Age and sex dependent changes of free circulating blood metabolite and lipid abundances, correlations and ratios

Supplementary Tables

Molecular features	Compound CHEBI codes
Choline	15354
Creatinine	16737
e-Caprolactam	28579
DL-2-Aminooctanoic acid	75145
Γ-Caprolactone	85235
L-Proline	17203
Betaine	17750
Salicylic acid	16914|15365
Theobromine	28946
Creatine	16919
L-Leucine	15603|18347
Hypoxanthine	17368
3-Pyridylacetic acid|trigonelline	86390|18123
Stachydrine	35280
Benzenebutanoic acid	41500
Indole-3-carbinol	24814

Acetaminophen	46195
2-Ketohexanoic acid	17308
S-(4,5-Dihydro-2-methyl-3-furanyl) ethanethioate	131456
L-Carnitine	16347
L-Phenylalanine	17295
Uric acid	17775
Indoleacetic acid	16411
Paraxanthine|Theophylline	25858|28177
L-Tyrosine|o-Tyrosine	17895|89461
Naproxen	7476
L-Tryptophan	16828
3-Indolepropionic acid	43580
1,3,7-Trimethyluric acid	691622
Caffeine	27732
Hippuric acid	18089
L-Acetylcarnitine	57589
Indolelactic acid	24813
Pantothenic acid	7916
Flavone	42491

Butyryl-L-carnitine|Isobutyryl-L-carnitine	21949|84838
Geranyl acetoacetate	85255
Dodecanedioic acid	4676
5a-Androst-3-en-17-one	86393
Propranolol	8499
γ-Glutamyl-leucine	68433
Myristic acid	28875
A-Linolenic acid	27432
L-Aspartyl-L-phenylalanine	73830
Pentadecanoic acid	42504
D-erythro-sphingosine	46964
Oleamide	116314
Piperine	28821
L-Octanoylcarnitine	18102
Palmitoleic acid	28716
2,6 dimethylheptanoyl carnitine	84095
4-Androsten-11Beta-ol-3,17-dione	27967|27967
Arachidonic acid	15843
Heptadecanoic aicd	32365

Phenylalanylphenylalanine	72723
Decanoyl-L-carnitine	28717
Fatty acid C20:5 methyl ester	91031
Linoleic acid	17351
Arachidonic acid methyl ester	78033
MAG(14:0)	87249
10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	86285|86329
Fatty acid C22:6	36005
4,8 dimethylnonanoyl carnitine	63874
Arachidonic acid ethyl ester	84873
MAG(18:0)	87255
C12 Carnitine	73054
Corticosterone	16827
MAG(16:1)	87253
MAG(16:0)	87251
MAG(18:3)	87258
Treprostinil	50861
Prostaglandin J2	27485
Hyodeoxycholic acid	52023

Deoxycholic acid	28834
Cortisol	17650
6-hydroxy-5-cholestanol|cholesterol	|16113
cis-5-Tetradecenoylcarnitine	73060
Cholic acid	16359
MAG(18:2)	87257
MAG(18:1)	87256
Stearic acid	28842
MAG(20:5)	86397
C16 Carnitine	73067
7-Ketocholesterol	64294
17-phenyl trinor Prostaglandin E2|17-phenyl trinor Prostaglandin D2	87820|87821
sodium glycochenodeoxycholate	87818
Deoxycholic acid glycine conjugate	27471
Chenodeoxycholic acid	16755
Linoleyl carnitine	73072
Oleoyl-L-carnitine hydrochloride	91318
A-Tocopherol	22470
3a,6b,7b-Trihydroxy-5b-cholanoic acid	81298

Barogenin	86509
Γ-Tocopherol	18185
Dodecanoic acid	30805
dehydroepiandrosterone sulfate	91028
LPE(16:0)	90452
1-palmitoyl-2-hydroxy-sn-glycero-3-PE	73134
GCA	17687
1-O-1'-(Z)-octadecenyl-2-hydroxy-sn-glycero-3-PE	87823
LPE(18:2)	91296
PC(15:2/0:0)|PE(18:2/0:0)	131590|91296
LPE(18:1)	64575
1-oleoyl-2-hydroxy-sn-glycero-3-PE	75168
LPE(18:0)	64576
1-Stearoyl-2-Hydroxy-sn-Glycero-3-PE	83047
2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	91006
PC(37:5)|PE(40:5)	85767|71745
LPC(0:0/16:1)	91298
LPC(16:1/0:0)	91305

LPC(0:0/16:0)	91297
1-palmitoyl-2-hydroxy-sn-glycero-3-PC	72998
LPE(20:4)	64569
PC(O-18:1/0:0)|PC(P-18:0/0:0)	64591|88779
LPC(18e:0/0:0)	75216
Lyso-PAF C-18	91144
PS(18:0)	131443
LPC(18:3)	64565
LPC(0:0/18:2)	91302
LPC(18:2/0:0)	91309
LPC(18:1)	64566
1-oleoyl-2-hydroxy-sn-glycero-3-PC	28610
LPC(0:0/18:0)	91299
1-stearoyl-2-hydroxy-sn-glycero-3-PC	73858
LPC(0:0/20:4)	91303
LPC(20:4/0:0)	91310
LPC(20:3)	64481
LPC(20:4)	64481
LPC(20:2)	67056

LPC(20:1)	67057
3-cis-Hydroxy-b,e-Caroten-3'-one	HMDB02890
Palmitic acid	15756
1-arachidoyl-2-hydroxy-sn-glycero-3-PC	74968
LPC(0:0/20:5)	91304
LPC(20:5/0:0)	91311
LPC(22:7)	74349
LPC(22:6)	74349
LPC(22:5)	74349
LPC(22:4)	91312
Biliverdin hydrochloride b	91027
Biliverdin hydrochloride a	91027
Biliribin I	16990
Biliribin II	16990
D-Urobilinogen|I-Urobilin	4260|36378
cis/trans-Oleic acid	36021
1-linoleoyl-2-stearoyl-sn-glycerol	86337
1-vaccenoyl-2-palmitoyl-sn-glycerol	86346
Ceramide PE(33:1)|SPM(30:1)	86515|72505

Ceramide PE(34:1)	86517
Ceramide PE(35:2)|SPM(32:2)	86523|72510
PC(28:2)	65292
Ceramide PE(35:1)|SPM(32:1)	86519|64586
PC(28:1)	65293
Ceramide PE(36:2)	86525
PC(29:1)	131438
Ornithine	18257
Ceramide PE(37:2)|SPM(34:2)	86527|64587
PC(30:2)	65301
N-palmitoyl-D-erythro-sphingosylphosphorylcholine	78646
PC(30:1)	65302
Ceramide PE(38:2)	86968
SPM(d18:2/18:1)	105799
N-(9Z-octadecenoyl)-sphing-4-enine-1-PC	84487
1,2-dipalmitoleoyl-sn-glycero-3-PC	83717
N-(octadecanoyl)-sphing-4-enine-1-PC	83358
PC(32:1)	66849
1,2-dipalmitoyl-sn-glycero-3-PC	72999

1,2-dilinoleoyl-sn-glycero-3-PC	42027
PC(33:1)|PE(36:1)	86472|71727
PC(34:5)|PE(37:5)	66854|131584
PC(34:4)	64423
PC(34:3)	64424
PC(34:2)|PE(37:2)	64516|131583
1-oleoyl-2-palmitoyl-sn-glycero-3-PC	74667
PC(34:0)	66855
C16-20:5 PC	unknown
PC(35:4)|PE(38:4)	91322|71737
1-stearoyl-2-arachidonoyl-sn-glycero-3-PE|C15-20:4 PC	79110|86344
PC(35:3)|PE(38:3)	131439|71736
PC(35:2)|PE(38:2)	85766|71735
PC(34:3)|PE(37:3)	64424|131581
PC(36:6)	66856
PC(36:5)	64504
1,2-dilinoleoyl-sn-glycero-4-PC	42027
PC(36:3)|PE(39:3)	64523|131585
SPM(40:2)	72529

1,2-dioleoyl-sn-glycero-3-PC|1,2-dipetroselenoyl-sn-glycero-3-PC	74669|86330
PC(36:1)	66857
SPM(41:2)	85762
PC(38:7)	64498
1-palmitoyl-2-docosahexaenoyl-sn-glycero-3-PC	74963
PC(38:5)|PE(41:5)	64525|131586
PC(38:4)	64526
PC(38:3)	64446
PC(38:2)	66859
N-(15Z-tetracosenoyl)-sphinganine-1-PC	91146
PC(40:6)	64431
SPM(42:3)	72535
LacCer(d18:1/14:0)	91034
PC(40:5)	64524
PC(42:7)	131440
Lactosyl ceramide(d18:1/16:0)	84758

Table S1: List of metabolites and lipids tested and CHEBI codes. Abbreviation: LPC = Lysophosphatidylcholine; LPE = lysophosphatidylethenolamine; PC = phosphatidylcholine; PE =

phosphatidylethanolamine; MAG = monoacylglycerol; GCA = glycocholic acid; SPM = sphingomyelin. See Figure 2 for an overview of the statistical procedure.

Women (n_1=804)				Men (n_2=1078)			
Group	Age range (min – max) years	Age mean±sd years	n. individuals per group	Group	Age range (min- max) years	Age mean±sd years	n. individuals per group
W_1	48.4-55.1	51.8±2.1	41	M_1	47.6-53.8	51.3±1.5	54
W_2	55.1-58.6	57.1±1.1	40	M_2	53.8-57.8	55.9±1.2	54
W_3	58.6-60.7	59.8±0.6	40	M_3	57.8-60.2	59.2±0.7	54
W_4	60.7-62.5	61.5±0.5	40	M_4	60.2-62.7	61.5±0.7	54
W_5	62.5-64.3	63.3±0.5	40	M_5	62.7-64.4	63.6±0.5	54
W_6	64.3-65.1	64.8±0.2	40	M_6	64.4-65.2	64.8±0.2	55
W_7	65.1-65.5	65.3±0.1	42	M_7	65.2-65.8	65.4±0.2	52
W_8	65.5-66.1	65.8±0.2	39	M_8	65.8-66.4	66.0±0.2	54
W_9	66.1-66.8	66.4±0.2	40	M_9	66.4-67.5	67.0±0.3	54
W_{10}	66.8-67.6	67.2±0.2	40	M_{10}	67.5-68.6	68.1±0.3	54
W_{11}	67.6-68.9	68.2±0.4	40	M_{11}	68.6-69.7	69.1±0.3	54

W_{12}	68.9-69.9	69.4±0.3	40	M_{12}	69.7-70.6	70.2±0.3	54
W_{13}	69.9-70.8	70.4±0.3	40	M_{13}	70.6-71.5	71.1±0.3	54
W_{14}	70.8-72.5	71.6±0.5	41	M_{14}	71.5-73.1	72.3±0.5	53
W_{15}	72.5-74.4	73.5±0.5	40	M_{15}	73.1-74.5	73.9±0.4	54
W_{16}	74.4-76.0	75.1±0.4	40	M_{16}	74.5-75.7	75.1±0.3	54
W_{17}	76.0-77.8	76.9±0.5	40	M_{17}	75.7-77.2	76.5±0.4	54
W_{18}	77.8-80.3	78.9±0.7	40	M_{18}	77.2-79.2	78.1±0.5	54
W_{19}	80.3-84.2	82.2±1.1	40	M_{19}	79.2-81.7	80.3±0.7	54
W_{20}	84.2-93.9	87.0±2.4	41	M_{20}	81.7-93.3	85.0±2.9	54

Table S2: Characteristics of the 20 groups resulting from the stratification of subjects by age using the 20 quantiles of the age distribution of women and men. For each group, the number of subjects per group, age-range, and age mean±standard deviation were reported. See figure 1 for a graphical illustration of the stratification procedure.

Association of abundance of molecular features a with age					
Women (n_w=804)	Molecular features	Correlation	*P*-value	*P*-value adjusted	Validation (>50%)
	1. C-16 Carnitine	0.79	$7x10^{-5}$	$9x10^{-4}$	79
	2. Pentadecanoic acid	0.58	$7x10^{-5}$	$9x10^{-4}$	22
	3. Palmitic acid	0.55	$8x10^{-5}$	$9x10^{-4}$	41
	4. Oleoyl-L-carnitine hydrochloride	0.72	$8x10^{-5}$	$9x10^{-4}$	32
	5. Heptadecanoic acid	0.67	$8x10^{-5}$	$9x10^{-4}$	32
	6. Myristic acid	0.67	$9x10^{-5}$	0.001	34
	7. cis/trans-Oleic acid	0.67	$9x10^{-5}$	0.001	42
	8. cis-5-Tetradecenoylcarnitine	0.57	$9x10^{-5}$	0.001	20
	9. Propranolol	0.52	$1x10^{-4}$	0.001	10
	10. Choline	0.51	$1x10^{-4}$	0.001	15
	11. Linoleyl carnitine	0.50	$1x10^{-4}$	0.001	26
	12. Corticosterone	0.58	$2x10^{-4}$	0.003	44
	13. L-Acetylcarnitine	0.57	$2x10^{-4}$	0.003	36
	14. Dodecanoic acid	0.57	$2x10^{-4}$	0.003	29

	15. 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.55	$2x10^{-4}$	0.003	41
	16. Barogenin	0.35	$3x10^{-4}$	0.003	37
	17. Dodecanedioic acid	0.52	$3x10^{-4}$	0.003	40
	18. PC(15:2/0:0)|PE(18:2/0:0)	0.52	$4x10^{-4}$	0.003	21
	19. LPC(20:1)	0.52	$4x10^{-4}$	0.003	17
	20. 5a-Androst-3-en-17-one	-0.52	$4x10^{-4}$	0.003	30
	21. MAG(16:0)	0.42	$4x10^{-4}$	0.003	12
	22. 4,8 dimethylnonanoyl carnitine	0.51	$4x10^{-4}$	0.003	32
	23. C12 Carnitine	0.51	$4x10^{-4}$	0.003	39
	24. 2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	0.51	$4x10^{-4}$	0.003	22
	25. gamma-Glutamyl-leucine	0.50	$4x10^{-4}$	0.003	19
	26. 7-Ketocholesterol	0.49	$4x10^{-4}$	0.003	16
	27. 3-Indolepropionic acid	-0.50	$4x10^{-4}$	0.003	26
	28. Naproxen	-0.49	$4x10^{-4}$	0.003	23
	29. Ceramide PE(38:2)	0.57	$4x10^{-4}$	0.003	20
	30. Theobromine	0.47	$4x10^{-4}$	0.003	5
	31. Paraxanthine|Theophylline	-0.46	$5x10^{-4}$	0.003	6

	32. PC(28:1)	0.46	$5x10^{-4}$	0.003	11
	33. Ceramide PE(35:1)|SPM(32:1)	0.46	$5x10^{-4}$	0.003	25
	34. Deoxycholic acid glycine conjugate	0.45	$6x10^{-4}$	0.003	27
	35. Ceramide PE(36:2)	0.44	$6x10^{-4}$	0.003	36
	36. MAG(14:0)	0.48	$7x10^{-4}$	0.004	28
	37. Uric acid	0.43	$7x10^{-4}$	0.004	15
	38. 1-Stearoyl-2-Hydroxy-sn-Glycero-3-PE	0.43	$8x10^{-4}$	0.004	18
	39. sodium glycochenodeoxycholate	0.42	$8x10^{-4}$	0.004	22
	40. L-Proline	0.42	$9x10^{-4}$	0.004	36
	41. Caffeine	-0.41	$9x10^{-4}$	0.004	45
	42. Indole-3-carbinol	0.41	$9x10^{-4}$	0.004	42
	43. L-Octanoylcarnitine	0.40	0.001	0.008	31
	44. Geranyl acetoacetate	0.40	0.001	0.008	22
	45. L-Leucine|L-Norleucine	0.40	0.001	0.008	29
	46. SPM(41:2)	-0.39	0.002	0.01	37
	47. 1-palmitoyl-2-hydroxy-sn-glycero-3-PE	0.39	0.002	0.01	42

	48. Biliverdin hydrochloride a	-0.39	0.002	0.01	24
	49. Linoleic acid	0.66	0.002	0.01	59
	50. α-Linolenic acid	0.65	0.003	0.01	66
	51. Butyryl-L-carnitine|Isobutyryl-L-carnitine	0.38	0.004	0.02	23
	52. Cholic acid	0.38	0.004	0.02	4
	53. Deoxycholic acid	0.38	0.004	0.02	16
	54. LPC(18e:0/0:0)	0.38	0.005	0.02	21
	55. LPE(18:1)	0.38	0.005	0.02	12
	56. LPE(18:2)	0.38	0.005	0.02	10
	57. PC(30:1)	0.38	0.005	0.02	37
	58. Creatine	0.38	0.005	0.02	22
	59. 1,3,7-Trimethyluric acid	0.38	0.005	0.02	6
	60. PC(42:7)	0.37	0.006	0.02	22
	61. Decanoyl-L-carnitine	0.37	0.006	0.02	15
	62. Stearic acid	0.37	0.007	0.02	30
	63. Palmitoleic acid	0.37	0.007	0.02	17
	64. N-palmitoyl-D-erythro-sphingosylphosphorylcholine	0.36	0.007	0.02	8
	65. Lactosyl ceramide(d18:1/16:0)	0.36	0.008	0.02	19

	66. Treprostinil	0.36	0.008	0.02	22
	67. PC(29:1)	0.36	0.008	0.02	19
	68. 4-Androsten-11Beta-ol-3,17-dione|11-Hydroxy-4-androstene-3,17-dione	-0.36	0.008	0.02	20
	69. Ceramide PE(37:2)|SPM(34:2)	0.36	0.009	0.02	20
	70. N-(octadecanoyl)-sphing-4-enine-1-PC	0.36	0.009	0.02	2
	71. PC(37:5)|PE(40:5)	0.35	0.009	0.02	14
	72. Hyodeoxycholic acid	0.35	0.009	0.02	12
	73. Pantothenic acid	0.34	0.009	0.02	13
	74. 1,4-dipalmitoyl-sn-glycero-3-PC	0.34	0.009	0.02	12
	75. LPE(16:0)	0.34	0.009	0.02	5
	76. MAG(18:0)	0.33	0.01	0.02	10
	77. Chenodeoxycholic acid	0.33	0.01	0.02	11
	78. 2,6 dimethylheptanoyl carnitine	0.33	0.01	0.02	6
	79. SPM(42:3)	-0.33	0.01	0.02	2
	80. Fatty acid C22:6	0.33	0.01	0.02	2

	81. Ornithine	0.33	0.01	0.02	1
	82. PC(30:2)	0.33	0.01	0.02	16
	83. Ceramide PE(34:1)	0.31	0.01	0.02	14
	84. N-(15Z-tetracosenoyl)-sphinganine-1-PC	-0.31	0.02	0.04	13
	85. 1-stearoyl-2-arachidonoyl-sn-glycero-3-PE|C15-20:4 PC	-0.31	0.02	0.04	18
	86. LPE(18:0)	0.31	0.02	0.04	22
	87. MAG(18:1)	0.31	0.02	0.04	29
	88. Lyso-PAF C-18	0.30	0.02	0.04	22
	89. Prostaglandin J2	-0.30	0.02	0.04	12
	90. LPE(20:4)	0.30	0.02	0.04	36
	91. PC(34:3)	0.30	0.02	0.04	17
	92. 2-Ketohexanoic acid	-0.28	0.02	0.04	15
	93. DL-2-Aminooctanoic acid	0.28	0.02	0.04	10
	94. LacCer(d18:1/14:0)	0.28	0.02	0.04	4
	95. Piperine	-0.27	0.02	0.04	13
	96. 1,2-dilinoleoyl-sn-glycero-3-PC	-0.27	0.03	0.06	2
	97. D-Urobilinogen|I-Urobilin	0.27	0.03	0.06	11

	98. C16-20:5 PC	-0.27	0.03	0.06	2
	99. Ceramide PE(33:1)|SPM(30:1)	0.26	0.03	0.06	12
	100. D-erythro-sphingosine	0.26	0.03	0.06	26
	101. 3a,6b,7b-Trihydroxy-5b-cholanoic acid	0.26	0.03	0.06	29
	102. LPC(20:4/0:0)	-0.25	0.04	0.08	14
	103. PC(35:3)|PE(38:3)	0.25	0.04	0.08	17
	104. LPC(16:1/0:0)	-0.24	0.05	0.09	11
	105. PC(O-18:1/0:0)|PC(P-18:0/0:0)	0.24	0.05	0.09	11
	106. 3-cis-Hydroxy-b,e-Caroten-3'-one	-0.23	0.05	0.09	3
	107. PS(18:0)	0.23	0.05	0.09	5
	108. Acetaminophen	0.23	0.05	0.09	19
	109. LPC(0:0/16:0)	0.23	0.05	0.09	2
	110. Arachidonic acid	0.22	0.05	0.09	17
	111. Biliribin I	-0.22	0.05	0.09	25
	112. Cortisol	0.22	0.05	0.09	12
	113. MAG(18:3)	0.22	0.05	0.09	1
	114. Glycocholic acid	0.22	0.05	0.09	1

	115. LPC(20:3)	0.22	0.05	0.09	3
	116. Indolelactic acid	0.22	0.06	0.10	5
	117. PC(38:7)	-0.22	0.06	0.10	5
	118. 1-palmitoyl-2-hydroxy-sn-glycero-3-PC	0.21	0.06	0.10	1
	119. Hippuric acid	0.21	0.07	0.12	1
	120. MAG(20:5)	0.21	0.07	0.12	1
	121. 1,3-dipalmitoleoyl-sn-glycero-3-PC	0.21	0.08	0.13	15
	122. Biliribin II	-0.21	0.08	0.13	26
	123. 3-Pyridylacetic acid|trigonelline	-0.20	0.09	0.14	4
	124. PC(38:4)	-0.20	0.09	0.14	6
	125. Gamma-Tocopherol	0.20	0.09	0.14	12
	126. MAG(18:2)	0.20	0.09	0.14	14
	127. 1-arachidoyl-2-hydroxy-sn-glycero-3-PC	0.20	0.10	0.16	14
	128. PC(34:4)	-0.20	0.10	0.16	2
	129. PC(36:5)	-0.19	0.10	0.16	2
	130. Creatinine	0.19	0.10	0.16	3

	131. N-(9Z-octadecenoyl)-sphing-4-enine-1-PC	0.19	0.11	0.17	15
	132. S-(4,5-Dihydro-2-methyl-3-furanyl) ethanethioate	-0.18	0.11	0.17	2
	133. SPM(d18:2/18:1)	0.18	0.11	0.17	15
	134. LPC(0:0/16:1)	-0.17	0.12	0.18	9
	135. 6-hydroxy-5-cholestanol|cholesterol	-0.17	0.12	0.18	10
	136. LPC(20:3)	0.17	0.12	0.18	13
	137. Alpha-Tocopherol	-0.17	0.13	0.19	14
	138. SPM(40:2)	-0.17	0.13	0.19	16
	139. LPC(18:3)	0,164388	0.13	0.19	2
	140. 1,2-dilinoleoyl-sn-glycero-3-PC	0,161861	0.14	0.20	4
	141. PC(38:2)	-0.16	0.14	0.20	5
	142. LPC(0:0/20:4)	-0.16	0.15	0.21	13
	143. 1-palmitoyl-2-docosahexaenoyl-sn-glycero-3-PC	0.16	0.15	0.21	21
	144. PC(36:1)	-0.15	0.16	0.22	12

	145. Arachidonic acid ethyl ester	0.15	0.16	0.22	10
	146. 1-stearoyl-2-hydroxy-sn-glycero-3-PC	0.14	0.17	0.23	8
	147. Oleamide	0.14	0.17	0.23	9
	148. PC(35:2)|PE(38:2)	0.14	0.17	0.23	9
	149. 1-vaccenoyl-2-palmitoyl-sn-glycerol	0.14	0.18	0.24	7
	150. 1,2-dioleoyl-sn-glycero-3-PC|1,2-dipetroselenoyl-sn-glycero-3-PC	-0.13	0.19	0.25	5
	151. Arachidonic acid methyl ester	-0.13	0.19	0.25	10
	152. LPC(0:0/18:0)	0.13	0.20	0.26	10
	153. LPC(22:4)	-0.12	0.20	0.26	12
	154. PC(34:3)|PE(37:3)	-0.12	0.20	0.26	4
	155. PC(33:1)|PE(36:1)	0.12	0.21	0.27	2
	156. MAG(16:1)	0.11	0.21	0.27	1
	157. Indoleacetic acid	0.10	0.25	0.32	2
	158. PC(40:6)	0.10	0.25	0.32	15

	159. Hypoxanthine	-0.11	0.25	0.32	1
	160. 1-O-1'-(Z)-octadecenyl-2-hydroxy-sn-glycero-3-PE	0.20	0.27	0.34	1
	161. LPC(20:2)	0.20	0.27	0.34	14
	162. PC(38:5)|PE(41:5)	-0.19	0.33	0.41	6
	163. Flavone	-0.18	0.35	0.43	4
	164. L-Tryptophan	0.19	0.35	0.43	4
	165. 17-phenyl trinor Prostaglandin E2|17-phenyl trinor Prostaglandin D2	0.18	0.35	0.43	10
	166. PC(32:1)	0.18	0.35	0.43	5
	167. LPC (22:5)	-0.18	0.38	0.46	5
	168. e-Caprolactam	0.18	0.39	0.47	9
	169. L-Phenylalanine	-0.17	0.40	0.48	2
	170. Benzenebutanoic acid	0.16	0.40	0.48	10
	171. Salicylic acid|Aspirin	0.16	0.41	0.48	1
	172. Phenylalanine	0.16	0.43	0.51	15
	173. Stachydrine	-0.15	0.45	0.52	13
	174. dehydroepiandrosterone sulfate	0.10	0.45	0.52	2

	175. LPC(22:5)	0.17	0.50	0.58	1
	176. LPC(20:5/0:0)	0.10	0.55	0.63	0
	177. PC(36:6)	0.14	0.58	0.66	1
	178. 1-oleoyl-2-hydroxy-sn-glycero-3-PC	0.17	0.59	0.67	6
	179. γ-Caprolactone	0.14	0.62	0.70	6
	180. L-Carnitine	0.11	0.63	0.70	8
	181. PC(36:3)|PE(39:3)	-0.29	0.73	0.81	6
	182. 1-oleoyl-2-hydroxy-sn-glycero-3-PE	0.29	0.74	0.82	1
	183. LPC (18:1)	0.29	0.77	0.85	10
	184. 1-oleoyl-2-palmitoyl-sn-glycero-3-PC	-0.29	0.78	0.86	3
	185. L-Tyrosine|o-Tyrosine	0.28	0.79	0.86	2
	186. PC(34:2)|PE(37:2)	-0.11	0.80	0.87	1
	187. Betaine	-0.10	0.82	0.88	13
	188. PC(34:5)|PE(37:5)	0.17	0.84	0.90	12
	189. 1-linoleoyl-2-stearoyl-sn-glycerol	-0.15	0.85	0.90	14
	190. PC(34:0)	-0.15	0.85	0.90	7

	191. L-Aspartyl-L-phenylalanine	0.13	0.85	0.90	1
	192. LPC(0:0/20:5)	0.16	0.86	0.91	1
	193. LPC(0:0/18:2)	-0.14	0.8	0.91	12
	194. PC(35:4)|PE(38:4)	-0.13	0.87	0.91	1
	195. PC(40:5)	0.12	0.87	0.91	2
	196. LPC(22:5)	0.11	0.90	0.92	4
	197. LPC(18:2/0:0)	-0.09	0.90	0.92	10
	198. Fatty acid C20:5 methyl ester	0.08	0.91	0.93	1
	199. Biliverdin hydrochloride b	-0.06	0.91	0.93	1
	200. PC(28:2)	0.05	0.92	0.93	1
	201. PC(38:3)	0.05	0.92	0.93	1
	202. Ceramide PE(35:2)|SPM(32:2)	-0.10	0.95	0.97	2
Men (n_M=1078)	1. 1,2-dipalmitoleoyl-sn-glycero-3-PC	-0.78	$9x10^{-5}$	0.005	6
	2. PC(34:4)	-0.76	$9x10^{-5}$	0.005	10
	3. PC(34:3)|PE(37:3)	-0.76	$9x10^{-5}$	0.005	18

	4. Hippuric acid	0.74	$9x10^{-5}$	0.005	3
	5. MAG(18:0)	-0.65	$2x10^{-4}$	0.005	53
	6. 1-palmitoyl-2-hydroxy-sn-glycero-3-PC	-0.67	$2x10^{-4}$	0.005	58
	7. PC(38:7)	-0.75	$2x10^{-4}$	0.005	20
	8. 2-Ketohexanoic acid	-0.70	$3x10^{-4}$	0.006	27
	9. LPC(16:1/0:0)	-0.67	$3x10^{-4}$	0.006	2
	10. LPC(0:0/16:0)	-0.69	$3x10^{-4}$	0.006	1
	11. Indole-3-carbinol	0.67	$4x10^{-4}$	0.006	46
	12. PC(38:3)	0.63	$4x10^{-4}$	0.006	37
	13. PS(18:0)	-0.63	$4x10^{-4}$	0.006	39
	14. LPC(0:0/18:0)	-0.65	$5x10^{-4}$	0.008	62
	15. LPC(22:5)	-0.63	$5x10^{-4}$	0.008	44
	16. PC(36:6)	-0.62	$5x10^{-4}$	0.008	48
	17. LPC(0:0/16:1)	-0.59	$5x10^{-4}$	0.008	42
	18. LPC(18:1)	-0.62	$8x10^{-4}$	0.008	44
	19. LPC(20:3)	-0.62	$8x10^{-4}$	0.008	6
	20. LPC(20:1)	-0.61	$8x10^{-4}$	0.008	38
	21. PC(36:5)	-0.61	0.001	0.008	10

	22. 1,2-dilinoleoyl-sn-glycero-3-PC	-0.62	0.001	0.008	20
	23. PC(36:3)|PE(39:3)	-0.62	0.001	0.008	15
	24. Indoleacetic acid	0.60	0.001	0.008	19
	25. MAG(16:0)	-0.58	0.002	0.01	22
	26. LPC(22:4)	-0.59	0.002	0.01	19
	27. PC(34:5)|PE(37:5)	-0.60	0.002	0.01	22
	28. LPC(0:0/20:4)	-0.57	0.002	0.01	3
	29. Corticosterone	-0.56	0.002	0.01	20
	30. PC(38:4)	-0.53	0.002	0.01	19
	31. PC(32:1)	-0.53	0.002	0.01	25
	32. Decanoyl-L-carnitine	0.53	0.002	0.01	41
	33. LPC(20:4/0:0)	-0.53	0.002	0.01	32
	34. Biliverdin hydrochloride a	-0.53	0.002	0.01	6
	35. Geranyl acetoacetate	-0.52	0.002	0.01	9
	36. Arachidonic acid ethyl ester	-0.52	0.002	0.01	18
	37. PC(34:2)|PE(37:2)	-0.52	0.002	0.01	17
	38. MAG(18:1)	-0.52	0.002	0.01	25

	39. 4-Androsten-11Beta-ol-3,17-dione|11-Hydroxy-4-androstene-3,17-dione	0.52	0.002	0.01	23
	40. PC(40:5)	-0.51	0.002	0.01	21
	41. LPC(22:5)	-0.51	0.002	0.01	15
	42. MAG(14:0)	-0.51	0.003	0.01	14
	43. Cholic acid	0.50	0.003	0.01	12
	44. L-Octanoylcarnitine	0.50	0.004	0.02	6
	45. LPC(22:5)	-0.49	0.004	0.02	9
	46. PC(35:4)|PE(38:4)	-0.49	0.004	0.02	5
	47. Prostaglandin J2	0.49	0.005	0.02	5
	48. PC(38:5)|PE(41:5)	-0.48	0.005	0.02	2
	49. LPE(18:1)	-0.48	0.005	0.02	1
	50. Gamma-Tocopherol	-0.47	0.005	0.02	10
	51. LPC(18:1)	-0.47	0.005	0.02	12
	52. LPC(20:5/0:0)	-0.46	0.005	0.02	15
	53. 1-oleoyl-2-hydroxy-sn-glycero-3-PC	-0.46	0.005	0.02	12
	54. L-Aspartyl-L-phenylalanine	0.46	0.005	0.02	12

	55. 1,2-dioleoyl-sn-glycero-3-phosphocholine|1,2-dipetroselenoyl-sn-glycero-3-PC	-0.46	0.005	0.02	13
	56. Treprostinil	0.45	0.005	0.02	21
	57. PC(36:1)	-0.45	0.005	0.02	24
	58. C16-20:5 PC	-0.44	0.005	0.02	31
	59. 1-stearoyl-2-arachidonoyl-sn-glycero-3-PE|C15-20:4 PC	-0.44	0.005	0.02	9
	60. 2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	0.44	0.005	0.02	19
	61. Biliribin II	-0.43	0.005	0.02	5
	62. MAG(18:2)	-0.42	0.005	0.02	2
	63. Piperine	-0.42	0.005	0.02	2
	64. Betaine	-0.41	0.005	0.02	10
	65. PC(34:0)	-0.41	0.005	0.02	15
	66. PC(42:7)	0.41	0.005	0.02	14
	67. LPE(18:0)	-0.41	0.005	0.02	14
	68. L-Tryptophan	-0.41	0.006	0.02	12
	69. Ceramide PE(35:2)|SPM(32:2)	0.41	0.006	0.02	21

	70. Dodecanedioic acid	0.40	0.006	0.02	21
	71. PC(28:2)	0.40	0.006	0.02	25
	72. LPC(0:0/18:2)	-0.40	0.006	0.02	5
	73. Butyryl-L-carnitine|Isobutyryl-L-carnitine	0.40	0.006	0.02	5
	74. 1-Stearoyl-2-Hydroxy-sn-Glycero-3-PE	-0.40	0.008	0.02	9
	75. PC(33:1)|PE(36:1)	0.39	0.009	0.02	3
	76. 3a,6b,7b-Trihydroxy-5b-cholanoic acid	0.39	0.009	0.02	1
	77. LPC(18:2/0:0)	-0.39	0.009	0.02	1
	78. Linoleic acid	-0.39	0.009	0.02	1
	79. Propranolol	0.39	0.01	0.02	2
	80. 1-arachidoyl-2-hydroxy-sn-glycero-3-PC	-0.38	0.01	0.02	10
	81. Stearic acid	-0.38	0.01	0.02	12
	82. Biliribin I	-0.38	0.01	0.02	11
	83. LPC(0:0/20:5)	-0.38	0.01	0.02	10
	84. 1-oleoyl-2-palmitoyl-sn-glycero-3-PC	-0.38	0.01	0.02	19

	85. L-Proline	-0.37	0.01	0.02	14
	86. cis-5-Tetradecenoylcarnitine	0.37	0.01	0.02	7
	87. Arachidonic acid methyl ester	-0.37	0.01	0.02	14
	88. Alpha-Tocopherol	-0.37	0.01	0.02	5
	89. Arachidonic acid	-0.36	0.01	0.02	21
	90. Uric acid	-0.35	0.02	0.04	10
	91. PC(34:3)	-0.35	0.02	0.04	1
	92. PC(35:3)|PE(38:3)	-0.35	0.02	0.04	2
	93. Ornithine	-0.35	0.03	0.06	1
	94. MAG(16:1)	-0.35	0.03	0.06	1
	95. C12 Carnitine	0.35	0.03	0.06	2
	96. Palmitic acid	-0.34	0.03	0.06	6
	97. 3-Pyridylacetic acid|trigonelline	0.33	0.03	0.06	3
	98. 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.32	0.04	0.08	3
	99. MAG(20:5)	-0.32	0.04	0.08	4
	100. 1-linoleoyl-2-stearoyl-sn-glycerol	-0.32	0.04	0.08	14

	101. Indolelactic acid	0.32	0.05	0.10	14
	102. 3-cis-Hydroxy-b,e-Caroten-3'-one	-0.31	0.06	0.12	12
	103. LPC(20:2)	-0.31	0.06	0.12	15
	104. 1,2-dilinoleoyl-sn-glycero-3-PC	-0.31	0.07	0.13	2
	105. Hypoxanthine	-0.30	0.07	0.13	1
	106. Alpha-Linolenic acid	-0.30	0.08	0.15	2
	107. Barogenin	0.30	0.08	0.15	2
	108. Fatty acid C20:5 methyl ester	-0.29	0.08	0.15	2
	109. dehydroepiandrosterone sulfate (sodium salt)	0.28	0.08	0.15	1
	110. Theobromine	-0.27	0.09	0.16	1
	111. cis/trans-Oleic acid	-0.27	0.09	0.16	1
	112. Creatinine	0.27	0.09	0.16	10
	113. sodium glycochenodeoxycholate	0.26	0.1	0.18	1
	114. Oleoyl-L-carnitine hydrochloride	0.26	0.1	0.18	1
	115. L-Tyrosine|o-Tyrosine	-0.26	0.11	0.19	4

	116. 1,3,7-Trimethyluric acid	-0.25	0.11	0.19	6
	117. 1-O-1'-(Z)-octadecenyl-2-hydroxy-sn-glycero-3-PE	-0.25	0.11	0.19	4
	118. LPE(20:4)	-0.25	0.12	0.20	3
	119. Choline	0.25	0.12	0.20	3
	120. Ceramide PE(34:1)	0.25	0.12	0.20	3
	121. LPE(18:2)	-0.24	0.12	0.20	2
	122. LPC(18e:0/0:0)	-0.24	0.13	0.21	1
	123. C16 Carnitine	0.24	0.13	0.21	1
	124. Deoxycholic acid glycine conjugate	0.23	0.13	0.21	1
	125. SPM(42:3)	0.23	0.13	0.21	1
	126. N-(15Z-tetracosenoyl)-sphinganine-1-PC	-0.23	0.13	0.21	1
	127. PC(28:1)	-0.23	0.13	0.21	10
	128. Gamma-Caprolactone	0.22	0.14	0.21	1
	129. Ceramide PE(35:1)|SPM(32:1)	-0.22	0.14	0.21	9
	130. Biliverdin hydrochloride b	-0.22	0.14	0.21	5

	131. gamma-Glutamyl-leucine	-0.21	0.14	0.21	5
	132. DL-2-Aminooctanoic acid	-0.21	0.14	0.21	12
	133. PC(40:6)	0.21	0.14	0.21	12
	134. D-erythro-sphingosine	0.21	0.15	0.22	5
	135. Deoxycholic acid	0.21	0.15	0.22	2
	136. PC(38:2)	0.21	0.15	0.22	14
	137. Ceramide PE(33:1)|Sphingomyelin(30:1)	0.20	0.15	0.22	10
	138. Acetaminophen	0.20	0.17	0.25	11
	139. Lactosyl ceramide(d18:1/16:0)	0.20	0.17	0.25	12
	140. Dodecanoic acid	0.19	0.18	0.26	10
	141. 1-palmitoyl-2-docosahexaenoyl-sn-glycero-3-PC	-0.19	0.18	0.26	1
	142. Stachydrine	0.19	0.2	0.26	1
	143. PC(35:2)|PE(38:2)	-0.19	0.2	0.28	12
	144. Creatine	-0.19	0.21	0.29	1

	145. D-Urobilinogen|I-Urobilin	0.18	0.21	0.29	4
	146. Ceramide PE(36:2)	0.17	0.22	0.30	6
	147. 1-oleoyl-2-hydroxy-sn-glycero-3-PE	-0.16	0.22	0.30	19
	148. Chenodeoxycholic acid	0.16	0.25	0.34	8
	149. 5a-Androst-3-en-17-one	-0.16	0.25	0.34	7
	150. Flavone	0.15	0.25	0.34	12
	151. LacCer(d18:1/14:0)	0.15	0.27	0.36	10
	152. Lyso-PAF C-18	-0.15	0.27	0.36	1
	153. Linoleyl carnitine	0.15	0.3	0.40	2
	154. L-Acetylcarnitine	0.15	0.31	0.41	2
	155. MAG(18:3)	-0.14	0.32	0.41	2
	156. L-Leucine|L-Norleucine	-0.14	0.32	0.41	3
	157. LPC(18:3)	-0.14	0.32	0.41	4
	158. Oleamide	0.14	0.32	0.41	5
	159. 6-hydroxy-5-cholestanol|cholesterol	-0.14	0.33	0.41	6
	160. 7-Ketocholesterol	-0.14	0.33	0.41	3

	161. e-Caprolactam	-0.13	0.33	0.41	2
	162. 1,2-dipalmitoyl-sn-glycero-3-PC	0.13	0.34	0.42	2
	163. LPC(20:1)	-0.13	0.34	0.42	4
	164. 1-vaccenoyl-2-palmitoyl-sn-glycerol	-0.13	0.34	0.42	1
	165. PC(O-18:1/0:0)|PC(P-18:0/0:0)	0.12	0.35	0.43	1
	166. Palmitoleic acid	-0.12	0.35	0.43	10
	167. Cortisol	-0.12	0.36	0.44	1
	168. Hyodeoxycholic acid	0.12	0.37	0.44	1
	169. 17-phenyl trinor Prostaglandin E2|17-phenyl trinor Prostaglandin D2	0.12	0.37	0.44	10
	170. Paraxanthine|Theophylline	0.11	0.38	0.45	1
	171. SPM(41:2)	0.11	0.4	0.47	2
	172. Phenylalanine	0.11	0.45	0.53	1
	173. PC(30:2)	-0.11	0.46	0.53	10
	174. SPM(d18:2/18:1)	-0.11	0.46	0.53	1
	175. Naproxen	0.11	0.46	0.53	1

	176. SPM(40:2)	-0.10	0.52	0.60	1
	177. Caffeine	-0.10	0.55	0.63	1
	178. S-(4,5-Dihydro-2-methyl-3-furanyl) ethanethioate	0.10	0.57	0.65	12
	179. PC(29:1)	0.10	0.58	0.65	1
	180. Ceramide PE(37:2)|SPM(34:2)	-0.10	0.58	0.65	2
	181. 2,6 dimethylheptanoyl carnitine	-0.10	0.61	0.68	3
	182. N-(9Z-octadecenoyl)-sphing-4-enine-1-PC	-0.10	0.62	0.69	3
	183. L-Phenylalanine	0.10	0.63	0.69	1
	184. PC(37:5)|PE(40:5)	0.10	0.63	0.69	2
	185. 4,8 dimethylnonanoyl carnitine	0.10	0.65	0.71	2
	186. Fatty acid C22:6	0.10	0.68	0.74	1
	187. Myristic acid	-0.10	0.71	0.77	5
	188. N-(octadecanoyl)-sphing-4-enine-1-PC	-0.10	0.73	0.78	9
	189. Ceramide PE(38:2)	-0.10	0.75	0.80	6

	190. LPE(16:0)	-0.10	0.83	0.882	7
	191. L-Carnitine	-0.10	0.85	0.90	1
	192. PC(15:2/0:0)|PE(18:2/0:0)	0.10	0.86	0.90	1
	193. Pantothenic acid	-0,09	0.87	0.90	1
	194. Heptadecanoic acid	-0,09	0.87	0.90	2
	195. Pentadecanoic acid	-0,09	0.87	0.90	2
	196. Salicylic acid|Aspirin	0,09	0.88	0.90	2
	197. 3-Indolepropionic acid	0,09	0.88	0.90	3
	198. 1-palmitoyl-2-hydroxy-sn-glycero-3-PE	0,09	0.89	0.90	4
	199. Benzenebutanoic acid	-0,09	0.89	0.90	2
	200. PC(30:1)	-0,09	0.9	0.90	1
	201. N-palmitoyl-D-erythro-sphingosylphosphorylcholine	0,09	0.93	0.93	1
	202. Glycocholic acid	0,09	0.95	0.95	1
Association of correlation among molecular features a with age					
Women	Molecular features	Correlation	*P*-value	*P*-value adjusted	Validation (>50%)

	1. Palmitoleic acid – Stearic acid	-0.75	$3x10^{-4}$	0.008	2
	2. Linoleic acid – Stearic acid	-0.73	$4x10^{-4}$	0.008	1
	3. Stearic acid – Palmitic acid	-0.72	$4x10^{-4}$	0.008	34
	4. Stearic acid – cis/trans-Oleic acid	-0.70	$4x10^{-4}$	0.008	1
	5. PC(32:1) – PC(35:3)|PE(38:3)	0.72	$5x10^{-4}$	0.008	54
	6. Ceramide PE(35:2)|SPM(32:2) – PC(32:1)	0.70	$5x10^{-4}$	0.008	2
	7. 1-Stearoyl-2-Hydroxy-sn-Glycero-3-PE – LPE(20:4)	-0.65	$6x10^{-4}$	0.008	27
	8. 1-2-dipalmitoyl-sn-glycero-3-PC – N-(15Z-tetracosenoyl)-sphinganine-1-PC	-0.69	$6x10^{-4}$	0.008	28
	9. PC(28:2) – PC(32:1)	0.69	0.001	0.008	57
	10. SPM(40:2) – Lactosyl ceramide(d18:1/16:0)	-0.67	0.001	0.008	25
	11. Heptadecanoic acid – Stearic acid	-0.64	0.001	0.008	4
	12. Biliverdin hydrochloride b – Bilirubin II	-0.63	0.001	0.008	25
	13. LPC(20:4/0:0) – PC(38:4)	-0.65	0.001	0.008	1

	14. N-(15Z-tetracosenoyl)-sphinganine-1-PC – Lactosyl ceramide(d18:1/16:0)	-0.65	0.002	0.01	20
	15. Deoxycholic acid – Deoxycholic acid glycine conjugate	-0.63	0.002	0.01	26
	16. N-palmitoyl-D-erythro-sphingosylphosphorylcholine – SPM(40:2)	-0.62	0.002	0.01	26
	17. PC(34:4) – PC(38:7)	0.62	0.002	0.01	2
	18. 1-2-dilinoleoyl-sn-glycero-3-PC – PC(38:4)	-0.62	0.003	0.01	20
	19. Ceramide PE(35:2)|SPM(32:2) – 1-oleoyl-2-palmitoyl-sn-glycero-3-PC	0.61	0.003	0.01	2
	20. PC(34:4) – PC(35:3)|PE(38:3)	0.61	0.003	0.01	37
	21. PC(30:1) – SPM(40:2)	-0.61	0.003	0.01	36
	22. Deoxycholic acid glycine conjugate – Chenodeoxycholic acid	-0.60	0.004	0.02	23
	23. Fatty acid C20:5 methyl ester – PC(34:5)|PE(37:5)	-0.60	0.004	0.02	1

	24. PC(28:2) – 1-oleoyl-2-palmitoyl-sn-glycero-3-PC	0.60	0.004	0.02	2
	25. PC(28:2) – PC(34:0)	0.59	0.004	0.02	13
	26. 1-palmitoyl-2-hydroxy-sn-glycero-3-PE – LPE(20:4)	-0.59	0.005	0.02	13
	27. Biliverdin hydrochloride b – Biliverdin hydrochloride a	-0.59	0.006	0.02	29
	28. Biliverdin hydrochloride b – Bilirubin I	-0.59	0.006	0.02	16
	29. Myristic acid – Stearic acid	-0.58	0.007	0.02	1
	30. LPC(20:5/0:0) – PC(34:5)|PE(37:5)	-0.58	0.007	0.02	26
	31. Fatty acid C20:5 methyl ester – PC(38:7)	-0.58	0.007	0.02	1
	32. 1-stearoyl-2-hydroxy-sn-glycero-3-PC – PC(40:5)	-0.52	0.007	0.02	12
	33. D-Urobilinogen|I-Urobilin – PC(40:5)	-0.51	0.008	0.02	13
	34. PC(36:6) – PC(38:7)	0.51	0.008	0.02	5
	35. PC(36:5) – PC(38:7)	0.50	0.008	0.02	28

	36. 4-8 dimethylnonanoyl carnitine – PC(40:5)	0.48	0.009	0.02	17
	37. MAG(18:3) –PC(40:5)	-0.42	0.009	0.02	9
	38. MAG(18:0) – PC(38:5)|PE(41:5)	-0.41	0.009	0.02	41
	39. Arachidonic acid – PC(38:5)|PE(41:5)	0.42	0.009	0.02	21
	40. Heptadecanoic acid – PC(38:5)|PE(41:5)	-0.43	0.009	0.02	22
	41. Phenylalanine – PC(38:5)|PE(41:5)	0.40	0.01	0.02	13
	42. 7-Ketocholesterol –Alpha-Tocopherol	-0.30	0.01	0.02	2
	43. 17-phenyl trinor Prostaglandin E2|17 – phenyl trinor Prostaglandin D2-Alpha-Tocopherol	-0.33	0.01	0.02	10
	44. sodium glycochenodeoxycholate – Alpha-Tocopherol	-0.30	0.01	0.02	6
	45. Deoxycholic acid glycine conjugate – Alpha-Tocopherol	-0.31	0.01	0.02	12

	46. Chenodeoxycholic acid – Alpha-Tocopherol	-0.30	0.01	0.02	15
	47. Linoleyl carnitine –Alpha-Tocopherol	-0.30	0.02	0.04	5
	48. Choline – Arachidonic acid	0.40	0.02	0.04	8
	49. Creatinine – Arachidonic acid	0.42	0.02	0.04	18
	50. LPC(20:4/0:0) – LPC(22:5)	-0.40	0.03	0.06	7
	51. LPC(20:3) – LPC(22:5)	-0.42	0.03	0.06	23
	52. LPC(20:5/0:0) – LPC(22:5)	-0.41	0.03	0.06	19
	53. LPC(22:4) – N-(9Z-octadecenoyl)-sphing-4-enine-1-PC	-0.39	0.04	0.07	2
	54. Biliverdin hydrochloride b – N-(9Z-octadecenoyl)-sphing-4-enine-1-PC	-0.21	0.04	0.07	1
	55. Biliverdin hydrochloride a – N-(9Z-octadecenoyl)-sphing-4-enine-1-PC	-0.19	0.04	0.07	1
	56. Biliribin I – N-(9Z-octadecenoyl)-sphing-4-enine-1-PC	-0.20	0.05	0.09	1

	57. Flavone – N-(octadecanoyl)-sphing-4-enine-1-PC	-0.23	0.05	0.09	23
	58. Geranyl acetoacetate – N-(octadecanoyl)-sphing-4-enine-1-PC	-0.22	0.07	0.12	12
	59. Dodecanedioic acid – N-(octadecanoyl)-sphing-4-enine-1-PC	-0.25	0.07	0.12	1
	60. 1-3-7-Trimethyluric acid – N-palmitoyl-D-erythro-sphingosylphosphorylcholine	0.25	0.07	0.12	14
	61. L-Aspartyl-L-phenylalanine – LPC(16:1/0:0)	-0.30	0.09	0.15	4
	62. Heptadecanoic acid – LPC(16:1/0:0)	-0.32	0.09	0.15	4
	63. Choline – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	-0.29	0.1	0.16	2
	64. 3-Pyridylacetic acid|trigonelline – Alpha-Linolenic acid	-0.28	0.12	0.19	3
	65. Stachydrine – Alpha-Linolenic acid	-0.29	0.12	0.19	5

	66. Benzenebutanoic acid – Alpha-Linolenic acid	-0.22	0.13	0.20	10
	67. Geranyl acetoacetate – Arachidonic acid	-0.30	0.15	0.22	1
	68. Dodecanedioic acid – Arachidonic acid	-0.28	0.15	0.22	1
	69. 5a-Androst-3-en-17-one – Arachidonic acid	0.25	0.15	0.22	6
	70. Caffeine – Barogenin	-0.26	0.19	0.27	7
	71. Hippuric acid – Barogenin	0.25	0.19	0.27	2
	72. L-Acetylcarnitine – Barogenin	-0.25	0.19	0.27	14
	73. Indolelactic acid – Barogenin	-0.28	0.20	0.28	11
	74. Geranyl acetoacetate – Biliribin I	0.25	0.20	0.28	10
	75. Dodecanedioic acid – Biliribin I	0.23	0.22	0.30	1
	76. 5a-Androst-3-en-17-one – Biliribin I	0.22	0.22	0.30	1
	77. Propranolol – Biliribin I	0.23	0.25	0.33	2
	78. L-Phenylalanine – Biliverdin hydrochloride a	-0.24	0.3	0.40	9

	79. 2-6 dimethylheptanoyl carnitine – Stearic acid	-0.22	0.35	0.45	8
	80. 4-Androsten-11Beta-ol-3-17-dione|11-Hydroxy-4-androstene-3-17-dione – Stearic acid	-0.13	0.35	0.45	5
	81. Arachidonic acid – Stearic acid	-0.20	0.37	0.47	11
	82. MAG(16:1) – Treprostinil	-0.23	0.4	0.50	15
	83. MAG(16:0) – Treprostinil	-0.25	0.42	0.52	10
	84. MAG(18:3) – Treprostinil	-0.23	0.45	0.55	1
	85. Choline – Uric acid	-0.22	0.47	0.56	1
	86. Betaine – Uric acid	-0.23	0.47	0.56	1
	87. Barogenin – LPC(22:4)	-0.23	0.49	0.57	1
	88. GCA – LPC(22:4)	-0.24	0.49	0.57	2
	89. Uric acid – D-Urobilinogen|I-Urobilin	0.15	0.5	0.57	5
	90. L-Leucine|L-Norleucine – 1-stearoyl-2-hydroxy-sn-glycero-3-PC	0.21	0.5	0.57	6
	91. Hypoxanthine – 1-stearoyl-2-hydroxy-sn-glycero-3-PC	0.22	0.55	0.62	4

	92. PC(O-18:1/0:0)|PE(P-18:0/0:0) – 1-stearoyl-2-hydroxy-sn-glycero-3-PC	0.22	0.58	0.64	2
	93. L-Tyrosine|o-Tyrosine – 1-vaccenoyl-2-palmitoyl-sn-glycerol	-0.23	0.58	0.64	2
	94. Naproxen – 1-vaccenoyl-2-palmitoyl-sn-glycerol	0.23	0.6	0.66	1
	95. Oleamide – 2-6 dimethylheptanoyl carnitine	-0.22	0.62	0.67	1
	96. Pentadecanoic acid – 2a-(3-Hydroxypropyl)-1a-25-dihydroxy-19-norvitamin D3	-0.23	0.62	0.67	1
	97. 3-Pyridylacetic acid|trigonelline – 7-Ketocholesterol	0.21	0.64	0.67	2
	98. Stachydrine – 7 -Ketocholesterol	0.22	0.64	0.67	1
	99. Flavone – 5a-Androst-3-en-17-one	0.25	0.64	0.67	1
	100. LPC(18:2/0:0) – 3-cis-Hydroxy-b-e-Caroten-3'-one	-0.20	0.69	0.71	2

	101. Indole-3-carbinol – 3a-6b-7b-Trihydroxy-5b-cholanoic acid	-0.15	0.72	0.73	3
	102. MAG(16:1) – LPC(0:0/16:1)	0.20	0.82	0.83	4
	103. LPC(18:3) – LPC(18:2/0:0)	0.25	0.93	0.93	2
Men (n_M=1078)	1. Palmitoleic acid – MAG(16:1)	-0.85	$1x10^{-5}$	0.001	21
	2. MAG(16:0) – LPC(16:1/0:0)	-0.81	$4x10^{-5}$	0.002	53
	3. PC(35:3)|PE(38:3) – PC(36:3)|PE(39:3)	0.81	$4x10^{-5}$	0.002	2
	4. MAG(16:0) – LPC(0:0/16:1)	-0.80	$6x10^{-5}$	0.002	59
	5. MAG(18:1) – LPC(16:1/0:0)	-0.78	$1x10^{-4}$	0.003	60
	6. MAG(18:0) – LPC(0:0/16:1)	-0.76	$2x10^{-4}$	0.004	53
	7. MAG(16:1) – LPC(16:1/0:0)	-0.76	$2x10^{-4}$	0.004	42
	8. MAG(16:1) – cis/trans-Oleic acid	-0.77	$2x10^{-4}$	0.004	35
	9. Ceramide PE(37:2)|SPM(34:2) – SPM(d18:2/18:1)	0.77	$2x10^{-4}$	0.004	2
	10. LPE(18:2) – LPC(18:3)	0.74	$4x10^{-4}$	0.004	13
	11. PC(30:2) – SPM(d18:2/18:1)	0.74	$4x10^{-4}$	0.004	9

	12. LPE(18:2) – LPC(0:0/18:2)	0.73	$5x10^{-4}$	0.005	18
	13. MAG(18:0) – PC(32:1)	-0.72	$6x10^{-4}$	0.005	49
	14. LPE(18:2) – LPC(18:2/0:0)	0.71	$8x10^{-4}$	0.005	45
	15. Palmitoleic acid – LPC(0:0/16:1)	-0.71	$8x10^{-4}$	0.005	16
	16. N-(9Z-octadecenoyl)-sphing-4-enine-1-PC – 1,2-dilinoleoyl-sn-glycero-3-PC	0.71	$9x10^{-4}$	0.005	1
	17. Palmitoleic acid – LPC(16:1/0:0)	-0.70	$9x10^{-4}$	0.005	1
	18. Arachidonic acid ethyl ester – LPC(16:1/0:0)	-0.71	$9x10^{-4}$	0.005	21
	19. LPC(0:0/16:1) – Palmitic acid	-0.70	$9x10^{-4}$	0.005	37
	20. MAG(16:1) – LPC(0:0/16:1)	-0.70	0.001	0.005	14
	21. LPC(18:3) – LPC(18:2/0:0)	0.70	0.001	0.005	42
	22. Salicylic acid|Aspirin – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.69	0.001	0.005	12
	23. Theobromine – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.69	0.002	0.009	32

	24. Creatine – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.68	0.002	0.009	24
	25. L-Leucine|L-Norleucine – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.68	0.002	0.009	28
	26. MAG(14:0) – LPE(18:0)	0.69	0.004	0.02	8
	27. 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid – LPE(18:0)	0.69	0.004	0.02	16
	28. Fatty acid C22:6 – LPE(18:0)	0.67	0.004	0.02	17
	29. 4-8 dimethylnonanoyl carnitine – LPE(18:0)	0.65	0.006	0.02	9
	30. Indole-3-carbinol – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.64	0.006	0.02	2
	31. Acetaminophen – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.65	0.006	0.02	1
	32. 2-Ketohexanoic acid – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.64	0.006	0.02	1

	33. S-(4-5-Dihydro-2-methyl-3-furanyl) ethanethioate – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.63	0.009	0.03	32
	34. L-Carnitine – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.63	0.009	0.03	31
	35. L-Phenylalanine – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.62	0.009	0.03	26
	36. Uric acid – 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid	0.62	0.009	0.03	21
	37. L-Tyrosine|o-Tyrosine – LPE(20:4)	0.60	0.01	0.03	20
	38. Naproxen – LPE(20:4)	0.60	0.01	0.03	15
	39. e-Caprolactam – DL-2-Aminooctanoic acid	-0.59	0.01	0.03	19
	40. Choline – Gamma-Caprolactone	-0.56	0.01	0.03	5
	41. Creatinine – Gamma-Caprolactone	-0.58	0.02	0.05	9

	42. e-Caprolactam – Gamma-Caprolactone	0.59	0.02	0.05	12
	43. DL-2-Aminooctanoic acid – Gamma-Caprolactone	-0.56	0.02	0.05	12
	44. Choline – L-Proline	0.53	0.03	0.07	5
	45. Creatinine – L-Proline	0.52	0.03	0.07	6
	46. e-Caprolactam – L-Proline	-0.52	0.03	0.07	13
	47. DL-2-Aminooctanoic acid – L-Proline	-0.51	0.05	0.12	21
	48. Gamma – Caprolactone-L-Proline	-0.50	0.05	0.12	13
	49. Benzenebutanoic acid – Alpha-Linolenic acid	0.49	0.06	0.13	21
	50. Geranyl acetoacetate – Arachidonic acid	0.48	0.06	0.13	5
	51. LPC(20:4/0:0 – PC(34:0)	-0.46	0.06	0.13	12
	52. LPC(20:2) – PC(34:0)	-0.45	0.07	0.15	11
	53. LPC(20:3) – PC(34:0)	-0.45	0.07	0.15	11
	54. 1-3-7-Trimethyluric acid – C16-20:5 PC	0.40	0.07	0.15	32

	55. Deoxycholic acid glycine conjugate – PC(35:3)|PE(38:3)	-0.39	0.09	0.18	18
	56. LPC(20:3) – Biliverdin hydrochloride a	-0.34	0.09	0.18	19
	57. Lyso-PAF C-18 – Biliverdin hydrochloride a	0.33	0.11	0.21	9
	58. LPC(20:2) – Biliverdin hydrochloride a	-0.32	0.11	0.21	8
	59. LPC(20:1) – Biliverdin hydrochloride a	-0.34	0.11	0.21	5
	60. PS(18:0) – Biliribin I	0.32	0.13	0.24	2
	61. L-Carnitine – LPC(22:5)	0.35	0.13	0.24	2
	62. Biliribin II – PC(34:2)|PE(37:2)	-0.33	0.15	0.27	2
	63. D-Urobilinogen|I-Urobilin – PC(34:2)|PE(37:2)	-0.31	0.15	0.27	1
	64. cis/trans-Oleic acid – PC(34:2)|PE(37:2)	0.30	0.15	0.27	1
	65. 1-linoleoyl-2-stearoyl-sn-glycerol – PC(34:2)|PE(37:2)	0.32	0.17	0.29	2
	66. 1-vaccenoyl-2-palmitoyl-sn-glycerol – PC(34:2)|PE(37:2)	-0.31	0.17	0.29	3

	67. Ceramide PE(33:1)|SPM(30:1) – 1-oleoyl-2-palmitoyl-sn-glycero-3-PC	0.31	0.18	0.30	5
	68. Ceramide PE(34:1) – 1-oleoyl-2-palmitoyl-sn-glycero-3-PC	0.31	0.18	0.30	6
	69. Stearic acid – cis/trans-Oleic acid	-0.30	0.19	0.31	5
	70. PC(32:1) – PC(35:3)|PE(38:3)	0.30	0.19	0.31	7
	71. Deoxycholic acid glycine conjugate – Chenodeoxycholic acid	0.35	0.21	0.33	10
	72. Fatty acid C20:5 methyl ester – PC(34:5)|PE(37:5)	0.34	0.21	0.33	1
	73. Cortisol – SPM(41:2)	0.35	0.21	0.33	2
	74. 6-hydroxy-5-cholestanol|cholesterol – SPM(41:2)	-0.36	0.25	0.39	2
	75. cis-5-Tetradecenoylcarnitine – SPM(41:2)	0.34	0.27	0.41	2
	76. 6-hydroxy-5-cholestanol|cholesterol – PC(38:7)	0.36	0.32	0.47	1

	77. cis-5-Tetradecenoylcarnitine – PC(38:7)	0.38	0.32	0.47	3
	78. Cholic acid – PC(38:7)	-0.37	0.34	0.48	14
	79. PC(36:5) – PC(38:7)	-0.38	0.34	0.48	12
	80. 1-2-dilinoleoyl-sn-glycero-3-PC – PC(38:7)	-0.39	0.34	0.48	11
	81. PC(36:3)|PE(39:3) – PC(38:7)	-0.35	0.35	0.48	11
	82. SPM(41:2) – N-(15Z-tetracosenoyl)-sphinganine-1-PC	0.38	0.35	0.48	10
	83. MAG(16:0) – C16-20:5 PC	-0.39	0.36	0.48	2
	84. MAG(18:3) – C16-20:5 PC	-0.40	0.36	0.48	2
	85. L-Leucine|L-Norleucine – 1-stearoyl-2-hydroxy-sn-glycero-3-PC	-0.40	0.36	0.48	1
	86. Hypoxanthine – 1-stearoyl-2-hydroxy-sn-glycero-3-PC	-0.41	0.41	0.53	3
	87. Caffeine – GCA	-0.40	0.41	0.53	1
	88. Creatinine – 1-Stearoyl-2-Hydroxy-sn-Glycero-3-PE	-0.40	0.41	0.53	1
	89. MAG(18:2) – LPC(0:0/18:2)	-0.41	0.45	0.57	2

	90. Deoxycholic acid – cis-5-Tetradecenoylcarnitine	0.42	0.45	0.57	2
	91. cis-5-Tetradecenoylcarnitine – 2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	0.39	0.46	0.57	3
	92. LPC(0:0/20:4) – Biliverdin hydrochloride b	-0.39	0.46	0.57	2
	93. LPC(20:4/0:0) – Biliverdin hydrochloride b	-0.38	0.52	0.64	4
	94. 4-Androsten-11Beta-ol-3-17-dione|11-Hydroxy-4-androstene-3-17-dione – PC(35:3)|PE(38:3)	0.37	0.55	0.67	10
	95. Arachidonic acid – PC(35:3)|PE(38:3)	0.36	0.57	0.68	1
	96. Myristic acid – PC(36:5)	0.33	0.58	0.68	10
	97. 1-vaccenoyl-2-palmitoyl-sn-glycerol – SPM(40:2)	0.30	0.58	0.68	12
	98. Ceramide PE(33:1)|SPM(30:1) – SPM(40:2)	-0.30	0.61	0.71	1
	99. Ceramide PE(34:1) – SPM(40:2)	-0.29	0.62	0.71	2

	100. Oleoyl-L-carnitine hydrochloride – PC(36:1)	0.28	0.63	0.71	1
	101. Alpha-Tocopherol – PC(36:1)	0.29	0.63	0.71	12
	102. 3a-6b-7b-Trihydroxy-5b-cholanoic acid – PC(36:1)	-0.26	0.65	0.72	10
	103. 1-O-1'-(Z)-octadecenyl-2-hydroxy-sn-glycero-3-phosphoethanolamine – PC(36:1)	-0.27	0.65	0.72	2
	104. D-erythro-sphingosine – PC(36:6)	0.25	0.68	0.75	5
	105. Oleamide – PC(36:6)	0.24	0.71	0.77	3
	106. Piperine – PC(36:6)	0.22	0.73	0.79	5
	107. dehydroepiandrosterone sulfate – PC(35:3)|PE(38:3)	0.22	0.75	0.80	3
	108. LPE(16:0) – PC(35:3)|PE(38:3)	0.20	0.83	0.88	2
	109. LPC(0:0/20:5) – 1,2-dipalmitoleoyl-sn-glycero-3-PC	-0.19	0.85	0.89	1

	110. DL-2-Aminooctanoic acid– LPE(18:1)	0.20	0.86	0.89	1
	111. L-Tyrosine|o-Tyrosine – Biliverdin hydrochloride b	-0.18	0.88	0.90	2
	112. Naproxen – Biliverdin hydrochloride b	-0.15	0.9	0.92	1
	113. L-Tryptophan – Biliverdin hydrochloride b	0.15	0.93	0.94	2
	114. 16. 1-O-1'-(Z)-octadecenyl-2-hydroxy-sn-glycero-3-PE – LPC(20:5/0:0)	0.12	0.97	0.97	2
Association of ratios among molecular features a with age					
Women (*n*=804)	Molecular features	Correlation	*P*-value	BH *P*-value adjusted	Validation (>50%)
	1. Acetaminophen/1-Stearoyl-2-Hydroxy-sn-Glycero-3-PE	-0.67	$2x10^{-4}$	0.002	15
	2. Arachidonic acid ethyl ester/1-vaccenoyl-2-palmitoyl-sn-glycerol	0.67	$2x10^{-4}$	0.002	21
	3. Deoxycholic acid glycine conjugate/N-palmitoyl-D-	0.66	$2x10^{-4}$	0.002	23

	erythro-sphingosylphosphorylcholine				
	4. 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid/PC(15:2/0:0)|PE(18:2/0:0)	-0.64	$2x10^{-4}$	0.002	11
	5. Paraxanthine|Theophylline/GCA	-0.64	$2x10^{-4}$	0.002	1
	6. Arachidonic acid/GCA	-0.63	$2x10^{-4}$	0.002	35
	7. Pantothenic acid/Ceramide PE(35:2)|SPM(32:2)	0.63	$2x10^{-4}$	0.002	3
	8. Acetaminophen/GCA	-0.62	$2x10^{-4}$	0.002	49
	9. Decanoyl-L-carnitine/LPC(0:0/18:2)	-0.67	$3x10^{-4}$	0.002	56
	10. LPC(0:0/20:5)/1,2-dipalmitoleoyl-sn-glycero-3-PC	0.62	$3x10^{-4}$	0.002	23
	11. DL-2-Aminooctanoic acid/LPE(18:1)	-0.61	$3x10^{-4}$	0.002	12
	12. 1-O-1'-(Z)-octadecenyl-2-hydroxy-sn-glycero-3-PE/ LPC(0:0/18:2)	-0.60	$3x10^{-4}$	0.002	2

	13. MAG(16:0)/PC(15:2/0:0)|PE(18:2/0:0)	-0.60	$4x10^{-4}$	0.002	1
	14. 6-hydroxy-5-cholestanol|cholesterol/ PC(15:2/0:0)|PE(18:2/0:0)	-0.60	$4x10^{-4}$	0.002	34
	15. L-Carnitine/1-Stearoyl-2-Hydroxy-sn-Glyce:ro-3-PE	-0.59	$4x10^{-4}$	0.002	33
	16. 1-O-1'-(Z)-octadecenyl-2-hydroxy-sn-glycero-3-PE/LPC(20:5/0:0)	-0.59	$4x10^{-4}$	0.002	25
	17. Arachidonic acid methyl ester/LPC(18:1)	0.60	$4x10^{-4}$	0.002	11
	18. Prostaglandin J2/1-palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	-0.59	0.001	0.005	10
	19. Caffeine/GCA	-0.59	0.001	0.005	42
	20. Creatinine/1-Stearoyl-2-Hydroxy-sn-Glycero-3-PE	-0.59	0.001	0.005	15
	21. 2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3/2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	-0.59	0.001	0.005	12

	22. Arachidonic acid methyl ester/PC(35:3)|PE(38:3)	0.66	0.002	0.009	2
	23. Indolelactic acid/GCA	-0.58	0.002	0.009	34
	24. Pantothenic acid/GCA	-0.58	0.002	0.009	63
	25. Dodecanedioic acid/GCA	-0.58	0.003	0.01	68
	26. Arachidonic acid methyl ester/PC(15:2/0:0)|PE(18:2/0:0)	-0.58	0.003	0.01	15
	27. MAG(20:5)/PC(15:2/0:0)|PE(18:2/0:0)	-0.58	0.004	0.01	2
	28. 7-Ketocholesterol/PC(15:2/0:0)|PE(18:2/0:0)	-0.58	0.004	0.01	2
	29. MAG(18:3)/2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	-0.58	0.004	0.01	1
	30. MAG(18:2)/ LPC(0:0/18:2)	-0.58	0.004	0.01	36
	31. Deoxycholic acid/cis-5-Tetradecenoylcarnitine	0.58	0.004	0.01	34
	32. cis-5-Tetradecenoylcarnitine/2a-(3-	-0.58	0.005	0.02	1

	Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3				
	33. LPE(16:0)/Palmitic acid	0.58	0.005	0.02	2
	34. Arachidonic acid ethyl ester/Biliverdin hydrochloride b	0.58	0.006	0.02	9
	35. Myristic acid/Biliribin II	-0.58	0.006	0.02	21
	36. L-Carnitine/LPC(22:5)	0.67	0.006	0.02	12
	37. Oleoyl-L-carnitine hydrochloride/PC(36:1)	0.68	0.006	0.02	32
	38. Alpha-Tocopherol/PC(36:1)	-0.67	0.006	0.02	21
	39. 3a-6b-7b-Trihydroxy-5b-cholanoic acid/PC(36:1)	-0.66	0.006	0.02	5
	40. 1-O-1'-(Z)-octadecenyl-2-hydroxy-sn-glycero-3-PE/PC(36:1)	-0.65	0.006	0.02	21
	41. Heptadecanoic acid/SPM(40:2)	0.64	0.007	0.02	22
	42. Phenylalanine/SPM(40:2)	0.63	0.007	0.02	31
	43. Ceramide PE(37:2)|SPM(34:2)/SPM(40:2)	0.62	0.007	0.02	15

	44. PC(30:2)/SPM(40:2)	0.62	0.007	0.02	26
	45. N-palmitoyl-D-erythro-sphingosylphosphorylcholine/SPM(40:2)	0.63	0.007	0.02	29
	46. Arachidonic acid/PC(35:3)|PE(38:3)	0.62	0.007	0.02	15
	47. Myristic acid/PC(36:5)	0.61	0.007	0.02	18
	48. 1-vaccenoyl-2-palmitoyl-sn-glycerol/SPM(40:2)	0.61	0.008	0.02	39
	49. Ceramide PE(33:1)|SPM(30:1)/SPM(40:2)	0.60	0.008	0.02	42
	50. Ceramide PE(34:1)/SPM(40:2)	0.60	0.008	0.02	12
	51. 3-cis-Hydroxy-b-e-Caroten-3'-one/N-(9Z-octadecenoyl)-sphing-4-enine-1-PC	-0.59	0.008	0.02	25
	52. Creatinine/1-Stearoyl-2-Hydroxy-sn-Glycero-3-PE	-0.58	0.009	0.02	26
	53. MAG(18:2)/LPC(0:0/18:2)	-0.58	0.009	0.02	15
	54. Deoxycholic acid/cis-5-Tetradecenoylcarnitine	-0.59	0.009	0.02	3

	55. cis-5-Tetradecenoylcarnitine/2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	-0.57	0.009	0.02	15
	56. LPC(0:0/20:4)/Biliverdin hydrochloride b	-0.56	0.009	0.02	19
	57. Lyso-PAF C-18/PC(34:3)	0.57	0.01	0.02	26
	58. PS(18:0)/PC(34:3)	0.56	0.01	0.02	2
	59. LPC(18:3)/PC(34:3)	0.56	0.01	0.02	4
	60. 6-hydroxy-5-cholestanol|cholesterol/Ceramide PE(37:2)|SPM(34:2)	-0.55	0.02	0.03	21
	61. cis-5-Tetradecenoylcarnitine/Ceramide PE(37:2)|SPM(34:2)	-0.55	0.02	0.03	10
	62. Cholic acid/Ceramide PE(37:2)|SPM(34:2)	-0.52	0.05	0.08	11
	63. MAG(18:2)/Ceramide PE(37:2)|SPM(34:2)	-0.53	0.07	0.13	11
	64. MAG(18:1)-Ceramide PE(37:2)|SPM(34:2)	-0.52	0.09	0.15	6
	65. Oleamide/PC(36:6)	0.51	0.10	0.16	9

	66. Piperine/PC(36:6)	0.52	0.10	0.16	15
	67. dehydroepiandrosterone sulfate/PC(35:3)|PE(38:3)	0.51	0.10	0.16	12
	68. Ceramide PE(35:2)|SPM(32:2)/PC(30:1)	0.50	0.14	0.21	3
	69. PC(28:2)/PC(30:1)	0.50	0.14	0.21	12
	70. Ceramide PE(35:1)|SPM(32:1)/PC(30:1)	0.49	0.15	0.22	1
	71. Hippuric acid – Barogenin	-0.48	0.25	0.25	5
	72. L-Acetylcarnitine – Barogenin	-0.47	0.17	0.25	4
	73. Ceramide PE(34:1)/PC(30:1)	0.46	0.19	0.27	7
	74. LPC(22:4)-Ornithine	-0.43	0.19	0.27	16
	75. Biliverdin hydrochloride b-Ornithine	-0.42	0.20	0.27	14
	76. Biliverdin hydrochloride a-Ornithine	-0.40	0.20	0.27	12
	77. LPE(18:2)/1-2-dioleoyl-sn-glycero-3-PC|1-2-dipetroselenoyl-sn-glycero-3-PC	0.41	0.21	0.28	2
	78. PC(15:2/0:0)|PE(18:2/0:0)/1-2-dioleoyl-sn-glycero-3-PC|1-2-	0.40	0.22	0.29	1

	dipetroselenoyl-sn-glycero-3-PC				
	79. LPE(18:1)/1-2-dioleoyl-sn-glycero-3-PC|1-2-dipetroselenoyl-sn-glycero-3-PC	0.39	0.23	0.30	2
	80. 1-oleoyl-2-hydroxy-sn-glycero-3-PE/1-2-dioleoyl-sn-glycero-3-PC|1-2-dipetroselenoyl-sn-glycero-3-PC	-0.39	0.24	0.31	3
	81. Stearic acid/Ornithine	-0.38	0.25	0.32	4
	82. Heptadecanoic acid/MAG(20:5)	0.37	0.27	0.34	54
	83. MAG(16:0)/PC(35:4)|PE(38:4)	-0.36	0.30	0.38	1
	84. 4,8 dimethylnonanoyl carnitine/2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	0.35	0.35	0.43	12
	85. 3-Pyridylacetic acid|trigonelline/1-2-dioleoyl-sn-glycero-3-PC|1-2-	-0.35	0.37	0.45	1

	dipetroselenoyl-sn-glycero-3-PC				
	86. Stachydrine/1-2-dioleoyl-sn-glycero-3-PC|1-2-dipetroselenoyl-sn-glycero-3-PC	-0.34	0.39	0.47	3
	87. Benzenebutanoic acid/1-2-dioleoyl-sn-glycero-3-PC|1-2-dipetroselenoyl-sn-glycero-3-PC	-0.34	0.40	0.49	5
	88. Myristic acid/SPM(d18:2/18:1)	-0.33	0.45	0.53	6
	89. LPC(0:0/16:1)/Ceramide PE(38:2)	-0.33	0.50	0.58	9
	90. LPC(0:0/16:0)/Ceramide PE(38:2)	-0.32	0.51	0.59	4
	91. LPC(18:3)/D-Urobilinogen|I-Urobilin	0.31	0.69	0.798	1
	92. LPC(0:0/18:2)/D-Urobilinogen|I-Urobilin	0.30	0.72	0.81	5
	93. LPC(18:2/0:0)/D-Urobilinogen|I-Urobilin	0.30	0.73	0.82	2

	94. 1-palmitoyl-2-hydroxy-sn-glycero-3-PC/cis/trans-Oleic acid	-0.29	0.75	0.83	1
	95. LPE(20:4)/cis/trans-Oleic acid	-0.29	0.77	0.84	3
	96. PC(O-18:1/0:0)|PC(P-18:0/0:0)/cis/trans-Oleic acid	-0.28	0.79	0.86	6
	97. LPC(18e:0/0:0)/cis/trans-Oleic acid	-0.28	0.81	0.87	5
	98. LPC(22:5)-D-Urobilinogen|I-Urobilin	-0.28	0.82	0.87	1
	99. 5a-Androst-3-en-17-one/PC(35:4)|PE(38:4)	-0.27	0.83	0.87	2
	100. Decanoyl-L-Carnitine/PC(35:4)|PE(38:4)	-0.24	0.91	0.93	1
	101. 4-Androsten-11Beta-ol-3,17-dione|11-Hydroxy-4-androstene-3,17-dione/2a−(3−Hydroxypropyl)−1a−25−dihydroxy−19−norvitamin D3	-0.23	0.91	0.93	1
	102. Gamma-Caprolactone/1-2-dilinoleoyl-sn-glycero-3-PC	-0.18	0.91	0.93	1

	103. Deoxycholic acid glycine conjugate/PC(32:1)	-0.16	0.92	0.93	2
	104. LPC(22:4)-Biliribin II	0.14	0.95	0.95	3
Men (n_M=1078)	1. Arachidonic acid ethyl ester/PC(35:4)|PE(38:4)	0.92	$1x10^{-7}$	$2x10^{-5}$	2
	2. Fatty acid C20:5 methyl ester/PC(35:4)|PE(38:4)	0.9	$4x10^{-7}$	$4x10^{-5}$	16
	3. Cortisol/PC(35:4)|PE(38:4)	0.9	$5x10^{-7}$	$4x10^{-5}$	19
	4. C16 Carnitine/PC(35:4)|PE(38:4)	0.9	$7x10^{-7}$	$4x10^{-5}$	6
	5. 4,8 dimethylnonanoyl carnitine/PC(35:4)|PE(38:4)	0.88	$2x10^{-6}$	$9x10^{-5}$	45
	6. Hippuric acid/PC(34:5)|PE(37:5)	0.87	$3x10^{-6}$	$1x10^{-4}$	43
	7. Deoxycholic acid glycine conjugate/PC(35:4)|PE(38:4)	0.86	$4x10^{-6}$	$1x10^{-4}$	12
	8. 1,3,7-Trimethyluric acid/PC(34:5)|PE(37:5)	0.86	$5x10^{-6}$	$1x10^{-4}$	10
	9. Barogenin/PC(35:4)|PE(38:4)	0.86	$5x10^{-6}$	$1x10^{-4}$	8
	10. 17-phenyl trinor Prostaglandin E2|17-phenyl trinor	0.85	$6x10^{-6}$	$1x10^{-4}$	13

	Prostaglandin D2/PC(35:4)|PE(38:4)				
	11. L-Acetylcarnitine/PC(37:5)|PE(40:5)	0.85	$7x10^{-6}$	$1x10^{-4}$	55
	12. L-Carnitine/PC(37:5)|PE(40:5)	0.85	$1x10^{-5}$	$2x10^{-4}$	51
	13. 2-Ketohexanoic acid/PC(37:5)|PE(40:5)	0.84	$1x10^{-5}$	$2x10^{-4}$	0
	14. Naproxen/PC(37:5)|PE(40:5)	0.85	$1x10^{-5}$	$2x10^{-4}$	46
	15. sodium glycochenodeoxycholate/PC(35:4)|PE(38:4)	0.84	$1x10^{-5}$	$2x10^{-4}$	2
	16. Arachidonic acid ethyl ester/2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	0.83	$2x10^{-5}$	$2x10^{-4}$	35
	17. MAG(16:1)/2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	0.83	$2x10^{-5}$	$2x10^{-4}$	12
	18. 1-oleoyl-2-hydroxy-sn-glycero-3-PE/ 2a−(3−Hydroxypropyl)−1a−25	0.83	$2x10^{-5}$	$2x10^{-4}$	2

	−dihydroxy−19−norvitamin D3				
	19. Indole-3-carbinol/PC(37:5)|PE(40:5)	0.82	$2x10^{-5}$	$2x10^{-4}$	41
	20. L-Phenylalanine/PC(37:5)|PE(40:5)	0.83	$2x10^{-5}$	$2x10^{-4}$	26
	21. L-Tryptophan/PC(37:5)|PE(40:5)	0.83	$2x10^{-5}$	$2x10^{-4}$	11
	22. Caffeine/PC(34:5)|PE(37:5)	0.84	$2x10^{-5}$	$2x10^{-4}$	2
	23. cis-5-Tetradecenoylcarnitine/PC(35:4)|PE(38:4)	0.83	$2x10^{-5}$	$2x10^{-4}$	13
	24. Cholic acid/PC(35:4)|PE(38:4)	0.83	$2x10^{-5}$	$2x10^{-4}$	27
	25. LPE(18:0)/ 2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	0.82	$3x10^{-5}$	$3x10^{-4}$	16
	26. S-(4,5-Dihydro-2-methyl-3-furanyl) ethanethioate/PC(37:5)|PE(40:5)	0.82	$3x10^{-5}$	$3x10^{-4}$	1
	27. Treprostinil/PC(35:4)|PE(38:4)	0.82	$3x10^{-5}$	$3x10^{-4}$	1

	28. Stearic acid/PC(35:4)|PE(38:4)	0.82	$3x10^{-5}$	$3x10^{-4}$	1
	29. Linoleic acid/2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	0.81	$4x10^{-5}$	$3x10^{-4}$	2
	30. Barogenin/2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	0.79	$4x10^{-5}$	$3x10^{-4}$	12
	31. MAG(18:3)/PC(35:4)|PE(38:4)	0.83	$4x10^{-5}$	$3x10^{-4}$	6
	32. Heptadecanoic acid/MAG(20:5)	-0.79	$5x10^{-5}$	$4x10^{-4}$	5
	33. MAG(16:0)/PC(35:4)|PE(38:4)	0.79	$5x10^{-5}$	$4x10^{-4}$	38
	34. 4,8 dimethylnonanoyl carnitine/2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	0.78	$5x10^{-5}$	$4x10^{-4}$	42
	35. 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid/PE(38:4)	0.78	$6x10^{-5}$	$4x10^{-4}$	16
	36. Prostaglandin J2/PC(35:4)|PE(38:4)	0.78	$6x10^{-5}$	$4x10^{-4}$	11
	37. PC(O-18:1/0:0)|PC(P-18:0/0:0)/LPC(20:1)	-0.76	$6x10^{-5}$	$4x10^{-4}$	54

	38. Oleoyl-L-carnitine hydrochloride/2a-(3-Hydroxypropyl)-1a,25-dihydroxy-19-norvitamin D3	0.73	$7x10^{-5}$	$4x10^{-4}$	36
	39. Pantothenic acid/PC(35:4)|PE(38:4)	0.73	$7x10^{-5}$	$4x10^{-4}$	10
	40. 5a-Androst-3-en-17-one/PC(35:4)|PE(38:4)	0.73	$7x10^{-5}$	$4x10^{-4}$	12
	41. Decanoyl-L-Carnitine/PC(35:4)|PE(38:4)	0.73	$7x10^{-5}$	$4x10^{-4}$	5
	42. 4-Androsten-11Beta-ol-3,17-dione|11-Hydroxy-4-androstene-3,17-dione/2a−(3−Hydroxypropyl)−1a−25−dihydroxy−19−norvitamin D3	0.72	$8x10^{-5}$	$4x10^{-4}$	52
	43. MAG(18:2)/PC(35:4)|PE(38:4)	0.71	$8x10^{-5}$	$4x10^{-4}$	54
	44. L-Octanoylcarnitine/LPC(22:5)	0.70	$8x10^{-5}$	$4x10^{-4}$	10
	45. 1-linoleoyl-2-stearoyl-sn-glycerol/Ceramide PE(36:2)	0.70	$9x10^{-5}$	$5x10^{-4}$	12
	46. PC(15:2/0:0)|PE(18:2/0:0)/PC(30:1)	0.70	$1x10^{-4}$	$5x10^{-4}$	36

	47. Flavone/PC(35:4)|PE(38:4)	0.70	$1x10^{-4}$	$5x10^{-4}$	22
	48. Butyryl-L-carnitine|Isobutyryl-L-carnitine/PE(38:4)	0.70	$1x10^{-4}$	$5x10^{-4}$	24
	49. L-Carnitine/LPC(22:5)	0.70	$2x10^{-4}$	0.001	35
	50. 10-nitro-9E-octadecenoic acid|9-nitro-9E-octadecenoic acid/LPC(22:5)	0.70	$2x10^{-4}$	0.001	5
	51. LPC(18e:0/0:0)/PC(40:6)	0.69	$2x10^{-4}$	0.001	10
	52. Lyso-PAF C-18/PC(40:6)	0.69	$3x10^{-4}$	0.001	2
	53. PS(18:0)/PC(40:6)	0.68	$3x10^{-4}$	0.001	6
	54. LPC(18:3)/PC(40:6)	0.69	$3x10^{-4}$	0.001	0
	55. LPC(0:0/18:2)-PC(40:6)	0.68	$3x10^{-4}$	0.001	24
	56. Flavone/SPM(42:3)	-0.68	$4x10^{-4}$	0.002	23
	57. Butyryl-L-carnitine|Isobutyryl-L-carnitine/SPM(42:3)	-0.67	$5x10^{-4}$	0.002	14
	58. Geranyl acetoacetate/SPM(42:3)	-0.67	$5x10^{-4}$	0.002	6
	59. N-(9Z-octadecenoyl)-sphing-4-enine-1-PC/SPM(42:3)	-0.68	$5x10^{-4}$	0.002	1
	60. 1-2-dipalmitoleoyl-sn-glycero-3-PC/SPM(42:3)	-0.66	$5x10^{-4}$	0.002	3

	61. Biliribin I/LacCer(d18:1/14:0)	0.69	$6x10^{-4}$	0.002	12
	62. PC(32:1)-SPM(42:3)	-0.65	$8x10^{-4}$	0.003	17
	63. L-Carnitine/LPC(22:5)	-0.68	$9x10^{-4}$	0.003	9
	64. Biliribin II/PC(34:2)|PE(37:2)	0.69	$9x10^{-4}$	0.003	4
	65. S-(4-5-Dihydro-2-methyl-3-furanyl) ethanethioate/PC(40:5)	0.67	$9x10^{-4}$	0.003	0
	66. L-Carnitine/PC(40:5)	0.69	0.001	0.004	11
	67. L-Phenylalanine/PC(40:5)	0.68	0.001	0.004	1
	68. Treprostinil/ LPC(0:0/18:2)	-0.68	0.001	0.004	9
	69. LPC(0:0/20:5)/1,2-dipalmitoleoyl-sn-glycero-3-PC	-0.67	0.001	0.004	19
	70. DL-2-Aminooctanoic acid/LPE(18:1)	0.65	0.005	0.02	21
	71. 1-O-1'-(Z)-octadecenyl-2-hydroxy-sn-glycero-3-PE/ LPC(0:0/18:2)	-0.67	0.005	0.02	17
	72. 1-O-1'-(Z)-octadecenyl-2-hydroxy-sn-glycero-3-PE/1-2-dioleoyl-sn-glycero-3-PC|1-2-	0.66	0.006	0.02	7

	dipetroselenoyl-sn-glycero-3-PC				
	73. LPE(18:2)/1-2-dioleoyl-sn-glycero-3-PC|1-2-dipetroselenoyl-sn-glycero-3-PC	-0.68	0.007	0.02	4
	74. PC(15:2/0:0)|PE(18:2/0:0)/1-2-dioleoyl-sn-glycero-3-PC|1-2-dipetroselenoyl-sn-glycero-3-PC	-0.66	0.007	0.02	2
	75. LPE(18:1)/1-2-dioleoyl-sn-glycero-3-PC|1-2-dipetroselenoyl-sn-glycero-3-PC	-0.65	0.007	0.02	3
	76. 1-oleoyl-2-hydroxy-sn-glycero-3-PE/1-2-dioleoyl-sn-glycero-3-PC|1-2-dipetroselenoyl-sn-glycero-3-PC	0.65	0.008	0.02	1
	77. Lyso-PAF C-18/PC(34:3)	-0.64	0.008	0.02	3
	78. PS(18:0)/PC(34:3)	-0.63	0.008	0.02	1
	79. LPC(18:3)/PC(34:3)	-0.62	0.008	0.02	10

	80. e-Caprolactam/1-2-dilinoleoyl-sn-glycero-3-PC	0.61	0.008	0.02	12
	81. DL-2-Aminooctanoic acid/1-2-dilinoleoyl-sn-glycero-3-PC	0.62	0.009	0.03	13
	82. Gamma-Caprolactone/1-2-dilinoleoyl-sn-glycero-3-PC	0.61	0.009	0.03	12
	83. Deoxycholic acid glycine conjugate/PC(32:1)	0.60	0.009	0.03	20
	84. Choline/PC(34:3)	-0.60	0.01	0.03	4
	85. Creatinine/PC(34:3)	-0.61	0.01	0.03	6
	86. e-Caprolactam/PC(34:3)	-0.59	0.02	0.06	0
	87. DL-2-Aminooctanoic acid/PC(34:3)	-0.62	0.02	0.06	1
	88. Oleoyl-L-carnitine hydrochloride/PC(36:1)	-0.58	0.02	0.06	22
	89. Alpha-Tocopherol/3a-6b-7b-Trihydroxy-5b-cholanoic acid	-0.62	0.03	0.08	12
	90. 3a-6b-7b-Trihydroxy-5b-cholanoic acid/PC(36:1)	-0.61	0.03	0.08	13
	91. 1-O-1'-(Z)-octadecenyl-2-hydroxy-sn-glycero-3-PE/PC(36:1)	-0.62	0.03	0.08	5

	92. MAG(20:5)/N-(octadecanoyl)-sphing-4-enine-1-PC	0.58	0.03	0.08	4
	93. Acetaminophen/PC(32:1)	0.57	0.03	0.08	2
	94. 2-Ketohexanoic acid/PC(32:1)	0.57	0.04	0.10	6
	95. S-(4-5-Dihydro-2-methyl-3-furanyl) ethanethioate/PC(32:1)	0.57	0.04	0.10	7
	96. L-Carnitine/PC(32:1)	0.56	0.04	0.10	1
	97. e-Caprolactam/Gamma-Caprolactone	-0.53	0.04	0.10	5
	98. DL-2-Aminooctanoic acid/Gamma-Caprolactone	-0.52	0.04	0.10	2
	99. e-Caprolactam/L-Proline	-0.50	0.05	0.12	3
	100. DL-2-Aminooctanoic acid/L-Proline	0.51	0.05	0.12	3
	101. gamma-Glutamyl-leucine/1-2-dipalmitoleoyl-sn-glycero-3-PC	-0.50	0.05	0.12	4
	102. 3-Pyridylacetic acid|trigonelline/1-2-dioleoyl-sn-glycero-3-PC|1-2-	0.50	0.09	0.21	14

	dipetroselenoyl-sn-glycero-3-PC				
	103. Stachydrine/1-2-dioleoyl-sn-glycero-3-PC|1-2-dipetroselenoyl-sn-glycero-3-PC	0.51	0.10	0.23	6
	104. Benzenebutanoic acid/1-2-dioleoyl-sn-glycero-3-PC|1-2-dipetroselenoyl-sn-glycero-3-PC	0.52	0.11	0.25	8
	105. C12 Carnitine/1-2-dipalmitoleoyl-sn-glycero-3-PC	-0.51	0.11	0.25	15
	106. Corticosterone/1-2-dipalmitoleoyl-sn-glycero-3-PC	-0.52	0.12	0.27	0
	107. LPC(0:0/16:1)/N-(9Z-octadecenoyl)-sphing-4-enine-1-PC	0.52	0.12	0.27	11
	108. LPC(16:1/0:0)/N-(9Z-octadecenoyl)-sphing-4-enine-1-PC	0.51	0.12	0.27	2

	109. LPC(0:0/16:0)/N-(9Z-octadecenoyl)-sphing-4-enine-1-PC	0.49	0.13	0.28	13
	110. Heptadecanoic acid/SPM(40:2)	0.48	0.13	0.28	27
	111. Phenylalanine/SPM(40:2)	0.48	0.13	0.28	16
	112. Decanoyl-L-carnitine/SPM(40:2)	-0.48	0.13	0.28	1
	113. 5a-Androst-3-en-17-one/SPM(d18:2/18:1)	0.49	0.14	0.29	1
	114. Propranolol/SPM(d18:2/18:1)	0.49	0.14	0.29	1
	115. gamma-Glutamyl-leucine/SPM(d18:2/18:1)	-0.47	0.14	0.29	2
	116. Myristic acid/SPM(d18:2/18:1)	-0.47	0.14	0.29	12
	117. LPC(0:0/16:1)/Ceramide PE(38:2)	0.46	0.15	0.30	23
	118. LPC(16:1/0:0)/Ceramide PE(38:2)	0.46	0.15	0.30	6

	119. LPC(0:0/16:0)-Ceramide PE(38:2)	0.45	0.15	0.30	9
	120. Oleamide/PC(36:6)	-0.42	0.18	0.36	14
	121. Piperine/PC(36:6)	-0.43	0.22	0.44	2
	122. dehydroepiandrosterone sulfate/PC(35:3)|PE(38:3)	-0.45	0.25	0.50	5
	123. LPC(22:4)/Ornithine	-0.44	0.26	0.51	1
	124. Biliverdin hydrochloride b/Ornithine	-0.44	0.26	0.51	1
	125. Biliverdin hydrochloride a/Ornithine	-0.42	0.27	0.51	1
	126. LPC(22:4)-Biliribin II	-0.41	0.27	0.51	2
	127. 6-hydroxy-5-cholestanol|cholesterol/LPC(20:5/0:0)	-0.40	0.27	0.51	4
	128. cis-5-Tetradecenoylcarnitine/LPC(20:5/0:0)	-0.40	0.27	0.51	12
	129. cis/trans-Oleic acid/PC(30:2)	0.40	0.28	0.51	10
	130. 1-linoleoyl-2-stearoyl-sn-glycerol/PC(30:2)	0.39	0.28	0.51	2

	131. 1-vaccenoyl-2-palmitoyl-sn-glycerol/PC(30:2)	0.38	0.28	0.51	6
	132. Ceramide PE(33:1)|SPM(30:1)/PC(30:2)	-0.39	0.28	0.51	12
	133. Arachidonic acid/1-arachidoyl-2-hydroxy-sn-glycero-3-PC	-0.37	0.28	0.51	3
	134. Heptadecanoic acid/1-arachidoyl-2-hydroxy-sn-glycero-3-PC	-0.37	0.28	0.51	1
	135. SPM(30:1)/PC(30:2)/1-arachidoyl-2-hydroxy-sn-glycero-3-PC	-0.36	0.29	0.52	1
	136. Decanoyl-L-carnitine-1-arachidoyl-2-hydroxy-sn-glycero-3-phosphocholine	-0.35	0.29	0.52	1
	137. 2-6 dimethylheptanoyl carnitine/3-cis-Hydroxy-b-e-Caroten-3'-one	0.34	0.30	0.52	2
	138. 4-Androsten-11Beta-ol-3-17-dione|11-Hydroxy-4-androstene-3-17-dione/3-cis-Hydroxy-b-e-Caroten-3'-one	0.34	0.30	0.52	5

	139. Arachidonic acid/3-cis-Hydroxy-b-e-Caroten-3'-one	0.33	0.30	0.52	2
	140. Decanoyl-L-carnitine/LPC(0:0/18:2)	0.34	0.33	0.56	2
	141. LPC(0:0/20:5)/1,2-dipalmitoleoyl-sn-glycero-3-PC	-0.34	0.33	0.56	3
	142. DL-2-Aminooctanoic acid/LPE(18:1)	-0.33	0.33	0.56	1
	143. MAG(18:3)/3-cis-Hydroxy-b-e-Caroten-3'-one	0.31	0.33	0.56	1
	144. Cholic acid/Ornithine	-0.31	0.33	0.56	2
	145. MAG(18:2)/Ornithine	-0.31	0.34	0.57	4
	146. MAG(18:1)/Ornithine	-0.30	0.35	0.58	1
	147. Stearic acid/Ornithine	-0.30	0.42	0.69	1
	148. L-Proline/Lyso-PAF C-18	0.31	0.43	0.70	5
	149. Betaine/Lyso-PAF C-18	0.29	0.44	0.72	6
	150. Salicylic acid|Aspirin/Lyso-PAF C-18	0.30	0.45	0.72	8

	151. Prostaglandin J2/LPC(20:1)	-0.29	0.45	0.72	2
	152. Hyodeoxycholic acid/LPC(20:1)	-0.32	0.45	0.72	2
	153. Deoxycholic acid/LPC(20:1)	-0.34	0.48	0.75	1
	154. Cortisol/LPC(20:1)	-0.32	0.48	0.75	1
	155. 4-8 dimethylnonanoyl carnitine/LPC(0:0/16:0)	-0.29	0.48	0.75	1
	156. Arachidonic acid ethyl ester/LPC(0:0/16:0)	-0.29	0.49	0.76	1
	157. MAG(18:0)/LPC(0:0/16:0)	-0.28	0.50	0.76	1
	158. 17-phenyl trinor Prostaglandin E2|17-phenyl trinor Prostaglandin D2/LPC(16:1/0:0)	0.27	0.50	0.76	1
	159. Sodium glycochenodeoxycholate/LPC(16:1/0:0)	0.28	0.50	0.76	1

	160. Deoxycholic acid glycine conjugate/LPC(16:1/0:0)	0.29	0.55	0.83	3
	161. Chenodeoxycholic acid/LPC(16:1/0:0)	0.28	0.60	0.89	1
	162. LPC(22:5)/D-Urobilinogen|I-Urobilin	-0.26	0.60	0.89	2
	163. MAG(16:0)/LPC(16:1/0:0)	0.25	0.60	0.89	15
	164. Ceramide PE(35:2)|SPM(32:2)/PC(30:1)	0.27	0.62	0.89	1
	165. PC(28:2)/PC(30:1)	-0.26	0.62	0.91	2
	166. Ceramide PE(35:1)|SPM(32:1)/PC(30:1)	0.26	0.63	0.91	3
	167. PC(30:1)/SPM(40:2)	-0.26	0.63	0.92	1
	168. Deoxycholic acid glycine conjugate/Chenodeoxycholic acid	0.24	0.65	0.92	1
	169. Fatty acid C20:5 methyl ester/PC(34:5)|PE(37:5)	0.25	0.65	0.93	1

	170. PC(28:2)/ 1-oleoyl-2-palmitoyl-sn-glycero-3-PC	0.28	0.67	0.93	1
	171. PC(28:2)/PC(34:0)	-0.25	0.67	0.95	3
	172. L-Phenylalanine/LPC(0:0/16:1)	0.21	0.67	0.95	2
	173. Uric acid/LPC(0:0/16:1)	0.21	0.69	0.95	2
	174. PC(32:1)/PC(35:3)|PE(38:3)	-0.24	0.69	0.95	2
	175. Stearic acid/Palmitic acid	0.22	0.69	0.95	3
	176. Stearic acid/cis/trans-Oleic acid	0.22	0.70	0.95	4
	177. Ceramide PE(35:2)|SPM(32:2)/PC(32:1)	-0.24	0.70	0.95	4
	178. PC(28:2)/PC(32:1)	-0.24	0.70	0.95	1
	179. Deoxycholic acid glycine conjugate/2a-(3-Hydroxypropyl)-1a-25-dihydroxy-19-norvitamin D3	-0.22	0.70	0.95	12
	180. Chenodeoxycholic acid/2a-(3-Hydroxypropyl)-1a-	-0.22	0.71	0.95	1

	25-dihydroxy-19-norvitamin D3				
	181. Linoleyl carnitine/2a-(3-Hydroxypropyl)-1a-25-dihydroxy-19-norvitamin D3	-0.22	0.71	0.95	2
	182. Oleoyl-L-carnitine hydrochloride/2a-(3-Hydroxypropyl)-1a-25-dihydroxy-19-norvitamin D3	-0.23	0.71	0.95	2
	183. Alpha-Tocopherol/2a-(3-Hydroxypropyl)-1a-25-dihydroxy-19-norvitamin D3	-0.22	0.72	0.95	8
	184. cis-5-Tetradecenoylcarnitine/LPC(0:0/16:1)	0.21	0.72	0.95	7
	185. Cholic acid/LPC(0:0/16:1)	0.22	0.72	0.95	11
	186. MAG(18:2)/LPC(0:0/16:1)	0.22	0.73	0.95	1
	187. MAG(18:1)/LPC(0:0/16:1)	0.22	0.74	0.96	2
	188. LPE(18:0)/1-Stearoyl-2-Hydroxy-sn-Glycero-3-PE	0.21	0.74	0.96	3

	189. Choline/2a-(3-Hydroxypropyl)-1a-25-dihydroxy-19-norvitamin D3	-0.21	0.75	0.96	1
	190. Creatinine/2a-(3-Hydroxypropyl)-1a-25-dihydroxy-19-norvitamin D3	-0.21	0.75	0.96	1
	191. Fatty acid C22:6/PC(15:2/0:0)|PE(18:2/0:0)	0.20	0.77	0.97	1
	192. 4-8 dimethylnonanoyl carnitine/PC(15:2/0:0)|PE(18:2/0:0)	0.21	0.77	0.97	5
	193. Arachidonic acid ethyl ester/PC(15:2/0:0)|PE(18:2/0:0)	0.21	0.78	0.97	3
	194. MAG(18:0)/PC(15:2/0:0)|PE(18:2/0:0)	0.20	0.78	0.97	1
	195. Cholic acid/PC(15:2/0:0)|PE(18:2/0:0)	0.20	0.80	0.97	12
	196. 1-palmitoyl-2-hydroxy-sn-glycero-3-PC/cis/trans-Oleic acid	-0.20	0.80	0.97	4

	197. LPE(20:4)/cis/trans-Oleic acid	-0.20	0.81	0.97	2
	198. PC(O-18:1/0:0)|PC(P-18:0/0:0)/cis/trans-Oleic acid	-0.22	0.81	0.97	3
	199. LPC(18e:0/0:0)/cis/trans-Oleic acid	-0.22	0.81	0.97	8
	200. LPE(16:0)/1-palmitoyl-2-hydroxy-sn-glycero-3-PE	0.22	0.82	0.97	7
	201. Choline/GCA	-0.20	0.82	0.97	7
	202. Creatinine/GCA	-0.19	0.82	0.97	6
	203. e-Caprolactam/GCA	-0.19	0.84	0.97	2
	204. DL-2-Aminooctanoic acid/GCA	-0.18	0.84	0.97	2
	205. Gamma-Caprolactone/GCA	-0.18	0.84	0.97	2
	206. C12 Carnitine/Gamma-Tocopherol	0.20	0.85	0.97	1
	207. Corticosterone/Gamma-Tocopherol	0.21	0.85	0.97	2
	208. MAG(16:1)/Gamma-Tocopherol	0.22	0.85	0.97	1

	209. MAG(16:0)/Gamma-Tocopherol	0.22	0.85	0.97	1
	210. Myristic acid/LPE(18:0)	-0.23	0.87	0.97	1
	211. Alpha-Linolenic acid/LPE(18:0)	-0.24	0.87	0.97	3
	212. L-Aspartyl-L-phenylalanine/LPE(18:0)	-0.24	0.87	0.97	2
	213. Propranolol/3a-6b-7b-Trihydroxy-5b-cholanoic acid	0.22	0.90	0.97	1
	214. gamma-Glutamyl-leucine/3a-6b-7b-Trihydroxy-5b-cholanoic acid	0.21	0.90	0.97	1
	215. Myristic acid/3a-6b-7b-Trihydroxy-5b-cholanoic acid	0.20	0.90	0.97	1
	216. Alpha-Linolenic acid/3a-6b-7b-Trihydroxy-5b-cholanoic acid	0.22	0.90	0.97	1
	217. 2-Ketohexanoic acid/Alpha-Tocopherol	0.20	0.91	0.97	1
	218. C12 Carnitine/PC(30:1)	-0.20	0.91	0.97	2

	219. Corticosterone/PC(30:1)	-0.21	0.91	0.97	2
	220. MAG(16:1)/PC(30:1)	-0.21	0.91	0.97	2
	221. MAG(16:0)/PC(30:1)	-0.22	0.92	0.97	1
	222. L-Carnitine/Linoleyl carnitine	-0.20	0.92	0.97	1
	223. L-Phenylalanine/Linoleyl carnitine	-0.18	0.92	0.97	1
	224. Uric acid/Linoleyl carnitine	-0.19	0.92	0.97	1
	225. Indoleacetic acid/Linoleyl carnitine	-0.18	0.92	0.97	2
	226. Paraxanthine|Theophylline/Linoleyl carnitine	-0.17	0.93	0.97	1
	227. MAG(18:0)/3a-6b-7b-Trihydroxy-5b-cholanoic acid	0.18	0.93	0.97	3
	228. PS(18:0)/D-Urobilinogen|I-Urobilin	0.19	0.93	0.97	1
	229. LPC(18:3)/D-Urobilinogen|I-Urobilin	0.19	0.93	0.97	3

	230. LPC(0:0/18:2)/D-Urobilinogen|I-Urobilin	0.19	0.94	0.97	5
	231. LPC(18:2/0:0)/D-Urobilinogen|I-Urobilin	0.18	0.94	0.97	5
	232. Caffeine/LPC(22:5)	-0.16	0.94	0.97	4
	233. Hippuric acid/LPC(22:5)	-0.19	0.94	0.97	1
	234. L-Acetylcarnitine/LPC(22:5)	-0.18	0.95	0.97	6
	235. Indolelactic acid/LPC(22:5)	-0.18	0.95	0.97	1
	236. 1-2-dioleoyl-sn-glycero-3-phosphocholine|1-2-dipetroselenoyl-sn-glycero-3-PC/PC(36:1)	0.17	0.95	0.97	4
	237. Indoleacetic acid/PC(2:7)	0.16	0.95	0.97	1
	238. Paraxanthine|Theophylline/PC(42:7)	0.16	0.96	0.97	3
	239. L-Tyrosine|o-Tyrosine/PC (42:7)	0.15	0.96	0.97	2
	240. Naproxen/PC(42:7)	0.13	0.97	0.97	1

	241. Prostaglandin J2/1-palmitoyl-2-hydroxy-sn-glycero-3-PE	0.12	0.97	0.97	1
	242. Caffeine/GCA	-0.10	0.97	0.97	1
	243. Creatinine/1-Stearoyl-2-Hydroxy-sn-Glycero-3-PE	0.15	0.97	0.97	1

Table S3: Association with age of molecular feature abundances, correlation and ratios for women and men. Compound names, Winsorized Pearson's correlation coefficient, the *P*-values, the Benjamini-Hochberg adjusted *P*-values, and the number of time that the association with age was validated are given. The correlation with age of abundances, correlation and ratios is given by Equations (6) – (8). An overview of the statistical procedure used to establish such association is given in Figure 2. Abbreviations: LPC = Lysophosphatidylcholine; LPE = lysophosphatidylethenolamine; PC = phosphatidylcholine; PE = phosphatidylethanolamine; MAG = monoacylglycerol; GCA = glycocholic acid; SPM = sphingomyelin.