

**Supplemental Table 5.** List of chemical compounds in Supplemental Figure 1.

No.	Compound name	Component 1	Component 2
1	2-Aminoadipic acid	0.003	0.114
2	GABA	0.020	0.112
3	2'-Deoxycytidine	-0.028	0.109
4	Mucic acid	-0.009	0.109
5	ADMA	-0.024	0.108
6	15(S)-HETE	0.024	0.107
7	<i>N,N</i> -Dimethylglycine	0.032	0.107
8	<i>S</i> -Methylmethionine	0.001	0.106
9	Linoleic acid	0.043	0.102
10	FA (24:5)	0.032	0.098
11	2-Hydroxyvaleric acid	-0.010	0.097
12	FA (17:0)	-0.022	0.095
13	FA (16:2)	-0.025	0.092
14	Taurodeoxycholic acid	0.052	0.091
15	AC (15:0)	0.022	0.090
16	Ophthalmic acid	-0.038	0.089
17	2-Hydroxybutyric acid	-0.049	0.089
18	Nicotinamide	-0.031	0.087
19	Stachydrine	0.053	0.085
20	Threonic acid	0.019	0.084
21	FA (22:4)	-0.050	0.084
22	Behenic acid	-0.017	0.083
23	Pyruvic acid	0.038	0.081
24	2-Aminobutyric acid	-0.069	0.077
25	AC (18:0)	-0.041	0.077
26	2-Hydroxyisobutyric acid	-0.011	0.076
27	Trigonelline	-0.063	0.072
28	cis-11,14-Eicosadienoic acid	-0.009	0.071
29	5-Hydroxylysine	0.023	0.070
30	<i>N</i> -Methylphenylethanolamine	0.071	0.068
31	Benzoic acid	-0.026	0.068
32	Pipecolic acid	0.078	0.067
33	<i>N</i> -Acetylhistidine	-0.063	0.067

34	Imidazolelactic acid	0.052	0.065
35	Ethyl arachidonate	0.041	0.063
36	Methionine sulfoxide	-0.030	0.062
37	Nervonic acid	-0.051	0.061
38	<i>S</i> -Sulfocysteine	-0.050	0.061
39	Sitosterol	-0.080	0.061
40	Pentadecanoic acid	0.082	0.060
41	Gluconolactone	-0.053	0.060
42	Ribulose 5-phosphate	0.081	0.059
43	Arachidonic acid	-0.072	0.059
44	FA (19:2)	-0.076	0.057
45	FA (16:3)	-0.073	0.056
46	<i>N</i> <sup>6</sup> , <i>N</i> <sup>6</sup> , <i>N</i> <sup>6</sup> -Trimethyllysine	-0.029	0.056
47	<i>N</i> <sub>ω</sub> -Methylarginine	0.006	0.052
48	Taurocholic acid	-0.079	0.051
49	Phosphocreatine	0.085	0.050
50	Deoxycholic acid	-0.041	0.048
51	AC (16:2)	-0.038	0.047
52	Betaine	-0.080	0.045
53	Sarcosine	-0.078	0.045
54	Carnitine	0.084	0.044
55	1-Methylnicotinamide	0.088	0.042
56	AC (17:0)	0.083	0.042
57	5-Hydroxytryptophan	-0.088	0.039
58	FA (22:5)	0.074	0.038
59	Dihydroxyacetone phosphate	0.091	0.037
60	3-Methylhistidine	0.088	0.036
61	AC (14:0)	-0.086	0.034
62	Heptadecanoic acid	0.090	0.033
63	AC (20:0)	-0.086	0.032
64	2-Amino-2-(hydroxymethyl)-1,3-propanediol	0.070	0.031
65	AC (20:1)	-0.087	0.031
66	Uric acid	0.081	0.030
67	AC (14:2)	-0.058	0.026
68	Corticosterone	-0.037	0.026

69	Phenaceturic acid	-0.012	0.025
70	Serotonin	-0.093	0.024
71	Ribose 5-phosphate	0.092	0.023
72	Myristic acid	-0.066	0.023
73	Taurine	0.029	0.023
74	1-Methyl-4-imidazoleacetic acid	0.014	0.023
75	FA (17:1)	0.017	0.022
76	Cystathionine	0.092	0.019
77	Urocanic acid	0.059	0.016
78	AC (12:0)	-0.090	0.013
79	SDMA	-0.003	0.013
80	Urea	0.088	0.013
81	<i>O</i> -Acetylcarnitine	0.075	0.012
82	$\alpha$ -Tocopherol	-0.090	0.012
83	Asn	-0.095	0.011
84	1-Methylhistamine	-0.014	0.011
85	Stearic acid	-0.094	0.010
86	Palmitoylcarnitine	-0.076	0.008
87	Hypotaurine	0.092	0.007
88	FA (19:1)	-0.092	0.007
89	Linolenic acid	0.094	0.007
90	Arachidic acid	-0.096	0.001
91	Erucic acid	-0.088	0.000
92	$\beta$ -Ala	-0.074	0.000
93	cis-11-Eicosenoic acid	-0.096	-0.002
94	N.D.	0.096	-0.003
95	<i>S</i> -Methylcysteine	-0.015	-0.005
96	Isovalerylalanine	-0.090	-0.006
97	AC (12:1)	-0.091	-0.008
98	Palmitic acid	-0.093	-0.009
99	Perillic acid	0.090	-0.009
100	AC (16:1)	-0.093	-0.012
101	Homoserine	0.020	-0.012
102	2-Oxoglutaric acid	-0.094	-0.012
103	Oleic acid	-0.094	-0.013

104	Testosterone	-0.067	-0.013
105	Linoleyl ethanolamide	0.090	-0.014
106	N.D.	-0.092	-0.014
107	AC (18:2)	0.000	-0.016
108	AC (14:1)	-0.094	-0.017
109	FA (14:1)	-0.095	-0.017
110	Glucose 6-phosphate	0.088	-0.017
111	Glucuronic acid	-0.060	-0.019
112	6-Hydroxyhexanoic acid	-0.057	-0.019
113	Guanosine	-0.080	-0.019
114	Palmitoleic acid	-0.088	-0.020
115	Met	0.083	-0.021
116	Cholic acid	-0.087	-0.022
117	Octanoic acid	-0.082	-0.022
118	N.D.	-0.063	-0.022
119	3-Phosphoglyceric acid	0.094	-0.023
120	His	-0.094	-0.023
121	AC (18:1)	-0.072	-0.023
122	Decanoic acid	-0.087	-0.026
123	2-Hydroxyglutaric acid	-0.091	-0.026
124	Trimethylamine <i>N</i> -oxide	-0.087	-0.026
125	2-Oxoisovaleric acid	-0.053	-0.027
126	Stearoyl ethanolamide	0.091	-0.027
127	Fructose 6-phosphate	0.090	-0.027
128	3-Hydroxytetradecanoic acid	-0.092	-0.028
129	Hecogenin	0.086	-0.028
130	Pantothenic acid	0.069	-0.030
131	Myristoleic acid	-0.089	-0.030
132	Glutathione (GSSG)_divalent	0.089	-0.030
133	cis-5,8,11,14,17-Eicosapentaenoic acid	0.073	-0.031
134	Inosine	0.027	-0.031
135	Ala	0.081	-0.031
136	Glycerophosphocholine	-0.090	-0.032
137	Citrulline	-0.038	-0.034
138	Stearidonic acid	-0.049	-0.034

139	Ricinoleic acid	-0.079	-0.035
140	Lauric acid	-0.086	-0.036
141	Creatinine	0.036	-0.036
142	Cholesterol sulfate	-0.073	-0.036
143	Isovalerylcarnitine	0.087	-0.036
144	5-Oxoproline	-0.038	-0.038
145	Sedoheptulose 7-phosphate	0.090	-0.038
146	Ethanolamine phosphate	0.086	-0.039
147	cis-4,7,10,13,16,19-Docosahexaenoic acid	0.004	-0.039
148	FA (20:3)	-0.086	-0.042
149	Butyrylcarnitine	-0.086	-0.042
150	Phosphoenolpyruvic acid	0.075	-0.042
151	Isethionic acid	0.085	-0.043
152	FA (14:2)	-0.088	-0.043
153	Cystine	-0.076	-0.043
154	FA (19:0)	0.004	-0.046
155	Lactic acid	0.072	-0.046
156	FA (22:3)	-0.083	-0.046
157	Cholesterol	0.068	-0.047
158	cis-8,11,14-Eicosatrienoic acid	-0.030	-0.048
159	Gluconic acid	-0.085	-0.050
160	N.D.	-0.084	-0.051
161	FA (14:1)	-0.071	-0.051
162	Hydroxyprogesterone caproate	0.078	-0.051
163	Hydroxyproline	-0.084	-0.052
164	Ethanolamine	0.065	-0.053
165	N <sup>6</sup> -Acetyllysine	-0.079	-0.054
166	8-Hydroxyoctanoic acid	-0.082	-0.054
167	Erythrose 4-phosphate	-0.065	-0.055
168	3-Aminobutyric acid	0.081	-0.055
169	3-Indoxylsulfuric acid	-0.072	-0.055
170	Glycerol 3-phosphate	-0.038	-0.055
171	Succinic acid	0.080	-0.056
172	Diethanolamine	0.060	-0.058
173	Gly	0.082	-0.059

174	Isocitric acid	-0.078	-0.059
175	Thr	-0.079	-0.060
176	Homovanillic acid	0.008	-0.060
177	<i>N</i> -Glycolylneuraminic acid	0.012	-0.061
178	$\gamma$ -Butyrobetaine	0.078	-0.065
179	Cytidine	0.034	-0.065
180	Acetoacetic acid	-0.052	-0.066
181	Ser	-0.074	-0.066
182	Lys	-0.071	-0.067
183	Phe	0.053	-0.069
184	Anserine_divalent	-0.034	-0.070
185	Palmitoylethanolamide	0.073	-0.070
186	FA (12:0)	0.064	-0.071
187	Tyr	-0.072	-0.071
188	<i>N</i> -Acetyl glycine	0.074	-0.071
189	Indole-3-carboxaldehyde	-0.033	-0.072
190	Glu	0.064	-0.072
191	Oleoyl ethanolamide	-0.041	-0.074
192	10-Hydroxydecanoic acid	-0.072	-0.075
193	Guanidoacetic acid	0.050	-0.075
194	Citric acid	-0.066	-0.076
195	Trp	0.070	-0.077
196	Spermidine	0.031	-0.078
197	Campesterol	-0.066	-0.079
198	Asp	0.054	-0.079
199	Carnosine	-0.062	-0.081
200	Hexylamine	0.048	-0.081
201	Pelargonic acid	-0.064	-0.081
202	Ascorbic acid	0.055	-0.081
203	5-Methoxyindoleacetic acid	-0.059	-0.083
204	Kynurenine	-0.030	-0.086
205	Histamine	0.023	-0.087
206	Arg	-0.054	-0.088
207	<i>N</i> <sup>6</sup> -Methyllysine	-0.004	-0.089
208	4-Acetamidobutanoic acid	-0.008	-0.089

209	Dyphylline	0.054	-0.090
210	3-Hydroxybutyric acid	-0.045	-0.090
211	Leu	0.048	-0.091
212	Cysteine glutathione disulfide	0.036	-0.091
213	Malic acid	-0.020	-0.091
214	<i>N</i> -Ethylmaleimide_+H <sub>2</sub> O	0.045	-0.092
215	Glyceric acid	-0.017	-0.094
216	Sphinganine	0.042	-0.094
217	Creatine	-0.048	-0.096
218	Pro	-0.050	-0.097
219	Adipic acid	0.035	-0.098
220	Val	0.046	-0.098
221	<i>N</i> -Acetylaspartic acid	0.046	-0.100
222	Putrescine	-0.016	-0.100
223	Uridine	0.046	-0.100
224	N.D.	0.045	-0.101
225	Hypoxanthine	0.038	-0.103
226	Glycerol	-0.041	-0.103
227	Ile	0.015	-0.103
228	Gln	-0.041	-0.103
229	<i>O</i> -Succinylhomoserine	-0.040	-0.104
230	Triethanolamine	0.039	-0.105
231	2-Hydroxy-4-methylvaleric acid	0.038	-0.105
232	Choline	0.038	-0.105
233	N.D.	0.032	-0.105
234	Hexanoic acid	-0.022	-0.106
235	N.D.	0.001	-0.106
236	<i>N</i> <sup>5</sup> -Ethylglutamine	0.018	-0.107
237	Sphingosine	0.025	-0.108
238	4-Methyl-2-oxovaleric acid/3-Methyl-2-oxovaleric acid	0.011	-0.109
239	<i>O</i> -Acetylhomoserine	-0.018	-0.111
240	11-Aminoundecanoic acid	0.010	-0.112
241	Ornithine	0.012	-0.112
242	<i>cis</i> -Aconitic acid	-0.017	-0.113

FA, Fatty acid; AC, Asylcarnitine; N.D., not determined.