

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

Lipid Species	Measurement*	Consensus Value**	Units	No. of labs
DAG 30:0	0.178 ± 0.038	0.83 ± 0.17	nmol/mL	7
DAG 34:1	49.49 ± 10.25	6.1 ± 2.4	nmol/mL	16
DAG 36:2	98.16 ± 20.31	6.2 ± 2.2	nmol/mL	16
DAG 36:3	161.6 ± 30.87	8.4 ± 3.3	nmol/mL	15
DAG 36:4	36.78 ± 10.52	2.8 ± 1.0	nmol/mL	12
TAG 46:2	43.34 ± 7.795	3.6 ± 1.3	nmol/mL	8
TAG 48:0	34.49 ± 12.89	4.5 ± 1.2	nmol/mL	10
TAG 48:1	74.69 ± 12.79	13 ± 3.2	nmol/mL	16
TAG 48:2	103.8 ± 16.77	16 ± 2.8	nmol/mL	15
TAG 48:4	235.8 ± 35.16	1.3 ± 0.23	nmol/mL	5
TAG 49:1	24.8 ± 2.353	2.0 ± 0.42	nmol/mL	9
TAG 49:2	30.15 ± 5.622	1.8 ± 0.56	nmol/mL	6
TAG 50:0	9.828 ± 2.134	3.8 ± 0.83	nmol/mL	11
TAG 50:1	55.95 ± 10.29	38 ± 10	nmol/mL	14
TAG 50:2	170.3 ± 32.99	47 ± 12	nmol/mL	15
TAG 50:3	165.7 ± 27.19	23 ± 6.6	nmol/mL	16
TAG 50:4	79.01 ± 16.99	8.7 ± 2.9	nmol/mL	15
TAG 50:5	15.8 ± 2.781	1.6 ± 0.64	nmol/mL	7
TAG 51:1	7.147 ± 3.01	1.8 ± 0.48	nmol/mL	7
TAG 51:2	17.31 ± 2.858	4.8 ± 1.1	nmol/mL	8
TAG 51:3	17.76 ± 3.09	4.8 ± 1.9	nmol/mL	5
TAG 52:1	23.14 ± 3.643	14 ± 2.9	nmol/mL	11
TAG 52:2	133.4 ± 22.13	44 ± 14	nmol/mL	16
TAG 52:3	331.1 ± 57.19	100 ± 29	nmol/mL	16
TAG 52:4	314.9 ± 47.26	48 ± 17	nmol/mL	15
TAG 52:5	141 ± 29.54	15 ± 5.7	nmol/mL	13
TAG 52:6	32.11 ± 10.75	4.0 ± 1.4	nmol/mL	8
TAG 52:7	6.449 ± 2.234	0.39 ± 0.13	nmol/mL	5
TAG 53:2	3.851 ± 1.391	1.9 ± 0.41	nmol/mL	9
TAG 53:3	7.06 ± 1.034	3.7 ± 1.1	nmol/mL	6
TAG 53:4	6.641 ± 1.643	2.4 ± 0.76	nmol/mL	6
TAG 54:1	2.161 ± 0.357	3.2 ± 0.91	nmol/mL	10
TAG 54:2	16.45 ± 2.89	8.2 ± 2.6	nmol/mL	13
TAG 54:3	72.95 ± 13.54	26 ± 9.8	nmol/mL	15
TAG 54:4	121.7 ± 20.45	36 ± 13	nmol/mL	15
TAG 54:5	123.5 ± 17.79	27 ± 11	nmol/mL	15
TAG 54:6	81.93 ± 15.22	14 ± 5.1	nmol/mL	16
TAG 54:7	36.25 ± 6.277	5.6 ± 1.5	nmol/mL	7
TAG 56:2	0.515 ± 0.024	0.69 ± 0.23	nmol/mL	5
TAG 56:4	3.261 ± 1.003	2.0 ± 0.56	nmol/mL	10
TAG 56:7	34.85 ± 6.133	13 ± 2.7	nmol/mL	8

TAG 56:9	11.28 ± 1.882	0.71 ± 0.27	nmol/mL	5
TAG 58:7	3.01 ± 0.275	2.0 ± 0.64	nmol/mL	5
TAG 58:8	0.744 ± 0.208	0.68 ± 0.21	nmol/mL	9
TAG 58:9	9.084 ± 0.997	1.2 ± 0.27	nmol/mL	6
LPC 14:0	1.375 ± 0.066	1.0 ± 0.20	nmol/mL	16
LPC 15:0	0.917 ± 0.016	0.52 ± 0.11	nmol/mL	9
LPC 16:0	164.4 ± 3.649	73 ± 11	nmol/mL	20
LPC O-16:0	4.355 ± 0.035	0.55 ± 0.16	nmol/mL	10
LPC P-16:0	2.717 ± 0.07	0.46 ± 0.13	nmol/mL	8
LPC 16:1	4.971 ± 0.134	2.4 ± 0.35	nmol/mL	19
LPC 17:0	1.359 ± 0.022	1.4 ± 0.24	nmol/mL	6
LPC 17:1	0.371 ± 0.015	0.25 ± 0.071	nmol/mL	6
LPC 18:0	53.73 ± 1.381	27 ± 3.3	nmol/mL	20
LPC O-18:0	1.32 ± 0.026	0.16 ± 0.058	nmol/mL	6
LPC 18:1	37.64 ± 0.349	18 ± 2.3	nmol/mL	19
LPC 18:2	56.79 ± 1.232	22 ± 2.9	nmol/mL	19
LPC 18:3	10.45 ± 0.452	0.44 ± 0.13	nmol/mL	18
LPC 20:0	0.256 ± 0.007	0.10 ± 0.034	nmol/mL	7
LPC 20:1	0.386 ± 0.024	0.19 ± 0.024	nmol/mL	13
LPC 20:2	0.498 ± 0.012	0.23 ± 0.044	nmol/mL	9
LPC 20:3	3.967 ± 0.167	1.8 ± 0.26	nmol/mL	18
LPC 20:4	15.49 ± 0.533	6.0 ± 0.60	nmol/mL	20
LPC 20:5	3.257 ± 0.659	0.33 ± 0.092	nmol/mL	15
LPC 22:0	0.096 ± 0.01	0.025 ± 0.0017	nmol/mL	5
LPC 22:1	0.139 ± 0.016	0.013 ± 0.0046	nmol/mL	5
LPC 22:4	0.344 ± 0.003	0.12 ± 0.041	nmol/mL	8
LPC 22:5	0.898 ± 0.07	0.43 ± 0.13	nmol/mL	12
LPC 22:6	2.083 ± 0.079	0.77 ± 0.14	nmol/mL	17
LPE 16:0	1.68 ± 0.023	0.91 ± 0.27	nmol/mL	14
LPE 18:0	3.619 ± 0.1	1.6 ± 0.55	nmol/mL	15
LPE 18:1	2.338 ± 0.018	1.4 ± 0.47	nmol/mL	14
LPE 18:2	4.694 ± 0.407	1.9 ± 0.56	nmol/mL	16
LPE 20:4	5.095 ± 0.184	1.1 ± 0.41	nmol/mL	14
LPE 22:6	2.082 ± 0.006	0.52 ± 0.18	nmol/mL	12
PC 30:0	5.731 ± 0.162	1.6 ± 0.32	nmol/mL	11
PC O-30:0/29:0	1.11 ± 0.16	0.072 ± 0.026	nmol/mL	7
PC 32:0	22.72 ± 0.636	7.2 ± 1.0	nmol/mL	18
PC O-32:0/31:0	28.08 ± 1.371	1.5 ± 0.41	nmol/mL	11
PC 32:1	41.45 ± 1.485	13 ± 1.9	nmol/mL	18
PC O-32:1/P-32:0/31:1	18.5 ± 0.975	1.6 ± 0.24	nmol/mL	11
PC O-32:2/P-32:1/31:2	2.625 ± 0.577	0.34 ± 0.093	nmol/mL	8
PC 32:3	0.164 ± 0.03	0.42 ± 0.14	nmol/mL	8
PC P-33:1/32:2	8.33 ± 2.414	2.6 ± 0.37	nmol/mL	16
PC 34:0	31.39 ± 1.571	2.1 ± 0.37	nmol/mL	12

PC O-34:0/33:0	5.899 ± 0.444	0.76 ± 0.17	nmol/mL	10
PC 34:1	338.6 ± 12.77	120 ± 21	nmol/mL	19
PC O-34:1/P-34:0/33:1	62.5 ± 3.335	4.9 ± 0.86	nmol/mL	17
PC O-34:2/P-34:1/33:2	53.99 ± 3.708	5.2 ± 1.3	nmol/mL	17
PC O-34:3/P-34:2/33:3	68.5 ± 3.918	4.7 ± 0.88	nmol/mL	12
PC P-35:1/34:2	31.35 ± 6.175	240 ± 47	nmol/mL	18
PC O-35:4/34:4	1.682 ± 0.123	1.0 ± 0.25	nmol/mL	9
PC 34:5	0.453 ± 0.009	0.034 ± 0.0045	nmol/mL	5
PC 36:1	90.3 ± 3.607	26 ± 4.6	nmol/mL	17
PC O-36:1/P-36:0/35:1	6.366 ± 0.509	3.5 ± 0.99	nmol/mL	16
PC 36:2	388.6 ± 18.39	140 ± 25	nmol/mL	18
PC O-36:2/P-36:1/35:2	23.48 ± 0.74	7.4 ± 1.7	nmol/mL	17
PC 36:3	147.2 ± 14.49	100 ± 14	nmol/mL	17
PC 36:4	291.4 ± 11.77	150 ± 28	nmol/mL	19
PC O-36:4/P-36:3/35:4	169.8 ± 11.2	12 ± 1.4	nmol/mL	17
PC 36:5	19.01 ± 0.426	11 ± 1.8	nmol/mL	16
PC O-36:5/P-36:4/35:5	78.36 ± 8.045	6.9 ± 1.6	nmol/mL	11
PC P-36:5/35:6	10.25 ± 0.941	0.30 ± 0.094	nmol/mL	5
PC 36:6	0.326 ± 0.007	0.28 ± 0.088	nmol/mL	8
PC O-38:2/37:2	6.382 ± 1.286	0.98 ± 0.32	nmol/mL	6
PC 38:3	83.19 ± 4.051	26 ± 5.2	nmol/mL	14
PC O-38:3/P-38:2/37:3	10.83 ± 0.789	1.5 ± 0.51	nmol/mL	14
PC 38:4	179.4 ± 8.391	84 ± 14	nmol/mL	18
PC O-38:4/P-38:3/37:4	75.14 ± 3.25	7.4 ± 2.0	nmol/mL	12
PC 38:5	40.93 ± 1.456	42 ± 7.9	nmol/mL	18
PC O-38:5/P-38:4/37:5	158.6 ± 11.57	11 ± 1.6	nmol/mL	16
PC 38:6	108.5 ± 4.194	41 ± 4.4	nmol/mL	18
PC O-38:6/P-38:5/37:6	22.28 ± 5.851	3.6 ± 1.0	nmol/mL	12
PC P-38:6/36:0	10.65 ± 0.663	1.2 ± 0.39	nmol/mL	10
PC 40:4	8.647 ± 0.282	2.9 ± 0.37	nmol/mL	18
PC O-40:2/P-40:1	1.822 ± 0.46	0.069 ± 0.021	nmol/mL	5
PC O-40:4/P-40:3/39:4	11.74 ± 0.801	0.95 ± 0.38	nmol/mL	8
PC 40:5	10.68 ± 0.681	6.7 ± 1.1	nmol/mL	18
PC 40:6	33.24 ± 0.791	14 ± 2.6	nmol/mL	17
PC 40:7	9.56 ± 0.354	3.5 ± 0.26	nmol/mL	16
PC 40:8	1.29 ± 0.036	0.73 ± 0.20	nmol/mL	14
PC O-42:5/P-42:4	20.98 ± 1.216	0.79 ± 0.12	nmol/mL	7
PE 34:1	1.381 ± 0.168	1.2 ± 0.17	nmol/mL	14
PE 34:2	3.84 ± 0.225	2.2 ± 0.26	nmol/mL	16
PE O-34:2/P-34:1	5.496 ± 0.301	0.78 ± 0.17	nmol/mL	11
PE O-34:3/P-34:2	2.213 ± 0.116	1.5 ± 0.41	nmol/mL	11
PE 36:0	4.213 ± 0.241	0.28 ± 0.10	nmol/mL	11
PE 36:1	23.39 ± 1.266	1.3 ± 0.26	nmol/mL	14
PE 36:2	25.52 ± 1.191	6.7 ± 0.79	nmol/mL	16

PE O-36:2/P-36:1/35:2	8.33 ± 2.414	0.93 ± 0.22	nmol/mL	12
PE 36:3	2.267 ± 0.266	2.4 ± 0.38	nmol/mL	16
PE O-36:3/P-36:2/35:3	5.743 ± 0.144	3.2 ± 0.76	nmol/mL	15
PE 36:4	4.228 ± 0.349	3.1 ± 0.39	nmol/mL	16
PE O-36:4/P-36:3	3.525 ± 0.814	1.6 ± 0.29	nmol/mL	14
PE O-36:5/P-36:4	8.523 ± 0.624	4.9 ± 1.9	nmol/mL	15
PE 38:3	9.887 ± 1.011	0.95 ± 0.20	nmol/mL	14
PE 38:4	13.66 ± 0.448	8.1 ± 1.2	nmol/mL	16
PE O-38:4/P-38:3/37:4	1.682 ± 0.123	0.94 ± 0.18	nmol/mL	9
PE O-38:5/P-38:4	18.77 ± 0.826	5.8 ± 1.9	nmol/mL	17
PE 38:6	7.554 ± 0.474	3.2 ± 0.59	nmol/mL	15
PE O-38:6/P-38:5	9.817 ± 0.718	4.9 ± 1.2	nmol/mL	16
PE O-38:7/P-38:6	3.789 ± 0.232	3.5 ± 0.98	nmol/mL	8
PE 40:4	19.2 ± 1.351	0.26 ± 0.082	nmol/mL	10
PE 40:5	4.64 ± 0.285	0.73 ± 0.23	nmol/mL	12
PE O-40:5/P-40:4/39:5	4.86 ± 0.131	0.73 ± 0.13	nmol/mL	12
PE 40:6	2.549 ± 0.141	1.8 ± 0.36	nmol/mL	14
PE O-40:6/P-40:5/39:6	2.124 ± 0.15	1.3 ± 0.31	nmol/mL	14
PE 40:7	0.825 ± 0.105	0.77 ± 0.26	nmol/mL	11
PE O-40:7/P-40:6/39:7	4.375 ± 0.311	2.5 ± 0.72	nmol/mL	14
PI 32:1	11.09 ± 1.752	0.56 ± 0.11	nmol/mL	10
PI 34:2	17.09 ± 2.841	2.8 ± 0.38	nmol/mL	14
PI 36:1	15.46 ± 3.207	2.1 ± 0.59	nmol/mL	13
PI 36:2	68.6 ± 16.17	7.7 ± 0.93	nmol/mL	15
PI 36:3	12.09 ± 2.065	2.2 ± 0.29	nmol/mL	14
PI 36:4	20.82 ± 4.196	3.0 ± 0.48	nmol/mL	14
PI 38:4	214.9 ± 46.61	19 ± 2.2	nmol/mL	17
PI 40:4	9.02 ± 1.867	0.30 ± 0.042	nmol/mL	7
PI 40:6	9.242 ± 3.314	0.84 ± 0.16	nmol/mL	12
PG 36:2	1.336 ± 0.116	0.67 ± 0.24	nmol/mL	6
HexCer d34:1	0.235 ± 0.03	0.86 ± 0.21	nmol/mL	6
HexCer d36:1	0.01 ± 0.002	0.13 ± 0.043	nmol/mL	5
HexCer d40:1	0.333 ± 0.106	2.4 ± 0.68	nmol/mL	5
HexCer d42:1	3.174 ± 0.258	2.7 ± 0.73	nmol/mL	6
CER d34:1	0.594 ± 0.066	0.28 ± 0.044	nmol/mL	17
CER d36:1	0.432 ± 0.033	0.12 ± 0.021	nmol/mL	14
CER d38:1	0.44 ± 0.037	0.11 ± 0.021	nmol/mL	16
CER d40:1	1.362 ± 0.162	0.65 ± 0.12	nmol/mL	18
CER d40:2	1.122 ± 0.067	0.15 ± 0.021	nmol/mL	6
CER d41:1	0.695 ± 0.109	0.67 ± 0.27	nmol/mL	7
CER d42:1	1.642 ± 0.327	1.9 ± 0.47	nmol/mL	19
CER d42:2	3.525 ± 0.309	0.82 ± 0.10	nmol/mL	19
SM d31:1	0.321 ± 0.028	0.19 ± 0.049	nmol/mL	5
SM d32:1	4.211 ± 0.061	8.4 ± 1.4	nmol/mL	14

SM d32:2	0.318 ± 0.004	0.66 ± 0.24	nmol/mL	10
SM d33:1	2.943 ± 0.019	4.7 ± 0.64	nmol/mL	14
SM d34:0	9.94 ± 1.147	5.8 ± 1.3	nmol/mL	14
SM d34:1	131.1 ± 3.516	100 ± 15	nmol/mL	21
SM d34:2	9.137 ± 0.16	16 ± 2.2	nmol/mL	17
SM d35:1	2.202 ± 0.08	2.5 ± 0.58	nmol/mL	9
SM d35:2	0.391 ± 0.002	0.52 ± 0.21	nmol/mL	6
SM d36:0	1.716 ± 0.187	2.0 ± 0.49	nmol/mL	11
SM d36:1	18.15 ± 0.524	20 ± 3.7	nmol/mL	22
SM d36:2	14.59 ± 0.153	9.6 ± 1.5	nmol/mL	22
SM d36:3	0.396 ± 0.019	1.3 ± 0.41	nmol/mL	13
SM d37:1	1.019 ± 0.07	1.0 ± 0.23	nmol/mL	11
SM d38:1	14.73 ± 0.436	11 ± 3.1	nmol/mL	17
SM d38:2	5.026 ± 0.27	5.2 ± 1.3	nmol/mL	17
SM d38:3	0.213 ± 0.023	0.61 ± 0.24	nmol/mL	8
SM d39:1	3.592 ± 0.13	3.6 ± 1.0	nmol/mL	14
SM d39:2	0.491 ± 0.024	0.61 ± 0.16	nmol/mL	9
SM d40:1	28.63 ± 1.794	20 ± 5.1	nmol/mL	17
SM d40:2	19.84 ± 0.455	12 ± 2.8	nmol/mL	15
SM d40:3	1.305 ± 0.174	2.2 ± 0.79	nmol/mL	8
SM d41:1	5.889 ± 0.512	7.7 ± 2.1	nmol/mL	14
SM d41:2	6.642 ± 0.222	5.8 ± 1.4	nmol/mL	14
SM d41:3	0.742 ± 0.009	0.77 ± 0.30	nmol/mL	7
SM d42:1	8.302 ± 0.973	20 ± 5.4	nmol/mL	21
SM d42:2	51.27 ± 2.319	44 ± 11	nmol/mL	18
SM d42:3	37.23 ± 1.08	17 ± 4.7	nmol/mL	12
SM d43:2	1.829 ± 0.222	1.0 ± 0.29	nmol/mL	10
SM d44:2	0.171 ± 0.02	0.40 ± 0.13	nmol/mL	9
CE 14:0	2 ± 0.379	16 ± 6.0	nmol/mL	7
CE 15:0	9.074 ± 2.168	5.3 ± 1.8	nmol/mL	6
CE 16:0	2.123 ± 0.493	210 ± 58	nmol/mL	13
CE 16:1	3.418 ± 0.979	100 ± 27	nmol/mL	11
CE 16:2	32.61 ± 2.209	1.9 ± 0.46	nmol/mL	5
CE 17:1	0.459 ± 0.137	8.2 ± 1.0	nmol/mL	9
CE 18:0	0.155 ± 0.018	15 ± 3.7	nmol/mL	7
CE 18:1	1.092 ± 0.213	450 ± 110	nmol/mL	14
CE 18:2	12.64 ± 2.376	1,700 ± 430	nmol/mL	14
CE 20:3	1.28 ± 0.127	35 ± 12	nmol/mL	13
CE 20:4	9.866 ± 1.422	350 ± 58	nmol/mL	14
CE 22:5	3.402 ± 0.861	4.1 ± 1.6	nmol/mL	6