

How to read an untargeted lipid analysis report based on LipidSearch 5.2.7.

Proteomics Resource Center, The Rockefeller University

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'Class_Summary_Normalized': Lipid class signals normalized to deuterated standards, per sample.

Class	Lipid Count	t-test A vs B	Log(2) Fold Change B vs A	t-test A vs C	Log(2) Fold Change A vs C	t-test D vs C	Log(2) Fold Change D vs C	t-test D vs B	Log(2) Fold Change B vs D	A_01	A_02	A_03	B_01	B_02
ACCA	4	0.35	-	0.01	0.67	0.12	-	0.01	1.37	1.20E-01	1.02E-01	1.22E-01	1.17E-01	1.17E-01
CER	40	0.37	-	0.34	-	0.71	-	0.33	-	3.11E+00	3.05E+00	3.69E+00	2.11E+01	3.62E+00
CHE	7	0.48	-	0.49	-	0.50	-	0.50	-	3.78E-01	4.00E-01	6.08E-01	3.85E-01	3.43E-01
CL	25	0.08	-	0.01	-0.41	0.64	-	0.82	-	9.47E-01	8.17E-01	1.06E+00	1.25E+00	1.03E+00
CO	2	0.48	-	0.03	-0.60	0.56	-	0.44	-	3.82E-01	3.43E-01	5.29E-01	6.36E-01	3.80E-01
DG	40	0.69	-	0.02	-0.19	0.21	-	0.07	-	9.89E+00	1.04E+01	1.06E+01	1.15E+01	9.81E+00
HEX1CER	5	0.78	-	0.00	1.55	0.37	-	0.01	1.38	3.74E-01	3.79E-01	3.64E-01	4.53E-01	2.89E-01
HEX3CER	9	0.82	-	0.01	0.40	0.57	-	0.13	-	1.16E+00	1.08E+00	1.30E+00	1.41E+00	1.02E+00
LPC	6	0.28	-	0.06	-	0.58	-	0.01	0.79	7.47E-02	7.48E-02	1.03E-01	1.03E-01	9.18E-02
LPE	5	0.01	0.51	0.83	-	0.69	-	0.06	-	1.25E-01	1.09E-01	1.49E-01	1.85E-01	1.71E-01
LPG	1	0.77	-	0.00	-1.15	0.03	-0.55	0.14	-	4.83E-03	5.72E-03	8.25E-03	8.61E-03	5.52E-03
LPI	1	0.14	-	0.12	-	0.94	-	0.01	0.81	8.40E-02	6.46E-02	1.05E-01	1.10E-01	9.84E-02
LPS	1	0.38	-	0.19	-	0.57	-	0.26	-	5.13E-02	4.96E-02	6.72E-02	6.77E-02	5.72E-02
MG	2	0.43	-	0.72	-	0.23	-	0.12	-	3.12E-02	3.66E-02	2.54E-02	2.93E-02	2.46E-02
PA	19	0.63	-	0.04	0.14	0.90	-	0.17	-	1.50E+00	1.54E+00	1.56E+00	1.66E+00	1.45E+00
PC	181	0.21	-	0.47	-	0.36	-	0.45	-	3.97E+01	3.86E+01	4.90E+01	4.88E+01	4.62E+01
PE	220	0.22	-	0.89	-	0.45	-	0.09	-	5.46E+01	5.31E+01	7.05E+01	7.45E+01	6.29E+01
PG	53	0.32	-	0.18	-	0.01	-0.56	0.04	0.53	2.37E+00	2.41E+00	3.11E+00	3.37E+00	2.69E+00
PI	53	0.65	-	0.63	-	0.69	-	0.62	-	2.71E+01	7.08E+01	3.50E+01	3.88E+01	3.11E+01
PS	86	0.15	-	0.70	-	0.59	-	0.07	-	2.52E+01	2.38E+01	3.31E+01	3.67E+01	2.94E+01
TG	118	0.32	-	0.00	0.44	0.19	-	0.05	-	6.58E+01	6.08E+01	6.44E+01	5.69E+01	4.96E+01

*) Based on pool sample(s)

#) Grades: From A to D. Typically only grade A and B are accepted.

\$) Typical criteria to pass: R² better than 0.9, CV better than 0.3, Scores A or B.

'Datatable_Normalized: Individual lipid signals normalized to deuterated standard, per sample.

ID	LipidID	Class	BaseRt	Adduction	Top_Grade	LipidMaps	Identifier	CV*	Percent_Backgroud	Rsq	QC_Status	t-test A vs B	Log(2) Fold Change B vs A	t-test A vs C	Log(2) Fold Change A vs C	t-test D vs C	Log(2) Fold Change D vs C	t-test D vs B	Log(2) Fold Change B vs D	A_01	A_02	A_03	B_01
135	AcCa(16:0)	ACCA	5.47	M+H	A	NA	acca(16:0)_5.4661	2.07	0	0.9969	Pass	0.39	-	0.01	0.75	0.12	-	0.01	1.49	8.13E-02	6.68E-02	7.61E-02	7.35E-02
107	AcCa(18:0)	ACCA	7.09	M+H	A	NA	acca(18:0)_7.0946	4.95	0	0.9977	Pass	0.30	-	0.05	0.51	0.16	-	0.01	1.11	2.11E-02	1.97E-02	2.53E-02	2.41E-02
528	AcCa(18:1)	ACCA	5.84	M+H	A	NA	acca(18:1)_5.8391	3.74	0	0.9986	Pass	0.27	-	0.01	0.83	0.14	-	0.00	1.59	1.42E-02	1.24E-02	1.64E-02	1.64E-02
118	AcCa(18:2)	ACCA	4.63	M+H	A	NA	acca(18:2)_4.6277	6.7	0	0.9987	Pass	0.89	-	0.28	-	0.22	-	0.48	-	3.59E-03	3.13E-03	3.88E-03	3.34E-03
906	Cer(d15:0_18:1)	CER	17.81	M+HCOO	B	NA	cer(d15:0_18:1)_17.8087	5.9	0	0.9971	Pass	0.52	-	0.00	1.10	0.59	-	0.03	1.20	2.55E-03	2.89E-03	3.36E-03	4.34E-03
1009	Cer(d15:0_24:1)	CER	21.86	M+HCOO	B	NA	cer(d15:0_24:1)_21.8631	9.43	0	0.9999	Pass	0.69	-	0.04	0.59	0.73	-	0.03	0.74	6.93E-04	6.75E-04	9.46E-04	9.94E-04
45	Cer(d18:0_16:0)	CER	20.13	M+H	A	LMSP02020001	cer(d18:0_16:0)_20.1275	6.38	1.25	0.9152	Pass	0.41	-	0.05	-	0.52	-	0.60	-	2.63E-01	2.78E-01	2.60E-01	2.16E+0
928	Cer(d18:0_16:0)	CER	20.21	M+HCOO	A	LMSP02020001	cer(d18:0_16:0)_20.2127	7.1	0	0.9933	Pass	0.89	-	0.06	-	0.27	-	0.15	-	5.06E-03	6.04E-03	7.13E-03	8.98E-03
162	Cer(d18:0_22:0)	CER	22.34	M+H2O	A	LMSP02020025	cer(d18:0_22:0)_22.3398	7.21	0.1	0.9982	Pass	0.55	-	0.47	-	0.50	-	0.06	-	3.75E-03	3.87E-03	6.39E-03	5.45E-03
895	Cer(d18:1_14:0)	CER	16.74	M+HCOO	A	LMSP02010001	cer(d18:1_14:0)_16.7417	7.47	0	0.9973	Pass	0.20	-	0.00	0.68	0.39	-	0.02	0.83	2.93E-03	3.17E-03	3.51E-03	4.65E-03
3	Cer(d18:1_16:0)	CER	18.88	M+H2O	A	LMSP02010036	cer(d18:1_16:0)_18.8839	6.65	0.81	0.9965	Pass	0.51	-	0.01	0.47	0.82	-	0.08	-	7.22E-02	7.64E-02	8.81E-02	1.13E-02
888	Cer(d18:1_16:0)	CER	18.53	M+HCOO	A	LMSP02010004	cer(d18:1_16:0)_18.5317	10.17	0	0.9931	Pass	0.71	-	0.00	0.84	0.45	-	0.04	0.71	2.43E-03	2.11E-03	2.72E-03	2.94E-03
891	Cer(d18:1_16:0)	CER	18.88	M+HCOO	A	LMSP02010004	cer(d18:1_16:0)_18.8809	6.39	0	0.9981	Pass	0.57	-	0.01	0.46	0.46	-	0.09	-	6.37E-02	7.21E-02	7.96E-02	9.74E-02
630	Cer(d18:1_17:0)	CER	20.01	M+HCOO	B	LMSP02010020	cer(d18:1_17:0)_20.0125	4.03	0	0.9966	Pass	0.71	-	0.26	-	0.12	-	0.30	-	5.01E-03	5.74E-03	7.00E-03	7.12E-03
900	Cer(d18:1_18:0)	CER	20.73	M+HCOO	A	LMSP02010006	cer(d18:1_18:0)_20.7261	9.08	0	0.9978	Pass	0.93	-	0.21	-	0.62	-	0.43	-	2.33E-02	2.43E-02	2.87E-02	3.41E-02
982	Cer(d18:1_20:0)	CER	21.57	M+HCOO	A	LMSP02010007	cer(d18:1_20:0)_21.5654	7.14	0	0.9994	Pass	0.69	-	0.03	0.52	0.58	-	0.03	0.66	3.95E-03	4.26E-03	5.31E-03	5.72E-03
148	Cer(d18:1_22:0)	CER	22.09	M+H2O	A	LMSP02010042	cer(d18:1_22:0)_22.0858	4.9	2.12	0.9983	Pass	0.83	-	0.09	-	0.20	-	0.02	0.61	1.45E-02	1.49E-02	1.95E-02	1.90E-02
953	Cer(d18:1_22:0)	CER	22.11	M+HCOO	A	LMSP02010008	cer(d18:1_22:0)_22.1078	7.69	0.29	0.9977	Pass	0.51	-	0.10	-	0.61	-	0.05	0.65	9.28E-03	1.02E-02	1.34E-02	1.49E-02
977	Cer(d18:1_23:0)	CER	22.30	M+HCOO	A	LMSP02010021	cer(d18:1_23:0)_22.3030	6.69	0	0.9973	Pass	0.69	-	0.05	0.70	0.81	-	0.01	0.85	3.09E-03	3.00E-03	4.48E-03	3.97E-03
598	Cer(d18:1_23:1)	CER	21.85	M+HCOO	A	NA	cer(d18:1_23:1)_21.8530	0.27	-	0.73	-	0.27	-	0.73	-	0.56	-	0.06	-	2.67E-03	2.64E-03	4.23E-03	4.37E-03
247	Cer(d18:1_24:0)	CER	22.34	M+H	A	LMSP02010012	cer(d18:1_24:0)_22.3430	0.41	-	0.13	-	0.41	-	0.13	-	0.47	-	0.35	-	2.98E-01	2.96E-01	2.27E-01	2.27E+0
248	Cer(d18:1_24:0)	CER	22.47	M+H2O	A	LMSP02010012	cer(d18:1_24:0)_22.4658	0.94	-	0.13	-	0.94	-	0.13	-	0.29	-	0.05	-	5.22E-02	5.29E-02	7.28E-02	7.07E-02
1005	Cer(d18:1_24:0)	CER	22.47	M+HCOO	A	LMSP02010012	cer(d18:1_24:0)_22.4658	4.64	0.38	0.9982	Pass	0.94	-	0.05	-	0.38	-	0.07	-	3.10E-02	3.24E-02	4.15E-02	4.35E-02
999	Cer(d18:1_24:1)	CER	21.97	M+HCOO	A	LMSP02010009	cer(d18:1_24:1)_21.9719	21.48	0	0.1547	Rsq < 0.9	0.35	-	0.26	-	0.31	-	0.01	1.17	1.01E-03	8.41E-04	1.61E-03	1.58E-03
1000	Cer(d18:1_24:1)	CER	22.10	M+HCOO	A	LMSP02010009	cer(d18:1_24:1)_22.0972	55.88	0	0.9986	CV > 30%	0.09	-	0.75	-	0.38	-	0.10	-	1.80E-02	1.92E-02	2.80E-02	3.40E-02
945	Cer(d18:2_18:0)	CER	19.40	M+HCOO	A	LMSP02010170	cer(d18:2_18:0)_19.4044	4.69	0	0.9904	Pass	0.88	-	0.04	1.11	0.83	-	0.05	-	2.04E-03	1.76E-03	1.22E-03	1.49E-03
639	Cer(d18:2_20:0)	CER	20.93	M+HCOO	B	LMSP02010026	cer(d18:2_20:0)_20.925	35.32	0	0.9906	CV > 30%	-	-	-	-	-	-	0.01	1.71	2.45E-03	2.50E-03	3.05E-03	4.25E-03
949	Cer(d18:2_22:0)	CER	21.58	M+H	A	LMSP02010029	cer(d18:2_22:0)_21.5752	10.04	0	0.7665	Rsq < 0.9	-	-	-	-	-	-	0.01	0.75	5.73E-04	6.69E-04	1.09E-03	1.14E-03
950	Cer(d18:2_22:0)	CER	21.68	M+HCOO	A	LMSP02010029	cer(d18:2_22:0)_21.6835	11.96	0	0.9994	Pass	-	-	-	-	-	-	0.00	1.96	5.68E-03	4.75E-03	8.92E-03	1.09E-03

*) Based on pool sample(s)

#) Grades: From A to D. Typically only grade A and B are accepted.

\$) Typical criteria to pass: R² better than 0.9, CV better than 0.3, Scores A or B.

'Class_Summary_Raw': Raw signals of lipid classes, per sample.

Lipid class

T-test p-value

LOG2 fold diff.

Summed signals (both polarities) for lipids in class, per sample.

Class	t-test A vs B	Log(2) Fold Change B vs A	t-test A vs C	Log(2) Fold Change A vs C	t-test D vs C	Log(2) Fold Change D vs C	t-test D vs B	Log(2) Fold Change B vs D	A_01	A_02	A_03	B_01	B_02	B_03	C_01	C_02
ACCA	0.42	-	0.03	0.70	0.05	-	0.00	1.50	3.42E+05	2.73E+05	3.98E+05	3.50E+05	3.77E+05	3.89E+05	2.36E+05	1.72E+
CER	0.78	-	0.90	-	0.23	-	0.48	-	3.81E+08	3.44E+08	3.76E+08	3.81E+08	3.65E+08	3.38E+08	3.48E+08	3.75E+
CH	0.70	-	0.69	-	0.24	-	0.99	-	1.15E+06	1.15E+06	2.36E+06	1.49E+06	1.31E+06	1.36E+06	1.63E+06	1.64E+
CH-D7	0.69	-	0.45	-	0.19	-	0.37	-	8.23E+06	6.05E+06	7.79E+06	7.02E+06	7.85E+06	8.16E+06	7.41E+06	7.79E+
CHF	0.46	-	0.72	-	0.21	-	0.75	-	1.07E+06	1.07E+06	1.99E+06	1.15E+06	1.11E+06	1.13E+06	1.42E+06	1.42E+
CHE-D7	0.57	-	0.52	-	0.09	-	0.07	-	2.03E+06	1.62E+06	1.94E+06	1.92E+06	1.91E+06	1.99E+06	1.85E+06	2.00E+
CL	0.19	-	0.11	-	0.28	-	0.43	-	2.09E+06	2.19E+06	3.47E+06	3.73E+06	3.32E+06	3.22E+06	3.37E+06	3.34E+
CO	0.11	-	0.09	-	0.16	-	0.77	-	1.08E+06	9.20E+05	1.73E+06	1.89E+06	1.23E+06	1.11E+06	1.69E+06	1.86E+
D5-DG	0.11	-	0.09	-	0.62	-	0.20	-	1.35E+08	1.25E+08	1.19E+08	1.16E+08	1.32E+08	1.36E+08	1.16E+08	1.26E+
D5-TG	0.11	-	0.09	-	0.00	-0.14	0.02	0.11	6.25E+08	5.38E+08	6.15E+08	5.98E+08	6.18E+08	6.26E+08	6.25E+08	6.28E+
DG	0.11	-	0.09	-	0.94	-	0.46	-	1.86E+08	2.08E+08	1.78E+08	2.03E+08	1.77E+08	1.51E+08	1.79E+08	1.97E+
HEX1CER	0.11	-	0.09	1.56	0.57	-	0.02	1.53	1.06E+06	1.02E+06	1.19E+06	1.35E+06	9.32E+05	8.05E+05	3.57E+05	3.66E+
HEX3CER	0.11	-	0.09	-	0.15	-	0.11	-	3.30E+06	2.90E+06	4.26E+06	4.22E+06	3.30E+06	2.43E+06	2.61E+06	2.38E+
LPC	0.24	-	0.09	-	0.38	-	0.01	0.90	1.02E+05	8.09E+04	1.23E+05	1.27E+05	1.17E+05	1.14E+05	6.89E+04	7.34E+
LPC-D5	0.78	-	0.81	-	0.19	-	0.17	-	2.90E+06	2.39E+06	2.63E+06	2.68E+06	2.80E+06	2.58E+06	2.61E+06	2.61E+
LPE	0.11	-	0.93	-	0.45	-	0.06	-	2.46E+05	2.13E+05	2.95E+05	3.54E+05	3.35E+05	2.73E+05	2.34E+05	2.38E+
LPE-D5	0.37	-	0.75	-	0.31	-	0.89	-	1.10E+07	9.92E+06	1.08E+07	1.04E+07	1.06E+07	8.58E+06	1.05E+07	1.00E+
LPG	0.27	-	0.01	-1.30	0.14	-	0.23	-	1.98E+03	1.67E+03	2.79E+03	3.23E+03	2.16E+03	2.79E+03	4.20E+03	6.55E+
LPG-D5	0.24	-	0.69	-	0.82	-	0.70	-	3.39E+06	2.73E+06	2.90E+06	3.18E+06	3.36E+06	3.32E+06	2.78E+06	3.49E+
LPI	0.76	-	0.23	-	0.79	-	0.20	-	1.52E+04	1.44E+04	2.17E+04	2.41E+04	1.83E+04	1.28E+04	1.21E+04	1.42E+
LPI-D5	0.81	-	0.30	-	0.75	-	0.26	-	6.49E+05	6.07E+05	5.99E+05	6.84E+05	6.26E+05	5.02E+05	6.07E+05	8.75E+
LPS	0.86	-	0.68	-	0.44	-	0.76	-	6.10E+03	5.60E+03	8.00E+03	8.06E+03	6.69E+03	4.21E+03	5.90E+03	6.19E+
LPS-D5	0.93	-	0.30	-	0.77	-	0.30	-	4.36E+05	3.70E+05	4.03E+05	4.52E+05	4.16E+05	3.29E+05	4.02E+05	5.93E+
MG	0.17	-	0.67	-	0.98	-	0.38	-	8.85E+04	9.80E+04	8.30E+04	8.72E+04	7.93E+04	7.24E+04	7.48E+04	8.63E+
PA	1.00	-	0.26	-	0.14	-	0.08	-	4.27E+06	4.12E+06	5.09E+06	4.96E+06	4.68E+06	3.84E+06	4.06E+06	3.72E+
PC	0.66	-	0.21	-	0.89	-	0.06	-	4.72E+09	4.15E+09	6.06E+09	4.83E+09	5.53E+09	5.43E+09	4.13E+09	3.50E+
PC-D5	0.66	-	0.21	-	0.89	-	0.06	-	4.72E+09	4.15E+09	6.06E+09	4.83E+09	5.53E+09	5.43E+09	4.13E+09	3.50E+

Deuterated (D7) lipid standard

*) Based on pool sample(s)

#) Grades: From A to D. Typically only grade A and B are accepted.

\$) Typical criteria to pass: R^2 better than 0.9, CV better than 0.3, Scores A or B.

'Datatable_Row': Individual, not normalized, lipid signals, per sample.

ID	LipidID	Class	BaseRt	Adduction	Top_Grade	LipidMaps	Identifier	CV*	Percent_Background	Rsq	QC_Status	t-test A vs B	Log2(2) Fold Change B vs A	t-test A vs C	Log2(2) Fold Change A vs C	t-test D vs C	Log2(2) Fold Change D vs C	t-test D vs B	Log2(2) Fold Change B vs D	A_01	A_02	A_03	B_01	B_02
135	AcCa(16:0)	ACCA	5.47	M+H	A	NA	acca(16:0)_5.4661	2.07	0.00	1.00	Pass	0.40	-	0.02	0.77	0.05	-	0.00	1.62	2.31E+05	1.79E+05	2.49E+05	2.19E	
107	AcCa(18:0)	ACCA	7.09	M+H	A	NA	acca(18:0)_7.0946	4.95	0.00	1.00	Pass	0.57	-	0.10	-	0.05	-	0.00	1.26	6.00E+04	5.29E+04	8.28E+04	7.19E	
528	AcCa(18:1)	ACCA	5.84	M+H	A	NA	acca(18:1)_5.8391	3.74	0.00	1.00	Pass	0.38	-	0.04	0.87	0.05	-	0.00	1.72	4.04E+04	3.31E+04	5.35E+04	4.89E	
118	AcCa(18:2)	ACCA	4.63	M+H	A	NA	acca(18:2)_4.6277	6.70	0.00	1.00	Pass	0.86	-	0.48	-	0.09	-	0.19	-	1.02E+04	8.38E+03	1.27E+04	9.95E	
906	Cer(d15:0_18:1)	CER	17.81	M+HCOO	B	NA	cer(d15:0_18:1)_17.8087	5.90	0.00	1.00	Pass	0.33	-	0.01	1.07	0.90	-	0.01	1.33	3.06E+04	3.03E+04	3.93E+04	4.82E	
1009	Cer(d15:0_24:1)	CER	21.86	M+HCOO	B	NA	cer(d15:0_24:1)_21.8631	9.43	0.00	1.00	Pass	0.94	-	0.02	0.65	0.53	-	0.05	-	1.15E+04	1.06E+04	1.40E+04	1.54E	
45	Cer(d18:0_16:0)	CER	20.13	M+H	A	LMSP02020001	cer(d18:0_16:0)_20.1275	6.38	1.25	0.92	Pass	0.94	-	0.01	-0.48	0.06	-	0.07	-	9.96E+04	1.07E+05	9.31E+04	1.50E	
928	Cer(d18:0_16:0)	CER	20.21	M+HCOO	A	LMSP02020001	cer(d18:0_16:0)_20.2127	7.10	0.00	0.99	Pass	0.68	-	0.07	-	0.99	-	0.28	-	2.21E+04	2.21E+04	2.83E+04	3.53E	
162	Cer(d18:0_22:0)	CER	22.34	M+H-H2O	A	1,LMSP02020025,L	cer(d18:0_22:0)_22.3398	7.21	0.10	1.00	Pass	0.63	-	0.42	-	0.26	-	0.05	0.55	3.21E+05	3.18E+05	5.19E+05	5.01E	
895	Cer(d18:1_14:0)	CER	16.74	M+HCOO	A	LMSP02010001	cer(d18:1_14:0)_16.7417	7.47	0.00	1.00	Pass	0.07	-	0.01	0.64	0.97	-	0.00	0.98	3.52E+04	3.33E+04	4.11E+04	5.16E	
3	Cer(d18:1_16:0)	CER	18.88	M+H-H2O	A	4,LMSP02010036,L	cer(d18:1_16:0)_18.8839	6.65	0.81	1.00	Pass	0.70	-	0.02	0.51	0.26	-	0.07	-	3.30E+06	3.10E+06	3.99E+06	4.69E	
888	Cer(d18:1_16:0)	CER	18.53	M+HCOO	A	LMSP02010004	cer(d18:1_16:0)_18.5317	10.17	0.00	0.99	Pass	0.57	-	0.02	0.84	0.77	-	0.01	0.86	2.35E+04	1.76E+04	2.54E+04	2.59E	
891	Cer(d18:1_16:0)	CER	18.88	M+HCOO	A	LMSP02010004	cer(d18:1_16:0)_18.8809	6.39	0.00	1.00	Pass	0.37	-	0.02	0.46	0.80	-	0.03	0.67	6.17E+05	6.01E+05	7.43E+05	8.57E	
23	Cer(d18:1_16:1)+D7:(s)	CER	17.06	M+H-H2O	A	NA	r(d18:1_16:1)+d7:(s)_17.05	3.77	0.01	1.00	Pass	0.55	-	0.39	-	0.05	-	0.66	-	8.07E+07	7.38E+07	8.20E+07	7.83E	
24	Cer(d18:1_16:1)+D7:(s)	CER	17.3	M+H-H2O	A	NA	cer(d18:1_16:1)+d7:(s)_17.3	24.28	0.22	0.0003	Rsq < 0.9	0.14	-	0.26	-	0.53	-	0.35	-	3.57E+06	3.15E+06	4.59E+06	4.33E	
25	Cer(d18:1_16:1)+D7:(s)	CER	17.38	M+H	A	NA	r(d18:1_16:1)+d7:(s)_17.3	14.41	0.00	1.00	Pass	0.22	-	0.30	-	0.75	-	0.32	-	3.79E+05	3.85E+05	3.58E+05	6.95E	
724	Cer(d18:1_16:1)+D7:(s)	CER	17.12	M+HCOO	A	LMSP02010008	cer(d18:1_16:1)+d7:(s)_17.12	0.04	0.00	1.00	Pass	0.44	-	0.68	-	0.37	-	0.26	-	1.20E+07	1.05E+07	1.17E+07	1.11E	
1	Cer(d18:1_17:0)	CER	20.01	M+HCOO	B	NA	cer(d18:1_17:0)_20.01	0.00	0.00	1.00	Pass	0.92	-	0.28	-	0.13	-	0.10	-	2.19E+04	2.10E+04	2.78E+04	2.80E	
1	Cer(d18:1_18:0)	CER	20.73	M+HCOO	A	NA	cer(d18:1_18:0)_20.73	0.00	1.00	Pass	0.67	-	0.30	-	0.33	-	0.17	-	1.02E+05	8.88E+04	1.14E+05	1.34E		
8:1)+D7:(s)	CER	19.15	M+H-H2O	A	NA	cer(d18:1_20:0)_21.5654	7.14	0.00	1.00	Pass	0.26	-	0.61	-	0.53	-	0.97	-	4.57E+07	4.06E+07	4.53E+07	4.16E		
8:1)+D7:(s)	CER	19.19	M+HCOO	A	NA	cer(d18:1_20:1)+d7:(s)_20.72	4.06	0.02	1.00	Pass	0.56	-	0.98	-	0.31	-	0.13	-	9.69E+06	8.34E+06	9.34E+06	8.80E		
1_20:0)	CER	21.57	M+HCOO	A	LMSP02010007	cer(d18:1_20:0)_21.5654	7.14	0.00	1.00	Pass	0.78	-	0.02	0.48	0.32	-	0.03	0.68	3.59E+04	3.37E+04	4.24E+04	4.40E		
8:1)+D7:(s)	CER	20.72	M+H-H2O	A	NA	cer(d18:1_20:1)+d7:(s)_20.72	4.06	0.02	1.00	Pass	0.95	-	0.32	-	0.11	-	0.65	-	2.72E+07	2.44E+07	2.90E+07	2.72E		
939	Cer(d18:1_20:1)+D7:(s)	CER	20.78	M+HCOO	A	NA	r(d18:1_20:1)+d7:(s)_20.77	7.93	0.04	1.00	Pass	0.39	-	0.95	-	0.39	-	0.19	-	4.37E+06	3.66E+06	3.97E+06	3.93E	
148	Cer(d18:1_22:0)	CER	22.09	M+H-H2O	A	8,LMSP02010042,L	cer(d18:1_22:0)_22.0858	4.90	2.12	1.00	Pass	0.92	-	0.06	-	0.15	-	0.10	-	1.24E+06	1.22E+06	1.58E+06	1.75E	
953	Cer(d18:1_22:0)	CER	22.11	M+HCOO	A	LMSP02010008	cer(d18:1_22:0)_22.1078	7.69	0.29	1.00	Pass	0.73	-	0.04	0.46	0.42	-	0.07	-	1.54E+05	1.60E+05	1.98E+05	2.31E	
174	Cer(d18:1_22:1)+D7:(s)	CER	21.53	M+H-H2O	A	NA	r(d18:1_22:1)+d7:(s)_21.53	3.09	0.04	1.00	Pass	0.38	-	0.70	-	0.76	-	0.82	-	6.49E+07	5.47E+07	6.11E+07	5.98E	
961	Cer(d18:1_22:1)+D7:(s)	CER	21.55	M+HCOO	A	NA	r(d18:1_22:1)+d7:(s)_21.55	4.18	0.07	1.00	Pass	0.66	-	0.79	-	0.41	-	0.81	-	9.09E+06	7.92E+06	7.98E+06	7.69E	
977	Cer(d18:1_23:0)	CER	22.30	M+HCOO	A	LMSP02010021	cer(d18:1_23:0)_22.3013	11.73	1.34	0.99	Pass	0.97	-	0.02	0.77	0.62	-	0.01	0.88	5.13E+04	4.71E+04	6.63E+04	6.16E	
500	Cer(d18:1_23:1)	CER	21.05	M+HCOO	A	NA	cer(d18:1_23:1)_21.0500	15.55	0.00	1.00	Pass	0.37	-	0.64	-	0.40	-	0.05	-	4.43E+04	4.15E+04	5.95E+04	5.77E	

*) Based on pool sample(s)

#) Grades: From A to D. Typically only grade A and B are accepted.

§) Typical criteria to pass: R² better than 0.9, CV better than 0.3, Scores A or B.