

Supplementary Table 1. List of metabolite concentrations determined using the Biocrates AbsoluteIDQ kit.

Metabolite class	Number	Metabolite name or abbreviation	Biological relevance (selected examples)
Amino acids	21	Alanine, arginine, asparagine, aspartate, citrulline, glutamine, glutamate, glycine, histidine, isoleucine, leucine, lysine, methionine, ornithine, phenylalanine, proline, serine, threonine, tryptophan, tyrosine, valine	Amino acid metabolism, urea-cycle, activity of gluconeogenesis and glycolysis, insulin sensitivity, neurotransmitter metabolism, oxidative stress
Carnitine	1	C0	
Acylcarnitine	25	C2, C3, C3:1, C4, C4:1, C5, C5:1, C6(or C4:1-DC), C6:1, C8, C9, C10, C10:1, C10:2, C12, C12:1, C14, C14:1, C14:2, C16, C16:1, C16:2, C18, C18:1, C18:2	
Hydroxy- and dicarboxyacylcarnitines	14	C3-OH, C4-OH(or C3-DC), C5:1-DC, C5-DC(or C6-OH), C5-M-DC, C5-OH(or C3-DC-M), C7-DC, C12-DC, C14:1-OH, C14:2-OH, C16:1-OH, C16:2-OH, C16-OH, C18:1-OH	Energy metabolism, fatty acid transport and mitochondrial fatty acid oxidation, ketosis, oxidative stress, mitochondrial membrane damage
Biogenic amines	19	acetylornithine, asymmetric dimethylarginine, total dimethylarginine, alpha-Amino adipic acid, carnosine, creatinine, histamine, kynurenone, methioninesulfoxide, nitrotyrosine, hydroxyproline, phenylethylamine, putrescine, sarcosine, serotonin, spermidine, spermine, taurine	
Lyso-phosphatidylcholines	14	lysoPC a C14:0/C16:0/C16:1/C17:0/C18:0/C18:1/C18:2/C20:3/C20:4/C26:0/C26:1/C28:0/C28:1	Degradation of phospholipids, membrane damage, signalling cascades, fatty acid profile
Diacyl-phosphatidylcholines	38	PC aa C24:0/C26:0/C28:1/C30:0/C30:2/C32:0/C32:1/C32:2/C32:3/C34:1/C34:2/C34:3/C34:4/C36:0/C36:1/C36:2/C36:3/C36:4/C36:5/C36:6/C38:0/C38:1/C38:3/C38:4/C38:5/C38:6/C40:1/C40:2/C40:3/C40:4/C40:5/C40:6/C42:0/C42:1/C42:2/C42:4/C42:5/C42:6	
Acyl-alkyl-phosphatidylcholines	38	PC ae C30:0/C30:2/C32:1/C32:2/C34:0/C34:1/C34:2/C34:3/C36:0/C36:1/C36:2/C36:3/C36:4/C36:5/C38:0/C38:1/C38:2/C38:3/C38:4/C38:5/C38:6/C40:1/C40:2/C40:3/C40:4/C40:5/C40:6/C42:0/C42:1/C42:2/C42:4/C42:5/C42:6	Dyslipidaemia, membrane composition and damage, fatty acid profile, activity of desaturases

		2:1/C42:2/C42:3/C42:4/C42:5/C44:3/C44:4/C44:5/C44:6	
Sphingomyelines	10	SM C16:0, SM C16:1, SM C18:0, SM C18:1, SM C20:2, SM C22:3, SM C24:0, SM 24:1, SM C26:0, SM C26:1	Signalling cascades, membrane damage (eg, neurodegeneration)
Hydroxysphingomyelines	5	SM (OH) C14:1, SM (OH) C16:1, SM (OH) C22:1, SM (OH) C22:2, SM (OH) C24:1	
Hexose	1	H1	Carbohydrate metabolism
Total	186		

aa, acyl-acyl; ae, acyl-alkyl; a, lyso; Cx:y, where x is the number of carbons in the fatty acid side chain; y is the number of double bonds in the fatty acid side chain; DC, decarboxyl; M, methyl; OH, hydroxyl; PC, phosphatidylcholine; SM, sphingomyelin.

Supplementary Table 2. The ρ for 168 metabolites between synovial fluid and plasma.

No.	Metabolites	ρ	p			
1	Creatinine	0.59	*	27	C0	0.36
2	PC aa C36:0	0.51	*	28	SM (OH) C22:1	0.35
3	PC ae C30:0	0.51	*	29	C8	0.35
4	Glycine	0.46	*	30	PC ae C30:1	0.35
5	Leucine	0.46	*	31	PC ae C34:1	0.35
6	lysoPC a C24:0	0.46	*	32	Kynurenine	0.34
7	Valine	0.45	*	33	C5-M-DC	0.34
8	Isoleucine	0.45	*	34	Sarcosine	0.34
9	C10	0.44	*	35	PC ae C30:2	0.34
10	PC aa C24:0	0.43	*	36	PC aa C36:5	0.34
11	Proline	0.42		37	PC aa C40:5	0.34
12	C12	0.42		38	PC aa C42:6	0.33
13	PC ae C36:2	0.41		39	PC ae C42:1	0.33
14	PC ae C38:0	0.41		40	PC aa C40:1	0.33
15	PC aa C26:0	0.41		41	lysoPC a C28:1	0.33
16	lysoPC a C28:0	0.40		42	PC aa C42:2	0.33
17	PC aa C40:6	0.40		43	PC ae C34:0	0.33
18	PC aa C38:6	0.40		44	Serine	0.33
19	PC aa C36:6	0.39		45	Tyrosine	0.32
20	Threonine	0.38		46	PC aa C38:5	0.31
21	PC aa C38:4	0.38		47	Glu	0.31
22	PC aa C36:4	0.38		48	SM (OH) C22:2	0.31
23	PC ae C38:3	0.38		49	PC ae C34:3	0.31
24	PC ae C36:1	0.38		50	PC ae C38:2	0.31
25	SM C20:2	0.37		51	C2	0.30
26	SM (OH) C14:1	0.37		52	C4	0.30
				53	PC aa C32:1	0.30
				54	PC aa C40:4	0.30
				55	Tryptophan	0.30
				56	PC ae C40:6	0.30
				57	PC aa C42:0	0.30

58	PC aa C28:1	0.29	89	PC aa C36:3	0.23
59	PC ae C36:3	0.29	90	PC ae C40:2	0.23
60	PC ae C36:0	0.29	91	SM C18:1	0.23
61	PC ae C38:4	0.29	92	PC ae C40:4	0.22
62	PC ae C34:2	0.29	93	SM C24:0	0.22
63	PC ae C32:2	0.29	94	C14:2	0.22
64	Acetylornithine	0.29	95	PC ae C42:3	0.21
65	lysoPC a C18:2	0.29	96	Asparagine	0.21
66	PC ae C44:4	0.29	97	lysoPC a C20:3	0.21
67	lysoPC a C26:0	0.28	98	PC ae C32:1	0.21
68	PC aa C38:3	0.28	99	PC aa C42:1	0.20
69	PC ae C44:5	0.27	100	C14	0.20
70	PC aa C30:0	0.27	101	PC aa C42:5	0.20
71	lysoPC a C20:4	0.27	102	SM (OH) C24:1	0.20
72	Phenylalanine	0.27	103	PC ae C42:2	0.19
73	PC aa C34:1	0.27	104	PC ae C42:4	0.19
74	Alanine	0.26	105	PC ae C38:6	0.19
75	alpha-AAA	0.26	106	PC ae C42:5	0.18
76	SM (OH) C16:1	0.26	107	PC ae C42:0	0.18
77	Lysine	0.26	108	PC aa C34:2	0.18
78	Ornithine	0.26	109	PC aa C36:2	0.18
79	C6 (C4:1-DC)	0.26	110	Histidine	0.18
80	lysoPC a C17:0	0.25	111	SM C16:1	0.17
81	PC aa C38:0	0.25	112	PC aa C40:2	0.17
82	PC ae C38:1	0.24	113	C9	0.17
83	PC aa C34:3	0.24	114	PC ae C36:4	0.17
84	PC ae C40:3	0.24	115	PC aa C32:3	0.17
85	total DMA	0.24	116	C10:2	0.17
86	PC aa C40:3	0.23	117	SM C18:0	0.17
87	Citrulline	0.23	118	C18:1-OH	0.16
88	PC ae C44:3	0.23	119	C12-DC	0.16

120	PC aa C36:1	0.16	146	C12:1	0.08
121	C10:1	0.16	147	lysoPC a C18:1	0.08
122	Taurine	0.15	148	lysoPC a C16:0	0.07
123	PC ae C40:1	0.15	149	C14:2-OH	0.07
124	lysoPC a C18:0	0.15	150	C16:1	0.06
125	C5-DC (C6-OH)	0.15	151	C16:2-OH	0.05
126	PC ae C44:6	0.14	152	lysoPC a C16:1	0.05
127	lysoPC a C14:0	0.14	153	C16	0.04
128	C7-DC	0.13	154	C14:1-OH	0.04
129	Nitrotyrosine	0.13	155	C3-DC (C4-OH)	0.04
130	C5-OH (C3-DC-M)	0.13	156	C4:1	0.03
131	PC aa C34:4	0.12	157	C16-OH	0.03
132	C3-OH	0.12	158	C18:2	0.02
133	C5	0.12	159	C3	0.02
134	C16:2	0.12	160	Spermidine	-0.01
135	PC ae C40:5	0.12	161	C16:1-OH	-0.01
136	PC aa C42:4	0.12	162	C6:1	-0.02
137	C5:1	0.11	163	C3:1	-0.03
138	PC ae C38:5	0.11	164	C5:1-DC	-0.04
139	SM C16:0	0.11	165	Glutamine	-0.06
140	lysoPC a C26:1	0.10	166	C14:1	-0.06
141	Hexose	0.10	167	C18:1	-0.09
142	Arginine	0.10	168	C18	-0.12
143	PC aa C32:0	0.10			
144	Methionine	0.10			
145	PC ae C36:5	0.08			

* p value $\leq 2.98 \times 10^{-4}$