

SUPPLEMENTARY DATA

Supplementary Table 1. Associations of the 365 baseline metabolites measured with incident diabetes

Metabolite	Inference category	Hazard Ratio (95% CI)	p-value*	Homogeneity P value	Coefficient of variation (CV)	Percent Measured (%)
1. Alpha-Glycerophosphocholine	Validation	1.08 (0.98, 1.19)	1.20×10^{-01}	3.21×10^{-01}	7.33	99.73
2. Asparagine	Validation	0.86 (0.77, 0.96)	6.77×10^{-03}	2.41×10^{-01}	14.91	99.73
3. Aspartate	Validation	1.05 (0.96, 1.14)	2.90×10^{-01}	7.23×10^{-02}	1.38	98.93
4. Betaine	Validation	0.81 (0.71, 0.92)	1.06×10^{-03}	8.32×10^{-01}	18.18	99.73
5. Glutamate	Validation	1.08 (0.98, 1.2)	1.32×10^{-01}	4.00×10^{-01}	2.66	99.73
6. Glutamine	Validation	0.85 (0.75, 0.95)	3.94×10^{-03}	7.22×10^{-01}	13.43	99.73
7. Isoleucine	Validation	1.14 (1.06, 1.22)	4.38×10^{-04}	6.81×10^{-01}	14.21	99.58
8. Leucine	Validation	1.09 (0.98, 1.21)	1.05×10^{-01}	6.02×10^{-01}	13.72	99.73
9. Methionine Sulfoxide	Validation	1.09 (1.01, 1.17)	2.46×10^{-02}	7.56×10^{-01}	7.06	99.73
10. Phenylalanine	Validation	1.04 (0.93, 1.16)	5.29×10^{-01}	7.24×10^{-01}	12.99	99.73
11. Serine	Validation	0.86 (0.77, 0.97)	1.10×10^{-02}	8.60×10^{-01}	10.42	99.73
12. Thiamine	Validation	0.91 (0.80, 1.03)	1.27×10^{-01}	8.29×10^{-01}	3.98	99.70
13. Tyrosine	Validation	1.02 (0.91, 1.15)	6.94×10^{-01}	7.37×10^{-01}	11.96	99.73
14. Valine	Validation	1.11 (1.00, 1.24)	6.02×10^{-02}	6.32×10^{-01}	16.74	99.73
15. 1-Methylhistamine	Discovery	1.05 (0.97, 1.15)	2.08×10^{-01}	9.25×10^{-01}	1.96	98.70
16. 1-Methylnicotinamide	Discovery	0.98 (0.86, 1.11)	7.25×10^{-01}	5.23×10^{-03}	20.21	99.73
17. 1,5-AG / 1-Deoxyglucose	Discovery	0.82 (0.73, 0.92)	1.15×10^{-03}	2.00×10^{-01}	3.38	98.82
18. 2-Hydroxybutyric Acid	Discovery	1.11 (1.01, 1.21)	2.52×10^{-02}	2.79×10^{-01}	4.99	98.82

SUPPLEMENTARY DATA

19. 2-Hydroxyglutaric Acid	Discovery	1.04 (0.98, 1.11)	2.16×10^{-01}	9.64×10^{-01}	7.62	98.82
20. 2-Ketoisovaleric Acid KIV	Discovery	1.01 (0.89, 1.13)	9.12×10^{-01}	3.87×10^{-01}	12.78	98.82
21. 3-Hydroxybutyric Acid	Discovery	0.97 (0.86, 1.08)	5.69×10^{-01}	3.05×10^{-02}	2.54	98.82
22. A-Ketoglutaric Acid	Discovery	1.06 (0.98, 1.16)	1.63×10^{-01}	6.64×10^{-01}	4.31	98.82
23. Acetoacetic Acid	Discovery	0.94 (0.84, 1.06)	3.08×10^{-01}	6.73×10^{-01}	7.41	98.82
24. Acetylglycine	Discovery	0.89 (0.77, 1.04)	1.54×10^{-01}	3.78×10^{-01}	2.62	99.62
25. Adenosine	Discovery	1.04 (1.00, 1.08)	3.63×10^{-02}	2.68×10^{-01}	0.60	94.25
26. Adma	Discovery	0.95 (0.85, 1.07)	4.18×10^{-01}	4.63×10^{-01}	9.00	99.73
27. Adp	Discovery	0.94 (0.81, 1.09)	4.28×10^{-01}	4.63×10^{-01}	21.07	91.39
28. Alanine	Discovery	1.05 (0.95, 1.17)	3.21×10^{-01}	8.89×10^{-01}	18.19	99.73
29. Allantoin	Discovery	1.08 (0.97, 1.2)	1.54×10^{-01}	7.99×10^{-01}	5.82	98.82
30. Aminoisobutyric Acid	Discovery	0.99 (0.89, 1.11)	9.11×10^{-01}	5.69×10^{-01}	4.30	99.73
31. Amp	Discovery	1.03 (0.94, 1.12)	5.43×10^{-01}	9.51×10^{-04}	17.08	98.82
32. Arginine	Discovery	1 (0.90, 1.11)	9.72×10^{-01}	8.05×10^{-01}	13.67	99.73
33. Beta-Alanine	Discovery	0.93 (0.84, 1.04)	1.98×10^{-01}	9.08×10^{-01}	4.57	99.73
34. Bilirubin	Discovery	0.78 (0.65, 0.92)	4.33×10^{-03}	2.27×10^{-02}	6.97	98.82
35. Butyrobetaine	Discovery	0.92 (0.80, 1.06)	2.37×10^{-01}	4.17×10^{-01}	15.00	99.73
36. C10 Carnitine	Discovery	0.94 (0.81 , 1.09)	4.17×10^{-01}	2.52×10^{-01}	12.92	99.73
37. C10:2 Carnitine	Discovery	1.00 (0.89, 1.11)	9.39×10^{-01}	3.99×10^{-01}	9.81	99.73
38. C12 Carnitine	Discovery	0.97 (0.85, 1.1)	5.93×10^{-01}	8.18×10^{-01}	8.99	99.73
39. C12:1 Carnitine	Discovery	0.92 (0.82, 1.03)	1.37×10^{-01}	6.22×10^{-01}	10.36	99.73

SUPPLEMENTARY DATA

40. C14 Carnitine	Discovery	0.98 (0.87, 1.1)	6.77×10^{-01}	5.29×10^{-01}	8.64	99.73
41. C14:0 CE	Discovery	1.11 (1.00, 1.22)	5.36×10^{-02}	7.31×10^{-01}	5.83	99.12
42. C14:0 LPC	Discovery	1.05 (0.95, 1.16)	3.69×10^{-01}	9.88×10^{-01}	14.46	99.73
43. C14:0 SM	Discovery	0.89 (0.79, 0.99)	3.41×10^{-02}	1.67×10^{-02}	20.99	99.73
44. C14:1 Carnitine	Discovery	0.89 (0.79, 1.01)	6.17×10^{-02}	7.87×10^{-01}	10.76	99.73
45. C14:2 Carnitine	Discovery	0.90 (0.79, 1.02)	1.05×10^{-01}	7.07×10^{-01}	10.79	99.73
46. C16-OH Carnitine	Discovery	0.97 (0.88, 1.08)	5.95×10^{-01}	2.97×10^{-01}	1.38	96.72
47. C16 Carnitine	Discovery	0.94 (0.83, 1.05)	2.82×10^{-01}	6.33×10^{-01}	10.92	99.73
48. C16:0 CE	Discovery	0.83 (0.74, 0.94)	3.61×10^{-03}	1.43×10^{-02}	19.33	99.73
49. C16:0 Ceramide (d18:1)	Discovery	0.98 (0.87, 1.1)	7.19×10^{-01}	3.87×10^{-02}	5.29	99.73
50. C16:0 LPC	Discovery	1.06 (0.95, 1.18)	3.09×10^{-01}	5.13×10^{-01}	24.25	99.73
51. C16:0 LPE	Discovery	1.10 (1.01, 1.21)	3.10×10^{-02}	4.65×10^{-01}	10.96	99.73
52. C16:0 SM	Discovery	0.82 (0.73 , 0.92)	1.10×10^{-03}	6.89×10^{-02}	21.66	99.73
53. C16:1 CE	Discovery	1.12 (1.01, 1.24)	3.76×10^{-02}	9.28×10^{-01}	18.23	99.73
54. C16:1 LPC	Discovery	0.95 (0.84, 1.07)	3.78×10^{-01}	4.09×10^{-01}	23.78	99.73
55. C16:1 MAG	Discovery	0.84 (0.30, 2.36)	7.48×10^{-01}	7.02×10^{-01}	3.61	99.73
56. C16:1 SM	Discovery	0.80 (0.70, 0.91)	8.15×10^{-04}	2.39×10^{-02}	21.54	99.73
57. C18 Carnitine	Discovery	0.98 (0.86, 1.12)	7.57×10^{-01}	3.84×10^{-02}	5.18	99.73
58. C18:0 CE	Discovery	0.93 (0.84, 1.03)	1.86×10^{-01}	1.12×10^{-01}	12.33	99.73
59. C18:0 LPC	Discovery	1.03 (0.92, 1.15)	6.08×10^{-01}	8.08×10^{-01}	22.20	99.73
60. C18:0 LPE	Discovery	1.11 (1.01, 1.23)	2.85×10^{-02}	8.78×10^{-01}	14.10	99.73

SUPPLEMENTARY DATA

61. C18:0 MAG	Discovery	1.04 (0.95, 1.13)	3.91×10^{-01}	2.86×10^{-01}	16.26	99.73
62. C18:0 SM	Discovery	0.87 (0.77, 0.99)	3.23×10^{-02}	7.06×10^{-01}	20.01	99.73
63. C18:1-OH Carnitine	Discovery	0.99 (0.8 , 1.10)	8.77×10^{-01}	8.29×10^{-01}	1.03	94.93
64. C18:1 Carnitine	Discovery	0.83 (0.73, 0.94)	3.19×10^{-03}	4.73×10^{-01}	10.84	99.73
65. C18:1 LPC	Discovery	0.94 (0.83, 1.08)	3.96×10^{-01}	9.13×10^{-01}	23.52	99.73
66. C18:1 LPE	Discovery	1.06 (0.93, 1.20)	4.02×10^{-01}	2.04×10^{-01}	13.40	99.73
67. C18:1 SM	Discovery	0.81 (0.70, 0.93)	3.24×10^{-03}	4.74×10^{-01}	20.29	99.73
68. C18:2 Carnitine	Discovery	0.88 (0.76, 1.01)	6.02×10^{-02}	9.96×10^{-01}	11.36	99.73
69. C18:2 CE	Discovery	0.83 (0.73, 0.93)	1.75×10^{-03}	4.02×10^{-03}	23.69	99.73
70. C18:2 LPC	Discovery	0.89 (0.78, 1.03)	1.14×10^{-01}	1.25×10^{-01}	22.25	99.73
71. C18:2 LPE	Discovery	0.98 (0.87, 1.11)	7.37×10^{-01}	3.81×10^{-02}	15.67	99.73
72. C18:2 SM	Discovery	0.79 (0.69, 0.91)	8.30×10^{-04}	5.16×10^{-01}	13.04	99.73
73. C18:3 CE	Discovery	1.01 (0.91, 1.13)	8.13×10^{-01}	6.99×10^{-02}	17.74	99.73
74. C2 Carnitine	Discovery	1.01 (0.91, 1.13)	7.90×10^{-01}	5.20×10^{-01}	16.16	99.73
75. C20 Carnitine	Discovery	0.95 (0.84, 1.08)	4.64×10^{-01}	5.42×10^{-01}	2.16	98.51
76. C20:0 SM	Discovery	0.87 (0.78, 0.97)	1.66×10^{-02}	1.25×10^{-01}	19.24	99.73
77. C20:3 CE	Discovery	0.96 (0.85, 1.08)	4.65×10^{-01}	7.85×10^{-01}	18.21	99.73
78. C20:3 LPC	Discovery	1.05 (0.94, 1.17)	3.81×10^{-01}	3.85×10^{-01}	21.00	99.73
79. C20:4 CE	Discovery	0.85 (0.74, 0.97)	1.70×10^{-02}	3.00×10^{-01}	19.41	99.73
80. C20:4 LPC	Discovery	0.98 (0.87, 1.1)	7.36×10^{-01}	5.67×10^{-01}	20.80	99.73
81. C20:4 LPE	Discovery	1.00 (0.89, 1.12)	1.00	2.50×10^{-02}	13.55	99.73

SUPPLEMENTARY DATA

82. C20:5 CE	Discovery	0.94 (0.83, 1.08)	3.92×10^{-01}	3.79×10^{-01}	15.40	99.73
83. C20:5 LPC	Discovery	0.98 (0.86, 1.11)	7.48×10^{-01}	8.48×10^{-01}	21.25	99.73
84. C22:0 Ceramide (d18:1)	Discovery	1.10 (0.99, 1.22)	8.47×10^{-02}	1.16×10^{-01}	11.16	99.73
85. C22:0 SM	Discovery	0.90 (0.81, 1.01)	6.53×10^{-02}	9.70×10^{-02}	20.40	99.73
86. C22:1 MAG	Discovery	1.00 (0.89, 1.11)	9.36×10^{-01}	6.50×10^{-01}	11.54	99.73
87. C22:1 SM	Discovery	0.82 (0.73 , 0.93)	1.74×10^{-03}	3.38×10^{-02}	22.04	99.73
88. C22:4 CE	Discovery	0.84 (0.72, 0.97)	2.02×10^{-02}	5.06×10^{-02}	5.87	98.10
89. C22:5 CE	Discovery	0.85 (0.74, 0.97)	1.67×10^{-02}	2.95×10^{-02}	10.54	99.73
90. C22:6 CE	Discovery	0.83 (0.72, 0.95)	9.53×10^{-03}	1.03×10^{-01}	15.18	99.73
91. C22:6 LPC	Discovery	0.97 (0.87, 1.09)	6.66×10^{-01}	2.60×10^{-01}	21.70	99.73
92. C22:6 LPE	Discovery	1.01 (0.90, 1.12)	9.29×10^{-01}	8.73×10^{-01}	6.61	99.73
93. C24:0 Ceramide (d18:1)	Discovery	1.06 (0.95, 1.17)	2.94×10^{-01}	1.43×10^{-01}	18.38	99.73
94. C24:0 SM	Discovery	0.92 (0.82, 1.03)	1.42×10^{-01}	3.75×10^{-01}	20.28	99.73
95. C24:1 Ceramide (d18:1)	Discovery	1.08 (0.97, 1.21)	1.37×10^{-01}	6.22×10^{-01}	12.69	99.73
96. C24:1 SM	Discovery	0.88 (0.78, 0.99)	3.74×10^{-02}	6.91×10^{-01}	20.24	99.73
97. C26 Carnitine	Discovery	1.03 (0.91, 1.17)	6.03×10^{-01}	1.06×10^{-01}	8.09	99.73
98. C3-Dc-Ch3 Carnitine	Discovery	1.09 (0.97, 1.22)	1.37×10^{-01}	9.06×10^{-01}	4.87	99.73
99. C3 Carnitine	Discovery	1.06 (1.00, 1.13)	4.11×10^{-02}	1.68×10^{-02}	15.26	99.73
100. C30:0 DAG	Discovery	1.16 (1.08, 1.25)	9.37×10^{-05}	1.31×10^{-01}	6.07	95.09
101. C30:0 PC	Discovery	1.11 (1.00, 1.23)	5.51×10^{-02}	5.18×10^{-01}	20.42	99.73
102. C30:1 PC	Discovery	1.10 (0.99 , 1.22)	8.03×10^{-02}	6.29×10^{-01}	18.42	99.70

SUPPLEMENTARY DATA

103. C32:0 DAG	Discovery	1.21 (1.13, 1.30)	1.58×10^{-07}	3.80×10^{-01}	11.48	99.73
104. C32:0 PC	Discovery	1.09 (0.98, 1.21)	1.32×10^{-01}	3.30×10^{-01}	21.93	99.73
105. C32:0 PE	Discovery	0.96 (0.86, 1.07)	4.66×10^{-01}	5.41×10^{-01}	1.75	94.97
106. C32:1 DAG	Discovery	1.18 (1.09, 1.27)	2.67×10^{-05}	5.24×10^{-01}	18.06	99.73
107. C32:1 PC	Discovery	1.11 (1.00, 1.23)	5.24×10^{-02}	4.54×10^{-01}	20.27	99.73
108. C32:2 DAG	Discovery	1.15 (1.06, 1.23)	3.08×10^{-04}	6.91×10^{-01}	4.52	97.18
109. C32:2 PC	Discovery	1.08 (0.96, 1.22)	1.97×10^{-01}	1.28×10^{-02}	22.51	99.73
110. C34:0 DAG	Discovery	1.12 (1.04, 1.20)	1.85×10^{-03}	5.36×10^{-01}	4.71	99.73
111. C34:0 PC	Discovery	0.98 (0.87, 1.11)	7.81×10^{-01}	1.28×10^{-01}	20.77	99.73
112. C34:0 PE	Discovery	0.97 (0.87, 1.08)	5.87×10^{-01}	5.53×10^{-01}	16.51	99.73
113. C34:0 PI	Discovery	1.00 (0.90, 1.11)	9.48×10^{-01}	4.43×10^{-03}	3.97	99.73
114. C34:0 PS	Discovery	0.97 (0.86, 1.10)	6.24×10^{-01}	7.88×10^{-01}	9.30	99.73
115. C34:1 PC	Discovery	1.03 (0.93, 1.16)	5.47×10^{-01}	4.09×10^{-02}	23.04	99.73
116. C34:1 PC Plasmalogen	Discovery	0.82 (0.72, 0.94)	3.38×10^{-03}	1.13×10^{-01}	20.63	99.73
117. C34:1 PC Plasmalogen-B	Discovery	0.87 (0.75, 1.00)	5.27×10^{-02}	8.37×10^{-01}	7.04	99.73
118. C34:1 PI	Discovery	1.11 (1.02, 1.21)	1.49×10^{-02}	9.54×10^{-01}	2.64	99.09
119. C34:2 DAG	Discovery	1.20 (1.09, 1.32)	2.52×10^{-04}	1.96×10^{-01}	17.24	99.73
120. C34:2 PC	Discovery	1.08 (0.95, 1.23)	2.40×10^{-01}	6.31×10^{-03}	21.15	99.73
121. C34:2 PC Plasmalogen	Discovery	0.82 (0.72, 0.93)	2.13×10^{-03}	2.19×10^{-01}	21.70	99.73
122. C34:2 PE	Discovery	1.24 (1.13, 1.35)	2.15×10^{-06}	4.02×10^{-01}	6.89	99.16
123. C34:2 PE Plasmalogen	Discovery	0.96 (0.85, 1.08)	4.79×10^{-01}	6.58×10^{-01}	6.66	99.66

SUPPLEMENTARY DATA

124. C34:3 DAG	Discovery	1.18 (1.06, 1.3)	2.21×10^{-03}	2.40×10^{-01}	19.19	99.73
125. C34:3 PC	Discovery	0.99 (0.87, 1.12)	8.82×10^{-01}	2.50×10^{-02}	22.82	99.73
126. C34:3 PC Plasmalogen	Discovery	0.92 (0.81, 1.04)	1.98×10^{-01}	1.04×10^{-01}	22.96	99.73
127. C34:3 PE Plasmalogen	Discovery	1.00 (0.89, 1.13)	9.84×10^{-01}	4.73×10^{-01}	9.38	99.62
128. C34:4 PC	Discovery	1.08 (0.96, 1.21)	2.20×10^{-01}	4.40×10^{-02}	21.79	99.73
129. C34:4 PC Plasmalogen	Discovery	0.83 (0.73, 0.95)	5.77×10^{-03}	9.27×10^{-01}	3.02	96.11
130. C34:5 PC Plasmalogen	Discovery	0.94 (0.84, 1.05)	2.94×10^{-01}	4.54×10^{-01}	3.10	97.64
131. C36:0 DAG	Discovery	1.04 (0.96, 1.13)	3.48×10^{-01}	8.42×10^{-02}	1.90	99.73
132. C36:0 PC	Discovery	0.89 (0.79, 1.00)	5.46×10^{-02}	4.81×10^{-02}	14.68	99.73
133. C36:0 PE	Discovery	0.94 (0.84, 1.05)	2.92×10^{-01}	6.74×10^{-01}	18.07	99.73
134. C36:1 DAG	Discovery	1.18 (1.10, 1.27)	1.00×10^{-05}	1.48×10^{-01}	19.70	99.73
135. C36:1 PC	Discovery	0.99 (0.90, 1.10)	9.19×10^{-01}	4.42×10^{-02}	20.56	99.73
136. C36:1 PC Plasmalogen	Discovery	0.83 (0.73, 0.94)	3.99×10^{-03}	3.40×10^{-01}	8.98	99.73
137. C36:1 PE	Discovery	1.20 (1.11, 1.30)	1.46×10^{-05}	4.99×10^{-01}	6.16	99.73
138. C36:1 PE Plasmalogen	Discovery	0.81 (0.71, 0.93)	2.63×10^{-03}	8.49×10^{-01}	4.76	98.86
139. C36:1 PS Plasmalogen	Discovery	0.89 (0.80, 0.99)	3.54×10^{-02}	1.01×10^{-01}	17.66	99.73
140. C36:2 DAG	Discovery	1.15 (1.05, 1.27)	4.66×10^{-03}	1.78×10^{-01}	24.57	99.73
141. C36:2 PC	Discovery	1.01 (0.90, 1.13)	8.40×10^{-01}	1.17×10^{-03}	20.79	99.73
142. C36:2 PC Plasmalogen	Discovery	0.85 (0.75, 0.97)	1.63×10^{-02}	2.17×10^{-01}	20.59	99.73
143. C36:2 PE	Discovery	1.26 (1.15, 1.38)	6.96×10^{-07}	2.66×10^{-01}	13.73	99.73
144. C36:2 PE Plasmalogen	Discovery	0.96 (0.85, 1.08)	4.54×10^{-01}	9.14×10^{-01}	7.89	99.73

SUPPLEMENTARY DATA

145. C36:2 PS Plasmalogen	Discovery	0.92 (0.82, 1.02)	1.27×10^{-01}	7.22×10^{-02}	18.37	99.73
146. C36:3 DAG	Discovery	1.12 (1.00, 1.26)	4.55×10^{-02}	3.81×10^{-01}	24.48	99.73
147. C36:3 PC	Discovery	1.01 (0.90, 1.14)	8.57×10^{-01}	3.19×10^{-02}	22.79	99.73
148. C36:3 PC Plasmalogen	Discovery	0.92 (0.81, 1.05)	2.29×10^{-01}	7.81×10^{-01}	20.18	99.73
149. C36:3 PE	Discovery	1.18 (1.07, 1.31)	1.66×10^{-03}	3.08×10^{-01}	10.12	99.73
150. C36:3 PE Plasmalogen	Discovery	1.04 (0.92, 1.17)	5.45×10^{-01}	4.80×10^{-01}	10.88	99.73
151. C36:3 PS Plasmalogen	Discovery	1.08 (0.97, 1.19)	1.53×10^{-01}	1.37×10^{-01}	6.77	98.90
152. C36:4 DAG	Discovery	1.08 (0.96, 1.21)	1.80×10^{-01}	6.81×10^{-01}	21.82	99.73
153. C36:4 Pc-A	Discovery	0.98 (0.87, 1.10)	7.25×10^{-01}	7.98×10^{-03}	20.68	99.73
154. C36:4 Pc-B	Discovery	1.08 (0.96, 1.22)	1.86×10^{-01}	5.07×10^{-01}	21.35	99.73
155. C36:4 PC Plasmalogen	Discovery	0.78 (0.68, 0.90)	4.68×10^{-04}	3.19×10^{-01}	13.43	99.73
156. C36:4 PE	Discovery	1.22 (1.11, 1.34)	2.27×10^{-05}	3.58×10^{-01}	11.08	99.70
157. C36:4 PE Plasmalogen	Discovery	0.97 (0.85, 1.09)	5.92×10^{-01}	3.36×10^{-01}	7.81	99.73
158. C36:5 PC Plasmalogen-A	Discovery	0.96 (0.86, 1.08)	5.25×10^{-01}	2.50×10^{-01}	15.29	99.73
159. C36:5 PC Plasmalogen-B	Discovery	0.93 (0.83, 1.04)	2.06×10^{-01}	2.63×10^{-01}	22.54	99.73
160. C36:5 PE Plasmalogen	Discovery	0.95 (0.85, 1.07)	4.37×10^{-01}	3.22×10^{-01}	15.55	99.73
161. C38:2 PC	Discovery	1.01 (0.90, 1.12)	9.19×10^{-01}	4.03×10^{-02}	22.45	99.73
162. C38:2 PE	Discovery	0.91 (0.79, 1.03)	1.42×10^{-01}	4.63×10^{-03}	20.80	99.73
163. C38:3 PC	Discovery	1.09 (0.98, 1.20)	1.16×10^{-01}	6.85×10^{-02}	22.26	99.73
164. C38:3 PE Plasmalogen	Discovery	1.00 (0.88, 1.13)	9.55×10^{-01}	9.64×10^{-01}	8.05	99.73
165. C38:4 DAG	Discovery	1.20 (1.10, 1.31)	4.89×10^{-05}	1.05×10^{-01}	3.76	99.73

SUPPLEMENTARY DATA

166. C38:4 PC	Discovery	0.96 (0.86, 1.08)	5.19×10^{-01}	5.26×10^{-02}	18.57	99.73
167. C38:4 PC Plasmalogen	Discovery	0.92 (0.81, 1.05)	2.17×10^{-01}	1.13×10^{-01}	21.53	99.73
168. C38:4 PE	Discovery	1.23 (1.11, 1.36)	6.01×10^{-05}	3.62×10^{-01}	14.02	99.73
169. C38:4 PI	Discovery	1.05 (0.94, 1.18)	3.87×10^{-01}	2.06×10^{-01}	8.26	99.73
170. C38:5 DAG	Discovery	1.16 (1.06, 1.26)	8.36×10^{-04}	1.05×10^{-01}	19.47	99.73
171. C38:5 PE	Discovery	1.13 (1.01, 1.27)	3.91×10^{-02}	2.39×10^{-01}	6.71	99.73
172. C38:5 PE Plasmalogen	Discovery	0.98 (0.88, 1.10)	7.32×10^{-01}	4.96×10^{-01}	17.35	99.73
173. C38:6 PC	Discovery	0.92 (0.81, 1.04)	1.66×10^{-01}	6.55×10^{-01}	20.62	99.73
174. C38:6 PC Plasmalogen	Discovery	0.87 (0.77, 0.98)	2.02×10^{-02}	3.94×10^{-01}	22.25	99.73
175. C38:6 PE	Discovery	1.17 (1.06, 1.29)	1.96×10^{-03}	9.40×10^{-01}	11.14	99.73
176. C38:6 PE Plasmalogen	Discovery	0.96 (0.85, 1.08)	4.73×10^{-01}	6.91×10^{-01}	17.06	99.73
177. C38:6 PS	Discovery	0.98 (0.87, 1.10)	6.97×10^{-01}	4.48×10^{-01}	1.71	90.29
178. C38:7 PC Plasmalogen	Discovery	0.91 (0.81, 1.02)	1.03×10^{-01}	1.15×10^{-01}	17.41	99.73
179. C38:7 PE Plasmalogen	Discovery	0.93 (0.83, 1.05)	2.24×10^{-01}	2.35×10^{-01}	15.19	99.73
180. C4-OH Carnitine	Discovery	1.06 (0.98, 1.15)	1.47×10^{-01}	4.50×10^{-01}	7.93	99.70
181. C4 Carnitine	Discovery	1.07 (0.98, 1.17)	1.12×10^{-01}	1.81×10^{-01}	13.64	99.73
182. C40:10 PC	Discovery	0.87 (0.76, 0.99)	3.40×10^{-02}	5.73×10^{-01}	10.91	99.73
183. C40:6 PC	Discovery	1.08 (0.98, 1.20)	1.31×10^{-01}	1.19×10^{-01}	22.70	99.73
184. C40:6 PE	Discovery	1.22 (1.1 , 1.34)	1.06×10^{-04}	8.04×10^{-01}	1.53	90.55
185. C40:6 PS	Discovery	1.00 (0.90, 1.11)	9.88×10^{-01}	6.49×10^{-01}	8.57	99.73
186. C40:7 PC Plasmalogen	Discovery	0.85 (0.75, 0.97)	1.45×10^{-02}	2.04×10^{-01}	20.29	99.73

SUPPLEMENTARY DATA

187. C40:7 PE Plasmalogen	Discovery	0.93 (0.83, 1.05)	2.32×10^{-01}	1.12×10^{-01}	10.85	99.73
188. C40:9 PC	Discovery	0.91 (0.80, 1.03)	1.19×10^{-01}	5.50×10^{-01}	19.09	99.73
189. C42:0 TAG	Discovery	1.19 (1.09, 1.30)	6.54×10^{-05}	5.65×10^{-01}	5.63	99.58
190. C44:0 TAG	Discovery	1.25 (1.15, 1.36)	1.07×10^{-07}	9.74×10^{-01}	10.48	99.73
191. C44:1 TAG	Discovery	1.24 (1.14, 1.34)	2.09×10^{-07}	8.80×10^{-01}	13.22	99.73
192. C44:13 PE Plasmalogen	Discovery	0.93 (0.82, 1.05)	2.19×10^{-01}	4.90×10^{-03}	4.52	99.66
193. C44:2 TAG	Discovery	1.22 (1.14, 1.31)	3.84×10^{-08}	8.72×10^{-01}	12.22	99.58
194. C46:0 TAG	Discovery	1.24 (1.14, 1.34)	1.52×10^{-07}	9.08×10^{-01}	17.16	99.73
195. C46:1 TAG	Discovery	1.27 (1.16, 1.39)	2.41×10^{-07}	9.69×10^{-01}	17.89	99.73
196. C46:2 TAG	Discovery	1.26 (1.16, 1.38)	1.72×10^{-07}	9.03×10^{-01}	19.75	99.73
197. C46:3 TAG	Discovery	1.24 (1.13, 1.35)	1.16×10^{-06}	9.16×10^{-01}	17.48	99.73
198. C46:4 TAG	Discovery	1.19 (1.10, 1.29)	1.63×10^{-05}	6.55×10^{-01}	3.96	99.35
199. C48:0 TAG	Discovery	1.28 (1.18, 1.38)	2.53×10^{-09}	6.43×10^{-01}	20.15	99.73
200. C48:1 TAG	Discovery	1.28 (1.17, 1.41)	1.66×10^{-07}	8.58×10^{-01}	22.52	99.73
201. C48:2 TAG	Discovery	1.24 (1.12, 1.38)	5.30×10^{-05}	8.02×10^{-01}	22.58	99.73
202. C48:3 TAG	Discovery	1.22 (1.10, 1.36)	2.21×10^{-04}	6.93×10^{-01}	20.56	99.73
203. C48:4 TAG	Discovery	1.23 (1.11, 1.35)	2.65×10^{-05}	7.97×10^{-01}	21.85	99.73
204. C48:5 TAG	Discovery	1.22 (1.11, 1.34)	2.54×10^{-05}	8.13×10^{-01}	5.19	99.66
205. C5-DC Carnitine	Discovery	1.20 (1.08, 1.33)	8.96×10^{-04}	7.79×10^{-02}	8.51	99.73
206. C5 Carnitine	Discovery	1.13 (1.04, 1.23)	5.63×10^{-03}	4.25×10^{-01}	15.15	99.73
207. C5:1 Carnitine	Discovery	1.03 (0.94, 1.13)	5.73×10^{-01}	3.03×10^{-01}	8.42	99.73

SUPPLEMENTARY DATA

208. C50:0 TAG	Discovery	1.26 (1.16, 1.36)	2.31×10^{-08}	4.03×10^{-01}	19.04	99.73
209. C50:1 TAG	Discovery	1.34 (1.21, 1.49)	5.20×10^{-08}	4.17×10^{-01}	23.13	99.73
210. C50:2 TAG	Discovery	1.29 (1.17, 1.44)	9.33×10^{-07}	4.44×10^{-01}	19.57	99.73
211. C50:3 TAG	Discovery	1.19 (1.05, 1.34)	4.70×10^{-03}	1.85×10^{-01}	23.25	99.73
212. C50:4 TAG	Discovery	1.11 (0.99, 1.24)	8.24×10^{-02}	1.92×10^{-01}	19.96	99.73
213. C50:5 TAG	Discovery	1.13 (1.01, 1.25)	2.63×10^{-02}	3.77×10^{-01}	23.34	99.73
214. C50:6 TAG	Discovery	1.22 (1.09, 1.35)	2.97×10^{-04}	7.46×10^{-01}	9.15	99.73
215. C52:0 TAG	Discovery	1.17 (1.08, 1.26)	1.14×10^{-04}	7.31×10^{-01}	8.21	99.73
216. C52:1 TAG	Discovery	1.26 (1.15, 1.39)	1.04×10^{-06}	3.66×10^{-01}	21.38	99.73
217. C52:3 TAG	Discovery	1.11 (0.99, 1.25)	6.96×10^{-02}	1.94×10^{-01}	24.58	99.73
218. C52:4 TAG	Discovery	1.05 (0.94, 1.18)	3.67×10^{-01}	3.07×10^{-01}	22.49	99.73
219. C52:5 TAG	Discovery	1.02 (0.91, 1.15)	6.85×10^{-01}	1.85×10^{-01}	21.23	99.73
220. C52:6 TAG	Discovery	1.07 (0.96, 1.19)	2.23×10^{-01}	3.54×10^{-01}	19.57	99.73
221. C52:7 TAG	Discovery	1.11 (0.99, 1.23)	7.36×10^{-02}	6.84×10^{-01}	13.11	99.73
222. C54:1 TAG	Discovery	1.17 (1.08, 1.27)	7.63×10^{-05}	6.94×10^{-01}	15.91	99.73
223. C54:10 TAG	Discovery	0.94 (0.84, 1.04)	2.05×10^{-01}	6.09×10^{-02}	8.63	99.73
224. C54:2 TAG	Discovery	1.18 (1.07, 1.3)	8.55×10^{-04}	4.76×10^{-01}	20.10	99.73
225. C54:3 TAG	Discovery	1.11 (0.99, 1.25)	8.55×10^{-02}	3.49×10^{-01}	24.08	99.73
226. C54:4 TAG	Discovery	0.99 (0.88, 1.11)	8.52×10^{-01}	3.54×10^{-01}	23.22	99.73
227. C54:5 TAG	Discovery	1.03 (0.91, 1.17)	6.02×10^{-01}	6.39×10^{-01}	21.55	99.73
228. C54:6 TAG	Discovery	1.16 (1.05, 1.29)	3.64×10^{-03}	4.65×10^{-01}	17.33	99.73

SUPPLEMENTARY DATA

229. C54:7 TAG	Discovery	1.11 (1.00, 1.24)	6.03×10^{-02}	9.46×10^{-01}	16.04	99.73
230. C54:8 TAG	Discovery	1.05 (0.95, 1.17)	3.33×10^{-01}	7.16×10^{-01}	13.72	99.73
231. C54:9 TAG	Discovery	1.05 (0.94, 1.18)	3.87×10^{-01}	8.62×10^{-01}	1.08	97.90
232. C56:10 TAG	Discovery	1.04 (0.93, 1.16)	5.13×10^{-01}	9.59×10^{-01}	2.52	99.50
233. C56:2 TAG	Discovery	1.09 (1.00, 1.18)	3.77×10^{-02}	7.04×10^{-02}	9.55	99.73
234. C56:3 TAG	Discovery	1.17 (1.07, 1.28)	4.32×10^{-04}	4.23×10^{-01}	21.50	99.73
235. C56:4 TAG	Discovery	1.15 (1.02, 1.28)	1.69×10^{-02}	3.75×10^{-01}	22.59	99.73
236. C56:5 TAG	Discovery	1.11 (1.00, 1.23)	6.07×10^{-02}	4.26×10^{-01}	11.25	99.73
237. C56:7 TAG	Discovery	1.12 (1.00, 1.27)	5.65×10^{-02}	8.39×10^{-01}	22.87	99.73
238. C56:8 TAG	Discovery	1.06 (0.94, 1.19)	3.72×10^{-01}	7.39×10^{-01}	19.11	99.73
239. C56:9 TAG	Discovery	1.04 (0.93, 1.16)	5.09×10^{-01}	9.41×10^{-01}	16.02	99.73
240. C58:10 TAG	Discovery	1.04 (0.92, 1.17)	5.32×10^{-01}	8.06×10^{-01}	16.95	99.73
241. C58:11 TAG	Discovery	1.04 (0.93, 1.16)	4.97×10^{-01}	8.02×10^{-01}	7.31	99.62
242. C58:6 TAG	Discovery	1.19 (1.09, 1.3)	1.49×10^{-04}	8.68×10^{-01}	15.78	99.73
243. C58:7 TAG	Discovery	1.09 (0.97, 1.23)	1.62×10^{-01}	6.30×10^{-01}	12.91	99.73
244. C58:8 TAG	Discovery	1.06 (0.93, 1.21)	3.71×10^{-01}	3.83×10^{-01}	6.33	99.73
245. C58:9 TAG	Discovery	1.04 (0.92, 1.18)	5.06×10^{-01}	5.17×10^{-01}	17.25	99.73
246. C6 Carnitine	Discovery	1.02 (0.90, 1.16)	7.50×10^{-01}	7.55×10^{-01}	10.79	99.73
247. C60:12 TAG	Discovery	1.02 (0.90, 1.16)	7.17×10^{-01}	4.00×10^{-01}	3.02	98.82
248. C7 Carnitine	Discovery	1.01 (0.90, 1.13)	8.79×10^{-01}	1.81×10^{-01}	2.17	99.66
249. C8 Carnitine	Discovery	0.96 (0.81, 1.14)	6.77×10^{-01}	1.39×10^{-01}	5.66	99.73

SUPPLEMENTARY DATA

250. C9 Carnitine	Discovery	0.95 (0.85, 1.07)	4.25×10^{-01}	5.40×10^{-01}	8.66	99.73
251. Carnitine	Discovery	1.05 (0.94, 1.18)	3.73×10^{-01}	3.38×10^{-01}	20.28	99.73
252. Choline	Discovery	1.03 (0.91, 1.16)	6.67×10^{-01}	7.09×10^{-01}	17.92	99.73
253. Citrulline (MGH)	Discovery	1.00 (0.89, 1.12)	1.00	8.60×10^{-01}	6.78	90.29
254. Citrulline	Discovery	0.96 (0.85, 1.09)	5.63×10^{-01}	5.37×10^{-01}	12.55	99.73
255. Cotinine	Discovery	1.12 (1.04, 1.20)	2.23×10^{-03}	7.10×10^{-01}	2.01	99.62
256. Creatine	Discovery	1.07 (0.96, 1.19)	1.99×10^{-01}	2.35×10^{-01}	13.23	99.73
257. Cyclic-AMP	Discovery	0.92 (0.82, 1.03)	1.47×10^{-01}	7.51×10^{-01}	15.38	98.82
258. Cytosine	Discovery	0.77 (0.67, 0.89)	4.93×10^{-04}	3.35×10^{-01}	2.50	99.70
259. D-Gluconic Acid	Discovery	1.04 (0.97, 1.13)	2.50×10^{-01}	8.17×10^{-01}	6.04	98.82
260. Deoxycholic Acid	Discovery	1.00 (0.90, 1.12)	9.66×10^{-01}	6.54×10^{-01}	3.41	98.82
261. Dimethylglycine	Discovery	1.06 (1.04, 1.08)	1.22×10^{-09}	5.41×10^{-01}	13.51	99.73
262. Dmgv	Discovery	1.07 (0.96, 1.20)	2.21×10^{-01}	3.26×10^{-01}	10.42	99.85
263. Fumaric Acid	Discovery	0.90 (0.80, 1.02)	9.51×10^{-02}	5.36×10^{-01}	24.89	98.82
264. Gaba	Discovery	0.95 (0.85, 1.06)	3.67×10^{-01}	8.07×10^{-01}	7.64	99.73
265. Glucose/Fructose/Galactose	Discovery	1.42 (1.25, 1.61)	5.54×10^{-08}	2.33×10^{-01}	2.67	98.82
266. Glutathione_reduced	Discovery	0.99 (0.89, 1.11)	9.02×10^{-01}	1.10×10^{-01}	15.93	96.88
267. Glyceric Acid	Discovery	0.94 (0.83, 1.08)	3.90×10^{-01}	1.50×10^{-01}	5.99	98.82
268. Glycine	Discovery	0.82 (0.72, 0.94)	3.12×10^{-03}	2.81×10^{-01}	16.84	99.73
269. Glycochenodeoxycholic Acid	Discovery	1.04 (0.94, 1.16)	4.40×10^{-01}	8.88×10^{-01}	3.33	98.82

SUPPLEMENTARY DATA

270. Glycocholic Acid	Discovery	1.06 (0.98, 1.14)	1.52×10^{-01}	2.56×10^{-02}	6.95	98.82
271. Hippuric Acid	Discovery	0.94 (0.84, 1.06)	3.44×10^{-01}	9.06×10^{-01}	2.98	98.82
272. Histamine	Discovery	0.98 (0.91, 1.06)	6.62×10^{-01}	9.97×10^{-01}	2.04	98.36
273. Histidine	Discovery	0.95 (0.85, 1.07)	3.99×10^{-01}	5.25×10^{-01}	10.67	99.73
274. Homogentisic Acid	Discovery	1.06 (0.95, 1.17)	3.23×10^{-01}	2.38×10^{-01}	16.68	98.82
275. Hydroxyphenylpyruvic Acid	Discovery	1.00 (0.90, 1.12)	9.69×10^{-01}	6.65×10^{-01}	12.81	98.82
276. Hydroxyproline	Discovery	1.03 (0.93, 1.15)	5.28×10^{-01}	1.32×10^{-01}	13.80	99.73
277. Hypoxanthine	Discovery	1.07 (0.96, 1.21)	2.18×10^{-01}	4.73×10^{-01}	3.36	98.82
278. Indole-3-Carboxylic Acid	Discovery	1.11 (1.02, 1.22)	1.68×10^{-02}	8.44×10^{-01}	11.80	98.82
279. Indole-3-Lactic Acid	Discovery	1.09 (0.99, 1.21)	9.46×10^{-02}	2.63×10^{-01}	4.06	98.82
280. Indole-3-Propanoic Acid	Discovery	0.94 (0.84, 1.07)	3.53×10^{-01}	8.91×10^{-03}	3.47	98.82
281. Indoxyl-Sulfate	Discovery	0.90 (0.80, 1.01)	7.73×10^{-02}	5.85×10^{-02}	2.43	98.82
282. Inosine	Discovery	1.08 (1.02, 1.15)	1.33×10^{-02}	4.96×10^{-01}	8.44	98.82
283. Keto-Isocaproic Acid KIC / Keto-Methylvalerate KMV	Discovery	1.03 (0.92, 1.15)	6.23×10^{-01}	6.38×10^{-02}	5.21	98.82
284. Kynurenic Acid	Discovery	0.88 (0.77, 0.99)	3.59×10^{-02}	1.39×10^{-01}	4.49	99.73
285. Kynurenic Acid (MGH)	Discovery	0.94 (0.82, 1.08)	3.69×10^{-01}	4.15×10^{-01}	5.78	98.82
286. Kynurenine	Discovery	1.01 (0.90, 1.13)	8.55×10^{-01}	7.76×10^{-01}	3.83	98.82
287. Lactic Acid	Discovery	1.09 (0.99, 1.20)	7.81×10^{-02}	3.15×10^{-01}	2.26	98.82
288. Lysine	Discovery	1.05 (0.95, 1.16)	3.51×10^{-01}	5.01×10^{-01}	12.83	99.73
289. Malic Acid	Discovery	1.07 (0.96, 1.19)	2.42×10^{-01}	6.64×10^{-01}	4.91	95.01

SUPPLEMENTARY DATA

290. Malonic Acid	Discovery	1.07 (0.98, 1.17)	1.28×10^{-01}	3.29×10^{-01}	10.48	98.82
291. Methionine	Discovery	0.98 (0.86, 1.11)	7.46×10^{-01}	4.60×10^{-01}	13.1	99.73
292. Methyl-Hydroxyisobutyric Acid	Discovery	1.00 (0.91, 1.1)	9.58×10^{-01}	2.17×10^{-01}	5.98	99.73
293. Methylthioadenosine	Discovery	0.96 (0.85, 1.09)	5.66×10^{-01}	3.34×10^{-02}	0.60	94.86
294. N-Carbamoyl-Beta-Alanine	Discovery	0.98 (0.91, 1.07)	6.94×10^{-01}	6.43×10^{-01}	3.46	99.73
295. Niacinamide	Discovery	0.97 (0.88, 1.07)	4.99×10^{-01}	3.02×10^{-01}	2.63	99.73
296. Nmma	Discovery	1.10 (1.00, 1.2)	4.19×10^{-02}	1.83×10^{-01}	6.80	99.73
297. Ornithine	Discovery	1.03 (0.93, 1.15)	5.91×10^{-01}	6.70×10^{-01}	12.29	99.73
298. Orotic Acid	Discovery	0.99 (0.90, 1.09)	8.53×10^{-01}	1.57×10^{-01}	6.32	98.82
299. Oxalic Acid	Discovery	0.93 (0.81, 1.07)	3.12×10^{-01}	5.63×10^{-01}	8.05	96.88
300. Oxaloacetic Acid	Discovery	1.05 (0.95, 1.16)	3.55×10^{-01}	3.23×10^{-01}	16.51	98.82
301. Pantothenic Acid	Discovery	0.95 (0.82, 1.1)	4.68×10^{-01}	6.04×10^{-02}	3.73	98.82
302. Phosphocholine	Discovery	1.05 (0.95, 1.15)	3.35×10^{-01}	9.78×10^{-01}	4.13	99.70
303. Pипecolic Acid	Discovery	1.03 (0.95 , 1.11)	4.54×10^{-01}	2.40×10^{-01}	9.75	99.73
304. Proline	Discovery	0.95 (0.84, 1.06)	3.50×10^{-01}	7.34×10^{-01}	17.25	99.73
305. Pseudouridine	Discovery	1.09 (0.97, 1.22)	1.59×10^{-01}	6.35×10^{-01}	3.07	98.82
306. Putrescine	Discovery	0.91 (0.79, 1.04)	1.52×10^{-01}	6.83×10^{-01}	3.98	99.05
307. Pyroglutamic Acid (MGH)	Discovery	1.01 (0.91, 1.13)	7.90×10^{-01}	5.96×10^{-02}	6.47	98.82
308. Pyroglutamic Acid	Discovery	1.03 (0.93, 1.14)	5.35×10^{-01}	4.47×10^{-02}	4.00	99.73
309. Pyruvic Acid	Discovery	1.00 (0.90, 1.10)	9.49×10^{-01}	2.64×10^{-01}	3.39	98.82
310. Quinolinic Acid	Discovery	0.98 (0.88, 1.1)	7.30×10^{-01}	6.91×10^{-01}	7.50	98.82

SUPPLEMENTARY DATA

		1.10)				
311. S-Adenosyl-L-Homocysteine	Discovery	1.11 (0.99, 1.24)	7.91×10^{-02}	1.45×10^{-01}	22.69	98.82
312. Sarcosine	Discovery	0.98 (0.87, 1.10)	7.22×10^{-01}	2.14×10^{-01}	4.29	99.73
313. Sdma	Discovery	0.97 (0.86, 1.10)	6.07×10^{-01}	4.05×10^{-01}	7.74	99.73
314. Serotonin	Discovery	0.98 (0.89, 1.09)	7.05×10^{-01}	4.37×10^{-01}	2.59	98.67
315. Spermidine	Discovery	0.86 (0.69, 1.09)	2.10×10^{-01}	3.45×10^{-01}	1.09	99.54
316. Sphingosine	Discovery	0.94 (0.78, 1.15)	5.68×10^{-01}	6.95×10^{-01}	4.39	99.70
317. Succinic Acid/methylmalonic Acid	Discovery	1.02 (0.96, 1.08)	5.54×10^{-01}	6.93×10^{-01}	4.63	98.82
318. Taurine	Discovery	0.95 (0.85, 1.07)	3.93×10^{-01}	5.77×10^{-01}	13.76	99.73
319. Taurine (MGH)	Discovery	0.96 (0.86, 1.08)	5.16×10^{-01}	2.85×10^{-01}	2.57	98.82
320. Taurocholic Acid	Discovery	1.06 (0.99, 1.13)	1.03×10^{-01}	2.32×10^{-02}	20.27	98.82
321. Taurodeoxycholic Acid / Taurochenodeoxycholic Acid	Discovery	1.02 (0.94, 1.11)	6.22×10^{-01}	5.85×10^{-01}	6.85	98.82
322. Threonine	Discovery	0.95 (0.85, 1.06)	3.43×10^{-01}	7.76×10^{-01}	5.56	99.73
323. Thyroxine	Discovery	0.98 (0.87, 1.10)	6.81×10^{-01}	2.47×10^{-01}	6.04	99.70
324. Trimethylamine-N-Oxide	Discovery	1.09 (1.01, 1.18)	1.91×10^{-02}	2.12×10^{-01}	20.91	99.73
325. Tryptophan	Discovery	0.99 (0.88, 1.11)	8.19×10^{-01}	2.83×10^{-01}	19.51	99.73
326. Uric Acid	Discovery	1.10 (0.98, 1.24)	9.49×10^{-02}	4.70×10^{-01}	2.52	98.82
327. Uridine	Discovery	0.95 (0.86, 1.06)	3.68×10^{-01}	6.42×10^{-01}	3.91	98.82
328. Xanthine	Discovery	1.04 (0.94, 1.15)	4.38×10^{-01}	2.43×10^{-01}	4.36	98.82
329. Xanthosine (MGH)	Discovery	1.01 (0.92, 1.11)	8.95×10^{-01}	3.79×10^{-02}	10.12	98.82

SUPPLEMENTARY DATA

330. Xanthosine	Discovery	0.95 (0.84, 1.07)	4.02×10^{-01}	3.36×10^{-01}	0.58	98.78
331. Xanthurenic Acid	Discovery	1.02 (0.91, 1.14)	7.38×10^{-01}	4.29×10^{-01}	3.84	98.78
332. 2-Aminoadipic Acid	Failed QC				34.93	98.82
333. 2-Deoxyuridine	Failed QC				9.78	52.46
334. 3-Aminoisobutyric Acid	Failed QC				25.93	98.82
335. 3-Phosphoglyceric Acid	Failed QC				8.66	22.17
336. 5-Aminolevulinic Acid	Failed QC				1.57	84.95
337. 5-Hydroxytryptophan	Failed QC				0.79	75.92
338. Acetylcholine	Failed QC				0.98	77.10
339. Aconitic Acid	Failed QC				4.59	46.36
340. Adipic Acid	Failed QC				14.90	52.46
341. Anserine	Failed QC				1.24	41.18
342. Anthranilic Acid	Failed QC				29.89	98.82
343. Arachidonoylglycerol	Failed QC				9.66	46.36
344. Atp	Failed QC				16.31	76.04
345. C18:1 CE	Failed QC				26.17	99.73
346. C20:4 Carnitine	Failed QC				1.31	78.1
347. C34:1 DAG	Failed QC				25.61	99.73
348. C38:4 PS	Failed QC				4.11	86.17
349. C42:11 PE Plasmalogen	Failed QC				2.21	84.15
350. C52:2 TAG	Failed QC				26.51	99.73
351. C56:1 TAG	Failed QC				3.15	81.56
352. C56:6 TAG	Failed QC				25.99	99.73
353. Citraconic Acid	Failed QC				6.39	52.46
354. Citric Acid/isocitric Acid	Failed QC				2.26	46.36
355. Creatinine	Failed QC				26.53	99.73
356. Glycerol-3-Phosphate	Failed QC				25.92	93.07
357. Glyoxylic Acid	Failed QC				10.89	52.46
358. Maleic Acid	Failed QC				18.33	52.46
359. Phosphocreatine	Failed QC				20.82	89.30
360. Udp-Glnac	Failed QC				48.90	87.39

SUPPLEMENTARY DATA

361. Udp-Glucose / - Galactose	Failed QC				54.26	98.82
362. Uracil	Failed QC				12.05	46.36

The HRs are expressed as incident diabetes risk for every SD increase in baseline metabolite levels using weighted Cox models adjusted for age, sex, race/ethnicity, hypertension status, baseline fasting plasma glucose, and baseline body mass index. Only metabolites that met QC criteria (<10% missing samples and an assay CV <25%) were included in the analysis. The metabolites are grouped according to their inference group (validation, discovery and failed QC).

*P-values for metabolites in the validation analysis were unadjusted. Benjamini-Hochberg false discovery rate adjustments were used to adjust for multiple hypothesis testing for p-values in the metabolites included in the discovery analysis. (A searchable html version of the table is available in [Supplemental Table 1.](#))

SUPPLEMENTARY DATA

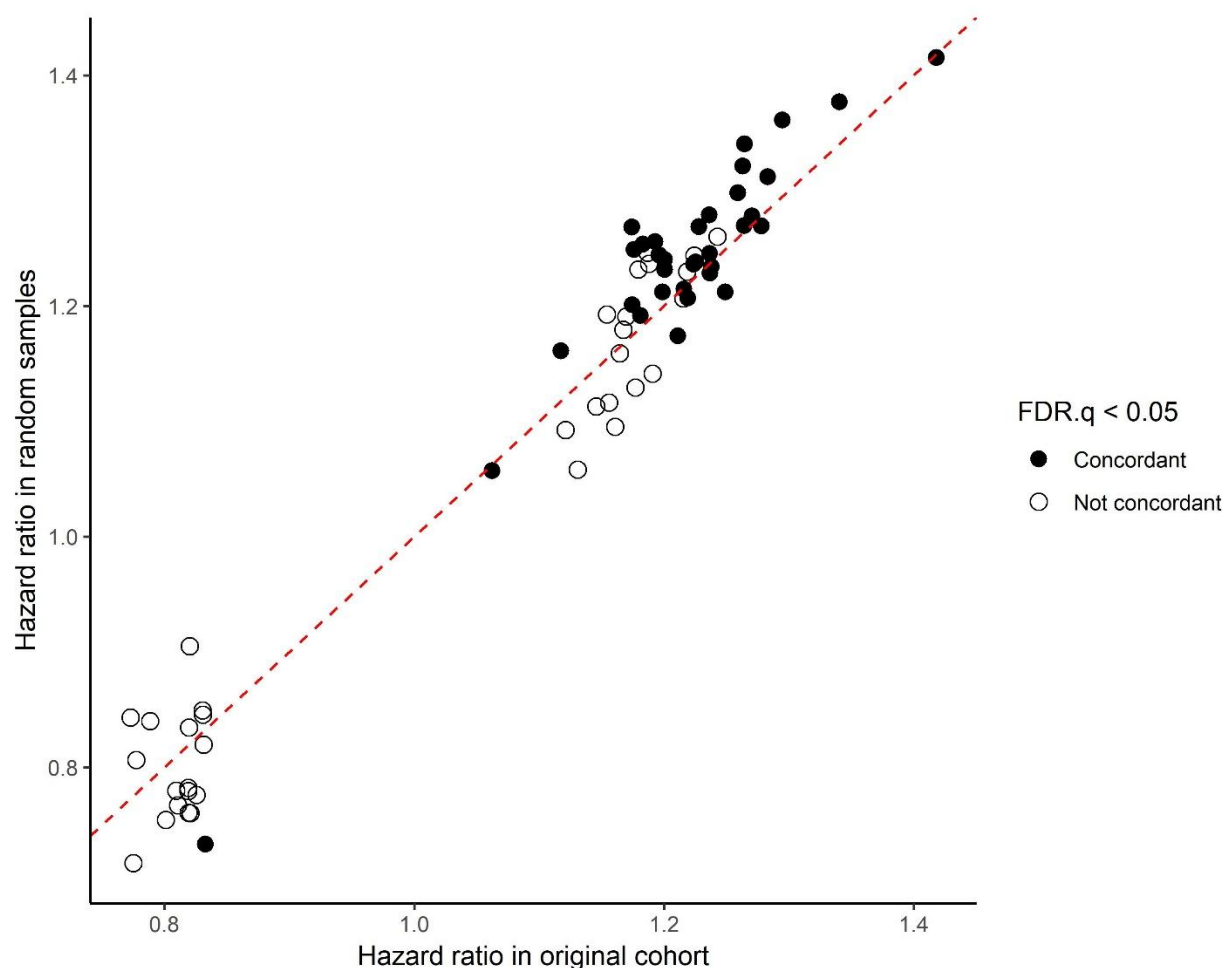
Supplementary Table 2. Metabolites associated with incident diabetes in the entire metabolite profiling cohort after multivariate adjustment including for clinically measured high-density lipoprotein (HDL) and triglycerides

Metabolite	Hazard Ratio (95% CI)	FDR-q	Homogeneity p-value
Glucose/fructose/galactose	1.45 (1.27-1.66)	6.70×10^{-06}	3.22×10^{-01}
Dimethylglycine	1.06 (1.04-1.09)	2.23×10^{-05}	1.63×10^{-01}
C16:1 SM	0.76 (0.66-0.87)	8.03×10^{-03}	2.71×10^{-02}
C5-DC Carnitine	1.20 (1.09-1.32)	8.03×10^{-03}	6.30×10^{-02}
C50:4 TAG	0.59 (0.46-0.77)	8.03×10^{-03}	1.08×10^{-01}
1,5-ag / 1-deoxyglucose	0.80 (0.71-0.90)	1.50×10^{-02}	2.03×10^{-01}
C48:0 TAG	1.22 (1.10-1.36)	1.50×10^{-02}	3.23×10^{-01}
C50:1 TAG	1.36 (1.15-1.62)	1.57×10^{-02}	4.15×10^{-01}
Cytosine	0.77 (0.66-0.89)	1.57×10^{-02}	2.55×10^{-01}
C22:1 SM	0.80 (0.70-0.91)	2.50×10^{-02}	3.55×10^{-02}
C38:4 PC	0.79 (0.68-0.91)	2.50×10^{-02}	1.40×10^{-01}
C18:0 CE	0.82 (0.73-0.92)	2.88×10^{-02}	2.32×10^{-02}
C18:2 SM	0.80 (0.69-0.91)	2.88×10^{-02}	4.93×10^{-01}
C16:0 SM	0.82 (0.73-0.93)	3.00×10^{-02}	6.23×10^{-02}
C36:0 PC	0.81 (0.71-0.92)	3.00×10^{-02}	1.17×10^{-02}
C44:0 TAG	1.18 (1.06-1.31)	3.11×10^{-02}	2.27×10^{-01}
C36:4 PC Plasmalogen	0.80 (0.69-0.92)	3.98×10^{-02}	4.46×10^{-01}
C52:5 TAG	0.77 (0.65-0.91)	3.98×10^{-02}	7.67×10^{-02}
C20:0 SM	0.83 (0.74-0.94)	3.98×10^{-02}	8.25×10^{-02}
Indole-3-carboxylic Acid	1.14 (1.05-1.25)	3.98×10^{-02}	8.53×10^{-01}
C18:1 SM	0.81 (0.70-0.93)	4.64×10^{-02}	4.90×10^{-01}
C14:0 SM	0.83 (0.73-0.94)	4.87×10^{-02}	1.57×10^{-02}
C40:10 PC	0.79 (0.67-0.93)	4.87×10^{-02}	3.84×10^{-01}
C42:0 TAG	1.14 (1.04-1.25)	4.87×10^{-02}	3.21×10^{-01}
C46:0 TAG	1.16 (1.05-1.29)	4.87×10^{-02}	2.65×10^{-01}
C5 Carnitine	1.13 (1.04-1.23)	4.87×10^{-02}	5.38×10^{-01}
C52:3 TAG	0.74 (0.60-0.91)	4.87×10^{-02}	4.60×10^{-01}
C50:0 TAG	1.19 (1.06-1.34)	4.96×10^{-02}	8.92×10^{-01}

The HRs are expressed as incident diabetes risk for every SD increase in baseline metabolite levels using weighted Cox models adjusted for age, sex, race/ethnicity, hypertension status, baseline fasting plasma glucose, baseline body mass index, HDL, and log-transformed triglycerides. Benjamini-Hochberg false discovery rate adjustment was applied to adjust for multiplicity. Phospholipids notation denotes (total number of carbon atoms:total number of double bonds). TAG: triglycerol. SM: sphingomyelin. PC: phosphatidylcholine. CE: cholesterol ester.

SUPPLEMENTARY DATA

Supplementary Figure 1. Metabolite associations with incident T2D in the random samples compared to associations in the whole metabolite profiling cohort



Concordance between hazard ratios for metabolite associations with incident diabetes between the 1,007 random samples and the whole metabolite profiling cohort (2,015 samples) are shown in this figure. Hazard ratios determined using weighted Cox-proportional hazards models (adjusting for sex, race/ethnicity, hypertension status, baseline fasting plasma glucose, and BMI) are expressed as incident diabetes risk for every 1 SD increase in metabolite concentration. Hazard ratios for metabolite associations in the whole metabolite profiling cohort are plotted on the x axis and in the random samples on the y axis. Metabolite associations with FDR $q < 0.05$ in both groups are represented by the filled circles, those with FDR $q < 0.05$ only in the whole metabolite profiling cohort are represented by the open circles.

SUPPLEMENTARY DATA

Supplementary Table 3. Metabolite associations with incident T2D in the whole metabolite profiling cohort and random samples

Metabolite	Whole Metabolite Profiling Cohort (n=2,015)		Random Samples (n=1,007)	
	Hazard Ratio (95% CI)	FDR <i>q</i>	Hazard Ratio (95% CI)	FDR <i>q</i>
Dimethylglycine	1.06 (1.04-1.08)	5.15×10⁻⁰⁷	1.06 (1.04-1.08)	2.42×10⁻⁰⁸
C48:0 TAG	1.28 (1.18-1.38)	8.01×10⁻⁰⁷	1.27 (1.12-1.44)	5.80×10⁻⁰³
C50:0 TAG	1.26 (1.16-1.36)	5.86×10⁻⁰⁶	1.30 (1.13-1.49)	6.86×10⁻⁰³
C44:2 TAG	1.22 (1.14-1.31)	6.95×10⁻⁰⁶	1.21 (1.09-1.34)	9.42×10⁻⁰³
C50:1 TAG	1.34 (1.21-1.49)	7.80×10⁻⁰⁶	1.38 (1.17-1.62)	5.80×10⁻⁰³
Glucose/Fructose/Galactose	1.42 (1.25-1.61)	7.80×10⁻⁰⁶	1.42 (1.18-1.69)	5.80×10⁻⁰³
C44:0 TAG	1.25 (1.15-1.36)	1.35×10⁻⁰⁵	1.21 (1.07-1.37)	2.12×10⁻⁰²
C32:0 DAG	1.21 (1.13-1.30)	1.56×10⁻⁰⁵	1.17 (1.07-1.29)	1.20×10⁻⁰²
C46:0 TAG	1.24 (1.14-1.34)	1.56×10⁻⁰⁵	1.23 (1.09-1.39)	1.30×10⁻⁰²
C46:2 TAG	1.26 (1.16-1.38)	1.56×10⁻⁰⁵	1.27 (1.11-1.45)	9.42×10⁻⁰³
C48:1 TAG	1.28 (1.17-1.41)	1.56×10⁻⁰⁵	1.31 (1.13-1.52)	9.28×10⁻⁰³
C44:1 TAG	1.24 (1.14-1.34)	1.77×10⁻⁰⁵	1.23 (1.09-1.40)	1.20×10⁻⁰²
C46:1 TAG	1.27 (1.16-1.39)	1.91×10⁻⁰⁵	1.28 (1.10-1.48)	1.28×10⁻⁰²
C36:2 PE	1.26 (1.15-1.38)	4.90×10⁻⁰⁵	1.32 (1.16-1.51)	2.46×10⁻⁰³
C50:2 TAG	1.29 (1.17-1.44)	6.22×10⁻⁰⁵	1.36 (1.16-1.60)	5.80×10⁻⁰³
C52:1 TAG	1.26 (1.15-1.39)	6.59×10⁻⁰⁵	1.34 (1.13-1.59)	1.06×10⁻⁰²
C46:3 TAG	1.24 (1.13-1.35)	7.01×10⁻⁰⁵	1.25 (1.10-1.41)	1.06×10⁻⁰²
C34:2 PE	1.24 (1.13-1.35)	1.18×10⁻⁰⁴	1.28 (1.12-1.47)	9.42×10⁻⁰³
C36:1 DAG	1.18 (1.10-1.27)	4.39×10⁻⁰⁴	1.19 (1.09-1.31)	5.80×10⁻⁰³
C36:1 PE	1.20 (1.11-1.30)	6.19×10⁻⁰⁴	1.23 (1.09-1.39)	1.06×10⁻⁰²
C46:4 TAG	1.19 (1.10-1.29)	6.62×10⁻⁰⁴	1.26 (1.10-1.44)	1.30×10⁻⁰²
C36:4 PE	1.22 (1.11-1.34)	8.47×10⁻⁰⁴	1.24 (1.09-1.40)	1.06×10⁻⁰²
C32:1 DAG	1.18 (1.09-1.27)	9.15×10⁻⁰⁴	1.13 (1.03-1.24)	6.92×10⁻⁰²
C48:4 TAG	1.23 (1.11-1.35)	9.15×10⁻⁰⁴	1.24 (1.08-1.42)	2.17×10⁻⁰²
C48:5 TAG	1.22 (1.11-1.34)	9.15×10⁻⁰⁴	1.23 (1.05-1.44)	5.97×10⁻⁰²
C38:4 DAG	1.20 (1.10-1.31)	1.50×10⁻⁰³	1.21 (1.07-1.38)	2.75×10⁻⁰²
C48:2 TAG	1.24 (1.12-1.38)	1.50×10⁻⁰³	1.26 (1.06-1.49)	5.11×10⁻⁰²
C38:4 PE	1.23 (1.11-1.36)	1.66×10⁻⁰³	1.27 (1.10-1.46)	1.18×10⁻⁰²
C42:0 TAG	1.19 (1.09-1.30)	1.73×10⁻⁰³	1.14 (1.02-1.27)	8.96×10⁻⁰²
C54:1 TAG	1.17 (1.08-1.27)	1.94×10⁻⁰³	1.20 (1.07-1.35)	2.02×10⁻⁰²
C30:0 DAG	1.16 (1.08-1.25)	2.24×10⁻⁰³	1.10 (1.01-1.19)	1.49×10⁻⁰¹
C40:6 PE	1.22 (1.10-1.34)	2.44×10⁻⁰³	1.21 (1.07-1.38)	2.31×10⁻⁰²
C52:0 TAG	1.17 (1.08-1.26)	2.54×10⁻⁰³	1.18 (1.04-1.33)	5.50×10⁻⁰²
C58:6 TAG	1.19 (1.09-1.30)	3.16×10⁻⁰³	1.25 (0.99-1.56)	1.97×10⁻⁰¹
C48:3 TAG	1.22 (1.10-1.36)	4.45×10⁻⁰³	1.24 (1.06-1.46)	5.49×10⁻⁰²
C34:2 DAG	1.20 (1.09-1.32)	4.99×10⁻⁰³	1.24 (1.09-1.41)	1.20×10⁻⁰²
C50:6 TAG	1.22 (1.09-1.35)	5.71×10⁻⁰³	1.21 (1.02-1.43)	1.39×10⁻⁰¹

SUPPLEMENTARY DATA

C32:2 DAG	1.15 (1.06-1.23)	5.83 ×10 ⁻⁰³	1.11 (1.01-1.22)	1.19×10 ⁻⁰¹
C56:3 TAG	1.17 (1.07-1.28)	7.71 ×10 ⁻⁰³	1.27 (1.17-1.38)	2.70 ×10 ⁻⁰⁶
C36:4 PC Plasmalogen	0.78 (0.68-0.90)	8.13 ×10 ⁻⁰³	0.81 (0.61-1.06)	3.34×10 ⁻⁰¹
Cytosine	0.77 (0.67-0.89)	8.32 ×10 ⁻⁰³	0.84 (0.70-1.02)	2.37×10 ⁻⁰¹
C16:1 SM	0.80 (0.70-0.91)	1.22 ×10 ⁻⁰²	0.75 (0.61-0.94)	6.82×10 ⁻⁰²
C18:2 SM	0.79 (0.69-0.91)	1.22 ×10 ⁻⁰²	0.84 (0.64-1.10)	4.52×10 ⁻⁰¹
C38:5 DAG	1.16 (1.06-1.26)	1.22 ×10 ⁻⁰²	1.12 (0.99-1.26)	2.38×10 ⁻⁰¹
C54:2 TAG	1.18 (1.07-1.30)	1.22 ×10 ⁻⁰²	1.23 (1.06-1.43)	4.31 ×10 ⁻⁰²
C5-DC Carnitine	1.20 (1.08-1.33)	1.26 ×10 ⁻⁰²	1.24 (1.14-1.36)	5.03 ×10 ⁻⁰⁵
C16:0 SM	0.82 (0.73-0.92)	1.48 ×10 ⁻⁰²	0.78 (0.63-0.97)	1.18×10 ⁻⁰¹
1,5-AG / 1-Deoxyglucose	0.82 (0.73-0.92)	1.49 ×10 ⁻⁰²	0.90 (0.75-1.09)	5.53×10 ⁻⁰¹
C36:3 PE	1.18 (1.07-1.31)	1.98 ×10 ⁻⁰²	1.25 (1.10-1.43)	1.20 ×10 ⁻⁰²
C18:2 CE	0.83 (0.73-0.93)	2.02 ×10 ⁻⁰²	0.78 (0.64-0.94)	6.11×10 ⁻⁰²
C22:1 SM	0.82 (0.73-0.93)	2.02 ×10 ⁻⁰²	0.76 (0.62-0.94)	6.19×10 ⁻⁰²
C34:0 DAG	1.12 (1.04-1.20)	2.04 ×10 ⁻⁰²	1.09 (0.99-1.20)	2.25×10 ⁻⁰¹
C38:6 PE	1.17 (1.06-1.29)	2.12 ×10 ⁻⁰²	1.19 (1.05-1.35)	4.86 ×10 ⁻⁰²
C34:2 PC Plasmalogen	0.82 (0.72-0.93)	2.21 ×10 ⁻⁰²	0.76 (0.62-0.93)	5.11×10 ⁻⁰²
C34:3 DAG	1.18 (1.06-1.30)	2.26 ×10 ⁻⁰²	1.25 (1.08-1.44)	2.31 ×10 ⁻⁰²
Cotinine	1.12 (1.04-1.20)	2.26 ×10 ⁻⁰²	1.16 (1.05-1.28)	2.17 ×10 ⁻⁰²
C36:1 PE Plasmalogen	0.81 (0.71-0.93)	2.48 ×10 ⁻⁰²	0.77 (0.62-0.96)	8.96×10 ⁻⁰²
Glycine	0.82 (0.72-0.94)	2.76 ×10 ⁻⁰²	0.78 (0.64-0.94)	6.19×10 ⁻⁰²
C18:1 Carnitine	0.83 (0.73-0.94)	2.79 ×10 ⁻⁰²	0.85 (0.70-1.02)	2.38×10 ⁻⁰¹
C18:1 SM	0.81 (0.70-0.93)	2.81 ×10 ⁻⁰²	0.78 (0.62-0.98)	1.49×10 ⁻⁰¹
C34:1 PC Plasmalogen	0.82 (0.72-0.94)	2.92 ×10 ⁻⁰²	0.83 (0.65-1.07)	3.69×10 ⁻⁰¹
C16:0 CE	0.83 (0.74-0.94)	3.05 ×10 ⁻⁰²	0.73 (0.61-0.89)	1.57 ×10 ⁻⁰²
C54:6 TAG	1.16 (1.05-1.29)	3.05 ×10 ⁻⁰²	1.16 (0.98-1.36)	2.43×10 ⁻⁰¹
C36:1 PC Plasmalogen	0.83 (0.73-0.94)	3.22 ×10 ⁻⁰²	0.85 (0.66-1.09)	4.51×10 ⁻⁰¹
Bilirubin	0.78 (0.65-0.92)	3.43 ×10 ⁻⁰²	0.72 (0.52-1.00)	1.81×10 ⁻⁰¹
C36:2 DAG	1.15 (1.05-1.27)	3.65 ×10 ⁻⁰²	1.19 (1.05-1.36)	5.11×10 ⁻⁰²
C50:3 TAG	1.19 (1.05-1.34)	3.66 ×10 ⁻⁰²	1.24 (1.04-1.47)	8.21×10 ⁻⁰²
C5 Carnitine	1.13 (1.04-1.23)	4.25 ×10 ⁻⁰²	1.06 (0.91-1.23)	7.36×10 ⁻⁰¹
C34:4 PC Plasmalogen	0.83 (0.73-0.95)	4.33 ×10 ⁻⁰²	0.82 (0.64-1.04)	2.92×10 ⁻⁰¹
C22:6 CE	0.83 (0.72-0.95)	6.23×10 ⁻⁰²	0.68 (0.54-0.85)	1.06 ×10 ⁻⁰²
C22:5 CE	0.85 (0.74-0.97)	9.19×10 ⁻⁰²	0.73 (0.60-0.89)	2.12 ×10 ⁻⁰²
C20:4 CE	0.85 (0.74-0.97)	9.27×10 ⁻⁰²	0.72 (0.59-0.89)	2.12 ×10 ⁻⁰²
C56:2 TAG	1.09 (1.00-1.18)	1.63×10 ⁻⁰¹	1.25 (1.16-1.35)	9.02 ×10 ⁻⁰⁷
C3 Carnitine	1.06 (1.00-1.13)	1.74×10 ⁻⁰¹	1.32 (1.09-1.6)	3.39 ×10 ⁻⁰²
S-Adenosyl-L-Homocysteine	1.11 (0.99-1.24)	2.63×10 ⁻⁰¹	1.36 (1.10-1.67)	2.93 ×10 ⁻⁰²
C4-OH Carnitine	1.06 (0.98-1.15)	3.89×10 ⁻⁰¹	1.17 (1.06-1.29)	2.12 ×10 ⁻⁰²
Glycocholic Acid	1.06 (0.98-1.14)	3.99×10 ⁻⁰¹	1.14 (1.04-1.25)	4.31 ×10 ⁻⁰²
Allantoin	1.08 (0.97-1.20)	4.00×10 ⁻⁰¹	1.35 (1.10-1.65)	2.93 ×10 ⁻⁰²
C8 Carnitine	0.96 (0.81-1.14)	8.53×10 ⁻⁰¹	1.16 (1.05-1.28)	2.75 ×10 ⁻⁰²

The hazard ratios are expressed as incident diabetes risk for each SD increase in baseline metabolite levels in Cox models adjusting for age, sex, race/ethnicity, hypertension status, baseline fasting plasma glucose, and BMI. FDR-*q* values <0.05 are in bold. Phospholipids notation denotes (total number of carbon atoms:total number of double bonds). TAG: triglycerol. DAG: diacylglycerol. SM: sphingomyelin. PC: phosphatidylcholine. CE: cholesterol ester.

SUPPLEMENTARY DATA

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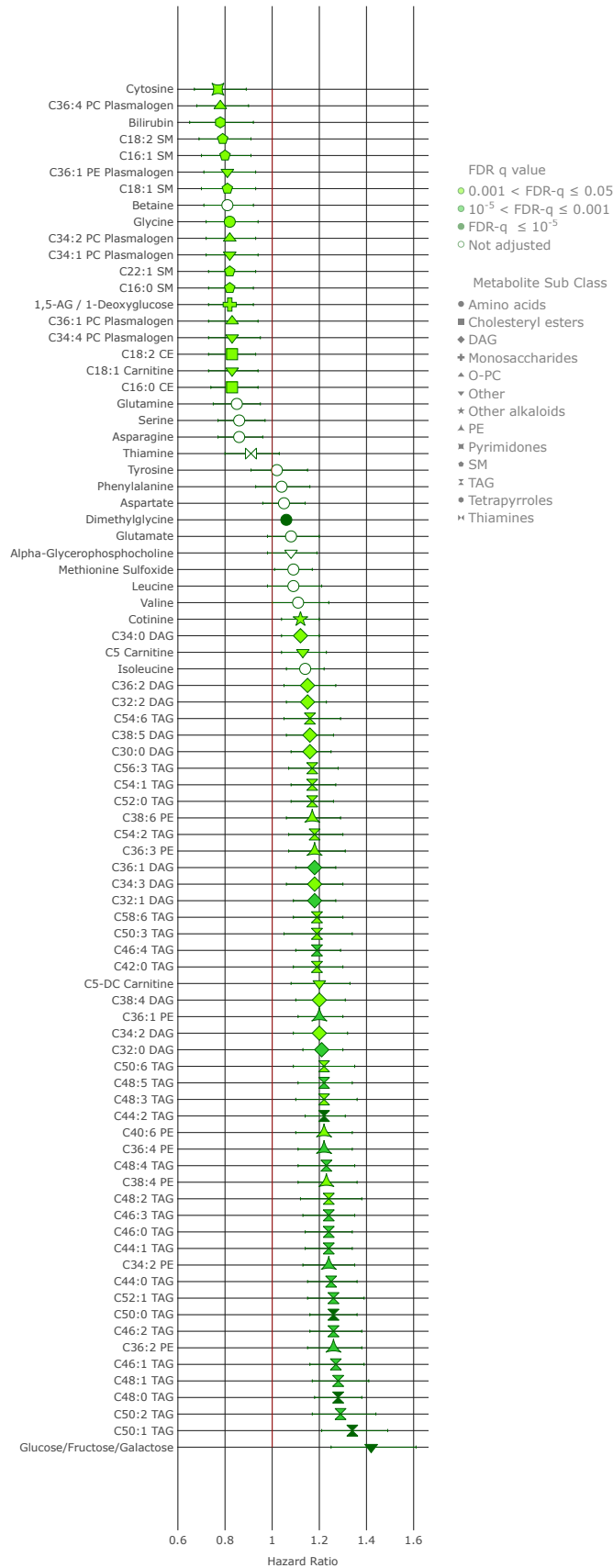
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Figure 1. Baseline metabolites associated with incident diabetes in the DPP

Figure 1. Baseline metabolites associated with incident diabetes in the DPP



The pooled HR and 95% CI are shown for baseline metabolite associations with increased or decreased risk of incident diabetes for every 1 SD increase in metabolite concentration in the entire metabolite profiling sub-cohort over an average follow-up of 2.8 years. Metabolites are arranged in increasing HR and color coded according to FDR-q value. All metabolites with FDR-q < 0.05 were included. Fourteen metabolites associated with incident diabetes in a smaller matched case-control metabolite profiling study in the DPP were not included in the FDR-q adjustment, these are uncolored. Association with FDR-q < 10⁻⁵ are in darkest green, q < 10⁻³ in medium green, q < 0.05 in lightest green, and unadjusted are in open circles. Weighted Cox models used are adjusted for treatment group, age, sex, race/ethnicity, hypertension status, baseline fasting plasma glucose, and baseline body mass index. Symbols represent metabolite subclasses. Phospholipids notation denotes (total number of carbon atoms:total number of double bonds). PC: phosphatidylcholine, DAG: diacylglycerol, PE: phosphatidylethanolamine, TAG: triacylglycerol.