.01281195
C22	2.04216886	1.58802602	2.47123414	2.32252041	3.92358272	4.83096952	1.57648296	-0.4242037	3.95049337	3.9378139	4.54410581	4.56908861	2.86794091	1.65567039	1.63510844	2.81572304	3.11891578	0.49286966	4.35804228	5.58063277	0.85968108	0.92389744
C23	1.91612181	1.19663149	3.21101989	2.4537614	4.86629284	5.41014256	1.4267666	0.73159332	3.97286081	4.21118343	4.117395	5.13204613	3.07755801	1.48239539	1.92939005	2.83986431	2.66058366	-0.2137633	4.02184026	1.72784145	1.51151284	1.5247915
C24	2.68681866	0.27255891	2.9216604	2.63229242	4.1625841	5.15645398	2.33045122	-0.5726879	4.11088539	4.45108322	4.90320863	4.65935365	3.29837164	1.34232018	2.04533269	2.74407644	2.15066151	0.76706194	4.70166353	1.95096027	0.86981999	2.02707258
C25	1.56058623	1.10357146	0.53093393	1.35908289	1.38712379	3.39281509	0.98810698	-0.4503703	2.93561275	1.76269082	5.04415904	2.8919646	2.05928666	0.91881255	1.45751589	2.58035787	2.27804128	0.73695629	4.75362513	2.20039899	1.23742412	0.57346864
C26	1.89319278	0.38155713	2.86316023	2.76126085	3.96391065	5.10999432	0.38604214	-0.6813386	3.85792015	3.93638418	4.9299539	4.51338686	3.34718367	1.38859255	1.76770582	2.65920794	2.33953592	0.83501704	4.65851675	1.29108034	1.38080348	1.34977819
C27	1.70613491	1.61017731	2.53532235	2.50689108	3.79520563	4.74522842	1.32787652	-1.3327555	4.27343362	3.10535533	5.19785808	4.05206271	2.81922473	1.92163665	2.21283722	3.34617624	2.37954644	1.2465498	5.01995451	1.74541279	2.18316666	1.61601036
C28	2.94405213	2.38006783	2.356871	1.8118843	3.25979417	3.86197799	2.01360918	-0.3077689	4.65759597	5.20531019	4.37749226	5.21030835	2.63435493	1.39612703	1.44490461	2.76912246	2.30069658	0.23775237	4.01481155	0.86389091	1.40646457	2.40433159
C29	2.46407358	0.71976477	2.92378926	2.57596266	4.20424006	5.01861764	2.21296825	-1.1305417	4.34536816	4.78602573	5.30059044	4.80673595	3.17457845	1.35962032	1.6536161	2.78885789	2.88002456	1.1220986	5.11061578	2.15904583	1.54836234	1.70815462
C30	2.08197972	1.29796291	2.33606434	2.52007074	3.68109295	4.79271186	-0.1787959	-0.5039634	2.70587313	1.74498239	4.22658141	4.16878914	2.05272858	0.82829202	1.58334876	2.48813215	2.31109891	-0.2175283	3.93514224	1.38435357	1.67165823	-0.2023209
C31	2.2419443	1.57932723	3.16110965	2.78608936	4.28305672	5.13859713	1.68850668	-0.6975947	3.94110609	4.38317141	6.06155163	5.03807723	3.28999367	1.71740571	1.99523036	2.80666382	2.4574142	1.69044977	5.83279349	2.77532852	1.33258038	1.6214128
C32	4.1749529	1.73591465	2.82156813	2.57813891	3.93810848	5.01133783	1.29923799	-0.4797313	3.4478666	3.42693847	4.71596455	4.67778602	2.92580089	1.25563439	1.93748883	2.55371174	1.05717452	0.27679677	4.36312989	0.89446512	1.2302965	0.87437633
C33	3.34302836	1.31698689	1.61724411	2.67806858	2.86875161	4.56770724	1.24877826	-0.4983742	3.8625807	3.6071213	4.64988951	4.07426354	2.83346482	1.1699957	1.70726916	2.81130497	1.93986973	-0.0588426	4.47179773	1.67401928	0.56631114	0.51204467
C34	1.98732159	0.80667073	1.70154737	2.18905785	2.86952086	4.29454481	1.47926716	-0.3287717	3.74603034	4.04213689	3.8408059	4.11482832	3.08145953	1.15503456	1.91458059	2.35293471	2.46616924	0.0850921	3.72677233	3.15949556	1.0612565	0.73487873
C35	2.01818252	1.25927059	2.86014731	2.74867779	3.93260921	5.27252367	1.99027977	-0.0357956	4.1033951	4.58322909	4.66008553	4.81001111	3.1502442	1.51251034	1.65061085	2.82843854	2.41663806	0.83160257	4.51048537	1.34705303	1.94016207	1.37688533
C36	3.42340008	1.28983276	3.16793368	2.58328975	4.41753318	5.35748903	1.88634098	-0.6572955	4.64739094	5.02803473	5.07008067	5.39925212	3.24305743	1.91149805	1.89522935	3.23067326	2.4534308	1.01913023	4.80480422	1.31420488	2.30872062	1.76051573
C37	1.71728854	-0.1971055	1.71053504	1.51489869	2.4574849	3.69115408	2.07906953	-1.1282876	3.81291973	4.2310398	3.98523459	3.61849825	1.83719904	0.71652768	0.45749065	1.6475677	2.71023314	-0.2470705	3.84575787	0.90954017	0.74728055	1.59008986
C38	2.23362502	1.43739935	1.46015135	1.75439338	2.2903913	3.72391044	1.71661696	-0.5540342	4.33068673	4.79271294	5.33660316	3.832813	2.35829143	1.15675994	1.85855641	2.57828398	2.66632589	0.93081298	5.03422097	2.05887571	1.56119622	1.56596285
C39	2.25583895	1.15835693	3.07764008	2.5779837	4.18625109	4.80599448	2.60625588	-0.3894122	4.3621819	4.76283753	4.88599086	4.61165927	2.70975369	0.99246271	1.6910179	2.63869192	2.61366436	-0.0824883	4.66702218	1.81935482	1.33433125	1.9787138
C40	3.77457932	1.74568561	2.83942719	2.33098372	4.00559414	4.84102715	1.13327248	-0.9119917	4.1983367	2.69377353	4.63656942	3.99781426	2.74528703	1.81122357	2.1527729	2.96946438	1.06562534	0.51366801	4.45637506	1.17337183	2.46227936	1.12554629

Table 8.36: Normalised data matrix for cholesterol ester for hair samples taken from patients with breast cancer.

	CE	CE(13:6)	CE(15:0)	CE(15:1)	CE(17:0)	CE(17:1)	CE(17:2)	CE(18:0)	CE(18:2)	CE(18:3)	CE(19:1)	CE(19:2)	CE(19:3)	CE(19:4)	CE(19:6)	CE(21:0)	CE(21:1)	CE(21:4)	CE(21:5)	CE(22:0)	CE(23:5)	CE(23:6)
P19	2.31040944	0.99530906	1.7805594	1.46274182	3.9840136	4.18038125	2.63378217	0.40829966	4.79815333	5.20255636	5.42086144	4.08513037	3.16572648	1.59312163	1.15002286	4.32140201	2.99712677	1.11752844	5.18995335	2.14729187	1.75770516	3.09990574
P20	3.07752215	0.50871236	2.69141653	2.32333926	3.60675399	4.82226058	1.78211541	-1.0691957	3.79506988	4.19636909	5.51189916	4.30845424	2.47490333	0.67557121	1.35796584	2.57419771	2.15816468	1.39367995	5.25390605	1.85900553	1.24318423	0.81973274
P21	1.65269169	1.65433343	2.24447614	2.15710381	2.85432875	4.45256593	1.34780131	0.28298917	3.92236187	3.56941046	4.40445309	3.89241524	2.61620143	1.32558184	1.90081725	3.25577943	1.58667362	0.37211759	4.12445621	0.91832865	2.09994333	0.95342686
P22	1.95648398	0.39883791	1.38039685	1.70383743	2.60470857	3.52767059	1.72614128	-0.7774253	4.19812569	4.52089656	4.33576012	3.3647831	2.42253073	0.87206082	1.47967411	2.50612077	2.12663974	0.40854185	4.21076036	1.02663083	0.92229679	1.91636317
P23	3.07744876	1.84066867	2.38768328	2.003104	3.5967299	4.14005339	2.1829346	-0.6686908	3.47569768	3.49082906	3.82597801	4.10092571	2.28366616	1.00653705	1.7855651	2.76188892	1.85841796	-0.0607794	3.60431052	2.92488072	1.59583277	0.60346037
P24	1.86761292	1.00907842	1.02176418	0.17681076	3.20865316	3.09395724	1.6145269	-0.4229247	4.59392444	5.05640676	5.07696239	3.35432533	2.17848842	0.90279087	0.81973952	2.84583387	2.01935757	0.97914278	4.87982143	0.98920584	1.34356849	1.99165223
P25	1.93973248	2.04253905	3.16341767	2.42246785	4.31649616	4.80210153	2.10439687	-1.2351931	4.16486418	4.41123738	4.3008055	4.48196739	3.07198781	1.36901822	1.77894906	2.99505413	2.6380345	-0.1963411	4.03827092	1.4215732	1.5271091	1.16180625
P26	2.74545595	0.98867602	2.32417456	1.48857065	3.53325005	4.41024422	1.51695244	-0.037455	3.93915447	4.36112018	4.64149782	5.48901305	3.66845617	1.79120317	1.22606074	2.89266387	2.35372171	0.69692425	4.37047872	1.16749662	1.65277901	0.12475749
P27	2.23323702	0.83782231	2.7153059	2.10908074	4.27033151	4.586293	2.05136995	-1.1267644	4.49351721	4.98428338	5.52685416	4.56611418	2.53990617	1.17516237	1.33946232	2.7601731	2.72370166	1.17852133	5.26526509	2.12350403	1.1651069	2.22828744
P29	2.85595153	2.87804865	2.85398213	2.05359754	3.96715303	4.47132863	1.09307548	-0.5183752	3.98678138	4.17439089	4.33599857	4.28484926	2.63705487	1.20940704	1.73802176	2.78270213	2.19891025	-0.0237706	4.13580836	0.65997062	1.63845037	1.66173222
P30	2.20893808	1.36514469	2.49886538	1.87350735	4.37637904	4.45571304	2.73271455	-0.1623922	4.97401817	5.45676805	5.24472341	4.61176114	3.32858331	1.4431146	1.20971251	3.89553962	2.36644116	0.82458371	4.95285487	1.66049677	1.70632303	3.33878062
P31	3.61877103	0.99974468	2.07011523	1.92434332	3.30311458	4.55461843	0.80963645	-0.9819559	3.57307656	3.49265211	4.3521333	3.89097263	2.47089352	0.9153606	1.81808711	2.86729972	1.49954729	-0.2536184	4.16019434	0.54073741	0.9686589	1.04039984
P32	2.43220644	-0.5230844	2.71231969	2.01606602	3.65934579	4.36086006	0.36248082	0.00450352	4.49745295	5.08553438	6.14987662	4.08593319	2.27978718	0.85678669	0.61238769	2.50880079	0.75978049	1.88272533	5.99635476	2.86842952	0.39188131	2.7977665
P33	3.76544574	1.25929364	2.65454243	2.04575733	4.30935911	4.60223639	2.03227927	0.47949753	4.55900081	4.97842421	5.56203027	4.35620018	2.5699492	1.2770075	1.62766928	2.8705409	2.59313145	1.3035618	5.31667413	1.99034488	0.28079502	1.12778151
P35	2.43270395	2.44248887	0.96773808	0.8807594	1.63331434	3.18846146	1.45531307	-1.8442609	3.67483916	3.9001085	4.85979768	3.05521418	1.87986764	1.55307521	1.08149898	2.31862083	1.76916658	0.82678033	4.66851073	1.43894463	0.78546995	1.58211682
P37	1.90407372	0.38467881	2.93129897	2.81736641	4.32616655	5.18923273	0.46909644	-1.0630838	3.88190768	4.01063448	3.17341924	4.65682906	3.17969302	1.17744749	1.77429715	2.75372354	2.67129057	-0.85063	2.99943237	1.48697377	0.62383888	1.42311569
P38	2.84110693	-0.1277217	2.11671324	1.65554296	3.88074312	4.37995704	1.79895667	-1.1809923	4.488308	4.83873891	5.81296831	3.8290478	2.5681692	1.27966279	1.46661995	2.59136707	2.00161375	1.3471632	5.60827233	2.42074922	1.17551578	1.37909734
P39	3.3403459	0.49126265	1.6256086	1.69107846	2.37805627	4.22214241	2.09307541	-0.1367891	3.55038403	3.49217992	4.65090811	3.37330006	2.34538353	0.96231926	1.32964181	2.54590431	1.903246	0.21456688	4.41446439	0.60751732	1.19922441	0.75125267
P40	2.08165663	1.54244529	2.85961046	2.47631694	3.97976848	5.07541725	2.31840767	0.18567832	4.52598229	4.94810137	5.52162889	4.66355693	3.27303674	1.38233478	1.52804898	3.57318394	2.48877052	1.672445	5.36730972	2.1754106	1.0799277	2.57064002
P41	3.16456324	2.36224847	2.57487367	2.89238593	3.23151857	4.79306956	3.41940478	-0.8873273	4.37195578	4.11294671	5.58201388	4.33685819	3.20300996	1.65753736	2.70552424	3.89140882	3.60695466	0.88515088	5.41710619	2.28132145	1.99015257	1.26414085

Table 8.37: Normalised data matrix for ceramide for hair samples taken from breast cancer free controls.

	Cer(d18:1/22:0)	Cer(d18:1/24:0)	Cer(d18:1/24:1)	Cer(d18:1/25:0)	Cer(d18:1/32:3)	Cer(d18:1/38:3)	Cer(d18:1/39:3)	Cer(d18:1/40:3)	Cer(d18:1/40:4)	Cer(d18:1/41:2)	Cer(d18:1/41:3)	Cer(d18:1/41:4)	Cer(d18:1/42:6)	Cer(d18:1/44:5)	Cer(d18:1/44:6)
C21	5.244916009	6.745967196	6.526909833	3.713336109	3.440135609	2.337349164	1.12246049	3.670102815	3.453926764	2.025902925	0.410707009	0.049474165	2.415991503	2.059869786	3.988771151
C22	3.912115858	5.324907898	4.518582901	3.50888679	1.274599341	0.725000505	1.309503948	1.357459386	0.933180156	-0.459776109	0.759092078	0.513802617	2.324086207	0.866375435	3.996573494
C23	4.572296084	5.876089775	5.382716266	3.696085473	1.728375531	0.61108884	2.205057508	2.311160589	1.182493246	0.637173026	1.66622287	1.031707319	3.760445336	4.526433978	4.859223217
C24	5.075128272	6.2725669	6.283241494	3.403671338	2.504978598	2.041721954	1.185814395	3.243797363	2.724152175	2.33226914	0.61685936	0.409599893	1.854453287	1.353616022	3.339477002
C25	2.224327633	3.870214025	2.507997102	2.38872748	2.545038116	1.055274339	1.069298654	2.079119121	2.669955661	0.163968865	0.615187417	-0.09836748	1.72817371	2.073878399	3.291876304
C26	4.284613942	5.619699436	4.923365823	3.213471917	1.375411187	0.217133527	2.331307623	1.435939715	0.608155581	0.317519962	1.923924999	1.419917707	1.304768818	1.505267059	2.989672282
C27	3.34594088	4.669586046	4.198994202	2.349113216	2.342202323	1.421866402	1.066230215	2.053478296	2.270158428	0.191202767	0.969804772	0.650349191	2.064640745	1.881676094	3.605369719
C28	5.180867695	6.40661191	6.415127959	3.338575377	2.584418149	1.940544368	0.995517152	3.464667238	2.869623704	1.346185043	0.67070589	0.457729536	3.205884643	0.977426479	4.036321068
C29	4.921173385	6.050442326	5.884108112	3.121326311	1.49103397	1.451352836	0.97182815	2.723299058	1.625363988	1.63923455	0.670554594	0.690649421	1.482617015	2.326981843	2.935947199
C30	2.859704612	4.260625052	3.157124379	2.941191709	1.048988497	0.381589632	1.337502589	1.134557588	0.900550786	0.818189265	0.928361636	0.639831195	1.657696317	1.381482966	3.079741923
C31	4.599911854	6.023802615	5.496133648	3.667521743	2.836406036	1.786144778	2.574966327	3.084774413	2.103359083	2.482646024	2.102568906	1.091933787	2.339946206	1.335312696	4.020430954
C32	3.681276643	5.148343052	4.592908127	3.210009516	0.851304834	0.302131413	2.00317531	1.669427118	0.691842941	0.115221566	1.44625675	0.793684047	2.694562589	1.095659912	3.747082242
C33	3.041165809	4.546640131	3.854857566	2.704069142	1.678068315	0.1354787	1.546241435	1.548815013	1.24564227	0.482088004	1.188553116	0.73823202	2.595199592	1.992878025	3.326392093
C34	3.96970409	5.406623161	5.194656884	3.030308675	2.687696475	1.603277801	1.173286959	2.560351042	2.167041948	0.551310719	0.871852817	0.598526856	3.069845984	2.175153766	4.227927089
C35	4.682354632	6.056483191	5.632187752	3.897828893	3.031325566	1.881745412	2.504417705	3.368317047	2.95482293	0.610202622	2.048903891	1.25310896	3.263099292	1.237133927	5.036152755
C36	5.151795495	6.43381287	6.04362362	4.100120417	2.60213072	1.273490673	2.379711286	2.976968478	2.29463942	1.565593336	2.154697473	1.209961257	3.850494508	2.346987589	4.761062379
C37	4.440073409	5.719623527	5.698462139	2.828025418	3.086855077	2.10951608	-0.028053453	3.328497122	2.857337699	1.869856272	0.044856414	0.712314	3.253191562	2.513760553	4.675376445
C38	5.010831743	6.332867248	5.817643448	3.738307421	2.732850461	1.877153159	1.443047956	3.224916228	2.606828329	2.281891574	1.056308877	0.63359017	2.805829829	3.647624045	4.179578354
C39	4.825305573	6.138132579	6.012856932	3.327578748	1.726926584	1.370041703	0.865128423	2.966322534	2.0428227	1.05092263	0.570221779	0.876255465	2.057467141	4.694612747	2.899530511
C40	2.840284086	4.056685529	3.746484395	2.030396189	1.158305384	0.004020478	1.459220321	1.013217786	1.050314503	-0.573454858	0.092116775	0.137937297	2.56373791	1.643364416	3.556841436

Table 8.38: Normalised data matrix for ceramide for hair samples taken from patients with breast cancer.

	Cer(d18:1/22:0)	Cer(d18:1/24:0)	Cer(d18:1/24:1)	Cer(d18:1/25:0)	Cer(d18:1/32:3)	Cer(d18:1/38:3)	Cer(d18:1/39:3)	Cer(d18:1/40:3)	Cer(d18:1/40:4)	Cer(d18:1/41:2)	Cer(d18:1/41:3)	Cer(d18:1/41:4)	Cer(d18:1/42:6)	Cer(d18:1/44:5)	Cer(d18:1/44:6)
P19	5.516268292	6.85569616	6.641167367	3.706021535	2.583196168	2.213419353	1.294181832	3.666382736	2.507069465	2.23057497	-0.400818204	0.927042124	2.074759035	1.79100583	3.383200954
P20	4.842306797	6.116727622	5.896633943	3.174942386	2.208746072	1.796614332	0.896377919	3.131616091	2.552355264	2.314774295	0.796058492	1.063300707	2.207860535	1.032970937	3.73816022
P21	3.699485952	5.080069757	4.810750604	2.528056219	1.514085089	0.936321624	1.106243809	1.772035875	0.834618841	0.600781234	0.598176943	0.466784167	0.492265153	0.984028149	2.022591011
P22	4.35550888	5.656902407	5.412950841	2.75704896	1.688449759	1.303011091	0.808240182	2.400826039	1.32378299	1.221813658	0.258160079	0.480902355	0.505234786	2.053761438	2.22192304
P23	4.143735003	5.430434453	5.312151641	3.094727746	2.632722975	1.598928083	1.557064006	2.717582252	2.229642774	0.531439767	1.160842926	0.3348442	3.158507591	1.440995754	4.694220465
P24	5.041234399	6.402578751	6.174228524	3.196496548	2.755389162	2.056110196	1.025134585	3.496059947	2.779214193	1.905956805	0.056479171	0.179960384	2.550471503	1.516972832	4.365359794
P25	4.845306284	6.08097419	6.082462806	2.907965119	2.423827124	1.958220278	1.373708391	3.243082546	2.756521853	1.828832363	0.802367902	0.576248218	3.234099295	1.320761024	4.550690349
P26	4.651673661	5.978062544	5.860140701	3.175788547	2.761797371	1.438975026	2.208176857	2.94374012	2.478653514	1.246786246	1.865935609	0.934038273	3.52563632	2.865964017	4.902924468
P27	5.415018804	6.687193603	6.654434834	3.729711549	2.642908165	2.141206689	1.42124968	3.561595736	2.953873772	0.784661814	1.087367005	1.069816216	3.696310758	1.185003074	4.686915539
P29	3.507155751	4.911198204	4.547613617	2.476261593	1.112578817	0.919751832	-0.4831477	2.143487628	1.284707183	0.430394776	0.453331138	0.165202744	0.830980195	3.404890339	2.256446234
P30	5.316163704	6.752285486	6.431033825	3.723421551	2.538152663	2.316811689	1.094128689	3.702434836	2.475119254	1.37387794	0.368381328	0.617220845	0.550448776	1.97104193	3.961960688
P31	3.330562687	4.743437784	4.303313623	2.448454565	1.805457145	1.034725407	1.509610211	1.887600729	1.50572923	0.626196054	0.899546478	0.537166545	2.368768284	2.74492804	3.651329799
P32	5.056221579	6.497788753	6.295692307	3.196931278	2.882031326	2.06294545	1.039662413	3.656304341	3.080927678	1.815797536	0.14769739	-0.187027786	2.726413659	1.43876739	4.101210478
P33	4.982845887	6.310929377	6.089292067	3.457989571	2.035160726	1.260405121	1.301451087	2.818169021	1.811675886	1.08624566	1.192736701	0.596504506	3.121213538	1.192650014	4.174602082
P35	4.015654433	5.374166708	5.019024981	2.443409243	2.350491831	1.55660264	0.409701953	2.737536994	1.871563687	1.00797959	0.110442269	-0.448741284	1.472811019	5.105350524	3.269055856
P37	4.078924932	5.449648297	4.998811475	3.304218466	1.351286997	0.232810573	1.663254326	1.624693828	0.670754252	-0.525790143	1.394237308	0.613988404	0.061719934	1.773826754	2.023618826
P38	4.94713672	6.114082407	6.080738053	3.085353885	3.078913883	1.742985152	1.498360143	3.160576996	2.757372051	1.431047331	0.946803497	1.869642349	3.502909317	1.382820538	4.955776113
P39	3.671273318	5.107916215	4.311929167	2.825335547	2.72721537	1.414867935	1.583206867	2.855848297	2.222287234	0.715350635	0.750868432	0.14628719	3.228094488	2.099962573	4.669205623
P40	4.910259191	6.239310118	5.803529993	3.329344786	1.981360509	1.779148116	1.146837548	3.235703132	2.052172664	1.396441824	1.070546068	0.383996532	1.879647703	3.596826202	3.036669967
P41	4.090855287	5.58472979	4.987903427	3.881162687	2.501503572	1.715767458	2.369781797	2.300465348	2.7326485	1.380814792	2.080143379	1.523767454	2.409270481	2.512686632	3.784634232

Table 8.39: Normalised data matrix for phosphatidic acid for hair samples taken from breast cancer free controls.

	PA-1	PA-2	PA-3	PA-4	PA-5	PA-6	PA-7	PA-9	PA(27:4)	PA(27:5)
C21	0.6461709	0.78544754	1.20744444	0.41706318	0.59388811	0.27284931	2.28489162	1.03911877	1.9215085	0.26800924
C22	0.96333379	0.52104678	1.00211188	1.76040701	0.69972727	0.57787661	2.17973765	1.20465471	2.32389009	0.81837702
C23	-0.7479627	-0.1033808	1.54951644	2.1748306	0.67355793	0.8263585	2.13442262	0.94963112	1.42291538	-0.0121074
C24	1.78382592	1.94624603	2.30939937	1.68469671	0.61787182	1.11217967	3.60053098	0.88854414	2.00500574	0.72399247
C25	0.85388467	3.32568164	0.86200543	2.2598757	1.4095482	1.39787832	1.77949987	-0.2662167	1.25484914	0.68671536
C26	0.49233777	0.52992604	2.06768436	0.31890212	0.1987361	0.78126489	2.16420463	1.6595694	2.31706344	0.86186974
C27	1.91240422	0.74009959	1.03484462	1.27346981	0.465512	1.08897915	0.9757714	0.62406238	1.95354975	1.3075811
C28	0.96299996	1.12653765	2.14427914	1.92544106	0.75916898	0.79667129	2.31577428	1.33729457	1.63234031	0.4028939
C29	1.4184417	0.5290114	1.53973867	1.4737041	0.55297542	0.77113778	1.31199214	1.16123827	1.26108134	1.25127513
C30	1.72065654	0.54188675	0.22668198	1.98870033	0.31655541	-0.321526	1.14028177	1.25402538	1.69231509	1.18861267
C31	-0.1649189	0.12448001	1.09026715	0.57575626	0.5957135	0.41674294	3.19207256	0.58438331	1.51885927	0.74855232
C32	1.49003348	0.50945451	1.10681359	1.20189166	1.19156942	1.75709024	3.87684094	1.21103661	3.1211561	0.64948039
C33	0.90186492	2.29733885	0.91797976	3.39215034	1.67733298	1.24890496	1.98058466	1.36637015	1.73111755	0.89519919
C34	1.59534276	1.5760476	1.35911724	1.88802097	0.25685256	0.90720687	2.42784475	0.1330061	2.68297962	0.93530874
C35	0.47134977	0.30621197	1.76323964	0.24765799	0.06593894	0.27362646	4.05792415	-0.0429659	2.35063733	0.68592395
C36	0.60824231	2.45317481	1.91080247	0.65440811	0.90293847	2.25356553	3.82869589	0.9476938	2.90559981	0.30455663
C37	0.465066	0.20432539	1.05221818	1.86729568	0.51181046	0.88161191	3.46947851	0.54604576	1.59466201	0.44040119
C38	0.95530525	1.20119151	0.88153702	1.07768426	0.16650221	0.42948772	3.4233464	1.00054083	2.60078238	0.705195
C39	1.34010886	1.96709785	0.73095664	1.57728808	0.88062978	1.39926726	4.03479479	0.61237087	2.34704243	0.20564015
C40	0.37196495	1.28720876	1.76994042	1.78178729	0.50417427	0.93417836	1.23751154	1.52837582	1.80404794	1.72898701

Table 8.40: Normalised data matrix for phosphatidic acid for hair samples taken from patients with breast cancer.

	PA-1	PA-2	PA-3	PA-4	PA-5	PA-6	PA-7	PA-9	PA(27:4)	PA(27:5)
P19	1.21322451	0.87050538	0.97893274	0.61231921	0.68145833	1.11973877	2.99851983	1.23649619	2.24379147	0.37637492
P20	0.62480004	2.14973288	1.14872943	1.96725944	0.53858837	1.41995755	3.86666856	0.55967293	3.31528346	0.47566216
P21	1.05611106	1.01679519	-1.4519764	1.71730913	0.54106935	0.81370731	1.98209102	1.35157628	2.75125541	1.47239424
P22	1.1024209	0.56979689	1.70151169	1.20438415	0.55254322	1.01147623	3.84152444	0.56565466	2.20611929	0.52348609
P23	0.52748876	0.8685858	-1.0866973	1.74008579	0.6044956	0.23536717	2.06005492	-0.029778	1.96411717	0.37537772
P24	0.22476315	0.50658134	-0.1495735	0.76718851	0.61866131	0.53930637	1.6800791	0.4531425	2.4796921	0.37235882
P25	0.78917262	0.50399922	2.05020155	1.31443404	0.50962617	2.04208848	1.48563926	1.05176865	3.01360256	0.47226054
P26	1.3247054	0.55343331	1.16956986	1.36957644	1.40113976	1.01094871	1.4515826	0.95829569	2.51474305	0.99621424
P27	0.88125132	1.36066561	1.18045434	1.26182624	1.35337562	1.31488898	1.72962528	1.14965982	2.40688908	1.3794499
P29	0.91300002	4.22630189	1.78350235	3.43928315	2.39381629	0.696125	3.53787481	0.37870595	2.66770547	0.82341256
P30	1.10907461	0.22171909	1.10616188	1.09024868	1.14834672	0.72620504	1.95278743	1.1956785	3.07573403	0.1761358
P31	1.47842041	0.7557449	0.91403121	1.18258758	0.54121903	0.96014173	2.07708954	0.74020858	2.50756591	1.21030273
P32	0.20556372	0.38184583	1.42698614	0.95207052	0.94990024	1.38903715	2.02845718	0.93051189	3.12057326	1.16194642
P33	0.93673601	0.24074769	0.92422347	2.10387192	0.88504034	0.70558028	2.77849713	0.96057689	2.3783129	1.57141853
P35	0.74151761	0.22412307	0.95015578	0.74887454	0.20480645	0.15850102	2.56579035	0.76494009	2.22318096	1.14375195
P37	0.81606503	0.42433898	1.02136388	0.48068787	0.49379877	0.34461815	1.79784599	0.46484203	0.79098114	0.96408864
P38	0.97071728	3.61888063	0.59414307	0.8549316	0.47745462	0.80715511	1.68104819	0.84792478	2.22012421	0.34635784
P39	1.40401499	2.55428223	2.00069591	2.56326442	1.19824213	0.48609226	4.32096122	0.7792872	1.74622899	0.09463463
P40	0.8978709	1.34021644	1.26411781	1.38193752	0.70110143	1.2749344	3.48833336	0.90228845	2.35377105	0.06675974
P41	1.6163556	1.80426566	1.99807443	3.39328561	2.35167759	1.82735985	4.35711558	1.80127791	1.50366064	2.2613064

Table 8.41: Normalised data matrix for lyso phosphatidylcholine for hair samples taken from breast cancer free controls.

	LPC(16:0)	LPC(17:0)	LPC(17:1)	LPC(17:2)	LPC(18:0)	LPC(18:1)	LPC(18:2)	LPC(18:3)	LPC(20:0)	LPC(20:1)	LPC(20:2)	LPC(20:3)	LPC(20:4)	LPC(20:5)	LPC(22:0)	LPC(22:1)	LPC(22:2)	LPC(22:4)	LPC(22:5)	LPC(22:6)	LPC(21:0)
C21	5.93683808	4.37535413	2.41574241	0.5721681	1.8160263	5.01786389	4.741118	0.50132598	3.69420731	2.32372929	0.29952819	2.42404288	1.9218334	-1.1236105	2.42067341	1.46838652	-0.4060627	-0.6046066	-0.8474099	1.78841952	4.88845339
C22	5.32592882	4.2207797	2.1625672	0.23347763	4.23736533	5.13737993	2.84168921	0.31642197	3.7507556	2.47200504	0.65104145	2.55420349	2.21508817	0.03271529	2.05756102	1.45718465	-2.6578886	-0.5267728	-1.9421934	1.56452265	4.64483762
C23	6.92550764	6.03147422	3.75778123	1.63177462	6.48048341	6.79314707	4.30372635	0.17752678	4.17834753	2.45344981	1.96936695	3.7247313	2.87433212	-0.1022387	2.84878683	1.44821299	-1.6095896	-0.5653064	-1.3139785	1.84400216	5.18766816
C24	6.09162393	5.21455426	3.23698686	2.31221276	2.58840328	5.70683326	3.9411156	0.49185706	4.02080945	2.19387578	1.18773282	3.23303023	2.11549322	0.27403893	2.93404742	1.62152072	-1.2104453	-0.6158	-1.1333263	2.14668706	5.18748258
C25	4.77567396	3.29372647	1.87766176	1.58807018	1.53413532	4.67242785	2.74377039	0.13442515	2.8813135	1.09357914	0.43641797	1.50881884	1.08988156	-0.1210447	1.20078228	0.53005832	-1.4602788	-2.509639	-1.1390401	0.15599677	3.24328297
C26	5.04523632	4.42170574	2.34519851	1.60131541	2.09542091	4.98169454	2.69218143	0.68969095	3.02522161	1.26424216	0.19547705	2.45553859	1.53534257	-0.1904737	0.97559619	0.38174901	-0.7819478	-0.8778251	-0.45201	0.29784685	3.59883562
C27	5.54881968	4.76420848	2.37184011	0.48955725	1.86822319	5.49093324	4.8249299	0.80403523	3.87256287	1.4860452	0.27490969	2.18854327	1.55875868	0.58036838	2.51523254	1.24684154	-0.9611685	0.17328957	-1.4164166	1.67390416	4.733958
C28	7.47464432	6.8035851	4.15037908	3.02979508	7.19102441	7.23758198	4.14913398	0.49823409	5.82515209	4.11725413	1.94418734	3.60083129	2.35135264	-1.078441	3.97216355	2.99360899	-1.0216003	-0.5060242	-1.0430806	3.41972299	6.65332645
C29	7.10369991	5.83513695	3.20017114	0.29346241	4.94275461	6.49603627	3.86163693	-0.028848	4.54819767	3.41274592	1.56385275	3.1998385	2.40719673	-1.5359224	3.05488483	2.01537996	-1.1447024	-0.9645278	-0.6217119	2.40340125	5.52102629
C30	4.82063116	4.09142807	2.2274703	0.5850572	3.70171837	4.96985398	2.89694707	0.48753147	2.89573416	1.14661391	0.66374217	1.86146331	1.25195141	0.27444841	1.41786073	0.33390827	-0.9806497	-2.1951307	-2.0009257	0.3580622	3.25717624
C31	6.01357597	5.40786802	3.11636929	0.68749104	1.72703404	6.01656998	3.5200099	0.55312568	4.4078422	2.82789023	1.55774096	3.07833065	2.74509187	0.21345585	2.6557446	1.96953963	-1.0091777	0.44192665	-1.4232966	2.06967608	5.20215134
C32	5.12094216	4.69989691	2.74355228	0.12356224	7.1552356	6.75741101	3.36811352	0.06178085	4.14470184	2.42088048	0.48520253	2.31127174	1.90720394	-0.8795138	2.95627851	1.12539713	-0.7740283	-2.9001447	-1.1999124	1.0841219	4.37621248
C33	4.86978584	4.45554606	3.2869893	3.08329315	4.54509789	5.27352848	2.39704375	0.32187043	4.03067753	2.11521975	0.34435149	2.27827043	1.07279596	-0.4833066	2.52363002	1.38467782	-1.1595564	-1.3877984	-1.4947814	1.91178437	4.95188335
C34	5.04857293	4.11908895	1.94647364	1.52744556	3.37899254	5.13835585	2.90202919	0.89886737	2.75834864	2.21260955	0.75879928	2.84732172	1.49363506	-0.9325163	1.32375437	0.80299673	-1.6961107	-1.7338944	-2.5439608	0.60568929	3.71653406
C35	5.71135844	4.88103394	2.6333799	0.36306238	2.62422627	5.63202594	3.65343026	0.1941601	3.95806239	2.00718062	1.46343224	3.24456727	2.61443686	-0.361854	2.80267973	1.73711121	-0.6054951	-0.0125871	-1.1625875	1.67941053	4.91067496
C36	4.97244009	4.19316209	2.08951529	0.61255962	3.24313378	5.25246429	3.34433109	1.37584897	3.3471871	2.13908594	0.65100892	2.19385269	1.34463226	-0.5131458	0.94098223	0.96320775	-2.2965605	-0.8528288	-1.3653392	0.7115709	3.95579224
C37	5.86947074	4.46492092	2.55264167	0.06570809	1.94727823	5.55288992	5.29803316	-0.1734298	3.48755439	1.72120216	0.47026146	2.91723601	2.12613105	-1.7495647	2.04968446	1.02154896	-0.6229977	-1.0788556	-1.3028972	1.39966023	4.55563954
C38	6.48182259	5.25681984	3.15423234	0.71914507	3.15752232	6.08343451	3.9564384	0.67630122	4.2302251	2.91067099	1.37780404	3.2744747	2.85795793	-0.7989285	2.67688861	1.8885219	-1.3450629	-0.7767311	-2.8556693	2.15657079	5.31559011
C39	5.7342299	4.94713786	3.01562753	2.09378445	2.58489521	5.39054835	3.09741498	0.17211125	3.39195093	1.97242135	1.65415216	3.13593294	1.67391111	-0.5096221	1.77147759	1.51886695	-0.8714267	0.13302049	-1.4525777	1.47340661	4.56516226
C40	4.67238997	3.72082197	1.89636908	0.49185052	1.31566715	4.68357063	2.28691359	0.58934682	3.051778	1.41382294	0.14921188	1.80764261	0.95158722	0.23660536	1.92301434	0.77152786	0.18630044	-0.6369815	-0.5479773	1.01762977	3.76406823

Table 8.42: Normalised data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.

	PC(22:0)	PC(22:1)	PC(22:2)	PC(23:0)	PC(23:1)	PC(23:2)	PC(24:0)	PC(24:1)	PC(24:2)	PC(25:1)	PC(25:2)	PC(26:0)	PC(27:0)	PC(27:1)	PC(27:2)	PC(27:3)	PC(28:3)	PC(28:4)	PC(28:5)	PC(28:6)	PC(31:0)	PC(31:1)	PC(31:2)
C21	3.97970684	0.54598016	-1.1345583	0.23194295	1.52224943	1.34724735	2.44441991	1.47358285	-1.0332629	0.05490212	-0.2916106	3.72488068	0.99337545	-0.4192648	1.01812782	-1.1376731	0.17093578	-0.9852688	0.6251255	-0.2643456	2.13667336	5.29304349	2.21216966
C22	3.05942574	0.91390655	0.00802293	-0.2291199	1.77983363	1.43146361	2.79509286	1.74530067	-1.2198888	-0.5261832	-0.7341821	2.55761686	0.85692948	-0.5852488	-1.3931667	-0.2731449	-0.2393237	-0.310784	1.13944595	-0.3857152	2.32872768	4.18611654	1.84689642
C23	3.77681761	0.41475868	-0.5034721	-0.7201583	1.94496825	1.34539609	2.59135587	1.67692046	-0.0346985	0.33473763	-0.2566544	2.71236818	0.43883303	-0.8636299	-0.57941	-0.5151513	0.01578539	-0.9791202	0.52064185	-0.3239418	2.50531795	4.36725298	1.8265371
C24	4.01061544	0.42142286	-0.6706124	0.19147173	2.11791906	1.05513369	2.48685942	1.79784463	-1.240118	0.95121704	0.10522613	3.3095241	1.26877424	-0.8843295	-0.8204097	-0.5948223	-1.2234333	-2.4614043	1.20031594	0.27992646	3.07793151	4.76208246	2.17586326
C25	2.1944503	-0.2166878	-0.8182984	-0.982714	1.51102305	0.35943575	2.53436278	1.76881338	-1.4694039	-0.6246464	0.14261798	0.72116643	-0.0155541	-0.9596184	0.20007653	-0.2857756	0.19100828	-0.3704727	0.27960023	-0.1282866	2.27890498	4.36564383	1.04190124
C26	2.97871603	0.53523423	0.47633733	-0.2349528	1.90472139	1.50301019	2.64108698	1.88848282	-0.4030475	0.02005642	-0.65711	2.63864653	0.3452048	-0.5917673	-1.4834615	-0.757437	-1.7073652	-1.8159265	1.26379631	-0.1850743	2.67042254	4.1218207	0.43306538
C27	3.29266749	0.81310082	-3.3021176	0.64091754	2.38033991	-0.2080777	2.44912295	1.89098417	0.62580385	0.55060236	-0.5867784	2.15185633	1.45190955	0.47107469	-0.7846495	-0.7889333	-0.3248459	0.04227514	0.49814333	0.10329	2.95402285	4.7763921	2.29691314
C28	4.90035232	1.33603271	-1.5797354	0.29320124	2.51214224	1.67424862	2.45095761	1.41278487	0.26049679	0.3873259	0.4684245	3.81314074	1.26437138	-0.3826553	-0.9255302	-0.1029056	-0.3852776	-2.4510034	0.52044301	-0.1635582	2.26127802	4.58909219	1.27048088
C29	4.12709028	1.10235345	-0.205489	0.6333873	2.0937849	1.30655469	2.66854306	1.91259483	-1.149273	-0.1617417	-0.3337679	3.60242259	1.24815457	-1.3345537	-0.586489	-0.8695581	-0.2393237	0.31354867	1.10109853	-0.0823985	2.21456747	4.73231824	1.51989312
C30	2.50259487	-0.2350186	-0.8414398	-0.338124	1.54901432	0.58935117	2.39654437	1.89028976	-0.6849039	-1.3857225	0.06809574	0.95056238	0.11363163	-1.1566864	1.17817711	-0.392823	-0.6619765	-1.2482298	-0.4743716	-0.271958	2.24046554	3.80665103	0.78921549
C31	3.78475967	1.5183433	-0.5984698	0.18502493	2.08325754	0.65275722	2.4661752	1.51172565	-0.467586	0.45633683	1.25242491	2.79436955	0.43128895	1.11936984	2.81034918	-1.2519965	-1.426618	0.78862419	1.71678406	0.13725368	2.98584436	5.29980858	2.17882631
C32	3.69082724	0.58888425	-1.2226227	0.84944822	1.68580645	0.59031167	2.10201622	1.50202159	-0.3862404	0.21511831	-0.9885021	1.7807155	-0.3169014	0.3999974	-0.1154482	0.15622056	-1.1677888	-0.8600864	-0.0038789	-0.9105487	1.76790767	3.01804632	0.51910214
C33	3.72076701	0.84019086	-1.254824	1.28833645	1.95821254	0.98937991	2.57224536	1.548176	-0.3447119	-2.0585516	0.21419878	1.95265407	0.34599875	-0.7108445	-0.1798684	0.12677516	-0.6019119	-1.2352062	-0.4177589	-1.1260777	2.45127647	4.08997974	1.37480923
C34	2.24147494	0.097612	-1.0147142	0.03406647	1.62046917	0.59540694	2.36953877	1.60799843	-0.3774289	-0.2322527	-1.4290308	3.25928364	0.62474803	-0.3874652	0.18682353	0.09254035	-0.3821865	-0.3711195	0.02301129	0.22819676	2.44639683	4.71252176	1.76369564
C35	3.74069956	0.62309051	-0.4145014	0.22009583	1.93085874	0.93258279	2.38004301	1.75882186	-0.9372988	0.29315711	-0.2968617	3.3011775	0.82754204	-0.2474237	-1.3762486	-1.2344689	-0.2238235	-0.2812221	0.14726884	-0.3741073	2.37858293	4.9335437	1.63021508
C36	2.79719714	1.13038202	-1.3452263	0.81789612	2.11514207	1.28798735	2.2861685	1.74259615	-0.8052423	-0.0604558	-0.3113182	3.62188768	0.98156361	0.03462915	1.39538804	-0.2398762	-0.8691281	0.28807848	0.96417371	0.60470789	1.70322658	3.79269126	1.58144234
C37	3.77771525	0.4237488	-0.7327294	0.85994165	1.97077576	1.33589913	2.46895783	1.46377912	0.10458818	1.03096791	0.21902585	3.02254291	0.76386676	0.32676684	1.18107863	-0.5010112	-0.3944943	-0.5313675	0.17084784	-1.0583598	2.50708626	4.91444624	1.9766304
C38	4.02344339	1.39087143	-0.6558933	0.1154537	2.13423689	1.68610794	2.4789803	1.51167184	-0.5453565	-0.0338567	0.09445458	3.23922148	0.74801463	-0.9786315	-1.1837859	0.96003208	-0.6311908	-0.1345215	1.51797366	-0.0293091	3.04917965	5.41586793	2.58227797
C39	2.91418056	0.93756294	0.00143904	0.15411881	2.06621408	1.43868953	2.57434791	1.923957	-0.297687	0.1141149	1.61139621	3.19198607	1.25995185	1.53479091	3.39265195	-1.0717488	1.05638902	0.77080934	-0.0142962	1.25268918	2.09209792	4.5095024	1.75743465
C40	2.46589762	0.11255468	0.38076028	0.70711303	1.48163714	1.11577331	2.65287877	1.42717049	-0.8916	0.51083888	-0.653993	2.40372167	1.20724838	-1.1244003	0.45127077	-0.1901292	-0.9995218	-1.0450917	0.45448919	0.59461807	2.21746349	3.63546856	0.64112647

Table 8.43: Normalised data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.

	PC(31:3)	PC(32:0)	PC(32:1)	PC(32:2)	PC(32:3)	PC(33:0)	PC(33:1)	PC(33:2)	PC(33:3)	PC(34:0)	PC(34:1)	PC(34:2)	PC(34:3)	PC(34:4)	PC(35:0)	PC(35:1)	PC(35:2)	PC(35:3)	PC(35:4)	PC(36:0)	PC(36:1)	PC(36:2)	PC(36:3)
C21	0.00563279	8.42216434	6.72091833	3.73808398	3.2043874	8.15860981	6.46222019	3.77851557	3.08313178	8.53327984	8.42180679	6.8338783	4.64016496	2.94418186	7.83159577	8.27239792	5.81602459	2.42242853	-0.2694132	11.4090015	9.7429993	7.86637592	6.2438777
C22	-0.0114875	7.49782146	5.42467661	2.5349103	3.00113773	6.17207341	4.55244925	2.56179143	3.26804989	6.68743345	6.71353733	6.39319266	4.60945504	1.88492118	5.71665397	5.92796652	4.20583499	-0.4999201	-0.9355509	11.3745728	9.55788585	6.85704532	4.99015011
C23	-0.0964594	7.27105789	5.59944319	2.94297573	3.19444016	6.69595169	5.20376449	3.29895016	2.88835547	7.14615762	7.51955973	6.27100911	4.48210279	1.52842138	6.27480401	7.08743454	4.75456799	1.96687089	-0.8179873	11.1002241	9.32720003	7.12939133	5.29401961
C24	-0.463323	8.03279452	6.17030651	2.94111483	2.968029	7.48809955	5.48945792	3.21728449	3.10933976	8.06488057	7.59686596	6.77771995	4.79010403	2.08473028	7.42914588	7.26099086	5.00419198	2.02667255	-1.9492809	11.5794378	9.71706644	7.44820944	5.70946372
C25	-0.9339848	6.34461567	5.90180916	2.74520483	2.53544127	4.50098635	4.32953415	2.24979301	3.00433314	5.36359272	6.5570416	6.31510073	4.43598323	1.7935961	3.77943449	4.66918592	3.99596079	-0.4566507	0.12476982	11.3181015	9.47525024	6.68733289	4.73576412
C26	-0.1269186	7.09480636	4.9010338	2.0228482	2.65920323	6.12984807	4.13947953	2.1949154	2.72433156	6.57432757	6.25218033	6.1878012	4.39629198	1.68958981	5.29553528	5.73396689	3.97998267	-1.1550865	-1.021074	11.2188405	9.37804841	6.55961055	4.72734566
C27	-0.2706946	7.28047192	5.68183938	2.98835502	2.80217493	5.8301585	4.05860609	2.14812312	3.21456996	6.58825849	6.44149277	6.11561173	4.26354087	1.56738777	5.76401682	5.40843243	3.72937599	-0.8289298	0.40360467	11.1287193	9.29618229	6.52518525	4.6159777
C28	-0.2189535	7.89105842	6.3058194	2.79403501	3.32982374	7.66121704	5.60574984	3.29406084	2.69998632	8.08820862	7.81090723	6.67993708	4.64471558	1.62598257	7.36181887	7.72043366	5.14826362	2.01187651	0.55780561	11.2042363	9.5173361	7.39398963	5.54828181
C29	-0.6327119	8.40676644	6.32110076	3.36039536	3.47694826	7.5145931	5.57759648	3.54327497	3.26978907	8.00443354	8.06639899	6.96861324	4.99686067	2.24891686	6.87167019	7.2391826	4.95193908	2.09896631	-1.1460427	11.5920434	9.81432143	7.61327953	5.67706225
C30	-1.0297406	6.12197383	4.21551225	1.65588186	2.57057168	5.64374395	3.24602167	2.12185519	2.98385179	6.09761097	5.67411233	6.02447903	4.19215671	1.51489043	5.13026338	5.26188211	3.60222429	-0.590353	-0.116236	11.0105267	9.18727479	6.30768065	4.21027882
C31	-0.1914572	7.66411782	6.05313218	3.1027232	3.22098632	6.93808334	5.03952123	2.9813508	3.40665049	7.55240734	7.24015388	6.6375882	4.74259969	1.98371568	6.83757197	6.94037913	4.54827049	-0.1896927	-1.4264871	11.3143687	9.44847914	7.10816808	5.11605316
C32	-0.961447	6.20406762	3.99410583	0.55453574	2.66831434	4.75427418	3.17849921	0.99374806	1.29691927	5.61850413	5.2761517	5.69634316	3.81508716	1.13852411	4.62639973	4.7107138	3.59588944	-0.3432834	-1.3771836	11.032293	9.16412136	6.2503032	4.33091293
C33	0.00548171	6.54083768	4.26755026	1.51547679	2.83479544	5.84752876	3.91547976	1.93296861	2.70946642	6.48458204	5.96522658	5.88154192	4.13164709	1.03497722	5.90433954	5.7111665	3.87817634	0.80218105	0.71976375	11.312151	9.48736531	6.63527192	4.5222837
C34	0.91096296	7.01395196	5.40826135	2.47603796	2.1354019	5.93233044	4.20427801	2.09657614	2.92147898	6.66154502	6.46276903	5.98705612	4.06304772	1.40347224	5.78866413	5.76726238	4.11228019	0.90851938	0.36532625	11.0881608	9.27757004	6.64524189	4.57218545
C35	-0.1976877	7.38420884	6.05443762	3.34372693	2.62186976	6.21535952	4.42570053	3.04834667	3.34884026	7.00460631	7.11046438	6.31482139	4.53714676	1.54915122	6.21101557	6.11320403	4.34936095	1.27732093	-0.1544191	11.2086689	9.41207115	6.87198711	4.98157966
C36	-0.6641236	7.26065	5.27019161	2.19239522	3.03104449	5.9066191	3.79718343	2.27765467	2.93244599	6.71890152	6.33270187	6.36738637	4.53470827	1.91147551	5.92349095	5.52073371	4.14252224	0.57743963	-0.7509301	11.4673331	9.64185457	6.89046108	4.88197253
C37	0.11177741	7.75019198	6.09692973	3.56935943	3.13733695	7.32672232	5.38278638	3.42204967	3.32777604	7.90243608	7.65808588	6.80047993	4.90432006	2.07736891	7.15982048	7.20143158	5.0845687	1.94699059	0.45007269	11.3044791	9.54750506	7.46146721	6.0559497
C38	0.51452017	7.90691585	6.30772127	3.49801615	3.25892614	7.59525939	5.6509427	3.71737457	3.62578137	8.08698739	7.93320455	6.87842676	4.93056225	2.09537422	7.40762779	7.65561476	5.10106507	2.46644024	0.68881837	11.4783186	9.73234104	7.49831532	5.54854782
C39	-0.8882599	7.48551007	5.51803212	2.60364978	3.37359886	6.54763456	4.70112215	2.67730985	2.84795157	7.12765036	6.86095371	6.67549736	4.84961981	1.94080838	6.44601211	6.32635245	4.86191166	0.59929014	0.24992208	11.5709397	9.75439883	7.07612086	5.32095605
C40	-0.2390241	7.06531786	4.67315559	0.50358788	2.33485847	5.15184469	3.4016214	1.43307074	1.75579839	5.97162997	5.63277681	5.80462944	4.08562589	1.23111055	4.90931293	4.65543598	3.70986499	-0.1153089	-1.6616461	11.2806861	9.43525932	6.50700497	4.50774622

Table 8.44: Normalised data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.

	PC(36:4)	PC(36:5)	PC(37:1)	PC(37:2)	PC(37:3)	PC(37:4)	PC(37:5)	PC(37:6)	PC(38:0)	PC(38:1)	PC(38:2)	PC(38:3)	PC(38:4)	PC(38:5)	PC(38:6)	PC(39:0)	PC(39:1)	PC(39:2)	PC(39:3)	PC(39:4)	PC(39:5)	PC(40:0)	PC(40:1)
C21	5.14466414	3.18188285	7.47750596	7.86770897	5.21273986	4.78796263	6.81395527	10.1857344	8.46495313	8.05204589	6.83448699	5.78616515	6.19881165	3.76702244	5.48790856	5.68088629	7.67425253	5.80794026	5.34961827	5.62552293	5.62193676	7.18106838	6.80500633
C22	3.89642514	2.57354685	5.38780552	5.85901445	2.90027348	3.15122554	6.73189859	10.1524782	6.88416825	6.7256597	4.95627116	4.07118438	3.8674932	3.11465937	4.64655719	4.19957556	5.21431985	3.20449212	3.02763261	4.21540436	5.04374165	5.93248068	5.09840677
C23	4.12499768	2.77598898	6.11713825	6.19787172	4.08634925	3.40929035	6.46978083	9.86290436	7.30041108	7.05033128	5.60755028	4.68371884	5.20107115	3.37256815	4.86668292	4.84665871	5.91664899	4.26229858	4.21652648	4.29946287	5.07975008	6.48168537	5.85042082
C24	4.25053743	2.78795101	6.87420317	7.4046064	3.96862022	3.56946828	6.95664622	10.3609215	7.84788054	7.56565436	6.23902543	4.96983598	5.41906587	3.79419565	5.4105238	5.54293268	6.9476678	4.88361959	4.46993055	4.99943195	5.83318561	6.55995375	6.08196935
C25	3.13672254	1.38632688	4.15733809	3.97735386	1.43817606	2.55814498	6.66563789	10.1036334	6.14193305	6.28301218	4.96498091	3.07319522	3.03908659	2.8684512	4.09805526	3.71688285	3.9310409	2.25924367	1.82768737	3.79254412	4.83141957	4.75319576	4.59274303
C26	3.08650325	1.3802896	4.92672419	5.73149704	2.70195931	2.86654836	6.59124615	10.0066759	7.00010178	6.36332866	4.45743507	3.32639542	3.68445805	3.0222998	4.34742686	4.24573967	5.23362065	2.8111966	2.64644762	3.61502164	4.61554907	6.17690821	5.27315247
C27	4.18133933	0.25010574	5.50784383	5.7301662	1.98560646	2.80526394	6.49017578	9.92091869	7.14380015	7.32185106	5.71853548	2.85538726	3.65820315	2.64049625	4.24656496	4.33026557	5.16849204	2.96212895	2.54217306	3.65833488	4.83393222	6.18043561	5.73664091
C28	4.30137499	3.40481152	6.71623668	7.13452637	4.3623712	3.7819087	6.63278611	10.0235879	7.94305424	7.50459146	6.20133291	5.11119715	5.54637922	3.70590426	5.40597783	4.89833228	6.52279928	4.74914576	4.76051886	5.06539839	5.66474675	6.79477716	6.32114127
C29	4.5860357	3.37086487	6.17516736	7.04718617	3.26339067	3.82588343	6.9582941	10.3660452	7.79615201	7.2915894	5.66957932	4.92377808	4.98657357	3.80607461	5.47107474	5.02606207	6.2972682	3.92799984	3.34893402	4.80566483	5.61257002	6.63002616	5.99765811
C30	2.88612034	-0.2740754	4.62763175	5.05455606	1.96217436	2.45200008	6.39798175	9.79483785	6.07892339	6.10709657	4.66086155	2.39872922	3.33150626	2.92287054	4.54061673	3.83407175	4.21107674	2.68105807	2.55199141	3.96713735	5.00832729	5.1745629	4.67183492
C31	4.08930898	2.65495393	6.40275384	6.75958158	3.65863354	3.43029523	6.69638916	10.0806223	7.61361067	7.22755494	5.73532508	4.65843293	4.94285803	3.23688599	4.83524044	5.07866774	6.44605624	4.38796845	4.19199966	4.79371427	5.28522556	6.76673618	6.14182722
C32	2.49185088	0.59922964	4.52344975	4.90641213	1.75186852	2.72765188	6.42476226	9.83306969	6.33463335	6.06851535	4.33795182	2.72848443	2.84390836	2.64536066	4.13552872	3.78828301	4.60012325	2.29966449	2.44019344	3.68188164	4.78805398	5.5435449	4.89622553
C33	2.84243714	-0.5442196	5.61703441	5.9715674	2.32276433	2.6741448	6.68006718	10.083639	7.26950894	7.08649582	5.22564261	3.02460101	3.60322359	3.18887386	4.6278934	4.25156659	5.46259855	2.96924908	2.99843111	4.21835808	5.28668268	6.2088268	5.74740157
C34	3.64552277	0.8401983	5.61833726	5.80353838	2.80156157	2.93392795	6.48057681	9.86639844	7.09434782	7.25484416	5.54530345	3.71009613	4.09318747	3.10372842	4.35609433	4.63361054	5.47391581	3.53929234	3.41375394	4.14320809	5.00268451	5.9897996	5.73303284
C35	3.71564056	1.99017946	5.85391078	6.48574055	3.31059235	2.87707585	6.57003337	9.99140248	7.58399688	7.43912437	5.92899425	4.03882984	4.77567434	3.38950554	4.67463409	4.43785301	6.02226713	4.45429008	3.78512913	4.52143213	5.3229728	6.61215919	6.0942249
C36	3.3067317	1.21814811	5.34119462	6.09320826	2.5124459	2.80799261	6.8499696	10.2501844	7.13384969	6.81655357	5.18728346	3.57562469	3.84814883	3.35816526	4.97995746	4.2038157	5.46916821	3.26918679	2.91451602	4.64208446	5.60490493	6.10908516	5.59764353
C37	6.11558504	4.7434237	6.53683827	7.12999346	3.89593024	3.48315278	6.68977009	10.0927993	7.89857252	7.52650837	6.22413719	4.88560542	5.40071187	3.44293304	5.20101821	5.38666447	6.63170533	4.79608075	4.31172072	4.74360311	5.43194369	6.74966441	6.2969042
C38	4.42908091	3.45700688	6.97683805	7.44267571	4.0934615	3.69706066	6.83614913	10.2660641	8.19903052	7.73005621	6.35415533	4.88459089	5.35749365	3.90709975	5.49482421	5.30587029	7.02728059	4.93516691	4.53734963	4.97264484	5.6571534	6.98665308	6.29691477
C39	3.95968221	1.52489372	5.81837293	6.39707945	3.28279826	3.32493829	6.97471564	10.3595309	7.44526839	7.31281424	5.67269026	4.33357279	4.53783943	3.54955411	5.03630542	4.72619059	5.67828097	3.92956256	3.87690841	4.76157023	5.76695724	6.55476173	6.02225765
C40	2.6878629	-0.6459413	4.76357373	5.11806031	1.02866593	2.69570995	6.65390337	10.0616798	6.50321515	6.85077641	5.00298673	2.34259154	2.76405592	2.73744944	4.05835757	3.97748761	4.56201222	2.44063414	1.82822982	3.65655084	4.83334359	5.64576619	5.30037972

Table 8.45: Normalised data matrix for phosphatidylcholine for hair samples taken from breast cancer controls.

	PC(40:2)	PC(40:3)	PC(40:4)	PC(40:5)	PC(40:6)	PC(41:0)	PC(41:1)	PC(41:2)	PC(41:3)	PC(41:4)	PC(41:5)	PC(41:6)	PC(42:0)	PC(42:1)	PC(42:2)	PC(42:3)	PC(42:4)	PC(42:5)	PC(42:6)	PC(43:0)	PC(43:1)	PC(43:2)	PC(43:3)
C21	5.4063845	4.58117122	4.86605101	4.20527264	5.29352078	5.47851459	5.66963265	3.1901038	5.41540908	5.29437221	3.91297155	4.41846505	5.43725383	5.09082982	3.7951246	3.63084439	3.67229256	3.3506059	3.80054409	1.06545112	3.46409502	2.69240165	4.14541368
C22	3.19833184	2.51325519	2.75226138	2.15658767	3.94908804	3.99629946	3.54901778	2.78013347	3.46608242	3.26772004	2.09634879	2.99485227	4.27615325	3.65966133	2.33804155	1.63224949	2.02333448	0.69350415	2.59892772	-0.2709677	1.94712876	1.65111339	2.11962446
C23	4.20461642	3.3628788	3.54604317	2.53490841	4.26478263	4.30893096	3.98599044	2.59523719	4.29965074	3.34637514	2.61420718	3.72008508	4.80041246	4.45318124	2.76023901	2.09781635	1.80984392	1.6833675	3.07191342	-0.3816171	1.91838036	1.43366998	2.83831018
C24	4.72159331	3.86214973	3.94355518	3.31250814	4.89578043	4.95467174	5.09273688	3.06570895	4.76633862	3.90997361	3.08902838	3.81016491	4.84295442	4.44687004	3.24815548	2.83788588	2.82597362	2.53128467	3.35880817	0.09890331	3.103041	2.233688	3.54013872
C25	2.92499769	1.28196447	1.65041009	0.83767793	2.40914932	2.13855573	2.0073883	1.26777161	0.91512835	1.40676607	0.62862273	1.83719874	2.88497463	3.00154869	1.31973953	0.2035945	0.11644877	0.20539126	1.07029906	-0.8678638	0.80585462	-0.4971695	0.05178572
C26	3.21250079	2.00882344	1.84875619	1.49967324	3.79263659	4.20159868	3.88501568	2.17639087	3.35980668	2.58450566	1.55255391	3.40593358	4.44740477	3.90893274	1.97897197	1.73562834	1.60724328	1.12707114	2.66929313	-0.4928542	1.94860287	1.68080534	2.68153167
C27	4.03256004	2.36869139	1.76295838	1.40231105	3.72887156	3.67609071	3.3818956	0.63497743	3.0183854	2.37576146	1.63146542	3.26216983	4.18848857	4.30298068	2.5725789	1.13622121	1.29299157	1.42677303	2.15186877	-0.5567361	1.75474904	1.01680279	1.6784265
C28	4.58765169	3.80697238	4.16114066	3.7117066	4.76366701	4.7509981	4.3171486	3.65867869	4.65007491	4.25964973	3.53653689	3.87588452	4.89749069	4.7267946	2.97865004	2.87141449	2.92168259	2.70982027	3.36166282	-0.3571264	2.36918042	1.88312771	3.48097663
C29	4.22388775	2.8339847	3.52562913	2.99019528	4.50676084	4.70954594	4.40735838	2.60249936	3.58304284	3.62907792	2.80493197	3.75438222	4.94380512	4.33520733	2.60886022	2.12546871	2.5411489	2.22894678	3.29037572	-0.7645383	2.38526017	1.76118882	2.17998026
C30	3.02663953	1.58990251	1.65442085	1.62840981	3.16558181	3.07705353	2.62145526	1.31626401	2.47232499	2.09335556	1.85767468	2.10695382	3.5079779	3.30038793	1.65961893	0.26245488	0.66850319	1.31216626	1.96820038	-0.8778224	1.26556055	0.73967691	0.70003672
C31	4.4451007	3.39060208	3.71467639	3.10441625	4.5001787	4.79358379	4.5825403	3.12446105	4.19953941	4.04997342	2.83651548	3.72087758	5.30829278	4.76913363	3.06847863	2.70091999	2.34250814	2.37912997	3.27512061	0.95602965	2.8410676	2.23243518	3.40492362
C32	2.97316707	2.04949929	1.85891129	1.21280545	3.34476212	3.54734476	2.99759496	0.78712088	3.16839254	2.86959308	1.05622647	2.61550625	3.99138187	3.58374187	1.68682922	1.98192386	1.93616262	0.77458979	2.31460439	-0.4549449	1.00550593	0.82388534	2.54529772
C33	3.88483066	2.38184654	1.76222976	0.99327245	3.98889022	3.98838249	3.40916311	0.83771978	3.19612805	2.38046063	1.55052623	3.2780236	4.36361471	4.39332732	2.4558461	1.90076597	1.02468862	0.80955793	2.67865773	-0.6528716	2.1634565	0.93257862	2.10654551
C34	3.9688936	2.72545323	2.63041054	1.34999211	3.81481143	3.85305347	3.48898095	1.97604845	3.77214719	2.87029004	2.14954922	3.04588242	4.22361374	4.35527226	2.26944373	1.99670238	1.68139987	1.5278472	2.32036051	-0.4566389	2.38097764	1.58754188	2.54349281
C35	4.38225567	3.55517813	3.51890136	2.48926081	4.11180231	4.59909936	4.4678055	2.91894878	4.43444853	3.88232652	2.14069571	3.64063477	4.87952718	4.68264598	3.04594836	2.77050782	2.84377508	1.71334764	2.50897924	-0.1446145	2.55512763	1.94576285	3.58829436
C36	3.73932159	2.45104145	2.42553521	2.19546451	4.14906966	4.10643123	3.79098194	1.53040422	3.32103968	2.82467428	1.99290577	3.15780548	4.32673235	4.2954028	2.56079256	2.02008804	1.35871274	1.17288953	2.83202274	-0.7152173	2.09120665	1.45517841	2.64391903
C37	4.67596398	3.72459097	3.74660621	3.58672255	4.69117	4.55940423	4.73588384	3.42870824	4.50542527	4.07679168	3.23210458	3.75335589	4.54049579	4.7406936	3.24683774	2.73417883	2.79581431	2.4886869	3.3046866	0.66553219	2.63352384	2.02873343	3.45174295
C38	4.65192961	3.86816789	4.06245554	3.51694779	4.871253	5.10655715	5.06579576	3.4155235	4.88222011	4.45618589	3.08698607	3.99250768	5.23927191	4.65943159	3.17027109	3.10389135	2.88157923	2.35879254	3.63528624	0.65619885	3.0614707	1.02289614	3.88845451
C39	4.22345913	3.13941619	3.13295813	1.67455653	4.26304958	4.53903324	4.06870864	2.82670783	4.01081142	3.23003839	1.56987155	3.7527805	4.7971573	4.48100188	2.83675907	2.56602277	2.10195474	1.78067158	3.37067103	0.1237319	2.52632046	2.83154403	2.81322892
C40	3.37223536	1.3197642	1.02370082	0.38923064	3.45657979	3.26800703	2.64562312	0.40755745	1.53731347	0.9778328	1.05340843	2.90882199	3.79200415	3.792309	1.7470869	0.84326188	0.74798237	1.302527	2.05718824	-0.6687478	1.69859399	-0.2382309	1.21722697

Table 8.46: Normalised data matrix for phosphatidylcholine for hair samples taken from breast cancer free controls.

	PC(43:4)	PC(43:5)	PC(43:6)	PC(30:0)	PC(30:1)	PC(30:2)	PC(d31)
C21	3.82767832	3.10114565	2.98657618	7.72103804	6.26219014	3.53681934	8.32101503
C22	2.18140775	1.51842733	1.87771649	6.98037106	5.4005782	2.47441657	8.29188241
C23	1.52280727	1.12924403	2.18252871	7.20645667	5.66513421	2.97442979	8.00512063
C24	2.79825041	2.17561497	2.52471749	7.01317395	5.68746627	3.15042607	8.49341903
C25	-0.6273949	-0.2794175	0.30817575	6.64341518	5.44857474	3.08367714	8.24297174
C26	1.63289301	1.320504	2.11197117	6.47931489	4.99584388	2.30580729	8.12509091
C27	0.78005717	0.62376796	1.68857686	7.70229363	6.25193102	3.68139766	8.04815396
C28	2.73304468	1.77471111	2.37221736	6.71843818	5.19566259	2.78608125	8.12118879
C29	2.52144062	1.78393782	2.33934784	7.15383287	5.46608506	2.62272878	8.50905628
C30	-0.7911414	0.10323928	1.09663785	6.38902822	4.8950503	2.1661222	7.94425835
C31	2.70886518	1.66661422	2.5662052	7.93484094	6.30469727	3.30766566	8.22802022
C32	1.94982733	-0.1984063	1.60121773	4.80421758	3.82916751	2.22962317	7.91251385
C33	0.62993374	-0.6265022	1.783181	6.74118297	5.25096819	2.47619079	8.21659196
C34	1.74800761	1.2807257	1.57049904	7.40019705	5.80953896	2.82252488	8.00600068
C35	2.85090398	1.29261161	2.50754388	7.51696959	5.97971254	3.28740684	8.14313762
C36	1.71688319	1.0686042	1.73749183	6.50575211	5.01895995	2.41076784	8.38450325
C37	2.73849324	2.17656298	2.0500676	7.50825836	5.97666686	3.32900765	8.22007797
C38	3.03638168	1.92777068	2.62963426	7.96583625	6.44569481	3.72020783	8.39658613
C39	1.56468118	0.8430924	2.09651572	6.9272858	5.42392893	2.61358715	8.48589061
C40	0.08608349	0.75737172	1.52424986	5.98757283	4.817338	2.12662087	8.20073436

Table 8.47: Normalised data matrix for lyso phosphatidylcholine for hair samples taken from patients with breast cancer.

	LPC(16:0)	LPC(17:0)	LPC(17:1)	LPC(17:2)	LPC(18:0)	LPC(18:1)	LPC(18:2)	LPC(18:3)	LPC(20:0)	LPC(20:1)	LPC(20:2)	LPC(20:3)	LPC(20:4)	LPC(20:5)	LPC(22:0)	LPC(22:1)	LPC(22:2)	LPC(22:4)	LPC(22:5)	LPC(22:6)	LPC(21:0)
P19	6.11098485	5.3070074	2.7147058	1.87013133	2.23349358	5.73931426	3.83905523	0.92704253	4.18010116	2.87741169	1.37228076	3.02097407	2.16376869	-0.0227571	2.99992129	2.08550217	-0.7987629	-0.3274209	-0.9606869	2.45610035	5.64945915
P20	5.01306328	4.16918031	2.29803152	1.17476544	2.60954062	5.09777193	2.9569104	0.63865663	3.3557065	2.04183585	0.47466138	2.15043022	1.43965868	-0.038906	1.68979391	1.01892631	-0.7715503	-2.3977836	-0.9338808	0.87569005	4.00714067
P21	5.28403938	4.50112937	1.94652481	0.73267879	0.82051498	4.5304004	1.81331503	0.1814186	3.3498805	1.85177003	0.28054584	1.77584331	0.59479627	0.00243843	2.25923368	1.02615565	-0.7259279	0.98776371	-1.2204459	1.15544795	4.55328017
P22	6.32427906	5.45339808	2.82593072	0.34462355	0.8804848	5.74787175	3.7995218	1.42E-05	4.37210691	2.10960552	1.44646982	3.40031485	2.54633379	-1.1689588	2.89342467	2.062254	-0.5947441	-0.7718641	-0.7150014	2.35096795	5.64543756
P23	5.46804419	4.36464775	2.39090364	1.27439822	2.0601295	5.34441034	3.21805651	0.56063137	3.16906996	1.79063111	0.76212779	2.81697578	1.93048683	-0.5665537	1.82735742	0.87393328	-0.739686	-3.5093783	-1.1650499	0.75358801	4.16323243
P24	5.26332909	3.71140867	1.83878363	0.61215523	1.79377499	5.05706763	2.53817155	0.37356061	3.48408401	1.16905824	-0.0209105	2.38659185	0.93616945	-2.0372143	1.9975328	1.52172208	-1.2008837	-0.083558	-0.3865813	1.39639663	4.50061857
P25	5.9379236	4.55801031	2.13614941	1.80832304	2.74045116	5.50613483	2.97850955	0.51412996	3.28303739	2.49193813	0.66418809	2.46591229	1.34892085	-0.5745973	1.85711603	1.08445096	-1.2197136	-1.1351214	-1.4104353	0.85780528	4.07164067
P26	4.96576723	4.05517719	1.91939696	1.91473563	3.04481502	4.79628208	2.69827841	1.19411635	3.65398263	1.29830233	0.17087222	1.90270137	1.12166709	0.07269597	2.73493077	1.56517774	-1.4603682	-3.3222338	-0.1716672	1.63569938	4.57402929
P27	5.46349064	4.52118672	2.32323722	1.89817467	2.50311815	5.30039774	2.82205758	0.56859395	3.47026581	1.99301004	0.57515528	2.43473761	1.52400141	-0.4520111	1.97001823	1.18001357	0.37507823	-1.2282006	-1.0319144	1.23991691	4.27254431
P29	5.39046963	4.49740834	3.79997515	3.24048053	1.10827131	4.9960577	3.2075392	0.84155504	3.52552976	1.54506172	0.1107192	2.3635791	1.25339202	-0.3842536	2.33798469	1.25256538	-0.6427827	0.69011266	-1.290863	1.93013735	4.99322247
P30	5.34400175	4.4425205	1.85184252	1.89734389	2.33974949	4.98696326	2.6752434	0.77025769	3.98151921	1.82312844	0.08435911	2.16876411	1.1171066	-1.7370736	2.95676395	1.47628342	-1.382881	-0.7765599	-1.9203007	1.98837198	5.09283978
P31	5.15385088	4.16244639	1.89020215	1.40473144	1.75774118	4.58033213	2.37767735	-0.2542098	3.49804441	1.60102767	0.37335067	1.76535657	1.56367052	-0.6820823	2.11656465	0.73519149	-1.027817	-0.9432429	-1.6756463	1.51027033	4.56763229
P32	5.47918362	4.29425136	2.24195141	0.36899617	2.26321448	5.27174959	3.04938692	0.21894669	4.04369107	2.33037579	0.66436575	2.5942398	1.5038562	1.18899178	2.6245249	1.69246303	-0.6791432	-1.1607138	-0.6257459	1.73733026	5.01145814
P33	6.27437412	5.37558384	2.86157966	0.57015595	6.09852606	6.25481387	3.59471859	0.66386159	4.14566534	3.22582321	1.44488507	3.63350111	2.51121106	-0.6850552	2.44803119	1.80976887	-0.736459	-0.3387373	-1.0196282	1.83183131	5.02442986
P35	6.15852161	4.25413426	2.27589481	1.79890382	1.76383823	5.08154733	3.23009721	0.13768096	3.77365438	1.72335852	0.43543695	2.2417614	1.71514419	-0.9758557	2.51575391	1.48528301	-1.0606583	-0.3625279	-1.0319144	1.11107593	4.49472708
P37	4.85971941	4.23018296	1.77924409	1.88024946	4.88505034	5.12179082	2.3546256	0.2605927	2.47184258	1.25822881	0.26885548	2.04035933	0.94811127	-0.8946705	1.39776039	0.40733846	-0.9400731	-0.4519108	-1.0381907	1.07821106	3.88424844
P38	6.23995366	4.95259537	2.56439332	1.88024946	2.50202971	5.88577829	3.6187688	0.49072968	3.91477594	2.88750706	1.41550471	2.98881742	2.31720935	-2.448532	2.23208981	1.66552767	-1.2239985	-1.2475885	-0.9505688	1.74389844	4.67079635
P39	4.82773461	3.32112859	2.90456446	2.9561444	3.61868455	4.96408444	3.06922069	-0.0476728	2.7970907	0.62493835	0.29362855	1.06077084	0.87425179	-0.3844957	1.30874162	0.55160281	-1.3563593	0.39454995	-1.2633815	0.3624108	3.38348007
P40	4.58901116	4.00411537	0.98688487	1.91473563	1.54980036	4.16833828	1.84664778	0.63842983	3.4605349	2.07473009	0.25355295	1.13417476	-0.1275377	0.10356177	2.71137759	1.24626734	-0.7907906	-0.4665356	-0.9160826	1.43989495	4.64712794
P41	5.94989791	4.69775401	2.6325487	2.77973307	7.6963405	7.35127839	3.47796126	1.15004407	3.5710999	2.5999021	1.62071201	2.41675013	1.22787787	0.68020814	2.0064864	1.2406032	-0.2026737	-0.2175142	-0.0510852	1.33745575	4.3487203

Table 8.48: Normalised data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.

	PC(22:0)	PC(22:1)	PC(22:2)	PC(23:0)	PC(23:1)	PC(23:2)	PC(24:0)	PC(24:1)	PC(24:2)	PC(25:1)	PC(25:2)	PC(26:0)	PC(27:0)	PC(27:1)	PC(27:2)	PC(27:3)	PC(28:3)	PC(28:4)	PC(28:5)	PC(28:6)	PC(31:0)	PC(31:1)	PC(31:2)
P19	4.07570014	0.52995478	-0.4948083	0.42690675	2.33755224	1.54962895	2.7942896	1.86294127	0.6626481	-0.0607846	-0.5985038	3.83461045	0.88251214	-1.2775285	-1.4292589	-0.2948966	-0.0291607	-1.0892093	0.69855208	-0.9207819	3.03628112	4.92274076	2.41551864
P20	2.8475319	0.57443091	-0.7211526	0.27408818	1.8189021	1.37924796	2.13641866	1.90084009	-0.9049792	-0.5567089	-0.8607459	2.78362233	0.60005529	0.09428168	0.17245302	-0.03989	-0.7863678	-0.8809498	1.17933978	-0.9269513	2.66733381	4.27194596	1.61423855
P21	3.20067421	0.44147729	-0.1087073	-0.5248968	1.93850885	0.89821672	2.236139	1.44526237	-0.6380024	1.07577082	1.50538515	2.5091094	0.47320671	1.89668668	3.74927879	-0.0047986	-0.3653509	1.60899108	1.11627325	1.17372327	2.803851	4.36389681	1.39040332
P22	4.17715718	0.92935436	-1.1055023	-0.3725669	1.99431065	1.47704377	1.87382461	1.21755478	-1.5445808	0.01086942	-0.2304255	3.34822915	0.96540437	0.47859923	0.41462192	-0.031805	-0.6199852	-2.5667538	0.02204611	0.0623891	2.3467831	4.53620845	1.56581541
P23	2.95066371	0.70294587	-0.3641754	0.05551255	1.7225374	0.99734793	2.5007427	1.70678275	-0.3426448	-0.2602605	-0.8414216	2.62356604	0.72582401	-1.20468	-0.4383598	-0.9401051	-0.8798216	-0.6271427	-1.0706968	-1.0060759	2.64574894	4.23856357	1.45596908
P24	3.44365998	0.7616726	-1.0607429	0.57880242	1.68000371	1.21744036	2.42219046	1.40334237	1.29646805	-0.290907	-0.0838896	3.77553733	1.18805347	-0.20289	1.41752972	1.18187846	-0.0556523	0.45767497	0.68036742	-0.0600684	2.66620223	4.71937698	0.60906935
P25	3.28684519	0.79203347	-1.9263607	-0.0563666	1.88350735	1.20520912	2.39537118	1.50763725	0.72451205	-0.4438929	-0.307609	3.15170041	0.73828273	-0.7448141	-1.0275199	-1.430328	-0.3810203	-1.2925941	1.28954649	-0.9603065	1.77574742	4.3957682	1.6868688
P26	3.21274253	0.63118305	-1.1097394	0.34174255	2.48166005	1.3263632	2.59155275	1.9680696	0.62765831	-0.177898	-0.0601419	3.55053494	0.44986436	-0.7558711	-0.2139732	-0.0224982	-0.0635007	-0.2527023	0.86748081	-0.4458545	2.68153387	4.64484165	1.68193546
P27	3.03995146	1.36315616	-0.7996351	0.34456405	2.35165485	1.47594848	2.42911145	1.76389284	-1.0823486	-0.2436178	-0.143077	3.82234315	1.16784662	-0.0041584	-0.8265018	-0.9801077	-0.8903898	-0.3584851	0.48768452	-0.4900344	2.56996291	4.67887316	1.48460596
P29	3.56356827	0.6475056	-1.5367042	0.91674306	1.76457576	1.09703709	2.48839697	1.59202884	1.2390736	-0.4438842	-0.9958561	2.83994724	0.52681594	-0.1143077	-0.1138842	0.23933999	-0.3980042	-0.7305886	0.6608135	-0.3844654	2.54024331	3.93722661	1.68001728
P30	3.52416957	0.97583666	-0.8366143	0.52319295	2.11355015	1.60501171	2.44604973	1.37316796	1.76397707	-2.5452668	-0.675253	3.85451715	0.28411427	0.25476979	-0.5997634	-0.4276251	2.00856768	-1.0710411	0.72499617	-1.3294838	2.56808541	4.50395144	1.88056995
P31	3.35998539	0.76804844	-1.7736553	0.57843031	1.66783306	0.82459775	2.3249631	1.09594357	-0.4272637	0.27846225	0.04803409	2.36414129	0.87296976	-0.1451918	-0.0927689	-0.9272218	-0.1311599	-0.9035017	0.20954461	0.1784292	2.24958545	3.79025517	1.03122056
P32	3.88431573	0.91694932	-0.8366143	-0.5905812	1.99551954	0.09328904	2.61376569	1.96044208	-0.9927589	0.79744958	-0.9512972	3.58545753	0.95445819	-0.4777494	-0.869078	-0.6211336	-0.9660905	-0.684058	0.74750534	2.37242283	2.18753603	5.08297534	1.64488982
P33	3.29226307	1.95951626	-0.7803339	0.29962082	2.47179374	1.55919094	2.42992083	1.52419028	-0.4996409	-0.6997941	0.04127398	3.84872448	1.29551505	0.129373	0.02144346	-0.8642779	-0.4491312	-1.2670676	1.14649167	0.23461864	2.91213855	4.58693321	1.3762388
P35	3.53838196	-0.0731572	-1.2418611	-0.4434974	2.00454796	0.76640041	2.01818794	1.22064279	2.11598288	-0.4279629	-0.6623216	2.49438103	0.72851843	-0.0041584	0.17318238	0.5452568	-0.1003882	-0.3756597	0.03138325	-0.7205516	2.4272473	4.18349654	1.28628668
P37	2.61660008	0.88016573	-1.1355757	0.1362244	1.44636086	1.21499542	2.66275342	1.636037	0.67276623	0.03917806	-0.2044288	2.7275518	0.40688643	-0.6483732	-0.9395631	-0.3638626	-1.1377738	-0.1974281	0.40941695	-0.7840285	2.49210398	4.44912589	2.02196065
P38	3.19657894	1.45381658	-0.8216754	0.74391316	2.28043255	1.13499729	2.35958058	1.55877046	0.79319597	-0.3371008	-0.7127362	3.68939221	0.70104511	-0.9394359	1.10393225	0.22842795	-0.7515147	-0.2633436	0.7629556	-0.2239645	2.36061003	4.80405368	1.2475552
P39	2.13436088	0.09759216	-0.8236212	0.37536399	2.17696348	1.10474638	2.61831129	1.87709167	0.78693277	-0.079892	-0.5244002	1.88086485	0.2418833	-0.4380457	-0.2479471	-1.0772289	-0.6385617	-0.6080811	0.05759189	-1.0681912	1.67176379	3.58899345	1.01157263
P40	3.48620814	0.64763254	-0.974491	0.18635053	2.15441451	1.52752387	2.03458456	1.33122566	-1.3694389	0.0484239	-0.7640674	3.44674604	0.80866134	-0.0433645	-0.2161468	-0.0224982	-0.4874227	-0.9339043	0.92709599	0.13105004	2.57179692	4.55350014	1.68775581
P41	2.51809238	1.01321841	0.46973307	1.87297882	3.33474131	2.21685475	3.35400411	2.28189338	0.51376975	0.6324892	-0.1893804	2.66264407	1.00793899	0.40947375	-0.2697647	1.23704298	0.42448817	-0.2262298	1.06514698	1.26896646	2.23843925	5.21907352	2.40449271

Table 8.49: Normalised data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.

	PC[31:3]	PC[32:0]	PC[32:1]	PC[32:2]	PC[32:3]	PC[33:0]	PC[33:1]	PC[33:2]	PC[33:3]	PC[34:0]	PC[34:1]	PC[34:2]	PC[34:3]	PC[34:4]	PC[35:0]	PC[35:1]	PC[35:2]	PC[35:3]	PC[35:4]	PC[36:0]	PC[36:1]	PC[36:2]	PC[36:3]
P19	0.19751963	8.48100867	6.36463307	3.4319204	3.16431154	7.28600766	5.37957907	3.28705703	2.94774008	8.21809507	7.81058331	6.77829765	4.77550104	2.00548884	6.92328978	7.38313534	4.98579816	1.67343881	-0.1342855	11.6199908	9.83502785	7.52228063	5.57406327
P20	0.14830118	7.10082186	5.47899168	2.23972937	2.65412464	6.44798756	4.90344193	2.98840254	2.80184891	6.90252771	7.13274047	6.32277241	4.41400572	1.62068574	6.15372356	6.47090936	4.53649114	-0.0058495	-1.1429358	11.4321739	9.62583405	7.01104469	5.14399829
P21	-1.018155	7.19981337	4.55141382	1.67272883	2.11420624	6.52388654	4.35557071	1.90233408	2.20955764	6.7416325	6.37882063	5.59401874	3.65701992	1.1112912	6.04427999	5.81063641	3.64094494	-0.0296599	-0.1700972	10.6971715	8.88388774	6.22252003	4.40812199
P22	0.26275552	8.3193965	5.93029823	2.48765106	2.43863053	7.27843418	5.28923356	3.16153929	2.73116675	7.91188565	7.52701089	6.24997982	4.14351398	1.6297374	7.02013893	7.44887179	4.93948704	1.92868788	0.92847131	11.0562804	9.33013091	7.24779009	5.43850229
P23	-0.8547684	7.39470068	5.65764711	2.642689	2.51574366	6.39749481	4.93439389	2.88696777	2.50500656	6.97735053	7.20592738	6.24471928	4.18577678	1.02613537	5.92252632	6.42725507	4.51959275	0.4749825	-0.8868142	11.3161278	9.5131539	7.02983339	5.23235237
P24	0.94587581	8.14018972	6.02736784	2.66787286	2.71255115	6.42137758	4.7322187	2.57388398	2.50547737	7.77310397	7.19717087	6.27071516	4.20501228	0.95649762	6.04843885	6.38459015	4.64543227	1.20646089	0.07729477	11.3862907	9.57831557	7.06230402	5.25651809
P25	-0.2264995	7.74476155	6.03831074	2.91174719	3.12310485	6.61726012	5.22829087	3.1360259	2.96091735	7.24970315	7.49518635	6.60753834	4.63801759	2.07572414	6.29484301	6.76123095	4.66952432	1.27319262	-0.0569973	11.4170594	9.6249737	7.19601977	5.36377576
P26	0.06974773	7.56262306	5.77815036	2.81049593	2.93018768	6.25245302	4.39763634	2.53894259	3.03908637	7.11938111	6.84814439	6.18073795	4.25205857	1.36347044	6.05119308	6.07273409	4.29677625	1.27369221	-0.9677556	11.3144992	9.50167	6.88346257	4.88853168
P27	-0.4314841	7.58428372	5.94501776	2.81681361	2.91324131	6.54427383	4.81449582	2.67599461	2.81669042	7.42788665	7.2357798	6.39271486	4.52672478	1.859161	6.50763331	6.56771191	4.60994853	1.25381466	-0.2778509	11.4613258	9.66091719	7.1693322	5.19599487
P29	-0.5015727	7.25318873	5.00438993	2.29964314	2.43453259	6.62745473	4.56124239	2.0755679	2.53047302	7.16077142	6.75065129	6.1090089	4.17302369	1.38819565	6.25876761	6.56611609	4.27875811	1.65001073	-0.0852008	11.2906995	9.48287491	6.88202096	4.91611645
P30	0.76984579	8.55134664	5.99732463	3.07974526	2.64548048	7.13414885	5.05361161	2.52682539	2.54447353	8.04715517	7.41666126	6.27195696	4.25246119	1.54838628	7.06446131	6.81150326	4.57066621	1.33988408	-1.1455587	11.3127581	9.52860184	7.06191808	5.23826401
P31	-0.8592378	7.17577008	4.91938065	1.54276467	2.35515437	5.88397755	4.03861313	1.8113826	1.84494833	6.52851796	6.16124208	5.66104558	3.69729235	1.13345134	5.62568308	5.54022525	3.90169223	-0.27851	0.08379361	11.0029065	9.16935426	6.38148081	4.5410814
P32	-0.5577489	7.84307445	6.47450679	3.5585665	3.27373271	7.30098685	5.48046482	3.52803628	3.20804537	7.89192997	7.88331355	6.83611377	4.91125885	2.14181888	7.07678187	7.49298223	5.20518391	2.07986216	-0.2951574	11.5531128	9.78006424	7.70706372	5.81645799
P33	0.20061546	8.00375607	5.82645958	2.66999071	3.54941017	7.34598014	5.52068131	3.45849798	2.92707866	7.99479376	7.79494964	6.59889643	4.64620297	1.74839335	6.91808529	7.58090145	4.90145322	1.66126575	-0.5851053	11.424777	9.65147362	7.36482382	5.56667353
P35	1.33515896	7.81756238	5.85999285	2.66680064	2.84807332	6.83458882	5.29280326	3.22829326	2.54858482	7.10118867	7.63962432	6.51095863	4.35343355	1.83781155	6.14649081	6.60962104	4.73733738	1.14946545	-0.0926134	11.1799067	9.38510689	7.02664754	5.39319373
P37	0.13120675	7.34269379	5.11179313	2.30906998	3.12639135	6.16429655	4.38944559	2.63440804	3.26358666	6.50770724	6.22394405	6.4003232	4.63937647	2.08147871	5.33538126	5.90516773	4.20599885	0.31959619	-1.1836691	11.3407622	9.51694747	6.76909021	4.75393037
P38	-1.2357788	8.57387816	6.56920882	3.04481023	2.82594572	7.15062125	5.56097492	3.08456199	2.66821785	8.00654915	7.85432904	6.65231242	4.47312753	1.83822661	6.65775661	7.30173318	5.08022153	1.40870859	-0.1231471	11.4442498	9.67587705	7.44389315	5.70247615
P39	-0.1533002	6.66534543	5.11376039	2.05484348	2.88415227	5.68679539	4.3342289	2.42626121	2.8562963	6.04293147	6.56121811	6.20392537	4.28110043	1.73102947	5.07977214	5.41855766	4.13593216	0.1445602	0.48807305	11.4365482	9.60600044	6.82844677	4.99587775
P40	-1.8982134	7.92054027	5.76149522	2.73202423	2.48347736	6.68565303	4.97368463	2.60918845	2.96742198	7.38870332	7.059488	6.31628572	4.43451723	1.73800292	6.39061395	6.79225366	4.37004567	0.97467635	0.203979	11.1928038	9.39986951	6.90085323	5.04865807
P41	1.33378457	7.33693971	6.28195004	3.47647576	4.44464065	5.35621742	4.45783435	3.44671045	4.22567563	6.44117683	6.86877936	7.55603712	5.74957759	2.98748211	5.06734882	5.27751371	4.9105283	-0.1667771	1.09148788	12.3212567	10.4790931	7.59678161	5.62856099

Table 8.50: Normalised data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.

	PC[36:4]	PC[36:5]	PC[37:1]	PC[37:2]	PC[37:3]	PC[37:4]	PC[37:5]	PC[37:6]	PC[38:0]	PC[38:1]	PC[38:2]	PC[38:3]	PC[38:4]	PC[38:5]	PC[38:6]	PC[39:0]	PC[39:1]	PC[39:2]	PC[39:3]	PC[39:4]	PC[39:5]	PC[40:0]	PC[40:1]
P19	4.44872512	2.51791431	6.55103717	7.23797744	3.97288798	3.66545359	6.9817967	10.3898667	8.1590896	7.61608302	6.21689263	4.70163774	5.25197067	3.8407926	5.29522334	5.21113898	6.97315103	5.0160665	4.2154396	5.07955563	5.89550402	6.79660207	6.334545
P20	3.88639323	1.9920054	5.86947185	6.26661565	2.85125887	3.11866542	6.8033092	10.2136323	7.34507679	7.15577002	5.7170682	3.89631043	4.29956044	3.38053185	4.91448256	4.77679307	5.95347705	3.93638356	3.23665178	4.40347593	5.40491172	6.17791259	5.83120574
P21	2.83799221	1.56982649	5.33876705	6.20181318	2.52956887	2.54469177	6.0724717	9.48284409	7.06680015	6.57967073	4.8667948	3.07834201	3.41738212	2.43197473	4.31252223	4.55966824	5.37048975	3.45531896	2.46103528	3.25621045	4.26714044	6.34735829	5.38104308
P22	4.22718789	2.57491799	6.74212355	6.79011139	4.12076764	3.64840404	6.40414526	9.82395633	7.41755204	7.28919534	6.10098159	4.97022938	5.54312566	3.30108709	4.9030384	4.83124061	6.61199177	5.28875815	4.72728008	5.05685943	5.3083513	6.3606932	5.59020102
P23	3.88663415	2.45562349	5.64156758	5.67084117	3.3450542	3.15374178	6.66894833	10.1059178	6.71711034	6.93987233	5.64994076	4.16234988	4.52615113	3.35521306	4.83016736	4.72352661	5.33164458	3.77704123	3.53806026	4.26961305	5.2246134	5.7059323	5.49032652
P24	3.82085596	1.57749003	5.74301263	6.62852926	3.22487603	3.32968802	6.74819173	10.1707709	7.91129448	7.38074938	5.97309223	4.42588747	4.83024309	3.59591098	5.0041123	5.2281354	6.1876414	4.15736752	3.38825197	4.57911602	5.37374925	6.77428794	6.26370143
P25	4.11157556	2.58737712	6.06609548	6.23402784	3.25204224	3.36962268	6.78374639	10.2104949	7.17039341	7.13991725	5.91470458	4.52827026	4.72634028	3.54006216	5.05578427	4.72859024	6.00187928	4.14030697	3.82326598	4.69077262	5.59341704	6.07357934	5.741434
P26	3.3132788	1.45673402	5.6989462	6.14301889	2.87476411	3.00719246	6.70872905	10.1001984	7.41452875	7.35675931	5.86036379	3.6827733	4.4363315	3.32596771	4.73870023	4.90442157	5.64344032	3.78467784	3.37715548	4.3888056	5.30873491	6.41691176	6.09715888
P27	3.61540553	1.50018567	6.16063868	6.553529	3.3343425	3.33306772	6.82905372	10.2357393	7.8091191	7.6034094	6.16599699	4.36490119	4.86704145	3.58117478	5.27173491	5.24829926	6.05472046	3.83977557	3.84115753	4.883735	5.76148878	6.68041971	6.34418723
P29	3.65831657	0.85962829	5.94322671	6.28996931	3.18538247	3.20477258	6.66802837	10.0722888	7.35191023	6.94285456	5.3161689	3.90555208	4.30661641	3.3952517	4.78478609	4.61886092	5.91959059	4.0026688	3.49807033	4.30982535	5.14424962	6.3203856	5.64478186
P30	4.09102423	2.75110187	6.43129754	7.15261699	3.23072645	3.28453522	6.70075272	10.0876957	7.8649491	7.41553137	6.10705084	4.25781257	4.69953349	3.30084464	4.90863788	4.99014348	6.56083399	4.32980135	3.63547546	4.66914432	5.53295577	6.4627963	5.81442133
P31	3.12917492	-0.0835606	5.08057369	5.70383548	2.27860956	2.89396616	6.36796814	9.79020979	7.02259722	6.64721996	5.01826711	3.26949515	3.51364906	2.47691948	4.28653855	4.05210337	5.22451263	3.30567107	2.54433427	3.86697764	4.72810522	6.24303729	5.50259215
P32	4.3758892	2.97174204	6.8248886	7.33116196	4.0895765	3.70178825	6.91351782	10.3335073	8.1622594	7.66365684	6.37749769	5.19067996	5.64404565	3.89768688	5.47688901	5.14806782	7.1946623	5.22522467	4.51941391	5.11296465	5.63052333	6.95037673	6.54833672
P33	4.38703192	2.86594255	6.47508263	6.77670386	4.19081407	3.56482179	6.80067358	10.2082432	7.72642365	7.52370192	6.10535903	4.99706917	5.44073308	3.7730423	5.47714332	5.20607951	6.36398053	4.71653075	4.67860974	4.94561014	5.61628689	6.58967845	6.20678226
P35	4.24848548	3.35040656	5.55331281	6.19025902	3.30832725	3.30117141	6.54635083	9.97673597	6.920558	6.54288443	5.17635846	4.28757134	4.2589807	3.09878002	4.26604559	4.07714449	5.60470133	3.94686433	2.89338371	4.13804575	4.97239803	5.86772312	5.18207046
P37	3.41381943	0.6393856	5.09623823	5.92051785	2.61118112	3.05243284	6.73544238	10.1276763	6.9028165	6.45674042	4.69988246	3.39606318	3.62844192	3.01235275	4.53750443	4.12065812	5.57101724	3.50092137	2.49732842	3.39094632	4.23096368	5.82944722	5.13818856
P38	4.32981645	1.94495813	6.34820006	6.55497782	4.05634278	3.82650531	6.82836774	10.2336765	7.66210965	7.4228206	6.16084626	5.0393567	5.40250879	3.68956634	5.23517722	4.94192911	6.24948634	4.2161425	4.32072538	4.88827157	5.59580873	6.64598183	6.17930921
P39	3.882622	1.57105701	4.68516758	5.30358092	2.19558064	3.04847015	6.79500911	10.2250017	6.71354445	6.3424485	4.6778132	3.34283068	3.14927081	3.06325959	4.241459	3.36456565	4.85332825	2.69979402	2.14056855	3.92770511	4.99777419	5.88467118	5.37872071
P40	4.18351111	1.89678115	6.10144895	6.32767907	3.42079277	3.17434783	6.57461602	9.97883149	7.47902394	6.98389713	5.51062671	4.26098302	4.72892508	3.26123789	4.88548082	4.85332153	6.01011373	4.01177849	4.21533953	4.71405078	5.38794446	6.42358182	5.78212787
P41	4.13840564	2.15582657	5.33465797	5.6879432	1.8963871	3.61551108	7.72021466	11.1094689	7.86473029	7.7391365	5.91197106	3.51306077	3.77519177	4.04059331	5.38246675	4.45048428	5.40540873	3.33155784	2.83716089	5.09459005	6.15888291	6.72152868	6.46727141

Table 8.51: Normalised data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.

	PC(40:2)	PC(40:3)	PC(40:4)	PC(40:5)	PC(40:6)	PC(41:0)	PC(41:1)	PC(41:2)	PC(41:3)	PC(41:4)	PC(41:5)	PC(41:6)	PC(42:0)	PC(42:1)	PC(42:2)	PC(42:3)	PC(42:4)	PC(42:5)	PC(42:6)	PC(43:0)	PC(43:1)	PC(43:2)	PC(43:3)
P19	4.80504357	3.6326595	3.88554173	3.26952758	4.60138946	4.99325868	4.96490907	3.23645918	4.85539425	4.36126518	2.92480732	4.02083923	5.20100595	4.6453514	3.17377117	3.20284128	3.05939278	2.28807245	3.3635388	0.8137944	2.93509598	2.29828257	3.8950861
P20	4.15174871	2.84658915	2.83840103	1.93343779	4.06663184	4.07705863	4.10974312	1.57953352	3.59653989	3.14699895	1.93747352	3.4002091	4.40542888	4.2230201	2.5910961	1.73126699	2.13796313	1.59538814	2.55413173	0.34100028	2.48793586	1.51471854	2.8656709
P21	3.42683929	2.15716515	2.0694033	1.78111174	4.09320443	4.50706981	3.9018525	1.80597921	3.22280183	2.43803906	2.21199337	3.49729841	4.78407032	3.88423108	2.46690552	2.10887069	1.28435871	1.2891736	2.92734325	0.7026054	2.45982429	2.99844218	1.72225195
P22	4.32067209	4.0402713	4.29993732	3.63754949	4.41145456	4.62052447	4.77854388	3.17031321	4.94229467	4.83217727	3.42296761	3.49687037	4.73765095	4.10836682	2.7992353	2.97217208	3.08788308	2.73879076	3.06528539	0.03249423	2.53552829	2.2219188	3.48212774
P23	3.87964336	2.74511528	3.09386612	2.55917354	3.87046965	3.42358446	3.27406116	2.33857907	3.61167745	3.13013838	2.44442313	2.60763485	3.72013131	3.80051016	2.31125523	1.95013397	1.55522841	1.1927395	2.42006126	-2.4327315	1.57349983	-0.1707793	1.80176843
P24	4.52278761	2.92786607	3.30747748	2.77400928	4.38523653	4.7684757	4.57472769	2.70102452	3.91363245	3.71307441	2.50807016	3.83531436	4.8834397	4.64865651	3.07529015	2.82444173	2.69544564	2.05914418	3.00496961	1.31976171	2.75373707	2.14720648	3.50508888
P25	4.0217447	3.27639189	3.31922348	2.05990972	4.09256079	4.05965765	4.10555042	2.06505279	4.19888517	3.57323306	2.4906562	3.09445212	4.27197055	4.10230388	2.64459645	2.2511327	2.30151038	2.11399001	2.62749592	-0.7516716	2.03811961	1.30837387	2.88928549
P26	4.31060243	2.80362823	2.89519535	1.74839696	3.90444639	4.15802353	3.92357389	1.68560075	3.73800844	3.23190676	1.91477901	3.51500386	4.54067805	4.68870239	2.99050995	2.32981635	2.12433661	1.87072132	2.50316835	-0.2354215	2.15628964	1.43121962	2.69551498
P27	4.47004797	3.22842042	3.33793447	2.66860513	4.42795677	4.47331742	4.12043651	1.99772802	3.90899576	3.72159342	2.24610912	3.6682357	4.81442777	4.58128877	2.93390546	2.54805612	2.38932187	2.16878655	3.08659289	0.32475595	2.33891643	1.66572272	2.72712435
P29	3.78597211	2.50973421	2.67627052	2.21945864	4.05425044	4.20417375	4.0389894	2.22822488	3.38419122	3.25731668	2.11926925	3.4646457	4.62933716	4.16511916	2.22594982	1.4558543	1.76217756	1.14943927	2.64938042	0.02943226	2.24328056	1.04248927	2.18351746
P30	4.25440826	3.09853456	3.36743859	2.51941046	4.53086923	4.88160455	4.69783714	2.81715915	4.13503048	3.7129906	3.0434205	3.76229408	5.04574186	4.12234928	2.73628117	2.69184493	2.47887555	2.21554946	3.22761765	1.22809963	2.63484673	1.72223715	3.00762609
P31	3.65613572	2.17390272	2.14026663	1.90069357	3.68781607	3.94025786	3.61009768	0.68084339	3.05738319	2.58746582	1.32811781	3.21140361	4.55443923	3.95566714	2.19888456	1.28534283	0.79804968	1.11308792	2.41414264	-0.1014059	2.15084429	0.86145571	1.73453858
P32	5.02204275	4.07329715	4.26164259	3.51190284	4.92139383	5.28912818	5.31291234	3.4871504	4.9815235	4.51217387	3.30851418	4.07462776	5.41318677	4.99313914	3.60382226	3.5412141	3.19460759	2.82093043	3.41099623	1.44975538	3.28514317	2.5854007	4.10869406
P33	4.45692127	3.64786402	4.04793854	3.16353166	4.58295763	4.64582818	4.38420983	3.25355948	4.49166757	4.04713179	2.8941677	3.67968684	4.79070253	4.73566006	3.0285554	2.35721571	2.89458827	2.36496756	3.32565161	0.13100491	2.65970741	1.80555374	3.02439698
P35	3.79864329	2.83805312	3.02693777	2.48879474	3.90779771	3.85328083	3.96349237	2.71064	3.20457114	3.24882687	2.39567215	3.15835119	4.10206746	3.41025925	2.22182667	1.7596132	1.85895972	0.98899	2.45813962	-0.5517539	1.91088149	1.12878592	2.21099749
P37	3.56655869	1.90140317	2.30108156	1.60362396	3.74066593	4.07024649	3.85660713	2.15578543	3.01367893	2.59222412	1.9422706	2.8190538	4.1146379	3.60508425	2.0261544	1.44004991	0.78518996	0.84512069	2.61496055	-0.3712927	2.19680227	0.81105812	2.0111052
P38	4.40878405	3.80127541	4.07026444	3.08771711	4.32551308	4.0602254	4.34532985	1.85143161	4.50054162	4.01434385	2.41987869	3.61235457	4.52647853	4.60641591	3.09949372	2.7178045	3.0890872	2.4357081	3.12504969	-1.4502327	2.33312871	1.85520875	3.41486991
P39	3.6183794	1.54138392	1.61092658	1.62146989	3.33533211	3.27904515	3.11896864	1.28510241	2.12782695	1.9090852	1.44981625	2.96338283	4.05115687	3.79020798	2.15850512	0.8558901	0.70876154	-0.0710948	2.20925454	-0.159129	1.22068294	0.23609983	0.82943175
P40	4.05607541	3.00523921	3.30735619	2.28287553	4.18146044	4.21637572	4.17202522	2.48929847	4.10070942	3.84483124	2.7673078	3.55332843	4.71773899	4.1898727	2.68399417	2.04054823	2.03117926	2.11967508	2.95232446	-0.4906943	2.12594473	1.57767034	2.99228468
P41	4.46111278	2.3729837	2.1748632	1.48622474	4.1604556	3.96085796	3.70398213	2.15015354	2.79910218	2.35869148	1.72619791	3.76792543	4.89534193	4.80915501	3.06989832	1.75798099	1.37381635	1.56158664	3.35868722	1.20914898	2.30522536	-0.360617	2.1364613

Table 8.52: Normalised data matrix for phosphatidylcholine for hair samples taken from patients with breast cancer.

	PC(43:4)	PC(43:5)	PC(43:6)	PC(30:0)	PC(30:1)	PC(30:2)	PC(d31)
P19	3.33177884	2.06358009	2.75184841	7.57626338	6.11291343	3.46936435	8.54158556
P20	1.27110331	-0.5373642	1.63610978	6.58356028	5.26050607	2.76894015	8.35409665
P21	0.63409023	0.45999143	2.16686524	6.98389052	5.34656213	2.21444274	7.62192679
P22	3.4454322	2.22960086	2.32648134	7.20187194	5.61316107	2.36852648	7.96409539
P23	1.09247458	0.96095753	1.29544494	6.85727755	5.56147188	3.25079081	8.25028835
P24	3.09941047	1.62902372	2.44978669	7.0381096	5.69864459	3.21734188	8.32381186
P25	2.19893314	0.75849366	2.11815803	6.79807862	5.52978178	3.0671832	8.33727893
P26	2.09207522	1.78357467	1.92959558	7.28776175	5.82165066	3.08732363	8.2213085
P27	2.4580475	1.25258692	2.43933654	7.00813884	5.60460198	2.77173141	8.37670613
P29	1.50320357	2.17279028	1.84850463	6.58951661	5.0376745	2.39178999	8.212161
P30	2.77329004	2.07775501	2.70749633	7.22283626	6.09092046	3.89331056	8.21753334
P31	1.23903885	-0.0206121	1.71398351	6.13550708	4.86637962	2.4305108	7.90674212
P32	3.50463502	2.50479382	3.11372584	7.40752245	5.90171449	3.22392178	8.46066077
P33	2.53032477	1.44809626	2.47197326	7.26014116	5.6869099	2.96974154	8.33459853
P35	1.83368643	1.75358494	1.95608009	6.74588328	5.23943286	2.70973553	8.08394281
P37	1.48039134	1.15949605	1.86896117	6.83490832	5.33934917	2.84100407	8.27629329
P38	2.66365454	1.57103097	1.67596695	7.13837414	5.7677006	3.26055073	8.36784462
P39	0.45644608	0.56894001	1.36338651	6.44201459	5.09486041	2.59857288	8.365062
P40	2.35105872	1.7187477	1.99763362	7.26220682	5.6823533	2.66240518	8.10898821
P41	0.72612998	-0.0233413	2.07172822	7.82991175	6.25337752	3.41793961	9.22893087

Table 8.53: Normalised data matrix for phosphatidylethanolamine for hair samples taken from breast cancer free controls.

	PE(34:0)	PE(34:1)	PE(34:2)	PE(35:1)	PE(36:1)	PE(36:2)	PE(36:3)	PE(38:1)	PE(38:2)
C21	0.77795076	1.83192002	1.7184531	1.33416866	2.73526863	2.91265788	1.46858994	1.49428709	1.42590708
C22	1.43679055	0.6529723	0.29274424	0.45672388	1.51333992	1.99215431	-0.1216835	0.27990189	0.55523478
C23	1.98368066	0.91512992	0.73722654	0.19754021	1.87769543	2.36261378	0.83375592	0.73195643	0.73362767
C24	2.02311359	1.62556317	1.39514839	1.43590493	2.58428291	2.76206015	1.00452412	1.63433495	1.33909274
C25	1.29830224	0.27230207	0.06788919	-0.169256	0.00074314	1.13468724	0.05167447	-1.2706422	-1.5067388
C26	2.17792849	0.19890004	-0.3575611	-0.493548	0.59364724	0.72030829	-0.4705958	-0.091432	-0.315725
C27	0.89314492	0.60756251	0.07605292	-0.7184684	0.74664755	0.72841779	-0.3061733	-0.0105207	0.11697251
C28	1.67461512	1.06545333	0.58986783	0.93731991	2.11003735	2.08591092	0.51791709	0.84115602	0.49093655
C29	0.83812376	2.3688195	1.36504792	0.99972154	2.967057	3.30622505	1.2693381	1.30979989	1.0419991
C30	1.50135057	-0.2596708	-0.5497236	-1.782376	0.26430401	0.31689976	-1.0054383	-0.0430518	-0.6951685
C31	2.34509876	1.38997975	1.07446474	1.02752124	2.08493308	2.64898092	0.97847649	0.45427313	0.48862027
C32	1.25630825	-1.0988191	-1.1452243	-1.9848589	-0.7744014	-0.1816194	-1.1888115	-1.7101389	-0.7970549
C33	1.99560133	-0.6516933	-0.1138733	-0.410602	0.59873554	0.54809894	-0.6539808	-0.406922	-0.5934969
C34	1.22512764	0.19524084	0.15564271	-0.4021193	1.18337923	1.23216574	-0.6005144	-0.4908965	-0.0548878
C35	2.31612102	0.77878766	0.48471056	-0.5349974	1.20202059	1.63287114	0.33472048	0.73125942	0.11979619
C36	0.71187113	0.26067365	0.84231248	-0.8712641	1.15141733	1.46022984	0.12849126	0.51776366	0.21573782
C37	0.63825334	1.26521634	1.9652411	0.55678084	2.19250568	2.52682138	1.38571162	0.94894204	0.8627622
C38	1.94425719	1.86683786	1.09535411	1.37515892	2.71807171	3.09153649	1.44843434	1.47482685	1.30975517
C39	0.27320557	1.10032194	0.69293605	0.85991946	2.03106018	2.15761113	0.18284611	0.84644829	0.47539877
C40	2.07952547	-1.6286025	-0.5430906	-2.595184	-1.1436956	-0.2090161	-1.1338805	-1.3498798	-1.9491654

Table 8.54: Normalised data matrix for phosphatidylethanolamine for hair samples taken from patients with breast cancer.

	PE(34:0)	PE(34:1)	PE(34:2)	PE(35:1)	PE(36:1)	PE(36:2)	PE(36:3)	PE(38:1)	PE(38:2)
P19	1.24787954	1.48121017	1.09073458	0.79319141	2.37847484	2.59206094	0.66764694	1.07664914	0.94982806
P20	1.27337952	1.22332908	0.5259296	0.66971266	1.59429277	2.0340771	0.47285946	0.28965943	0.3606649
P21	1.73292023	0.70835946	-0.0356494	0.23662089	1.0164114	1.39467079	-0.0759558	0.642767	0.24888927
P22	1.48728247	1.02268957	1.17308641	0.85335161	2.24090386	2.31721814	0.88106153	0.91912734	0.9498655
P23	2.27474778	0.7841611	0.70135315	0.27064652	1.51330335	2.07521344	0.69258024	0.47675731	0.36101449
P24	1.28391324	-0.0879066	-0.3404809	-0.3163506	1.10809982	0.80535041	-0.6059986	-0.3842458	0.19540552
P25	0.5833904	1.75497876	1.17482432	1.16905115	2.25820327	2.83483441	1.11219056	0.93577661	0.53082493
P26	1.16750753	-0.0756579	0.07284276	-0.1703555	1.11565569	1.18536496	0.13820772	0.72783842	-0.2525046
P27	1.26012775	0.987413	0.64038076	0.65949667	1.95423079	2.07893868	0.6510304	0.78921276	0.70582275
P29	2.15148272	0.42310854	0.17851054	0.19444667	1.3235203	1.34725002	-0.0946865	0.02880374	0.02935521
P30	1.29545152	1.71795702	0.93128126	1.26984191	2.65830465	2.6810305	0.65845578	1.39185216	1.26304588
P31	1.47110053	-0.5761294	-0.3398306	-0.4631857	0.60014766	0.4437977	-0.2114433	-0.4276178	-0.49638
P32	0.05029314	2.01231946	1.55966506	1.49692236	2.88819065	3.19163532	1.72916542	1.47373431	1.08476047
P33	1.27537776	1.53759353	1.15393661	0.54188607	2.60652781	2.90916508	1.32300744	1.27934429	1.00920063
P35	1.615397	0.65325737	0.4881217	0.27960422	1.30102153	1.67611185	0.14050623	-0.5790822	0.25143213
P37	0.80367079	0.64413852	0.20682675	0.50702995	1.01097329	1.44595102	0.06489863	-0.2350146	-0.112387
P38	0.17892313	1.19888599	0.94103427	0.73649399	2.05699185	2.2240781	0.25850284	0.89966929	0.54716082
P39	0.51575559	0.06974259	0.07821356	-0.766517	0.48825788	0.90699768	-0.0906713	-0.5636991	-0.8291387
P40	-0.366214	0.75525512	0.94884827	0.63822404	1.99901513	2.22258981	0.48486848	0.74062153	0.48775307
P41	2.99845191	0.68169435	1.31770989	0.65088317	1.74904477	2.27176671	0.18456903	-0.1361921	-0.6612771

Table 8.55: Normalised data matrix for phosphatidylglycerol for hair samples taken from breast cancer free controls.

	PG(16:0)	PG(18:0)	PG(26:0)	PG(19:5)	PG(19:6)	PG(28:0)	PG(30:0)	PG(30:1)	PG(31:0)	PG(32:0)	PG(32:1)	PG(34:1)	PG(36:1)	PG(36:2)	PG(36:3)
C21	4.73579412	5.05461995	3.89583988	3.17974455	0.61807135	3.44353796	3.28347126	2.92794308	2.77689658	3.50082626	3.35777425	3.04104297	1.82650479	2.30577998	2.12122036
C22	2.30776416	2.40352743	2.37786681	2.80743583	1.07077238	2.06566901	1.91418726	1.12895904	1.2759213	2.48186363	1.91078089	1.69483352	0.56478201	0.48534077	0.30454709
C23	1.85508968	1.97905337	1.39489984	2.98862027	0.83737843	0.94877855	1.13081886	-0.0257867	0.18307156	1.65988274	0.50180777	1.02873415	0.26351084	0.21781806	1.52414053
C24	2.42900182	2.47988353	2.40413114	3.13949644	2.09395264	2.00476902	1.73489834	1.22338688	0.83923128	2.18841111	1.36975909	1.87956769	1.16246905	0.8729485	1.67052145
C25	2.01177005	2.35684772	2.32847115	2.34184566	1.1256844	2.06441849	2.17706886	1.87778576	1.50751301	1.896239	1.97029371	1.59641066	-0.1780177	0.23084539	-1.3116875
C26	1.11493501	1.89170636	1.84408728	2.997865	0.55215949	1.8685456	1.81117095	1.01664152	0.93571159	2.40199383	0.97089255	1.59659445	0.66394835	0.44773246	0.74597996
C27	2.35720553	1.2111903	1.69257474	1.70820084	0.45391381	2.03814129	2.11458396	1.799008	1.74026828	2.31663188	2.22333109	1.945979	0.35229948	0.52499622	-0.0655935
C28	6.00725181	6.26917972	4.0622719	3.06661363	0.42397181	3.41506833	3.32051855	2.68770702	2.54080528	3.60929748	3.1717705	3.33791053	2.23365274	3.12245248	1.34550773
C29	1.82086625	1.7195273	1.67077354	2.94394826	1.70008986	1.5434759	1.56751933	0.85097019	-0.1213971	2.35919832	0.79473953	1.42611843	0.65457526	0.54581901	0.87014357
C30	2.79657487	2.68954738	2.47676291	2.53630455	-0.2547761	2.34139854	2.75481719	2.1643795	1.78279119	2.96979757	2.57209886	2.63273236	1.43263013	1.5145992	-0.2856777
C31	2.41373283	2.72700893	1.6996379	3.25387768	1.19693592	1.64251056	1.43894537	0.99289986	0.33185669	1.69780644	0.87472627	1.07473148	0.27858772	0.42969013	1.42422668
C32	2.41139025	2.66187681	2.41240642	3.0117334	0.55824924	1.79980835	1.63501381	1.50071129	0.61678765	1.78896291	1.08334033	1.30747033	0.1534279	0.76247875	-0.3668623
C33	2.6626686	2.5553931	3.20937329	2.92411063	0.33210887	2.89762766	2.39162477	2.47616359	2.08444491	2.4375934	2.49981673	2.00635588	0.29243489	1.02150226	0.25035991
C34	6.45129254	6.8737963	6.08688483	2.43548873	1.96002196	5.21779514	4.9350362	4.60949965	4.68906289	4.8722369	4.94073414	4.78762938	3.98055925	4.38805387	0.66611162
C35	1.96323393	2.16702005	1.64470913	2.98649972	0.8750002	1.31953972	1.44698548	0.66237256	0.56345048	2.13900678	0.74813372	1.14350054	0.57029327	0.01924834	1.33373351
C36	3.74308047	4.207224	3.32715474	2.99633631	1.32052806	2.78997637	2.09302663	1.91974256	1.06346695	2.35444102	1.54900985	1.7453623	1.38033916	1.71210731	0.51782204
C37	6.97252861	6.66304815	4.37377595	2.21327048	0.8491402	3.58373859	3.28094053	2.90510687	2.77709423	3.58280368	3.5198298	3.44301255	2.41126724	3.24420897	1.63779056
C38	2.60398387	3.31891893	4.14037095	2.96737279	1.38946253	3.59338969	3.35137526	2.86582815	1.97654968	2.67735893	2.65017111	2.16714952	1.01389978	1.59923431	1.91483903
C39	2.54211047	2.82712162	2.06781917	3.19559795	1.96781038	2.19088146	2.28513257	1.68720658	1.44486022	2.59091335	2.00413813	2.15940219	1.14395029	1.16350838	1.02698235
C40	2.32663952	2.13904253	1.16409679	2.5381125	0.17627654	1.01225395	0.87571127	0.68290382	1.15069521	1.75170789	1.09338436	0.96319749	0.21658207	0.16587757	-0.6526018

Table 8.56: Normalised data matrix for phosphatidylglycerol for hair samples taken from patients with breast cancer.

	PG(16:0)	PG(18:0)	PG(26:0)	PG(19:5)	PG(19:6)	PG(28:0)	PG(30:0)	PG(30:1)	PG(31:0)	PG(32:0)	PG(32:1)	PG(34:1)	PG(36:1)	PG(36:2)	PG(36:3)
P19	2.58628062	2.74960277	2.4876077	3.30899378	1.04457887	2.55324248	2.5492758	1.59235593	1.1366352	3.09456689	1.87718159	2.39891915	1.85520679	1.77774903	2.40361864
P20	5.33700188	5.66911191	4.2326776	3.1633026	0.95173376	3.4775746	3.09062183	3.01674968	2.7835406	3.30533516	3.2564926	3.29060443	1.94948994	2.81032956	0.85982255
P21	1.72028584	1.84994639	2.47080471	2.10712662	-0.0790162	2.40258491	2.80981074	2.16774999	2.36796946	3.12041148	2.87530042	2.81023711	1.2901541	1.91467903	0.67672558
P22	4.54412264	5.29720996	4.68162504	2.67794221	-0.1925489	4.13085689	3.72454678	3.36743309	2.83372171	3.40020334	3.45965026	3.06276337	1.1935963	2.1016743	2.82730874
P23	1.71470089	2.39318964	1.63163828	2.63069467	0.67915766	1.48052363	1.37941803	0.64648446	0.9907817	1.65058249	1.34001282	1.24910266	0.26354113	0.68956028	1.42837337
P24	4.07589591	4.1648512	4.52069125	2.67282548	0.99237145	4.20193597	3.68288916	3.49088762	1.94837443	3.61495005	3.09670849	3.08500944	2.03162045	2.71939303	1.07119519
P25	2.39488156	2.554673	2.33590027	2.5333773	1.7436042	2.39917951	2.35900478	1.60175485	0.93683657	2.46468812	1.89797404	2.24358929	1.19112245	1.35853404	1.68765765
P26	2.65472221	2.75082554	3.12658539	2.26159167	0.83863336	2.86649021	2.19621042	2.01091332	0.6370928	2.13316314	1.37303313	2.12289334	0.92578795	2.50283963	0.80057503
P27	1.7779167	2.12363485	2.07239293	3.28025428	1.31676675	1.98261956	1.72911582	0.90069855	0.73531876	2.33738831	0.90375499	1.5280916	1.05606572	0.98764465	1.22435798
P29	4.55355538	4.95972409	4.44571688	3.09021645	0.35997048	3.84443937	3.12892811	2.60418462	2.55814087	3.24819345	2.74972716	2.99986614	2.32385312	3.05871995	0.77421864
P30	3.30015028	3.65303535	3.16197278	2.94017546	0.91277283	2.82608638	2.42981304	2.62552904	0.61563102	2.29152136	1.61815772	2.21315261	1.6263208	1.66473168	2.0124711
P31	3.76940778	4.36906105	3.92576554	2.77838797	0.3250939	3.13464023	2.71997937	2.31412702	2.1672415	2.96015487	2.84632047	2.69765106	1.74641073	1.96309838	0.3869534
P32	4.25296852	3.98359644	2.90172072	2.8938477	1.89987653	2.62888309	2.42460832	1.68921746	1.44416225	3.00110145	1.96890097	2.32679113	2.0032301	1.66026475	1.92569739
P33	3.2563351	3.64003466	3.54790112	3.15043362	1.34573089	2.85548881	2.59408265	2.03654662	2.20447718	3.0546142	2.36440027	2.38357801	1.80918065	1.95204537	1.79271794
P35	6.47160021	6.97591692	5.33337386	2.60483807	0.89519988	4.35223642	4.03318981	3.42093965	3.448173	3.98131939	3.87411415	3.85566989	2.80780975	3.86260328	1.23764299
P37	1.64869578	1.66340786	2.61360963	2.937913	0.53115055	2.35541487	1.85332429	1.42766888	0.72129475	2.43431189	1.35607713	1.11960951	-0.0133669	-0.1551681	0.68284686
P38	5.2018511	5.54216898	4.64028493	3.08788586	1.1261648	3.56174114	3.10097051	2.88020443	2.39633041	3.01000335	3.05130487	2.62582513	1.47133239	2.35967966	2.15779364
P39	5.69356511	6.32521371	5.03760149	3.27210266	0.47100982	3.90129163	3.73363274	3.40354546	3.29623996	3.78574208	3.8690689	3.40508695	1.94743042	2.94369942	0.28331093
P40	2.50441024	2.50297805	2.81454481	2.92570898	1.44596001	2.52123632	2.58265246	2.10083904	1.58070483	2.75901789	2.44882092	2.43407155	1.69165154	1.81771558	1.33204657
P41	4.35573442	4.81158668	5.79889387	4.01628557	2.12886048	4.89274863	5.10482758	4.62708977	4.9873131	5.2045871	5.28278346	4.67070345	3.13190154	3.89952523	1.2536364

Table 8.57: Normalised data matrix for phosphatidylinositol for hair samples taken from breast cancer free controls.

	PI(16:0)	PI(32:0)	PI(32:1)	PI(33:0)	PI(34:1)	PI(36:0)	PI(36:1)	PI(36:2)	PI(36:3)	PI(38:1)	PI(38:2)	PI(38:3)	PI(38:4)	PI_Cer_1	PI_Cer_2	PI(34:2)
C21	2.5067386	3.49579847	1.47396955	1.17808426	3.77255112	3.81672881	4.44764759	4.05149989	1.52736331	2.52747495	1.66064463	2.58613022	2.33865796	0.20438488	0.83125023	2.16247306
C22	0.90490762	2.29380631	1.5394997	0.81381019	2.86352511	2.90311698	3.10060165	2.01753954	1.0754119	2.12025182	1.23390359	1.37886235	1.88486918	1.00700726	1.86775775	-0.0324088
C23	1.0916119	3.18468515	1.01142095	2.06835627	3.39503018	3.59530582	3.96750102	3.06777143	1.33974743	1.99805769	0.49953324	1.84879461	1.37480246	0.47320297	1.7101816	0.98758217
C24	1.80538185	2.55575786	1.90225269	1.80741277	2.97668478	3.11906092	3.71818341	3.13476565	0.77739422	2.20409926	2.00699791	1.82991635	1.45656753	1.6858268	1.32742981	1.5931788
C25	2.06386443	1.26505924	2.17661713	0.95707904	2.81996733	1.95668088	3.15519238	3.02015656	2.7057392	1.94744562	2.26010225	2.10409925	1.53532599	1.5708065	0.66146639	2.00840476
C26	0.98738273	2.49660573	2.11225314	1.89100633	2.61243611	2.8050668	3.26280799	2.40454132	1.44417719	2.16312071	2.51065507	2.23009002	1.36434097	1.54769725	1.34052176	1.28204249
C27	1.00173181	2.89060925	2.35489754	3.02762196	3.17241886	3.40217199	3.71211086	3.57558683	1.9664018	2.6704112	1.31626934	2.2433212	2.04543583	0.83719501	1.34378635	2.85188878
C28	1.6576259	2.94758736	1.65125201	0.6903903	2.91349869	3.55975334	3.74912921	3.13225131	0.38786253	1.70019397	0.65787016	1.28234831	1.52404408	0.28935891	0.63062309	1.17478045
C29	0.99907079	3.62038445	1.84103931	1.13716886	3.38156436	3.88388371	4.22283729	2.71003537	0.99725038	2.72369222	0.7717801	1.72674655	1.90879725	1.43108163	1.57481689	1.04221199
C30	1.52275714	2.97830787	2.1592255	0.80156748	2.56621618	3.70104002	3.64253371	2.0829887	2.20989283	1.96079424	0.90914112	0.35199423	1.53826582	1.85969605	2.09390754	1.44787937
C31	0.91723404	2.75836282	1.19569835	1.49150213	3.15979213	3.25863113	3.90239291	3.43451912	0.9187128	2.26401869	1.5611211	1.53971263	1.88516158	0.82860367	1.12303251	1.43936701
C32	1.06775111	1.96515192	0.94558621	0.18604062	1.41462977	0.45307729	1.20571095	0.84633226	0.46285099	0.15030893	-0.3838744	-1.2778809	-0.3544643	1.68040804	1.00566158	0.30297555
C33	0.92486167	2.04723953	1.80749601	1.21115297	2.20647689	3.17556605	3.06095442	1.93775228	1.08033436	1.37663835	1.07565104	-0.2814214	0.18823162	0.55532188	1.10174636	0.12848955
C34	1.92575754	2.44538133	2.21621173	1.39924726	2.88803759	2.07522329	2.94917713	2.68740554	0.66045766	2.09478492	1.53918153	1.10094805	0.340099	1.35155147	0.82412792	1.51827066
C35	1.62877277	2.69212111	2.39643034	1.62931544	3.19409579	3.25248058	3.85040163	3.70205493	1.91308671	2.4855343	2.14816916	2.29872112	1.43970486	0.41475721	0.58093092	2.0013755
C36	-0.291143	2.22364426	1.07951212	-0.1764913	2.41965196	2.27106828	2.3978618	1.85311991	0.56452649	0.47352782	0.25270498	0.31134251	-0.1443855	1.58013991	-0.1673398	1.14968427
C37	1.37512982	3.00591572	1.7965213	1.37782511	3.69011592	3.44565352	4.18609383	3.84515049	1.31677301	2.50966863	2.12300802	2.43962561	1.75949951	0.20040127	0.49817159	3.14596217
C38	0.46173482	2.88823451	2.1909009	1.67470305	3.03755269	3.7151848	4.13237872	3.35671776	0.29193711	2.3173656	1.75600668	1.87481427	2.09712016	0.10656606	0.30987443	0.54396689
C39	1.89123772	2.27017821	0.93135448	1.22823172	2.75734089	3.08087376	3.24389142	2.53667855	0.05674084	0.35105064	0.2628257	0.32815467	0.35886255	1.68462853	0.75432241	1.00219792
C40	-0.0948446	1.7812617	2.36931875	2.38746312	2.72947336	0.74197986	2.15541706	2.43059188	2.82259456	2.63608736	1.03173962	1.6546605	0.66467422	0.67465038	0.16834034	1.62974391

Table 8.58: Normalised data matrix for phosphatidylinositol for hair samples taken from patients with breast cancer.

	PI(16:0)	PI(32:0)	PI(32:1)	PI(33:0)	PI(34:1)	PI(36:0)	PI(36:1)	PI(36:2)	PI(36:3)	PI(38:1)	PI(38:2)	PI(38:3)	PI(38:4)	PI_Cer_1	PI_Cer_2	PI(34:2)
P19	1.8885669	3.30840754	2.17792963	1.89705773	3.76401572	3.38840642	3.9718083	3.12529738	1.04936447	2.21279365	1.76324088	1.48945271	1.70736638	1.09812112	1.00079348	1.18951272
P20	1.9678625	2.79553107	1.74715098	1.12213236	2.83697522	3.0141389	3.52303451	3.00442558	0.31660626	1.76816196	0.67812456	1.28795321	1.18009269	1.32763005	1.18965003	2.03333622
P21	1.9125665	3.52449787	2.82790875	3.1213734	3.40721981	3.23031218	4.24518636	3.13475792	4.28461456	3.47258893	2.33508686	2.35892863	1.98426756	1.94665222	2.31527389	1.86362432
P22	2.06589424	3.30778635	2.38150659	1.35475455	3.8407191	3.53821602	4.20668424	3.63497859	0.60364265	2.51225002	1.21796775	2.10516576	2.53722899	1.56077907	0.68192572	1.53505093
P23	1.50182219	2.30762954	1.97217234	1.01621664	2.67600286	2.1991227	3.56435163	2.84059878	1.25915833	1.82380996	1.53596683	1.37284994	1.39277928	1.38450509	1.48532426	1.56721511
P24	1.75060041	2.22025862	2.29269253	1.18448413	3.03266798	3.07469869	2.98530357	1.9797178	-0.2511212	1.23530141	0.83797442	0.57293288	1.89909059	1.24577879	0.31775236	1.35319371
P25	0.25658931	2.89582514	2.44842536	1.45152591	3.2174013	3.11628204	3.41264527	2.78588771	0.66011385	1.8428743	1.27841227	0.02184483	1.4781479	1.78607669	-0.060963	-0.3072369
P26	1.11909694	2.47049571	1.83203226	0.8924926	3.14237211	2.35010059	3.03112431	3.20312121	1.01264917	1.96966926	1.41792392	1.90473408	1.87636664	0.59420075	0.61276831	0.70069407
P27	2.15305533	2.62161729	1.50397739	1.253568	2.97813204	3.33635048	3.61459981	2.97381237	0.38877875	2.14876826	0.95176163	1.9309361	1.567936	1.51978737	0.07975805	1.50842695
P29	1.54077425	3.33640937	2.9821982	2.32671232	3.9531369	2.6315604	3.12113637	3.08362424	1.84026081	2.80984683	1.45396658	0.77913545	1.90296609	1.09288841	1.03352078	2.62621672
P30	0.86790862	3.0794782	3.3165466	1.44949821	3.29470762	3.29496663	3.67575229	2.69768355	-0.1611608	1.6533789	0.84379568	1.08923397	0.85694917	1.02323455	0.50325497	0.59916612
P31	1.4951012	2.78179526	2.56508291	2.09736815	2.91993023	2.147878	2.63716355	2.65302299	1.25471345	2.12429793	0.99609285	1.27556	0.7927635	1.13621651	1.01378805	1.58597883
P32	2.37204553	3.06687646	2.04323085	2.06470898	3.40509529	4.0083372	4.17784843	3.65572492	0.24311925	2.53904265	1.6817605	1.93047439	1.21330499	1.58089936	0.75844727	1.59388308
P33	1.86525441	3.41955627	1.1829414	1.52940937	3.29717367	3.59790103	4.03183535	2.97331082	0.9212868	2.08837297	0.932902	1.75876514	1.72806123	1.50659961	0.86327114	0.3047367
P35	2.21086309	2.63280119	2.36709129	0.79876344	3.15419089	2.89052574	3.52819716	2.76056754	1.00138757	2.56959935	1.99326263	1.69949055	1.87617817	2.54094405	0.57802213	1.34616305
P37	1.2445277	2.30813509	1.96688761	0.47374662	2.73254216	3.13961614	3.2374016	2.20317782	1.97117804	2.45650659	1.54886134	0.5568342	0.96019148	0.78923056	1.04095924	0.06052731
P38	1.42187171	3.67332461	2.67776478	2.23989291	4.30450224	3.51132411	4.0521514	3.46636155	0.61295686	2.74331547	1.60784817	1.98776475	2.64197486	1.08818067	1.21646161	1.76628983
P39	1.74841632	2.61097537	2.46866263	1.51726231	2.90469547	1.8695948	2.50994879	2.38967718	1.25809262	0.98103861	-0.8112955	0.17310361	-0.5769781	1.7646146	1.41480199	1.10795305
P40	1.52659849	4.293562	2.44098959	3.00103992	4.71412227	4.35071519	5.07081611	4.15047796	1.68487473	3.1386701	2.34011206	2.61325872	2.7192659	0.85994833	1.15154646	2.23177666
P41	2.60098824	3.94085112	2.9773939	2.26556403	3.48382214	3.34226828	3.81957725	3.3944891	2.61527192	2.43538518	2.69884014	1.92786498	2.06142607	2.65890372	2.65678439	2.19265396

Table 8.59: Normalised data matrix for sphingomyelin for hair samples taken from breast cancer free controls.

	SM(30:0)	SM(32:0)	SM(32:0)(2)	SM(32:1)	SM(33:0)	SM(33:1)	SM(34:0)	SM(34:1)	SM(34:2)	SM(d31)
C21	-1.0001629	3.08238498	2.28428559	-0.9377645	3.58366854	3.5857025	8.59795741	6.17247214	1.85304576	8.42216434
C22	-0.1903313	1.88740776	2.08427023	-0.7545255	2.59095736	2.58708316	7.89600976	5.03891049	0.98214457	7.47501243
C23	-0.3033491	2.32990653	2.79580183	-0.7930591	3.51240049	3.51240049	8.11182154	5.65789126	1.11359988	7.27060471
C24	0.88512956	2.32873628	2.53434656	-1.2777092	3.71902226	3.71902226	7.83309554	5.81559221	2.33810054	8.03279452
C25	0.76856582	2.72281274	2.1253596	0.21848719	3.57838865	3.57838865	7.46155742	5.72570881	1.85066355	6.34461567
C26	-0.2761146	1.87054846	2.55802965	-0.3863708	3.31653096	3.31653096	7.40918063	5.04184543	1.03111094	7.09480636
C27	-0.1180084	3.00911815	1.9458641	-1.5563734	3.97553773	3.97553773	8.62196341	6.2729326	2.31585026	7.29658992
C28	-0.4463278	2.71940818	3.00543195	-0.9004794	3.21621314	3.21621314	7.44846804	5.16919111	1.6670052	7.89105842
C29	0.43434079	1.76121723	2.45256666	-1.1474631	2.86406476	2.86406476	8.0013701	5.08997016	1.19003129	8.40676644
C30	0.23803946	2.26195938	2.03371653	-1.219108	2.97426289	2.97426289	7.28379007	4.86835759	0.71915252	6.11567907
C31	-0.6787836	2.82342626	2.58802466	-1.3179147	4.15818318	4.15818318	8.8317658	6.01544642	1.68419688	7.6650225
C32	-0.6064472	1.59060403	1.77412981	-1.0232237	2.16273259	2.1963083	5.74144369	4.44613574	0.57994111	6.20406762
C33	-0.7148918	1.50854467	2.6467265	-0.4445337	2.97452095	2.98679543	7.65885693	5.06048243	0.36651848	6.54083768
C34	-0.0946702	2.60977194	2.79148694	-0.8973882	3.45765147	3.45765147	8.32622214	5.45657877	1.64852251	7.01395196
C35	-0.3114373	2.97808667	2.03716892	-0.9718344	3.88493796	3.88493796	8.42441318	5.74286119	2.38449419	7.38420884
C36	-0.6610554	1.32890998	1.88200316	-0.5770035	2.60743075	2.62062483	7.42912457	5.07134036	-0.4972759	7.26065
C37	-0.4273537	2.8279879	2.40032104	-1.3864522	3.65010151	3.64279796	8.3843357	5.82193519	1.90817638	7.75019198
C38	-0.86539	3.31183404	2.85747873	-1.3609396	4.1270099	4.1270099	8.8797343	6.31529198	2.95408627	7.90691585
C39	0.85119438	2.27767092	2.25044726	-1.2636795	3.12315214	3.12315214	7.86645078	5.5901266	1.31973607	7.47604225
C40	0.0481925	1.67508084	2.81080629	-0.4655386	2.6557801	2.67443365	6.96064087	5.13399485	-0.5559441	7.06531786

Table 8.60: Normalised data matrix for sphingomyelin for hair samples taken from patients with breast cancer.

	SM(30:0)	SM(32:0)	SM(32:0)(2)	SM(32:1)	SM(33:0)	SM(33:1)	SM(34:0)	SM(34:1)	SM(34:2)	SM(d31)
P19	0.00525451	2.63625489	2.74776905	0.01509817	3.92663179	3.92663179	8.48200756	6.06851759	1.65061193	8.48100867
P20	0.03202318	2.28415094	2.93802867	-0.4183957	3.34567488	3.34567488	7.46688056	5.46430761	-0.2599645	7.09201317
P21	1.52383904	1.64882162	2.67795499	0.72261733	3.10696844	3.10696844	7.91298175	5.05178859	0.70554203	7.19722162
P22	-0.0506685	2.54365839	2.8425516	-0.39526	3.14570491	3.14570491	8.10022571	5.07710286	1.34502168	8.3193965
P23	-1.0109087	2.6338057	2.97042143	-1.0699891	3.93101567	3.93101567	7.77412418	5.82698598	1.98778952	7.37774309
P24	0.46645675	2.94204029	2.24386017	-0.7086591	3.43154271	3.43154271	7.95226427	5.88401983	1.38498138	8.13234304
P25	-0.358918	2.28998906	1.77230861	-0.1087794	3.333769	3.333769	7.68958841	5.74598321	1.45599255	7.74380453
P26	-0.065689	2.79644972	2.32582063	-0.3359809	3.73465536	3.73465536	8.18965853	5.67639598	1.59457301	7.55549007
P27	-0.4728328	2.29373626	2.16782544	-0.0561293	3.44011241	3.44011241	7.90747448	5.57433665	1.05610319	7.58428372
P29	-0.1140129	2.01485594	3.13507709	-0.7806854	3.83833316	3.83833316	7.5207755	5.03744178	0.40903192	7.25318873
P30	-0.7488118	3.34353549	2.34584754	1.35027698	4.31305765	4.31305765	8.13482119	6.49717231	2.76677729	8.55134664
P31	-0.7362441	2.19153979	1.95862796	-0.8140352	3.18413822	3.18413822	7.02850894	5.16915284	0.90311747	7.17577008
P32	-0.2112107	2.77861929	2.61803238	1.28642945	3.36588417	3.36588417	8.22707218	5.76174677	1.74006644	7.84307445
P33	0.0671145	2.38006607	2.81587307	-0.7298	3.59744429	3.59744429	8.11999262	5.71018108	0.81308087	8.00375607
P35	-0.7831169	2.34180095	2.23484137	-1.386435	3.23506063	3.23506063	7.61659545	5.31609522	0.78782175	7.81756238
P37	-0.1414595	1.95218466	2.91248044	-0.314089	3.45733728	3.45157609	7.74676801	5.27783642	0.39781563	7.34269379
P38	-0.1209858	2.88593446	2.13571866	-1.3513564	3.53954415	3.53954415	8.0048786	5.88198683	0.84885063	8.57387816
P39	0.24079682	1.90087087	2.6247451	0.07740206	2.78123783	2.78123783	7.35986895	5.19483773	0.98006966	6.66534543
P40	-0.3441319	2.38854562	2.18020111	0.05970248	3.26649975	3.26649975	8.1988471	5.3401891	1.35562234	7.91597785
P41	0.48728088	2.80617201	3.81655928	0.27659716	3.58954748	3.68489024	8.72464031	6.18137457	0.89775995	7.37731323

8.3.3. Heteroscadascity plots for hair samples

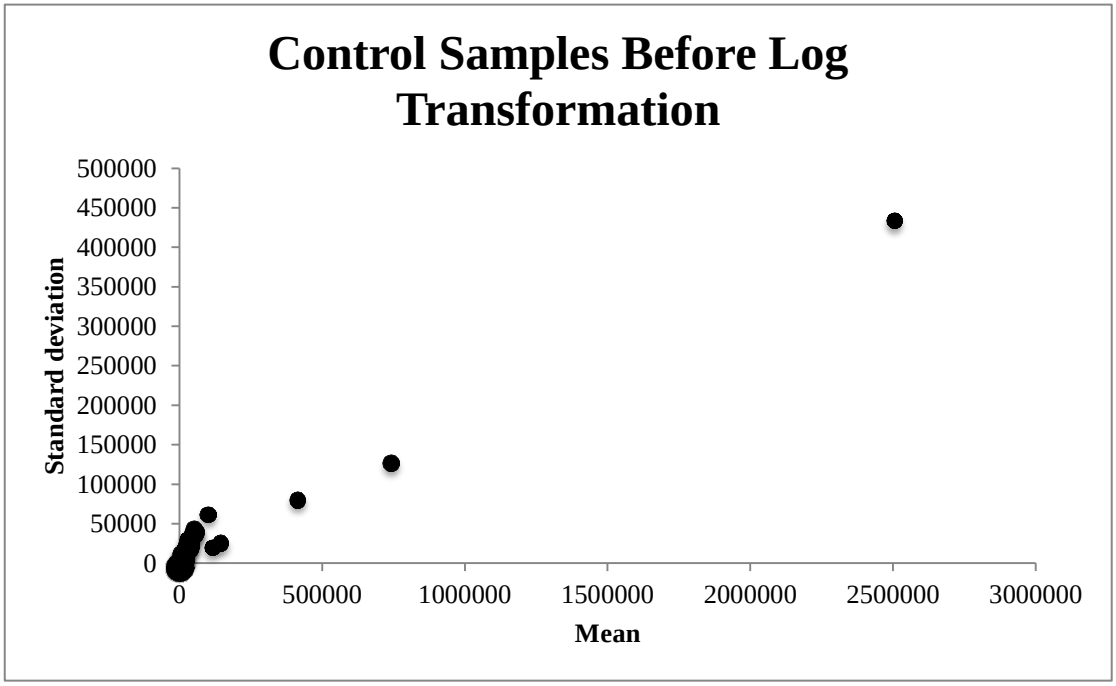


Figure 8.1: Heteroscadascity plot of the average of the control hair samples for all lipid species before log transformation

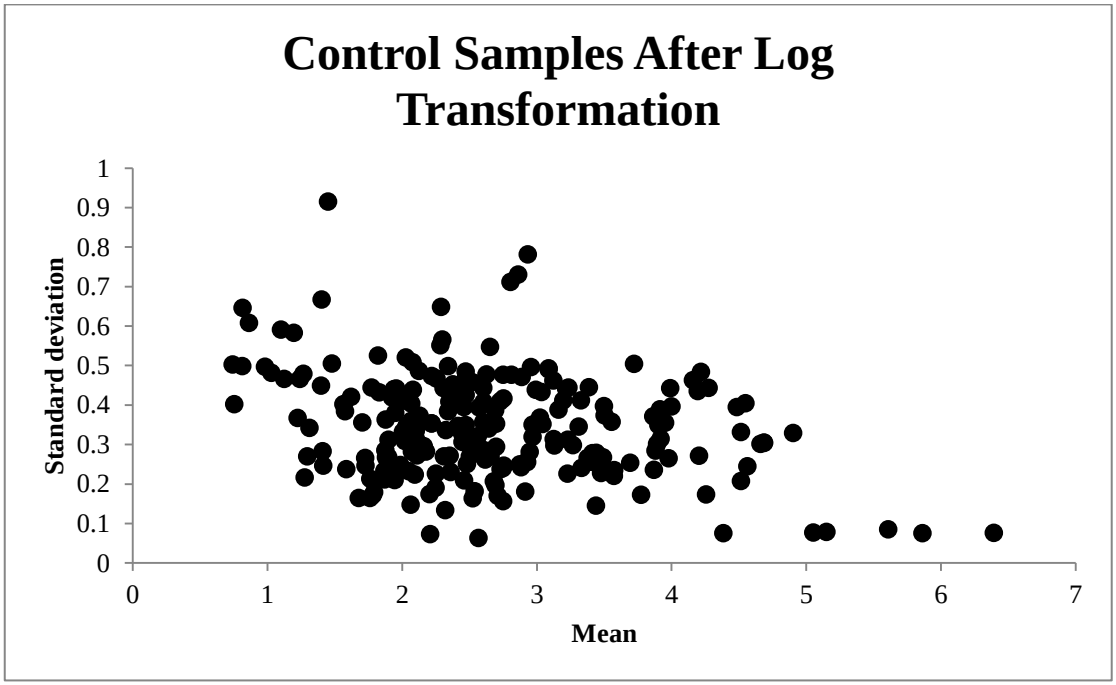


Figure 8.2: Heteroscadascity plot of the average of the control hair samples for all lipid species after log transformation

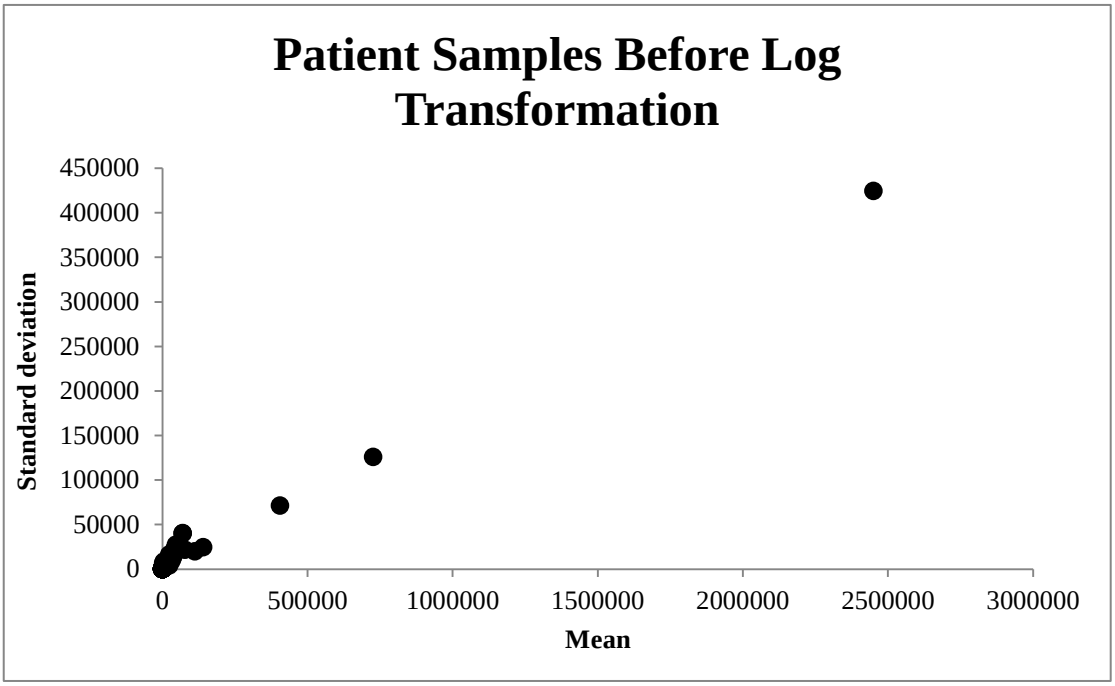


Figure 8.3: Heteroscadascity plot of the average of the patient hair samples for all lipid species before log transformation

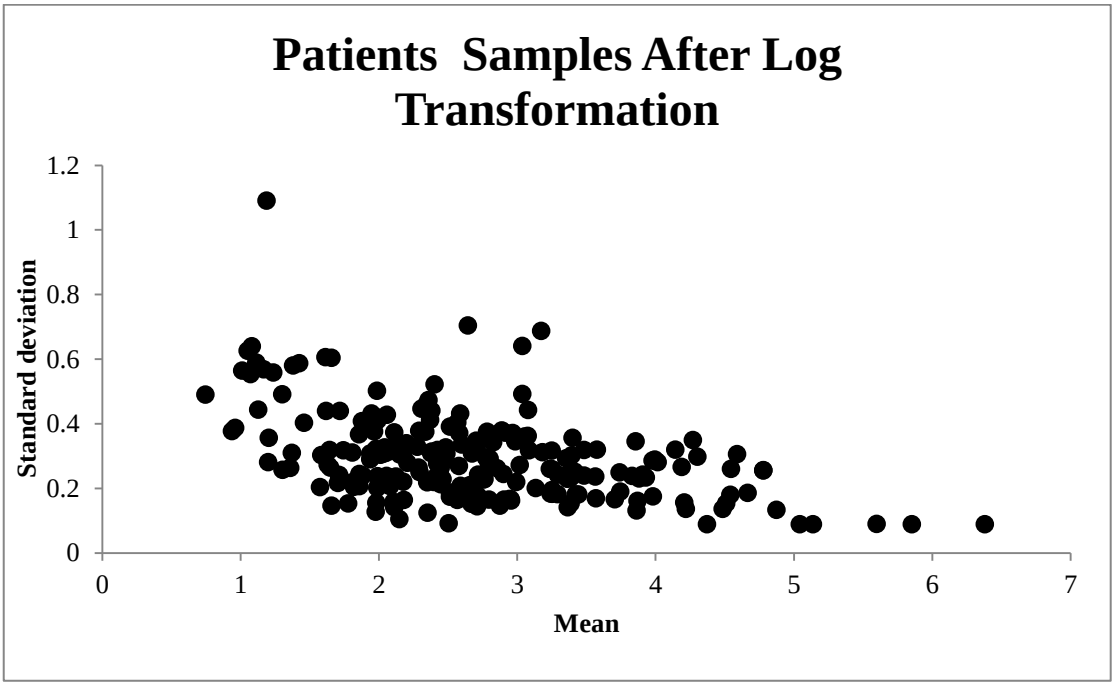


Figure 8.4: Heteroscadascity plot of the average of the patient hair samples for all lipid species after log transformation

8.3.4. Two sided t-test

Table 8.61: Data generated from a two sided t-test comparing control hair samples to the breast cancer patient hair samples. Those species with an adjusted p-value < 0.05 and fold change > 2 were considered significantly different (in red with pink fill) between the two groups.

Phospholipid specie	Fold change	logFC	T statistic	p value	Adjusted p value
CE(15:1)	0.749935437	-0.28776816	-1.846655366	0.071225612	0.686856721
CE(18:3)	1.449233965	0.371035117	1.710645771	0.093872687	0.686856721
CE(21:0)	1.192204707	0.175804288	1.494412325	0.141885571	0.686856721
CE(19:2)	0.826844221	-0.190138968	-1.329706257	0.190160875	0.686856721
CE(17:1)	0.81927296	-0.199337966	-1.324812829	0.191766526	0.686856721
CE(18:2)	1.168000968	0.155293713	1.286517464	0.204689428	0.686856721
CE(17:2)	1.224525368	0.202553314	1.101241211	0.276511545	0.686856721
CE(22:0)	0.768709795	-0.263041761	-1.030899618	0.307969197	0.686856721
CE(19:4)	0.901351408	-0.103860077	-1.022593953	0.311839161	0.686856721
CE	1.23071931	0.207598803	0.994452945	0.325196523	0.686856721
CE(23:5)	0.862670042	-0.147722999	-0.930555082	0.356933998	0.686856721
CE(19:6)	0.882776858	-0.124682819	-0.896494298	0.374649121	0.686856721
CE(21:4)	1.136785397	0.128204452	0.736722017	0.465026302	0.717594335
CE(19:3)	0.930065493	-0.072500273	-0.634914404	0.528624715	0.717594335
CE(21:5)	1.116033158	0.109780575	0.632465855	0.530208833	0.717594335
CE(19:1)	1.110593613	0.104894659	0.599404681	0.551839316	0.717594335
CE(23:6)	1.124394955	0.117245073	0.570407979	0.571172402	0.717594335
CE(21:1)	0.911768601	-0.092369048	-0.546847102	0.587122637	0.717594335
CE(18:0)d6	0.921373445	-0.081889847	-0.46360485	0.645113614	0.746973658
CE (13:6)	1.050018655	0.048807931	0.219139517	0.827509257	0.872910827
CE(17:0)	0.969190579	-0.03129401	-0.166941285	0.868146765	0.872910827
CE(15:0)	0.973738983	-0.026611996	-0.160855	0.872910827	0.872910827
Cer(d18:1/40:3)	1.279433116	0.246417102	1.765236206	0.08427408	0.41954386
Cer(d18:1/38:3)	1.248129021	0.221645647	1.649982959	0.105874206	0.41954386
Cer(d18:1/24:1)	1.372597364	0.316704831	1.611103756	0.114113801	0.41954386
Cer(d18:1/25:0)	0.828610225	-0.188005409	-1.5528905	0.127418437	0.41954386
Cer(d18:1/42:6)	0.702129568	-0.353637322	-1.502770166	0.139847953	0.41954386
Cer(d18:1/39:3)	0.760222622	-0.274143965	-1.314856607	0.195185221	0.487963052
Cer(d18:1/24:0)	1.1748289	0.16112252	1.129143915	0.264789642	0.518700138
Cer(d18:1/22:0)	1.181657823	0.166918387	1.083104913	0.28450154	0.518700138
Cer(d18:1/41:4)	0.841800546	-0.172212174	-1.024129056	0.311220083	0.518700138
Cer(d18:1/41:3)	0.841203878	-0.172921225	-0.794556291	0.431020664	0.646530996
Cer(d18:1/44:6)	0.894493586	-0.111497546	-0.589548525	0.558426627	0.730404131
Cer(d18:1/40:4)	1.095281071	0.091011016	0.551031936	0.584323305	0.730404131
Cer(d18:1/32:3)	1.061550952	0.059731001	0.428757171	0.670134906	0.773232584

Phospholipid specie	Fold change	logFC	T statistic	p value	Adjusted p value
Cer(d18:1/41:2)	1.037371708	0.036690311	0.20314757	0.839930745	0.899925798
Cer(d18:1/44:5)	0.972560325	-0.027823175	-0.0833076	0.933974529	0.933974529
PA-3	0.674641913	-0.393573228	-1.945558266	0.057772825	0.415790023
PA-5	1.228605355	0.205879668	1.627892748	0.11031164	0.415790023
PA(27:4)	1.33445766	0.288524962	1.56343648	0.124737007	0.415790023
PA-9	0.876460043	-0.131864163	-0.82655441	0.412714783	0.85524896
PA-7	0.915041614	-0.088785735	-0.339616672	0.735675836	0.85524896
PA-2	1.088462649	0.084766287	0.33335244	0.740368138	0.85524896
PA-1	0.950082152	-0.051206822	-0.31574749	0.753608331	0.85524896
PA(27:5)	1.05525598	0.053783373	0.309244592	0.758518206	0.85524896
PA-4	1.060377581	0.058625053	0.291552601	0.771926609	0.85524896
PA-6	0.974189539	-0.026149396	-0.183442713	0.85524896	0.85524896
LPC (18:2)	0.518856753	-0.65612744	-3.833390342	0.000416625	0.052911388
LPC (20:4)	0.580451126	-0.543949675	-3.447368904	0.001298587	0.082460296
LPC (20:3)	0.658138312	-0.418340169	-3.07688453	0.003673204	0.155498948
LPC (17:0)	0.669913661	-0.400606439	-2.541085748	0.014831229	0.365025793
LPC (17:1)	0.647658739	-0.434391359	-2.448141772	0.018616492	0.365025793
PC (32:0)	1.296881339	0.259962412	2.393541142	0.021229281	0.365025793
PC (24:2)	1.989292576	0.687779086	2.376932414	0.022087286	0.365025793
LPC (20:2)	0.706708434	-0.347137097	-2.360005548	0.022993751	0.365025793
PC (26:0)	1.350545536	0.300508611	2.010312826	0.050845533	0.68163999
LPC (20:1)	0.731142847	-0.313146425	-1.98521978	0.05367244	0.68163999
LPC (18:1)	0.692376584	-0.367625275	-1.915679198	0.062226991	0.718438894
LPC (20:0)	0.768015495	-0.26394537	-1.85886564	0.070059174	0.741459591
LPC (22:5)	1.42242802	0.352365285	1.74673022	0.087990844	0.85960286
LPC (16:0)	0.788437509	-0.237702129	-1.661210387	0.104115665	0.944477817
PC (22:0)	0.80321973	-0.219126966	-1.616027973	0.113572616	0.961581478
LPC (17:2)	1.585132247	0.46066784	1.509087428	0.138759623	0.994927471
PC (33:1)	1.21125878	0.191660133	1.499229833	0.141290188	0.994927471
PC (34:1)	1.201963279	0.183956286	1.436738592	0.158196717	0.994927471
LPC (22:2)	1.268251345	0.237639058	1.168910858	0.249028176	0.994927471
PC (39:2)	1.196933327	0.179762725	1.164355611	0.250848244	0.994927471
LPC (22:1)	0.882493207	-0.125004187	-1.155903927	0.254250588	0.994927471
LPC (18:0)	0.535267531	-0.624988599	-1.146992719	0.257873815	0.994927471
LPC (22:6)	0.851343987	-0.160939017	-1.122656044	0.267957469	0.994927471
PC (22:1)	1.156640641	0.145519804	1.097634852	0.278614166	0.994927471
PC (34:3)	0.881262289	-0.12639998	-1.080788652	0.285955312	0.994927471
PC (34:0)	1.147694331	0.137755	1.066686488	0.292203966	0.994927471
PC (41:1)	1.142462775	0.133186261	1.045782262	0.301640352	0.994927471
LPC(21:0)	0.85866136	-0.15238066	-1.041432473	0.303630028	0.994927471
PC (25:2)	0.806119526	-0.215523252	-0.996619077	0.324654201	0.994927471
PC (27:1)	1.283484991	0.249579028	0.994718672	0.325566986	0.994927471
PC (35:1)	1.174389196	0.160748179	0.92598574	0.359741345	0.994927471

Phospholipid specie	Fold change	logFC	T statistic	p value	Adjusted p value
PC (33:3)	0.871554942	-0.137476373	-0.900446357	0.373014637	0.994927471
PC (23:1)	1.123552234	0.116495304	0.890633142	0.3781973	0.994927471
PC (42:2)	1.070378648	0.068012463	0.883961386	0.381746972	0.994927471
PC (23:2)	1.137572366	0.128896488	0.860365895	0.394469918	0.994927471
PC (36:3)	1.072299349	0.069805267	0.846712018	0.401952247	0.994927471
PC (40:2)	1.073428029	0.070857293	0.837651119	0.40696599	0.994927471
PC (35:2)	1.068776683	0.066514707	0.83684544	0.407413667	0.994927471
PC (34:4)	0.893783086	-0.112292166	-0.836284234	0.407725682	0.994927471
PC (27:3)	1.220318258	0.199111692	0.835711858	0.408044058	0.994927471
PC (25:1)	0.825004262	-0.192366727	-0.831300091	0.410503194	0.994927471
PC (32:1)	1.110951508	0.105216863	0.803421842	0.426252527	0.994927471
PC (31:2)	0.895611837	-0.110248177	-0.797562904	0.429608308	0.994927471
PC (38:3)	1.125682308	0.118389347	0.785669454	0.436469143	0.994927471
PC (39:1)	1.109406528	0.103825213	0.75457175	0.454714325	0.994927471
PC (38:2)	1.078913708	0.075954709	0.752942307	0.455682455	0.994927471
PC (38:0)	1.059209675	0.05752304	0.738839012	0.464111952	0.994927471
PC (43:0)	1.167936524	0.155238537	0.735038591	0.466398746	0.994927471
PC (22:2)	0.836953544	-0.177986713	-0.730407746	0.469193962	0.994927471
PC (33:0)	1.11088087	0.105153277	0.701695187	0.486737768	0.994927471
PC (40:4)	1.127698882	0.120179169	0.682160458	0.498880761	0.994927471
PC (33:2)	1.08402425	0.080680274	0.68132578	0.499403297	0.994927471
PC (24:0)	0.90471034	-0.100140453	-0.666327526	0.50884382	0.994927471
PC (32:3)	0.917503257	-0.086099149	-0.665848674	0.509146818	0.994927471
PC (40:0)	1.051728764	0.050435252	0.655537741	0.515694839	0.994927471
PC (35:4)	1.173370341	0.159880241	0.637515031	0.527248126	0.994927471
PC (43:2)	0.882418611	-0.12508872	-0.610862177	0.544581183	0.994927471
PC (24:1)	0.907965294	-0.096549124	-0.610011475	0.545139212	0.994927471
PC (40:1)	1.051959649	0.050654757	0.594512739	0.555357028	0.994927471
LPC (20:5)	0.841767497	-0.172251434	-0.591388494	0.557428422	0.994927471
PC (41:5)	1.083012463	0.079746476	0.589794542	0.558486722	0.994927471
PC (28:3)	1.137443365	0.128783082	0.585577154	0.561291714	0.994927471
PC (41:4)	1.109307855	0.103736267	0.583468915	0.562696551	0.994927471
PC (35:3)	1.13435838	0.126067187	0.577208993	0.566878215	0.994927471
LPC (22:0)	0.909271383	-0.095111679	-0.570194779	0.571582012	0.994927471
PC (37:4)	1.044916611	0.043937084	0.555974013	0.581177201	0.994927471
PC (42:0)	1.04858017	0.04743703	0.523212077	0.603575046	0.994927471
PC (42:1)	0.953060357	-0.048077044	-0.520403462	0.605513749	0.994927471
PC (31:1)	0.950493373	-0.050774089	-0.483177327	0.631477969	0.994927471
PC (36:2)	1.036018446	0.035384949	0.47925711	0.634240621	0.994927471
PC (38:6)	1.037060462	0.036390232	0.478073434	0.635075821	0.994927471
PC (38:4)	1.076087265	0.073331559	0.465377494	0.644064151	0.994927471
PC (34:2)	0.956006888	-0.04499016	-0.443241875	0.659864554	0.994927471
PC (31:3)	1.100235446	0.095524199	0.440328855	0.661955824	0.994927471

Phospholipid specie	Fold change	logFC	T statistic	p value	Adjusted p value
PC (37:3)	1.075492278	0.072778489	0.421605071	0.675462385	0.994927471
PC (43:4)	1.103819084	0.098776061	0.414477165	0.680633055	0.994927471
PC (43:1)	1.041577411	0.040736306	0.400741467	0.690640899	0.994927471
PC (41:6)	1.033896718	0.033334885	0.400602188	0.69074267	0.994927471
PC (40:5)	1.071903015	0.069435587	0.396999728	0.693376966	0.994927471
PC (43:6)	1.033663399	0.03310919	0.343321923	0.733068142	0.994927471
PC (43:3)	0.942307668	-0.059423447	-0.31107166	0.757284142	0.994927471
PC (39:0)	1.028062228	0.027675699	0.307929873	0.759656945	0.994927471
PC (41:2)	0.947806772	-0.053604625	-0.300931215	0.764951011	0.994927471
PC (38:5)	1.025210134	0.024897601	0.28798274	0.774775643	0.994927471
PC (37:2)	1.034394615	0.033816342	0.252221152	0.802099783	0.994927471
PC (37:1)	1.028590981	0.028189887	0.229983645	0.81922041	0.994927471
PC (39:5)	0.976421856	-0.023860556	-0.225716322	0.822516334	0.994927471
PC (28:4)	1.06938727	0.06708584	0.220767395	0.826342767	0.994927471
PC (42:6)	1.016295768	0.016164417	0.196857495	0.844888143	0.994927471
PC(30:0)	0.973795957	-0.026553487	-0.195002053	0.846331166	0.994927471
PC (36:1)	1.02256134	0.022310597	0.185992701	0.853345467	0.994927471
PC (36:5)	1.050287117	0.049063571	0.173994125	0.86270564	0.994927471
PC(d31)	1.020779243	0.0205663	0.159423056	0.874099414	0.994927471
PC (37:6)	1.020467942	0.020261289	0.15711422	0.875907346	0.994927471
PC (36:0)	1.018751592	0.018577948	0.144474019	0.885816891	0.994927471
PC (27:0)	0.982714762	-0.017436371	-0.134986458	0.893267123	0.994927471
PC (39:3)	0.981766289	-0.018401994	-0.109729766	0.913146076	0.994927471
PC (37:5)	1.013988047	0.013891117	0.108633756	0.914010091	0.994927471
PC (36:4)	0.984918066	-0.015196823	-0.107442459	0.914949343	0.994927471
PC (31:0)	0.985094652	-0.015017549	-0.101941005	0.919288417	0.994927471
PC (28:6)	0.976649496	-0.023627447	-0.094679667	0.925019328	0.994927471
PC (42:3)	1.012944567	0.012861502	0.087747855	0.930493935	0.994927471
PC (23:0)	1.018100834	0.017938965	0.085856105	0.931988604	0.994927471
PC (40:6)	1.006192758	0.006173662	0.08518247	0.932520903	0.994927471
PC (28:5)	1.014602867	0.014497272	0.082638824	0.934531142	0.994927471
PC (41:3)	1.014194515	0.014094717	0.075330531	0.940309236	0.994927471
PC (38:1)	0.994556649	-0.00545822	-0.064564266	0.948827121	0.994927471
PC (35:0)	1.008940973	0.008901239	0.056002499	0.955605262	0.994927471
PC (42:5)	0.993647393	-0.006372871	-0.045795327	0.963690336	0.994927471
PC (32:2)	1.00616106	0.006142159	0.039793049	0.968446588	0.994927471
PC (43:5)	1.007892498	0.007861515	0.039446883	0.968720929	0.994927471
PC(30:2)	1.005037461	0.005024815	0.037817825	0.970012033	0.994927471
LPC (18:3)	0.99519768	-0.004813888	-0.028504832	0.977394468	0.994927471
PC (42:4)	1.004092021	0.004083671	0.025589825	0.979705646	0.994927471
PC (27:2)	1.009542879	0.009497633	0.023364768	0.981469912	0.994927471
PC (40:3)	1.002825305	0.002821321	0.020020444	0.98412183	0.994927471
PC (41:0)	1.002127664	0.002125404	0.019287881	0.984702748	0.994927471

Phospholipid specie	Fold change	logFC	T statistic	p value	Adjusted p value
PC (39:4)	0.998186052	-0.001815595	-0.019211283	0.984763491	0.994927471
LPC (22:4)	0.997971583	-0.002030477	-0.006783529	0.994619672	0.994927471
PC(30:1)	0.999199887	-0.000800433	-0.00639545	0.994927471	0.994927471
PE (35:1)	1.356505755	0.304912096	2.628577375	0.011920025	0.107280222
PE (36:1)	1.145240898	0.135615006	1.352419063	0.183467111	0.687178388
PE (34:0)	0.680213145	-0.385349081	-1.220536243	0.229059463	0.687178388
PE (34:2)	0.940246403	-0.061613307	-0.653751154	0.516830117	0.836700001
PE (36:2)	1.053025612	0.051667556	0.543549648	0.589620569	0.836700001
PE (36:3)	1.038847117	0.038111557	0.442046911	0.660719615	0.836700001
PE (38:2)	0.959126467	-0.041732339	-0.401292737	0.690235924	0.836700001
PE (38:1)	0.964364026	-0.036286435	-0.329072982	0.743733335	0.836700001
PE (34:1)	0.994689101	-0.005325052	-0.057692236	0.95426696	0.95426696
PG (26:0)	1.495297002	0.402324851	2.47799831	0.017385872	0.20891241
PG(36:2)	1.356587033	0.304972011	2.187375761	0.034425947	0.20891241
PG(19:6)	0.561663278	-0.576852757	-2.060114079	0.045720646	0.20891241
PG(28:0)	1.233113442	0.209542225	1.940908978	0.059109536	0.20891241
PG(19:5)	0.618138427	-0.481042854	-1.893651553	0.065285128	0.20891241
PG(32:0)	0.912975401	-0.091046342	-0.892778233	0.377144568	0.782170569
PG (18:0)	1.258393733	0.229836092	0.781689797	0.438851866	0.782170569
PG(30:1)	1.115027127	0.108878734	0.779766179	0.439970945	0.782170569
PG(32:1)	1.08928418	0.085520765	0.544254238	0.589190775	0.94270524
PG(30:0)	1.046955096	0.045886043	0.444765206	0.658809854	0.958268879
PG(34:1)	1.031261887	0.030783185	0.310547773	0.757705077	0.984745152
PG(36:3)	0.932519465	-0.069865253	-0.234551056	0.815715252	0.984745152
PG (16:0)	1.049985659	0.048776506	0.175361317	0.861652008	0.984745152
PG(31:0)	1.002334344	0.002331624	0.013184522	0.989544014	0.999459842
PG(36:1)	1.000083488	8.35E-05	0.000681095	0.999459842	0.999459842
PI (32:1)	1.369933477	0.314762182	1.92292767	0.060384854	0.584685749
PI (34:1)	1.183428438	0.168415682	1.459959719	0.150763415	0.584685749
PI (36:3)	0.734719762	-0.308266128	-1.300619183	0.199548981	0.584685749
PI(34:2)	0.792487846	-0.23257811	-1.262233671	0.212914458	0.584685749
PI (32:0)	1.182310401	0.167470491	1.22261206	0.227397839	0.584685749
PI_2	0.809778805	-0.210994149	-1.141372808	0.259331842	0.584685749
PI (16:0)	1.21144209	0.19181146	1.05787813	0.295363579	0.584685749
PI (38:2)	0.849905515	-0.162630094	-1.000530683	0.322030942	0.584685749
PI (38:3)	0.84562491	-0.167679387	-0.979156563	0.3323728	0.584685749
PI_1	1.240413413	0.215444722	0.955782722	0.343932794	0.584685749
PI (38:4)	1.082273217	0.07906366	0.499738051	0.619524424	0.857834418
PI (38:1)	1.058467594	0.056822196	0.437432118	0.663744183	0.857834418
PI (36:1)	0.95025862	-0.0510211	-0.369662925	0.713246563	0.857834418
PI (36:0)	0.932381332	-0.070013394	-0.365780403	0.716123184	0.857834418
PI (33:0)	1.052560615	0.051225876	0.311296092	0.756912722	0.857834418
PI (36:2)	0.989420234	-0.01063613	-0.083813603	0.933550413	0.933550413

Phospholipid specie	Fold change	logFC	T statistic	p value	Adjusted p value
SM (32:1)	1.723258625	0.544217048	2.728162701	0.009240405	0.092404054
SM (34:2)	0.690882713	-0.369785205	-2.159813089	0.036509074	0.182545372
SM (34:0)	0.87188394	-0.13709896	-1.216341148	0.23060749	0.768691632
SM(d31)	1.158068363	0.146753413	0.969211693	0.337956006	0.770867915
SM (34:1)	0.933557724	-0.068752482	-0.877023736	0.385433957	0.770867915
SM (32:0)	0.958088458	-0.042815169	-0.447469962	0.656821836	0.93415038
SM (30:0)	0.918438179	-0.085080683	-0.440726599	0.661658078	0.93415038
SM (33:0)	0.99181284	-0.008220859	-0.099706443	0.921049037	0.93415038
SM (33:1)	0.993252351	-0.006770517	-0.083117914	0.93415038	0.93415038

8.3.1. Weight of hair samples

Table 8.62: Weight (mg) of each hair sample for LCMS analysis. Hair was cut from as close to the scalp as possible and then cut finely, washed in acetone, dried and weighed to 30mg (or as close as possible).

Sample	Weight (mg)	Sample	Weight (mg)
C21	30.9	P19	29.8
C22	28	P20	29
C23	29.1	P21	28
C24	29.3	P22	31.5
C25	30.4	P23	29.2
C26	30	P24	30.6
C27	30.5	P25	31.7
C28	32.4	P26	28.5
C29	28	P27	32
C30	31.1	P29	31
C31	32	P30	29
C32	29.5	P31	33
C33	28.3	P32	29
C34	32.3	P33	28
C35	32.2	P35	32
C36	29.6	P37	29.5
C37	32.7	P38	29.5
C38	31.9	P39	28
C39	27	P40	28.5
C40	28	P41	12

8.3.1. Principle component analysis for hair samples including pooled biological quality controls

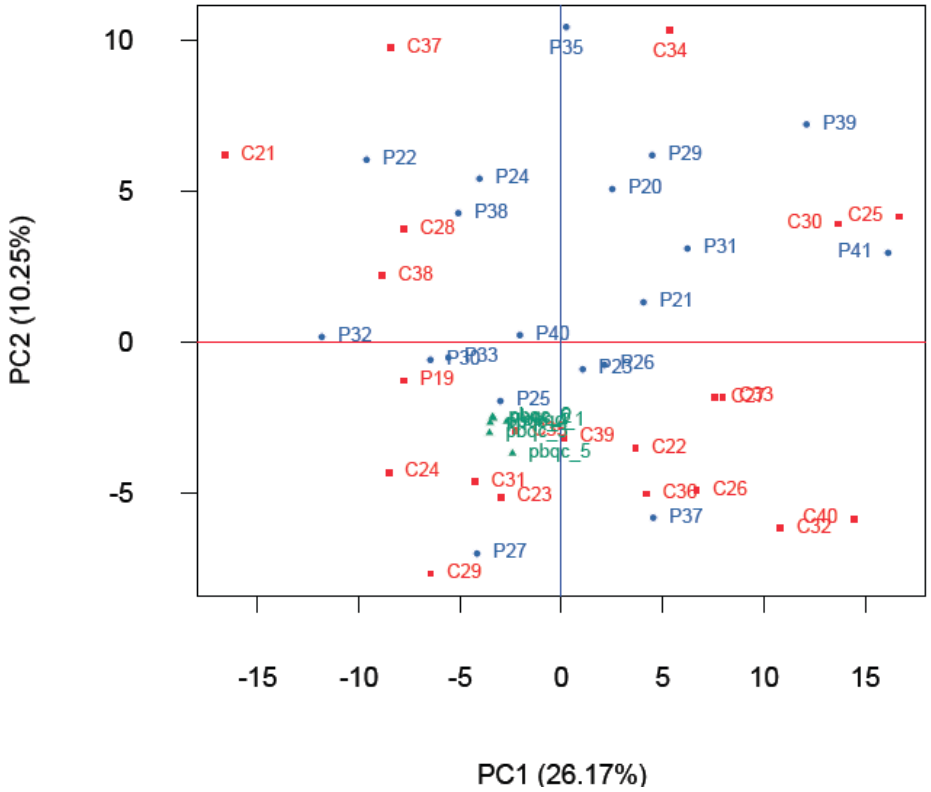


Figure 8.5: PCA with the PBQC's, which are clustering (in green), compared to the controls samples in red and the patient's samples in blue. This indicates that the data is robust.

8.3.2. Lipids from along the hair fibre

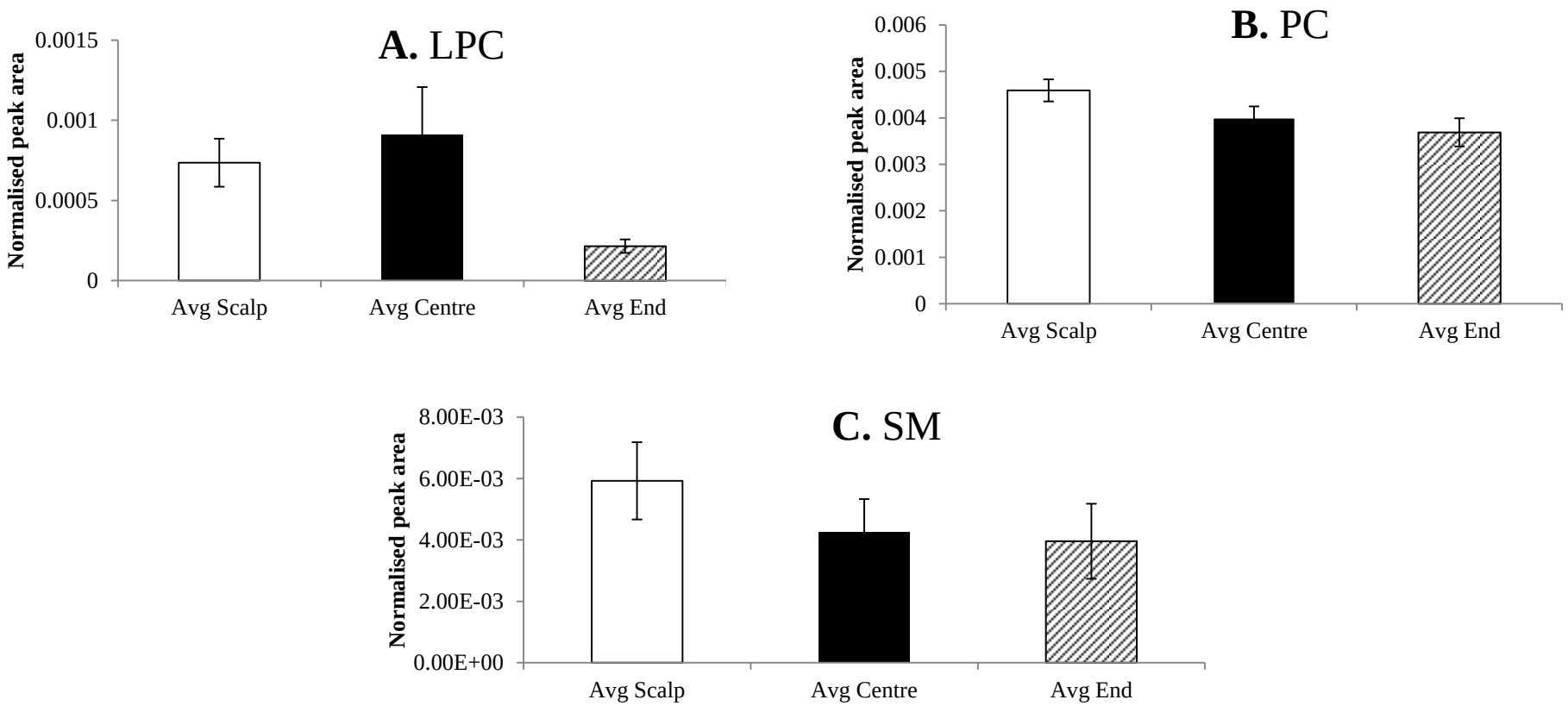


Figure 8.6 (A-C): Analysis of the levels of LPC (A), PC (B) and SM (C) along the hair fibre where shoulder length hair from three individuals was split equally into three sections and profiled for lipids (scalp, centre, end). The average of the three participants was graphed for each section and results showed variation in the amount of lipids between the three sections.

8.3.3. Optimization of the method of extraction of lipids from hair

A set of variables were compared in order to establish the optimal method of extraction from hair. Optimal was defined as the highest amount of lipid from a sample. Variables in this study were:

1. Amount of hair: 7mg, 15mg, 30mg
2. Amount of solvent during homogenization of hair: 0ul, 750ul, 1500ul
3. Number of cycles in the cryomill: 3 cycles, 9 cycles
4. Time in the shaker: 5 minutes, 15 minutes, 30 minutes

Data shown is for one lipid species (SM 34:1) but another 10 species of lipid were also analysed (data can be provided upon request).

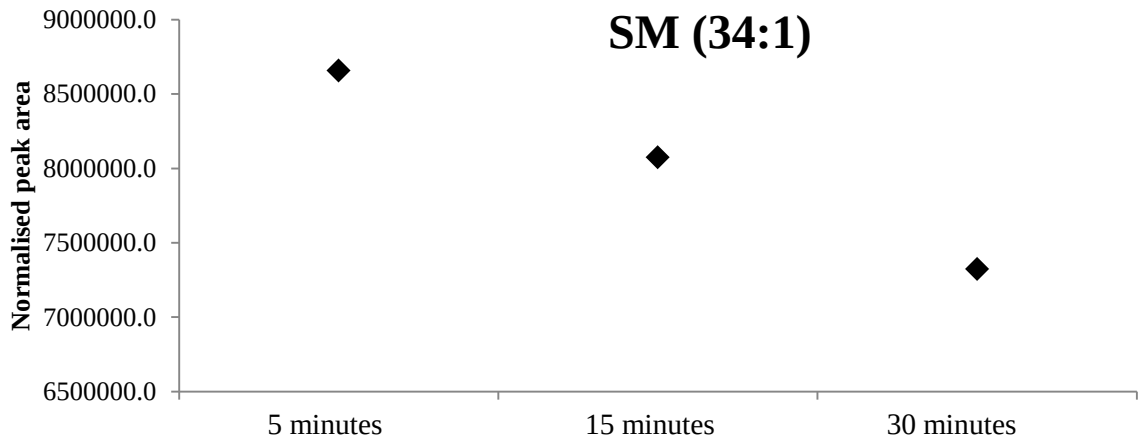


Figure 8.7: Average (of four replicates) for each sample shaken for 5, 15 and 30 minutes. The highest amount of lipid was obtained from shaking for 5 minutes.

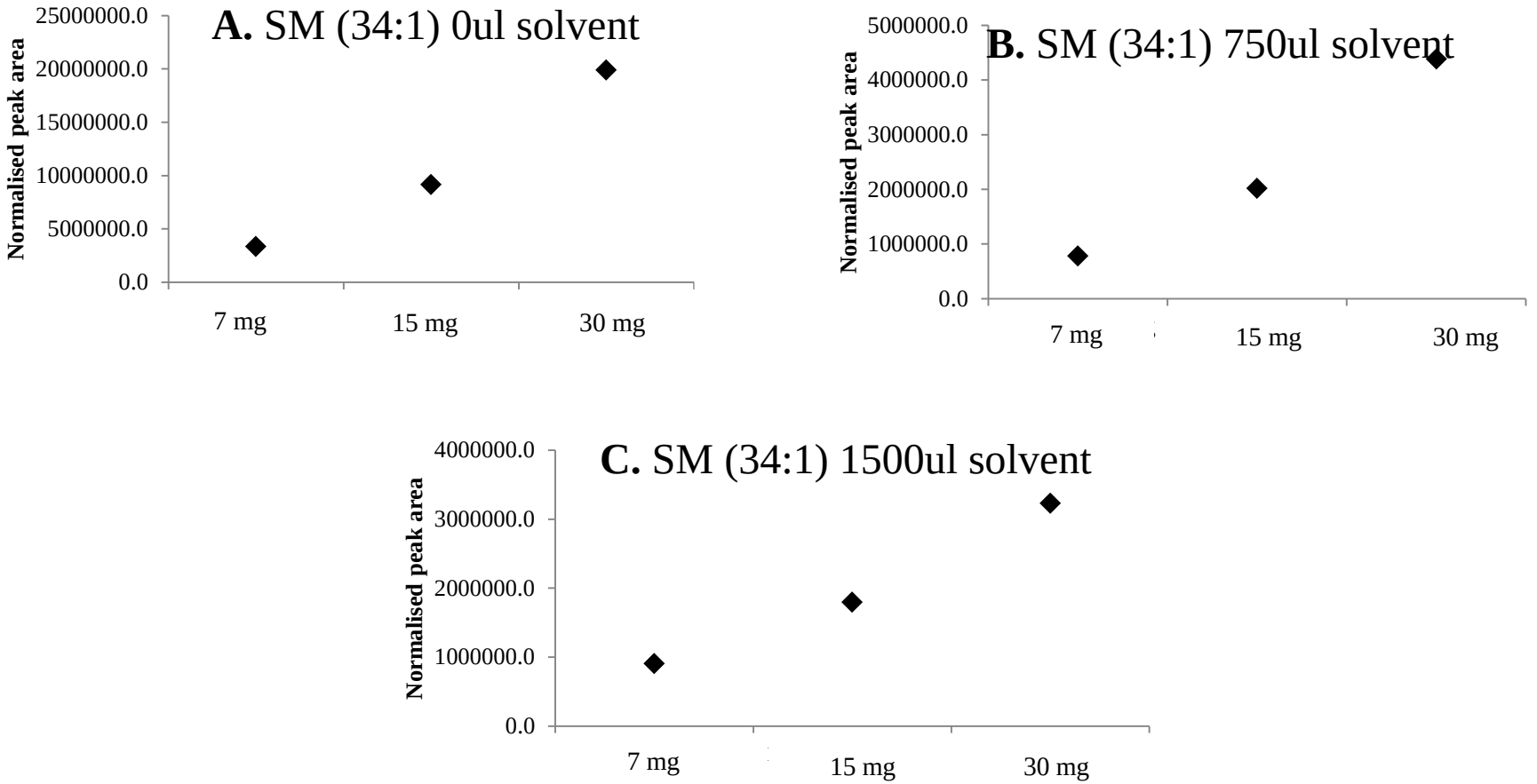


Figure 8.8: The various weights of samples (7mg, 15mg, 30mg) were compared for three solvent amounts, 0ul (A), 750ul (B) and 1500ul (C) to determine the ideal weight of a sample. This was an average of four replicates for each weight. The optimal sample weight, for which the highest amount of lipid was extracted, was found to be 30mg of hair.

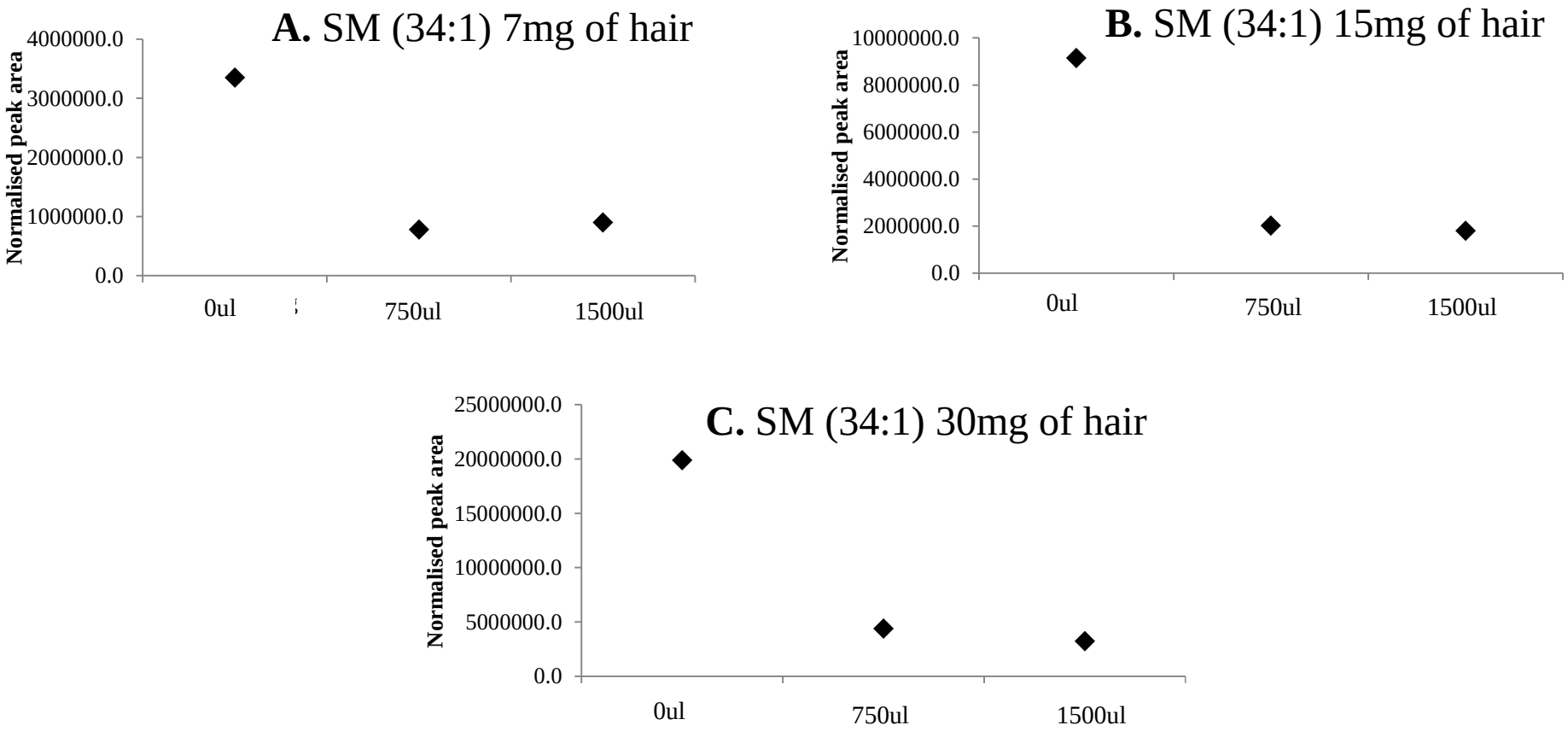


Figure 8.8: The different amounts of solvent (0ul, 750ul, 1500ul) were compared for three sample weights, 7mg of hair (A), 15mg of hair (B) and 30mg of hair (C), to determine the ideal amount of solvent required to homogenise the hair but also extract the maximum amount of lipid. This was an average of four replicates for each solvent amount. The optimal sample amount of solvent, for which the highest amount of lipid was extracted, was found to be 0ul during homogenization.

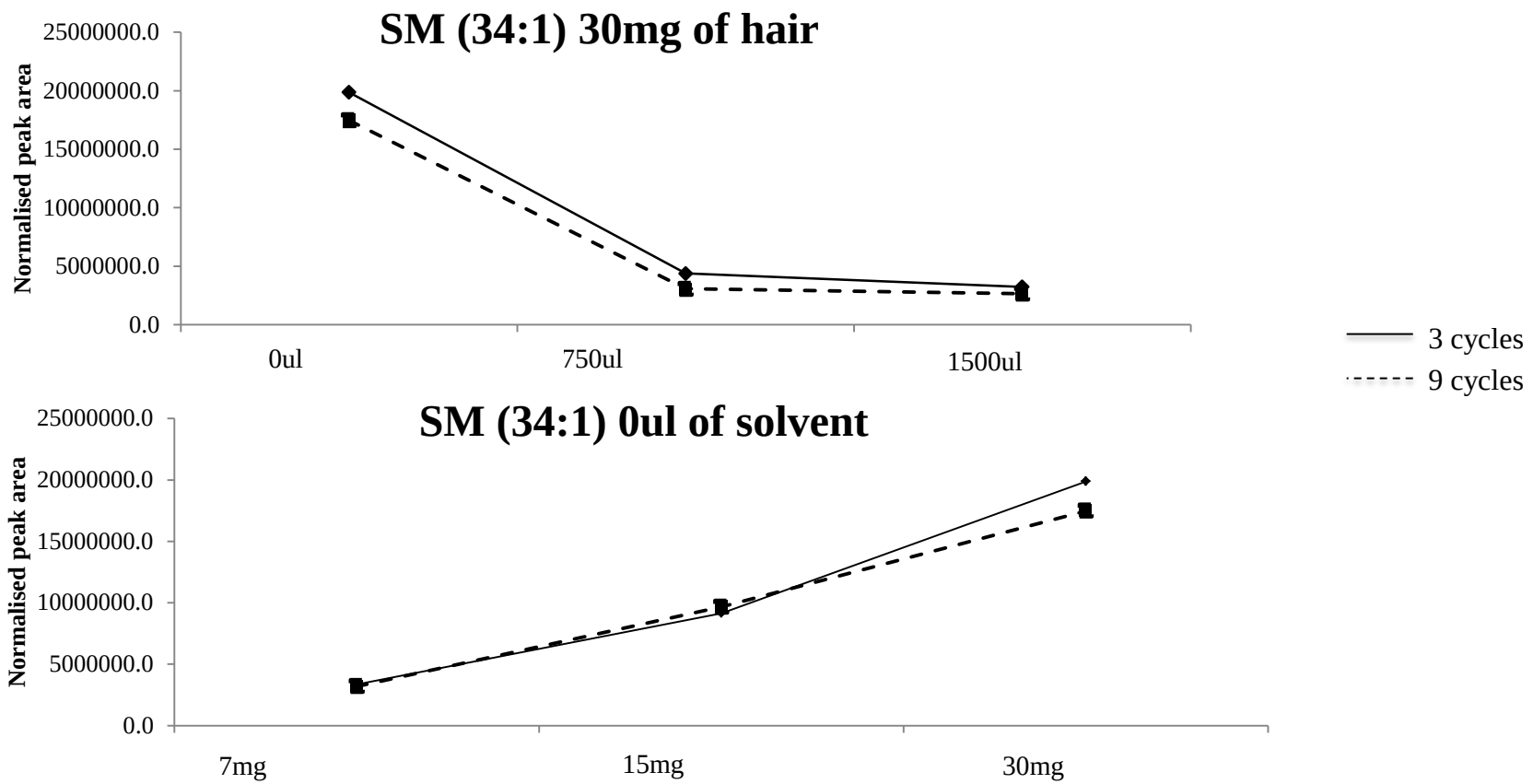


Figure 8.9: To determine the ideal number of cycles in the cryomill (3 or 9) to fully homogenise the hair sample and for maximum lipid extraction the number of cycles were compared for the optimal amount of hair (30mg) in 0ul, 750ul and 1500ul of solvent (A) and also for the optimal amount of solvent (0ul) for 7mg, 15mg and 30mg of hair (B). This was an average of four replicates for each solvent amount and hair amount. The optimal number of cycles, for which the highest amount of lipid was extracted, was found to be 3 cycles for full homogenization of the hair.

8.4. From Chapter 5

8.4.1. Raw peak area data

Table 8.63: Raw peak area data matrix for cholesterol ester for serum samples taken from breast cancer free controls.

Samples	Cholesterol	CE	CE(10:0)	CE(13:6)	CE(13:2)	CE(24:0)	CE(24:1)	CE(24:2)	CE(24:3)	CE(24:4)	CE(24:5)	CE(24:6)	CE(14:0)	CE(14:1)	CE(15:0)	CE(16:0)	CE(16:1)	CE(16:2)	CE(17:0)	CE(17:1)	CE(17:2)	CE(17:3)	CE(17:5)
C-1	92.596974	1989.46527	19.4624997	255.473311	105.40472	3776.46711	3821.09185	1405.06795	310.214273	239.3674	296.024077	908.993794	24.6099436	1072.51455	300.019391	1220.76236	671.553429	42.2055932	11.1512206	66.8599123	98.1747905	85.3858168	141.55714
C-10	49.5117829	2116.82907	65.5969756	132.619857	95.1691976	2242.38914	1425.19964	733.270405	200.481157	61.5110155	244.245531	469.311013	48.0313903	125.580754	652.004799	902.363794	434.278731	90.6703516	53.0681262	94.3883652	55.8736011	84.0763808	55.3209063
C-11	98.0297827	1993.99975	12.3147001	225.610563	167.523213	1232.30038	2681.62438	513.056443	345.026757	146.791936	191.463575	729.75027	48.7228222	536.640741	238.767999	1125.46471	594.210078	31.0305085	23.9617805	57.0921664	57.7915839	41.3630995	33.3554849
C-12	24.4282841	1986.79542	38.0066469	108.485107	128.503631	3340.19457	4113.35088	878.732888	312.442821	137.6911	323.023933	946.517073	14.3553947	868.537919	150.352419	608.575996	215.96111	70.8162382	59.13937	42.4571223	28.0617877	16.3705643	45.1927198
C-13	70.7101284	2136.39066	11.239729	44.7790195	74.1545072	800.959468	1960.17336	350.412661	335.181506	119.839316	311.332789	534.824862	10.2986937	119.139095	319.787563	516.498373	379.327037	81.5831713	19.1624781	47.6725945	30.1728048	72.5703363	56.2037127
C-14	23.8627282	1654.0313	30.8699333	57.433682	140.807614	1410.09511	1592.41154	346.127212	198.221428	53.8599117	117.684152	345.869001	12.290475	62.1074801	458.271895	258.943675	61.6786257	17.741925	6.61783241	14.7309549	40.5206362	13.9536814	11.4162433
C-15	159.189897	1711.64683	32.1525063	291.973698	53.0510556	1655.49724	2854.15373	475.046402	283.417074	197.189687	287.090597	861.586651	43.0205964	205.406264	346.844531	1278.22885	1122.67538	55.2312024	12.5491021	129.625326	46.5579828	79.8065505	104.451099
C-16	59.7688456	2590.17482	11.660528	64.8843942	133.31476	1179.82351	2339.2695	284.608585	331.167998	166.153328	328.516494	464.614019	11.4126835	1026.94327	22.0250325	668.074993	266.783013	20.0387418	12.7742099	120.026903	221.813285	36.0118736	39.1411094
C-17	103.668306	1996.25482	41.5052816	285.640965	138.720087	3061.85847	2903.05314	1182.98519	222.639045	166.52979	164.72529	689.261541	68.9084196	1093.72752	290.267365	1931.96415	2001.38	20.8964984	19.5772842	189.469807	14.7203431	43.1449253	39.7518558
C-18	53.4671182	2224.78872	45.4892564	165.021039	112.904781	867.750379	1397.10055	239.509545	249.185302	142.367064	123.712769	338.15494	25.0785881	524.185114	203.740947	774.691585	421.311391	43.2372508	14.5539813	30.5399973	41.7126438	46.8532436	55.1631917
C-19	56.4007094	1911.99708	27.3586982	224.336616	98.5057605	1159.43305	1619.39119	327.478079	304.712638	135.949646	296.125902	471.868111	41.149371	441.076453	351.9069	958.863407	507.429656	95.9221434	50.8814341	129.05997	72.0450014	104.243162	65.6574371
C-2	45.7499949	2495.10004	10.6955093	268.464946	110.877144	2121.02333	2725.50558	772.511198	331.722141	215.987007	308.870083	617.001842	44.0241896	789.274281	170.571278	1222.64046	1532.85344	31.8911693	9.49760193	116.549651	40.1401944	147.887855	138.877876
C-20	79.5170524	2232.29515	14.8872967	431.196611	102.594778	6999.63365	5362.12571	2799.7057	522.657362	187.186286	443.40621	1035.93254	28.715783	925.363567	247.887307	1253.0109	427.367035	47.3432995	21.4345144	64.2640328	40.8836727	78.8069913	83.2703368
C-3	49.2795375	1932.14466	40.6465928	90.8551219	132.618434	1454.94813	2040.63291	491.49731	393.924633	203.995519	186.600898	432.013029	30.0041059	518.974736	273.794372	1034.92897	632.496286	45.9161195	8.26269871	75.6650886	64.680657	46.8772939	33.8560108
C-4	48.2526439	1360.10093	26.5012504	146.60242	64.1783334	1009.42036	1226.59722	205.367227	195.577034	164.004233	192.605499	367.633471	6.97399278	200.286479	156.781765	678.840175	350.241258	59.2425651	11.041498	41.4106263	69.3781221	35.8662619	52.7139139
C-5	107.557192	2102.95766	27.2017694	116.370694	100.928762	1500.04336	1828.51032	372.379702	248.119162	125.898541	288.489846	359.747442	20.2337958	209.880095	602.879829	1152.18386	640.566728	35.5162637	19.5898421	82.4251733	44.8824234	74.7214909	39.1070675
C-6	84.8936336	2535.65921	61.5044457	211.12745	119.935233	737.784254	1170.42231	230.86793	232.747835	80.0417997	129.881456	318.569785	24.4637485	247.559058	453.77419	833.299645	416.651176	64.4680145	10.9771567	17.1153378	93.3920318	51.2099116	109.091398
C-7	43.9393719	1668.97794	53.3770353	270.855056	90.616258	989.917477	1647.22473	241.486185	221.001007	194.069992	356.109738	471.502991	10.1713084	605.652941	256.225191	956.990567	328.643202	53.763223	10.2564464	12.7338082	83.5040491	83.3326156	84.2740327
C-8	57.6770012	2523.91268	37.6493903	163.485603	180.720413	998.311449	1564.60966	357.167314	273.699257	104.681989	209.551618	346.06852	43.683919	715.814665	320.542005	1132.88794	1716.70385	11.9352917	24.7352366	151.1279	83.4283836	41.9574926	35.9447814
C-9	46.2701207	2595.07454	22.6712804	125.655594	147.808042	860.377022	1601.21073	249.610426	270.286269	101.609882	150.477772	264.573266	18.0656368	200.206182	406.548707	850.661113	418.494384	37.6394878	33.8486183	86.0720135	27.6430376	67.6359776	28.5431611
C-21	53.3524546	2398.57098	32.3713995	156.885775	61.5955141	1883.20145	2609.50814	420.209898	274.421077	52.5908357	235.024427	784.876053	16.3254427	219.926766	185.858487	612.340498	521.850605	59.2605176	27.6532779	68.0974837	137.929474	34.0073248	81.8934087
C-22	91.3454441	2678.17077	19.9484939	189.027696	161.243148	1735.02176	2673.71213	425.449078	274.662174	103.534381	349.339302	627.102663	40.9413245	447.378053	217.958111	752.819132	1265.43873	71.550327	44.3574889	82.3663785	179.36201	40.1215786	17.4251309
C-23	48.9588262	2040.79271	14.379862	229.03951	115.804689	1179.20745	1276.8092	352.422615	228.579564	101.451316	216.879791	310.13054	61.8284903	235.742026	192.121115	712.217489	571.25029	37.6671869	13.3912975	110.196255	28.9944702	71.5883516	57.1100932
C-24	97.2256145	1514.72574	11.5844245	84.8269575	79.7571287	1398.92354	1965.50571	351.914723	311.472479	202.172265	312.331588	394.611878	76.0672809	130.709957	144.48441	762.50387	1271.99817	50.2703288	14.0374252	116.845977	28.5947181	67.5978784	28.0070277
C-25	26.1372682	2229.22476	13.2532665	235.389672	117.396703	2343.2969	3123.13087	1125.28117	533.969922	222.575324	273.153027	717.953882	22.925214	222.543412	98.5743428	470.86072	995.373528	62.2028483	11.3558819	145.315795	94.1368132	90.0030702	45.2703101
C-26	109.731262	2591.89636	14.7790644	133.969632	217.129864	1798.48464	2291.55234	461.639385	339.78242	133.470471	332.040667	563.958535	47.6703759	254.1072	73.4385131	823.243437	646.049998	74.0187133	8.69344084	69.9537167	24.264183	67.8666383	38.1478231
C-27	62.7764463	3080.82556	42.0369184	77.7069335	163.460396	758.649058	1661.87482	237.72627	240.147352	107.167344	139.061115	336.710495	81.4852224	131.830813	203.95227	508.792904	681.904723	56.2537577	25.9492222	66.5295946	50.0719497	78.3839341	45.644243
C-28	48.2798513	2261.06568	14.5448152	565.919489	135.884575	4341.40207	2764.12432	1831.27605	406.784647	90.4657795	300.889281	692.15734	24.3197251	444.939391	183.026118	1688.69236	849.160184	45.0682292	12.5590223	146.138556	49.0072404	94.811701	167.076706
C-29	66.9265516	2206.00755	13.4607981	133.972201	97.0851275	2650.25252	3692.02254	881.892154	336.566189	260.687589	285.981541	777.796316	52.0917972	555.860112	251.751702	1549.46696	910.425095	51.5928324	24.800958	173.926912	82.7656946	75.4966207	80.0528627
C-30	10.0532984	11.5012305	16.342543	13.6433416	29.9732363	47.7455264	55.1843347	36.9598505	8.45102861	9.09138509	48.9489481	30.7604335	8.75735322	28.3916932	20.0665586	127.521751	110.299927	23.3203269	12.7150236	13.5418831	18.0021437	12.5143923	13.4417087
C-31	45.8849487	3198.92316	21.1797	70.948992	180.544721	1031.7099	1376.17585	248.488329	144.630181	48.1501149	138.225024	464.29581	8.92027762	99.0603892	262.231814	609.748078	226.27191	67.2729618	42.718023	99.1706316	86.0913693	147.092981	14.7051352
C-32	70.1788425	2397.15877	42.1400654	170.47691	50.6736184	3273.3521	4326.43289	1317.40224	382.486636	117.870934	371.973006	921.701447	42.4704146	154.980879	124.403904	931.460939	399.960454	91.0416887	19.5446299	59.8949514	61.8220655	120.652571	69.7780597
C-33	77.0521327	2686.61728	14.2309422	490.316759	109.426071	1837.02332	2318.4696	726.537244	536.83711	125.499094	293.742076	616.287267	18.0224891	1396.47151	75.8955934	744.605407	797.153208	45.4821738	12.8352729	38.8798808	76.6665941	182.988593	211.687903
C-34	60.0102765	2339.49278	11.6743295	169.758283	164.329841	2236.15698	3677.09907	766.828205	281.980216	160.682408	368.30664	795.541915	56.4486381	623.676499	142.903568	1208.93742	1289.31872	49.5514518	27.36584	147.01469	92.7469025	49.7087958	86.7293089
C-35		10.6218852	10.2942465	4.18521533	13.5075739	28.8994015	27.0223354	10.2718808	16.6216745	24.9849986	45.1182246	17.2867116	8.59882489	31.415107	31.1709769	31.8216437	14.0137563	20.6202649	9.76669136	18.3113762	15.6917522	12.6706841	22.9691863
C-36	73.7224092	2620.80409	10.150959	363.504888	124.921416	4774.19062	9223.72743	1472.04292	1148.61902	170.685977	723.796488	1872.19722	40.3977839	677.201616	115.423422	1123.34448	420.156447	111.417213	35.9759717	109.903565	27.2268786	85.6072658	190.823162
C-37	82.1408854	2376.50346	10.3610349	180.385548	144.199093	8478.28771	6616.85142	2987.0048	627.239952	110.276539	782.267926	2115.89574	65.9994541	452.262734	115.55961	1410.59694	482.993379	60.8797986	17.9104736	115.022874	40.882526	95.5954744	91.5942851
C-38	97.6804485	2157.12159	19.7550582	122.064144	103.152171	6257.63835	6256.38738	1692.48741	688.375137	57.5731249	896.041436	1687.52331	40.9731927	258.848774	135.521598	830.270389	1607.52951	81.2526322	12.4128391	124.034902	72.7079231	65.5521008	73.9073745
C-39	124.674868	2545.93874	18.1553247	64.4403143	156.8704	1432.6756	2896.6779	234.194329	270.862357	89.2902418	281.059512	556.139848	11.6980754	75.0614977	170.874077	613.685301	370.526858	42.9906564	15.3896209	37.7370927	99.7666967	66.5362684	22.3789214
C-40	57.0978757	3207.40322	9.19064223	362.008775	114.018715	3561.31157	5483.08702	788.170515	620.158159	170.40477	641.078427	1147.74592	14.7338976	1017.57023	64.6306946	840.504573	421.261093	24.4605049	25.1373662	51.8367975	20.0128113	119.775801	70.1207804

Table 8.64: Raw peak area data matrix for cholesterol ester for serum samples taken from breast cancer free controls.

Samples	CE(18:0)	CE(18:1)	CE(18:2)	CE(18:3)	CE(18:4)	CE(18:6)	CE(20:0)	CE(20:1)	CE(20:3)	CE(20:4)	CE(20:5)	CE(22:0)	CE(22:1)	CE(22:2)	CE(22:3)	CE(22:4)	CE(22:5)	CE(22:6)
C-1	393.687712	11665.6015	65108.9922	2283.06655	57.4503424	10.9887792	595.38722	1490.14632	23.2378292	345.176388	1658.20252	872.755059	512.503659	813.458544	5141.65314	5653.5864	532.384793	5836.11594
C-10	372.267321	10452.6988	60210.4129	3919.6225	175.178816	9.43847327	194.351194	665.378763	65.1027256	719.222996	3079.11545	646.156723	329.186635	444.976743	2373.18316	2719.05882	255.551676	8239.03247
C-11	390.289263	11059.7918	68339.2147	2089.53756	77.0577191	30.6527154	485.137673	996.131076	11.0774787	246.589416	716.24982	548.874732	521.818709	719.532595	4014.91262	4262.90614	350.711128	4145.22279
C-12	156.485482	3698.06412	20088.283	1117.29926	53.6650481	13.1019573	632.323638	1619.76085	18.6006668	101.598689	209.849005	1703.62828	265.834738	1055.91674	5647.39779	6364.53516	442.728029	1088.26993
C-13	387.35952	8108.42934	51079.5444	3197.13628	94.9298077	28.1975716	237.010861	704.088851	43.009721	182.631407	573.129459	601.883726	371.01253	607.174174	2952.61635	3150.81241	288.858973	2629.04352
C-14	155.396613	983.048395	6348.63821	186.595035	15.1836392	56.5033225	348.65847	755.733616	15.7212947	22.5220611	44.1710552	823.725853	521.224943	604.88813	2813.39594	2776.54446	277.695209	440.910881
C-15	437.671865	13810.0491	72828.9114	4680.77101	190.678618	21.6158196	623.672552	857.789846	46.3631286	388.616144	886.660138	1156.7697	577.929943	1171.00187	5189.92344	4805.75206	470.239298	3676.40453
C-16	316.501819	7176.50663	42821.1006	1918.16086	70.8026341	11.7336753	586.308548	1031.8116	26.6211573	95.3671065	297.625599	700.717276	410.431682	1211.15458	5614.75638	5929.65455	334.754773	1596.85845
C-17	554.288213	19031.921	76741.3775	4800.65485	266.358932	19.2100359	641.39534	873.149783	66.0742788	593.278984	2378.83226	917.771806	572.178038	989.179767	4165.2411	3285.85351	414.09492	6144.7389
C-18	329.238004	9683.41104	73518.4086	2199.43311	35.0665418	15.62134	385.358312	984.014137	14.4854618	112.96782	472.895403	417.111156	610.125221	511.637006	3261.1328	4641.81344	218.318357	3127.15164
C-19	384.046933	12733.5882	66034.149	3727.30731	160.460635	34.3520091	243.895598	711.017062	49.7694503	411.945698	1081.48611	548.095756	960.975885	494.101604	3412.97015	3714.56421	351.434657	6270.52119
C-2	385.698594	13386.1882	59098.5894	3637.55557	210.837039	17.0984749	570.964503	710.968418	61.192298	442.99238	1652.07536	562.331874	426.424809	1019.73139	4565.70073	3879.98855	310.869228	5540.10908
C-20	292.068862	7544.88284	52457.6987	1877.71376	97.3721582	29.2258649	1292.92672	3414.26425	12.4687773	247.007871	1030.50474	2023.64906	542.156454	1000.63365	7615.18026	9077.53872	808.538214	3207.25806
C-3	287.762549	10914.9269	84116.1455	3614.30584	53.808719	16.4521841	528.478379	1119.66192	60.965733	393.896988	891.511438	836.289684	588.585584	570.118111	3853.51714	4916.72576	323.933878	4869.1729
C-4	289.731808	6068.94468	43304.366	3005.50379	199.381802	31.8715214	268.067008	822.066393	17.8229465	193.209935	557.151767	484.433693	239.974431	691.060457	3484.56568	4200.62833	325.222734	3163.47672
C-5	559.680743	11220.859	80437.6053	3981.34988	210.646127	12.3897511	298.456386	848.375814	40.7758655	677.958914	2258.35295	535.528403	718.885994	616.153518	3087.91918	3703.60742	330.721506	7928.66655
C-6	409.070067	8639.87592	54306.1442	2226.14186	73.8799685	21.8820935	227.370656	655.360333	44.7369128	235.138204	973.631095	349.718062	699.062123	510.337249	2421.82297	2821.77507	185.581884	5753.15471
C-7	305.888357	12275.9664	97773.8103	3633.3314	134.961684	31.9284298	437.424369	1175.41994	36.4281698	211.528715	688.709395	551.090316	396.587383	490.709654	3492.30364	4447.09022	306.930134	3812.01136
C-8	375.823471	10946.8276	65446.0578	4405.35271	249.542798	12.2599612	434.244136	823.413959	49.8452681	429.011427	1278.18641	635.58848	629.880143	663.755023	3017.01688	3036.57209	287.52203	4167.9833
C-9	414.674843	7531.73069	43813.2196	3306.43786	141.549496	13.6679119	294.164897	731.549352	42.6591508	274.915397	534.444504	670.587295	541.968059	552.746252	2500.78633	2818.03278	188.358374	3002.44107
C-21	355.627029	9052.03364	46869.0458	3147.57424	87.6430607	34.0770869	506.891824	1071.31193	81.1657443	318.458548	953.977071	871.907327	738.834734	1202.24233	5951.99591	5225.75579	415.49294	3574.83296
C-22	414.475315	10951.7468	39498.5315	3178.6804	198.652861	22.3736017	542.219232	500.496837	25.5448752	400.867404	1187.76684	777.448845	508.581565	1177.02839	5822.13211	3710.2314	257.114642	4180.21124
C-23	345.981815	9254.0053	78345.4858	4450.74953	161.040845	41.0473965	256.346909	838.583544	14.0571989	370.449341	1060.03005	512.976799	470.800937	776.120088	3475.83056	4141.7201	257.456034	4967.24077
C-24	377.263306	12720.3648	91687.8298	5969.56587	242.368898	20.3857073	288.967837	859.933454	18.0175007	284.821633	1001.98458	849.184975	328.759328	885.378853	4029.04934	4284.48188	492.459647	5257.31565
C-25	354.172464	9101.5915	59593.8847	3107.1847	233.033853	9.24480058	483.011619	992.12624	32.8968293	536.751453	1464.64283	945.460641	198.341817	1314.0254	6417.85141	5875.51418	615.868898	4051.91899
C-26	320.959491	9236.28723	60398.9879	2310.28602	132.810865	34.2356117	304.951285	1013.24698	35.9966774	246.054183	1164.43865	518.931518	373.07847	925.250457	5327.31834	5727.26831	412.293238	5058.03082
C-27	226.406727	7180.76522	43611.7424	3673.53326	234.016135	78.6699684	158.980585	600.085853	23.7498672	353.29672	821.891814	486.371244	439.641641	465.190417	2231.6337	2672.71493	240.944525	2826.82009
C-28	593.989433	18561.7896	118281.803	3040.62585	170.323796	43.3261166	452.186822	1163.24941	80.8389894	1631.45436	5639.69164	475.7791	792.752643	937.721667	5064.60328	6054.57246	416.347667	11731.0513
C-29	632.482729	18019.5728	101525.044	4861.44922	337.290143	15.862774	354.146255	1189.55067	67.5658747	846.435117	3126.68525	1173.0196	794.408649	582.093163	4086.21794	4703.51983	419.871719	9957.97257
C-30	143.358393	833.407772	8408.86612	588.332018	10.5843083	10.6965554	18.9865445	84.7085069	28.6684462	21.8365949	109.743677	16.7413587	5.66376814	21.3744311	239.771182	160.543619	41.6363175	427.869219
C-31	288.480048	5921.67334	35664.9074	2470.52258	98.7951918	8.60472045	220.702672	487.920416	30.0130099	225.119502	960.497833	329.361675	718.511008	403.489407	2479.98563	2815.30714	149.701735	4867.24132
C-32	393.947953	8257.51617	43884.1284	2312.75855	142.952702	11.2070148	550.4551	1745.56644	15.9478508	325.085063	977.678392	1558.77947	748.147271	1594.74679	7648.26179	8887.49952	641.129953	4085.00816
C-33	334.380446	8033.66659	59525.8426	4044.7462	266.203249	42.0523694	437.266582	1174.13112	19.7309757	358.328996	1044.93622	1480.95433	646.572418	933.844738	4668.16386	5214.13362	528.133254	3412.23944
C-34	499.979193	13969.7706	67163.1102	6535.76789	647.234325	26.494625	584.013939	757.924694	38.6777839	430.759082	1517.4972	1780.58731	647.821884	1295.98855	5697.17689	4943.90277	398.632593	5188.9993
C-35	151.410732	163.070743	1117.58968	114.846665	16.7442293	11.4692196	28.989997	4.06560453	10.650038	8.38967957	18.4504441	11.5945598	7.41212566	11.2673451	21.0080158	21.9453742	24.969266	53.5804886
C-36	465.213067	12454.1857	101109.11	3025.5924	59.3852874	14.2398696	1650.27138	4392.13947	33.4945527	210.945925	527.976389	3256.74399	791.789986	3078.04655	20118.3825	28259.6106	1758.98831	4498.5192
C-37	479.338178	13402.5219	82081.7007	3400.32021	170.284322	47.6931048	1269.37328	3157.01921	52.7294842	422.641041	1727.04279	3005.35231	948.299037	3196.14042	15886.0067	22240.9472	1422.02665	6461.74205
C-38	495.279037	11767.3103	64409.8925	4587.07739	223.72295	14.3897587	1336.85839	2263.1818	24.4666926	516.010698	948.564153	3113.7406	572.218061	3203.29706	15579.0205	15565.6534	1514.34713	3925.09637
C-39	360.735123	6861.06435	39428.0776	1673.92991	42.9475387	19.3325908	398.479934	1098.16762	45.0687317	152.066923	423.527901	758.339959	465.749353	1459.64981	6265.13229	6434.39737	337.906256	3193.12471
C-40	289.511969	7002.56174	35193.6699	1924.69097	26.620175	33.0692148	1309.67642	2463.04129	34.2788997	57.856058	219.268751	2969.8233	794.823915	4023.63045	17655.8481	16457.1435	1157.79561	1415.45707

Table 8.65: Raw peak area data matrix for cholesterol ester for serum samples taken from patients with breast cancer.

Samples	Cholesterol	CE	CE(10:0)	CE(13:6)	CE(3:2)	CE(24:0)	CE(24:1)	CE(24:2)	CE(24:3)	CE(24:4)	CE(24:5)	CE(24:6)	CE(14:0)	CE(14:1)	CE(15:0)	CE(16:0)	CE(16:1)	CE(16:2)	CE(17:0)	CE(17:1)	CE(17:2)	CE(17:3)	CE(17:5)
P-1	33.662625	2417.60491	18.498329	210.350376	67.004436	1756.81647	2802.16957	606.317046	258.752409	153.845622	267.812781	594.005975	41.0101708	915.133556	236.954851	1092.01865	1629.30464	61.9278181	49.4749061	118.751906	40.5619131	43.9880243	30.7549625
P-10	77.9620924	2376.54479	14.3064639	191.590138	101.632889	1460.09918	1418.72719	803.278198	312.290792	91.2451617	201.096878	310.980637	5.38904445	314.363609	440.120597	874.011389	336.019195	53.0568668	10.8440374	69.8099182	40.6280974	101.823825	132.882036
P-11	89.8135003	1964.5252	17.9157149	133.637727	121.013719	719.146153	1214.32143	194.709238	259.068758	172.847854	128.005153	229.027867	18.203675	93.4130201	273.185717	873.719117	427.097884	39.2629012	16.9822363	45.9651585	51.0769776	41.3593839	42.5759387
P-12	110.257577	1663.83653	74.5819363	169.000793	91.5522507	912.156991	2733.54276	318.738857	282.194565	101.253678	262.590731	636.757661	24.8587917	712.236766	234.724705	1385.59884	849.744298	38.2544039	13.8878178	108.54614	56.5897512	82.8469621	103.495814
P-13	62.1369931	3110.8658	12.6333293	215.772876	175.534217	1098.45713	1713.03072	264.55854	244.501001	135.47429	226.499352	339.283309	47.6806178	478.865593	347.629279	750.497716	1028.30905	94.6402275	20.8603676	36.5153701	27.8748303	25.9295069	46.5532397
P-14	84.3214633	1948.99129	28.7267249	372.686694	96.2104167	1480.83473	2922.5234	294.134436	163.734897	64.2738523	449.950485	575.34136	29.0281178	489.8824	498.489702	888.735499	1314.97012	16.9087522	28.3107564	140.50825	51.1912662	48.6702244	35.2521834
P-15	67.5162835	1517.16609	31.2878699	90.620886	46.6031554	566.283901	1379.60007	236.343431	284.556835	139.918379	392.244009	346.857857	30.4134488	112.728602	576.91384	730.447495	418.988552	106.18849	11.3260994	43.5010128	94.6187999	97.6401483	52.5488714
P-16	76.8498377	2837.65671	15.4167196	344.83402	144.565094	2018.78833	2127.77267	648.821523	372.336312	137.369242	187.707353	335.237477	63.2411762	728.134614	397.407376	1051.43819	958.909766	62.899214	28.6645551	76.4950999	60.111286	96.2235341	75.5713965
P-17	61.1956644	2006.78744	39.5596815	126.00905	111.008824	1148.65963	1623.66756	344.864518	290.18326	111.020004	107.391781	449.522929	14.5704401	250.046554	328.1633	991.024174	499.97174	49.9147064	16.140871	148.836986	38.5961656	49.6588419	55.7957211
P-18	34.301991	1728.87031	12.0321089	333.131643	104.898128	971.270482	1506.23398	299.684924	234.697604	134.685286	204.764836	348.578113	23.0813851	1003.42012	119.654675	1033.5812	915.636521	57.6066928	19.3355439	135.541221	41.4561855	152.902221	84.395147
P-19	85.2734609	2546.41991	26.6611925	43.1942933	141.578334	3948.97366	4827.28289	1898.48234	2257.37856	400.091979	4375.29577	829.168074	39.8828439	94.1549989	475.271257	1334.73899	1087.809	15.6056612	28.3225007	160.680626	24.8787833	65.6032786	178.732922
P-2	44.5432454	2041.83765	21.2170388	108.350205	101.428113	1404.47583	2172.31841	373.224889	339.142085	267.76647	306.864544	396.314079	31.3902674	554.960567	222.308626	935.560484	546.546319	54.9443619	11.3071056	89.0905762	54.223585	83.6034761	59.4482395
P-20	68.7287076	2702.12464	38.8253238	399.09202	128.563853	1101.36696	1758.61389	846.542772	1459.3143	237.586739	2771.42903	394.452777	36.0318453	962.371329	129.173956	928.452876	795.462455	28.7393989	34.5612551	63.8730763	53.8600324	46.116807	147.77323
P-3	34.2257026	2821.6515	21.1730933	167.827349	109.886114	560.600278	1062.56164	231.271493	145.655815	60.83813	136.255839	150.577016	26.24306	219.272123	266.414786	621.365217	249.088634	47.6826687	7.28078017	19.764551	30.2866421	5.9412292	74.0088441
P-4	38.5618952	2595.01511	23.8896645	237.114492	84.0674438	3491.50725	2883.85661	1436.25634	305.726033	89.6911916	317.433995	651.660341	27.6727396	418.531654	502.142371	1088.56186	460.905565	38.1809186	21.2556831	35.5400924	47.6579329	34.4710145	117.992372
P-5	80.3111223	2431.74391	16.9971197	244.071002	200.316048	1280.82601	1399.2609	244.040333	260.258383	175.413258	395.690458	321.812148	15.0998921	524.449486	236.595816	816.62354	430.700232	78.2416041	21.3344097	99.3771732	29.9787784	113.403005	97.391944
P-6	10.0895559	7.99788773	9.14276618	13.2418073		44.7882521	96.0423402	23.376525	19.3406127	18.2077053	55.2032669	36.0979798	9.74910226	25.7978802	78.0187396	71.2327063	89.5392661	16.2786935	18.386614	8.4778691	13.5956573	16.8789652	10.7728321
P-7	99.5598561	1850.76897	14.9894555	181.494468	74.9761585	1679.63314	3520.63958	482.645942	386.439496	199.547992	209.200861	501.596605	84.8644673	549.145745	270.989546	1423.05732	1102.39912	38.200777	27.3340617	103.500327	73.8618018	106.038603	80.8619395
P-8	98.4791735	1657.08746	13.7853845	285.889153	89.3466743	923.486219	1554.33415	409.493694	253.018937	163.318974	350.552898	240.004424	38.7474995	199.614497	460.98429	820.648785	647.534319	59.7243078	46.0339752	45.0813521	53.0541204	93.9141649	67.8684903
P-9		15.8222973	15.1755755	15.5626158		197.698406	164.958272	59.5137468	22.0131048	9.65876996	78.0525887	74.6715469	9.97561118	21.1866296	61.95281	65.8570377	32.754311	15.6561647	17.8640302	18.6912571	12.3633139	12.4011907	12.8015346
P-21	46.4304214	1901.40093	20.548721	270.383484	117.995962	1073.72212	1553.92565	914.01269	1671.77395	353.77783	4123.60173	314.677842	25.5434046	370.392434	334.002039	472.232682	786.517423	54.1212038	11.4308073	72.138884	65.5856128	86.4415216	141.212408
P-22	65.4416379	2821.70613	25.0966244	194.073757	124.455925	1103.80705	1272.0668	444.948491	950.455487	239.552671	2033.29933	110.755254	56.804385	375.569809	260.548697	358.517879	1048.8079	68.4893442	24.5559189	88.9247445	103.757084	236.927325	123.268589
P-23	61.212322	2028.3263	16.6246161	186.190423	160.092738	2282.04369	1982.15584	1184.71936	1587.95375	223.030744	3112.95804	593.697985	41.3015898	214.334464	306.788264	743.551792	534.314332	20.7225161	12.2395242	99.8042088	82.2191433	117.98787	124.249352
P-25	49.3241383	2495.08681	13.6620227	478.927138	177.371743	2099.41805	2573.61546	1005.58063	1709.50964	302.149589	3319.22065	514.338325	76.5262048	387.870423	143.248043	1013.55271	706.563075	53.3706676	9.30766214	82.3286338	59.2016139	30.5433205	233.031934
P-26	49.0044732	2402.34864	13.9937947	169.138526	180.765979	1825.35507	2727.92201	760.058573	1265.96338	211.372142	2446.69747	606.34827	42.5672375	608.347752	140.906711	1342.69832	621.38291	72.2131252	51.7868174	93.6587744	90.5035457	100.738739	154.339502
P-27	49.6693392	2910.94166	36.6959726	104.327142	100.442655	1864.98426	2568.71679	720.353892	1113.55081	269.811126	2152.0809	738.669684	67.6603256	418.53469	251.266939	901.996572	1325.87821	82.4622391	26.0844222	72.5144638	91.942678	135.3977	124.155295
P-28	86.8463688	2250.58959	10.8486278	169.010464	112.094382	1540.20663	1804.09203	976.07823	884.037802	157.469895	1236.30898	436.16946	13.8269582	82.9357705	92.3405057	947.161311	298.304001	29.1980352	18.7422641	92.1184546	44.3970884	20.4126244	107.916172
P-29	118.761555	2538.77058	31.2105673	105.924687	106.03057	2786.77478	3550.78507	991.505515	611.820571	96.0609912	434.883954	597.232064	26.4420059	703.641337	227.351067	1669.68213	959.112836	47.634741	23.3707535	93.2507196	24.1524157	56.2055813	215.69691
P-30	69.2044472	2023.91909	14.990665	175.611131	112.82888	2178.14013	1595.6723	824.775377	347.84373	118.876742	95.6454201	343.968248	56.1857971	140.847537	365.380588	755.156001	749.735847	33.2650798	33.0700573	85.5731928	40.4442611	158.329419	40.6410423
P-31	86.556081	2954.19655	23.0229672	166.000639	184.320595	1195.02646	3040.68309	334.850147	379.897403	147.478535	294.380745	769.317636	14.9408017	420.87537	122.678975	928.916908	479.02022	89.8099795	17.1941072	39.6575963	37.9515351	47.3866155	88.651303
P-32	26.2405437	2977.87899	17.5949234	101.374061	131.151013	1611.19043	1215.98864	535.396111	179.886724	101.09277	130.630639	318.773532	6.4794554	173.51037	338.153461	647.113834	204.152739	23.8051822	12.6517724	19.5788003	29.9217488	63.2156813	16.6477091
P-33	97.3154096	2112.90001	25.7819882	195.655358	121.384342	1143.55576	2083.78555	469.588365	470.224909	190.245421	703.329421	396.413726	28.5980484	356.975075	158.48929	649.323974	544.757425	34.1048856	13.6573463	127.708466	50.2376384	142.077127	60.2422535
P-35	67.4578078	2025.93385	29.5264701	314.863063	100.976827	5654.13341	4438.97324	2105.56947	471.383711	314.996438	325.023592	930.475597	110.848065	610.577565	157.66554	691.855326	2752.34077	28.1603588	31.713685	158.120526	65.9273274	128.646294	75.8207574
P-36	107.430429	2324.09987	19.6484966	183.724615	189.690739	3064.84576	2670.45345	1449.97818	491.51019	84.5801231	307.027344	549.477741	22.9417257	252.507717	179.646324	359.751313	482.417528	57.2214518	13.3099839	67.5246999	28.4117447	82.3322521	37.0288535
P-37			17.5735185	5.52561806		56.9941014	28.6742923	10.192137	25.069884	24.069203	50.2694564	12.5705954	13.5066187		25.0673121	23.8423513	72.2545084	23.748041	10.3775682	11.7033764	8.80171515	4.69989884	11.2827142
P-38	79.9950819	1577.74972	13.5983212	161.707511	122.083758	932.104291	1817.82817	229.544289	300.758049	181.343215	272.047583	388.600082	68.4726645	333.931487	175.787648	1299.15878	1114.38219	49.6647086	32.8804915	82.9214149	46.4023675	91.5674639	94.9835347
P-39	113.649756	1872.75953	22.9902494	150.593008	127.813023	2450.56712	2502.76861	1137.55513	312.074244	173.409098	194.781131	733.893417	9.30936098	93.7996339	305.470919	604.338544	555.19258	24.8256438	19.3556459	112.636767	36.0783997	47.2416828	52.4979732
P-40	85.4153751	2420.58304	25.4441487	59.6738861	85.1171946	1123.90968	1855.84765	333.978978	289.289714	66.8285945	171.914694	504.282842	13.1911617	162.568297	167.79116	891.095872	215.519978	108.030236	14.9251637	55.5315606	16.0557131	64.6481778	48.6467922
P-41	87.4849896	2199.95268	9.79577045	293.254004	126.106165	2125.36044	3450.61258	661.59758	364.976527	124.753268	286.041697	754.343032	25.2783822	591.179017	132.018173	1191.14453	1065.03343	54.9614582	17.9993801	86.4732342	30.9292795	54.4373174	78.6055674

Table 8.66: Raw peak area data matrix for cholesterol ester for serum samples taken from patients with breast cancer.

Samples	CE(18:0)	CE(18:1)	CE(18:2)	CE(18:3)	CE(18:4)	CE(18:6)	CE(20:0)	CE(20:1)	CE(20:3)	CE(20:4)	CE(20:5)	CE(22:0)	CE(22:1)	CE(22:2)	CE(22:3)	CE(22:4)	CE(22:5)	CE(22:6)
P-1	484.082081	11809.0547	55950.1247	3696.54168	180.316469	36.5844977	368.85758	800.870027	41.7338046	591.745096	1783.4623	716.329884	315.023662	845.817871	4134.58956	2996.73295	344.880842	5433.79115
P-10	324.94301	10706.6781	77014.7833	2042.23721	68.2538746	68.5625958	240.763266	758.950775	51.2650323	774.234165	2134.29664	228.007451	1205.26039	551.364926	3185.21554	4078.1309	303.973837	10947.8287
P-11	500.450851	9686.43687	71376.9429	3325.51042	98.5099472	17.9766222	283.421853	650.389348	11.6966666	160.708851	553.37581	387.852258	569.401981	539.676262	2741.11756	3431.75649	231.965834	5923.2273
P-12	405.884675	15776.4	91636.3068	2750.26261	62.2215556	10.4794672	267.897825	786.235615	22.1182468	303.882451	1008.64828	409.481984	466.212612	686.399004	3080.59113	3884.95722	317.98099	8983.3092
P-13	307.806018	10236.3327	55204.5802	4303.16854	170.471274	20.7489756	327.9653	775.673183	53.2316261	267.399642	907.322795	588.898928	613.171569	594.95639	3026.64418	2678.34643	338.74563	2873.96765
P-14	376.138805	13195.6479	60047.8041	3498.12878	124.157753	16.6432792	398.631457	538.314465	97.0798239	500.056008	1331.58776	781.844525	815.589118	728.412949	3465.50203	2776.8085	297.698193	4014.86888
P-15	356.837683	10050.5266	57646.5223	2507.07888	70.830019	9.24560259	176.47757	568.360401	48.1584496	157.840224	761.166942	262.69336	603.203321	430.583935	1981.96861	2182.45561	156.958247	5817.59577
P-16	463.938593	11247.8749	67018.718	3622.53282	135.069329	27.0174179	402.103899	872.82259	102.192045	422.536808	1808.99519	617.526309	801.045301	541.701246	3751.32475	3649.56691	333.365875	3675.93852
P-17	492.229255	9646.35229	61947.9476	2411.79885	85.5348845	20.5363489	399.212024	829.869666	25.7394517	293.308474	983.69024	352.91146	325.070636	646.270764	3630.14125	3788.15264	232.025046	5410.73529
P-18	377.927938	12937.6594	76791.4987	4468.95463	207.008374	13.2995539	264.322311	620.590379	30.1076174	255.40266	1098.01639	628.367679	740.982476	652.305677	3416.49755	3357.30391	246.765678	4742.67038
P-19	533.714232	13592.5858	90067.3639	4983.77607	224.525311	13.8695867	875.163992	2794.89689	101.932225	445.279557	1967.34053	1718.0481	417.903087	1282.91846	6329.31287	6373.88939	517.490547	6885.33982
P-2	322.284854	11163.9307	81504.1084	3914.57444	133.027566	54.3941103	395.828363	1071.6937	92.8367868	337.4084	904.630958	747.729379	514.326122	576.957873	3619.89391	4464.49271	338.225611	4969.17275
P-20	636.33269	13155.0136	63456.2844	3559.00008	130.446941	16.6279921	640.298223	1606.39294	19.2231068	167.616325	565.104736	846.203461	481.766847	1052.29996	5249.95333	4328.04349	346.604893	2073.58099
P-3	344.410718	8926.41283	47353.9399	2218.76719	52.0553539	44.5214976	216.544627	534.533271	30.4361462	157.470012	578.237947	276.54149	435.861725	452.628153	2575.60413	2589.02998	249.815785	4947.80387
P-4	333.349222	9544.82077	66141.4823	2318.23069	203.334658	18.9379947	448.743727	900.187207	39.9525331	663.362746	2668.95172	811.034721	551.700547	558.493917	2928.29094	3923.11054	354.581739	5962.45191
P-5	396.069643	12915.4699	83952.795	2104.62748	32.2349226	16.4548493	378.005554	1129.55766	18.7984497	212.460155	841.538159	541.355667	504.748902	853.437741	4269.06375	5661.56717	514.501059	3719.69814
P-6	121.331392	577.785091	3490.16462	254.584001	22.8092941	18.8889833	32.7365811	81.7335003	45.9437623	11.152346	86.0188403	26.5786495	11.3332635	18.8627753	127.107918	127.623369	26.913943	221.879808
P-7	400.013984	14594.9673	84130.5009	4775.65373	144.406624	27.630682	550.117578	1134.98208	49.7621507	374.085043	1109.07283	1131.11653	464.670779	740.005399	4565.41253	4201.096	476.212039	4615.92991
P-8	469.902319	14354.4323	109719.761	2533.50583	51.9114665	19.1194847	283.284802	814.361873	40.8647029	701.507058	2174.58405	340.78781	771.849895	547.139683	2686.11999	3417.18541	254.739404	9241.77782
P-9	142.630154	720.945638	5489.85039	214.549676	11.9453469	12.7079545	43.6120043	119.473967	13.2367071	11.6182918	132.664685	19.5234067	10.6597473	91.7825798	315.79424	394.213831	32.3377267	573.355616
P-21	426.41783	14824.955	102852.064	4894.03466	147.85447	11.4930978	427.421028	1795.71214	36.990249	489.990177	1632.44489	531.667785	324.970529	411.780168	3119.17013	2941.26288	401.447176	6927.08613
P-22	335.172959	9956.96231	78189.6262	5499.25837	275.449381	11.7500534	223.948699	1156.98664	16.5897197	355.432227	990.795653	579.546409	112.294696	580.625336	3513.85675	3295.89408	452.948893	4497.22692
P-23	394.254831	10678.087	59775.6193	2588.38868	191.001391	18.340556	367.151816	1429.78945	60.0164085	725.21683	2883.68672	453.62199	254.87864	685.542529	4263.42507	3903.5411	317.188508	5891.17179
P-25	505.114645	13566.7129	85156.6105	3241.48429	91.888472	15.7143102	428.750314	2056.6148	89.6630954	314.869784	1198.422	811.917151	702.541884	971.045247	6162.22338	6520.15405	535.284008	3907.71775
P-26	381.130409	12960.0766	91740.9596	6488.75159	256.430592	15.7949772	421.068143	2026.51994	50.59489	292.694615	899.725876	1427.45296	445.482813	892.943658	5976.66822	7287.86523	563.163501	4275.42988
P-27	416.347155	9322.6415	51677.9309	3945.97835	201.310239	30.6734766	372.228051	1134.95856	29.5856925	421.900586	1136.07848	865.58595	590.109186	878.074824	4901.48655	3492.31036	325.891967	4062.07037
P-28	350.07942	6719.06122	45468.7672	3049.01487	116.19782	10.8024732	347.761909	950.813609	37.3899219	437.280231	1464.42599	524.471606	390.874289	587.099233	3793.95288	3664.27238	324.030542	5140.42793
P-29	630.006375	24012.0349	121272.289	4777.66663	296.09486	19.9208574	645.743933	1468.6199	79.9060884	929.251236	2337.02464	1135.59449	411.70189	1355.86784	6391.47446	6355.02113	417.195904	9880.11097
P-30	564.559095	12415.432	68757.4985	3275.2036	247.322598	26.4295737	198.50573	420.057142	55.2629218	1295.93993	4603.60836	370.160776	632.105772	455.804922	2479.11356	2290.9855	235.251476	9275.05677
P-31	360.391979	9427.50435	59807.1037	2567.55821	59.574719	9.3827889	402.009813	894.053649	82.6838776	176.579478	822.936981	477.200187	545.080375	1030.48888	5067.59296	4867.93163	265.846436	5032.45662
P-32	219.151945	5875.19711	32918.511	1269.53323	71.3317356	48.5411578	185.16567	552.18766	26.4869667	343.860614	1328.88557	279.230439	680.816006	494.931578	2292.47239	2740.52484	178.059627	4236.0963
P-33	417.794209	13036.9282	95749.0684	3815.68617	127.496025	95.6285089	263.64764	1073.09926	53.7309763	246.437854	772.826152	720.671097	186.205938	655.697936	3726.32741	3725.21182	502.697965	5116.11983
P-35	487.175732	15468.0296	62509.087	6220.19921	655.688535	22.0218909	703.548788	1040.72272	70.6854128	998.431559	2846.92319	2505.38223	187.897631	1659.65163	7089.46162	5112.24976	593.125973	6507.41547
P-36	328.442494	6829.15203	37719.3043	2318.82159	246.66646	64.5891423	377.306427	641.644277	9.37966001	737.133406	2032.23607	762.730599	258.234533	979.782805	4460.83975	4503.00408	392.754827	5262.63254
P-37	177.563454	625.594298	5074.6947	180.282708	15.5831605	11.27906	14.3044761	32.5162616	11.0749876	12.3573508	124.807996	13.8216588	11.6765699	17.0056995	53.7589645	73.6850223	26.510825	377.276124
P-38	679.905027	21947.361	110413.791	5983.3241	242.532927	35.163985	423.541785	520.585151	62.1273414	228.233185	738.320961	542.185286	448.057136	717.961823	3271.60735	3044.43527	370.998206	3594.11834
P-39	377.148017	13105.0264	72075.9252	2921.01945	95.329046	37.9909747	378.62895	864.774842	125.036296	934.237822	2881.78755	559.339537	615.632183	827.467666	3935.55892	4087.80097	335.17316	7898.97781
P-40	365.49101	10011.7636	56769.2772	3518.81891	153.711679	12.7278244	309.47124	758.322702	43.4321817	232.060613	858.259388	619.385191	845.04522	954.285598	4106.07252	4221.74811	414.2239	5988.98853
P-41	337.099978	12350.9004	77796.8518	4007.67333	126.740581	38.5465119	351.527576	1335.63472	10.5871411	278.380961	1095.44589	957.882913	475.106952	1394.88927	6276.44617	6476.11452	495.982234	5408.46001

Table 8.67: Raw peak area data matrix for ceramide for serum samples taken from breast cancer free controls.

Samples	Cer(d18:1/16	Cer(d18:1/17	Cer(d18:1/22	Cer(d18:1/24	Cer(d18:1/24	Cer(d18:1/25	Cer(d18:1/32	Cer(d18:1/32	Cer(d18:1/38	Cer(d18:1/39	Cer(d18:1/39	Cer(d18:1/39	Cer(d18:1/40	Cer(d18:1/40	Cer(d18:1/41	Cer(d18:1/42	Cer(d18:1/44	Cer(d18:1/44	modCer576.	modCer614.	modCer632.	modCer651.
C-1	1596.2247	1826.20452	54924.1004	83161.0373	111753.102	4482.09259	5083.42282	4713.67954	6686.07106	4994.56577	405.607878	915.196917	16557.7804	6391.62168	3868.27375	578.009043	782.272243	10948.287	660.514005	3296.45883	19338.1736	5354.77024
C-10	2208.67549	1977.37814	77585.5351	175472.044	180185.817	10455.5263	6582.20809	7047.11609	7294.61522	3839.3025	929.8714	1470.74185	21638.7045	9275.82646	2642.3944	1616.50239	1647.66016	22658.7896	896.48035	3721.4126	41592.9135	10523.4012
C-11	1432.51961	2318.68052	54422.2253	88484.2782	133218.696	4647.89471	5974.95286	6898.44533	6115.07225	3242.69546	692.517656	1221.65903	12090.4758	6505.70639	2228.20006	744.269926	1027.1064	14479.605	867.935696	3343.68521	20605.7742	7969.96556
C-12	342.607203	610.858165	16177.6261	22945.3263	19948.259	996.275098	1907.86444	3937.74413	5619.33894	2826.53975	140.60977	421.60569	8565.27185	3529.58923	1449.55535	503.439516	581.53136	7852.88181	247.761203	546.801103	5019.59879	2907.51322
C-13	1963.70357	1216.47858	67573.6563	159492.981	100917.592	9112.33026	7167.25599	6165.10037	8406.26287	4257.34538	442.338109	798.92942	17597.7547	6707.16867	3542.44779	1240.8612	1873.28496	26031.6778	461.117591	2546.20507	37344.6005	8428.33388
C-14	945.254345	446.559258	25171.2398	62435.973	8131.97661	4025.28054	2286.63464	2463.62621	3206.81062	2006.87412	141.696962	184.58265	6173.12351	737.981041	1610.44091	474.757175	509.769811	7118.96438	208.212338	1380.41487	15104.8278	4543.96536
C-15	3182.88032	2196.02527	82939.9665	189212.805	143173.951	10784.0752	7514.5712	8504.06711	9216.34999	5876.18621	809.618173	859.734792	19440.2584	8181.2318	3679.33347	2080.46177	2097.06981	26789.1077	1008.86882	4587.27104	46637.2812	11035.4667
C-16	1083.39383	1200.97854	37369.7594	55759.253	62518.169	3162.36281	4344.36222	7580.52793	9723.95966	6081.3978	337.538055	817.694289	19317.3963	7060.55903	2125.74867	962.071549	867.539592	14188.2873	433.502914	1715.39409	13966.2566	5401.3138
C-17	1712.09779	2156.81602	56525.9679	92116.493	139372.68	4944.36382	6227.90614	6636.35246	7669.57228	5563.95664	924.748268	1355.51429	20627.1846	9011.1948	3295.07601	958.527772	769.718515	11694.5516	889.301453	2754.77267	23461.5408	7648.38183
C-18	2403.27728	2267.93127	60794.9667	121920.76	125682.836	8532.28392	6119.69398	8429.48032	7760.54273	5802.57265	708.951794	1002.42966	16736.5853	7172.4241	2336.72177	909.99252	882.328048	14477.3141	632.301445	2797.46657	30734.2484	9436.82746
C-19	2649.04481	2781.66947	86093.5844	151582.563	197541.599	8148.67344	7100.41087	8367.28606	6879.62867	4814.4928	851.452476	1519.02296	16493.9404	7570.49322	2231.95529	1436.38804	2275.89181	28146.4534	971.57057	3570.48443	35713.2044	11220.4716
C-2	1062.13717	1338.94777	38622.3036	69524.275	92922.4065	4500.18433	5454.56885	6013.41349	6357.48837	3640.99898	408.387771	891.39805	13972.7012	7846.46602	2182.07814	649.937751	952.515687	12691.3867	540.162774	1350.6454	16834.3348	5253.5002
C-20	1155.69311	1718.56975	35250.6953	46470.3683	51503.8601	3427.09483	4460.32267	5939.7947	7114.26097	6243.56426	460.437995	672.415207	16061.3883	4820.9015	2635.81445	786.049814	968.747134	13306.7157	485.90171	1801.41061	10419.4905	5424.70405
C-3	2235.61634	1961.72573	74311.7365	123965.018	134237.242	5847.26261	6488.28747	8918.65521	9398.63791	5260.85455	670.054272	1164.23358	18229.1634	7668.60254	2405.35693	999.602743	1555.58935	19318.6973	974.336501	3179.59301	29395.0543	7992.5561
C-4	1647.56398	1337.09076	53968.4347	135200.216	63084.104	5663.34962	4173.34908	6988.83154	8610.45561	4277.01982	336.599625	1128.91102	17305.5362	5444.61905	3458.64389	1197.02595	1227.96865	16926.2439	356.125794	3107.01847	32062.4343	9658.38958
C-5	2756.76098	2312.9366	74131.1232	174149.984	138834.925	12339.6181	7354.94064	4987.38612	8236.87863	4704.2611	657.317563	1064.38377	15210.9999	8123.04569	2673.16789	1691.85068	2058.36173	29211.9411	946.786872	3656.28166	42585.487	11601.5849
C-6	2039.14534	2355.75727	66315.7585	120328.171	124357.951	8327.76471	6159.07667	9614.75869	9248.99121	5476.44321	440.491792	1612.06708	20143.6854	8642.94218	2538.863	1399.95274	1922.64938	27496.0312	1175.9013	3738.47319	28946.5347	11464.6227
C-7	1869.38725	2281.64649	57531.313	101864.576	132506.212	5969.94089	6078.25908	8159.52664	10585.0929	7879.51841	548.300361	1498.55564	25264.8659	11096.8052	3811.86704	1036.39021	1388.21052	18166.69	580.176054	3540.2186	23919.4158	6259.49537
C-8	1591.16688	1341.60254	48382.4514	108063.377	123986.643	5849.10551	4872.06852	6656.72765	6515.67276	4038.89346	616.702076	1266.53636	17602.7488	7201.2367	1629.78614	1206.70178	939.9511	15477.9282	786.427104	4065.64345	27100.9281	7500.98398
C-9	1957.35972	1761.35651	53381.8349	112499.246	106371.948	7069.18876	4175.65363	9815.58474	6324.30341	4088.6662	430.804178	1133.91653	13600.203	7044.22838	2039.95126	1188.3412	1457.78263	20778.7096	901.78601	3826.51249	26935.7106	9283.11406
C-21	2311.11615	2040.77306	77841.4221	165133.503	138481.483	9477.09713	6434.62933	8491.04814	9120.95897	5601.10495	651.559627	1332.47055	19788.3355	7499.23396	5652.51539	741.501453	1205.44235	18940.9841	1501.6824	7885.73074	40611.414	11695.3691
C-22	2007.06406	1474.86583	75343.183	206081.38	176807.509	9493.18881	5016.61604	4736.80521	7831.49244	4393.67641	555.393253	847.419058	18017.4546	7478.89216	2913.53391	1141.01102	962.529762	15945.1335	1161.53672	7729.39706	50244.2556	6530.12576
C-23	2600.96693	2529.50175	70742.327	152436.556	132648.917	9552.875	6753.05734	7681.60363	7391.11112	5295.87041	657.264936	805.838376	16625.1184	7803.0646	2073.80247	1398.44026	1452.51988	25363.2186	894.087273	4290.84334	34976.0686	11060.5905
C-24	3032.13825	1786.38328	106814.037	211010.043	167726.162	9553.47328	8593.60627	4898.18526	11096.1045	4783.07129	705.619882	958.598479	18591.3042	7261.89144	3575.76884	1221.34838	1641.91022	25275.1498	931.035933	3052.03054	51284.7376	8404.23586
C-25	1908.1066	1103.66637	46864.5658	113202.509	69673.3307	6284.97646	6857.81493	4681.98735	7133.83796	4915.21338	364.558372	397.219852	16510.5353	5208.67026	4460.65031	932.355288	1272.53879	17560.4592	366.144491	1304.57296	27030.8102	4482.13019
C-26	2558.63717	2199.03253	63538.9547	147401.617	122627.004	8672.23237	7662.78484	5765.5336	7689.76519	4904.87084	363.649911	650.451991	15987.3844	8202.97866	2626.85051	1255.00295	1950.29465	28243.3195	556.233579	2361.51407	35141.5403	7965.35903
C-27	2045.80523	1269.62128	58218.4572	115873.387	108888.178	6830.38511	5842.18793	5613.96474	6968.95052	4873.32199	393.684723	482.879963	14915.868	6992.4423	2547.86085	1178.03219	1691.68963	25663.7425	477.033919	1876.98017	28176.8336	5935.24786
C-28	3344.6871	4971.73843	99291.8382	162145.912	224684.894	12139.8396	10083.332	9523.34964	11328.9482	8566.5781	1555.88269	2185.1562	30070.9318	12360.512	3901.54798	1648.86859	1652.01105	26413.5397	1165.83989	4224.42147	38895.784	11162.7346
C-29	2317.01517	3754.09844	83202.2986	146608.752	188520.525	7382.21215	9928.06605	7006.08929	9009.98354	4028.28394	1143.22851	2195.04226	22776.2469	11457.0453	2968.9482	1598.70588	1695.18478	21671.0582	843.162635	3368.01682	34954.1938	7505.97266
C-30	14.58907	16.9736323	1041.85625	2432.53017	1847.93189	107.632061	71.5358455	35.6389966	30.2364796	32.5024569	13.4795467	11.5960097	143.802367	38.4415316	38.9286956	16.4397228	11.4762867	63.8759669	27.13697	66.2446424	410.524979	93.08954
C-31	2426.61443	2692.8255	67665.1403	153262.586	116295.197	8099.00297	7059.74001	7242.18341	4523.09191	2690.41145	481.438457	790.586864	7844.73653	3970.84217	2684.45806	1082.00567	1501.5052	22377.514	1007.59685	3740.6135	38134.0267	13805.0362
C-32	2331.85397	1627.52445	64023.9993	148059.451	80716.2227	11754.9054	8144.44436	8387.57156	12692.9014	8252.05665	594.981707	925.281698	28534.6056	7715.31335	4290.68892	1884.2826	1954.97158	31778.6472	596.815371	2490.97689	37179.8394	11708.0569
C-33	1968.3983	1724.73087	57195.8305	73175.6636	111390.283	3645.98148	5811.1008	4420.917	10847.8985	8794.66901	619.549898	1152.13801	25436.698	8965.32524	4063.45783	894.153918	1097.14887	15303.6038	656.705873	2021.70447	18158.153	2871.15729
C-34	3407.45824	3000.90611	104724.016	171690.851	141291.362	8141.38628	7441.88819	9271.77742	11790.5372	6221.05854	1068.20951	1459.33027	23067.3336	10193.3597	3700.2638	1237.88583	1779.76236	28448.2411	1302.20344	3924.02527	42048.9235	8680.15262
C-35	24.7231683	14.5457865	250.930906	480.306362	345.464815	46.86764	43.0780111	14.2973592	9.57643562	19.2765482	9.89403793	15.9474154	48.4051144	16.876686	17.6914926	11.2875503	15.6100952	42.8678042	17.8614298	12.4545831	188.505487	47.5134049
C-36	2631.58199	3403.872	89545.6189	139979.571	122680.997	7233.15911	8622.83511	11038.2006	14062.3786	9422.87483	441.947464	1179.2456	29610.0957	8899.79085	3215.04511	1302.97445	1697.36801	25888.1512	1158.004	5358.03015	34363.6663	9125.86994
C-37	3217.23817	4680.375	99421.7031	158091.796	185922.557	9773.47514	9278.97213	10797.3364	16204.8362	10318.1924	1267.27684	1657.01489	32759.7094	12251.2951	3832.81891	2488.67344	2112.89397	33401.6152	1190.95493	2849.56129	36813.7268	11665.8713
C-38	2853.2916	1069.91719	84153.7768	225726.893	146793.709	10978.2383	7474.48256	6610.45647	10955.9223	5033.95696	625.687654	898.600371	20843.9571	8842.69329	6752.5964	1078.70631	1734.81435	23256.1596	876.774611	4205.52294	55320.6108	9114.43963
C-39	3238.93968	2856.87958	89698.5389	189271.263	148265.325	13243.5648	8006.52894	10602.8929	10581.9267	6065.34764	738.834545	888.915839	18830.6994	10208.0152	4078.56767	1652.7128	2493.39637	34349.2544	1046.079	3078.73051	45400.525	13866.4063
C-40	1372.64491	1939.34493	49579.1273	87125.0993	55564.2923	4202.17485	5366.56229	9306.67299	14460.9705	8336.51756	413.310309	997.189239	28028.7816	7913.41116	4663.08919	1387.13599	1757.1192	23583.0395	418.277222	1518.66378	21397.2005	7412.61098

Table 8.68: Raw peak area data matrix for ceramide for serum samples taken from breast cancer free controls.

Samples	modCer703.	modCer731.	modCer766.	modCer769.	modCer798.	modCer875.	modCer883.	modCer886.	modCer910.	modCer921.
C-1	859.602259	450.24493	548.475822	4805.89052	1209.48006	381.971487	1159.73811	795.484614	589.253614	314.21476
C-10	1577.01823	420.408507	794.659854	4264.2172	1464.66224	866.528111	1158.10083	995.215453	775.400943	223.889461
C-11	1487.24359	560.612819	1147.59167	3356.52992	1387.49795	726.525178	1154.84015	1051.39404	711.742817	289.178839
C-12	387.077723	292.386711	335.032452	3082.07969	405.242456	91.1462676	345.873742	151.8861	303.89254	188.118596
C-13	896.963014	597.133204	470.795346	4077.86421	1119.64735	707.723338	989.69021	404.622327	658.197433	173.903442
C-14	535.769066	186.593168	243.744232	2157.529	638.908793	195.412461	235.611528	51.9071381	72.1619565	28.1926114
C-15	1393.77288	679.932047	850.116236	6117.58436	1458.68069	962.761812	1416.48814	1242.10946	852.201917	349.334601
C-16	629.656961	615.516491	728.806625	6572.68783	570.20893	204.311184	676.122502	783.759758	588.295064	234.516678
C-17	1418.51484	753.982836	568.238558	6210.45902	1579.5643	681.611495	1750.3175	934.558049	838.042352	568.203596
C-18	1101.36875	487.818429	659.244822	6016.42681	1266.38427	641.522813	1137.76824	1144.27428	815.425322	370.878504
C-19	1536.99348	290.467426	805.963606	5225.45814	1723.5951	1030.61136	1192.13402	965.85483	710.812616	158.802551
C-2	996.243938	438.978894	606.610389	4531.07963	901.534056	235.150875	1174.89922	784.129464	682.090541	144.13721
C-20	766.587628	628.82557	444.767591	6277.25519	860.162253	485.021227	742.176129	422.622866	609.516169	264.537935
C-3	1330.30206	716.544165	715.702273	5592.14349	1586.38527	579.399132	1262.87855	1353.55436	869.793894	175.189078
C-4	937.153998	427.987866	558.383273	5048.28791	1169.30591	347.380191	763.997043	372.428146	427.218086	114.33384
C-5	1792.60167	486.338659	810.904472	4914.70886	1505.42826	836.985131	1590.38416	1077.03069	1094.47054	332.236789
C-6	1315.79208	604.907186	838.930161	5787.3144	1711.52549	835.846985	977.030213	995.425134	989.231338	177.764967
C-7	1036.36147	609.880124	663.16858	7820.45128	1185.09413	536.116706	1213.01846	1333.17111	602.030392	301.919208
C-8	951.863897	454.404915	601.319136	4317.67226	1399.72877	570.317483	827.67978	541.623937	672.050604	307.952067
C-9	1590.72548	418.233786	636.131939	4301.22509	1147.1287	503.819561	970.604188	672.636041	626.585045	227.362267
C-21	1620.21688	635.239325	803.588528	5414.10345	1339.43405	820.249524	1323.26828	1098.11224	922.912397	195.645804
C-22	1133.04123	547.60787	825.951456	4621.29451	1391.77349	696.531434	1275.61203	1135.81507	766.45094	373.629023
C-23	1165.18198	419.354561	980.075285	5029.64678	1571.02021	783.66534	1181.66018	1017.91528	848.254205	306.114268
C-24	1613.01433	550.223562	936.775421	5033.52156	1328.54334	1121.72519	1609.26582	746.710735	898.055474	198.060094
C-25	796.352217	316.991154	308.842639	5117.8433	684.294615	268.803158	1271.72541	264.705015	448.678587	289.191566
C-26	992.329421	397.285257	536.318614	5477.27483	1025.12232	562.502592	987.209193	542.980508	699.563276	183.721871
C-27	971.041086	438.563631	550.288358	5287.61664	990.072016	467.563558	1193.38629	462.693397	464.814492	261.599154
C-28	1846.78007	888.405394	1311.31327	9960.90611	2234.71137	1457.82659	2285.15396	1209.35851	1497.529	583.29058
C-29	978.934009	603.124495	999.382183	4997.5573	1878.18208	1176.49942	1749.24924	1058.00173	1411.2191	102.425424
C-30	28.3715892	18.554041	56.3828951	13.8171698	38.5249199	12.2542242	11.4610033	11.061051	15.6304009	8.52091976
C-31	1914.40438	356.597955	566.309492	2706.99728	1529.29989	788.86144	1010.30114	580.03871	817.771549	97.9229892
C-32	1187.16574	655.298303	747.492372	8578.4273	1384.90817	941.448678	855.512047	418.454882	759.799316	304.603821
C-33	731.198591	647.096107	784.957119	8492.62763	1390.52011	387.166739	1531.53613	482.895988	1017.87481	409.096471
C-34	1452.98297	540.028304	1066.88584	6790.43268	1545.46695	924.998908	1481.44636	831.434855	1449.17485	211.500018
C-35	14.3507594	10.4771379	10.8762687	20.5575458	15.4006871	13.2203432	28.4891264	26.7298013	16.6316461	7.46441258
C-36	897.450942	752.95333	1163.38381	9531.32201	1767.66332	672.352178	1365.64097	1243.28314	1158.51852	263.838442
C-37	1876.66896	747.434395	1457.29941	10950.4146	1764.38282	1403.18549	1800.37632	1794.2479	1256.36599	369.978211
C-38	1316.77177	370.724055	678.833422	5628.83597	1567.05085	1044.3314	1382.01316	491.088985	738.793281	247.148147
C-39	2043.54547	597.008642	867.962891	6398.50199	1647.66353	1249.1904	1525.98362	687.194001	1122.31172	367.909579
C-40	924.049662	630.288114	642.337151	8765.39722	948.202921	335.02782	753.081217	555.086754	600.900571	249.136536

Table 8.69: Raw peak area data matrix for ceramide for serum samples taken from patients with breast cancer.

Samples	Cer(d18:1/16	Cer(d18:1/17	Cer(d18:1/22	Cer(d18:1/24	Cer(d18:1/24	Cer(d18:1/25	Cer(d18:1/32	Cer(d18:1/32	Cer(d18:1/38	Cer(d18:1/39	Cer(d18:1/39	Cer(d18:1/39	Cer(d18:1/40	Cer(d18:1/40	Cer(d18:1/41	Cer(d18:1/42	Cer(d18:1/44	Cer(d18:1/44	modCer576.	modCer614.	modCer632.	modCer651.
P-1	1544.67103	1331.87981	46230.861	87566.3553	115722.132	5471.58425	5004.96468	7091.37862	6241.10344	4009.40394	534.542817	996.680002	16211.8002	7528.29058	2630.32075	609.897255	1048.03037	14608.6152	858.914303	3487.14271	21467.5126	6846.34245
P-10	2636.13585	3231.61953	76964.5269	136082.772	147363.258	7988.95542	6968.70844	9228.30919	9791.32117	6499.45758	739.921104	1501.24008	20960.7976	9188.26966	2439.38876	669.630316	1472.18099	21026.5985	904.916226	3080.18255	33372.6274	11578.5099
P-11	2381.87988	2152.26791	68058.7846	155795.08	134941.687	8345.90402	7933.97117	6418.45835	11301.8639	6028.02769	878.788346	1390.57444	21393.965	10986.6998	4647.38663	1177.88391	1713.83224	26058.4653	798.920283	2401.43822	38164.5213	13974.0096
P-12	1705.26103	2767.08429	67563.6979	111554.062	215501.589	7619.95347	8302.86755	8856.49956	13327.2793	5976.12813	1115.75449	1911.66111	30021.1025	16627.6241	3112.90215	1646.11676	1685.75983	27308.5279	932.631607	2765.41229	26408.438	8751.71461
P-13	1925.34232	1602.67766	57550.0355	126527.013	96292.6837	5312.00433	4829.6682	4864.7934	4532.28679	2612.79413	473.906587	716.457727	10315.9751	4065.0799	3228.1994	634.200837	900.512747	11021.1247	559.064829	4083.61479	31226.2445	6800.43861
P-14	1841.1385	1661.68825	63532.9078	136942.438	154916.509	5819.56979	5900.1491	4337.75595	4260.10477	1979.34538	429.848862	878.699271	10553.8133	4835.05448	1605.98343	896.46091	876.731555	16923.2239	698.706454	2444.8017	33672.0782	5572.92938
P-15	2472.38548	2257.69211	103917.575	204938.374	247480.803	9927.86492	7433.98305	5563.09316	8251.10894	3930.74532	1154.15443	1688.28731	26589.9367	9359.365	2813.55773	962.829326	1621.17666	26306.3298	1276.21288	4093.64857	49887.815	14337.0713
P-16	1624.49235	1381.9224	41672.2315	74358.4661	77058.4201	4810.56458	5091.32747	6148.93472	7223.68871	5493.01542	588.887473	917.621215	17045.7492	5983.61121	2745.33307	901.089595	1336.20042	17997.8062	512.014102	2081.4823	18291.4705	6208.63915
P-17	3434.35804	2683.47524	94614.837	165433.599	147432.055	10658.071	6405.8684	7219.64326	7852.17069	4756.56034	694.259698	1203.33351	12911.7057	6975.74814	3196.8252	1021.49122	1674.63673	22971.1869	1445.45361	5278.94091	39133.1236	8796.37119
P-18	1834.85836	1506.01353	55644.3961	114530.246	117321.53	6794.96886	5202.28299	7641.65676	8094.54014	5521.3043	498.024079	1101.31112	20499.1696	8951.45475	3485.06302	1039.29463	1243.6292	15261.7293	640.244517	3290.71358	26628.8428	6016.17061
P-19	631.264127	415.194574	22250.5586	44638.8816	40402.2852	2596.34854	5679.50866	4161.63311	6316.77748	3574.17591	375.015334	757.618322	10076.1112	4610.60903	2703.30753	815.289955	1175.57134	18874.3962	187.02736	1813.5146	10645.9415	7341.0443
P-2	2276.18177	2377.00198	90723.9778	146889.318	159080.159	7125.31322	6286.20149	8500.26283	8590.07798	4825.70543	660.073628	1236.37478	16640.6541	7443.23168	2413.04833	1141.14128	1549.14156	19874.8903	1292.80049	5673.19264	35463.6204	8770.11457
P-20	1656.71557	1827.86457	48574.691	76593.0906	70431.9777	2935.58685	4672.14382	7156.78439	10113.3898	5903.71556	695.074335	1006.74341	18149.7357	6857.12872	3930.0014	986.852042	1092.43508	16140.0247	589.612097	1638.56056	18551.7461	7384.17974
P-3	1007.51726	1196.78227	40933.453	71067.5362	108293.769	3908.08863	4272.82248	6581.63435	7908.95306	4444.44852	591.045937	981.252403	15580.2758	9234.13149	1560.27131	1462.76841	1528.6303	21362.1444	868.342435	2368.04898	16784.2158	7335.04087
P-4	1701.05286	2200.86065	51669.8001	84459.4645	118092.843	5535.03694	5408.95517	6668.59762	7576.41824	5173.00234	583.449367	960.892071	17096.6507	7678.01481	2973.93213	933.043069	906.517415	13875.2584	592.584706	2051.89968	20047.3654	6834.06049
P-5	1391.16933	2062.37949	49436.3029	106258.653	133407.326	6054.50547	6274.58011	8986.64919	9590.08544	5663.95077	607.537339	1260.52145	20904.5636	10479.7282	1675.60575	1213.57868	1645.97652	22604.4189	860.862126	3522.7114	25551.7404	8058.80084
P-6	29.7917065	17.9687628	890.442027	2658.68333	1603.25306	110.020886	25.5482036	70.1680628	48.9306877	36.2348231	23.9577435	19.3393343	81.5896119	48.6468424	40.0892147	18.8347697	9.87146994	54.6615416	21.7181551	117.477453	516.292995	60.9732786
P-7	2578.53145	2127.45603	80904.724	141456.621	133757.297	8803.751	7029.68749	6683.11397	8301.06347	5257.70368	592.433865	904.517305	17227.0909	7746.625	2834.72763	1258.34853	1400.35216	21918.7138	1042.84959	4601.57072	33638.5977	6676.94128
P-8	2397.55005	4127.54953	78388.7211	146956.239	214987.096	9813.86352	9364.14431	9724.18366	11881.5409	6929.29256	1289.06003	1515.11529	24808.5827	15388.6658	2479.24371	1806.02311	2118.17966	31361.5343	837.731332	3018.7366	34883.8984	13371.969
P-9	112.189533	20.1213804	1079.17005	2398.55252	2159.96516	243.460639	82.013107	51.484281	74.6591867	21.7238023	11.5350067	14.8720664	223.401886	73.5887553	72.6631161	17.8913997	9.75821796	92.227425	48.9836229	30.0907206	505.927037	129.242649
P-21	2174.3382	1617.07761	58468.992	133467.269	138401.612	8429.73763	8467.48568	5211.64672	9095.3548	5554.40783	541.377979	728.830496	19488.8463	8924.04822	3017.33688	1660.24576	2177.2813	30427.2514	337.2363	1610.49136	30874.2877	5457.47977
P-22	1469.46191	795.250529	37938.9004	112167.03	88934.0099	7317.06443	7805.08176	3882.50655	5973.03101	3395.90413	355.889611	368.459338	13061.6951	6721.79124	2826.71701	1268.69092	1737.56344	23218.7912	180.001986	1383.73762	26183.6179	4425.84474
P-23	2034.4275	1582.23758	43634.4576	114368.939	116988.08	7170.01103	7250.35844	5305.4116	6450.20419	5059.88827	465.478824	654.313369	13916.5989	9204.50512	4212.13937	1713.90911	1904.66828	25621.9773	419.78178	2188.06937	27250.0848	5807.77201
P-25	2183.36596	2702.35117	70331.2997	109700.605	139907.778	6399.39969	7243.1164	8962.47367	9492.74234	6238.39857	765.38205	942.964169	19287.3772	9732.73182	4436.65049	1565.42176	1859.80009	25734.9073	825.60675	2300.54046	25500.0515	9621.04806
P-26	2469.47191	2529.79042	88391.998	135698.44	167385.694	6147.44017	8245.87661	9096.58459	13365.5941	8983.07176	1037.34535	1771.55651	32311.0314	13453.5434	3157.71528	1338.51656	1460.56444	21993.5253	599.176377	3169.35233	33358.2402	9228.21315
P-27	1871.50332	1585.9126	77719.3705	130890.397	124279.118	6474.92393	7059.35625	7034.01787	9638.0861	4794.06357	503.722836	876.623705	17145.5176	7686.90023	4217.20055	1385.73363	1712.55521	22641.8871	775.885769	2272.39003	31171.1513	8306.33087
P-28	2135.92514	1958.43705	58408.9049	120623.171	103511.597	7226.57599	6106.53697	6018.89775	6516.35139	4975.97089	528.457559	566.873115	15200.6152	5814.75601	3133.32713	1020.44952	1479.15932	23074.708	623.406079	2951.96756	28968.8213	10159.8429
P-29	1833.35748	1439.0289	55422.8286	90669.3727	152114.745	6324.93808	9265.28892	6556.84959	9970.40473	5800.58854	908.102622	1953.20031	20880.8802	11980.2455	3673.63224	1127.88646	1669.59817	25917.815	680.461743	2774.37914	21525.7406	9343.0872
P-30	2637.68394	2230.36391	67458.3748	154903.945	160985.22	9773.01634	8052.94719	5857.99463	10305.0625	5481.08557	621.23405	835.86486	18467.0863	11063.5168	5166.79673	2139.42723	2205.24243	29394.5751	681.567651	2060.95416	37532.5347	6866.85183
P-31	1819.24115	2631.41878	64406.3005	112245.613	126032.465	6064.73747	6346.78403	9391.05	10022.3149	5735.19558	549.589989	1043.2305	19652.4152	9605.9525	2470.04313	1126.91169	1805.77018	27031.066	941.438825	4068.84868	26099.0296	8329.56412
P-32	1117.2299	1117.04426	31511.7246	69297.5209	77475.942	4707.69743	5106.42236	5338.10296	7123.21065	4833.57994	424.949413	652.863867	17167.0694	7377.42282	2001.79854	1095.0234	1732.21028	23796.4311	283.710008	1202.41898	16757.263	8137.62171
P-33	1575.35307	1129.49435	50300.6267	112012.742	80555.6865	5958.24672	7550.26395	5204.02589	9622.33655	5378.01039	283.018617	628.457138	19328.8681	5888.56037	4019.02337	858.505308	1988.15504	25793.1187	223.803958	1409.02721	28457.3526	5146.76997
P-35	1697.15837	649.901495	40182.2543	113485.387	91190.3433	7872.03415	6539.01342	4866.74208	6574.37142	4451.27236	328.947176	631.058707	19632.5005	7001.20464	1428.03961	1074.3029	1607.67245	21597.1131	343.800433	1628.83157	28248.8766	3550.06468
P-36	7371.8755	921.489185	36213.6055	91009.2941	53879.2339	8890.98805	5179.83664	5408.0876	8331.17792	6594.90126	474.634439	729.868292	19725.7699	6204.83615	3860.41481	1392.60012	1805.19566	27689.425	322.145376	1393.18418	21164.907	4210.92711
P-37	33.886819	15.683554	650.672798	1969.30957	941.392765	169.821024	57.7553614	46.1638911	116.159684	55.8908973	18.9692085	25.1190454	178.308381	44.9576572	22.4547533	9.155348	9.21104385	98.3645265	28.4488657	135.539252	482.732447	102.963741
P-38	3400.45139	3575.94024	127798.378	271346.374	248919.514	11205.7077	9554.30608	6840.68451	9509.45	5255.3399	977.530151	1764.94784	27664.0299	9261.07201	3482.31309	1467.71801	1952.4554	25263.51	1396.26775	6626.04667	64370.6363	10793.8034
P-39	2518.00016	2479.54992	63324.2323	128055.309	111589.643	7323.35471	8189.23355	6359.03248	11889.0303	7080.65454	875.552072	738.702845	22074.6356	9662.272	3623.28375	2070.11315	2464.97962	33903.1789	453.555425	1626.36782	30365.883	8744.26273
P-40	2756.02907	2111.78915	81439.5335	167280.225	145023.819	13781.5775	6764.15254	6541.57657	6828.83641	3934.30674	445.00039	559.194912	14465.5307	7010.54243	2420.96051	744.776815	1436.34051	23677.806	956.760288	3670.77432	42118.0358	9569.84264
P-41	2983.13326	2790.23703	84579.4251	146217.664	138098.661	8114.21492	8393.95413	9195.60381	10298.3009	7586.23912	662.090657	1020.37699	23276.3313	9031.75216	4775.61914	1343.30673	1846.08782	25390.876	903.591051	3171.69808	36665.5439	9060.51228

Table 8.70: Raw peak area data matrix for ceramide for serum samples taken from patients with breast cancer.

Samples	modCer703.	modCer731.	modCer766.	modCer769.	modCer798.	modCer875.	modCer883.	modCer886.	modCer910.	modCer921.
P-1	1172.66639	547.580027	549.06369	4093.53693	1112.18158	327.418798	1089.28397	622.611019	614.715347	320.219322
P-10	1996.49399	535.520238	937.892883	6181.59062	1540.24653	938.083746	1309.60064	1197.49743	1132.78631	324.787133
P-11	1853.28482	646.648518	935.808613	6153.62366	1595.20386	1268.48464	1164.11311	547.520573	632.362917	306.625056
P-12	1400.83837	831.317781	751.396975	6642.20146	1827.57554	1022.79222	1565.94353	789.29973	1448.5477	494.025113
P-13	901.580802	405.099669	508.03737	2691.10836	953.558175	442.684098	979.977449	721.100539	498.870129	149.292946
P-14	1157.7632	274.49101	701.444265	2118.78264	1344.80375	645.935809	1380.14831	942.863747	979.980945	115.857654
P-15	3014.23153	503.666028	1223.23313	3779.57439	2186.37288	1863.98666	1620.70799	812.132181	1129.17489	245.414091
P-16	901.88651	323.999467	428.113917	5508.28774	681.903677	282.02715	1029.06058	322.91974	368.704227	229.441876
P-17	2100.92276	533.461435	825.156067	5092.059	971.957405	420.038952	1725.39841	688.797618	1042.83156	208.150284
P-18	850.079316	456.595919	792.031446	5734.12973	1432.46407	312.482693	1110.35808	797.42312	635.605407	277.469997
P-19	1129.21321	619.115178	713.175853	3917.61	546.709527	665.991261	760.596065	370.586469	835.466359	209.063534
P-2	1500.41496	616.296403	817.612316	4993.33092	1388.58092	739.538849	1509.72936	1364.26734	1323.55754	289.75858
P-20	1328.93423	521.618469	697.661397	5980.43412	1271.31087	345.286202	740.584788	672.21333	729.530155	254.627065
P-3	1154.51733	328.034601	379.011615	4437.32223	1143.07143	445.901106	783.03675	649.333006	636.015529	218.108323
P-4	1093.47895	396.988323	742.980206	5396.14294	1144.88836	457.763028	997.336319	680.278421	632.148887	247.887078
P-5	952.564588	440.266309	455.310656	5854.8778	1149.96034	469.689059	1291.30399	989.090203	680.705563	290.841698
P-6	25.3278748	14.4935976	20.284507	34.0394358	11.1404335	12.0732723	15.6038783	15.3480237		7.60553546
P-7	1098.97403	455.615583	842.931943	5129.16265	1344.28109	619.225293	1599.01855	1094.72805	1185.91852	270.297874
P-8	1647.98907	585.122092	947.54515	7184.82128	2058.6019	1212.83878	1473.59578	1430.18595	1204.47912	382.234439
P-9	35.334447	12.1076959	10.1534605	94.7636746	19.8475571	15.7037689	27.586002	13.6410654	38.4397469	15.439196
P-21	726.683255	321.673223	350.906567	6071.89672	913.773906	621.804475	1110.11828	714.81277	421.436898	354.189993
P-22	562.693057	377.160611	234.284291	3551.00871	632.11381	415.417866	1025.00684	490.585466	277.589582	139.700855
P-23	736.535162	416.181536	364.183388	4419.44978	839.221319	455.795153	1040.9817	788.101138	431.405574	361.310807
P-25	1413.23112	887.982923	804.693151	6513.92004	1697.80602	779.500849	1439.86179	1025.67235	929.924844	261.678999
P-26	1384.00819	864.390831	1249.49147	9480.07915	1869.99948	796.17368	1765.14575	1430.2238	1240.27027	319.814051
P-27	1127.04312	561.476449	816.984506	5208.68259	1155.36018	671.507768	1367.41406	616.148601	1055.91281	225.338086
P-28	1160.4253	295.007629	346.740497	5124.02793	1198.32594	604.606955	1067.58668	262.623508	650.943218	346.826877
P-29	1181.18865	591.938215	1141.81701	5676.52485	1590.69379	1131.90614	1621.10591	1008.20064	2031.10712	201.004173
P-30	1029.05847	340.362572	458.515353	6633.98798	1045.17374	747.241349	1378.38197	552.999413	781.967893	374.465446
P-31	1419.31454	556.648107	595.362407	5786.4939	1181.45028	527.205497	1184.42452	544.916501	883.925861	290.137364
P-32	1062.12643	383.330691	320.487808	4729.41881	802.890371	585.641351	628.986882	328.862817	509.203951	249.044955
P-33	769.065522	431.418403	340.803649	5082.9104	968.43919	372.878429	850.313015	263.792055	387.65633	168.443732
P-35	547.35284	365.310558	299.735772	4518.0543	517.800551	448.03198	1047.57647	342.951447	343.332927	264.336585
P-36	559.238765	420.573793	325.365887	6930.46074	803.879303	321.27137	624.937667	266.429134	262.516383	238.235014
P-37	9.71315141	9.10854208	29.7244078	36.7101313	16.194859	12.7508802	28.3048002	10.706657	12.0491142	7.40847835
P-38	1102.12167	507.710473	1260.92588	4960.14581	2468.23993	1131.00388	1940.30957	1371.34896	1329.70459	276.708681
P-39	1215.37095	410.245293	641.478656	7229.12799	1195.86318	718.780611	1356.62916	456.361625	753.066173	293.829996
P-40	1532.90503	444.807104	668.076016	3876.17186	1026.76113	651.713306	962.697715	809.588218	704.210221	223.936859
P-41	1197.1967	616.327032	815.789686	7645.31706	1284.67237	678.15723	1464.43395	807.198367	1078.10764	488.504188

Table 8.71: Raw peak area data matrix for phosphatidic acid and lyso-phosphatidic acid for serum samples taken from breast cancer free controls.

Samples	LPA 12:0	LPA 14:0	LPA 16:0	LPA 17:0 (IS)	LPA 18:0	LPA 18:1	LPA 18:2	LPA 18:3	LPA 20:0	LPA 20:1	LPA 20:2	LPA 20:4	LPA 22:0	LPA 22:1	LPA 22:2	LPA 22:5	LPA 22:6	PA 17:0/17:0	PA 32:0	PA 32:1	PA 34:1	PA 36:0
C-1	76.6606404	4467.58774	382246.754	18033.4987	156960.846	66972.3343	87833.1283	186.045539	16458.2766	897.170876	1502.9341	47194.497	3473.96605	2302.83469	5157.45847	6290.89714	14733.9941	119.697368	19.0219539	24.5521781	367.537266	174.407158
C-10	33.0686007	7766.38414	718206.157	15298.2348	253810.737	221155.204	403678.068	3737.3552	28010.0017	2361.96925	6665.24199	245969.538	4985.08516	5404.55126	15049.1944	31311.7092	76181.7069	128.83482	57.9565137	43.586593	332.428322	142.805733
C-11	41.78517	2553.92796	367742.798	17683.5981	108517.748	70023.3412	94554.1085	57.7267979	18350.378	985.611787	3153.78209	73466.9524	2782.55105	2237.17127	7090.47718	3442.04373	14565.2715	147.143061	76.0388649	13.976652	384.712988	134.529244
C-12	50.7530796	970.810081	102225.386	4194.42057	51102.1689	11302.3727	11244.9442	94.6157831	2829.98381	282.925265	597.243908	9750.23456	575.433283	271.170609	399.821229	1234.21872	2057.07485	98.1684514	60.5632072	70.3384118	227.23662	30.4806887
C-13	16.6389999	6731.61853	919086.612	5643.16579	385378.915	358172.029	506683.223	1613.95243	15519.3711	3565.51251	17111.3089	294772.788	2310.39552	2977.28571	7198.12003	13859.8114	56328.0272	262.0553	15.025679	15.3858081	361.35155	94.4040342
C-14	12.7944607	1527.90846	121695.477	1138.00244	75450.1431	18940.8493	14710.5732	185.602666	4833.8778	558.676895	7125.80581	8151.10996	660.24698	398.93818	383.159687	1221.20109	4430.44395	102.079123	31.8885825	17.4536955	131.384981	87.8275633
C-15	16.5924044	7005.27323	685411.604	20976.5494	191725.434	224240.575	245114.186	178.717796	29722.1096	1930.10872	5522.37391	235975.954	4842.33299	6558.66401	11452.8047	18977.4794	22818.3585	216.147474	14.0195754	29.611759	288.192375	138.436703
C-16	16.5037428	2020.55288	309184.638	14832.2564	138271.73	57138.3491	93275.0857	30.8489629	13715.0499	871.202148	1257.72004	34042.3087	2836.45843	1824.07661	5041.73257	4045.43139	3183.64455	17.3616251	67.0814383	22.3047757	185.301205	47.1405533
C-17	13.5290285	5731.65933	639223.194	18926.9868	210254.722	129275.606	151652.158	156.490106	22731.6207	947.479766	2340.94969	107966.429	4219.94427	4298.99765	7423.61215	17267.8152	18578.9823	141.944648	18.1304784	43.577183	464.940444	137.79227
C-18	15.8442474	5503.50946	524861.958	16506.2204	218773.86	142192.407	223728.383	283.424148	22662.0486	1957.15111	3926.46302	78284.9418	4324.21612	3400.72535	12102.3979	7691.73475	14313.8687	110.327053	32.3129285	78.6971528	451.766656	43.0921499
C-19	60.6664358	3499.1371	559128.972	16191.0942	215843.373	161341.431	263180.141	491.152332	23557.955	2094.9283	4411.48537	149264.873	5127.6068	5023.51615	12877.2274	10204.5321	42449.8584	204.803945	54.2771235	35.2390525	216.896492	110.83903
C-2	12.7366294	3540.65936	418225.632	13446.5232	155191.729	120598.711	87480.9809	124.456128	14681.8867	976.582505	2450.5888	92648.2877	2849.2128	2525.25239	4241.62889	10428.4088	7905.27965	52.9810659	59.3369858	20.9319347	242.041915	43.0568085
C-20	27.3989558	1948.61181	290691.92	12028.817	154680.985	36627.2139	59009.2638	198.757902	12320.8753	470.788836	1672.31906	27870.2938	2923.4885	875.244592	2632.7965	4427.46863	10073.7099	70.3989639	15.704657	39.6626523	257.134132	48.7199759
C-3	48.3606922	4320.30662	433003.729	19642.2193	199599.62	108231.207	196114.726	238.390358	21716.4199	1295.81765	2838.84506	83992.163	5163.52285	3102.90973	10330.6843	8943.92918	17168.2902	100.258401	40.1223936	16.6072961	302.642812	70.8728176
C-4	25.9841847	7764.88609	634504.184	14113.3321	283530.247	213095.136	381889.793	263.333474	25298.155	2022.52104	7177.21696	131496.867	5089.05324	3783.86341	14025.8381	13429.3124	25318.3122	161.607276	36.515163	45.9862868	177.851206	146.141182
C-5	12.3482187	5724.42786	702729.14	7627.50825	289547.129	247011.791	402013.584	146.996096	19818.2253	2204.68767	10543.2688	189242.459	3395.01833	3550.22026	10067.2756	24779.3947	44785.1037	157.13558	12.7558276	19.774109	432.294763	57.6881884
C-6	37.2400303	2152.56991	446108.814	13691.2624	167403.1	139736.68	194706.001	487.748479	21218.7248	1223.32722	3112.16767	123184.202	3771.82687	4047.59917	10440.9351	12943.7397	36106.036	80.1863879	11.4291577	50.5440397	351.984982	118.357266
C-7	23.8420659	2116.04473	464946.558	14825.7855	194087.481	91987.2388	164449.214	306.525157	19611.1616	1253.25022	3072.24609	67121.2103	4227.32657	2975.41564	9676.67908	7644.20118	11090.695	24.8571258	44.4530358	64.2779751	404.303328	96.8833417
C-8	76.5799105	6938.49157	467089.865	21988.7905	144578.938	121240.085	180163.365	180.242633	25393.3154	1265.17904	2993.20546	74821.5053	4612.9647	4354.45433	11928.748	9439.31563	21091.0811	100.24119	32.501988	10.5144747	181.728489	16.8480203
C-9	21.7589587	2331.52388	286208.155	9684.31602	145405.024	88437.243	115445.083	268.157896	13842.4624	1314.18601	2485.10039	65924.7478	2994.26692	2143.71819	7005.51387	5968.5351	11730.1426	229.353938	71.9501555	25.9623083	236.684647	171.157673
C-21	10.5482073	2419.04009	306093.462	14476.1242	131872.027	122661.849	176599.725	439.290214	18848.1247	1203.93162	3412.44183	98612.9225	3861.50567	4668.57111	9786.03105	8184.06407	17044.9084	126.770243	40.0896914	51.8644773	419.797745	100.867454
C-22	9.86749837	5256.9398	526603.131	20048.613	226321.257	237583.881	189232.435	4533.59658	25867.6865	1546.32141	3811.27524	145839.495	6967.97801	9420.94286	11246.3971	16662.8567	38493.1265	58.5031826	78.1154567	21.4429988	257.531086	172.546041
C-23	15.7615674	4473.27025	481058.234	14479.0346	172654.486	146074.733	224576.557	314.041842	19196.6456	1549.85761	4478.16513	88119.0215	4150.89197	4333.40362	12638.2992	13774.2405	19641.0245	69.923306	14.4700272	29.0691021	282.135064	67.7325982
C-24	34.9294043	12948.3474	1580792.14	12155.6635	538983.145	494447.565	915480.393	20818.5974	20586.7946	4070.24373	21015.9572	338684.847	5276.38045	4441.79171	14682.1777	32870.3742	93142.7757	110.026052	56.3587418	39.1368175	425.118325	143.266947
C-25	7.20234869	8633.08336	1493067.4	4844.53126	513423.161	375187.458	498484.026	6256.08074	9310.72601	3094.7987	12049.1302	258172.512	2120.29103	1583.56193	3724.58452	23048.3022	64998.6552	83.5858719	69.6990767	37.9900381	128.213561	25.8085322
C-26	53.2122205	6680.47081	1128819.02	6842.48418	407723.446	441123.068	587178.929	1011.63061	17650.7131	3670.07816	15374.6367	250280.065	2977.00834	3686.43061	9323.51146	23781.6861	109727.941	112.681851	73.3607967	45.3042959	326.293088	77.7562447
C-27	24.9179319	6379.04246	936879.679	5815.28617	458496.326	365340.114	517151.395	1298.18996	10850.4888	3029.83403	12920.4802	284074.246	2995.50135	2353.80716	5669.56897	25296.4781	58530.5059	294.686164	34.4734363	50.1824751	287.932143	81.40596
C-28	9.98725048	4437.62047	558707.684	21543.6491	248619.302	190898.378	324605.367	250.357474	27507.3446	2720.78278	3364.16677	136733.825	6969.31176	6388.76282	18491.0737	21624.8317	38462.2233	84.3759023	18.6103716	15.5791472	200.090448	150.76273
C-29	9.11141248	8139.55725	946523.947	35634.9851	317691.82	229149.884	374971.039	238.383531	34829.5764	2500.22778	4779.29455	210263.679	10165.4368	7148.61799	16951.5397	29766.5943	27308.7402	152.60125	56.3162003	55.53551	643.442308	49.1725003
C-30	13.4352828	6507.32883	620950.687	4343.73778	289258.735	248246.588	309327.105	1908.12753	15966.2858	1681.47386	13614.7381	164293.114	2606.93659	2637.37499	5661.94064	23063.9424	47283.355	134.148046	24.0064849	46.8844813	209.394877	107.080755
C-31	11.0159021	2178.45033	231142.093	4218.41331	143098.252	126168.663	145441.443	332.561227	11803.9133	1427.3059	4756.10255	97049.4643	2416.87079	2113.66489	5438.54876	5163.86212	27279.1297	189.042013	37.7258027	93.8256933	234.823062	157.226616
C-32	73.7394558	5168.47812	472695.809	6748.57202	254574.824	221644.268	279600.751	605.214243	17952.749	2079.3077	11099.0042	117975.519	2728.57888	2257.7464	5817.89336	14710.8361	34889.2525	118.99579	23.9870555	93.0340979	160.805194	171.048953
C-33	39.9706455	2519.80735	260584.114	16855.6712	92793.2944	38892.7067	51822.5469	41.7464126	11446.7181	811.143943	834.562362	41643.2505	2572.96172	1610.47528	2822.85294	3551.63869	3206.31818	71.3264939	38.7724001	39.5609066	410.374596	80.4567873
C-34	54.3704193	7743.4783	618866.982	23083.7504	247023.737	230544.459	251987.005	4459.8169	28389.3376	1742.8295	6202.86226	205794.609	7156.04225	7539.90109	12693.0679	18662.7209	22901.5935	65.5769468	12.0331702	43.6716992	318.23526	135.440782
C-35	12.33206	116.752332	1701.18459	81.1174451	27482.3457	5912.55418	5005.51259	12.3429512	428.525608	238.109744	307.148438	1722.6629	65.6209672	64.2377851	13.8312106	27.9983226	201.608448			11.8469482	4.94213092	25.5191804
C-36	59.5542854	3227.76543	469341.551	25759.9217	217032.056	98774.8817	262357.207	234.660874	26766.8251	1483.03706	3426.74893	80834.6749	7621.9581	4413.54139	17943.2886	8569.06663	16358.5829	24.2984867	16.0282546	33.5955173	253.538095	93.9327966
C-37	14.4719626	5861.53621	747657.876	19777.8842	312794.237	227054.153	423766.527	351.442325	32192.0206	3055.90071	5072.02123	127794.584	7846.75529	6406.89795	20629.7865	23918.5155	65517.991	34.5307273	42.4360105	64.4357715	175.48934	75.244106
C-38	10.5585295	8643.6769	909488.384	15503.0422	302543.557	406548.539	475510.779	6645.92801	25118.2807	2039.89501	11730.0294	217998.853	4263.25083	6496.27127	14210.0952	20730.7148	41553.7349	50.472993	41.0423397	12.1269525	75.948236	39.5446432
C-39	26.4657346	2196.52671	312105.601	3660.93095	169100.679	168706.337	188324.41	208.831868	13632.5867	2180.66378	9148.0232	117708.14	2285.25926	2387.99893	4951.53918	9546.36496	33108.4242	205.145513	16.4010048	92.9424192	287.335397	87.7488945
C-40	12.3604923	2562.33276	264835.014	9817.60895	125143.747	63967.7142	68004.9129	135.50092	13307.9468	596.432365	2510.62573	28118.702	2891.33701	1979.56414	4505.10812	4554.54893	5351.96693	20.7850255	17.9188148	10.656197	90.4338272	42.6959774

Table 8.72: Raw peak area data matrix for phosphatidic acid and lyso-phosphatidic acid for serum samples taken from breast cancer free controls.

Samples	PA 36:1	PA 36:2	PA 38:4	PA 38:5	PA-1	PA-2	PA-3	PA-4	PA-5	PA-6	PA-7	PA-8	PA-9	PA(24:0)	PA(24:0)	PA(26:1)	PA(26:2)	PA(26:3)	PA(27:4)	PA(27:5)	PA(27:6)
C-1	12.8651055	34.6873123	49.5145318	18.7590119		33.2674694	13.5052879	18.32669	13.9948136	21.4662891		59.5377853	17.4677642	10.1872543	34.3941564	17.586006	19.2414369	15.986609	42.6764681	52.1707723	8.17969922
C-10	17.7945674	45.5348614	158.270971	17.7198985	22.584806		12.0815439			35.3931212	22.266039	59.3817928	20.8824734	23.0157779	53.0322641	21.7153692		30.3972045	54.29088	16.9664288	
C-11	40.2754231	66.0616118	28.4002557	43.2638655	18.2259587		13.6640706	17.1061471		20.9950246	22.7362568	4.47836419	27.6682803		24.4804824		15.7471058	34.4658447	16.1657209	28.8276289	
C-12	25.8353705	49.4492555	78.4503767	72.3599105	45.6833363	22.9870695	50.9041447	52.8968726	29.08978	24.3406358	43.4306021	51.1022257	39.5174722	32.016788	19.7456993	17.8158031	32.2201941	40.8556926	54.9069921	33.937956	41.4773525
C-13	27.4212715	27.7181708	42.0688295	165.249209	21.0043251	15.5790018	18.2740745			18.4978717		20.6073257	15.7749118		173.146364	33.205828	18.7113497	11.5632282	11.6079658	37.5874528	29.7900244
C-14	11.1902854	44.6252877	142.495682	90.8245649		30.4234028	9.74168373	27.5471507	54.7918527	9.79559169	19.024946	17.1000259	16.0739883	17.3324073	198.982329	17.7165326		15.7257956	13.2742001		
C-15	28.1588564	22.2435096	113.435797	18.7614413	11.0370779	15.2184906	23.1038306		13.7985595	18.7704912		91.989378			92.2472122	13.8148302		24.3778763	13.5487669	14.5577195	19.2892289
C-16	21.8562489	26.611852	47.2042842	13.7026163	9.98482581		21.1739292		14.5131176		12.8391684	31.24885	30.0289974		87.0715791			18.738497			
C-17	40.2748481	34.7250598	106.119838	30.2604433	13.4637395			33.9949206		16.0016745	22.8629275	63.7677946	24.7356869		24.6663882	12.7707134		11.3830475	53.3941631	13.9875293	31.773328
C-18	21.4241191	8.03526968	104.047926	9.14569158		9.91469576	17.0768704	17.9661384		17.8799065	21.7964084	94.6980031	14.8571225	24.6359432	65.8841763	11.7970353	36.2260507	41.6814372	19.550343	19.4378988	25.2401606
C-19	23.9963327	53.3833959	203.307958	27.7287076	15.7393852		17.7545924				13.4794575	71.545661		58.6494855	131.863219	32.5557105		12.3950233	15.3446624		15.5296443
C-2	33.8461689	54.4162999	53.2007868	71.8172713			42.3233257	48.0058853	15.2159541	21.2476197		30.8763058		21.8211768	84.5613862	16.5699279	20.3587746	10.5636751	44.5313525		32.0248107
C-20	20.6896736	38.3136006	46.1750254	13.3713942	25.9722422	24.9649648	34.1211219		12.8379511	20.0732674		86.913314	25.0361664	34.2950127	46.3414531		29.6331876	13.2562389	14.1452667	17.0314072	
C-3	18.8645729	13.00938	42.2764429	25.0366434		34.1316576	28.549193	14.2469448	29.9667262	29.6590708	13.3055331	45.1943471		13.2776338	75.929079	27.2819078	48.1338861	26.1541155	13.6804686		36.2403666
C-4	33.1040117	52.4273363	115.692919	19.7631166		18.7398552	16.8855547	16.7790562	22.035218	19.2005503		26.6164573	49.647735	29.6158537	121.112505		29.4415193	29.3121696	32.8521411	16.5568939	37.1547816
C-5	10.5639058	16.3578077	270.686146	55.8223071	30.5667637	10.7730834	21.062633	14.8697726	16.7017276	36.1541294	19.1989407	47.9942629		43.6080151	188.471519	23.293259	17.5660871		17.0702231		
C-6	12.6610184	29.093482	165.704414	17.0721764		30.110328	20.428014	31.9583512	15.6803955	22.0619818		94.1704541	47.9609068	20.3805344	78.1541808	35.5223488	32.797237	8.90687929	57.9832518	10.2976426	8.60774898
C-7	26.650994	26.9870734	156.745289	39.3202379	14.3363058		14.5779514		10.729902	27.5721254	13.5522324	65.2671219	16.5322973		21.0210105	9.56306599		25.0137165	74.6867713	23.4578849	42.881132
C-8	8.78196944	4.79490859	186.957416	35.0537486	17.1565816	24.2156241	17.141978		14.5071963	9.77606727	21.3211252	50.1830867		14.4063114	120.876604	26.8337937	19.6806558		99.7026052		26.4887278
C-9	20.5367702	42.9049083	497.259017	14.2114584			62.4628456	12.0410248	26.6336245	19.4003143	37.6307268	137.094249	33.1978069	23.2661559	56.7183518	13.8921512	22.7367167		15.0289037		11.5744269
C-21	24.8112992	14.9182086	25.8219597	62.5847843		22.4874128	8.48324661		15.7914746	16.7246477	9.60036838	79.41669	23.3113514	27.2960854	69.8124614	23.1511329	10.2766496	26.4413968		27.8407964	17.4834565
C-22	43.6340701	12.8796472	64.4363485	83.5865264		16.2242376		12.6957572	15.2358896	44.9631128	15.4217564	137.777102			77.3515673		14.3241035		25.7135234		27.6121121
C-23	14.8687608	9.40220487	31.283484	5.65962664		25.4782194	35.2629255		12.0514169	21.4573239	20.1808277	57.0322902			74.7847027	20.6535566			9.01586547	36.6858929	35.1656486
C-24	60.9243304	17.8071815	69.7336209	7.75882048					11.7425889	23.6344332	17.512573	19.59798	58.0991235		161.027057		20.6866595	16.6601831	50.7762561		23.707435
C-25	16.4343602	23.4076975	44.8172718	15.3182741	20.54393		23.4807977		12.5693724	26.067159	35.7954106	16.0241506	31.7615008	34.7297132	238.499075	27.9266886	70.7404805		17.396623	14.9909638	
C-26	19.7591728	33.5434957	55.5966309	18.5158261		22.1807668	36.7326663		10.1144972	78.5904456		127.355125	25.751194	15.4337673	130.757557			42.983037	121.240255	39.0088433	
C-27	14.0585097	42.1418007	23.2697605	58.5657487	14.8965565	18.6422764	29.405755	19.2914782	10.0934686	12.5312818	34.9285358	41.7933813	16.4409252	23.9024689	78.1404501		15.2806295	19.4386146	32.5393063	23.5777253	31.8711489
C-28	57.7693687	29.0993938	63.5475243	16.7626247		28.5126536	12.7672549	23.3355417	16.3891911	21.9540058		154.546698		15.6120359	142.526308	19.6285325		31.5855888	51.6436215	19.1469343	24.5371114
C-29	40.6362507	24.714793	120.327038	19.3645656			8.99943107	20.0545546	17.4866116	20.9307001		123.841441	10.3197348		34.3947389	19.2955346		10.8932094	12.216569	16.1114498	
C-30	14.7638496	48.9280103	60.3519106	58.6336079	11.958371	11.6728473	11.4714488	19.412899	17.519639	31.7558288		9.38022182	10.3410073	11.9154087	201.369926	26.0473933	8.82869881	39.9639972	32.6849968	28.3321928	40.663082
C-31	16.909467	42.2948702	229.468887	44.7842933	33.7373728		19.4773628	26.4727097		17.5320282		92.4818208		22.7557595	173.170852	42.1434959			37.0624249		33.6452161
C-32	26.1702307	11.3245418	87.7291909	24.8910267	11.9049217		30.5471488			10.969211		51.9838288		12.1160406	109.406272	25.446316	23.1000033	15.3016188	20.8616425	29.2706493	
C-33	22.1311496	50.1895211	97.5858296	30.0574416	13.289611		37.0845897			34.102004	20.3136349	12.3264767	29.3756158	10.2915349	19.7370385	21.0597605	18.0263245		24.0164226	40.0621049	
C-34	29.0818004	6.21277786	110.480142	69.2104036		20.6269465		35.2485515	15.2010485		32.6556047	25.4733111		24.435829	24.249907	38.5455842		12.7883492	29.0315924		
C-35		2.64441683	27.0473576	9.82446571	17.8041145	22.7733797	18.0388486	13.8564843	20.8096285	11.2932168	15.6434439	33.9292864		76.6188787	20.6067663	13.2808778		28.9085212	23.2495213	16.7856977	19.6972663
C-36	70.7085223	25.7975859	45.187838	13.6149165	25.7258096	28.4047365	59.3572501		129.734983	13.956869	23.8210628	84.2020248		14.8890178	50.3497163		21.5099991		42.1554428	23.2050313	29.6009879
C-37	10.3460919	18.7359713	19.1285677	76.0289501	16.3725066		15.0964795			21.5632321		33.2504434		13.9205137	43.5608341		13.0669142		23.0306809	22.507011	25.182312
C-38	33.4747373	16.7526907	40.1492264	16.5836744	14.9637319	43.100993	20.4873934	9.653953	15.7370573	8.74923219		27.5394568		44.8188391	128.34961	39.0829245		12.2201311	18.9062382		25.8129348
C-39	41.494278	9.56473303	95.3628958	20.5544317	27.4556024		70.2835023		11.9131907	22.0037645	16.5499058	172.013206	12.0925995	13.7457455	61.8952474	59.1171312	15.117611		21.7603719	20.2123875	21.3085201
C-40	24.257986	17.9840154	12.5790644	24.486231	30.7325639		32.1973586	26.3568579		23.8957821	8.32848446	27.9145582	13.6653195		114.342189	13.0001764	30.7721715		23.1114936	27.4045606	16.8154666

Table 8.73: Raw peak area data matrix for phosphatidic acid and lyso-phosphatidic acid for serum samples taken from patients with breast cancer.

Samples	LPA 12:0	LPA 14:0	LPA 16:0	LPA 17:0(IS)	LPA 18:0	LPA 18:1	LPA 18:2	LPA 18:3	LPA 20:0	LPA 20:1	LPA 20:2	LPA 20:4	LPA 22:0	LPA 22:1	LPA 22:2	LPA 22:5	LPA 22:6	PA 17:0/17:0	PA 32:0	PA 32:1	PA 34:1	PA 36:0
P-1	23.0867781	3971.87726	460693.697	17615.0396	143205.946	130234.192	108558.016	145.497039	18397.3727	1295.90837	2674.58553	81293.9164	3260.10565	4020.60324	6215.74489	13760.3622	10108.09	53.2508154	15.4873529	70.6923657	436.677692	27.9992221
P-10	44.6440958	1126.18512	550870.267	13922.3941	235046.949	179527.538	276009.449	158.405067	22171.5756	1784.36631	3901.3768	126372.162	4772.58958	4720.56624	11050.9128	22253.5835	94006.8561	219.507328	81.9601392	31.5221635	404.224217	134.154013
P-11	84.4758065	5124.75467	664501.865	5004.56797	264011.259	274075.078	493594.891	1406.70826	16572.9424	2568.54035	15949.5565	152874.317	2756.65483	2920.77428	8939.93317	11588.3589	87153.2877	142.281183	60.2639264	44.3496835	238.974167	159.254351
P-12	13.1770415	3532.65004	556227.172	20458.4889	224986.976	135351.213	196737.225	268.382243	22124.5941	2158.79782	3735.22414	142276.452	5302.47449	4005.56379	9421.02418	9779.17758	36941.5451	235.317985	50.6570546	69.4360946	298.527365	173.070404
P-13	143.989229	3861.58623	487899.702	17676.6007	216896.654	149030.846	201379.558	562.762217	22093.781	1845.97384	4314.56301	115688.032	5027.75122	4565.02946	11538.0877	11715.189	18708.5495	252.629556	24.9235992	29.8660766	296.584198	135.951557
P-14	27.6912521	9785.71682	1106505.01	25703.6489	265408.701	302604.526	378013.097	284.911041	37050.4617	2504.93324	5304.79968	399347.121	5990.13094	8315.92412	14104.8295	15261.1259	48263.6815	245.372455	25.6413857	222.699304	616.297158	131.605516
P-15	22.1210039	2277.18673	551881.987	7067.39657	194039.756	221203.574	308911.784	148.437927	17486.5707	2505.84251	11192.6958	262343.737	2709.71282	3566.13205	8623.90734	9373.26764	55337.1182	88.9694271	11.531997	124.827663	339.356315	223.087714
P-16	7.39319484	5121.19678	535010.582	16579.9235	242642.59	176413.01	258251.638	152.861186	17915.0934	1569.94548	3758.51113	110634.03	3502.46939	2718.57154	8663.76468	12355.0686	9964.59281	31.6175555	35.327227	33.6809661	349.191517	192.297616
P-17	10.1240274	3463.7454	386250.864	15684.6374	182100.22	144651.199	246586.067	397.673312	19991.3688	1212.84025	3620.79065	100503.775	4218.51674	4236.28804	14005.5881	8948.49192	32979.3445	132.367613	32.7054461	36.6085369	439.150832	11.4057603
P-18	11.5752707	3679.49667	523993.053	15432.7015	165485.421	126351.953	142949.363	169.630305	18074.2989	2067.33661	2721.54281	87368.7829	2810.80233	3193.1677	6981.9586	9350.80989	10466.33	63.2807645	27.1775336	16.530753	157.830868	152.385675
P-19	28.6885113	7207.23411	734402.099	8875.29194	263964.533	207211.069	267199.705	415.66446	16527.691	1843.91256	16842.2514	141784.173	3972.35067	2396.5427	6355.54917	15310.1342	31684.8194	29.4603832	22.2413027	70.547888	245.600935	115.113727
P-2	29.1894251	3340.04523	454554.896	20793.6698	201583.208	107262.034	205439.625	1066.01047	24243.5256	1375.1035	3260.00242	77777.5545	5424.16361	3484.61083	12048.5361	9025.60226	27124.4735	53.4062625	28.4922194	18.8174424	597.510805	21.5950421
P-20	9.49194247	3615.29027	346351.035	10721.9293	159049.525	95600.9918	128153.104	125.550521	15473.4578	1217.20561	1992.47888	56034.7274	3534.44157	2372.57807	5419.39681	6711.47958	8838.32049	70.2555941	83.0405863	22.418968	170.494681	21.7664984
P-3	12.0033888	3241.02208	409294.916	15126.431	155943.469	145948.041	182427.196	181.969388	18766.1352	1762.39298	2480.1963	80985.5441	3590.49985	3811.84047	9405.77324	8566.4987	22619.6822	66.7079063	15.6122302	80.2443107	345.1296	143.681144
P-4	53.2522739	3617.13344	499638.211	14043.493	196921.224	100321.403	156236.179	118.190181	18704.4574	1319.6119	2180.95519	92837.0474	3904.50445	2613.64267	7160.90646	9817.62792	29915.5818	55.6367773	14.2818412	21.9938685	176.683007	64.2147948
P-5	17.8805992	2242.32366	476307.433	17412.8768	141666.145	109649.85	199004.199	169.888027	20689.9555	1657.70182	3455.13307	58380.8656	3283.09739	3854.13481	10912.2917	10548.4211	11668.9898	289.829555	41.0105958	24.791723	119.541289	37.2179952
P-6	11.3708274	4483.94533	781841.595	20185.3398	295087.437	180448.48	317691.496	155.670658	24939.5791	2907.44563	3761.92745	171025.821	5866.79168	3898.46972	12707.8246	16230.2336	60618.4024	445.973295	23.412324	23.3443993	274.262129	101.338927
P-7	13.9973107	6715.75091	655494.373	20697.7853	241418.256	168663.047	276380.183	3072.18652	26996.805	1777.43378	4756.57353	164852.862	5209.73268	4083.36861	12283.0189	12116.681	23077.5581	96.2365516	41.5680358	41.1403806	428.532931	78.0172765
P-8	39.4339085	5223.8643	769581.677	19531.5225	272272.519	240477.843	574918.963	112.174102	30699.1909	3352.06293	6226.32519	175295.936	6011.22897	6793.89627	23871.3359	24725.5173	54557.6083	53.5446732	20.4346611	33.7891094	317.689017	30.8718638
P-9	32.2212541	6466.08646	772368.883	6000.49194	273801.473	337399.05	390073.859	1513.19338	21555.8627	3402.44751	11313.8112	122789.813	3170.00903	4767.50985	10164.4902	8351.97729	41887.3777	100.442484	34.6611937	47.8609596	372.335233	120.628105
P-21	25.0395107	12366.7842	2000155.75	9796.60609	715665.735	712132.999	1136710.43	17110.8558	20855.708	7490.18214	19652.3708	438331.203	3363.34392	4108.0136	10334.4538	43319.3304	149152.89	43.2521937	84.5338546	40.0624185	175.12272	111.088933
P-22	8.49629366	15884.6326	2171533.13	8649.76698	620513.246	671903.912	941478.403	18207.277	14102.4832	5598.83291	23415.8047	229078.152	3098.96025	2046.08103	6911.06899	29252.9637	96280.8846	86.8692146	64.3231089	83.3618652	251.22464	22.8496438
P-23	14.9900895	6812.05807	1260540.17	5790.214	501636.573	421921.701	512355.295	2084.23596	18799.6869	4641.04457	13935.1607	304203.117	2910.05013	2380.45753	5670.31396	33882.7881	110983.703	190.544211	37.2053816	159.187466	271.464606	126.119655
P-25	72.7018731	5078.50485	471907.649	17957.165	208037.425	143003.313	210273.245	170.682817	21993.9842	1360.68869	3275.18234	101179.924	4967.39912	3875.33966	11447.8486	10451.612	19636.9429	36.2105844	22.9124154	22.396283	202.900987	94.4700572
P-26	25.9839138	5151.78143	740470.662	22940.7337	263160.152	153619.016	375142.908	3396.57492	26230.5146	1834.10875	3275.05997	149207.151	5439.11337	4100.11002	13629.3895	11686.9003	29013.6553	203.635703	22.7501568	21.5400284	151.470195	44.4435473
P-27	235.748294	7066.27576	924193.126	17291.423	331385.683	274470.681	330743.602	240.832677	26754.1079	1619.28993	6856.98396	240588.239	6352.02804	5781.47694	13302.7981	19982.5402	40708.4301	45.5349322	66.9624397	33.7772899	351.781439	68.0076054
P-28	44.2485765	4186.37159	489081.092	6096.07687	210064.167	183019.722	269483.393	800.172284	13342.9302	1842.59387	7339.7542	152592.046	2271.26472	2299.35552	6851.87363	13931.1912	53539.4854	55.8238032	30.7339162	51.2482086	371.247863	57.5462833
P-29	47.2367413	5370.71041	753173.344	26125.7362	232559.185	235015.909	324139.933	75.2565894	29286.5615	2597.25848	4086.83803	166414.934	6245.34425	6144.1679	14784.9611	20424.8792	23252.9975	27.6816426	33.9114172	11.0529951	210.741389	99.8585852
P-30	20.1991323	16765.6456	1781987.03	12126.3802	750585.819	756204.179	1024124.94	1208.65572	26852.3214	4169.22507	16005.1438	543023.733	6337.78245	7272.2852	13722.9394	59168.3884	166719.911	84.1656262	22.7398065	24.4978583	300.565274	201.166296
P-31	22.2993171	2125.88553	321062.833	12609.351	129857.09	104259.64	145884.665	196.8383	14416.1626	1412.57104	2000.44028	108940.337	2300.35399	3078.27958	7639.14581	7889.70502	23741.0069	100.98267	62.9186768	24.5490244	291.430627	28.5308159
P-32	15.6753353	2668.00639	572613.079	4835.33256	217192.421	167785.581	216565.227	134.948487	11692.4223	2329.49662	9419.75513	121587.608	1863.71598	2257.61247	3533.99525	12498.3971	43751.7822	26.8382573	45.6679987	21.4592029	344.890297	36.3807163
P-33	32.359971	7530.50095	1126493.77	7508.52214	504503.934	389185.63	591749.451	4326.96894	9308.9743	2969.37543	10871.7845	281390.232	1964.61484	1076.69576	5171.18852	19384.775	60001.6326	21.3793079	35.218934	104.854298	247.601806	123.591529
P-35	8.73033553	13741.6103	1842941.85	15507.4359	414293.631	490006.511	427808.535	8866.0218	14892.8192	2747.78372	11282.7748	257007.586	1709.48476	2178.73118	3844.22572	36096.5134	112624.241	34.9643477	27.595528	53.3506591	86.3975371	69.0256956
P-36	11.7564259	8830.26891	812224.946	4957.36972	318672.117	248265.604	284072.502	823.400112	6808.31624	2688.31673	10930.0228	181933	1098.68326	1140.4	1994.98355	20623.4171	87573.0609	124.988836	45.0041103	27.6017267	262.423032	107.970744
P-37	21.1411848	13565.7352	1940397.64	10389.4021	757043.296	607454.73	1130852.4	6881.64568	20411.8695	7134.71148	19222.7655	264448.416	3863.38567	3924.2544	11652.2755	41884.7615	51275.2466	31.5666606	24.8636512	74.280743	343.489727	133.074803
P-38	34.492568	5525.54736	778879.69	27687.7312	298082.945	346032.078	507495.723	3137.52738	35295.3786	3233.58764	5916.81218	291411.394	8363.16161	11517.0828	21689.3481	14505.2658	21739.713	189.952362	96.048269	22.7143363	423.837639	70.9758123
P-39	12.5497218	6280.2578	1297784.64	5623.79363	542893.171	534773.609	711547.751	4521.28634	23922.2617	4607.32297	18584.7614	467687.377	3338.60403	4077.93109	8514.80214	46056.9343	176647.189	155.246492	26.9958498	17.7494757	294.498492	40.3299254
P-40	64.9982422	3312.52783	545590.793	8183.80058	269508.26	280896.645	269383.334	643.335068	16527.1357	2679.40993	7666.04557	154678.176	3742.02436	4613.7278	7702.88535	15767.2844	50984.4917	63.5600237	25.5534771	11.4622902	213.785226	50.7787124
P-41	20.2663905	6327.02347	586518.488	19037.968	293868.732	220301.224	304922.861	567.752537	24894.4155	1860.96769	4406.68772	150138.508	6469.86012	6132.2961	15888.5915	13589.1658	32817.5866	136.999919	13.1566303	39.8505184	218.919626	34.3126655

Table 8.74: Raw peak area data matrix for phosphatidic acid and lyso-phosphatidic acid for serum samples taken from patients with breast cancer.

Samples	PA□6:1□	PA□6:2□	PA□8:4□	PA□8:5□	PA-1□	PA-2□	PA-3□	PA-4□	PA-5□	PA-6□	PA-7□	PA-8□	PA-9□	PA(24:0)□	PA(24:0)□	PA(26:1)□	PA(26:2)□	PA(26:3)□	PA(27:4)□	PA(27:5)□	PA(27:6)□
P-1	35.9367281	16.2274003	120.365357	28.579055			10.5084713	19.7734198		47.2850925		50.3657966		28.2349944	23.0349279	20.7126389			46.9633364		
P-10	74.8472352	60.404089	171.943106	32.2224647		10.0846575	38.4090229	46.798472		22.7903917	67.6037532	38.8400605	20.9883448	25.5294927	15.6454477	25.3217679	22.3939651		39.4601761	35.8841455	
P-11	17.1281432	17.4895848	235.781679	90.7413704	30.8482952	19.0137677	20.5570392	36.6427572	17.8048112	10.8792681	20.0070605	97.8088774	7.38739643	24.5149811	330.724898	24.0635017		10.813045	52.9334504		17.1310072
P-12	32.7996407	26.5674149	241.426269	85.9542221	18.6680798	32.1549565	13.1746635		18.3709548	24.0244538	16.8062183	130.181912	10.3339237		32.037765					27.7041704	
P-13	23.8838293	7.19107502	196.371839	24.5435359	32.7299879	28.5255506	17.9668106	21.2627879	21.6403107	31.6876156	15.4884283	45.238972	21.0600746	24.7624526	168.326662	30.4037412	32.151926		22.6774703		
P-14	57.0765737	65.8856417	150.061533	101.531645	18.5686443		30.2203158	22.3164239	9.67856544	33.7234602		70.9873052	16.2529891		99.4454741	29.7131499		20.9513662	17.691545	23.943195	
P-15	15.4090192	50.5489721	340.074935	65.8292556		11.2896591	30.2375286	26.9454519		40.5877461	37.6605242	115.616034	18.0133868		157.888439				37.8809011	23.4923819	
P-16	21.9158923	11.5127373	70.9050035	35.9181913			18.1248968		19.6715076		31.8872544	54.7759225		25.3617929	113.034896				14.3800988	34.8668772	
P-17	17.9387946	37.8949432	13.6506776	43.3026189	37.1988196		15.2333672	10.5458426	36.2943699			29.8645659			132.677996	16.0004317		9.14698828	111.013457	9.32515171	
P-18	36.723376	20.9150223	58.8893606	25.4780177	17.1672705		15.77684	19.0962985	25.6181509	33.7361668	34.548002	83.4841577			53.2994308		15.0363551	30.5323556	17.3407342	22.3411719	
P-19	28.50959	16.7239321	90.2222844	153.451013	15.0997248		11.6394368	18.632549	28.9567352	25.1670399		28.457266		34.0226184	198.977584	27.7802841	15.3371806	27.5646543	18.442109		32.8171168
P-2	14.9569617	25.3615232	78.3612769	39.6532269		26.9048762	39.195434		28.333248	11.1958614		188.085046	31.7140994		51.2310669	10.1098035	16.1640644	18.7896376	58.8304729		
P-20	15.9737423	32.0874748	76.2449626	11.2562159	34.1113058	21.6468552		46.4138996	16.9381771	43.1470568		18.715874		12.6173761	16.4639157	56.2162117		13.0784931	37.748347	26.571081	
P-3	41.0518846	30.2847606	111.086401	62.7682821	12.0423639	19.3933385	22.9660134	46.0195471	17.248345	22.5388991		161.388831		33.5584146	81.5692408	34.8185617		18.7659128	22.8698331	29.3092974	47.4203587
P-4	9.53080711	12.6233734	199.115145	10.9310338	23.8266837	37.6076356	17.2531352	17.5448122		12.4517139	35.6892372	75.5863522	9.11707098	25.7347018	17.3096643	15.232721	14.3293444	19.7331772	30.1764171	10.629246	
P-5	11.3367402	3.31560708	35.1206041	11.4139018		15.676807	15.682941	9.56620972			16.8836108	22.3421131	36.1049219		77.8028844		14.5746692	24.3191539	37.1026918	26.5269329	
P-6	18.8507612	13.5225806	175.754111	18.6490587			18.2843023	15.573574	9.99260107	62.0398795	16.8372299	7.63721732	22.9887335	15.0744706	32.5855636	10.5730905	15.7236245	18.7891368	11.8243594	23.3873489	17.0670085
P-7	29.3870655	17.6145338	122.93859	39.2528265	60.9198511	12.1694015	16.6976728			37.4883209	25.1794067	36.8811689		11.0058069	38.12815	19.5321949	20.4608428		28.8616705	11.764001	
P-8	14.9224057	64.281116	164.458585	15.5010695	29.6007403	34.913014	23.9025799	14.3054937	13.1111752			187.580338	38.2443674	21.3780111	162.811108			20.4143993	15.9607884		
P-9	18.7354702	38.4511466	185.09369	31.2773795	10.1985584	18.6628102	21.0665939	22.5993986		47.5585287		38.4681227	19.8915643	17.032991	169.010182	20.2028042	23.9271786	37.6838753	13.5633914		
P-21	17.8674958	5.56464138	169.318966	82.7126348			17.1816715	15.790073		35.4121623		48.2788802		39.635337	244.127534	14.146063	24.6113119	31.2156125	30.5048391	9.96676429	
P-22	52.843182	13.0184693	24.9910679	88.0306528		18.0211823	12.1128138			27.2544086	12.6294076	33.8739387	12.8648436		169.450353		12.3155949		41.5036794		25.2537722
P-23	38.0058222	13.0245179	80.784631	144.343265	17.7265067		50.2186268	35.342972	27.9606636	30.1996587		14.0306181	15.8999297		155.354714	41.6180148	19.3144892		26.9625475	13.5826586	
P-25	17.1656106	20.9981725	51.4117823	51.228502		19.300827	16.071496	27.6694633		9.76924366	17.1407381	55.8853724			54.7529263	12.2407114	15.9440278	20.6372138	49.2285453	21.1878267	
P-26	20.3030922	8.12456126	107.767688	30.130883	9.58605648	34.7529419	22.2574617	16.1432527	10.1402956	23.4765711		164.434804	28.2566124		18.2127597	19.4830245		29.948334	29.6247104		
P-27	35.460112	39.3427718	196.745418	14.9015601			28.7672893	17.4710665			11.3234488	18.9863038	12.8395247	20.9321171	20.8250368	24.0150843			55.149115	25.1196897	18.7305779
P-28	10.1450358	8.09830655	60.9687935	62.7404864	54.3568613	18.5018462	30.7875385	24.1509123	10.6464462	23.2018154		26.3973996		24.5329026	248.653732	28.3758275		32.9211484	17.7730724		
P-29	22.4262607	19.5383668	74.1882123	12.3842144	40.9423404	40.8695753	12.082651		26.5461287	33.0333791	56.4883923	52.5128042	41.7542317		48.746984	26.2316034			15.8214499	23.1770567	
P-30	15.1325791	40.4973724	139.248773	90.8358344	12.0029397		11.8604147	23.9599675	9.96955563	24.3388028		67.2961251		43.513294	160.752939		20.6276753	27.0793517	31.4032996	24.1014335	
P-31	54.1763833	22.9091389	84.0180847	20.8705811	13.379365		28.283269		39.3223185	14.309202	18.9284179	129.263458		26.609493	30.6680736		15.6294753	27.8053789	16.3656205	8.6643627	16.1814334
P-32	12.5231074	28.111773	146.173976	26.1708124			10.9863731		12.732602	19.5941142		69.544852	33.4491494	9.6987917	96.3042403	15.3057003			34.6988759		24.7554395
P-33	12.1218513	15.1479665	14.6961377	44.8320204	10.6616866	26.7255469	24.1370109	13.5253708		23.1216406	30.8744164	20.1473031	25.9151293		131.775199	12.5417571	22.1302243		13.9417554		
P-35	13.136325	15.7129418	32.4598274	15.5580644	26.4268632	15.4239587	13.2124958			16.6496924	23.1786879	13.7081609	11.2766656	19.1408484	127.656944			13.4713815	68.8363302	24.395054	
P-36	29.7401954	14.42602	27.7489668	81.2765379					23.786527	21.999127		11.803907	38.724623	28.8314409	224.761156	31.1899915	21.7719437		13.5937663		10.15279
P-37	14.509146	27.0993315	20.0302769	62.062673	12.883251		38.9997686	18.743254	25.7083301	26.6297658		21.6099302		18.3466068	130.907463	12.1045924	13.5584112	16.6302342	18.9291413	17.2536397	
P-38	17.5390458	28.0649018	132.287678	19.2465693	55.6725597	9.96071398	9.29036832	41.7689994	19.2119979			103.248082		34.5149297	225.412444		20.5312043	10.8069624	11.8661974	28.2539323	
P-39	20.2451057	71.3097824	163.5371	56.5712334	37.7807985	22.2291642	74.7220829		45.4411445	76.2142421	42.4446895	116.049771		27.2859093	143.420891	10.9536332	23.1654587	12.1160321	47.9067389	20.5048735	
P-40	26.7903737	37.4116709	56.3581212	48.8378322	70.5409238	12.131166		23.2242775	12.9166025	20.0740096	20.4064425	73.7414698	26.4816738		32.0459849				9.46075004	13.6160853	10.6259586
P-41	15.943974	56.9249281	31.5702038	35.5618129			43.4528576	16.009421	30.334109	42.0220359		76.1857828		23.7524459	29.4694412		26.242599		27.5750993	21.9261521	34.9248922

Table 8.75: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls.

Samples	LPC(14:0)	LPC(15:0)	LPC(16:0)	LPC(16:1)	LPC(17:0)	LPC(17:1)	LPC(17:2)	LPC(18:0)	LPC(18:1)	LPC(18:2)	LPC(18:3)	LPC(20:0)	LPC(20:1)	LPC(20:2)	LPC(20:3)	LPC(20:4)	LPC(20:5)	LPC(22:0)	LPC(22:1)	LPC(22:2)	LPC(22:3)	LPC(22:4)
C-1	44817	26231	3085911	52015	121327	9776	743	2158486	1251870	1887581	55337	34967	16646	49714	310150	808302	221893	2363		51276	132465	30937
C-10	40594	36314	3382751	75512	99580	13777	1107	1870996	2044686	3476914	89366	25216	21971	108501	706037	1914746	931137	2050		39677	102696	63449
C-11	15953	25934	2438083	39745	72054	6951	886	879568	971794	1748502	40012	24708	14256	59742	377730	920806	92732	1025	6693	34781	84393	23902
C-12	10970	18261	1642540	12988	53653	2979	735	913592	213349	309725	26211	21436	2836	9487	74616	186997	26610	1189	8162	29109	73889	7098
C-13	23563	26144	2229236	63625	61333	7800	855	1337588	1563282	2833606	68536	31776	17494	79633	633340	1539440	157935	2515	10306	51006	126504	48377
C-14	6516	4532	369767	3726	11125	1960	381	210433	70359	110628	14979	19326	611	2958	24064	45375	11358	182	7573	23683	59314	964
C-15	39001	34560	3464846	134899	128368	22511	896	1572129	2181923	2576710	88653	40477	19306	105192	809501	1966298	275488	2088	13253	65458	156030	90205
C-16	19975	25613	3048644	43731	109176	7740	822	1873936	863632	1846291	52394	29512	12850	34820	286035	631867	52227	2231	8460	41707	108189	30263
C-17	44779	32471	3959806	120372	142598	17567	977	2525787	1977074	2147937	74876	45745	18997	59413	425515	1400437	477168	2240	11066	63194	171686	64049
C-18	30605	27832	2959188	59032	114881	11687	916	1556328	1461832	2882875	68978	35257	16783	59502	372101	735512	71708	2183	6054	48667	123812	34637
C-19	15873	32173	2727265	63159	102492	11225	1062	1770944	1715089	2967819	67063	20876	21514	91826	750756	1663002	238226	2143	6882	39676	102905	53153
C-2	26408	27630	3090776	116341	97697	12716	865	1486948	1437309	1388307	46042	29045	13748	51344	447329	1103902	208729	1420	8399	48980	129098	34701
C-20	18769	32097	2708894	30898	131853	8225	763	1715128	571002	1162561	49876	28998	7881	27973	170051	397878	172067	2252	11197	40927	103892	14865
C-3	19241	27060	2595169	52281	77698	7826	738	1628168	1168705	2443700	65437	28379	14421	56230	362153	940204	171207	2110	6457	37540	92267	33396
C-4	38437	32465	2984198	76913	90231	13377	971	1815728	1574241	3061799	93593	33139	15928	97644	671140	985573	126795	2934	11214	55732	128926	46815
C-5	22624	33688	2745176	63250	125527	13664	994	1655455	1580657	2958162	67409	21585	17447	83096	591314	1292363	320032	1705	7139	32269	78709	41218
C-6	12491	29724	2489313	60931	106920	10724	1043	1347632	1324269	2415110	52925	27391	15079	51957	435168	1138828	159876	2061	5961	41025	99213	33492
C-7	19218	30132	3545803	49190	100714	8594	1119	2370690	1588292	3353406	62521	28523	24963	78214	419228	978591	142021	2755	5543	43318	112019	42575
C-8	61174	20617	2942361	118422	63013	11937	795	1345461	1681393	2521300	80170	37560	15380	73392	430490	1103132	250879	1636	6653	54341	141930	51999
C-9	8859	16566	1116501	19039	40829	6548	750	708616	638352	1170892	41318	22083	6021	29283	214710	510840	60486	900	4244	23174	59874	18930
C-21	11449	21509	1604053	41272	40556	7131	736	866611	1239146	1832351	54590	24766	10411	49655	394605	967024	144648	1003	8917	29897	67852	37197
C-22	34235	16016	2673662	192189	85833	18785	659	1953146	2950800	2511874	82213	45994	22977	97539	694482	1689517	357114	2402	11606	64813	162128	89172
C-23	32404	24693	2858924	77943	107032	13284	945	1474684	1563297	3016568	73723	19599	18760	97011	782665	962461	191690	1610		31797	72153	44212
C-24	32591	22203	2589271	120358	69939	15120	714	1596039	2078230	3953503	117579	25700	21030	164472	1430041	1450426	213031	1209		36289	81756	89629
C-25	37503	29841	3611643	140066	165149	21337	897	2222871	2095990	3337021	62789	29209	23617	117271	907129	1631077	585541	1393	11234	48662	133410	56736
C-26	21252	23275	2308166	87220	107952	15643	857	1368809	1856724	3123638	61129	26882	20792	107888	882527	1293417	250573	1015	9178	39204	99813	54231
C-27	20486	18497	2233364	88661	96141	16886	863	1581287	1781632	2898587	74643	23630	18522	104609	866230	1660689	177897	893	7691	37051	93582	94800
C-28	26104	32587	3704339	79339	200399	17643	1663	2639098	2495718	4535113	86769	29771	42000	74715	341347	1380387	977964	3878	7183	42893	103244	35899
C-29	50073	31346	4968907	146430	190668	18209	1283	3373068	2559081	4257831	106284	30720	39239	123419	826750	2277003	598652	3434	8039	43697	121662	85551
C-30	19669	18556	1584503	44552	65398	13653	830	928653	1182520	1900236	58318	29174	9878	68423	649337	924027	155141	828	7122	38663	94802	39982
C-31	8688	10755	841003	23944	29471	5189	840	465845	631264	1077736	31229	12579	6329	32074	265325	719980	89337	562	5578	13220	28696	17292
C-32	24222	29928	2453125	43727	79120	11033	825	1311943	1292117	2193102	58144	32780	13022	55119	341625	833612	221992	1534	14624	46984	104995	31185
C-33	45558	26971	4156641	102754	134990	15141	1135	2419694	1436208	2195757	60569	26389	25405	71956	523756	850455	186954	2142	5575	37311	85806	40442
C-34	52184	27043	3569916	135655	132014	23506	977	2344950	2582145	2743976	112891	35096	25601	140649	999805	2088654	390825	2533	11937	57409	138596	97395
C-35	51966	46297	4705744	118072	252451	23142	1290	3729914	2828728	5949109	117366	38783	35482	131815	741764	1563665	265524	3230	14571	63784	180258	79581
C-36	22774	38528	3265490	51992	127360	10704	1343	2533778	1559134	4210139	91295	28826	21016	83970	463899	999670	132659	3592	16904	43704	135872	37313
C-37	26508	39199	3351840	85056	170254	17255	1375	2169631	2055509	4061790	101872	32041	22796	87853	595579	1123960	522962	2668	18011	54904	136074	45231
C-38	33022	25165	3323709	216938	61501	17395	685	1584880	2445581	3415280	109745	35069	19101	128101	882921	1527158	430801	1383	21246	57372	143977	56098
C-39	4690	17663	802080	24974	34848	5153	867	450977	640981	1210611	24184	14998	7173	33219	257573	649832	55374	354	9042	14235	36992	22377
C-40	19589	23871	2260229	41550	79853	11366	970	1209913	994768	1256682	43014	35923	9989	50245	328363	457953	56498	1852	12920	54591	116407	30473

Table 8.76: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls.

Samples	LPC(22:5)	LPC(22:6)	LPC(21:0)	PC(22:0)	PC(22:1)	PC(22:2)	PC(23:0)	PC(23:1)	PC(23:2)	PC(24:0)	PC(24:1)	PC(24:2)	PC(25:1)	PC(25:2)	PC(26:0)	PC(27:0)	PC(27:1)	PC(27:2)	PC(27:3)	PC(28:3)	PC(28:4)	PC(28:5)
C-1	178097	628301	8541	920	1808	590	76	868	207	5050	650	1116	618	315	24632	1474	2752	2540	5480	2733	1624	18
C-10	425148	1375712	10794	810	3372	1888	198	916	198	2301	1512	1632	481	418	10662	2452	6975	6026	6413	3225	1788	172
C-11	81672	404516	5259	678	2659	811	235	533	150	819	284	420	401	114	2789	1218	2073	1321	6056	3432	2248	87
C-12	24937	72476	3917	1131	689	259	61	232	80	219	124	205	220	59	1864	1482	1671	1708	2429	1134	771	24
C-13	157883	475516	6034	473	3058	1136	325	587	221	875	1124	1295	569	469	3474	1824	6599	6578	2772	1098	818	28
C-14	5588	18095	2180	123	42	38	22	30	9	205	171	307	109	65	917	303	954	807	977	471	310	29
C-15	274796	639192	10357	873	3379	1100	299	787	298	540	1339	1376	797	569	5243	2725	12563	9986	9134	4435	2826	136
C-16	96533	182467	6194	1570	2954	812	110	858	220	885	294	508	351	153	4381	1782	4583	3094	3958	2191	1495	40
C-17	304551	843639	13504	927	2635	656	269	1173	259	785	602	958	514	203	6281	1527	7573	6225	7764	3561	2543	44
C-18	124408	383078	8007	895	2539	1098	123	1053	230	537	371	596	443	191	3795	2033	5451	5202	6673	3450	2456	41
C-19	221170	910335	9547	725	3928	1565	169	776	205	229	255	508	415	171	1985	1404	5465	5428	6869	3401	2401	17
C-2	162254	510613	9818	1073	2452	441	139	592	156	383	526	455	321	129	2311	1095	5302	3647	4621	2302	1723	31
C-20	103403	331044	7814	1091	1734	597	86	672	199	265	279	283	462	133	1734	1645	6373	4662	3454	2271	1718	18
C-3	154662	584083	7194	849	2745	1272	89	764	240	279	175	352	217	58	2579	1359	1685	1110	5328	2725	1854	24
C-4	154946	515132	8464	875	2738	1330	114	790	273	2500	1708	1548	771	706	16277	3300	7506	6701	6634	3285	2387	91
C-5	265263	977529	8287	1018	3095	990	128	757	158	481	1132	1182	620	543	3063	2076	11288	8731	3932	2384	1922	109
C-6	208231	782643	8608	599	3535	1280	106	740	143	172	295	520	424	152	1677	2507	5619	4709	6223	4127	2982	25
C-7	164201	563620	5980	945	3415	1297	131	1567	300	157	285	516	417	222	2608	2210	5480	4394	5993	3100	2132	32
C-8	200899	617344	10908	714	2238	562	88	1031	222	17573	2367	1972	595	358	52099	3532	3115	1999	6371	2209	1446	60
C-9	72125	199286	3513	396	1944	616	39	282	62	274	382	407	344	177	1388	1240	1727	1118	4016	2569	1674	45
C-21	149405	435011	5484	343	1606	702	196	477	141	440	747	736	228	132	2336	739	2151	1631	6547	3708	2175	58
C-22	336699	802361	12686	606	2210	544	235	923	254	411	735	760	447	140	2639	797	3403	2857	6750	2516	1886	173
C-23	233287	703765	7918	737	2247	878	151	672	164	343	449	479	405	238	2652	1494	7861	6101	6414	3761	2950	92
C-24	306455	831814	9183	442	1893	636	294	485	131	408	1327	1103	560	344	3673	1413	3590	2942	3681	1500	861	26
C-25	255847	875269	9402	809	2668	784	141	616	190	195	687	708	513	258	2704	1459	10135	8601	1334	695	522	27
C-26	242883	839515	9012	513	2683	1028	149	762	204	356	570	491	381	260	2416	1377	5012	3756	2465	1598	1198	68
C-27	308486	443750	5882	504	2490	784	106	578	175	169	392	441	363	157	1382	793	6684	6196	2155	963	804	48
C-28	393039	1537661	11183	1337	5592	1678	133	2939	291	423	914	1069	729	624	3193	1363	13085	9607	8727	5300	3675	85
C-29	440716	1394902	13184	1911	5497	1514	297	2575	395	519	776	846	487	302	4337	2040	8998	6987	6916	3267	2492	112
C-30	165452	439642	6042	308	1352	461	155	281	68	394	659	620	371	265	2793	917	6095	4906	2177	1286	995	40
C-31	90228	353347	3229	165	984	354	61	145	18	124	570	526	375	268	1573	578	3270	2464	6721	3587	2822	15
C-32	160858	646034	9979	810	2758	910	138	895	203	345	476	729	511	279	3293	1824	6901	6123	2250	1342	1246	15
C-33	148571	409772	8374	1977	3552	1201	94	1918	189	1704	1015	936	584	323	10548	2086	9699	7332	4432	2201	1495	23
C-34	317302	870778	10811	999	3708	1059	139	1016	171	420	840	935	534	307	5940	1302	10291	9400	8626	4523	3100	191
C-35	326312	966314	10785	1702	7389	2850	245	2238	432	1268	1860	1718	1062	800	9300	2523	17728	14192	1878	1044	716	18
C-36	156714	558655	9489	886	4041	1918	121	1209	284	298	397	684	438	315	2675	1656	7813	6449	6560	3476	2845	29
C-37	360817	1255708	18569	1285	5941	2017	90	1206	296	448	458	521	514	182	3818	2574	10052	7507	6391	4786	3629	78
C-38	232200	832422	17506	374	1853	463	182	737	180	158	398	554	370	161	2099	1058	6500	5147	3355	1366	889	12
C-39	95253	321361	4865	317	1599	535	47	303	85	88	617	705	353	274	1105	568	3197	2458	5341	3308	2191	24
C-40	85903	171053	6289	868	2011	618	67	748	103	210	303	552	371	193	1721	1615	6027	4533	4425	2622	1848	21

Table 8.77: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls.

Samples	PC(28:6)	PC(31:0)	PC(31:1)	PC(31:2)	PC(31:3)	PC(32:0)	PC(32:1)	PC(32:2)	PC(32:3)	PC(33:0)	PC(33:1)	PC(33:2)	PC(33:3)	PC(33:4)	PC(34:0)	PC(34:1)	PC(34:2)	PC(34:3)	PC(34:4)	PC(34:5)	PC(35:0)	PC(35:1)
C-1	32	3075	183496	148569	10958	659391	778642	326979	295194	74204	118418	71857	11610	2005	418627	5723751	6260168	570075	85014	23216	22481	283476
C-10	130	5690	211013	174844	16298	778078	1002086	479750	483146	82186	207151	89349	21921	4876	507910	6796645	7261246	748749	111513	43036	24000	280053
C-11	98	3915	171562	154058	9841	525654	754496	262691	240054	64092	167797	82502	19977	3360	433113	5751826	7148300	498175	61884	9565	33952	268916
C-12	86	5262	94730	59574	3404	534222	302551	68821	94720	67435	87970	30333	4855	1925	209769	2840026	3113582	321724	33774	4432	12063	160300
C-13	142	5168	200261	161745	13266	470488	882915	336486	374637	47935	201639	67928	8373	2216	350639	4917327	5987823	650436	77789	10026	23977	234253
C-14	39	1362	62977	37120	1080	110255	178429	15982	58076	14197	7147	7094	5656	2387	26340	412542	267888	162155	18856	682	8328	61295
C-15	179	5197	288197	248921	16363	659759	1525007	451058	399442	94888	195865	104573	28657	3236	612979	8189917	6890517	842916	133278	17343	33885	469954
C-16	172	6478	141006	111099	6971	668038	530720	205725	170758	78382	198186	102411	8505	1726	384275	5423089	8589308	560273	52477	5325	18526	250508
C-17	168	3194	204429	176388	14549	776352	1195148	403157	381817	101125	154177	77941	20327	3254	572802	7608801	6216693	709424	108499	28697	26037	336127
C-18	127	5296	215554	158696	12110	656010	774538	345166	277837	84844	238184	148727	16221	3843	468389	6538460	8903810	793844	86291	9893	27778	318110
C-19	30	4885	226231	196480	18467	518247	888736	406735	468539	66990	210481	119659	22487	4387	444675	6118255	7729233	819068	91283	12820	24096	286163
C-2	43	3891	177285	148267	11509	682024	1620225	388999	324949	89235	182671	87378	12089	2130	687088	8998696	6914873	812765	108435	20561	30293	346926
C-20	229	5408	192140	160660	8850	614104	537371	178414	219112	102119	126579	64962	10620	2898	271465	3821226	5294708	494548	53664	11984	25620	310113
C-3	184	3967	159434	137410	8583	510656	750044	280167	240859	53874	157055	80052	18353	3064	372342	5327511	7138812	609664	63674	11097	18354	212691
C-4	264	5726	212263	184246	11895	773758	1020984	294569	254752	85477	195313	85883	22834	3725	474994	6571147	8296090	663640	72869	10119	25857	302535
C-5	157	7213	311455	306292	23026	697045	1177803	491140	569181	96394	203000	143508	14609	4808	425833	6010065	6972766	779073	82922	15341	29079	382127
C-6	160	6506	229679	209111	14867	638077	884725	298486	331116	86283	229449	116641	22175	4650	447291	6070331	6972831	658489	58638	8358	29851	314959
C-7	90	5249	214676	175877	12954	617079	747059	361684	339443	58632	210341	115267	18664	2652	513276	7269009	9976935	704290	66604	8696	23693	294671
C-8	168	3780	140768	94501	6970	725600	1330390	359557	232988	65168	165792	60138	15294	2446	569199	7568104	7836922	739130	123627	23809	18005	232989
C-9	80	3936	153234	109650	7680	346678	492190	162182	194482	50123	121459	42945	16181	4238	250224	3353320	3875071	427241	42428	5474	12664	188460
C-21	59	3884	171505	166759	9708	473874	903392	257445	260241	47638	147264	43416	22866	2750	406176	5505438	5602922	438205	39031	8888	19332	247859
C-22	37	2213	148173	143308	11018	472169	1650872	427217	343092	54241	104611	63680	19732	2288	620179	8400366	6288277	840497	109078	18832	22942	301618
C-23	121	5492	257157	261715	17371	580847	1187201	533611	377903	79789	227348	182634	22740	3226	555798	7696671	10303689	1051093	108906	18420	38350	415957
C-24	88	4257	221565	221839	15247	500022	1604504	507808	457845	52208	134254	113959	13222	2109	449878	6113720	7378512	837537	81667	10762	24000	276606
C-25	19	3551	256750	272518	19755	540764	1397633	493632	447119	81580	158141	156407	3736	1884	500251	7219206	8519599	738418	86350	22274	32207	464008
C-26	70	4642	245438	258590	18055	473098	1125756	409187	402045	67458	195983	131712	8838	2205	407547	5808737	7070756	658701	64949	10574	23596	349145
C-27	41	3956	229770	240334	19962	491421	1320327	427488	473903	72285	136051	122193	6392	1612	463081	6400115	7674969	701951	76965	8160	23361	360740
C-28	88	4185	332633	345969	28915	644065	1064363	578252	575813	87601	240726	180783	26202	3173	476324	6906655	9657478	781641	76945	31592	36322	425993
C-29	48	2913	246005	222346	19175	637174	1341096	696413	504623	75073	172139	185280	24872	2929	611104	8451446	9821829	1243949	171001	33645	23552	330605
C-30	72	4235	193935	174186	11286	443089	897949	243888	286350	76985	134966	74061	9253	2591	360960	4833559	4803896	460482	48969	7886	15308	304613
C-31	36	3444	205873	197412	13546	338328	832039	235126	276801	44709	113641	45897	24452	4388	241656	3336810	3166211	324739	37494	7243	10912	215912
C-32	165	6786	227172	218263	10488	751315	978944	256730	250595	83556	180954	58988	9791	1794	416003	5820729	6624800	454046	44604	13190	25557	334451
C-33	20	3942	218366	205168	14609	622127	1440778	526067	343125	82116	147319	135076	16455	1581	623925	8749075	10056314	989408	124646	25074	33783	418349
C-34	85	3803	285488	285607	19766	720016	1880456	566996	455368	100192	155199	137507	35878	3323	695386	9345661	7680401	1051043	167037	26486	34686	479010
C-35	127	5922	329286	327319	22389	687855	1361896	634219	516865	94603	232338	214918	6813	1129	537800	7678220	11682414	917451	88995	12823	34809	482211
C-36	150	5519	190117	195010	11823	537102	668320	303037	221498	64661	192714	109518	26363	2300	380359	5666631	10185185	577521	53189	9456	23991	302963
C-37	223	7646	291458	304154	17997	640902	1064615	398529	335035	91737	242300	172683	25964	2765	478129	6796054	9114212	748432	59731	17939	32180	423140
C-38	86	4463	194662	177381	9832	693167	2039001	481866	342732	53577	152109	70803	12097	1869	665322	9105526	8800467	910118	99325	22111	20657	317375
C-39	22	6202	236394	224919	15179	335510	905418	213254	264574	46615	190632	52150	17576	2492	198665	2840393	3040855	233940	20688	3987	15436	256812
C-40	104	6901	175659	160520	6497	560131	810734	164104	134136	89737	193658	63813	11887	1193	484548	6545785	6339311	391074	32935	4811	27938	375198

Table 8.78: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls.

Samples	PC(35:2)	PC(35:3)	PC(35:4)	PC(35:5)	PC(35:6)	PC(36:0)	PC(36:0)_1	PC(36:1)	PC(36:2)	PC(36:3)	PC(36:4)	PC(36:5)	PC(36:6)	PC(37:1)	PC(37:2)	PC(37:3)	PC(37:4)	PC(37:5)	PC(38:0)	PC(38:1)	PC(38:2)	PC(38:3)
C-1	246048	14265	226431	78510	26466	345751	82006	3656250	6928638	2485441	2341082	1233029	65423	769629	288845	414562	301609	283708	51290	860609	2095692	2905432
C-10	240856	21423	435014	53306	26577	347745	79496	3642518	6848999	3304726	3680569	3594541	113532	1059940	428791	247735	372400	540723	75000	1120110	3332934	3504396
C-11	229966	19831	370012	68430	13642	212355	49875	2205732	4832416	2888152	3110611	629273	31064	715659	270853	279794	380488	393030	41696	777736	2113683	2459563
C-12	113840	6269	155904	45517	15790	123584	30274	1262457	3144502	1293259	1525207	279441	14036	194817	67012	404337	200005	157485	21528	313155	527659	1696569
C-13	193392	9287	453348	129916	11504	221052	55712	2755831	5609308	3076436	2874014	580601	29670	1006403	379921	244871	425545	534494	45053	924625	2698755	2824715
C-14	13340	3457	29904	54076	3929	52502	10868	489337	329982	165251	96372	16804	2356	365527	114791	129654	52006	23591	11831	161602	212130	98727
C-15	265042	23890	469521	126442	21811	368413	83706	3918657	5920289	3882910	4474628	1346645	70195	1391651	530602	613422	677432	482168	70959	1145267	2902520	3723156
C-16	340530	11929	282027	95274	25655	288335	71285	3412245	9166883	3553291	2522591	439977	22527	572604	219209	383464	400860	424009	39897	660062	1624996	3338450
C-17	223343	23919	272113	117491	27511	447297	102705	4605097	7015771	2876882	3400259	2340362	104139	843583	307449	731214	362875	359312	59708	917133	2561918	4159831
C-18	378402	21730	296349	52280	20972	316406	73462	3451416	8499887	3536507	2001119	454536	38232	906203	362770	376361	417652	441503	56291	863725	2358993	2340953
C-19	289381	27263	486008	47689	16521	312926	74075	3481228	7416911	3898388	3552383	1155988	52771	929055	394954	239616	517328	597684	61606	1059129	3064120	3961161
C-2	243877	13153	367157	60441	19258	370667	91925	4000057	6833790	3675285	4381077	1928952	87547	591663	229754	807492	432304	383759	44043	715192	2081073	4807319
C-20	270660	16119	217679	85921	24047	234336	49271	2300854	5419717	1761731	1486076	988127	37931	760065	282562	376201	267868	257308	52081	711635	1442433	1898427
C-3	229236	22725	290182	62284	16445	261956	65295	3052724	6990936	2650047	2408391	863263	39720	761650	286397	298872	318771	366023	44206	798162	2074706	2693865
C-4	246981	25878	415721	122488	23588	374100	87004	3995885	7614271	3520551	2416917	615389	33614	1184797	437653	449663	423148	493262	76627	1244408	2788216	2460896
C-5	370595	11132	523717	64142	23056	291800	65791	3107479	6469618	3260224	2752991	1347061	51167	1206848	469875	222262	541419	596047	52642	898624	2790938	2913517
C-6	345212	17309	454493	73579	19363	264110	61157	2855021	6418665	3057865	2815622	859170	36440	842481	333016	296719	469600	612417	47510	750321	2274041	3232499
C-7	324017	24272	274537	72547	28426	428620	101113	4766650	11077995	3559410	2394297	869098	36138	1003303	415437	275353	423849	385395	71701	1153439	3082740	3291242
C-8	170319	13218	253321	35212	18895	290672	76632	3389592	6720573	3007895	3135466	1427543	68064	608986	245339	687594	338470	305181	42794	724469	2029579	2665227
C-9	171410	11867	333554	35317	12170	156059	38697	1813217	3732314	1761873	1525685	315053	14323	569290	218936	153871	270903	333010	25258	442896	1462640	1517666
C-21	162245	15760	457111	98898	12370	250461	60799	2847612	4914278	2485734	2563926	702809	24978	937345	344086	207583	333789	416070	42016	824771	2292721	2283095
C-22	178998	14187	234747	76948	14903	479015	124575	5529450	6612646	3269192	3375638	1572095	84418	720886	278521	609358	245569	271803	39432	805209	2572174	3900788
C-23	418188	21285	375790	62220	19225	341602	82081	3918494	8873822	4995817	2831398	1292076	85374	1250568	458739	296712	419921	497012	63026	1104121	2990432	3087354
C-24	204791	12841	319892	93702	11317	334613	79785	3625779	6393968	4178252	2271665	757074	39678	1569968	572107	294941	292571	375005	78311	1552905	3471242	2388182
C-25	370307	5153	281721	114107	15188	340323	85559	4023362	7736078	3971128	3448081	2356450	91711	1471144	526530	397249	236820	391252	67601	1239571	2802992	3631550
C-26	329378	8821	312289	95830	11752	245118	62313	3083929	6143831	3628947	2476831	979466	51394	1248383	482677	269383	366998	414540	44958	893103	2744041	2736576
C-27	314974	5816	356387	71207	12332	289757	72461	3518317	6745941	3687478	3587702	787375	27951	1092027	429773	281733	376883	381226	47065	874385	2750734	3710373
C-28	510652	35690	222810	124469	25759	481087	108521	5107004	9996415	3275082	2404082	3762782	131929	1709236	666818	260260	291177	454850	110714	1885951	4111914	3365507
C-29	355877	34235	281461	109437	26667	510738	119359	5452058	9808449	4058976	4086219	2911956	151306	1326929	505229	452450	392947	440077	103985	1851543	4368543	5544022
C-30	218256	9135	366675	82993	11445	261595	61105	2751146	4601011	2859803	2038075	571324	21692	1240471	450202	232592	371904	365254	50149	817788	1969112	1996775
C-31	146380	10230	354195	83159	7634	162736	37999	1736135	2990419	1670695	1828876	386411	18337	859577	305913	113448	236450	405446	27685	565061	1753571	1512071
C-32	212116	9088	418411	137892	20117	295479	67258	3199548	5609490	2372236	2275922	952303	36284	1340591	461532	317565	431151	455249	66191	1140583	2362404	2075546
C-33	343552	24361	215483	94407	26130	538158	126888	5809009	10309604	4258217	2988177	1722243	95447	1253612	480065	761327	453106	275915	96462	1483292	3083040	3884753
C-34	260701	38973	352424	117525	22381	589449	140948	6185340	7639293	4003468	4538402	2002140	91591	1639782	582964	649761	534536	380640	101743	1635589	3357021	5075281
C-35	531893	10913	306280	178122	27130	499092	115438	5608590	11800959	4101018	2529980	994976	61336	1813930	690067	453993	554010	452995	101769	1774535	3721422	3284256
C-36	376421	28271	339147	138896	25427	419886	98188	4745831	11060413	3524139	2215208	618288	38842	1329919	534614	257432	462430	454023	71489	1284286	2590783	2787484
C-37	450813	28267	349458	121025	22846	399922	91413	4454089	8992209	3241328	2155722	1974159	87911	1559522	611573	353724	525811	516997	81151	1373532	3023880	2794287
C-38	174721	12489	348639	127151	17298	382414	95295	4463419	6784562	3879606	3292142	1895753	83461	1637195	553585	745452	331528	349953	82050	1699599	3499348	2907440
C-39	178726	9973	578765	114742	6428	139878	36221	1851943	3126209	1584119	1383040	209999	13017	1198906	426923	123504	377389	638291	37773	713058	2171016	1449166
C-40	228166	11700	291280	104261	17298	337615	78255	3572762	5882549	2743903	1888258	386958	20720	763800	276197	491549	426004	325469	51173	809005	1566012	2166148

Table 8.79: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls.

Samples	PC(38:4)	PC(38:5)	PC(38:6)	PC(39:0)	PC(39:1)	PC(39:2)	PC(39:3)	PC(39:4)	PC(39:5)	PC(40:0)	PC(40:1)	PC(40:2)	PC(40:3)	PC(40:4)	PC(40:5)	PC(40:6)	PC(41:1)	PC(41:2)	PC(41:3)	PC(41:4)	PC(41:5)	PC(41:6)
C-1	2450701	1662632	2056835	228564	247343	175957	150275	1643748	115211	426776	432463	41783	115921	248460	622248	1381987	274957	620801	826460	60768	98353	54751
C-10	3203433	2820847	2978298	129048	141020	207581	172182	1029429	230708	333940	275367	35636	106943	229520	618057	1228381	148077	292738	343354	91903	243431	122233
C-11	2157885	969660	1437495	193932	221205	189794	146039	1908745	160829	311648	368151	23443	87760	163368	269828	637744	193595	358482	382578	59072	145717	60158
C-12	965512	629032	705262	295476	380003	13679	93124	2327914	43175	469606	461296	21232	73523	92775	200546	472250	353378	847629	1071290	63201	23597	10645
C-13	2720165	1207047	1057032	138271	145955	185424	145823	1199632	181556	205814	225308	31696	97453	188009	282940	510146	205251	346218	313513	77592	216845	52508
C-14	146770	32263	26601	61862	66910	22982	47904	509906	16698	65440	57247	20549	50665	22466	11033	34663	91016	188394	178439	31069	15001	4973
C-15	3255300	1769373	1793251	189173	235687	240069	212786	2299442	287040	341281	336292	31014	129735	308323	481181	719892	169401	430493	537926	103682	374267	104692
C-16	2483350	1265256	1034477	242909	288556	109166	145125	3855340	165377	498299	588055	25155	101953	242133	442327	618992	426944	901431	912142	104945	167115	42113
C-17	3013277	2645707	2568805	266582	296061	230150	182046	1823114	150781	434024	399745	35361	125568	360677	919481	1675613	236992	661962	1012253	68663	159518	79515
C-18	2391523	1063549	1322035	209908	250342	163006	167310	1817817	161108	399909	513960	40353	117400	195889	322169	610061	295589	549314	640890	85641	168539	69767
C-19	3583639	1733922	2300987	150703	154838	199165	234954	1192010	261630	312871	336222	41505	117896	250998	480350	1131381	162162	350524	405395	109945	313862	99109
C-2	3226407	2179692	2554541	272438	316297	164903	158533	1664919	170036	367777	364327	28401	107547	266449	610125	1285719	195267	544887	807303	59434	152312	59605
C-20	1619126	1355432	1454816	238350	284824	128449	140978	2516494	109174	642292	492881	42875	125732	159179	436095	960853	386186	787616	834936	86741	79541	51052
C-3	2226649	1331517	1750728	163036	178742	145321	134252	1794032	174617	331603	378905	28485	90483	204042	424592	944256	242369	458286	460646	70184	161353	71177
C-4	3020467	1065749	1335857	175433	213586	146128	162064	2565152	180676	305813	329324	30940	114562	228844	397748	861047	256827	570622	590622	95790	233014	85607
C-5	2833203	1852908	2293799	142839	126123	260251	190839	988555	246818	215564	206167	29395	110368	181696	428889	1022531	167790	287817	296038	79048	236647	73556
C-6	2560526	1637167	2221128	176368	190766	189290	166786	1508749	254673	282334	312607	28499	102395	203350	448760	1098403	195037	378853	393617	84611	257502	110792
C-7	3187043	1426361	1806185	185978	216186	199791	215922	2051951	169513	477794	584121	51634	142020	282548	495277	1051878	281750	573956	659819	108662	217887	76009
C-8	2193459	1581246	1862647	207917	258882	121792	127226	1348990	135631	331242	389308	28392	98724	220772	448997	863846	214287	425478	586572	51862	116088	45124
C-9	1531370	684316	656728	108185	129050	113278	98899	639935	121675	145908	162666	24142	71263	113619	178866	354428	149880	316752	387204	56896	117952	40289
C-21	2236411	1168546	1234943	121323	140385	195620	125400	1683534	127935	177312	173623	14681	77126	184062	347156	613644	135437	330140	348773	61471	117782	40612
C-22	3486264	2180554	2009172	171595	186149	185592	141722	1651666	114403	255194	226240	21022	107423	348875	742349	1142425	141665	481223	747837	52850	167694	46105
C-23	3828820	1902943	2474830	139163	153062	265747	199188	2035568	213758	278125	278168	22866	106561	247287	592060	1136298	163235	362429	348905	77634	198454	80531
C-24	3720041	1225739	1384238	87559	100639	244263	160553	1397238	148726	187211	171455	20897	91957	219553	424437	710295	124270	244703	201063	69185	174693	41934
C-25	3486148	2151956	2290729	142151	159359	224395	160851	2310423	179149	374151	279599	17997	91374	221534	499534	1050688	168917	404092	400578	56771	139746	54181
C-26	3124195	1479684	1811299	108757	122197	210309	171475	1763396	184606	219855	195520	16271	90586	185749	373186	762062	145302	304176	283058	66960	191405	67257
C-27	3531417	1643998	1134717	111936	116260	250578	176571	1061602	172871	175467	193692	19247	95940	305339	565491	641767	128435	299355	330822	63612	183780	48994
C-28	3047580	3157750	3398715	132114	125650	332309	236904	2322554	269143	429232	347715	49661	145559	237654	824013	1962779	182669	405600	403877	103248	311743	147965
C-29	4819796	2874204	3229838	151631	150549	279357	246539	2304493	251289	450057	475175	47528	158986	438131	1038087	2027316	171479	382134	437308	124100	391647	116889
C-30	2254751	1086813	1024294	136747	152367	169294	133113	1042400	147131	168448	159454	22092	80392	155806	290406	562447	168785	366354	388641	60102	130967	48762
C-31	1552784	806989	920003	60532	64968	173759	115602	544099	113426	73406	66694	11727	49252	86883	158450	384557	83154	157951	121839	34555	93599	34915
C-32	1986286	1343205	1817427	190511	201126	171437	136311	3247231	190542	293392	227020	18422	105341	187380	386694	916248	252131	579612	572721	81662	182945	70856
C-33	4500413	1805460	1922747	191324	231966	265187	275299	3083656	223741	538096	554559	41318	158653	361169	691148	1229291	246186	629709	821623	113658	275030	80469
C-34	4406425	2132538	2275812	167735	191056	230496	217537	2255201	218352	377331	323659	31983	137015	431051	778820	1344325	151651	495543	705945	102645	302522	73601
C-35	3470398	1566257	1908123	156303	167137	288534	306993	4543097	255114	423667	443371	37507	143158	295417	595443	1073145	263681	613604	580907	175915	477883	117355
C-36	2576644	1153459	1516582	146310	157337	171201	211845	5789534	192776	432107	405964	25756	125224	254584	409417	816165	320868	732135	570430	135991	292881	115475
C-37	2908951	2185620	2783618	160671	172264	309368	274781	4816081	330615	629306	310317	24569	140744	242649	697157	1487181	232946	555596	511142	137408	406839	153528
C-38	3276001	1661941	2025301	173530	199853	187310	140980	3971509	139609	513526	263457	17103	106693	221527	446969	903347	171178	471853	458151	94627	141066	38325
C-39	1800751	653222	677685	72605	62290	211034	123338	999847	174658	78619	70920	10704	63594	104978	163552	345364	97089	199878	136134	49195	192335	61176
C-40	2216581	913061	844224	269975	349290	111986	190672	4816480	141844	375584	284334	15991	105561	230441	364744	570886	304633	936527	1196885	135601	121499	37167

Table 8.80: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from breast cancer free controls.

Samples	PC(42:0)	PC(42:1)	PC(42:2)	PC(42:3)	PC(42:4)	PC(42:5)	PC(43:0)	PC(43:4)	PC(43:5)	PC(43:6)	PCIS	PCIS_2	PC(30:0)	PC(30:1)	PC(30:2)	PC(d31)
C-1	60964	45623	21694	54816	19400	61320	2663273	389001	783487	1050970	7386.93996	588.650658	40370	2233558	1246337	10854
C-10	166841	48349	21326	57575	19324	55385	1913833	247037	461368	610209	4960.27746	324.946406	54045	3147809	1749267	10504
C-11	60785	37539	12185	32887	10296	45827	2385982	508936	682850	883577	5160.09571	456.296453	43359	2264010	1196899	6606
C-12	26284	38906	12133	33276	11815	23927	3029484	563116	769101	1001248	3915.11771	417.037471	19849	978559	508026	3986
C-13	64064	36445	17081	42827	13971	33636	1583601	540261	387417	504519	4126.72015	308.744393	56000	2967854	1735714	6688
C-14	9483	19744	14633	43897	14654	13317	524060	389160	78735	101640	1438.79404	140.353512	12441	641932	333798	1857
C-15	98039	48584	11803	30798	11138	54309	1833251	558263	510865	636537	4724.80623	356.044452	72911	3560550	1863907	11506
C-16	65706	56616	13186	27859	9681	49679	3555240	579237	1116332	1445414	5877.1984	600.895357	38418	2072524	1140057	8663
C-17	88802	47006	15809	42441	15222	77457	2558613	491876	738147	963275	7501.63583	624.304164	52126	2771239	1521635	13826
C-18	80763	56006	24838	61532	20585	48124	3716526	359593	949727	1285425	4978.11099	371.641998	52411	2766693	1468103	9601
C-19	119203	49130	25558	66115	22744	49698	2249084	268618	554863	744014	5868.52825	421.144071	54801	2949229	1699888	9463
C-2	73484	35685	13342	33482	12371	49063	2232600	353942	662831	858925	7219.18408	462.518618	44083	2331632	1254611	11210
C-20	66502	63145	22633	64568	22227	45251	3114323	676529	830974	1121929	5085.68802	544.235885	39592	2048668	1173805	7287
C-3	87933	44392	15474	37072	12955	47258	2484962	394533	656560	842633	6348.35648	537.855596	37102	2291482	1207689	8086
C-4	102088	51018	18342	43574	14124	46892	2323797	565187	572419	761959	3613.10688	291.964236	65147	3294622	1717649	11304
C-5	120005	43655	14917	40801	14448	36323	1601302	300316	337358	451468	4113.06508	288.210681	63169	3542293	1933687	8406
C-6	134765	56239	14549	36551	13152	45349	2386749	398616	586510	786974	3952.78058	423.381701	46741	2744276	1516617	8239
C-7	101322	57355	30013	61484	21497	64982	3857257	325115	1167270	1574595	7680.93108	514.583249	53214	3014524	1662366	13017
C-8	56080	32817	17841	45939	16040	48203	2610119	245469	723058	963588	6101.60838	270.454022	36798	1985360	1092857	8831
C-9	49736	32694	14119	38775	13052	24952	1393111	304929	271497	356936	3318.97886	281.655902	32953	1642885	857924	4674
C-21	46225	27381	6214	13907	5205	33799	927800	570376	196960	239837	4658.81912	317.303863	50119	2756885	1428867	7593
C-22	61719	26686	8178	15093	5395	57322	1341621	411915	324690	388937	7213.37575	509.345982	43732	2465612	1407693	14549
C-23	94601	36891	11355	26695	9767	43356	2087381	367110	485751	653490	5134.53582	465.477934	56505	3304791	1742422	10404
C-24	58273	23900	8728	24433	8547	35882	1260607	411864	256607	325789	6680.57068	482.663054	64105	3294296	1792753	10354
C-25	68356	31674	8469	18989	6689	39598	1398098	522165	362267	437820	5478.62036	274.913223	63312	3172434	1810757	10957
C-26	85198	35142	6523	14779	6748	37910	1209955	500390	274639	335663	4309.6911	361.956672	56676	3155949	1731615	7484
C-27	53778	27726	9308	22421	8569	34594	1405920	352699	289126	359751	4719.54827	193.473715	50420	2767975	1600717	8683
C-28	225555	56786	19593	34643	13268	80481	2053243	463680	634650	824399	8950.71447	744.888073	61058	4063822	2243337	15062
C-29	207652	53807	23202	43464	16266	108073	2587888	355508	844774	1097690	8747.22318	636.446753	60219	3903182	2059717	15263
C-30	50938	33172	11314	31502	11390	27231	1301809	492083	237487	297746	35.3558189	11.9338105	46446	2428133	1408090	8261
C-31	44448	22842	6086	14981	5578	20011	512050	376808	97048	123831	3005.41726	204.532295	56094	2754116	1475283	5136
C-32	98557	47204	8276	17962	8761	44543	1258314	981844	273200	338488	4211.26871	444.275418	63875	3448265	1849115	8928
C-33	97497	49130	22404	40123	14291	77801	3226276	414477	1054454	1375365	12432.0126	746.292874	54927	2800654	1473299	17196
C-34	98110	37447	13611	29193	12034	63571	1691627	449931	466340	580475	9740.3225	413.183849	70641	3597406	1878709	18466
C-35	207649	63278	14390	26388	10375	64227	2448186	617922	685288	878317	25.3418755	9.35072288	73385	4342181	2322638	14798
C-36	127343	59469	11270	12862	6032	58911	1388690	701116	418208	497439	8570.22041	762.751599	53861	3280576	1857732	12891
C-37	246346	64472	9547	13831	6379	71785	1435280	748460	321093	398784	6541.12969	621.924045	62011	3700158	2051403	12309
C-38	53577	44740	6534	13452	5442	42460	916264	824795	190500	221750	5916.87916	314.924228	66220	3587401	1906353	11919
C-39	69604	32919	3577	8248	4922	27498	385321	683584	66128	82195	3080.54536	180.706151	63344	3110898	1633928	4350
C-40	38943	39803	6320	10809	5597	42479	1285943	947106	318976	381645	6223.53081	607.240252	45984	2513028	1371296	10300

Table 8.81: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer.

Samples	LPC(14:0)	LPC(15:0)	LPC(16:0)	LPC(16:1)	LPC(17:0)	LPC(17:1)	LPC(17:2)	LPC(18:0)	LPC(18:1)	LPC(18:2)	LPC(18:3)	LPC(20:0)	LPC(20:1)	LPC(20:2)	LPC(20:3)	LPC(20:4)	LPC(20:5)	LPC(22:0)	LPC(22:1)	LPC(22:2)	LPC(22:3)	LPC(22:4)
P-1	28259	28780	3294307	143892	93459	14118	878	1535478	1772053	1665415	50550	33143	16356	67088	530236	1211786	262007	1337	8266	54029	141127	39601
P-10	6228	37918	2773516	49252	123187	9057	1422	1677854	1648638	2715102	53546	28861	19333	53230	239969	1121359	454446	2292	5700	39594	111183	34003
P-11	17700	22012	2031740	52630	76326	10387	852	1091132	1406524	3162281	66092	22719	15267	88590	456367	924932	111650	1205	5643	30599	77356	41549
P-12	27236	38872	3733851	119770	134042	12343	1345	2395732	2017994	2883380	60469	30885	33629	87967	565779	1854624	167644	3863	5865	44522	126925	71877
P-13	17759	21239	2315451	91841	73596	13473	834	1398415	1419347	2056183	64460	35436	10683	62812	555637	1074197	180021	1425	6670	50033	128153	49884
P-14	46253	32466	4316323	216231	155969	24585	912	2131201	3084917	3324328	87813	47388	30033	137758	1171911	2888156	339865	2259	10902	77589	217600	95897
P-15	7846	20452	1564191	41264	48431	6284	756	674256	1126508	2040118	38126	16479	11714	60544	557551	1518774	86171	754	5456	18269	47348	25409
P-16	28738	29708	3291654	80620	105656	11874	1007	1870363	1497359	2421698	64361	31470	13373	57031	407549	913162	260266	1929	7353	47767	123968	28457
P-17	13701	19602	2105280	58269	78891	12331	708	1147699	1396281	2517426	56983	23553	12155	59579	430532	871232	141905	1122	5598	31673	81332	29336
P-18	31151	39443	3695918	99672	113097	16218	1293	1922043	1912498	2612136	62414	29462	30658	80858	592909	1114839	213141	2540	5524	46334	113984	48542
P-19	33234	28577	2733195	67774	73679	9865	794	1426992	1293344	2097045	64529	37710	14225	64553	519993	982349	186695	1436	11611	62651	153527	40221
P-2	22909	27046	2787181	64487	94408	10460	751	1838542	1364076	2798508	72080	27848	17862	77619	528552	1091740	182161	1938	7798	43257	105443	41434
P-20	25388	27984	2634389	58233	94253	11244	953	1514966	1347800	2008123	70893	32535	14142	44686	367650	712645	111485	1856	6205	51519	129737	29408
P-3	17462	22960	2684992	64973	83578	11746	999	1318094	1535022	2379640	55561	30658	15992	50476	343755	933425	98478	1605	5371	47411	125403	36891
P-4	28229	27826	2940137	64970	125437	10970	1129	1825986	1184998	2056851	57802	30621	15511	44331	329068	1112748	598701	1891	6781	39261	103568	25186
P-5	11319	27801	2464900	43677	80841	8443	873	1089199	1322899	2514712	50453	29609	17552	66182	339324	577757	107410	1376	4231	40421	106605	27249
P-6	23332	31553	3385285	92428	146343	13125	1669	2338590	1872408	3361751	70482	27604	35439	83600	478532	1558584	639731	2588	5644	38216	114361	40805
P-7	38689	32495	2993639	88600	100935	12479	693	1950153	1678879	2654390	89452	35405	16929	85534	679056	1566518	225775	1791	8604	49660	126547	59798
P-8	18403	42818	2517760	58799	110205	10710	1307	1606629	1779808	4145701	71639	26192	27747	91343	331096	1129597	366046	1989	4343	30141	85272	34006
P-9	19729	23940	1984083	64189	61941	10548	915	922232	1437910	2274442	57016	31033	14363	72475	476033	588187	66159	1294	6866	36457	93447	23041
P-21	44284	41879	4157979	133533	209701	22456	1203	3169441	3454440	5657551	145577	32956	52626	176483	916928	2135481	442332	2862	5924	48582	129264	93481
P-22	43102	23101	3350235	159944	105675	18005	779	1942615	2525577	4013213	131444	32953	30412	168955	702368	902016	282415	1491	5007	48395	119984	47965
P-23	23140	27868	2893156	85093	165352	18484	964	1775442	2045848	3056312	61816	27409	27798	113447	795314	1526088	652060	1415	6279	39639	95705	44387
P-25	22673	34481	2413932	59664	110202	12861	1179	1562733	1477131	2454938	63476	28497	17218	64451	420593	947792	176124	1904	6368	34989	81354	35551
P-26	39878	40443	4276594	99689	131777	13562	1412	2714517	2197422	4547148	143626	27773	27389	98471	691313	1593106	250886	3476	7371	43317	98968	64464
P-27	33142	29868	3594611	176884	84175	17674	981	2362705	2250339	2909435	81552	33773	18876	103525	975878	1957215	316214	2153	9336	48484	124325	77256
P-28	9894	14890	1311741	35328	50870	7686	693	687190	905959	1677306	35425	14197	9135	43215	392846	967802	210544	701	5709	18999	49750	23277
P-29	35669	37019	4446135	107581	110354	12679	1440	2440774	2615925	3650003	72556	32898	36053	98098	610129	1712572	631132	3038	8159	51542	135620	56064
P-30	34940	29493	2873204	131281	154665	21808	981	2457512	2946178	3598221	87022	27809	29380	118641	822517	2097364	1244517	1708	5576	34517	92420	51398
P-31	10103	21400	1820962	45395	66370	7526	1003	915559	1013940	1686895	33597	18001	10039	35810	321844	1149793	88431	878	6998	21175	57956	34823
P-32	10297	19144	1798763	34937	75183	7831	996	949432	947409	1560568	27385	24143	12922	44254	246588	834358	289771	1005	5612	30498	84975	21995
P-33	24758	34037	3158765	70303	116810	14616	1074	2189033	2138392	3731063	58344	24683	21275	108962	759214	1743254	159274	1681	8953	37752	95091	81476
P-35	62268	24362	4324866	285656	82388	20129	729	1882340	3082656	2879853	129965	44897	24144	116292	665299	1783892	998280	1466	16552	66807	169793	68894
P-36	26546	25452	1936665	73559	78309	12356	798	1016347	1191781	1800616	37737	23781	12432	66508	481930	1079468	474350	879	11440	29183	68870	36876
P-37	46278	44239	4490086	135644	154455	22074	1152	3174232	2819773	5468999	123848	33777	41090	171377	901611	1322180	358109	2287	6098	60270	144938	72209
P-38	21759	36285	3075255	127989	110209	15216	839	2191032	3405143	4268050	100986	38721	41200	145740	1171230	2504433	209149	2910	6893	49047	128654	113643
P-39	12654	32677	2172377	51228	121391	12532	1028	1453009	1892665	2777579	44496	24506	21775	79922	555041	1768036	583811	1305	7189	29124	69898	51158
P-40	13799	19034	1994100	51129	72586	9556	930	1275154	1597784	2146486	56619	22225	18146	79847	533528	1056996	128340	1178	6486	25606	60253	40253
P-41	41466	33873	3460100	115379	164232	24674	1068	2490479	2332318	3671471	99939	35312	24022	114745	878604	1563274	243893	2633	10686	54541	125068	67894

Table 8.82: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer.

Samples	LPC(22:5)	LPC(22:6)	LPC(21:0)	PC(22:0)	PC(22:1)	PC(22:2)	PC(23:0)	PC(23:1)	PC(23:2)	PC(24:0)	PC(24:1)	PC(24:2)	PC(25:1)	PC(25:2)	PC(26:0)	PC(27:0)	PC(27:1)	PC(27:2)	PC(27:3)	PC(28:3)	PC(28:4)	PC(28:5)
P-1	195837	638316	11084	974	2813	665	131	808	208	303	263	518	314	113	2695	1137	5067	3189	4983	2372	1583	29
P-10	376912	1653141	12095	874	3265	1614	108	1173	250	228	167	213	361	89	888	1138	4031	3621	5191	3936	2700	49
P-11	196296	854920	7550	469	1930	954	103	457	193	441	637	756	439	323	2154	1389	6944	5370	3988	1700	1373	18
P-12	240218	1142631	13526	1583	7058	2871	248	2709	630	523	568	844	673	310	3887	1404	5508	5068	6005	3699	2875	47
P-13	167377	413595	8210	491	1483	447	203	442	124	236	693	732	449	250	2398	1397	3141	2276	6693	2989	2247	29
P-14	233931	726731	12541	557	3007	753	308	1134	238	340	386	687	417	237	3312	1469	6285	6047	6240	2585	2225	116
P-15	115646	675477	5874	260	1732	660	196	314	85	119	240	594	328	221	1599	1944	3265	2769	4963	2242	1537	33
P-16	140758	426133	7072	1202	3030	731	246	921	173	335	162	318	207	127	3253	1867	5283	4582	4546	2253	1400	40
P-17	163900	670784	7038	557	2298	655	183	438	98	352	500	557	418	183	1842	1060	3161	2896	6711	4281	2840	56
P-18	168964	560140	9120	1634	4127	1334	183	2253	225	311	241	632	354	129	3778	1510	5215	4320	5258	2725	1791	35
P-19	181360	592489	14596	573	1792	781	56	673	152	529	541	1087	471	305	3770	1630	6978	4727	3163	1309	873	39
P-2	173727	613999	8199	800	3063	984	151	720	147	267	394	519	248	123	3104	1202	2857	2069	6170	3236	2209	16
P-20	115046	253540	9774	872	2834	637	79	733	177	2334	526	671	256	211	7483	2873	4588	4345	4560	2529	1655	45
P-3	164490	579928	8336	660	3411	1163	101	1071	181	652	1069	974	582	287	3573	3209	5065	3743	4787	2831	1967	62
P-4	189034	828882	9780	970	2881	1130	92	1175	205	398	567	559	512	239	2401	1129	6617	5759	5175	2562	2159	63
P-5	119777	351837	4589	883	4168	1588	199	901	149	223	170	422	396	115	1677	1494	1844	1753	4327	2454	1612	14
P-6	267958	1383992	11677	1124	4775	1518	220	2590	297	105	181	552	390	175	1728	1224	4002	3623	6708	4228	2878	131
P-7	198012	642377	8559	879	2916	818	162	721	177	2186	1531	1412	611	386	9393	1549	3192	2233	4627	2634	1534	19
P-8	271399	1104690	8390	1002	6041	2106	97	1406	276	622	302	586	430	187	3374	1549	3386	2241	7367	4364	2999	28
P-9	96127	388785	6374	255	1578	541	74	592	155	235	1041	1289	698	448	2609	1730	7854	6742	5463	2781	1927	23
P-21	410368	1270180	17714	1117	6245	1961	206	2055	327	506	878	1158	754	430	5652	1828	13058	9813	2001	849	762	25
P-22	216933	750638	10968	699	3301	981	113	1037	210	334	376	553	296	155	2563	1192	2711	2380	1041	692	265	20
P-23	314630	1066165	17160	664	3457	1001	144	1253	232	533	887	1136	671	482	3143	1424	11014	10072	1864	1165	674	12
P-25	155874	526531	12471	830	4319	1415	183	887	171	586	731	835	678	396	4286	1569	4909	3755	5506	4619	2685	162
P-26	210084	718301	14307	998	4980	1961	233	1604	378	633	1479	1411	755	421	6395	2762	8796	6684	9651	4961	3451	87
P-27	264241	775611	18055	1337	4234	1059	432	923	118	1175	1748	1692	634	359	4323	1044	7549	7032	7003	3198	2100	102
P-28	137476	584947	9131	227	1390	360	91	342	67	159	992	1057	471	426	1611	781	4296	3449	3617	2298	1363	28
P-29	292732	1306672	13782	1567	4724	1238	209	2925	417	898	931	995	391	295	4840	1119	7520	5505	5556	3461	2143	27
P-30	409958	1760700	12364	1049	5314	1195	173	1074	251	921	1513	1442	978	665	5226	1506	7588	5339	3691	1606	1372	30
P-31	138463	430631	5837	430	3000	952	135	445	112	205	275	447	370	213	1609	1572	2321	1958	4047	2527	1714	35
P-32	153831	643226	6028	552	1765	554	61	745	151	159	140	316	240	138	1081	1422	4566	3529	1498	878	642	13
P-33	240590	702973	6087	621	3068	1145	195	794	207	576	506	643	429	216	3038	1445	6584	5850	1137	584	441	17
P-35	408795	1364452	18433	950	2920	688	197	1271	343	516	637	774	373	194	5303	1644	5830	4805	1553	410	303	36
P-36	260513	959314	8929	745	2885	748	106	449	97	70	427	517	312	225	1445	1161	2513	1855	1152	709	508	11
P-37	312020	974469	10321	1658	4918	1635	188	1531	297	699	1207	1233	663	391	5336	2492	11242	8380	1915	1039	639	73
P-38	264898	526877	8336	616	4604	1245	439	1480	235	382	326	601	376	191	2934	2289	4580	3296	8067	5025	3326	85
P-39	358305	1390251	9466	491	3159	1008	110	671	157	203	466	704	495	301	1886	2904	4452	3142	3071	1788	1205	27
P-40	191754	729027	6326	256	1970	476	114	437	123	261	280	418	316	148	1032	537	5141	3477	3573	2266	1472	26
P-41	277488	738735	10405	1421	4589	1138	403	873	188	1135	1580	1538	678	466	8624	1491	11810	11468	7402	4202	3227	74

Table 8.83: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer.

Samples	PC(28:6)	PC(31:0)	PC(31:1)	PC(31:2)	PC(31:3)	PC(32:0)	PC(32:1)	PC(32:2)	PC(32:3)	PC(33:0)	PC(33:1)	PC(33:2)	PC(33:3)	PC(33:4)	PC(34:0)	PC(34:1)	PC(34:2)	PC(34:3)	PC(34:4)	PC(34:5)	PC(35:0)	PC(35:1)
P-1	68	3791	207823	150732	11298	722637	1838526	414232	333910	85628	204358	83355	13568	3103	752308	9714535	7199651	856383	108152	22000	29929	330632
P-10	45	5219	270603	260742	19933	600704	864333	386017	487020	75426	235969	82511	23580	5446	434191	6060460	6749812	600988	47879	12065	30743	335969
P-11	66	5044	264189	223156	16172	524249	1043639	363185	399097	63435	173209	110393	13767	3625	377901	5257467	6903371	662982	59587	8577	28476	307322
P-12	31	5285	266867	201484	18024	807837	1315842	547129	533662	76556	273372	115821	18084	3777	523985	7192549	7523545	892599	112846	12323	20519	250299
P-13	85	3452	170346	145509	9573	469163	1007854	249544	264781	63220	143302	73196	18470	3135	463522	6105846	5590057	622663	73437	10835	23331	275282
P-14	39	3231	216123	192639	16845	665391	1776903	488475	456590	89257	154705	100233	20306	3019	706333	9312362	7111553	885408	161474	18511	30843	367591
P-15	184	5440	245212	214886	17266	441293	1188691	420784	536562	49372	175113	73742	20676	5851	297437	4071450	4485934	474847	59824	8600	25439	220872
P-16	103	5167	220331	163274	12035	819237	1060850	335469	332957	87209	191760	92686	14144	3571	539648	7331419	8244179	763286	87701	17912	28997	362865
P-17	72	3766	310557	306123	19791	507485	1280849	448835	469135	75980	161956	146651	22691	3784	467901	6164782	7191205	619718	54274	8903	31154	336586
P-18	155	5224	207366	163245	12190	798302	1324232	389630	311054	97159	235988	119369	18469	2843	692642	9286109	9656837	896593	104543	18562	31896	389355
P-19	96	5776	202703	164645	10189	750467	1075449	328771	326983	77980	157211	69080	10086	3024	418233	5744900	5850780	617010	72183	12975	19480	267294
P-2	82	3960	193788	180575	12466	531087	950381	362497	333328	64102	161808	106860	23119	3215	419839	5829071	7956745	706206	76721	11942	23345	254702
P-20	124	5657	193039	142697	8108	644481	869881	283600	244800	86728	240734	127407	13206	2807	519786	7164637	7806574	781554	75546	9992	24190	316044
P-3	193	6206	194334	142959	12160	673624	963617	324138	350544	81951	257395	105147	13718	3887	576053	7649781	8338237	707985	63325	8255	25492	393073
P-4	67	4391	238090	191920	16320	682875	826646	342982	355486	87791	161529	114097	14527	3720	397710	5338661	6232655	707595	105237	33396	26579	305940
P-5	108	5131	200205	145552	11308	554878	685958	263274	309689	65187	218825	77258	12936	3995	459602	6339958	8185442	631848	51670	7677	24267	254379
P-6	37	3600	257747	246145	23050	602764	988521	477931	454997	64619	190482	144040	19369	3106	425541	5959493	7786290	795415	88978	30848	25160	295481
P-7	98	4399	245795	217267	13080	576079	1188155	466325	388212	68114	147187	85822	15346	2183	428102	5842669	6377124	751012	130004	16000	20305	280217
P-8	129	6118	327948	285448	21000	508773	873908	412196	394173	64854	262916	136549	22865	3836	370461	5252852	8265645	760081	75719	22198	30600	290685
P-9	80	7286	252290	199457	13115	717655	1047641	306088	361186	73437	275243	70989	19785	4941	369001	5122617	5295802	553038	50691	6335	26566	290732
P-21	125	3762	315450	313813	27219	602284	1424052	666889	642659	81580	199063	208972	4926	1619	587042	8205198	10218852	1200095	115978	19762	35305	417619
P-22	73	2735	177131	143087	12074	515081	1395443	506692	372390	55935	158396	114099	2894	1356	570928	7787719	9162824	1096091	86675	15574	19768	268599
P-23	20	4377	276864	281622	22400	484612	1175153	520270	557944	76823	168792	145308	6686	1612	452494	6308347	7749494	687701	73445	19894	29366	416322
P-25	139	5444	253011	257721	17060	508183	962672	388677	343362	74669	226859	124784	17445	2590	422539	5752293	7285295	662172	69982	11018	24769	348438
P-26	239	4972	217513	192185	15330	643114	1138305	525567	391243	72367	245522	159006	28574	2665	546539	7937199	11014053	1233623	130198	22182	25153	315888
P-27	137	5540	242517	199556	12906	791210	1923691	456722	397937	75766	197453	93368	18790	2560	610314	8201391	7728829	863409	103202	15628	22003	293933
P-28	34	4608	215574	217144	16917	470792	839000	274132	331136	57851	153000	82936	8715	1843	298921	4116911	4913415	382149	40252	7534	29052	283651
P-29	71	4108	234216	218536	20172	752303	1372601	686360	558925	62923	241507	121767	19841	3111	703164	9551571	9738003	858818	125237	36114	34234	352957
P-30	97	3198	253440	239255	24964	449339	1296278	531415	551085	66332	168233	139099	8205	2043	457395	6191037	6090913	739302	97121	35974	22562	348299
P-31	87	5225	215181	220192	14665	525364	963740	350895	366949	67829	229878	99591	13643	2892	396206	5280258	6244959	484584	48863	5766	27418	280125
P-32	77	4986	195529	174964	10628	634399	735144	214250	248947	76381	162026	64401	5351	2167	333696	4658566	5336699	394158	34523	8946	23550	274064
P-33	71	3752	265237	262567	16622	520596	1255391	471683	412279	70166	184913	141195	3954	1701	602805	8264305	10357540	736536	91103	12512	40858	397428
P-35	90	3082	159083	137867	9619	942301	2112302	421390	309529	72123	120792	58618	3406	1221	792622	10725315	7176318	907854	130907	46701	20925	295634
P-36	41	4173	163280	139802	8834	440647	871071	235854	208054	63845	139737	65743	3964	761	326138	4452624	4589720	362695	51986	18477	18989	293757
P-37	209	4212	294112	308384	21086	646119	1599355	653087	517929	80180	214937	177672	5976	1427	649001	9163563	12343352	1153186	112218	22916	32293	436251
P-38	163	3255	260879	243237	17659	459576	1336087	456449	428942	50785	212200	114208	25320	3216	554364	7636491	7524411	907583	97015	9376	24839	309156
P-39	219	4574	302823	315310	22656	429755	1096078	380139	433625	72388	178769	99228	10686	2366	357371	4871662	5072396	410499	46522	17046	24393	369336
P-40	62	4283	231068	239893	18854	500940	1149064	417319	442375	62884	183310	91691	13790	2670	482372	6547661	5984368	559094	50901	6850	23487	332342
P-41	102	5150	301550	296448	22032	689012	1382391	511165	454230	106387	188036	170442	18793	1791	526445	7342704	8667088	889567	109603	15213	30946	441897

Table 8.84: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer.

Samples	PC(35:2)	PC(35:3)	PC(35:4)	PC(35:5)	PC(35:6)	PC(36:0)	PC(36:0)_1	PC(36:1)	PC(36:2)	PC(36:3)	PC(36:4)	PC(36:5)	PC(36:6)	PC(37:1)	PC(37:2)	PC(37:3)	PC(37:4)	PC(37:5)	PC(38:0)	PC(38:1)	PC(38:2)	PC(38:3)
P-1	213985	13855	366789	70625	22153	400779	100314	4318247	6747016	3798141	4042888	2090649	96219	679263	255059	917514	449215	387534	50070	804241	2358295	4451615
P-10	312190	25457	412174	93152	21892	299040	67872	3263117	6515373	2276455	2302328	1832001	51373	1085628	436751	194668	353798	632061	60383	1044135	2905076	2768468
P-11	322622	12884	420136	103353	13151	239012	58865	2835364	5772356	2713800	1839425	445690	33377	1505426	538983	191659	307013	463466	64345	1240836	3394060	1977676
P-12	291160	27709	371283	76325	22151	333513	79350	3724689	7441495	3206276	3700252	998738	61558	753904	338338	504835	516661	633667	69431	1249809	3649074	4677084
P-13	201090	13529	282440	52200	13375	283763	68833	3033875	5522697	2901055	2628969	886366	33082	699799	253538	506015	319001	316063	37384	602295	1687263	2602102
P-14	217963	24272	350562	47817	20693	381653	91643	4087978	5816968	4120216	5309184	1532812	60242	992589	379646	822769	491811	326563	69908	1228048	3109983	4206931
P-15	188234	22601	521310	57659	8945	220037	49688	2179220	3600150	2474689	2764561	365246	21471	1275125	496632	133835	342246	503052	63871	1293950	3697429	2065910
P-16	286060	14607	305148	54183	27491	339843	80501	3712643	7574694	3287522	2824783	1527524	54447	864025	319364	463022	366546	379162	46271	825497	2232075	2876080
P-17	306173	19868	289191	64230	13126	280518	66116	3032409	5958227	2657955	2151499	717679	33049	1210630	450760	265176	362508	337592	50953	876273	2326340	2122237
P-18	325523	24378	459114	40852	27840	506010	123366	5535438	9780553	4492007	3393652	1708448	74702	927219	361752	548084	573412	514278	75892	1206576	2842071	3749356
P-19	173844	8842	326459	137514	17673	257049	60697	2730590	5106646	2703671	2350383	766659	39145	924563	339537	551505	316491	357016	53146	939095	2345612	2407130
P-2	285332	24041	283520	79164	17179	305812	79763	3528430	7673662	3147279	2697815	936553	44921	882282	362311	364066	349829	362439	53062	922759	2400787	2968817
P-20	297798	15873	290973	54425	19931	370723	84278	3920336	7719132	3433262	2403868	789551	41990	601485	252064	458199	490362	396748	42082	650560	1634009	2699207
P-3	295040	10308	367933	34560	18085	287576	72589	3248767	7309605	3137743	2865280	658255	28036	485062	199564	365308	504892	545288	31194	512600	1950345	2833933
P-4	282105	17346	300027	62528	21824	291576	68452	3059690	6373514	2409558	2889475	2776627	112554	857271	317431	378407	310662	396099	56476	860167	2391259	3332127
P-5	300477	12076	294453	38452	17016	221698	55611	2742939	6310878	2801071	1719550	662177	21748	554082	248997	238349	354548	386244	34919	701353	2211045	1631915
P-6	343449	26144	262845	112857	19655	326473	77906	3754734	7583556	2872839	2899944	2587065	113814	1142106	467721	332129	278948	415112	67549	1226401	3574961	3744962
P-7	213234	18169	352445	89992	17942	314683	75200	3421385	6018198	3015646	3249033	996710	61282	1194010	436183	471700	469063	411008	64936	1100968	2534181	3201245
P-8	373979	22667	509966	39512	16181	275392	64039	3030209	7357761	2873954	1996428	1410245	72328	1003455	429476	181285	456485	677380	63039	1034872	3086408	2323230
P-9	216748	15431	336885	139182	15752	230626	55615	2637671	4673725	2816322	1262312	269276	21935	1350318	507865	292167	283314	433550	58010	1108503	2999826	1458118
P-21	450306	6919	385014	61679	19550	442776	106978	5052023	9664191	4280240	3283844	1675151	80011	1405152	556381	314622	457295	476904	82463	1490105	3984979	3697834
P-22	279312	3491	188731	66314	12292	311549	80091	3706672	7363426	3688476	1865266	1258640	66902	868801	331499	436030	232994	265099	43446	903096	3001596	1934223
P-23	401374	5041	321726	97294	14497	278769	64515	3213586	6432104	3515035	3160903	2536632	91216	1107105	435191	258413	358189	439484	48040	859236	2914763	3232298
P-25	328249	17430	405294	97053	16859	325587	76224	3611784	6788948	2944873	2390864	903918	55555	1054291	422698	305093	438270	464721	62654	971494	2648418	2527789
P-26	331027	46177	370996	110796	23439	417780	104210	5023538	10818759	4333011	3328842	1416504	81530	1338948	533124	414425	535575	517057	84037	1581574	3461848	3774754
P-27	185567	18294	379816	111137	19739	442478	110713	4786718	7144217	4122811	4299287	1565005	71720	1060288	414932	725940	535985	449100	56546	1016080	2835438	4545092
P-28	224718	6790	384307	89526	8858	195111	45648	2151657	4138086	2306945	2389320	869919	28131	1075396	404127	146899	380046	454628	38871	771505	2271643	2176336
P-29	267601	24336	384738	143618	24025	473225	113161	5265252	9067068	3724956	3782421	3482784	138742	1377210	552568	458141	342668	493689	86332	1639780	4420974	4409839
P-30	289725	6649	308072	57201	12203	334679	82968	3809914	5900723	2898589	2984010	3493619	138258	1242504	481766	223624	359084	485511	52176	955289	3169303	3217601
P-31	258624	10178	442999	77748	11813	201287	49974	2398386	5155100	2582164	3464650	564808	25062	771716	304832	219921	483511	588420	38361	731718	2256940	3290430
P-32	247112	7513	331749	72525	15118	181766	45482	2104844	4569332	2111625	2408752	1284719	30503	709806	249376	217644	274816	448432	31678	626236	1986705	2289551
P-33	388425	5940	466743	68917	17820	441136	110418	5111122	9594325	4172342	3797226	864513	49115	1342452	497082	238207	580564	495462	87135	1517765	3136978	4171304
P-35	138365	3984	211592	97239	25294	401026	97099	4374737	5904947	3078430	3795433	3996353	144034	1041002	381720	967743	307515	268290	65100	1239462	2872002	3126337
P-36	190869	5138	338622	65003	9141	169483	42086	2118202	3897421	2079124	2277614	1641790	64905	1027341	358352	247272	276416	406508	39115	777493	1780984	2104325
P-37	421808	8225	331007	97702	20891	500373	124332	5931667	11922525	4382045	2360554	1753416	85898	1454831	583755	498009	445646	377011	86229	1513810	3609173	3034440
P-38	239471	34170	496307	73582	14480	406979	99711	4677098	7335683	4114018	3704550	916727	35366	1378005	546680	324992	540154	499407	79493	1497584	3458827	3747975
P-39	287690	9824	484945	77657	11613	282235	64423	3006802	4847506	2429423	2672298	1808499	56212	1512642	554552	147158	477656	552610	67937	1192814	2817693	2728674
P-40	253412	8538	384813	95772	14376	278536	69395	3348892	5884808	3055948	2515655	603838	29652	1149946	422140	186097	370827	528085	39594	788864	2612358	2723623
P-41	382013	21544	364313	171348	22787	504459	119544	5319006	8920425	4170763	3238004	1120318	66235	1442570	559074	515248	507195	439770	81824	1313514	3027226	3766112

Table 8.85: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer.

Samples	PC(38:4)	PC(38:5)	PC(38:6)	PC(39:0)	PC(39:1)	PC(39:2)	PC(39:3)	PC(39:4)	PC(39:5)	PC(40:0)	PC(40:1)	PC(40:2)	PC(40:3)	PC(40:4)	PC(40:5)	PC(40:6)	PC(41:1)	PC(41:2)	PC(41:3)	PC(41:4)	PC(41:5)	PC(41:6)
P-1	3410236	2202929	2661432	271282	324922	180042	169797	1738967	188071	386703	373587	27692	110965	274839	646324	1359970	195610	545681	796436	61128	172045	67740
P-10	2329585	2478270	3920530	171988	164794	210826	163512	1326823	231123	279194	268651	36068	106133	183209	683938	1933045	176891	355371	386417	80573	195290	103232
P-11	2670619	1085370	1643996	123353	113471	238490	157335	1191899	130802	174534	186681	27562	97640	151906	309488	736425	163405	288143	213263	79381	155822	62725
P-12	3754289	1730291	2730726	187049	189853	235137	225066	1293011	291189	349207	420944	54329	142986	331665	627910	1690634	174898	346006	405445	138799	475616	133047
P-13	2307788	1273193	1152714	174596	210949	138207	121274	1135138	125480	269372	289058	27862	91588	220312	372705	639673	196302	419602	535109	50598	92418	28256
P-14	3599282	1426364	1541195	187444	235235	232859	200064	1284002	146066	384858	449433	43336	123270	277845	427361	762553	155388	345107	484494	88899	205773	46251
P-15	2774224	800655	1166134	76868	75531	300932	185293	467710	141737	117739	123614	36038	86404	92628	161728	449717	40181	161570	96375	89704	219848	50296
P-16	2622557	1644162	1706557	212579	256374	149984	195736	1522239	134374	369299	389998	39108	113333	193346	394573	818294	230253	521445	700432	73327	121999	46032
P-17	2229664	1146876	1689854	121913	145004	254140	167425	1385182	173805	213519	222839	25040	82906	149323	334961	828240	146815	286753	260695	59731	149451	46671
P-18	3666004	1808227	2298788	215515	250421	195182	213434	1829212	260931	425495	473714	42745	156794	321774	560344	1113733	207061	528469	770513	100451	282034	90212
P-19	2504897	1308526	1478294	249043	274199	151599	179775	1991714	119856	330001	327167	31856	116507	197665	423424	876989	301570	574583	582138	76242	123539	47378
P-2	2842657	1377691	1721331	168940	188255	178168	201203	1996060	180377	359117	397187	30310	98576	223438	468956	965615	246582	475203	478197	76261	173091	65729
P-20	2251057	1271501	1133158	229192	280921	103464	148745	1942561	190168	364753	432581	27737	101464	206657	354218	577960	255343	633017	855577	63308	157629	47923
P-3	2335321	1403208	1986741	191279	240910	173025	164292	1377317	246027	312209	384653	27090	98675	202855	422213	958974	204310	425849	605278	75954	240143	95235
P-4	2470300	2569832	2623442	177889	193563	207339	157127	1205226	178286	439572	381193	45950	118553	184743	480962	1316518	212083	445211	539154	72240	144138	75392
P-5	2118762	906722	1130786	170584	218279	123164	167142	1314784	180773	335524	405273	30926	99016	156223	266077	470060	204834	365277	454708	94166	191286	79701
P-6	3289877	2426911	3103445	136854	148217	263000	195644	1765990	188240	400422	374545	40989	136611	237550	589557	1711586	187220	377887	391811	83312	241788	99169
P-7	2787666	1347570	1539780	151135	174886	223167	183398	1546339	199865	320891	363219	36280	103080	230422	390052	784168	196768	411614	455679	82076	220691	53901
P-8	2374765	1636553	2174703	103157	106916	302803	280994	999824	274418	261813	328358	37984	114795	179466	445428	1011174	167590	264110	255136	118867	354913	135703
P-9	2395084	731591	877145	127941	145345	190074	181433	1406649	141725	153843	158544	26724	99870	120599	185755	390776	183383	328521	300377	69024	134724	40277
P-21	3802061	1989812	2341282	125778	120719	306635	249457	1108653	235388	293885	343473	41880	139625	307749	592767	1128062	163210	314034	375646	119706	330880	93244
P-22	2833615	1291450	1691283	121043	145887	169443	138204	1290867	121045	238939	259558	20417	83204	170560	366138	731857	148152	286911	363588	57762	122097	43260
P-23	3324906	2342435	2483546	123285	134207	255164	173936	1375915	203459	266341	214228	16488	98115	200969	491332	1099150	137477	301859	315095	65690	215017	89964
P-25	2668251	1312060	1567084	140157	159847	228443	195401	1962117	217826	250928	259647	25262	94439	196833	369232	742020	179144	439729	591246	94147	271232	106809
P-26	3662878	1510470	1933034	147515	166473	182851	219442	2881637	269740	408009	461778	38358	120637	293520	489048	998190	210513	441494	472189	121832	362731	90470
P-27	4074473	1908292	1989681	156279	183826	200456	188860	2023621	242085	319426	306795	24549	110837	327754	624569	1180079	170008	450833	608670	87149	314159	80269
P-28	2138886	1264753	1491871	84149	87496	216111	124647	925639	157161	121013	110984	16257	64492	118193	250274	635038	98795	211600	170497	40385	126828	45407
P-29	4184875	2636755	3579440	177777	207184	261791	238747	2648755	230424	498423	418776	39582	148383	298921	722691	1757037	179138	429802	539754	119018	345408	114712
P-30	3107232	2831704	2764460	85552	84449	262446	165786	618413	231596	194116	162378	21738	87039	170769	529401	1409411	101167	210728	257951	67787	262435	87393
P-31	2343726	1334277	1505834	115946	125232	193431	140044	1418189	219242	163842	188419	17515	77367	171736	316030	644766	124437	260318	233524	62092	239207	82530
P-32	1919817	1699923	2091884	147280	164625	154687	106685	1316460	154417	204254	183422	20847	80205	133389	335406	891689	183237	370732	430826	45960	111901	74245
P-33	3528769	1670903	1996336	133549	141747	268221	206168	1771331	222039	248669	291396	28283	114967	306297	528987	989739	165359	387091	453458	85185	242291	71919
P-35	2688513	2610812	3166022	218061	254314	158415	156929	2299849	146118	595080	348390	17178	108827	241671	721347	1485952	147869	419492	586381	50268	144969	60042
P-36	1860157	1816806	2137172	104854	116553	127061	95372	1127916	159032	200367	144345	13960	66526	140490	401960	982982	117997	252505	250400	37815	116006	60289
P-37	4013649	1668784	2117033	147629	183803	266156	284577	2562608	217196	431090	480382	39165	141154	296990	645612	1281744	215630	496467	548205	122639	277441	71253
P-38	3503391	1479792	1130939	108374	123332	236176	274934	1276261	225534	241545	280949	37325	124521	294241	365070	454493	122230	283430	345929	133998	437142	73346
P-39	2333796	2021037	2360453	92236	87598	342964	195562	954378	243211	162172	139815	20968	93133	164284	422138	969421	105656	224090	210718	69969	244231	97551
P-40	2802822	1425997	1854098	105831	120077	200448	127700	1248905	171410	129373	128569	15445	74610	182937	406354	1034935	118549	290502	314772	46001	141255	50113
P-41	3835390	1682748	1848557	159313	169133	280595	243918	2835752	260338	359390	354627	28142	121996	309201	634750	1076174	202954	540997	636167	111018	331648	85516

Table 8.86: Raw peak area data matrix for phosphatidylcholine and lyso-phosphatidylcholine for serum samples taken from patients with breast cancer.

Samples	PC(42:0)[2]	PC(42:1)[2]	PC(42:2)[2]	PC(42:3)[2]	PC(42:4)[2]	PC(42:5)[2]	PC(43:0)[2]	PC(43:4)[2]	PC(43:5)[2]	PC(43:6)[2]	PC_IS[2]	PC_IS_2[2]	PC(30:0)[2]	PC(30:1)[2]	PC(30:2)[2]	PC(d31)[2]
P-1	84888	39697	12595	34096	11638	51936	2237660	379475	673608	866969	6930.97525	625.80559	50781	2528635	1382977	11795
P-10	164625	61137	17065	45585	15686	46000	1977599	433753	503904	660338	5039.72789	431.360719	58737	3274688	1824161	8811
P-11	77191	40045	15018	41377	13897	34041	1613288	528546	324090	429217	3662.09797	243.884941	65367	3617284	1992285	7387
P-12	193080	65710	26601	63490	21816	74714	2716279	284806	818333	1084348	6135.9412	579.757186	66442	3472835	2021738	10378
P-13	39546	34532	14503	40443	13204	30499	2126853	255459	516645	678142	5503.45889	469.020278	35819	2027318	1087409	8658
P-14	56676	34150	24553	68783	22754	52876	2615203	220003	735577	986239	6036.22052	243.695708	53616	2844267	1637029	11795
P-15	67227	28775	19778	58602	19567	24134	1006252	318345	194948	258672	4938.36644	356.457173	58264	3110071	1783139	6706
P-16	58401	43739	20913	53336	17525	37398	2879419	314268	706456	951775	5719.3839	542.394021	47442	2575845	1381377	10162
P-17	75546	36493	9866	27142	9335	30130	1690079	336141	396095	518232	5461.58215	413.705576	54076	2859504	1493162	8795
P-18	132599	56476	26265	55834	19095	75781	3031950	244630	939388	1257670	9125.10791	520.354619	47193	2761937	1471003	15049
P-19	76618	49278	16689	46929	16897	53071	2471887	778938	517191	660848	2812.0908	261.484774	54621	2853683	1538226	7783
P-2	82353	44447	15508	40857	13712	50509	2567574	409048	720956	940436	6308.65577	533.000087	45807	2577161	1424919	9305
P-20	58532	44434	14899	35423	12942	42803	2776214	315901	795877	1048330	7060.44131	511.037272	42072	2230891	1268800	10739
P-3	107000	49223	15886	35612	12586	40141	2719818	209239	710999	963509	3926.57372	310.595357	38728	2113547	1159039	8579
P-4	91878	50459	22987	63409	22254	52553	2474610	364169	677032	900342	4998.13444	305.467895	41573	2538492	1436778	9094
P-5	87599	42413	19649	48908	16049	40363	2822754	250179	789369	1077297	5010.8354	415.396848	44336	2414351	1292333	6543
P-6	155552	50780	17972	37462	13544	71943	2198289	446445	674088	904975	120.513568	10.6834348	52300	3503381	1996624	10192
P-7	81351	41072	16925	45663	15638	41454	2170953	405233	618767	796537	6703.55325	595.45968	49304	2909033	1479045	9408
P-8	196820	57667	17864	45170	15235	59845	2219501	243524	543392	727778	5422.55706	444.980578	56571	3400332	1736207	8585
P-9	54697	39088	14509	40880	14164	36126	1318119	744980	245931	326329	40.0555388	12.1048295	68002	3620319	2059199	6992
P-21	128729	40592	20984	48396	17137	66375	2661788	231652	525708	695762	6463.14895	377.925786	76003	3878456	2145276	13102
P-22	61439	26082	10371	24602	8410	40404	2081943	275398	438694	576972	5330.92812	279.619897	54107	2783608	1458759	9542
P-23	111181	36602	7149	15733	5835	41891	1375684	449394	316620	410261	3631.71298	240.565736	55065	3205735	1855960	8359
P-25	108824	45626	9851	22397	8596	43090	1632229	532243	402741	509446	6625.57857	327.226853	53630	2946777	1545334	9863
P-26	113639	44954	17568	33136	13334	61420	2759389	414063	841425	1089002	8676.91639	588.860733	61585	3737773	2120446	12933
P-27	106131	37248	10296	25475	9878	45547	1877305	457337	467360	580386	6536.85306	328.252292	64910	3349836	1797194	13300
P-28	49454	23950	5347	16306	8677	20729	749368	478767	150681	188182	3797.51156	314.996847	52429	2834109	1586373	5794
P-29	162016	46227	19112	37483	13490	77337	2525866	521685	725954	943661	7506.88862	648.60688	74043	3923240	2119770	14315
P-30	164732	32667	7958	21924	7357	42831	1037212	194238	234852	297245	5769.44217	290.815614	66759	3359943	1825914	10210
P-31	77740	33898	6693	17789	6528	26944	1159402	467577	260239	324288	5027.68484	509.734645	50152	2641563	1401372	6172
P-32	68987	36804	11083	27381	10154	34379	1475694	657330	283637	359019	2818.06994	151.560141	46988	2492458	1308497	5419
P-33	76252	34503	15648	32635	12120	35564	1948885	363485	417028	536013	8317.70234	388.392855	62680	3560872	1921711	14071
P-35	81180	26906	7624	15500	5579	46484	1322427	527430	340928	407108	5728.2097	345.321378	51733	2888210	1602374	12514
P-36	68177	27913	5483	13176	5437	25989	675659	466357	164688	197796	3670.32734	238.963996	41347	2160568	1130469	5307
P-37	121188	46266	16396	39325	13770	70546	3313558	359237	852123	1136501	74.8687597	20.7748899	70819	3747460	1983437	14592
P-38	82108	33159	14760	36525	12307	50680	1921220	259465	437972	566183	7821.28285	537.071432	69488	3861646	2060390	11669
P-39	118074	33304	8091	21156	7688	38524	830713	400550	182561	225164	5220.77466	486.356204	62765	3342177	1811193	8767
P-40	59401	27059	6067	14271	5640	30050	887305	470979	175883	217644	4432.36269	312.547283	59603	3290344	1864622	8348
P-41	124217	46498	10001	22061	8685	55785	2022421	490705	541638	688949	8415.7366	520.934291	68270	3850007	2153803	14872

Table 8.87: Raw peak area data matrix for phosphatidylethanolamine and lyso-phosphatidylethanolamine for serum samples taken from breast cancer free controls.

Samples	LPE(17:0)	LPE(18:0)	LPE(18:1)	LPE(18:2)	LPE(20:4)	LPE(18:1)-la	PE(32:0)-M	PE(34:0)	PE(34:1)	PE(34:2)	PE(34:3)	PE(35:0)	PE(35:1)	PE(35:2)/PE(	PE(35:3)	PE(35:4)	PE(36:1)	PE(36:2)	PE(36:3)	PE(36:4)	PE(36:5)	PE(37:1)	PE(37:2)	PE(37:3)	PE(37:4)
C-1	453.896116	13715.6126	4155.41599	5315.75317	2673.37266	13.4497752	325.554708	295.246512	2819.94239	3448.41026	307.865378	122.223087	504.579795	702.148192	51.3600701	579.067425	4424.11777	11753.178	3485.30971	3177.95926	725.822428	371.132249	716.25525	43.904719	1510.47811
C-10	191.768144	4749.5483	2042.93915	2457.07398	1633.56018	45.6672186	436.17081	59.9054368	750.604883	694.655136	203.939598	49.2109504	345.540538	283.324225	63.1031411	471.871002	1056.76824	2184.33041	929.609408	1177.7602	639.176496	167.807146	319.391922	33.1300405	611.040191
C-11	281.49383	7129.50511	2870.46106	4495.51787	3292.16269		315.545017	302.511011	2304.70159	2972.9573	424.45287	91.0541706	415.986033	617.462005	105.334624	1596.23081	1824.99077	6623.13682	2281.71513	3237.14175	277.579012	330.468605	540.789754	29.1410304	1665.35954
C-12	328.431828	6891.73278	1325.56771	1343.95803	887.874779	11.2291352	317.64427	238.295728	1019.37671	1237.81251	169.706356	31.0939854	340.772132	387.369687	61.5033704	546.326966	2321.62303	5173.09911	1224.24619	1462.78263	149.371062	246.020325	378.689797	17.7060445	1004.54321
C-13	257.911665	2117.52352	1160.56818	2033.36412	714.00515	12.9715169	256.18547	69.66406	274.594268	521.21595	190.268827	18.0670669	185.841408	292.758305	61.7037302	623.156001	744.020316	1321.06329	634.123226	673.701466	86.2886246	248.135462	195.309991	12.9430302	831.275381
C-14	48.7257239	453.331017	19.981854	221.53611	62.9704484	32.7700521	168.750278	23.7299191	68.3412842	56.4110526	45.6950297	36.0605385	51.0048923	93.6096165	47.2848057	44.1198625	164.605538	158.072012	41.6033772	76.391732	20.169563	157.817249	84.76086	6.45344529	128.829015
C-15	313.279195	6031.12312	1832.6311	2622.22101	2121.77887	22.7826967	334.01342	140.746534	943.14019	1335.77793	111.21059	10.5429564	331.154889	467.49688	65.9174897	865.785096	1126.99674	3199.39501	1264.68439	1788.53149	385.946109	301.529803	671.196977	27.4656267	1195.873
C-16	344.277776	9711.73258	5815.48018	6117.68882	1997.72898	12.7426219	526.198034	484.332342	2447.24598	3852.86918	338.81185	49.6135097	412.605329	944.96492	103.022777	495.330005	7164.52362	19962.3477	6143.23029	3426.29111	203.636723	292.797148	1046.94256	39.5177487	1329.62943
C-17	273.609773	8082.76751	2131.66926	2542.0175	2175.41198	12.3645751	229.095578	218.759436	1088.40854	997.477473	115.827838	51.4801432	382.032989	312.65737	14.5460507	635.899816	1826.15901	4251.90952	1326.17026	2109.34578	525.735215	354.444705	292.273257	15.9491302	1326.84393
C-18	279.286461	6967.55218	2686.61941	5038.14044	1871.01946	8.55836563	358.612338	169.306425	1467.08912	2381.67358	195.134813	26.9068928	494.470842	957.160557	18.8532105	977.666779	2127.45895	8714.10939	2513.88789	1982.5353	277.331032	305.417997	422.934348	43.7335574	1788.64004
C-19	246.423573	3515.16606	1507.47558	2002.51886	1334.61358	23.9993082	304.194145	93.7572846	510.771866	545.009501	199.88178	3.59723767	214.851838	311.789148	37.0619292	1021.55009	967.587717	2993.67823	1218.46051	920.99977	112.670143	293.591906	376.670774	42.0644457	1331.33823
C-2	388.778759	8660.11353	3698.12543	3293.44038	3653.6285	22.8710546	280.110543	280.598109	1952.57081	2043.28112	207.084837	14.9809098	464.176389	621.408089	56.5019854	1104.84605	3002.85855	6667.20418	2071.05639	2698.27671	475.087674	358.109791	669.799288	18.2869884	2003.76207
C-20	445.43958	7503.09892	1300.81672	2518.45984	1305.62905	11.3764386	497.791549	117.440525	609.664712	1106.8833	300.962051	104.688919	277.621529	393.984878	74.3153503	594.32106	1451.57681	4617.96138	979.904381	1234.46707	508.044727	314.165152	484.157248	16.0066241	840.728868
C-3	290.61658	8755.02541	3158.3921	4437.74886	2399.99867	10.9730105	299.22102	176.221317	1420.01611	2252.77829	279.694105	35.710136	325.907786	490.363619	55.4221753	966.09179	2574.77688	8084.20044	2403.95482	2161.09102	430.620914	385.729207	474.172769	38.5612725	1055.65418
C-4	190.104642	2786.8524	1484.94691	2119.83751	685.701646	10.5142693	247.464723	233.486368	1477.21306	2443.16808	107.791369	21.5295962	302.194108	502.971979	21.6432366	628.323135	1842.19264	5562.63824	2105.90663	1711.6663	322.814241	221.578292	279.792042	8.81898612	1033.50904
C-5	165.270402	2787.94394	945.718812	1744.84772	895.321668	8.95738734	177.705813	23.3122881	239.914515	519.461672	193.357188	26.6172604	186.333997	257.480457	39.7152757	323.582883	669.520478	1357.8365	466.700191	589.324418	129.992032	248.299301	330.639349	18.2322193	630.345228
C-6	133.559194	2365.45268	1226.03276	1926.49142	859.044766	10.6763875	263.473528	81.8792403	481.459201	765.830606	147.603238	15.3741804	193.917049	324.625008	40.3924119	775.99618	778.663098	2181.41513	760.759113	922.450112	133.20556	146.429278	352.56218	9.05221321	926.243639
C-7	433.014952	13624.6552	5168.7267	9160.22046	3384.56298	10.7657247	381.786362	311.663948	2548.40189	3953.28528	355.126205	26.0953867	386.849609	810.297838	45.6760041	548.593092	4780.46508	16046.4019	3625.47896	3536.88778	480.010808	280.951679	660.387782	68.8372916	1426.19619
C-8	164.252307	5300.84132	2556.15764	3687.15974	1742.76234	17.2269948	267.646093	176.432688	1598.19724	2359.60786	56.7764684	53.4167214	369.661329	456.862207	21.4476988	860.718361	2421.47613	5632.10857	2288.33074	2355.28805	391.710755	268.07925	413.593396	16.2491065	1151.18641
C-9	101.582889	2531.93586	1087.51122	1569.93782	611.230026	14.6999407	266.354095	60.9619077	392.952918	529.374725	73.3715888	61.6780403	206.187014	408.052815	38.8350953	857.238549	1077.89561	2742.71071	935.666123	560.268269	142.795509	224.927371	338.619103	27.183336	1254.21945
C-21	170.251538	4154.93587	1984.92497	2417.48553	1821.36638	15.2506995	314.596434	149.34245	1584.03955	1530.03289	68.438114	26.3056878	265.649731	407.316975	71.3357015	1133.99696	1456.96418	4348.34168	1696.36729	1862.55161	280.319776	383.625598	435.038758	27.9250858	1137.42815
C-22	418.825618	15601.9607	6417.96328	5268.95067	4254.50492	21.8335141	349.984379	315.782591	2828.96761	2605.4918	182.527939	48.0783286	288.205248	441.106823	32.3043133	594.875501	4439.15831	9565.58551	3672.46657	3716.7783	734.280432	385.384317	588.872766	77.1486606	720.611307
C-23	260.412135	5155.57066	2343.6384	3587.60541	1901.92277	20.9212621	443.302553	115.290169	1157.51198	1596.06215	244.984645	56.2050204	291.813737	577.536106	24.460624	917.376824	1797.2776	5328.81491	1796.80856	1486.94033	455.918782	374.161445	506.500692	42.9040511	1173.03923
C-24	122.748949	4659.96466	2175.61477	3933.55039	1706.53782	14.8876529	246.190495	34.9003489	626.018594	850.680141	193.186633	88.5642592	204.389224	403.278384	21.2334092	482.43468	1022.44852	2760.89787	1022.23993	1013.8995	148.88049	349.00998	473.448235	17.0797458	1059.14465
C-25	358.870824	10048.5444	3684.53114	4979.74944	2855.23846	25.0241108	288.11783	130.545904	1225.28827	1402.16024	167.459868	72.7380075	310.265793	404.542483	31.7038561	538.49167	2138.77276	5323.07576	1377.04833	1621.26586	477.71142	446.656941	766.220472	20.3474944	873.066067
C-26	221.024451	4906.68744	2663.13275	3805.92516	1763.39639	23.1765264	240.510586	175.850237	708.574858	1092.54093	89.1771243	26.5802269	175.527101	385.185808	58.6607413	507.325662	1164.45645	3601.90298	1571.80765	1137.56972	241.428009	227.787665	541.805226	11.8616979	972.672507
C-27	267.897886	5380.42771	2315.23894	3285.06608	1695.54826	13.1384656	125.157948	76.554368	775.287194	921.908385	175.114608	25.546353	236.322475	320.325218	51.8666197	601.65974	1118.99828	3676.20325	1149.42655	1196.57427	211.069514	248.626316	545.248488	17.7268734	1140.5527
C-28	397.161947	9169.64781	7172.24179	7007.60338	2391.78945	12.8124075	495.370055	178.970306	1194.84884	1971.41313	109.007169	37.8010251	225.314033	475.009715	48.3086826	421.371852	3210.43174	8812.22105	3310.41798	1905.17061	1015.00251	360.186794	606.029929	39.2851869	807.967956
C-29	544.826257	13320.2741	5040.5395	8488.59587	5670.29764	27.4768432	473.286231	303.769597	1917.77974	2600.84277	315.406602	22.1354306	319.713403	534.998583	20.2507795	513.44967	2804.64646	7812.05357	2623.18741	2761.23639	580.003776	224.043388	490.999682	56.8754784	1087.7147
C-30	28.0360566	34.6218406	28.6651257	42.1239368	22.535615	11.7658578	46.7745758	27.3519347	58.0962236	119.974717	4.51523237	7.50811675	15.5756165	123.153465	6.21810859	32.3328725	167.456581	412.556961	136.649201	79.4712752	50.8057633	29.6050761	61.0907346	7.32864859	117.840489
C-31	197.584579	1912.31331	687.721573	1170.60652	724.051908	19.1383275	204.233195	41.8259286	350.288854	582.340877	118.499268	8.70510761	175.974161	238.284606	21.9783878	350.168139	528.772289	1191.7723	376.290446	483.567355	76.216125	178.564441	255.723265	25.9686438	500.290231
C-32	161.806613	1806.73732	804.198173	1280.70925	557.518352	11.9276144	271.040526	98.9773289	428.608028	426.57486	64.6703034	9.98816245	281.656008	388.468356	37.9074074	899.41088	805.456266	1269.46022	516.58275	685.074972	211.1984	377.17164	351.704644	19.1699786	1519.70836
C-33	514.25062	17964.5206	6713.2948	12997.8817	4738.50167	82.2854326	359.631736	626.43444	4142.92222	5409.14209	261.888319	65.0613216	639.946498	909.358179	47.2776142	691.965487	7723.997	24937.5091	5319.96502	4408.80349	837.883293	510.330079	892.654371	6.02359761	1446.97342
C-34	448.500725	11658.2116	3655.87626	5357.28326	3320.29891	10.34924	298.869556	221.421805	1886.29572	2124.7337	267.505487	20.5589301	372.997263	316.436425	33.9526007	384.765216	2051.96757	5742.50827	1863.84167	2630.41621	511.466471	337.93909	484.846709	24.7105057	926.428695
C-35	70.2830196	30.4159235	12.0003533		21.9113686	24.3353609	20.3192411	41.546435	34.4916815	103.547656	10.5619975	15.1895402		48.2591526	1.12632213		27.9366433	211.457153	11.5978745	46.9678796	10.8163832	14.8755337	23.4989797	5.85453189	18.1925383
C-36	307.061231	10095.2817	4948.04313	8091.45153	3096.89638		549.676221	205.23424	1425.98171	2747.45641	309.975441	83.6460147	653.755255	1165.05001	74.3705736	2049.26613	4121.70745	12300.9051	3905.61632	2709.6275	340.887851	433.280756	715.357617	68.1497801	3388.28023
C-37	450.645564	9312.18526	4258.20956	6600.94075	1987.10897	10.6248532	380.824849	113.048014	999.048603	1850.58573	329.858523	25.2060062	311.729316	305.737453	24.8365816	435.882203	2068.96119	6622.50756	2387.38364	2063.03394	548.092677	249.506156	474.289719	42.1418051	933.698345
C-38	191.356091	3978.85106	995.663733	2372.61104	829.074575	10.375813	319.444067	86.3442987	533.710814	824.426098	111.207492	19.1124015	239.192754	394.147766	69.6606494	704.808234	742.33753	2294.52043	596.384247	1023.93362	327.321311	416.952279	374.651468	29.0158728	756.357261
C-39	139.036097	1026.76176	579.281442	926.891107	633.999391	21.6048029	261.565611	9.03223234	246.296027	282.96	73.4509487	4.81182655	141.898206	217.156097	32.0198787	522.838396	421.144981	1101.03486	466.248302	321.707074	32.3177102	306.337157	416.404369	14.2409249	693.073562
C-40	210.690272	4175.14929	1623.23518	2457.05823	1052.87845	15.6651244	385.721028	183.669997	976.373991	1636.69835	139.382132	106.494057	325.560021	581.118356	43.8471646	967.819872	1843.57837	5357.01867	1692.13474	1671.75724	274.33944	338.020265	628.742426	16.3920991	1713.54445

Table 8.88: Raw peak area data matrix for phosphatidylethanolamine and lyso-phosphatidylethanolamine for serum samples taken from breast cancer free controls.

Samples	PE(37:5)	PE(37:6)	PE(38:1)	PE(38:2)	PE(38:3)	PE(38:4)	PE(38:5)	PE(38:6)	PE(39:5)	PE(39:6)	PE(40:4)	PE(40:5)	PE(40:6)	PE(41:3)	PE(43:3)	PE(unknown	PE(unknown	PE(unknown	PE(unknown	PE(16:6)	PE(21:5)	PE(21:6)	PE(38:0)	PE(d31)
C-1	1376.56022	1285.80403	84.4120096	1376.39631	2866.98672	11268.9621	150.52154	11424.7995	906.355772	1791.91204	591.52807	2307.37253	9521.21622	5655.39211	139.182562	865.982624	151.883313	66.7498815	175.253583	5785.51975	1243.63639	5242.05763	325.554708	465
C-10	1179.85178	1301.25074	120.900497	963.002272	1051.0492	2791.54729	190.426761	4122.20372	497.785379	892.803639	192.070732	703.011237	3217.59622	801.650493	83.6415059	1210.75487	360.161023	134.882296	151.156137	2440.44547	745.040219	4326.06849	389.709123	590
C-11	1532.72007	1827.87534	123.947934	1198.56189	2421.35981	7841.98349	414.456583	7383.36295	716.351842	1508.6591	374.685585	1170.83901	5652.93719	3450.56679	183.238987	1012.07538	138.093021	87.2327027	140.520071	4408.62899	720.512479	4563.46101	338.434596	379
C-12	799.813411	608.07426	167.97779	816.335181	2309.9558	7765.8275	106.96616	3605.83348	470.885474	637.211125	696.175834	1249.10003	3536.12429	10546.4952	204.457963	444.78216	31.9248049	72.7693337	35.3706962	3167.18377	359.554207	975.302039	328.217782	266
C-13	636.40315	443.493729	87.5566498	699.503177	848.366278	1373.70799	63.7632771	770.523479	360.248272	429.970064	47.3974212	187.606087	704.706861	593.939353	88.0513988	1471.50899	326.580047	115.418799	217.7203	962.192734	216.254795	869.179145	406.638697	310
C-14	40.1247081	63.0355969	10.6364628	314.142279	199.34541	212.599247	20.4490746	69.3361112	97.9953254	43.9041428	19.1007438	122.27396	149.601768	387.12918	139.26478	548.140721	64.9580252	117.657649	107.226098	284.892183	11.161988	36.497832	225.494455	61
C-15	1366.20641	785.160518	160.585563	1114.3338	1475.91879	5005.59378	225.263848	3986.54932	649.178522	641.960743	419.325859	927.303312	2432.9109	1305.13141	126.44802	1491.14943	244.39854	119.732896	190.7368	2482.22577	685.445987	2494.46407	356.570497	467
C-16	890.468754	611.742916	318.985117	1281.67631	3469.34374	10267.4197	67.5953203	3466.99865	835.430949	676.430435	533.397852	1315.6669	2902.54042	8921.75123	326.058981	896.918338	100.068464	46.1467934	70.5489971	4023.99835	565.861675	1471.00266	548.274285	726
C-17	1561.54413	1272.36421	72.8981719	978.307742	1668.29669	6445.20886	131.010411	6161.38834	889.300607	1469.72816	335.731275	1733.72821	4940.17914	2989.66302	126.7859	1045.92839	209.394034	131.80639	102.763865	3238.66674	993.029511	4186.40249	188.89329	414
C-18	1667.97094	1205.45572	187.12769	902.593552	2291.07774	5892.23311	152.633726	4884.96468	804.274577	1211.89072	301.949055	894.752935	2850.57086	3449.12983	134.717398	1361.2489	233.149108	92.9029693	179.00828	3073.28066	485.683224	2629.49498	358.612338	611
C-19	1312.80169	1599.86434	159.561209	780.000964	1298.11894	2895.73123	94.1303756	2120.94921	598.489289	1122.04652	215.213041	474.976789	2201.26722	1573.11949	103.996255	1327.65762	265.817974	125.390822	224.009121	1048.41211	432.407552	1969.79601	285.653434	226
C-2	1724.49351	1496.25464	233.537221	1093.65863	3724.41385	11282.2772	245.439364	8004.98055	1274.01972	1438.85861	544.387113	2249.74844	6626.61027	4971.90629	119.919805	867.354969	212.18154	127.472479	145.689925	3309.08066	1294.89884	4862.17682	306.664408	406
C-20	1019.09525	1182.80306	185.739033	982.026788	1599.40802	5257.59752	100.348431	4639.14148	919.907459	1222.02985	164.076107	1268.64715	4248.1838	6103.1161	167.944043	879.531454	161.691563	82.9888448	93.1845562	3208.33348	562.996053	2362.68339	381.567369	153
C-3	1355.6963	1904.56894	58.2911681	1090.49599	2228.02843	7346.25653	173.795863	5492.30247	778.348745	1542.73668	427.555686	1548.41082	5356.90808	3507.11733	161.838994	1226.43171	141.576073	88.5756923	168.607623	3494.2985	755.427185	3818.60926	299.22102	338
C-4	1017.23296	1483.27808	108.45183	558.947059	1743.26156	3020.61722	129.495835	2970.23596	594.33968	1129.98469	139.170717	665.415304	1951.46135	1875.69311	89.6280582	857.114398	205.437373	78.9996623	148.08897	1538.83526	322.002556	943.222874	226.784428	532
C-5	716.481035	573.917821	52.5248144	841.638765	876.877155	1856.51987	140.312078	1750.10582	537.480434	599.072691	203.542065	358.979863	1181.75864	449.352544	108.122818	1508.55413	422.178921	147.483687	200.522835	1389.33506	421.27852	2142.82156	179.909486	500
C-6	965.647775	1269.60167	32.9598781	773.034481	908.651494	2337.76471	133.035316	1729.86207	415.362577	1016.81472	132.847674	534.52767	1515.67618	1218.96986	133.085302	993.56032	256.24613	195.974088	211.319503	1163.94107	339.272405	1295.89505	306.228673	235
C-7	1245.28046	1283.54442	65.3552172	1327.95061	3470.20022	13911.7359	299.052966	9188.74798	871.583761	1507.09985	507.766135	2194.43027	6795.21883	4387.90838	154.022528	1250.92615	281.209068	98.4681869	210.737107	5419.717	1173.44918	5553.52244	410.213033	616
C-8	1110.1706	1581.6926	32.2642694	876.344786	1899.09495	5529.4168	197.260676	4708.1332	697.874318	1024.09363	441.854235	991.380097	3117.93513	3023.1552	126.595832	742.264034	220.348383	81.5740966	103.959479	2954.53721	470.842045	2163.25518	261.876266	368
C-9	1612.64191	1060.04302	99.5664472	727.730066	1032.79418	2107.26511	90.1664309	899.307492	669.550134	1105.28433	120.734878	450.630946	928.803906	1928.12344	95.4487253	837.287489	185.120852	81.1502464	135.440066	794.331167	186.89933	744.342512	258.725243	218
C-21	1961.75365	1296.89034	85.3492525	1113.10227	1681.99577	4988.92531	201.873755	3668.09787	526.780013	794.568074	414.384818	1078.7137	2584.25717	1841.74915	113.226684	1424.72979	303.440642	136.783166	168.692533	1867.92577	469.500107	2198.62734	314.596434	540
C-22	1044.33973	919.216576	124.818431	1574.74008	3814.0648	14658.2318	631.614702	11204.0758	614.150126	769.163506	936.922766	3670.43543	11082.3348	2742.30519	106.831504	972.222216	227.288862	86.720162	124.872779	4870.59861	2081.2741	8547.26091	369.652136	1055
C-23	1374.19865	1320.88517	95.7755259	1200.721	1614.06233	4152.13199	160.593978	3627.63182	749.303862	998.708704	367.499518	951.230454	2988.78444	2051.06998	159.422869	1332.40102	329.988301	151.665195	167.639786	1959.79093	565.712768	2466.77847	419.421737	596
C-24	847.706625	530.567783	63.8090078	921.434814	1032.00502	2070.79044	194.988582	1809.09862	400.576772	557.951939	219.308372	512.123152	1809.15174	628.295427	67.2172617	1508.52368	362.160723	214.91128	290.582814	2098.00259	707.591739	3410.08542	245.277174	370
C-25	958.7189	1141.66724	172.705312	1314.32282	1722.70483	5641.73042	224.022688	5705.44131	454.967257	903.688351	344.280024	1064.51358	4549.81985	1911.07725	94.3488725	1399.86988	409.630751	129.172216	162.88889	3762.30168	1022.92661	5700.23942	275.730227	672
C-26	911.573024	864.788781	90.882574	928.41891	1425.33634	3275.7773	154.326683	2895.29763	385.646273	751.413057	215.28412	772.761768	2137.27881	1206.18001	62.6786647	1834.03743	349.770264	92.746679	219.04651	2064.21482	683.91478	3476.58839	318.156344	533
C-27	972.135688	478.836272	113.338369	919.796864	1337.49227	3690.89973	115.539849	1521.76185	796.309211	405.087247	422.540302	596.64743	1564.93182	1073.70304	36.9830776	1442.7124	284.36495	167.513408	119.868786	1839.93984	783.663273	1477.3858	146.005601	518
C-28	1196.40845	1751.12378	95.3487564	1383.28734	1393.45545	4961.5305	298.050001	7467.78496	847.403103	1459.28968	229.080242	1417.3534	5779.87296	2605.11262	81.3193526	1700.80398	305.124456	163.139149	224.935794	3722.07714	1346.93095	8046.80325	531.036121	725
C-29	953.611382	1286.53109	132.388339	1370.29367	2609.95873	9374.54151	299.447017	8199.8437	841.814956	1458.40886	391.932089	2032.60713	7394.35877	2466.33756	178.027951	1653.20333	407.777544	98.5955355	221.311935	5312.1508	1797.44274	10549.6589	460.602368	716
C-30	92.614799	50.107627	8.49873807	137.95725	100.363717	234.127888	3.13915168	72.7870441	51.1303522	70.620657	19.978909	41.5710065	173.848374	84.5521782	18.181374	8.60215791		14.8106138	22.1027282	93.7642524	50.1291599	45.1611604	41.8281023	276
C-31	635.347866	641.007219	62.7144686	663.245719	714.052261	1773.00458	213.598006	1638.64373	354.715076	627.154441	54.5957817	496.757417	1235.68713	652.208829	70.5219169	1603.27982	274.035689	124.189172	162.639976	933.094011	360.345921	1409.38363	200.377166	264
C-32	1562.13065	1628.9608	92.6421378	793.271856	935.335659	1337.14172	109.679519	1675.24126	681.542738	1135.82955	96.834827	592.735335	1306.73341	1022.96308	75.8065455	1715.25852	148.908803	120.189931	273.954639	1108.61006	234.456385	1205.65078	353.017253	465
C-33	1250.82156	1464.13834	214.227159	1638.03372	6829.81984	17826.4474	681.030214	9112.20239	942.099392	1418.09887	984.79251	3366.1006	10353.7325	5950.2898	214.203586	1094.64018	210.251625	110.768188	142.396988	6276.5714	1971.77538	7027.62836	359.631736	933
C-34	1024.70011	800.919645	62.7416001	1101.54263	2237.37463	7721.47683	258.263765	6907.54928	549.068886	793.292287	460.832662	1851.82672	6563.9389	2212.32355	110.568015	1343.28223	261.372238	156.380098	100.155978	4600.44038	1187.63383	5901.50982	298.547338	561
C-35	8.5349935	32.247506	3.57934823	58.52166	27.5799043	106.962315	19.611631	26.0575927	22.9709395	18.0942168	9.58768477	27.514371	22.8078673	63.357363	11.3861006	14.0622655		6.44204196	13.7466586	14.8266417	42.7844066	35.3948866	20.4462504	842
C-36	2323.34337	2153.03092	66.7157401	1507.42355	2192.20485	7677.74604	313.386451	4560.03144	1314.68439	2626.01108	692.539689	1395.10179	3880.50556	4247.97776	96.4661715	1622.27946	116.240576	91.1833089	179.690045	3484.2948	863.989008	4138.01256	538.418883	463
C-37	880.85124	1007.41895	89.3887154	1050.18664	1665.39768	4782.01393	167.237352	5761.51105	728.53194	1190.51052	106.85028	1231.93566	4336.70408	2224.64871	73.6517454	1391.93594	268.945716	128.435727	212.005355	3878.36136	1064.33986	5977.7982	325.99688	566
C-38	1139.82114	1236.37398	107.606538	1115.59526	1087.18619	2745.72556	185.065587	2527.77194	442.000802	806.844446	102.295955	609.983284	2043.76964	862.803666	73.5079203	1565.70481	289.314791	166.49735	254.741654	1582.86424	455.625513	2155.42262	319.444067	236
C-39	549.770117	647.914364	149.623197	1013.68124	613.073486	1137.84215	55.0702412	647.998243	396.321744	468.117915	109.949381	362.160326	670.193992	251.847303	81.2570889	1599.60663	357.958564	174.145426	137.355086	611.562078	209.541789	691.041418	326.413715	225
C-40	1494.22856	963.681042	60.6146586	1076.4853	2136.98068	4650.37653	289.897788	1716.59651	833.277649	873.256508	451.151505	1104.70954	1881.8409	6010.85354	344.824318	1318.61599	85.5954842	86.5280654	104.273732	1660.48084	363.513521	770.648136	375.280118	379

Table 8.89: Raw peak area data matrix for phosphatidylethanolamine and lyso-phosphatidylethanolamine for serum samples taken from patients with breast cancer.

Samples	LPE(17:0)	LPE(18:0)	LPE(18:1)	LPE(18:2)	LPE(20:4)	LPE(18:1)pla	PE(32:0)aM	PE(34:0)	PE(34:1)	PE(34:2)	PE(34:3)	PE(35:0)	PE(35:1)	PE(35:2)/PE(	PE(35:3)	PE(35:4)	PE(36:1)	PE(36:2)	PE(36:3)	PE(36:4)	PE(36:5)	PE(37:1)	PE(37:2)	PE(37:3)	PE(37:4)
P-1	350.612982	7191.10766	3203.85017	2562.96859	2569.06886	9.9119023	422.355157	234.389869	1940.03524	1490.92594	112.749893	68.1370221	457.753627	624.785554	71.7746355	1021.9266	2455.69291	5074.85736	1774.82183	2312.5627	501.000673	269.516979	678.779539	12.4533049	1764.38612
P-10	276.719146	3781.5373	1841.42516	2365.58954	1379.61653	10.3755335	268.764037	178.286062	752.110744	938.497388	164.32081	45.4082773	263.056726	524.825999	39.3432858	1272.45014	1206.68095	2979.99307	1113.20356	1136.64489	367.968346	331.118711	565.990603	8.34757293	1191.84683
P-11	103.197276	1430.74827	900.242071	1334.47049	602.89096	25.8963134	200.771598	27.5679443	206.660978	335.04845	138.401005	67.6231969	226.991678	353.106843	9.10156501	644.793099	590.387688	1134.00563	472.820322	243.658792	84.0498511	326.005677	410.197112	7.06245932	893.75434
P-12	216.20275	6818.85118	2615.27912	3679.0937	2738.86035	10.234758	360.625023	117.056656	904.077108	1278.93867	245.524519	22.3466903	195.731486	328.885813	23.8303214	294.537136	1234.75083	3490.06829	1372.51498	1543.01979	235.372046	221.128697	395.963446	25.8591328	798.391719
P-13	214.722133	6478.63377	2427.85346	3353.47126	2296.88809	15.9701203	411.165696	91.1162798	1203.01573	1324.45808	149.279514	26.0997946	284.816286	486.181669	89.0797965	462.099801	1357.34764	4464.43507	1326.57903	1849.30482	244.949194	365.604246	595.390763	29.7196728	946.902384
P-14	487.60802	15341.6042	6949.07799	6494.50708	4714.21437	12.6312206	434.442646	339.090806	2602.30984	2529.6672	361.053824	68.0166961	484.070784	571.60747	110.711789	770.09431	2792.20465	6646.04226	2491.60949	3985.99847	476.750806	362.256745	626.693084	7.35488782	1768.56598
P-15	173.480173	2153.23445	1078.90843	1440.44935	848.758207	54.9592041	352.569666	24.2722102	244.146325	391.686944	150.063332	20.5483937	74.674572	161.262331	30.955379	359.692575	469.600021	1029.12918	453.484642	561.21031	125.160443	161.510716	276.61317	31.9600969	599.956953
P-16	338.557166	10408.2181	4170.305	4949.1183	2066.37058	18.7064531	414.375783	349.574236	1875.29045	2715.54649	227.808726	24.420416	488.684819	691.496692	79.8198961	730.954138	3943.02792	10979.646	3796.50154	2741.37097	582.474989	230.41024	773.669454	50.5573092	1106.6001
P-17	161.179759	5210.58691	2378.48543	3545.64647	1352.72553	8.14465527	297.140178	104.481479	1232.62905	1410.75787	343.503097	60.7082	232.926448	480.202172	79.8625948	581.685634	1474.95355	5077.66832	1515.59899	989.906601	184.315593	281.200545	742.560412	26.7379166	807.059137
P-18	271.230582	10166.0365	4893.98874	6413.77135	3167.11249	10.4786008	497.071663	329.415706	2725.26832	3476.63594	222.281642	86.3158815	739.94538	819.220937	98.752988	923.717478	5595.99281	14015.9994	4128.87602	3335.45143	548.459749	447.207433	708.724484	68.1916065	2347.48342
P-19	200.378564	1471.69122	568.017259	962.363874	549.504118	8.03751048	273.498582	28.1482918	160.966703	251.890527	149.654406	21.1571758	146.900935	177.198847	29.4800692	601.590983	322.439884	827.800214	283.317614	282.849212	103.819258	222.563038	236.458824	15.744815	699.606917
P-2	330.752909	8908.23665	3054.91173	4910.67668	2701.46249	12.1696355	546.876251	182.545336	1491.25003	2288.63996	269.674773	60.0181188	316.873778	493.084686	69.7564352	752.175244	3091.78546	7053.53279	1923.6962	2258.92597	296.727022	318.263933	519.240672	88.0080775	1320.38974
P-20	300.907383	7038.09654	3003.7182	3815.07437	1939.79911	11.9341154	350.919146	199.940638	1541.00849	2334.95344	128.293349	83.4883317	437.475424	632.475336	40.9647598	788.363229	2769.85283	8279.80286	2828.71185	2854.6301	300.293373	325.933137	518.6315	21.1135898	1475.17741
P-3	181.923711	2711.72624	1273.019	2349.20523	928.736081	8.11844291	294.877435	114.712794	737.124926	1206.07732	168.506946	23.2684738	238.623565	329.938989	77.6425195	840.27541	1037.6409	2793.67687	1149.67655	1225.88509	99.7067286	142.798939	392.125311	18.8264601	1406.30401
P-4	354.757893	7556.82541	2250.75453	2600.13217	1761.30723	8.57546896	335.331014	109.92247	919.734473	1100.36282	288.112164	48.3699034	195.433401	550.408503	14.7502739	545.230732	1708.28454	5078.97918	1605.96655	1726.65214	721.971862	271.877089	596.670507	12.2383929	953.333235
P-5	330.817788	4280.99589	3351.80998	5638.06181	1890.07885	16.6325418	244.084403	153.111654	1226.18826	2191.44029	185.611127	19.5472986	444.668678	521.258049	56.8039843	619.695451	2116.08476	6687.02146	2677.92822	1613.09876	347.374278	213.494376	576.774026	42.604879	982.182825
P-6	51.4781185	20.1725443	26.3338414	16.8249911	19.1627333	16.0851515	41.8917997	13.2791541	53.8054278	70.6720638	2.19213464	5.61766213	47.3579355	25.7584977	3.01237034	18.7613463	114.917064	401.034686	84.3415176	110.897414	42.2419298	16.5291286	51.7202377	13.6118455	75.9806832
P-7	319.03012	10509.1696	3155.96465	4980.60329	3492.31805	11.9431622	202.691115	147.634774	1275.34959	1582.88281	236.739727	53.326947	343.136317	401.919661	72.9960549	720.665322	1671.90287	5024.23396	1657.3284	2381.59076	443.704394	496.007718	555.017962	6.18964855	1389.90958
P-8	357.383543	5616.79485	3895.32326	5152.48962	2286.9443	8.23281575	330.306445	199.829259	681.576148	1316.2883	56.4770535	93.6330958	510.760723	622.900952	40.9084115	1096.1571	1811.51991	5476.21694	1860.57219	1404.91784	575.631539	259.513448	347.409403	10.976275	1830.52235
P-9	33.2653362	26.083923	23.826515	25.9651	47.1674464	9.19142664	14.4752977	12.9742195	47.5243773	106.553679	4.20386269	8.40126328	12.7793684	60.5600663	3.3532548	17.7462372	149.259155	241.784069	88.2808979	54.128479	16.7286713	15.7229179	37.8960533	4.2331902	31.7011956
P-21	312.097723	6861.62862	3859.72456	5553.02417	3103.9268	19.1003266	318.302575	81.3656325	967.241959	1251.07495	105.569305	29.2003258	346.365574	516.615954	22.9944785	749.455227	1305.70861	4058.40409	1560.14309	1531.39808	321.437142	349.770078	491.050454	33.9784387	1695.12058
P-22	272.423947	10231.1905	3827.51346	8091.24996	2067.08764	16.2489741	224.928727	112.416274	1007.3147	2368.30391	130.048943	18.2728609	181.402372	492.343379	23.4522342	289.746986	1679.9328	7696.61121	1814.3517	1293.12088	528.954101	204.034554	419.116629	4.83250866	443.611596
P-23	466.662716	8654.8387	3542.57503	4191.63128	2732.70085	24.7049297	204.309199	138.362323	1012.26378	1288.37054	246.274044	37.2784061	249.331508	534.371361	74.3580887	531.142797	1623.41179	4280.59593	1471.06549	1603.73908	678.40379	355.721879	625.508835	25.76272	885.3997
P-25	173.837963	4872.47741	2159.29977	3109.86636	1941.18533	36.4294845	316.990239	121.898463	774.623509	1188.69294	89.8606594	49.4247618	308.102652	418.335363	60.9698204	566.660175	1665.55092	4338.44905	1298.7507	1643.75281	287.297045	297.527761	505.374149	26.6202364	970.765981
P-26	371.692704	12652.0177	8106.78579	9507.44711	4722.98543	10.9944303	466.916438	212.008797	2056.4613	3761.35345	219.586918	48.9822107	720.697933	916.81603	120.474254	1983.69375	4796.51719	13814.5996	4109.63528	3383.94678	566.59971	484.088637	724.278283	37.0049705	3620.00888
P-27	218.506567	5829.7079	2786.895	3466.05252	2030.76879	23.623296	275.526526	134.595392	1135.46921	1009.15677	356.240267	21.6947748	196.17187	401.126787	37.5319785	411.960118	1558.5568	3942.12503	1474.60678	1809.76355	336.303987	293.714035	486.377038	50.3545878	844.606799
P-28	131.37297	1849.66347	641.335998	846.958704	733.883361	16.6323634	262.648989	33.9363109	227.339138	336.649235	67.0585573	31.9395479	214.657781	299.081517	53.8822412	461.805756	669.728979	1236.24972	525.989745	596.852325	134.787102	434.396395	366.974857	34.803195	942.219998
P-29	141.9055	6794.06744	2331.63328	3561.03421	1956.14712	25.0066649	270.033389	75.8136427	915.348937	1216.23491	136.953857	28.2346188	245.004877	392.803824	67.1337745	719.355992	1267.55989	3550.96231	1096.96842	1305.02505	324.372042	288.596281	493.774047	16.5922466	662.977225
P-30	431.203442	10173.292	4522.06599	4845.14526	3217.47916	12.5787554	339.269031	103.640546	645.388558	984.359772	129.607068	22.2678907	235.982112	294.524336	9.60520409	343.150039	1495.15916	3881.78339	1236.86436	1349.87635	922.330873	285.345516	400.76113	54.538857	696.967216
P-31	335.275223	3314.0888	1140.91911	2086.5361	1786.76509	11.7196373	257.031541	166.435599	795.579953	896.441974	180.844617	31.8284206	233.842299	280.244838	34.5825806	945.879785	806.253921	2732.48107	951.297851	1476.5683	103.142544	339.770648	480.525168	42.0412495	1179.9619
P-32	135.335356	1815.36883	587.401879	915.493469	449.805481	14.5122852	211.069714	61.4673535	320.10034	417.187183	61.5391442	11.6004661	167.088324	182.929681	11.7342514	442.432019	671.92523	1287.87473	492.863353	736.223176	214.654872	271.216486	310.694976	6.36903118	457.173754
P-33	183.050457	4377.26365	2932.44948	4180.79218	2583.19887	10.4116154	503.035948	90.8034985	784.723001	1107.6513	100.80774	41.3843585	360.980032	588.174492	70.8036533	1057.06536	1704.54631	4521.37684	1058.29204	1273.91057	174.098654	488.370508	673.276732	14.602103	1824.92098
P-35	150.073878	4446.49356	2160.07481	2362.67998	1874.42836	8.70276349	332.585709	142.753626	894.808441	919.238851	70.9762351	28.2555925	299.098944	380.929355	14.1709479	741.659773	855.737646	2055.52938	678.165333	1222.3703	564.588683	313.516136	431.302768	39.1523662	796.693362
P-36	150.46377	2879.1875	921.60082	1467.28059	1099.65385	25.0932946	240.757234	23.453334	587.40276	563.610832	66.9854236	30.5283046	223.313596	311.078668	64.7059553	644.072688	634.331845	1678.7144	646.171251	958.57065	512.045415	257.098093	417.360991	25.6426759	788.002792
P-37	46.2679275	34.6102491	11.1955183	79.5255424	36.4362529	13.5910185	16.000674	33.5909614	84.8480615	107.032195	5.90459393	5.87055514	62.5946471	114.77017	12.4475313	34.8322244	29.2183348	187.072909	35.0822335	70.4502411	17.0050946	26.1784679	25.1185772	9.47550527	10.6171936
P-38	200.04406	6459.7057	3974.16988	4563.81771	3027.86899	15.8212544	404.20873	99.0160401	1055.92986	1162.71744	121.834084	106.268912	471.843821	501.741291	43.8190048	1113.46832	1515.14663	4638.38137	1471.01169	1715.14297	228.647814	362.408707	463.206783	59.5032477	1523.82475
P-39	260.377354	2593.43088	1785.25873	1641.33527	1270.53375	13.9507502	453.043496	25.5244439	396.001031	280.365035	160.45539	78.1672273	380.386405	320.606725	22.2913834	950.810925	862.571978	1663.60104	716.675147	891.422793	295.720046	369.214499	301.709073	21.3627464	1524.54367
P-40	146.980892	2463.63285	1206.00804	1853.85643	823.744918	17.2547795	311.14927	95.5522109	505.526494	629.571701	192.17775	21.7561073	256.151004	295.468649	33.480062	194.95456	674.060921	1988.82159	500.751138	737.837286	123.67138	385.730096	455.70552	29.9052216	489.920242
P-41	461.964482	8972.58866	4010.51811	5631.89068	2782.4026	20.3394108	242.354106	200.472452	1683.12529	2308.83235	210.349704	55.4154731	333.837263	644.682211	33.5332498	1106.53153	2709.40734	8101.13499	2838.98914	2334.2263	325.929452	363.207024	645.542847	29.4761926	1739.16129

Table 8.90: Raw peak area data matrix for phosphatidylethanolamine and lyso-phosphatidylethanolamine for serum samples taken from patients with breast cancer.

Samples	PE(37:5)	PE(37:6)	PE(38:1)	PE(38:2)	PE(38:3)	PE(38:4)	PE(38:5)	PE(38:6)	PE(39:5)	PE(39:6)	PE(40:4)	PE(40:5)	PE(40:6)	PE(41:3)	PE(43:3)	PE(unknown	PE(unknown	PE(unknown	PE(unknown	PE(16:6)	PE(21:5)	PE(21:6)	PE(38:0)	PE(d31)
P-1	1806.18422	1637.36832	103.632647	1316.60757	2302.6029	8070.3072	510.0194	7273.79648	945.684748	1537.78768	545.169593	1487.34793	5836.1723	3749.50467	148.51597	1150.6891	138.924708	139.956612	140.651692	3185.83344	821.876087	4050.5873	385.285068	410
P-10	1659.5772	2308.93478	91.7004055	890.302648	869.390779	2933.46897	332.815485	5214.75703	828.779129	1941.63255	138.179126	955.997912	3547.82693	1602.99538	84.0175793	1205.14543	201.880326	149.666375	236.520443	2315.44819	576.273676	4481.61225	243.286902	250
P-11	542.635256	851.676656	191.633908	1161.0427	675.049061	743.310968	107.480349	988.821989	396.924763	592.996099	111.093249	289.913334	791.404455	394.617527	218.825019	1483.42449	295.784093	155.005631	208.708114	768.487735	237.930846	1273.07489	251.954118	303
P-12	750.289866	648.262129	98.8588257	1100.43023	1655.33199	5174.81994	93.4403108	4619.54813	517.271475	624.891567	167.857224	815.184038	3147.35717	2429.25	34.6095219	1341.45792	377.629186	124.688886	204.587046	2816.27334	757.405482	4601.3823	237.110227	183
P-13	964.74635	925.217056	162.97053	969.265048	1765.10838	5251.73445	165.334851	3430.02253	601.901768	676.283131	272.497772	1121.58394	3345.45607	2177.17848	180.031567	997.182478	180.719368	164.618733	127.197009	2669.91891	734.550111	2416.17234	342.128604	324
P-14	1433.25134	1149.55509	98.3539744	1317.05739	2719.2167	10979.5334	194.135421	6477.90567	785.782656	807.360383	481.830651	1600.88128	5345.64032	1807.94333	160.90332	1207.56544	308.177282	170.42104	293.765038	6115.31747	1518.79602	6146.26429	449.716152	751
P-15	486.760007	591.718952	69.0286761	778.753346	672.141905	1442.86743	74.6730502	1103.4076	174.506946	332.038004	109.017568	249.60791	835.809673	428.691352	54.6263516	1389.86094	322.375372	170.392276	168.600626	825.617698	229.554042	1461.15665	288.608195	133
P-16	1346.43365	1229.23879	167.395612	1000.69206	2187.18626	8041.70202	89.2369487	5670.34779	648.429133	1164.21483	292.24262	1274.03511	4583.05952	4455.33088	199.632294	1158.39232	275.612817	89.7039862	126.482041	3619.84611	757.20923	3177.38835	414.375783	758
P-17	928.66275	1006.75483	168.852293	1022.10691	1262.98527	3595.33614	103.070541	2416.50781	589.806864	533.423652	229.136427	797.0278	2465.64557	1636.5967	148.153159	1328.83987	358.819415	116.944829	141.434088	1839.84919	551.582089	2432.27346	299.256533	197
P-18	1668.28062	1938.60273	242.66022	1728.47557	3604.11383	10796.0404	481.662818	8652.98429	921.869959	1743.84656	360.55271	1979.9176	7098.6181	4047.59805	160.674006	1124.69335	184.914636	154.523694	205.040176	3921.73056	1180.12043	5168.21179	483.183499	711
P-19	778.279498	755.380371	106.80768	826.238312	728.232399	1097.27239	132.142187	962.423837	329.541582	486.105433	138.500928	334.805884	658.789318	709.263137	137.8043	998.564233	166.390161	109.762864	171.329496	910.534981	206.146952	1418.54628	268.46706	261
P-2	1150.17879	1345.41851	105.311877	1278.80749	2084.02139	6830.07577	123.389661	4612.09945	595.961745	1213.24362	436.671741	1480.9996	4673.77147	3243.07722	164.921906	1038.01174	198.297514	108.951637	185.012561	3245.27963	923.920144	3657.37835	570.77363	458
P-20	1413.04023	830.87368	18.6147393	1118.1629	2448.08677	9004.70599	454.316371	4423.86199	996.400489	1063.39691	363.246334	1278.86185	2842.26201	4843.68151	70.4663223	1014.08236	69.6756745	84.2216614	104.412067	2802.40734	676.932153	2010.66321	359.019836	513
P-3	1208.62215	822.336465	161.656384	955.001177	1110.14989	3113.24937	79.5775395	1932.88016	634.397052	881.29368	126.123877	510.703206	1379.88582	2328.3655	88.1145516	961.633923	255.112407	129.576	166.924491	1279.01663	253.5911	1538.83764	298.841386	258
P-4	1019.16257	1455.74653	105.589543	1020.26198	1742.38777	6162.64821	162.457179	5639.12299	566.123779	1286.05444	236.294328	1340.46119	5748.81223	3787.4011	183.799774	1046.46977	268.23156	109.490726	194.709054	2937.05801	690.858339	4539.03179	294.584057	348
P-5	1113.16678	977.219252	72.8563077	1392.46162	1909.01163	3308.54929	197.148536	2822.57799	712.458913	1046.92384	309.480561	807.864472	1625.88608	3746.84053	87.3839373	1077.84536	214.514741	166.055109	101.918416	2513.3439	516.432174	2472.17605	173.88501	343
P-6	12.3574258	35.9158643	16.2084966	87.8851274	90.8281326	346.75735	13.02424	199.335748	31.6701588	26.6163606	3.2615303	69.3102831	142.576285	85.7337487	9.62734755	13.2010105	11.6332887	1.52561255	9.36132712	34.2044672	17.4402834	7.33280531	42.5937246	320
P-7	1221.76345	1148.55896	81.4299048	1149.68257	2200.0903	7735.36934	193.657279	5312.94768	571.932983	764.156074	350.052968	1161.11781	4249.05563	2356.83265	155.306553	1380.16407	191.060895	158.282021	205.57714	4278.89797	1110.62389	4731.96086	202.691115	321
P-8	1893.51886	2551.30972	70.487626	1022.97396	1110.82306	3812.02141	219.797954	4085.2698	703.453885	2045.54082	263.790358	759.056434	3166.95927	1395.7131	262.815559	1454.00853	227.30094	153.36478	202.990033	2767.95297	609.345348	4466.6525	339.971923	326
P-9	49.80168	16.3060595	10.7087789	47.0771801	56.2179166	192.790742	6.66034318	92.2452395	28.2886467	31.2225776	23.132727	86.2464902	91.3843817	104.04689	8.84705326	21.9195765	10.9580396	11.6333175	12.7093234	29.0766123	28.4977932	20.6376286	9.44462224	418
P-21	1378.72564	1316.47246	91.5502306	1220.90686	1410.50822	3668.50558	223.629229	3578.63095	595.524747	962.936992	102.520038	929.372716	2498.61835	1024.90034	121.427514	1553.33502	411.021423	174.022347	178.502279	2440.39052	1168.11817	5335.12719	318.302575	421
P-22	644.1945	623.145315	163.505986	1091.36247	1653.14055	3334.99045	164.164652	4238.19354	399.852508	704.188561	163.411714	800.880821	3004.69715	1059.81254	84.8128506	1519.48499	318.353322	165.088638	123.501366	3450.2374	995.013887	4903.59052	224.928727	504
P-23	828.717209	1067.555	133.906524	1194.9687	2233.83824	5537.80974	268.350194	6895.58666	440.953132	713.846709	231.60462	1276.47373	5377.25775	1165.46031	150.491695	1379.15601	207.193625	148.124558	135.195807	3851.32208	969.106141	6733.18327	195.030152	740
P-25	1005.54596	1156.59681	108.879144	1048.2098	1654.97325	3894.02397	66.5518629	2981.94084	537.563216	773.177858	283.98325	582.829415	2447.24662	2947.38825	128.058569	1027.66638	239.142242	116.864613	167.929086	1524.09236	500.562453	2469.19458	314.814944	308
P-26	2956.66548	2424.79244	58.5404705	1605.14846	2774.85382	9121.88122	298.308387	6958.52676	1312.42227	2447.82263	477.969855	1671.01073	5115.5072	3340.13824	80.0639965	1375.85135	227.332318	207.637	293.361879	4382.14544	1649.54231	7188.49575	665.491303	723
P-27	949.401682	918.472289	53.2576124	782.315629	1439.53034	5077.9158	201.267521	3021.09055	492.246309	783.518409	246.95785	754.645036	2911.37024	1712.95883	58.232729	1342.18588	310.674746	140.481194	197.232173	2252.91502	575.869879	2686.25117	272.549194	477
P-28	815.595038	793.277502	89.3274718	1144.04831	1003.25188	1856.0034	116.138725	1295.70936	391.578767	602.555231	101.020497	363.91733	1113.68981	813.369854	92.6688225	1361.22485	199.354342	143.079598	196.864014	633.409943	191.045071	898.517607	266.082103	166
P-29	902.300304	1593.34535	152.397408	1276.0644	1890.2458	4584.05436	109.644549	5643.52074	459.981235	776.575107	159.317113	1035.21245	4212.20331	1815.57496	124.697442	1625.98501	453.588992	120.485971	108.571761	2750.7312	691.579404	5411.1658	258.377741	389
P-30	800.809106	797.7644	110.796422	1035.93331	1477.58394	4691.47682	160.778786	4934.20233	642.65324	865.641197	109.164178	1021.269	5141.50451	753.112073	229.861496	1540.6016	430.045228	305.093398	148.783568	3747.89722	1186.94779	8016.5975	306.119204	552
P-31	1422.89099	1222.61616	92.9523942	1115.4195	1385.85395	5023.51085	103.509333	3423.35956	574.370757	818.941913	133.191259	749.344149	2516.77262	2320.93233	43.3413596	1325.12403	295.198546	142.775297	116.214123	1548.06004	415.667314	2061.74358	220.48085	211
P-32	649.282513	932.621635	52.291233	887.230768	1057.16174	2235.12589	172.592949	3068.14145	355.367768	628.10083	92.278841	566.523319	1869.55625	1172.70983	195.233677	1159.66551	143.231784	107.5599	166.425846	1232.90555	213.692823	1433.63603	211.765815	330
P-33	1536.13943	1389.11084	68.4571534	1159.39162	1364.46959	3882.31775	151.910156	2227.95388	965.737399	1155.05801	142.498183	659.560856	1815.68052	1495.03311	174.402102	1639.52198	349.963479	199.027655	283.989188	1573.81002	1004.94159	3052.53283	433.732343	395
P-35	1711.35499	1788.71404	60.1890723	651.715458	1131.98814	2541.96235	198.152772	3322.47186	721.980013	1048.99385	210.64313	781.375609	2369.44532	1377.99236	11.4178014	977.195407	244.631541	106.758034	129.935173	2292.30844	985.518925	4389.71787	332.585709	377
P-36	1210.57003	1322.31556	177.192434	791.385387	914.953619	2977.03809	99.85303	4013.35512	602.961986	936.51488	136.641652	772.528891	3106.68078	1096.18766	110.913924	1059.72892	179.95499	85.1074358	164.373615	1525.40826	437.579191	3039.33495	240.757234	200
P-37	8.69161007	34.1010963	10.7107908	65.2795314	75.057207	178.114399	3.33162087	95.8748032	61.4437473	18.2087361	33.1962912	43.7386311	80.2628624	56.0903821	13.9529313	13.6844935	16.9768957	4.79891694	20.6254062	41.0914604	24.5865548	10.4589834	15.1776349	609
P-38	1192.95761	622.536489	162.61412	1078.33824	1817.38265	5100.22288	111.459096	1865.81248	486.265119	406.778846	373.832044	865.488416	1621.19427	1319.82677	70.6528091	2120.01204	310.545122	149.558345	226.234253	2214.75422	882.399019	1873.92027	404.20873	361
P-39	1665.58291	1614.28072	98.5502788	1098.79608	720.985724	1691.07935	94.615502	1682.7267	894.252699	1114.1508	102.148892	496.050382	1419.13999	605.344979	85.636798	1559.73706	279.72365	187.968248	206.76317	1413.34564	442.91949	2938.05458	453.043496	267
P-40	627.423059	439.441606	79.6560351	1042.34417	1101.96655	2429.72763	92.8982484	1888.72841	349.268241	502.290219	140.824821	492.541997	1665.415	1075.56417	71.9664733	1550.79917	343.499799	152.428548	203.788981	1151.77287	328.398822	1609.28488	315.019803	208
P-41	1514.89589	1249.13822	91.4595493	1184.36796	2296.33621	6915.6998	245.30961	3865.00087	937.645068	907.762838	392.044124	1262.86615	3881.16164	2784.73495	233.456553	1634.68065	332.202595	178.429587	205.943172	3295.5687	929.471663	3686.59096	242.354106	857

Table 8.91: Raw peak area data matrix for phosphatidylglycerol and lyso-phosphatidylglycerol for serum samples taken from breast cancer free controls.

Samples	LPG(16:0)	LPG(17:0)	LPG(18:0)	LPG(20:5)	LPG(20:6)	LPS(18:0))	PG(26:0)/die	PG(28:0)	PG(30:0)	PG(30:1)	PG(31:0)	PG(32:0)	PG(32:1)	PG(34:0)	PG(34:1)	PG(34:2)	PG(36:0)	PG(36:1)	PG(36:2)	PG(36:3)
C-1	1517.31395	291.314468	497.258604	224.196921	290.232228	26.1975904	136.970702	366.872798	828.044948	155.280866	113.92911	1449.23835	42.9396499	392.300568	2236.31863	523.426734	56.6549101	195.75376	668.105863	164.100772
C-10	1662.21453	175.189457	262.576898	317.908832	319.515206	42.9789041	104.881565	99.3870768	164.583668	55.0044089	102.660683	346.091865	187.176424	41.8394197	516.507226	256.44086	12.199863	89.9589413	145.888746	68.4973862
C-11	1511.63496	176.448844	530.540719	366.211629	260.304382	11.5375471	147.911524	169.547122	195.557226	91.8531737	93.6228991	247.8077	96.32121	79.6056959	446.888057	211.449449	12.246475	33.6656293	77.0141504	52.610442
C-12	757.147832	503.97669	672.648041	169.144708	259.897793	34.6362832	94.6289298	66.7369861	40.7336407	31.8047659	12.3628337	69.5658109	58.4479643	57.7392429	76.4294358	44.6266847	10.1424552	16.8464386	20.9249216	19.5033963
C-13	1104.14892	170.979727	114.520539	406.535268	294.11884	18.0695269	27.5958534	23.0846178	43.3750014	26.3622793	50.2219141	14.2776706	31.2099185	77.4456674	28.8159028	9.64944362	18.5897549	26.751384	14.229937	16.8366981
C-14	1573.52173	171.089975	264.219373	334.20379	473.012962	21.8512124	36.5639761	39.6763513	27.0905378	14.2479813	35.2965947	69.0383723	17.0230101	77.0806174	15.2977561	14.0588499	12.0328724	12.0208748	48.1545261	
C-15	1940.26263	422.309763	577.634861	286.083471	326.314946	28.13211	24.8660093	47.2249845	94.8183053	14.2934731	33.0927689	174.071741	88.5817071	95.905402	222.622788	68.5538647	19.4027547	30.289739	82.0330466	18.7944062
C-16	1446.29643	571.892426	920.796154	220.16836	196.640373	71.8854558	390.399112	473.42089	629.295419	346.188404	165.608298	941.867505	662.552875	695.288847	1688.35067	680.932014	82.8111002	505.222088	1466.42017	541.400603
C-17	1991.31068	739.588893	998.645784	450.611487	396.06876	58.4460395	100.296988	54.0673859	99.0639423	34.1497469	91.6920442	121.493927	42.9965118	25.1833207	231.715277	19.2531138	14.8932058	16.6910681	34.6327731	15.0597073
C-18	1716.42881	260.339836	605.301422	207.152576	182.646543	31.9971754	211.115371	132.866428	338.774393	59.2714643	115.312025	572.451835	232.949419	247.443021	450.928109	142.490079	57.69498	156.984838	165.306637	82.9162994
C-19	1834.16255	121.336875	328.583907	146.109499	151.214637		78.3320197	20.9726859	14.1487197	16.0568567	68.7662744	70.2660181	24.8612677	33.1221248	23.6985681	12.394734	28.0094465	56.9528209	39.8183025	15.7004056
C-2	1398.04125	516.291281	834.49983	363.495751	292.221002	15.5505612	192.721166	124.618711	291.846281	19.1529639	25.8742865	374.478769	13.526861	172.137693	530.026108	186.510232	63.5018255	26.2148678	150.049384	40.5691842
C-20	1339.20458	585.35022	818.894177	275.855191	342.74821	15.1510484	129.439979	134.034938	169.685747	52.5614762	43.5486659	233.271562	59.204852	125.453418	152.271799	67.6713707	51.9573013	31.5631777	39.5636217	5.84829786
C-3	1565.32666	292.541782	686.432506	244.458915	340.123892	20.4361155	128.790487	50.0446218	95.693096	51.0630516	46.9440521	238.613484	131.255444	165.576789	489.296337	178.65204	20.3406093	63.4637617	145.61036	31.2024441
C-4	1668.23991	161.372592	403.963807	174.994714	165.850943	42.1324785	195.827741	177.852972	255.931205	144.393728	28.1623368	516.910898	173.177564	126.634378	494.520157	190.531969	33.1852064	89.328606	162.774326	48.0391135
C-5	1920.94386	175.496993	256.218781	430.816715	354.711849	18.9097665	62.6156291	90.9039769	169.068998	66.6751517	66.8243294	329.752625	98.4800332	177.590302	309.668557	84.4581561	10.7526948	98.8529054	54.187921	42.1319586
C-6	2250.586	151.708926	223.716012	311.557062	402.076201	11.7607547	115.998155	12.7818811	23.9332794	29.5382719	54.8385338	72.7556519	4.38673259	54.4068258	10.9946567	16.5008962	11.0915661	15.7327491	14.4912763	21.048572
C-7	1687.64047	537.768023	575.765652	131.704299	169.745487	54.5802074	83.2396108	78.8710946	64.5232049	7.14153963	70.331632	140.913182	105.862124	64.6436314	142.746591	75.9263933	9.58904442	16.805628	41.7384578	14.9392484
C-8	3638.11963	412.895317	508.095914	222.198295	255.649133		174.986304	380.042327	579.706576	189.397014	53.406841	1268.10158	353.922506	386.202201	720.656534	151.739398	38.9510931	198.010779	139.018184	29.5662739
C-9	2373.26002	157.350049	241.888586	214.867838	234.600933		61.9592567	49.5106536	77.12571	36.0790816	51.3869605	178.388388	32.6042701	13.6694724	108.833894	19.092134	13.8661091	10.5005252	58.280968	18.2758369
C-21	1533.31091	263.539916	438.045786	265.171957	386.964332	20.2351817	98.9425531	53.053844	101.25401	43.5733763	51.1362642	176.626443	97.6998116	79.1327374	209.0165	50.1055324	14.2474323	25.1147062	35.8339535	12.6673882
C-22	1833.94037	165.222201	285.946082	328.860636	350.835978	61.0878586	254.059437	206.938921	432.218491	185.209143	47.2626252	843.61202	463.256312	416.986159	971.145237	233.106522	41.4309418	232.528545	379.219372	162.745445
C-23	1346.79913	166.234533	286.786578	291.188741	312.91471	18.1184471	69.1597389	5.35099712	42.9878079	63.0552538	123.316008	97.0537425	22.0498777	56.1320884	70.0189904	36.8347837	15.0524345	90.3811645	75.3150366	42.6007857
C-24	894.427961	118.325958	226.332892	376.784411	337.316786	43.3325056	32.9972436	6.03755582	68.7930798	22.0826671	63.9325934	136.850343	68.4342696	32.5381041	195.237723	65.2029567	13.3652208	21.762133	44.4457549	11.5822088
C-25	646.106418	219.217032	295.359694	336.81467	236.017492	17.6920166	135.991519	45.1249806	78.213164	39.286817	50.6748847	269.183287	196.246609	110.902239	481.827993	102.875514	36.7740354	55.6265824	162.496573	83.6420946
C-26	248.091044	167.19014	244.695304	271.918105	298.12746	15.5514823	130.066627	34.9393279	78.4399639	101.413815	31.3571963	200.851582	93.8177816	82.7378635	210.978545	104.474242	17.6345325	33.518127	126.801821	47.7456177
C-27	1230.46994	225.313251	228.266978	286.722252	289.067821	11.1756007	117.045059	17.394865	109.616737	39.9399059	135.217352	145.267532	49.5429947	68.2191536	202.064331	48.8719354	55.9307758	42.9450735	71.1260731	69.6704007
C-28	1027.56323	271.785593	404.462875	302.959118	344.973975	12.4468765	157.177493	91.8733296	48.002884	25.3579813	125.478371	51.2642224	39.0139328	37.6753242	92.2096045	51.5550618	33.0748627	58.5207693	116.912325	29.1916182
C-29	1295.82328	293.228313	311.870759	371.525616	273.028907	22.7294723	32.8644594	13.4803316	45.5392298	12.7238133	105.583262	51.8937423	80.9066962	39.17307	225.010297	136.813311	33.5622211	33.8143152	98.7838108	55.6949721
C-30	30.6472131	171.220538	421.481155	58.2231992	120.953331	25.8515517	82.4414591	70.0002585	9.28980333	4.93424602	14.5816286	66.3670649	8.26110934	15.6597963	23.005237	14.6100162	9.37707563	11.7313873	10.4700979	11.2016779
C-31	1540.50306	136.963434	163.325202	400.079837	404.916195	25.6151001	105.586584	37.2183039	40.880984	12.5826787	102.375291	87.1590272	55.3855456	44.1740056	57.9382142	51.2488733	58.1181405	64.5135935	18.4002385	17.6936772
C-32	984.555849	141.586978	325.173897	318.682827	419.947003	15.6747883	99.2714892	18.1068755	19.2160846	46.2690275	18.7473907	43.8855409	19.4162993	17.72475	11.2536287	19.5250912	25.7947964	55.31619	19.5449694	15.683231
C-33	855.154776	414.740077	304.501265	164.785605	207.59839	35.7962906	799.084798	1192.93365	2493.15247	882.145124	224.049391	3605.84027	2085.12657	1171.14516	3714.36421	1685.78617	47.7659498	292.827126	883.908637	459.281077
C-34	1742.00446	134.320672	165.682588	415.494011	389.819711	75.6179412	78.0287671	90.7748038	302.204291	86.6509386	52.498053	931.005593	474.872258	273.277295	1370.17976	432.538586	43.9721114	108.862063	163.14973	39.9741763
C-35	36.4982494	204.862888	386.507326	76.1929403	32.2600465	27.5084583	94.3666088	69.6497208	16.8152942	5.12397746	9.28471517	32.4422194	9.70225307	19.218763	16.6903012	11.6742101	12.4904652	22.3745006	25.0409893	20.5461536
C-36	1127.56902	308.329526	473.170775	167.101336	158.12983	47.4758439	60.9026332	18.2618237	39.1246138	13.5997719	26.802381	77.3045697	67.6341929	28.0063106	150.852657	12.8294431	33.0643177	43.8776186	61.41122	108.375147
C-37	935.167027	139.581423	112.316593	351.566393	298.880046	19.5894884	50.4453585	27.1539355	57.7400431	16.2401543	50.40553	91.5801012	46.1490344	11.0604382	130.668089	75.4029827	13.636336	25.9224217	58.640452	36.9104485
C-38	953.721052	131.895064	352.685316	224.523531	215.87671	14.8127778	136.15119	23.308461	25.4091938	8.64674924	28.1545606	81.7322356	66.6617601	16.2227128	68.6137657	20.4707687	10.1012452	22.8825497	9.0286516	13.5483026
C-39	877.839508	115.65619	234.563452	346.334509	460.839433		103.730983	38.2863425	84.2748879	47.7789617	72.7159311	144.301777	31.6162359	74.9909669	49.8865782	9.77162348	17.5599686	69.2156781	11.3107328	19.2145779
C-40	1245.10778	136.739416	193.621174	210.651846	217.88603	15.3724618	78.4166119	60.1971885	88.0011755	18.8242282	28.9594416	183.327569	103.105366	73.1165941	124.497464	36.9287003	33.7359414	77.9838414	45.7654858	13.6809196

Table 8.92: Raw peak area data matrix for phosphatidylglycerol and lyso-phosphatidylglycerol for serum samples taken from patients with breast cancer.

Samples	LPG(16:0)	LPG(17:0)	LPG(18:0)	LPG(20:5)	LPG(20:6)	LPS(18:0))	PG(26:0)/die	PG(28:0)	PG(30:0)	PG(30:1)	PG(31:0)	PG(32:0)	PG(32:1)	PG(34:0)	PG(34:1)	PG(34:2)	PG(36:0)	PG(36:1)	PG(36:2)	PG(36:3)
P-1	1929.19989	340.573513	582.207462	338.124257	262.855791	8.44680908	131.94799	89.1916509	172.745473	46.3348945	11.3140432	272.464577	94.8030213	70.4647294	378.574815	177.591215	62.7386983	11.5730517	144.42216	24.8585648
P-10	1597.92466	158.447248	333.858726	419.286132	532.965259	18.5537312	75.6054703	6.82878456	23.4743869	64.1216285	97.2721461	29.2569824	19.3599213	57.7360325	54.6457936	15.3538735	17.1853504	35.7226319	9.48793661	19.5853054
P-11	965.605152	141.437741	167.806501	369.395489	446.235723	31.4959803	81.0384218	41.4723111	19.2879339	26.8124925	99.5143243	47.9195627	40.7182563	129.367493	51.0465005	18.0718355	24.32199	10.7227619	29.5860582	7.67853492
P-12	1370.44581	404.466735	821.459745	251.23925	183.050013	22.244114	81.0898896	29.6537688	31.3297058	23.4719191	36.3285661	91.0491365	64.7414263	70.3968751	87.1273183	29.2465326	12.6666334	18.1796284	48.829563	10.6106304
P-13	2203.47939	491.653721	603.96512	387.341117	214.488681	18.927412	47.0411698	58.6851497	38.1521186	35.8402192	46.4207732	189.001632	54.1550428	15.2082197	243.422293	72.342837	59.6786557	64.3549154	28.1668896	14.0757642
P-14	2719.16244	131.939935	200.908502	326.555674	217.527311	76.4830019	105.294121	41.3585763	147.359612	48.3504636	79.9252083	329.03547	260.199336	89.6639664	495.794883	246.70649	19.296484	62.9970678	194.227168	60.0894453
P-15	2448.4085	62.4999154	147.953202	257.446763	332.805082	20.1856065	90.0447453	24.98988	64.85212	30.1268513	33.3545868	52.0618618	28.0591914	30.4491887	33.9291732	7.48012213	9.72810358	13.5092018	30.9620036	19.2206786
P-16	2285.10857	887.647548	988.061335	187.676157	328.520964	21.096137	200.997575	123.582075	648.712197	205.158643	85.9903253	1361.21892	523.449156	624.176976	1502.49057	410.711187	108.45141	326.767356	654.185357	116.576979
P-17	1499.11155	160.925513	246.897027	334.487579	277.169834	25.3826758	134.192154	141.314953	269.02346	85.6466791	133.891774	626.262465	187.412981	270.848378	815.392107	282.661155	53.951424	96.8665383	227.141111	127.975327
P-18	1562.02006	166.867521	214.772201	146.252165	177.375708		62.5204519	91.1010638	159.689223	51.1835157	50.1412251	432.398489	220.553501	128.627061	810.263531	282.954243	25.6159786	57.3946164	206.120589	157.116615
P-19	1840.23548	117.230832	91.8619209	679.91954	708.828604	16.9358021	115.594571	24.9355534	55.5621237	34.2400073	50.8677195	114.890441	70.2875177	40.3085751	146.775682	18.319597	16.9351219	49.7176977	35.9797971	27.5708497
P-2	2209.6804	283.906687	429.470622	275.321915	335.07872	15.593268	76.2957882	20.3634714	153.368411	61.334242	21.8003593	255.560206	189.260739	91.9259528	386.817914	100.478923	59.6069752	88.2697071	138.140297	13.8218493
P-20	1572.12042	525.930462	570.858346	194.583261	209.743709	11.8049558	69.7233354	25.565319	120.047722	48.2757839	22.0264641	38.9536497	55.0946933	79.100105	174.82357	40.3207538	25.2485506	50.7654506	131.329111	47.6609478
P-3	1850.85266	73.6453431	247.639266	245.275239	239.035811	31.9597753	75.9450604	15.2064253	55.0709234	23.8074876	53.8537576	72.8517625	64.9538868	20.7053032	91.1486284	52.7018138	11.6936202	31.9419161	50.4578017	18.3791146
P-4	1813.10913	147.51754	315.496384	341.014336	303.426884	21.2207168	91.1731597	35.9271944	24.1487698	12.3973124	55.6521573	42.4510752	33.3716469	30.8766673	45.5908608	11.898695	17.2205099	14.6378674	43.0299225	21.2427055
P-5	1365.11351	239.901467	434.130642	146.463864	169.435753	23.8891753	116.6551	46.4497626	70.6222373	54.0425094	32.3604392	73.3111017	14.803658	66.2424704	89.3329202	10.0274152	15.103306	13.8097464	32.9105995	18.3336356
P-6	39.8717116	256.383445	392.659673	47.6875958	58.4549979	16.9058411	68.0926722	19.549177	40.5833579	21.0603674	9.22976002	45.5519364	19.6548326	23.812083	12.5103284	23.5071095	19.3297655	14.7945155	9.99858863	15.7387181
P-7	1546.15473	367.830335	516.105694	443.632663	437.639541	46.8929334	114.655524	66.2090819	259.450229	81.8089768	48.0113107	294.512649	110.464516	113.989124	526.414719	128.027742	41.7677948	15.8640058	71.5273208	46.7802307
P-8	1637.25696	153.945157	235.206519	417.121452	330.03162	13.7229736	77.3889344	24.0105356	68.1097745	44.6751196	53.3852616	74.9634117	48.3967714	78.8610652	103.076107	55.6953175	28.2204619	34.1689277	109.915182	33.5143874
P-9	30.4155389	165.197227	293.24886	66.0936169	50.8574143	24.1810176	73.3861215	68.2662441	62.4635341	8.42934361	25.0553701	19.8781786	3.32028757	12.6953637	20.9646067	15.1615041	12.5533376	16.5906909	17.2318033	21.9612738
P-21	1248.45375	114.133452	258.202717	305.707916	144.892698	22.555992	46.2845198	13.5135591	81.4489658	23.7363169	43.7268297	106.039841	90.0256971	41.6529665	158.743947	61.5448075	11.4044899	63.0636038	111.487875	26.715586
P-22	593.607855	265.1834	504.772163	323.874557	311.343889	38.7498138	70.9800848	2.19836112	103.864953	22.9415428	21.9534807	325.493575	115.339618	113.259023	365.70057	115.714998	20.8246534	57.5595702	98.5556603	72.5276921
P-23	921.615145	205.364832	328.310168	316.904167	377.381312	30.2478894	98.7004598	34.60315	65.1654741	26.4773136	46.0462543	84.1662386	58.9665625	30.2973714	182.815876	59.7986749	50.8200455	36.7526673	107.662098	65.9801582
P-25	1706.50637	428.504991	532.628067	211.183214	305.50652	19.6243147	77.2891389	43.2763611	41.5184208	25.410319	29.053803	66.7541098	17.0708242	78.9716013	75.8447434	36.3843701	32.7092661	19.7664273	54.8164331	17.7060828
P-26	2384.00156	325.133339	265.008709	274.833737	204.007883	13.2087229	79.6785157	47.9433341	111.960663	69.1792366	47.0889918	423.281981	193.027382	182.921466	896.865931	387.058631	40.6814743	229.502203	334.107294	86.9426388
P-27	2181.0212	243.110563	279.181336	329.816131	315.031545	55.8711881	121.365298	19.6300533	69.2620927	5.20069113	60.2242867	189.332894	111.275744	34.7613378	196.67609	100.951222	50.4358988	51.8934845	79.5133178	27.8641184
P-28	1068.40609	159.147196	198.263432	235.426365	255.557683	11.7428458	33.0650268	22.5608243	14.1157565	11.3265731	42.0822048	57.8569172	17.097518	49.6607942	16.48691	18.5820471	39.3064603	11.469259	20.164791	17.6942175
P-29	1807.92354	287.796822	313.831393	347.610223	384.514175	12.871548	17.4751199	13.6999633	69.918781	43.4053386	15.0913557	82.4102565	40.9615618	46.4947606	136.455848	31.4015455	41.5038544	15.2976249	61.1601455	6.93912745
P-30	1117.74958	144.334068	206.986898	456.063687	430.140076	11.9587297	127.631234	135.555972	203.05695	173.832317	78.3334041	422.952682	405.294631	204.914345	945.958019	300.413103	14.3107718	227.981037	598.315396	223.052949
P-31	1283.81194	197.817805	382.852905	249.291513	274.374454	26.2081032	117.401469	31.4149524	45.3308984	8.95366035	77.5021685	92.2971138	57.0009528	53.5963226	66.3474627	28.0964788	7.23669682	39.8547221	21.9946057	21.7020827
P-32	1105.47189	95.4667309	287.158531	283.277309	344.443302	31.0050078	71.0440902	7.2990029	72.5685835	34.0327641	53.8844299	37.2910323	45.3076255	19.3454657	35.0593555	12.876327	35.4386888	36.4844257	13.2559548	9.57556078
P-33	820.732436	317.731427	501.38615	193.116476	206.973429	41.4036957	94.3391868	101.932327	191.343842	14.4972454	81.9222957	501.239461	141.253739	206.442175	376.898813	107.199698	63.1026615	101.881563	179.366729	55.5739186
P-35	763.87247	273.793512	447.909264	370.562714	344.527826	31.407994	73.652992	59.8374077	137.592931	56.8077069	46.8183045	337.737517	136.758279	53.6158435	366.109929	115.081397	67.2646706	60.6566981	90.9164592	19.4666295
P-36	869.009969	93.3081227	225.267066	339.07037	447.258393	23.6164906	40.0270798	24.141342	77.1791924	13.078796	37.5194652	64.2102516	38.1921994	13.7592864	14.2331884	11.3709639	14.6327023	28.8046274	15.4231545	
P-37	33.5321893	227.718685	453.986883	42.1233489	45.2320766	57.4042266	171.070042	59.6817601	34.1547058	5.97634159	14.0292383	46.5611829	19.4210029	8.61384753	17.0655915	9.7830967	17.1067916	12.3692586	16.7748709	19.8455169
P-38	1646.10153	124.375535	235.296043	244.565924	254.899234	32.2607514	117.014298	36.3018788	75.8328661	26.3631229	58.937626	170.318561	55.9067671	83.6623383	262.68035	85.2357139	24.8367289	30.8974944	57.3958916	51.3091443
P-39	1067.38207	102.736353	220.01009	440.095477	541.834288	39.6530356	85.9861819	35.1356453	11.992611	30.3831156	41.4574092	89.0002582	51.6562648	86.0291804	75.425185	40.720535	23.908665	68.1186578	42.242136	21.7923263
P-40	1374.49871	691.843907	972.149937	210.375735	294.069503	28.161759	160.072009	100.07968	57.9777519	6.9709701	17.5327115	29.766273	63.2791938	46.0099598	26.546282	10.4422759	27.7155152	17.4004773	50.8231094	39.5297094
P-41	1265.78832	160.313846	312.588079	263.459937	387.156445	19.3192919	132.624833	137.496859	363.62678	139.134158	32.7099941	634.609081	291.409721	399.934731	994.992756	220.57951	141.590227	154.859699	377.103134	86.8606919

Table 8.93: Raw peak area data matrix for phosphatidylinositol for serum samples taken from breast cancer free controls.

Samples	PI(16:0)	PI(32:0)	PI(32:1)	PI(33:0)	PI(34:1)	PI(34:2)	PI(36:0)	PI(36:1)	PI(36:2)	PI(36:3)	PI(36:4)	PI(38:0)	PI(38:1)	PI(38:2)	PI(38:3)	PI(38:4)	PI(38:5)	PI(38:6)	PI(16:0/16:0)	PI(30:0)	PI(30:1)	PI(32:1)	PI(34:0)	PI(34:1)	PI(36:0)	PI(36:1)	PI_Cer_1	PI_Cer_2	PI(34:2)
C-1	40.8404518	36.5491285	16.219		414.589104	25.3397367	29.205872	493.310242	972.41021	278.313069	433.360652		34.7065402	16.0295679	1419.28216	4407.08266	282.214612		21.5990907	10.4759326	35.1190898	19.8917791	54.1836437	99.9836869	101.120016	401.045018		23.7869026	283.574896
C-10	16.015322	11.5765141		14.9605267	51.2491556	39.9201569	19.6487172	16.9967208	49.4229431	76.4875538	15.5880036				34.2202536	364.156382	97.9568022		11.808743	34.6036521	11.3129425		25.1868226	27.8844946	43.0680866	58.6852328		21.6985923	32.863754
C-11	21.4894134	73.3116696	32.4091704	14.6646769	238.106712	11.1535075	56.3164418	350.901662	679.869599	217.394408	142.429345		48.9811152	39.0294074	592.915008	2153.51795	79.949393	9.38211859	107.165839	9.39810273	18.3798841	25.9397887	20.0751403	58.8420148	22.5780481	251.668742	17.6246073	15.6962349	319.966871
C-12	47.9534212	146.738395	22.333421	21.8792506	230.257902	43.0369126	95.4880374	220.120865	1061.09451	321.761894	236.658823	26.4286744	38.9948758	41.4323373	537.153795	2326.39867	215.152195	28.1656431	13.7146607	24.57612	33.2177611	17.3770044	56.9346212	157.555714	37.343595	106.953132	28.943807	13.5996889	199.262491
C-13			12.8681948	46.4240827	7.34597419	2.41714241	4.55533148	5.88184424	41.7308942	15.0079231	50.1402903			14.4798638	28.786343	26.5396137	10.5988903	16.9718545			24.4236632		2.94182899	2.55114582	4.82551912	13.0135403	15.2940377	16.9544059	15.7076583
C-14		20.8401868		26.8361565	14.821424	1.4925853	3.41111182	8.25677401	21.3570039	12.7636424	6.19759493				1.98457449	27.7174715	31.4645572			26.5780489		24.1011115	3.64209896	3.23558237	18.442737	1.90232247		13.4516497	2.42218373
C-15	29.6509054	30.510055			194.475446	1.72385364	25.1502629	120.915221	132.374929	11.9108318	95.4536815	21.7636474	25.9081012	46.5877476	97.9701721	267.982465	61.815965		24.9917157	17.8455821	20.0256469		24.0430557	11.1004169	6.87836136	111.097063		10.2444941	16.5173992
C-16	28.9728576	86.2767134	17.910057	22.4206923	532.927662	65.6237868	67.5169628	548.323239	1537.50428	345.143147	321.057766		49.9462771	21.4085686	840.8214	3631.91143	390.453074		92.4068005	19.8699555		12.6689493	125.831328	62.7123138	160.930649	119.767428		64.9150946	259.251493
C-17	92.0133894	71.4962651		20.5206148	237.674318	81.9993362	9.00538529	248.565126	609.416125	326.62272	262.193597				710.512779	2141.42719	242.516877	10.7810558	17.0443684	24.6268537		22.2041384	80.6704435	33.5425733	165.181793	221.441124	12.997578	14.4215695	250.636507
C-18	17.3690123	29.0924446		22.2417462	95.9503377	63.5878558	126.927896	196.799428	623.395651	265.666054	178.894561	21.6365614	43.6991808		330.176382	1209.48079	65.1216503	16.926496	19.0099889	19.7721699	23.7943954	15.7834529	2.00139447	13.4527085	32.8804621	42.4617332		20.9910118	35.8382383
C-19	14.8094383	10.4546738		8.05545469	81.5511027	15.0510671	11.8089756	51.906758	144.709572	77.1917844	64.4452355	10.7350168	16.3001766		210.097356	453.19255	57.1725854	18.7482119	20.5090896	30.1340341		24.0713453	2.97909945	31.1006778	44.6344205	66.0018437		26.3034721	59.7304625
C-2	36.4337177	167.642404	27.5546234	14.3942791	709.859306	38.3205676	79.9905352	534.653644	869.571397	505.825883	629.436522	34.6509191	17.6071515		991.578664	4006.79916	332.570106	18.7325133	39.552474			16.2363617	8.75066622	47.322173	219.680207	227.907854		19.4570309	152.158335
C-20	67.8830616	74.7338558	39.7075643	18.6970599	405.68246	17.610318	34.611374	307.166225	834.419477	303.879803	216.222688		62.1038217	28.4955444	401.02355	1861.08947	199.049805	28.1354112	69.1012987		13.0129655	16.2125813	14.9174964	48.9386687	145.952208	289.137164		29.448403	280.146357
C-3	21.6621017	66.227505		20.9734689	185.913596	18.7423594	130.534265	532.878196	871.115964	214.671619	268.674043				461.542145	2149.67846	317.784362	27.2962314	23.6211601	19.15547	43.1979292		8.1404013	23.3427339	76.6440291	124.288845	23.6869649	66.9759555	211.533203
C-4	26.8682271	38.2777411		12.4642649	54.33757	0.78081112	2.40051007	143.737596	23.4415643	97.8329328	98.0885684		22.4551695		74.9280573	211.323559	28.4028905	18.8750471	50.0369513	30.227234		24.7475066	1.1338183	8.77019199	1.30405913	8.66579486		24.0409392	87.3732797
C-5	15.6407409			27.7466674	29.0048915	1.7281485	10.4216017	75.7265468	28.2544842	69.8890511	14.9369845	10.3413916			14.8627998	46.3970744	50.9993016		13.4408385		8.57640068		16.6882274	11.7019411	11.5614724	28.3040205	19.1676978	23.065414	9.19807973
C-6	27.1809368		17.5484853		19.7001402	1.79126942	2.41992794	115.348176	214.6848	43.0212331	28.6178606		26.2413869	32.3108006	159.886971	104.122875	60.717726	10.7833141	8.44369244			16.0916549	3.77035001	26.5800919	3.2708156	8.76995873		30.6890368	5.02720755
C-7	15.4581056	49.2928838		16.0221758	349.382418	40.2380042	42.5610087	541.668217	1326.43495	611.972524	552.316233	15.4026904	30.4890649		1021.76195	4283.82517	329.331591	39.5854013	29.6380665	24.8695971	37.9397438	18.1240466	75.2024098	101.021009	98.087422	365.505368	19.2471422	50.3745081	543.874247
C-8	32.7335478	44.9111252		13.3367879	281.191137	38.5018738	5.33756166	320.545668	459.193559	167.893623	119.603766		30.7366161	21.6707187	242.925564	804.335213	208.305879		66.1634077	15.251473	20.6723661	14.3378762	12.5027557	19.232518	25.2058	87.1144245	28.4813226	12.0950361	49.8720141
C-9	49.9678263	18.1720933	15.5580583		18.9661102	33.9164598	3.27316113	37.1183928	85.138252	29.5154537	32.0612008	18.25453			69.6368025	98.7683063	14.6616624			17.5804117			2.23551105	2.55900227	14.8252992	11.3013184		9.5283726	20.3266439
C-21	31.8902006			21.2210575	19.8477314	1.64028162	6.41506565	89.8003076	73.3915698	23.3372948	53.4442784		23.6239327		6.79589088	157.579113	43.5066963	11.6837361					3.2748733	8.17489787	3.52858951	8.9636986		23.596447	27.3018893
C-22	16.9245921	23.1370446			36.8626089	3.68995883	2.06205226	26.0825971	212.630443	97.2321496	154.881771		44.9080909		509.278145	1752.7863	122.894985		36.4033624		27.0514536	19.155458	1.566954	15.38135	76.3220363	12.030058		19.9102703	30.1251755
C-23	30.4955737	18.4424353	7.92370264	49.7164806	138.744873	28.9663774	16.8386352	52.1272751	321.543764	25.6546347	85.1109525				213.998346	716.157698	35.452911		24.0348205	16.1878342	8.773797	19.1555951	20.124075	44.0506628	69.9076117	83.8069791		3.82778228	81.5098429
C-24	10.7948309	46.51668			11.8374334	3.02996957	15.0033699	72.945908	56.6574946	12.2562549	34.3928107				144.01019	182.202348	12.2307599			16.2438983		27.778843	10.0871223	9.2544022	1.00936284	29.6496247		47.4705624	22.2510359
C-25	24.3829279	37.5063519	25.2152682	20.3940032	101.291827	1.80945114	26.2012566	152.545196	319.239075	102.747203	132.243211		34.8005761		326.237562	775.347465	95.9803369	18.4297091	45.0766328	20.2257383	17.7959725		1.80972453	37.4130789	60.932312	68.566104	17.5108928	30.174419	68.8427986
C-26	12.0080499	11.9110063			36.3307432	10.916631	11.8158286	63.8233928	115.255716	33.456424	22.6323746	24.3847801	22.9805408	19.8981143	18.9858356	245.345403	17.8573257	22.9451647	9.47986625		26.0658886	27.0743845	17.675843	2.73477389	47.8807528	13.037761		7.80142777	44.7029475
C-27				13.6189104	19.0824509	0.73232436	2.55896166	74.7757662	73.4025879	128.089812	5.39746212			17.7601779	68.8302808	216.513778	6.88475741			9.97313035	14.3378486		29.1637989	39.8405618	57.593635	18.740265	19.7347398	16.7438654	22.6245236
C-28	30.2288251	29.7702238	26.2895475		232.319095	25.2064134	64.0475043	259.897629	707.236616	245.994681	354.878281	17.8178073	11.5415396	14.178483	376.234114	1576.34032	307.361099		28.7892887		20.0105378		5.01547198	10.3852459	71.3945829	319.414626		32.2261396	144.27409
C-29	68.6509982			36.7853437	433.288704	2.25401517	0.79819025	416.749183	1188.66415	335.998731	529.480033			19.6662351	1112.78348	3662.70304	599.291787	18.4534319	64.9909917		28.4492195	37.9549202	72.542004	20.5514136	97.4852369	269.464051	29.6996183	27.0247463	311.645599
C-30	18.3271569	21.7097628			6.36180468	14.4437349	13.1915009	13.917779	31.5337687	3.31485929	5.85869287			10.6687236	26.0223399	93.0112429	12.4241931	12.3173429		42.2108122	21.1696855	18.604346	25.976863	26.6111581	15.3504486	5.79391752		31.7823738	10.4763788
C-31	15.1324945				4.7840323	4.32079047	3.0967149	19.9847191	18.3974511	24.0715408	6.31221216	39.5887196			35.1398716	68.4165389	8.64766416		36.7761446	20.03815			1.56908817	14.5340996	16.6425826	15.067126		2.78709562	7.40838571
C-32					8.318231	2.83868789	0.75530938	16.0592796	58.0790354	36.1285634	3.81655971				3.57941865	40.1103727	9.88468142		32.4337954	12.2470698	28.2197701		22.6140956	1.97955736	47.4257635	35.056954		45.7470631	21.6337773
C-33	13.8975807	241.55518	15.5366004		1241.05967	175.990747	65.089342	1171.78804	3742.12032	1528.28484	2327.04094	12.5102319	30.3023666		4538.76069	12426.7068	1490.48816	10.6575074	378.831918	31.035744		20.2238797	327.014642	150.499627	638.385136	556.379493		16.655222	1430.70452
C-34	56.7678471	25.0879922		16.4492539	202.663401	22.3601298	33.9255112	127.362345	222.802483	95.2208386	360.562113	11.8602688			315.659743	1507.05797	115.794194		48.4456693	27.4892984	20.1371141		48.4580174	15.3720565	115.555775	35.5311109		75.5428236	163.07112
C-35					13.6314877	1.70720023	4.08075699	22.1884524	12.9577364	3.27290061	8.94700937				2.98153604	3.12935061	10.3374764						18.5939385	3.31599516	3.44941692	4.83179474		8.50349214	21.8941192
C-36	8.53286646	25.2123066		20.4695994	401.543702	39.6867882	13.6133244	360.117762	1316.11221	387.737046	381.773308	20.3882191	34.1030831	13.7172637	515.018227	2182.73949	207.502291	30.3818241	42.3393064		24.7333494	21.6399871	99.637994	47.2367139	64.2069343	144.407329		10.8465961	224.63739
C-37	18.7821256	24.4213737	13.0060767	10.7040512	66.3662392	3.40548929	0.76108201	184.722722	479.546484	144.08181	165.00472		30.4315568	20.9461638	160.036508	505.931897	33.746112	11.0522085	19.6352806	7.40438367		23.1774318	44.8728557	16.0988353	61.955014	48.7743562	19.9336271	1.81679686	63.4540191
C-38	36.5307205	17.8203586			103.718667	0.90771717	0.30751121	23.0090243	95.5796794	59.9549191	6.86802841		15.803137		70.0805255	157.960071	56.3378463	12.4592825	24.277991				13.0216805	41.8149889	9.93293186	21.4112103		11.031303	95.226424
C-39				25.3854566	27.8525067	1.87761227	14.0803157	20.7193434	58.8083767	13.4514183					2.60089061	22.2770635	17.2885423		21.3496484		15.6042935		23.2646764	22.1865625	12.7678862	4.47299901	17.0655797	1.73446411	5.98444057
C-40	17.914102	25.8689103		22.8583815	208.191099	2.30578578	2.42431163	437.049851	268.3688	194.348381	198.544098	20.5921643	10.5665972		476.428734	1612.80737	106.578198		17.5735804		23.1728952	16.9216629	43.3747574	35.2975974	30.5519464	171.409298		26.9604236	100.133396

Table 8.94: Raw peak area data matrix for phosphatidylinositol for serum samples taken from patients with breast cancer.

Samples	PI(16:0)	PI(32:0)	PI(32:1)	PI(33:0)	PI(34:1)	PI(34:2)	PI(36:0)	PI(36:1)	PI(36:2)	PI(36:3)	PI(36:4)	PI(38:0)	PI(38:1)	PI(38:2)	PI(38:3)	PI(38:4)	PI(38:5)	PI(38:6)	PI(16:0/16:0)	PI(30:0)	PI(30:1)	PI(32:1)	PI(40:3)	PI(40:4)	PI(40:5)	PI(40:6)	PI_Cer_1	PI_Cer_2	PI(34:2)
P-1	14.8604806	19.9997487		19.4768478	408.459931	2.13604908	98.9581988	303.939094	465.776067	205.310382	515.056416		38.388156	12.5588705	942.530093	2274.91403	264.928513	23.4224207	59.5751419	19.0887923	9.6842501	20.7690649	16.5314993	9.81655203	191.018167	159.793887	12.7644364	15.196882	337.729824
P-10	18.5972351		24.9297115	35.5601232	19.8765144	2.9545071	1.76178352	80.9434698	146.460104	70.210463	161.584187	23.6546887	27.0098839		80.7410753	578.842838	130.812068	9.66044149	8.79546308	24.347319		17.4026124	20.8298375	23.5152723	51.6279929	145.867499		24.3325252	49.6257427
P-11		8.61797935		20.0411406	25.3820943	4.28059819	0.98924641	3.23388545	87.035753	12.0490365	16.0064612				3.11093962	78.1967195	19.48245		16.8545673			23.8304153	3.93919029	2.61529389	0.68432298	47.97289		21.8409337	9.53077421
P-12	23.444401	21.4030318	27.5851753	15.1378638	355.70643	0.98462471	38.1677359	496.451459	606.849147	505.688163	604.273152	22.9239776	26.348541	42.0761764	868.599543	4623.69909	324.958039	12.7093591	11.4669354			27.1667623	1.7766294	32.1928426	193.045973	394.135942	16.9519469	12.876339	304.605739
P-13	26.0223936	16.1234891	16.6852185	28.9916029	42.5054698	1.16063874	13.6641135	117.306467	230.646581	96.9505451	116.691681			9.39659472	302.687484	690.062348	126.373469		18.8042831	19.6055529	14.0474846	47.5517099	23.7753444	44.6396108	31.3781906	62.3901195	31.3804022	44.4046237	20.824999
P-14	15.0468982	10.1190465	16.8457681	35.62161	125.607968	27.060014	49.3933633	147.976183	437.850188	105.922942	258.012628	11.9430568	22.1990268	54.3642751	422.497634	1218.84755	169.526856	14.0419536	27.5765829			26.362636	18.6119141	12.3376101	43.5212853	77.7201535		28.8186684	61.0095854
P-15		27.7726532			43.2489735	2.39773493	15.7549556	30.7995162		8.66364814	31.3279671				0.44788808	13.7009611	53.7091485			13.7348001	14.2217687	13.9510336	8.95060612	33.9638725	4.05876199	6.99152314	16.8597137	27.8090632	6.20983992
P-16	22.4853454	25.9748817		16.7556813	119.154566	28.4240627	19.4450804	250.793023	604.013413	89.760542	199.000211	11.1462654		27.3390166	517.597711	1922.99019	119.393168		34.1425569	13.3740822		13.4716463	9.94844223	66.0180301	20.4082197	108.33383		2.25091497	158.053942
P-17	11.775302	12.0499904		27.4141361	83.0904229	2.6692573	17.9178683	52.245056	295.813183	83.3493106	66.388713			15.6148059	57.9229251	356.310605	65.3613161		23.6466235		24.469901		28.3786535	20.4474171	20.0835783	24.8527858	13.4143238	49.3935808	9.63205101
P-18	47.2941318	58.9670788	18.7408161	23.2793187	793.055477	38.179256	220.469997	780.745093	1740.03858	709.057134	603.118657		53.7122	26.4152517	1242.14467	4493.01432	441.815894	13.682058	65.7775248		29.4838863	41.6952541	67.6302558	50.7602756	255.504679	418.710349	30.5212837	67.8677487	402.814054
P-19	27.2893302		11.6293804	11.6756349	11.5481603	1.60210955	2.38472606	37.2500577	45.571395	61.8301685	6.08512893		9.25377399	46.2171879	6.29953389	10.0595888	9.41870158	25.1596753		13.7455318	21.6335816		1.82571872	10.4726365	20.4342829	9.96132929		19.0180769	20.7271636
P-2	39.2500636	11.6259015	14.3887226		147.633709	106.414343	15.3993944	181.592385	680.813366	117.100677	280.409877	11.0422122	16.8651384		379.283227	1969.57205	152.888865	13.5462837	27.4399633	10.2303215	8.8546461	16.5141178	17.3268928	39.174997	116.305744	185.389092		35.3817332	97.5788882
P-20	14.6757162	25.7385057			251.474989	113.133839	28.3250755	651.888634	961.479449	264.138445	179.129419	19.4352384	21.2150642		662.459176	1875.30711	117.517723	25.9731802	26.7313128	42.7640044	14.7659172		68.2989803	48.4469935	132.651228	83.0615208	24.6880373	74.2802881	127.525661
P-3	52.2743138	13.070085			75.5173433	17.3879897	4.27075173	57.9225381	137.993601	29.1983565	30.5028124	23.4913897			113.632118	711.133467	65.8727253		18.2102934	32.8522877	24.9106279	26.9657742	11.2956054	20.8500382	34.1920696	125.911805	13.134599	32.4887725	20.0869185
P-4	17.7043242	100.017244			167.895889	95.054321	3.51279555	336.689738	671.943667	206.391784	293.055376	11.3017434		19.5394335	265.267423	1605.95946	240.26927		14.9449803	17.070614	19.6479127	24.3517564	1.46081181	64.4336769	128.652647	185.458753		11.0574869	121.247024
P-5	18.6059244	33.3421195		21.5851793	119.954129	1.21952301	41.6585465	556.014058	883.006206	199.161655	328.479356	18.1134375	33.984098		699.088655	1438.14343	187.423719	17.5671593	49.8517025	13.6057232	19.7419528	12.9097223	27.9922671	27.5853703	122.403686	118.203747	15.7976135	1.97477031	107.681909
P-6	22.6331523	16.4138925		50.4228536	226.656385	25.6264707	5.2196288	198.764761	958.088461	360.086626	346.013187	30.8271408	36.0524505		612.37128	3443.15527	302.153214	9.09072983	49.9006162	25.0131433	17.7508434	17.5958316	22.3622819	21.4431448	64.063756	182.696626		17.7510869	131.083882
P-7	22.378962			20.6085505	233.576117	14.7744971	9.32100624	237.064508	446.104793	215.921907	328.794473	34.2709178	19.405697	15.3370913	429.26633	1654.46772	99.1982951	17.0071029	93.3551149	15.2680057	21.1764878	21.9614491	71.5881873	20.6478795	4.68763653	77.7009808		28.4266632	96.563468
P-8	46.3904355			35.9110345	81.8419797	1.81552162	5.27847794	104.724849	361.282933	124.746598	166.801831				103.9165	524.112273	64.6577714	23.6827225			20.7842078		43.4924058	3.94543403	17.7984463	27.9505387		15.8678671	60.7683791
P-9			30.8159683		36.9456385	2.44661192	4.25964025	5.5335387	62.5749533	15.9720382	21.2358382	15.5658258	19.2083666		11.7043931	20.5295241	44.9255013					35.5176668	5.99793027	11.9901529	15.5494269	5.36656084	21.6820812	5.04719865	11.1001389
P-21	61.2315236	17.1358771		23.5623124	98.260875	2.12916303	17.8684133	56.1334942	258.523049	49.493704	49.7494198	20.7763932		16.4788889	212.344143	846.347542	325.624936		10.7551171				25.2449231	36.9885163	23.6365074	196.301085		20.4948898	12.7127934
P-22	21.1186501	25.9578378	11.8438011		73.9007353	26.8261266	9.61688979	159.109666	333.871578	147.552933	160.229668		41.1611419		397.458123	813.364505	199.396954	14.1319602		22.9128911		25.2798645	19.0265701	31.3920812	75.5578114	57.9251792	26.3726423	18.6901042	178.389076
P-23	24.6855908	16.1776298		24.5669182	20.3649558	1.35476305	67.2460567	61.8965734	201.089025	50.6119584	39.1366815				152.564792	242.112537	36.7676888	26.9419567	16.6681077	16.1149748		18.726208	17.2047035	11.4750771	26.0236917	29.9021617		80.255341	15.3625004
P-25	27.052496	10.9607136			126.75535	16.8197765	8.81180261	366.750294	359.127558	141.331431	144.331781				344.775359	1463.68935	158.957016		11.1975619				89.4231119	2.47529168	45.0151731	30.1707942	34.4032708	24.1452372	29.9076438
P-26	24.5983504	48.0844078	16.2261428		506.984026	49.6887486	49.1919872	540.643983	1448.57421	857.43888	665.634678	27.0960934	16.0728477		1042.54488	4225.28589	514.693065	19.3604408	11.1696751		14.4822249	23.343606	86.6612401	57.7142726	108.651676	245.406796		84.1846335	370.158138
P-27	44.9380924	31.5505157			172.101299	15.4946598	20.1988249	168.456472	295.030795	131.586783	144.352634	26.8824647	26.7679013	25.6839322	210.246382	1039.53043	106.802252		71.6100355	42.9013441	11.308229		0.76585515	43.9927545	41.5694174	45.8124016		4.05655074	164.18211
P-28	22.4424673				18.7980078	2.72229592	4.01583231	42.7805892	34.6038114	16.1176322	12.3795188		11.2731607		51.3078727	183.662494	37.042128		13.4404779	24.6973318	26.5216841	23.7697313	2.58835557	14.1838537	2.80011345	31.1346461		2.89272005	6.86688505
P-29	22.9818728	21.6406758	18.9983935	18.6001918	236.521282	0.8865173	4.98743147	267.826023	562.974926	315.831766	176.62433		9.13301043	19.219832	657.720054	2371.45478	219.044456	14.9614704	10.6320479		9.19234182	18.1523218	16.1019462	5.08482006	129.819886	175.744046		15.5687931	84.5393814
P-30	13.950479	41.9166848		22.1601054	3.77564073	1.39509228	33.9491728	17.6853391	191.620106	129.649037	145.97276			9.85979801	80.2795988	475.188972	19.2018256		17.5419787		33.3086256		0.95668652	12.6903177	23.4405589	46.9548156		18.0771819	5.78444982
P-31	19.9356577	21.3354137			39.9038352	38.0163633	0.72805963	95.1197797	214.112993	90.548435	102.193389		20.8123128		330.985032	1111.51953	38.0378589		10.4976263	12.6133582			16.9554959	110.50325	26.0823728	21.4233585		2.38838492	60.8980161
P-32		23.9072528	14.126567		16.0210518	1.36021781	3.30905719	12.3642076	33.2568164	29.4294621	2.45818097				74.1349353	54.5501815	12.6492812		26.1814357	47.4099828	15.0972356	21.1154468	22.3244814	7.49108432	16.4747481	3.49904248		13.5308371	8.22710717
P-33	20.8678912	23.5332127		21.8712877	195.732322	1.61378781	51.8416269	208.654409	384.575239	112.586611	39.4319786		18.8938841		353.295355	1025.28379	64.7447787	13.173535			12.8440648	13.4557979	2.19367959	25.3913901	62.4554436	16.8475166		16.3383728	150.066655
P-35	16.662501	36.8793958			253.076734	11.7508869	47.0992711	206.641441	259.920833	95.9060439	262.577469	17.5065727	21.9670941	26.6128984	315.974722	1504.38884	227.254991	28.6102985	51.0072396	23.4669186	44.6651695		26.8016112	60.2508011	78.6230204	184.803633		23.4892154	172.739257
P-36	25.8559891	33.7815641		39.2777561	5.25320505	18.5229185	20.1790551	33.4631985	49.6376138	20.4446254	29.8994442		46.020994		107.766374	169.182436	8.71534499	34.4971444				9.85513722	15.1922088	13.8456092	41.5901657	20.1607695		22.5711865	9.74247944
P-37	34.6519601				36.3299054	1.53968183	27.4648615	120.66234	402.512192	155.01145	107.255599		10.997303	10.8881927	449.384862	1338.32903	169.607636	18.052861		12.0702801			21.0424845	57.9663238	73.8157755	134.715223		15.7718194	87.1498787
P-38	29.1201368	61.7875068			165.438736	2.91059924	11.1806118	322.541969	314.214502	120.21797	81.6719877		9.68698432	20.9256636	269.708322	764.407204	157.964355		24.2895836	30.2571672	10.4095806	17.3193531	18.553574	14.8502835	32.7505668	52.7439845		45.7307525	157.123422
P-39	21.3260128	29.088815		16.1455799	20.4712352	1.5698419	0.61700078	5.23805695	27.7947426	8.58486923	39.2486277			15.399305	5.08829938	86.2640376	5.06787752		18.7898066	14.714884			2.2168808	22.5508227	8.17770999	29.7245783		51.0292454	52.7544341
P-40	36.355056		23.5677598		17.2146637	2.52282326	3.09091648	68.4820453	76.837387	69.6143139	24.4621739		9.55704277	24.0402153	52.9445988	301.953224	44.5956674				10.4602532		16.2313419	7.40166975	4.40205611	43.3106463		16.5385291	57.8246204
P-41	16.600461	26.6927596			169.332467	39.1355938	40.7294639	260.004398	429.019274	165.035825	196.438976		25.8128158	15.4067738	396.674046	1241.38558	154.034285	22.9262372	10.8978698		21.467415	22.0081509	18.2593871	8.2203463	165.788703	70.4963466		1.41064837	157.240673

Table 8.95: Raw peak area data matrix for phosphatidylserine for serum samples taken from breast cancer free controls.

Samples	PS(32:1)	PS(32:2)	PS(34:0)	PS(34:1)	PS(34:2)	PS(36:0)	PS(36:1)	PS(36:2)	PS(38:1)	PS(38:2)	PS(38:3)	PS(38:4)	PS(38:5)	PS(40:4)	PS(40:5)	PS(40:6)
C-1	48.2653822	15.0621092	529.841455	30.2680196	20.8192113	546.304101	74.1954503	62.7772561	38.3728214	24.9195298	11.5785929	273.420446	24.9588943	35.9153897	46.9727239	25.5610911
C-10	49.1855156	34.6950461	478.656786	14.3505121	40.0717732	1252.94527	209.086059	19.5839468	13.3245361	27.1913767	63.8293181	363.269857	64.91662	285.564901	156.845625	23.5015372
C-11	15.628614	37.1714602	453.957123	11.377218	21.1696552	754.345266	172.23504	12.9591297	15.0088704	17.4648934	25.5574917	299.258423	45.909982	38.2929091	135.098907	40.845851
C-12	149.393809	55.9573656	405.596146	40.8377486	80.0239188	642.118921	756.666672	86.1244542	51.7110506	49.4527065	82.416553	481.544983	41.5790976	50.7014206	63.6938315	46.2792428
C-13	18.5918859	21.3799913	863.121056	9.90913854	29.0710919	2636.23005	80.5750664	14.5722116	13.8608187	38.9570468	22.6224616	69.0879125		34.7566869	1.36492405	12.1092935
C-14	44.446904	27.448002	2564.43266		16.7839559	5134.31054	15.4783218	62.2416803	21.5932386		36.6987007	35.2888569	38.0918396	13.705949	0.36620755	47.8624367
C-15	30.0795261	14.5294914	565.050926	15.7426829	26.6606064	777.575727	1.99758253	21.887973	28.606182		27.3545374	139.4589	17.0947845	13.6583246	23.1771583	
C-16	65.6613593	19.190134	157.835616	24.0393914	15.6426039	383.248354	15.9573295	36.7875013	16.9650534	32.8819125	0.7401188	102.531325	55.31539	27.6577411	1.37327363	13.2491179
C-17	57.0531702	44.951322	295.476782	64.7522536	53.5788532	422.447832	63.1479106	20.3279158	36.0234216		47.6282479	125.538117	99.6908889	15.6590005	43.8342068	16.5013974
C-18	10.3201446	20.999334	663.927956	41.1432672	15.2932688	1601.49809	48.0009623	17.4769461	22.8475313	14.2176778	12.5058427	71.2076581	11.5246722		75.3324549	71.1689483
C-19	27.6650441	26.083829	684.568911	31.239556	19.2049423	1582.35727	36.2524942	7.66105751	18.2330985	13.1405663	10.6628962	78.9188195	55.8537139		4.63060459	29.2445584
C-2	54.840935	27.9707821	263.272738	15.405209	68.033223	429.012868	25.4969969	49.1415283	12.4015657	11.5922044	21.688897	148.687193			49.3834013	33.029955
C-20	27.9741658	24.4152428	857.465169	53.9940842	18.2145003	1698.28864	13.4086233	12.2911733	25.0139477	24.5567651	67.545736	90.6730235	64.602395		1.03250105	47.4646156
C-3	60.5874013	49.458702	573.6301	15.1060364	11.3888958	943.390568	254.619591	14.9319656	11.8107436	26.8567226	55.1126414	300.331822	34.9965833	54.6644495	19.3188616	14.9449556
C-4	14.7608139	10.4590136	524.186021	65.2630448	78.3573311	1198.20443	34.8908746	18.9242613	13.3371209	38.5851578	43.4781544	172.117053	23.3566439	21.6118416	46.8547657	36.0197406
C-5	14.8247948	12.8179346	537.966437		13.8164203	1682.52153	50.3118741	17.0976867	13.0154076	68.9913458	51.5036179	164.709678		104.956039	2.35955961	53.6357348
C-6	89.4791078	25.7567199	504.343312	18.7788452	25.6936865	1444.9194	164.412405	22.3564565	15.3740601	33.1119103	57.037467	281.821651	17.7230252	18.2045631	4.25454839	36.1012612
C-7	18.6125816	21.6429997	704.694164	36.3850347	33.5914324	1135.16586	434.880867	146.795941	22.5442072	22.3979882	85.6967697	1311.85485	20.727879	56.0502785	114.540132	9.56622697
C-8	23.8428141	23.854909	797.059254	19.8989122	157.641424	648.084038	136.78814	12.8142497	44.1092225	22.973593	12.3492944	336.258605	39.4711783	64.7624985	98.531076	12.6450178
C-9	28.9445572	23.6208426	936.878248	50.1931352	11.3870477	1850.21343	56.6382254	30.3968525	16.6105071	33.491747	9.43003826	122.914795	32.7647876	10.5445092	3.97310838	51.4125882
C-21	14.0075224	22.6280821	326.890142	25.7007397	17.9781426	670.517881	86.2647974	17.596585	22.2321215	11.8371911	24.3135732	100.512981	12.0470634	18.0947446	2.37171983	21.605882
C-22	12.831314	26.5097891	316.801541	45.0584435	18.0065532	346.504246	187.19823	11.0321273	17.505422	44.3969239	17.7544149	245.825283	22.7820383	12.5840898	25.5368867	
C-23	24.7197805	11.2071455	211.553768	19.9652256	16.3618155	364.576684	127.286677	21.1937412		25.5462034	106.121493	160.252048	30.2389343	45.2545001	32.2131923	16.9204496
C-24	15.5135751	44.8941325	395.389774	27.2727486		639.585371	5.49990838	5.35180348	39.7308926	36.0249041	24.4443504	332.096782	14.5146401	677.226365	27.6808539	34.4413562
C-25	57.4066797	12.685358	266.348531	55.3189669	65.3168455	605.733414	17.0955767	33.0710875	14.3326156	13.1287872	50.4223863	133.212333	12.8114149	10.2892146	58.4687089	12.8813017
C-26	34.4007965	23.163973	441.393193	15.7019817	14.5472163	563.001145	108.938486	0.50910898	50.7989533		36.583838	222.423649	10.9437435		4.39821619	20.4468629
C-27	26.7274384		824.232081	32.0086247	55.3353847	1232.46973	39.0719039	29.7126965	12.755628	13.9545954	20.6805752	69.7657038	38.8131886	22.3845813	15.1250519	22.1403557
C-28	157.918002	14.9973188	288.469771	40.8854188	19.5944133	439.471619	49.9620824	29.2038481	12.3231599	43.6719685	21.913329	162.795413	15.623505	36.5666638	3.2550682	21.3796415
C-29	90.3065089	24.1332131	133.092449	19.3097015	16.5949367	287.429708	68.8806296	86.550088	50.0232024		50.7732727	300.293498	22.0624121	55.5997374	12.5710018	17.9310416
C-30	64.7237417	17.0863577	850.158775	15.4453054	33.0850321	2068.78506	121.999876	15.4143985	29.3146431	13.375925	26.0013929	362.79449	17.1345519	18.3890278	28.266386	35.8798862
C-31	70.8005972		463.461302	20.0925753	45.9255168	1919.72235	2.72850559	47.7920479	24.8587542	27.9554667	32.437454	90.7841585		31.953037	1.50456152	22.7801558
C-32	96.8454085	39.5579643	95.5122918	36.3243523	20.1220064	796.106072	41.0623147	14.7523427	24.8043117		19.6336482	32.6258351	22.3348743	17.5370815	1.50430983	27.6960868
C-33	67.8047749		277.333684	51.5506105	46.0960242	73.1794102	274.58102	36.1001986	14.5788992	21.75393	77.7166335	406.874886	14.2923375	36.9832168	19.1831977	8.12101455
C-34	34.3038061	29.9366095	586.785067	22.2038773	18.3868083	201.30997	164.847782	44.0924827	22.8403738	14.3893508	20.1396318	142.439082	55.00657	9.83260759	93.3252749	15.5184858
C-35		11.4601376	2.95084071		17.3734439	61.7737743	3.9487384	16.1664732	21.8495461			25.7740563			24.7562053	12.8858884
C-36	22.3985134	20.7301125	122.937201	41.2420083	30.10939	182.462204	84.6979719	76.3267357	21.1423534		24.1634044	196.135198	38.0038938	12.6248992	49.242044	18.4367405
C-37	216.69792	22.5338791	147.575485	38.4539721	38.1719252	118.410061	100.194893	52.0130072	15.9683139	25.330565	49.6887928	93.7793589	16.6568376	11.7054453	1.16627625	26.2954606
C-38	93.7360482	25.4483798	113.942849		34.1846094	151.203875	15.6126301	5.30570066	42.1500158	68.8596258	27.0669082	105.646794	26.0715633	31.6112039	0.24509636	23.1076092
C-39	97.5032312		244.916114	30.2096551		868.089258	36.2646172	60.1707509	48.8541032	19.8140419	32.5569572	24.5908765	12.9775496	9.01176369	26.7727961	25.3157686
C-40	41.3647886	7.91629212	122.317074	13.5184983	27.8356726	379.138014	138.982533	28.6414172	39.7843975	25.019438	23.7990274	141.596894	17.2999341	39.0151558	29.0595419	36.2340474

Table 8.96: Raw peak area data matrix for phosphatidylserine for serum samples taken from patients with breast cancer.

Samples	PS(32:1)	PS(32:2)	PS(34:0)	PS(34:1)	PS(34:2)	PS(36:0)	PS(36:1)	PS(36:2)	PS(38:1)	PS(38:2)	PS(38:3)	PS(38:4)	PS(38:5)	PS(40:4)	PS(40:5)	PS(40:6)
P-1	38.9566033	44.3323872	552.140275	50.9998958	47.6624051	329.516226	33.5440693	10.941397	52.2984365	26.7619943	12.4584895	258.610152	15.3492247	20.7286705	35.0961475	32.2921121
P-10	80.6975813	24.2879534	422.133713	34.1452742	18.8766242	1221.93129	50.8402436	12.9101155	23.8747229	19.5985932	37.3304444	114.309459	31.4185434		1.62356231	29.3608122
P-11	10.5904748	45.2254386	898.970587	13.4834474		2869.21377	26.4541687	3.98081098	11.4692161	25.1761317	3.39571935	137.739194	11.9506694	19.5542435	1.49952622	
P-12	25.7320204	16.046188	506.355014	10.3355774	97.6331319	1274.093	125.872619	26.661559	16.0453965	8.73962831	2.34434097	244.557207	16.564235	12.7334338	4.08699056	21.6272099
P-13	8.75111375	13.43434	858.243733	52.8009827	28.467201	1577.26909	40.7001042	18.1090304	29.1331848	32.5404229	32.5374397	132.737062	27.4022667	81.7614778	29.731536	29.5765677
P-14	8.18612895	26.8978603	719.478004	21.88665	229.966842	986.1436	67.7439957	21.7283871	15.2836788	68.3251835	24.5080025	162.515936	38.3818413	46.8919362	30.327337	77.0170184
P-15	10.6428981	14.9583455	1219.26644	14.6690593	24.7393194	2542.76323	13.1195118	17.5308352	9.31248102	20.7314807	41.4720417	7.31526601	41.4183581	13.3177059	1.01462212	16.417274
P-16	60.466783	18.2443742	670.351398	30.255477	41.8692002	1244.21747	83.1238161	19.3303319	13.764923	45.7384667	65.0202371	234.352891	18.5570613	19.4705813	23.6970222	16.7986401
P-17	36.990903	19.926859	657.48969	20.2948647	48.0873128	1317.01886	88.6481913	17.9692226	27.4942845	29.8588264	14.9820709	34.6308981	15.0623555	17.8950133	72.3577584	17.5959496
P-18	11.0033184	25.8757012	484.763541	15.0654368	21.1855726	393.819041	64.5153081	21.0645869	17.8649881	44.8469532	33.9894528	264.427723	21.9229147	19.2173597	3.07193369	23.4258011
P-19	53.8457848	15.5579906	531.047026	27.3433504	23.0186203	1397.95095	23.2316839	10.1725658	18.0442151	19.1898387	3.55987482	83.1237006	23.4346091	12.2080434	5.98617851	28.0902575
P-2	30.8065944	15.1781954	835.550664	9.55464549	11.3095511	718.314966	69.1118491	68.199191	59.9875684	20.8307879	29.8206641	142.34013	14.5991506	32.5479182	40.67979	7.4014226
P-20	36.6590465	40.2443804	414.898262	12.354944	29.7310958	1053.94773	144.980099	9.19664419	33.2612493	42.4217206	34.2075463	245.192197	28.2839171	16.9887864	23.939331	44.3785355
P-3	12.3585325	8.78775052	500.74442	23.2857631	16.408014	1078.95135	14.7545981	9.88913076	11.4547385	15.5870821	18.9916322	53.6941877	15.8900331	28.5530594	23.6982528	20.660858
P-4	20.6763138	14.8115842	991.59005	33.4907552	57.2485056	1427.7396	26.9389646	14.3399586	57.2207423	13.9270859	31.6930957	43.2117916	27.1596854		57.4388495	77.4296091
P-5	7.33083006	26.5561084	779.270848	9.40254567	34.1039973	1449.53975	3.4957354	14.7530155	26.6213861	11.2168275	9.64503586	14.7132091	14.5507418		20.9308954	32.7920475
P-6	85.4979925	28.2528186	535.23907	52.8003311	38.9302465	483.40083	13.7798012	21.3788664	77.0335132	9.45671451	25.4004592	11.7374412	20.2957053	15.6929196	22.1138367	29.4052396
P-7	13.9804374	33.7560218	878.50543	24.0248701	21.2598544	1119.5758	24.2464359	15.11843	13.9518414	19.9833974	19.0524533	45.4083109	32.2540333	48.9656603	1.79499588	30.3067596
P-8	36.0321189	10.200944	640.079391	20.2795912	40.6923578	760.205284	37.6856997	19.8312803	70.204783	23.6946904	20.5920992	41.9725459	19.8085485	27.110257	4.92347818	18.126879
P-9	11.722857		747.430335	28.4736985	13.9427292	2258.25818	36.1699754	72.0561458	53.0971142	35.4619394	25.8491076	53.6784592	11.890204	15.9617061	0.70254495	35.1830306
P-21	14.8594178	24.9810022	620.596585	14.2870237	58.6467048	865.888393	59.6176578	21.6919827	14.2922953	78.85436	6.55708913	27.3382912	47.6091087	12.9535189	4.50402951	47.9485905
P-22	20.3861184	16.9539423	568.257889	40.1564868	12.7876177	917.81894	9.52106294	7.55649937	12.8916402		16.7607158	76.9871167		17.6753604	2.15333447	24.4988662
P-23	34.8300423	12.6507931	817.977097	37.0682649	16.8418364	1118.88004	42.8272784	16.8814045	14.6442773		14.1462726	134.669271	30.2830644	38.2624176	27.2877787	16.1759425
P-25	174.892889	15.6034827	295.783708	22.724253	17.3248945	447.501578	1.25686119	12.1768378			9.62601093	18.4910105	19.9297254	25.1075985	1.38943137	25.1747928
P-26	85.3601912	68.8801655	414.576736	23.4699005	19.7073849	197.125796	206.726361	42.1285278		23.2459731	10.2034814	268.323021	41.5456711	9.07309089	36.4153521	9.19722809
P-27	42.879367	12.6404041	572.081995	50.8976436	40.3336836	892.984525	87.9465605	14.2696878	9.86183561	13.3360621	14.2830023	151.913385	27.6165406	32.7911263	4.15421042	15.6348867
P-28	47.8240494	37.4881909	851.86121	30.1670603		929.680483	36.175349	11.0722568		27.2201365	18.5335192	46.1542324	19.1129132	15.6345151	3.53906864	
P-29	96.1253865	26.2173219	148.477874	82.9763536	27.9203834	267.470793	66.4446298	20.4532981	40.7319992		9.65625028	26.6235339	54.3437548	19.1613644	3.53919276	17.6922412
P-30	34.9612117	58.6086753	579.622001	43.4609616	9.84048625	1047.28456	16.5985633	44.4938104	26.5736478	8.85823613	10.3013259	22.4002112	37.7020869		12.4339145	41.4580408
P-31	53.7941844	15.8620131	240.319859		14.7439349	657.359568	42.6597965	5.54319809			29.0745363	11.0887924	14.0416581	20.9333664	0.54097505	
P-32	26.608794	21.856624	547.555078	56.2700008	31.2233007	1223.98528	2.53086163	32.4124509	21.2079909	40.1789756	28.8648407	61.3160247	10.2750876	29.6020699	2.41985329	27.1200348
P-33	51.6869718	26.9934354	335.32582	32.3538286	68.7244617	736.612999	27.8220683	11.0838336	30.6266121		16.875119	202.745513	9.92242382	36.5873094	35.2500378	41.4242094
P-35	80.5324371	63.6008905	135.440912	62.138424	53.3100009	167.069971	48.9139707	71.0362966	25.7874123	10.1474729	17.6459017	103.656729	10.2923968		0.6525145	28.337333
P-36	46.4071112	20.8290179	400.066249	53.3901653	24.0185895	674.032248	18.6923625	27.6396123	21.8705214		52.5086027	21.5811745	46.8023861		14.791016	
P-37	45.0187583	20.6281827	480.679089	24.5468037	43.0029333	658.65901	17.1670548	5.49228536	39.6278864	28.6653713	4.53473246	104.144062		37.2036793	1.82657039	27.9262405
P-38	22.1036053	33.7392172	801.239223	10.2592006	22.3795592	917.664894	2.98571297	18.8389073	36.8849862	24.2770981	42.4177834	44.1866674	29.6227858	14.3166376	14.4584308	12.0394775
P-39	36.2106324	21.056242	726.658088	16.8731077	38.5449918	1219.52858	2.88088903	19.5470854	15.3778649	23.6852902	13.8008702	24.1520649	10.8596821	20.5839771	4.07221174	21.6664445
P-40	81.9141848	60.6742602	288.975494	14.8888519	22.3847189	740.332984	57.2633374	12.4492468	10.771105	14.8183363	12.4220386	44.262873	32.1277426	16.9534092	1.03573227	38.8358131
P-41	42.609323	33.8827718	496.851854	25.7543664	14.8263341	410.888122	87.7684169	23.5387552	11.896269	14.7058981	4.74758201	23.9352451	14.1489889	11.4585017	1.25699924	98.0643512

Table 8.97: Raw peak area data matrix for sphingomyelin for serum samples taken from breast cancer free controls.

Samples	SM(30:0)	SM(30:1)	SM(30:2)	SM(32:0)	SM(32:1)	SM(33:0)	SM(33:1)	SM(34:0)	SM(34:1)	SM(34:2)	SM(46:7)_1	SM(d31)
C-1	1378	142	595	799285	16546	900073	900073	518758	5670889	899676	64165.9302	727858
C-10	3715	14	689	954545	53317	1066503	1072930	729303	8124703	1593229	14643.7395	869435
C-11	1010	12	477	651324	9580	864087	870622	554655	5850907	703272	52911.0678	571415
C-12	607	119	259	261643	6939	364974	364974	231470	2522592	184100	64613.8647	608042
C-13	3454	58	270	937450	44516	1082438	1086508	570615	7712098	1395220	9277.30083	518351
C-14	668	18	235	264825	3781	282953	283509	152638	1684501	78173	2462.85238	124635
C-15	4865	168	1034	1593254	46996	1768982	1768982	643427	9402791	1346592	16487.0256	723896
C-16	1280	26	415	489552	18399	756516	756516	394975	5434170	589249	67005.8897	736063
C-17	2692	202	789	1013044	42900	1157584	1157584	713572	7072508	1181181	42310.4765	864498
C-18	1830	278	719	731953	29195	955769	955769	834832	6921212	865865	44615.6188	726883
C-19	1777	26	599	854656	37098	1105971	1104745	715818	7731528	1351565	25696.3108	574390
C-2	1838	111	384	607502	33958	759095	759095	510985	6012101	855971	49769.0182	746369
C-20	1347	105	498	644232	20913	1008213	1008213	525066	5375550	532358	64493.9253	688755
C-3	565	66	372	625605	9218	720074	720545	536998	5867162	748457	51548.853	569157
C-4	4711	301	611	963137	45160	1111725	1111206	845104	8418630	1106279	10233.8912	852624
C-5	6052	172	515	1030024	76378	1678335	1678335	677769	9222480	1528236	8652.39697	761482
C-6	1598	37	610	714891	23840	1071848	1077793	613018	7208518	945900	20612.6337	721419
C-7	2160	69	675	916098	30927	1202330	1202330	674452	7776719	1247484	68273.5602	683595
C-8	2084	23	774	707920	15161	638565	637910	571014	5012419	664341	47716.4049	813553
C-9	905	32	445	376279	7996	581627	584243	351083	4303981	522612	16199.6515	385191
C-21	940	22	497	840537	9631	932941	944752	538034	7227406	949799	9838.04462	521796
C-22	1711	9	527	888239	20028	779561	784002	443816	6361156	995518	16801.4994	508407
C-23	2214	50	684	914860	37611	1379319	1379319	735783	8391568	1130090	18898.5279	643832
C-24	2090	98	326	1299593	17794	1290539	1301910	744152	8369506	1432681	7724.34436	544693
C-25	2650	15	144	1220324	43811	1517983	1517983	491496	8344017	1307827	9467.21023	590750
C-26	1393	48	296	1058574	16695	1505308	1509849	549372	8239452	1174889	8641.64469	521278
C-27	2117	51	191	954883	39817	1243799	1253952	483806	7288750	1205600	7336.86422	533670
C-28	4034	129	849	1564747	59279	2083181	2083181	889174	10517958	1939133	32823.5421	704718
C-29	3189	41	762	1310020	60418	1534558	1534558	906132	10100348	2122628	44729.6936	704555
C-30	1836	14	317	690126	22515	963146	969283	501857	6331702	717270	170.881925	495616
C-31	2041	17	885	854852	13062	1257238	1267163	527561	7208891	979565	4304.66701	373550
C-32	2326	23	314	897957	26188	1306131	1306131	717897	8890719	804257	6241.90524	829823
C-33	3189	36	565	1121895	44618	1328564	1328564	619395	7241181	1116717	96368.2316	676876
C-34	3547	30	958	1391579	50982	1808989	1808989	674980	9236265	1532368	19861.2813	800078
C-35	6152	191	268	1983106	76540	2401009	2401009	903180	11295220	1833119	78.3501261	744788
C-36	2529	37	701	1110947	26191	1412354	1412354	760207	8623170	967293	26833.48	588245
C-37	3248	23	723	1032873	41812	1957751	1957751	606085	9674887	1137445	16708.1587	713228
C-38	2559	11	315	1147623	42104	1180635	1180635	592090	9329799	1361492	4768.24421	760686
C-39	1542	10	468	1011650	12769	1537918	1541820	341503	8236156	1032978	2813.65154	373266
C-40	1360	68	464	693889	14045	1012753	1012753	475692	6682998	446203	18586.4859	621462

Table 8.98: Raw peak area data matrix for sphingomyelin for serum samples taken from patients with breast cancer.

Samples	SM(30:0)	SM(30:1)	SM(30:2)	SM(32:0)	SM(32:1)	SM(33:0)	SM(33:1)	SM(34:0)	SM(34:1)	SM(34:2)	SM(46:7)_1	SM(d31)
P-1	1483	68	468	699645	25859	831733	831733	555249	6584686	948726	38944.7542	778819
P-10	1345	97	593	692393	21707	1179894	1179894	945289	8492277	1322077	21337.3176	661475
P-11	2703	175	458	1088928	43969	1312834	1319373	715131	9481104	1462908	6525.05028	573192
P-12	2065	32	664	920115	41839	1265881	1265881	891337	9012706	1851527	57100.1541	882673
P-13	1654	29	635	834901	13389	941335	946476	505345	5276319	766628	34717.9126	514349
P-14	1899	58	746	1104951	35689	1276051	1284494	692513	7294843	1348153	31991.1569	726065
P-15	1291	24	359	869047	18629	1044370	1053053	667466	8237020	1514360	7061.09585	482313
P-16	1264	205	402	771374	29614	973115	973115	593202	6696135	956314	40705.1766	905989
P-17	1409	17	670	881692	12427	1355409	1344740	646604	7461574	1083012	23009.0776	565951
P-18	1597	94	414	710961	25856	941575	941575	680259	7232305	972181	54762.5088	882393
P-19	4144	218	352	878147	41706	982244	982244	648113	7418270	931180	12498.3156	807396
P-2	935	29	631	724901	11436	916210	913159	564538	6694525	919760	50010.5107	588156
P-20	1820	18	295	576739	17154	768161	769848	481820	5790248	632317	53678.2699	714682
P-3	2477	100	480	586790	35172	765278	767080	462013	5529397	863318	29506.301	737481
P-4	1657	32	614	792437	30016	1161159	1161159	699300	6582493	1003531	35998.1455	766047
P-5	853	74	332	620916	11730	830952	829467	452626	6344192	948349	54359.34	622261
P-6	1384	43	925	1102279	19750	1555144	1555144	731495	9152156	1678994	127.738492	676829
P-7	1993	68	569	1045424	17182	1260237	1260237	702163	7481902	1200954	43701.93	642649
P-8	1459	22	612	1013821	14067	1533392	1545413	847006	8782438	1247084	28925.6136	569419
P-9	3989	20	667	1028834	34555	1319620	1327007	714339	9643431	1207549	485.108312	800130
P-21	2735	28	327	1603724	63738	1913663	1913663	882553	10021222	2074470	13627.7091	679248
P-22	1019	21	104	849898	14771	966131	966131	597015	7065569	1462286	18678.7651	567206
P-23	3795	10	197	1103631	52334	1517683	1517683	495799	8458698	1397103	8911.54332	544922
P-25	1352	49	683	878460	14008	1425814	1433125	554467	7672120	1100838	25384.0195	553721
P-26	3616	88	880	1410652	39746	1577056	1577056	859849	9590534	1540384	53256.3085	711505
P-27	3285	196	694	1224278	47162	1322476	1322476	670773	8603911	1362831	18440.6817	863608
P-28	1919	56	271	1003161	15161	1375696	1374595	521344	7170579	1110863	4765.95708	514281
P-29	3351	59	371	1334730	56173	1577344	1577344	764210	10278614	2152660	36857.7565	822323
P-30	2250	19	438	1444475	29126	1857251	1870575	535179	8697478	1993402	8781.40681	500430
P-31	904	32	378	654220	10081	1009087	1009087	448535	6818031	1010071	15756.7524	590533
P-32	1332	19	180	570412	16590	841897	846249	434498	6455032	629127	4994.09073	708404
P-33	2675	12	112	1049635	39790	1392537	1392537	761955	9186071	1238929	13961.6829	573893
P-35	2053	11	116	1191104	26422	1021736	1021736	596047	7449782	1009409	11760.7384	1025337
P-36	862	36	152	664721	8682	789893	789893	374555	5651007	657612	6273.79424	491476
P-37	5031	75	234	1597709	69483	1885476	1885476	689551	9745053	1638644	195.535333	688728
P-38	2124	71	654	1353417	19074	1796262	1799960	846307	9868517	1730016	24695.0255	504231
P-39	1539	49	317	1138797	14151	1526487	1528618	609293	8935945	1236025	5840.00157	474978
P-40	1519	32	275	769296	24047	1180868	1182560	562862	8543497	1278050	6380.67898	553149
P-41	4262	29	726	1744468	54839	2035296	2035296	822460	9778222	1754574	25862.4541	729380

8.4.1. Normalised to the mean data matrix

Table 8.99: Normalised data matrix for cholesterol ester for serum samples taken from breast cancer free controls.

	Cholesterol	CE	CE(10:0)	CE(13:6)	CE(13:2)	CE(24:0	CE(24:1	CE(24:2	CE(24:3	CE(24:4	CE(24:5	CE(24:6	CE(14:0)	CE(14:1)	CE(15:0)	CE(16:0)	CE(16:1)	CE(16:2)	CE(17:0)	CE(17:1)	CE(17:2)	CE(17:3)
C_1	-1.5483183	1.51904646	-3.1080852	-0.5334568	-1.4187673	2.15996951	2.17171677	1.17126623	-0.3393115	-0.5985751	-0.3861339	0.73576355	-2.8734241	0.9011865	-0.3727276	1.03065611	0.43301887	-2.334022	-3.6650257	-1.8739751	-1.4898252	-1.6293947
C_10	-2.0103524	1.74511146	-1.7290335	-1.0250763	-1.3569067	1.80273409	1.34950411	0.68495147	-0.6118428	-1.7933468	-0.4143891	0.23870262	-2.0407083	-1.0796141	0.56748885	0.89245469	0.1611235	-1.4053327	-1.9409866	-1.3651453	-1.8894711	-1.4808374
C_11	-1.2575076	1.75511888	-3.3319853	-0.4239686	-0.721657	1.27385898	2.05139906	0.39760692	0.00084303	-0.8537628	-0.5880814	0.74992344	-1.9566314	0.44254992	-0.3672866	1.18317236	0.54445398	-2.4078081	-2.6663189	-1.798112	-1.7859358	-2.1203898
C_12	-2.4796968	1.91883988	-2.0376773	-0.9888255	-0.8194812	2.43834594	2.64655487	1.10304257	0.06898308	-0.7504256	0.10228802	1.17735061	-3.0113126	1.09137284	-0.6624564	0.73568339	-0.3003401	-1.4153501	-1.5955415	-1.9269437	-2.3410296	-2.8799535
C_13	-1.3664561	2.04182819	-3.2055902	-1.8233052	-1.318894	1.06076546	1.95574331	0.2340666	0.18962731	-0.8388931	0.11581751	0.65689444	-3.2930278	-0.8447532	0.14261202	0.62202725	0.31335384	-1.2234219	-2.6720908	-1.7606882	-2.2181039	-1.3404886
C_14	-1.7989285	2.43972458	-1.5414635	-0.9206153	-0.0238517	2.28016621	2.40175862	0.87556015	0.31813851	-0.9848598	-0.2032419	0.87481387	-2.4624216	-0.8423798	1.15621644	0.58536435	-0.8493088	-2.0953157	-3.0814783	-2.2812952	-1.2694348	-2.3355028
C_15	-1.006438	1.36867548	-2.6060454	-0.399872	-2.105281	1.33532092	1.8799949	0.08687672	-0.4296162	-0.7923696	-0.4167379	0.68223987	-2.3148568	-0.751546	-0.2276591	1.07669493	0.94693408	-2.0650077	-3.5468866	-1.2118876	-2.2358373	-1.6969302
C_16	-1.5424783	2.22651784	-3.1767534	-1.4603557	-0.7402499	1.44015733	2.12463116	0.01815204	0.16966298	-0.5200518	0.16162423	0.50824418	-3.1982375	1.30137915	-2.5407832	0.87143762	-0.0465272	-2.6352953	-3.0855345	-0.8452469	-0.2311268	-2.0491141
C_17	-1.5179776	1.43985404	-2.4333534	-0.5044384	-1.2267159	1.86760328	1.8143442	0.91662227	-0.7536222	-1.0439999	-1.0548949	0.37644672	-1.9263957	0.83817281	-0.4883716	1.40711838	1.44241815	-3.1195925	-3.1848041	-0.9149444	-3.4699437	-2.3946093
C_18	-1.633805	2.09454539	-1.7953957	-0.5067989	-0.886327	1.15303225	1.62928249	-0.1342786	-0.094675	-0.6544632	-0.7949093	0.21063235	-2.3908574	0.64897305	-0.2960225	1.03959315	0.43050036	-1.8461694	-2.9350073	-2.1938346	-1.8820676	-1.7658516
C_19	-1.9552795	1.56814235	-2.6787267	-0.5746135	-1.3976462	1.0679252	1.40204433	-0.1963401	-0.2683921	-1.0754767	-0.2969765	0.1689383	-2.2705526	0.101457	-0.1243946	0.87798741	0.24159687	-1.4242244	-2.0582631	-1.127484	-1.7104703	-1.341035
C_2	-2.21911	1.77978239	-3.6724778	-0.4495814	-1.3338789	1.61735224	1.86810751	0.60734479	-0.238004	-0.6670835	-0.309381	0.38257029	-2.2575625	0.62881218	-0.9031485	1.06646639	1.29258455	-2.5799726	-3.7912624	-1.2839843	-2.3499235	-1.0458475
C_20	-1.7884204	1.54639361	-3.4638837	-0.0978278	-1.5336049	2.68922115	2.42272382	1.77287764	0.09453417	-0.9322876	-0.0699056	0.77866536	-2.806945	0.66579476	-0.6514177	0.96891271	-0.1067487	-2.3069666	-3.0993895	-2.0013918	-2.4536612	-1.7973902
C_21	-1.9275692	1.87813926	-2.4272139	-0.8489712	-1.7839001	1.63623936	1.96242788	0.13626519	-0.2898254	-1.9419473	-0.4447997	0.76103666	-3.1117644	-0.5111945	-0.6795036	0.51279935	0.3528922	-1.8225459	-2.5847449	-1.6835489	-0.9777467	-2.3779132
C_22	-1.4560004	1.92224048	-2.9774952	-0.7287553	-0.8877354	1.48812642	1.92057428	0.08249645	-0.3551069	-1.3307451	-0.1146052	0.47046145	-2.2585089	0.13275518	-0.5863459	0.65317619	1.17252535	-1.7002477	-2.1783673	-1.5594715	-0.7812426	-2.2787345
C_23	-1.8853985	1.84471539	-3.1105494	-0.3424837	-1.0244731	1.29621964	1.37574122	0.08845286	-0.3444939	-1.1567992	-0.397035	-0.0393849	-1.6520139	-0.3136401	-0.5182522	0.79200512	0.57144925	-2.1475889	-3.1817732	-1.0741153	-2.4092731	-1.5054458
C_24	-1.2633645	1.48259098	-3.3907372	-1.3997853	-1.4614126	1.40305963	1.74310616	0.02299019	-0.0990877	-0.5312786	-0.0963333	0.137504	-1.5087805	-0.9674179	-0.8672271	0.79620889	1.30794561	-1.9229837	-3.1986717	-1.0795421	-2.4871767	-1.6268221
C_25	-2.697949	1.74809795	-3.3770672	-0.5000689	-1.1957524	1.79800294	2.08528005	1.06447701	0.3190283	-0.5560456	-0.351279	0.61509413	-2.8290739	-0.556189	-1.3705002	0.19325113	0.94180686	-1.8309104	-3.5315754	-0.9824019	-1.416562	-1.4614674
C_26	-1.1570817	2.00502903	-3.1619044	-0.9575029	-0.4746204	1.63958368	1.8818687	0.27966799	-0.0268106	-0.9612358	-0.0498586	0.47986469	-1.9908059	-0.3173598	-1.5586675	0.85813591	0.61576085	-1.5507981	-3.6925472	-1.6072822	-2.6661147	-1.6375715
C_27	-1.5774882	2.31588475	-1.9785199	-1.3641236	-0.6204974	0.91447116	1.69863352	-0.2459482	-0.2358154	-1.0426766	-0.7821546	0.10215536	-1.3166465	-0.8355488	-0.3991821	0.51497293	0.80782181	-1.6871953	-2.4609265	-1.5194213	-1.8036072	-1.3554492
C_28	-2.3768541	1.46972316	-3.5766338	0.08458346	-1.3420626	2.12208427	1.6706108	1.25889993	-0.2455844	-1.7488967	-0.547126	0.28594493	-3.0625806	-0.1559303	-1.0442395	1.17784139	0.49037948	-2.4456908	-3.723429	-1.2693132	-2.3619003	-1.7019755
C_29	-2.0129559	1.48238792	-3.6167701	-1.3189194	-1.6409635	1.6658585	1.997378	0.56551807	-0.3977569	-0.653229	-0.5606244	0.43991298	-2.2635442	0.10396496	-0.6881084	1.12911455	0.59735993	-2.2731689	-3.0056694	-1.0579165	-1.800538	-1.8924638
C_3	-1.9719859	1.69689105	-2.1645798	-1.3602287	-0.9820188	1.41323069	1.75152045	0.32796163	0.10666476	-0.5513968	-0.6405227	0.19896091	-2.4681606	0.38236036	-0.2571175	1.07259323	0.58017951	-2.0426786	-3.7577436	-1.543178	-1.7000326	-2.0219614
C_30	-1.3359542	-1.2014009	-0.8500832	-1.0306033	-0.2435501	0.22203045	0.36682419	-0.0340227	-1.5095668	-1.4365277	0.24692295	-0.2176257	-1.4739612	-0.2977583	-0.6448002	1.20443202	1.05934833	-0.4945295	-1.1010707	-1.0380676	-0.7533641	-1.1169756
C_31	-1.71497	2.52946241	-2.4880639	-1.2791459	-0.3451286	1.39786569	1.68595669	-0.0257112	-0.5669271	-1.6667836	-0.6122242	0.59941476	-3.35278	-0.9453775	0.02812178	0.87193877	-0.1193697	-1.3323487	-1.7864862	-0.9442652	-1.0856979	-0.5500422
C_32	-1.7809598	1.75003282	-2.2910077	-0.8934068	-2.1066012	2.06156319	2.34049201	1.15141042	-0.0853129	-1.2624164	-0.1131854	0.79421471	-2.2831989	-0.9887049	-1.2084731	0.8047476	-0.040641	-1.5206891	-3.0593061	-1.9394144	-1.9077463	-1.2390916
C_33	-1.7035181	1.84803782	-3.3925817	0.14705128	-1.3527512	1.46790144	1.70066225	0.5402894	0.23769437	-1.2157018	-0.3652983	0.37571285	-3.15638	1.19370364	-1.7186417	0.56485408	0.63304655	-2.2306799	-3.4958033	-2.3875234	-1.7085343	-0.8385765
C_34	-2.0881219	1.57505168	-3.7252454	-1.0482622	-1.0807621	1.52987629	2.02724168	0.45962505	-0.5408008	-1.1032079	-0.2737219	0.49638579	-2.1493066	0.25299406	-1.2204677	0.91485935	0.97923149	-2.2796262	-2.8733422	-1.1921052	-1.6527634	-2.2764558
C_35	1.15038809	-0.7084633	-0.7397947	-1.6398216	-0.4681292	0.29244108	0.22528396	-0.7419697	-0.2606723	0.14689579	0.73790646	-0.2214417	-0.9197543	0.37590909	0.36810763	0.38876688	-0.4313404	-0.0451055	-0.792402	-0.1638573	-0.3182446	-0.5320888
C_36	-2.0914263	1.47950334	-4.0741649	-0.4959404	-1.5640482	2.07924662	2.7378014	0.90267335	0.65458253	-1.2519076	0.19277715	1.14313489	-2.6929582	0.12623592	-1.6431258	0.63233255	-0.351106	-1.6784513	-2.8088819	-1.6921298	-3.0875284	-1.941963
C_37	-2.0415895	1.32336013	-4.1119733	-1.2549289	-1.4788305	2.59523837	2.3473495	1.55200101	-0.0086963	-1.7470342	0.21217188	1.2072081	-2.2603789	-0.3357621	-1.7002389	0.80174284	-0.2700225	-2.341124	-3.5646398	-1.7048944	-2.7393227	-1.8898999
C_38	-1.7343154	1.36051322	-3.3326072	-1.5114701	-1.6798115	2.42554134	2.42534141	1.11793778	0.21831716	-2.2629609	0.48196987	1.11500044	-2.6030988	-0.7597728	-1.4068858	0.40573463	1.06643703	-1.9184536	-3.7972854	-1.4954538	-2.0295664	-2.1331715
C_39	-0.847616	2.16892939	-2.7743614	-1.5075859	-0.6179053	1.59397369	2.29799448	-0.2171741	-0.0717145	-1.1814331	-0.0347589	0.64769446	-3.213901	-1.3550176	-0.5323984	0.74615693	0.2416006	-1.9123425	-2.939632	-2.0426818	-1.0704909	-1.4755781
C_4	-1.6898593	1.64900431	-2.289118	-0.5785856	-1.4046442	1.35082167	1.54568925	-0.2415102	-0.2903555	-0.4664176	-0.3056658	0.34077656	-3.624122	-0.2665611	-0.5114551	0.95407584	0.29231235	-1.4846696	-3.1646492	-1.8427724	-1.3267383	-1.9865128
C_40	-1.9682899	2.06016007	-3.794871	-0.1213884	-1.2766943	2.16482732	2.59636669	0.6566576	0.41691769	-0.8748802	0.45009495	1.03249838	-3.3229061	0.91211609	-1.8443674	0.72094554	0.03019596	-2.8159971	-2.7887014	-2.0649566	-3.0166842	-1.2274352
C_5	-1.2358362	1.73724117	-2.6105769	-1.1570781	-1.2994439	1.39939042	1.597398	0.00605516	-0.3999498	-1.0783825	-0.249199	-0.0284566	-2.9065046	-0.5673225	0.48785901	1.13555555	0.54849442	-2.3438682	-2.9388477	-1.501968	-2.1098126	-1.6000911
C_6	-1.2574631	2.13934668	-1.5797528	-0.3464003	-0.9119104	0.9047892	1.36625766	-0.2570164	-0.2489066	-1.3163133	-0.8322401	0.06497931	-2.5016699	-0.1872131	0.41873745	1.02653105	0.33338711	-1.532693	-3.3030458	-2.8588872	-1.1620562	-1.7629291
C_7	-2.0147065	1.62244947	-1.8201366	-0.1959334	-1.2908836	1.10010435	1.60932993	-0.310705	-0.39935	-0.5292984	0.0777217	0.35840821	-3.4779464	0.60878988	-0.2514605	1.0662763	-0.0025446	-1.8129276	-3.4696108	-3.2532567	-1.3726221	-1.3746772
C_8	-1.8603937	1.91831346	-2.2869354	-0.8185272	-0.718301	0.99081313	1.44013948	-0.0370478	-0.3032223	-1.2643251	-0.5702821	-0.0686154	-2.1382721	0.65816912	-0.1452388	1.11727318	1.5329092	-3.4357525	-2.7070234	-0.8971257	-1.4912636	-2.1785951
C_9	-1.8231658	2.20370833	-2.5365632	-0.8241174	-0.6617478	1.09970851	1.72085314	-0.1377608	-0.0581805	-1.0365214	-0.6438468	-0.079544	-2.7636506	-0.3583144	0.35004156	1.08835164	0.37900128	-2.0296085	-2.135764	-1.2024779	-2.3382883	-1.4435221

Table 8.100: Normalised data matrix for cholesterol ester for serum samples taken from breast cancer free controls.

	CE(17:5)	CE(18:0)	CE(18:1)	CE(18:2)	CE(18:3)	CE(18:4)	CE(18:6)	CE(20:0)	CE(20:1)	CE(20:3)	CE(20:4)	CE(20:5)	CE(22:0)	CE(22:1)	CE(22:2)	CE(22:3)	CE(22:4)	CE(22:5)	CE(22:6)
C_1	-1.1238713	-0.1010167	3.28782503	5.00724323	1.65670008	-2.0256537	-3.6797	0.31263727	1.23005488	-2.9307932	-0.2325192	1.33691476	0.69508023	0.16273314	0.62472025	2.46855522	2.56347067	0.20079181	2.59524606
C_10	-1.8994122	0.00704913	3.34205242	5.09303752	2.36118756	-0.7467558	-3.6677688	-0.6428963	0.58779338	-1.7365967	0.66560839	2.11983458	0.55847901	-0.1159382	0.18545895	1.85942437	1.99547801	-0.3691384	3.10407513
C_11	-2.3355567	0.12410922	3.46829251	5.28946009	1.80191911	-1.4982242	-2.4200577	0.34165377	1.06109991	-3.4378648	-0.3350543	0.73125007	0.4650913	0.41454128	0.73582288	2.45499192	2.51492745	0.01718394	2.48693287
C_12	-1.8645024	-0.6224752	2.54012635	4.23245359	1.34323128	-1.6926765	-3.1026768	0.77396295	1.71459539	-2.752241	-1.0544078	-0.3290502	1.76507713	-0.0925636	1.28672621	2.96351175	3.08305808	0.41751725	1.3169061
C_13	-1.5960621	0.33430836	3.37561457	5.2160945	2.44496589	-1.0719071	-2.285809	-0.1569389	0.93185967	-1.8636187	-0.4175749	0.72606673	0.77501939	0.29119095	0.7837708	2.36540207	2.43037072	0.0408937	2.24933049
C_14	-2.536209	0.07473442	1.91941213	3.78474939	0.25769446	-2.2510277	-0.9369468	0.88284663	1.65644273	-2.2162301	-1.8567509	-1.1831765	1.74259155	1.28493548	1.43379731	2.97090133	2.95771621	0.65527792	1.11759655
C_15	-1.4278168	0.0049337	3.45661604	5.11933253	2.37468236	-0.8259464	-3.0031103	0.35908971	0.67782337	-2.2400313	-0.1139437	0.71092599	0.97685089	0.28291689	0.9890792	2.47793846	2.40103306	0.07670595	2.13315476
C_16	-1.9657895	0.12436617	3.24560519	5.03182345	1.9261593	-1.3730666	-3.1704999	0.74088337	1.30610855	-2.3512565	-1.0752291	0.0628735	0.91914167	0.38424667	1.46636656	3.00019066	3.05475842	0.18043543	1.74283069
C_17	-2.4765175	0.15851072	3.69469883	5.08902224	2.31733354	-0.5743293	-3.2037412	0.30447195	0.61293304	-1.9683945	0.22649068	1.61519093	0.66277471	0.19027613	0.73770201	2.17535537	1.93820764	-0.1330789	2.56417746
C_18	-1.6025759	0.18390906	3.56529765	5.59241927	2.08308308	-2.0556244	-2.8642339	0.34130174	1.27876842	-2.9397263	-0.8857688	0.54600238	0.4204809	0.80079237	0.62474356	2.47695805	2.82998855	-0.2269175	2.435006
C_19	-1.8033103	-0.0369965	3.4642373	5.11016608	2.23568013	-0.9097126	-2.4511007	-0.491021	0.57893521	-2.0803599	0.03313032	0.99833018	0.31868879	0.8801881	0.21497995	2.14757698	2.23225543	-0.1257374	2.75585354
C_2	-1.1087068	-0.0872455	3.459677	4.94466062	2.15676547	-0.6912162	-3.2033124	0.30502533	0.52432629	-1.9282804	0.05125085	1.36748585	0.28979048	0.01313434	0.88499281	2.38402557	2.22128576	-0.3029294	2.57746775
C_20	-1.7422996	-0.4874023	2.7642329	4.70337044	1.37341829	-1.5858516	-2.7893378	1.00027176	1.97132536	-3.6411642	-0.6549717	0.77341206	1.44826568	0.13116268	0.74399678	2.77350699	2.94916643	0.530836	1.90877972
C_21	-1.4990706	-0.0306066	3.20625557	4.85062358	2.1498982	-1.4312167	-2.3758639	0.32380847	1.07215013	-1.5079959	-0.1409968	0.95615049	0.86619399	0.70058511	1.18745455	2.78699274	2.65686556	0.12497647	2.27718458
C_22	-3.1127353	0.05636461	3.33060543	4.61336996	2.09357261	-0.6790899	-2.862767	0.32502159	0.24495247	-2.7302121	0.0229819	1.1091814	0.68536903	0.26097679	1.10009942	2.698773	2.24820071	-0.4211268	2.36746825
C_23	-1.7313973	0.07000801	3.35643354	5.49250543	2.62444959	-0.6947202	-2.0616508	-0.2298466	0.95533601	-3.1332436	0.1383385	1.18967433	0.46385241	0.37805716	0.87792906	2.37721053	2.55248826	-0.2255292	2.73424158
C_24	-2.5079432	0.09254468	3.61056083	5.58574624	2.8540308	-0.3499378	-2.8255647	-0.1740833	0.91645632	-2.9490551	-0.1885356	1.0693392	0.90387835	-0.0450727	0.94561695	2.46088704	2.52235622	0.35901383	2.72697715
C_25	-2.1486598	-0.0915272	3.15489336	5.03399703	2.08016114	-0.5101275	-3.7372499	0.2187295	0.93853915	-2.4679349	0.32422393	1.32805548	0.89036105	-0.6713193	1.21953932	2.80552746	2.71723765	0.4617229	2.34563466
C_26	-2.2136473	-0.0838011	3.27577923	5.15361158	1.89001057	-0.96619	-2.3218497	-0.134964	1.06579924	-2.2716894	-0.3495643	1.20487836	0.39665588	0.06667273	0.97494842	2.72548722	2.79787792	0.16661879	2.67361648
C_27	-1.8961906	-0.2947351	3.1620931	4.96601358	2.49184109	-0.2616781	-1.3518066	-0.648286	0.6800046	-2.5494912	0.15024014	0.99454064	0.46990408	0.36889181	0.42537869	1.99342106	2.17378193	-0.2325014	2.22983958
C_28	-1.1354153	0.13299316	3.57499206	5.42695686	1.76595028	-1.1161671	-2.4851128	-0.1397729	0.80510422	-1.861409	1.14335878	2.3837163	-0.0889147	0.42164288	0.58958481	2.27616272	2.45470068	-0.2223477	3.11612619
C_29	-1.8338645	0.23310121	3.58266212	5.31150909	2.27254016	-0.3956082	-3.4525766	-0.3468417	0.86477923	-2.0034487	0.52448185	1.83117699	0.85078485	0.4610463	0.15007881	2.09882341	2.2395147	-0.1766025	2.98957707
C_3	-2.3473783	-0.2073592	3.42839173	5.47045897	2.32316025	-1.8840593	-3.0690366	0.40050705	1.15128722	-1.7591829	0.10659458	0.92342343	0.85948022	0.5082275	0.47634871	2.38724671	2.63090325	-0.0889554	2.62118452
C_30	-1.0454925	1.32149282	3.08166812	5.39318699	2.73343652	-1.2844824	-1.2739332	-0.7001244	0.7953611	-0.2880578	-0.5602677	1.05429251	-0.8259727	-1.9097655	-0.5816595	1.83583013	1.43471075	0.08511788	2.41496266
C_31	-2.8529103	0.12351881	3.14526723	4.94081538	2.27107786	-0.9480582	-3.3887962	-0.1442907	0.6490452	-2.1394762	-0.1244757	1.32634461	0.25604935	1.03607391	0.45904312	2.27490093	2.40171953	-0.5324622	2.94917548
C_32	-1.786687	-0.0557879	2.98687246	4.65730134	1.71418961	-1.0694928	-3.6154668	0.27873873	1.43282773	-3.2626826	-0.2479198	0.85317412	1.31965175	0.58559319	1.34246359	2.91022703	3.06039436	0.43122552	2.28307235
C_33	-0.6928873	-0.2357209	2.94339597	4.94616548	2.25717374	-0.4637402	-2.3090846	0.03254269	1.02028334	-3.0658106	-0.1665488	0.90371078	1.25244163	0.42368486	0.79130985	2.40052075	2.51112788	0.22134828	2.08712374
C_34	-1.7198459	0.03192874	3.36201329	4.93224168	2.60240738	0.29007066	-2.9056959	0.18728711	0.44794629	-2.5273724	-0.1170888	1.14217993	1.30206079	0.29097805	0.9843913	2.46508831	2.32327259	-0.1945976	2.3716584
C_35	0.06277379	1.94861642	2.02280431	3.94754977	1.67221809	-0.2533261	-0.6317129	0.29557104	-1.6688174	-0.7058163	-0.9443775	-0.1562914	-0.6208438	-1.0682625	-0.6494711	-0.0264757	0.01717657	0.14626591	0.90980518
C_36	-1.140386	-0.2492376	3.03807893	5.13222239	1.62312907	-2.3076866	-3.7356874	1.01696191	1.99583862	-2.8803503	-1.0401313	-0.1226815	1.69675009	0.28256307	1.64031733	3.51765612	3.85745576	1.08076099	2.01977044
C_37	-1.9326565	-0.2776191	3.05317275	4.86544496	1.68159947	-1.3125559	-2.5852386	0.69625316	1.60735816	-2.4848506	-0.4035022	1.00414044	1.55812466	0.40464448	1.61967383	3.2231685	3.55966492	0.80981293	2.32362881
C_38	-2.0132042	-0.1108955	3.05706386	4.75700572	2.11498158	-0.9056083	-3.6495	0.88206086	1.40851019	-3.1187041	-0.0698893	0.53893263	1.72756326	0.03350335	1.7559191	3.33766366	3.33680527	1.0067229	1.95912939
C_39	-2.5652058	0.21481863	3.16029253	4.90890814	1.74960405	-1.913346	-2.711533	0.31433182	1.32807294	-1.8651366	-0.6490046	0.37529407	0.95780645	0.47032229	1.6126265	3.06942965	3.09608814	0.14944318	2.39542992
C_4	-1.6014304	0.10264582	3.14463013	5.10969886	2.44189061	-0.2710883	-2.104597	0.0249271	1.14551128	-2.6858231	-0.3025325	0.7565278	0.61667069	-0.0857775	0.97191743	2.58978881	2.77667952	0.21820041	2.49311705
C_40	-1.7628377	-0.3448602	2.84097447	4.45556466	1.54946385	-2.7313875	-2.5144541	1.16447853	1.79609531	-2.4785269	-1.9550987	-0.6227587	1.98320088	0.66506375	2.28688302	3.76576549	3.69545806	1.04121628	1.24215092
C_5	-2.2475557	0.41350764	3.41167086	5.3813782	2.37551733	-0.5636793	-3.3969893	-0.2152351	0.82946484	-2.2057685	0.60522781	1.80853217	0.36939505	0.66384391	0.50963727	2.12139386	2.30320373	-0.1125822	3.06438127
C_6	-1.0066762	0.31502421	3.36528125	5.2035304	2.00916301	-1.3964205	-2.6131936	-0.2722807	0.78632296	-1.8980633	-0.2386888	1.18217023	0.15826505	0.85087736	0.53620953	2.09341358	2.24625917	-0.475366	2.95864138
C_7	-1.3634435	-0.074297	3.61788144	5.69289479	2.40038801	-0.8925263	-2.3340204	0.28338658	1.27186352	-2.2021749	-0.4431565	0.73730217	0.51438147	0.18537917	0.39833538	2.36079963	2.60248804	-0.0708971	2.44839501
C_8	-2.3332683	0.01386737	3.38555281	5.17372937	2.47532344	-0.3956217	-3.4089134	0.15835473	0.79820689	-2.0063286	0.14623139	1.23794532	0.53929914	0.53027738	0.58266097	2.09677166	2.10323239	-0.2539527	2.41993541
C_9	-2.3062448	0.36983252	3.26921795	5.03002868	2.44596453	-0.7050127	-3.0426113	0.0264783	0.9375025	-1.9044204	-0.0411988	0.62356571	0.8504917	0.63754488	0.65723685	2.16669831	2.28613214	-0.4193158	2.34951874

Table 8.101: Normalised data matrix for cholesterol ester for serum samples taken from patients with breast cancer.

	Cholesterol	CE	CE(10:0)	CE(13:6)	CE(13:2)	CE(24:0	CE(24:1	CE(24:2	CE(24:3	CE(24:4	CE(24:5	CE(24:6	CE(14:0)	CE(14:1)	CE(15:0)	CE(16:0)	CE(16:1)	CE(16:2)	CE(17:0)	CE(17:1)	CE(17:2)	CE(17:3)
P_1	-2.4790792	1.79506523	-3.077787	-0.6466928	-1.7907086	1.47579124	1.94268185	0.41193564	-0.4395957	-0.9595177	-0.4051792	0.39142199	-2.2816473	0.82360263	-0.5275978	1.00031585	1.40044121	-1.8694979	-2.0940018	-1.2184309	-2.2926379	-2.21155
P_10	-1.5004056	1.91677466	-3.1959168	-0.6012699	-1.2352611	1.42963136	1.40088712	0.83207282	-0.1126935	-1.3430783	-0.5528415	-0.1168976	-4.1722602	-0.106078	0.23042049	0.91646512	-0.03946	-1.885264	-3.4730129	-1.6108522	-2.1521684	-1.2333842
P_11	-1.0911513	1.9941193	-2.7032083	-0.693754	-0.7929827	0.98917804	1.51305414	-0.3173792	-0.0317931	-0.4364748	-0.736816	-0.1550429	-2.6872631	-1.0518558	0.02126528	1.18387238	0.46812666	-1.9186065	-2.7567187	-1.7610029	-1.6555527	-1.8665872
P_12	-1.1867281	1.52733408	-1.577649	-0.7596439	-1.3726374	0.92626482	2.02380646	-0.1251752	-0.2469505	-1.2719183	-0.3189506	0.56684185	-2.6763358	0.6788631	-0.4311339	1.3443404	0.85538818	-2.2452886	-3.2585353	-1.202372	-1.8537194	-1.4725522
P_13	-1.6782073	2.23510751	-3.2712103	-0.4333225	-0.6397149	1.19411301	1.63847058	-0.2294863	-0.3083294	-0.898767	-0.3848068	0.01928663	-1.9430239	0.36387111	0.04358777	0.81318776	1.12812218	-1.2574662	-2.7696978	-2.2098156	-2.4798247	-2.5521673
P_14	-1.4993792	1.64105156	-2.5761878	-0.0132776	-1.367478	1.36634555	2.04618704	-0.2499787	-0.835767	-1.7708628	0.17512188	0.42094787	-2.5657507	0.2601497	0.27756727	0.855784	1.24755355	-3.1061843	-2.5907738	-0.9887495	-1.9984467	-2.0489482
P_15	-1.4061269	1.70610373	-2.1752653	-1.111811	-1.7768275	0.72059981	1.6110532	-0.1532098	0.03243728	-0.6774365	0.35338839	0.23041933	-2.2036108	-0.8935126	0.7391972	0.97516162	0.41934787	-0.95328	-3.191386	-1.8457115	-1.0686395	-1.037207
P_16	-1.7223138	1.88656676	-3.3287145	-0.2211039	-1.0904373	1.54608564	1.59866389	0.41099054	-0.1443696	-1.1414946	-0.829283	-0.249328	-1.9172115	0.52631881	-0.0792052	0.89374708	0.80162985	-1.9226335	-2.7085058	-1.7269404	-1.9679695	-1.4974932
P_17	-1.6315333	1.85868075	-2.0677992	-0.909256	-1.036	1.30074132	1.64683312	0.09754196	-0.075097	-1.0358993	-1.069126	0.36257718	-3.0666149	-0.2239626	0.04790167	1.15312925	0.4689419	-1.835294	-2.9642551	-0.742758	-2.0924567	-1.8404332
P_18	-2.3130518	1.6069683	-3.3606764	-0.0397174	-1.1952655	1.03034981	1.46911259	-0.1455235	-0.3899573	-0.9453143	-0.526393	0.00560717	-2.7092287	1.06291439	-1.0636453	1.09252977	0.9713643	-1.7946164	-2.8863101	-0.9389794	-2.1236181	-0.8184565
P_19	-1.8901856	1.50639477	-3.0528399	-2.5703405	-1.3831958	1.94516207	2.14599011	1.21276115	1.38591056	-0.3443545	2.04768047	0.38437395	-2.6501027	-1.7911066	-0.1721632	0.86044211	0.65587194	-3.5884152	-2.9923924	-1.2566302	-3.1220336	-2.1524233
P_2	-2.1383573	1.68678767	-2.8800132	-1.2494492	-1.3154675	1.31260162	1.74873244	-0.0126367	-0.1083987	-0.3447026	-0.2084114	0.0473892	-2.4883199	0.38407924	-0.5307512	0.90632798	0.36880124	-1.9284968	-3.5093865	-1.4451643	-1.9417019	-1.5087327
P_20	-1.8340037	1.83762293	-2.405098	-0.0749787	-1.207745	0.94013667	1.40811051	0.67699002	1.22155123	-0.5936379	1.86294765	-0.0866713	-2.4797676	0.80522966	-1.2030107	0.76934892	0.61475294	-2.7059017	-2.5214375	-1.9072728	-2.077782	-2.2329933
P_21	-2.216243	1.49614837	-3.0313992	-0.4543566	-1.2835475	0.92468865	1.29434183	0.7636466	1.36744273	-0.1855287	2.27028441	-0.3026485	-2.8138187	-0.1396348	-0.2430508	0.10327398	0.61341702	-2.0629718	-3.6178858	-1.7756047	-1.8708415	-1.5947297
P_22	-1.7902932	1.97364511	-2.7487185	-0.7032136	-1.1475002	1.03506856	1.17694638	0.12650665	0.88548945	-0.4926786	1.64596316	-1.264129	-1.9318384	-0.0430075	-0.4086621	-0.0894733	0.98395758	-1.7447737	-2.770499	-1.4836614	-1.3293994	-0.5036984
P_23	-1.9746085	1.52600927	-3.2780725	-0.862187	-1.0132037	1.6438697	1.50298336	0.98830422	1.28124454	-0.6816474	1.95437171	0.29741377	-2.368056	-0.7214193	-0.3627992	0.52248144	0.19202732	-3.0577361	-3.5842866	-1.4857466	-1.6795688	-1.3183752
P_25	-2.2867914	1.63687385	-3.570585	-0.0136565	-1.0069572	1.46421051	1.66786203	0.72811544	1.2587569	-0.4742827	1.92228034	0.05767632	-1.8475717	-0.2245336	-1.2206273	0.73601202	0.37520752	-2.2079437	-3.954367	-1.774486	-2.1042561	-2.7660589
P_26	-2.3397656	1.55252494	-3.5930632	-1.1009591	-1.0344739	1.2778526	1.67961823	0.4017183	0.91191147	-0.8780569	1.57081722	0.17577732	-2.4805923	0.17906948	-1.2835792	0.97075934	0.20027029	-1.9520554	-2.2845416	-1.6920191	-1.7262882	-1.6191468
P_27	-2.2581127	1.81273141	-2.5608335	-1.5159689	-1.5539135	1.3675074	1.68766126	0.41624212	0.85180862	-0.5657783	1.51069002	0.44135036	-1.9490005	-0.1267407	-0.6369846	0.64111023	1.02632983	-1.75116	-2.9021622	-1.8797144	-1.6423352	-1.2552841
P_28	-1.3224951	1.93231175	-3.4025971	-0.6566751	-1.0672945	1.55303611	1.71117696	1.09690699	0.99786407	-0.7274015	1.33324984	0.29139509	-3.1600156	-1.3685693	-1.2611529	1.06683367	-0.0885226	-2.4125343	-2.8558547	-1.2635605	-1.9934619	-2.7704822
P_29	-1.4830381	1.57927936	-2.8193991	-1.5974275	-1.5964284	1.67248436	1.91476815	0.63906866	0.1562832	-1.6951725	-0.1850766	0.1321499	-2.985202	0.29611291	-0.8336605	1.16023269	0.60585287	-2.3965935	-3.1086705	-1.7248641	-3.0757714	-2.2311398
P_3	-1.8777981	2.53430266	-2.3580438	-0.2878392	-0.7113305	0.91823316	1.55766294	0.03281734	-0.4295286	-1.3025582	-0.4962407	-0.3963003	-2.1433734	-0.0204614	0.17427947	1.02114405	0.10703382	-1.546207	-3.425537	-2.426885	-2.0000682	-3.6288589
P_30	-1.6815484	1.69417753	-3.2111859	-0.7503415	-1.1927412	1.76761312	1.45643691	0.79649756	-0.0668602	-1.1405264	-1.3579657	-0.0780642	-1.8899495	-0.9709355	-0.017674	0.70831083	0.70110742	-2.4141053	-2.4199853	-1.4692415	-2.2186888	-0.8539357
P_31	-1.3808293	2.1493602	-2.7051295	-0.7296302	-0.6249452	1.24430181	2.17821567	-0.0279387	0.09827942	-0.8479392	-0.1567478	0.80388214	-3.137526	0.20071496	-1.0320508	0.99239749	0.33012101	-1.3439257	-2.9970551	-2.1613393	-2.2053118	-1.983282
P_32	-2.1883414	2.54331952	-2.5880366	-0.8368298	-0.5792976	1.92908152	1.64766566	0.82735981	-0.2633197	-0.8396085	-0.5832733	0.30883386	-3.5870106	-0.2994097	0.36785276	1.01687516	-0.1367786	-2.2857438	-2.9178497	-2.4811997	-2.0570615	-1.3090947
P_33	-1.3781565	1.6997028	-2.7064378	-0.6797592	-1.157152	1.08578388	1.6858276	0.1957426	0.19709721	-0.707799	0.59971148	0.02634453	-2.6027754	-0.0784479	-0.8904269	0.51981789	0.34422671	-2.4266732	-3.3418363	-1.1063638	-2.0393494	-0.9997438
P_35	-2.167346	1.23493768	-2.9935612	-0.6267105	-1.7639573	2.26129378	2.01933002	1.27349288	-0.2231759	-0.626287	-0.5949506	0.45684749	-1.6706879	0.03555698	-1.3183724	0.16052851	1.54135866	-3.0409331	-2.9221001	-1.3154908	-2.1902953	-1.5217816
P_36	-1.219411	1.85483366	-2.9182536	-0.6828165	-0.6508594	2.1314981	1.99374914	1.38304936	0.30122825	-1.4585551	-0.1693176	0.41271384	-2.7632971	-0.3648126	-0.7052644	-0.0108414	0.28255555	-1.8493256	-3.30774	-1.683761	-2.5494518	-1.4854915
P_37	0.59945202	4.01820901	-0.7674541	-1.9244522	1.14172308	0.40910051	-0.2778463	-1.3122307	-0.41218	-0.4529141	0.2835504	-1.1024869	-1.0306674	2.34211006	-0.4122826	-0.4623838	0.64634746	-0.4663472	-1.2942007	-1.1739699	-1.4589007	-2.0863063
P_38	-1.5730782	1.40871152	-3.345097	-0.8692542	-1.150336	0.88240134	1.55035439	-0.5189474	-0.2487372	-0.7546519	-0.3490664	0.00750738	-1.7286088	-0.1441075	-0.7857666	1.21442887	1.06101207	-2.0497488	-2.4621638	-1.53715	-2.1176929	-1.4379674
P_39	-1.2224643	1.57958259	-2.8205155	-0.9410048	-1.1050173	1.84848904	1.86956713	1.0810509	-0.2123446	-0.7999322	-0.6837092	0.64277809	-3.7245653	-1.4144248	-0.2337311	0.44854883	0.36372933	-2.7437086	-2.9926016	-1.2314175	-2.3698914	-2.1003091
P_4	-2.3185959	1.89048708	-2.7974146	-0.5023174	-1.5392412	2.18722826	1.99602323	1.2989347	-0.2481712	-1.474488	-0.2105906	0.50866293	-2.6504127	0.06589198	0.24802315	1.02175217	0.16233263	-2.3285247	-2.9142362	-2.4001991	-2.1068114	-2.4307417
P_40	-1.2687119	2.07552565	-2.4797523	-1.6273436	-1.272209	1.30833061	1.80985876	0.09483999	-0.0488094	-1.514107	-0.5692397	0.50689924	-3.136691	-0.6251399	-0.593518	1.07621396	-0.3431845	-1.0338269	-3.0131894	-1.6992865	-2.9401733	-1.5472781
P_41	-1.5263194	1.69840451	-3.7158359	-0.3167475	-1.1606625	1.66391007	2.14852044	0.49687087	-0.0979536	-1.1714487	-0.341649	0.6280606	-2.767837	0.38433226	-1.114847	1.08488329	0.97297485	-1.9911544	-3.1074493	-1.5379517	-2.5660833	-2.0007367
P_5	-1.4573065	1.95314933	-3.0101707	-0.3457554	-0.5433182	1.31204586	1.40048484	-0.3458811	-0.2815397	-0.6760699	0.13741762	-0.0692466	-3.128527	0.4191345	-0.3768613	0.8619636	0.22219772	-1.4834131	-2.7828934	-1.2442922	-2.4427249	-1.1122667
P_6	-1.3416587	-1.5739821	-1.4401966	-1.0697805	1.12241079	0.14878631	0.91162957	-0.5014273	-0.6909524	-0.7513147	0.35786257	-0.0669227	-1.3759844	-0.4028672	0.70378949	0.61279251	0.84151769	-0.8633025	-0.7415367	-1.5157004	-1.0434091	-0.8270914
P_7	-1.4852037	1.43739377	-3.3786157	-0.8847375	-1.7687925	1.34036796	2.08043523	0.09332062	-0.1289874	-0.789908	-0.7426679	0.1318335	-1.6449072	0.22240116	-0.4838825	1.17460015	0.91928138	-2.4431069	-2.7778291	-1.446388	-1.7837669	-1.4221595
P_8	-1.3008389	1.52213278	-3.2670751	-0.2350799	-1.39816	0.93747186	1.45811852	0.12423749	-0.3572197	-0.7949788	-0.0311724	-0.4100267	-2.2336178	-0.594296	0.24267995	0.81941121	0.58248778	-1.8009449	-2.0613043	-2.0822153	-1.9193715	-1.3483028
P_9	0.34341298	-1.1284661	-1.170199	-1.1450147	0.88568404	1.39685636	1.21580624	0.19632102	-0.7982484	-1.62202	0.46749651	0.42321282	-1.5897431	-0.836516	0.23648666	0.29759999	-0.4008517	-1.1390216	-1.0070971	-0.9618304	-1.3751528	-1.3720938

Table 8.102: Normalised data matrix for cholesterol ester for serum samples taken from patients with breast cancer.

	CE(17:5)	CE(18:0)	CE(18:1)	CE(18:2)	CE(18:3)	CE(18:4)	CE(18:6)	CE(20:0)	CE(20:1)	CE(20:3)	CE(20:4)	CE(20:5)	CE(22:0)	CE(22:1)	CE(22:2)	CE(22:3)	CE(22:4)	CE(22:5)	CE(22:6)
P_1	-2.569416	0.18678709	3.38115448	4.93674855	2.21968559	-0.8007539	-2.3958428	-0.0850568	0.69023128	-2.2641559	0.38760857	1.49084448	0.5786734	-0.2428196	0.74483667	2.33167596	2.00981057	-0.1522684	2.60492497
P_10	-0.9671665	-0.0729785	3.42199467	5.39512439	1.76517288	-1.6333941	-1.6288811	-0.3728141	0.77530864	-1.9196194	0.79524609	1.80926415	-0.42725	1.23782263	0.45576861	2.20964696	2.45676577	-0.1396866	3.44426814
P_11	-1.8375973	0.62662283	3.58959536	5.5868436	2.52049189	-0.998729	-2.6998144	0.05804987	0.88868462	-3.1295827	-0.5092922	0.72715079	0.37173792	0.75570009	0.70208288	2.32723442	2.55194094	-0.1422965	3.09775017
P_12	-1.2500161	0.11652177	3.77672314	5.53603554	2.02990438	-1.7588458	-3.5401295	-0.2989416	0.77770921	-2.7931444	-0.1729063	1.02681908	0.12534561	0.25509448	0.6419118	2.14332948	2.37531995	-0.1275557	3.2135763
P_13	-1.9669523	-0.0780791	3.42614985	5.11125235	2.55955805	-0.6689821	-2.775052	-0.014641	0.84618242	-1.8328962	-0.2188045	1.00294943	0.57070572	0.61109593	0.58093926	2.2076609	2.08540603	0.01770062	2.15589996
P_14	-2.3714882	-0.0040574	3.55362669	5.0688806	2.2259678	-1.1124627	-3.1220092	0.05402166	0.35442723	-1.3584821	0.28070444	1.26011165	0.72764024	0.76989503	0.65685246	2.21659712	1.99504186	-0.2379355	2.36374431
P_15	-1.6567521	0.25878528	3.59688458	5.34358947	2.20837783	-1.3582128	-3.3943477	-0.4453019	0.72426	-1.7439991	-0.5569124	1.01635698	-0.0475083	0.78375859	0.44664655	1.97335015	2.06971022	-0.5625159	3.05014663
P_16	-1.7390893	0.07558507	3.26376736	5.0485601	2.1307616	-1.1583789	-2.7676854	-0.0674566	0.70756518	-1.4373133	-0.0178906	1.43635969	0.36155454	0.62175037	0.23054751	2.16569719	2.13819665	-0.2549265	2.14539663
P_17	-1.7239125	0.45333489	3.42872544	5.28844008	2.04251848	-1.2966854	-2.7234132	0.24388298	0.97565898	-2.4975848	-0.0643848	1.14570137	0.12060752	0.03843282	0.72560887	2.45141716	2.49402407	-0.2987644	2.8505306
P_18	-1.4127453	0.08644836	3.61964249	5.40059404	2.55665462	-0.5154959	-3.2605247	-0.2710859	0.58241607	-2.443477	-0.3054138	1.15300537	0.5948703	0.7597218	0.63225811	2.28811602	2.27063835	-0.339816	2.61610045
P_19	-1.1501563	-0.0561884	3.18123083	5.07226423	2.1778942	-0.9220605	-3.7063505	0.43836236	1.59950157	-1.7117408	-0.2373466	1.248389	1.11289517	-0.3007994	0.82084388	2.41689803	2.42391621	-0.0870577	2.50110084
P_2	-1.8497118	-0.159382	3.38562556	5.37359089	2.33764408	-1.0442615	-1.9385619	0.04616287	1.04217776	-1.4039749	-0.1135238	0.87270926	0.6822233	0.30803972	0.42295143	2.25938218	2.46909305	-0.1111047	2.57619083
P_20	-1.0684918	0.39155081	3.42038752	4.9939358	2.1130642	-1.1932041	-3.2530832	0.39776333	1.31757583	-3.1080577	-0.9424931	0.27284038	0.67658912	0.11328957	0.89456277	2.50180376	2.30870016	-0.2159852	1.57286163
P_21	-1.1039327	0.00122183	3.54986933	5.4868491	2.44157447	-1.0579694	-3.6124512	0.00357168	1.4389591	-2.4435435	0.14018749	1.34363625	0.22182097	-0.2704634	-0.0337082	1.9911244	1.93239646	-0.0591219	2.78899668
P_22	-1.1570863	-0.1568052	3.23457544	5.29544038	2.64091664	-0.353048	-3.5075941	-0.5600349	1.0821223	-3.1626687	-0.0981173	0.92705643	0.39079387	-1.2503252	0.39265381	2.19301762	2.12898088	0.14432742	2.43976437
P_23	-1.2666665	-0.1119595	3.186992	4.90939617	1.76983385	-0.8366763	-3.1798422	-0.1831815	1.1763255	-1.994339	0.49751371	1.87786788	0.02830725	-0.5481695	0.44125356	2.26887114	2.18068242	-0.3294607	2.59225322
P_25	-0.7340295	0.03958047	3.33016954	5.16704237	1.89858167	-1.6646294	-3.4306332	-0.1243302	1.44361166	-1.6891457	-0.4330458	0.90355602	0.51419335	0.36950007	0.69316811	2.54098798	2.59744833	0.09759251	2.08550383
P_26	-1.1925225	-0.2885356	3.23795168	5.19504703	2.54614823	-0.6848192	-3.4719852	-0.1888825	1.38239809	-2.3078266	-0.5525474	0.57041293	1.03196979	-0.1325185	0.56284628	2.46394134	2.66228875	0.10189279	2.12896273
P_27	-1.3419673	-0.1319811	2.9767008	4.68928561	2.11695171	-0.8586533	-2.7401022	-0.2439938	0.87085092	-2.7762096	-0.1187308	0.87183719	0.59990619	0.21680709	0.61423132	2.33379333	1.9948183	-0.3769346	2.14594758
P_28	-1.105281	0.07152429	3.02606797	4.93814519	2.23593807	-1.0313417	-3.4068606	0.06488233	1.0706823	-2.1652346	0.2939385	1.50258288	0.47575554	0.18175025	0.58855811	2.45452798	2.41974931	-0.005798	2.75825586
P_29	-0.8862816	0.18557408	3.82615458	5.44563776	2.2115517	-0.569476	-3.2683886	0.21024718	1.03192254	-1.8793038	0.57422328	1.49647802	0.77475572	-0.2398563	0.95204115	2.50256441	2.49684465	-0.2266	2.93812317
P_3	-1.1065904	0.43105992	3.68599492	5.35463033	2.29393203	-1.4584673	-1.6148028	-0.0329783	0.870619	-1.9951441	-0.3515399	0.94921048	0.21158589	0.66655008	0.70429596	2.44306443	2.44826359	0.10994882	3.09592412
P_30	-2.2138351	0.41743154	3.50808197	5.21972755	2.17552179	-0.40792	-2.6441299	-0.6277956	0.12177723	-1.9065113	1.248378	2.51598218	-0.0046761	0.53044322	0.20345139	1.89704282	1.81812383	-0.4579585	3.21647048
P_31	-1.3569111	0.04557047	3.30976489	5.15725793	2.00908881	-1.7543905	-3.6027448	0.1548547	0.95414398	-1.4265972	-0.6678507	0.87125783	0.32631428	0.45931146	1.09616681	2.68899942	2.64880261	-0.258703	2.68204174
P_32	-2.6433744	-0.0658818	3.22284783	4.94614336	1.69075751	-1.1883057	-1.573235	-0.2343961	0.85824089	-2.1789943	0.38458932	1.7364489	0.17639033	1.06764503	0.74877247	2.2817391	2.46025767	-0.2735286	2.89575038
P_33	-1.8577399	0.07887509	3.51942735	5.51337228	2.29076189	-1.1080287	-1.3956429	-0.3815004	1.02219235	-1.9721242	-0.449004	0.69394023	0.62406896	-0.7292606	0.52958632	2.26706452	2.2667651	0.26387563	2.58403769
P_35	-2.0504763	-0.1902235	3.26768221	4.66421886	2.35670885	0.10683752	-3.2868114	0.17728887	0.56882231	-2.1206091	0.52733725	1.57514575	1.44734823	-1.1429511	1.03551464	2.48751632	2.16054649	0.00655845	2.40184929
P_36	-2.284557	-0.1018927	2.93270136	4.64167287	1.85255997	-0.3882174	-1.7282081	0.03680323	0.56777964	-3.6577109	0.70651446	1.72063755	0.74065046	-0.3423862	0.99107649	2.50683789	2.5162456	0.07693114	2.67213224
P_37	-1.2105754	1.54548076	2.80485481	4.89817438	1.56067895	-0.8876564	-1.2108994	-0.9732748	-0.1521069	-1.2291581	-1.1195962	1.19292926	-1.0076104	-1.176263	-0.8002987	0.35066317	0.66595229	-0.3562941	2.29913008
P_38	-1.4013398	0.56690976	4.04135882	5.65694695	2.7416882	-0.4639059	-2.395021	0.09360881	0.2999101	-1.8258572	-0.5246755	0.64933527	0.34056443	0.14987739	0.62137303	2.13799332	2.06602733	-0.0388461	2.23201063
P_39	-1.9948112	-0.022948	3.52516542	5.22988964	2.02410225	-1.3982512	-2.3182371	-0.019029	0.80688346	-1.1269817	0.88414532	2.01058034	0.37117097	0.46706397	0.76278432	2.32222247	2.36017673	-0.1409384	3.01890292
P_4	-1.2002406	-0.1616699	3.19289342	5.12869086	1.777699	-0.6560074	-3.0296903	0.13559142	0.83174221	-2.2831685	0.52646143	1.91858052	0.72745032	0.34214487	0.35438318	2.01131369	2.30377958	-0.0999216	2.72237653
P_40	-1.8316522	0.18500362	3.49527798	5.2305125	2.44964261	-0.6811594	-3.1724476	0.0186271	0.91487096	-1.9450374	-0.2692395	1.03866831	0.71248929	1.02315208	1.14472493	2.60398419	2.6317665	0.31016858	2.98143975
P_41	-1.6333441	-0.1774071	3.42369763	5.26406963	2.29817952	-1.1556443	-2.345921	-0.1354985	1.19937529	-3.6381465	-0.3687961	1.00113015	0.86693893	0.16575332	1.24278369	2.74677259	2.77808938	0.20875349	2.59793306
P_5	-1.2644711	0.13837545	3.62296648	5.49479535	1.80867915	-2.3701642	-3.0425944	0.09169428	1.18636678	-2.9094402	-0.4844601	0.89201675	0.45086188	0.38084647	0.90605798	2.51593521	2.79824141	0.399983	2.37818319
P_6	-1.2761321	1.14536602	2.70604242	4.50454462	1.88647128	-0.5259915	-0.7145807	-0.1646664	0.7503044	0.17425853	-1.2415097	0.80140678	-0.3730513	-1.2254175	-0.7159691	1.19187691	1.19592394	-0.3605151	1.74897627
P_7	-1.6932195	-0.0944632	3.50246932	5.25416173	2.38532343	-1.1133296	-2.7670359	0.22416931	0.94840941	-2.1787081	-0.1614796	0.92531693	0.94499778	0.05536643	0.52069476	2.34030143	2.257138	0.07990049	2.3513059
P_8	-1.6731122	0.26184082	3.68113003	5.71500075	1.94667531	-1.9411443	-2.9399761	-0.2442313	0.81172081	-2.1804173	0.66254694	1.79390867	-0.059424	0.75810608	0.41402011	2.00516903	2.2458885	-0.3504429	3.24080553
P_9	-1.3403213	1.07036864	2.69067743	4.72076998	1.47865499	-1.4095445	-1.3476582	-0.1145539	0.8932122	-1.3068925	-1.4373056	0.99793848	-0.9182722	-1.5234116	0.62953621	1.86520456	2.08700718	-0.4136517	2.46161984

Table 8.103: Normalised data matrix for ceramide for serum samples taken from breast cancer free controls.

	Acyl[3	Cer(17:0	Cer(d18:1/16	Cer(d18:1/17	Cer(d18:1/22	Cer(d18:1/24	Cer(d18:1/24	Cer(d18:1/25	Cer(d18:1/32	Cer(d18:1/32	Cer(d18:1/38	Cer(d18:1/39	Cer(d18:1/39	Cer(d18:1/39	Cer(d18:1/40	Cer(d18:1/40	Cer(d18:1/41	Cer(d18:1/42	Cer(d18:1/44	Cer(d18:1/44
C_1	2.02653277	-0.5931789	-0.4585804	2.94513203	3.35995872	3.65547177	0.43926982	0.56516461	0.48964861	0.8392062	0.54753026	-1.9631886	-1.1494362	1.74603589	0.79416781	0.29198813	-1.608986	-1.3063727	1.33236279	
C_10	1.9379522	-0.615528	-0.7261492	2.94345999	3.75955872	3.78606762	0.93920965	0.47644925	0.54469745	0.57921542	-0.0626303	-1.48063	-1.0221541	1.66656257	0.81949069	-0.4362355	-0.9276562	-0.9085648	1.71262682	
C_11	1.96172636	-0.8322596	-0.3506962	2.80507815	3.29113042	3.70029764	0.3447199	0.59588174	0.7396016	0.61906211	-0.0152896	-1.559116	-0.9914847	1.30072355	0.68098523	-0.3905004	-1.487046	-1.1649489	1.48104664	
C_12	1.74637928	-1.2301038	-0.6518236	2.62469604	2.97418113	2.83420873	-0.162665	0.48705139	1.21167486	1.56728089	0.88012012	-2.1207	-1.0226179	1.98878273	1.10224836	0.21232372	-0.8452248	-0.7010235	1.90194743	
C_13	2.04747077	-0.5163145	-0.9951865	3.02207141	3.88085312	3.42315747	1.01848167	0.77837608	0.62775762	0.93783021	0.25749902	-2.0068275	-1.4156295	1.67662453	0.71203011	0.07367116	-0.9753411	-0.5634532	2.06816738	
C_14	2.27586733	-0.1219191	-0.8718011	3.16008417	4.06852371	2.03018613	1.32697672	0.76146325	0.83601644	1.09965897	0.63096045	-2.0196825	-1.7552758	1.75458706	-0.369455	0.4108901	-0.8105697	-0.7394139	1.89714437	
C_15	1.8967402	-0.3680847	-0.7392222	2.89224583	3.71700111	3.43818911	0.8521993	0.49097274	0.61467331	0.69510786	0.24503672	-1.7370638	-1.6770025	1.44147487	0.5759715	-0.2231396	-0.7932814	-0.7853302	1.76212415	
C_16	1.8472325	-0.8370117	-0.7339736	2.70375155	3.10393312	3.21834697	0.23420922	0.55176871	1.10847259	1.35748266	0.88812432	-2.0031873	-1.118377	2.0438958	1.03741398	-0.1629862	-0.9557767	-1.0592044	1.73530653	
C_17	1.83938157	-0.7669892	-0.5360756	2.72999151	3.21834537	3.63244286	0.29353968	0.52433155	0.58785385	0.73255222	0.41160085	-1.3829424	-1.0005277	1.72190122	0.89375904	-0.1122794	-1.3470654	-1.566439	1.15441443	
C_18	1.9466977	-0.4008755	-0.4588408	2.82979812	3.52566244	3.55605268	0.8661482	0.53380321	0.85402624	0.77134339	0.4805925	-1.6216766	-1.2752822	1.53988818	0.6925348	-0.4289599	-1.3720278	-1.4029002	1.394874	
C_19	2.02681914	-0.4408342	-0.391982	3.04040161	3.60609716	3.87091591	0.68282187	0.54511937	0.70929631	0.5135314	0.15659742	-1.5758449	-0.9969659	1.38795978	0.60922494	-0.6121553	-1.0529016	-0.5926613	1.92238808	
C_2	1.97961026	-0.871658	-0.640057	2.72188882	3.30973487	3.59982371	0.57217726	0.76451248	0.86205146	0.91769229	0.36031699	-1.8274792	-1.0469053	1.70516441	1.12812214	-0.1516634	-1.3628198	-0.9805898	1.60898245	
C_20	1.85247466	-0.7611049	-0.3643128	2.65668008	2.93300969	3.03585158	0.32590773	0.58941593	0.87586939	1.05629618	0.92574604	-1.6813823	-1.3026844	1.87061297	0.66715576	0.06338704	-1.1465403	-0.9375568	1.68246367	
C_21	1.91174901	-0.6106442	-0.7350461	2.90629896	3.65837951	3.48236187	0.80050331	0.41331949	0.6906377	0.7622002	0.27458914	-1.8767611	-1.16134	1.5367179	0.56642613	0.2837259	-1.7474529	-1.2615282	1.4929533	
C_22	1.96518781	-0.6425257	-0.9506316	2.98285479	3.98907248	3.83586296	0.91137591	0.27355695	0.21616424	0.71895444	0.14096767	-1.9272775	-1.5047586	1.55214233	0.67288601	-0.2698319	-1.2072839	-1.377389	1.42995501	
C_23	1.84212926	-0.4159774	-0.4438383	2.88718343	3.65488783	3.51584527	0.8849815	0.53813469	0.66696768	0.62841743	0.2950667	-1.7915287	-1.5877327	1.43905406	0.6826559	-0.6424768	-1.0365031	-0.9985608	1.86143939	
C_24	2.24139966	-0.3331303	-0.8622053	3.22869097	3.90950734	3.67993428	0.8145064	0.70862009	0.1464664	0.96419572	0.12268449	-1.791077	-1.4846814	1.48029557	0.54024194	-0.1682182	-1.2424429	-0.9465381	1.78742331	
C_25	1.96330102	-0.2839539	-0.8314276	2.91719657	3.79911304	3.31375232	0.9080968	0.99532357	0.61365737	1.03478408	0.66226987	-1.9391339	-1.8533307	1.87393338	0.7202593	0.56522927	-1.0001066	-0.6890513	1.93558444	
C_26	1.89240364	-0.2673081	-0.4187653	2.94487036	3.78637813	3.60236443	0.95334342	0.82959265	0.54511489	0.83310743	0.38344594	-2.2183465	-1.6368706	1.56501711	0.89771452	-0.2409972	-0.9796449	-0.5388024	2.13407413	
C_27	1.95296417	-0.376728	-0.8538008	2.97168302	3.65997868	3.59780204	0.82886163	0.67258595	0.63273777	0.84894522	0.49125641	-2.0247243	-1.8205066	1.60990619	0.85231047	-0.1572653	-0.928674	-0.5667916	2.15255977	
C_28	1.79667328	-0.5713609	-0.1749645	2.81932931	3.30976256	3.63596489	0.71775851	0.5321497	0.47501258	0.64862718	0.3691343	-1.336691	-0.9970468	1.62482492	0.73577281	-0.4173607	-1.2786447	-1.2767407	1.49514268	
C_29	1.89881606	-0.6396503	-0.1570819	2.94134489	3.5078374	3.7592768	0.51914326	0.81543561	0.46684958	0.71840316	-0.0865896	-1.3460738	-0.6937288	1.6457881	0.95867476	-0.3917223	-1.0107356	-0.9521383	1.59604756	
C_3	2.10215322	-0.5331358	-0.6638282	2.97061617	3.48234668	3.56195597	0.42832089	0.53234589	0.85049244	0.90291205	0.32264075	-1.7380493	-1.1855897	1.56536996	0.69948167	-0.4599544	-1.3380501	-0.8957983	1.62342067	
C_30	1.70819529	-1.1475053	-0.9961168	3.12098133	3.96890929	3.69404447	0.85094064	0.44242073	-0.2543375	-0.4187288	-0.3464622	-1.2266044	-1.3771169	1.14066197	-0.1786395	-0.1660463	-1.0280774	-1.387495	0.32916526	
C_31	2.0054718	-0.3082215	-0.2041275	3.01985261	3.83743417	3.56141324	0.89702244	0.7596897	0.78520421	0.31447728	-0.2050244	-1.9256954	-1.4296983	0.86512428	0.18425968	-0.2072397	-1.1159021	-0.7882505	1.91333809	
C_32	1.77161696	-0.5553342	-0.9149377	2.75726017	3.59561605	2.98894175	1.0622728	0.69533819	0.7247532	1.13904506	0.70846463	-1.9212225	-1.4796549	1.94911975	0.64120927	0.05444948	-0.7684507	-0.7316222	2.05679676	
C_33	1.92588555	-0.5131174	-0.6452665	2.85614345	3.10252535	3.52270254	0.10328804	0.56943247	0.29600959	1.19363382	0.98380819	-1.6690996	-1.0487182	2.04585538	1.00302683	0.21169674	-1.3022149	-1.0976227	1.53775079	
C_34	2.06953986	-0.32938	-0.4564324	3.0959818	3.59034881	3.39547748	0.5416138	0.45177794	0.67162843	0.91195061	0.27259341	-1.4893628	-1.1773691	1.58307082	0.76638983	-0.2469426	-1.3419417	-0.9788668	1.79273967	
C_35	0.58744102	-0.0665024	-0.5969418	2.25093444	2.90018097	2.57064762	0.57308428	0.4887695	-0.6141683	-1.0149377	-0.3153539	-0.9823108	-0.5049464	0.60536229	-0.44831	-0.4011593	-0.8505428	-0.5263253	0.48387788	
C_36	1.97074901	-0.5659194	-0.308591	2.96124359	3.40799188	3.27608286	0.44517128	0.62090932	0.86785743	1.10999843	0.70963562	-2.3500689	-1.3686297	1.85461076	0.65252317	-0.3656632	-1.2688549	-1.0044258	1.72028077	
C_37	1.80009737	-0.5927392	-0.2178842	2.83810796	3.30191338	3.46406776	0.51840963	0.46648831	0.61803701	1.02404726	0.57264612	-1.5243921	-1.2562447	1.72793692	0.74436918	-0.4176619	-0.8495127	-1.0132039	1.74734179	
C_38	2.00903794	-0.3625274	-1.3434195	3.02164508	4.00832511	3.57802754	0.98491425	0.60049417	0.47765199	0.98287944	0.20520563	-1.8799047	-1.5179176	1.62606336	0.76859078	0.49892636	-1.3352383	-0.8601003	1.7355693	
C_39	1.82626646	-0.4055615	-0.5310776	2.91564696	3.66237372	3.41819588	1.00270424	0.4994498	0.78031935	0.77833999	0.22178434	-1.8834888	-1.6985602	1.35468096	0.74236569	-0.1750617	-1.0783895	-0.6671617	1.95577279	
C_4	1.95391697	-0.5417072	-0.7505089	2.94739427	3.8657517	3.10346376	0.69301046	0.38771379	0.90330832	1.11197217	0.4122514	-2.1298662	-0.9197516	1.8100214	0.65362273	0.19987151	-0.861165	-0.8356438	1.78786025	
C_40	1.78976294	-0.8484079	-0.5027971	2.7384226	3.30219768	2.85239344	0.27045489	0.51504021	1.06558434	1.506306	0.95549824	-2.0487039	-1.167962	2.16808457	0.90341161	0.37453082	-0.8379061	-0.6014717	1.99538046	
C_5	1.9059271	-0.4372679	-0.6128063	2.85451116	3.7085926	3.48196134	1.06149077	0.54404798	0.15558765	0.65729717	0.09714442	-1.8709123	-1.3889283	1.27069454	0.64338087	-0.4680601	-0.9255013	-0.7294139	1.92325327	
C_6	1.8347089	-0.6818522	-0.5375208	2.80004455	3.39583976	3.4287811	0.72521207	0.42354387	0.86891627	0.83013148	0.30607283	-2.2142465	-0.9168658	1.60850785	0.76236005	-0.4626667	-1.0579445	-0.7406789	1.91965867	
C_7	1.79668372	-0.6932362	-0.4939496	2.73348245	3.30479732	3.5677826	0.4678901	0.48587139	0.78033923	1.04059975	0.74541986	-1.919779	-0.9143452	1.9105678	1.08781032	0.01927218	-1.2831032	-0.9908314	1.58074277	
C_8	1.82469929	-0.6736513	-0.8442541	2.74101822	3.54459893	3.68205489	0.6281698	0.44539965	0.75750907	0.73609152	0.25785181	-1.6214882	-0.901833	1.72993612	0.83613383	-0.6496701	-0.9502281	-1.2000464	1.60129607	
C_9	1.9190673	-0.5166479	-0.6221601	2.78922612	3.53470213	3.4786975	0.76750133	0.24102651	1.09572701	0.6561555	0.21997441	-2.030346	-1.0625668	1.42184033	0.76396422	-0.4753185	-1.015686	-0.8113279	1.84568449	

Table 8.104: Normalised data matrix for ceramide for serum samples taken from breast cancer free controls.

:6)	modCer576.	modCer614.	modCer632.	modCer651.	modCer703.	modCer731.	modCer766.	modCer769.	modCer798.	modCer875.	modCer883.	modCer886.	modCer910.	modCer921.
C_1	-1.4755572	0.1320286	1.90126083	0.61716758	-1.2121057	-1.8587838	-1.6614323	0.50902214	-0.8706296	-2.0232295	-0.912626	-1.289624	-1.5897188	-2.2184988
C_10	-1.5171999	-0.0938177	2.32000878	0.94568044	-0.9523852	-2.2744494	-1.6377621	0.0423376	-1.0262964	-1.5511817	-1.2611396	-1.4127171	-1.6622961	-2.9045238
C_11	-1.3333321	0.01537908	1.83387687	0.8839857	-0.79477	-1.7704192	-1.0540289	0.01921321	-0.8641924	-1.5111766	-1.0477325	-1.1415775	-1.5317331	-2.4324044
C_12	-1.554223	-0.7626033	1.45441687	0.90836501	-1.1080629	-1.3886111	-1.252461	0.96667145	-1.0622029	-2.5542229	-1.2206146	-2.0435575	-1.3500143	-1.8296158
C_13	-1.965249	-0.2565428	2.42904154	0.94045232	-1.2998874	-1.7067619	-1.9444786	0.21442658	-1.078133	-1.5368488	-1.2015101	-2.095948	-1.6093971	-2.9404019
C_14	-1.6348148	0.25676619	2.64939652	1.44818216	-0.68967	-1.7444425	-1.4772537	0.70334569	-0.5136115	-1.6982607	-1.5111888	-3.0239169	-2.6944602	-3.6343132
C_15	-1.5170415	-0.0025859	2.31652902	0.8752431	-1.1938569	-1.9116336	-1.6882534	0.28529608	-1.1483388	-1.5638205	-1.1776906	-1.3090601	-1.685803	-2.5775963
C_16	-1.752967	-0.3774674	1.71953392	0.76953197	-1.3796904	-1.4024038	-1.2334571	0.9658126	-1.4788627	-2.5052213	-1.3084913	-1.160763	-1.4476369	-2.3673388
C_17	-1.4220276	-0.2913737	1.85065389	0.72978547	-0.9550982	-1.5870943	-1.8699226	0.52152618	-0.8475596	-1.6880041	-0.7449114	-1.3723902	-1.4813953	-1.8699841
C_18	-1.7360979	-0.2489947	2.14766874	0.96691097	-1.1811552	-1.9955209	-1.6943692	0.51678465	-1.0415431	-1.7216194	-1.1486402	-1.1429383	-1.4817543	-2.2695896
C_19	-1.4438747	-0.142332	2.16048721	1.00270665	-0.9852051	-2.6512971	-1.63075	0.2385092	-0.870621	-1.3848811	-1.2392883	-1.449775	-1.7563797	-3.2551269
C_2	-1.5478259	-0.6313585	1.89147944	0.72695346	-0.9357042	-1.755245	-1.4318097	0.57901914	-1.0355986	-2.3794691	-0.7707587	-1.1751222	-1.314534	-2.8689307
C_20	-1.6275541	-0.3172352	1.43787296	0.78515817	-1.1716114	-1.3697066	-1.7160086	0.93112763	-1.0564394	-1.6293678	-1.2039739	-1.7670802	-1.400895	-2.2355758
C_21	-1.0417887	0.61668015	2.25567441	1.01081821	-0.9658147	-1.9021282	-1.6670427	0.24063255	-1.1561276	-1.6465214	-1.1682701	-1.3547822	-1.5285957	-3.0798241
C_22	-1.1894548	0.7058322	2.57769756	0.53722754	-1.2142933	-1.9413945	-1.5304179	0.1914762	-1.0086198	-1.700841	-1.0957726	-1.2118481	-1.6051832	-2.3236906
C_23	-1.4838125	0.08462265	2.18280342	1.03152773	-1.2189834	-2.2408992	-1.3919865	0.24348911	-0.9201354	-1.6156339	-1.2049403	-1.354104	-1.5364356	-2.5556575
C_24	-1.5138558	-0.3265913	2.49499481	0.68633746	-0.9642937	-2.039829	-1.5077101	0.17372147	-1.1583153	-1.3275305	-0.9666203	-1.7344758	-1.5499218	-3.0615832
C_25	-1.9347925	-0.6641895	2.36691204	0.57003313	-1.157779	-2.0789467	-2.1049887	0.70266782	-1.309432	-2.2438412	-0.6896907	-2.2592045	-1.7315138	-2.1707313
C_26	-1.7933498	-0.3474799	2.35260109	0.8683192	-1.214483	-2.1298835	-1.8298097	0.49382486	-1.1819709	-1.7821424	-1.2196561	-1.8174647	-1.5640819	-2.9011151
C_27	-1.8326871	-0.4628552	2.24598071	0.68838937	-1.1219059	-1.9167698	-1.6898323	0.57284818	-1.102497	-1.8527394	-0.9157245	-1.8632101	-1.8586363	-2.4334613
C_28	-1.6252923	-0.3378517	1.8821518	0.6338469	-1.1652904	-1.8970612	-1.5077049	0.51993398	-0.974622	-1.4017874	-0.9523007	-1.588644	-1.3749176	-2.3178039
C_29	-1.6505255	-0.265606	2.07410837	0.53576897	-1.5012211	-1.9855617	-1.4805481	0.12901917	-0.8496258	-1.3173867	-0.9207434	-1.4235481	-1.1354761	-3.7585504
C_3	-1.3636513	-0.1808995	2.04317371	0.74085789	-1.0522467	-1.6709681	-1.6721437	0.38370994	-0.8761947	-1.8834164	-1.1042591	-1.0349187	-1.4771517	-3.0795422
C_30	-0.5268809	0.36557666	2.18965885	0.7057839	-0.4823897	-0.9070903	0.20438791	-1.2018659	-0.1764726	-1.3219072	-1.3888277	-1.4243479	-1.0785601	-1.6852536
C_31	-1.1871504	0.12453111	2.44638845	1.43031494	-0.545312	-2.2258648	-1.7633331	-0.1988785	-0.7699085	-1.4318831	-1.1844701	-1.739379	-1.3958908	-3.5182925
C_32	-1.9181453	-0.4893229	2.21376883	1.0582794	-1.2304291	-1.8246626	-1.693029	0.74725277	-1.076364	-1.4623333	-1.5580529	-2.273184	-1.6766988	-2.5907411
C_33	-1.6108566	-0.4863966	1.70878211	-0.1356224	-1.5034077	-1.625598	-1.4324637	0.9488609	-0.8606597	-2.1392374	-0.7640663	-1.9182915	-1.1726206	-2.0841418
C_34	-1.2912889	-0.1882287	2.18348712	0.60569244	-1.181728	-2.1714804	-1.4906027	0.36016799	-1.1200206	-1.6333094	-1.1623278	-1.739949	-1.1843523	-3.1088769
C_35	-0.3915996	-0.7521545	1.96488393	0.5867687	-0.6104403	-0.9250476	-0.8876599	-0.2510151	-0.5398311	-0.6924864	0.0752793	0.01153592	-0.4629359	-1.2640964
C_36	-1.3868068	0.14509179	2.00349518	0.67760862	-1.6417014	-1.8172566	-1.3821718	0.72107882	-0.9638461	-1.9304776	-1.2218807	-1.315749	-1.3863626	-2.8659229
C_37	-1.586507	-0.7140974	1.84460832	0.69540512	-1.1317641	-2.0523712	-1.3846775	0.63211485	-1.1934615	-1.4225175	-1.1732668	-1.1766765	-1.533039	-2.7555736
C_38	-1.542506	0.02539793	2.60214483	0.79885921	-1.1358176	-2.403298	-1.7983802	0.31690195	-0.9618053	-1.3676238	-1.0874595	-2.1221307	-1.7137378	-2.8087681
C_39	-1.5357586	-0.4562902	2.23471615	1.04866158	-0.8661212	-2.0966312	-1.7224138	0.27525638	-1.0814493	-1.3583119	-1.1581683	-1.9559462	-1.4654169	-2.5807256
C_4	-2.0734763	0.09265851	2.42668001	1.22682186	-1.1059127	-1.8896655	-1.6237147	0.5780441	-0.8845947	-2.0983405	-1.3101964	-2.0287162	-1.8914657	-3.2096378
C_40	-2.0367582	-0.7473165	1.89811277	0.83803541	-1.2441368	-1.6267256	-1.6077893	1.00566451	-1.2183341	-2.258689	-1.4487295	-1.7537782	-1.6744731	-2.5549015
C_5	-1.5060056	-0.1548776	2.30018922	0.99981742	-0.8676563	-2.1721744	-1.6609293	0.14090822	-1.0422469	-1.6292733	-0.9873487	-1.3771164	-1.3610536	-2.5532316
C_6	-1.2323481	-0.0757057	1.97106749	1.044883	-1.1199442	-1.8970633	-1.5700108	0.36128534	-0.8569979	-1.5736927	-1.4176207	-1.3989684	-1.4052101	-3.121676
C_7	-1.8632706	-0.0546585	1.85584358	0.51525264	-1.2831309	-1.8133398	-1.729573	0.73789533	-1.1490247	-1.9422503	-1.1257351	-1.0312865	-1.8262943	-2.5164427
C_8	-1.3783742	0.26445307	2.16144902	0.87691526	-1.1874522	-1.9268855	-1.6467484	0.32459748	-0.8018405	-1.699681	-1.3272479	-1.7513023	-1.5355406	-2.3159301
C_9	-1.2916224	0.15370941	2.10520854	1.03995266	-0.7240542	-2.0599591	-1.6405937	0.27065549	-1.0509824	-1.8737815	-1.2180809	-1.5847953	-1.6557152	-2.669455

Table 8.105: Normalised data matrix for ceramide for serum samples taken from patients with breast cancer.

	AcylCer	Cer(d17:0	Cer(d18:1/16	Cer(d18:1/17	Cer(d18:1/22	Cer(d18:1/24	Cer(d18:1/24	Cer(d18:1/25	Cer(d18:1/32	Cer(d18:1/32	Cer(d18:1/38	Cer(d18:1/39	Cer(d18:1/39	Cer(d18:1/39	Cer(d18:1/40	Cer(d18:1/40	Cer(d18:1/41	Cer(d18:1/42	Cer(d18:1/44	Cer(d18:1/44
P_1	1.8536148	-0.6566621	-0.8048818	2.74217447	3.38092376	3.65971881	0.60809511	0.51895726	0.86740667	0.7396839	0.29716949	-1.7178165	-1.0947986	1.69426629	0.92719491	-0.1243673	-1.5859379	-1.0445605	1.59013834	
P_10	1.9177478	-0.4874927	-0.2838235	2.88653775	3.45645644	3.53609381	0.62125314	0.48462303	0.76546897	0.82468953	0.41491185	-1.7580186	-1.0505154	1.58584704	0.76112076	-0.5650594	-1.8578364	-1.0700619	1.58898136	
P_11	1.75171866	-0.5842714	-0.6856393	2.76821035	3.59638009	3.45268127	0.66960942	0.61899222	0.40701649	0.97280619	0.34425841	-1.5813727	-1.1224445	1.61094741	0.94452397	0.08414358	-1.2884419	-0.9134295	1.80818121	
P_12	1.76003508	-1.010194	-0.526118	2.66915863	3.17059713	3.82905608	0.48685806	0.57268874	0.6372394	1.04590081	0.24386069	-1.4343813	-0.8959396	1.85798835	1.26715321	-0.4083567	-1.0454932	-1.0216958	1.76328683	
P_13	2.16738522	-0.3262382	-0.5096662	3.07131278	3.85911386	3.58605037	0.68862726	0.5934358	0.60068228	0.52988465	-0.0209218	-1.728087	-1.314778	1.35235171	0.42109143	0.19058255	-1.4367316	-1.0861329	1.41847189	
P_14	2.20444761	-0.4383487	-0.5408987	3.10282516	3.87082783	3.99415348	0.7124935	0.72624478	0.41862431	0.40056091	-0.3659667	-1.8930545	-1.1780454	1.3077544	0.52715955	-0.5749965	-1.1580334	-1.1802873	1.77995403	
P_15	1.96027293	-0.6622755	-0.7531158	3.07613912	3.7552504	3.94387409	0.72788652	0.43860287	0.14869535	0.54288868	-0.1986299	-1.4240909	-1.0437443	1.7130739	0.66891852	-0.5330091	-1.605338	-1.0843067	1.70235066	
P_16	1.91091021	-0.4865887	-0.6483085	2.75805093	3.33711346	3.37277977	0.59903038	0.65575453	0.84449478	1.00558165	0.73169329	-1.5013042	-1.0577547	1.86411679	0.8172402	0.03811833	-1.0759347	-0.681954	1.9184658	
P_17	2.17283299	-0.1784327	-0.42515	3.13755157	3.69630717	3.5811047	0.95405472	0.44495178	0.56454281	0.64852728	0.14726206	-1.7771719	-1.2271671	1.14587159	0.53017685	-0.2501045	-1.3909992	-0.8966665	1.72197796	
P_18	1.90725841	-0.5935628	-0.791064	2.81845131	3.54030888	3.56438822	0.7156524	0.4485675	0.83308437	0.89065971	0.50808406	-1.8976369	-1.1040287	1.81985432	0.991286	0.04795606	-1.1619878	-0.9824962	1.52481828	
P_19	1.91988829	-1.2353414	-1.6543185	2.32705659	3.02329474	2.92357582	0.17879553	0.9615542	0.65059705	1.06789866	0.49842411	-1.7560989	-1.0528861	1.53485687	0.75304943	0.21916551	-0.979522	-0.6135562	2.16249578	
P_2	2.14400727	-0.6141734	-0.5708327	3.07114893	3.55300661	3.63273546	0.52698093	0.40168423	0.70342432	0.71393506	0.13728417	-1.8520767	-1.2244892	1.37517599	0.57063236	-0.5557819	-1.3046439	-0.9989718	1.55278438	
P_20	1.88066749	-0.6069225	-0.5086112	2.77134303	3.22674727	3.14288778	-0.0348522	0.42985842	0.85630117	1.20210066	0.66382231	-1.4754961	-1.1050388	1.7868964	0.8135292	0.25688018	-1.1249948	-1.0233504	1.66954259	
P_21	1.85464039	-0.4107756	-0.7068794	2.8809966	3.70635631	3.74265972	0.94426568	0.94873365	0.46339591	1.02026386	0.52709185	-1.8011375	-1.5038141	1.78234235	1.00124972	-0.0831254	-0.6805343	-0.409423	2.22783867	
P_22	1.82914758	-0.4592334	-1.0732277	2.79184733	3.87585945	3.64376498	1.14607956	1.21064538	0.51235131	0.94312485	0.37844038	-1.8772643	-1.8425546	1.72555426	1.06122502	0.19498632	-0.6061441	-0.2916458	2.30083226	
P_23	1.68586078	-0.4154383	-0.6668127	2.65019443	3.61377681	3.63641933	0.84425447	0.85539819	0.54307464	0.73845907	0.49569168	-1.8903414	-1.5498216	1.50742958	1.09404033	0.31231796	-0.5868759	-0.4813449	2.11779775	
P_25	1.8820423	-0.6459904	-0.4327359	2.82635887	3.27089682	3.51412542	0.42934613	0.5531935	0.76618821	0.82366948	0.40386545	-1.6942382	-1.4855851	1.53259279	0.84863656	0.06304164	-0.9787028	-0.8063891	1.82099027	
P_26	1.9375622	-0.6653554	-0.6412232	2.91242177	3.34107539	3.55094102	0.24667609	0.54035359	0.63853935	1.02332413	0.62598221	-1.5326948	-0.9975011	1.90604903	1.02988284	-0.4195109	-1.2777977	-1.1905367	1.52138843	
P_27	2.05192068	-0.6712671	-0.8368491	3.05509545	3.57635123	3.52452091	0.56992778	0.65634479	0.652749	0.96771347	0.26936932	-1.9837382	-1.4296865	1.5437277	0.74150853	0.14116245	-0.9717794	-0.7600226	1.82179252	
P_28	1.91625549	-0.384606	-0.4713591	2.9239625	3.64916553	3.49617779	0.83425948	0.66585397	0.65139828	0.73080875	0.46111464	-1.7812986	-1.7111256	1.57783004	0.61689296	-0.0014104	-1.1232626	-0.752032	1.99523126	
P_29	1.98057469	-0.8133688	-1.0555492	2.59547385	3.0877019	3.60511741	0.42498252	0.80675732	0.46099252	0.88010345	0.33844166	-1.5159156	-0.7500485	1.61931619	1.06374136	-0.1183368	-1.2991722	-0.9069347	1.83541284	
P_3	1.66347138	-1.0319757	-0.8598284	2.67248277	3.22416575	3.64538274	0.32358353	0.41280973	0.84481821	1.02853053	0.45219091	-1.5653264	-1.0583904	1.70654086	1.18344168	-0.5946052	-0.6591341	-0.6150928	2.02215552	
P_30	1.80273872	-0.3902484	-0.5579848	2.85136114	3.68265562	3.72116296	0.91947556	0.72588854	0.40765773	0.97248568	0.34115358	-1.836197	-1.5394379	1.55584043	1.04350332	0.28210331	-0.5996115	-0.5693122	2.02066054	
P_31	1.84595158	-0.7180157	-0.348912	2.84877626	3.40425423	3.52010433	0.48605605	0.53151303	0.9233219	0.9883789	0.43018665	-1.915018	-1.2741131	1.66176503	0.94594775	-0.4121996	-1.1969543	-0.725448	1.98055159	
P_32	1.44711205	-0.7993258	-0.7994919	2.5401816	3.32823104	3.43978937	0.63902083	0.72032095	0.76469225	1.05318047	0.66540929	-1.7659632	-1.3365647	1.93281489	1.08824628	-0.216132	-0.8194024	-0.3607799	2.25935753	
P_33	2.00757473	-0.5215217	-0.8542311	2.94201643	3.74261152	3.41294759	0.80877515	1.04558141	0.67343143	1.28808601	0.70631738	-2.2382437	-1.4404886	1.98559862	0.79701044	0.41503782	-1.1285635	-0.288794	2.27410663	
P_35	1.85674044	-0.3759353	-1.3358251	2.78853485	3.82678347	3.6080584	1.15842589	0.97289569	0.67753413	0.97828836	0.58829937	-2.0167487	-1.365247	2.07229577	1.04119162	-0.548588	-0.8332186	-0.4301032	2.16766904	
P_36	1.63574732	1.00892731	-1.0705091	2.60069005	3.52221679	2.99800029	1.19629334	0.65602868	0.69915069	1.13126001	0.89755197	-1.7339552	-1.303636	1.99318105	0.83658417	0.3620298	-0.6575723	-0.3980759	2.33230573	
P_37	0.974273	-0.3312732	-1.1016867	2.62370759	3.73113897	2.99306113	1.28044577	0.20191687	-0.0221014	0.90066652	0.16910221	-0.9114823	-0.630673	1.32921521	-0.0485782	-0.742797	-1.6399611	-1.6338961	0.73438092	
P_38	2.14991034	-0.456548	-0.406228	3.16999767	3.92293995	3.83667342	0.73596708	0.57653577	0.24243162	0.57182986	-0.0212115	-1.7031823	-1.112335	1.63967683	0.54536363	-0.4327594	-1.2967474	-1.0113684	1.54890488	
P_39	1.83310756	-0.4234411	-0.438829	2.80136202	3.50555623	3.3679222	0.64416247	0.75591426	0.50297019	1.1287101	0.6104603	-1.4798067	-1.6497656	1.74752319	0.92132277	-0.0595253	-0.6193028	-0.4447225	2.17660273	
P_4	1.92055938	-0.5934911	-0.33589	2.82013498	3.31153321	3.64673262	0.58635974	0.56331745	0.77267109	0.90030206	0.51871475	-1.6635361	-1.1646317	1.71414408	0.91362253	-0.0348535	-1.1940424	-1.2228835	1.50536878	
P_40	2.0535648	-0.2576315	-0.5238868	3.12843845	3.84824803	3.70547562	1.35191036	0.64021461	0.60675583	0.64973192	0.09831232	-2.0811025	-1.8526796	1.40034625	0.67599271	-0.387258	-1.5660931	-0.9093238	1.89311578	
P_41	1.93902282	-0.3958549	-0.4627025	2.94886196	3.49626728	3.43913929	0.60478838	0.63868262	0.72989645	0.84314985	0.53750689	-1.9011819	-1.4686569	1.65860795	0.71191731	0.07469455	-1.1936948	-0.8757604	1.74556082	
P_5	1.75277984	-0.9230118	-0.5292961	2.64752856	3.41271977	3.64025058	0.54764623	0.5833501	0.94258358	1.00757333	0.48096519	-1.7514981	-1.021631	1.78681102	1.09628627	-0.7369817	-1.0595829	-0.7548226	1.86498894	
P_6	1.1754614	-0.5510698	-1.056665	2.84641815	3.94028644	3.43449015	0.75537037	-0.7047328	0.30559341	-0.0548951	-0.3552792	-0.7690083	-0.9831588	0.4564021	-0.060713	-0.2541925	-1.0095952	-1.6556511	0.05586053	
P_7	2.16974354	-0.4238311	-0.6161242	3.0222211	3.58094199	3.52497583	0.80412677	0.57909114	0.52853293	0.74533252	0.28864326	-1.8945671	-1.471405	1.47543208	0.67620615	-0.3291053	-1.1412509	-1.0343274	1.71628967	
P_8	1.74475075	-0.7541235	-0.210887	2.73310915	3.36156395	3.74200711	0.65522513	0.60831706	0.64604504	0.84641511	0.30718682	-1.3746576	-1.2130794	1.58261877	1.10506035	-0.7206173	-1.0374436	-0.8780138	1.81701122	
P_9	1.3531159	0.62803726	-1.0903695	2.89179511	3.69046828	3.58569493	1.40280285	0.31472664	-0.1508759	0.22078114	-1.0137439	-1.646766	-1.3926677	1.31681989	0.2063398	0.19368148	-1.2078323	-1.8140426	0.4321051	

Table 8.106: Normalised data matrix for ceramide for serum samples taken from patients with breast cancer.

i:6)	modCer576.	modCer614.	modCer632.	modCer651.	modCer703.	modCer731.	modCer766.	modCer769.	modCer798.	modCer875.	modCer883.	modCer886.	modCer910.	modCer921.
P_1	-1.2435592	0.1576096	1.97506766	0.83224147	-0.932193	-1.6937198	-1.6910139	0.31793628	-0.9851496	-2.2079883	-1.0059525	-1.5653064	-1.5780691	-2.2302222
P_10	-1.5567198	-0.331818	2.05092915	0.99234391	-0.7654142	-2.0813235	-1.5209264	0.36476875	-1.0248644	-1.5207229	-1.1870846	-1.276573	-1.3321265	-2.5813922
P_11	-1.6766556	-0.5760936	2.18974486	1.18503768	-0.8352018	-1.8881138	-1.5185058	0.36487966	-0.9851599	-1.2143385	-1.3002019	-2.0545167	-1.9104533	-2.6342911
P_12	-1.6136572	-0.5267225	1.72977138	0.62533744	-1.2068413	-1.7286553	-1.8297334	0.34953125	-0.940922	-1.5213758	-1.0954237	-1.7805213	-1.1733507	-2.2490811
P_13	-1.5628318	0.42564061	2.45991694	0.93564514	-1.0849476	-1.8849641	-1.6585422	0.00861117	-1.0288968	-1.7962408	-1.0015677	-1.3083187	-1.6767514	-2.8831868
P_14	-1.4072574	-0.1547688	2.46793611	0.66918799	-0.902243	-2.3415696	-1.4033467	-0.2978911	-0.7524848	-1.485788	-0.7265419	-1.1075663	-1.068955	-3.2041258
P_15	-1.3235619	-0.1580223	2.34231786	1.09538966	-0.464114	-2.2533008	-1.3659615	-0.2378475	-0.785215	-0.9447414	-1.0845958	-1.7755511	-1.4459717	-2.9722673
P_16	-1.6411872	-0.2387038	1.93465079	0.85415766	-1.0750507	-2.0987975	-1.82015	0.73446975	-1.3546509	-2.237536	-0.9431377	-2.1021355	-1.9695446	-2.4438896
P_17	-1.0438395	0.25146276	2.25470653	0.76207654	-0.6698861	-2.0406312	-1.6044455	0.21541954	-1.440706	-2.2796706	-0.8668047	-1.7850705	-1.3703231	-2.9817577
P_18	-1.6464352	-0.0094256	2.08146488	0.59392088	-1.3629557	-1.9844865	-1.4336842	0.54590593	-0.841134	-2.3637363	-1.0958475	-1.4268999	-1.6537074	-2.4825725
P_19	-2.4518109	-0.1800438	1.58986822	1.21817058	-0.6537894	-1.2547745	-1.1133378	0.59017125	-1.3791482	-1.1817893	-1.0489634	-1.767979	-0.9550757	-2.3404276
P_2	-1.179862	0.29907928	2.13183464	0.73467711	-1.030931	-1.9207	-1.6380398	0.17143045	-1.1083905	-1.7384012	-1.0247424	-1.1260552	-1.1563495	-2.6753799
P_20	-1.64005	-0.6179415	1.80880431	0.88758024	-0.8273823	-1.7625785	-1.471781	0.67673356	-0.8717111	-2.1751412	-1.4120748	-1.5089391	-1.4271142	-2.4797149
P_21	-2.2744714	-0.7109606	2.24242376	0.50948714	-1.5067645	-2.321719	-2.2347352	0.61617107	-1.2776721	-1.6626296	-1.0830334	-1.5232346	-2.0515852	-2.2254218
P_22	-2.558917	-0.5193414	2.42100429	0.64333151	-1.4191506	-1.8192138	-2.2953496	0.42310205	-1.3028155	-1.7226	-0.8194304	-1.5562854	-2.1257412	-2.8123815
P_23	-1.993673	-0.3426331	2.17940392	0.6335443	-1.431451	-2.0022865	-2.1357504	0.36036248	-1.3009335	-1.9113645	-1.0854885	-1.3637816	-1.9663593	-2.1436694
P_25	-1.6184948	-0.593714	1.81182241	0.83709515	-1.0809794	-1.5456608	-1.6441523	0.44708337	-0.8975212	-1.6759596	-1.0623109	-1.4015097	-1.4995096	-2.7674948
P_26	-2.0815589	-0.4158324	1.93794515	0.65290576	-1.2443759	-1.7150899	-1.346623	0.67983299	-0.9434215	-1.7972976	-1.0011264	-1.2115287	-1.3540304	-2.7093752
P_27	-1.5517591	-0.4771769	2.14148395	0.8190089	-1.1784116	-1.8751945	-1.5001442	0.35231788	-1.1535969	-1.6962388	-0.9850877	-1.7822762	-1.2436035	-2.7881625
P_28	-1.616063	-0.0610339	2.22271426	1.17493711	-0.9947193	-2.3642599	-2.2026845	0.49043497	-0.9625803	-1.6466826	-1.0781052	-2.4805397	-1.5728387	-2.2024354
P_29	-1.8045014	-0.3990907	1.64973173	0.81511901	-1.2529965	-1.9438707	-1.2868969	0.3168215	-0.9553475	-1.2956147	-0.9364091	-1.4113505	-0.7109367	-3.0239473
P_3	-1.180634	-0.1773985	1.78097402	0.9531981	-0.8957825	-2.1541011	-2.0096533	0.45058621	-0.905746	-1.847123	-1.2840405	-1.4712745	-1.4919972	-2.5622283
P_30	-1.7435094	-0.6369805	2.26505855	0.56655615	-1.3315053	-2.4378934	-2.1399111	0.53205653	-1.3159665	-1.6515167	-1.0392393	-1.9525479	-1.6060912	-2.3424053
P_31	-1.3767811	0.08692488	1.94546293	0.80337592	-0.9662612	-1.9022572	-1.8350202	0.43909136	-1.1496925	-1.9566001	-1.1471782	-1.9235579	-1.4398173	-2.553836
P_32	-2.1699807	-0.7258427	1.90865369	1.18631988	-0.8499051	-1.8690353	-2.0480891	0.64362423	-1.1297152	-1.4452258	-1.373823	-2.0222927	-1.5850847	-2.3002999
P_33	-2.4729859	-0.6331016	2.37240546	0.66236822	-1.2385802	-1.816678	-2.0524499	0.6498829	-1.0080707	-1.962504	-1.1381519	-2.3085953	-1.9236372	-2.7571546
P_35	-1.9725845	-0.4170277	2.43616308	0.36207522	-1.5075522	-1.9118981	-2.1097446	0.60319083	-1.5630558	-1.7077813	-0.8584112	-1.975057	-1.9739453	-2.2354227
P_36	-2.1214972	-0.6571529	2.06359963	0.44893799	-1.5699236	-1.8548802	-2.1115498	0.94718145	-1.207051	-2.124214	-1.4588482	-2.3113918	-2.3261866	-2.4232425
P_37	-0.506191	1.05496197	2.32516325	0.78007758	-1.5808185	-1.6450867	-0.4623308	-0.2512465	-1.0696055	-1.308699	-0.5112679	-1.4834336	-1.3653082	-1.8516742
P_38	-1.3466534	0.21055216	2.48420139	0.69851602	-1.5832191	-2.3583001	-1.4486099	-0.079021	-0.7769509	-1.5573506	-1.0176087	-1.3646613	-1.3954994	-2.9652462
P_39	-2.1375439	-0.8605569	2.06641366	0.82149175	-1.1518567	-2.2379061	-1.7908854	0.63121237	-1.1680378	-1.6771051	-1.041903	-2.1313758	-1.6305082	-2.57166
P_4	-1.648	-0.4059725	1.87335925	0.79718051	-1.0353742	-2.0485869	-1.4218244	0.56094593	-0.9894314	-1.9061421	-1.1274057	-1.5099916	-1.5833688	-2.5195205
P_40	-1.3156248	0.02898025	2.46905368	0.98719439	-0.8442577	-2.0815369	-1.6747757	0.08342566	-1.2450131	-1.6995729	-1.3094382	-1.4826519	-1.6221007	-2.7678135
P_41	-1.5902075	-0.334562	2.11300838	0.71509659	-1.3088463	-1.9728066	-1.6924278	0.54526424	-1.2383254	-1.8772052	-1.1073603	-1.7030149	-1.4136218	-2.2052363
P_5	-1.4029774	0.0060745	1.98754896	0.83360829	-1.3017538	-2.073532	-2.0399318	0.51411865	-1.113429	-2.0088409	-0.9975039	-1.2641262	-1.6377819	-2.4881326
P_6	-0.8671513	0.82094657	2.30137457	0.16513586	-0.7133943	-1.2715928	-0.9354425	-0.4177801	-1.5347187	-1.4543057	-1.1977804	-1.2143131	2.72052372	-1.9164235
P_7	-1.3290942	0.15534659	2.14462304	0.52760888	-1.2766741	-2.157157	-1.5419202	0.26389131	-1.0751918	-1.8503372	-0.9016611	-1.2805451	-1.2005335	-2.6792818
P_8	-1.8056287	-0.5237325	1.92345446	0.96458975	-1.1290151	-2.1645056	-1.6824516	0.34339975	-0.9065438	-1.4356072	-1.2408654	-1.2707664	-1.4425237	-2.590292
P_9	-0.2006664	-0.6879356	2.13424003	0.7695392	-0.5272941	-1.5983112	-1.7743379	0.45923372	-1.1040715	-1.3382517	-0.774844	-1.4790677	-0.4430604	-1.355243

Table 8.107: Normalised data matrix for phosphatidic acid and lyso phosphatidic acid for serum samples taken from breast cancer free controls.

8/9.05	LPA 12:0	LPA 14:0	LPA 16:0	LPA 17:0(IS)	LPA 18:0	LPA 18:1	LPA 18:2	LPA 18:3	LPA 20:0	LPA 20:1	LPA 20:2	LPA 20:4	LPA 22:0	LPA 22:1	LPA 22:2	LPA 22:5	LPA 22:6	LPS(18:0))	PA 17:0/17:0	PA 32:0	PA 32:1	PA 34:1
C_1	-1.1755436	2.88967188	7.33888963	4.28505435	6.44881966	5.59710289	5.86826202	-0.2889405	4.19365176	1.28431434	1.80024254	5.24710057	2.63812017	2.22696411	3.03326719	3.23192697	4.08298063	-2.2492646	-0.7299654	-2.5693382	-2.3141314	0.39189272
C_10	-2.5583152	2.90066054	7.4276125	3.5785933	6.38744471	6.24972058	6.85147355	2.16923404	4.1834175	1.71035154	2.74776211	6.35606355	2.45730633	2.53809727	3.56218031	4.29484797	5.18397721	-2.29619	-1.1983683	-1.9972065	-2.2821498	-0.2504752
C_11	-1.7623455	2.35050086	7.32025208	4.28550586	6.09978204	5.66169694	5.96204055	-1.4391655	4.32251848	1.39837558	2.5614707	5.70970398	2.43623646	2.21808055	3.37162095	2.64893371	4.09150834	-3.0492803	-0.5034817	-1.1636424	-2.8574988	0.4576106
C_12	-1.2615517	1.68960685	6.34641131	3.15298648	5.65305821	4.14424395	4.1391499	-0.6386997	2.75950226	0.45665878	1.20380158	3.99652262	1.16659929	0.41422417	0.80249351	1.92966943	2.44051627	-1.6436222	-0.6018391	-1.0848364	-0.935206	0.23746785
C_13	-3.0670849	2.93573663	7.85230138	2.75936624	6.98314807	6.90993442	7.25680702	1.50760711	3.77101001	2.30022882	3.86866061	6.71512587	1.86633975	2.11993307	3.0027409	3.65791441	5.06011325	-2.9846073	-0.3102787	-3.1690736	-3.1453887	0.01101705
C_14	-2.5216023	2.26104041	6.63866246	1.96641511	6.16061271	4.77846155	4.52570713	0.15299354	3.41278963	1.25495665	3.80086344	3.93529474	1.42199933	0.91819182	0.87783719	2.0369755	3.32564042	-1.9863582	-0.4448664	-1.6083666	-2.2110632	-0.1924828
C_15	-2.9800251	3.06544838	7.64880473	4.16219031	6.37484951	6.53150467	6.62050936	-0.6031621	4.51067639	1.77636153	2.82759302	6.5825151	2.69618182	2.99957212	3.55701984	4.06203818	4.2463506	-2.4520585	-0.4130092	-3.1485155	-2.4007985	-0.1253419
C_16	-2.5313115	2.27622774	7.3067952	4.26966087	6.50207737	5.61833207	6.1084096	-1.9057956	4.19135033	1.43497533	1.80215716	5.10046069	2.61541281	2.17393046	3.19060635	2.97044476	2.73088319	-1.0598248	-2.4806364	-1.1289913	-2.2300979	-0.1129161
C_17	-3.1342702	2.91465248	7.62890108	4.10923618	6.51696716	6.03059401	6.19023687	-0.6861151	4.29240434	1.11469771	2.0192041	5.85046774	2.60846933	2.62702929	3.17331315	4.01749178	4.09067836	-1.671004	-0.7836707	-2.8415135	-1.9645742	0.40280144
C_18	-2.9078107	2.94252403	7.50027335	4.04087536	6.62517665	6.19431918	6.6475708	-0.0236727	4.35782972	1.90862796	2.60487709	5.59749333	2.70136894	2.46112681	3.73054167	3.2772844	3.89836697	-2.2049696	-0.9671681	-2.1951498	-1.3050102	0.44254858
C_19	-1.798264	2.25661709	7.33048086	3.78856204	6.37865371	6.0876235	6.57693944	0.29309974	4.16356425	1.74362002	2.48831215	6.00982309	2.63873973	2.61823081	3.55956113	3.32693263	4.75242427	-2.5306882	-0.5816014	-1.9095517	-2.3414997	-0.5242343
C_2	-3.0329871	2.59459905	7.36630716	3.92900666	6.3749474	6.12275468	5.80170749	-0.7535159	4.01690062	1.30659004	2.22661441	5.85909656	2.37732883	2.2566271	2.77523345	3.67481978	3.39781693	-2.8333725	-1.6075346	-1.4942364	-2.5361932	-0.0883583
C_20	-2.0473486	2.21701899	7.22216577	4.03720695	6.5912666	5.15069328	5.62759621	-0.065766	4.06119677	0.79655615	2.06411309	4.87746315	2.62267936	1.41664987	2.51794835	3.03772977	3.85983081	-2.6397838	-1.103675	-2.6038962	-1.6774435	0.19174435
C_21	-3.2683684	2.16680178	7.00732146	3.95593165	6.16526293	6.09286235	6.4573167	0.46083597	4.21984439	1.46902353	2.51085909	5.87463328	2.63448815	2.82428402	3.56438694	3.38561983	4.1192825	-2.6169015	-0.781948	-1.9332051	-1.6756902	0.41544873
C_22	-3.642532	2.63552604	7.24242416	3.97413694	6.39793245	6.44649771	6.21895304	2.48749254	4.22897153	1.41185579	2.31394081	5.95848363	2.91730205	3.21891214	3.39602479	3.78915906	4.62645666	-1.8194652	-1.8626972	-1.5735904	-2.8663801	-0.3806379
C_23	-2.8468866	2.80141391	7.4792825	3.97599588	6.45458658	6.28741252	6.71751083	0.14506512	4.25802972	1.74145723	2.80250756	5.78198258	2.72661741	2.76964746	3.84002599	3.92609439	4.28091463	-2.7075305	-1.3570621	-2.9323817	-2.2347853	0.03792479
C_24	-2.6325827	3.28281174	8.08752492	3.21963876	7.01152787	6.92528468	7.54129252	3.75769026	3.7464934	2.12554645	3.76712558	6.54691359	2.38508391	2.2129014	3.40847793	4.21441534	5.25597711	-2.4170087	-1.4851945	-2.1541743	-2.5188481	-0.1335442
C_25	-3.8753546	3.21359526	8.36658147	2.63584403	7.29909391	6.98541932	7.26956508	2.89154744	3.2891606	2.18771639	3.54698601	6.61162154	1.80954689	1.51767023	2.37294884	4.19558564	5.23236011	-2.9766483	-1.4238872	-1.6055747	-2.2124378	-0.9960644
C_26	-2.1182489	2.71440672	7.84414551	2.73836911	6.82580738	6.90454216	7.19054785	0.82678175	3.68599445	2.11543122	3.54793744	6.33779881	1.90613714	2.11987693	3.04775758	3.98413405	5.5132223	-3.3483811	-1.3679687	-1.7971473	-2.2791352	-0.304741
C_27	-2.6490699	2.8961157	7.88565256	2.8035877	7.17104998	6.94392644	7.29143336	1.30406865	3.42730783	2.15160554	3.60191137	6.69233333	2.14020931	1.89913178	2.77821079	4.27376288	5.11264579	-3.4509247	-0.1787466	-2.3244685	-1.9489917	-0.2019327
C_28	-3.534962	2.5616023	7.39711041	4.14156506	6.58740681	6.32322523	6.85409419	-0.3133815	4.38593704	2.07240362	2.28466431	5.98952015	3.01300047	2.92602463	3.98877211	4.14532627	4.72116054	-3.3148016	-1.4009894	-2.9125522	-3.090338	-0.5375018
C_29	-3.6695109	3.12545245	7.88151293	4.60204454	6.78979845	6.46309297	6.95556545	-0.4051578	4.57918358	1.9450985	2.59300961	6.37707902	3.34771008	2.99563571	3.85907533	4.42210343	4.33592347	-2.7553762	-0.8512103	-1.8480564	-1.862016	0.58779375
C_3	-1.803356	2.68903827	7.29645823	4.20339319	6.52202535	5.90998164	6.50441172	-0.2081339	4.30378055	1.48485378	2.26910919	5.65643539	2.86733096	2.35805219	3.56083042	3.41668689	4.06877598	-2.6647397	-1.0742925	-1.9901088	-2.8722013	0.03050989
C_30	-3.1705939	3.01220611	7.57052872	2.60801227	6.80659862	6.65369961	6.87367636	1.78539947	3.90975642	1.65894776	3.75042994	6.24092917	2.09745286	2.10906116	2.87304376	4.27754752	4.99543539	-2.5161076	-0.8695342	-2.5901542	-1.9207915	-0.4242564
C_31	-3.3459569	1.94107225	6.60549113	2.60191755	6.12598995	6.00007809	6.14223204	0.06152719	3.63088959	1.51824716	2.72188702	5.73767927	2.04493212	1.91088183	2.85597073	2.80414325	4.46858041	-2.5021148	-0.5033275	-2.1149525	-1.2038581	-0.2864645
C_32	-1.4708974	2.77889819	7.29477199	3.04565085	6.67591471	6.53739362	6.76968261	0.63414715	4.02406317	1.86835492	3.54317531	5.90679706	2.14010083	1.95068707	2.89725815	3.82490429	4.68849875	-3.0193818	-0.9923473	-2.593921	-1.2384693	-0.6912417
C_33	-1.6806975	2.46309491	7.10183817	4.36359963	6.06928684	5.19971921	5.48673779	-1.6372293	3.97661552	1.32960271	1.35806465	5.26805177	2.48397012	2.0154418	2.57666052	2.80632156	2.70403576	-1.7909985	-1.101575	-1.7111342	-1.6910014	0.64822757
C_34	-1.9499179	3.00886809	7.38990747	4.10114604	6.47150154	6.40246084	6.49139463	2.45712482	4.30803075	1.51752706	2.78702795	6.28889574	2.92997418	2.98222618	3.50307312	3.88854511	4.09322361	-1.6200446	-1.762514	-3.4580711	-2.1690379	-0.1829472
C_35	-1.4461497	0.80170282	3.48072806	0.437546	6.26294706	4.72648115	4.55994306	-1.4452669	2.10199845	1.51437963	1.7689791	3.49327453	0.22554322	0.20423955	-1.3314244	-0.6262074	1.34797539	-0.6438585	0.7972385	-0.320138	-1.4862818	-2.3605554
C_36	-1.7243036	2.26835348	7.24789415	4.34538326	6.47660846	5.68940673	6.66627036	-0.3530505	4.38372665	1.49065545	2.32817537	5.48896941	3.1275967	2.5812408	3.98377955	3.24472221	3.8913161	-1.9509709	-2.6207778	-3.0368388	-2.2967992	-0.2756778
C_37	-3.1244229	2.87953091	7.72806468	4.09568355	6.85666478	6.53630774	7.16030185	0.06540953	4.58283781	2.22819357	2.7348586	5.96154335	3.1712193	2.96849441	4.13785517	4.28577206	5.29344397	-2.821643	-2.2547865	-2.0486388	-1.6309671	-0.6290578
C_38	-3.4671561	3.2404932	7.89654737	3.82470142	6.7958904	7.09136847	7.24805469	2.97766948	4.30726104	1.79656348	3.54581731	6.46815494	2.53369712	2.9548935	3.73761778	4.11528155	4.81065255	-3.1286	-1.9026517	-2.1094859	-3.3286597	-1.4940381
C_39	-2.4144666	2.00431515	6.9607794	2.51515528	6.34793208	6.34559736	6.45560387	-0.348788	3.82990081	1.99706712	3.43097562	5.98564597	2.04391729	2.08789355	2.81713628	3.47359826	4.71722556	-2.317351	-0.3665979	-2.8929749	-1.1583373	-0.0296673
C_4	-2.6582509	3.04162806	7.44486015	3.63913616	6.63933508	6.35375498	6.93714834	-0.3423178	4.22274774	1.69636104	2.96292797	5.87099929	2.61910808	2.32276182	3.63291748	3.58945608	4.22354421	-2.1749201	-0.8305698	-2.3180114	-2.0873958	-0.7347917
C_40	-2.7323041	2.60186396	7.24005293	3.94512349	6.49040894	5.81932438	5.88052584	-0.337831	4.24930725	1.14415646	2.5814779	4.99738079	2.72266492	2.34382258	3.16615778	3.17707238	3.33841003	-2.5142317	-2.2125766	-2.3609581	-2.8806678	-0.742191
C_5	-3.2980556	2.8409305	7.65115941	3.12794911	6.76450597	6.60562396	7.09267377	-0.8211614	4.08278987	1.88677374	3.45167552	6.33921693	2.31849705	2.36319754	3.40547801	4.30620034	4.89806347	-2.8718889	-0.7544584	-3.2655792	-2.8271939	0.25754029
C_6	-2.1041338	1.95289964	7.28680011	3.80299506	6.30664188	6.125997	6.45772794	0.46828179	4.24112124	1.38781159	2.32155669	5.99991802	2.51379667	2.58436112	3.53197135	3.74684945	4.77269726	-3.25675	-1.3371643	-3.2853503	-1.798673	0.14207044
C_7	-2.4850048	2.00084763	7.39322145	3.94766691	6.51960797	5.77294884	6.35390077	0.06884353	4.22739785	1.47703933	2.3737079	5.45779908	2.69286876	2.34168272	3.52101775	3.28524633	3.65740545	-1.656785	-2.4433118	-1.862023	-1.4932393	0.34570911
C_8	-1.3077746	3.19873033	7.4081676	4.35217874	6.23547157	6.05941869	6.45550995	-0.4518054	4.4961319	1.49685958	2.35799081	5.57675128	2.79051669	2.73284524	3.74059722	3.50652941	4.31049619	-2.2731429	-1.0385302	-2.1648081	-3.2933565	-0.4435956
C_9	-2.5883368	2.08591496	6.89611224	3.50990055	6.218916	5.72168606	5.98818782	-0.0767864	3.86713373	1.51261035	2.14970594	5.42790679	2.33609231	2.00193468	3.18609042	3.0258944	3.7015547	-2.295396	-0.233096	-1.3923888	-2.4117166	-0.2016337

Table 8.108: Normalised data matrix for phosphatidic acid and lyso phosphatidic acid for serum samples taken from breast cancer free controls.

	PA 36:0	PA 36:1	PA 36:2	PA 38:4	PA 38:5	PA-1	PA-3	PA-4	PA-5	PA-6	PA-8	PA(24:0)	PA(24:0) 1	PA(26:1)	PA(26:3)	PA(27:4)	PA(27:5)
C_1	-0.3535394	-2.9604134	-1.968558	-1.6126658	-2.5832577	-2.5085474	-2.9118507	-2.6065735	-2.8762452	-2.4484482	-1.4283208	-3.1937946	-1.9770453	-2.6478285	-2.7431806	-1.7612843	-1.5604096
C_10	-1.0954142	-3.1780062	-2.2384212	-0.9925909	-3.1822112	-2.9396221	-3.5652204	-2.9093873	-2.9898303	-2.4903819	-1.9729118	-2.9207195	-2.0859989	-2.9788792	-2.6425488	-2.0625432	-3.2256628
C_11	-0.5931054	-1.7991455	-1.3042992	-2.1484888	-1.7275692	-2.5920401	-2.8801172	-2.6554491	-2.4278179	-2.4506015	-3.9956291	-2.2705228	-2.2970108	-2.316398	-1.9549181	-2.711994	-2.1335527
C_12	-1.7714307	-1.9367795	-1.287577	-0.8260577	-0.9068716	-1.3667904	-1.2585797	-1.2201798	-1.8181371	-1.9963768	-1.254696	-1.7222636	-2.2055883	-2.3084381	-1.4784778	-1.1828833	-1.66399
C_13	-1.3312505	-2.5675152	-2.5567461	-2.1395272	-0.7713796	-2.8341059	-2.9733509	-2.7313222	-2.8117652	-2.9611786	-2.8531876	-2.6544701	-0.724697	-2.3761089	-3.4310042	-3.4271427	-2.252164
C_14	-0.5952393	-2.6555686	-1.272314	-0.111303	-0.5616849	-2.0642301	-2.7942007	-1.7547155	-1.0670731	-2.7886822	-2.2315347	-2.2180366	0.22260137	-2.1961164	-2.3153123	-2.4847923	-1.8592343
C_15	-0.8585569	-2.4511082	-2.6869198	-1.0577331	-2.8571663	-3.3877098	-2.6489717	-2.641458	-3.1644059	-2.8566841	-1.267297	-2.5646059	-1.264498	-3.1632274	-2.5952941	-3.1826745	-3.1108487
C_16	-1.4817651	-2.2504118	-2.053542	-1.4804141	-2.7173119	-3.0338322	-2.282128	-2.1873866	-2.6598458	-2.1994515	-1.8929161	-2.1105345	-0.8681682	-2.1564097	-2.4043186	-1.8172026	-2.1235184
C_17	-0.8133606	-2.0433807	-2.1916463	-1.0745389	-2.3292665	-3.1391078	-2.4939081	-2.2128968	-2.6720388	-2.9664145	-1.5838596	-2.5147437	-2.5336664	-3.1919533	-3.3069827	-1.7614064	-3.1009417
C_18	-1.9072764	-2.6060999	-3.5867767	-1.0257656	-3.4573343	-2.6642326	-2.8328923	-2.7821284	-2.6035481	-2.7869397	-1.1199243	-2.4664107	-1.4827189	-3.202769	-1.9405613	-2.6976244	-2.7033925
C_19	-1.1955756	-2.7257536	-1.9261548	-0.5889327	-2.5811863	-3.1474884	-3.0270104	-2.7561425	-2.8365855	-2.7682074	-1.6333187	-1.8320758	-1.0218894	-2.4207018	-3.3863595	-3.1728869	-2.6922743
C_2	-1.8149488	-2.0556434	-1.5808055	-1.603396	-1.3033442	-2.5710846	-1.8321308	-1.7061456	-2.8551247	-2.5212243	-2.1474801	-2.4945883	-1.1399915	-2.7698797	-3.220048	-1.7812757	-2.3660889
C_20	-1.4717644	-2.3282188	-1.7120486	-1.5254144	-2.7647358	-2.1008252	-1.8279369	-2.2103414	-2.8054478	-2.3584646	-0.8929423	-1.8228536	-1.5218166	-2.1793645	-2.7733852	-2.7084735	-2.5227944
C_21	-1.010517	-2.4130251	-2.9217418	-2.373099	-1.4878021	-2.6179397	-3.4862311	-2.4768122	-2.8648541	-2.8074408	-1.2496158	-2.317581	-1.3785118	-2.4822806	-2.3493935	-2.1066282	-2.2978219
C_22	-0.7811142	-2.15594	-3.37613	-1.7661004	-1.505896	-2.9253937	-2.6865786	-3.3905105	-3.2081245	-2.1259359	-1.0061411	-2.7074141	-1.5834175	-2.7532893	-2.8215037	-2.6847613	-2.720398
C_23	-1.3888935	-2.9051987	-3.3635169	-2.1613708	-3.8711032	-2.5980765	-2.041629	-2.456949	-3.1152789	-2.5383951	-1.5608435	-2.3800969	-1.2898478	-2.5765736	-2.4941864	-3.4054753	-2.0020688
C_24	-1.2212021	-2.0762791	-3.3063099	-1.9412291	-4.1370814	-3.1795271	-2.940712	-3.0383996	-3.7226894	-3.023207	-3.2104852	-2.9615475	-1.1043393	-3.0074227	-3.3728901	-2.2584829	-2.9745314
C_25	-2.5990566	-3.0503875	-2.6966968	-2.0471682	-3.1207152	-2.8271962	-2.6935788	-2.7022496	-3.3184987	-2.5890855	-3.0756647	-2.3021661	-0.3753963	-2.5201789	-2.7394871	-2.9934856	-3.1423141
C_26	-1.7389582	-3.1089192	-2.579694	-2.0744144	-3.1739112	-3.0861524	-2.4888706	-2.9450249	-3.7785673	-1.7282869	-1.2455576	-3.3559792	-1.2191921	-2.914048	-2.3317315	-1.2947629	-2.4287486
C_27	-1.4652091	-3.2214297	-2.1236174	-2.7175029	-1.7945075	-3.1635275	-2.4834672	-2.9049941	-3.552769	-3.3364295	-2.1319196	-2.6906758	-1.5061497	-2.6861686	-2.8973961	-2.3822088	-2.7043552
C_28	-0.820564	-1.7798126	-2.4655539	-1.6844832	-3.0171196	-2.8298867	-3.2893876	-2.6862937	-3.0396492	-2.7473217	-0.795775	-3.0882291	-0.8767447	-2.859287	-2.3835703	-1.8919046	-2.8841287
C_29	-1.9837041	-2.1743781	-2.6716366	-1.0888253	-2.9155937	-2.872654	-3.6818773	-2.8805823	-3.0176031	-2.8378216	-1.0600366	-2.6546745	-2.341135	-2.9191649	-3.490899	-3.3762455	-3.0995084
C_3	-1.4211564	-2.7447577	-3.1163727	-1.9378134	-2.4617029	-2.6756588	-2.3304147	-3.0255009	-2.2819557	-2.2922754	-1.8710714	-3.0959624	-1.3522437	-2.3758196	-2.4180368	-3.0660742	-2.4706631
C_30	-1.094895	-3.0762966	-1.8781282	-1.6682856	-1.6971702	-3.2870467	-3.328617	-2.8025405	-2.9051557	-2.3104019	-3.5298748	-3.2906458	-0.4633346	-2.5085605	-2.0804992	-2.2815621	-2.4244795
C_31	-0.6876086	-2.9174232	-2.000631	-0.3095293	-1.9434393	-2.2266906	-2.7760439	-2.4691824	-2.6782277	-2.8812674	-1.2182847	-2.6204785	-0.5910181	-2.0042164	-2.6350221	-2.1326931	-2.5339165
C_32	-0.6294856	-2.5068128	-3.3444632	-1.2971807	-2.556928	-3.2944835	-2.352164	-2.6239233	-2.7043663	-3.376343	-1.8205027	-3.2769051	-1.0763671	-2.5348644	-3.0434767	-2.7335232	-2.3948501
C_33	-0.9811226	-2.2718567	-1.4530366	-0.7881105	-1.9657325	-2.7818602	-1.7556413	-2.2213307	-2.3017737	-1.8394867	-2.8570933	-3.0375211	-2.3863458	-2.3214787	-2.2585682	-2.1901049	-1.6784119
C_34	-1.0372037	-2.5756256	-4.1191301	-1.2409024	-1.708587	-2.9393536	-2.7005384	-2.3833137	-3.2243738	-2.8102909	-2.7081069	-2.7496877	-2.7573254	-2.2938966	-3.3972036	-2.5773535	-2.7343578
C_35	-0.7189217	-0.6758749	-2.9859015	-0.6607627	-1.6734763	-1.0789225	-1.0658244	-1.3295987	-0.9229363	-1.5341498	-0.4340735	0.38049146	-0.9327326	-1.3720268	-0.5942156	-0.8120675	-1.1378248
C_36	-1.2686123	-1.5526258	-2.560911	-2.0003639	-3.2000259	-2.5636971	-1.7276176	-2.6636798	-0.9456981	-3.1752201	-1.3779729	-3.110568	-1.8921989	-2.6327029	-2.7009172	-2.0698281	-2.6668228
C_37	-1.4758985	-3.4600272	-2.8661908	-2.8454532	-1.4655219	-3.0010326	-3.0821745	-2.649124	-2.729567	-2.7256464	-2.292568	-3.1632725	-2.0224776	-2.6181471	-2.6863614	-2.6598088	-2.6828092
C_38	-2.1466599	-2.3132991	-3.0055313	-2.131487	-3.0156714	-3.1184607	-2.8042804	-3.5567227	-3.0680719	-3.6551242	-2.5084704	-2.0214616	-0.9693323	-2.1584045	-3.3210055	-2.8845982	-2.6127098
C_39	-1.2158382	-1.9647619	-3.4322348	-1.1326279	-2.6672409	-2.3777472	-1.4377804	-2.5428054	-3.2126712	-2.5991039	-0.5427462	-3.0695881	-1.5648741	-1.6107967	-2.5800428	-2.610227	-2.6840218
C_4	-0.9311659	-2.4160845	-1.9563109	-1.1647996	-2.9319216	-2.9093544	-3.0892805	-3.0956076	-2.823097	-2.9608001	-2.6342093	-2.5274292	-1.1190191	-2.73725	-2.5377362	-2.4237221	-3.1089364
C_40	-1.4927047	-2.0580635	-2.3573261	-2.7147755	-2.0486984	-1.8214866	-1.774925	-1.9750809	-2.1797403	-2.0731074	-1.917661	-2.0224452	-0.5076138	-2.6818465	-2.1365347	-2.1064793	-1.9360999
C_5	-1.7565149	-3.4541243	-3.0168621	-0.2106074	-1.7893938	-2.3916541	-2.7640669	-3.1122369	-2.9960552	-2.2237762	-1.9404859	-2.0363264	-0.5726205	-2.6634034	-2.7012927	-2.9742318	-2.6001871
C_6	-0.9478103	-3.1829902	-2.3510039	-0.6113125	-2.884068	-2.7151335	-2.7046109	-2.2570845	-2.9691068	-2.6276622	-1.1764116	-2.7069378	-1.3628345	-2.151356	-3.5346941	-1.6613639	-3.3896031
C_7	-1.0829487	-2.3736299	-2.3610983	-0.6018342	-1.984717	-2.9936611	-2.9769461	-2.5089442	-3.2834219	-2.339651	-1.4779679	-2.4320921	-2.6109339	-3.3985479	-2.437032	-1.3431533	-2.5012496
C_8	-2.8218762	-3.4734087	-4.0785547	-0.4152285	-2.0892268	-2.8037275	-2.804579	-2.4985972	-2.9714645	-3.3661721	-1.7304313	-2.9784429	-0.8513391	-2.3564473	-2.5358347	-1.0439175	-2.434729
C_9	-0.5257772	-2.6461455	-1.9093762	0.54074865	-3.0143138	-2.6619778	-1.5337905	-3.1800428	-2.3861879	-2.7030731	-0.7476938	-2.5213626	-1.6302646	-3.0370384	-2.5580877	-2.9583871	-2.4569821

Table 8.109: Normalised data matrix for phosphatidic acid and lyso phosphatidic acid for serum samples taken from patients with breast cancer.

	LPA 12:0	LPA 14:0	LPA 16:0	LPA 17:0(IS)	LPA 18:0	LPA 18:1	LPA 18:2	LPA 18:3	LPA 20:0	LPA 20:1	LPA 20:2	LPA 20:4	LPA 22:0	LPA 22:1	LPA 22:2	LPA 22:5	LPA 22:6	LPS(18:0))	PA 17:0/17:0	PA 32:0	PA 32:1	PA 34:1
P_1	-2.3602987	2.78743531	7.54092986	4.27694952	6.37248024	6.27753077	6.0954812	-0.5194031	4.32040433	1.66740836	2.39199089	5.80626765	2.58995607	2.79962841	3.23528204	4.02998862	3.72153256	-3.3657701	-1.5245457	-2.7595351	-1.2412212	0.57963656
P_10	-2.0334592	1.19440996	7.38707336	3.70907266	6.53535931	6.26590264	6.69600913	-0.7670258	4.17438512	1.65463737	2.43690355	5.91480525	2.63846308	2.62750279	3.47808707	4.17807708	5.61894175	-2.9115103	-0.4407956	-1.4259482	-2.3814903	0.16978847
P_11	-1.5401816	2.56519114	7.43014617	2.54145958	6.50710024	6.54451057	7.13282361	1.2723609	3.73887988	1.87444627	3.70053951	5.96072461	1.94512642	2.00295723	3.1216366	3.38110954	5.39877699	-2.5267869	-1.0188415	-1.8779131	-2.1845412	-0.5002913
P_12	-3.1931017	2.39822583	7.45735432	4.15457542	6.55222004	6.0440505	6.41804648	-0.1791655	4.23286737	1.90572902	2.45398535	6.09394953	2.80435112	2.52386186	3.37912133	3.41643291	4.74551432	-2.6695003	-0.31064	-1.8464993	-1.5311709	-0.0727162
P_13	-0.7543643	2.53473051	7.37376232	4.05589424	6.56307346	6.18780577	6.48884394	0.60875438	4.27894863	1.79665943	2.64564852	5.93454966	2.79862528	2.70207744	3.62930601	3.64453868	4.11263308	-2.7834916	-0.1921786	-2.5082877	-2.3273795	-0.0317717
P_14	-2.73766	3.12990254	7.85794037	4.09561164	6.43024959	6.56140544	6.78390752	-0.4065996	4.46125949	1.76724076	2.51759069	6.8388097	2.63909195	2.96715093	3.49549594	3.57428749	4.72565802	-1.7217081	-0.5559993	-2.8145689	-0.6529541	0.36495265
P_15	-2.7309114	1.90325716	7.3936506	3.03580855	6.34837944	6.4793998	6.81337212	-0.827272	3.94174957	1.99894138	3.49557778	6.64997199	2.07715903	2.35179792	3.23485464	3.31817814	5.09376027	-2.8224691	-1.3391461	-3.3823134	-1.0005048	-0.0003883
P_16	-3.610619	2.92996444	7.57886281	4.10476882	6.78816582	6.46940418	6.85051073	-0.5816488	4.18221985	1.74761718	2.62059919	6.00280401	2.55004454	2.29668286	3.45572563	3.81064268	3.59561437	-2.5620891	-2.1574665	-2.046525	-2.0942461	0.24444153
P_17	-3.2556862	2.57950806	7.29364463	4.08983929	6.54171476	6.31148289	6.84486866	0.41503313	4.33245819	1.5301225	2.62384998	5.94735286	2.77664115	2.78084499	3.97661397	3.52864259	4.83303901	-2.3365308	-0.6850147	-2.0830561	-1.9703163	0.51424522
P_18	-3.0775393	2.68412097	7.64282343	4.11783374	6.4902281	6.2204163	6.34383547	-0.3927889	4.27583598	2.10760612	2.38254393	5.85148305	2.41481497	2.54235844	3.32467448	3.61680796	3.72950844	-2.2318119	-1.3788289	-2.2240196	-2.7211878	-0.4648863
P_19	-2.4727868	3.053557	7.67752844	3.26174297	6.65428649	6.41220967	6.66646808	0.20059481	3.88350896	1.69036145	3.90236244	6.03277774	2.45782977	1.9524989	2.92780006	3.80698671	4.53430942	-2.9998537	-2.4462371	-2.7273325	-1.5729918	-0.3255755
P_2	-2.2610316	2.47890153	7.39223587	4.30756578	6.57911942	5.94819194	6.59806937	1.33684033	4.46106677	1.59144618	2.45464512	5.62677007	2.96378089	2.52127355	3.76186035	3.47298241	4.57335358	-2.8879988	-1.6569101	-2.2852071	-2.7000539	0.75793427
P_20	-3.1293351	2.81314906	7.37542972	3.90026802	6.59719254	6.0881601	6.38120258	-0.5470701	4.26710306	1.72453466	2.21735644	5.55394854	2.79053223	2.39195407	3.21796143	3.43179634	3.70707378	-2.9112589	-1.1276384	-0.9604489	-2.269871	-0.2410743
P_21	-2.8965394	3.30577501	8.39174116	3.07279684	7.36397404	7.35902552	7.82665461	3.63047393	3.8283885	2.80435394	3.76895881	6.87373562	2.00369652	2.20370043	3.12624417	4.55935979	5.79573272	-3.0009937	-2.3499465	-1.6798424	-2.4265558	-0.9515075
P_22	-3.9103987	3.62307873	8.54091531	3.01525898	7.28827355	7.36784194	7.70517801	3.75954794	3.50407749	2.58028476	4.01113781	6.29178982	1.98879325	1.57365287	2.79085092	4.23370749	5.4249964	-2.3929027	-1.585625	-1.8861097	-1.6268377	-0.5236812
P_23	-3.269322	2.8497383	8.07033963	2.68721327	7.14891992	6.97586377	7.17006233	1.66544636	3.86488423	2.46598348	3.56545921	6.64873964	1.99921432	1.79833672	2.6662885	4.45395118	5.64042739	-2.5672849	-0.726827	-2.3602578	-0.9066287	-0.3728795
P_25	-1.2833587	2.96304631	7.49481272	4.22601861	6.6757474	6.30089721	6.68643726	-0.4299189	4.42879838	1.64602037	2.52440296	5.95492976	2.9409258	2.69266272	3.77583123	3.68478564	4.31544205	-2.5929565	-1.9803744	-2.4380469	-2.4608309	-0.2570078
P_26	-2.4531066	2.83651362	7.80445707	4.33008515	6.76993384	6.23164667	7.12447809	2.4199386	4.46409447	1.80372972	2.38350724	6.20250667	2.89078712	2.60818486	3.80939951	3.65563963	4.56493764	-3.1297068	-0.3942516	-2.5860122	-2.6406712	-0.6901953
P_27	-0.4652164	2.93510772	7.80869521	3.82998474	6.78305705	6.59461859	6.7811176	-0.4438787	4.26646217	1.46176188	2.90504183	6.46286106	2.82854828	2.73443332	3.56774854	3.97463305	4.68620935	-1.9049323	-2.1095014	-1.7238493	-2.4081925	-0.0649711
P_28	-1.8798086	2.6699579	7.43065182	3.04576894	6.58553655	6.44771743	6.83463027	1.01519529	3.82911018	1.8492978	3.23142886	6.2658915	2.05846033	2.07075238	3.16264565	3.87225381	5.21854294	-3.2063876	-1.6474314	-2.244265	-1.7329511	0.24723816
P_29	-1.8366116	2.89693183	7.84026705	4.47889253	6.66511639	6.67562485	6.99714695	-1.3708802	4.5931004	2.1704281	2.62374321	6.33045591	3.04780791	3.03147496	3.90958216	4.23272537	4.36240569	-3.1367643	-2.3710142	-2.1680319	-3.2890822	-0.3411519
P_3	-3.3005359	2.29791915	7.13646638	3.83847402	6.17152398	6.10528109	6.32838158	-0.5818864	4.05408434	1.68870295	2.03036813	5.51630109	2.40032184	2.46014255	3.36335409	3.26988951	4.24085084	-2.3212468	-1.5854014	-3.0376703	-1.400649	0.05819513
P_30	-3.0752819	3.64616565	8.31231809	3.32221702	7.44768776	7.45514518	7.75842757	1.01634253	4.11718603	2.25456394	3.59974392	7.12398679	2.6733627	2.81090434	3.4459026	4.90722118	5.94314899	-3.59946	-1.6481349	-2.9568045	-2.8823358	-0.3752566
P_31	-2.4655294	2.0918583	7.10930671	3.87210854	6.20410441	5.98455419	6.32048621	-0.2877028	4.00601985	1.68308134	2.03103716	6.02847023	2.17073288	2.46204073	3.37095566	3.40322861	4.50487367	-2.3040168	-0.9551365	-1.4282424	-2.3694133	0.10471658
P_32	-2.8524479	2.2845504	7.65342911	2.87916878	6.68400256	6.42590573	6.68111065	-0.6996433	3.76215983	2.14887108	3.54602797	6.10385393	1.92579121	2.1175267	2.5656479	3.82881928	5.08175122	-2.1703877	-2.314708	-1.7831386	-2.5383828	0.23868998
P_33	-2.2464107	3.20338391	8.21128758	3.20046101	7.40799798	7.14847877	7.56750567	2.64928963	3.41540126	2.27277398	3.5705932	6.82416478	1.85971856	1.25831921	2.8275249	4.14891031	5.27879412	-1.9999628	-2.6609094	-2.1617491	-1.0707612	-0.2115111
P_35	-3.5752559	3.78612407	8.684814	3.90701524	7.19227057	7.36011427	7.22437134	3.34792179	3.86657476	2.17649026	3.5889728	6.7148012	1.70188761	1.94443827	2.5122678	4.75189187	5.88975257	-2.2949972	-2.1877308	-2.424406	-1.7651734	-1.2831005
P_36	-3.2889859	3.33255486	7.85414672	2.75524469	6.91853212	6.66886855	6.80359888	0.96005636	3.07251423	2.14328464	3.54588278	6.35800788	1.24848181	1.28574847	1.84500519	4.18079657	5.62684282	-2.5914407	-0.9251615	-1.9466321	-2.4355076	-0.1834281
P_37	-2.9147085	3.54937087	8.51247192	3.28260998	7.57124417	7.35110138	7.97255068	2.87068155	3.95794029	2.90679554	3.89791901	6.51946993	2.29336764	2.3090001	3.3973252	4.6767458	4.87903184	-1.9158136	-2.51383	-2.7525246	-1.6580798	-0.1267744
P_38	-2.4528444	2.62354936	7.57202364	4.23515644	6.61153883	6.76069852	7.14365533	2.05760208	4.47791908	2.08775929	2.69196487	6.58890304	3.03800358	3.35799844	3.99098831	3.58867879	3.99330773	-2.5197369	-0.7468149	-1.4287374	-2.870592	0.05576222
P_39	-3.590365	2.62510282	7.95610576	2.51469825	7.08460435	7.06953529	7.35513432	2.29648833	3.96250127	2.31533878	3.71003375	6.93549186	1.99324455	2.19328156	2.92949787	4.61757012	5.96184625	-2.439896	-1.0750494	-2.8243803	-3.2437075	-0.4347896
P_4	-1.4522762	2.76612041	7.69432282	4.12259772	6.76324233	6.08881762	6.53180739	-0.6550217	4.40920042	1.75777624	2.2602015	6.01128434	2.84256944	2.44118347	3.44907513	3.7646181	4.87881804	-2.3723388	-1.4084723	-2.7683278	-2.336553	-0.2529595
P_40	-1.5696267	2.36147993	7.46563757	3.265925	6.76036738	6.80175513	6.75990374	0.72267875	3.96877196	2.14936493	3.20056925	6.20511501	2.48339508	2.6928045	3.20536332	3.92170553	5.09528984	-2.4060219	-1.5920022	-2.5032135	-3.3049244	-0.379015
P_41	-2.8449874	2.89863393	7.42800822	4.00023933	6.73693721	6.44879984	6.77386286	0.4877344	4.26844753	1.67490065	2.53692735	6.06536228	2.92095852	2.86737328	3.81940537	3.66307687	4.54476858	-2.8928471	-0.9339709	-3.2770254	-2.1688158	-0.4652466
P_5	-2.5368278	2.29472388	7.65327472	4.34442119	6.64068441	6.18450331	6.78053713	-0.2854045	4.51685955	1.9926434	2.72707218	5.5541994	2.67599851	2.83635776	3.87710104	3.8431874	3.94414609	-2.2471186	0.24874894	-1.7067136	-2.2100342	-0.6368822
P_6	-3.2629911	2.71421638	7.87536523	4.21866966	6.90098478	6.40915837	6.97479384	-0.6462996	4.43016914	2.28098798	2.53864452	6.35552761	2.98302099	2.57429717	3.75593098	4.00058885	5.31831159	-2.866383	0.40621686	-2.5407797	-2.5436851	-0.0799579
P_7	-3.1143962	3.0589495	7.63988357	4.18452056	6.64102478	6.28239677	6.77627124	2.27688338	4.45021238	1.72966448	2.71402141	6.25954718	2.8050224	2.56141614	3.66271158	3.64907695	4.29335448	-1.9053944	-1.1864522	-2.0259299	-2.0362713	0.30710616
P_8	-2.1735604	2.71280621	7.70541589	4.0315985	6.66637227	6.54219676	7.41379789	-1.1281343	4.4838051	2.26914475	2.8883551	6.22604441	2.85319801	2.9755934	4.2322472	4.2674046	5.05882597	-3.2291151	-1.8676702	-2.830954	-2.3280479	-0.0871135
P_9	-2.3776693	2.92403073	7.70692194	2.84930114	6.66986297	6.87872603	7.02379578	1.47168192	4.12810751	2.28195471	3.48348389	5.86793374	2.21119411	2.6192838	3.37635997	3.17995799	4.79244421	-2.6647277	-1.2407103	-2.3046749	-1.9819955	0.06949901

Table 8.110: Normalised data matrix for phosphatidic acid and lyso phosphatidic acid for serum samples taken from patients with breast cancer.

	PA□6:0	PA□6:1	PA□6:2	PA□8:4	PA□8:5	PA-1	PA-3	PA-4	PA-5	PA-6	PA-8	PA(24:0)	PA(24:0)□1	PA(26:1)	PA(26:3)	PA(27:4)	PA(27:5)
P_1	-2.1673821	-1.917799	-2.7128576	-0.7090271	-2.1468847	-2.1383164	-3.1473771	-2.5152202	-2.4442585	-1.6433637	-1.5802465	-2.1589967	-2.3625471	-2.4688147	-2.4217011	-1.6501916	-2.4053875
P_10	-0.9331928	-1.5167321	-1.7311244	-0.6850176	-2.3595174	-2.4709388	-2.1838888	-1.9863307	-2.7768809	-2.7058422	-2.172729	-2.5923469	-3.0820013	-2.6005168	-2.7543235	-2.1568893	-2.2518857
P_11	-0.9061442	-3.1359239	-3.1150412	-0.5137405	-1.4686334	-2.5475653	-2.9534434	-2.375431	-3.0971781	-3.5897878	-1.3936314	-2.7773624	-0.1753599	-2.7959506	-3.5958935	-2.0076113	-2.8824755
P_12	-0.6178793	-2.2811602	-2.4918923	-0.2850136	-1.3177629	-2.8447627	-3.1932822	-2.6183948	-2.8608069	-2.5925055	-0.902645	-2.5678201	-2.3046624	-2.6515096	-2.69372	-2.3236784	-2.4499948
P_13	-0.8118042	-2.5509012	-3.7512621	-0.4440928	-2.5236543	-2.2358111	-2.8355766	-2.6671443	-2.649545	-2.2681769	-1.9121439	-2.5147743	-0.5981963	-2.3095371	-2.6462451	-2.6027309	-2.6299315
P_14	-1.1789677	-2.0143828	-1.8708561	-1.0477312	-1.4384061	-3.1373022	-2.6502622	-2.9534537	-3.7888629	-2.5405829	-1.7962755	-2.8550189	-1.4591671	-2.6671869	-3.0165727	-3.1856898	-2.8830924
P_15	-0.4198739	-3.0924859	-1.9044963	0.00172708	-1.6403746	-2.4661965	-2.4183551	-2.5336244	-2.7721386	-2.1239727	-1.0771643	-2.6236812	-0.7655502	-2.7073707	-2.7495812	-2.1929919	-2.6707627
P_16	-0.3521347	-2.5239669	-3.167725	-1.349838	-2.0299351	-2.2499365	-2.7138925	-2.457996	-2.6320077	-2.2402195	-1.6079283	-2.3779352	-0.8834824	-2.4911108	-2.5333212	-2.9453338	-2.0596417
P_17	-3.1364792	-2.683632	-1.93578	-2.9568086	-1.8023846	-1.9543207	-2.8471095	-3.214866	-1.9789351	-2.1996382	-2.173925	-2.36684	-0.6826726	-2.797982	-3.357173	-0.8609463	-3.3378825
P_18	-0.4999956	-1.9229968	-2.4859426	-1.4507498	-2.2885942	-2.6834056	-2.7678672	-2.5769158	-2.2831092	-2.0078398	-1.1017534	-2.3226526	-1.5504846	-2.4063421	-2.1076233	-2.673352	-2.419979
P_19	-1.083363	-2.479043	-3.0124428	-1.3270071	-0.7959022	-3.114607	-3.3748845	-2.9043735	-2.4634807	-2.6037483	-2.48088	-2.302258	-0.5360914	-2.504957	-2.5127492	-2.914647	-2.7351123
P_2	-2.5623743	-2.9296612	-2.4016049	-1.2735082	-1.9546658	-2.2735957	-1.9662778	-2.4816551	-2.2908021	-3.2192939	-0.3979439	-2.4310804	-1.698492	-3.3213325	-2.7015326	-1.5601781	-2.5406668
P_20	-2.2994064	-2.6088321	-1.9113126	-1.045827	-2.9588579	-1.8501495	-2.176919	-1.5421794	-2.5502083	-1.6151642	-2.4504063	-2.8447035	-2.5786073	-1.3505732	-2.8088092	-1.7488367	-2.0999549
P_21	-1.4066634	-3.2340113	-4.4005619	-0.9852101	-1.7016221	-2.755752	-3.2731512	-3.357613	-3.0616941	-2.5499391	-2.2400003	-2.4372734	-0.6193037	-3.4675581	-2.6760761	-2.6991091	-3.8177385
P_22	-2.9210932	-2.0827	-3.4836596	-2.8315102	-1.5723436	-2.6887862	-3.5557648	-2.8968457	-2.9947284	-2.7448134	-2.5273827	-2.846271	-0.9174687	-2.9299605	-2.9721709	-2.3242466	-2.9558574
P_23	-1.1394802	-2.3389719	-3.4098777	-1.5849245	-1.004517	-3.1016502	-2.0603253	-2.4116117	-2.6459126	-2.5688806	-3.3354693	-2.7729536	-0.9310003	-2.2481781	-2.8988535	-2.6822625	-3.3679174
P_25	-1.0214429	-2.7268179	-2.5252905	-1.6298585	-1.6334298	-2.2084834	-2.7926786	-2.2493965	-2.5144256	-3.2904868	-1.5464232	-2.3659682	-1.5668951	-3.0649585	-2.5426299	-1.6732522	-2.5162991
P_26	-1.9163644	-2.699811	-3.6156925	-1.0306064	-2.3050336	-3.4502746	-2.6079069	-2.9290821	-3.3940671	-2.5545813	-0.6080701	-2.5068266	-2.8084618	-2.7410407	-2.3111105	-2.3219754	-2.6164129
P_27	-1.7083616	-2.3595727	-2.2556689	-0.6460705	-3.2265152	-2.5667387	-2.5687422	-3.067435	-2.8726808	-2.5570216	-2.9842633	-2.8866965	-2.8918252	-2.749299	-2.8501234	-1.9179404	-2.7043291
P_28	-1.6170422	-3.3526473	-3.5779768	-1.5592696	-1.5306248	-1.6740609	-2.2425218	-2.4853096	-3.3044056	-2.5254012	-2.3963663	-2.4696166	-0.1535705	-2.3240941	-2.1755165	-2.7919472	-2.5754605
P_29	-1.0880286	-2.581551	-2.7194036	-1.3851784	-3.175361	-1.9796189	-3.200013	-2.5386006	-2.4128997	-2.1942651	-1.7307266	-2.488026	-1.8051403	-2.4248187	-2.6139259	-2.930417	-2.5486208
P_3	-0.8181283	-2.0708881	-2.3750802	-1.0754166	-1.646275	-3.2972941	-2.6517094	-1.9566586	-2.9380087	-2.6704822	-0.7019083	-2.2724372	-1.3842726	-2.2355742	-2.8536828	-2.6559062	-2.4078201
P_30	-0.7767896	-3.3640715	-2.3796844	-1.1446595	-1.5718677	-3.5957699	-3.6077152	-2.9045371	-3.7813855	-2.8888496	-1.8718189	-2.307855	-1.0010529	-2.9608533	-2.78215	-2.6340086	-2.8986502
P_31	-2.2191007	-1.5778403	-2.4385495	-1.1390533	-2.5317449	-2.9763718	-2.227815	-2.4169024	-1.8982932	-2.9091826	-0.7082328	-2.2888174	-2.1468632	-2.4500172	-2.2448559	-2.7749026	-3.410867
P_32	-2.0104975	-3.0769609	-2.268348	-0.6197389	-2.3398916	-2.243294	-3.2078807	-2.4513534	-3.0603706	-2.6293072	-1.3625645	-3.3325351	-1.0370241	-2.8763111	-2.5266787	-2.0578291	-2.5103651
P_33	-0.9063509	-3.2283232	-3.0054666	-3.0357482	-1.9204103	-3.3566763	-2.5395866	-3.1187657	-2.6680326	-2.5825639	-2.7202625	-2.5195753	-0.8422355	-3.1942693	-2.6454752	-3.0884446	-2.6291617
P_35	-1.5075809	-3.1666784	-2.987575	-2.2620564	-2.9974806	-2.4676786	-3.1608967	-2.5888767	-2.6867594	-2.9296679	-3.1240683	-2.790235	-0.8927131	-2.6219915	-3.1414921	-1.510328	-2.5476793
P_36	-1.0715256	-2.3608864	-3.0843524	-2.4301873	-1.3555285	-2.3921434	-2.5505265	-2.6002029	-2.5842666	-2.6623831	-3.2849553	-2.3919194	-0.3383476	-2.3132886	-2.6755281	-3.1437746	-2.6592146
P_37	-1.0750202	-3.2911523	-2.6664225	-2.9686866	-1.8377868	-3.4100035	-2.3023758	-3.0350977	-2.7191165	-2.6839019	-2.8927786	-3.0564869	-1.0914409	-3.4723466	-3.1547092	-3.025229	-3.1179084
P_38	-1.7312491	-3.1291586	-2.6590685	-1.1086093	-3.0362554	-1.9741009	-3.76461	-2.2614338	-3.0380533	-2.6226287	-1.3564536	-2.4521963	-0.5756564	-2.87352	-3.6133976	-3.5198944	-2.6523556
P_39	-2.4229697	-3.1121504	-1.85303	-1.0230236	-2.0845629	-2.4882625	-1.8062878	-2.9668805	-2.3036455	-1.7865151	-1.3660443	-2.8136931	-1.1542799	-3.7263923	-3.6255339	-2.2508073	-3.0994009
P_4	-1.2650831	-3.1727873	-2.8917666	-0.1334334	-3.0357108	-2.2565106	-2.5793228	-2.5625584	-2.3720164	-2.9054584	-1.102041	-2.1794764	-2.5760517	-2.7038709	-2.4450154	-2.020256	-3.0637075
P_40	-1.8165097	-2.4559443	-2.1220042	-1.7122606	-1.8554817	-1.4877939	-2.5411275	-2.5987888	-3.1854734	-2.744561	-1.4434216	-2.5402293	-2.276815	-2.6239187	-2.6661292	-3.4968353	-3.1327351
P_41	-2.3184367	-3.0848703	-1.8122179	-2.4017375	-2.2826789	-2.4927088	-2.0822746	-3.0807739	-2.4416785	-2.1157571	-1.5207764	-2.6862657	-2.4705974	-2.7338831	-2.7760935	-2.5370381	-2.7662712
P_5	-1.8037517	-2.9924953	-4.2219033	-1.8617561	-2.985712	-2.0593016	-2.6679705	-3.162307	-2.3652438	-2.0495845	-2.3140707	-2.2167864	-1.0663656	-2.3004759	-2.2292798	-1.8068546	-2.1423835
P_6	-1.0755716	-2.7574889	-3.0896813	-0.5249563	-2.7682465	-2.3327998	-2.7879993	-2.9484667	-3.3921973	-1.5662648	-3.6610089	-2.9810396	-2.2101729	-3.3357301	-2.7607633	-3.2238804	-2.541847
P_7	-1.3963311	-2.3727068	-2.8845371	-0.9415765	-2.083238	-1.6437023	-2.9379921	-2.6000784	-2.6979611	-2.129232	-2.1455603	-3.3548384	-2.1123086	-2.7811973	-2.6754037	-2.390747	-3.2882173
P_8	-2.4183413	-3.1453227	-1.6849206	-0.7455277	-3.1072775	-2.4603871	-2.6742001	-3.1875428	-3.2747215	-2.4772269	-0.6139793	-2.7858236	-0.7555958	-2.7281183	-2.831946	-3.0780515	-2.7540152
P_9	-1.0575833	-2.9198771	-2.2009071	-0.6294335	-2.4074005	-3.5280492	-2.802607	-2.7323723	-2.7949953	-1.9883345	-2.2004657	-3.0151435	-0.7203366	-2.8444742	-2.2210633	-3.2429212	-2.7561243

Table 8.111: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls.

	LPC(14:0)	LPC(15:0)	LPC(16:0)	LPC(16:1)	LPC(17:0)	LPC(17:0)d2	LPC(17:1)	LPC(17:1)d2	LPC(17:2)	LPC(17:2)d2	LPC(18:0)	LPC(18:1)	LPC(18:2)	LPC(18:3)	LPC(20:0)	LPC(20:0)d2	LPC(20:0)d3	LPC(20:1)	LPC(20:2)	LPC(20:3)	LPC(20:4)	LPC(20:5)
C_1	-0.3750066	-0.9106522	3.85700805	-0.226062	0.62089523	-1.5761645	-1.8976637	-1.7348993	-4.4746534	-5.5018531	3.49956818	2.95479957	3.36545725	-0.1641524	-0.6231894	-2.1921886	-1.9764882	-1.3654242	-0.2713076	1.55946191	2.51734161	1.22460114
C_10	-0.6856832	-0.7971001	3.73714113	-0.0650119	0.2116579	-1.797862	-1.7663029	-1.3570946	-4.2876498	-5.6949399	3.14492275	3.23369607	3.76459696	0.10343686	-1.1618247	-1.9906812	-2.2329009	-1.29958	0.29745595	2.17036421	3.16803682	2.44710298
C_11	-1.2189541	-0.7330461	3.81036639	-0.3061169	0.28881487	-1.5724194	-2.0497154	-1.5741168	-4.1096393	-5.885721	2.79082991	2.89054288	3.47791373	-0.2994216	-0.7814739	-2.1655043	-2.3176917	-1.3314231	0.10143432	1.94557869	2.83664841	0.54111265
C_12	-1.038526	-0.5289226	3.97030887	-0.8696644	0.54884716	-1.2702523	-2.3421026	-2.3478255	-3.741575	-5.6409651	3.38369385	1.92923909	2.30199458	-0.1675111	-0.3686185	-1.846907	-1.9637443	-2.3912956	-1.1837678	0.87866473	1.79740234	-0.1524031
C_13	-0.9117783	-0.8078363	3.63795824	0.08155051	0.04486206	-1.6739244	-2.0173322	-1.337933	-4.2281098	-6.1589297	3.1271673	3.28308677	3.87784942	0.15590319	-0.6127447	-2.0702463	-1.8128228	-1.209598	0.30597261	2.37955143	3.26771802	0.99072759
C_14	-0.4060531	-0.7691505	3.63255928	-0.9649785	0.12888103	-1.4357339	-1.6073693	-3.0163685	-3.2452697	-6.0100152	3.06885352	1.97329691	2.42585943	0.42633543	0.68113755	-1.1007361	-2.1678784	-2.7729721	-1.1958004	0.90040315	1.5346475	0.14960855
C_15	-0.7786872	-0.8995775	3.70814899	0.46225188	0.41262667	-1.5550744	-1.3282704	-1.6138372	-4.5520893	-5.7224086	2.91791156	3.24568741	3.4119942	0.0424554	-0.7415406	-1.5136975	-2.3597128	-1.4818585	0.21351278	2.25414354	3.14163339	1.1762696
C_16	-1.0825266	-0.833908	3.94544412	-0.2989508	0.61595319	-1.539509	-2.0306064	-1.710885	-4.2730229	-5.4434998	3.45878825	2.68413869	3.44392598	-0.118216	-0.6922111	-2.3984173	-1.6377091	-1.5236643	-0.5268161	1.57910612	2.37167086	-0.1214085
C_17	-0.5836105	-0.9050024	3.8986005	0.40523714	0.57467967	-1.7400974	-1.5193277	-1.56409	-4.4086184	-5.4437803	3.44895816	3.20402344	3.28691331	-0.0695164	-0.5622673	-1.949896	-2.0737059	-1.4410687	-0.3008368	1.66795039	2.8591898	1.78251882
C_18	-0.8037437	-0.8987207	3.76776304	-0.1468275	0.51898967	-1.6310714	-1.76643	-1.4276258	-4.3126461	-5.6603917	3.12517734	3.06253858	3.7416362	0.00888047	-0.6622431	-1.7672004	-1.9917793	-1.4045407	-0.1388972	1.69425818	2.37565971	0.04769517
C_19	-1.5127706	-0.8062625	3.63366444	-0.1317348	0.35239463	-1.5419842	-1.8592467	-1.2315828	-4.2172362	-5.5539336	3.2018779	3.16983014	3.71819251	-0.0717576	-1.2387899	-1.8993266	-2.1389724	-1.2086862	0.24250537	2.34369059	3.13898957	1.19582969
C_2	-0.8867615	-0.8415264	3.87574897	0.59609703	0.42144235	-1.6970009	-1.6175675	-1.7381955	-4.3054543	-5.735465	3.14405247	3.11009939	3.07541179	-0.3308745	-0.7915822	-2.3851372	-2.3970685	-1.5395351	-0.2218804	1.94286584	2.84617795	1.18060825
C_20	-1.1142688	-0.5777128	3.85782037	-0.6157839	0.83521233	-1.2680909	-1.939297	-1.9878745	-4.3169726	-5.6312206	3.40076765	2.30091737	3.01190527	-0.1369354	-0.6792485	-1.644588	-2.0143875	-1.9820205	-0.7152356	1.08962305	1.93967009	1.1014086
C_21	-1.4226875	-0.7921185	3.51969892	-0.1404056	-0.1579062	-1.8261457	-1.8961384	-1.5383002	-4.1671151	-5.9643241	2.90400029	3.2615878	3.65276521	0.1392608	-0.6511182	-1.949567	-2.3737717	-1.517727	0.04450918	2.11729535	3.0136334	1.11371329
C_22	-0.5950987	-1.354759	3.7628571	1.13013202	0.3240563	-2.2582388	-1.1952886	-1.5709649	-4.545379	-5.2339842	3.44884944	3.86148435	3.70043712	0.28096619	-0.2998363	-2.4546208	-2.0632582	-0.9938535	0.45190505	2.414819	3.30385072	1.74970781
C_23	-0.7680348	-1.0397968	3.71188396	0.10966114	0.42681121	-1.7996312	-1.6597563	-1.5343408	-4.302887	-5.9123249	3.04988236	3.10823568	3.76555839	0.05399818	-1.2708381	-2.0841437	-2.331013	-1.3145897	0.32850773	2.41638811	2.6231769	1.00956284
C_24	-0.5825559	-0.9663647	3.79253953	0.72387852	0.18103132	-1.8594172	-1.3505737	-1.3960361	-4.4034644	-5.7594116	3.3086881	3.57267973	4.21576518	0.70051833	-0.8201011	-2.4468079	-2.2928269	-1.0206421	1.03614823	3.19886628	3.21302047	1.29484558
C_25	-0.5308489	-0.7593866	4.0366482	0.78684387	0.95157822	-1.5120071	-1.0948272	-1.2517625	-4.2639693	-5.6693976	3.55128501	3.4925114	3.9575639	-0.01549	-0.780793	-1.7219197	-2.2621579	-0.9933031	0.60921762	2.65501479	3.24172594	2.21726633
C_26	-1.0002979	-0.9093691	3.68745967	0.41168479	0.62493781	-1.6145758	-1.3067253	-1.3251124	-4.2110662	-5.9406236	3.16494742	3.46982005	3.99000475	0.05623751	-0.765292	-1.6583992	-2.3920655	-1.0221806	0.62434478	2.72604051	3.10829396	1.46700142
C_27	-0.9772812	-1.0794144	3.71424131	0.48779717	0.56879293	-1.7297542	-1.1705381	-1.5138678	-4.1443635	-5.4976064	3.36897142	3.48826214	3.97495572	0.31569381	-0.8345058	-2.0360834	-2.3656279	-1.0780637	0.65320666	2.76712753	3.41796492	1.1841818
C_28	-1.2770808	-1.0552559	3.67809078	-0.1654395	0.76114105	-1.6208042	-1.6688302	-1.247043	-4.0305461	-5.5918527	3.33902314	3.28316241	3.88043595	-0.0759199	-1.1456346	-1.5653249	-1.7592327	-0.8014997	-0.2254885	1.29373023	2.69094984	2.34630353
C_29	-0.6441135	-1.1125088	3.95335972	0.42895205	0.69293824	-1.80368	-1.6556795	-1.314027	-4.3083944	-5.4370722	3.56598254	3.28980804	3.7989197	0.10851931	-1.1326815	-2.6187099	-1.7518138	-0.8879243	0.25798962	2.1599069	3.17301993	1.83708501
C_3	-1.0783679	-0.7373547	3.82599557	-0.0787783	0.31741817	-1.6160215	-1.9779598	-1.4468206	-4.3392228	-5.4793348	3.35979939	3.02824023	3.76585722	0.1456765	-0.6897619	-2.1956557	-1.8924083	-1.3667259	-0.0059609	1.85665543	2.81068553	1.10746201
C_30	-0.9068781	-0.9651287	3.48210418	-0.0892649	0.29456978	-1.6109136	-1.2719626	-1.8576421	-4.0722515	-6.229329	2.94781325	3.18948114	3.66381147	0.1799889	-0.512644	-1.5976386	-2.6243408	-1.5956118	0.33978713	2.59002995	2.94281939	1.15841248
C_31	-1.3410482	-1.1276202	3.23160428	-0.3272732	-0.1195842	-1.8589584	-1.85645	-1.603424	-3.6773443	-6.1066811	2.64086201	2.94473321	3.47962687	-0.0616438	-0.9709622	-2.1146986	-2.7596261	-1.6578487	-0.0349452	2.07796454	3.07623248	0.98942478
C_32	-0.9241076	-0.7125744	3.6937491	-0.3334031	0.25959679	-1.4821455	-1.7104781	-1.6746026	-4.3037408	-6.0423904	3.06789562	3.05266834	3.58170336	-0.0484462	-0.6215503	-1.461301	-2.1855157	-1.5447287	-0.1018744	1.72234474	2.61439917	1.29127245
C_33	-0.5832087	-1.1074327	3.93026766	0.23014287	0.50300579	-1.7028492	-1.6847886	-1.9637686	-4.2755623	-5.6539584	3.38920145	2.86756667	3.29208723	-0.2984117	-1.1292477	-2.075698	-2.0138909	-1.1672489	-0.1261401	1.85883101	2.34357659	0.82866768
C_34	-0.5263676	-1.1837154	3.6991538	0.42897135	0.40176443	-1.6900398	-1.3238878	-1.6684331	-4.5044122	-5.6951667	3.27887581	3.37523218	3.43601969	0.2452792	-0.9230564	-2.2433103	-2.0742885	-1.2385121	0.46512388	2.42641671	3.16313157	1.48711634
C_35	-0.6024529	-0.7179654	3.9034966	0.21825204	0.9781746	-1.2744272	-1.4113934	-1.1192167	-4.2984004	-5.4920903	3.67109789	3.39453985	4.13795417	0.21225469	-0.8950606	-1.5432102	-1.7881081	-0.984017	0.32835686	2.05598856	2.80174514	1.02866266
C_36	-1.1704471	-0.6446814	3.79509845	-0.3449768	0.55095107	-1.3252933	-1.9254492	-1.2309016	-4.0011607	-5.3631803	3.54140009	3.05581916	4.04918429	0.21802937	-0.9347889	-1.6809362	-1.5181795	-1.2507826	0.13439294	1.8436002	2.61135857	0.59171527
C_37	-1.180886	-0.7896814	3.65893212	-0.0150227	0.67895883	-1.3213178	-1.6102307	-1.3471756	-4.1398789	-5.7493168	3.22397977	3.16994617	3.85104643	0.16538451	-0.9913163	-1.936853	-2.0724179	-1.3317475	0.01733235	1.93120143	2.56628083	1.80117619
C_38	-0.6235168	-0.8952367	3.98814581	1.2589208	-0.0016374	-1.9995077	-1.264508	-1.5924054	-4.4990272	-5.9595419	3.24757318	3.68134721	4.01532397	0.5774687	-0.5633732	-1.949012	-2.186275	-1.1709501	0.73212822	2.66254493	3.21047298	1.94495547
C_39	-2.0448921	-0.7188526	3.09688368	-0.3724894	-0.0393289	-1.5195455	-1.9507456	-1.2094831	-3.733041	-6.2214138	2.52109167	2.87267514	3.5085558	-0.4046334	-0.8824078	-1.6302299	-2.7414566	-1.6200007	-0.0872027	1.9609785	2.8863892	0.4237855
C_4	-0.6853383	-0.8541963	3.66672747	0.00831607	0.16801421	-1.7007449	-1.740822	-1.5526865	-4.3637877	-5.7449459	3.16988293	3.02716969	3.69239909	0.20459675	-0.833648	-1.8725502	-1.9188916	-1.5662803	0.24696937	2.17461892	2.55886436	0.50821277
C_40	-0.9883541	-0.7906579	3.75989918	-0.2364247	0.41686521	-1.3492897	-1.5326958	-1.8205538	-3.9937814	-5.689294	3.1349815	2.93918731	3.17290796	-0.2017966	-0.3819445	-1.6932603	-2.0250123	-1.6618377	-0.0464112	1.83079747	2.16344432	0.07088301
C_5	-1.1578085	-0.7596781	3.64078068	-0.1297247	0.55570108	-1.3994207	-1.6620552	-1.4069909	-4.2828379	-5.6751867	3.13501138	3.08877607	3.71550362	-0.0660413	-1.2048212	-1.5147234	-2.3151769	-1.4176521	0.14317678	2.10552739	2.88740781	1.4916012
C_6	-1.6617283	-0.7947819	3.63302536	-0.0769946	0.48534421	-1.5872373	-1.8142525	-1.3699517	-4.1446355	-5.776372	3.01936757	3.0018792	3.60276343	-0.2178609	-0.8765222	-1.8903709	-2.1400766	-1.4734336	-0.2363202	1.88899548	2.85101826	0.88766183
C_7	-1.3476701	-0.8979297	3.87000253	-0.4078271	0.30876742	-1.5707095	-2.1524531	-1.4470472	-4.191082	-5.3251686	3.46741893	3.0668971	3.81421442	-0.1680149	-0.9528066	-2.1797002	-1.6414413	-1.0861227	0.05593126	1.73489752	2.58259638	0.65245753
C_8	-0.0394543	-1.1270606	3.833791	0.62107792	-0.0098355	-2.0432059	-1.6735338	-1.7340537	-4.3825898	-6.030494	3.05131539	3.2742013	3.67935332	0.23097278	-0.5272369	-2.4886825	-2.0734851	-1.4201086	0.14263834	1.9117475	2.85273209	1.37179415
C_9	-1.4543841	-0.8284656	3.38213694	-0.6893285	0.07357459	-1.5722518	-1.7566584	-1.6995254	-3.9235001	-5.7395523	2.92749575	2.82307183	3.42970311	0.08548022	-0.5410099	-1.9392854	-2.3833408	-1.8405647	-0.2588109	1.73347026	2.6002384	0.46659391

Table 8.112: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls.

	LPC(22:0)	LPC(22:1)	LPC(22:2)	LPC(22:3)	LPC(22:4)	LPC(22:5)	LPC(22:6)	LPC(21:0)	LPC(21:0)(2)	PC(22:0)	PC(22:1)	PC(22:2)	PC(23:0)	PC(23:1)	PC(23:2)	PC(24:0)	PC(24:1)	PC(24:2)	PC(25:1)	PC(25:1)(2)	PC(25:2)	PC(26:0)
C_1	-3.3176621	-3.9283931	-0.2403713	0.70872431	-0.7456413	1.0047342	2.26542521	-2.032716	-3.9456891	-4.2609758	-3.5853729	-4.7052269	-6.7546161	-4.3191577	-5.7526306	-2.5582059	-4.6083771	-4.0678433	-4.658861	-5.2623035	-5.3327768	-0.9735477
C_10	-3.6714636	-3.8952171	-0.7085318	0.24246973	-0.239067	1.66313391	2.83742326	-2.010313	-4.0094981	-4.6000245	-3.1737974	-3.7537854	-6.0087917	-4.4770424	-6.0087917	-3.5559596	-3.9758702	-3.8994972	-5.1211914	-5.7211096	-5.2615773	-2.0226174
C_11	-3.9639084	-4.2978472	-0.4395297	0.44688349	-0.8146388	0.41411026	2.01409032	-2.3286601	-3.9228132	-4.377209	-3.0106509	-4.1980882	-5.4367707	-4.6178348	-5.885721	-4.1882722	-5.247382	-4.8561015	-4.9023948	-5.4240856	-6.1601578	-2.9629179
C_12	-3.2605776	-4.7246744	-0.0626428	0.86887374	-1.4738772	-0.2173376	0.84956524	-2.0683642	-3.4356922	-3.310588	-3.8062042	-4.7846174	-6.2305716	-4.8947081	-5.9594189	-4.9523738	-5.5211639	-5.0184355	-4.947818	-5.6593143	-6.2639081	-2.8109655
C_13	-3.1491832	-4.1835055	-0.1395127	0.76881796	-0.1924315	0.99039828	2.09294456	-2.2740458	-3.8114021	-4.8201159	-2.9536949	-3.9439426	-5.1953861	-4.6041864	-5.5810485	-4.2049874	-3.9545622	-3.8129453	-4.6353308	-5.7113531	-4.8286085	-2.8261493
C_14	-3.9840624	-6.6231197	0.8844437	1.80253157	-2.3169778	-0.5596924	0.61532186	-1.5009889	-4.2113353	-4.3758847	-5.4503995	-5.5504829	-6.0970266	-5.7868717	-6.9908445	-3.8650591	-4.0464055	-3.4612213	-4.4967212	-6.6231197	-5.0136818	-2.3669616
C_15	-3.7060678	-4.0707109	-0.2608658	0.60777383	0.05981039	1.17375453	2.01793041	-2.1046119	-3.800947	-4.5780942	-3.2246947	-4.3469643	-5.6495862	-4.6818015	-5.6529363	-5.0584606	-4.1503514	-4.1230937	-4.6691751	-5.3387626	-5.0061493	-2.7853806
C_16	-3.2745582	-4.1517316	-0.3463391	0.60687163	-0.6670822	0.49287685	1.12956127	-2.253427	-3.5173923	-3.6259324	-2.9938479	-4.285263	-6.284283	-4.2301592	-5.5911358	-4.1991757	-5.3011836	-4.7542819	-5.1239771	-5.1587632	-5.9543254	-2.5997311
C_17	-3.5788739	-3.8695366	-0.2391405	0.76031742	-0.2257014	1.33348875	2.35237487	-1.7823639	-4.0062287	-4.4611515	-3.4164666	-4.8069443	-5.6983937	-4.2257852	-5.736277	-4.6274214	-4.8928476	-4.4282573	-5.0508818	-5.1110202	-5.9798991	-2.5478206
C_18	-3.4442071	-4.0450887	-0.339906	0.59385714	-0.6799847	0.59865934	1.72333148	-2.144591	-3.8321896	-4.3358387	-3.2931368	-4.1314168	-6.3204781	-4.1732639	-5.6945831	-4.8466643	-5.2164604	-4.7424218	-5.0390927	-5.2521294	-5.880389	-2.8912227
C_19	-3.5151834	-3.5302283	-0.5966436	0.35641612	-0.3042156	1.12154152	2.53642255	-2.0211631	-3.6323833	-4.5989737	-2.9092597	-3.8295043	-6.0552467	-4.5309929	-5.8621354	-5.7514234	-5.6438818	-4.9546639	-5.1568669	-5.1986934	-6.0434818	-3.5917712
C_2	-3.8097716	-4.2043804	-0.2690165	0.7001433	-0.61366	0.9287345	2.07518346	-1.8762111	-3.8692525	-4.08997	-3.2635245	-4.9791389	-6.1337099	-4.6846772	-6.0183278	-5.1201488	-4.8028826	-4.9478864	-5.2967427	-5.1546808	-6.2083714	-3.3227482
C_20	-3.2346566	-4.1083507	-0.3346853	0.59687656	-1.3474659	0.59215864	1.75577596	-1.9905583	-3.6166429	-3.9593806	-3.4960445	-4.5623135	-6.4998833	-4.4439723	-5.6609258	-5.3745008	-5.3230188	-5.3087837	-4.8186657	-5.1859096	-6.0638815	-3.4960445
C_21	-3.8575944	-4.1090513	-0.4628318	0.35673895	-0.2443618	1.14607083	2.21478141	-2.1587552	-4.264057	-4.9306147	-3.3868433	-4.2144118	-5.4902305	-4.6008287	-5.8195853	-4.6815705	-4.15228	-4.1671151	-5.3389996	-5.7313926	-5.8855433	-3.0121498
C_22	-3.2520455	-3.674092	0.04315895	0.9600389	0.36221984	1.69084211	2.55921138	-1.5878482	-4.6730744	-4.6292225	-3.3353547	-4.7371533	-5.576517	-4.2084733	-5.4987683	-5.0175093	-4.436232	-4.4027841	-4.9335439	-5.0572168	-6.0944601	-3.1579472
C_23	-3.7700825	-4.0271811	-0.7869447	0.03247222	-0.4573204	1.20595281	2.31012785	-2.177178	-4.2798734	-4.551484	-3.4367207	-4.3764253	-6.1367921	-4.6438136	-6.0542055	-5.3163415	-5.047049	-4.9823713	-5.1501849	-5.3764196	-5.6818013	-3.2710026
C_24	-3.8767985	-4.0546635	-0.4750775	0.33714708	0.42908681	1.65847881	2.65701674	-1.8492382	-4.1445537	-4.8830375	-3.4284292	-4.5191488	-5.2907676	-4.7901985	-6.0991501	-4.9630802	-3.7836714	-3.9685584	-4.6464106	-5.3467263	-5.1337057	-2.7655834
C_25	-3.8238102	-3.705469	-0.2703714	0.73815722	-0.1168609	1.38930974	2.6192614	-1.9143474	-3.8648416	-4.3672262	-3.1739407	-4.3986161	-6.1142653	-4.6397782	-5.8160011	-5.7900256	-4.5306909	-4.5005811	-4.8227493	-5.128131	-5.5100656	-3.1605377
C_26	-4.0418603	-3.9641697	-0.3879701	0.54654956	-0.0634962	1.43583097	2.67607547	-1.8581919	-4.0146477	-4.7242283	-3.0698133	-4.0291337	-5.9605578	-4.3285576	-5.6463842	-5.0895734	-4.6188678	-4.76806	-5.0217048	-5.2877504	-5.4038225	-3.1746356
C_27	-4.1101916	-4.0233669	-0.3847276	0.54181512	0.55474647	1.73465353	2.09823841	-2.2251261	-3.936869	-4.6822019	-3.0847402	-4.2403692	-6.2413391	-4.5452043	-5.7399922	-5.7748795	-4.9335164	-4.8157333	-5.0103754	-5.3753491	-5.8485324	-3.6734912
C_28	-3.1838498	-2.5598244	-0.7804607	0.09792579	-0.9584599	1.43473951	2.79884838	-2.1247746	-3.7032214	-4.248741	-2.8178323	-4.0215667	-6.5565755	-3.4610999	-5.7736013	-5.3995524	-4.629094	-4.4724457	-4.8552509	-4.6236385	-5.0107742	-3.3782084
C_29	-3.3238697	-3.5438151	-0.780316	0.24365126	-0.1084828	1.53080523	2.68298399	-1.9785915	-3.7040316	-3.9099688	-2.853393	-4.1428403	-5.7716186	-3.6117459	-5.486465	-5.2134468	-4.8111982	-4.7248314	-5.2770866	-4.7958526	-5.7549237	-3.0904126
C_3	-3.2887234	-3.8801185	-0.4100043	0.4892752	-0.5269752	1.00583075	2.33463175	-2.062164	-3.7472294	-4.1991074	-3.0256303	-3.7948209	-6.4545303	-4.3045988	-5.4625277	-5.3119548	-5.7783807	-5.0795354	-5.5632693	-5.2098253	-6.8827236	-3.0880096
C_30	-4.074664	-4.5076791	-0.2310388	0.66586861	-0.1974925	1.22275923	2.20003886	-2.0871868	-4.0460907	-5.0635774	-3.5843369	-4.6602791	-5.7502521	-5.1553225	-6.5741695	-4.8173263	-4.3029536	-4.3639577	-4.8774751	-6.4116505	-5.2139474	-2.8588056
C_31	-4.0792444	-4.4167848	-0.9212601	-0.1462332	-0.652747	0.99934885	2.36445963	-2.3308185	-4.1588423	-5.3048008	-3.5191203	-4.5414493	-6.2998724	-5.4340125	-7.5203745	-5.5904647	-4.0651099	-4.145445	-4.4838202	-6.8272273	-4.8197593	-3.0500063
C_32	-3.6834902	-3.976838	-0.2615618	0.54254383	-0.6714317	0.96915309	2.35948323	-1.810886	-3.5807406	-4.3220899	-3.0968631	-4.2056796	-6.0918705	-4.2223005	-5.7059182	-5.1755798	-4.8537063	-4.4274504	-4.7827546	-5.2476831	-5.3879124	-2.9195699
C_33	-3.6404549	-3.0543815	-0.7829067	0.04989402	-0.7023261	0.59886805	1.61340599	-2.2770632	-3.7020721	-3.7206144	-3.1346841	-4.2190404	-6.7666554	-3.7509119	-6.0682032	-3.8692165	-4.3873063	-4.4683347	-4.9400492	-4.6253385	-5.5322979	-2.0462586
C_34	-3.5517392	-4.0167808	-0.4309425	0.45041968	0.09763133	1.27871045	2.28824352	-2.1005794	-4.0136431	-4.482144	-3.1706509	-4.4238185	-6.4544249	-4.4652702	-6.2472353	-5.3486441	-4.6554969	-4.5483523	-5.108503	-5.2841056	-5.6620511	-2.6994344
C_35	-3.3805604	-3.4753135	-0.3975402	0.64134659	-0.1762672	1.23481141	2.32044626	-2.1748863	-3.3725431	-4.0212385	-2.5530502	-3.5057236	-5.9595396	-3.74746	-5.3923723	-4.3156017	-3.9324661	-4.0118817	-4.4928886	-4.7514935	-4.7761861	-2.3230282
C_36	-3.0173575	-3.9013255	-0.518627	0.61564661	-0.6767249	0.75835583	2.02946545	-2.0459334	-3.5944554	-4.417105	-2.8995745	-3.6447837	-6.4080314	-4.1062731	-5.5548477	-5.5067284	-5.2198857	-4.675864	-5.121603	-5.0012864	-5.4512493	-3.3121173
C_37	-3.4770035	-3.7557303	-0.4527464	0.45486624	-0.6465499	1.43003829	2.67712222	-1.5368391	-3.4001952	-4.2075739	-2.6764551	-3.7567214	-6.8662782	-4.2710235	-5.6757284	-5.2612947	-5.2392187	-5.1103378	-5.1238646	-4.9608594	-6.1620812	-3.1186059
C_38	-3.7964357	-3.9585719	-0.0711344	0.84896277	-0.0935906	1.32690827	2.60364873	-1.2581471	-4.3425851	-5.1041903	-3.5038848	-4.890719	-5.8244394	-4.4258582	-5.8354892	-5.965851	-5.0419941	-4.7112814	-5.1149431	-4.9858132	-5.9470417	-3.3792298
C_39	-4.628783	-4.195461	-0.934621	0.020377	-0.482291	0.96621184	2.18224043	-2.008258	-3.9413016	-4.7391782	-3.1209462	-4.2158132	-6.6479323	-4.7843471	-6.0554287	-6.0207431	-4.0732109	-3.9398821	-4.6316119	-5.8159487	-4.8849518	-3.4904793
C_4	-3.2579922	-4.0476773	-0.3138044	0.52487975	-0.4881552	0.70871783	1.91006434	-2.198537	-3.9858169	-4.4678902	-3.3271311	-4.0491799	-6.5059157	-4.5700812	-5.6326423	-3.4180681	-3.7990357	-3.8973951	-4.5944257	-5.384181	-4.6824989	-1.5446058
C_40	-3.3470561	-4.4994657	0.0365468	0.79377044	-0.5464812	0.48989652	1.17865122	-2.1245202	-3.645596	-4.1048858	-3.2646901	-4.4445891	-6.6663849	-4.2536745	-6.2363485	-5.52397	-5.1573447	-4.5575295	-4.9548755	-5.5383587	-5.6083873	-3.4204167
C_5	-3.7432547	-4.0796096	-0.8027128	0.08893772	-0.5579447	1.303902	2.60820817	-2.1621318	-3.7206385	-4.2589799	-3.1470319	-4.2868701	-6.3325448	-4.5552118	-6.12198	-5.0087078	-4.1528338	-4.1096119	-4.7548556	-5.3468446	-4.8874658	-3.157425
C_6	-3.4635454	-3.9684047	-0.472555	0.41053237	-0.6754301	1.15191135	2.47593997	-2.0340447	-3.6490744	-4.6992304	-2.9240234	-3.9398766	-6.4310529	-4.4878418	-6.1316473	-5.9469975	-5.4075166	-4.8406632	-5.0447585	-5.5415324	-6.0706114	-3.6697302
C_7	-3.2901	-3.568269	-0.5349491	0.4151511	-0.5522502	0.79757389	2.03086286	-2.5150968	-3.8448275	-4.3600878	-3.0753399	-4.0434635	-6.3360754	-3.8543544	-5.5074902	-6.1550269	-5.5587835	-4.9651659	-5.1781865	-4.5130046	-5.8085953	-3.3449338
C_8	-3.6609224	-3.8390961	-0.1578976	0.80215738	-0.2019521	1.1496257	2.27224981	-1.7636801	-4.2730869	-4.4900489	-3.347594	-4.72943	-6.5835951	-4.1226474	-5.6582545	-1.286813	-3.2915533	-3.4741283	-4.6723705	-4.9673621	-5.1803989	-0.2000308
C_9	-3.7411785	-4.5496119	-0.4927871	0.45642433	-0.6950701	0.6425827	1.65892295	-2.3793477	-3.7213759	-4.5621591	-2.9710703	-4.1203263	-6.8800117	-4.9016662	-6.4164389	-4.9304452	-4.5981527	-4.5347601	-4.7029316	-6.7823732	-5.3674236	-3.3079542

Table 8.113: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls.

	PC(27:0)	PC(27:1)	PC(27:2)	PC(27:3)	PC(28:3)	PC(28:4)	PC(28:5)	PC(28:6)	PC(31:0)	PC(31:1)	PC(31:2)	PC(31:3)	PC(31:3)(d2)	PC(32:0)	PC(32:1)	PC(32:2)	PC(32:2)(d2)	PC(32:3)	PC(33:0)	PC(33:0)(d2)	PC(33:1)	PC(33:1)(d2)
C_1	-3.7896144	-3.1652662	-3.2454301	-2.476489	-3.1721942	-3.6927019	-8.1949777	-7.6196135	-3.0542892	1.03459872	0.82345535	-1.7835244	-2.4357254	2.31372254	2.47995723	1.6123018	1.16047264	1.51003862	0.12922391	-0.4613184	0.37474472	0.59662659
C_10	-3.4923994	-2.4469711	-2.59322	-2.5309763	-3.2183705	-3.8082058	-6.1495642	-6.4295243	-2.6505932	0.96261631	0.77459071	-1.598261	-2.0828259	2.26752334	2.52053567	1.7839617	1.28094294	1.79101545	0.01968153	-0.3873483	0.2610313	0.94414456
C_11	-3.7913908	-3.2596041	-3.7102119	-2.1875515	-2.7554578	-3.17856	-6.4304481	-6.3113888	-2.6237856	1.15634375	1.04872819	-1.7020436	-1.6055425	2.27604223	2.63744901	1.58237747	1.3954674	1.49226293	0.17171858	-0.2860405	0.547937	1.13415395
C_12	-3.0402977	-2.920268	-2.8983671	-2.5462106	-3.307939	-3.6937571	-7.1633917	-5.8870982	-1.773179	1.11734051	0.65352901	-2.208739	-1.969972	2.84712125	2.27855963	0.7978187	0.98851819	1.11723494	0.77747394	-0.0636052	0.60074508	1.04330562
C_13	-3.4704241	-2.1845378	-2.1877252	-3.0518869	-3.9779656	-4.2723489	-7.6470067	-6.0233842	-2.4289702	1.22816555	1.01456505	-1.4862516	-2.6582763	2.08231448	2.71177296	1.74710057	1.62945906	1.85450159	-0.20161	-0.3262198	0.44010659	1.235023
C_14	-3.4743363	-2.3274054	-2.4947454	-2.3035824	-3.033211	-3.4514968	-5.8207732	-5.5245074	-1.9713596	1.86245579	1.33384211	-2.2033528	-1.3186674	2.42248207	2.90387697	0.49114929	1.98981713	1.7814387	0.37271688	0.34804364	0.72417999	-0.3136211
C_15	-3.439806	-1.9115185	-2.1410904	-2.2302708	-2.9527469	-3.4034122	-6.4373749	-6.1626439	-2.7941929	1.2213698	1.07486111	-1.6472518	-2.0540623	2.04960015	2.88747981	1.66932146	1.39207125	1.5477941	0.11042278	-0.2964766	0.73127867	0.83515118
C_16	-3.4992717	-2.5546543	-2.9475433	-2.7012692	-3.29265	-3.6748819	-7.2958839	-5.8372689	-2.2085962	0.87179438	0.63341363	-2.1352494	-2.396739	2.42733699	2.19722651	1.24953226	0.80055288	1.06323928	0.28458624	-0.0243192	0.39540757	1.21219792
C_17	-3.9620448	-2.3607605	-2.5567764	-2.3358521	-3.1153084	-3.4520053	-7.5089155	-6.1691411	-3.2240758	0.93487092	0.7873363	-1.7078275	-2.1080825	2.26925621	2.70067549	1.61397625	1.06337266	1.55959162	0.23100756	-0.7581064	0.50145168	0.65275148
C_18	-3.5153946	-2.5291081	-2.575864	-2.3268376	-2.9865329	-3.3263731	-7.4190904	-6.2884753	-2.5579553	1.14830432	0.84208328	-1.7308756	-2.0915694	2.26126889	2.42735958	1.61911832	1.01462578	1.40212747	0.21590713	-0.1168076	0.59194921	1.24813634
C_19	-3.9380648	-2.579026	-2.5858194	-2.3503716	-3.0533206	-3.4015048	-8.351932	-7.783948	-2.6912208	1.14416649	1.00317053	-1.3614048	-1.9472871	1.97306185	2.51241012	1.73077176	1.40614884	1.87222923	-0.0728468	-0.436949	0.39362399	1.07200528
C_2	-4.0696741	-2.4923444	-2.8665236	-2.6298174	-3.3266502	-3.6163615	-7.6341966	-7.3069837	-2.8017623	1.0173301	0.8385862	-1.7172992	-2.1668172	2.36463634	3.2298918	1.80314827	1.30079397	1.62323974	0.33084483	-0.4961748	0.80152762	1.04725821
C_20	-3.548735	-2.194405	-2.5070308	-2.8069424	-3.2262551	-3.5053145	-8.0638589	-5.5205086	-2.358596	1.21174894	1.03281499	-1.8660579	-2.2955379	2.37368896	2.24021339	1.13763135	1.14849615	1.34310768	0.57966346	-0.0654861	0.57233145	0.79439128
C_21	-4.1630473	-3.0946571	-3.3713966	-1.981583	-2.5500973	-3.0835612	-6.7079022	-6.6908077	-2.5037244	1.28402251	1.25595974	-1.5876396	-1.3446692	2.30035155	2.94556666	1.69021619	1.76393288	1.70101821	0.00304085	-0.3027022	0.70761541	1.13163698
C_22	-4.3552478	-2.9036899	-3.0785751	-2.2188047	-3.2056769	-3.4938891	-5.8828109	-7.4251846	-3.3339982	0.87003326	0.83664891	-1.7288169	-2.1598373	2.02898973	3.28071166	1.92894483	1.51039169	1.70965139	-0.1349102	-1.0092918	0.62225573	0.52190146
C_23	-3.8448596	-2.1844028	-2.437864	-2.3878335	-2.9216318	-3.1645115	-6.6322834	-6.3582814	-2.5430242	1.30337015	1.32093948	-1.3915145	-1.9186488	2.11817074	2.83303707	2.03335046	1.49259807	1.6883209	0.133069	-0.2297535	0.86146955	1.18016524
C_24	-3.720877	-2.7884399	-2.9875025	-2.7634077	-3.661127	-4.2162529	-7.7162509	-6.4970106	-2.6180274	1.33412388	1.33535978	-1.3422094	-2.2375369	2.14805998	3.31397784	2.16351131	2.03037594	2.05993858	-0.1113564	-0.4102359	0.75457615	0.83314141
C_25	-3.7775186	-1.8392751	-2.0033914	-3.8670879	-4.5191133	-4.8053576	-7.7671883	-8.1185862	-2.8880406	1.39283298	1.45243479	-1.1718632	-3.614109	2.13771308	3.0872655	2.04652043	1.7742448	1.94755491	0.24631426	-0.3419628	1.03193715	0.90821717
C_26	-3.7368417	-2.4449138	-2.7333943	-3.1545571	-3.587996	-3.8760954	-6.7449964	-6.7160089	-2.5216036	1.44629549	1.49849492	-1.1633262	-2.5967395	2.10255368	2.96946121	1.95742339	1.85437834	1.93981515	0.15475631	-0.2199021	0.87350032	1.22127905
C_27	-4.228955	-2.0973063	-2.173119	-3.2292322	-4.0347248	-4.2151789	-7.0335772	-7.1912061	-2.6217895	1.44005587	1.48500669	-1.0031925	-2.6876096	2.20027826	3.18861178	2.06090328	1.98643464	2.16397972	0.2835937	-0.4708095	1.11420553	0.91600688
C_28	-4.2294812	-1.9677028	-2.2766773	-2.3727477	-2.8714625	-3.2376162	-7.0042734	-6.9695878	-3.1076626	1.26787045	1.30717985	-1.1748088	-2.1930459	1.92863032	2.43096245	1.82084043	1.40100192	1.81661363	-0.0663769	-0.4775202	0.48644653	0.94449003
C_29	-3.8446456	-2.3605931	-2.6135442	-2.6237579	-3.3737233	-3.6445099	-6.7468519	-7.5941497	-3.488412	0.94775641	0.84663928	-1.6039881	-2.627089	1.89944732	2.64364702	1.98834742	1.05112881	1.66621616	-0.2391345	-0.7091088	0.29774962	0.59070684
C_3	-3.7286622	-3.5136458	-3.9310513	-2.3624354	-3.0329429	-3.4180659	-7.7651128	-5.7282309	-2.6574012	1.0362187	0.88755781	-1.8856278	-1.7388443	2.20028483	2.58472053	1.59997451	1.29735576	1.44880036	-0.0487634	-0.3628391	0.41845909	1.02118472
C_30	-3.9725697	-2.0784531	-2.295463	-3.1079741	-3.6343853	-3.8909344	-7.1047977	-6.5170111	-2.4425386	1.38160115	1.2742018	-1.4623589	-2.1177723	2.20784876	2.91419138	1.61078721	1.86781831	1.77129294	0.4576887	-0.1003696	1.0887822	1.019101
C_31	-4.0511724	-2.318201	-2.6012049	-1.597754	-2.2256748	-2.4655451	-7.702696	-6.8272273	-2.2663574	1.82426852	1.78230196	-0.8968997	-0.6890804	2.32102489	3.22088836	1.95713059	2.22557844	2.12030788	0.29718387	-0.203531	1.05273686	1.2300534
C_32	-3.510337	-2.1797026	-2.2993167	-3.3004387	-3.8172079	-3.8914305	-8.311074	-5.9131787	-2.1965072	1.31433854	1.27433186	-1.7611372	-2.4882253	2.51045611	2.77510554	1.43665605	1.69524089	1.41246919	0.31414817	-0.053671	0.74379707	1.08687396
C_33	-3.6669466	-2.1301721	-2.4099466	-2.913344	-3.6132831	-4.0000687	-8.174456	-8.3142179	-3.0305067	0.98397764	0.92163424	-1.7205571	-2.674974	2.03094934	2.87074361	1.86323367	1.10877921	1.4358999	0.00593797	-0.2525576	0.59661069	0.59040539
C_34	-4.217242	-2.1498738	-2.2404339	-2.3263627	-2.9719681	-3.3497414	-6.1366254	-6.9462476	-3.1453533	1.17305645	1.17347319	-1.4971803	-2.1150204	2.09812989	3.05812603	1.8592087	1.51264829	1.63996234	0.1259448	-0.4089594	0.82866257	0.56356462
C_35	-3.6275939	-1.6778973	-1.9003641	-3.9228352	-4.5099831	-4.8871177	-8.5704261	-6.6166108	-2.7743683	1.24388411	1.23789266	-1.4444728	-3.6367518	1.98053549	2.66359056	1.89935175	1.44334235	1.69473915	-0.0033534	-0.0217127	0.5783048	0.89515064
C_36	-3.7916616	-2.2402776	-2.4321416	-2.4150761	-3.0501844	-3.2505036	-7.8365261	-6.1931866	-2.58787	0.95157302	0.97698418	-1.8260199	-2.2232722	1.99012136	2.20870044	1.41778825	1.17930006	1.1043469	-0.1269084	0.01686442	0.30226017	0.96514057
C_37	-3.5128715	-2.150561	-2.4424967	-2.6034419	-2.8926376	-3.1693755	-7.0093791	-5.9589161	-2.42415	1.2165633	1.25920154	-1.5681275	-2.0079311	2.00454395	2.5120359	1.52944766	1.34052365	1.35590239	0.06059318	-0.0295297	0.58734159	1.03184402
C_38	-4.0643105	-2.2488886	-2.4822768	-2.910239	-3.808804	-4.2383488	-8.5435394	-6.5740988	-2.6248696	1.15057393	1.05760917	-1.8350484	-2.4473396	2.42058016	3.49952447	2.05697527	1.69757743	1.71625801	-0.1395709	-0.4847112	0.71185398	0.90390657
C_39	-4.1559585	-2.4281118	-2.6909767	-1.9149118	-2.3939809	-2.8059666	-7.3200261	-7.4070375	-1.7654529	1.87517523	1.82541567	-0.8704118	-1.0241453	2.22532709	3.21807204	1.77215927	2.26116204	1.98779631	0.25159771	0.36818108	1.0536623	1.6600202
C_4	-3.1404364	-2.3186561	-2.4321021	-2.4421509	-3.1449922	-3.4643215	-6.7312546	-5.666165	-2.5893416	1.02346723	0.88191298	-1.8582407	-2.1822479	2.31690032	2.5941633	1.35115443	1.07335986	1.20593168	0.11388849	-0.2246004	0.44768475	0.94024456
C_40	-3.4839873	-2.1670729	-2.4519383	-2.476052	-2.9993848	-3.3492183	-7.8265551	-6.2266866	-2.0316559	1.20522238	1.11509631	-2.0919817	-2.1230901	2.36484845	2.73461778	1.13717814	1.36727838	0.93553198	0.53356094	0.2330222	0.9985149	1.30277148
C_5	-3.5463768	-1.8530796	-2.1099399	-2.9076716	-3.40804	-3.6234535	-6.4932272	-6.1283293	-2.3009348	1.46443508	1.44771911	-1.1401958	-2.1706146	2.27003018	2.79458633	1.91990943	1.75681065	2.0673787	0.29162417	-0.1571487	0.89642176	1.03638619
C_6	-3.2676499	-2.460583	-2.6372611	-2.3584846	-2.7691859	-3.0941425	-7.8756161	-6.0193182	-2.3140119	1.249946	1.15612853	-1.4875927	-1.7023302	2.27172228	2.59854018	1.51198634	1.3739411	1.61573208	0.27089591	-0.1196263	0.73211952	1.2489441
C_7	-3.5105249	-2.6024123	-2.8232774	-2.5129253	-3.1721153	-3.5464569	-7.7455368	-6.711463	-2.6454798	1.06561251	0.86626749	-1.7421128	-2.4590074	2.12147965	2.31262676	1.5872535	1.11643778	1.52378864	-0.2322368	-0.0662565	0.18304941	1.04521262
C_8	-2.8913123	-3.0169474	-3.4605295	-2.3014202	-3.3606367	-3.7843755	-6.9665873	-5.9369679	-2.8234526	0.79393655	0.39543382	-2.2115614	-2.2783022	2.4338223	3.04005081	1.73169612	0.95717733	1.29781035	0.02379195	-0.5125162	0.36320609	0.95755739
C_9	-3.4207066	-3.0894322	-3.5242767	-2.2455316	-2.6923013	-3.1206021	-6.7369108	-6.1615467	-2.265653	1.39614814	1.06147545	-1.5971985	-1.2782714	2.21257837	2.5630468	1.45290114	1.49301503	1.63452159	0.27866196	-0.0790995	0.80583273	1.16375873

Table 8.114: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls.

	PC(33:2)	PC(33:3)	PC(33:4)	PC(33:4)(2)	PC(34:0)	PC(34:0)(2)	PC(34:1)	PC(34:2)	PC(34:3)	PC(34:4)	PC(34:4)(2)	PC(34:5)	PC(35:0)	PC(35:0)(2)	PC(35:0)(3)	PC(35:1)	PC(35:1)(2)	PC(35:2)	PC(35:2)(2)	PC(35:3)	PC(35:4)	PC(35:4)(2)
C_1	0.09708389	-1.7257274	-3.4819501	-2.5226094	1.85938616	1.57638702	4.47478549	4.56436816	2.16817379	0.2652218	0.37979237	-1.0327525	-1.0649236	-0.7140795	-2.6930394	1.46953332	0.01363511	1.32793249	0.71618518	-1.5197852	1.24484612	-0.8444258
C_10	0.10324661	-1.3018584	-2.8049782	-2.1587515	1.84100083	1.3239342	4.43488095	4.50100328	2.22910038	0.32483774	0.21105519	-0.6272665	-1.2112496	-0.8823056	-2.4280825	1.24567543	0.28661408	1.09489581	0.8921424	-1.3248383	1.68607478	-0.2506868
C_11	0.42422157	-0.9940194	-2.77666	-1.8480643	2.0823977	1.08616026	4.66867168	4.88602888	2.22235045	0.1366607	0.3268317	-1.7304904	-0.4636532	-1.1681749	-2.693326	1.6057981	0.30709133	1.44933051	1.05680928	-1.0013546	1.92493447	-0.3907683
C_12	-0.021454	-1.8536811	-2.7787643	-2.7236859	1.9123167	1.6980175	4.51787826	4.60983888	2.34000381	0.08600105	0.90584635	-1.9448393	-0.9435473	-0.4892513	-2.0088966	1.64335683	-0.4964879	1.30110372	0.85236226	-1.5980734	1.6155502	-1.3024868
C_13	0.14699235	-1.9464437	-3.2757522	-2.744381	1.78830123	0.80747483	4.4290644	4.62602722	2.40618694	0.28254406	0.54535619	-1.7662743	-0.8943609	-1.4354031	-2.8107248	1.38494576	0.343812	1.19326325	1.12912177	-1.8428404	2.04520407	-0.9970049
C_14	-0.3210644	-0.5475969	-1.4102764	-1.4991557	0.9907749	1.06941484	3.74202422	3.31025519	2.80823887	0.65651737	1.94743924	-2.6630394	-0.1606905	-0.5488353	-2.2853263	1.83538448	0.24549485	0.31045325	1.0136324	-1.0399126	1.11767846	-1.5042051
C_15	0.20761092	-1.0868767	-3.2679365	-1.9701154	1.97605621	1.09591376	4.56838457	4.39562693	2.29459284	0.4501627	-0.1584121	-1.5890855	-0.919302	-0.8555939	-2.3418056	1.71036035	0.47184258	1.13761383	1.00302652	-1.2688145	1.70943855	-0.416655
C_16	0.55198606	-1.9363538	-3.5312015	-2.7533873	1.87435038	1.64384783	4.52141279	4.98126539	2.2514161	-0.1166331	-0.0261627	-2.4045954	-1.1578329	-0.682936	-2.3896836	1.44648279	0.09095864	1.75349516	0.98596664	-1.5980357	1.56499475	-1.1913139
C_17	-0.0293977	-1.3733998	-3.2054648	-2.2921286	1.9651903	1.43098128	4.55171107	4.34964356	2.17910356	0.30139114	0.02589576	-1.0285572	-1.1258312	-0.7035453	-2.7178317	1.43213925	-0.0409601	1.02335889	0.5275771	-1.2106767	1.22086761	-0.5046936
C_18	0.77720527	-1.4386004	-2.8786538	-2.2230218	1.924392	1.26289771	4.5605498	4.86932741	2.45197983	0.23281816	0.63506804	-1.9330797	-0.9006628	-0.7663532	-2.3864231	1.53749009	0.3222525	1.71104998	1.20189578	-1.1462133	1.46663067	-0.5841156
C_19	0.50725592	-1.1644527	-2.7987445	-1.9507956	1.81995357	0.99240432	4.44164209	4.6753748	2.430777	0.23657446	0.51640671	-1.7263837	-1.0953443	-0.9568968	-2.3922921	1.37917147	0.34270809	1.39035405	1.0067624	-0.9718596	1.90883497	-0.2405511
C_2	0.30981503	-1.6681326	-3.4043065	-2.5466002	2.37203387	1.35059816	4.94440645	4.68100137	2.54001351	0.52572241	0.15018268	-1.1370324	-0.7495118	-0.8323755	-2.8960193	1.68868299	0.12591288	1.33623549	0.89382806	-1.5837786	1.74536104	-0.9297032
C_20	0.12732715	-1.6837363	-2.9824545	-2.3723739	1.55735788	1.48429808	4.20185125	4.52798777	2.15716888	-0.063733	0.80124095	-1.5629029	-0.803102	-0.5424206	-2.3863443	1.69046141	-0.0151948	1.55438808	0.97030769	-1.2664766	1.33654616	-1.1315194
C_21	-0.0897619	-0.7309388	-2.848989	-1.5771876	2.14619665	1.20228989	4.7529017	4.77045361	2.22209693	-0.1962337	-0.2019893	-1.6758879	-0.8988282	-0.9688857	-2.9479057	1.65227012	0.49619583	1.22851763	1.20807527	-1.1031148	2.26433634	-0.0597667
C_22	0.02552329	-1.1461056	-3.3006692	-1.8938269	2.3016609	1.17947481	4.90768331	4.61809514	2.60564614	0.56371598	-0.5297481	-1.1927897	-0.995378	-0.9311037	-3.0994424	1.58081407	0.0702372	1.05902739	0.58797068	-1.4760212	1.33016109	-0.3277475
C_23	0.9611675	-1.1221912	-3.0750737	-2.007204	2.07408827	1.18839177	4.70222653	4.99394062	2.71126921	0.44416848	-0.1677628	-1.3328796	-0.5995621	-1.0023971	-2.7638034	1.78426524	0.53386511	1.78961444	1.23276273	-1.188314	1.68271383	-0.3260477
C_24	0.66924662	-1.48471	-3.3203782	-2.3981309	2.04238432	0.89783168	4.65169859	4.83973515	2.66387332	0.33605789	-0.3161473	-1.6905707	-0.8885383	-1.1876184	-2.5578589	1.55600199	0.43296196	1.25539783	1.00994951	-1.5139489	1.70139132	-0.6325727
C_25	0.89719171	-2.8372544	-3.5218727	-3.4879535	2.0598401	1.15627463	4.72923038	4.89485468	2.44924019	0.30313893	-0.463046	-1.0518498	-0.6830861	-0.7285347	-2.5701247	1.98463192	0.38215666	1.75906252	1.12671484	-2.5156908	1.48564735	-1.3132717
C_26	0.82386885	-1.8776883	-3.2660214	-2.7178082	1.95340739	0.93962521	4.61036957	4.80697381	2.43352084	0.11685347	-0.3032762	-1.6983507	-0.8956717	-0.86582	-2.8077071	1.79873843	0.64042603	1.74045715	1.25058274	-1.8796136	1.68718017	-1.1118363
C_27	0.80857883	-2.1419757	-3.5195473	-2.9546283	2.14087905	1.04506581	4.7670483	4.9486966	2.55684067	0.34632784	0.17193423	-1.8977788	-0.845955	-0.8074935	-2.6484304	1.89113454	0.3446113	1.75546716	1.13345549	-2.2364102	1.87899428	-1.2410719
C_28	0.65812809	-1.2733336	-3.3844918	-2.1791647	1.62692896	1.20352612	4.30107139	4.63631849	2.12222623	-0.1960785	-0.590448	-1.0862654	-0.9467457	-0.7314185	-2.2941074	1.51525358	0.4680401	1.69651901	0.97786983	-0.9642988	0.86715006	-0.4658952
C_29	0.66427274	-1.3438528	-3.4829344	-2.3161414	1.85767171	1.24914365	4.48449738	4.63476719	2.56845082	0.58407395	-0.7626008	-1.041731	-1.3983847	-0.8660944	-2.6476086	1.24332886	0.34297941	1.31698971	0.57571165	-1.0243469	1.08239844	-0.3831928
C_3	0.34726508	-1.1256183	-2.9156901	-1.9545957	1.88440144	1.27462212	4.54522808	4.83789031	2.37749664	0.11836497	0.16795203	-1.6287365	-1.1255638	-0.9189227	-2.6734097	1.32442906	0.25797532	1.3993407	0.98389954	-0.9119457	1.63509697	-0.4596726
C_30	0.41896718	-1.6609741	-2.933878	-2.4150566	2.00284525	1.04833619	4.59741643	4.59126064	2.24635187	0.00526555	0.28754187	-1.8208329	-1.1575463	-0.3469936	-2.6592096	1.83312022	0.49208417	1.49974679	1.25608663	-1.6738087	2.018554	-0.9615245
C_31	0.3234088	-0.3062789	-2.0241174	-1.219181	1.98452428	0.92223884	4.60977959	4.55729993	2.28003083	0.12118997	0.41077054	-1.5229555	-1.1131279	-0.4695295	-2.8418506	1.87187997	0.75375587	1.48321503	1.33536024	-1.1776664	2.36685666	0.14504047
C_32	-0.0340349	-1.8299053	-3.5269211	-2.6439555	1.91932357	1.39649601	4.55781189	4.68720656	2.00682962	-0.3135454	-0.2267993	-1.5319099	-0.8704576	-0.7922496	-2.4255257	1.70112148	0.4018066	1.2457644	1.25254892	-1.904414	1.9250953	-0.8335452
C_33	0.50364267	-1.6015655	-3.9441374	-2.487628	2.03383526	1.38927787	4.67450835	4.81376106	2.49491187	0.42328281	-0.7310976	-1.1803635	-0.8822372	-0.6181871	-2.2440577	1.6341211	0.51005548	1.43714357	0.88687483	-1.2092114	0.97068711	-0.9753623
C_34	0.44253128	-0.9010193	-3.2802756	-1.7807224	2.06332354	1.14853301	4.6615239	4.46528349	2.47639474	0.6370718	-0.6859016	-1.2045273	-0.9348074	-0.7887453	-2.3491096	1.69057793	0.50646192	1.08223061	0.77067428	-0.8182745	1.38369145	-0.3864157
C_35	0.81721399	-2.63421	-4.4317103	-3.5531463	1.73444418	1.24996363	4.39310046	4.81279734	2.2685566	-0.0644624	-0.9264907	-2.0018021	-1.0031666	-0.6937876	-1.9857882	1.62533921	0.70990665	1.72339977	1.14338291	-2.1630878	1.17145715	-1.6076041
C_36	0.40002226	-1.0241051	-3.4631575	-1.8515481	1.64504889	1.43192051	4.34628338	4.93262284	2.06267815	-0.322215	-0.9891067	-2.0494172	-1.1183879	-0.6134317	-2.2631928	1.41754403	0.57601896	1.63464154	1.34252286	-0.9542301	1.53036699	-0.5647505
C_37	0.69312493	-1.2016216	-3.441292	-2.0219162	1.71154796	1.18135213	4.36576482	4.65925762	2.15964774	-0.3684815	-1.1283091	-1.5713555	-0.9869875	-0.8110046	-2.1209597	1.58937048	0.64840649	1.65272001	1.13439539	-1.1166376	1.39805077	-0.5683507
C_38	0.13921058	-1.6277333	-3.4952873	-2.5162654	2.37958034	1.29499619	4.99594597	4.96186927	2.69288347	0.47770651	-0.8985802	-1.0246156	-1.0926366	-1.2063855	-2.8093894	1.63939325	0.29123439	1.04249962	1.0157251	-1.5958425	1.73334621	-0.7938219
C_39	0.36379951	-0.7237903	-2.6772391	-1.5899263	1.70129532	0.67976431	4.36137303	4.42956933	1.86474	-0.5607708	-0.1902613	-2.2072856	-0.8536222	-0.8901722	-2.4340726	1.95801963	1.00202367	1.59552924	1.52740563	-1.2904432	2.77057185	0.11403435
C_4	0.11862706	-1.2061082	-3.019292	-2.0632644	1.82894333	1.28101127	4.45608484	4.68918076	2.16338099	-0.0456955	0.12032561	-2.019944	-1.0817775	-0.8181972	-2.5234506	1.37783813	0.29263154	1.17495257	1.06200133	-1.0809657	1.69565552	-0.3868722
C_40	0.1926347	-1.4878769	-3.7868511	-2.374087	2.21989426	1.43188588	4.82325438	4.79120313	2.00557457	-0.4687863	-0.6695245	-2.3924173	-0.6333345	-0.5675395	-2.3605062	1.96413165	0.55864024	1.4667512	1.34092253	-1.5037334	1.71096277	-1.2413034
C_5	0.68957099	-1.595182	-2.7065386	-2.4485677	1.77722746	1.28595196	4.42437105	4.57294748	2.38128496	0.14108062	0.54764656	-1.5462908	-0.9068035	-0.6875949	-2.6465993	1.66893322	0.43666654	1.63829003	1.19043834	-1.8669959	1.98413167	-0.6862425
C_6	0.57236416	-1.0877712	-2.6498695	-1.9121396	1.9164727	1.17701724	4.52443173	4.6630399	2.30321113	-0.1153537	0.3102022	-2.0635175	-0.7905183	-0.849829	-2.41535	1.56570579	0.47231544	1.65742204	1.16402132	-1.3355101	1.93244583	-0.4055972
C_7	0.44373378	-1.3769209	-3.3282033	-2.2064816	1.93729631	1.47677848	4.58785785	4.90451381	2.2536728	-0.1047528	0.17337613	-2.1406543	-1.1383378	-0.8059498	-2.189916	1.38234208	0.39116437	1.47727858	1.15297824	-1.114194	1.31156864	-0.469975
C_8	-0.0565347	-1.425716	-3.2587226	-2.1980236	2.19105351	1.27397364	4.77852126	4.81342484	2.45229722	0.66409237	0.20976915	-0.9831129	-1.2625271	-1.0060116	-2.9047086	1.29781465	0.1725971	0.98449655	0.80210101	-1.5715971	1.38148086	-0.7041737
C_9	0.1241022	-0.8519803	-2.1917266	-1.7104022	1.88653849	1.16412093	4.48188815	4.62650124	2.42153023	0.1119905	0.98939986	-1.9358084	-1.0970547	-0.603079	-2.6462768	1.60306776	0.43166908	1.50824032	1.23645901	-1.1620566	2.17398675	-0.121411

Table 8.115: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer controls.

	PC(35:5)	PC(35:5)(d2)	PC(35:5)(d3)	PC(35:6)	PC(35:6)(d2)	PC(36:0)	PC(36:0)_1	PC(36:1)	PC(36:2)	PC(36:3)	PC(36:4)	PC(36:4)(d2)	PC(36:5)	PC(36:6)	PC(37:1)	PC(37:2)	PC(37:2)(d2)	PC(37:3)	PC(37:3)(d2)	PC(37:4)	PC(37:4)(d2)	PC(37:5)
C_1	0.18563186	-0.3150766	-1.6151094	-1.664262	-0.9017333	1.66812472	0.22919827	4.02659917	4.66582439	3.64061124	1.97492789	3.58077435	2.93963488	0.00327973	2.46831444	1.44595032	1.48829607	1.8496284	1.33721671	0.80747032	1.53153733	1.47035139
C_10	-0.4132545	0.61926305	-1.2280991	-1.6319553	-1.1092573	1.46216602	-0.0135967	3.81112704	4.44255435	3.71380541	2.21579961	3.8215192	3.79786815	0.3427813	2.57666414	1.58549551	1.67166618	1.12305619	1.46903535	0.99542096	1.53066511	1.9036037
C_11	0.23721036	-0.1917644	-1.3485441	-1.487329	-1.3754477	1.36965844	-0.0790811	3.71021374	4.49450086	3.97977116	1.78331668	4.05397348	2.45596422	-0.5525514	2.58460283	1.57243829	1.61297527	1.64545265	1.67547694	1.1927218	1.95285367	1.98528498
C_12	0.38439565	-0.5007913	-2.182643	-1.3400993	-0.6743134	1.38323086	-0.023401	3.70712487	4.61972058	3.73123044	1.07839929	3.89619519	2.19910095	-0.7920648	1.83837043	1.13269755	0.77118148	2.56855846	1.41331179	1.0418609	1.86465214	1.62563999
C_13	0.79543212	-0.6674625	-1.82048	-1.5747855	-1.6287612	1.326942	-0.0512604	3.85001834	4.56072667	3.96007109	2.06081345	3.89200897	2.2926078	-0.6813195	2.8426819	1.71875493	1.86850737	1.42927557	1.66364428	1.05682013	1.98191473	2.20986454
C_14	1.71007667	-0.7912372	-1.360031	-0.5116524	-0.9119289	1.68053747	0.1055089	3.91273762	3.51872431	2.82715174	-0.096287	2.28790191	0.54130316	-1.4233485	3.62102635	0.84640288	2.46279929	2.58455557	1.48302357	0.24373344	1.6710453	0.88055149
C_15	0.39750923	-0.6210737	-1.497625	-1.7257271	-1.35986	1.46693012	-0.0149638	3.8312298	4.24386607	3.82206568	1.78365134	3.96390403	2.76309712	-0.1909974	2.79597162	1.61662206	1.83173774	1.97677865	1.64704928	1.01883329	2.07603471	1.73601813
C_16	0.47974889	-1.3565683	-2.2279235	-1.8289848	-0.8322696	1.58711493	0.18967786	4.05811765	5.04634453	4.09862143	2.53055927	3.75603376	2.00971439	-0.9622935	2.27318631	1.40143679	1.31301755	1.87223768	1.5669147	1.2257345	1.91660417	1.97274662
C_17	0.38101192	-0.1252366	-1.371483	-1.6483235	-1.0707639	1.71787299	0.24651099	4.0495692	4.47056608	3.57911254	1.81944025	3.74625707	3.37271109	0.26037673	2.35230849	1.43680812	1.34295941	2.20935636	1.35989445	0.80752926	1.50870861	1.49884128
C_18	-0.2682933	-1.2343382	-1.5433378	-1.5807201	-1.1817189	1.53211906	0.07186112	3.92163272	4.82290101	3.94598765	2.47466462	3.37655466	1.89436998	-0.5812343	2.5843562	1.57039957	1.66886188	1.70564165	1.6105379	0.99432373	1.80974141	1.86527767
C_19	-0.4126894	-0.253629	-1.1506734	-1.6188103	-1.4727578	1.46857663	0.02768798	3.87775027	4.63412783	3.9909283	2.11708654	3.89798381	2.77532056	-0.3114283	2.55677783	1.66562446	1.70137919	1.20164753	1.74786456	1.26064863	1.97128699	2.11567207
C_2	-0.0587608	-0.0467716	-1.8166055	-1.3156354	-1.2025019	1.75487558	0.36054452	4.13363538	4.6692062	4.04895745	2.08103961	4.22462136	3.40430362	0.31174729	2.22250871	1.43959587	1.27658067	2.53350464	1.65373486	1.38009359	1.90870054	1.78958625
C_20	0.40695293	0.17364982	-1.764195	-1.594178	-0.8664651	1.41028065	-0.1491397	3.6945603	4.55132354	3.42757679	1.55065319	3.25741903	2.84933589	-0.4107066	2.58692862	1.51491758	1.59742266	1.88364824	1.44966367	0.90428256	1.54401898	1.50379847
C_21	0.7334991	0.12590957	-1.3691215	-1.5510292	-1.3453157	1.66271331	0.24698343	4.09364612	4.63931021	3.95773335	1.86940597	3.98870504	2.69449525	-0.6425945	2.9824615	1.72297782	1.98030171	1.47494135	1.66710354	1.0108676	1.94991914	2.1702636
C_22	0.21478262	-0.5737709	-1.3288732	-1.4976102	-1.4267847	2.04338466	0.6965607	4.48949638	4.66839191	3.96395089	2.04732458	3.99599238	3.23181716	0.3074334	2.45213376	1.43773898	1.50114621	2.2840587	1.3944328	0.83990233	1.37523072	1.47673029
C_23	-0.1156402	-0.3068925	-1.395668	-1.6175983	-1.2901051	1.58732967	0.16138992	4.02714603	4.84454423	4.27003959	2.69274542	3.70220921	2.91768886	0.20072496	2.88503648	1.86090667	1.88216477	1.44644532	1.91039747	1.2196527	1.79374995	1.96229752
C_24	0.47352742	-0.7067724	-1.8600775	-1.633242	-1.6402861	1.74638252	0.3127434	4.12923232	4.69651821	4.27105614	2.37455855	3.6616762	2.56286889	-0.3857952	3.2922184	1.67008663	2.28273392	1.62018322	1.7750955	0.97169077	1.61211525	1.86034724
C_25	0.58186673	-0.0657704	-3.1132279	-1.6169014	-1.4347642	1.67462529	0.29393632	4.14460328	4.79838025	4.13153559	2.31576026	3.99030325	3.60964166	0.36337246	3.13852574	1.94386003	2.11103844	1.82929342	1.8661466	1.31203049	1.31203049	1.81408198
C_26	0.50582691	-0.3936745	-1.9793093	-1.7993704	-1.5927254	1.44499085	0.0754212	3.97721084	4.66645489	4.13994893	2.23363623	3.75798632	2.83025865	-0.1172274	3.07285552	1.91891144	2.12259882	1.53938528	1.96213627	1.27896061	1.84860752	1.9704206
C_27	0.26856819	-0.7818339	-2.0833409	-1.5103678	-1.4848254	1.67201971	0.28602555	4.16871509	4.81967333	4.2156751	1.87918226	4.18824423	2.67168169	-0.66657	2.99876795	1.9963423	2.06623423	1.64393688	2.01136756	1.47807567	1.93491186	1.94636944
C_28	0.28488736	0.19159332	-1.3380909	-2.000485	-1.2903853	1.6368788	0.14777437	3.99919888	4.67081248	3.55492886	2.57556597	3.24575407	3.69374453	0.34309457	2.90463244	1.78682092	1.96334781	1.0225118	1.43455885	0.88302359	1.134762	1.58079836
C_29	0.13775359	-0.6319457	-1.3818777	-1.9865111	-1.2741686	1.67826129	0.22454031	4.04615298	4.63340398	3.75109055	2.29334288	3.75777992	3.41898485	0.46170882	2.63302708	1.46098073	1.66741634	1.55708181	1.31496449	0.93979406	1.41607929	1.52935426
C_3	0.09629323	-0.1385223	-1.428951	-1.6411591	-1.2353899	1.53276521	0.14350412	3.98837824	4.81695839	3.84692131	2.26468798	3.75130282	2.72530805	-0.3535565	2.60007579	1.37507332	1.62196762	1.66460404	1.42799664	0.92020442	1.72906163	1.86728483
C_30	0.53283437	-0.3155163	-1.8212134	-1.4642213	-1.4483689	1.68087561	0.2266718	4.03385093	4.54810944	4.07258612	1.94990879	3.73383912	2.46203458	-0.8089784	3.23732453	1.76775605	2.22377447	1.56336395	1.93671859	1.29667031	2.03271386	2.0146711
C_31	0.91776349	-0.2034572	-0.8935831	-1.3246095	-1.470379	1.5891383	0.13456889	3.95642571	4.50017784	3.91800403	1.55081877	4.0084659	2.45391062	-0.5940701	3.25344946	1.93550566	2.2203098	1.22835363	1.91810584	1.54917009	1.96274582	2.50199674
C_32	0.81510187	0.4689039	-2.4663708	-1.6840914	-1.1098037	1.57722887	0.09716707	3.95939593	4.52084619	3.66021935	1.85162415	3.61877162	2.74751436	-0.519992	3.08949694	1.64099737	2.02318249	1.64931362	1.57548103	0.79777985	1.95508948	2.00947562
C_33	0.14542031	-0.6502468	-1.894223	-1.7464912	-1.1391108	1.88595728	0.44110989	4.26497035	4.83863625	3.95441089	2.42552749	3.60022387	3.04918788	0.15637621	2.73158935	1.57993369	1.7717266	2.23286805	1.59796175	0.77031544	1.71393118	1.21789793
C_34	0.28550753	-0.7876746	-1.4555127	-1.7482707	-1.3729312	1.89804465	0.46724748	4.24879371	4.45991679	3.81377272	1.92567208	3.9391867	3.12082834	0.03618947	2.92117504	1.49380791	1.88698189	1.99546105	1.48686556	0.92971648	1.80025553	1.4607105
C_35	0.62942614	-1.0773254	-2.9372251	-2.0710568	-1.2524024	1.65974788	0.19569102	4.07901206	4.82289351	3.76594795	2.50920305	3.28292411	2.34967605	-0.4366756	2.95020847	1.6974557	1.98374613	1.56503921	1.58098218	0.75697113	1.76414017	1.56283852
C_36	0.6376588	-0.6529171	-1.5852204	-2.0580201	-1.0602551	1.74391659	0.29081735	4.16895517	5.01506096	3.87132477	2.84168941	3.40703493	2.13088771	-0.6365645	2.89680666	1.45221106	1.98547833	1.25468895	1.52555515	0.81610184	1.84042854	1.8220812
C_37	0.33766452	0.11434537	-1.6225931	-2.0845438	-1.3295566	1.53293692	0.05705509	3.94324522	4.6457812	3.62540579	2.19965276	3.21754837	3.12956515	0.01799233	2.89380203	1.50764488	1.95770171	1.41018434	1.59038618	0.83835843	1.80660922	1.78970446
C_38	0.72468456	-0.1051369	-1.9842784	-1.4963121	-1.2700999	1.825813	0.43628655	4.28297955	4.70171422	4.14279809	2.45689236	3.9786029	3.42668061	0.30368866	3.2800489	1.75131995	2.19572451	2.49329995	1.63290672	0.66244983	1.68302148	1.73710807
C_39	1.15236146	-0.1139889	-1.1595223	-1.7599857	-1.7296612	1.35044594	-0.0006856	3.93366597	4.4572517	3.77745902	1.23271116	3.64171458	1.7567781	-1.0240685	3.49884008	2.10819397	2.466279	1.22594887	2.13029198	1.67885221	2.34295181	2.86846962
C_4	0.47365422	-0.3244472	-1.4965678	-1.7599924	-1.1736207	1.5901643	0.13159525	3.95866152	4.60342069	3.83201395	2.24232658	3.4558892	2.08789575	-0.8194162	2.74296789	1.45508743	1.74706752	1.77413957	1.49067915	0.88559149	1.71336316	1.86668163
C_40	0.68357514	-0.9019427	-2.2858519	-1.5989837	-1.1127313	1.85858396	0.39665049	4.21777201	4.71642322	3.9538144	1.83935792	3.58008776	1.99499393	-0.9322228	2.67498374	1.41930411	1.65779215	2.2342394	1.67893938	1.04124133	2.0911265	1.82194499
C_5	-0.1157204	0.18954799	-1.59197	-1.5011109	-1.1388938	1.39924885	-0.0903367	3.76474728	4.49805255	3.81273139	1.96572444	3.64362345	2.92886067	-0.341725	2.81894749	1.92554365	1.87564691	1.12703708	1.85038558	1.24274734	2.01737368	2.11349973
C_6	0.11162297	-0.1747598	-1.3520538	-1.490152	-1.2233727	1.389629	-0.0732924	3.77009779	4.58022875	3.83873555	2.0280134	3.75620179	2.56923012	-0.5910696	2.54961442	1.52774501	1.62145385	1.50604888	1.66366532	1.40115222	1.96514458	2.23067674
C_7	-0.0192828	-0.7573542	-1.4010524	-1.7109529	-0.9562132	1.75705334	0.3127213	4.16588163	5.00919859	3.87383268	2.63116507	3.47732754	2.46393849	-0.7161725	2.60753544	1.71382442	1.72581358	1.31453651	1.50705756	0.72856622	1.74585986	1.65075138
C_8	-0.5917897	-0.4466046	-1.5431068	-1.4971217	-1.2142793	1.51901889	0.18583815	3.97528824	4.6597521	3.85581918	2.05967195	3.89735649	3.11053347	0.06727184	2.25861868	1.2351597	1.34946433	2.38002195	1.3159547	0.55067988	1.67125887	1.56772845
C_9	-0.0714536	-0.2736734	-1.0295053	-1.3173596	-1.1368441	1.41441612	0.01994405	3.86703987	4.58896567	3.8383147	1.94910208	3.69438074	2.11692285	-0.9739514	2.70857195	1.7205654	1.75296142	1.40029656	1.80954772	1.30544575	1.9659428	2.17235449

Table 8.116: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls.

	PC(37:5)(2)	PC(38:0)	PC(38:1)	PC(38:2)	PC(38:3)	PC(38:4)	PC(38:5)	PC(38:6)	PC(39:0)	PC(39:0)(2)	PC(39:1)	PC(39:1)(2)	PC(39:2)	PC(39:3)	PC(39:4)	PC(39:4)(2)	PC(39:5)	PC(39:5)(2)	PC(40:0)	PC(40:0)(2)	PC(40:1)	PC(40:2)
C_1	1.30679607	-0.2400983	2.58004613	3.47004494	3.79674322	3.62653524	3.23856302	3.45132953	1.04514802	1.25422211	0.82272142	1.33318189	0.9926455	0.8348728	3.22714013	1.2070477	0.56917108	0.3875454	1.87866514	0.28055985	1.89190263	-0.4451046
C_10	1.06902597	-0.0718153	2.63187874	3.72230484	3.77247002	3.68267489	3.55548904	3.60980384	0.43392539	0.47088099	0.01474151	0.55959829	0.94621819	0.75924862	2.54745612	1.1044409	1.0518494	-0.7011242	1.4216579	-0.253721	1.22880132	-0.8159471
C_11	1.40665253	-0.2581958	2.66778617	3.66758624	3.819138	3.68828289	2.88834453	3.28205633	0.9369774	1.27890662	1.01856164	1.41048891	1.25733831	0.99527274	3.56560027	1.40527655	1.09174072	-0.731043	1.75327338	0.14523671	1.91989221	-0.834029
C_12	1.87582916	-0.3643358	2.31300805	2.83476001	4.00267303	3.4389683	3.0104919	3.12487914	1.36082678	2.25489739	2.13769925	2.50648892	-0.8178284	1.10024171	4.31903764	0.99389516	0.33157139	0.75192607	2.71820382	0.93603607	2.70034969	-0.3781808
C_13	0.88500469	-0.2636164	2.75793228	3.82908987	3.87470678	3.83699185	3.02447619	2.89176429	1.15281112	0.85775956	0.67076815	0.91184239	1.15118913	0.91093759	3.01831415	1.54356086	1.13010818	-0.6210241	1.25551688	0.09590669	1.34601239	-0.6152655
C_14	2.23954902	0.19040941	2.80482273	3.0768855	2.31204467	2.70855294	1.19360727	1.00063502	-0.6551994	1.8445923	1.72499917	1.92303464	0.85439751	1.58888521	3.9539126	1.43481803	0.53497516	1.33661306	1.9008199	0.88275329	1.76706145	0.74249848
C_15	1.20239828	-0.1801722	2.60111861	3.53106013	3.7800525	3.64576524	3.03610605	3.04951098	0.60209214	0.80038747	0.49182529	1.02023018	1.03865191	0.91801249	3.29814729	1.53376167	1.21734711	-0.6061826	1.39043171	-0.0954606	1.37570536	-1.0078358
C_16	1.28721876	-0.3907069	2.41532571	3.31625257	4.03625384	3.74035567	3.06602169	2.8646432	1.17522348	1.41567882	1.4593927	1.58788111	0.6158616	0.90058738	4.18020641	1.16283237	1.03121965	0.46792368	2.13419223	0.28569558	2.29981242	-0.8519514
C_17	1.50346997	-0.2958838	2.43590269	3.46316166	3.94787992	3.62543366	3.49534379	3.46584628	1.00496316	1.20033208	0.68707648	1.3052157	1.05338146	0.81890959	3.1229515	1.06814485	0.63047864	0.25174531	1.68775002	0.15259023	1.60547703	-0.8197403
C_18	1.27285517	-0.1943725	2.53634729	3.54108297	3.53340625	3.55477854	2.74445957	2.96202035	0.92546111	1.1217622	0.86244225	1.29792084	0.86887987	0.89494124	3.28048447	1.28565055	0.8571678	0.11445987	1.76632988	0.10962162	2.0172383	-0.5272414
C_19	1.11439027	-0.1566308	2.68781204	3.75012558	4.00690233	3.90674393	3.18075106	3.46370333	0.95883374	0.7379209	0.2328978	0.7649893	1.01674351	1.18199964	2.80600612	1.48237879	1.28954118	-0.6162416	1.46840085	0.11724421	1.54038154	-0.5515762
C_2	1.36765841	-0.3752621	2.41212253	3.4802104	4.31746632	3.91869591	3.52651036	3.68519933	1.27195199	1.44698256	0.87275727	1.59625314	0.94492892	0.90553427	3.25710325	1.29842057	0.97558167	-0.3797906	1.74704827	0.21647252	1.73762331	-0.8140042
C_20	1.28492374	-0.0936751	2.5210898	3.22761121	3.50230559	3.34316644	3.16540016	3.23615937	1.10926989	1.42726484	1.41299102	1.60539611	0.8090566	0.90212851	3.7841466	0.87816624	0.6464676	0.51367656	2.41856769	0.49763826	2.15379243	-0.2881864
C_21	1.29512072	-0.1225394	2.85451586	3.87690469	3.87269735	3.85203772	3.20292561	3.25819018	1.01827244	0.9378665	0.92773482	1.08379874	1.41558409	0.97091872	3.56806052	1.32662828	0.99093241	-0.6377221	1.31732098	-0.0720688	1.29629637	-1.1740358
C_22	1.3582489	-0.4537696	2.56275462	3.72415949	4.14058662	4.02823871	3.558987	3.47713073	1.15870693	1.0167898	0.67203604	1.09820018	1.09520347	0.82552014	3.28119251	1.06890592	0.61138006	0.15309909	1.41367679	-0.1388263	1.29324914	-1.0827777
C_23	0.92268329	-0.1027693	2.76048817	3.75685649	3.78875304	4.00399529	3.30484027	3.56761034	1.20073102	0.68932926	0.49980608	0.78452642	1.33622808	1.04793245	3.37221353	1.3043535	1.11852789	-1.0615355	1.381754	-0.0844692	1.3819086	-1.1166656
C_24	0.7789012	0.29409596	3.28129053	4.08567562	3.71169557	4.15489785	3.04470709	3.16631297	0.75176825	0.40572073	0.36759993	0.54494774	1.4316534	1.01203199	3.17566059	1.3013306	0.93551357	-0.8580495	1.16564421	-0.2393648	1.07772872	-1.0269865
C_25	0.74596714	0.0583529	2.96725076	3.78317282	4.04214496	4.00128281	3.5188626	3.58135551	1.10522101	0.80162	0.72859209	0.91588965	1.25813802	0.9252086	3.58991603	1.47880162	1.03294799	-0.816409	1.76938959	0.08687669	1.47808656	-1.2650648
C_26	0.80302477	-0.2510202	2.73795304	3.86043806	3.85771391	3.99018305	3.24283496	3.44505067	1.21662497	0.63236716	0.54839131	0.74888562	1.291829	1.08768861	3.4182479	1.28291195	1.16147495	-0.9677995	1.33621936	0.12909559	1.2189138	-1.2673645
C_27	0.79007706	-0.1454933	2.77649785	3.92260013	4.22186475	4.17243155	3.40786342	3.03711562	0.77256787	0.72090434	0.66136569	0.75880613	1.52674731	1.17670013	2.97051143	1.49635533	1.15552272	-0.7042649	1.17042806	-0.2140841	1.26924633	-1.0396677
C_28	0.83299776	0.16778097	3.00301815	3.78247456	3.58216457	3.48293378	3.5184457	3.59198337	1.1808014	0.34449586	0.17418239	0.29433093	1.26689593	0.92848567	3.21125339	0.90452895	1.05607351	-0.7294006	1.52282824	0.13207882	1.31221385	-0.6339494
C_29	1.0091753	0.08665121	2.96617917	3.82458937	4.06288006	3.92289143	3.40593559	3.52259181	1.0158771	0.46385449	-0.0831036	0.45669316	1.07489508	0.94992474	3.18502052	1.3454094	0.96900822	-0.7124818	1.55177879	0.05386491	1.60608771	-0.6962764
C_3	1.28712535	-0.2465508	2.64690024	3.60216339	3.8633209	3.6728417	3.15866283	3.43237564	1.1124784	1.05855969	0.84307065	1.15053208	0.94353374	0.86430729	3.45680954	1.10359371	1.12718366	-0.3331715	1.76852713	0.17223214	1.90187417	-0.6860337
C_30	0.97187297	0.02907668	2.82068124	3.69941606	3.71336676	3.83487293	3.10508294	3.04583698	0.92963887	1.03221061	0.88646467	1.14037019	1.24571495	1.00527649	3.06335913	1.38872758	1.10540145	-0.4899716	1.2407052	0.0267409	1.18583358	-0.7907063
C_31	1.12251113	-0.1821002	2.83394274	3.96641861	3.81824456	3.84481378	3.19031909	3.32138598	0.95125169	0.6001812	0.52419834	0.67090389	1.65467833	1.24716231	2.79614026	1.26508859	1.22815969	-1.0683255	0.79301472	0.04662644	0.69712404	-1.0410971
C_32	0.97293189	0.0811756	2.92792591	3.65606612	3.52661063	3.48265294	3.09144493	3.39380814	1.26092357	1.13834104	1.29552481	1.19256268	1.03284695	0.80357014	3.97418901	1.39312896	1.13850374	-0.5804014	1.5701407	0.31972167	1.31366922	-1.1978233
C_33	1.15290966	0.16695424	2.89982431	3.63147649	3.86261977	4.00972954	3.09637577	3.15931526	0.75101575	0.85177341	0.63648347	1.0443959	1.17824032	1.21566287	3.63167627	1.48357017	1.00829422	-0.2375938	1.88584207	-0.2081709	1.91597829	-0.6808967
C_34	1.08107152	0.14130648	2.91861472	3.6376657	4.05099362	3.90967543	3.18392455	3.24894864	0.67255837	0.6412418	0.37878513	0.77142303	0.95908996	0.9012254	3.23985084	1.45461007	0.90496489	-0.3441866	1.45197924	-0.1064563	1.29854694	-1.015939
C_35	0.72883033	0.06966297	2.92825113	3.66881856	3.54385285	3.598982	2.80340141	3.00083275	0.88423642	0.49875386	0.47214631	0.56577127	1.11177036	1.17378238	3.86832165	1.56885796	0.98866794	0.17237872	1.4959052	0.26015753	1.54136432	-0.928515
C_36	0.94126852	-0.0265231	2.86189154	3.56364877	3.63682802	3.5581764	2.75445388	3.02814774	1.00200568	0.689661	0.8468359	0.76232335	0.84677165	1.05978822	4.36774043	1.1800077	0.96546224	0.46544039	1.77260659	0.46242529	1.71019783	-1.047399
C_37	0.94236534	-0.062021	2.76680819	3.55596344	3.47699964	3.5172152	3.23132221	3.47317419	1.06460721	0.62102618	0.68139926	0.69069557	1.2761989	1.15764181	4.02138319	1.54590995	1.34262194	-0.7655109	1.98628501	0.51044543	1.27926174	-1.2568471
C_38	1.155657	0.28663802	3.31745683	4.03964115	3.85433745	3.97368796	3.29505068	3.49278282	1.08031689	1.0356597	0.99989845	1.1768913	1.1120742	0.82792724	4.16621061	0.64687031	0.81815486	-0.6234865	2.12060987	-0.058181	1.45319937	-1.2814369
C_39	1.05824977	0.04126989	2.97923809	4.09262587	3.68841883	3.90563441	2.89159237	2.92835791	1.08226114	0.69470912	0.56552256	0.54147623	1.76169459	1.22460388	3.3172776	1.75028561	1.57250511	-1.0622787	0.77428873	0.38232296	0.67122781	-1.2197072
C_4	1.05046186	0.00459065	2.79205635	3.5987984	3.47392195	3.67880789	2.63707427	2.86296947	0.72035075	0.83289836	0.86607554	1.02968072	0.65012411	0.75363248	3.51541417	1.06046798	0.86234653	0.08420462	1.38861496	0.13323751	1.46268323	-0.902309
C_40	1.4990042	-0.0281102	2.73248286	3.39296531	3.71738352	3.74039896	2.85348046	2.77509563	1.10487102	1.63500713	1.64921811	1.89258029	0.75505163	1.28723244	4.51647642	0.8986893	0.99140563	0.41096201	1.96515991	0.45436108	1.68682737	-1.1912962
C_5	0.81933243	-0.3133055	2.52404491	3.65731323	3.70029643	3.67234336	3.24769179	3.46114488	1.1830125	0.68489833	0.27877142	0.56043783	1.28482676	0.97461035	2.61942449	1.48246361	1.23183143	-0.9052916	1.09643806	0.03130462	1.05186673	-0.8959952
C_6	1.18572758	-0.3257965	2.43376443	3.54257702	3.89427412	3.6612313	3.2139859	3.51903377	1.22319808	0.98583604	0.75364065	1.06431086	1.05654354	0.92997487	3.13229942	1.39314407	1.35324368	-0.8086715	1.45635408	0.25900391	1.55821012	-0.8368677
C_7	1.26147033	-0.0310127	2.74698579	3.73005669	3.79550288	3.76333141	2.95936432	3.19545476	1.03179705	0.92211099	0.58840192	1.07262175	0.99375442	1.07139983	3.32302893	1.24082767	0.82941222	0.27881395	1.86566228	0.07038885	2.06659075	-0.359337
C_8	1.38789085	-0.3967787	2.43226238	3.46240706	3.73486791	3.54005843	3.21279183	3.37657728	0.79986489	1.18396236	0.7669795	1.40319576	0.64913807	0.69278844	3.05393485	0.81057671	0.75676137	-0.265098	1.64967263	-0.353494	1.81119421	-0.8070692
C_9	1.41609996	-0.4066751	2.45751695	3.65218028	3.68911088	3.69810001	2.89260177	2.8514519	0.6562839	1.0480247	0.96985204	1.2243819	1.09402695	0.9582811	2.82554858	1.39738731	1.16553553	-0.1907633	1.34715826	0.12823847	1.45588099	-0.451865

Table 8.117: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls.

	PC(40:3)	PC(40:3)(2)	PC(40:4)	PC(40:4)(2)	PC(40:5)	PC(40:6)	PC(41:1)	PC(41:1)(2)	PC(41:2)	PC(41:3)	PC(41:3)(2)	PC(41:4)	PC(41:4)(2)	PC(41:5)	PC(41:6)	PC(41:6)(2)	PC(42:0)	PC(42:1)	PC(42:2)	PC(42:3)	PC(42:4)	PC(42:5)
C_1	0.57531478	0.27079357	1.33768772	-0.4564411	2.25574458	3.05368345	1.43902058	0.85251693	2.25341643	2.53955737	0.80773702	-0.0705308	-0.562765	0.4109689	-0.1747985	-0.4547965	-0.0673106	-0.3571822	-1.1005584	-0.173612	-1.2123211	-0.0614881
C_10	0.28299254	-0.1114297	1.04668673	-0.9109907	2.03727725	2.72414888	0.60842897	0.05527537	1.28997457	1.44945855	0.37836818	0.13143024	-0.6874831	1.1055301	0.41662562	0.02500886	0.72773783	-0.5108579	-1.3293765	-0.336215	-1.4279556	-0.3749946
C_11	0.48600485	-0.0958831	1.10740436	-0.7851637	1.60918375	2.46933598	1.27716738	0.61016878	1.89327748	1.95833159	0.34301356	0.09015607	-0.4923662	0.99306542	0.10837347	-0.3011475	0.11874208	-0.3632206	-1.4883953	-0.4955235	-1.6568455	-0.1637275
C_12	0.86390805	0.66930018	1.09648698	-0.2453561	1.86735342	2.72381828	2.43384808	1.52032533	3.30875281	3.54292858	1.30949254	0.71262989	0.64201503	-0.2725706	-1.0685999	-0.9733325	-0.1647298	0.22745825	-0.9377612	0.07114619	-0.9643203	-0.2586827
C_13	0.50791424	0.06129166	1.16503386	-0.673932	1.57377889	2.16324099	1.25277765	0.08600423	1.77561267	1.67638486	0.5478735	0.28000836	-0.5673711	1.30772684	-0.1104904	-0.2001925	0.08842661	-0.4756517	-1.2334892	-0.3142872	-1.4344722	-0.555859
C_14	1.64492154	1.89624036	0.83168926	1.02209403	0.12057699	1.26535904	2.23072152	1.57841391	2.95822172	2.90393301	2.38355917	1.15589674	0.63062283	0.42780307	-0.6762905	-0.6789081	-0.0308131	0.70253585	0.40296546	1.50153219	0.40439954	0.30872762
C_15	0.42321944	-0.4929557	1.28887346	-1.0989534	1.73396903	2.13682673	0.68999421	0.23295335	1.62265659	1.84544653	0.13036219	0.19905405	-0.4933797	1.48269498	0.20874823	-0.1821613	0.14309089	-0.5589802	-1.9739207	-1.0148247	-2.0319118	-0.4475845
C_16	0.54750386	-0.3327885	1.4124791	-1.0000645	2.01504136	2.35108428	1.97964479	1.13971957	2.72697544	2.73878762	0.46160557	0.57642834	0.41596719	1.04167413	-0.3366516	0.04655544	0.10818218	-0.0407164	-1.4978524	-0.749852	-1.8068429	-0.1714258
C_17	0.44749763	-0.131796	1.50263301	-0.8737447	2.43845957	3.03858454	1.08267657	0.88167295	2.10985834	2.53458401	0.61033427	-0.1561393	-0.6856293	0.68680696	-0.0094041	-0.6064697	0.10105936	-0.5350746	-1.6247704	-0.6372349	-1.6626081	-0.0356269
C_18	0.54067976	0.22995165	1.05264103	-0.5052318	1.55016911	2.18865181	1.46406283	0.7787371	2.08376308	2.23795069	0.70313609	0.225257	-0.3221873	0.90226003	0.02025398	-0.5085828	0.1666118	-0.1994483	-1.0125324	-0.1053498	-1.2003445	-0.3511261
C_19	0.49241277	0.28834254	1.24805486	-0.4390567	1.89712489	2.75380418	0.81120572	0.30500263	1.58203907	1.72747179	0.62421126	0.42259013	-0.1301053	1.47156329	0.31883014	-0.0534803	0.50343781	-0.3829203	-1.0364397	-0.0859945	-1.1530887	-0.3714254
C_2	0.51749946	-0.1647999	1.42475435	-0.9318004	2.25323535	2.99864487	1.11393935	0.77729195	2.14014993	2.53327056	0.1737725	-0.0755621	-0.4751555	0.86550254	-0.072689	-0.6124216	0.13663919	-0.5856981	-1.5695116	-0.6494205	-1.6450735	-0.2673233
C_20	0.78767732	0.55224409	1.02355402	-0.221711	2.03138477	2.82134609	1.90984378	0.98667133	2.62253532	2.68087974	0.79959187	0.41645133	-0.247733	0.32979727	-0.1136306	-0.4694217	0.15075668	0.09895833	-0.9270663	0.12124359	-0.9451676	-0.2342506
C_21	0.48485054	-0.7785882	1.35468275	-1.5690658	1.98918433	2.55882504	1.04791668	0.30756258	1.93892689	1.99383137	0.05785245	0.25797561	-0.5323217	0.90824555	-0.1565263	-0.3520939	-0.0270691	-0.5507406	-2.0337851	-1.2281976	-2.2109702	-0.3401587
C_22	0.54842706	-0.8441707	1.72636644	-1.6311827	2.48147224	2.91256123	0.82511787	0.66051023	2.04798353	2.48883779	0.17218458	-0.1608895	-1.1579328	0.99379364	-0.2974258	-0.5677558	-0.0057554	-0.8442082	-2.0268996	-1.4141162	-2.4428746	-0.0796628
C_23	0.42240094	-0.5042756	1.26423296	-1.2569546	2.13729133	2.78921424	0.84887423	0.1981095	1.64651194	1.60848303	-0.0368593	0.10568883	-0.7174886	1.04424069	0.14232556	-0.2966126	0.3033514	-0.638349	-1.8166585	-0.9618404	-1.9673073	-0.4768715
C_24	0.45472896	-0.3930801	1.32500154	-1.147363	1.98417147	2.49908826	0.7558645	-0.0426521	1.43345311	1.23702617	0.37422216	0.17019196	-0.7513521	1.09643803	-0.3304952	-0.3295656	-0.0014533	-0.8927137	-1.9000559	-0.8706574	-1.9210118	-0.4863563
C_25	0.3596911	-0.7758411	1.2453062	-1.3468918	2.05840579	2.80193059	0.9741376	0.16994829	1.8463727	1.83763863	-0.0732341	-0.1162442	-0.7641902	0.78455662	-0.1629396	-0.3426032	0.06945947	-0.6997737	-2.0188574	-1.21141	-2.2548055	-0.4764913
C_26	0.4495508	-0.8063356	1.16764743	-1.5293416	1.86532808	2.57927904	0.92206546	0.0002226	1.66085761	1.58890295	-0.0316651	0.14734655	-0.7016652	1.19764273	0.15177223	-0.1849855	0.38822908	-0.4973519	-2.1814145	-1.3635416	-2.1475027	-0.4215339
C_27	0.56670006	-0.3196848	1.7243997	-0.9939179	2.34067145	2.46720237	0.8584	0.16360862	1.70460723	1.80455753	0.33585285	0.1557792	-0.5634552	1.21671646	-0.1053251	-0.3619135	-0.0121585	-0.6746523	-1.7661487	-0.8870249	-1.8488719	-0.4533427
C_28	0.44141217	-0.5485755	0.9316465	-1.2993934	2.17501698	3.04294727	0.66850644	0.12491107	1.46619812	1.46194105	-0.0008657	0.09796453	-0.6297297	1.2030098	0.45780643	0.2589161	0.8793947	-0.4998795	-1.563997	-0.9940736	-1.9538142	-0.1511482
C_29	0.5112207	-0.4276907	1.5249225	-1.1571984	2.38753942	3.05687258	0.58686536	0.24226943	1.38817588	1.5230423	0.08425376	0.26349224	-0.3231412	1.41276547	0.20362931	0.17061504	0.77826815	-0.5721919	-1.413357	-0.7856624	-1.7685184	0.12521147
C_3	0.46975064	-0.0470571	1.28291451	-0.8588586	2.01571736	2.81498597	1.45505001	0.71014667	2.0920821	2.09721851	0.42488335	0.21570902	-0.3723113	1.04818317	0.22975839	-0.3476075	0.44116382	-0.2423521	-1.2962501	-0.4225494	-1.4739295	-0.1797894
C_30	0.50099277	0.02504055	1.16268975	-0.700727	1.78535805	2.44637501	1.24270382	0.30215584	2.01767818	2.07673414	0.69354066	0.21012122	-0.4708545	0.98902349	0.00102942	-0.4664917	0.04468731	-0.3842158	-1.459881	-0.4358709	-1.4531861	-0.5815659
C_31	0.39395902	-0.3314164	0.96157143	-1.1253912	1.56244813	2.44910107	0.91770336	-0.1235281	1.55929391	1.29970955	0.39092918	0.03956131	-0.6910613	1.03602875	0.04992558	-0.2276214	0.29132901	-0.37439	-1.6969999	-0.7962082	-1.7841607	-0.5067088
C_32	0.54583381	-0.8512744	1.12176974	-1.5320616	1.84626478	2.70891817	1.41857989	0.35062352	2.25099001	2.23902979	-0.1291298	0.29121988	-0.1206826	1.09781666	0.14928075	0.08955543	0.47926616	-0.2568903	-1.9980091	-1.2231105	-1.9410588	-0.3149139
C_33	0.66452451	-0.2504309	1.48715108	-1.0367629	2.13615907	2.71199795	1.10389243	0.78026257	2.04306289	2.30908674	0.2520035	0.33099903	-0.2282693	1.21468527	-0.0143229	-0.210391	0.1776267	-0.5077251	-1.2929554	-0.7102452	-1.7425649	-0.0480406
C_34	0.43894686	-0.5621251	1.58508286	-1.2134395	2.17663641	2.72250376	0.54043828	0.37001915	1.72451058	2.07839378	-0.0153619	0.15013288	-0.4106137	1.23101045	-0.1824849	-0.1053865	0.10494575	-0.8582169	-1.8702653	-1.1072146	-1.9934076	-0.3289862
C_35	0.41090635	-0.7907733	1.13534535	-1.2475121	1.8362631	2.4253063	1.02169747	0.40897655	1.8663072	1.81154811	0.20600683	0.61695836	-0.2699251	1.61632336	0.21216096	0.18000179	0.78280659	-0.4055049	-1.886509	-1.2801332	-2.2136435	-0.3906189
C_36	0.53403748	-1.201168	1.24356418	-1.6111486	1.71866754	2.40854988	1.47496317	0.61035561	2.29989827	2.05032381	0.23919595	0.61652205	-0.4395564	1.38369973	0.4529874	0.07987903	0.55081758	-0.2106115	-1.8739223	-1.7417894	-2.498988	-0.2200388
C_37	0.48861003	-1.3688368	1.03328334	-1.7990526	2.08867802	2.84630505	0.99247406	0.25978226	1.8617088	1.77831483	-0.2504511	0.46462199	-0.5602463	1.55008492	0.57555035	0.62224533	1.04840444	-0.2921016	-2.2021056	-1.8314202	-2.6053213	-0.1846571
C_38	0.54926476	-1.2515427	1.27985368	-1.6981916	1.98179845	2.68541596	1.02201316	0.33864404	2.0359767	2.00650803	-0.2598558	0.42925205	-1.8995327	0.82853707	-0.4745884	-0.6552674	-0.1395709	-0.3198228	-2.2436715	-1.521563	-2.4265442	-0.3721283
C_39	0.56219446	-0.8305679	1.06342613	-1.5295564	1.50680631	2.25427426	0.98530341	-0.1356813	1.70738251	1.32331502	0.04034287	0.30546732	-0.4190018	1.66891397	0.52343028	0.15455697	0.65249737	-0.0962747	-2.3158002	-1.4803539	-1.9966097	-0.2762114
C_4	0.40675732	-0.2111677	1.09868171	-1.0020829	1.6514598	2.42379025	1.21404386	0.42648943	2.01236815	2.04681738	0.31590898	0.22779945	-0.6174266	1.1167397	0.11540821	-0.4775526	0.29147634	-0.4021803	-1.4251653	-0.5598982	-1.6864834	-0.4865118
C_40	0.69596675	-1.0960485	1.47667263	-1.517503	1.9358735	2.38386731	1.75578554	1.04038915	2.87885612	3.12415539	0.14461289	0.94639452	-0.2624648	0.8365838	-0.347901	-0.4239003	-0.3012232	-0.2793799	-2.119603	-1.5829431	-2.2410915	-0.2143124
C_5	0.42700045	-0.1078472	0.92551517	-0.7770448	1.78437835	2.65321642	0.84589341	0.06162062	1.38550507	1.41366803	0.45115193	0.09323547	-0.4986025	1.18974979	0.02122723	0.17010468	0.51071362	-0.500502	-1.5743183	-0.5681132	-1.6062638	-0.6843686
C_6	0.4421012	-0.1260351	1.12819195	-0.8900853	1.91975154	2.8148759	1.0864526	0.43656807	1.75041158	1.78864167	0.33514971	0.2513276	-0.4119089	1.3642908	0.52091788	-0.04527	0.71679584	-0.1571262	-1.5092144	-0.5880281	-1.6101628	-0.3723486
C_7	0.65245049	0.2034775	1.34033105	-0.5290338	1.9015998	2.65481502	1.33750275	0.81551779	2.04903534	2.18844815	0.60245343	0.38472475	-0.2674554	1.08045918	0.02733435	-0.3043447	0.31478616	-0.2542574	-0.9018868	-0.1847404	-1.235604	-0.1294071
C_8	0.43915148	-0.030763	1.2439539	-0.8284644	1.95383961	2.60821792	1.21413964	0.63246343	1.90003665	2.22111883	0.3181993	-0.2045903	-0.7876409	0.60117193	-0.3437623	-0.6878783	-0.1263974	-0.6622299	-1.2716774	-0.3258622	-1.378091	-0.2777553
C_9	0.63055923	0.43631501	1.09703272	-0.4004785	1.5508189	2.2346872	1.37401695	0.62439402	2.12230111	2.32313366	0.91687922	0.40540701	-0.272738	1.13445974	0.06026045	-0.3879661	0.27091099	-0.1486265	-0.9882966	0.02195768	-1.0668766	-0.418864

Table 8.118: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from breast cancer free controls.

	PC(43:0)	PC(43:4)	PC(43:4)(2)	PC(43:5)	PC(43:5)(2)	PC(43:5)(2)	PC(43:6)	PC(43:6)(2)	PC(43:6)(3)	PC(30:0)	PC(30:0)(2)	PC(30:0)(3)	PC(30:1)	PC(30:2)	PC(d31)
C_1	3.70971695	1.78598777	-1.2682916	2.48616032	0.10112542	1.50205273	2.77987468	1.07912488	0.14392583	-0.4795072	0.52575483	1.77152381	3.53375696	2.95036998	-1.7930605
C_10	3.16755988	1.12023469	-1.1727102	1.74489255	0.41169666	0.69459471	2.02449808	0.30548805	0.85434653	-0.3994864	0.72944458	1.62546495	3.6651585	3.07764868	-2.0375473
C_11	3.78876509	2.24372131	-0.8131338	2.53767425	0.53249172	1.53677229	2.79537747	0.95224828	0.18726214	-0.2190867	0.96913975	0.99608726	3.73629189	3.09888836	-2.1006226
C_12	4.58245736	2.89979542	-0.044363	3.21153207	-0.3960486	2.91387059	3.47531227	2.74442814	-1.3407157	-0.4455366	0.54860483	1.3132399	3.45239085	2.7968424	-2.050902
C_13	3.29600068	2.22059639	-0.8648147	1.88804566	0.56882071	1.6838811	2.15214953	1.191659	0.50593184	-0.0461043	0.90124898	0.92836776	3.92413844	3.38771817	-2.1711411
C_14	3.98129239	3.68367678	0.14058753	2.08577399	-3.0743869	3.08145244	2.34112336	2.47513673	-4.8186212	0.24068368	1.33806272	1.57386821	4.18416859	3.53022223	-1.6613515
C_15	3.0715717	1.88255571	-0.7722721	1.7938309	0.57186136	1.33105894	2.01376808	0.80833789	0.54428669	-0.153035	0.51333425	1.23830079	3.73539583	3.08815563	-1.9994058
C_16	4.09916979	2.28470366	-0.3971946	2.94079553	0.83552917	1.91447898	3.199143	1.58134111	-0.1469487	-0.428482	0.53454173	0.83498484	3.5595144	2.96182548	-1.917947
C_17	3.46187078	1.81287684	-1.2159584	2.21879318	0.27970119	1.25034296	2.48498913	0.82004602	0.36624701	-0.4316859	0.71944955	1.51991939	3.54169998	2.94219088	-1.7587989
C_18	3.9956375	1.66006569	-0.8741262	2.63126743	0.39423498	1.11766632	2.93393754	0.60277439	0.15744444	-0.2657907	1.17752697	1.09478025	3.70050088	3.06681923	-1.9630399
C_19	3.44088819	1.31590018	-0.5227229	2.04133112	0.89071606	1.11699624	2.33466974	0.7716258	0.74857376	-0.2736817	0.89108049	0.65736436	3.71190895	3.16092753	-2.0300007
C_2	3.5504936	1.70870455	-0.7099649	2.33609155	0.52041486	1.35523162	2.5952531	1.1015827	0.23245152	-0.3743543	0.70234076	1.21725903	3.59389522	2.97415234	-1.7436223
C_20	3.99729173	2.47049998	-0.9908246	2.67612317	-0.0878741	2.20817429	2.97632947	1.85639294	0.14490519	-0.3678483	0.86481833	0.85248324	3.57846977	3.02153055	-2.0603834
C_21	2.97222628	2.48570588	-1.001193	1.42241075	0.24773973	1.85870824	1.61936961	1.30958722	0.2882744	0.05381027	1.04452189	1.20000312	4.06126679	3.40404719	-1.8333631
C_22	3.07328662	1.89246977	-1.321176	1.65452363	0.10090692	1.48801649	1.83507013	1.0618391	0.08395811	-0.3502671	0.47993808	1.28552401	3.68184808	3.12136023	-1.450825
C_23	3.3973488	1.65934488	-0.784934	1.9393795	0.23463861	1.11739512	2.23601058	0.35518682	0.31225447	-0.2119875	0.95290388	1.21509698	3.85681186	3.21671473	-1.9041263
C_24	3.07275651	1.95410108	-1.0076973	1.48095361	0.02223726	1.34637895	1.71965782	0.50869601	0.28320829	0.09393025	1.08859364	1.42346894	4.03335565	3.42491559	-1.7292192
C_25	3.08759815	2.10271376	-1.0254439	1.73711164	-0.0110564	1.68888016	1.92653799	1.23138799	0.24730666	-0.007195	0.60525313	1.12379332	3.90698452	3.3462304	-1.7612914
C_26	3.04158957	2.15863892	-0.7869518	1.55870863	0.3732819	1.65310182	1.75935881	1.01476826	0.51610471	-0.019398	0.79851054	1.04554752	4.00029565	3.4000609	-2.0439815
C_27	3.25142424	1.86859207	-1.0492212	1.66983964	0.40039711	1.37823695	1.88838919	0.87173385	0.31400435	-0.076635	0.7769022	1.11135594	3.92884835	3.381184	-1.8356558
C_28	3.08800644	1.60002533	-1.1178752	1.91390434	0.45679893	0.89468804	2.17548531	0.42119671	1.15268563	-0.4273451	0.90081686	0.66952416	3.77070986	3.17655044	-1.8269943
C_29	3.30100193	1.3159523	-0.5260842	2.18147368	0.93105298	0.81969944	2.4433678	0.49784111	1.00944668	-0.4596075	0.91851657	1.20082356	3.71195195	3.07272842	-1.8321639
C_3	3.7826013	1.94229144	-0.9308695	2.45160274	0.4368444	1.35872062	2.70112017	0.91721341	0.57838156	-0.4217405	0.94460665	1.05614012	3.7015427	3.06105255	-1.9452772
C_30	3.28558822	2.3127255	-1.1568933	1.58419099	0.05736719	1.74110552	1.81031888	1.08674843	0.10650068	-0.0476316	0.95051079	1.27799513	3.90895603	3.36406756	-1.7743763
C_31	2.73543132	2.42874482	-1.1159728	1.07221475	0.16159581	1.66060574	1.31592678	1.00627388	0.12995287	0.5240379	1.345196	1.14817502	4.41786085	3.79361416	-1.8667164
C_32	3.02615911	2.77806354	-0.8551588	1.49883523	0.53118377	2.21056239	1.71311974	1.65537898	0.57205778	0.04555915	1.05455357	1.37409171	4.03425759	3.41109353	-1.9221765
C_33	3.6768889	1.62482257	-0.3317845	2.55858346	0.87615441	1.21657056	2.82427952	0.66236022	0.6124656	-0.3961899	0.54299122	1.24811646	3.53541333	2.89306447	-1.5575181
C_34	2.95230252	1.62795069	-0.8920568	1.66377143	0.64859539	1.24202644	1.88270319	0.85273882	0.58096402	-0.2235328	0.52757658	1.76404225	3.70682476	3.05719657	-1.5652123
C_35	3.25006005	1.87331967	-0.6542467	1.97679662	0.88546708	1.37699063	2.22496501	0.93559346	1.03827272	-0.257323	0.84982398	1.2265336	3.82308947	3.19741632	-1.8585505
C_36	2.94004948	2.2566067	-0.6283342	1.73991226	0.75929341	1.97905312	1.91340628	1.7295819	0.91240806	-0.30966	1.07977641	0.78492769	3.79970764	3.23104501	-1.7395373
C_37	2.81078262	2.15968515	-0.5678193	1.31339819	0.82103636	1.78495623	1.53008731	1.36095475	1.14018934	-0.3310208	0.61689745	0.80478754	3.75779819	3.16794662	-1.9480019
C_38	2.69961374	2.59444408	-1.0877591	1.1289614	-0.0470082	2.21960502	1.28085983	1.72051756	0.12717568	0.07229174	0.83782982	1.3952831	4.06449247	3.43225648	-1.642557
C_39	2.36375208	2.93702487	-0.4159442	0.60126759	0.55353995	2.34078459	0.8187698	1.61266502	0.63504815	0.55825552	0.860108	0.52597706	4.45234204	3.80841754	-2.1201488
C_4	3.41659892	2.00279781	-1.0877122	2.0155124	0.27294906	1.45374027	2.30153391	0.76915945	0.56375704	-0.1577126	0.88514256	1.74109293	3.76568788	3.11435293	-1.9092022
C_40	3.19592535	2.89008879	-0.5198	1.80179363	0.38115828	2.64044813	1.98116862	2.1373285	0.0748928	-0.1350287	0.84607776	1.20802502	3.86592145	3.26018932	-1.6311783
C_5	3.10175254	1.42801546	-1.1413691	1.54432489	0.33182435	1.01972601	1.83568471	0.63506274	0.53272694	-0.1310061	0.8138336	1.19410544	3.89570975	3.29036403	-2.1478741
C_6	3.59095078	1.80126186	-0.8524629	2.18745303	0.69311392	1.14346203	2.48145853	0.58482044	0.72853976	-0.342115	0.92985495	0.66189719	3.73053588	3.13750079	-2.0778577
C_7	3.95419419	1.48066157	-0.7908383	2.75890557	0.51620756	0.99973278	3.05823597	0.56980029	0.59645445	-0.3291959	0.86527198	0.85890578	3.70767982	3.11247977	-1.7372612
C_8	3.7139745	1.34999407	-1.1722027	2.43031284	0.13027202	0.82109895	2.71748722	0.38322212	-0.174112	-0.5477331	0.4950435	2.22417601	3.44037894	2.84337405	-1.9749083
C_9	3.60347663	2.08426094	-0.7778547	1.96813306	0.50622086	1.4561453	2.24173847	0.91038741	0.31172655	-0.1407357	0.87862845	0.95691514	3.7683911	3.11869749	-2.0938028

Table 8.119: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer.

	LPC(14:0)	LPC(15:0)	LPC(16:0)	LPC(16:1)	LPC(17:0)	LPC(17:0)d2	LPC(17:1)	LPC(17:1)d2	LPC(17:2)	LPC(17:2)d2	LPC(18:0)	LPC(18:1)	LPC(18:2)	LPC(18:3)	LPC(20:0)	LPC(20:0)d2	LPC(20:0)d3	LPC(20:1)	LPC(20:2)	LPC(20:3)	LPC(20:4)	LPC(20:5)
P_1	-0.8800703	-0.8618016	3.8784688	0.74758071	0.31604053	-1.7385777	-1.5740317	-1.6310902	-4.351591	-5.8927956	3.1151147	3.25841173	3.19634731	-0.2985194	-0.7206508	-2.44653	-2.3472216	-1.4268875	-0.0154771	2.05183988	2.87836827	1.34688891
P_10	-2.4091771	-0.6028064	3.68963874	-0.3412824	0.57547116	-1.4786022	-2.0346944	-1.0298918	-3.886168	-5.7343416	3.18703851	3.16947241	3.66835244	-0.2576913	-0.8757412	-1.9823197	-2.0659838	-1.2764189	-0.2636102	1.24227738	2.78406426	1.88084673
P_11	-1.1752835	-0.9572603	3.56779976	-0.0855618	0.28616555	-1.860328	-1.7082931	-1.5438937	-4.2090168	-6.0007763	2.94612288	3.2000286	4.01020079	0.14219962	-0.9256465	-1.7331494	-2.3357711	-1.3231545	0.4351709	2.07444922	2.78087213	0.66652089
P_12	-1.1438154	-0.7880809	3.77684035	0.33721817	0.44979811	-1.4806108	-1.935266	-0.8939217	-4.1519611	-5.6163174	3.33308903	3.16150416	3.51836343	-0.3462242	-1.0180844	-2.580252	-1.9036084	-0.9329663	0.02860667	1.88984847	3.07708219	0.67348761
P_13	-1.0972545	-0.9183078	3.77321288	0.54591194	0.32444379	-1.7557046	-1.3734592	-1.6057741	-4.1556688	-5.7171162	3.26894785	3.2838053	3.65445975	0.19189799	-0.4064186	-1.8026961	-2.0892007	-1.6054932	0.16599925	2.34596832	3.0051818	1.21892663
P_14	-0.5114743	-0.8654072	4.02455857	1.03074668	0.70405667	-1.4995291	-1.1434641	-1.3557858	-4.4377159	-5.6888355	3.31884035	3.68867944	3.76342223	0.12960896	-0.4872316	-1.8643674	-2.1089417	-0.9433038	0.57989793	2.72079043	3.62277292	1.48294788
P_15	-1.8233304	-0.8652535	3.47178984	-0.1633437	-0.0031941	-1.709947	-2.0453275	-1.3638651	-4.1630481	-5.9312771	2.63027566	3.14354366	3.73742873	-0.2424377	-1.0812474	-2.2740963	-2.6719886	-1.4225495	0.22003618	2.44021978	3.44232451	0.5729995
P_16	-0.8304656	-0.7972696	3.91045952	0.20106083	0.4715026	-1.5315081	-1.7143348	-1.5600398	-4.1817103	-5.5670121	3.34520188	3.12277224	3.6035383	-0.0241781	-0.7396512	-1.6959765	-2.0282406	-1.5954482	-0.145091	1.82147524	2.62822737	1.37301826
P_17	-1.4111607	-1.0529979	3.62357423	0.03644069	0.33943762	-1.5866304	-1.5165131	-1.6358382	-4.3739407	-5.9125043	3.01688482	3.21293802	3.8023627	0.01412345	-0.8693763	-2.0801513	-2.4776685	-1.5308889	0.05867363	2.03639212	2.74127877	0.92652829
P_18	-0.9527978	-0.7167875	3.82334012	0.21024067	0.33660173	-1.5518642	-1.6055224	-1.4144323	-4.134679	-5.7581359	3.16949984	3.1645214	3.47627943	-0.2578545	-1.0085428	-2.1737458	-1.96578	-0.9687505	0.00105041	1.99339681	2.62482116	0.9703098
P_19	-0.6333362	-0.7843074	3.7763169	0.079269	0.16280818	-1.8548334	-1.8479165	-1.7885867	-4.3675815	-5.9147662	3.12641438	3.02807676	3.51137485	0.0302051	-0.5069843	-2.0836837	-2.377157	-1.4819087	0.03057696	2.11690571	2.75303701	1.09256663
P_2	-1.0202718	-0.8542625	3.78098432	0.014662	0.39582416	-1.6646475	-1.8042432	-1.5290189	-4.4381513	-5.4176499	3.36492649	3.0664309	3.78504004	0.12597496	-0.8250405	-2.2799995	-2.0420734	-1.2691261	0.20001059	2.11833954	2.84372638	1.05308926
P_20	-0.9121697	-0.8148134	3.72996023	-0.0819941	0.39953633	-1.3484945	-1.7266117	-1.5204019	-4.1945867	-5.5777381	3.17670195	3.05978259	3.45850941	0.11472537	-0.6641299	-1.616646	-2.0233468	-1.4972972	-0.3467861	1.76068508	2.42253708	0.56744373
P_21	-0.6499406	-0.7057796	3.89222034	0.45378456	0.90511863	-1.3870347	-1.3290062	-0.9127928	-4.2557456	-5.570667	3.62074643	3.70685156	4.20018231	0.54014108	-0.9453907	-1.3636667	-1.7327139	-0.4773538	0.73266048	2.38046487	3.22588311	1.65149665
P_22	-0.2224014	-0.8460949	4.13081497	1.08885296	0.67439755	-1.6868918	-1.0953213	-1.109867	-4.235715	-5.5000985	3.58581948	3.84825403	4.31137665	0.89261011	-0.4908885	-1.5771356	-1.7972265	-0.5711335	1.14366161	2.56848669	2.81866146	1.65740682
P_23	-1.0309877	-0.8450714	3.79755277	0.27119432	0.93552608	-1.5344221	-1.255645	-1.3084656	-4.2092144	-5.7572958	3.30925423	3.4510172	3.85241378	-0.0483882	-0.861679	-1.216547	-2.2713389	-0.8475864	0.55878531	2.50618655	3.15791242	2.30758613
P_25	-1.1039577	-0.6847241	3.56387971	-0.1364037	0.47718253	-1.4617738	-1.670933	-1.3268477	-4.0604659	-5.7763015	3.12905897	3.07272445	3.58072427	-0.0744706	-0.8753337	-1.5647331	-2.1301868	-1.3791772	-0.0592273	1.8165331	2.62900255	0.94605577
P_26	-0.8068746	-0.7928058	3.86821281	0.10935597	0.38841173	-1.4498927	-1.8854276	-1.1189074	-4.1476922	-5.5774088	3.41366995	3.20234077	3.92955613	0.47451333	-1.168635	-2.2911508	-1.8593727	-1.1825579	0.09706272	2.04589332	2.88074148	1.03229928
P_27	-0.8616335	-0.9656471	3.82475624	0.81305933	0.07046315	-1.6088378	-1.4903402	-1.3827811	-4.3816176	-5.6141983	3.40512761	3.35640133	3.61327936	0.03880603	-0.8427732	-2.4515599	-2.1905281	-1.4245435	0.27737831	2.52090276	3.216843	1.39398438
P_28	-1.4612601	-1.0524988	3.4259219	-0.1885128	0.17608471	-1.6458888	-1.7137882	-1.6073743	-4.1199139	-6.1283444	2.77942217	3.05580541	3.67175557	-0.1857709	-1.100158	-1.6758744	-2.6656373	-1.5410755	0.01299901	2.22022903	3.12183888	1.59650601
P_29	-0.9302934	-0.8931441	3.89521507	0.17366866	0.19911799	-2.0671972	-1.9646283	-1.2474024	-4.1399323	-5.7152372	3.29549509	3.36479765	3.69790788	-0.2202167	-1.0111635	-2.4417715	-1.9544273	-0.9195853	0.08139159	1.90909502	2.94117622	1.94293964
P_3	-1.2947726	-1.0210461	3.74063339	0.01917216	0.27098069	-1.6374258	-1.6912869	-1.4565305	-4.1558001	-5.7106968	3.02914239	3.18150035	3.61990485	-0.1373181	-0.731906	-2.2019139	-2.1798856	-1.382711	-0.2333017	1.68512955	2.68406097	0.43503353
P_30	-0.6883487	-0.8578281	3.72120206	0.63535906	0.79928048	-1.3138319	-1.1597041	-0.9446638	-4.2611638	-5.3090946	3.56492373	3.74628301	3.94621383	0.22417996	-0.9166213	-1.5709406	-2.0958158	-0.8616668	0.53412112	2.47038815	3.40645559	2.88452178
P_31	-1.5847623	-0.8342038	3.60952551	-0.0821927	0.29765044	-1.5083733	-1.879231	-1.2107	-3.8945992	-5.8637076	2.9219401	3.02400431	3.53305014	-0.3831579	-1.0071674	-2.0638939	-2.4596571	-1.5911172	-0.3193675	1.87647225	3.1497425	0.58462788
P_32	-1.5060007	-0.8858639	3.65700122	-0.2843068	0.48207187	-1.682377	-1.7797631	-1.6477652	-3.8418613	-5.9834346	3.01801064	3.01587762	3.51495187	-0.5278579	-0.6538588	-1.771497	-2.3148451	-1.278922	-0.0479075	1.66986566	2.8888093	1.83123769
P_33	-0.9817788	-0.6634793	3.86700893	0.06188699	0.5696212	-1.3460181	-1.5088107	-1.1923493	-4.1195375	-5.4049506	3.50028769	3.47688194	4.03352098	-0.124571	-0.9848127	-1.9488358	-2.1375733	-1.1333948	0.50007172	2.44135621	3.27258128	0.87969851
P_35	-0.0371773	-0.9756004	4.20351151	1.48616337	0.24281487	-1.9573879	-1.1664634	-1.591671	-4.4847065	-5.81369	3.37164604	3.86492192	3.79686961	0.69864026	-0.3642539	-1.7439992	-2.2635368	-0.984589	0.58747935	2.33161164	3.31792785	2.73740887
P_36	-0.4828813	-0.5249661	3.8069623	0.5363274	0.59890214	-1.4317547	-1.2476186	-1.2558264	-3.9874071	-5.742262	3.1622097	3.3214437	3.7341237	-0.1311194	-0.5928735	-1.7865689	-2.4448161	-1.2414866	0.43556184	2.41603847	3.2224632	2.40018504
P_37	-0.630087	-0.6751469	3.94487346	0.44528013	0.57514911	-1.4448655	-1.3703532	-1.2592874	-4.3232541	-5.4349728	3.59806731	3.47965799	4.1420972	0.35430133	-0.9449736	-2.0372113	-1.9670953	-0.7489889	0.67911213	2.33942948	2.72228349	1.41608373
P_38	-1.2453857	-0.7340087	3.70572993	0.52653115	0.37696539	-1.3487618	-1.6030657	-0.8755209	-4.5009578	-5.5461931	3.36671477	3.80762904	4.03349915	0.28956872	-0.6690311	-1.9076262	-1.7633912	-0.6069749	0.65641104	2.74039658	3.50040446	1.01763374
P_39	-1.5608116	-0.6121135	3.5847923	-0.1624987	0.70023181	-1.1658327	-1.5704996	-1.1662587	-4.0711698	-5.5993684	3.18260692	3.44695623	3.83055003	-0.3033856	-0.899867	-1.232023	-2.3609538	-1.0180224	0.28226622	2.22025705	3.37883967	2.27079236
P_4	-0.8997697	-0.9141487	3.74609193	-0.0661939	0.59168411	-1.669341	-1.8449553	-1.6195172	-4.1187872	-5.8445699	3.26975586	2.83737683	3.38881192	-0.1830962	-0.8184335	-1.8770039	-1.9928358	-1.4985701	-0.4484353	1.55614488	2.77446838	2.15464278
P_40	-1.283075	-0.9614443	3.69027699	0.02668074	0.37710096	-1.6928249	-1.6505019	-1.2491614	-3.9802418	-5.8456131	3.24315112	3.46870184	3.76391626	0.12867351	-0.8064533	-2.1562129	-1.9894258	-1.009221	0.47244119	2.37184044	3.05551509	0.94701188
P_41	-0.7300917	-0.9323473	3.69408724	0.29325683	0.64631453	-1.511369	-1.2492155	-1.4494315	-4.3891778	-5.7905668	3.36526481	3.29965237	3.75338214	0.14959447	-0.8907427	-1.8672015	-2.2750002	-1.2759955	0.28774674	2.32336875	2.89957209	1.04176407
P_5	-1.5970764	-0.6984871	3.78634742	-0.2467375	0.36892516	-1.4312191	-1.8902214	-1.318714	-4.1593788	-5.9968404	2.96963874	3.16402172	3.80635446	-0.1025169	-0.6354807	-1.9643203	-2.1171326	-1.1583912	0.16884942	1.8033963	2.33559426	0.65309419
P_6	-1.1981703	-0.8963275	3.77919725	0.17843384	0.63795706	-1.7307463	-1.7734773	-1.2120238	-3.8357715	-5.4035489	3.40930734	3.18698446	3.77222112	-0.0926388	-1.0300354	-1.8864434	-1.8040347	-0.7801832	0.0780474	1.82272696	3.00353687	2.11305165
P_7	-0.5752183	-0.7496874	3.77347134	0.25335821	0.3837031	-1.3134895	-1.7067264	-1.3489943	-4.5974989	-5.6454675	3.34488947	3.19510794	3.65319651	0.26292852	-0.6639206	-2.1254207	-2.1301823	-1.4017455	0.21814031	2.28992995	3.12583696	1.18876528
P_8	-1.3805163	-0.5360714	3.53809495	-0.2189051	0.40931232	-1.3810598	-1.9218521	-0.8996967	-4.0252955	-5.8117135	3.08886352	3.19123082	4.03679722	-0.0213903	-1.0275759	-1.4529578	-2.1451123	-0.9699022	0.2215917	1.50937841	2.73658626	1.60972906
P_9	-1.0313143	-0.8378532	3.57950819	0.14842793	0.11277839	-1.8028245	-1.6574677	-1.3166843	-4.1022351	-6.1937714	2.81339289	3.25754202	3.7160861	0.029928	-0.5783528	-1.4808983	-2.3021317	-1.3487485	0.26983774	2.15208325	2.36364099	0.178657

Table 8.120: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer.

	LPC(22:0)	LPC(22:1)	LPC(22:2)	LPC(22:3)	LPC(22:4)	LPC(22:5)	LPC(22:6)	LPC(21:0)	LPC(21:0)(2)	PC(22:0)	PC(22:1)	PC(22:2)	PC(23:0)	PC(23:1)	PC(23:2)	PC(24:0)	PC(24:1)	PC(24:2)	PC(25:1)	PC(25:1)(2)	PC(25:2)	PC(26:0)
P_1	-3.931054	-4.1252635	-0.2319614	0.72817788	-0.5426279	1.05580037	2.23735115	-1.8159797	-3.8750597	-4.2478263	-3.1872308	-4.6294506	-6.2540403	-4.4346755	-5.7916995	-5.4155048	-5.5570836	-4.8792623	-5.3798446	-5.0795041	-6.4018498	-3.2300841
P_10	-3.4088076	-3.6176559	-0.5595548	0.47294513	-0.7117836	1.69377938	3.17220003	-1.7454402	-3.7582784	-4.3729073	-3.0549726	-3.7595168	-6.4638564	-4.0786678	-5.6245267	-5.716642	-6.0279938	-5.7846955	-5.2571097	-5.0367401	-6.6573513	-4.3570159
P_11	-3.8623685	-3.9553577	-0.6278808	0.29957005	-0.3219746	1.23077564	2.70215981	-2.0273005	-4.446345	-4.8060006	-3.3913281	-4.0959397	-6.3218744	-4.83192	-5.6939132	-4.8675585	-4.4998337	-4.328562	-4.872104	-5.4431746	-5.178951	-3.2815215
P_12	-3.096911	-3.4255445	-0.6523716	0.39524129	-0.1733987	1.03319177	2.59273371	-1.8437413	-3.6180581	-3.9890333	-2.4941933	-3.3936947	-5.8426816	-3.4517755	-4.9103905	-5.0965289	-5.0139889	-4.6179579	-4.844365	-4.442373	-5.6195381	-3.0907174
P_13	-3.6199751	-4.2698611	-0.0614641	0.87907798	-0.0644466	1.14610187	2.05074035	-1.868794	-4.1296318	-4.685458	-3.5800798	-4.7793436	-5.5686962	-4.7905923	-6.0616206	-5.4180704	-4.3408722	-4.2861217	-4.7748793	-5.6037875	-5.3604412	-3.0995118
P_14	-3.5306784	-3.897076	0.00582507	1.03705792	0.2176741	1.1094256	2.2429558	-1.8165973	-4.3025411	-4.9307906	-3.2446577	-4.6292906	-5.5232561	-4.2198494	-5.7810852	-5.4244103	-5.2975185	-4.7210216	-5.2202697	-5.3534585	-5.7852957	-3.1480484
P_15	-4.1656971	-4.3049287	-0.9781286	-0.0258096	-0.6482308	0.8671996	2.63208491	-2.1127984	-4.0928214	-5.2304078	-3.3340574	-4.2988496	-5.5129748	-5.0416965	-6.3484382	-6.011966	-5.3104506	-4.4042102	-4.9980759	-6.9409419	-5.3929268	-3.4139558
P_16	-3.5316842	-4.1257111	-0.3223509	0.63133754	-0.8402918	0.75835617	1.86606557	-2.2325426	-3.6233721	-4.0046991	-3.0801233	-4.5020277	-5.5911097	-4.2709812	-5.9431496	-5.2823107	-6.0088449	-5.3343898	-5.7637224	-5.0609598	-6.2522541	-3.0091083
P_17	-3.9135167	-4.0457757	-0.5731649	0.36991001	-0.6498141	1.07062696	2.47981765	-2.0773055	-3.8836638	-4.6138196	-3.1965904	-4.4517496	-5.7268987	-4.8541659	-6.3514173	-5.0727536	-4.7217767	-4.6138196	-4.9009034	-6.459048	-5.7268987	-3.4177776
P_18	-3.45948	-2.793065	-0.5557681	0.34441396	-0.5092147	0.73804155	1.93654263	-2.1811743	-3.7807922	-3.9006131	-2.9740934	-4.1034622	-6.0899133	-3.5793815	-5.883299	-5.5596065	-5.8146025	-4.85051	-5.4301025	-4.8664593	-6.439587	-3.0624494
P_19	-3.7750482	-3.5375238	0.00067001	0.89696681	-0.4425204	1.06357437	2.24742267	-1.4561621	-4.1259697	-4.6937792	-3.5535773	-4.3840898	-7.0193132	-4.5329196	-6.0207844	-4.7736765	-4.7512456	-4.053488	-4.8898068	-5.7023307	-5.3243531	-2.8098346
P_2	-3.4901451	-3.9135725	-0.3846426	0.50636887	-0.4276999	1.00568345	2.26819165	-2.0477895	-3.9628356	-4.3749452	-3.0324068	-4.167931	-6.0422771	-4.4803057	-6.0691243	-5.4723083	-5.083206	-4.8076531	-5.5461282	-5.5065973	-6.2473726	-3.0191101
P_20	-3.5280227	-4.082533	-0.2044957	0.719063	-0.7651796	0.59888573	1.38907528	-1.8667205	-3.5072275	-4.2834122	-3.1047572	-4.5974319	-6.6847538	-4.4570559	-5.8780519	-3.2988628	-4.7889004	-4.5454325	-5.5090242	-5.8894156	-5.7023435	-2.1338125
P_21	-3.3890434	-3.1330424	-0.557311	0.42129275	0.09719413	1.57649024	2.70634982	-1.5662088	-3.8516669	-4.3299176	-2.6087829	-3.7671095	-6.0204432	-3.7202882	-5.5583592	-5.1217827	-4.5706728	-4.2938697	-4.722927	-4.9025995	-5.2845342	-2.7085546
P_22	-3.5865238	-3.631799	-0.1065743	0.8013876	-0.1154992	1.39361775	2.63495271	-1.5909889	-3.8646385	-4.3440753	-2.7917453	-4.0051536	-6.1663383	-3.9496389	-5.5466185	-5.0825851	-4.9641369	-4.5783681	-5.2033666	-4.7452578	-5.850301	-3.0447924
P_23	-3.8254209	-3.5001163	-0.492737	0.38872009	-0.3796038	1.57884689	2.79927292	-1.3299694	-3.861396	-4.5820236	-2.9321493	-4.171551	-6.1104924	-3.9470098	-5.6335684	-4.8017843	-4.2924608	-4.0450371	-4.5715366	-5.1375064	-4.9023616	-3.0273727
P_25	-3.5811756	-4.0084095	-0.6700988	0.17367748	-0.6541642	0.82391547	2.04117769	-1.7017266	-3.9008775	-4.4114621	-2.7621086	-3.878003	-5.9234016	-4.3450428	-5.9912242	-4.759568	-4.5384743	-4.4054561	-4.6137405	-5.283563	-5.1514736	-2.7697786
P_26	-3.2468172	-3.6848851	-0.7241542	0.1020972	-0.3265924	0.85480808	2.08418933	-1.8319504	-3.6498399	-4.4947014	-2.8872695	-3.8192448	-5.9494162	-4.0201989	-5.4655605	-4.9499842	-4.1013332	-4.1484007	-4.7737369	-4.6081102	-5.3578218	-2.6371829
P_27	-3.5955726	-4.153796	-0.481201	0.46046429	-0.0153102	1.21442675	2.29121629	-1.4690122	-3.4790806	-4.0720065	-2.9192876	-4.3051098	-5.2017645	-4.4425609	-6.4995055	-4.2011667	-3.8039625	-3.8365236	-4.8181411	-5.6497892	-5.3868677	-2.8984852
P_28	-4.108436	-4.2791279	-0.8088023	0.15382182	-0.6057229	1.17026071	2.6183326	-1.5415134	-3.9838605	-5.2359939	-3.4238849	-4.7748399	-6.1500844	-4.8261332	-6.4562513	-5.5920397	-3.7612208	-3.6977539	-4.5060858	-5.6110879	-4.6065046	-3.2763335
P_29	-3.393376	-3.3731733	-0.5621784	0.40528146	-0.4780815	1.17468212	2.67066333	-1.881212	-3.9570322	-4.0554124	-2.9519195	-4.2910782	-6.0699964	-3.4312809	-5.3792445	-4.6121606	-4.5760714	-4.5095879	-5.4436231	-4.2639849	-5.7253553	-2.9276607
P_3	-3.6816759	-3.9236879	-0.2959454	0.67673291	-0.546832	0.94805014	2.20810432	-2.0342162	-3.792242	-4.5703151	-2.9277941	-4.0037968	-6.4474344	-4.0862069	-5.8640579	-4.5825104	-4.088076	-4.1811436	-4.6960845	-4.9205175	-5.4030727	-2.8813941
P_30	-3.7066579	-3.6886708	-0.700529	0.2843624	-0.3023817	1.77407371	3.23148573	-1.727192	-3.4891508	-4.1941437	-2.5716362	-4.0638348	-5.9964447	-4.170591	-5.6242833	-4.3242762	-3.8278866	-3.87595	-4.2642266	-5.2776185	-4.6499492	-2.5883348
P_31	-4.0277034	-3.9908071	-0.8447735	0.1620894	-0.3473166	1.03300844	2.16765687	-2.1333777	-3.8564528	-4.7415648	-2.7989824	-3.9467849	-5.9000752	-4.7072757	-6.0868511	-5.48234	-5.1885789	-4.7027914	-4.891847	-5.3372898	-5.4440578	-3.4219818
P_32	-3.8328657	-3.6731866	-0.4201922	0.60450383	-0.7470381	1.19800133	2.62864287	-2.041438	-3.824937	-4.4320605	-3.2697026	-4.4284439	-6.6347347	-4.1322243	-5.7283287	-5.6767043	-5.8039661	-4.9898663	-5.2649696	-5.2649696	-5.8183549	-3.7599667
P_33	-3.6715386	-4.0390651	-0.559889	0.36390685	0.20938102	1.29216676	2.364391	-2.3847721	-3.8768469	-4.6673517	-3.0699016	-4.0555228	-5.8256832	-4.4215993	-5.765964	-4.7425751	-4.8721461	-4.632538	-5.0372258	-5.1172686	-5.7234044	-3.0797281
P_35	-3.7860873	-3.4556751	0.03318294	0.96595512	0.06394417	1.84458888	3.04988324	-1.2544824	-3.9383072	-4.2199182	-3.0970413	-4.5425914	-5.7931765	-3.9288209	-5.2386498	-4.8302734	-4.6196105	-4.4248083	-5.1548018	-4.6962577	-5.808522	-2.5003522
P_36	-3.8907308	-4.1141588	-0.3881741	0.47046027	-0.1541995	1.80089236	3.10445804	-1.572456	-3.5266883	-4.0561315	-2.7022355	-4.0521127	-6.0060766	-4.5624928	-6.0948047	-6.4210204	-4.6127317	-4.4214728	-4.9265125	-5.1282521	-5.2534153	-3.3936511
P_37	-3.6375128	-3.0382775	-0.3659192	0.51155239	-0.185189	1.27831361	2.41713903	-2.130573	-3.7242459	-3.9591416	-2.8718517	-3.9731109	-6.136067	-4.0388326	-5.6787768	-4.8228582	-4.2766157	-4.2553035	-4.875734	-5.3514856	-5.4038014	-2.7902774
P_38	-3.2572601	-3.4354664	-0.4326342	0.53171345	0.40764878	1.25393167	1.94155395	-2.2048297	-3.7640846	-4.8099215	-2.7984877	-4.1062776	-5.148669	-3.9333711	-5.7735829	-5.2877478	-5.4462711	-4.8345735	-5.3035793	-5.101942	-5.980895	-3.2490465
P_39	-3.8325819	-3.4454186	-0.7272224	0.1482521	-0.1638661	1.78259964	3.13845465	-1.8510785	-3.803879	-4.8100961	-2.9485294	-4.0908168	-6.3060598	-4.4977711	-5.9502944	-5.6933342	-4.8623546	-4.4497619	-4.8019825	-5.5598028	-5.29943	-3.4643268
P_4	-3.6030137	-3.4507535	-0.5698879	0.40010887	-1.0138312	1.00180736	2.47995827	-1.95978	-3.9079422	-4.2705787	-3.1819821	-4.1179019	-6.6260862	-4.0788514	-5.8248648	-5.1614228	-4.8075155	-4.8217253	-4.9095502	-4.9994065	-5.6714113	-3.3642342
P_40	-3.743853	-4.0469332	-0.6648444	0.19088125	-0.2124866	1.34854219	2.68403966	-2.063003	-4.3066573	-5.2702489	-3.2296376	-4.6500085	-6.0792279	-4.7354932	-6.003242	-5.250906	-5.1806368	-4.779945	-5.0596842	-5.557931	-5.8182141	-3.8761724
P_41	-3.4868417	-3.9033819	-0.4560128	0.37389206	-0.2370179	1.17081216	2.14997373	-2.1126791	-3.891927	-4.1036047	-2.9313034	-4.3256932	-5.3637843	-4.5907853	-6.1262789	-4.3283329	-3.9975407	-4.0244827	-4.8435735	-5.5575858	-5.2185352	-2.3004165
P_5	-3.7043784	-3.7301435	-0.3242097	0.64557131	-0.7185423	0.76207258	1.8396089	-2.499897	-3.4593823	-4.1479892	-2.5961228	-3.5610837	-5.6380096	-4.1278091	-5.9273681	-5.5241426	-5.7955159	-4.8863091	-4.9499002	-4.9858938	-6.1863823	-3.5065526
P_6	-3.3971107	-2.6505473	-0.7047418	0.39136399	-0.6391915	1.24283413	2.88473123	-1.890375	-3.7641059	-4.2311024	-2.7846022	-3.9306024	-5.8621239	-3.3963382	-5.5620193	-6.6017911	-6.0572544	-4.9422034	-5.2896047	-4.6627069	-6.0909654	-3.8010315
P_7	-3.6479995	-4.1050224	-0.3255739	0.60984014	-0.1398014	1.05755399	2.23440171	-2.0837903	-3.7030909	-4.359744	-3.1605608	-4.4316666	-6.0509326	-4.5578898	-5.9623792	-3.4487003	-3.8048525	-3.8857665	-4.723432	-5.2250259	-5.1826916	-1.9908089
P_8	-3.605398	-3.5453946	-0.8871436	0.1528162	-0.766493	1.31056011	2.71429008	-2.1659894	-3.5553875	-4.2910319	-2.4944604	-3.5482395	-6.6260743	-3.9522812	-5.5803844	-4.7678451	-5.4903582	-4.8274654	-5.137	-5.141662	-5.9696766	-3.076931
P_9	-3.7556657	-4.0204285	-0.4172704	0.5239905	-0.8761287	0.5522663	1.94962256	-2.1611767	-4.1937275	-5.3798957	-3.5572457	-4.6277399	-6.6170941	-4.5376526	-5.8777341	-5.4615737	-3.9732221	-3.7595372	-4.3729401	-5.6954125	-4.816366	-3.0544369

Table 8.121: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer.

	PC(27:0)	PC(27:1)	PC(27:2)	PC(27:3)	PC(28:3)	PC(28:4)	PC(28:5)	PC(28:6)	PC(31:0)	PC(31:1)	PC(31:2)	PC(31:3)	PC(31:3)(d2)	PC(32:0)	PC(32:1)	PC(32:2)	PC(32:2)(d2)	PC(32:3)	PC(33:0)	PC(33:0)(d2)	PC(33:1)	PC(33:1)(d2)
P_1	-4.0930891	-2.5987334	-3.0617749	-2.6154502	-3.3577488	-3.7621605	-7.7619418	-6.9097299	-2.8888525	1.11520445	0.79402111	-1.7968566	-2.2191918	2.36142471	3.29523713	1.80494389	1.30307381	1.58938918	0.22853002	-0.464477	0.74060679	1.09839105
P_10	-4.10896	-2.8442179	-2.9514821	-2.591306	-2.8680674	-3.2449806	-7.2541673	-7.3393252	-2.5859266	1.36242044	1.32529905	-1.2458557	-1.6738216	2.15986994	2.52372575	1.71764905	1.68569718	1.95007283	0.08491968	-0.286854	0.44937459	1.22546808
P_11	-3.720264	-2.1109701	-2.3680202	-2.6655582	-3.5182198	-3.73185	-8.0662316	-6.7669486	-2.4306487	1.52781667	1.35902299	-1.2655667	-2.0292893	2.21311867	2.90162083	1.84606426	1.90432771	1.94035641	0.10116767	-0.3373025	0.71295826	1.10565087
P_12	-4.1090298	-2.7421535	-2.8254088	-2.6557626	-3.1402926	-3.3923024	-7.5059627	-7.9221231	-2.7834825	1.13839534	0.8573549	-1.5566509	-2.2434931	2.24600524	2.73387697	1.85632954	1.29545548	1.83140761	-0.1103326	-0.3741792	0.16504119	1.16247843
P_13	-3.6398198	-2.8296057	-3.1517274	-2.0730847	-2.879208	-3.1645509	-7.5146063	-6.4392509	-2.7351931	1.16368478	1.00609106	-1.7152003	-1.9265831	2.17680337	2.94143171	1.54548837	1.28690985	1.60475618	0.17247382	-0.3348254	0.76981956	0.99080741
P_14	-3.9610187	-2.5074348	-2.5460383	-2.5146204	-3.3958751	-3.5458437	-6.4997657	-7.5897942	-3.1728089	1.03024709	0.91521737	-1.5215467	-2.4171273	2.15477424	3.13702664	1.8456877	1.33034466	1.77818524	0.14591925	-0.4832722	0.58018099	0.69591948
P_15	-3.2185865	-2.7000744	-2.864848	-2.2813238	-3.0759659	-3.4535017	-7.2945819	-5.5761537	-2.1895551	1.61878894	1.48677346	-1.0345949	-1.1347821	2.20637486	3.19727378	2.15878544	2.28646689	2.40184792	0.01604926	-0.2104063	0.68763784	1.28209728
P_16	-3.5643531	-2.5241918	-2.6665503	-2.6744382	-3.3764233	-3.8522137	-7.4075618	-6.4617122	-2.5463937	1.20644503	0.90674384	-1.7008669	-2.3278669	2.51968749	2.77813982	1.62684362	1.28602714	1.61932742	0.27962161	-0.0722701	0.63088571	1.06755866
P_17	-3.9703606	-2.8777411	-2.9652991	-2.1248816	-2.5744429	-2.9848255	-6.9110331	-6.6597187	-2.7026161	1.70973793	1.69535745	-1.0434022	-1.2132807	2.20083763	3.12664889	2.07802581	1.96641361	2.12226105	0.30184062	-0.0686929	1.18223818	1.05869516
P_18	-3.9795345	-2.740105	-2.9283887	-2.7318934	-3.3891757	-3.80887	-7.7440513	-6.2559743	-2.7383807	0.94284122	0.70360802	-1.8910282	-2.4389002	2.29084285	2.79694382	1.57355345	1.02959859	1.34832241	0.18470469	-0.2921628	0.59741337	1.07213683
P_19	-3.6483296	-2.1941473	-2.5836189	-2.9853887	-3.8676461	-4.2727294	-7.3811033	-6.4803167	-2.3831982	1.17483222	0.96688201	-1.8156009	-2.4018969	2.48378604	2.84358389	1.65845182	1.62082426	1.65299855	0.21954275	-0.3889361	0.58581245	0.92067922
P_2	-3.9678148	-3.1020295	-3.4247363	-2.3321028	-2.9774637	-3.3592617	-8.2869682	-6.6528377	-2.7755576	1.11496312	1.04434455	-1.6287967	-1.7096285	2.1231242	2.7050613	1.74121454	1.46234054	1.65732534	0.00867391	-0.3459617	0.55058598	0.93460879
P_20	-3.0910895	-2.6230021	-2.6774206	-2.6291237	-3.2186224	-3.6426453	-7.2475391	-6.23392	-2.4135526	1.11644592	0.81427718	-2.0535951	-2.269121	2.32199902	2.6219101	1.50111847	1.16057803	1.35399523	0.31633046	0.16206832	0.74242803	1.33724627
P_21	-3.8373416	-1.8711631	-2.156856	-3.746917	-4.6042602	-4.7123728	-8.1294435	-6.5200056	-3.1156133	1.31343611	1.30823319	-1.1366488	-3.8406293	1.96016502	2.82069753	2.06205954	1.48810443	2.02505018	-0.0389799	-0.5644377	0.63478472	0.85305728
P_22	-3.8103382	-2.9886532	-3.1188703	-3.945789	-4.3541401	-5.3139963	-7.8979938	-6.6032666	-2.9798394	1.19091877	0.97748204	-1.4949164	-3.701544	2.25835337	3.25499641	2.24193253	1.51137364	1.93397089	0.0382195	-0.6470744	0.81173527	1.07912743
P_23	-3.8190806	-1.7733833	-1.8627912	-3.5498257	-4.0198294	-4.5670756	-8.5953991	-8.0845735	-2.6961869	1.45097595	1.46801529	-1.0634895	-2.977114	2.01079811	2.89660317	2.08179745	1.81666156	2.15170814	0.16895362	-0.5488497	0.94650866	0.95611673
P_25	-3.774694	-2.6340623	-2.9020442	-2.5192941	-2.6949543	-3.2374518	-6.0452915	-6.1984139	-2.5306184	1.30830045	1.32674509	-1.388396	-1.9844228	2.0057091	2.64458023	1.73761615	1.46173436	1.61365277	0.08793249	-0.1613674	0.8081054	1.19919616
P_26	-3.4767443	-2.3184023	-2.5929828	-2.2256378	-2.891092	-3.2540353	-6.9345465	-5.9239911	-2.8888772	0.88955925	0.76575908	-1.7628877	-2.2280238	1.97362263	2.54459622	1.77177831	1.14043172	1.47662948	-0.210949	-0.2377819	0.21088526	1.01068719
P_27	-4.3193753	-2.3410197	-2.4119637	-2.4160962	-3.1999092	-3.6204975	-6.6452173	-6.3502092	-2.6504403	1.12863699	0.93366008	-1.8047425	-2.2381394	2.3111286	3.1995662	1.76164007	1.49467228	1.62385888	-0.0347852	-0.2617603	0.63315452	0.92306576
P_28	-4.0003688	-2.2955043	-2.5151043	-2.4675437	-2.9211495	-3.4435005	-7.3287394	-7.1345834	-2.2253947	1.62011559	1.62737208	-0.9248696	-1.9719847	2.40122774	2.97902206	1.8604211	1.98433804	2.04934052	0.3046821	0.04384991	1.01037748	1.27724928
P_29	-4.39214	-2.4870093	-2.7989186	-2.789697	-3.2630178	-3.7423687	-8.1164938	-7.1496508	-3.0916391	0.95166837	0.88237537	-1.5002799	-2.6068056	2.11856378	2.71988737	2.02682688	1.33723128	1.8214399	-0.3626636	-0.6725051	0.17395677	0.98232306
P_3	-2.9888403	-2.5324455	-2.8349122	-2.5888957	-3.1141696	-3.4782901	-6.9354205	-5.7998647	-2.3292831	1.11477869	0.80775823	-1.6566478	-2.0742337	2.35787245	2.71589427	1.62636971	1.24672392	1.70468659	0.25132187	-0.2028254	0.74171092	1.39581223
P_30	-3.8325239	-2.215413	-2.5669426	-2.9360836	-3.7682344	-3.9257115	-7.7485389	-6.5750253	-3.0794554	1.29314611	1.23554893	-1.0245462	-3.0146824	1.86579661	2.92527136	2.03356226	1.6298297	2.06990806	-0.0473086	-0.4485389	0.81917629	0.88336892
P_31	-3.445246	-3.0555966	-3.2256712	-2.4996188	-2.9705619	-3.3587649	-7.2500019	-6.3394419	-2.2441399	1.47388483	1.49690519	-1.212131	-1.7015931	2.36649665	2.97322684	1.96289233	1.85017914	2.00762817	0.31939513	-0.0428195	0.93052702	1.53995403
P_32	-3.4857889	-2.3192157	-2.5768387	-3.4337224	-3.967962	-4.2810202	-8.1806592	-6.4018031	-2.2312193	1.43785544	1.32672697	-1.4743612	-2.4697229	2.61482482	2.76221313	1.52929029	1.66400476	1.67938675	0.4978807	-0.2894435	0.85246656	1.24990355
P_33	-3.8228182	-2.306285	-2.4244858	-4.0625343	-4.7287818	-5.0096379	-8.2654694	-6.8360029	-2.8686385	1.38969628	1.37957881	-1.3802004	-3.6120694	2.06404683	2.94427487	1.96537967	1.83910612	1.83077282	0.05993638	-0.0354408	0.84458252	1.02895796
P_35	-3.6714926	-2.4056079	-2.5989679	-3.7284364	-5.060223	-5.3626474	-7.4928613	-6.5765705	-3.0430462	0.90080115	0.75766453	-1.9048846	-3.6147398	2.67969983	3.4869087	1.87493385	1.44741136	1.56642686	0.10974807	-0.7046093	0.60214444	0.62544513
P_36	-3.6124787	-2.8402831	-3.1438757	-3.6202608	-4.1056602	-4.4390342	-8.2716204	-6.9559436	-2.3331252	1.33370612	1.17846673	-1.5831525	-2.9384625	2.3264837	3.00796309	1.70145257	1.70065515	1.57603726	0.39469787	-0.2528154	1.00715146	1.17800168
P_37	-3.5516681	-2.0450969	-2.3389058	-3.8150361	-4.426495	-4.9126045	-7.0820495	-6.0301747	-3.0268161	1.21920697	1.26659208	-1.4161444	-3.6065159	2.00623002	2.91260202	2.01695667	1.47978696	1.78508449	-0.0804796	-0.2533374	0.6701208	0.90559128
P_38	-3.4972981	-2.8037142	-3.1327036	-2.2376315	-2.7109877	-3.1236428	-6.7905172	-6.1394183	-3.1452209	1.23864352	1.1686231	-1.4541676	-2.2734713	1.80489115	2.87208729	1.7980638	1.49164441	1.73590853	-0.3978121	-0.303711	0.48157069	1.03211605
P_39	-3.0326958	-2.6054315	-2.9539254	-2.9767817	-3.5176873	-3.9123054	-7.7107033	-5.6174685	-2.5783968	1.61436354	1.65477135	-0.9783602	-2.1224842	1.96443034	2.9007087	1.84175204	1.93755976	1.97339517	0.1832556	-0.1963881	0.90203569	1.08730953
P_4	-4.1187872	-2.3504774	-2.4893557	-2.5962802	-3.2993313	-3.4704744	-7.0047401	-6.9431822	-2.7605625	1.23252922	1.01695909	-1.4477282	-2.124105	2.2861923	2.47725702	1.59755844	1.24500515	1.63336634	0.23483946	-0.4431483	0.62868334	0.84456516
P_40	-4.5294283	-2.2704235	-2.6615013	-2.6342655	-3.0896549	-3.5210491	-7.5573299	-6.688292	-2.4530174	1.53504093	1.57252188	-0.970946	-1.6924975	2.30881522	3.13903187	2.12617981	2.06227865	2.18448683	0.23362065	-0.2500244	1.04528564	1.3035076
P_41	-4.0555185	-1.9860189	-2.015405	-2.4532153	-3.0194049	-3.2834126	-7.0586557	-6.737748	-2.8159688	1.25397031	1.23690629	-1.3624696	-2.4958572	2.08029315	2.77660435	1.7817269	1.39796944	1.66363814	0.21211786	-0.2900693	0.78464693	0.7816679
P_5	-3.622102	-3.411622	-3.4622305	-2.5586846	-3.1258398	-3.5460835	-8.2922571	-6.2491832	-2.3882585	1.27578274	0.95697431	-1.5980487	-2.0556079	2.29518917	2.5072573	1.54963621	1.32998955	1.71200947	0.15370096	-0.1108763	0.52389722	1.36471322
P_6	-4.1458719	-2.9612019	-3.0606937	-2.4446953	-2.9062671	-3.2909005	-6.3805541	-7.6448335	-3.0670623	1.20398236	1.15792467	-1.2103304	-2.0803131	2.05352962	2.54821376	1.82147025	1.34815396	1.7722947	-0.1794876	-0.6821039	0.44070322	0.90156158
P_7	-3.7931641	-3.070126	-3.4274277	-2.6988649	-3.26227	-3.8028949	-8.1940899	-6.5535614	-2.7493964	1.27372421	1.15035337	-1.6596893	-2.1938482	2.12547116	2.84938332	1.91410917	1.50288797	1.73077794	-0.0095909	-0.3219959	0.54294029	0.76093024
P_8	-3.8554204	-3.0733807	-3.4861078	-2.2960194	-2.8196409	-3.1947511	-7.8685807	-6.3409728	-2.4817947	1.49982511	1.36102993	-1.2485075	-1.836437	1.93897199	2.47994516	1.72846901	1.37836706	1.68375995	-0.1208914	-0.3154627	0.43360537	1.27880464
P_9	-3.4652825	-1.952381	-2.1050473	-2.3154058	-2.9905934	-3.3574395	-7.785665	-6.5391326	-2.0274492	1.51717529	1.28219474	-1.4396473	-1.64064	2.56258502	2.94089232	1.71046871	1.88088319	1.87598913	0.28302396	0.1220026	0.77709994	1.60425041

Table 8.122: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer.

	PC(33:2)	PC(33:3)	PC(33:4)	PC(33:4)(d2)	PC(34:0)	PC(34:0)(d2)	PC(34:1)	PC(34:2)	PC(34:3)	PC(34:4)	PC(34:4)(d2)	PC(34:5)	PC(35:0)	PC(35:0)(d2)	PC(35:0)(d3)	PC(35:1)	PC(35:1)(d2)	PC(35:2)	PC(35:2)(d2)	PC(35:3)	PC(35:4)	PC(35:4)(d2)
P_1	0.20162628	-1.6137682	-3.0891129	-2.4475474	2.4016635	1.33341725	4.95989619	4.66030552	2.5312354	0.46205533	0.03735922	-1.1304399	-0.8226544	-0.8928198	-2.7205209	1.57952366	0.2626044	1.14442361	0.89605631	-1.5928361	1.68330444	-0.8350264
P_10	0.17469925	-1.0778335	-2.543351	-1.8942175	1.83525217	1.28395629	4.47130862	4.57903757	2.1603426	-0.3695554	0.44438948	-1.7479237	-0.81257	-0.7801192	-2.5444533	1.57878653	0.47848814	1.50537961	1.20097674	-1.0012416	1.78321323	-0.2295365
P_11	0.65519864	-1.4265737	-2.7609938	-2.2456542	1.88578417	0.88829135	4.51855654	4.79091703	2.44789975	0.03858934	0.5583201	-1.8997639	-0.6997865	-1.1303749	-2.9569248	1.67904797	0.48328893	1.72763327	1.22841927	-1.4928619	1.99173038	-0.7459621
P_12	0.30369083	-1.5533275	-3.119425	-2.288717	1.81310799	1.09164493	4.43244584	4.47743765	2.34578236	0.27766899	0.30443308	-1.9368876	-1.4270038	-1.1176875	-2.5428206	1.07430113	0.32485179	1.22551787	0.77990994	-1.1265978	1.4686095	-0.3869126
P_13	0.31899389	-1.0579991	-2.8315177	-1.8440122	2.16470696	1.00082669	4.74285507	4.65459788	2.45985856	0.32228101	0.50930754	-1.5913653	-0.8243639	-0.8290898	-2.9760919	1.64364914	0.28516112	1.32960568	1.02901388	-1.3693114	1.66931925	-0.4532424
P_14	0.26189688	-1.3346842	-3.2406749	-2.1730103	2.2144862	1.15327519	4.79349745	4.52387533	2.44044796	0.73874354	0.15992603	-1.4272354	-0.9166908	-0.7153041	-2.7383651	1.56137031	0.34615087	1.03872473	0.81072109	-1.1562772	1.51393698	-0.5249475
P_15	0.41723832	-0.8543606	-2.1167216	-1.6145127	1.81186824	0.62100962	4.42842028	4.52536781	2.27965845	0.20807272	0.75067609	-1.731572	-0.6470508	-1.2075317	-2.5864176	1.51424915	0.65485181	1.35435167	1.15322872	-0.76534	2.37301068	0.11675463
P_16	0.34053151	-1.5393954	-2.9158403	-2.3155001	2.10223115	1.58516661	4.71123843	4.82857673	2.44894687	0.28524737	0.59173924	-1.3032151	-0.8214936	-0.7966975	-2.5479432	1.70534494	0.24368918	1.46751565	1.03673273	-1.5071851	1.53211098	-0.7179625
P_17	0.95942609	-0.9066612	-2.6978479	-1.7881326	2.11962721	0.93723153	4.69797853	4.8519845	2.40063501	-0.0345842	0.19650935	-1.8422412	-0.5896869	-0.8203699	-2.675892	1.79022416	0.70494267	1.69552077	1.1574146	-1.0395191	1.63845784	-0.22982
P_18	0.39057541	-1.4755505	-3.3467843	-2.326048	2.14886915	1.44039377	4.74463078	4.78377732	2.4069579	0.25795435	-0.013864	-1.4705276	-0.9291635	-0.7327343	-2.4139585	1.5728474	0.41308159	1.393789	0.96645516	-1.197963	1.73765442	-0.6744202
P_19	0.09835562	-1.8257613	-3.0303292	-2.6211233	1.89912906	1.19682796	4.51915815	4.53742063	2.2879756	0.14229493	0.46809054	-1.5738852	-1.1675213	-0.8605954	-2.8277663	1.45143954	1.45143954	1.02124871	0.92647622	-1.9573965	1.65139473	-1.1869072
P_2	0.51971791	-1.0111469	-2.9839743	-1.8135599	1.88806965	1.12468924	4.51881126	4.82997362	2.40810533	0.18837381	0.14727806	-1.6717401	-1.0014188	-1.0211889	-2.69156	1.38829258	1.38829258	1.50185176	0.90142687	-0.9720409	1.49548101	-0.4056916
P_20	0.70094036	-1.5657751	-3.11433	-2.3420997	2.10697087	1.34921667	4.73046635	4.81627515	2.51483792	0.17829542	0.32036943	-1.8446616	-0.960507	-0.6457958	-2.3039937	1.60943512	0.66820653	1.54996908	1.22161164	-1.3818268	1.52678416	-0.8635446
P_21	0.90163619	-2.8460368	-3.9587554	-3.2972972	1.93453229	1.03142924	4.57195906	4.79142545	2.64959192	0.31283644	-0.0276082	-1.4568032	-0.8765395	-0.9374421	-2.6825338	1.59400545	0.51481217	1.66936327	1.10726999	-2.5062928	1.51271562	-1.3008613
P_22	0.75109569	-2.9233312	-3.6814316	-3.6836464	2.36129231	1.09666263	4.97433249	5.13693891	3.0135347	0.47619469	0.02403155	-1.2403679	-1.0019063	-1.083396	-2.9794738	1.60724876	0.32435842	1.64635864	1.07128723	-2.7357826	1.25435192	-1.4580845
P_23	0.80630517	-2.2725347	-3.6950748	-3.135459	1.94222405	0.99000446	4.5770785	4.78283237	2.36080369	0.12398637	-0.1049435	-1.1821323	-0.7927129	-0.8348965	-2.9092715	1.85890854	1.85890854	1.8223432	1.12359956	-2.554946	1.6011498	-1.1005518
P_25	0.60145172	-1.3660794	-3.2734746	-2.2574609	1.82114923	1.08659453	4.43222132	4.66848069	2.27039282	0.02310555	-0.2011031	-1.8256022	-1.0155396	-0.7633419	-2.4752373	1.62832779	0.58736886	1.56863995	1.24824259	-1.3669397	1.77948021	-0.4090919
P_26	0.57624257	-1.1402022	-3.5124953	-1.9520427	1.8109063	1.19124428	4.48661635	4.81422791	2.62501128	0.376357	-0.4885713	-1.3934182	-1.2677222	-1.0204845	-2.2835462	1.26268835	0.48693362	1.30950057	1.05325121	-0.6602175	1.42349191	-0.3397086
P_27	0.17411385	-1.42911	-3.4224276	-2.2511313	2.05153876	1.18036088	4.64962423	4.59027782	2.39845369	0.27425341	-0.312739	-1.6133706	-1.271256	-1.0229001	-2.512721	1.32091703	0.4032543	0.86098118	0.82735034	-1.4558617	1.57725211	-0.6546355
P_28	0.66488058	-1.588143	-3.141794	-2.4118917	1.94699068	0.94821856	4.56966976	4.74653585	2.19262194	-0.058029	0.17761686	-1.7337625	-0.3841013	-1.1525752	-2.6908946	1.89455596	0.72628225	1.66165764	1.32088457	-1.8377377	2.19825307	-0.5401297
P_29	0.29753399	-1.5168249	-3.3696312	-2.3180748	2.05101476	1.25838438	4.65988553	4.67921595	2.25098163	0.32563255	-0.5320784	-0.9178948	-0.9713561	-1.1922457	-2.6835808	1.36177084	1.36177084	1.08492167	0.89509748	-1.3126187	1.44798719	-0.4746982
P_3	0.50055973	-1.5360908	-2.797162	-2.3585503	2.20140003	1.22964496	4.78763266	4.87380744	2.40762327	-0.0065194	0.39104508	-2.0439806	-0.916435	-0.9896622	-2.8499865	1.8191957	0.38184542	1.5323113	1.08441507	-1.8218794	1.75310121	-0.6168594
P_30	0.69320491	-2.1372373	-3.5275617	-3.0477556	1.88356635	0.78716851	4.48887688	4.47257226	2.36372549	0.33397662	-0.1328956	-0.6591845	-1.1257139	-0.9089197	-2.7631075	1.6110803	0.57194168	1.42695119	0.90246814	-2.3475145	1.48835252	-0.8497907
P_31	0.7034771	-1.2843681	-2.8356464	-2.2524036	2.08433957	1.04587462	4.67413554	4.84193515	2.28569609	-0.0085742	0.00593231	-2.1456161	-0.586395	-1.1727529	-2.7269719	1.73764123	0.60130344	1.65778057	1.25908421	-1.5773662	2.19597281	-0.3289638
P_32	0.32727589	-2.1605698	-3.0645095	-3.1258843	1.97237713	1.30802362	4.60860968	4.74450931	2.13889857	-0.2962275	0.52254106	-1.6466468	-0.6787275	-0.7029244	-2.7683266	1.77550839	1.77550839	1.67198841	1.09168765	-1.8212184	1.96652539	-2.0028747
P_33	0.75921443	-2.8161998	-3.6597112	-3.5058125	2.21066628	1.22609694	4.82877344	5.05454255	2.41103063	0.32106325	-0.0200849	-1.6642393	-0.4808248	-1.0974335	-2.4202214	1.7940863	0.66576378	1.77117262	1.34342202	-2.4092183	1.9548513	-1.6490893
P_35	-0.0975831	-2.9430863	-3.9689547	-3.455185	2.50672151	1.65030898	5.11173719	4.70991679	2.64245865	0.70586222	-0.7094732	-0.3248593	-1.1276803	-0.8711967	-2.6879299	1.52049728	0.0337815	0.7612702	0.74408143	-2.7863386	1.18603497	-2.0215247
P_36	0.4239928	-2.3845068	-4.0348823	-3.3589655	2.0255602	0.94147979	4.63948846	4.6698139	2.13180186	0.18921405	-0.3039307	-0.8452337	-0.8179005	-0.7948907	-2.7688791	1.92099249	0.53260919	1.48982693	1.22023533	-2.1250965	2.06312404	-2.0290435
P_37	0.71518548	-2.6770022	-4.1091793	-3.6141755	2.01068058	1.11634125	4.65823668	4.95611922	2.58553015	0.25568973	-0.4389557	-1.3329183	-0.9899032	-0.8522694	-2.3691928	1.61346409	0.66194465	1.57979656	1.25261936	-2.3575754	1.33738584	-1.40708
P_38	0.41260817	-1.0938186	-3.1572748	-1.9619211	1.99240833	0.86909802	4.61528031	4.60049464	2.48537185	0.24945243	-0.0930473	-2.0872599	-1.1129982	-1.0751162	-2.397667	1.40843283	0.76615673	1.15301915	1.07544273	-0.7940651	1.88178151	-0.1656086
P_39	0.4986353	-1.7298505	-3.2375842	-2.593597	1.77998952	0.83316062	4.3924055	4.43278363	1.91858856	-0.2588596	-0.1140321	-1.2628694	-0.9044887	-0.4200316	-2.6431977	1.81292186	0.79777793	1.56309858	1.26924038	-1.8139566	2.08525055	-0.724856
P_4	0.49692943	-1.5641105	-2.9263959	-2.3641721	1.74560357	1.21383313	4.34261062	4.49743815	2.32175236	0.41609542	0.59922118	-0.7316834	-0.9599981	-0.7679978	-2.728074	1.48326947	0.05281629	1.40215981	0.7643233	-1.3867576	1.46375294	-0.7501789
P_40	0.61075312	-1.2837274	-2.9255926	-2.1124178	2.27104449	1.26015595	4.87919206	4.78923491	2.41864651	0.02221146	-0.1259618	-1.9834225	-0.751224	-0.9059568	-2.9684454	1.89849345	0.52181147	1.62734551	1.29054411	-1.7631443	2.04508639	-0.4499989
P_41	0.68342953	-1.5214811	-3.8721914	-2.4240579	1.81118133	1.19001129	4.44649691	4.61232261	2.33576929	0.24189921	-0.5065335	-1.7328152	-1.0227218	-0.5626352	-2.3870906	1.63611129	0.46105134	1.49048911	0.89552199	-1.3848682	1.44304785	-0.6614558
P_5	0.32359137	-1.463545	-2.6385155	-2.2540452	2.1068018	1.23062872	4.73106832	4.98655339	2.42508976	-0.0786818	0.76047668	-1.9853303	-0.8344417	-0.8796224	-2.5029524	1.51526618	0.49782722	1.68181211	1.39794446	-1.5323391	1.6615603	-0.5869624
P_6	0.62209491	-1.3843223	-3.2146604	-2.1358829	1.70536518	1.08109947	4.34474456	4.61212365	2.33086787	0.14039302	0.02286845	-0.9189242	-1.1227407	-0.9021441	-2.7733567	1.34060841	0.21116154	1.4910425	0.79158339	-1.0843764	1.22356838	-0.3628528
P_7	0.22150174	-1.4999188	-3.4500736	-2.3708883	1.82858784	1.09456046	4.44216935	4.52969885	2.39064799	0.63679157	0.13456451	-1.4581849	-1.2199065	-0.9370872	-2.8323037	1.40479066	0.3746765	1.13161651	0.8166949	-1.3310568	1.63412094	-0.7130088
P_8	0.62365357	-1.1634226	-2.9485998	-2.0458519	1.62171823	0.90745957	4.2734965	4.7268331	2.34039506	0.03399917	0.4317882	-1.1930278	-0.8720299	-0.8476881	-2.544178	1.37921026	0.65587886	1.6311697	1.35938203	-1.1721198	1.94131411	-0.264932
P_9	0.249121	-1.0284799	-2.4158362	-1.8670049	1.89739542	1.17290867	4.52801679	4.56126578	2.30202278	-0.0876556	0.55363854	-2.1673141	-0.7337717	-0.9335603	-2.4162411	1.65899795	0.66753214	1.36533146	1.44653046	-1.2770255	1.80633769	-0.3954836

Table 8.123: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer.

	PC(35:5)	PC(35:5)(2)	PC(35:5)(3)	PC(35:6)	PC(35:6)(2)	PC(36:0)	PC(36:0)_1	PC(36:1)	PC(36:2)	PC(36:3)	PC(36:4)	PC(36:4)(2)	PC(36:5)	PC(36:6)	PC(37:1)	PC(37:2)	PC(37:2)(2)	PC(37:3)	PC(37:3)(2)	PC(37:4)	PC(37:4)(2)	PC(37:5)
P_1	0.03590188	0.01308785	-1.7349104	-1.3123433	-1.1235094	1.77192784	0.38682296	4.1491225	4.5953733	4.0207847	2.11739795	4.08323226	3.42374751	0.34514453	2.29952608	1.39033837	1.32001258	2.60018553	1.63465208	1.17170878	1.8860193	1.73832128
P_10	0.2960002	0.75419144	-1.0943387	-1.5049044	-1.1521111	1.46234498	-0.0206088	3.85220579	4.54368738	3.49214232	2.05653167	3.5034437	3.27493173	-0.2991196	2.75168154	1.73359819	1.84113088	1.03306318	1.52002567	1.1306087	1.63049377	2.21075355
P_11	0.58930222	-0.3030922	-1.5144372	-1.4770759	-1.4723503	1.42766567	0.0263986	3.90107751	4.61198751	3.85725706	1.93872389	3.46836021	2.05077555	-0.540981	3.2679831	1.95387781	2.24083594	1.20686966	1.79952811	1.18170957	1.678042	2.08988494
P_12	-0.1133545	-1.2097551	-1.3204986	-1.8105128	-1.3504724	1.36132677	-0.0744866	3.77438357	4.46647198	3.62451035	1.86278065	3.76780113	2.45813741	-0.3283753	2.17690997	1.34877202	1.37569033	1.77587657	1.45905373	1.06730103	1.79903188	2.00316851
P_13	-0.0190644	-0.4142947	-1.3482472	-1.4183159	-1.3807596	1.6739925	0.2575364	4.04344907	4.64247472	3.99868286	1.88664789	3.90020015	2.81298307	-0.4751576	2.57664627	1.46990585	1.56136683	2.25241943	1.58227183	0.94866943	1.79104735	1.78179468
P_14	-0.4782194	-0.559481	-1.3353739	-1.4527874	-1.3158051	1.59891122	0.1723	3.97020515	4.32293385	3.97806027	1.82471073	4.23159283	2.98925864	-0.2472308	2.55471608	1.44562788	1.59363864	2.36707488	1.64794429	1.05488068	1.8524939	1.44302229
P_15	0.17121215	-0.2243986	-0.8932679	-1.0729079	-1.6922395	1.51046152	0.02242926	3.8033881	4.30539659	3.93053581	1.3369027	4.04130293	2.0172369	-0.816631	3.26746529	2.02378088	2.32451511	1.0132735	2.02412626	1.47799553	1.95219558	2.33735935
P_16	-0.1963187	-0.0222998	-1.5640173	-1.3529464	-0.8748273	1.63979782	0.19958368	4.03081337	4.7438823	3.90920344	2.30891376	3.7575009	3.14271747	-0.1914582	2.57291577	1.73987077	1.57764559	1.94908864	1.58904689	0.98910652	1.7154381	1.74927763
P_17	0.13384086	-0.5161591	-1.2138797	-1.3658557	-1.4540345	1.60800837	0.16278125	3.9884831	4.6638987	3.85668278	1.72685316	3.64529056	2.54739287	-0.5306382	3.07026664	1.7975741	2.08230552	1.55176423	1.79198145	1.01492461	1.86441701	1.79320854
P_18	-0.6816883	-0.1740942	-1.6666713	-1.6206817	-1.0651703	1.83491231	0.42351142	4.22728185	4.79650718	4.01841075	2.42503042	3.73801778	3.05169651	-0.0781373	2.44054566	1.42051432	1.49931477	1.91478444	1.63109862	1.11341908	1.95996036	1.85111985
P_19	0.78681609	-0.280928	-1.8598475	-1.3864387	-1.2648716	1.41235709	-0.0310154	3.77536335	4.40138847	3.76545612	1.55678883	3.62542394	2.50513248	-0.4696369	2.69241156	1.50284974	1.69067329	2.17574127	1.50918016	0.74181581	1.62038517	1.74087096
P_2	0.21972	-0.4709796	-1.2790848	-1.697612	-1.3081139	1.57116888	0.22725808	4.01680664	4.79374757	3.9024919	2.14843537	3.74839581	2.69040446	-0.3468963	2.63071008	1.40536226	1.74070131	1.74553352	1.5405322	0.90426579	1.70564281	1.74105453
P_20	-0.1496227	-0.8421637	-1.7490057	-1.5488809	-1.15417	1.76900883	0.28767453	4.12748632	4.80501088	3.99481979	2.21018551	3.63838806	2.52501811	-0.4090148	2.25295527	1.38936316	1.3832367	1.98085726	1.63096139	1.02389562	2.04869757	1.836855
P_21	-0.3186206	-0.2920786	-2.3927422	-1.7686939	-1.4675888	1.65249992	0.23205913	4.08697996	4.7356186	3.92120028	2.5151677	3.65620589	2.98309451	-0.0584	2.80733668	1.84075455	1.88088923	1.31080784	1.70075264	1.04435733	1.68476462	1.72675113
P_22	0.20843024	-0.5305062	-2.4253031	-1.4065118	-1.4770222	1.75558583	0.39719269	4.23191892	4.91830979	4.22699785	2.81861046	3.54518815	3.15181625	0.21725806	2.7811433	1.86598453	1.817654	2.09174025	1.7322207	0.80602744	1.4650419	1.59413254
P_23	0.40518687	0.28450248	-2.2036216	-1.7203392	-1.4986087	1.45783303	-0.0056527	3.90259227	4.59650652	3.99225431	2.00276573	3.88606257	3.66604204	0.34067986	2.83695332	2.02925605	1.90323456	1.38200862	1.9220346	1.4107541	1.70851032	1.91305086
P_25	0.3501247	-0.1632939	-1.5231004	-1.8619228	-1.4002479	1.56049719	0.10854386	3.96682459	4.59791876	3.76268845	2.14171415	3.55427757	2.58160613	-0.207759	2.73549126	1.74439312	1.82152546	1.49548413	1.75599882	1.08084543	1.85770264	1.91630471
P_26	0.2149913	-0.8607078	-1.3327671	-1.9249079	-1.3382981	1.54225561	0.15370873	4.02919038	4.79633748	3.88131859	2.60336037	3.61768041	2.76324777	-0.0917283	2.70694014	1.45889325	1.78605467	1.53419265	1.41670335	0.77863213	1.79064157	1.75545375
P_27	0.34832886	-0.7895837	-1.6841568	-1.6942349	-1.3798384	1.72995593	0.34450645	4.11116546	4.51162368	3.96185567	2.02060211	4.00376965	2.99320948	-0.0896652	2.60386103	1.3213252	1.66567983	2.22503255	1.42767213	0.79985662	1.92167136	1.74481076
P_28	0.74134044	0.10213702	-1.6471052	-1.5270527	-1.5718676	1.52037998	0.06777115	3.92080488	4.5748	3.99049077	1.60692442	4.02557544	3.01521146	-0.4163165	3.2272556	2.09361712	2.24854054	1.23655663	2.06131495	1.50169916	2.18710365	2.36629086
P_29	0.4625816	0.1765368	-1.4651134	-1.7353047	-1.3254804	1.65499557	0.22423619	4.06430889	4.60782883	3.71823493	2.28782403	3.73354417	3.65101186	0.4280407	2.7232396	1.62728133	1.81000111	1.6226016	1.33013592	0.77883136	1.33218666	1.69733037
P_3	-0.6121027	-0.9116606	-1.4586871	-1.3484135	-1.2597168	1.50668753	0.13001375	3.93123118	4.74214487	3.89645939	2.04701699	3.80562171	2.33479275	-0.8213102	2.02947708	1.47678483	1.14133534	1.74594119	1.63931702	1.14002162	2.0695449	2.14651445
P_30	-0.1954096	0.41263627	-1.9260849	-1.7658629	-1.7402992	1.57119086	0.17647399	4.00338089	4.44084916	3.72999834	2.35476762	3.75904231	3.91671244	0.6871405	2.88290297	1.88580043	1.93547752	1.16798507	1.70542455	1.20374292	1.64157534	1.94322094
P_31	0.45587812	-0.6974125	-1.4254356	-1.5944098	-1.4283941	1.40713705	0.01390817	3.88495659	4.65014709	3.95878838	1.59446212	4.25277219	2.43889115	-0.6762419	2.7510219	1.87166647	1.8221661	1.49567369	1.87865416	1.52911588	2.28347936	2.47984627
P_32	0.44607806	0.70207415	-2.1320149	-1.4253381	-1.1219672	1.36486688	-0.0205366	3.81414336	4.58926903	3.8173598	1.86968547	3.94901078	3.32044203	-0.4200282	2.72713842	1.8355456	1.68110853	1.54500743	1.71230394	1.41945458	1.77824851	2.26790378
P_33	0.0419754	-0.3458566	-2.6886294	-1.500634	-1.3106061	1.89842574	0.51334568	4.34824675	4.97799957	4.14530531	2.42430335	4.0510986	2.57123886	-0.296763	3.01132559	1.69595958	2.01782752	1.28221256	1.79401082	1.26588398	2.17307256	2.01456318
P_35	0.40854694	0.30517154	-3.2852707	-1.3228438	-0.9380577	1.82540134	0.40710615	4.21497676	4.51492083	3.86355008	2.19775274	4.07292886	4.12451255	0.80142446	2.77931407	1.41058401	1.77606243	2.70634163	1.12504164	0.48270339	1.55989894	1.42344356
P_36	0.41267302	0.7967269	-2.148729	-1.6503358	-1.5489906	1.37099222	-0.0220453	3.89656249	4.50630993	3.87794153	1.7888942	3.96912328	3.64178199	0.41116426	3.17296879	1.8828204	2.11975534	1.74872854	1.79391642	1.3745967	1.86014657	2.24584321
P_37	0.11716835	-0.2912899	-2.4993211	-1.7213363	-1.4254352	1.75060014	0.35820173	4.22330689	4.92143107	3.92051711	2.61247514	3.30189794	3.00456749	-0.0115931	2.81789134	1.65186445	1.9047277	1.74586447	1.63833498	0.70176223	1.63477124	1.46752069
P_38	-0.0270127	-0.8716233	-1.297601	-1.8145951	-1.6526448	1.68334841	0.27686283	4.12501993	4.57509262	3.99674227	2.18334553	3.8919039	2.49539654	-0.7596623	2.9029789	1.49022964	1.97845045	1.45838739	1.68335824	0.99726992	1.96644111	1.88800822
P_39	0.25351676	0.83439319	-1.7636359	-1.6083934	-1.6466598	1.54395512	0.06668578	3.9098474	4.38743469	3.69662412	1.92380272	3.79190912	3.40146756	-0.0696547	3.22282813	1.89167411	2.21937565	0.8927219	1.85021825	1.41607827	2.07010587	2.21586757
P_4	-0.1045051	0.2405413	-1.4938748	-1.6174094	-1.1571093	1.43518116	-0.0139868	3.78594935	4.51978671	3.54707908	1.98377333	3.72871057	3.68887263	0.48331358	2.51363456	1.61185304	1.52014094	1.6958508	1.47881425	1.10107053	1.49858597	1.74154465
P_40	0.65429926	-0.6961422	-1.523506	-1.436103	-1.242111	1.72187621	0.33214371	4.20871371	4.77245828	4.11717402	1.95465239	3.92261738	2.49563484	-0.5181415	3.13979915	1.97849959	2.1376659	1.31859693	1.87616023	1.32247448	2.00806454	2.36158615
P_41	0.68873104	-0.8793668	-1.7203383	-1.9657349	-1.3287753	1.76852103	0.32871897	4.12407619	4.64113334	3.88088874	2.19688925	3.62774684	2.56640232	-0.2617565	2.81921599	1.55646339	1.87131631	1.7896828	1.64863055	0.98085906	1.77393001	1.63128633
P_5	-0.3741484	-0.2132145	-1.4425093	-1.3326551	-1.189405	1.37775699	-0.0051781	3.89322615	4.72647099	3.91419802	2.36590778	3.42625881	2.47197379	-0.9440373	2.29375359	1.5828347	1.49388175	1.45017688	1.71312932	1.05913015	1.84728464	1.93291019
P_6	0.37812541	0.03942842	-1.266132	-1.8490222	-1.3696644	1.44035113	0.00750685	3.8827766	4.58574137	3.61505989	2.114637	3.62445058	3.51028318	0.38656941	2.69263308	1.71720901	1.79987584	1.45752732	1.48151404	1.00970274	1.28302926	1.68055224
P_7	0.26894713	-0.843709	-1.7159037	-1.7547396	-1.3436293	1.52079214	0.08937759	3.90702707	4.47176951	3.7807957	1.78012091	3.85533905	2.67368621	-0.1152875	2.85429902	1.4329088	1.84728824	1.92556955	1.57645852	0.93819215	1.91996344	1.78783903
P_8	-0.6164255	0.5005267	-1.2993498	-1.7584605	-1.5091922	1.32516559	-0.1335377	3.72335692	4.610481	3.67041411	2.48360588	3.30608491	2.95848878	-0.0118186	2.61817437	1.64518412	1.76953591	0.90704043	1.59587294	1.0737168	1.83052589	2.22520246
P_9	0.9223785	-0.6174536	-1.3128484	-1.4955462	-1.2564366	1.42739342	0.00504902	3.86424768	4.43630775	3.92978313	1.88024931	3.12729631	1.58233294	-0.9253204	3.19469147	1.85670057	2.21681173	1.66392163	1.78359563	1.09662411	1.63315189	2.0586032

Table 8.124: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer.

	PC(37:5)(2)	PC(38:0)	PC(38:1)	PC(38:2)	PC(38:3)	PC(38:4)	PC(38:5)	PC(38:6)	PC(39:0)	PC(39:0)(2)	PC(39:1)	PC(39:1)(2)	PC(39:2)	PC(39:3)	PC(39:4)	PC(39:4)(2)	PC(39:5)	PC(39:5)(2)	PC(40:0)	PC(40:0)(2)	PC(40:1)	PC(40:2)
P_1	1.4185933	-0.3080603	2.46841666	3.54421187	4.17953992	3.91305447	3.47606081	3.66513729	1.24841159	1.38167656	0.93022421	1.56210284	0.97170785	0.9131213	3.23956423	1.20062667	1.01533724	-0.4285131	1.73617465	0.02047734	1.7016686	-0.9003387
P_10	1.14108879	-0.1375248	2.71271171	3.73598247	3.68781701	3.51521306	3.57708365	4.03574976	1.81438608	0.90919234	0.45590063	0.86646385	1.11280079	0.85865402	2.95231028	0.89986343	1.20471767	-0.6108826	1.39367452	0.37530274	1.35518078	-0.6528263
P_11	0.96270678	0.11541114	3.07469254	4.08093403	3.54082961	3.84121747	2.94082813	3.35603705	1.26603628	0.76620207	0.58344103	0.68269921	1.42547929	1.0095292	3.03445502	1.35108228	0.82483664	-0.1777096	1.11327148	0.00620109	1.18055319	-0.7324101
P_12	1.2493758	-0.2080216	2.68239095	3.75387365	4.00207505	3.78229913	3.00768981	3.46396772	1.03632152	0.78301554	0.05535808	0.79789502	1.01181325	0.96803862	2.71637382	1.45702313	1.22561747	-0.5679879	1.4073098	0.10890556	1.59414474	-0.4532969
P_13	1.44976294	-0.3529041	2.42660047	3.45671608	3.88992797	3.76989788	3.17513631	3.07572756	0.78189719	1.18832785	0.87671864	1.37746951	0.95460568	0.82390556	3.06036262	1.15714731	0.8579995	-0.0782939	1.62194644	-0.1595383	1.69248047	-0.6468831
P_14	1.46918345	-0.0984205	2.7675806	3.69677194	3.99888809	3.84288906	2.91728323	2.99471277	0.4710939	0.88787954	0.34855984	1.11498442	1.10483252	0.95303672	2.81213645	1.24955306	0.63845798	0.03209166	1.60727384	-0.5081503	1.76238619	-0.5766169
P_15	1.15865763	0.27353123	3.28212064	4.33205879	3.74999189	4.04479215	2.80209595	3.17811509	1.0373691	0.45875547	0.06808258	0.44120897	1.82355013	1.33860416	2.26451425	1.4911476	1.07063903	-0.07903	0.88513611	0.06475069	0.93382961	-0.2987603
P_16	1.22825412	-0.3541705	2.5272997	3.522001	3.77549761	3.68321915	3.21630018	3.25354724	0.88983229	1.17062775	0.92428932	1.35795139	0.82184269	1.08808088	3.13925163	1.29412979	0.71194103	0.0788974	1.72292068	-0.274605	1.77745568	-0.5223589
P_17	1.17715031	-0.0977259	2.74704816	3.72342197	3.63159647	3.68097665	3.01616747	3.40376789	0.88855918	0.77467815	0.68320432	0.9481318	1.50925577	1.09190596	3.20495729	1.15557244	1.12930445	-0.7496374	1.33509629	-0.0388865	1.37782001	-0.808155
P_18	1.16548505	-0.0623328	2.70389775	3.56064417	3.83769525	3.8152134	3.10845796	3.34849318	1.02727009	0.98138639	0.50209774	1.13149938	0.88228833	0.97168353	3.11999643	1.42151579	1.17261188	-0.4414009	1.66160907	-0.0231081	1.76895964	-0.6363919
P_19	1.23911849	-0.1638668	2.70800701	3.62339199	3.64928081	3.68909326	3.03974696	3.16173436	1.28225274	1.38071594	1.07524508	1.47694448	0.88432924	1.05479643	3.45984122	1.41439354	0.64938139	0.1558622	1.66218605	0.33228045	1.65356111	-0.6756839
P_2	1.24054325	-0.1803406	2.67556644	3.63175023	3.84411718	3.8006928	3.07636253	3.29905145	0.958504	0.97774197	0.77623433	1.08599577	1.03092527	1.15251269	3.44712886	1.10833086	1.04324745	-0.3454281	1.73184659	0.07062825	1.83260555	-0.740324
P_20	1.3038193	-0.4068262	2.33138721	3.25234546	3.75426698	3.57270884	3.00150705	2.88631738	0.88293221	1.28811376	1.06069829	1.49162717	0.4927774	0.85578711	3.42531616	1.39180485	1.10146157	-0.1332576	1.75277409	0.01709776	1.92332327	-0.8236791
P_21	0.6427267	-0.0282144	2.86603779	3.84972324	3.77493844	3.80273449	3.15523136	3.31788984	1.13345513	0.39395437	-0.0824076	0.35290145	1.28509404	1.07872248	2.57033696	1.34144407	1.02067114	-0.6567154	1.24262445	-0.2315227	1.39854443	-0.7057557
P_22	1.02154631	-0.214452	2.81985806	4.02092863	3.58149018	3.96333776	3.1775501	3.44727189	1.05999946	0.81017506	0.67496517	0.99686155	1.14654579	0.94276006	3.17709857	1.14363202	0.81019158	-0.517364	1.49023749	-0.4149181	1.57300939	-0.9696029
P_23	0.70738372	-0.3005165	2.58349317	3.80499334	3.90839816	3.93664623	3.58639581	3.6448922	1.27354015	0.64194829	0.48147656	0.72683293	1.36935602	0.98613696	3.05432379	1.11614073	1.14291405	-0.9638866	1.41222699	0.07316951	1.19449041	-1.3699176
P_25	1.02349553	-0.087505	2.65370257	3.65658524	3.60996777	3.66404596	2.95422118	3.13183933	0.86360514	0.7176307	0.58705184	0.84908459	1.20615421	1.04992134	3.35664675	1.71263321	1.15856406	-0.6207222	1.30003353	-0.0010471	1.3341905	-0.9958312
P_26	1.09262609	-0.0614422	2.87347646	3.65685846	3.74339113	3.71330509	2.82747677	3.0741467	0.59822476	0.5012305	0.29699827	0.62213377	0.71597225	0.89838859	3.47341445	1.4431679	1.10475916	-0.7170231	1.51858986	-0.3091694	1.64238489	-0.8457363
P_27	1.03274607	-0.3273804	2.56127255	3.58751688	4.05936843	3.95006187	3.19152906	3.23329478	0.69986903	0.68920805	0.50210284	0.85155484	0.93815995	0.87857118	3.25020894	1.46528358	1.12685408	-0.4681685	1.40409082	-0.046735	1.36374495	-1.1617637
P_28	0.74042409	-0.0929402	2.89515451	3.97506999	3.93220936	3.91485177	3.38944348	3.55459767	1.2355827	0.67940039	0.65484681	0.71840443	1.62260352	1.0722971	3.07729567	1.551076	1.30408211	-1.2860218	1.04270933	0.03621465	0.9561974	-0.9646651
P_29	1.14596452	-0.0463751	2.89774197	3.88953992	3.88701807	3.83465672	3.37272888	3.67838625	1.09422057	0.67595456	0.33613321	0.82903189	1.06297108	0.97082902	3.3772696	1.12399132	0.9353457	-0.7538015	1.70687372	0.02081538	1.53276078	-0.8262009
P_3	1.28618848	-0.7145739	2.08469617	3.42096192	3.79462114	3.60110499	3.09171668	3.43945124	1.10982132	1.09893345	0.77013977	1.32962378	0.99863645	0.94684569	3.07309304	1.38591866	1.35064164	-0.5768797	1.58887319	0.14326097	1.79754199	-0.855635
P_30	0.67060035	-0.2873584	2.62003291	3.81928597	3.83441033	3.79950657	3.70665293	3.68261959	1.22264286	0.20714337	-0.1588491	0.1941668	1.32806434	0.8687168	2.18557552	1.26816413	1.20301347	-0.6961062	1.02647492	0.01245371	0.84794595	-1.1629191
P_31	1.06549465	-0.2505534	2.69780049	3.82417049	4.20117883	3.86190255	3.29855015	3.41950747	0.99951349	0.85552986	0.76493832	0.93257331	1.36732616	1.04436196	3.35954128	1.63910156	1.49258144	-1.1260065	1.20130785	0.21170415	1.3410735	-1.034537
P_32	0.9765887	-0.3822308	2.60187403	3.7563795	3.89825774	3.72213188	3.60048496	3.8079671	1.49426148	1.15448227	1.03812238	1.26581689	1.20355045	0.8320273	3.34484832	0.87635964	1.20180347	-0.7354663	1.48151105	0.30623338	1.37393624	-0.8006432
P_33	0.64797796	0.27653116	3.13406666	3.86008771	4.14505649	3.97777688	3.230192	3.4081413	1.06600523	0.70354097	0.54969974	0.7631163	1.40088379	1.13776389	3.28855904	1.47291802	1.21192556	-0.7415751	1.32519521	-0.046825	1.48375568	-0.8486666
P_35	1.35781956	0.00729963	2.95380777	3.7941397	3.87899239	3.72811861	3.69879164	3.89160627	1.03025325	1.21614992	0.87099295	1.3699448	0.89659325	0.88716855	3.57197382	0.73190528	0.81578959	-0.5219486	2.22007093	0.18935233	1.68469762	-1.3249954
P_36	0.84527804	-0.0952544	2.89431424	3.7231609	3.88998963	3.76665577	3.74307489	3.90547834	1.32700192	0.8908085	0.84980926	0.9965857	1.08290688	0.79602463	3.26636656	1.04745206	1.30734504	-1.0883707	1.53839028	0.22811214	1.21044586	-1.1255643
P_37	0.76630681	-0.0077471	2.85763125	3.72648026	3.55302849	3.8327024	2.95509682	3.19301718	0.85472324	0.52994869	0.51284865	0.74911085	1.11932892	1.18625019	3.38402709	1.21567828	0.91604649	0.03590008	1.60156321	-0.1409125	1.70982794	-0.7969702
P_38	1.13436381	0.05025579	2.98619525	3.82327162	3.9035578	3.83607346	2.97424364	2.70539036	0.51232006	0.36017503	-0.004398	0.48946673	1.13916411	1.29111789	2.82627681	1.6279756	1.09305775	-0.4181213	1.16164261	-0.34133	1.31275998	-0.7057498
P_39	0.64069759	0.11979587	2.98528556	3.84488881	3.81278612	3.65646647	3.51258109	3.66782389	1.21140665	0.42556557	0.07312234	0.37397323	1.73884055	1.17709253	2.76227488	1.5545495	1.39514444	-0.9758915	0.98987256	0.12070806	0.84153518	-1.0557875
P_4	1.11912829	-0.2063038	2.51700702	3.53945575	3.87124659	3.57197535	3.61147627	3.63212294	0.98905674	0.94104023	0.54223403	1.02548351	1.0942356	0.81693486	2.85430285	1.04945977	0.94326947	-0.3965467	1.84568199	0.20579698	1.70318628	-0.4125657
P_40	1.0499009	-0.2289935	2.76292283	3.96033743	4.00204715	4.03071094	3.35495539	3.61748249	1.39454365	0.75417237	0.66845124	0.88046209	1.39288375	0.94201265	3.22235134	1.15719981	1.23638724	-0.7862758	0.9550286	-0.1068479	0.94879462	-1.1703858
P_41	0.91199131	-0.0503949	2.72549573	3.56043643	3.77883291	3.79706087	2.97321792	3.06719508	0.72280435	0.61590529	0.50214943	0.67571985	1.18194681	1.04186657	3.4950969	1.33816087	1.10701525	-0.3761916	1.42944262	0.11185876	1.416101	-1.1177024
P_5	1.34808307	-0.470528	2.52945223	3.67766143	3.37395035	3.63502813	2.7862768	3.00710914	1.03462114	1.11566874	0.83717536	1.36221496	0.7899577	1.09528465	3.15786857	1.61888683	1.173683	-0.4106432	1.79213439	0.0807853	1.98100181	-0.5919618
P_6	1.18744265	-0.1351429	2.76384302	3.83371342	3.88017062	3.75060933	3.44637841	3.69227194	1.20181899	0.57091854	0.28546993	0.65068129	1.22415791	0.92830056	3.12847059	0.93706882	0.88972162	-0.5458773	1.64452287	0.10266999	1.57771583	-0.6346924
P_7	1.15414793	-0.0573715	2.77317143	3.60685214	3.84052143	3.70218632	2.97528461	3.10862118	0.74840538	0.78739983	0.58919336	0.93336069	1.17714673	0.98088501	3.11287184	1.43596441	1.06686849	-0.2337479	1.54032786	-0.0126492	1.66423231	-0.639507
P_8	1.03658742	-0.1492764	2.64900308	3.74173328	3.45768379	3.47962381	3.10731753	3.39161743	1.06290989	0.34322215	0.04614137	0.37901353	1.42005248	1.34530337	2.61454931	1.4382769	1.32162254	-0.8970796	1.27460056	0.23628458	1.50107453	-0.6558649
P_9	1.24774102	0.04721148	2.9973618	3.99290563	3.27149791	3.76776965	2.58181768	2.76326838	1.08381265	0.83816529	0.88897778	0.9657063	1.23400954	1.18748251	3.23556163	1.20147748	0.94048463	0.01780557	1.02252867	-0.022921	1.05262823	-0.7278419

Table 8.125: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer.

	PC(40:3)	PC(40:3)(2)	PC(40:4)	PC(40:4)(2)	PC(40:5)	PC(40:6)	PC(41:1)	PC(41:1)(2)	PC(41:2)	PC(41:3)	PC(41:3)(2)	PC(41:4)	PC(41:4)(2)	PC(41:5)	PC(41:6)	PC(41:6)(2)	PC(42:0)	PC(42:1)	PC(42:2)	PC(42:3)	PC(42:4)	PC(42:5)
P_1	0.48773253	-0.2833238	1.39470316	-0.9034129	2.24981862	2.99373561	1.05464057	0.76582977	2.08055225	2.45866446	0.24294195	-0.1085123	-0.5454095	0.92627376	-0.0058055	-0.2466723	0.21985043	-0.5402067	-1.6881824	-0.6923022	-1.7672067	-0.2714701
P_10	0.42646066	0.06246219	0.97239521	-0.7638155	2.28963491	3.3286194	0.93730136	0.31336826	1.63492995	1.71868473	0.45286778	0.15093124	-0.6273685	1.03625327	0.39874652	0.16814536	0.8654378	-0.1251151	-1.4012028	-0.4186536	-1.4854638	-0.409591
P_11	0.53243916	0.01024919	0.97441382	-0.7259727	1.68607123	2.55295931	1.04738369	0.11888633	1.6146088	1.31367806	0.68504947	0.32541096	-0.6740289	0.99986624	0.089912	-0.3722437	0.29743478	-0.3588443	-1.3395986	-0.3261229	-1.4171751	-0.5212824
P_12	0.51439165	0.04121345	1.35577035	-0.6565581	1.99404177	2.98450382	0.71584788	0.31600451	1.39810105	1.55663016	0.31793006	0.48467177	-0.2266586	1.71625574	0.44234738	-0.1513962	0.81474954	-0.263104	-1.1674063	-0.2974727	-1.3657114	-0.1346876
P_13	0.54315337	0.21503805	1.42089784	-0.6018978	1.94664034	2.48681022	1.3055074	0.71394801	2.06515976	2.30832358	0.75477957	-0.0502348	-0.7317499	0.55217488	-0.6328411	-1.171878	-0.2966823	-0.4322605	-1.2997914	-0.2742533	-1.3936271	-0.556453
P_14	0.46877648	0.21939322	1.28146281	-0.575049	1.71202849	2.29107142	0.70032462	0.44269083	1.49825392	1.83750445	0.67425209	0.1419003	-0.6392497	0.98117302	-0.5115175	-0.6322969	-0.3082498	-0.814838	-1.1447666	-0.114644	-1.2208596	-0.377651
P_15	0.57569977	0.5091748	0.64525727	-0.2983441	1.20258171	2.2252843	-0.18994	0.90038377	1.20160429	0.68491263	1.02387944	0.61318116	-0.3735814	1.5096022	0.03459135	-0.3481014	0.32474076	-0.5238272	-0.898764	0.18743463	-0.9094897	-0.6997126
P_16	0.54164446	0.28556659	1.0757954	-0.5065794	1.78911824	2.51853576	1.25049278	0.66948948	2.06791787	2.36301136	0.60175147	0.10624296	-0.4776048	0.61532692	-0.3593491	-0.6524624	-0.1213529	-0.4104458	-1.148315	-0.2120744	-1.3250575	-0.5670687
P_17	0.38907791	-0.0927142	0.97748222	-0.8928745	1.78538458	2.69067344	0.96054376	0.20074114	1.62999169	1.53472161	0.48451308	0.06122162	-0.6892721	0.97833905	-0.1855065	-0.0009947	0.29611221	-0.4315091	-1.739535	-0.7275472	-1.7948588	-0.6231082
P_18	0.66328872	-0.064615	1.38220531	-0.7876147	1.93690676	2.62382859	0.94136931	0.66361393	1.87834002	2.2554124	0.27752381	0.21802592	-0.2922789	1.25038351	0.11051833	-0.0793562	0.49568541	-0.3578284	-1.1234069	-0.3692611	-1.4422176	-0.0637965
P_19	0.62104172	0.10306368	1.14966404	-0.6080816	1.91146441	2.63958481	1.57209253	0.70744279	2.21673492	2.2297979	0.66616834	0.19700286	-0.6605429	0.67964726	-0.2787517	-0.6507279	0.2019224	-0.2394319	-1.3221598	-0.2882738	-1.3097735	-0.165279
P_2	0.43902617	-0.0415017	1.25733232	-0.8014415	1.99870729	2.72096355	1.35589294	0.5896636	2.01194043	2.01822113	0.44385341	0.18236001	-0.4504009	1.00201581	0.03373857	-0.3350568	0.25921323	-0.3575042	-1.4104456	-0.4417235	-1.5335303	-0.2296501
P_20	0.47325773	-0.090046	1.18461409	-0.8523888	1.72346622	2.21305834	1.39616142	1.00144342	2.30405095	2.60532977	0.39093741	0.00156538	-0.2779991	0.91379785	-0.2768508	-0.6221173	-0.0768727	-0.3524414	-1.4451522	-0.579085	-1.5859685	-0.3898381
P_21	0.49839618	-0.1653295	1.28872044	-0.9349166	1.94423732	2.58769232	0.65447364	0.23228345	1.30893718	1.48808313	0.33076441	0.34447466	-0.5142241	1.36119169	0.09465563	-0.2508639	0.41714534	-0.7369931	-1.3968038	-0.5611469	-1.5993242	-0.2452436
P_22	0.43532463	-0.4757397	1.15311634	-1.2494627	1.91703951	2.60961434	1.01226798	0.34538077	1.67320127	1.91005056	0.21649546	0.07036032	-0.8972492	0.81884501	-0.2187424	-0.5853402	0.13207401	-0.7247254	-1.6469573	-0.7831431	-1.8565493	-0.287042
P_23	0.4135898	-0.7914537	1.13060021	-1.4878371	2.02456961	2.82974198	0.75090617	-0.0430801	1.53740956	1.58032372	-0.151996	0.01239625	-0.8535759	1.19816664	0.32685913	0.11582462	0.53860905	-0.5724476	-2.205578	-1.41679	-2.4086762	-0.4374795
P_25	0.3228216	-0.5762421	1.05722313	-1.4051236	1.68629265	2.38424368	0.96305743	0.427465	1.86102611	2.15709966	0.33792317	0.31972487	-0.7070117	1.37784202	0.44590967	-0.1360015	0.46459938	-0.4046548	-1.9375595	-1.1162055	-2.0738355	-0.4618416
P_26	0.30008667	-0.5454637	1.18924641	-1.2129166	1.69976128	2.41324427	0.85684804	0.42657328	1.59746506	1.66467996	0.12875747	0.30994368	-0.3457465	1.40096214	0.01231894	-0.1701972	0.24032739	-0.6870596	-1.6266203	-0.9920791	-1.9023822	-0.3749639
P_27	0.34562583	-0.609642	1.42982851	-1.2878914	2.07462699	2.71090185	0.77341068	0.34706835	1.74866216	2.04884143	0.19209449	0.10518448	-0.4034137	1.38746441	0.02294867	-0.0683245	0.30223936	-0.7448366	-2.0306793	-1.1247372	-2.0721248	-0.5436901
P_28	0.41335254	-0.4403854	1.01913024	-1.0940486	1.76936767	2.7004962	0.83985835	-0.0558699	1.60150906	1.38552906	0.15713291	-0.0547302	-0.6090795	1.08964319	0.06247763	-0.1699753	0.1478543	-0.5772203	-2.076653	-0.9616555	-1.5925128	-0.721655
P_29	0.49522138	-0.4846491	1.19560393	-1.2034931	2.07840635	2.96680875	0.68358107	0.26524445	1.55874924	1.78653809	0.17261774	0.27469935	-0.6063268	1.34015093	0.23784925	-0.1239873	0.5831197	-0.6710114	-1.554259	-0.8806879	-1.9026267	-0.1564029
P_3	0.43703198	-0.1036758	1.1576918	-0.8955115	1.89071028	2.71106432	1.16483881	0.58683139	1.89928518	2.25088821	0.2253878	0.17532825	-0.4042843	1.32643494	0.40154788	-0.3510971	0.51802919	-0.2584386	-1.3893614	-0.582117	-1.6222146	-0.4624014
P_30	0.22437529	-0.5682152	0.89833076	-1.3325694	2.02976518	3.00894616	0.37479161	-0.0921387	1.1085872	1.31078864	0.13425389	-0.0256106	-0.7381669	1.32802243	0.22843418	0.39638215	0.86233891	-0.7556156	-2.1678033	-1.1543991	-2.2463288	-0.4847189
P_31	0.45096563	-0.4973311	1.24836371	-1.1595974	1.85824244	2.57129276	0.92620486	0.07435621	1.66430926	1.55569015	0.03929651	0.23102245	-0.386109	1.57973458	0.51556716	-0.2968363	0.45577522	-0.3742387	-1.9965325	-1.0190144	-2.0214941	-0.6038341
P_32	0.54673259	-0.1635039	1.0554164	-0.9757095	1.97748847	2.95526415	1.37292713	0.33827095	2.07762616	2.22785103	0.34651479	-0.0100818	-0.4847613	0.87976128	0.46951717	-0.134849	0.39606481	-0.2322467	-1.4324409	-0.5280039	-1.5199856	-0.3004074
P_33	0.55371765	-0.2954811	1.53362774	-1.0005334	2.08003637	2.70651379	0.91719139	0.28275494	1.76773233	1.92597517	0.27892686	0.25389788	-0.3799853	1.299212	0.084613	-0.2792645	0.14311616	-0.6498812	-1.4405844	-0.7055422	-1.6960705	-0.6195936
P_35	0.52113454	-1.0943126	1.31895237	-1.7900051	2.41249537	3.135186	0.82770182	0.34928658	1.87041953	2.20534482	-0.2126616	-0.2512562	-0.9907378	0.807895	-0.0735806	-0.1663774	0.22804399	-0.8762756	-2.1373238	-1.4277849	-2.4496154	-0.3295168
P_36	0.43583245	-0.7887851	1.18337591	-1.6095332	2.23459218	3.12883041	1.0088988	-0.0681671	1.76967065	1.76129924	-0.2111378	-0.1290546	-0.41904	0.99188151	0.33738926	-0.0394704	0.46034686	-0.4326679	-2.060108	-1.1833634	-2.068533	-0.504087
P_37	0.48509781	-0.3513584	1.22894479	-1.0634563	2.00544503	2.69122325	0.9088103	0.46197088	1.74276334	1.84189563	0.28514869	0.3444914	-0.443948	1.16085462	-0.1985168	-0.1636389	0.33258938	-0.6303463	-1.6677163	-0.7928932	-1.8422614	-0.2084887
P_38	0.4990612	-0.2408833	1.35898598	-0.9716918	1.57467594	1.79376934	0.48049134	0.19778745	1.321552	1.52082037	0.49709172	0.5724117	-0.4149113	1.75484491	-0.0302252	-0.3621839	0.08262228	-0.824099	-1.6334924	-0.7274162	-1.815245	-0.3998818
P_39	0.43524364	-0.5919971	1.0028117	-1.3220175	1.94654734	2.77791405	0.5614036	-0.2579572	1.31326282	1.25173581	0.16443001	0.14926735	-0.7609889	1.39932956	0.48159038	0.21461483	0.67252661	-0.5931074	-2.0080326	-1.0468614	-2.0591243	-0.4475035
P_4	0.53524059	0.34689687	0.97884614	-0.4928533	1.93566873	2.94262612	1.11685818	0.52492208	1.8584288	2.04988171	0.66255929	0.03987438	-0.2119504	0.73065164	0.08258164	-0.3285166	0.28034208	-0.3189584	-1.1051907	-0.0905137	-1.1375978	-0.2782973
P_40	0.40460344	-0.70184	1.30147072	-1.4088616	2.09955359	3.03442279	0.86765527	0.11155471	1.76393935	1.84417746	-0.0210069	-0.079008	-0.7195019	1.04289566	0.00660935	-0.3137894	0.17663995	-0.6096514	-2.1048069	-1.2494416	-2.177787	-0.5048084
P_41	0.34902272	-0.7696173	1.27902602	-1.3633323	1.99826569	2.5262019	0.85801382	0.38862295	1.8384482	2.00049557	0.03627419	0.25472682	-0.4618419	1.34910863	-0.006262	-0.1116797	0.3670645	-0.6155562	-2.1522804	-1.3611542	-2.2933681	-0.4334605
P_5	0.57172235	0.24626421	1.02772537	-0.568284	1.56022664	2.12930124	1.29864079	0.6611706	1.87709687	2.09609635	0.63564462	0.52150008	-0.3185111	1.23021059	0.35472303	-0.5050232	0.44921048	-0.2761042	-1.0455327	-0.1336181	-1.2479126	-0.3256456
P_6	0.56914135	-0.2478849	1.122382	-0.9848814	2.03137528	3.09717958	0.88428827	0.28818812	1.58659908	1.62278346	0.23064526	0.07459647	-0.7182565	1.14006518	0.24882934	-0.0955373	0.69898396	-0.4204935	-1.4591811	-0.724669	-1.7420525	-0.072122
P_7	0.40473174	0.07917949	1.20913877	-0.6806679	1.73550642	2.43384964	1.05125173	0.42723564	1.78931237	1.89101497	0.64098265	0.176872	-0.381371	1.16598989	-0.2436246	-0.1973475	0.16799948	-0.515447	-1.4019818	-0.4094853	-1.4810698	-0.5061893
P_8	0.45011798	-0.1028602	0.89695582	-0.8587525	1.80600567	2.62583736	0.82849057	0.12038633	1.28333573	1.24876679	0.37731918	0.48497527	-0.3698099	1.57884274	0.61743872	0.14913884	0.98925965	-0.2383449	-1.4102424	-0.4825968	-1.5694345	-0.2012721
P_9	0.59046541	0.00917606	0.77906706	-0.8155475	1.21102467	1.95473057	1.19817293	0.18927173	1.78119683	1.69163442	0.6212668	0.22105034	-0.7678862	0.88982431	-0.3176233	-0.6597874	-0.0115951	-0.3475884	-1.3386348	-0.302763	-1.3627004	-0.4263911

Table 8.126: Normalised data matrix for phosphatidylcholine and lyso phosphatidylcholine for serum samples taken from patients with breast cancer.

	PC(43:0)	PC(43:4)	PC(43:4)(2)	PC(43:5)	PC(43:5)(3)	PC(43:5)(2)	PC(43:6)	PC(43:6)(2)	PC(43:6)(3)	PC(30:0)	PC(30:0)(2)	PC(30:0)(3)	PC(30:1)	PC(30:2)	PC(d31)
P_1	3.49170365	1.71730641	-0.8257666	2.29116603	0.55834682	1.28344264	2.54352091	0.90428956	0.3693658	-0.29396	0.72758959	1.35365586	3.6139526	3.01051139	-1.7538066
P_10	3.3514064	1.83424288	-1.1807467	1.98415341	0.20059985	0.83970014	2.25451946	0.50703884	0.81822998	-0.1651625	1.39076191	0.06905726	3.85574551	3.27064307	-2.0622314
P_11	3.33718152	2.22128175	-0.6872235	1.73217317	0.21273259	1.4506453	2.01311453	0.64761513	0.56480601	0.13116945	1.11263529	1.11240594	4.14463066	3.54818941	-2.0491264
P_12	3.45866314	1.20345318	-0.290801	2.25891427	1.27654942	0.79459757	2.54037909	0.49323735	1.17044669	-0.2520257	0.97127244	1.03501761	3.70437147	3.16335775	-2.1086669
P_13	3.68825182	1.56891504	-1.3851055	2.2732091	-0.2376208	1.07344374	2.54520982	0.6967455	-0.6486074	-0.3956684	0.8493553	1.16405454	3.64032213	3.0174062	-1.8156631
P_14	3.52349641	1.04804059	-1.1008621	2.25505463	0.13153165	0.67036049	2.54829812	0.39952282	0.13793289	-0.3637531	0.67199707	1.50363772	3.60746007	3.0550377	-1.8779249
P_15	3.03065362	1.8798015	-1.0836168	1.38939866	0.3486396	1.23406662	1.67222665	0.66492696	0.54310398	0.18165021	1.32377755	0.63337629	4.15906664	3.60279638	-1.9803316
P_16	3.77665789	1.5615602	-1.0635495	2.37157499	0.24814844	1.0465159	2.66964273	0.61000948	-0.2093408	-0.329178	0.79339213	1.43474296	3.66524699	3.04215018	-1.8700307
P_17	3.40390102	1.78890119	-1.2190461	1.95302455	0.05229201	1.06454996	2.22179349	0.4154325	0.29488042	-0.0382391	1.07530787	0.91623626	3.92977393	3.28002177	-1.8544462
P_18	3.62531713	1.10810274	-0.6189522	2.45358448	0.77095088	0.68132727	2.74537196	0.24805309	0.70065103	-0.5373985	0.67807107	1.47310858	3.5320434	2.90205564	-1.6803326
P_19	3.67582747	2.52102182	-0.7869705	2.11150261	0.12002135	1.98594714	2.35661422	1.36167562	0.34669161	-0.1364912	0.94541356	1.47450167	3.81945608	3.20147545	-2.0849678
P_2	3.69891511	1.86203085	-0.8674752	2.42877646	0.46419966	1.35217124	2.69454194	0.83419253	0.39320443	-0.3273647	0.82736361	1.07322971	3.70264203	3.1100686	-1.9212498
P_20	3.78239708	1.60898255	-0.6624715	2.53299833	0.43305728	1.19397222	2.80850738	0.79138169	0.1948104	-0.4070639	0.63914361	1.29691034	3.56371001	2.99938053	-1.7725643
P_21	3.44618928	1.00467217	-0.6963209	1.82418185	0.70865565	0.58235545	2.10444357	0.22053265	0.73810226	-0.1097913	0.86677745	1.4091756	3.82262834	3.23045941	-1.8677992
P_22	3.65508607	1.63224653	-1.1717604	2.09783133	0.09594687	1.03105073	2.37182294	0.32255729	0.18581309	0.00499277	0.89203175	1.63081485	3.94553241	3.29937056	-1.7302677
P_23	3.05415588	1.93534955	-1.1695447	1.58515186	0.14109027	1.38060678	1.84424309	0.80032066	0.56417417	-0.1640362	0.68777345	0.98395562	3.90014622	3.35360691	-2.0492117
P_25	3.17256933	2.05196763	-0.5901023	1.77316116	0.7923857	1.43612512	2.00819134	0.79608657	0.71792319	-0.2430239	0.72242097	0.94700919	3.76333479	3.11786283	-1.9363421
P_26	3.43006519	1.53331877	-0.6992122	2.24239751	0.88805476	1.00120534	2.50031759	0.48284746	0.75985674	-0.372281	0.85832904	1.15935112	3.73354589	3.16668235	-1.9329172
P_27	3.1751577	1.76298572	-0.8092892	1.78466502	0.71615814	1.32866423	2.00125858	0.89454479	0.52570134	-0.1894331	0.650837	1.43428836	3.75423185	3.13154702	-1.7746708
P_28	2.86604154	2.4180254	-0.735646	1.26197637	0.21770686	1.79097266	1.48422094	1.18682388	0.08301107	0.20627123	1.10793298	1.02028024	4.19629424	3.61601691	-1.9963657
P_29	3.32976386	1.75248856	-0.573397	2.08291126	0.85424894	1.117762	2.3451916	0.60368256	0.81935611	-0.1999294	0.805962	0.98450695	3.77009773	3.15448748	-1.8432675
P_3	3.7535206	1.1886775	-0.5816959	2.41187138	0.76724485	0.83508177	2.71578219	0.55008012	0.38925017	-0.4982368	0.57233151	1.09833729	3.50132322	2.90054685	-2.0054823
P_30	2.70231062	1.02710321	-1.2279669	1.21697453	0.47197184	0.6378696	1.45257571	0.24486725	0.81911924	-0.0408919	0.56005447	1.29089847	3.87769829	3.26785496	-1.9186134
P_31	3.15806493	2.24996934	-0.8022886	1.66400574	0.81481423	1.65255085	1.88403731	1.26365933	0.63951075	0.01746369	0.86250015	0.83817383	3.98153136	3.34761233	-2.0775718
P_32	3.4590304	2.65033291	-0.5639591	1.80984198	0.49228779	1.99895547	2.04552204	1.42866378	0.41652464	0.01203898	0.85393488	0.9262163	3.98317138	3.33878116	-2.147942
P_33	3.38408521	1.70481055	-0.8634484	1.84222588	0.63936829	1.24051244	2.09323093	0.83654526	0.53729185	-0.0528851	1.10273909	1.07920129	3.98683326	3.37004373	-1.5468115
P_35	3.01859904	2.09939123	-1.2557309	1.66304639	0.13312668	1.57019324	1.84045358	1.10934176	0.44792032	-0.222529	0.53180089	2.02668006	3.79976729	3.21061663	-1.6417769
P_36	2.75392811	2.38319103	-0.7290696	1.34229237	0.54253439	1.84903652	1.52547579	1.36710227	0.52103964	-0.0397605	0.65487295	1.48222749	3.91636603	3.26862747	-2.0927337
P_37	3.64102414	1.41922866	-0.5889176	2.2829772	0.62771963	0.89212972	2.57095584	0.30989764	0.49367562	-0.2046264	0.6267363	1.2940219	3.76407988	3.1278328	-1.7842802
P_38	3.2353025	1.23320864	-0.6052531	1.7567418	0.84532079	0.61313876	2.01350417	0.11009498	0.73317383	-0.0842591	1.07134129	0.87520315	3.93343562	3.30523739	-1.8684774
P_39	2.62349943	1.89405367	-1.2001144	1.10829943	0.35648054	1.26853597	1.31804409	0.82997486	0.76931858	0.04061266	0.95505671	0.66682753	4.01559273	3.40295609	-1.9277903
P_4	3.57371856	1.65749851	-1.0662411	2.27759901	0.36795643	1.2092523	2.56265516	0.9044579	0.37253259	-0.5126686	0.97621742	1.07961191	3.59920595	3.03003885	-2.0325047
P_40	2.88051767	2.2471424	-0.8295757	1.26214789	0.06429864	1.66821739	1.47518959	1.07890371	0.03214214	0.1800348	1.05557204	0.97682634	4.19107629	3.62314252	-1.7856491
P_41	3.15708505	1.7408776	-0.8062572	1.83963235	0.69394074	1.32103217	2.08020171	0.84867265	0.61859448	-0.2314951	0.87411379	1.41990621	3.80086471	3.22002486	-1.7554853
P_5	3.92190918	1.49861756	-0.2244585	2.64767479	0.91731874	1.03827615	2.9586513	0.59954923	0.85064536	-0.2317621	0.7399046	0.78433966	3.76562669	3.14064529	-2.1451633
P_6	3.34743848	1.75332009	-1.0009382	2.16536454	0.67620014	1.14702636	2.45991119	0.60923839	0.88748793	-0.3909998	0.94898535	0.81593234	3.81348766	3.25121691	-2.026393
P_7	3.45214788	1.77368857	-1.1487719	2.19695514	0.33351205	1.21245759	2.44949994	0.69355548	0.31672506	-0.3327684	0.90064463	1.37654198	3.74480236	3.06837824	-1.9892133
P_8	3.41200772	1.20218555	-0.5039885	2.00480102	1.03718329	0.52629955	2.29696611	0.04717158	1.2255789	-0.2575335	1.12727493	0.72024851	3.8385984	3.16642818	-2.1430135
P_9	3.17055707	2.59995344	-1.0141778	1.49164708	-0.1732637	1.80248327	1.77450214	0.82101911	0.00285296	0.20613319	1.14794185	1.33121956	4.18091349	3.61666842	-2.0686373

Table 8.127: Normalised data matrix for phosphatidylethanolamine and lyso phosphatidylethanolamine for serum samples taken from breast cancer free controls.

	LPE(17:0)	LPE(18:0)	LPE(18:1)	LPE(18:2)	LPE(20:4)	LPE(18:1)/pla	PE(32:0)/PM	PE(34:0)	PE(34:1)	PE(34:2)	PE(34:3)	PE(35:0)	PE(35:1)	PE(35:2)/PE(	PE(35:3)	PE(35:4)	PE(36:1)	PE(36:2)	PE(36:3)	PE(36:4)	PE(36:5)	PE(37:1)	PE(37:2)	PE(37:3)
C_1	-0.7268089	2.68161285	1.48749059	1.73375276	1.0464189	-4.2457148	-1.0591467	-1.1568666	1.09979451	1.30099138	-1.1150146	-2.0388293	-0.6209512	-0.2905327	-2.9058162	-0.4832583	1.55014894	2.52720173	1.31163496	1.2193173	-0.2573718	-0.9281188	-0.2706406	-3.0626554
C_10	-1.0057473	2.20377046	1.36011047	1.54469214	1.13648273	-2.4406536	-0.1840004	-2.1692671	0.35884505	0.28138118	-0.9442105	-2.3659182	-0.4169244	-0.6154424	-2.1172638	-0.1053287	0.70093636	1.42703027	0.57273017	0.80933544	0.19814628	-1.139219	-0.4956154	-2.7615939
C_11	-1.0809434	2.15094316	1.241174	1.68978221	1.37824604	-3.7973402	-0.9667526	-1.0089363	1.02165254	1.27625852	-0.670253	-2.2095993	-0.6904023	-0.2954364	-2.0639118	0.65434644	0.78827627	2.07727043	1.01162875	1.3613921	-1.0949483	-0.9205423	-0.4280234	-3.3489068
C_12	-0.4306757	2.61307287	0.96459116	0.97836934	0.56382577	-3.8064932	-0.4640728	-0.7514925	0.7019417	0.89609604	-1.0909353	-2.7879905	-0.3937909	-0.2656254	-2.105913	0.07821268	1.52501685	2.32622228	0.88507563	1.06309086	-1.2185714	-0.7195908	-0.2882876	-3.3510989
C_13	-0.1686735	1.93671191	1.33537434	1.89615628	0.84959955	-3.1585347	-0.175389	-1.4776061	-0.105996	0.53487382	-0.4728527	-2.8271999	-0.496397	-0.0419433	-1.5989462	0.71350626	0.89077771	1.46490159	0.73095267	0.79149646	-1.2635929	-0.2073158	-0.4467026	-3.1607332
C_14	-0.4149112	1.81550428	-1.3062937	1.0994673	-0.1584528	-0.8116033	0.82730167	-1.1343816	-0.0766043	-0.2684532	-0.4791288	-0.7159192	-0.3691967	0.23801482	-0.4449293	-0.5142082	0.80243363	0.7619324	-0.572937	0.03475617	-1.2969436	0.76031941	0.13871558	-2.4365042
C_15	-0.6219236	2.33567013	1.14448957	1.50275855	1.29099171	-3.2430171	-0.5578372	-1.4220578	0.48019654	0.82825072	-1.6575928	-4.0135604	-0.5664322	-0.2216257	-2.1806146	0.39461832	0.65829322	1.70169861	0.77355948	1.12013177	-0.4133207	-0.6601495	0.14004425	-3.0560831
C_16	-0.8698474	2.46979381	1.95698247	2.00764349	0.88847013	-4.1663437	-0.4456185	-0.5285248	1.09142241	1.54527722	-0.8858512	-2.807033	-0.6888047	0.13985163	-2.0763461	-0.506072	2.16560068	3.19030699	2.01180982	1.42793748	-1.3949585	-1.0318161	0.24233318	-3.0345463
C_17	-0.7963172	2.58946953	1.25664057	1.43269326	1.27695327	-3.8931845	-0.9738808	-1.0200474	0.58445178	0.49720949	-1.6559151	-2.4668239	-0.4625131	-0.6629121	-3.7307006	0.04702096	1.10195007	1.94710339	0.78203049	1.24611305	-0.1432224	-0.5374677	-0.7303309	-3.6386158
C_18	-0.8904611	2.32632018	1.37333989	2.00209327	1.01153966	-4.3757898	-0.6404571	-1.3909888	0.76833646	1.25285964	-1.2490084	-3.2303166	-0.3192109	0.34127208	-3.5860158	0.36246983	1.1399845	2.54999969	1.30688673	1.06943269	-0.8974872	-0.8010177	-0.4754821	-2.7445834
C_19	-0.6105328	2.04725737	1.20060705	1.48457642	1.0788124	-2.9395597	-0.3999185	-1.5768753	0.11833836	0.18321855	-0.8198586	-4.8374184	-0.747636	-0.3752575	-2.5049944	0.81149176	0.7572214	1.88667341	0.98775878	0.70787511	-1.3931202	-0.435394	-0.1862132	-2.3783818
C_2	-0.7754378	2.32803488	1.4771331	1.36123977	1.46502783	-3.6085761	-1.1032639	-1.1015248	0.83845392	0.88386395	-1.4053197	-4.0316715	-0.5981836	-0.3064602	-2.7041725	0.26901305	1.26887173	2.06650766	0.89736586	1.16192036	-0.5749489	-0.8576086	-0.2314701	-3.8322584
C_20	-0.2863767	2.5376331	0.78530929	1.44596451	0.78900193	-3.9538939	-0.1752569	-1.6195063	0.02747085	0.6238652	-0.6784541	-1.734445	-0.7591795	-0.4091258	-2.0771208	0.00198137	0.8949674	2.05227032	0.50201669	0.73295632	-0.1548688	-0.6355195	-0.2030286	-3.6124357
C_21	-1.2266762	1.96809913	1.22938324	1.42653009	1.14338911	-3.6393278	-0.6126625	-1.3577112	1.0037804	0.96909136	-2.1380233	-3.094168	-0.7817745	-0.3543615	-2.0965562	0.66955066	0.92015707	2.01359668	1.0722912	1.16574951	-0.7280221	-0.4142861	-0.288518	-3.0344277
C_22	-0.8110131	2.80668408	1.91838831	1.72111871	1.50726589	-3.7650217	-0.9905793	-1.0934138	1.09919933	1.01690893	-1.6415645	-2.9756363	-1.1847949	-0.7591807	-3.373267	-0.4601157	1.54975227	2.3174593	1.36015101	1.37214473	-0.2495768	-0.8942267	-0.4702577	-2.5027336
C_23	-0.9049898	2.08057779	1.29220457	1.71798494	1.08336533	-3.4264893	-0.3730028	-1.7198031	0.58677283	0.90803942	-0.9660598	-2.4382492	-0.7911396	-0.1084843	-3.2701907	0.35426302	1.02677305	2.11362885	1.02651204	0.83722051	-0.3449406	-0.5425679	-0.2397296	-2.708289
C_24	-1.2935798	2.34304213	1.58134554	2.17357669	1.33850092	-3.4031888	-0.5976154	-2.5512242	0.33565906	0.64231518	-0.8400643	-1.6199926	-0.7836949	-0.1040939	-3.0481452	0.07512452	0.82623452	1.81959021	0.82603049	0.81783805	-1.1005771	-0.2486205	0.05632157	-3.2658277
C_25	-0.6513219	2.68089868	1.67761418	1.97885047	1.42262626	-3.3144446	-0.8709149	-1.6625595	0.57664704	0.71148497	-1.4135407	-2.2474203	-0.7968551	-0.5315276	-3.0778461	-0.2455124	1.13370308	2.04552218	0.69341321	0.85667814	-0.3652776	-0.4324936	0.10718557	-3.5213266
C_26	-0.8186938	2.28138725	1.67029135	2.0273473	1.25802991	-3.0738271	-0.734203	-1.0473344	0.34628862	0.77929431	-1.7263425	-2.9367995	-1.0491736	-0.2632413	-2.1451964	0.01218604	0.8430426	1.9722505	1.14301452	0.81968235	-0.7303958	-0.7885532	0.07793949	-3.7436525
C_27	-0.5255879	2.47432937	1.63107439	1.98094826	1.31956764	-3.5406495	-1.2866173	-1.7781926	0.53703975	0.71025207	-0.9507531	-2.8756992	-0.6509965	-0.346857	-2.1675184	0.28349829	0.90399539	2.09344199	0.93082466	0.97102419	-0.7640063	-0.6002428	0.18504785	-3.241112
C_28	-0.6860191	2.45329094	2.20761033	2.18438782	1.10943387	-4.1199492	-0.4650581	-1.4831433	0.41541175	0.91614267	-1.9789496	-3.038027	-1.2528681	-0.507028	-2.7927519	-0.6268475	1.40379749	2.41353158	1.43446652	0.88196362	0.25228315	-0.7837404	-0.2634338	-2.9995157
C_29	-0.506223	2.69035262	1.71857849	2.23978897	1.83630698	-3.4933463	-0.6469896	-1.0904204	0.75223351	1.05690091	-1.0528273	-3.7095104	-1.0392649	-0.5244258	-3.7984966	-0.5655379	1.13234287	2.15673324	1.06545552	1.11674392	-0.4436553	-1.3948502	-0.6102464	-2.7658256
C_3	-0.9170867	2.4882916	1.4687268	1.80881097	1.19413191	-4.1936529	-0.8879091	-1.4173509	0.66933195	1.13082798	-0.955395	-3.013657	-0.8024771	-0.3939444	-2.5741118	0.2841673	1.26442661	2.40857532	1.19577895	1.08927693	-0.5238634	-0.633956	-0.4275198	-2.9368431
C_30	-0.3835306	-0.1725373	-0.3613408	0.02359415	-0.6019251	-1.2518201	0.1283178	-0.4082347	0.34507866	1.07025903	-2.2095653	-1.7010373	-0.9713154	1.09640926	-1.8895562	-0.2409376	1.4037021	2.30535228	1.20039506	0.65837364	0.2109878	-0.3290762	0.39533821	-1.7252309
C_31	-0.3954276	1.87447464	0.85178976	1.38368298	0.90326878	-2.7299013	-0.3623319	-1.9480779	0.1771638	0.68546167	-0.9066875	-3.5176844	-0.5112571	-0.2081285	-2.5915347	0.17681913	0.58896358	1.4016025	0.248767	0.4995963	-1.3480213	-0.4966448	-0.1374984	-2.4247045
C_32	-0.8187567	1.59411936	0.78468717	1.25001076	0.41833687	-3.4263023	-0.3028902	-1.3102677	0.15538427	0.15062933	-1.7358564	-3.6037579	-0.2644721	0.05705317	-2.270012	0.89658142	0.78625036	1.24118852	0.34207694	0.62436973	-0.5523606	0.02754181	-0.0423668	-2.9518131
C_33	-0.8759564	2.67748687	1.693178	2.35387454	1.34480912	-2.7084731	-1.2335866	-0.678623	1.21048953	1.47717864	-1.550749	-2.9433369	-0.6572826	-0.3059281	-3.2626302	-0.5791311	1.83342011	3.0054612	1.46055486	1.27269147	-0.3877883	-0.8836094	-0.3244677	-5.3229825
C_34	-0.4509524	2.80690338	1.6472284	2.02934959	1.55094741	-4.2199496	-0.8568555	-1.1567932	0.98550757	1.10453907	-0.9677226	-3.5335673	-0.6352916	-0.7997403	-3.0318972	-0.6042294	1.06969172	2.09878869	0.97353237	1.31803468	-0.3195807	-0.733997	-0.3730299	-3.3496342
C_35	0.89870347	0.06113952	-0.8688907	4.89243238	-0.2668211	-0.1618963	-0.3422585	0.37298496	0.18689142	1.2862052	-0.9965643	-0.6332197	2.36414309	0.52275875	-3.2348692	3.19604241	-0.0238875	2.00019564	-0.9030049	0.4956372	-0.9727648	-0.6541089	-0.1968698	-1.5866107
C_36	-1.1432546	2.34952163	1.63644565	2.12826161	1.16785392	-3.9465881	-0.5609724	-1.5461498	0.39231397	1.04812902	-1.1338087	-2.443708	-0.3875688	0.19021749	-2.5612415	0.75493522	1.45372098	2.54712632	1.39986907	1.03426465	-1.0387483	-0.7989159	-0.2975192	-2.6485939
C_37	-0.36991	2.65848789	1.87601289	2.31437628	1.11384491	-4.1173953	-0.5382516	-1.7527785	0.42621226	1.04266631	-0.6819273	-3.2535089	-0.7384559	-0.7578644	-3.2682735	-0.4032191	1.15421075	2.31763819	1.29736216	1.15134179	-0.1741468	-0.9611076	-0.3187728	-2.7395509
C_38	-0.8451571	2.18945526	0.80411646	1.67245321	0.62101699	-3.7598157	-0.3327109	-1.6409503	0.18056102	0.61539438	-1.3878954	-3.1489557	-0.6220234	-0.1225672	-1.8556575	0.45863264	0.51051091	1.63898602	0.29159205	0.83211385	-0.3083508	-0.0663213	-0.1732969	-2.7314501
C_39	-0.5666366	1.432795	0.86041823	1.33046588	0.95067778	-2.4284546	0.06531495	-3.3005707	0.00516396	0.14393533	-1.2047524	-3.9302935	-0.5462603	-0.1207538	-2.0350133	0.75790221	0.54160694	1.50263558	0.64334812	0.27227121	-2.0257548	0.22331611	0.53028662	-2.8452504
C_4	-0.8842717	1.80082173	1.17128796	1.52724838	0.39859628	-3.779113	-0.6205783	-0.6787226	1.16606619	1.66920453	-1.4516487	-3.0624178	-0.4207768	0.08868812	-3.0571533	0.31120824	1.38686545	2.49198144	1.52065502	1.31337628	-0.3547693	-0.7310703	-0.4977997	-3.9549394
C_40	-1.0114873	1.97502891	1.03029998	1.44484359	0.59740659	-3.6104396	-0.4067621	-1.1487358	0.52196922	1.03855981	-1.4246572	-1.6937873	-0.5763296	0.00307796	-2.5811664	0.5131695	1.15758725	2.2242864	1.07186969	1.05975411	-0.7475103	-0.5387706	0.08184519	-3.565077
C_5	-0.7019616	2.12351509	1.04240071	1.65487799	0.98763849	-3.617066	-0.6294151	-2.660564	-0.3292619	0.44324846	-0.5450054	-2.5279847	-0.5820038	-0.2586008	-2.1278087	-0.0300893	0.69701718	1.40410333	0.33614249	0.56943225	-0.9420714	-0.2949097	-0.0085164	-2.9063543
C_6	-1.0295147	1.84466521	1.18747935	1.63939622	0.83176155	-3.556025	-0.3501066	-1.518814	0.25276201	0.71690152	-0.9295316	-3.19137	-0.656629	-0.1413888	-2.2254175	0.73008811	0.73351899	1.7636696	0.71025728	0.90297381	-1.032166	-0.9375169	-0.0588325	-3.7210502
C_7	-0.7889965	2.65986753	1.69061287	2.26285674	1.26721129	-4.4834013	-0.9149076	-1.1178433	0.98345294	1.42253344	-0.9872956	-3.5980102	-0.9017328	-0.1623669	-3.0381957	-0.5524118	1.61252433	2.82347113	1.3359729	1.31123368	-0.6859602	-1.2215861	-0.3669416	-2.6280232
C_8	-1.263806	2.21041111	1.48105077	1.847402	1.09801696	-3.5187321	-0.7755442	-1.1922703	1.01142183	1.401041	-1.2260878	-2.3870859	-0.4526225	-0.2408279	-3.2995924	0.39255762	1.42692288	2.27102945	1.37036818	1.39920859	-0.394686	-0.7739271	-0.3403264	-3.5771718
C_9	-1.2724029	1.94346141	1.09836904	1.46551325	0.52219532	-3.2054346	-0.3084514	-1.7830288	0.08041176	0.3784185	-1.5977413	-1.7713501	-0.5644945	0.11811857	-2.2339537	0.86043819	1.08948786	2.02342398	0.94798066	0.43513768	-0.9318644	-0.4775005	-0.0684022	-2.5906739

Table 8.128: Normalised data matrix for phosphatidylethanolamine and lyso phosphatidylethanolamine for serum samples taken from breast cancer free controls.

	PE(37:4)	PE(37:5)	PE(37:6)	PE(38:1)	PE(38:2)	PE(38:3)	PE(38:4)	PE(38:5)	PE(38:6)	PE(39:5)	PE(39:6)	PE(40:4)	PE(40:5)	PE(40:6)	PE(41:3)	PE(43:3)	PE(unknown	PE(unknown	PE(unknown	PE(unknown	PE(16:6)	PE(21:5)	PE(21:6)	PE(38:0)
C_1	0.47550429	0.38266584	0.31446228	-2.4089675	0.38254676	1.11633961	2.48513028	-1.830571	2.49886444	-0.0352453	0.64636128	-0.4619681	0.8991875	2.31660065	1.7956875	-1.9088908	-0.0808124	-1.8215647	-2.6437247	-1.6784433	1.81843626	0.28111771	1.71979215	-1.0591467
C_10	0.1531284	0.81110976	0.90904685	-1.4670665	0.60802143	0.69550984	1.67231696	-1.0127667	2.06210884	-0.0518653	0.53233233	-1.0041706	0.29333854	1.8143555	0.42463838	-1.8354945	0.83696496	-0.3754831	-1.3576318	-1.243721	1.53790153	0.35140386	2.1103801	-0.2966337
C_11	0.69674237	0.61374532	0.78985561	-1.9011924	0.36782375	1.07103062	2.24619313	-0.6940857	2.18593056	-0.1468825	0.59792258	-0.7949667	0.34442193	1.9188766	1.42523984	-1.5102627	0.19870439	-1.7931264	-2.2524747	-1.7757036	1.67026509	-0.1410912	1.70478266	-0.8967231
C_12	0.68728325	0.45937351	0.18529206	-1.1011732	0.47982008	1.51997872	2.73248335	-1.5524924	1.96530327	-0.07039	0.23209609	0.32059731	0.90517364	1.94578162	3.03854393	-0.9046426	-0.1274203	-2.7616217	-1.9377103	-2.6591213	1.83559312	-0.34014	0.65774226	-0.4313276
C_13	1.0016705	0.73454162	0.37339303	-1.2490046	0.82907971	1.02202185	1.5039783	-1.5661132	0.9257795	0.16550281	0.34242496	-1.8627228	-0.4869461	0.83649129	0.66548659	-1.2433699	1.57275305	0.06738446	-0.9727234	-0.3380794	1.14792415	-0.3448333	1.04625863	0.28663444
C_14	0.55736776	-0.609126	-0.1574187	-1.9368303	1.4487277	0.99392075	1.05829062	-1.2831807	-0.0621524	0.28380147	-0.5191096	-1.351391	0.50514579	0.70685858	1.65764013	0.63525871	2.00541374	-0.127377	0.46666083	0.37382137	1.3509925	-1.8886042	-0.7038654	1.11717727
C_15	0.71761335	0.85077473	0.29686978	-1.2901915	0.64699362	0.92801758	2.14929292	-0.951746	1.92166291	0.10668935	0.09550876	-0.3303701	0.46326231	1.42782532	0.80504061	-1.5291871	0.93828413	-0.8702181	-1.583755	-1.1181239	1.44789253	0.1610513	1.45281078	-0.4924864
C_16	0.48135938	0.08045184	-0.2949841	-0.9461517	0.44462794	1.44042456	2.52543485	-2.4977574	1.43974838	0.01665153	-0.1944666	-0.4320286	0.4708028	1.26204547	2.38495136	-0.9242179	0.08766865	-2.1054416	-2.8794687	-2.4549887	1.58873513	-0.3729465	0.58240336	-0.4045205
C_17	0.78253835	0.94541036	0.74061195	-2.1189565	0.47780421	1.01153837	2.36307225	-1.5327433	2.31803734	0.38241525	0.88481266	-0.591709	1.05000933	2.0971368	1.59489589	-1.5655202	0.54464011	-1.0638023	-1.526686	-1.7755863	1.67489695	0.49274031	1.93157698	-1.1668378
C_18	0.96651179	0.89666409	0.5719139	-1.2909078	0.28257328	1.21407855	2.15869127	-1.494658	1.97121827	0.16724166	0.57723793	-0.8124408	0.27384856	1.43257549	1.62317819	-1.6195198	0.6934588	-1.0710209	-1.9911435	-1.335267	1.50780182	-0.3371425	1.35184802	-0.6404571
C_19	1.07635522	1.06233415	1.26008944	-1.0451571	0.54171047	1.05108684	1.85340826	-1.5729039	1.54203433	0.27682395	0.90532486	-0.7459563	0.04568126	1.5792038	1.24323118	-1.4732298	1.0735868	-0.5347729	-1.2861493	-0.7058979	0.83744734	-0.0482161	1.46810059	-0.4628054
C_2	0.8643335	0.71424044	0.57227213	-1.2851068	0.25883566	1.48421653	2.59254015	-1.2353983	2.24937096	0.41148408	0.53315722	-0.4387876	0.98012545	2.06040045	1.77311037	-1.951625	0.02700008	-1.381006	-1.8905477	-1.7569677	1.36597745	0.42773963	1.75079329	-1.0126942
C_20	0.34883091	0.54123219	0.69020407	-1.1610957	0.50418028	0.99195055	2.18199115	-1.7767899	2.0568463	0.43883477	0.72283026	-1.2851079	0.76026807	1.96880852	2.33111645	-1.2618075	0.39395102	-1.2997477	-1.9667321	-1.8508563	1.68806861	-0.0521657	1.38211498	-0.4411509
C_21	0.67257184	1.21764092	0.80377148	-1.9172015	0.65095309	1.06378318	2.15102265	-1.0563106	1.84347537	-0.0971701	0.31384552	-0.3371581	0.619571 45	1.49324024	1.15451787	-1.6345613	0.8977843	-0.6487671	-1.4455562	-1.2358754	1.16863073	-0.2122846	1.33163536	-0.6126625
C_22	-0.2683679	0.10267233	-0.024946	-2.0216077	0.51337771	1.39798298	2.74428956	-0.4001882	2.47556511	-0.4282284	-0.2031642	-0.0058669	1.35959779	2.46463987	1.06808636	-2.1772149	0.0311166	-1.4222461	-2.3857814	-2.0211723	1.64250433	0.79226774	2.20489836	-0.9359054
C_23	0.60009799	0.75837074	0.71880207	-1.9052481	0.62342219	0.91925417	1.86412191	-1.388376	1.72908002	0.15188929	0.43920785	-0.5605333	0.39050106	1.53536674	1.15886157	-1.3956951	0.72748257	-0.6681981	-1.4455799	-1.3454378	1.11333778	-0.1291688	1.34341301	-0.4283784
C_24	0.86149592	0.6388136	0.17022671	-1.9478266	0.72221102	0.8355378	1.53196466	-0.83078	1.39686299	-0.1108156	0.22055181	-0.7132422	0.13484411	1.39689235	0.33928947	-1.8957909	1.21516574	-0.2116329	-0.7334957	-0.4318324	1.54502001	0.45814627	2.03077161	-0.6013321
C_25	0.23772685	0.33131353	0.50596058	-1.3826976	0.64679246	0.91736653	2.10366173	-1.1225371	2.11489123	-0.4140589	0.27220017	-0.692829	0.43598885	1.88855853	1.02113798	-1.9872851	0.70985018	-0.5190282	-1.6731379	-1.4412161	1.69850182	0.39613863	2.11397907	-0.9148614
C_26	0.66308036	0.59820462	0.54551821	-1.7073988	0.61651595	1.045196	1.87734338	-1.1778954	1.75387611	-0.2620465	0.40498842	-0.8450084	0.43300372	1.45032163	0.87824654	-2.078946	1.29730798	-0.3596905	-1.6870952	-0.827683	1.41553811	0.31086623	1.93683966	-0.4544242
C_27	0.92307446	0.76330161	0.05516494	-1.385816	0.70795906	1.08235792	2.09743175	-1.3665783	1.21143027	0.56379378	-0.1120913	-0.069909	0.27513259	1.23940375	0.86267495	-2.5057333	1.15808645	-0.4659353	-0.9951304	-1.3297961	1.40129437	0.54778565	1.18183567	-1.1325488
C_28	0.02415918	0.41671618	0.7976498	-2.1128219	0.56185486	0.56917866	1.83910633	-0.973102	2.24799049	0.07181328	0.61534186	-1.2362909	0.5861834	1.99177377	1.19486797	-2.2719792	0.76849313	-0.9496435	-1.5757597	-1.2545482	1.55167395	0.5352207	2.32266696	-0.3955332
C_29	0.18514427	0.05356633	0.3530149	-1.9209503	0.41609045	1.06039978	2.33906304	-1.1047524	2.20518047	-0.0711297	0.4784114	-0.8356013	0.81038465	2.10178276	1.00379966	-1.6247493	0.60378019	-0.7959681	-2.2156639	-1.4071167	1.77106218	0.68743033	2.4571589	-0.6741548
C_3	0.37282438	0.62297892	0.96291943	-2.523641	0.40529636	1.11978081	2.3128546	-1.4312101	2.02201129	0.06808313	0.75222164	-0.531007	0.75589286	1.99705069	1.57345816	-1.5024896	0.52277263	-1.6362544	-2.1052341	-1.4615173	1.56979637	0.03819185	1.65855002	-0.8879091
C_30	1.05230992	0.81142694	0.19715123	-1.5771043	1.20992186	0.89177875	1.73884549	-2.5730694	0.57051597	0.2173563	0.54030069	-0.7223448	0.01038096	1.44116151	0.72034684	-0.8166243	-1.5650089	1.7728492	-1.0216779	-0.621321	0.82376168	0.19758087	0.09321543	0.01654642
C_31	0.53359408	0.77257836	0.78144641	-1.5430021	0.81555123	0.88936185	1.79883658	-0.3174985	1.72002988	0.18972056	0.75959852	-1.6816377	0.52650751	1.43778817	0.79877049	-1.4256708	1.69821239	-0.068336	-0.8597883	-0.5900553	1.15691165	0.20547015	1.56931344	-0.3813929
C_32	1.42111518	1.44864742	1.490539	-1.3764145	0.77100744	0.93574691	1.29313102	-1.2075959	1.51855392	0.61920041	1.12996	-1.3321518	0.47958944	1.27012717	1.02530013	-1.5769739	1.54216054	-0.9018245	-1.1160853	-0.292196	1.10570376	-0.447889	1.18961622	-0.0386416
C_33	0.15856221	0.01288872	0.17035504	-1.7516302	0.28258471	1.71038643	2.6697713	-0.5950605	1.99870257	-0.2705564	0.13840529	-0.2262362	1.00284312	2.12643522	1.57252806	-1.7517402	-0.1204862	-1.7703621	-2.4112275	-2.1600483	1.62591201	0.46802248	1.73893743	-1.2335866
C_34	0.2744744	0.37529259	0.12889794	-2.417838	0.44760419	1.15619573	2.39489824	-1.0028813	2.28350751	-0.2486388	0.11932905	-0.4238277	0.96706516	2.23248346	1.14493594	-1.8512318	0.64600864	-0.9909171	-1.5045731	-1.9501339	1.87704463	0.52285555	2.12610081	-0.8579342
C_35	-0.4528152	-1.2096522	0.11961395	-2.078646	0.71557019	-0.0367394	1.31864982	-0.3777039	-0.0935176	-0.2195968	-0.4582344	-1.0933473	-0.0391183	-0.2267212	0.79496437	-0.9214334	-0.7103318	2.13604445	-1.4909812	-0.733031	-0.6574011	0.40234695	0.21274061	-0.3360272
C_36	1.25777596	0.88046073	0.80433006	-2.6698609	0.44785541	0.82236129	2.07577949	-1.1228647	1.55478299	0.31105011	1.00291947	-0.3299363	0.37042086	1.39341892	1.48389652	-2.3011094	0.52128571	-2.1146398	-2.3574299	-1.6790684	1.28571915	-0.1087418	1.45766909	-0.581665
C_37	0.35856224	0.30029759	0.43455567	-1.9875967	0.476132	0.93722805	1.99202589	-1.3611771	2.17836388	0.1104403	0.60154633	-1.8091626	0.63575075	1.89427874	1.22676313	-2.1812433	0.75785965	-0.8860816	-1.6251626	-1.1239796	1.78257684	0.48951886	2.21521641	-0.6937034
C_38	0.52922071	0.93933351	1.02064504	-1.4208117	0.91785028	0.89205504	1.81850752	-0.8785828	1.73580041	-0.0079814	0.59383777	-1.471423	0.31413843	1.52325812	0.66089404	-1.8019	1.25679823	-0.4317778	-0.9843137	-0.5590432	1.26769817	0.02237811	1.57644897	-0.3327109
C_39	1.03976593	0.80813001	0.97238832	-0.4932501	1.41997356	0.9171146	1.53551868	-1.4927607	0.97251777	0.48085616	0.64735001	-0.8013501	0.39071679	1.006197	0.02745275	-1.1037521	1.87614281	0.37904703	-0.3414795	-0.5788008	0.91464626	-0.156447	1.03682955	0.28679543
C_4	0.80886879	0.79299509	1.1701635	-1.4455402	0.19420842	1.33166676	1.88137013	-1.2681976	1.86455034	0.25560467	0.89811302	-1.196145	0.36856503	1.44448744	1.40488719	-1.6361779	0.62172506	-0.8067051	-1.7624028	-1.1340331	1.20693474	-0.3572869	0.71745626	-0.7078464
C_40	1.0844428	0.94748886	0.50888389	-2.2573397	0.61958018	1.30527273	2.08282699	-0.6923481	1.08622235	0.36349042	0.41035285	-0.2500733	0.64546123	1.1781293	2.33944555	-0.5188414	0.82246149	-1.912244	-1.9014077	-1.714857	1.05298602	-0.46606	0.28535541	-0.4342038
C_5	0.63672308	0.7648072	0.54294164	-1.8482589	0.92580633	0.96682234	1.71691441	-0.8656755	1.65788696	0.47734778	0.58583837	-0.4936719	0.07372172	1.26521441	0.29826318	-1.1262768	1.50936237	0.23588463	-0.815827	-0.5086164	1.42703596	0.23374961	1.86033415	-0.6170907
C_6	0.90707782	0.94873966	1.222399	-2.4287685	0.72626417	0.88790214	1.83289101	-1.0334449	1.53173747	0.10509233	1.00037071	-1.0348563	0.35732401	1.39955746	1.18170192	-1.0330692	0.97723529	-0.3779211	-0.646077	-0.5706883	1.13550752	-0.0972561	1.24289741	-0.1997274
C_7	0.40299738	0.26734727	0.29761182	-2.6799315	0.33162335	1.29219878	2.68071929	-1.1591481	2.26596618	-0.0894568	0.45817367	-0.6297478	0.83390895	1.96420574	1.52683916	-1.8226699	0.27187069	-1.2206704	-2.2700353	-1.5091574	1.73803009	0.20793392	1.76241889	-0.8430922
C_8	0.68333863	0.64705925	1.0010411	-2.8912493	0.41054988	1.18392299	2.25262791	-1.0806836	2.09183704	0.18282931	0.56635351	-0.2742297	0.53388829	1.67971652	1.64884661	-1.5242101	0.2444953	-0.9699999	-1.963698	-1.7212085	1.62588758	-0.210687	1.31415967	-0.7973376
C_9	1.24099067	1.49235101	1.07278673	-1.2924528	0.69665215	1.04674516	1.75986819	-1.3916208	0.90834697	0.613328	1.11457985	-1.099681	0.21737066	0.94061959	1.67102445	-1.3346888	0.83688944	-0.6722692	-1.4969757	-0.9847488	0.78422242	-0.6627079	0.71922325	-0.3375114

Table 8.129: Normalised data matrix for phosphatidylethanolamine and lyso phosphatidylethanolamine for serum samples taken from patients with breast cancer.

	LPE(17:0)	LPE(18:0)	LPE(18:1)	LPE(18:2)	LPE(20:4)	LPE(18:1)pla	PE(32:0)DM	PE(34:0)	PE(34:1)	PE(34:2)	PE(34:3)	PE(35:0)	PE(35:1)	PE(35:2)/PE(	PE(35:3)	PE(35:4)	PE(36:1)	PE(36:2)	PE(36:3)	PE(36:4)	PE(36:5)	PE(37:1)	PE(37:2)	PE(37:3)
P_1	-0.7859599	2.23495756	1.42646561	1.20327854	1.20565587	-4.3519066	-0.5997964	-1.1886571	0.92481849	0.66150971	-1.9204709	-2.4241222	-0.5193118	-0.2082345	-2.3721118	0.28380202	1.16052131	1.88641076	0.83581238	1.10046865	-0.4290355	-1.0490115	-0.1253465	-4.1236569
P_10	-0.6993503	1.91553248	1.19594168	1.44642913	0.90720744	-3.9829029	-0.7285196	-1.1389641	0.30053016	0.52192665	-1.2205327	-2.506659	-0.7499837	-0.0592866	-2.6500281	0.82634614	0.77327544	1.67732284	0.69264381	0.7134827	-0.4143565	-0.5198765	0.01622406	-4.2003826
P_11	-1.0613697	1.56794074	1.10465158	1.49827774	0.70372424	-2.4439115	-0.3958442	-2.3813585	-0.3669325	0.11626303	-0.7678568	-1.484061	-0.2730988	0.16875857	-3.4895657	0.77091738	0.68276731	1.33549934	0.46070334	-0.2022433	-1.266602	0.08890268	0.31862569	-3.7432188
P_12	-0.8652018	2.58602788	1.6277077	1.96900331	1.67387877	-3.9156288	-0.3535797	-1.4787604	0.56549624	0.91236744	-0.7380216	-3.1347402	-0.9646747	-0.4457078	-3.0704596	-0.5560133	0.87720606	1.91625817	0.98298168	1.10007826	-0.780251	-0.8426735	-0.2600965	-2.9887546
P_13	-1.0087423	2.39817789	1.41667575	1.73966424	1.36122344	-3.6073675	-0.3590908	-1.8659506	0.71449975	0.81067162	-1.3722666	-3.1161596	-0.7262427	-0.1915047	-1.8885545	-0.2423062	0.83520077	2.02581092	0.81227171	1.14447803	-0.8770362	-0.4765356	0.01113089	-2.9862778
P_14	-0.6190333	2.82977852	2.03781914	1.97016691	1.64979243	-4.2723736	-0.7344812	-0.9822772	1.0556096	1.02729791	-0.9195181	-2.5887919	-0.626314	-0.4600926	-2.1016148	-0.1620321	1.12604163	1.99323168	1.01213904	1.48199799	-0.6415512	-0.9161919	-0.3680882	-4.81318
P_15	-0.4889323	2.02973076	1.33870948	1.62771477	1.09877873	-1.6384045	0.22025261	-2.4556635	-0.1472279	0.32546729	-0.6339382	-2.6222128	-1.331856	-0.5619632	-2.2124488	0.24025408	0.50688569	1.29147264	0.47196578	0.6851001	-0.8153992	-0.5604241	-0.0223756	-2.1805075
P_16	-0.8596393	2.56601876	1.65141223	1.8226325	0.94921678	-3.7554637	-0.657559	-0.8276163	0.85218661	1.22241628	-1.2558259	-3.4889127	-0.4926145	-0.1454739	-2.3045594	-0.0899815	1.59537199	2.61946625	1.55750305	1.23188121	-0.317046	-1.2444708	-0.0331875	-2.7612247
P_17	-1.2108232	2.2651043	1.48087571	1.88013231	0.91653327	-4.1959816	-0.5991395	-1.6443337	0.82356113	0.95853886	-0.4541473	-2.1872647	-0.8426207	-0.1191363	-1.9130359	0.07258668	1.0030383	2.23926397	1.03022254	0.60426712	-1.076694	-0.6542754	0.31676076	-3.0072608
P_18	-1.3575919	2.26624644	1.53520169	1.80564148	1.10001431	-4.6112261	-0.751827	-1.1632408	0.94976092	1.19325917	-1.556616	-2.5025476	-0.3539849	-0.2522074	-2.3679396	-0.132155	1.6692448	2.58739352	1.36519925	1.15180206	-0.6534474	-0.8575387	-0.3970944	-2.7382398
P_19	-0.2822203	1.71173878	0.75972308	1.2869639	0.72658754	-3.4983093	0.02886771	-2.2449421	-0.5012312	-0.0534342	-0.5741001	-2.5304496	-0.5926703	-0.4051562	-2.1987143	0.81714906	0.19348799	1.13634311	0.06413985	0.06248521	-0.9397772	-0.1772183	-0.1166546	-2.8259176
P_2	-0.8310132	2.46234675	1.39212113	1.86678218	1.26916372	-4.1334409	-0.3281623	-1.4253863	0.67498515	1.10332817	-1.0351682	-2.5377384	-0.8738813	-0.4317039	-2.3873752	-0.0094155	1.40411918	2.22889903	0.92961887	1.0902599	-0.9395722	-0.8695038	-0.3800173	-2.1549562
P_20	-0.7808583	2.37143223	1.5199454	1.75905463	1.08267889	-4.0082597	-0.627105	-1.1896403	0.85253154	1.26808643	-1.6333414	-2.0629539	-0.4066403	-0.0380196	-2.7749486	0.18229813	1.43888867	2.53391364	1.45991591	1.46903675	-0.7829009	-0.7009685	-0.2364672	-3.4377439
P_21	-0.667971	2.42241277	1.84706378	2.21081063	1.62913597	-3.4615819	-0.6482849	-2.0123343	0.46316135	0.7204711	-1.7519197	-3.0371075	-0.5637925	-0.1639876	-3.2760332	0.20805925	0.76321384	1.89725777	0.9412455	0.92264905	-0.6384853	-0.5540113	-0.2147404	-2.8855612
P_22	-0.6709992	2.95483751	1.97161193	2.72017979	1.35553724	-3.4903289	-0.8625751	-1.55615	0.63668464	1.49157061	-1.4104479	-3.3729418	-1.0776411	-0.0791823	-3.123393	-0.6093506	1.14815035	2.67017669	1.22512478	0.88645515	-0.0074571	-0.9600694	-0.2402095	-4.702993
P_23	-0.3549511	2.56531602	1.67205134	1.84028745	1.41248791	-3.293555	-1.1809233	-1.570682	0.41938665	0.66057574	-0.9941129	-2.8821436	-0.9817744	-0.2194668	-2.1916654	-0.2255269	0.89172745	1.8612897	0.79318443	0.87953529	0.01918486	-0.6264086	-0.0619924	-3.2516293
P_25	-1.1345147	2.19871949	1.38490096	1.74969673	1.27841576	-2.6972598	-0.5337673	-1.4894499	0.35973881	0.78797131	-1.7943781	-2.3921868	-0.5622053	-0.2563549	-2.1822593	0.04712148	1.12527293	2.0826339	0.87651978	1.1120989	-0.6321216	-0.5971308	-0.0673393	-3.0109666
P_26	-1.0708238	2.45668075	2.01156551	2.17093944	1.47130515	-4.5915024	-0.8427409	-1.6322635	0.63985073	1.2436429	-1.5971431	-3.0974341	-0.4086711	-0.1679844	-2.1974552	0.60382468	1.48675411	2.54459002	1.33219833	1.13790676	-0.6492382	-0.8066232	-0.4037155	-3.377839
P_27	-0.9196695	2.36423659	1.62619776	1.84428603	1.30968412	-3.1442522	-0.6878017	-1.4042124	0.72831566	0.61038479	-0.4308802	-3.2294142	-1.0274944	-0.312208	-2.6812923	-0.285559	1.04502996	1.97298961	0.98966105	1.19446589	-0.4884701	-0.623879	-0.1195015	-2.3873959
P_28	-0.8934235	1.75129516	0.69208966	0.9701881	0.82688627	-2.9601134	-0.2006453	-2.2469783	-0.3450209	0.04757771	-1.5658976	-2.3076188	-0.4024188	-0.0707477	-1.7846629	0.36368053	0.73540929	1.34837382	0.49381788	0.62020589	-0.8677673	0.30249363	0.1338295	-2.2217546
P_29	-1.3795984	2.48904529	1.41956449	1.84304651	1.24397228	-3.1156174	-0.7362142	-2.0064815	0.48454556	0.76875544	-1.4151157	-2.9942109	-0.8334817	-0.3614495	-2.1280725	0.24359657	0.8100892	1.84021413	0.66554589	0.83921773	-0.5528687	-0.669731	-0.1326818	-3.5258243
P_3	-0.8612201	1.84053315	1.08433898	1.6970248	0.76901706	-3.9706692	-0.3782478	-1.322376	0.53794983	1.03032093	-0.9378306	-2.9177082	-0.5899203	-0.2658998	-1.7126923	0.66892216	0.8798975	1.87030633	0.98242837	1.04661084	-1.4625744	-1.1033699	-0.0932261	-3.1295442
P_30	-0.3236931	2.83724801	2.02645113	2.09545939	1.68608035	-3.8582638	-0.5634797	-1.7493445	0.07957943	0.50171834	-1.5257658	-3.2871274	-0.9265171	-0.7049115	-4.1279681	-0.5521053	0.91971482	1.87377685	0.7300616	0.81749516	0.43663091	-0.7365723	-0.3969076	-2.3913597
P_31	-0.3604555	1.93053072	0.86418217	1.46785332	1.31275477	-3.7141414	-0.6262085	-1.0607988	0.50366407	0.62302629	-0.9777691	-2.7150477	-0.7207603	-0.5397436	-2.6320572	0.67670821	0.51699145	1.73755801	0.68241993	1.12206868	-1.5392953	-0.3471365	-0.0005277	-2.436756
P_32	-0.8039872	1.79230097	0.66396625	1.10772026	0.39707226	-3.0367474	-0.3595545	-1.5932368	0.05689154	0.32179204	-1.5920695	-3.2606977	-0.5932204	-0.5026411	-3.2492309	0.38054386	0.7984041	1.44900568	0.488489	0.88979033	-0.3427115	-0.1088256	0.02706868	-3.8602956
P_33	-1.1728276	2.00158961	1.60100389	1.95566656	1.47419432	-4.0396674	-0.1619278	-1.8738917	0.28274133	0.62740764	-1.7693743	-2.6596865	-0.4937668	-0.0055658	-2.1226789	0.58066236	1.05846479	2.03398237	0.58182214	0.76725717	-1.2229673	-0.1915151	0.12956697	-3.7014239
P_35	-1.1444732	2.24427021	1.52229724	1.61195095	1.38045812	-3.9919603	-0.3487033	-1.1944806	0.64100877	0.6679451	-1.8932558	-2.8143095	-0.4548265	-0.212987	-3.5044069	0.45328972	0.59636295	1.47268781	0.36379022	0.95294623	0.18049658	-0.4077501	-0.0887906	-2.48814
P_36	-1.0293131	1.92222798	0.78307674	1.24813059	0.95971529	-2.8204348	-0.5592463	-2.8880228	0.33267528	0.29132856	-1.8385604	-2.6243812	-0.6344584	-0.3029896	-1.8731822	0.42477615	0.4095368	1.3827481	0.42802913	0.82240783	0.19537789	-0.4935777	-0.0090839	-2.7987774
P_37	0.51129682	0.22099766	-0.9076386	1.05292606	0.27241204	-0.713743	-0.5505213	0.19110483	1.11770995	1.34997748	-1.5474215	-1.553203	0.81352757	1.41977941	-0.8016299	0.22739075	0.05164422	1.90834623	0.23454264	0.93175447	-0.4896392	-0.058215	-0.0995445	-1.0744421
P_38	-1.1108236	2.36397777	1.8782099	2.0165535	1.60625307	-3.648007	-0.4074299	-1.8140794	0.55281577	0.64915389	-1.6067011	-1.7433885	-0.2527132	-0.1912766	-2.6292937	0.60587376	0.91390622	2.03275947	0.88434439	1.03789045	-0.9771784	-0.5165887	-0.2711877	-2.3233304
P_39	-0.5123384	1.78626658	1.41284827	1.32879501	1.07272201	-3.4389371	0.04151778	-2.8348338	-0.0930535	-0.4383779	-0.9964544	-1.7156199	-0.1332828	-0.3042551	-2.9702702	0.78284486	0.68544824	1.34226947	0.5001523	0.71834847	-0.3850571	-0.1630926	-0.3650071	-3.0128218
P_4	-0.5526168	2.5061541	1.29496843	1.4392652	1.0497592	-4.2751467	-0.6089342	-1.7242771	0.40003266	0.57934288	-0.7607025	-2.5451746	-1.1488327	-0.1133916	-3.7327907	-0.1228433	1.0191926	2.10881321	0.95742871	1.02988728	0.15793381	-0.8187023	-0.0326873	-3.9194744
P_40	-0.9234339	1.8956558	1.18133453	1.61128679	0.80012441	-3.0656473	-0.1734637	-1.3540637	0.31186394	0.53130324	-0.6553158	-2.833842	-0.3679694	-0.2251738	-2.4027864	-0.64097	0.59958398	1.68156107	0.30237274	0.68998681	-1.0961086	0.04140138	0.2081103	-2.5157034
P_41	-0.5313679	2.43507361	1.62981982	1.96934459	1.26421419	-3.6542955	-1.176456	-1.3661791	0.76155174	1.07764131	-1.3180845	-2.651997	-0.8562023	-0.1980984	-3.1543184	0.34212976	1.2376293	2.33290356	1.28434744	1.08857987	-0.8801749	-0.7718829	-0.1967643	-3.283273
P_5	-0.5958708	1.96450241	1.71981724	2.2398571	1.1469353	-3.5860774	-0.8999245	-1.3662711	0.71422713	1.29487574	-1.1737848	-3.4246014	-0.3001091	-0.1411933	-2.3578321	0.03178962	1.25988432	2.4104853	1.49536019	0.98847377	-0.5470357	-1.033828	-0.039988	-2.6454698
P_6	0.61735876	-0.3194756	-0.0529432	-0.5009327	-0.3708307	-0.5459015	0.41129202	-0.7376026	0.66157627	0.93425228	-2.5389223	-1.5978825	0.53393632	-0.0750335	-2.2210708	-0.3919994	1.4204126	2.67024985	1.11107617	1.3848075	0.41961525	-0.5186739	0.62205107	-0.7128577
P_7	-0.7597863	2.73493162	1.53197766	1.98823448	1.63324917	-4.0449129	-1.2133886	-1.5303303	0.62590378	0.8419312	-1.0581105	-2.54863	-0.686944	-0.5288196	-2.2346664	0.05510302	0.89664587	1.99695645	0.88789037	1.25045211	-0.4299133	-0.3184803	-0.2060713	-4.7021935
P_8	-0.5986303	2.15607659	1.79009206	2.06979542	1.25753195	-4.3693118	-0.677419	-1.1799766	0.0469681	0.70513128	-2.4436055	-1.938056	-0.2415387	-0.0430524	-2.7661042	0.52212591	1.02448162	2.13072992	1.05119946	0.77029422	-0.1219721	-0.9186314	-0.626936	-4.0817038
P_9	0.22887881	-0.0143179	-0.1048381	-0.0188838	0.57806687	-1.0573659	-0.6031935	-0.7126728	0.58560569	1.3930118	-1.8396333	-1.147255	-0.7278051	0.82799861	-2.0657056	-0.3994636	1.730047	2.21240796	1.20488666	0.71572337	-0.458513	-0.5205177	0.35920988	-1.8326812

Table 8.130: Normalised data matrix for phosphatidylethanolamine and lyso phosphatidylethanolamine for serum samples taken from patients with breast cancer.

	PE(37:4)	PE(37:5)	PE(37:6)	PE(38:1)	PE(38:2)	PE(38:3)	PE(38:4)	PE(38:5)	PE(38:6)	PE(39:5)	PE(39:6)	PE(40:4)	PE(40:5)	PE(40:6)	PE(41:3)	PE(43:3)	PE(unknown	PE(unknown	PE(unknown	PE(unknown	PE(16:6)	PE(21:5)	PE(21:6)	PE(38:0)
P_1	0.82991517	0.8533288	0.75520261	-2.0047905	0.53717075	1.09615253	2.35030389	-0.4111942	2.24639071	0.20626633	0.69245716	-0.344546	0.65910697	2.0261875	1.58373609	-1.6449504	0.40247332	-1.7117108	-1.7043105	-1.6993564	1.42082628	0.0659467	1.66097423	-0.6916594
P_10	0.76090593	1.09196473	1.42218814	-1.8038266	0.46920804	0.44543929	1.66158753	-0.5147652	2.23689436	0.39760027	1.248931	-1.3938026	0.54040231	1.85173714	1.05727585	-1.8913274	0.77200211	-1.0146783	-1.3139448	-0.8563188	1.42500513	0.03422926	2.08538472	-0.828112
P_11	1.09741884	0.59842526	1.04919483	-0.4424253	1.35906165	0.81677326	0.91310238	-1.0207041	1.19850221	0.28573464	0.68717571	-0.9876422	-0.0284301	0.97579705	0.2799049	-0.3097397	1.60409643	-0.0083823	-0.6545507	-0.3570754	0.94641249	-0.226032	1.45117831	-0.1687651
P_12	0.44118094	0.37904121	0.23287672	-1.6477256	0.76203809	1.17033846	2.31014141	-1.7040956	2.19663376	0.00714942	0.19615973	-1.1183046	0.46199549	1.81289997	1.55391943	-2.6972896	0.96009389	-0.3075057	-1.4155967	-0.9204249	1.70175137	0.38848034	2.19269363	-0.7728933
P_13	0.47510897	0.49377818	0.45194132	-1.2845177	0.49845106	1.09788033	2.18822663	-1.2701142	1.76223507	0.02200721	0.13852478	-0.7704566	0.64441015	1.73727126	1.307698	-1.1849548	0.52684674	-1.1811417	-1.2744549	-1.5323499	1.51171634	0.22117118	1.41185285	-0.5429003
P_14	0.66937919	0.45915568	0.23858514	-2.2199722	0.37461015	1.09955401	2.49524309	-1.5399892	1.96760741	-0.1418649	-0.114775	-0.6309524	0.56976443	1.77549149	0.69140007	-1.7277414	0.28781645	-1.0778699	-1.670273	-1.1257649	1.91000684	0.51712808	1.91505462	-0.6999285
P_15	0.75186229	0.54277558	0.73803616	-1.4104736	1.01269874	0.86547386	1.62939206	-1.3318764	1.36116287	-0.4830311	0.16025381	-0.9534866	-0.1251043	1.0834053	0.41574158	-1.6444792	1.59196335	0.13072099	-0.5068923	-0.5174629	1.07113621	-0.2088571	1.641988	0.02007442
P_16	0.3247154	0.52088242	0.42981816	-1.5639723	0.22411488	1.00603896	2.30806381	-2.193037	1.95867351	-0.2097795	0.37546995	-1.0067479	0.46561217	1.74578985	1.71752439	-1.3878551	0.37045617	-1.0653352	-2.187817	-1.8442319	1.50985457	-0.0546926	1.37948264	-0.657559
P_17	0.40005347	0.54040217	0.62114392	-1.1643192	0.6362779	0.84788999	1.89404929	-1.6579299	1.49673525	0.08645166	-0.0140275	-0.8590259	0.38754608	1.51686547	1.10703071	-1.2950969	0.89871809	-0.4105242	-1.5316412	-1.3415097	1.22409541	0.0194472	1.5032382	-0.5920423
P_18	0.8005379	0.45898755	0.6091615	-1.4688991	0.49443388	1.22926995	2.32637347	-0.7833169	2.10509829	-0.1341571	0.50328737	-1.0729231	0.63024925	1.90709416	1.34531766	-1.8811837	0.06470445	-1.740667	-1.9202138	-1.6373553	1.31372705	0.11281052	1.58972077	-0.7801648
P_19	0.9680899	1.07465698	1.0447927	-0.9113989	1.13445452	1.0081915	1.41815401	-0.6985502	1.2870262	0.21527382	0.60399681	-0.6515517	0.23112219	0.90797506	0.98179787	-0.6565942	1.32388975	-0.4680933	-0.8841065	-0.4388401	1.23160359	-0.2538395	1.67495915	0.0102995
P_2	0.55329738	0.41528784	0.57207556	-1.9754586	0.52129843	1.00966982	2.1967062	-1.8170375	1.8040536	-0.2422084	0.46866789	-0.5532031	0.6680877	1.81733678	1.45189307	-1.5269128	0.31267753	-1.3426163	-1.9414808	-1.4119611	1.45257195	0.1962408	1.57211703	-0.2853922
P_20	0.80887274	0.76583805	0.23481697	-3.5637071	0.53178155	1.31540129	2.61784181	-0.368867	1.90710754	0.41648847	0.4815629	-0.5925796	0.66606498	1.4646947	1.99776955	-2.2325259	0.4340786	-2.2438095	-2.0542087	-1.8393155	1.45057329	0.02991025	1.1185591	-0.6042832
P_21	1.02422183	0.81762757	0.77142373	-1.8943995	0.69606187	0.84041803	1.79625233	-1.0012979	1.77144826	-0.0218444	0.45870065	-1.7812291	0.42322253	1.41220587	0.52106333	-1.6119698	0.9368722	-0.392642	-1.2521036	-1.226686	1.38862603	0.651862	2.17078068	-0.6482849
P_22	-0.1834093	0.18964198	0.15642103	-1.1815091	0.71682345	1.1320734	1.83386638	-1.1774888	2.07353369	-0.287263	0.27868745	-1.1820859	0.40735343	1.72957334	0.68748861	-1.8379116	1.04776801	-0.5151969	-1.1718762	-1.4621065	1.8678396	0.62439798	2.21936426	-0.8625751
P_23	0.28548137	0.21932116	0.47256845	-1.6034158	0.58531746	1.21091876	2.11879653	-0.908265	2.33807906	-0.4116192	0.07011043	-1.0555261	0.65129884	2.089376	0.56031359	-1.4866499	0.72866919	-1.1669041	-1.5025043	-1.5938337	1.75561395	0.37581633	2.31424549	-1.2274036
P_25	0.58544713	0.62064761	0.76059889	-1.6023998	0.66220073	1.11890182	1.97456004	-2.0946568	1.70769135	-0.0055919	0.35787081	-0.643723	0.07525624	1.51008054	1.69603641	-1.4401506	0.64240755	-0.8155798	-1.5316222	-1.1690965	1.03651604	-0.0769059	1.51900899	-0.5406533
P_26	1.20534052	1.00292615	0.80460997	-2.9191729	0.3920803	0.93946211	2.1295401	-1.2907634	1.85883182	0.19073854	0.81406295	-0.8193436	0.43229272	1.5511406	1.12487624	-2.606065	0.23793675	-1.5624783	-1.6530999	-1.3074843	1.39640247	0.4193619	1.89134598	-0.4883657
P_27	0.4323856	0.54934639	0.51622615	-2.3313448	0.35577269	0.9655866	2.22617059	-1.0018506	1.70688757	-0.1075064	0.35730897	-0.7972679	0.3197619	1.66989353	1.13949188	-2.242038	0.89556923	-0.5677391	-1.361412	-1.022104	1.41349463	0.04939614	1.58941629	-0.6986665
P_28	1.07677496	0.93245412	0.90470927	-1.2791548	1.27086456	1.13953805	1.75471691	-1.0166785	1.39534976	0.19872285	0.6297155	-1.1561404	0.12546289	1.24397009	0.9297221	-1.2424317	1.44467637	-0.47638	-0.8080627	-0.4889506	0.679654	-0.5189545	1.02928247	-0.1876589
P_29	0.16198085	0.47018761	1.03883129	-1.3082682	0.81677615	1.20970237	2.09557933	-1.637516	2.30350361	-0.2035741	0.32013358	-1.2638632	0.60760216	2.01098136	1.16939769	-1.5088694	1.05910928	-0.2175683	-1.5432265	-1.6473484	1.58486226	0.20421819	2.26146005	-0.7803372
P_3	1.18391272	1.03242872	0.64734209	-0.9793346	0.79690502	0.94744277	1.97861472	-1.6880757	1.50195893	0.38786747	0.71658337	-1.227543	0.17098106	1.16494849	1.68811425	-1.5861699	0.80382629	-0.5231033	-1.20054	-0.947266	1.08903925	-0.5290844	1.27397508	-0.3648946
P_30	0.15646526	0.29534948	0.2915402	-1.6825786	0.55278493	0.90789045	2.06322958	-1.3102437	2.11367319	0.07533218	0.37319738	-1.6974201	0.53852814	2.15482791	0.23394094	-0.9527962	0.94965515	-0.3263827	-0.6696552	-1.3877804	1.8386771	0.68886729	2.59899624	-0.6662985
P_31	0.89783015	1.08503871	0.93334095	-1.6433198	0.84157856	1.05866452	2.34647706	-1.5357455	1.9629704	0.17786783	0.53260588	-1.2836211	0.44379108	1.65532537	1.57431697	-2.4062999	1.01385406	-0.4877591	-1.2141352	-1.4199729	1.16935056	-0.1455221	1.45590002	-0.7795964
P_32	0.41332056	0.76412496	1.12625662	-1.7549142	1.07636215	1.25160002	2.00030987	-0.560807	2.3170843	0.16141025	0.73095775	-1.1869281	0.62777528	1.82171341	1.35532948	-0.4375458	1.34414392	-0.7472788	-1.0336951	-0.5971931	1.40538593	-0.3472034	1.55622621	-0.356262
P_33	1.1267025	0.95443822	0.85382967	-2.1563814	0.67306121	0.83593159	1.88159815	-1.3593002	1.32624943	0.49030249	0.66931638	-1.4232602	0.10898478	1.12162615	0.92731417	-1.2212259	1.01957054	-0.5247607	-1.0891457	-0.7336533	0.97866526	0.53009524	1.64113749	-0.3101618
P_35	0.52486897	1.28943984	1.33365134	-2.0581101	0.32400716	0.87612989	1.68509075	-0.8665626	1.95286343	0.42639657	0.79998586	-0.8054355	0.50545508	1.61481027	1.07278202	-3.7204272	0.72908575	-0.6558477	-1.485036	-1.2885652	1.58171375	0.73756744	2.23141935	-0.3487033
P_36	0.6264662	1.0558112	1.14410425	-0.8657991	0.63074963	0.77583794	1.95564872	-1.439336	2.25434742	0.35881872	0.79912998	-1.1256736	0.60663397	1.99827473	0.95655824	-1.334281	0.92273299	-0.8503287	-1.599121	-0.9408935	1.28698193	0.03822226	1.97635857	-0.5592463
P_37	-0.9606775	-1.160794	0.20617734	-0.9519005	0.85552634	0.99509839	1.85927384	-2.1196933	1.23989101	0.79496988	-0.4212507	0.17928596	0.45507952	1.06215483	0.70381216	-0.6874626	-0.7068889	-0.4912989	-1.7547619	-0.2966286	0.39264813	-0.1209525	-0.9756909	-0.6033292
P_38	0.91961747	0.67482962	0.02444097	-1.3179812	0.57381519	1.09579137	2.12767825	-1.6957036	1.12209061	-0.2226073	-0.4010916	-0.4855547	0.35393272	0.98155709	0.7758945	-2.1515834	1.24981577	-0.6710321	-1.4016747	-0.9877903	1.29353544	0.37328308	1.12642664	-0.4074299
P_39	1.25498005	1.34346007	1.3121744	-1.4839035	0.92750002	0.50614897	1.35865191	-1.524649	1.35370043	0.72151803	0.94137741	-1.4480389	0.13220714	1.18333597	0.33132815	-1.6243553	1.27780217	-0.4406682	-0.8381973	-0.7428963	1.17924461	0.01891765	1.91103257	0.04151778
P_4	0.43591216	0.5026842	0.85922177	-1.764493	0.50376236	1.03895938	2.30220951	-1.3336379	2.21343148	-0.0852396	0.73528188	-0.9589742	0.77671665	2.23269619	1.81538298	-1.2102054	0.52912529	-0.8322017	-1.7282125	-1.1525459	1.56111132	0.11388244	1.99641665	-0.738488
P_40	0.2805061	0.52788454	0.17176833	-1.5360187	1.03549095	1.09111512	1.88179793	-1.3822317	1.62992257	-0.0578963	0.30544157	-0.9662198	0.28584322	1.50409311	1.0668641	-1.6375362	1.43278916	-0.07455	-0.8870406	-0.5966515	1.13532115	-0.1195077	1.46980867	-0.161101
P_41	0.79430236	0.6562461	0.46335328	-2.1509591	0.41010865	1.07221428	2.17469355	-1.1643348	1.59286129	0.17651559	0.14412726	-0.6954815	0.47428324	1.59703389	1.26505209	-1.2138599	0.73234685	-0.8611109	-1.4826618	-1.3392556	1.43347813	0.16776043	1.54560156	-1.176456
P_5	0.49233894	0.61752566	0.48727251	-2.1089494	0.84138988	1.15690238	1.70682656	-1.1134811	1.5479674	0.17128371	0.55617294	-0.6625432	0.29695578	0.99636969	1.83122971	-1.9271271	0.58528076	-1.0290601	-1.2851188	-1.7732659	1.43193084	-0.1504946	1.4154155	-1.2390443
P_6	1.00668106	-0.8095409	0.25738102	-0.5382625	1.15223251	1.18517099	2.52482718	-0.7569858	1.9711925	0.1315768	-0.042272	-2.1416016	0.9147952	1.63607912	1.12744847	-1.0591903	-0.7435047	-0.8699274	-2.9014021	-1.087211	0.20855818	-0.4650154	-1.3314399	0.42790886
P_7	0.71192215	0.58297872	0.52119153	-2.1253292	0.52216933	1.17118186	2.42848669	-1.2589818	2.05283026	-0.17605	0.11370023	-0.6669873	0.53206663	1.82938021	1.24000208	-1.4796709	0.70488584	-1.2724796	-1.4606934	-1.1992505	1.83637895	0.48760538	1.93702313	-1.2133886
P_8	1.03491676	1.06875232	1.36692224	-2.2220027	0.45302943	0.53541663	1.768475	-1.0847311	1.83770317	0.07856244	1.14597761	-0.9022852	0.15463624	1.5830873	0.76372086	-0.9059874	0.80463964	-1.051165	-1.4446206	-1.164283	1.44842344	-0.0650547	1.92695464	-0.6485768
P_9	0.1807173	0.63241163	-0.4841003	-0.9045732	0.57615129	0.75359842	1.98596827	-1.3794661	1.24881359	0.06682346	0.16550438	-0.1343887	1.18157227	1.23943749	1.36920458	-1.0955527	-0.188257	-0.8815637	-0.8217639	-0.7333012	0.09429706	0.07418956	-0.2485211	-1.0301916

Table 8.131: Normalised data matrix for phosphatidylglycerol and lyso phosphatidylglycerol for serum samples taken from breast cancer free controls.

	LPG(16:0)	LPG(17:0)	LPG(18:0)	LPG(20:5)	LPG(20:6)	PG(26:0)/die	PG(28:0)	PG(30:0)	PG(30:1)	PG(31:0)	PG(32:0)	PG(32:1)	PG(34:0)	PG(34:1)	PG(34:2)	PG(36:0)	PG(36:1)	PG(36:2)	PG(36:3)
C_1	1.56056836	-0.0897252	0.44498167	-0.3516038	-0.0934472	-0.8443615	0.14088664	0.95493888	-0.718893	-1.0285521	1.51466487	-2.0043329	0.20789975	1.94845777	0.49626851	-1.7271499	-0.487271	0.74031809	-0.6636479
C_10	2.39001114	0.13997309	0.54464908	0.73586975	0.74090996	-0.3730631	-0.4268728	0.07752416	-1.0184816	-0.3944657	0.82080934	0.20615671	-1.292056	1.22119438	0.52100317	-2.5244702	-0.5265415	-0.0430506	-0.7990993
C_11	2.32408694	0.17617084	1.27703655	0.90635122	0.56499148	-0.0002459	0.13627073	0.27899289	-0.4766688	-0.4575852	0.51579288	-0.4291716	-0.6197745	1.10544797	0.35712579	-2.491622	-1.4803828	-0.652871	-1.0339455
C_12	2.41166971	2.00464121	2.29333341	0.9128658	1.34239964	0.33207443	-0.0171295	-0.5108345	-0.7582727	-1.7031941	0.02438441	-0.149752	-0.1619518	0.1184791	-0.4195568	-1.9011587	-1.3937495	-1.1769479	-1.2473002
C_13	3.12468129	1.25939617	0.85860537	2.12552186	1.80183508	-0.5644833	-0.7429823	-0.1122656	-0.6102146	0.03430265	-1.223452	-0.4414129	0.4674278	-0.5212214	-1.6152486	-0.9595382	-0.5955626	-1.2268008	-1.0585879
C_14	3.3267561	1.10787416	1.54246428	1.77743552	2.12480736	-0.4352519	-0.3535601	-0.7351309	-1.3777002	-0.4705289	0.20034704	-1.1997495	0.31053642	-1.3066093	-1.3910633	-1.5466732	-1.5476707	-0.1599003	0.13361751
C_15	3.00449069	1.47965115	1.79285401	1.09019569	1.22177507	-1.3525862	-0.7111648	-0.0141254	-1.9062849	-1.0667731	0.59337959	-0.0821626	-0.0027256	0.83939087	-0.3384682	-1.6006729	-1.1552789	-0.1589658	-1.6325287
C_16	1.02809585	0.10028537	0.57657315	-0.854273	-0.967289	-0.281496	-0.0886807	0.19593528	-0.4016824	-1.1390402	0.59919908	0.24743483	0.29566183	1.18284187	0.27479694	-1.8321034	-0.0236674	1.04191392	0.04549396
C_17	3.04878471	2.05833086	2.35863652	1.5628419	1.43382421	0.06037204	-0.5575325	0.0480019	-1.0170084	-0.029328	0.25210066	-0.7866446	-1.3215817	0.89774574	-1.5900908	-1.8468585	-1.7328899	-1.0029632	-1.8357408
C_18	2.08626214	0.20024885	1.04398756	-0.0282834	-0.1541862	-0.0093342	-0.4723947	0.46359538	-1.279611	-0.6140973	0.98818961	0.08908235	0.14944134	0.74956893	-0.4024666	-1.3065688	-0.3055898	-0.2539368	-0.9439073
C_19	3.53367595	0.81790344	1.8141249	1.00368901	1.03803294	0.38028913	-0.9374464	-1.3310432	-1.2045314	0.2500461	0.27162097	-0.7673563	-0.4804658	-0.8152527	-1.4633956	-0.6481255	0.06155589	-0.2963407	-1.2269808
C_2	2.23917823	1.2430219	1.72318334	0.89211841	0.67386117	0.25759521	-0.1783904	0.67257803	-2.0511917	-1.7503995	0.92188591	-2.3989718	0.1446455	1.26927707	0.2248369	-0.8525805	-1.7373225	0.00731527	-1.3006404
C_20	2.41983413	1.59221335	1.92795788	0.83987908	1.05699912	0.08322031	0.11810351	0.3539512	-0.8180135	-1.0061179	0.67220629	-0.6989935	0.05193753	0.24567009	-0.5653338	-0.8295747	-1.3280058	-1.1020869	-3.0138463
C_21	2.76653161	1.00555178	1.51367038	1.01172545	1.38967946	0.02588635	-0.5973457	0.04897925	-0.7942067	-0.6341591	0.60538395	0.01324657	-0.1975264	0.77376013	-0.6545216	-1.9120764	-1.3451995	-0.9897572	-2.0296222
C_22	1.86202535	-0.5449056	0.00360648	0.14343727	0.20812202	-0.1146286	-0.3197731	0.41673443	-0.4307111	-1.796477	1.0854959	0.4860837	0.38085624	1.22627924	-0.2007013	-1.9281688	-0.2031838	0.28591806	-0.5600095
C_23	2.84382694	0.75174053	1.2970792	1.31231254	1.38427155	-0.1252402	-2.6843762	-0.6007426	-0.2176477	0.45309112	0.21360576	-1.2683521	-0.3339515	-0.1128926	-0.7552165	-1.6501194	0.14237678	-0.0399793	-0.6097864
C_24	2.61102952	0.58828833	1.23685204	1.74651833	1.63586766	-0.6887308	-2.3871556	0.04594831	-1.0903618	-0.0273255	0.7337331	0.04071887	-0.702743	1.08906306	-0.00765	-1.592499	-1.1049834	-0.3908854	-1.7356847
C_25	1.57382619	0.49292422	0.79105588	0.92239481	0.56676789	0.01545449	-1.087702	-0.5377001	-1.226249	-0.9717076	0.69825448	0.38223405	-0.188489	1.28044916	-0.2636184	-1.292346	-0.8784768	0.19351888	-0.4705911
C_26	0.90140826	0.5067442	0.88762625	0.99311341	1.08513359	0.25565931	-1.0587745	-0.250054	0.00682179	-1.1669437	0.69017871	-0.0710331	-0.1967102	0.73936892	0.03655302	-1.7425285	-1.1003011	0.23023787	-0.7465002
C_27	2.44186108	0.7442013	0.75722554	0.98522362	0.99337097	0.08926862	-1.8171153	0.02369971	-0.9859144	0.23359314	0.30528673	-0.7704495	-0.450565	0.63529575	-0.7840871	-0.6491756	-0.9133684	-0.4088364	-0.4295148
C_28	2.35526373	1.02533174	1.42287819	1.13391611	1.26378722	0.47769394	-0.059271	-0.7084207	-1.3465882	0.25245164	-0.6426887	-0.9157629	-0.9506764	-0.0556175	-0.6370314	-1.0809082	-0.5103	0.18174254	-1.2058001
C_29	2.68136641	1.19541643	1.25705377	1.43208271	1.12404257	-0.9931433	-1.8843034	-0.666961	-1.9420598	0.17396476	-0.5363369	-0.0922385	-0.8175456	0.93061106	0.43308221	-0.972134	-0.9646509	0.10739863	-0.4656452
C_3	2.38569501	0.7084527	1.56135311	0.52889246	0.85915514	-0.1119678	-1.0572398	-0.4090086	-1.0370936	-1.1211983	0.50469022	-0.0930094	0.13928027	1.22281352	0.21528521	-1.9575355	-0.8196857	0.01077949	-1.5296584
C_30	0.10807681	1.8284875	2.72931015	0.74981897	1.48093986	1.09762353	0.93403402	-1.0855475	-1.718265	-0.6347025	0.880736	-1.202906	-0.5633682	-0.178743	-0.6327576	-1.076197	-0.852197	-0.9659415	-0.8984013
C_31	2.98303196	0.56288164	0.73891098	1.63483178	1.64684778	0.30269898	-0.7400317	-0.6461673	-1.8245112	0.27181304	0.11090201	-0.3425137	-0.5686958	-0.2974552	-0.4201387	-0.2943545	-0.1899564	-1.4444687	-1.483625
C_32	2.96309515	1.02381873	1.85526463	1.83510086	2.11103304	0.66876293	-1.0328038	-0.9733478	-0.0946227	-0.9980409	-0.1475106	-0.9629826	-1.0541335	-1.5084049	-0.9573951	-0.6789227	0.08397015	-0.9563775	-1.1765034
C_33	0.23920255	-0.4844279	-0.7934047	-1.4074347	-1.1764745	0.17138715	0.57209088	1.30922332	0.27027666	-1.1002134	1.67823018	1.13050492	0.5536574	1.70788288	0.91790738	-2.6457669	-0.8324975	0.27227378	-0.3824175
C_34	2.11404536	-0.4485163	-0.2386725	0.68072185	0.616938	-0.9916688	-0.8403646	0.36235689	-0.8868585	-1.3879703	1.48751893	0.81429948	0.26174066	1.87395087	0.72092518	-1.5651908	-0.6586647	-0.254078	-1.6605127
C_35	0.22804847	1.95312509	2.58793499	0.96405298	0.10461369	1.17797146	0.87426286	-0.546927	-1.7352848	-1.1408463	0.11024481	-1.0968577	-0.4133288	-0.554388	-0.9118337	-0.8442503	-0.2612939	-0.1487018	-0.3465421
C_36	2.75280667	1.45615649	1.88444376	0.84358782	0.78840379	-0.1657362	-1.3701999	-0.6082608	-1.6649596	-0.9865219	0.07274046	-0.0608989	-0.9425827	0.74129097	-1.7232698	-0.7765579	-0.4936082	-0.1574201	0.41058618
C_37	2.65415543	0.75207838	0.53475188	1.67582885	1.51347259	-0.265679	-0.8850477	-0.1306188	-1.3990829	-0.2664688	0.33064429	-0.3546937	-1.7831951	0.68609071	0.13627711	-1.5738317	-0.9314614	-0.115145	-0.5780751
C_38	2.96163916	0.98327457	1.96684414	1.51524845	1.47597539	1.01503389	-0.7499156	-0.663621	-1.7415486	-0.5610227	0.50471642	0.30089941	-1.1123198	0.32976111	-0.8797341	-1.5860734	-0.7683575	-1.698329	-1.2924708
C_39	2.50078795	0.47394607	1.1810503	1.57072926	1.85637384	0.36512501	-0.6315826	0.15740809	-0.4100904	0.00988466	0.69523094	-0.8230051	0.04069183	-0.3669238	-1.9971932	-1.411054	-0.0394484	-1.8509238	-1.3210066
C_4	2.27480085	-0.0610076	0.85660173	0.02003221	-0.0336341	0.13251185	0.03623365	0.40018512	-0.1721798	-1.806738	1.10314696	0.00959389	-0.3034195	1.05886436	0.10509644	-1.6426194	-0.6524018	-0.0523588	-1.272708
C_40	2.69696985	0.48806952	0.83589601	0.92019923	0.9539646	-0.0679717	-0.3323819	0.04734265	-1.4948627	-1.0641112	0.78126702	0.20574391	-0.1379522	0.39427782	-0.8210185	-0.9114437	-0.0735059	-0.6064773	-1.8140054
C_5	2.67469154	0.2817415	0.66015129	1.17980234	0.98542536	-0.7488655	-0.3760767	0.2444265	-0.6860481	-0.6838132	0.91246235	-0.2960266	0.29359882	0.84962215	-0.4496242	-2.510724	-0.2922475	-0.8934224	-1.1450738
C_6	3.84516812	1.14818594	1.53659966	1.86780472	2.12286384	0.8797965	-1.3257492	-0.6985079	-0.488091	0.13061533	0.41332881	-2.3951931	0.12271183	-1.4763684	-1.0703631	-1.4675928	-1.1180333	-1.200231	-0.8269451
C_7	3.0177949	1.87413552	1.94240896	0.46726749	0.72100842	0.00843156	-0.045477	-0.2462668	-2.4473634	-0.1600701	0.53485221	0.24884577	-0.2444022	0.54777921	-0.0835274	-2.1526705	-1.5915779	-0.6818688	-1.7092999
C_8	2.62371334	0.44768518	0.65516133	-0.1719387	-0.031703	-0.4108012	0.36477373	0.78701317	-0.3316635	-1.5975701	1.56976734	0.29356907	0.38085216	1.00465374	-0.5533443	-1.9132021	-0.2871874	-0.6409042	-2.1888746
C_9	3.56567891	0.85213202	1.28213632	1.16368222	1.251545	-0.0798639	-0.304153	0.13909578	-0.6206277	-0.2669565	0.97762222	-0.7218976	-1.5911759	0.4834819	-1.2570645	-1.5768932	-1.8549156	-0.1410653	-1.3007611

Table 8.132: Normalised data matrix for phosphatidylglycerol and lyso phosphatidylglycerol for serum samples taken from patients with breast cancer.

	LPG(16:0)	LPG(17:0)	LPG(18:0)	LPG(20:5)	LPG(20:6)	PG(26:0)/die	PG(28:0)	PG(30:0)	PG(30:1)	PG(31:0)	PG(32:0)	PG(32:1)	PG(34:0)	PG(34:1)	PG(34:2)	PG(36:0)	PG(36:1)	PG(36:2)	PG(36:3)
P_1	2.70969152	0.97546189	1.51165774	0.96824434	0.71643645	0.02723872	-0.3643817	0.29665015	-1.0192738	-2.4291244	0.7523395	-0.3033678	-0.6000568	1.08124461	0.32431525	-0.7161907	-2.4064898	0.11757157	-1.6419668
P_10	3.29843059	0.98739133	1.73268754	1.96052319	2.20042586	0.24749825	-2.1568837	-0.9221205	0.08275134	0.4994823	-0.7019121	-1.1148254	-0.0221489	-0.0771581	-1.3466626	-1.2339731	-0.502246	-1.8280092	-1.1032508
P_11	2.75779865	0.83690327	1.00785518	1.7969115	1.98589098	0.27996703	-0.3899304	-1.1554766	-0.8260884	0.48534524	-0.2454325	-0.4082798	0.74770078	-0.1822194	-1.2206017	-0.9235755	-1.7425876	-0.7276531	-2.0765276
P_12	2.9534504	1.73312853	2.44164196	1.2569647	0.94031844	0.12611732	-0.8798517	-0.8248743	-1.1136362	-0.6768366	0.24195835	-0.0990397	-0.0152921	0.19792951	-0.8936799	-1.7304697	-1.3691393	-0.381105	-1.9075846
P_13	3.14116651	1.64114823	1.84689003	1.40267932	0.81163054	-0.7056033	-0.4844397	-0.9150451	-0.9775557	-0.7188794	0.68512923	-0.5647753	-1.8347904	0.93817134	-0.27521	-0.467652	-0.3922131	-1.2184793	-1.912172
P_14	2.91167925	-0.1140532	0.30644966	0.79220052	0.38592447	-0.3396424	-1.2741201	-0.003524	-1.1179241	-0.6153086	0.79976562	0.56504808	-0.500331	1.20976237	0.5117994	-2.036477	-0.8533118	0.27262851	-0.9005657
P_15	3.87668854	0.20866025	1.07039106	1.624308	1.88105202	0.57380176	-0.708034	0.24560464	-0.5210881	-0.4193097	0.02592771	-0.5921887	-0.5104456	-0.4022297	-1.9142558	-1.651486	-1.3231339	-0.4937442	-0.9705182
P_16	1.74552222	0.79992816	0.90709818	-0.7539287	-0.1940459	-0.6853538	-1.1717411	0.48634256	-0.664863	-1.5344118	1.22748924	0.27179331	0.44778735	1.32623279	0.02924366	-1.3023444	-0.1993981	0.49474413	-1.2300948
P_17	1.91297084	-0.3187155	0.10931429	0.41294268	0.22497337	-0.5003843	-0.448666	0.19514152	-0.9494266	-0.5026253	1.04011249	-0.1663424	0.20190211	1.30401204	0.24459178	-1.411573	-0.8263229	0.02591439	-0.5478196
P_18	2.30538065	0.06884569	0.32122342	-0.0630222	0.1299156	-0.9128608	-0.536385	0.02487505	-1.112937	-1.133511	1.02099307	0.34778578	-0.1914373	1.64900502	0.59693068	-1.8051382	-0.998404	0.28010686	0.00863378
P_19	3.11977205	0.36626814	0.12240981	2.12409769	2.16573698	0.35221221	-1.1815821	-0.380375	-0.864482	-0.4686482	0.34610221	-0.1452826	-0.7013125	0.59102868	-1.4899054	-1.5684871	-0.4915158	-0.8149192	-1.0811177
P_2	2.83630128	0.78434373	1.19825145	0.75363913	0.9500636	-0.5296842	-1.8505592	0.16854106	-0.7479636	-1.7823754	0.67915613	0.37882375	-0.3433185	1.09365219	-0.2543539	-0.7765293	-0.3839049	0.06396793	-2.2380513
P_20	2.80056688	1.7055553	1.7875274	0.71124645	0.78627265	-0.3150786	-1.318377	0.22827565	-0.6826836	-1.4673691	-0.8972412	-0.5505603	-0.1888995	0.6041636	-0.8627474	-1.3308449	-0.6323977	0.31809278	-0.6955013
P_21	2.78437168	0.392079	1.20845561	1.37734073	0.63070406	-0.5104818	-1.7415958	0.05468725	-1.1782832	-0.5673275	0.31852549	0.15480576	-0.6159168	0.72200312	-0.2255239	-1.9112823	-0.2011456	0.36862645	-1.0600422
P_22	1.78061501	0.97481775	1.61850325	1.17475236	1.13529414	-0.3432046	-3.8178918	0.03748761	-1.4726545	-1.5166782	1.17973881	0.14227707	0.12407352	1.29621097	0.14552635	-1.5694664	-0.5527835	-0.0149824	-0.3216355
P_23	2.26419243	0.76285277	1.2320235	1.19666412	1.37132082	0.03015431	-1.0179906	-0.3850055	-1.285647	-0.7322889	-0.1291414	-0.4849648	-1.1508743	0.64654421	-0.4709518	-0.6336444	-0.9577245	0.1170623	-0.3725812
P_25	3.12744178	1.74554067	1.96306165	1.03796435	1.4072094	0.03279172	-0.5471552	-0.5886245	-1.0796064	-0.9456123	-0.1137459	-1.4773909	0.05432659	0.01392668	-0.7206224	-0.8271033	-1.3307768	-0.3107717	-1.4408535
P_26	2.52255819	0.53025788	0.3257852	0.36218883	0.06418114	-0.8759775	-1.3839577	-0.5358299	-1.0172767	-1.4019382	0.79406108	0.00885456	-0.0449206	1.54492889	0.70459869	-1.5482047	0.18193513	0.55748469	-0.7887289
P_27	3.10343552	0.90940336	1.04774855	1.21442235	1.16855981	0.21469202	-1.6070512	-0.3462152	-2.9353214	-0.4860373	0.65939384	0.12789833	-1.0356072	0.6974452	0.03052448	-0.6634098	-0.6349197	-0.2081884	-1.2567732
P_28	3.16960345	1.26550981	1.48527688	1.65707846	1.73912842	-0.3058436	-0.6881048	-1.1570281	-1.3771682	-0.0646948	0.25365329	-0.9653864	0.10089604	-1.001753	-0.8821238	-0.1329308	-1.3646494	-0.8003817	-0.9310818
P_29	3.30230188	1.46462238	1.55122351	1.65344943	1.75434828	-1.3368542	-1.5802392	0.04970193	-0.4270499	-1.4835103	0.21407753	-0.4849983	-0.3582927	0.71836873	-0.7507753	-0.4718461	-1.4699348	-0.0841366	-2.2604563
P_3	3.35207524	0.12793444	1.34064665	1.33105454	1.30528691	0.15868372	-1.4496084	-0.1627046	-1.0013263	-0.1850543	0.11710026	0.00235112	-1.1409366	0.34116499	-0.2066766	-1.7122831	-0.7074073	-0.2501891	-1.2601115
P_30	1.54931952	-0.4976226	-0.1370976	0.65287935	0.5943578	-0.620608	-0.5603685	-0.1562666	-0.311662	-1.108779	0.5775072	0.53486118	-0.147161	1.38244508	0.23540543	-2.8087406	-0.0404907	0.92436492	-0.0623439
P_31	2.94665922	1.07641664	1.73672107	1.30769316	1.40356401	0.55466963	-0.7636458	-0.3969409	-2.0188674	0.13937613	0.31408308	-0.1678618	-0.2294493	-0.0160243	-0.8752855	-2.2317649	-0.5256889	-1.1201326	-1.1335216
P_32	3.04590119	0.59665144	1.69790805	1.68429992	1.87980311	0.30117429	-1.9743886	0.32240571	-0.4348027	0.02471518	-0.3433735	-0.148651	-0.9996683	-0.4050839	-1.4067359	-0.3943223	-0.3652409	-1.3776795	-1.7029123
P_33	1.66442218	0.71543148	1.17160159	0.21751854	0.28681545	-0.4988783	-0.4214658	0.20829706	-2.3718163	-0.6400038	1.17130898	-0.0952171	0.28424538	0.88620178	-0.3710815	-0.901012	-0.421964	0.1436575	-1.028061
P_35	1.77117902	0.74515239	1.23736885	1.04780087	0.97495303	-0.5678571	-0.7755908	0.05707772	-0.8275498	-1.0209476	0.95504719	0.05099315	-0.8853772	1.03571181	-0.1215822	-0.6585867	-0.7619918	-0.3572808	-1.8985201
P_36	2.86518099	0.63373356	1.51511305	1.92403406	2.20096288	-0.2126174	-0.7182478	0.44395629	-1.3311813	-0.2773137	0.25998928	-0.2595423	-1.2804596	-1.2465972	-1.4711105	-1.2189147	-0.5416376	-1.1663037	-0.1190443
P_37	0.08920008	2.00480526	2.69476254	0.31729642	0.38850072	1.7187673	0.66572068	0.10759461	-1.6354972	-0.7821622	0.41746144	-0.4569507	-1.2699347	-0.5862415	-1.1426497	-0.5838302	-0.9080915	-0.6034238	-0.4353276
P_38	2.82736742	0.24450785	0.88204683	0.92068726	0.96207066	0.18349849	-0.9869281	-0.2502659	-1.3068315	-0.5023179	0.55887293	-0.5551122	-0.1520087	0.99214025	-0.1333771	-1.3664741	-1.1481226	-0.5288249	-0.6409287
P_39	2.64900206	0.30820381	1.0697112	1.76302949	1.970998	0.1302244	-0.7647461	-1.8396715	-0.9100752	-0.5992956	0.16467706	-0.3793507	0.13072434	-0.000821	-0.6172297	-1.1497213	-0.1027111	-0.580544	-1.2424043
P_4	3.45317393	0.94432262	1.70452275	1.78230005	1.66551621	0.46313609	-0.46813	-0.865391	-1.5321448	-0.0305036	-0.3012722	-0.5419178	-0.6196237	-0.2299172	-1.5731957	-1.2035234	-1.3660126	-0.2877287	-0.9936109
P_40	2.96251095	2.27602694	2.61617663	1.08556173	1.42048272	0.81229035	0.34263325	-0.2032741	-2.321579	-1.3992651	-0.8699574	-0.1157768	-0.4344755	-0.9844437	-1.9174709	-0.9413411	-1.4068358	-0.3349823	-0.5862809
P_41	1.64666678	-0.4196502	0.24810268	0.07711771	0.46204526	-0.6092593	-0.5731825	0.39934441	-0.561345	-2.0091029	0.95622558	0.17794665	0.49451776	1.40595185	-0.1005254	-0.5438464	-0.4542641	0.43573511	-1.032478
P_5	3.06441989	1.32565531	1.91877254	0.83220576	0.97790084	0.60464874	-0.3162016	0.1027721	-0.164802	-0.6776363	0.14013908	-1.4596987	0.03874883	0.33779709	-1.8492501	-1.4396593	-1.5291984	-0.6607782	-1.2458356
P_6	0.22930407	2.09031114	2.51658025	0.4083083	0.61189417	0.76450659	-0.4834298	0.24699506	-0.4089701	-1.23393	0.36249012	-0.4780398	-0.2861699	-0.9298084	-0.2990601	-0.4947169	-0.7621065	-1.1539191	-0.7002392
P_7	2.3277808	0.89187628	1.23056607	1.07925138	1.0656501	-0.2738133	-0.8229279	0.54281938	-0.6113585	-1.1443089	0.66957645	-0.3110512	-0.2796425	1.25034383	-0.1634985	-1.2836199	-2.2516928	-0.745666	-1.1702848
P_8	2.89770675	0.53352563	0.95739315	1.53030665	1.29611768	-0.154227	-1.3245781	-0.28195	-0.703654	-0.5255361	-0.1860706	-0.6236377	-0.1353831	0.13239684	-0.4831747	-1.1630235	-0.9717541	0.19663822	-0.991096
P_9	0.04142071	1.73360716	2.30748869	0.81753926	0.55549301	0.92220192	0.8498825	0.76105002	-1.241814	-0.1524447	-0.3839103	-2.1734815	-0.8322961	-0.3306973	-0.6547733	-0.8435463	-0.5646912	-0.5267762	-0.2842523

Table 8.133: Normalised data matrix for phosphatidylinositol for serum samples taken from breast cancer free controls.

	PI(16:0)	PI(32:0)	PI(34:1)	PI(34:2)	PI(36:0)	PI(36:1)	PI(36:2)/IS	PI(36:3)	PI(36:4)	PI(38:1)	PI(38:3)	PI(38:4)	PI(38:5)	PI(16:0/16:0)	PI30:0	PI30:1	PI32:1	PI40:3	PI40:4	PI40:5	PI40:6	PI_Cer_2	PI(34:2)
C_1	-0.8414358	-0.9524515	1.47617903	-1.3187351	-1.1767391	1.65002938	2.32866885	1.07763774	1.52046141	-1.0041807	2.70679762	3.83985933	1.09155893	-1.4784577	-2.2020284	-0.992364	-1.5608024	-0.5587298	0.05389815	0.0651992	1.4429648	-1.3819738	1.09636738
C_10	-0.4107481	-0.7353155	0.7524052	0.50258744	-0.2062819	-0.3512735	0.71612081	1.15283409	-0.4377923	0.24156904	0.34852374	2.71328946	1.40023265	-0.7154538	0.35966529	-0.7583465	-0.148792	0.04202701	0.14377685	0.57848833	0.88789418	-0.1070466	0.30807641
C_11	-1.1726317	0.05452768	1.23252682	-1.8284381	-0.2092056	1.6203139	2.28170889	1.14152113	0.71865393	-0.3487573	2.14485894	3.43466591	0.14120172	0.43418541	-1.9996843	-1.3289353	-0.9844141	-1.2407099	-0.165336	-1.123214	1.28792158	-1.4867713	1.52802534
C_12	-0.6266554	0.49176586	0.94231448	-0.7348273	0.06211547	0.89729127	2.4701707	1.2769263	0.96973403	-0.8334553	1.78939894	3.25519121	0.87446015	-1.8784201	-1.2951103	-0.9938008	-1.6417378	-0.4549819	0.56289362	-0.8767241	0.17550521	-1.8868386	0.79773749
C_13	0.6858075	1.2189031	-0.7155383	-1.8271047	-1.1933924	-0.9378203	1.02155102	-0.0011124	1.20513418	0.71617229	0.65021037	0.56894777	-0.3489414	1.10986504	0.34056896	0.48586177	0.32581122	-1.6306592	-1.7731481	-1.1357724	-0.1437003	0.12083703	0.04445768
C_14	1.17346063	0.81484561	0.47403614	-1.8215279	-0.9949993	-0.1110036	0.83934217	0.32456312	-0.3978763	1.20382542	-1.536633	1.10002539	1.22682418	1.59751817	1.05804808	0.89625673	0.96022039	-0.9294774	-1.0478286	0.69263306	-1.5789621	0.37706418	-1.3373681
C_15	-0.0507571	-0.0221935	1.83005611	-2.8956875	-0.2153815	1.35483984	1.44538846	-0.9628016	1.11839132	-0.1856941	1.14441326	2.15067175	0.68391186	-0.2217054	-0.5584938	-0.443236	-0.4047479	-0.2604036	-1.0332671	-1.5118694	1.27015445	-1.1135094	-0.6358355
C_16	-1.380385	-0.2891847	1.53164127	-0.5628062	-0.5343656	1.56012054	2.59117136	1.09721482	1.02487664	-0.8357965	1.98763484	3.45076992	1.22056336	-0.2205439	-1.7575356	-1.6284501	-2.2075904	0.08819791	-0.6081866	0.33422909	0.03880733	-0.5736643	0.81105418
C_17	0.29912786	0.04683897	1.24809509	0.18390491	-2.0249835	1.29289865	2.18969509	1.56599951	1.34627691	-0.7969433	2.34318069	3.44642156	1.26826507	-1.3869864	-1.0189688	-1.1045119	-1.1225276	0.16756602	-0.7099908	0.8842404	1.17735051	-1.5540813	1.30119747
C_18	-0.7612312	-0.2454404	0.9479118	0.53650356	1.22770023	1.66626613	2.81926244	1.96632114	1.57087764	0.16141041	2.18370806	3.4820275	0.56033812	-0.6709544	-0.6316436	-0.4464689	-0.8569568	-2.9220748	-1.0167385	-0.1230403	0.13268433	-0.5718246	-0.0369035
C_19	-0.6141118	-0.9623274	1.09185334	-0.5979276	-0.8405166	0.64007248	1.66535227	1.03691652	0.85643929	-0.5182006	2.03819451	2.80694058	0.73669799	-0.2885083	0.09627872	-0.1910822	-0.1283544	-2.2177555	0.1278531	0.48912881	0.88030616	-0.0396756	0.78046564
C_2	-0.7916831	0.73465542	2.17788905	-0.741191	-0.0052694	1.8944414	2.3808227	1.83901477	2.05764727	-1.5188726	2.51212054	3.90857025	1.41967294	-0.7095495	-1.3369181	-1.2688834	-1.5999245	-2.2180479	-0.5301988	1.00499515	1.04176366	-1.4189692	0.63774392
C_20	-0.24207	-0.1459233	1.54571423	-1.5913715	-0.9156741	1.26753255	2.26687974	1.25677573	0.91645234	-0.331049	1.53416365	3.06906082	0.83369857	-0.224283	-1.4095968	-1.8939103	-1.6740689	-1.7573217	-0.5692887	0.52342272	1.20704469	-1.0772168	1.17545567
C_21	0.65747988	1.12377491	0.18327082	-2.3099509	-0.9461697	1.69276951	1.49099018	0.34523382	1.17382069	0.3574414	-0.8885007	2.25510874	0.96809597	1.01473685	0.24544076	0.3134754	0.23068303	-1.6185397	-0.7037507	-1.5439207	-0.611636	0.35627726	0.50213701
C_22	-0.4514728	-0.1388055	0.32695723	-1.9746252	-2.5565388	-0.0189722	2.07931515	1.29686091	1.76242155	0.52437747	2.95275382	4.18872147	1.53108971	0.31442064	-0.2299808	0.01750024	-0.3276528	-2.8311069	-0.5470848	1.05472121	-0.7928322	-0.2890048	0.12512072
C_23	-0.0881828	-0.5911101	1.42687245	-0.1396286	-0.6820884	0.44792398	2.26736931	-0.2610401	0.93819138	-0.0799014	1.86020393	3.06813604	0.06244101	-0.3262607	-0.7215044	-1.3339947	-0.5531695	-0.5038475	0.27957605	0.74141019	0.92275194	-2.1634788	0.89495943
C_24	-0.466217	0.99452657	-0.3740176	-1.7367318	-0.1370095	1.44443379	1.19173989	-0.339248	0.69256317	0.5805786	2.12459968	2.35983349	-0.3413303	0.97427135	-0.057567	0.27300991	0.4789903	-0.5340248	-0.620185	-2.8359651	0.54416508	1.01482539	0.25710418
C_25	-0.3969469	0.03368018	1.02717561	-2.9978066	-0.3250227	1.4366308	2.17511016	1.04144151	1.29381262	-0.0411962	2.19679571	3.06248115	0.97331323	0.21753387	-0.5838742	-0.711858	-0.5553282	-2.9976555	0.03119023	0.51893349	0.63696818	-0.1838356	0.64099551
C_26	-0.6156447	-0.623759	0.49144238	-0.7109345	-0.6317819	1.05489786	1.64593136	0.4090219	0.01815947	0.03342589	-0.1575287	2.40144511	-0.2188081	-0.8520517	-0.0509623	0.15940559	0.19736614	-0.229023	-2.0951732	0.76749168	-0.5333721	-1.0469152	0.69881752
C_27	0.27132742	0.80442303	-0.1754017	-3.4357025	-2.1845692	1.19032307	1.17178842	1.7285609	-1.4382419	0.30169221	1.107473	2.25348341	-1.1948609	0.69538496	-0.8242763	-0.461268	-0.0886689	0.2487574	0.56071476	0.92924128	-0.1934964	-0.3061388	-0.0051363
C_28	-0.7498949	-0.7651822	1.28942096	-0.9315924	0.00093419	1.40159694	2.40267441	1.34661904	1.71308398	-1.7127382	1.77152071	3.20417031	1.5693324	-0.7986875	-1.1084312	-1.1624319	-1.123189	-2.5461633	-1.8183047	0.10953112	1.60779915	-0.685913	0.81302402
C_29	-0.2052232	-0.5056651	1.63714535	-3.6215458	-4.6596672	1.59822565	2.64632648	1.38284847	1.83763654	-1.0083959	2.58036088	3.77169778	1.96148969	-0.2600102	-1.3839993	-1.0861382	-0.7978598	-0.1500932	-1.4113292	0.14544204	1.16217608	-1.1375059	1.30760773
C_3	-1.1256264	-0.0080948	1.02409135	-1.2704045	0.67044508	2.0771022	2.56858443	1.16791883	1.39230823	-0.7753277	1.93338269	3.47188288	1.56018237	-1.0390478	-1.2486024	-0.4353981	-1.1656888	-2.1043512	-1.0509049	0.13798103	0.62141757	0.00314301	1.1531913
C_30	0.05478494	0.22416305	-1.0032869	-0.1833383	-0.2740263	-0.2204319	0.59745999	-1.6551838	-1.0856725	0.57226398	0.40535639	1.67912137	-0.3339534	0.96595673	0.8890774	0.19897123	0.0697962	0.40360725	0.4277316	-0.1224543	-1.0967903	0.60531285	-0.5044759
C_31	0.29050238	1.5022518	-0.8610582	-0.9629036	-1.2960002	0.56862594	0.48587013	0.75468826	-0.5838558	0.99952099	1.13299443	1.79927259	-0.2690528	1.17850739	0.57129596	0.6919523	0.60915993	-1.9758473	0.25015558	0.38562263	0.28617329	-1.4013419	-0.4237294
C_32	0.81756383	1.35065943	-0.4594848	-1.5345924	-2.8585622	0.19835248	1.4838704	1.00914942	-1.2385849	0.84792862	-1.302734	1.1137006	-0.2869481	0.90126658	-0.0726477	0.76208843	0.45756756	0.54063905	-1.8950611	1.28123125	0.97903963	1.24519323	0.49632149
C_33	-2.6251154	0.2302678	1.86689073	-0.0863987	-1.0810693	1.80945596	2.97057752	2.07507123	2.49552262	-1.8456043	3.16357914	4.17077308	2.05002884	0.68026248	-1.8216906	-2.1385358	-2.2499661	0.53317481	-0.2428695	1.20211163	1.06462047	-2.4441063	2.00909214
C_34	0.08188622	-0.7346945	1.3544626	-0.8498044	-0.4329166	0.88995226	1.44920178	0.59911494	1.93058037	-0.5312209	1.797581	3.36083079	0.79473055	-0.0766409	-0.6432871	-0.9545193	-0.921582	-0.0763861	-1.2245325	0.79266944	-0.3866752	0.36761582	1.13710255
C_35	1.19059881	1.72369441	0.407483	-1.6700447	-0.7986169	0.8946726	0.35679362	-1.0192228	-0.0135801	1.22096359	-1.1124608	-1.0640739	0.13087639	1.61465635	0.84536027	0.9133949	0.83060253	0.71793625	-1.0061416	-0.9666942	-0.6296814	-0.0644225	0.88131868
C_36	-2.2002918	-1.116885	1.65109918	-0.6631989	-1.7331681	1.5422139	2.83822018	1.6161102	1.6006098	-0.8148294	1.8999851	3.34411882	0.99092519	-0.5985013	-1.2939575	-1.1360647	-1.2696743	0.25732636	-0.4890458	-0.182106	0.62842079	-1.9603659	1.0702703
C_37	-0.5047787	-0.2422257	0.75750409	-2.2122958	-3.7106985	1.78117151	2.73515644	1.53269687	1.66828969	-0.0222043	1.63771758	2.78871768	0.08118082	-0.4603564	-1.4356122	-0.3193901	-0.2945053	0.36614867	-0.6589375	0.68872415	0.4495203	-2.8406094	0.71263115
C_38	0.74979179	0.03197977	1.79332034	-2.9451842	-4.0276055	0.28752472	1.71159846	1.24523116	-0.9214847	-0.0881533	1.40128317	2.21398051	1.18300476	0.34120844	0.20189788	0.26993252	0.18714015	-0.2817461	0.88489309	-0.5525061	0.21555285	-0.4476248	1.70789569
C_39	0.78595796	1.31905356	0.71738273	-1.9795393	0.03523753	0.42152749	1.46474406	-0.0104557	2.78683019	0.81632274	-1.6536863	0.49401737	0.24050374	0.45149503	0.44071941	0.13800586	0.42596168	0.53739594	0.48994657	-0.0626071	-1.1114811	-2.0588417	-0.8203774
C_4	0.40979221	0.76371633	1.11406366	-3.1285742	-2.005471	2.08683716	0.27335847	1.70210903	1.7047186	0.23036863	1.43537619	2.47223819	0.46533869	1.03160953	0.52759108	0.23714207	0.32757251	-2.7555613	-0.7097935	-2.6156704	-0.7217686	0.29860595	1.58903729
C_40	-0.8048281	-0.4373744	1.64804011	-2.8549948	-2.8048687	2.38963097	1.90194586	1.57923603	1.60059493	-1.3327185	2.47590186	3.69531535	0.97846267	-0.8240196	-0.6401566	-0.547433	-0.8618217	0.07946135	-0.1266014	-0.2709879	1.45363796	-0.3960463	0.91608696
C_5	-0.0746022	1.10411252	0.54298321	-2.2774307	-0.4806005	1.50264751	0.5167709	1.42242772	-0.120641	0.60138171	-0.1256198	1.01275513	1.10733066	-0.2261836	0.22577838	-0.675467	0.21102065	-0.0097778	-0.3647265	-0.3768031	0.51852258	0.31385299	-0.6054865
C_6	0.26368926	0.88976719	-0.0582009	-2.4559021	-2.1550888	1.70912856	2.3303443	0.72286718	0.31520441	0.22851121	2.03564052	1.60674508	1.06740907	-0.9054069	0.01143305	0.07946769	-0.2605258	-1.7116588	0.2413359	-1.8537872	-0.8674945	0.38507887	-1.4239619
C_7	-1.8038128	-0.6441665	1.31422082	-0.8471343	-0.7910077	1.75270741	2.64830388	1.87474113	1.77217451	-1.1245782	2.38733757	3.82065537	1.25511886	-1.1528867	-1.3283002	-0.905947	-1.6447067	-0.221763	0.07338225	0.04391289	1.35933471	-0.622461	1.7567718
C_8	-0.4267774	-0.1104923	1.72385678	-0.2644709	-2.2404089	1.8548469	2.21429396	1.20815272	0.86900647	-0.4897232	1.57757722	2.77483826	1.42382971	0.2769497	-1.1905018	-0.88638	-1.2522731	-1.3892288	-0.9585754	-0.6881037	0.55204462	-1.4223827	-0.0057179
C_9	1.07206194	0.0605697	0.10333633	0.68458305	-1.6535612	0.77479522	1.60495904	0.54559659	0.62832921	0.5865456	1.40397581	1.75345938	-0.1540813	0.98023835	0.02746793	0.27897691	0.19618454	-2.0348475	-1.8996999	-0.1429823	-0.414398	-0.5850435	0.17261515

Table 8.134: Normalised data matrix for phosphatidylinositol for serum samples taken from patients with breast cancer.

	PI(16:0)	PI(32:0)	PI(34:1)	PI(34:2)	PI(36:0)	PI(36:1)	PI(36:2)/IS	PI(36:3)	PI(36:4)	PI(38:1)	PI(38:3)	PI(38:4)	PI(38:5)	PI(16:0/16:0)	PI30:0	PI30:1	PI32:1	PI30:3	PI40:4	PI30:5	PI40:6	PI_Cer_2	PI(34:2)
P_1	-1.5031354	-1.2061211	1.81055304	-3.4428829	0.39285674	1.51498655	1.94186419	1.12268211	2.04243566	-0.5540918	2.64672706	3.52785676	1.37761924	-0.1146024	-1.2527394	-1.9313399	-1.1683762	-1.3965732	-1.9177708	1.05052775	0.87204399	-1.4807505	1.62040546
P_10	-0.3734062	0.03999991	-0.3068802	-2.2130873	-2.7300924	1.0973319	1.69033396	0.95507824	1.78860719	-0.0002162	1.09482833	3.0646119	1.5773426	-1.1221831	-0.1039974	-0.3605848	-0.4397988	-0.2600326	-0.138769	0.64764492	1.68627957	-0.1046052	0.6080906
P_11	1.01813439	-0.1087368	0.97145651	-0.8084947	-2.2733993	-1.0889031	2.20373152	0.22639722	0.51040499	0.90170357	-1.1276627	2.09664023	0.70692659	0.56203421	0.83212278	0.67324679	0.90837525	-0.8916123	-1.301211	-2.6419128	1.60804859	0.82119843	-0.0080615
P_12	-1.0590968	-1.150196	1.66037722	-4.2292233	-0.571738	1.99375718	2.1945517	2.01219167	2.1902978	-0.9423156	2.55315366	4.2252218	1.56996753	-1.7742608	-1.1190183	-1.2778943	-0.9117343	-3.6390106	-0.7419844	1.04919983	1.76296734	-1.6583371	1.50528975
P_13	-0.3827837	-0.861464	0.10789165	-3.4927706	-1.0269682	1.12304877	1.799145 47	0.93245989	1.11779414	-0.4774501	2.07095975	2.89504084	1.19750045	-0.7076565	-0.6659283	-0.9992978	0.22007663	-0.473092	0.15688048	-0.195628	0.4916658	0.15160249	-0.605587
P_14	-1.2734906	-1.6702431	0.84850318	-0.6866054	-0.0848464	1.01238883	2.09721431	0.67804936	1.56834602	-0.8846141	2.06152134	3.12099855	1.14834885	-0.6676955	-0.8899523	-1.0488283	-0.7127148	-1.0608606	-1.4720102	-0.2114124	0.36845209	-0.6236391	0.12636848
P_15	0.65789921	0.70122919	1.14415086	-1.7482981	0.13433232	0.80467634	3.3753678	-0.4636867	0.82168857	0.5414684	-3.4260346	-0.0053567	1.36076071	0.72327564	-0.0028899	0.03195115	0.01273096	-0.4311014	0.90247474	-1.2219446	-0.6781242	0.70253934	-0.7966875
P_16	-0.7999827	-0.6557165	0.86757507	-0.5656104	-0.9452524	1.61178154	2.49074995	0.58429903	1.38045943	-0.7485554	2.33635187	3.64879019	0.86957552	-0.3823018	-1.3195278	-0.9770122	-1.3122593	-1.6154305	0.27708143	-0.8969087	0.77237103	-3.1015097	1.15008992
P_17	-0.9605753	-0.9375157	0.9933499	-2.4447793	-0.5407811	0.52936572	2.26314858	0.9964608	0.76894751	-0.2622885	0.63253371	2.44922329	0.75335104	-0.2633592	-0.3318693	-0.2291357	-0.3198512	-0.0809423	-0.408723	-0.4266771	-0.2136097	0.47324093	-1.1614834
P_18	-1.1326568	-0.9120637	1.68685015	-1.3467507	0.40671859	1.67120568	2.47261953	1.57489308	1.41307092	-1.0054029	2.13555171	3.42123607	1.10185023	-0.8027648	-1.8943328	-1.6051991	-1.2586557	-0.7749876	-1.061929	0.55419769	1.04813636	-0.7714821	1.00943202
P_19	0.67875983	0.70868306	-0.1812098	-2.1564147	-1.7586517	0.98991753	1.19154426	1.49665545	-0.821888	-0.4027045	-0.7872603	-0.3192097	-0.3850387	0.71836233	-0.0070222	0.44651085	0.47899239	-2.0257622	-0.2789701	0.38947806	-0.3290254	0.31765398	0.40370913
P_2	-0.2461308	-1.4628484	1.07865039	0.75125649	-1.1817557	1.28568065	2.60720433	0.84695017	1.7201685	-1.0908352	2.02219935	3.66948768	1.11362741	-0.6040834	-1.5907279	-1.7351416	-1.1118682	-1.0638241	-0.2480452	0.84013856	1.30637294	-0.3498882	0.66457728
P_20	-1.5296962	-0.9679023	1.31145313	0.51268112	-0.8721429	2.26398334	2.65258279	1.36058297	0.97221815	-1.1611789	2.28006853	3.32063731	0.55069875	-0.9300548	-0.4601937	-1.5235688	-1.1091621	0.00800443	-0.3354201	0.67183293	0.20369114	0.09195521	0.6324272
P_21	0.4652685	-0.8082193	0.93823228	-2.8936647	-0.7663591	0.37833903	1.9055912	0.25245182	0.25760515	-0.4851026	1.70881462	3.09153643	2.13635257	-1.274012	-0.5546834	-0.7135594	-0.5426653	-0.4207686	-0.0387862	-0.4866012	1.63025598	-0.6292181	-1.1067848
P_22	-0.709782	-0.5034649	0.54278427	-0.4705622	-1.4964176	1.30965518	2.05081791	1.23424847	1.3166697	-0.0424439	2.22515107	2.94124085	1.53535907	-0.4138402	-0.6282388	-0.8241043	-0.5299303	-0.8141021	-0.3133828	0.56495957	0.29921365	-0.8319443	1.42402847
P_23	0.01623943	-0.4063509	-0.1761647	-2.8863537	1.01837811	0.93548455	2.11376745	0.73420761	0.4770799	-0.0256892	1.8376091	2.29942237	0.41463916	-0.3764831	-0.4102313	-0.254146	-0.2600562	-0.3447975	-0.7498028	0.06902707	0.2079505	1.19523304	-0.4580508
P_25	-0.2904266	-1.1938885	1.25405299	-0.7656505	-1.4121138	2.31647536	2.29547178	1.36290185	1.38390882	-0.4239148	2.25468721	3.70050962	1.48042797	-1.1725098	-0.4934956	-0.6523716	-0.4814775	0.90517331	-2.6818476	0.21879375	-0.1813315	-0.4041187	-0.1900918
P_26	-1.3203956	-0.650117	1.70540452	-0.6172965	-0.6273442	1.76968602	2.75526007	2.23087493	1.97766602	-1.7459436	2.42634503	3.82576723	1.72049576	-2.1098724	-1.4283647	-1.8501529	-1.3727519	-0.0610682	-0.4675705	0.16507216	0.97984225	-0.0900626	1.39085534
P_27	-0.0261283	-0.3798242	1.31666915	-1.0909187	-0.8257897	1.29526329	1.85566564	1.04825248	1.14084505	-0.5442106	1.51686599	3.11511028	0.83956491	0.43982113	-0.0725109	-1.4058834	-0.7246858	-4.0981763	-0.0473891	-0.1040494	-0.0068593	-2.4310811	1.26956214
P_28	0.5151395	0.74060349	0.33793537	-1.5943399	-1.2055709	1.16026895	0.94814831	0.18409832	-0.0797721	-0.1733908	1.34202868	2.61728428	1.01624034	0.00245537	0.61087969	0.68214714	0.57259745	-1.6447928	0.05628873	-1.5661556	0.8425057	-1.5336183	-0.6691049
P_29	-0.6598715	-0.7200026	1.67146095	-3.9150319	-2.1876562	1.79576036	2.53865785	1.96063245	1.37944781	-1.5826819	2.69420215	3.97668163	1.59469747	-1.4307044	-0.699867	-1.5762065	-0.8957788	-1.0156371	-2.1683176	1.07157076	1.37445141	-1.0493088	0.64264024
P_3	0.58439353	-0.8017856	0.95225075	-0.5163319	-1.9203217	0.68699498	1.55509573	0.00200083	0.0457073	-0.2078206	1.3608546	3.19474854	0.81561289	-0.4701246	0.11990979	-0.1568171	-0.0775432	-0.9476978	-0.3347558	0.15988214	1.46347011	0.10878298	-0.3720428
P_30	-0.4896283	0.61054176	-1.7965721	-2.7921816	0.3997223	-0.2524062	2.13037261	1.7396889	1.85827784	0.03914885	1.26037334	3.03857037	-0.1701368	-0.2605454	-0.0304319	0.3806742	-0.0184138	-3.1694217	-0.5843029	0.02932562	0.72404358	-0.2304917	-1.3699689
P_31	-0.2632676	-0.1954093	0.43069487	0.38223912	-3.5731499	1.29935937	2.11072632	1.25010734	1.37108942	-0.2202328	2.54629559	3.75770574	0.38280438	-0.9046284	-0.7210211	-0.3199433	-0.1490492	-0.4251855	1.44926737	0.00548215	-0.1912957	-2.3851602	0.85342303
P_32	0.72914353	0.62260356	0.22232527	-2.2439335	-1.354915	-0.0367725	0.95268143	0.83041797	-1.6521567	0.61271272	1.75430856	1.44754272	-0.0139779	0.71347228	1.30725449	0.16293334	0.49842653	0.55410558	-0.5378648	0.25025047	-1.299089	0.05339299	-0.4441439
P_33	-0.4368108	-0.3166097	1.8017256	-2.9964383	0.47317102	1.86565692	2.47711703	1.24870038	0.19955471	-0.5361841	2.39228199	3.45770231	0.69543064	-0.1289241	-0.3803122	-0.9221406	-0.8756123	-2.6894421	-0.2406123	0.65943098	-0.6508192	-0.6815059	1.53605714
P_35	-1.4182674	-0.6237751	1.30226459	-1.7674994	-0.3791706	1.09955697	1.32894895	0.33194086	1.33911801	-1.1418825	1.52423407	3.08471386	1.19464455	-0.2994606	-1.0758364	-0.4322342	-1.1246998	-0.9429661	-0.1329123	0.13323639	0.98786567	-1.0748867	0.92035513
P_36	0.28626227	0.55363522	-1.3074416	-0.0472712	0.0383652	0.54416629	0.9384689	0.05144004	0.4315599	0.86281769	1.71368568	2.16469764	-0.8011947	0.37981829	0.12843025	-0.0304457	-0.6782871	-0.2454973	-0.3383118	0.76158375	0.03745862	0.15039417	-0.6897843
P_37	-0.2811744	-0.4901097	-0.2338875	-3.3949529	-0.5136213	0.96646733	2.17119665	1.21697025	0.84868603	-1.4288787	2.28135094	3.37264839	1.30695901	-0.4804304	-1.3357825	-0.8906945	-0.7198004	-0.7799853	0.23333348	0.47504373	1.07663435	-1.068304	0.64110064
P_38	-0.4489785	0.30329278	1.28819254	-2.7520494	-1.4062272	1.95582485	1.92966747	0.9688981	0.58230266	-1.5496253	1.77693267	2.81869222	1.24196099	-0.6303608	-0.4106753	-1.4776818	-0.9685839	-0.899746	-1.1223895	-0.3314881	0.14504131	0.00236258	1.23662321
P_39	0.4246923	0.73511845	0.38378545	-2.1842604	-3.1181203	-0.9792847	0.6896116	-0.485234	1.03468119	0.52905575	-1.0082916	1.82217751	-1.0123132	0.29807924	0.05362421	0.30059897	0.47149306	-1.8391341	0.48053626	-0.5338231	0.75673897	1.29716362	1.33041254
P_4	-1.204638	0.52689573	1.04489719	0.47600164	-2.8220347	1.74071496	2.43172762	1.25132934	1.6019147	-0.9141558	1.50229157	3.30302977	1.40331337	-1.3740714	-1.2410884	-1.1004758	-0.8858429	-3.6994546	0.08718954	0.77866923	1.14438562	-1.6753391	0.7193831
P_40	0.4503528	0.19343853	-0.2972189	-2.2176019	-2.0145128	1.08359111	1.19871084	1.09998972	0.05414751	-0.8857021	0.82626557	2.56729163	0.65465622	0.2031178	-0.0482702	-0.7953978	-0.0362521	-0.3560364	-1.1412749	-1.6609088	0.62541799	-0.3372877	0.91443415
P_41	-1.1335339	-0.658572	1.18889966	-0.275932	-0.2360126	1.61773416	2.11853747	1.16319819	1.33738745	-0.6920933	2.04015052	3.18101905	1.09421083	-1.554397	-0.8482541	-0.8764282	-0.8515515	-1.0382851	-1.836352	1.16774972	0.31259651	-3.5989149	1.1148132
P_5	-0.8926441	-0.3093027	0.97098528	-3.6176643	-0.0866176	2.50466945	2.9672081	1.4779927	1.97834986	-0.2902314	2.73365343	3.45498414	1.4172478	0.09292852	-1.2056336	-0.8333782	-1.2581434	-0.4841958	-0.4988386	0.99120035	0.95628567	-3.135672	0.86305747
P_6	-0.9172833	-1.238571	1.38673606	-0.7930733	-2.3842728	1.25542294	2.82824103	1.84964555	1.8097778	-0.4517242	2.38063968	4.10744448	1.67423514	-0.1266657	-0.8172977	-1.1602661	-1.169037	-0.9293234	-0.9712941	0.12317969	1.17112791	-1.1602523	0.83913836
P_7	-0.880582	-0.6522843	1.46480471	-1.2958008	-1.7564327	1.47962899	2.11185059	1.38621351	1.80672956	-1.0231366	2.07337425	3.42253132	0.60841753	0.54770737	-1.2629438	-0.9358118	-0.8994147	0.28222678	-0.9610907	-2.4437748	0.36416459	-0.6413757	0.5814972
P_8	0.42617532	-0.074499	0.99387233	-2.8145452	-1.7472802	1.24041844	2.47874342	1.41536648	1.70588849	-0.2466269	1.23266971	2.85078794	0.75819032	-0.0648197	-0.3162077	-0.3767245	-0.3041896	0.36166836	-2.038359	-0.5318068	-0.0804815	-0.6466219	0.69615159
P_9	0.70541452	0.76111168	1.03414027	-1.6806032	-1.1261226	-0.8644798	1.56105776	0.19553225	0.4803829	0.38003861	-0.1153431	0.44655672	1.22969826	0.77079095	0.51940291	0.36052692	0.99472289	-0.7838929	-0.0912216	0.16871645	-0.8951201	-0.956474	-0.1683497

Table 8.135: Normalised data matrix for phosphatidylserine for serum samples taken from breast cancer free controls.

	PS(32:1)	PS(32:2)	PS(34:0)/IS	PS(34:1)	PS(34:2)	PS(36:0	PS(36:1	PS(36:2	PS(38:1	PS(38:2	PS(38:3	PS(38:4	PS(38:5	PS(40:4	PS(40:5	PS(40:6
C_1	-0.0526053	-1.2171376	2.34325792	-0.5192282	-0.8934437	2.37385588	0.37738293	0.21027294	-0.2819705	-0.7136681	-1.480162	1.6816908	-0.7120897	-0.348154	-0.0797528	-0.6882486
C_10	-0.4420329	-0.7910351	1.83335178	-1.6738464	-0.6469599	2.79562023	1.00511389	-1.3629218	-1.7480249	-1.0347321	-0.1814194	1.55751393	-0.1645284	1.31683729	0.71763	-1.1805662
C_11	-1.1822823	-0.3158445	2.18661701	-1.4997728	-0.8788169	2.69446444	1.21747432	-1.3695852	-1.2227444	-1.071193	-0.6904553	1.76992175	-0.1047032	-0.286121	0.97462141	-0.2215805
C_12	0.33435065	-0.6476451	1.33312276	-0.9626283	-0.2899096	1.79253833	1.95668764	-0.2164418	-0.7265637	-0.7712184	-0.2604489	1.50476446	-0.9446376	-0.7462813	-0.5181475	-0.8375416
C_13	-0.6266852	-0.4869549	3.21114451	-1.255953	-0.1796662	4.32769472	0.83977881	-0.870294	-0.9203444	0.11304923	-0.4304672	0.68596934	-0.1124843	-0.0010385	-3.2383117	-1.0554372
C_14	0.08668645	-0.3953155	4.14188368	-0.2799618	-0.8871854	4.83609198	-0.9681684	0.42341601	-0.6352286	-0.3644798	-0.1048675	-0.1440416	-0.0676088	-1.0897789	-4.7121639	0.16072213
C_15	-0.0799528	-0.807617	2.85311835	-0.7274218	-0.2006104	3.17238353	-2.7918598	-0.3978602	-0.1301747	-0.1406684	-0.1749151	1.45397243	-0.6450241	-0.8694483	-0.3406303	-0.1732914
C_16	0.97567937	-0.254435	1.85272284	-0.0291375	-0.458833	2.73985198	-0.438913	0.3963269	-0.3776757	0.28409149	-3.5097758	1.42133712	0.80421993	0.11107441	-2.8916338	-0.6249003
C_17	0.01562543	-0.222778	1.66023205	0.14221029	-0.0472038	2.01770775	0.11712155	-1.0163631	-0.4441889	-0.6852292	-0.1649322	0.80425122	0.57371607	-1.2773124	-0.2479437	-1.2249131
C_18	-1.4211794	-0.7107865	2.74289644	-0.0382169	-1.0278644	3.62341758	0.11594386	-0.8943946	-0.6264341	-1.1007911	-1.2290813	0.51032317	-1.3107871	0.29054105	0.56663385	0.5097794
C_19	-0.2855506	-0.3444047	2.92306906	-0.1640351	-0.6505526	3.7609507	-0.0152121	-1.5695702	-0.7024817	-1.0300162	-1.2389502	0.76269946	0.41701576	0.44009799	-2.0730328	-0.2300267
C_2	0.19288589	-0.4803905	1.76163951	-1.0768453	0.40844515	2.2499359	-0.5729903	0.08315346	-1.2937283	-1.3612182	-0.7347505	1.19029371	-0.3746249	0.23426724	0.08806335	-0.3141361
C_20	-0.4162337	-0.5523075	3.00646544	0.24135937	-0.8452971	3.68986122	-1.1516171	-1.2386337	-0.5280815	-0.5465277	0.46528982	0.75974477	0.42073636	0.29830313	-3.7155311	0.11246938
C_21	-0.7486801	-0.2690829	2.40134958	-0.1417548	-0.4991179	3.11977579	1.06914703	-0.5205697	-0.2867364	-0.9170282	-0.1972398	1.22201231	-0.8994537	-0.492653	-2.5246592	-0.315309
C_22	-1.1364377	-0.4108123	2.06994921	0.11963407	-0.7975906	2.15956875	1.54384179	-1.2875146	-0.8258157	0.10484387	-0.8116921	1.81629473	-0.5623539	-1.155893	-0.4482024	-0.3778202
C_23	-0.5605926	-1.3516448	1.58628288	-0.7742043	-0.973246	2.1305406	1.07824553	-0.7144904	-0.5476694	-0.5277076	0.89638828	1.30855156	-0.359066	0.0441058	-0.2958202	-0.9396734
C_24	-0.5605926	-1.3516448	1.58628288	-0.7742043	-0.973246	2.1305406	1.07824553	-0.7144904	-0.5476694	-0.5277076	0.89638828	1.30855156	-0.359066	0.0441058	-0.2958202	-0.9396734
C_25	0.38346531	-1.1262469	1.91811036	0.34642048	0.51255462	2.73974462	-0.8278756	-0.1680359	-1.0041576	-1.091888	0.25373989	1.22524899	-1.1163588	-1.3355991	0.40179636	-1.1109186
C_26	0.05285582	-0.3426257	2.60471218	-0.731437	-0.8078242	2.84805776	1.20555947	-4.1603171	0.44265185	-0.1420948	0.11438266	1.91935999	-1.092456	0.56059435	-2.0040249	-0.4673944
C_27	-0.4581008	-0.5334475	2.97066064	-0.2777861	0.26962108	3.37298385	-0.0783879	-0.352217	-1.1978189	-1.1079826	-0.7145966	0.50135104	-0.0850314	-0.6354191	-1.0274391	-0.6463895
C_28	1.40269869	-0.9515058	2.00521307	0.05139626	-0.6841327	2.42619591	0.25188713	-0.2850767	-1.1478968	0.11732921	-0.5722822	1.43311705	-0.9106007	-0.0602402	-2.479164	-0.5969381
C_29	0.62075011	-0.6988704	1.00858457	-0.9218518	-1.0733618	1.77851891	0.34991558	0.57826387	0.03002752	-0.5393304	0.04491066	1.8223009	-0.7885841	0.13571905	-1.3510667	-0.995926
C_3	0.1482488	-0.0547002	2.39614659	-1.2407438	-1.5231993	2.8936422	1.58393246	-1.2523339	-1.4868286	-0.665322	0.05354094	1.74904976	-0.4005877	0.0453754	-0.9947563	-1.2514644
C_30	0.23497258	-1.0968752	2.81026762	-1.1978504	-0.4360745	3.69956128	0.86886452	-1.1998535	-0.5570684	-1.3416991	-0.6770054	1.95868102	-1.0940585	-1.0234013	-0.5934822	-0.3549786
C_31	0.64523865	-0.4042848	2.5240941	-0.6142784	0.2123921	3.94530706	-2.6108747	0.25223047	-0.4014188	-0.284016	-0.135315	0.89385601	-0.1777027	-0.1503616	-3.2061273	-0.488739
C_32	1.12266263	0.22731369	1.1088016	0.14203503	-0.4486393	3.22927908	0.26463743	-0.7590515	-0.2394359	-0.1073243	-0.4732085	0.03465111	-0.344304	-0.5861358	-3.0421191	-0.1291622
C_33	0.3566595	-0.6496292	1.7652483	0.08259094	-0.0292464	0.43294098	1.75527325	-0.2736748	-1.1803979	-0.7801787	0.49309619	2.14853261	-1.2002496	-0.2495089	-0.9059383	-1.765518
C_34	-0.2675535	-0.4037277	2.57184879	-0.7025429	-0.8911763	1.50203605	1.3022127	-0.0165205	-0.6742801	-1.1363214	-0.8001202	1.1561046	0.20464282	-1.5171056	0.73328116	-1.0607779
C_35	0.94440986	-0.598154	-1.9549386	0.39061838	-0.1820859	1.08645022	-1.6636326	-0.2540891	0.04715146	0.30610037	0.56599149	0.21233973	0.39989744	1.00878956	0.17204749	-0.4808959
C_36	-0.6347374	-0.7121446	1.06794168	-0.0242746	-0.3388949	1.46281107	0.69535967	0.5912913	-0.6924537	-0.4006029	-0.5588927	1.53507223	-0.1060434	-1.208061	0.15301583	-0.8293865
C_37	1.79990302	-0.4635814	1.41573852	0.07086071	0.06349901	1.1955524	1.02851593	0.37289254	-0.8079949	-0.3465895	0.32717812	0.96234349	-0.7657805	-1.1185471	-3.4247853	-0.309205
C_38	1.2099904	-0.0938404	1.40520457	0.09715464	0.20128309	1.68813666	-0.5824122	-1.6617106	0.41074262	0.90157759	-0.0321806	1.32960897	-0.0696472	0.12301918	-4.7365963	-0.1903305
C_39	0.85983918	-0.5097024	1.78086942	-0.3118848	-0.1940964	3.0462482	-0.1292038	0.37714003	0.16879203	-0.7336555	-0.2370553	-0.5176708	-1.1568254	-1.5215155	-0.43266	-0.4886189
C_4	-1.1981076	-1.5426194	2.37176308	0.2883424	0.47119599	3.19849586	-0.3378582	-0.9496388	-1.2995324	-0.2372159	-0.1178249	1.25809124	-0.7392021	-0.8168422	-0.0430308	-0.3060164
C_40	0.01897968	-1.6345274	1.10316632	-1.0993913	-0.3771319	2.23444997	1.23089794	-0.3485965	-0.0199755	-0.4837973	-0.5338056	1.24953393	-0.8527476	-0.0395001	-0.3341034	-0.1134511
C_5	-1.0881233	-1.2335791	2.50337179	-0.3567773	-1.1585666	3.64362447	0.13381673	-0.9454812	-1.2182905	0.44955668	0.15722767	1.31976001	-0.3474983	0.8691172	-2.9259494	0.19779115
C_6	0.59658973	-0.6487199	2.32584177	-0.9646845	-0.6511701	3.37839338	1.2049625	-0.7903003	-1.1647338	-0.3975224	0.14629293	1.74385899	-1.0225508	-0.9957432	-2.4494268	-0.3110876
C_7	-1.430832	-1.2799877	2.20309411	-0.7605122	-0.8403987	2.67986427	1.72040234	0.63437368	-1.2391916	-1.2456986	0.09614535	2.82452754	-1.3231902	-0.3284207	0.38625547	-2.0964309
C_8	-0.9063189	-0.9058117	2.60312728	-1.0871367	0.98252124	2.39621863	0.84063156	-1.5272439	-0.2911329	-0.9434563	-1.5642028	1.74007878	-0.402231	0.09292496	0.51257024	-1.5405385
C_9	-0.3367189	-0.5399716	3.14045229	0.21377722	-1.2696245	3.82095523	0.33458307	-0.287762	-0.8920656	-0.190802	-1.4582009	1.10939034	-0.2127467	-1.3464958	-2.3225523	0.237782

Table 8.136: Normalised data matrix for phosphatidylserine for serum samples taken from patients with breast cancer.

	PS(32:1)	PS(32:2)	PS(34:0)/IS	PS(34:1)	PS(34:2)	PS(36:0	PS(36:1	PS(36:2	PS(38:1	PS(38:2	PS(38:3	PS(38:4	PS(38:5	PS(40:4	PS(40:5	PS(40:6
P_1	-0.1740606	-0.0447934	2.47729326	0.09531472	0.02763406	1.96111672	-0.3236488	-1.4439554	0.1204576	-0.5495261	-1.3141066	1.71881285	-1.1054439	-0.8049911	-0.2784175	-0.3616859
P_10	0.72158035	-0.4791478	2.37619386	-0.1385041	-0.7312039	3.43905965	0.25955998	-1.1111171	-0.496308	-0.6936705	-0.0493191	1.06978107	-0.22173	-0.4712016	-3.1845056	-0.2894674
P_11	-0.9450311	0.50667363	3.49626422	-0.7035233	0.29652556	4.65680722	-0.0295723	-1.9235005	-0.8653195	-0.0790897	-2.0824705	1.62037589	-0.8241988	-0.3317938	-2.8998369	0.10768994
P_12	-0.2249963	-0.6972611	2.7545056	-1.1371404	1.10848447	3.67725741	1.36253801	-0.1895096	-0.6973104	-1.3048648	-2.6207281	2.02671683	-0.6654866	-0.9285013	-2.0649235	-0.3987802
P_13	-1.7384442	-1.309811	2.84726298	0.05890465	-0.5588726	3.45582506	-0.2013945	-1.0112144	-0.5357473	-0.4251421	-0.4252337	0.98074504	-0.5969994	0.49618105	-0.5154169	-0.5206427
P_14	-1.9711419	-0.7815363	2.50494289	-0.9877062	1.36435207	2.82021892	0.14215277	-0.9949635	-1.3467975	0.15069535	-0.8745834	1.017193	-0.4259986	-0.2257373	-0.6615335	0.27044335
P_15	-0.8509216	-0.510545	3.89019027	-0.5300739	-0.0074206	4.62519225	-0.6417138	-0.3518531	-0.9844589	-0.1841611	0.5092051	-1.225851	0.50790981	-0.62672	-3.2012982	-0.4174803
P_16	0.15714157	-1.0410958	2.56284944	-0.5352754	-0.2104021	3.18130947	0.47537865	-0.9832771	-1.3228291	-0.1220129	0.22974596	1.51187545	-1.0241022	-0.9760479	-0.7796032	-1.1236547
P_17	-0.1542711	-0.7728746	2.72348601	-0.7545752	0.1080753	3.41818295	0.71973255	-0.8762826	-0.4509649	-0.3684626	-1.0580889	-0.2201968	-1.0527445	-0.880421	0.51667961	-0.8972743
P_18	-1.1580832	-0.3029758	2.62738112	-0.8438769	-0.5029597	2.41961141	0.61062242	-0.5086868	-0.6734373	0.24697554	-0.0302298	2.02128784	-0.4687477	-0.6004661	-2.4339729	-0.4024421
P_19	0.58132746	-0.6602223	2.87005392	-0.0963233	-0.2684932	3.83796617	-0.2592796	-1.0851022	-0.5119715	-0.4504158	-2.1350713	1.01553321	-0.2505827	-0.9027016	-1.6153434	-0.0693739
P_2	-0.319052	-1.0269209	2.9813102	-1.4897533	-1.3211332	2.83012735	0.4889454	0.47565191	0.34735656	-0.7103487	-0.3515792	1.21143869	-1.0658174	-0.2640674	-0.0410494	-1.7451086
P_20	-0.3243594	-0.2310493	2.10201367	-1.4119634	-0.5338262	3.03427847	1.05057681	-1.707181	-0.4216266	-0.1783592	-0.3935734	1.57602271	-0.5837263	-1.0934662	-0.7504969	-0.1332638
P_21	-0.8652796	-0.3457979	2.86676774	-0.9045618	0.50761788	3.19984252	0.5240383	-0.4869708	-0.9041929	0.8036891	-1.6833667	-0.2556252	0.29911059	-1.002546	-2.0589411	0.3062159
P_22	-0.2704296	-0.4547834	3.0572916	0.40750024	-0.7368064	3.53671639	-1.0317773	-1.2628757	-0.7287047	-0.0261255	-0.4662459	1.05835434	-0.0640789	-0.4131121	-2.5182662	-0.0866569
P_23	-0.1667469	-1.1795073	2.98960714	-0.104466	-0.8933611	3.30285631	0.03994805	-0.8910145	-1.0331776	-0.4580689	-1.067776	1.18559474	-0.3066386	-0.072759	-0.4107883	-0.9337021
P_25	2.04356641	-0.3731132	2.56902115	0.00282545	-0.2684629	2.98307274	-2.8919898	-0.6210717	0.18937052	0.13855096	-0.8561384	-0.2033226	-0.128395	0.10256321	-2.7917127	0.10523589
P_26	0.61461667	0.40010509	2.19499491	-0.6765444	-0.8512697	1.45157891	1.49913282	-0.091538	-0.5222853	-0.6861313	-1.5095342	1.75992838	-0.1054698	-1.6269502	-0.2372727	-1.613361
P_27	0.14934476	-1.0721476	2.74023633	0.32077063	0.08814094	3.18552325	0.86768337	-0.9509084	-1.3203737	-1.0185742	-0.9499758	1.41426453	-0.2906311	-0.1188881	-2.1849236	-0.8595413
P_28	0.25397919	0.01047652	3.13387416	-0.2067988	-0.0120378	3.22129151	-0.0251715	-1.2091069	-0.3035716	-0.3095924	-0.6939685	0.21843922	-0.6631853	-0.8640685	-2.3496859	-0.2008734
P_29	1.00410534	-0.2951278	1.43888785	0.85700757	-0.2321911	2.02746227	0.63482086	-0.543404	0.1454659	-0.3023898	-1.2939427	-0.2797525	0.43378159	-0.6086521	-2.2976494	-0.6884219
P_3	-0.8131156	-1.1541035	2.88863352	-0.1796202	-0.5296924	3.65628257	-0.6359075	-1.0360261	-0.8890588	-0.5810198	-0.3834638	0.65584245	-0.5617702	0.02430178	-0.162061	-0.2992213
P_30	-0.0445015	0.47214204	2.76363548	0.17312242	-1.3122356	3.35521528	-0.7894245	0.1966094	-0.3188206	-1.417393	-1.2664681	-0.4896703	0.03097476	-0.400814	-1.0783129	0.12594117
P_31	0.79081839	-0.4304198	2.28762381	0.21264923	-0.5035152	3.29388419	0.55890997	-1.4817754	0.11563087	0.06481131	0.17551578	-0.7884121	-0.5523185	-0.1530026	-3.8087291	0.21832907
P_32	-0.2054731	-0.4022109	2.81874815	0.54344664	-0.0455503	3.62315253	-2.5581551	-0.0081723	-0.4323369	0.20662896	-0.1240906	0.62932631	-1.1569926	-0.0988706	-2.603008	-0.1864422
P_33	0.12672015	-0.5228919	1.99661705	-0.3417532	0.4116196	2.78357705	-0.4926561	-1.412998	-0.3966163	-0.5593273	-0.9926453	1.49346596	-1.5236884	-0.2187842	-0.256019	-0.0946201
P_35	0.8666433	0.63061072	1.38651872	0.60734779	0.4541072	1.59639596	0.36804631	0.74117422	-0.2721303	-1.2047921	-0.6515132	1.119068	-1.1906113	-0.3240901	-3.9489387	-0.1778366
P_36	0.13056641	-0.6705392	2.28474386	0.27074026	-0.5280582	2.80639166	-0.7787713	-0.3876363	-0.6217466	-0.447728	0.25409072	-0.6350649	0.13904789	-0.5089596	-1.0128663	-0.2942103
P_37	0.37147217	-0.4089489	2.73959279	-0.2350254	0.32566124	3.05459888	-0.592615	-1.7322626	0.24392599	-0.0799173	-1.923841	1.21016807	-0.2144023	0.18080058	-2.833167	-0.1060403
P_38	-0.349962	0.07295819	3.24045687	-1.1175278	-0.3375547	3.3761296	-2.3518641	-0.5097784	0.16210191	-0.2561692	0.30186501	0.34272042	-0.0571588	-0.7842804	-0.774425	-0.9575116
P_39	0.3120963	-0.2300594	3.31119957	-0.4515354	0.37456969	3.82896316	-2.2191576	-0.3044303	-0.5443274	-0.1124023	-0.6525248	-0.0928866	-0.8921994	-0.2527435	-1.8730702	-0.2014918
P_4	-0.8588591	-1.1924382	3.01146193	-0.3765784	0.1595537	3.37599994	-0.5942741	-1.2247979	0.15906862	-1.2540123	-0.431749	-0.1217344	-0.5861141	-0.6899212	0.16287306	0.46152142
P_40	0.99692612	0.6967735	2.25759583	-0.7081333	-0.3003675	3.19835401	0.63891453	-0.8870859	-1.031879	-0.7128807	-0.8892739	0.38140019	0.06097385	-0.5782771	-3.3736374	0.25059678
P_41	0.44706439	0.21789799	2.90328321	-0.0564045	-0.6086038	2.71331228	1.16969303	-0.1463605	-0.8287839	-0.61676	-1.7473732	-0.1296566	-0.6553655	-0.8662767	-3.0762814	1.28061522
P_5	-1.2568734	0.03029761	3.40939649	-1.0079817	0.28045242	4.03003919	-1.9974184	-0.5575147	0.0327527	-0.8315471	-0.9825188	-0.5602165	-0.5713202	-0.0510355	-0.2077359	0.24122385
P_6	0.81745205	-0.2898476	2.65167267	0.33547662	0.03073065	2.54980534	-1.007837	-0.568638	0.71319972	-1.3843158	-0.3962736	-1.168257	-0.6206315	-0.8778312	-0.5348373	-0.249868
P_7	-0.8529897	0.02851011	3.28757337	-0.3115592	-0.4338282	3.53005643	-0.3023791	-0.7747342	-0.8550372	-0.4957469	-0.5434528	0.32504643	-0.0170056	0.40047053	-2.905646	-0.0792779
P_8	0.00376725	-1.2581632	2.88094874	-0.5710285	0.12539682	3.05294503	0.04863722	-0.593383	0.67077296	-0.4153925	-0.555736	0.15637225	-0.5945299	-0.2807313	-1.9866283	-0.6832476
P_9	-1.1125037	-0.2687765	3.04259684	-0.2250635	-0.9390861	4.14830482	0.0141851	0.70340136	0.39807832	-0.0055843	-0.3217682	0.40896753	-1.0983294	-0.8038518	-3.9270902	-0.0134804

Table 8.137: Normalised data matrix for sphingomyelin for serum samples taken from breast cancer free controls.

	SM(30:0)	SM(30:1)	SM(30:2)	SM(32:0)	SM(32:1)	SM(33:0)	SM(33:1)	SM(34:0)	SM(34:0)(2)	SM(34:1)/IS	SM(34:2)	SM(d31)/IS
C_1	-4.2681894	-6.5407508	-5.1080164	2.09489504	-1.7826782	2.21365334	2.21365334	1.24604376	1.66261496	4.05427864	2.21321216	2.00128344
C_10	-3.4646816	-9.0457582	-5.1495743	2.08417452	-0.800805	2.19508009	2.20108824	1.35260196	1.81502902	4.22560419	2.59645779	1.99078331
C_11	-4.2200053	-8.6528043	-4.9701944	2.24905155	-1.9702781	2.5317178	2.53925224	1.51652545	2.08839064	4.44439631	2.32578807	2.11816008
C_12	-4.2731044	-5.9025097	-5.1248051	1.79310309	-1.8367202	2.12594823	2.12594823	1.28443584	1.67057239	4.05916433	1.4416012	2.63636607
C_13	-3.4774839	-7.5643292	-6.0263502	2.12614652	-0.9211682	2.26995428	2.27370726	1.39887081	1.62969783	4.23352864	2.52379049	1.53363572
C_14	-3.6176587	-7.2315751	-4.6623614	2.36487765	-1.8842031	2.43108922	2.43305228	1.38193786	1.81387752	4.21503307	1.14473273	1.61119788
C_15	-3.5578752	-6.9237332	-5.1065071	2.23359184	-1.2898794	2.33821762	2.33821762	1.12218508	1.32686668	4.00881994	2.06539033	1.44470583
C_16	-4.0387646	-7.9352834	-5.1651014	1.90786605	-1.3733283	2.34309905	2.34309905	1.50146291	1.69319784	4.31483744	2.09322421	2.31569108
C_17	-3.9484449	-6.5382169	-5.1757182	1.98198566	-1.1798575	2.11536107	2.11536107	1.11377392	1.63155406	3.92524115	2.13554078	1.82341971
C_18	-4.1898983	-6.0743485	-5.1241082	1.801502	-1.4202168	2.06830195	2.06830195	1.12525197	1.9330162	4.04813187	1.9695147	1.79455123
C_19	-4.0833446	-8.3079299	-5.1707648	2.09242792	-1.0447081	2.35020783	2.34909869	1.35928262	1.91515481	4.29479066	2.55074733	1.69503748
C_2	-3.962404	-6.7693071	-5.5281948	1.83827344	-1.0459576	2.0610449	2.0610449	1.32450192	1.6652582	4.13044752	2.18115447	2.04413809
C_20	-4.2019458	-6.7536206	-5.1969809	1.96823321	-1.4594547	2.41610903	2.41610903	1.14551165	1.76369827	4.08979047	1.77749049	2.03505992
C_21	-4.4324531	-8.1872905	-5.0697429	2.3634633	-2.1055906	2.46776429	2.48034478	1.67873116	1.91734408	4.51505779	2.48567271	1.88669903
C_22	-3.8121917	-9.0598004	-4.9898245	2.43997113	-1.3521384	2.30946122	2.31514185	1.55853872	1.74614034	4.40869568	2.55399349	1.88201259
C_23	-4.0088477	-7.7993808	-5.1834459	2.01512256	-1.1763519	2.42569669	2.42569669	1.38269593	1.79728675	4.23133418	2.22640407	1.66378933
C_24	-4.015157	-7.0751088	-5.8731789	2.41748537	-1.8734597	2.4104942	2.41926665	1.38682185	1.85992427	4.2800291	2.51498175	1.54790129
C_25	-3.6415669	-8.8158316	-6.5540685	2.49074516	-0.8362416	2.70901125	2.70901125	1.61917793	1.58132729	4.41317352	2.55999575	1.7652664
C_26	-4.2771061	-7.6451201	-5.8259617	2.35611217	-1.7934566	2.70818697	2.71119909	1.5497322	1.70020997	4.40812328	2.46036312	1.64771766
C_27	-3.8666583	-7.5925879	-6.2721401	2.24493054	-0.9323643	2.50926741	2.51739717	1.40850697	1.56502573	4.27742907	2.47807437	1.6631194
C_28	-3.806788	-7.2494893	-5.3652425	2.15393299	-1.1192913	2.44010489	2.44010489	1.13392793	1.5887465	4.05929292	2.3684498	1.35625128
C_29	-3.8534045	-8.2072951	-5.2849206	2.16468585	-0.9118248	2.32288583	2.32288583	1.2519479	1.79607315	4.20721332	2.64729838	1.54445456
C_3	-4.8397377	-6.9869087	-5.2576696	2.16991103	-2.0476501	2.31054583	2.31119971	1.49025133	2.01718621	4.40831816	2.3492056	2.07534816
C_30	-3.748604	-8.6248912	-5.5050468	2.18068091	-1.2420115	2.51401173	2.52036335	1.57737729	1.86212194	4.39713108	2.21925906	1.84960816
C_31	-3.7942664	-8.5822483	-4.629874	2.24322203	-1.9379991	2.62896621	2.6368295	1.50469991	1.76055818	4.37536408	2.37940227	1.41534554
C_32	-3.7936778	-8.4100889	-5.7961901	2.16229435	-1.3725265	2.53699678	2.53699678	1.60728619	1.93849827	4.45493537	2.05209104	2.08338459
C_33	-3.6174911	-8.1014348	-5.348128	2.24557605	-0.9790611	2.41465549	2.41465549	1.22810243	1.65154474	4.11034114	2.24094996	1.74028964
C_34	-3.7255946	-8.4982547	-5.0346043	2.24649758	-1.0602241	2.50882664	2.50882664	1.35645922	1.52298629	4.13919609	2.34287276	1.69301245
C_35	-3.4374277	-6.9096867	-6.5709732	2.3382147	-0.9163914	2.52943946	2.52943946	1.18927433	1.55171699	4.07793002	2.25956928	1.35889473
C_36	-3.8332999	-8.0579612	-5.1163712	2.25184426	-1.495708	2.49188928	2.49188928	1.36476891	1.87246695	4.30108423	2.11337763	1.61601971
C_37	-3.6974106	-8.6477111	-5.1997961	2.06464951	-1.1422666	2.70410163	2.70410163	1.52548162	1.53157023	4.30183883	2.16108979	1.69435113
C_38	-3.7160024	-9.1654789	-5.8108016	2.3898292	-0.9154762	2.41818878	2.41818878	1.62884354	1.72803972	4.48534982	2.56071751	1.97860173
C_39	-3.9947008	-9.0329513	-5.1870681	2.49155687	-1.8807607	2.91040376	2.91293775	1.77956875	1.4055754	4.58850794	2.5124201	1.49451023
C_4	-3.4714077	-6.2219529	-5.5139662	1.84888779	-1.2110961	1.99236026	1.99189331	1.13577492	1.71815182	4.01689451	1.98744953	1.72701077
C_40	-4.1388199	-7.1345522	-5.2141753	2.09600739	-1.8040382	2.47412303	2.47412303	1.52760931	1.71846597	4.36101735	1.65446939	1.98577015
C_5	-3.3149568	-6.8756064	-5.778934	1.8219918	-0.7796509	2.31021193	2.31021193	1.15277295	1.40346094	4.01405368	2.21652383	1.51992095
C_6	-4.1231339	-7.8887241	-5.0861831	1.98024332	-1.4205219	2.38525278	2.39078395	1.3950601	1.82650754	4.2911319	2.2602501	1.98933335
C_7	-4.0120642	-7.4558212	-5.175215	2.03795091	-1.3505428	2.30984419	2.30984419	1.3356538	1.73172807	4.17671737	2.34671157	1.7451932
C_8	-3.6523747	-8.1589249	-4.6428472	2.17566728	-1.6679375	2.07255966	2.07153339	1.2816849	1.96074991	4.1330101	2.11213176	2.31474726
C_9	-4.1330107	-7.4752097	-4.8428713	1.89714054	-1.9542489	2.332639	2.33712665	1.53029888	1.82783232	4.33410534	2.22564897	1.92054897

Table 8.138: Normalised data matrix for sphingomyelin for serum samples taken from patients with breast cancer.

	SM(30:0)	SM(30:1)	SM(30:2)	SM(32:0)	SM(32:1)	SM(33:0)	SM(33:1)	SM(34:0)	SM(34:0)(d2)	SM(34:1)/IS	SM(34:2)	SM(d31)/IS
P_1	-4.1773035	-7.2596182	-5.3306576	1.97920248	-1.3187119	2.15214089	2.15214089	1.46347189	1.74804608	4.22113135	2.28374945	2.08640809
P_10	-4.4430928	-7.0725311	-5.2620477	1.80066692	-1.661852	2.33369309	2.33369309	1.34958303	2.11200391	4.30742565	2.44747247	1.7549854
P_11	-3.9458111	-6.6831426	-5.7210594	2.05277567	-1.1566885	2.2397701	2.24473857	1.36118661	1.63229241	4.21688271	2.34800818	1.4110474
P_12	-4.1179622	-8.2851118	-5.2525655	1.98140626	-1.1092635	2.3004312	2.3004312	1.34916988	1.94963018	4.26329824	2.68067358	1.9398624
P_13	-3.9038287	-7.9474848	-4.8611556	2.32028783	-1.8125919	2.44027375	2.44572028	1.2657514	1.81821604	4.16395865	2.23497635	1.83587669
P_14	-4.1584249	-7.6470646	-5.0927821	2.20780389	-1.2249099	2.35177305	2.35836776	1.17486606	1.74057463	4.09517056	2.40673841	1.78788716
P_15	-4.2694174	-8.254536	-5.5492674	2.24256268	-1.600115	2.42633458	2.43461431	1.64793856	1.97865392	4.49155938	2.79791366	1.65375875
P_16	-4.4631495	-6.2821761	-5.608734	1.95074255	-1.3091836	2.18307147	2.18307147	1.26914662	1.68810419	4.11185498	2.16565552	2.11159637
P_17	-4.1813494	-8.5987715	-4.9247072	2.25761319	-2.0043581	2.68762893	2.67972636	1.46587152	1.94750445	4.39329206	2.46327173	1.8142779
P_18	-4.1810877	-7.0136751	-5.5311039	1.917403	-1.3966719	2.19833942	2.19833942	1.33434883	1.87325903	4.23709849	2.23032742	2.13342295
P_19	-3.4228183	-6.3677401	-5.8886039	1.93333417	-1.1138348	2.04535992	2.04535992	1.23082941	1.62958523	4.06722132	1.99197276	1.84933442
P_2	-4.475002	-7.9482527	-4.8682426	2.17824188	-1.9710269	2.41245238	2.4091168	1.54772804	1.92821448	4.40125209	2.41631955	1.969199
P_20	-3.6960788	-8.3122988	-5.5156952	2.06247455	-1.4526839	2.34908407	2.35127782	1.53085177	1.88265533	4.36901513	2.15447558	2.27692242
P_21	-3.947081	-8.5287632	-6.0710076	2.42687124	-0.7984315	2.60356202	2.60356202	1.37041146	1.82960638	4.25924786	2.68424852	1.56777384
P_22	-4.3088387	-8.1908933	-6.5910248	2.41745593	-1.6349946	2.54563902	2.54563902	1.64424917	2.06428182	4.53532841	2.96009583	2.01306214
P_23	-3.3116625	-9.2505171	-6.2698985	2.36101401	-0.6877007	2.67959319	2.67959319	1.58904616	1.56082368	4.39760362	2.59680917	1.65529574
P_25	-4.3258841	-7.6434041	-5.0087295	2.15070128	-1.9878405	2.63502907	2.64014356	1.46601715	1.6905382	4.31787917	2.3763579	1.68919186
P_26	-3.754855	-7.4706419	-5.1680568	2.21158389	-1.3577142	2.3230917	2.3230917	1.221936	1.71653339	4.12830845	2.29956362	1.52715905
P_27	-3.8390656	-6.6580729	-5.3937156	2.08167428	-1.1748438	2.15882873	2.15882873	1.23325404	1.47999849	4.03153986	2.18888715	1.73268668
P_28	-3.9323281	-7.4665359	-5.8897688	2.32677898	-1.865406	2.64258275	2.64178211	1.48961013	1.67227778	4.29360937	2.42876015	1.65863749
P_29	-3.7923071	-7.8317837	-5.9931191	2.19491842	-0.9731297	2.36193181	2.36193181	1.41456491	1.63727674	4.23625482	2.67289368	1.71056738
P_3	-3.6746717	-6.8843049	-5.315689	1.79294718	-1.0214695	2.05851935	2.06087128	1.19322606	1.55387321	4.03611423	2.17906329	2.02152051
P_30	-3.951642	-8.7258886	-5.5881086	2.51292895	-1.390941	2.76428045	2.77142889	1.49177564	1.52002901	4.30821611	2.83502574	1.45289547
P_31	-4.4642674	-7.8053609	-5.3362026	2.12010221	-2.052689	2.55345977	2.55345977	1.65274983	1.74264524	4.46398453	2.55443443	2.01768404
P_32	-3.9668134	-8.2168113	-5.9682934	2.09286392	-1.4446949	2.48216269	2.48731865	1.69409342	1.82069635	4.51912027	2.19083815	2.30951956
P_33	-3.5989121	-9.0057101	-6.7721179	2.37333631	-0.8992458	2.65602109	2.65602109	1.6862765	2.05302605	4.54258214	2.53914113	1.76958152
P_35	-3.7390147	-8.9681769	-6.612482	2.62431902	-1.1841199	2.47094155	2.47094155	1.61470232	1.93200265	4.45762318	2.45880342	2.47445975
P_36	-4.2908757	-7.466612	-6.0262504	2.35699173	-1.9811238	2.52952182	2.52952182	1.6669733	1.78336298	4.49721337	2.34623942	2.05503744
P_37	-3.4078793	-7.6137652	-6.4759322	2.35282798	-0.7824159	2.51843756	2.51843756	1.32725505	1.51254264	4.16101703	2.37812633	1.51134839
P_38	-4.1373886	-7.5357651	-5.3153376	2.31969807	-1.9423636	2.6027734	2.60483001	1.34940483	1.85019246	4.30641515	2.56519622	1.33234478
P_39	-4.2069514	-7.6540193	-5.7869378	2.39964344	-1.988299	2.69264002	2.69403506	1.60916524	1.77421499	4.45975291	2.48157159	1.52518421
P_4	-4.1222996	-8.0693277	-5.1150687	2.04780464	-1.2255778	2.42986556	2.42986556	1.23919935	1.92277147	4.16486046	2.28397169	2.01393516
P_40	-4.1458673	-8.0059389	-5.8549037	2.08155626	-1.3839093	2.51008549	2.51151731	1.68846013	1.76911493	4.48900613	2.5891712	1.75170785
P_41	-3.6002665	-8.5904645	-5.3702103	2.41419985	-1.0456034	2.56839148	2.56839148	1.29319324	1.66229479	4.13790788	2.41997631	1.54218979
P_5	-4.5381749	-6.9828694	-5.4817995	2.05201662	-1.9170295	2.34339285	2.34160414	1.54113302	1.73588699	4.37611584	2.47554339	2.05418044
P_6	-4.4842982	-7.9558312	-4.8872376	2.19585905	-1.8261226	2.54004734	2.54004734	1.45443642	1.7858143	4.31246868	2.616674	1.70814257
P_7	-4.023738	-7.4016266	-5.2772539	2.23879876	-1.8695167	2.42567601	2.42567601	1.30462273	1.8407865	4.20686325	2.37749245	1.75221963
P_8	-4.2681354	-8.4625995	-5.1369097	2.27559493	-2.0020551	2.68935084	2.69715975	1.49574416	2.09582107	4.43462261	2.48267659	1.69872983
P_9	-3.4306752	-8.7262387	-5.219181	2.12196567	-1.2716635	2.37088336	2.37646557	1.50879465	1.7571419	4.3598165	2.28213223	1.87055848

8.4.2. Heteroscadascity plots for serum samples

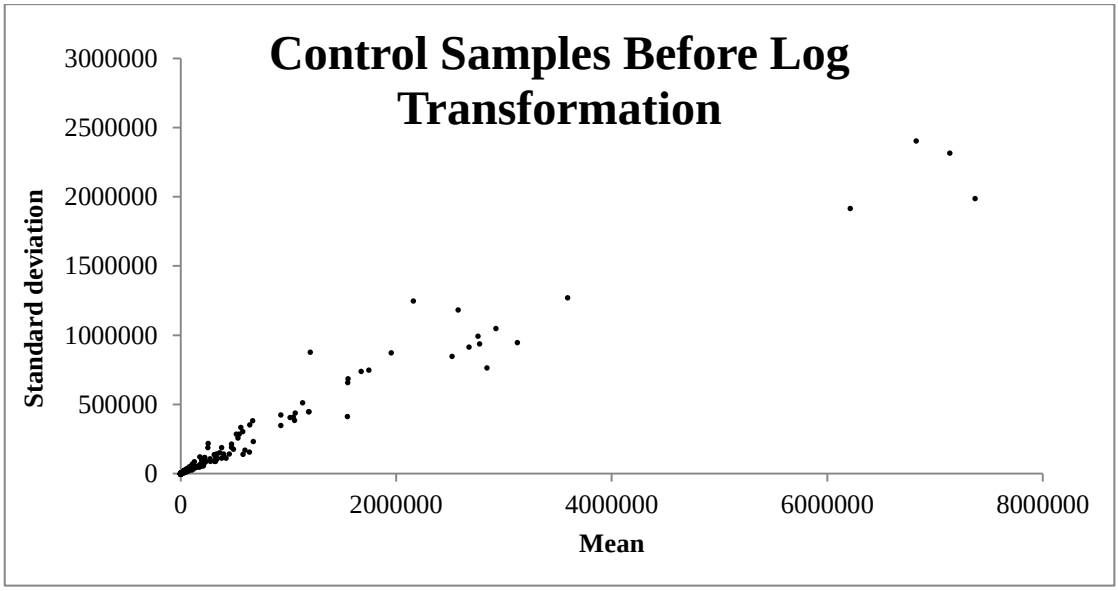


Figure 8.10: Heteroscadascity plot of the average of the control serum samples for all lipid species before log transformation

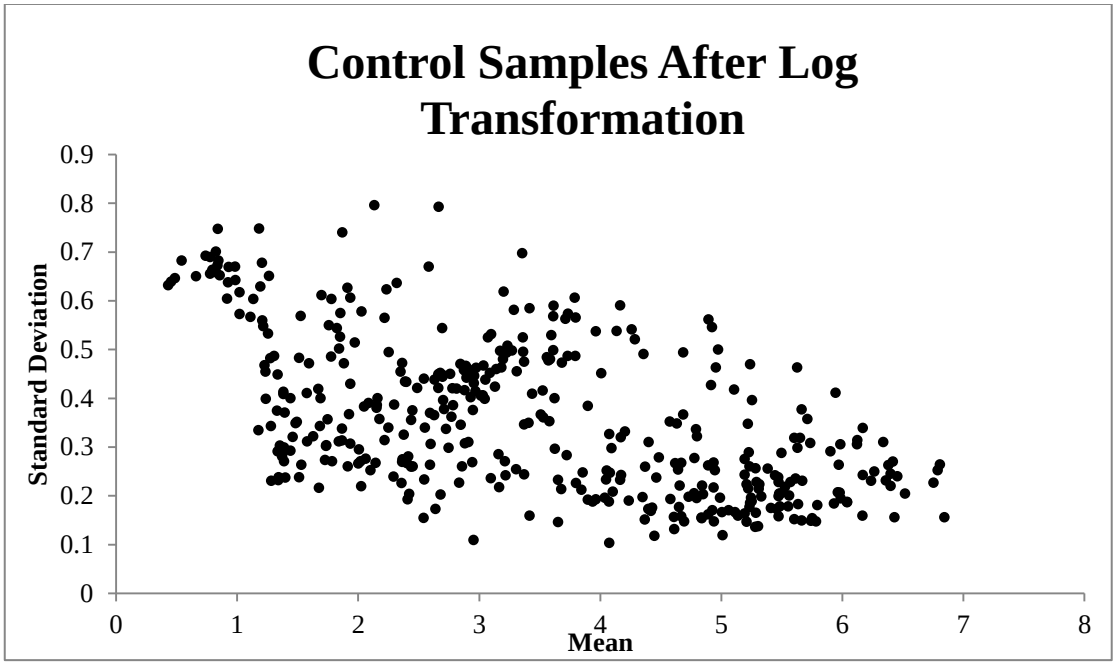


Figure 8.11: Heteroscadascity plot of the average of the control serum samples for all lipid species after log transformation

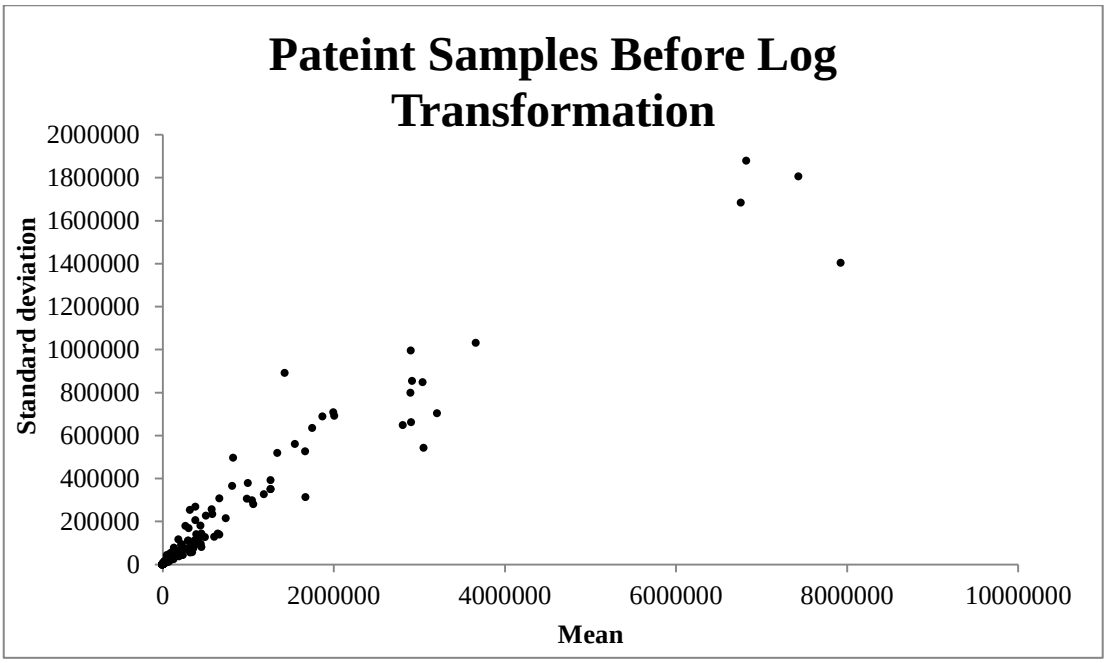


Figure 8.12: Heteroscadascity plot of the average of the patient serum samples for all lipid species before log transformation

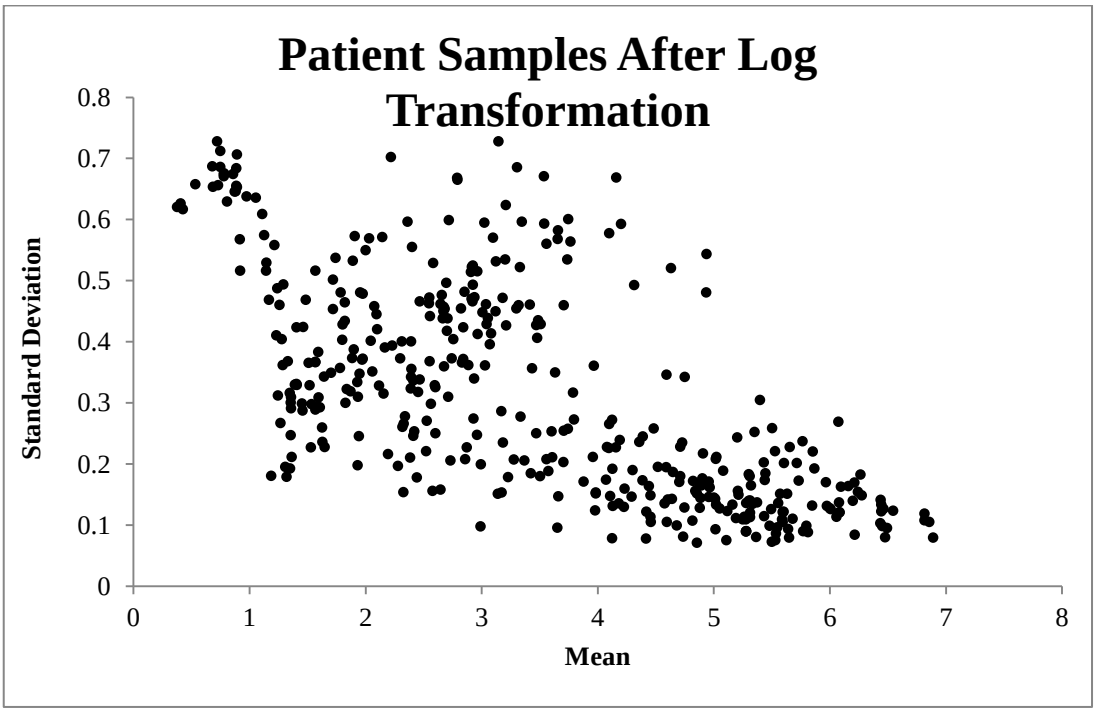


Figure 8.13: Heteroscadascity plot of the average of the patient serum samples for all lipid species after log transformation

8.4.3. Two sided t-test

Table 8.139: Data generated from a two-sided t-test comparing control serum samples to the breast cancer patient serum samples. Those species with an adjusted p-value < 0.05 and fold change > 2 were considered significantly different (in red) between the two groups.

Phospholipid specie	Log Fold Change	T statistic	P value	Adjusted P value	Fold change
CE	0.005742719	0.034458544	0.972589333	0.972589333	1.00575924
CE (10:0)	-0.046710877	-0.285764491	0.775728293	0.865506723	0.954363286
CE (13:6)	0.038246935	0.328089569	0.743621212	0.865506723	1.038987763
CE (3:2)	0.110324437	0.83986269	0.403255285	0.612350618	1.116640292
CE 24:0	-0.225511863	-1.957507923	0.053448246	0.146091874	0.798107593
CE 24:1	-0.216903808	-2.008423497	0.047656007	0.139564022	0.805007401
CE 24:2	-0.0604406	-0.461478626	0.6455909	0.865506723	0.941349683
CE 24:3	0.263024784	2.274263055	0.025375355	0.104038956	1.300858959
CE 24:4	0.135891628	1.344076034	0.18236953	0.373857537	1.14555774
CE 24:5	0.422717264	2.597908525	0.010989959	0.085139476	1.526102751
CE 24:6	-0.351390489	-3.70003191	0.000374439	0.015351981	0.70370891
CE(14:0)	0.036398673	0.255491377	0.798938226	0.865506723	1.037069216
CE(14:1)	-0.040194158	-0.251286422	0.802176963	0.865506723	0.960602912
CE(15:0)	0.216008612	1.462971112	0.14702835	0.317271702	1.241113068
CE(16:0)	-0.082198989	-0.99699612	0.3214927	0.569625857	0.921088654
CE(16:1)	0.104880086	0.917798803	0.361226153	0.569625857	1.110577428
CE(16:2)	-0.058791068	-0.41797825	0.676978472	0.865506723	0.942903752
CE(17:0)	0.082028984	0.53917942	0.591120969	0.835722749	1.085487271
CE(17:1)	-0.020016179	-0.174287553	0.862038746	0.906245861	0.980182814
CE(17:2)	-0.219319828	-1.62615544	0.107483007	0.259223723	0.803064834
CE(17:3)	-0.009670488	-0.076177466	0.939450369	0.962936628	0.990376121
CE(17:5)	0.25711544	2.091572659	0.039350815	0.134448619	1.293194405
CE(18:0)	0.090289214	0.94236451	0.348579072	0.569625857	1.09449078
CE(18:1)	0.169195773	2.051012045	0.043231615	0.136345862	1.184351981
CE(18:2)	0.160183283	1.873417742	0.064321075	0.164822754	1.173725975
CE(18:3)	0.073211621	0.782148204	0.436221386	0.638752744	1.075958208
CE(18:4)	0.034038714	0.259684414	0.795712168	0.865506723	1.034624661
CE(18:6)	0.047472624	0.284054004	0.777034497	0.865506723	1.048617494
CE(20:0)	-0.277863852	-3.046498515	0.00305333	0.041728844	0.757399933
CE(20:1)	-0.1074317	-0.962905443	0.338226464	0.569625857	0.898137863
CE(20:3)	0.229334729	1.498412836	0.137595208	0.313411307	1.257762979
CE(20:4)	0.171840804	1.281886009	0.203240677	0.384384727	1.187488774
CE(20:5)	0.333576928	2.531232001	0.013137863	0.085139476	1.39595243
CE(22:0)	-0.388515169	-3.127608624	0.00238762	0.041728844	0.678062936
CE(22:1)	-0.17519859	-1.273301993	0.206255219	0.384384727	0.83929033
CE(22:2)	-0.261061675	-2.299219743	0.023853724	0.104038956	0.770233414
CE(22:3)	-0.254945768	-2.194580125	0.030820056	0.114874753	0.774958524
CE(22:4)	-0.293905274	-2.467398491	0.01554051	0.085139476	0.745347092
CE(22:5)	-0.213925488	-2.617075869	0.010434159	0.085139476	0.807408544
CE(22:6)	0.262463148	2.441732411	0.016612581	0.085139476	1.300128555
Cer(d18:1/16:0)D31	0.052724009	0.738677109	0.462063537	0.851548176	1.054138672
Cer(d18:1/17:	-0.08236042	-1.283045014	0.202836337	0.851548176	0.920939974

0)					
Phospholipid specie	**log Fold Change**	**T statistic**	**P value**	**Adjusted P value**	**Fold change**
Cer(d18:1/22:0)	-0.038362415	-0.857260302	0.393623563	0.851548176	0.962364102
Cer(d18:1/24:0)	0.00310706	0.049521441	0.960615682	0.981473794	1.003111892
Cer(d18:1/24:1)	0.122681994	1.792128391	0.076540218	0.851548176	1.13052485
Cer(d18:1/25:0)	0.03535896	0.511573681	0.610227362	0.87970875	1.035991522
Cer(d18:1/32:2)	0.033540993	0.61233006	0.541894294	0.851548176	1.034109834
Cer(d18:1/32:3)	-0.041811528	-0.617614127	0.538420523	0.851548176	0.959050518
Cer(d18:1/38:3)	0.036255847	0.450108455	0.65373622	0.898887303	1.036921106
Cer(d18:1/39:3)	-0.038925274	-0.507414023	0.613130341	0.87970875	0.96182258
Cer(d18:1/39:4)	0.095999443	1.48029342	0.142357002	0.851548176	1.100758451
Cer(d18:1/39:5)	-0.011155565	-0.16816513	0.866838251	0.981473794	0.988906428
Cer(d18:1/40:3)	0.001546407	0.023287166	0.981473794	0.981473794	1.001547603
Cer(d18:1/40:4)	0.118265936	1.639308844	0.104709944	0.851548176	1.125543394
Cer(d18:1/41:2)	-0.008654623	-0.116635318	0.907414124	0.981473794	0.99138272
Cer(d18:1/42:6)	-0.004688923	-0.074157203	0.941053167	0.981473794	0.995322053
Cer(d18:1/44:5)	0.062273379	0.878457454	0.382081517	0.851548176	1.064253249
Cer(d18:1/44:6)	0.076358846	0.8270715	0.410427762	0.851548176	1.079349825
Cholesterol	0.060009463	0.442349617	0.659318633	0.865506723	1.061846595
LPA 12:0	-0.025717328	-0.152736874	0.878964248	0.878964248	0.974610546
LPA 14:0	0.189466269	1.650350205	0.102525984	0.314008345	1.208604355
LPA 16:0	0.416461152	3.16657589	0.002135912	0.013883427	1.516585084
LPA 17:0 (IS)	0.098843507	0.620756456	0.53640471	0.697326123	1.103893534
LPA 18:0	0.236852093	2.921082886	0.004456149	0.024827114	1.267253668
LPA 18:1	0.45716057	3.668364806	0.000422705	0.005860726	1.579582498
LPA 18:2	0.50352258	3.612216267	0.000510492	0.005860726	1.654539264
LPA 18:3	0.375562894	1.268303625	0.208118685	0.352896901	1.45581065
LPA 20:0	0.099854698	1.014296186	0.313292008	0.48781036	1.105010347
LPA 20:1	0.373283684	4.21879628	6.07E-05	0.002366202	1.452496331
LPA 20:2	0.273909986	1.905559682	0.060054889	0.234214065	1.315096419
LPA 20:4	0.463694609	3.495461759	0.000751375	0.005860726	1.589937344
LPA 22:0	0.049190171	0.423678836	0.672859852	0.77180983	1.050420091
LPA 22:1	0.177235886	1.39577818	0.16638132	0.314008345	1.193912688
LPA 22:2	0.27045515	1.573688019	0.119238468	0.314008345	1.310560817
LPA 22:5	0.41936964	2.672597418	0.009006554	0.043906949	1.521002475
LPA 22:6	0.604941348	3.553740387	0.000620151	0.005860726	1.831144806
LPC (14:0)	-0.102557593	-1.095911799	0.276331148	0.536781196	0.902526169
LPC (15:0)	0.055894226	1.504224465	0.136372241	0.411551942	1.057485823
LPC (16:0)	0.028327066	0.670890613	0.504178831	0.718080724	1.028732093
LPC (16:1)	0.188272813	1.870144344	0.065038292	0.297066795	1.2071628

Phospholipid specie	log Fold Change	T statistic	P value	Adjusted P value	Fold change
LPC (17:0)	0.042296269	0.741582449	0.460462692	0.692235841	1.043203502
LPC (17:1)	0.058395764	0.924747237	0.357815496	0.609893606	1.060134476
LPC (17:2)	0.008513041	0.164974945	0.869370425	0.92523504	1.00854938
LPC (18:0)	0.019318839	0.34866379	0.728236908	0.840690181	1.019506655
LPC (18:1)	0.203951948	2.799607216	0.006380058	0.107822988	1.226239229
LPC (18:2)	0.153424417	2.100574506	0.038755656	0.265786642	1.165819668
LPC (18:3)	-0.021214335	-0.348509128	0.728352601	0.840690181	0.979009106
LPC (20:0)	-0.052122073	-0.826242702	0.411068188	0.651137347	0.949212986
LPC (20:1)	0.222266589	2.882906907	0.005031812	0.106290101	1.248904277
LPC (20:2)	0.156255283	1.76042899	0.082070238	0.315224322	1.169124623
LPC (20:3)	0.104917148	1.109686192	0.27038357	0.535085661	1.11061859
LPC (20:4)	0.182268009	2.197196619	0.030832762	0.23685167	1.199935744
LPC (20:5)	0.254095473	1.779829796	0.078814947	0.31142819	1.289294891
LPC (22:0)	-0.042119612	-0.64317606	0.52190754	0.718080724	0.958755095
LPC (22:1)	0.278093874	2.542049089	0.01290565	0.137547586	1.320610162
LPC (22:2)	-0.088705685	-1.36336837	0.176504472	0.448938972	0.915114866
LPC (22:3)	-0.060123589	-0.905037673	0.368101466	0.609893606	0.941648149
LPC (22:4)	0.087641844	0.910717665	0.365118151	0.609893606	1.09159709
LPC (22:5)	0.154668633	1.68628237	0.095549433	0.331659719	1.167271101
LPC (22:6)	0.282350267	2.71678227	0.008041675	0.113229086	1.326243177
LPC(21:0)	0.123790949	2.034179763	0.045171617	0.290567927	1.131779247
LPE (17:0)	0.008566596	0.091235903	0.9275225	0.985565687	1.008603394
LPE (18:0)	-0.088921443	-0.61132783	0.542634483	0.952482211	0.914917444
LPE (18:1)	0.101061051	0.700817368	0.485354993	0.952482211	1.106344183
LPE (18:2)	-0.135576151	-0.984620214	0.327639984	0.952482211	0.873212665
LPE (20:4)	0.146040977	1.406513217	0.163262886	0.952482211	1.157243607
LPG (16:0)	0.129761788	0.712234713	0.477690473	0.830141833	1.138557133
LPG (17:0)	0.055069975	0.361379163	0.718446233	0.830141833	1.056614549
LPG (18:0)	0.092057379	0.579315898	0.56345298	0.830141833	1.096427732
LPG(20:5)	0.154263597	1.009419743	0.314787593	0.830141833	1.166798411
LPG(20:6)	0.141987332	0.91241485	0.363364621	0.830141833	1.152562048
LPS (18:0))	-0.174417996	-1.435059276	0.154903977	0.314008345	0.83994573
modCer 576.5/7.68	-0.099132192	-1.072480925	0.286428725	0.851548176	0.905622984
modCer 614.6/5.72	-0.056437292	-0.6526256	0.515694484	0.851548176	0.94512575
modCer 632.6/9.22	-0.009308664	-0.152593992	0.879066879	0.981473794	0.990734527
modCer 651.6/7.56	-0.040505044	-0.697209419	0.487504793	0.851548176	0.960304321
modCer 703.6/5.87	-0.013264711	-0.211936453	0.832645425	0.981473794	0.986822878
modCer 731.6/6.22	-0.084318553	-1.205181413	0.231355702	0.851548176	0.919138415
modCer 766.6/7.17	-0.141561078	-1.735494461	0.086144533	0.851548176	0.868002158
modCer 769.6/8.01	-0.028364201	-0.358282196	0.720987927	0.951704063	0.972034286
modCer 798.7/7.29	-0.117769588	-2.295168307	0.024095256	0.795143446	0.888900842
modCer 875.7/9.23	-0.006107017	-0.079331841	0.936948333	0.981473794	0.993911593
modCer 883.8/7.75	0.05031703	0.902694627	0.369145795	0.851548176	1.051604434
modCer	-0.062128757	-0.66820109	0.505749513	0.851548176	0.939761878

886.8/9.06					
Phospholipid specie	**log Fold Change**	**T statistic**	**P value**	**Adjusted P value**	**Fold change**
modCer 910.8/8.98	0.11960711	0.950591341	0.344408544	0.851548176	1.127053956
modCer 921.8/9.05	0.121563568	1.246068154	0.216037825	0.851548176	1.129261149
PA 17:0/17:0 (IS)	-0.239696102	-1.459107992	0.148185276	0.314008345	0.786866952
PA 32:0	-0.087352391	-0.62337449	0.534691407	0.697326123	0.916354123
PA 32:1	0.031455336	0.224255484	0.823091449	0.878964248	1.031955283
PA 34:1	0.048936257	0.429923128	0.668328956	0.77180983	1.050153409
PA 36:0	-0.21058627	-1.498248985	0.137737255	0.314008345	0.810109164
PA 36:1	-0.172016942	-1.40731134	0.162945965	0.314008345	0.841964909
PA 36:2	-0.178431006	-1.14253329	0.256409328	0.416665158	0.836581774
PA 38:4	0.085985628	0.496706492	0.620665781	0.756436421	1.089790666
PA 38:5	0.225530605	1.386840668	0.169081417	0.314008345	1.252987382
PA-1	0.167551276	1.42010074	0.159200353	0.314008345	1.182405918
PA-3	-0.175550263	-1.39320918	0.167154036	0.314008345	0.838995226
PA-4	-0.096271763	-0.939279681	0.350222823	0.48781036	0.908217163
PA-5	-0.024262066	-0.196217953	0.844903381	0.878964248	0.976029892
PA-6	0.141604906	1.351383092	0.180123698	0.319310191	1.152121363
PA-8	-0.056948578	-0.312902813	0.755113484	0.841412168	0.944642643
PA(24:0)	-0.06430643	-0.559181193	0.577494153	0.726524903	0.93771761
PA(26:1)	-0.16072089	-1.632830007	0.106167956	0.314008345	0.851529709
PA(26:3)	-0.107938208	-0.965112851	0.337199543	0.48781036	0.897683065
PA(27:4)	-0.135604672	-0.951425888	0.344059611	0.48781036	0.87318776
PA(27:5)	-0.239260521	-2.338941928	0.021661829	0.093867926	0.787209771
PC (22:0)	-0.044859061	-0.514869116	0.608031969	0.790441559	0.956132228
PC (22:1)	0.224904868	2.694023935	0.008562807	0.113229086	1.252203586
PC (22:2)	0.114566499	1.358675323	0.177981722	0.448938972	1.12138721
PC (23:0)	0.135959159	1.438999883	0.153963412	0.432412249	1.145635104
PC (23:1)	0.187250186	1.953910111	0.054127035	0.290567927	1.205928954
PC (23:2)	0.068337902	0.824133499	0.412258557	0.651137347	1.070727049
PC (24:0)	-0.225964385	-1.240055048	0.218497941	0.48498819	0.797746513
PC (24:1)	-0.155548605	-1.105243277	0.272292111	0.535085661	0.855945472
PC (24:2)	-0.022416982	-0.226920756	0.821051099	0.895210553	0.977832412
PC (25:1)	-0.060329751	-0.907995579	0.366545955	0.609893606	0.941454037
PC (25:2)	-0.025981248	-0.236145378	0.813909726	0.895210553	0.974353361
PC (26:0)	-0.218476298	-1.653550126	0.102049144	0.331659719	0.80374253
PC (27:0)	-0.057636982	-0.746376997	0.457577929	0.692235841	0.943992572
PC (27:1)	-0.115596839	-1.292105048	0.199956641	0.481221765	0.8908343
PC (27:2)	-0.112379577	-1.164506882	0.247601253	0.520380083	0.893704964
PC (27:3)	-0.187909027	-1.684385877	0.095916583	0.331659719	0.828690093
PC (28:3)	-0.155652623	-1.27755562	0.205017556	0.481221765	0.855856444
PC (28:4)	-0.189826219	-1.555314288	0.123729187	0.387226528	0.827102856
PC (28:5)	-0.218321944	-1.478425342	0.143131675	0.424372861	0.8038666
PC (28:6)	-0.064260601	-0.456359452	0.649340056	0.826451198	0.937760587
PC (31:0)	-0.079182882	-1.010676787	0.315149286	0.591780326	0.923870949
PC (31:1)	0.065378693	1.233361106	0.22097095	0.48498819	1.067563227
PC (31:2)	0.06340294	0.969942544	0.334932364	0.602165633	1.065456068
PC (31:3)	0.159978513	2.240832607	0.027745412	0.23685167	1.173485656
PC (32:0)	-0.009078485	-0.19877776	0.842929472	0.90784957	0.9909626
PC (32:1)	0.104173963	1.585647777	0.11667495	0.372038993	1.109793501
PC (32:2)	0.166949157	2.644347051	0.009808661	0.118404556	1.181694183
PC (32:3)	0.172500973	2.858101301	0.005402996	0.106290101	1.188272977

Phospholipid specie	log Fold Change	T statistic	P value	Adjusted P value	Fold change
PC (33:0)	-0.039752305	-0.805547258	0.422837751	0.661662777	0.961027451
PC (33:1)	0.031521854	0.577780305	0.564998422	0.754463592	1.032023929
PC (33:2)	0.11423255	1.800509247	0.075463645	0.31142819	1.121012786
PC (33:3)	-0.232261866	-1.93264609	0.056738116	0.290567927	0.792738505
PC (33:4)	-0.06084845	-0.558239882	0.578204297	0.757492451	0.940965833
PC (34:0)	0.074545154	1.455421292	0.149377063	0.432412249	1.077393991
PC (34:1)	0.061236287	1.295738585	0.198707361	0.481221765	1.063150093
PC (34:2)	0.038038812	0.72281688	0.471852554	0.693418102	1.038771549
PC (34:3)	0.044854923	0.987236148	0.326436017	0.59964877	1.045876116
PC (34:4)	0.039813206	0.615199503	0.540129516	0.730255106	1.040616375
PC (34:5)	0.11040077	1.106426654	0.271782853	0.535085661	1.11672553
PC (35:0)	0.033072641	0.642062247	0.522626799	0.718080724	1.033625621
PC (35:1)	-0.015580805	-0.341807864	0.733371438	0.840690181	0.984539948
PC (35:2)	0.038884476	0.618677155	0.53784689	0.730255106	1.039650372
PC (35:3)	-0.190892382	-1.802350768	0.07517104	0.31142819	0.826221499
PC (35:4)	0.050549756	0.657368177	0.51278838	0.718080724	1.051849198
PC (35:5)	-0.184317404	-1.976571972	0.05145743	0.290567927	0.831671786
PC (35:6)	0.037197385	0.685857878	0.494740673	0.718080724	1.037897866
PC (36:0)	-0.028717191	-0.737617821	0.462855917	0.692235841	0.971691229
PC (36:1)	-0.013282298	-0.33800369	0.73622572	0.840690181	0.986805522
PC (36:2)	-0.011045652	-0.229678399	0.818914618	0.895210553	0.989015127
PC (36:3)	0.014069109	0.285229678	0.776188621	0.862999191	1.014168544
PC (36:4)	0.041368214	0.437982783	0.662552331	0.829417363	1.042235801
PC (36:5)	0.221273634	1.706058818	0.091788717	0.331659719	1.247664787
PC (36:6)	0.144365818	1.413051006	0.161431902	0.432412249	1.155306663
PC (37:1)	-0.030563476	-0.406272662	0.685602423	0.833477292	0.969898865
PC (37:2)	0.067331973	1.262926672	0.21020113	0.48498819	1.069650514
PC (37:3)	-0.072639044	-0.752188056	0.454095446	0.692235841	0.929936435
PC (37:4)	0.054464262	0.90970441	0.365649215	0.609893606	1.055974737
PC (37:5)	0.082766428	1.186158501	0.238991158	0.511259566	1.086288053
PC (38:0)	-0.036473804	-0.788323523	0.432784512	0.671014518	0.964183351
PC (38:1)	0.0058724	0.112585879	0.910634517	0.946989831	1.005889676
PC (38:2)	0.098100607	1.878514496	0.063870733	0.297066795	1.103073756
PC (38:3)	0.030210984	0.505439655	0.614608329	0.792891661	1.030671966
PC (38:4)	0.040887939	0.84836054	0.39871116	0.647905635	1.041735361
PC (38:5)	0.092604049	1.203984576	0.23206549	0.502808561	1.097027281
PC (38:6)	0.166956987	1.961648917	0.053202447	0.290567927	1.181703436
PC (39:0)	0.084925528	1.254018631	0.213404541	0.48498819	1.088635991
PC (39:1)	-0.223553554	-2.538649527	0.013022257	0.137547586	0.799672065
PC (39:2)	0.107151296	1.405172499	0.163753751	0.432412249	1.11310265
PC (39:3)	0.017243421	0.448700197	0.654833496	0.826451198	1.017392947
PC (39:4)	-0.320515751	-3.511235529	0.000728511	0.040056477	0.725774622
PC (39:5)	0.080275788	1.541930993	0.126947469	0.390074951	1.083585866
PC (40:0)	-0.14913117	-1.937936437	0.056078716	0.290567927	0.861456111
PC (40:1)	-0.078007255	-0.979155926	0.330387924	0.600382357	0.924957716
PC (40:2)	0.007789545	0.109126922	0.913368891	0.946989831	1.007819962
PC (40:3)	-0.069350012	-1.777264632	0.079239125	0.31142819	0.933000062
PC (40:4)	-0.079895114	-1.715412815	0.090052613	0.331659719	0.923213174
PC (40:5)	-0.011365001	-0.156579021	0.875962168	0.92523504	0.988699336
PC (40:6)	0.067793937	0.909088366	0.365972335	0.609893606	1.070144769
PC (41:1)	-0.240653518	-2.841802478	0.00566042	0.106290101	0.786113954
PC (41:2)	-0.26355311	-3.19155542	0.002007676	0.056549552	0.768316816
PC (41:3)	-0.226512774	-2.225846959	0.028773635	0.23685167	0.797309157

Phospholipid specie	log Fold Change	T statistic	P value	Adjusted P value	Fold change
PC (41:4)	-0.093023566	-1.656051589	0.101540091	0.331659719	0.911172027
PC (41:5)	0.108535673	1.433050812	0.155651574	0.432412249	1.11464467
PC (41:6)	0.072126665	1.012033526	0.314504103	0.591780326	1.074791473
PC (42:0)	0.07343104	1.063133131	0.290847816	0.55856001	1.07619432
PC (42:1)	-0.114676326	-1.994144098	0.049465416	0.290567927	0.891654703
PC (42:2)	-0.02892512	-0.291787441	0.771187326	0.862999191	0.971489207
PC (42:3)	0.04840681	0.411968783	0.681439102	0.833477292	1.049597555
PC (42:4)	0.004853703	0.046957567	0.96266142	0.980058915	1.004865501
PC (42:5)	-0.100191469	-2.329487488	0.022297784	0.209351414	0.904664186
PC (43:0)	-0.014018136	-0.161831758	0.871837123	0.92523504	0.98607966
PC (43:4)	-0.290235549	-2.687827372	0.00870993	0.113229086	0.748087335
PC (43:5)	-0.02085941	-0.198191155	0.843386878	0.90784957	0.979356643
PC (43:6)	-0.008804729	-0.079776681	0.936609581	0.965164751	0.991233919
PC(30:0)	0.020096533	0.382046505	0.703416902	0.83505877	1.020299828
PC(30:1)	0.02766163	0.574858291	0.566963765	0.754463592	1.028047765
PC(30:2)	0.03158841	0.653403874	0.515327109	0.718080724	1.032092619
PC(d31)	-0.045578526	-1.158450673	0.250048705	0.520380083	0.955444572
PE (32:0)	0.029191359	0.340295887	0.734483769	0.968669182	1.029621603
PE (34:0)	-0.163172399	-1.20938582	0.229909578	0.952482211	0.849444732
PE (34:1)	-0.05776251	-0.640714801	0.523453172	0.952482211	0.943874082
PE (34:2)	-0.105937028	-1.099682185	0.274614205	0.952482211	0.899481288
PE (34:3)	-0.100263699	-0.912765449	0.363979837	0.952482211	0.904598845
PE (35:0)	0.197557872	1.214568149	0.227936253	0.952482211	1.218423576
PE (35:1)	0.010502118	0.09960091	0.920898638	0.985565687	1.010557459
PE (35:3)	0.066020601	0.459820747	0.646833562	0.952482211	1.068248724
PE (35:4)	-0.049930228	-0.394622345	0.694122415	0.968669182	0.951295796
PE (36:1)	-0.110618012	-1.22941771	0.22234994	0.952482211	0.89528067
PE (36:2)	-0.10251718	-1.015562653	0.312755749	0.952482211	0.902562643
PE (36:3)	-0.054569977	-0.528359554	0.598643838	0.952482211	0.946892246
PE (36:4)	-0.016099664	-0.211705988	0.832849551	0.968669182	0.984029243
PE (36:5)	0.100566595	0.917330036	0.361597661	0.952482211	1.10579728
PE (37:1)	0.040556364	0.471415328	0.638567038	0.952482211	1.041390005
PE (37:2)	0.093815461	1.490980607	0.139714713	0.952482211	1.098357038
PE (37:3)	0.0284962	0.167007034	0.867766142	0.968669182	1.028906101
PE (37:4)	0.004044733	0.042877475	0.965901026	0.985565687	1.004052924
PE (37:5)	0.018518901	0.171219857	0.864462929	0.968669182	1.01869144
PE (37:6)	0.072885538	0.773883591	0.441173577	0.952482211	1.075607413
PE (38:1)	0.118104524	0.927394071	0.356380665	0.952482211	1.125361733
PE (38:2)	0.073482485	1.110049802	0.27014714	0.952482211	1.076249686
PE (38:3)	-0.046645608	-0.765718645	0.445991325	0.952482211	0.954425578
PE (38:4)	-0.023786362	-0.273605894	0.785059544	0.968669182	0.976494304
PE (38:5)	-0.049936985	-0.480951191	0.631802348	0.952482211	0.951289368
PE (38:6)	0.09487435	0.837993449	0.404413977	0.952482211	1.099520692
PE (39:5)	-0.024080784	-0.362633881	0.717789795	0.968669182	0.976206845
PE (39:6)	-0.041065426	-0.471058554	0.638820731	0.952482211	0.959766334
PE (40:4)	-0.193358686	-1.843424848	0.068795778	0.952482211	0.824186297
PE (40:5)	-0.05437921	-0.747634176	0.456770028	0.952482211	0.947072899
PE (40:6)	-0.002754384	-0.027678767	0.977984052	0.985565687	0.997249406
PE (41:3)	-0.150339809	-1.253225343	0.213603019	0.952482211	0.86041555
PE (43:3)	-0.034251568	-0.25532484	0.799096731	0.968669182	0.966328377
PE unknown-1	0.061617522	0.448661951	0.65483152	0.952482211	1.063555481
PE unknown-2	-0.002997745	-0.01814569	0.985565687	0.985565687	0.997006744
PE unknown-3	0.1770884	1.386200525	0.16935659	0.952482211	1.193736615

Phospholipid specie	log Fold Change	T statistic	P value	Adjusted P value	Fold change
PE unknown-4	0.113858546	0.936195427	0.351858005	0.952482211	1.120593602
PE(16:6)	-0.063663519	-0.659110528	0.511628739	0.952482211	0.938320673
PE(21:5)	0.052533601	0.56096412	0.576316285	0.952482211	1.053937975
PE(21:6)	0.126886882	0.78434978	0.435042581	0.952482211	1.135288589
PE(38:0)	-0.042535836	-0.459237174	0.647250815	0.952482211	0.958356122
PG (26:0)/diether PG14:0	-0.025446117	-0.185175707	0.853401244	0.858328327	0.974874907
PG(28:0)	-0.342825937	-2.04418565	0.043105232	0.409499708	0.709761744
PG(30:0)	-0.052680349	-0.390491317	0.696859867	0.830141833	0.948683212
PG(30:1)	-0.047149122	-0.328954826	0.742758482	0.830141833	0.953945133
PG(31:0)	-0.115860828	-0.785728908	0.433562182	0.830141833	0.890599161
PG(32:0)	-0.219183886	-1.610402556	0.109915621	0.696132267	0.803174012
PG(32:1)	0.082019302	0.54281938	0.588252604	0.830141833	1.085476761
PG(34:0)	-0.047863359	-0.350468331	0.726596605	0.830141833	0.953264033
PG(34:1)	-0.062941473	-0.36301404	0.717227745	0.830141833	0.938998429
PG(34:2)	-0.100634956	-0.643962942	0.520818188	0.830141833	0.904263068
PG(36:0)	0.316245623	2.319472569	0.02204589	0.409499708	1.371967201
PG(36:1)	-0.084269746	-0.621712326	0.535300628	0.830141833	0.919183277
PG(36:2)	0.101631387	0.71045605	0.478788417	0.830141833	1.106975351
PG(36:3)	0.025819391	0.178883524	0.858328327	0.858328327	1.026155599
PI (16:0)	-0.084996982	-0.461773469	0.645299042	0.920733433	0.918515057
PI (32:0)	-0.501260329	-2.935829642	0.004171955	0.095954968	0.605766713
PI (34:1)	-0.070281727	-0.377834708	0.706395926	0.920733433	0.932131177
PI (34:2)	-0.307214034	-1.157119407	0.250123617	0.743943637	0.735493164
PI (36:0)	0.090642935	0.358755171	0.720573991	0.920733433	1.094877993
PI (36:1)	-0.023322418	-0.126975766	0.899227843	0.951178048	0.976947448
PI (36:2)/IS	0.230511658	1.405926646	0.163006909	0.743943637	1.259244147
PI (36:3)	0.080380259	0.45815366	0.647887912	0.920733433	1.083699076
PI (36:4)	0.148201352	0.715349535	0.476146831	0.920733433	1.15974639
PI (38:1)	-0.318192811	-1.861215182	0.065804854	0.504503882	0.727462512
PI (38:3)	0.159849151	0.593225112	0.554439642	0.920733433	1.173333862
PI (38:4)	0.268800116	1.1361203	0.258763004	0.743943637	1.308393587
PI (38:5)	0.209577856	1.254894058	0.212594345	0.743943637	1.23315738
PI 16:0/16:0 (IS)	-0.370960815	-1.997199546	0.048663044	0.504503882	0.690070982
PI 30:0	0.011073549	0.061389353	0.951178048	0.951178048	1.011135088
PI 30:1	-0.220439417	-1.270759131	0.206916142	0.743943637	0.802166235
PI 32:1	0.017255595	0.09891665	0.921412788	0.951178048	1.017405332
PI 40:3	-0.151451307	-0.612118759	0.541920902	0.920733433	0.859459731
PI 40:4	-0.024047145	-0.131308439	0.895808883	0.951178048	0.976239683
PI 40:5	0.083759067	0.395848875	0.69310377	0.920733433	1.08736688
PI 40:6	0.194051951	1.060852023	0.291445663	0.744805584	1.214159359
PI_Cer_2	-0.045154419	-0.196484887	0.844650209	0.951178048	0.95584987
PI(34:2)	-0.111072195	-0.590053897	0.556554859	0.920733433	0.894874141
PS (32:1)	-0.063662879	-0.353517616	0.724588249	0.772894132	0.938321274
PS (32:2)	0.276826531	2.463245955	0.015814951	0.046223865	1.318937556
PS (34:0)/IS	0.648784331	3.826880408	0.000249215	0.001993718	1.913213581
PS (34:1)	0.137262109	1.062837833	0.290908754	0.423140006	1.147128782
PS (34:2)	0.27125136	2.110277246	0.037816087	0.075632173	1.311604714
PS 36:0	0.477751115	2.604754564	0.010875734	0.046223865	1.61244412
PS 36:1	-0.536612437	-2.247691899	0.027222475	0.0622228	0.584725696
PS 36:2	-0.12445538	-0.727023741	0.469237575	0.536271514	0.882977659
PS 38:1	0.245966344	2.016152301	0.046987372	0.083533107	1.278856531

Phospholipid specie	log Fold Change	T statistic	P value	Adjusted P value	Fold change
PS 38:2	0.090853428	0.772129189	0.442210032	0.536271514	1.095108481
PS 38:3	-0.411263037	-2.42775047	0.017333949	0.046223865	0.662812565
PS 38:4	-0.667547883	-3.849830076	0.000230195	0.001993718	0.512964887
PS 38:5	-0.028465011	-0.240123372	0.810821038	0.810821038	0.971936301
PS 40:4	-0.134696321	-0.993245424	0.323449743	0.431266324	0.873981281
PS 40:5	-0.493161689	-1.563062116	0.121806724	0.194890758	0.610692519
PS 40:6	0.311169418	2.44278734	0.016675231	0.046223865	1.36502046
SM (30:0)	-0.116379854	-1.613564121	0.110569194	0.298539592	0.890137037
SM (30:1)	-0.112470765	-0.620340751	0.536800808	0.585600882	0.893623472
SM (30:2)	-0.231663816	-2.159075948	0.033847476	0.203084858	0.793212744
SM (32:0)	0.044867774	1.025177607	0.308376602	0.411168803	1.045889557
SM (32:1)	-0.07525408	-0.836900626	0.405147368	0.486176842	0.927507795
SM (33:0)	0.052809745	1.220827853	0.225745666	0.350102855	1.054229054
SM (33:1)	0.052079081	1.200744568	0.233401904	0.350102855	1.053459048
SM (34:0)	0.055485633	1.456164774	0.149269796	0.298539592	1.05705383
SM (34:0) (2)	0.057227695	1.513454697	0.134114315	0.298539592	1.058896888
SM (34:1)/IS	0.056578867	1.585766128	0.11674679	0.298539592	1.058210069
SM (34:2)	0.200254625	3.365428571	0.001177186	0.014126235	1.221713797
SM(d31)/IS	0.016465096	0.273635186	0.785071887	0.785071887	1.016601393

8.4.4. Principle component analysis for serum samples including pooled biological quality controls

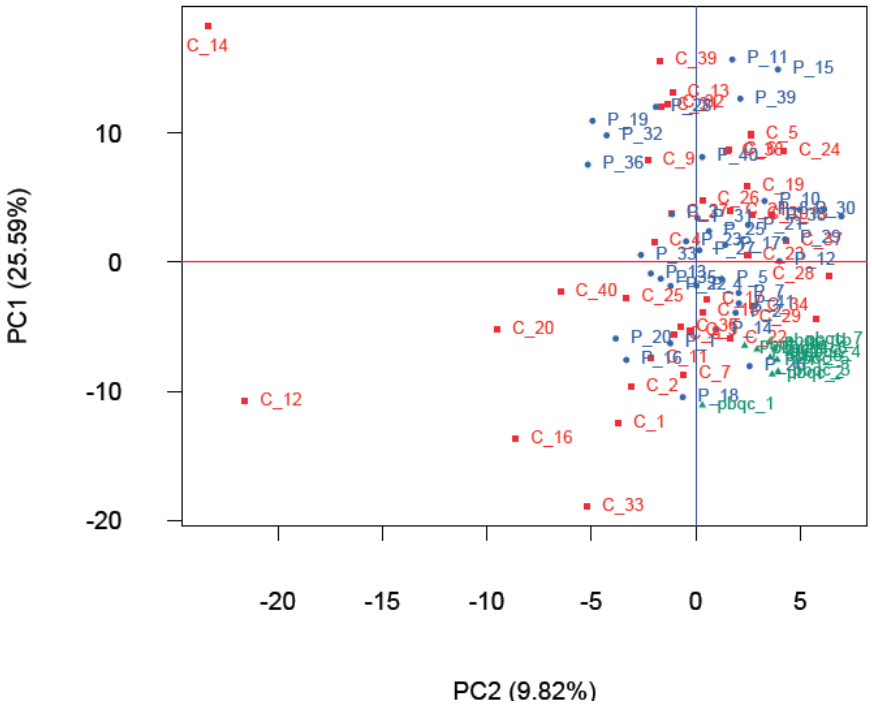


Figure 8.14: PCA with the PBQC's, which are clustering (in green), compared to the controls samples in red and the patient's samples in blue. This indicates that the data is robust.

8.5. From Chapter 4 and 5

8.5.1. Clinical data

Table 8.140: Clinical data for the 40 healthy control individuals who participated in the studies, which extracted lipid from, scalp hair and serum.

Expt Assigned name	DOB	Reason for examination	Other comment	Risk level	Previous history	Family history of cancer	Family history of breast cancer	Hair length
C1	29/11/28	Family History		Potentially high	No	Yes	Yes	n/a
C2	1/07/51	Family History		Average	No	Yes	Yes	n/a
C3	6/08/76	Lumpy	cysts	Mod increased	n/a	Yes	Yes (mother @ 42 bilateral, died @ 52 metastatic)	n/a
C4	25/09/44	8mm lump	fat lobule	Average & Mod increased	History of cysts	Yes	No	n/a
C5	10/06/50	nil		n/a	No	No	No	n/a
C6	18/01/75	15mm Lump	Benign Fibroadenoma	n/a	lump & discomfort for 9 months, unchanged for 10yrs	n/a	n/a	n/a
C7	24/07/72	20mm lump similar to past cysts.	Benign Fibrocystic change	n/a	No	n/a	n/a	n/a
C8	28/12/69	Lumpy	dense glandular tissue	Average	n/a	Yes	Yes	n/a
C9	31/05/65	nil		n/a	No	n/a	n/a	n/a
C10	24/03/50	Family History		Mod increased	No	Yes	Yes	n/a
C11	11/05/53	nil		n/a	No	No	No	n/a
C12	2/10/69	Family History		Mod increased	n/a	Yes	Yes	n/a
C13	1/06/57	Family History		Average	No	Yes	Yes	n/a
C14	27/09/55	Family History		Mod increased	No	Yes	Yes	n/a
C15	30/09/58	Family History (implants)		Average	No	Yes	Yes	n/a
C16	31/05/73	Lumpy (painful)	Due to mirena (drug)	Average	n/a	Yes	Yes	n/a
C17	1/07/44	Family History		Average	No	Yes	Yes	n/a
C18	13/03/56	Family History		Mod increased	n/a	Yes	Yes	n/a
C19	16/12/70	30mm thickening/lump	cyst	Average & Mod increased	No	Yes	Yes	n/a
C20	11/05/43	Previous History		n/a	1990 malignancy - conserving surgery	n/a	n/a	n/a
C21	8/07/38	Previous History		Mod increased	1996 malignancy, surgery, clearance, adjuvant Chem - Radi - Hormonal	Yes	Yes	Short
C22	31/05/47	Previous History, tenderness		n/a	1997 wide local excision, clearance (invasive breast cancer), adjuvant Chem - Radi, ceased Hormonal (side effect)	n/a	n/a	Long

C23	9/10/65			n/a	No	No	No	Short
C24	5/08/44	Previous History, tenderness		Mod increased	1999 malignancy; 2009 left 9th rib fracture	Yes	Yes (2 nieces)	Short
C25	16/12/63	Previous History, tenderness		0	2009 upper outer quadrant pain	No	No	Long
C26	9/12/63	Family History	Minor cystic changes	Mod increased & Potentially high	n/a	Yes	Yes	Long
C27	8/07/57	nil		n/a	No	No	No	Long
C28	24/04/47	Previous History		Average	2005 (R) microdochectomy (benign breast disease, remove duct?)	Yes	Yes	Long
C29	17/07/32	tender lumpy	multiple cysts	n/a	2006 malignancy; 2011 tender lumpy area	n/a	n/a	Short
C30	22/08/74	soft lump	fat lobule	Mod increased	No	Yes	Yes	Long
C31	20/02/51	Family History		n/a	n/a	Yes	Yes (sister @ 49, maternal grandmother, maternal aunt & paternal aunt)	Short
C32	28/04/60	Lumpy (painful)	Cyst	n/a	2011 March - upper outer quadrant pain	n/a	n/a	Long
C33	6/09/59	Lumpy (painful)	ternder cyst	n/a	2010 Nov fibrocystic changes with a tense cyst	n/a	n/a	Long
C34	20/01/53	Family History		Average	n/a	Yes	Yes	Long
C35	4/11/55	nil		n/a	n/a	n/a	n/a	Long
C36	15/05/74	Previous History	lump (indeterminate)	Average	2011 March lump	Yes	Yes	Long
C37	30/12/67	nil	Annual surveillance	n/a	No	No	No	Short
C38	18/02/44	nil		n/a	n/a	n/a	n/a	Short
C39	5/07/36	nil	Extremely lumpy	n/a	n/a	n/a	n/a	Short
C40	20/09/75	Family History		Mod increased	n/a	Yes	Yes (mother @ 40)	Long

Table 8.141: Clinical data, for the 40 individuals with breast cancer, who participated in the studies, which extracted lipid from, scalp hair and serum.

Expt Assigned name	Type of breast cancer	Grade	Size	Clinical (mammo, US, biopsy)	Exam reason	Previous history	Family history of Breast Cancer	Family history of other cancers	Age at Exm/Opr	DOB	Hair length
P0	Invasive ductal	n/a	n/a	Lumpy, suggestive of inflammatory carcinoma, small scattered cysts	skin nodules, fungal growth, increasing mass	n/a	No	No	52	8/02/59	
P1	n/a	n/a	7x7x6mm	Thickening, suspicious appearance, 7x7x6mm	Thickening	n/a	No	No	82	10/12/28	
P2	Invasive ductal	n/a	4mm	Normal adjacent tissue, 4mm, Biopsy malignant		n/a	No	No	55	24/11/56	
P3	Invasive ductal	3	30mm, 15mm	15mm, Indeterminate, 30mm, Malignant	Thickening	n/a	No	No	40	13/10/71	
P4	Invasive ductal	2	n/a	Fibroadipose breast tissue, poor tubule formation, numerous intraluminal calcifications	Cores	n/a	n/a	n/a	64	17/08/47	
P5	Malignant	n/a	n/a	dense fibroglandular tissue, cluster of indeterminate microcalcification, 10x9x7mm solid lump, malignancy	Lump	n/a	n/a	n/a	64	6/05/47	
P6	DCIS	n/a	n/a	Biopsy Intraductal carcinoma	Lump	n/a	n/a	n/a	69	19/11/41	
P7	Invasive ductal	2	7mm	malignant cells, microcalcification in lump, discrete mass, 7mm suspicious lump	Lump	n/a	No	No	60	26/04/51	
P8	Malignant	n/a	18x13x17 mm	dense fibroglandular tissue, solid hypoechoic lump, 18x13x17mm palpable lump	Lump	2009 Cysts, scattered benign calcifications	n/a	n/a	49	14/06/62	
P9	Invasive ductal with tubular features	1	9x5mm	Simple breast cysts, fibroglandular tissue with interspersed fat, 9x5mm lump	Lump	n/a	Yes	n/a	66	1/02/45	
P10	Invasive ductal	n/a	n/a	Biopsy invasive duct carcinoma	Cores (4)	n/a	n/a	n/a	60	20/01/51	
P11	Invasive ductal (not otherwise specified)	3		suspicious microcacification l& small spiculated mass, 2 main cores contain invasive ductal NOS, poor tubule formation, with patchy necrosis	Cores (3)	n/a	n/a	n/a	60	13/06/51	
P12	Invasive ductal	1		Invasive duct carcinoma, mucinous stroma	Lump, Cores (2)	n/a	n/a	n/a	90	3/01/21	
P13	Invasive ductal	1	7-11mm	7-11mm, Invasive duct carcinoma	Lump, Cores (3)	n/a	n/a	n/a	72	29/07/38	
P14	Invasive duct	n/a	6mm, 5mm	Stellate solid lump, 6mm & 5mm, Invasive duct carcinoma, focal microcalcification.	Cores (2)	n/a	n/a	n/a	52	8/09/59	

P15	Malignant	n/a	n/a	Lump,□simple□breast□cysts,□malignant□lump	Lump	n/a	Yes	n/a	43	21/03/68	
P16	Invasive□ductal	1	1.5mm	□1.5mm,□infiltrated□by□invasive□ductal□carcinoma□	Cores□(3)	n/a	n/a	n/a	52	6/11/59	
P17	Invasive□ductal□(not□otherwise□specified)□and□DCIS	3	20mm,□22mm,□8mm	□20mm,□22mm,□8mm,□hormone□receptor□+ve,□high□grade,□Metastatic□carcinoma□in□5/26□lymph□nodes,□minor□DCIS	Mastectomy,□sentinel□node□biopsy,□Tissue□expander□reconstruction	2010□□Cyst□removed	Yes,□Mother□@□78,□Maternal□grandmother□@□early□40s□&□died□early□50s	Yes,□Father□died□@42□□Stomach/Esophagus,□2□nuts□&□1□uncle□□Thyroid□cancer	56	10/08/55	
P18	Invasive□ductal	2	23mm	n/a	wide□local□excision,□□sentinel□node□biopsy□	dense□fibroglandular□tissue,□15mm□small□□nodule	No	Yes,□Father□□Prostate	58	26/01/54	
P19	Invasive□ductal□and□DCIS	2	15mm,□10mm	15mm,□>10mm□DCIS	back□wall□echo,□□sentinel□node□biopsy□	Nil	Yes,□Paternal□aunt□@□70□□Lumpectomy□lived□till□90s	No	71	1/01/40	long
P20	n/a	2	□1.2x1x0.8cm	□1.2x1x0.8cm,□solid□lump□	back□wall□echo,□□sentinel□node□biopsy□	n/a	No	No	46	23/04/65	long
P21	Invasive□ductal	2	9mm	9mm	Lumps	n/a	Yes,□Mother□@□57,□died□of□intraabominal□malignancy□@□64;□sister□@□54,□died□@□57	No	57	3/10/54	long
P22	Mucinous□breast□cancer	n/a	19mm,□12mm	19mm□&□12mm	mucinous□breast□cancer□condition	2010□□Pancreatic□cyst	Yes,□Niece□@□40's;□maternal□niece□@□40's	Yes,□Sister□@□48□□Uterus	87	23/10/24	long

P23	Invasive ductal	2	8mm	Solid, likely malignant, Stellate lesion, 8mm	back wall echo, Sentinel node biopsy	n/a	Yes, Maternal grandmother @ 60 bilateral synchronous cancer; maternal aunt @ 60 Unilateral breast cancer	Yes, Mother Pancreatic, Lung	65	13/08/46	long
P24	Invasive ductal and DCIS	1	15mm, 24mm	15mm, 24mm high grade DCIS	back wall echo, Sentinel node biopsy	Nil	No	Yes, half-brother @ 13 died from Ewings Sarcoma	50	10/10/61	long
P25	Invasive ductal, (not otherwise specified)	2	14mm	Discrete mass, Solid, likely malignant, 14mm, Suspicious lump, biopsy malignant invasive	back wall echo, Sentinel node biopsy	n/a	n/a	n/a	48	17/03/63	long
P26	Invasive	2	13mm, 10mm, 7mm length & 1mm diameter each, 10.5mm	13mm, 10mm, 7mm length & 1mm diameter each, 10.5mm	back wall echo, Sentinel node biopsy	n/a	Yes, Cousin @ 30 bilateral breast malignancy	Yes, Father Lung (smoker), (mother ovarian @ 67, also @ 65 Lung)	47	11/05/64	long
P27	Invasive & Lobular	2	16mm	16mm	back wall echo, Sentinel node biopsy	2002 Left DCIS + breast-conserving surgery & radiotherapy;	No	Yes, Mother Brain tumour	72	22/06/39	short
P28	Invasive ductal and DCIS	3	28x22x17 mm	28x22x17mm, DCIS	back wall echo, Sentinel node biopsy	Hysterectomy + one ovary removed	Yes, Mother @ 81; niece	No	73	22/05/38	short
P29	Invasive ductal	3	100mm, 45mm	Lump, multifocal with axillary metastases	Mastectomy + Axillary Lymphnode Dissextion	n/a	No	No	75	16/03/36	long

P30	Invasive Apocrine and DCIS	2	10mm	no significant abnormality, Discrete mass, Solid, likely malignant, 8mm, Focal apocrine DCIS	back wall echo, Sentinel node biopsy, Mastectomy	n/a	No	Yes, Mother Skin cancer, DVT, died @ 84 renal failure; Father @ 70's Skin, died oesophagial stricture, NIDDM, CCF (post op)	69	24/04/42	short
P31	Invasive ductal (not otherwise specified)	3	11mm & 14mm	Malignant lump, 11mm & 14mm (cores of fibrofatty tissue), DCIS	back wall echo, Sentinel node biopsy	2011 Nov noticed lump; 1997 Cervical Intraepithelial Neoplasia 3	No	No	49	8/11/62	long
P32	Invasive Tubular, Ductal and DCIS	2	3.8mm	38mm DICS, Indetermination calcifications, MRI shows indetermination lump (benign)	back wall echo, Sentinel node biopsy, DCIS	2011 new calcification - no further intervention, Invasion carcinoma = DCIS >38mm Grade 1, clear lymph glands	No	Yes, Brother @ 47 Prostate; Aunt Pancreatic	65	10/01/46	short

P33	Ductal (not specific type)	2	58mm	1 lymph node contained disease with extra nodal spread,	back wall echo, sentinel node biopsy, mastectomy, tissue expander	drain seroma fluid around implant until Chemo start, 2010 Feb Marinua Removed	No	Yes, Mother @69 Rip Lung	52	3/11/59	short
P35	Invasive ductal with DCIS	2	19mm	dense	back wall echo, sentinel node biopsy	1985 benign lump removed	Yes, Mother's sister @ old age	No	64	18/12/47	long
P36	Extensive DCIS	3	1-3.5mm, 75mm	dense fibroglandular tissue, multiple cysts, DCIS 75mm, isolated tumour cells in one lymph node	back wall echo, sentinel node biopsy, mastectomy	n/a	No	No	46	9/11/65	n/a
P37	Invasive ductal (not otherwise specified) with papillary subtype	2	9mm	Lump, Discrete mass, Malignant lump, 9mm	Lump	1992 Mastectomy	Yes, Maternal grandmother @ 86, Mother, Daughter #1 @ 39, Daughter #3 @ 44 & Maternal aunt	Yes, Brother Prostate, mother ovarian	80	9/10/31	short
P38	Invasive ductal	n/a	11-13mm & 13-18mm	no solid lump, 3mm cyst, 2 cysts, 8mm & 3mm, 11-13mm & 13-18 lump, benign, abnormal lymph node	Lump	1994 Melanoma, 43mm	No	Yes, Father Melanoma & Pancreatic	57	23/10/54	n/a
P39	Invasive ductal (not otherwise specified) and DCIS	3	27mm, 8mm, 110mm	27mm lump, 8mm infractlavicular, 110mm DCIS, pagets disease, 16 nodes with metastatic breast cancer	Mastectomy, Tissue expander reconstruction	n/a	No	Yes, Uncle Lung; Grandmother Bowel	52	30/03/60	long
P40	Intracystic papillary & ductal, (not otherwise specified)	3	30x17mm	highly proliferative papillary lump, tumoure incompletely excised, palpable undersacrs of breast reduction, solid & cystic mass 30x17mm	wide local excision, sentinel node biopsy	1990 breast reduction	No	Yes, Maternal Uncle Stomach	60	18/10/51	short
P41	High graded DCIS	3 (DCIS)	40mm	pleomorphioc calcification, indeterminate lesion, unremarkable, high graded DCIS	Mastectomy, sentinel node biopsy	n/a	No	No	63	14/01/49	n/a

8.6. From all chapters

8.6.1. LCMS technical data (ion scans and chromatograms of standards)

Table 8.142: Electrospray ionisation mode and ion scans for LCMS used in this study

Lipid		ESI Mode	Ion scan
Phospholipids	Phosphatidylcholine (PC)	Positive	184 Precursor scan mode
	Phosphatidylethanolamines (PE)	Positive	141 Neutral loss scan mode
	Phosphatidylserines (PS)	Negative	87 Neutral loss scan mode
	Phosphatidylinositols (PI)	Negative	241 Precursor scan mode
	Phosphatidic acid (PA)	Negative	153 Precursor scan mode
	Phosphatidylglycerol (PG)	Positive	189 Neutral loss scan mode
	Lysophosphatidylcholine (LPC)	Positive	184 Precursor scan mode
Sphingolipids	Ceramide (Cer)	Positive	264 Precursor scan mode
	Sphingomyelin (SM)	Positive	184 Precursor scan mode
Sterol Lipids	Cholesterol Ester (CE)	Positive	369 Precursor scan mode

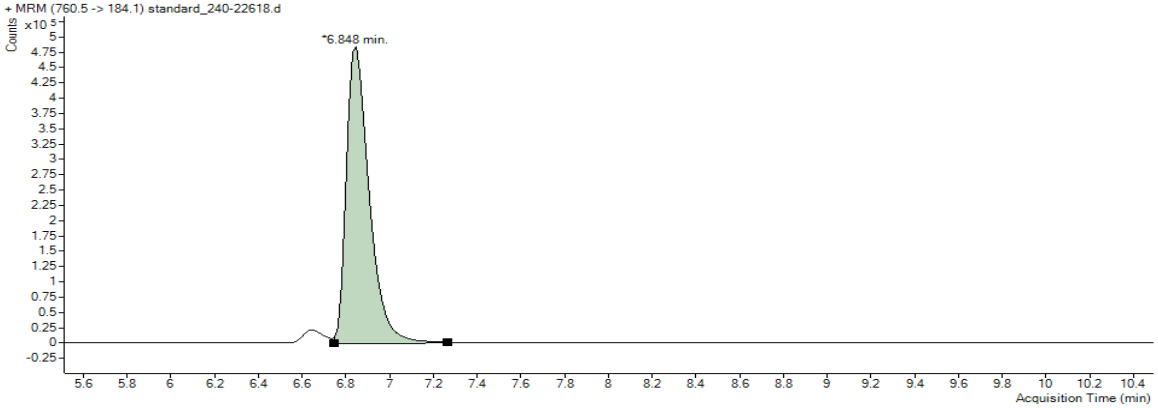


Figure 8.15: Chromatogram of PC(34:1) standard (MRM 760.5 > 184.1 , RT = 6.84 min)

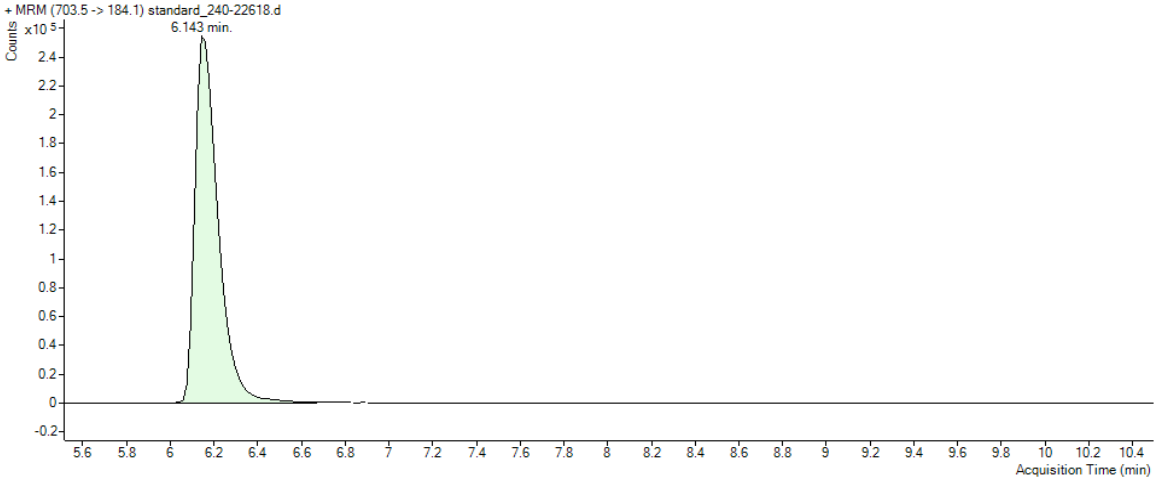


Figure 8.16: Chromatogram of SM(34:1) standard (MRM 703.5 > 184.1 , RT = 6.14 min)

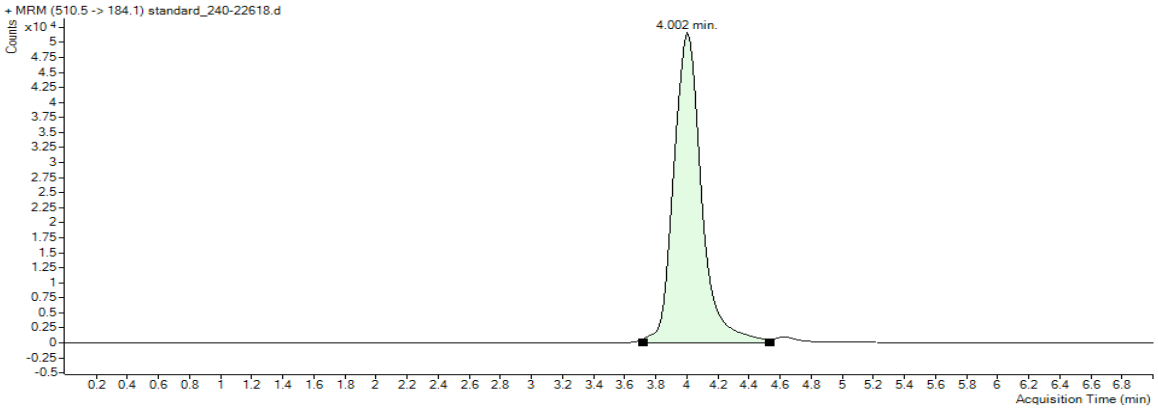


Figure 8.17: Chromatogram of LPC(17:0) standard (MRM 510.5 > 184.1 , RT = 4.00 min)

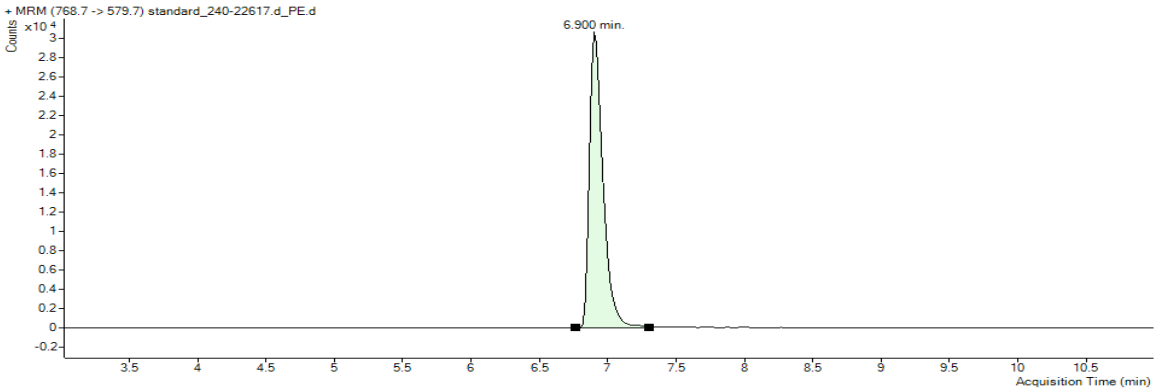


Figure 8.18: Chromatogram of PG(34:0) standard (MRM 768.7 > 579.6 , RT = 6.9 min)

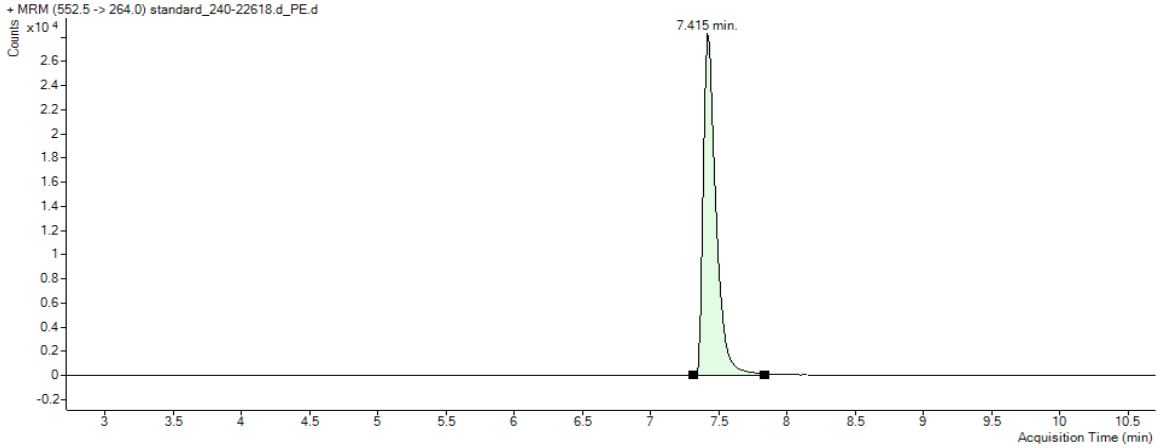


Figure 8.19: Chromatogram of Cer(d18:1\17:0) standard (MRM 552.5 > 264 , RT = 7.4 min)

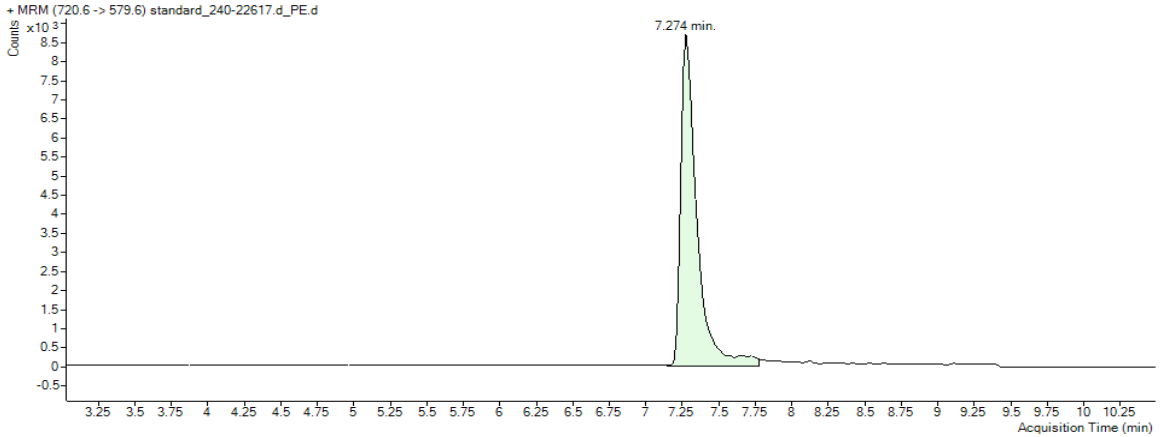


Figure 8.20: Chromatogram of PE(34:0) standard (MRM 720.5 > 579.6 , RT = 7.27 min)

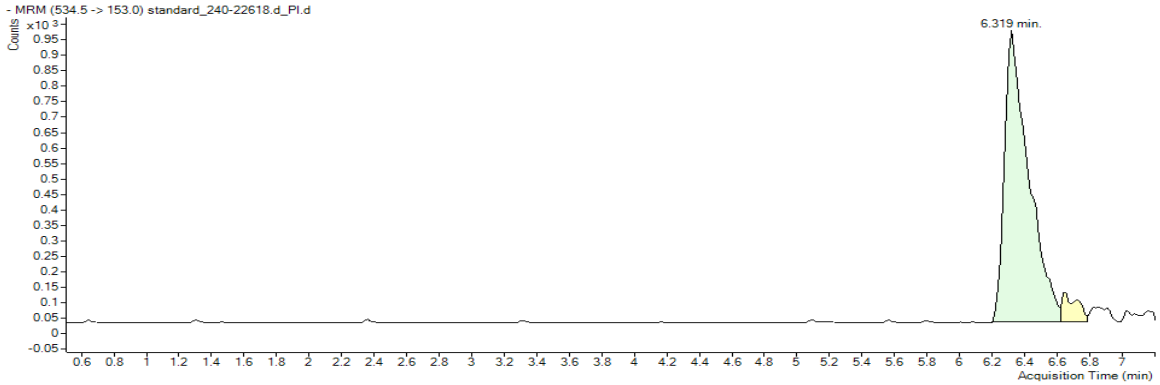


Figure 8.21: Chromatogram of PA(24:0) standard (MRM 534.5 > 153 , RT = 6.3 min)

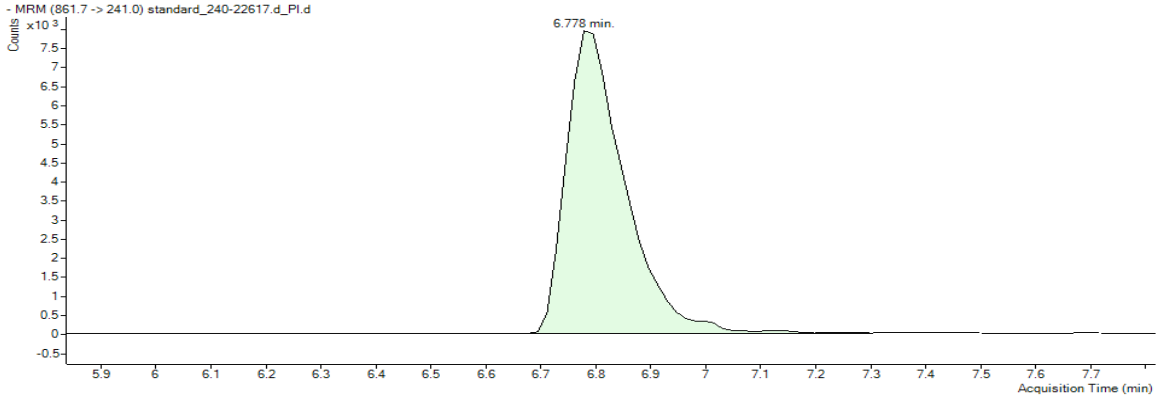


Figure 8.22: Chromatogram of PI(36:2) standard (MRM 861.7 > 241 , RT = 6.77 min)

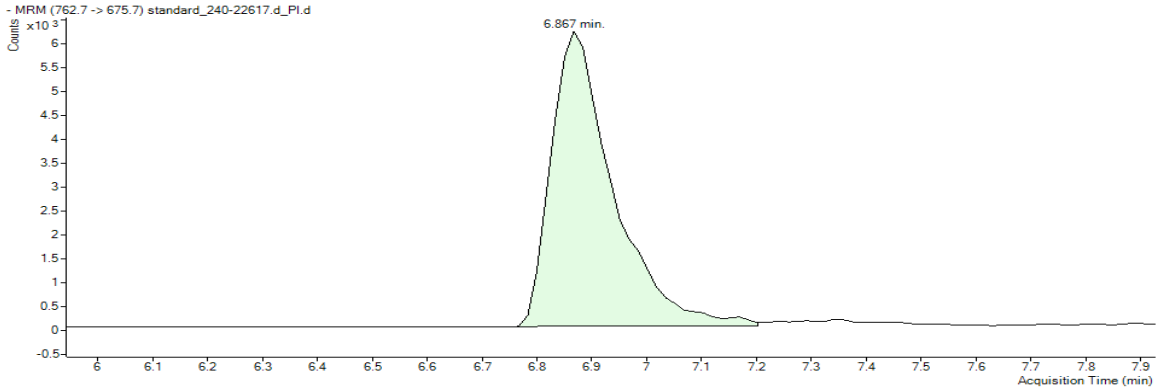


Figure 8.23: Chromatogram of PS(34:0) standard (MRM 762.7 > 675.7 , RT = 6.87 min)

8.7. Ethics approval letter

Subject: Fwd: Final Approval- Ethics application reference-5201100091
Date: Monday, 9 May 2011 11:29 AM
From: DHARMICA MISTRY <dharmica.mistry@students.mq.edu.au>
To: <dmistry@sbcresearch.com.au>

---------- Forwarded message ----------
From: Ethics Secretariat <ethics.secretariat@mq.edu.au>
Date: Mon, May 2, 2011 at 10:20 AM
Subject: Final Approval- Ethics application reference-5201100091
To: Prof Mark Connor <mark.connor@mq.edu.au>
Cc: Miss Dharmica April Mistry <dharmica.mistry@students.mq.edu.au>

Dear Prof Connor

Re: "The identification and characterization of breast cancer-associated lipid (s) in hair and blood and their use in the development of a diagnostic test for breast cancer" (Ethics Ref: 5201100091)

Thank you for your recent correspondence. Your response has addressed the issues raised by the Human Research Ethics Committee and you may now commence your research.

The following personnel are authorised to conduct this research:

Prof Mark Connor- Chief Investigator/Supervisor
Ms Dharmica Mistry- Co-Investigator

NB. STUDENTS: IT IS YOUR RESPONSIBILITY TO KEEP A COPY OF THIS APPROVAL EMAIL TO SUBMIT WITH YOUR THESIS.

Please note the following standard requirements of approval:

1. The approval of this project is conditional upon your continuing compliance with the National Statement on Ethical Conduct in Human Research (2007).

2. Approval will be for a period of five (5) years subject to the provision of annual reports. Your first progress report is due on 02 May 2012.

If you complete the work earlier than you had planned you must submit a Final Report as soon as the work is completed. If the project has been discontinued or not commenced for any reason, you are also required to submit a Final Report for the project.

Progress reports and Final Reports are available at the following website:

http://www.research.mq.edu.au/for/researchers/how_to_obtain_ethics_approval/human_research_ethics/forms <http://www.research.mq.edu.au/for/researchers/how_to_obtain_ethics_approval/%0Ahuman_research_ethics/forms>

3. If the project has run for more than five (5) years you cannot renew approval for the project. You will need to complete and submit a Final Report and submit a new application for the project. (The five year limit on renewal of approvals allows the Committee to fully re-review research in an environment where legislation, guidelines and requirements are continually changing, for example, new child protection and privacy laws).

4. All amendments to the project must be reviewed and approved by the Committee before implementation. Please complete and submit a Request for Amendment Form available at the following website:

http://www.research.mq.edu.au/for/researchers/how_to_obtain_ethics_approval/human_research_ethics/forms <http://www.research.mq.edu.au/for/researchers/how_to_obtain_ethics_approval/%0Ahuman_research_ethics/forms>

5. Please notify the Committee immediately in the event of any adverse effects on participants or of any unforeseen events that affect the continued ethical acceptability of the project.

6. At all times you are responsible for the ethical conduct of your research in accordance with the guidelines established by the University. This information is available at the following websites:

http://www.mq.edu.au/policy/

http://www.research.mq.edu.au/for/researchers/how_to_obtain_ethics_approval/human_research_ethics/policy <http://www.research.mq.edu.au/for/researchers/how_to_obtain_ethics_approval/%0Ahuman_research_ethics/policy>

If you will be applying for or have applied for internal or external funding for the above project it is your responsibility to provide the Macquarie University's Research Grants Management Assistant with a copy of this email as soon as possible. Internal and External funding agencies will not be informed that you have final approval for your project and funds will not be released until the Research Grants Management Assistant has received a copy of this email.

If you need to provide a hard copy letter of Final Approval to an external organisation as evidence that you have Final Approval, please do not hesitate to contact the Ethics Secretariat at the address below.

Please retain a copy of this email as this is your official notification of final ethics approval.

Yours sincerely
Dr Karolyn White
Director of Research Ethics
Chair, Human Research Ethics Committee