

Table 1 Measurement accuracy summary compared against SRM 1950 - "Metabolites in Frozen

Lipid Species	Measurement*	Consensus Value**	Units	No. of labs
FFA 20:4	0.194 ± 0.022	4.7 ± 1.5	nmol/mL	7
FFA 20:5	0.012 ± 0.004	0.42 ± 0.056	nmol/mL	7
FFA 22:6	0.254 ± 0.01	1.5 ± 0.17	nmol/mL	8
LPC 14:0	0.323 ± 0.004	1.0 ± 0.20	nmol/mL	16
LPC 15:0	0.226 ± 0.029	0.52 ± 0.11	nmol/mL	9
LPC 16:0	48.85 ± 0.768	73 ± 11	nmol/mL	20
LPC O-16:0	0.29 ± 0.011	0.55 ± 0.16	nmol/mL	10
LPC P-16:0	0.131 ± 0.006	0.46 ± 0.13	nmol/mL	8
LPC 16:1	1.311 ± 0.036	2.4 ± 0.35	nmol/mL	19
LPC 17:0	0.486 ± 0.029	1.4 ± 0.24	nmol/mL	6
LPC 17:1	0.08 ± 0.013	0.25 ± 0.071	nmol/mL	6
LPC 18:0	19.68 ± 0.957	27 ± 3.3	nmol/mL	20
LPC 18:1	8.885 ± 0.214	18 ± 2.3	nmol/mL	19
LPC 18:2	16.02 ± 0.275	22 ± 2.9	nmol/mL	19
LPC 20:0	0.065 ± 0.003	0.10 ± 0.034	nmol/mL	7
LPC 20:1	0.12 ± 0.025	0.19 ± 0.024	nmol/mL	13
LPC 20:2	0.13 ± 0.004	0.23 ± 0.044	nmol/mL	9
LPC 20:3	1.014 ± 0.068	1.8 ± 0.26	nmol/mL	18
LPC 20:4	4.685 ± 0.151	6.0 ± 0.60	nmol/mL	20
LPC 20:5	0.19 ± 0.003	0.33 ± 0.092	nmol/mL	15
LPC 22:0	0.021 ± 0.002	0.025 ± 0.0017	nmol/mL	5
LPC 22:4	0.114 ± 0.022	0.12 ± 0.041	nmol/mL	8
LPC 22:5	0.379 ± 0.016	0.43 ± 0.13	nmol/mL	12
LPC 22:6	0.838 ± 0.125	0.77 ± 0.14	nmol/mL	17
LPC 24:0	0.049 ± 0.002	0.046 ± 0.015	nmol/mL	5
LPE 16:0	0.572 ± 0.05	0.91 ± 0.27	nmol/mL	14
LPE 18:0	4.737 ± 0.216	1.6 ± 0.55	nmol/mL	15
LPE 18:1	0.65 ± 0.027	1.4 ± 0.47	nmol/mL	14
LPE 18:2	1.538 ± 0.136	1.9 ± 0.56	nmol/mL	16
LPE 20:4	1.677 ± 0.127	1.1 ± 0.41	nmol/mL	14
LPE 22:6	1.79 ± 0.214	0.52 ± 0.18	nmol/mL	12
PC 30:0	5.741 ± 1.624	1.6 ± 0.32	nmol/mL	11
PC O-30:1/P-30:0	0.19 ± 0.054	0.047 ± 0.0096	nmol/mL	7
PC 32:0	7.466 ± 1.357	7.2 ± 1.0	nmol/mL	18
PC O-32:0/31:0	1.653 ± 0.312	1.5 ± 0.41	nmol/mL	11
PC 32:1	8.982 ± 1.801	13 ± 1.9	nmol/mL	18
PC O-32:1/P-32:0/31:1	0.926 ± 0.259	1.6 ± 0.24	nmol/mL	11
PC P-33:1/32:2	0.698 ± 0.172	2.6 ± 0.37	nmol/mL	16
PC 34:0	13.87 ± 2.736	2.1 ± 0.37	nmol/mL	12
PC O-34:0/33:0	0.399 ± 0.054	0.76 ± 0.17	nmol/mL	10
PC 34:1	122.4 ± 25.31	120 ± 21	nmol/mL	19

PC O-34:1/P-34:0/33:1	3.912 ± 0.776	4.9 ± 0.86	nmol/mL	17
PC O-34:2/P-34:1/33:2	2.539 ± 0.51	5.2 ± 1.3	nmol/mL	17
PC O-34:3/P-34:2/33:3	3.773 ± 0.731	4.7 ± 0.88	nmol/mL	12
PC P-35:1/34:2	3.262 ± 0.583	240 ± 47	nmol/mL	18
PC 34:5	0.047 ± 0.011	0.034 ± 0.0045	nmol/mL	5
PC 36:1	36.99 ± 7.267	26 ± 4.6	nmol/mL	17
PC O-36:1/P-36:0/35:1	0.577 ± 0.11	3.5 ± 0.99	nmol/mL	16
PC 36:2	155 ± 31.67	140 ± 25	nmol/mL	18
PC O-36:2/P-36:1/35:2	1.304 ± 0.351	7.4 ± 1.7	nmol/mL	17
PC 36:3	52.74 ± 10.44	100 ± 14	nmol/mL	17
PC 36:4	75.15 ± 14.31	150 ± 28	nmol/mL	19
PC O-36:4/P-36:3/35:4	8.813 ± 1.657	12 ± 1.4	nmol/mL	17
PC 36:5	8.206 ± 1.459	11 ± 1.8	nmol/mL	16
PC O-36:5/P-36:4/35:5	4.947 ± 0.991	6.9 ± 1.6	nmol/mL	11
PC P-36:5/35:6	0.082 ± 0.006	0.30 ± 0.094	nmol/mL	5
PC 36:6	0.187 ± 0.046	0.28 ± 0.088	nmol/mL	8
PC 38:2	4.668 ± 1.095	2.3 ± 0.20	nmol/mL	15
PC O-38:2/37:2	1.022 ± 0.083	0.98 ± 0.32	nmol/mL	6
PC 38:3	35.39 ± 7.219	26 ± 5.2	nmol/mL	14
PC O-38:3/P-38:2/37:3	0.75 ± 0.188	1.5 ± 0.51	nmol/mL	14
PC 38:4	68.63 ± 12.31	84 ± 14	nmol/mL	18
PC O-38:4/P-38:3/37:4	5.23 ± 1.016	7.4 ± 2.0	nmol/mL	12
PC 38:5	11.45 ± 2.2	42 ± 7.9	nmol/mL	18
PC O-38:5/P-38:4/37:5	7.624 ± 1.349	11 ± 1.6	nmol/mL	16
PC 38:6	23.33 ± 4.473	41 ± 4.4	nmol/mL	18
PC O-38:6/P-38:5/37:6	1.895 ± 0.295	3.6 ± 1.0	nmol/mL	12
PC P-38:6/36:0	0.28 ± 0.065	1.2 ± 0.39	nmol/mL	10
PC 40:4	4.034 ± 0.883	2.9 ± 0.37	nmol/mL	18
PC O-40:4/P-40:3/39:4	0.873 ± 0.212	0.95 ± 0.38	nmol/mL	8
PC 40:5	3.855 ± 0.756	6.7 ± 1.1	nmol/mL	18
PC O-40:5/P-40:4/39:5	1.252 ± 0.236	1.7 ± 0.45	nmol/mL	12
PC 40:6	11.01 ± 2.209	14 ± 2.6	nmol/mL	17
PC 40:7	1.367 ± 0.185	3.5 ± 0.26	nmol/mL	16
PC O-40:7/P-40:6/39:7	0.518 ± 0.108	1.1 ± 0.23	nmol/mL	9
PC 40:8	0.606 ± 0.115	0.73 ± 0.20	nmol/mL	14
PC O-42:5/P-42:4	1.523 ± 0.262	0.79 ± 0.12	nmol/mL	7
PE 34:1	0.376 ± 0.007	1.2 ± 0.17	nmol/mL	14
PE 34:2	0.778 ± 0.04	2.2 ± 0.26	nmol/mL	16
PE O-34:2/P-34:1	0.356 ± 0.015	0.78 ± 0.17	nmol/mL	11
PE O-34:3/P-34:2	0.487 ± 0.03	1.5 ± 0.41	nmol/mL	11
PE 36:0	0.873 ± 0.1	0.28 ± 0.10	nmol/mL	11
PE 36:1	1.908 ± 0.084	1.3 ± 0.26	nmol/mL	14
PE O-36:2/P-36:1/35:2	0.385 ± 0.004	0.93 ± 0.22	nmol/mL	12
PE 36:3	0.386 ± 0.066	2.4 ± 0.38	nmol/mL	16

PE O-36:3/P-36:2/35:3	1.523 ± 0.033	3.2 ± 0.76	nmol/mL	15
PE 36:4	0.692 ± 0.036	3.1 ± 0.39	nmol/mL	16
PE O-36:4/P-36:3	0.43 ± 0.027	1.6 ± 0.29	nmol/mL	14
PE O-36:5/P-36:4	2.187 ± 0.059	4.9 ± 1.9	nmol/mL	15
PE 38:3	0.797 ± 0.007	0.95 ± 0.20	nmol/mL	14
PE 38:4	3.154 ± 0.185	8.1 ± 1.2	nmol/mL	16
PE O-38:4/P-38:3/37:4	0.519 ± 0.027	0.94 ± 0.18	nmol/mL	9
PE 38:5	0.382 ± 0.018	2.7 ± 0.47	nmol/mL	12
PE O-38:5/P-38:4	5.419 ± 0.185	5.8 ± 1.9	nmol/mL	17
PE 38:6	0.679 ± 0.019	3.2 ± 0.59	nmol/mL	15
PE O-38:6/P-38:5	2.406 ± 0.178	4.9 ± 1.2	nmol/mL	16
PE O-38:7/P-38:6	0.8 ± 0.013	3.5 ± 0.98	nmol/mL	8
PE 40:4	0.796 ± 0.023	0.26 ± 0.082	nmol/mL	10
PE 40:5	0.176 ± 0.008	0.73 ± 0.23	nmol/mL	12
PE O-40:5/P-40:4/39:5	2.437 ± 0.227	0.73 ± 0.13	nmol/mL	12
PE 40:6	0.506 ± 0.022	1.8 ± 0.36	nmol/mL	14
PE O-40:6/P-40:5/39:6	2.94 ± 0.186	1.3 ± 0.31	nmol/mL	14
PE 40:7	0.209 ± 0.008	0.77 ± 0.26	nmol/mL	11
PE O-40:7/P-40:6/39:7	1.081 ± 0.035	2.5 ± 0.72	nmol/mL	14
PI 32:1	0.456 ± 0.03	0.56 ± 0.11	nmol/mL	10
PI 34:1	1.056 ± 0.346	2.4 ± 0.42	nmol/mL	14
PI 34:2	2.733 ± 0.217	2.8 ± 0.38	nmol/mL	14
PI 36:1	1.749 ± 0.07	2.1 ± 0.59	nmol/mL	13
PI 36:2	6.338 ± 0.532	7.7 ± 0.93	nmol/mL	15
PI 36:3	1.064 ± 0.068	2.2 ± 0.29	nmol/mL	14
PI 36:4	2.666 ± 0.148	3.0 ± 0.48	nmol/mL	14
PI 38:3	2.911 ± 0.237	3.4 ± 0.54	nmol/mL	14
PI 38:4	15.83 ± 1.142	19 ± 2.2	nmol/mL	17
PI 38:5	0.928 ± 0.045	2.5 ± 0.44	nmol/mL	15
PI 38:6	0.777 ± 0.106	0.32 ± 0.031	nmol/mL	10
PI 40:4	1.277 ± 0.139	0.30 ± 0.042	nmol/mL	7
PI 40:6	0.385 ± 0.005	0.84 ± 0.16	nmol/mL	12
PG 36:2	0.41 ± 0.087	0.67 ± 0.24	nmol/mL	6
HexCer d42:1	0.012 ± 0.003	2.7 ± 0.73	nmol/mL	6
SM d31:1	0.043 ± 0.003	0.19 ± 0.049	nmol/mL	5
SM d32:1	3.624 ± 0.364	8.4 ± 1.4	nmol/mL	14
SM d32:2	0.239 ± 0.02	0.66 ± 0.24	nmol/mL	10
SM d33:1	2.289 ± 0.192	4.7 ± 0.64	nmol/mL	14
SM d34:0	4.05 ± 0.221	5.8 ± 1.3	nmol/mL	14
SM d34:1	43.58 ± 3.71	100 ± 15	nmol/mL	21
SM d34:2	7.613 ± 0.789	16 ± 2.2	nmol/mL	17
SM d35:1	0.85 ± 0.096	2.5 ± 0.58	nmol/mL	9
SM d35:2	0.22 ± 0.019	0.52 ± 0.21	nmol/mL	6
SM d36:0	0.958 ± 0.027	2.0 ± 0.49	nmol/mL	11

SM d36:1	8.982 ± 0.905	20 ± 3.7	nmol/mL	22
SM d36:2	4.48 ± 0.34	9.6 ± 1.5	nmol/mL	22
SM d36:3	1.746 ± 0.07	1.3 ± 0.41	nmol/mL	13
SM d37:1	0.423 ± 0.075	1.0 ± 0.23	nmol/mL	11
SM d38:1	9.126 ± 0.875	11 ± 3.1	nmol/mL	17
SM d38:2	2.521 ± 0.291	5.2 ± 1.3	nmol/mL	17
SM d39:1	3.08 ± 0.339	3.6 ± 1.0	nmol/mL	14
SM d39:2	0.393 ± 0.028	0.61 ± 0.16	nmol/mL	9
SM d40:1	18.37 ± 1.588	20 ± 5.1	nmol/mL	17
SM d40:2	14.62 ± 1.515	12 ± 2.8	nmol/mL	15
SM d40:3	1.247 ± 0.093	2.2 ± 0.79	nmol/mL	8
SM d41:1	5.686 ± 0.957	7.7 ± 2.1	nmol/mL	14
SM d41:2	5.168 ± 0.547	5.8 ± 1.4	nmol/mL	14
SM d41:3	0.431 ± 0.026	0.77 ± 0.30	nmol/mL	7
SM d42:1	8.041 ± 1.284	20 ± 5.4	nmol/mL	21
SM d42:2	33.71 ± 2.501	44 ± 11	nmol/mL	18
SM d42:3	23.96 ± 1.99	17 ± 4.7	nmol/mL	12
SM d43:2	1.07 ± 0.207	1.0 ± 0.29	nmol/mL	10
SM d44:2	0.179 ± 0.037	0.40 ± 0.13	nmol/mL	9
CDCA	0.23 ± 0.006	0.30 ± 0.11	nmol/mL	7
CA	0.04 ± 0.006	0.12 ± 0.034	nmol/mL	9
DCA	0.23 ± 0.006	0.35 ± 0.083	nmol/mL	9
GCDCA	0.419 ± 0.013	1.1 ± 0.18	nmol/mL	8
GDCA	0.419 ± 0.013	0.43 ± 0.069	nmol/mL	7
GLCA	0.008 ± 0.002	0.025 ± 0.0018	nmol/mL	6
GUDCA	0.419 ± 0.013	0.15 ± 0.024	nmol/mL	6
UDCA	0.23 ± 0.006	0.11 ± 0.024	nmol/mL	8