

Supplementary Materials

Supplementary Table 1: Lipids significantly altered in SWCNT-Fed LMB.

<i>Gut</i>				
Lipid Class	Lipid Species	HMDB ID	FDR p	Fold Change ^a
Hydroxyceramides	HCER(20:0)	HMDB04973	0.031	0.632
Hydroxyceramides	HCER(20:1)		0.014	0.592
Hydroxyceramides	HCER(22:1)		0.042	0.658
Hydroxyceramides	HCER(24:0)	HMDB04978	0.031	0.544
Hydroxyceramides	HCER(24:1)	HMDB04975	0.042	0.614
Hydroxyceramides	HCER(26:0)		0.031	0.661
Hydroxyceramides	HCER(26:1)		0.031	0.665
Diacylglycerols	DAG(14:0/16:1)		0.036	0.399
Lysophosphatidylcholines	LPC(22:5)	HMDB10403	0.020	2.240
Lysophosphatidylethanolamines	LPE(22:4)		0.036	0.452
Lysophosphatidylethanolamines	LPE(22:5)	HMDB11495	0.020	0.450
Lysophosphatidylethanolamines	LPE(16:0)	HMDB11503	0.014	0.350
Lysophosphatidylethanolamines	LPE(16:1)		0.014	0.346
Lysophosphatidylethanolamines	LPE(18:1)	HMDB11476	0.012	0.358
Lysophosphatidylethanolamines	LPE(18:2)	HMDB11477	0.042	0.439
Lysophosphatidylethanolamines	LPE(18:3)		0.014	0.295
Lysophosphatidylethanolamines	LPE(20:0)		0.036	0.536
Lysophosphatidylglycerols	LPG(20:1)		0.031	2.194
Lysophosphatidylglycerols	LPG(20:2)		0.036	2.448
Phosphatidylcholines	PC(14:0/22:6)	HMDB07892	0.036	1.865
Phosphatidylcholines	PC(16:0/16:1)	HMDB07969	0.001	10.51
Phosphatidylcholines	PC(16:0/18:0)	HMDB07970	0.031	1.939
Phosphatidylcholines	PC(16:0/20:3)	HMDB07981	0.001	4.542
Phosphatidylcholines	PC(16:0/20:4)	HMDB07982	0.020	1.899
Phosphatidylcholines	PC(16:0/22:5)	HMDB07990	0.012	3.068
Phosphatidylcholines	PC(18:0/18:0)	HMDB08036	0.026	2.015
Phosphatidylcholines	PC(18:0/20:0)	HMDB08043	0.036	2.197
Phosphatidylcholines	PC(18:0/20:1)	HMDB08044	0.001	10.79
Phosphatidylcholines	PC(18:0/20:2)	HMDB08045	0.001	4.583
Phosphatidylcholines	PC(18:0/20:3)	HMDB08047	0.005	3.970
Phosphatidylcholines	PC(18:0/20:4)	HMDB08048	0.014	2.013
Phosphatidylcholines	PC(18:0/22:4)	HMDB08054	0.010	2.384
Phosphatidylcholines	PC(18:0/22:5)	HMDB08056	0.014	2.481

Phosphatidylcholines	PC(18:0/22:6)	HMDB08057	0.014	2.231
Phosphatidylcholines	PC(18:1/20:3)	HMDB08113	0.007	3.612
Phosphatidylcholines	PC(18:1/20:4)	HMDB08114	0.014	2.594
Phosphatidylcholines	PC(18:2/20:1)	HMDB08144	0.020	2.873
Phosphatidylcholines	PC(20:0/18:1)	HMDB08269	0.020	2.264
Phosphatidylethanolamines	PE(P-18:0/22:6)	HMDB11394	0.014	0.315
Phosphatidylethanolamines	PE(P-18:1/22:6)		0.010	0.224
Phosphatidylethanolamines	PE(P-18:2/22:6)		0.018	0.352
Phosphatidylethanolamines	PE(16:0/16:0)		0.020	2.343
Phosphatidylethanolamines	PE(18:0/22:5)	HMDB09011	0.031	1.717
Phosphatidylglycerols	PG(18:0/22:6)		0.012	1.776
Phosphatidylglycerols	PG(20:0/20:5)		0.018	2.135
Phosphatidylserines	PS(18:1/20:4)		0.014	2.081
Phosphatidylserines	PS(20:0/20:2)		0.001	23.47
Phosphatidylserines	PS(20:0/20:3)		0.001	17.96
Phosphatidylserines	PS(20:0/20:5)		0.018	2.061
Phosphatidylserines	PS(20:0/22:4)		0.042	1.940
Phosphatidylserines	PS(20:0/22:5)		0.042	1.951
Phosphatidylserines	PS(18:0/20:4)		0.001	2.334
Triacylglycerols	TAG(50:3/FA18:3)	HMDB01388	0.036	0.755
Triacylglycerols	TAG(50:4/FA16:0)	HMDB00220	0.020	0.699
Triacylglycerols	TAG(50:4/FA18:3)	HMDB01388	0.014	0.763
Triacylglycerols	TAG(50:5/FA20:4)	HMDB01043	0.012	0.542
Triacylglycerols	TAG(50:5/FA20:5)		0.018	0.420
Triacylglycerols	TAG(52:2/FA20:0)	HMDB02212	0.020	0.683
Triacylglycerols	TAG(52:6/FA20:4)	HMDB01043	0.042	0.722
Triacylglycerols	TAG(52:6/FA22:6)	HMDB02183	0.031	0.638
Triacylglycerols	TAG(52:7/FA16:0)	HMDB00220	0.042	0.657
Triacylglycerols	TAG(52:7/FA22:6)		0.036	0.655
Triacylglycerols	TAG(52:8/FA16:1)	HMDB03229	0.020	0.586
Triacylglycerols	TAG(52:8/FA18:2)	HMDB00673	0.014	0.645
Triacylglycerols	TAG(46:3/FA14:0)	HMDB00806	0.026	0.605
Triacylglycerols	TAG(53:2/FA17:0)	HMDB02259	0.026	1.519
Triacylglycerols	TAG(54:2/FA18:0)	HMDB00827	0.014	1.854
Triacylglycerols	TAG(54:3/FA18:0)	HMDB00827	0.042	1.360
Triacylglycerols	TAG(54:3/FA18:1)	HMDB00207	0.018	1.496
Triacylglycerols	TAG(54:4/FA18:2)	HMDB00673	0.014	1.459
Triacylglycerols	TAG(46:3/FA18:3)		0.042	0.415
Triacylglycerols	TAG(54:8/FA18:3)	HMDB01388	0.014	0.707
Triacylglycerols	TAG(56:3/FA18:1)	HMDB00207	0.036	1.668

Triacylglycerols	TAG(56:3/FA18:2)	HMDB00673	0.042	2.044
Triacylglycerols	TAG(56:6/FA20:4)	HMDB01043	0.042	1.339
Triacylglycerols	TAG(47:2/FA16:1)	HMDB03229	0.026	0.517
Triacylglycerols	TAG(57:10/FA22:6)		0.014	0.509
Triacylglycerols	TAG(58:10/FA20:5)	HMDB01999	0.036	0.688
Triacylglycerols	TAG(48:2/FA16:1)	HMDB03229	0.036	0.616
Triacylglycerols	TAG(48:3/FA14:0)	HMDB00806	0.020	0.637
Triacylglycerols	TAG(50:1/FA20:1)		0.042	0.716
<i>Liver</i>				
Lipid Class	Lipid Species	HMDB ID	FDR <i>p</i>	Fold Change^a
Triacylglycerols	TAG(51:0/FA17:0)	HMDB02259	0.0311	3.334

^aFold change from control group.

Supplementary Table 2: EquiSPLASH LIPIDOMIX internal standard mix.

Catalog Number	Mixture Component	Molecular Weight	Conc. (µg/mL)
791637	15:0-18:1(d7) PC	753.11	100
791643	18:1(d7) Lyso PC	528.72	100
791638	15:0-18:1(d7) PE	711.03	100
791644	18:1(d7) Lyso PE	486.64	100
791640	15:0-18:1(d7) PG (Na Salt)	764.02	100
791641	15:0-18:1(d7) PI (NH ₄ Salt)	847.13	100
791639	15:0-18:1(d7) PS (Na Salt)	777.02	100
791648	15:0-18:1(d7)-15:0 TAG	812.37	100
791647	15:0-18:1(d7) DAG	587.98	100
791646	18:1(d7) MAG	363.59	100
791645	18:1(d7) Chol Ester	658.16	100
791649	d18:1-18:1(d9) SM	738.12	100
860681	C15 Ceramide-d7	530.92	100

Supplementary Table 3. Scan information for lipids in positive ion mode. Declustering potential = 60V, entrance potential = 10V, and collision exit potential =15V for all lipids in positive mode.

Positive Mode (+)				
Q1 (m/z)	Q3 (m/z)	Retention Time (min)	Lipid ID	Collision Energy (V)
738.663	184.2	11.8	SM(18:1)+H_d9_SPLASH.IS	43
675.5	184.1	11.8	SM(14:0)+H	43
703.6	184.1	11.8	SM(16:0)+H	43
731.6	184.1	11.8	SM(18:0)+H	43
729.6	184.1	11.8	SM(18:1)+H	43
759.6	184.1	11.8	SM(20:0)+H	43
757.6	184.1	11.8	SM(20:1)+H	43
787.7	184.1	11.8	SM(22:0)+H	43
785.7	184.1	11.8	SM(22:1)+H	43
815.7	184.1	11.8	SM(24:0)+H	43
813.7	184.1	11.8	SM(24:1)+H	43
843.7	184.1	11.8	SM(26:0)+H	43
841.7	184.1	11.8	SM(26:1)+H	25
754.7	369.4	2.3	CE(24:0)+H	25
714.6	369.4	2.3	CE(22:6)+H	25
698.7	369.4	2.3	CE(20:0)+H	25
696.7	369.4	2.3	CE(20:1)+H	25
716.6	369.4	2.3	CE(22:5)+H	25
614.6	369.4	2.3	CE(14:0)+H	25
642.6	369.4	2.3	CE(16:0)+H	25
640.6	369.4	2.3	CE(16:1)+H	25
670.6	369.4	2.3	CE(18:0)+H	25
668.6	369.4	2.3	CE(18:1)+H	25
666.6	369.4	2.3	CE(18:2)+H	25
664.6	369.4	2.3	CE(18:3)+H	25
694.6	369.4	2.3	CE(20:2)+H	25
692.6	369.4	2.3	CE(20:3)+H	25
690.6	369.4	2.3	CE(20:4)+H	25
688.6	369.4	2.3	CE(20:5)+H	25
726.7	369.4	2.3	CE(22:0)+H	25
724.7	369.4	2.3	CE(22:1)+H	25
722.7	369.4	2.3	CE(22:2)+H	25
718.6	369.4	2.3	CE(22:4)+H	25
752.7	369.4	2.3	CE(24:1)+H	43
510.6	264.4	2.3	CER(14:0)+H	43

538.6	264.4	2.3	CER(16:0)+H	43
566.7	264.4	2.3	CER(18:0)+H	43
564.8	264.4	2.3	CER(18:1)+H	43
594.6	264.4	2.3	CER(20:0)+H	43
592.6	264.4	2.3	CER(20:1)+H	43
622.7	264.4	2.3	CER(22:0)+H	43
620.7	264.4	2.3	CER(22:1)+H	43
650.8	264.4	2.3	CER(24:0)+H	43
648.8	264.4	2.3	CER(24:1)+H	43
678.9	264.4	2.3	CER(26:0)+H	43
676.9	264.4	2.3	CER(26:1)+H	43
512.6	266.4	2.3	DCER(14:0)+H	43
540.6	266.4	2.3	DCER(16:0)+H	43
568.7	266.4	2.3	DCER(18:0)+H	43
566.8	266.4	2.3	DCER(18:1)+H	43
596.7	266.4	2.3	DCER(20:0)+H	43
594.4	266.4	2.3	DCER(20:1)+H	43
624.8	266.4	2.3	DCER(22:0)+H	43
620.4	266.4	2.3	DCER(22:1)+H	43
652.9	266.4	2.3	DCER(24:0)+H	43
650.9	266.4	2.3	DCER(24:1)+H	43
680.5	266.4	2.3	DCER(26:0)+H	43
678.5	266.4	2.3	DCER(26:1)+H	43
644.5	264.4	7	HCER(18:1/12:0)+H_d_CER.IS	43
672.5	264.4	7	HCER(14:0)+H	43
700.7	264.4	7	HCER(16:0)+H	43
728.8	264.4	7	HCER(18:0)+H	43
726.7	264.4	7	HCER(18:1)+H	43
756.7	264.4	7	HCER(20:0)+H	43
754.7	264.4	7	HCER(20:1)+H	43
784.9	264.4	7	HCER(22:0)+H	43
782.8	264.4	7	HCER(22:1)+H	43
812.9	264.4	7	HCER(24:0)+H	43
810.9	264.4	7	HCER(24:1)+H	43
840.9	264.4	7	HCER(26:0)+H	43
838.9	264.4	7	HCER(26:1)+H	43
871.9	264.4	7	HCER(d18:0/18:0)+H	43
834.9	264.4	7	HCER(d18:0/20:0)+H	43
862.9	264.4	7	HCER(d18:0/22:0)+H	43
890.2	264.4	7	HCER(d18:0/24:0)+H	43
888.2	264.4	7	HCER(d18:0/24:1)+H	43
918.2	264.4	7	HCER(d18:0/26:0)+H	43
916.2	264.4	7	HCER(d18:0/26:1)+H	43
806.6	264.4	8	LCER(18:1/12:0)+H_d_CER.IS	43

944.2	264.4	8	LCER(14:0)+H	43
974.8	264.4	8	LCER(16:0)+H	43
972.9	264.4	8	LCER(18:0)+H	43
1002.4	264.4	8	LCER(18:1)+H	43
1000.4	264.4	8	LCER(20:0)+H	43
730.7	266.4	8	LCER(20:1)+H	43
758.7	266.4	8	LCER(22:0)+H	43
786.8	266.4	8	LCER(22:1)+H	43
814.9	266.4	8	LCER(24:0)+H	43
812.9	266.4	8	LCER(24:1)+H	43
842.9	266.4	8	LCER(26:0)+H	43
840.9	266.4	8	LCER(26:1)+H	38
892.7	266.4	8	LCER(d18:0/18:0)+H	43
920.7	266.4	8	LCER(d18:0/20:0)+H	43
948.7	266.4	8	LCER(d18:0/22:0)+H	43
976.8	266.4	8	LCER(d18:0/24:0)+H	43
974.7	266.4	8	LCER(d18:0/24:1)+H	43
1004.9	266.4	8	LCER(d18:0/26:0)+H	43
1002.9	266.4	8	LCER(d18:0/26:1)+H	43
829.37	570.5	2.2	TAG(15:0/18:1/15:0)+NH4d7_SPLASH.IS	38
712.645	467.409	2.2	TAG(40:0/FA14:0)+NH4	38
712.645	439.378	2.2	TAG(40:0/FA16:0)+NH4	38
740.676	495.441	2.2	TAG(42:0/FA14:0)+NH4	38
740.676	467.409	2.2	TAG(42:0/FA16:0)+NH4	38
738.661	493.425	2.2	TAG(42:1/FA14:0)+NH4	38
738.661	465.394	2.2	TAG(42:1/FA16:0)+NH4	38
738.661	467.409	2.2	TAG(42:1/FA16:1)+NH4	38
738.661	439.378	2.2	TAG(42:1/FA18:1)+NH4	38
736.645	439.378	2.2	TAG(42:2/FA18:2)+NH4	38
768.708	523.472	2.2	TAG(44:0/FA14:0)+NH4	38
768.708	495.441	2.2	TAG(44:0/FA16:0)+NH4	38
768.708	467.409	2.2	TAG(44:0/FA18:0)+NH4	38
766.692	521.456	2.2	TAG(44:1/FA14:0)+NH4	38
766.692	493.425	2.2	TAG(44:1/FA16:0)+NH4	38
766.692	495.441	2.2	TAG(44:1/FA16:1)+NH4	38
766.692	467.409	2.2	TAG(44:1/FA18:1)+NH4	38
764.676	519.441	2.2	TAG(44:2/FA14:0)+NH4	38
764.676	491.409	2.2	TAG(44:2/FA16:0)+NH4	38
764.676	493.425	2.2	TAG(44:2/FA16:1)+NH4	38
764.676	465.394	2.2	TAG(44:2/FA18:1)+NH4	38
764.676	467.409	2.2	TAG(44:2/FA18:2)+NH4	38
762.661	465.394	2.2	TAG(44:3/FA18:2)+NH4	38
782.723	537.488	2.2	TAG(45:0/FA14:0)+NH4	38
782.723	509.456	2.2	TAG(45:0/FA16:0)+NH4	38

780.708	507.4	2.2	TAG(45:1/FA16:0)+NH4	38
780.708	481.4	2.2	TAG(45:1/FA18:1)+NH4	38
796.7	551.503	2.2	TAG(46:0/FA14:0)+NH4	38
796.7	523.472	2.2	TAG(46:0/FA16:0)+NH4	38
796.7	495.441	2.2	TAG(46:0/FA18:0)+NH4	38
794.7	549.5	2.2	TAG(46:1/FA14:0)+NH4	38
794.7	521.4	2.2	TAG(46:1/FA16:0)+NH4	38
794.7	523.472	2.2	TAG(46:1/FA16:1)+NH4	38
794.7	493.425	2.2	TAG(46:1/FA18:0)+NH4	38
794.7	495.441	2.2	TAG(46:1/FA18:1)+NH4	38
792.7	547.5	2.2	TAG(46:2/FA14:0)+NH4	38
792.7	519.441	2.2	TAG(46:2/FA16:0)+NH4	38
792.7	521.4	2.2	TAG(46:2/FA16:1)+NH4	38
792.7	493.425	2.2	TAG(46:2/FA18:1)+NH4	38
792.7	495.441	2.2	TAG(46:2/FA18:2)+NH4	38
790.7	545.5	2.2	TAG(46:3/FA14:0)+NH4	38
790.7	517.4	2.2	TAG(46:3/FA16:0)+NH4	38
790.7	519.441	2.2	TAG(46:3/FA16:1)+NH4	38
790.7	491.409	2.2	TAG(46:3/FA18:1)+NH4	38
790.7	493.425	2.2	TAG(46:3/FA18:2)+NH4	38
790.7	495.441	2.2	TAG(46:3/FA18:3)+NH4	38
788.7	491.409	2.2	TAG(46:4/FA18:2)+NH4	38
810.7	565.5	2.2	TAG(47:0/FA14:0)+NH4	38
810.7	537.4	2.2	TAG(47:0/FA16:0)+NH4	38
810.7	523.472	2.2	TAG(47:0/FA17:0)+NH4	38
808.7	563.5	2.2	TAG(47:1/FA14:0)+NH4	38
808.7	535.4	2.2	TAG(47:1/FA16:0)+NH4	38
808.7	537.4	2.2	TAG(47:1/FA16:1)+NH4	38
808.7	521.4	2.2	TAG(47:1/FA17:0)+NH4	38
808.7	509.4	2.2	TAG(47:1/FA18:1)+NH4	38
806.7	561.5	2.2	TAG(47:2/FA14:0)+NH4	38
806.7	535.4	2.2	TAG(47:2/FA16:1)+NH4	38
806.7	507.4	2.2	TAG(47:2/FA18:1)+NH4	38
806.7	509.4	2.2	TAG(47:2/FA18:2)+NH4	38
824.7	579.5	2.2	TAG(48:0/FA14:0)+NH4	38
824.7	551.4	2.2	TAG(48:0/FA16:0)+NH4	38
824.7	523.472	2.2	TAG(48:0/FA18:0)+NH4	38
822.7	577.5	2.2	TAG(48:1/FA14:0)+NH4	38
822.7	549.4	2.2	TAG(48:1/FA16:0)+NH4	38
822.7	551.4	2.2	TAG(48:1/FA16:1)+NH4	38
822.7	521.4	2.2	TAG(48:1/FA18:0)+NH4	38
822.7	523.472	2.2	TAG(48:1/FA18:1)+NH4	38
820.7	575.5	2.2	TAG(48:2/FA14:0)+NH4	38
820.7	547.4	2.2	TAG(48:2/FA16:0)+NH4	38

820.7	549.4	2.2	TAG(48:2/FA16:1)+NH4	38
820.7	519.441	2.2	TAG(48:2/FA18:0)+NH4	38
820.7	521.4	2.2	TAG(48:2/FA18:1)+NH4	38
820.7	523.472	2.2	TAG(48:2/FA18:2)+NH4	38
818.7	573.5	2.2	TAG(48:3/FA14:0)+NH4	38
818.7	545.4	2.2	TAG(48:3/FA16:0)+NH4	38
818.7	547.4	2.2	TAG(48:3/FA16:1)+NH4	38
818.7	519.441	2.2	TAG(48:3/FA18:1)+NH4	38
818.7	521.4	2.2	TAG(48:3/FA18:2)+NH4	38
818.7	523.472	2.2	TAG(48:3/FA18:3)+NH4	38
816.7	571.5	2.2	TAG(48:4/FA14:0)+NH4	38
816.7	543.4	2.2	TAG(48:4/FA16:0)+NH4	38
816.7	545.4	2.2	TAG(48:4/FA16:1)+NH4	38
816.7	517.4	2.2	TAG(48:4/FA18:1)+NH4	38
816.7	519.441	2.2	TAG(48:4/FA18:2)+NH4	38
816.7	521.4	2.2	TAG(48:4/FA18:3)+NH4	38
816.7	495.441	2.2	TAG(48:4/FA20:4)+NH4	38
814.7	517.4	2.2	TAG(48:5/FA18:2)+NH4	38
814.7	519.441	2.2	TAG(48:5/FA18:3)+NH4	38
838.8	565.5	2.2	TAG(49:0/FA16:0)+NH4	38
838.8	551.503	2.2	TAG(49:0/FA17:0)+NH4	38
838.8	537.5	2.2	TAG(49:0/FA18:0)+NH4	38
836.8	591.6	2.2	TAG(49:1/FA14:0)+NH4	38
836.8	563.5	2.2	TAG(49:1/FA16:0)+NH4	38
836.8	565.5	2.2	TAG(49:1/FA16:1)+NH4	38
836.8	549.5	2.2	TAG(49:1/FA17:0)+NH4	38
836.8	537.5	2.2	TAG(49:1/FA18:1)+NH4	38
834.8	589.6	2.2	TAG(49:2/FA14:0)+NH4	38
834.8	561.5	2.2	TAG(49:2/FA16:0)+NH4	38
834.8	563.5	2.2	TAG(49:2/FA16:1)+NH4	38
834.8	547.5	2.2	TAG(49:2/FA17:0)+NH4	38
834.8	535.5	2.2	TAG(49:2/FA18:1)+NH4	38
834.8	537.5	2.2	TAG(49:2/FA18:2)+NH4	38
832.8	559.5	2.2	TAG(49:3/FA16:0)+NH4	38
832.8	561.5	2.2	TAG(49:3/FA16:1)+NH4	38
832.8	535.5	2.2	TAG(49:3/FA18:2)+NH4	38
832.8	537.5	2.2	TAG(49:3/FA18:3)+NH4	38
852.8	607.6	2.2	TAG(50:0/FA14:0)+NH4	38
852.8	579.5	2.2	TAG(50:0/FA16:0)+NH4	38
852.8	551.503	2.2	TAG(50:0/FA18:0)+NH4	38
850.8	605.6	2.2	TAG(50:1/FA14:0)+NH4	38
850.8	577.5	2.2	TAG(50:1/FA16:0)+NH4	38
850.8	579.5	2.2	TAG(50:1/FA16:1)+NH4	38
850.8	549.5	2.2	TAG(50:1/FA18:0)+NH4	38

850.8	551.503	2.2	TAG(50:1/FA18:1)+NH4	38
850.8	523.472	2.2	TAG(50:1/FA20:1)+NH4	38
848.8	603.6	2.2	TAG(50:2/FA14:0)+NH4	38
848.8	575.5	2.2	TAG(50:2/FA16:0)+NH4	38
848.8	577.5	2.2	TAG(50:2/FA16:1)+NH4	38
848.8	547.5	2.2	TAG(50:2/FA18:0)+NH4	38
848.8	549.5	2.2	TAG(50:2/FA18:1)+NH4	38
848.8	551.503	2.2	TAG(50:2/FA18:2)+NH4	38
848.8	523.472	2.2	TAG(50:2/FA20:2)+NH4	38
846.8	601.6	2.2	TAG(50:3/FA14:0)+NH4	38
846.8	573.5	2.2	TAG(50:3/FA16:0)+NH4	38
846.8	575.5	2.2	TAG(50:3/FA16:1)+NH4	38
846.8	545.5	2.2	TAG(50:3/FA18:0)+NH4	38
846.8	547.5	2.2	TAG(50:3/FA18:1)+NH4	38
846.8	549.5	2.2	TAG(50:3/FA18:2)+NH4	38
846.8	551.503	2.2	TAG(50:3/FA18:3)+NH4	38
846.8	523.472	2.2	TAG(50:3/FA20:3)+NH4	38
844.6	599.4	2.2	TAG(50:4/FA14:0)+NH4	38
844.6	571.3	2.2	TAG(50:4/FA16:0)+NH4	38
844.6	573.3	2.2	TAG(50:4/FA16:1)+NH4	38
844.6	545.3	2.2	TAG(50:4/FA18:1)+NH4	38
844.6	547.3	2.2	TAG(50:4/FA18:2)+NH4	38
844.6	549.3	2.2	TAG(50:4/FA18:3)+NH4	38
844.6	521.3	2.2	TAG(50:4/FA20:3)+NH4	38
844.6	523.3	2.2	TAG(50:4/FA20:4)+NH4	38
842.6	597.4	2.2	TAG(50:5/FA14:0)+NH4	38
842.6	569.3	2.2	TAG(50:5/FA16:0)+NH4	38
842.6	571.3	2.2	TAG(50:5/FA16:1)+NH4	38
842.6	543.3	2.2	TAG(50:5/FA18:1)+NH4	38
842.6	545.3	2.2	TAG(50:5/FA18:2)+NH4	38
842.6	547.3	2.2	TAG(50:5/FA18:3)+NH4	38
842.6	521.3	2.2	TAG(50:5/FA20:4)+NH4	38
842.6	523.3	2.2	TAG(50:5/FA20:5)+NH4	38
840.7	519.441	2.2	TAG(50:6/FA20:4)+NH4	38
866.8	593.5	2.2	TAG(51:0/FA16:0)+NH4	38
866.8	579.5	2.2	TAG(51:0/FA17:0)+NH4	38
866.8	565.5	2.2	TAG(51:0/FA18:0)+NH4	38
864.8	591.5	2.2	TAG(51:1/FA16:0)+NH4	38
864.8	577.5	2.2	TAG(51:1/FA17:0)+NH4	38
864.8	563.5	2.2	TAG(51:1/FA18:0)+NH4	38
864.8	565.5	2.2	TAG(51:1/FA18:1)+NH4	38
862.8	589.5	2.2	TAG(51:2/FA16:0)+NH4	38
862.8	591.5	2.2	TAG(51:2/FA16:1)+NH4	38
862.8	575.5	2.2	TAG(51:2/FA17:0)+NH4	38

862.8	563.5	2.2	TAG(51:2/FA18:1)+NH4	38
862.8	565.5	2.2	TAG(51:2/FA18:2)+NH4	38
860.8	589.5	2.2	TAG(51:3/FA16:1)+NH4	38
860.8	573.5	2.2	TAG(51:3/FA17:0)+NH4	38
860.8	563.5	2.2	TAG(51:3/FA18:2)+NH4	38
860.8	565.5	2.2	TAG(51:3/FA18:3)+NH4	38
858.8	587.5	2.2	TAG(51:4/FA16:1)+NH4	38
858.8	561.5	2.2	TAG(51:4/FA18:2)+NH4	38
858.8	563.5	2.2	TAG(51:4/FA18:3)+NH4	38
858.8	537.5	2.2	TAG(51:4/FA20:4)+NH4	38
856.8	559.5	2.2	TAG(51:5/FA18:2)+NH4	38
856.8	561.5	2.2	TAG(51:5/FA18:3)+NH4	38
880.8	607.5	2.2	TAG(52:0/FA16:0)+NH4	38
880.8	579.5	2.2	TAG(52:0/FA18:0)+NH4	38
880.8	551.503	2.2	TAG(52:0/FA20:0)+NH4	38
878.8	605.5	2.2	TAG(52:1/FA16:0)+NH4	38
878.8	607.5	2.2	TAG(52:1/FA16:1)+NH4	38
878.8	577.5	2.2	TAG(52:1/FA18:0)+NH4	38
878.8	579.5	2.2	TAG(52:1/FA18:1)+NH4	38
878.8	549.5	2.2	TAG(52:1/FA20:0)+NH4	38
878.8	551.503	2.2	TAG(52:1/FA20:1)+NH4	38
876.8	631.6	2.2	TAG(52:2/FA14:0)+NH4	38
876.8	603.5	2.2	TAG(52:2/FA16:0)+NH4	38
876.8	605.5	2.2	TAG(52:2/FA16:1)+NH4	38
876.8	575.5	2.2	TAG(52:2/FA18:0)+NH4	38
876.8	577.5	2.2	TAG(52:2/FA18:1)+NH4	38
876.8	579.5	2.2	TAG(52:2/FA18:2)+NH4	38
876.8	547.5	2.2	TAG(52:2/FA20:0)+NH4	38
876.8	549.5	2.2	TAG(52:2/FA20:1)+NH4	38
876.8	551.503	2.2	TAG(52:2/FA20:2)+NH4	38
874.8	629.6	2.2	TAG(52:3/FA14:0)+NH4	38
874.8	601.5	2.2	TAG(52:3/FA16:0)+NH4	38
874.8	603.5	2.2	TAG(52:3/FA16:1)+NH4	38
874.8	573.5	2.2	TAG(52:3/FA18:0)+NH4	38
874.8	575.5	2.2	TAG(52:3/FA18:1)+NH4	38
874.8	577.5	2.2	TAG(52:3/FA18:2)+NH4	38
874.8	579.5	2.2	TAG(52:3/FA18:3)+NH4	38
874.8	545.5	2.2	TAG(52:3/FA20:0)+NH4	38
874.8	547.5	2.2	TAG(52:3/FA20:1)+NH4	38
874.8	549.5	2.2	TAG(52:3/FA20:2)+NH4	38
874.8	551.503	2.2	TAG(52:3/FA20:3)+NH4	38
872.8	627.6	2.2	TAG(52:4/FA14:0)+NH4	38
872.8	599.5	2.2	TAG(52:4/FA16:0)+NH4	38
872.8	601.5	2.2	TAG(52:4/FA16:1)+NH4	38

872.8	571.5	2.2	TAG(52:4/FA18:0)+NH4	38
872.8	573.5	2.2	TAG(52:4/FA18:1)+NH4	38
872.8	575.5	2.2	TAG(52:4/FA18:2)+NH4	38
872.8	577.5	2.2	TAG(52:4/FA18:3)+NH4	38
872.8	543.5	2.2	TAG(52:4/FA20:0)+NH4	38
872.8	547.5	2.2	TAG(52:4/FA20:2)+NH4	38
872.8	549.5	2.2	TAG(52:4/FA20:3)+NH4	38
872.8	551.503	2.2	TAG(52:4/FA20:4)+NH4	38
872.8	523.472	2.2	TAG(52:4/FA22:4)+NH4	38
870.8	625.6	2.2	TAG(52:5/FA14:0)+NH4	38
870.8	597.5	2.2	TAG(52:5/FA16:0)+NH4	38
870.8	599.5	2.2	TAG(52:5/FA16:1)+NH4	38
870.8	571.5	2.2	TAG(52:5/FA18:1)+NH4	38
870.8	573.5	2.2	TAG(52:5/FA18:2)+NH4	38
870.8	575.5	2.2	TAG(52:5/FA18:3)+NH4	38
870.8	547.5	2.2	TAG(52:5/FA20:3)+NH4	38
870.8	549.5	2.2	TAG(52:5/FA20:4)+NH4	38
870.8	551.503	2.2	TAG(52:5/FA20:5)+NH4	38
870.8	523.472	2.2	TAG(52:5/FA22:5)+NH4	38
868.8	623.6	2.2	TAG(52:6/FA14:0)+NH4	38
868.8	595.5	2.2	TAG(52:6/FA16:0)+NH4	38
868.8	597.5	2.2	TAG(52:6/FA16:1)+NH4	38
868.8	569.5	2.2	TAG(52:6/FA18:1)+NH4	38
868.8	571.5	2.2	TAG(52:6/FA18:2)+NH4	38
868.8	573.5	2.2	TAG(52:6/FA18:3)+NH4	38
868.8	547.5	2.2	TAG(52:6/FA20:4)+NH4	38
868.8	549.5	2.2	TAG(52:6/FA20:5)+NH4	38
868.8	523.472	2.2	TAG(52:6/FA22:6)+NH4	38
866.7	593.4	2.2	TAG(52:7/FA16:0)+NH4	38
866.7	567.4	2.2	TAG(52:7/FA18:1)+NH4	38
866.7	547.4	2.2	TAG(52:7/FA20:5)+NH4	38
866.7	521.4	2.2	TAG(52:7/FA22:6)+NH4	38
864.8	593.5	2.2	TAG(52:8/FA16:1)+NH4	38
864.8	567.5	2.2	TAG(52:8/FA18:2)+NH4	38
894.8	621.5	2.2	TAG(53:0/FA16:0)+NH4	38
892.8	619.5	2.2	TAG(53:1/FA16:0)+NH4	38
892.8	605.5	2.2	TAG(53:1/FA17:0)+NH4	38
892.8	591.5	2.2	TAG(53:1/FA18:0)+NH4	38
892.8	593.5	2.2	TAG(53:1/FA18:1)+NH4	38
890.8	617.5	2.2	TAG(53:2/FA16:0)+NH4	38
890.8	603.5	2.2	TAG(53:2/FA17:0)+NH4	38
890.8	591.5	2.2	TAG(53:2/FA18:1)+NH4	38
890.8	593.5	2.2	TAG(53:2/FA18:2)+NH4	38
888.8	615.5	2.2	TAG(53:3/FA16:0)+NH4	38

888.8	601.5	2.2	TAG(53:3/FA17:0)+NH4	38
888.8	591.5	2.2	TAG(53:3/FA18:2)+NH4	38
886.8	613.5	2.2	TAG(53:4/FA16:0)+NH4	38
886.8	599.5	2.2	TAG(53:4/FA17:0)+NH4	38
886.8	589.5	2.2	TAG(53:4/FA18:2)+NH4	38
886.8	591.5	2.2	TAG(53:4/FA18:3)+NH4	38
886.8	565.5	2.2	TAG(53:4/FA20:4)+NH4	38
884.8	563.5	2.2	TAG(53:5/FA20:4)+NH4	38
882.8	561.5	2.2	TAG(53:6/FA20:4)+NH4	38
908.8	635.5	2.2	TAG(54:0/FA16:0)+NH4	38
908.8	607.5	2.2	TAG(54:0/FA18:0)+NH4	38
906.8	633.5	2.2	TAG(54:1/FA16:0)+NH4	38
906.8	605.5	2.2	TAG(54:1/FA18:0)+NH4	38
906.8	607.5	2.2	TAG(54:1/FA18:1)+NH4	38
906.8	577.5	2.2	TAG(54:1/FA20:0)+NH4	38
906.8	579.5	2.2	TAG(54:1/FA20:1)+NH4	38
904.8	631.5	2.2	TAG(54:2/FA16:0)+NH4	38
904.8	603.5	2.2	TAG(54:2/FA18:0)+NH4	38
904.8	605.5	2.2	TAG(54:2/FA18:1)+NH4	38
904.8	607.5	2.2	TAG(54:2/FA18:2)+NH4	38
904.8	575.5	2.2	TAG(54:2/FA20:0)+NH4	38
904.8	577.5	2.2	TAG(54:2/FA20:1)+NH4	38
904.8	579.5	2.2	TAG(54:2/FA20:2)+NH4	38
902.8	629.5	2.2	TAG(54:3/FA16:0)+NH4	38
902.8	631.5	2.2	TAG(54:3/FA16:1)+NH4	38
902.8	601.5	2.2	TAG(54:3/FA18:0)+NH4	38
902.8	603.5	2.2	TAG(54:3/FA18:1)+NH4	38
902.8	605.5	2.2	TAG(54:3/FA18:2)+NH4	38
902.8	607.5	2.2	TAG(54:3/FA18:3)+NH4	38
902.8	575.5	2.2	TAG(54:3/FA20:1)+NH4	38
902.8	577.5	2.2	TAG(54:3/FA20:2)+NH4	38
902.8	579.5	2.2	TAG(54:3/FA20:3)+NH4	38
900.8	627.5	2.2	TAG(54:4/FA16:0)+NH4	38
900.8	629.5	2.2	TAG(54:4/FA16:1)+NH4	38
900.8	599.5	2.2	TAG(54:4/FA18:0)+NH4	38
900.8	601.5	2.2	TAG(54:4/FA18:1)+NH4	38
900.8	603.5	2.2	TAG(54:4/FA18:2)+NH4	38
900.8	605.5	2.2	TAG(54:4/FA18:3)+NH4	38
900.8	573.5	2.2	TAG(54:4/FA20:1)+NH4	38
900.8	575.5	2.2	TAG(54:4/FA20:2)+NH4	38
900.8	577.5	2.2	TAG(54:4/FA20:3)+NH4	38
900.8	579.5	2.2	TAG(54:4/FA20:4)+NH4	38
900.8	551.503	2.2	TAG(54:4/FA22:4)+NH4	38
898.8	625.5	2.2	TAG(54:5/FA16:0)+NH4	38

898.8	627.5	2.2	TAG(54:5/FA16:1)+NH4	38
898.8	597.5	2.2	TAG(54:5/FA18:0)+NH4	38
898.8	599.5	2.2	TAG(54:5/FA18:1)+NH4	38
898.8	601.5	2.2	TAG(54:5/FA18:2)+NH4	38
898.8	603.5	2.2	TAG(54:5/FA18:3)+NH4	38
898.8	573.5	2.2	TAG(54:5/FA20:2)+NH4	38
898.8	575.5	2.2	TAG(54:5/FA20:3)+NH4	38
898.8	577.5	2.2	TAG(54:5/FA20:4)+NH4	38
898.8	579.5	2.2	TAG(54:5/FA20:5)+NH4	38
898.8	549.5	2.2	TAG(54:5/FA22:4)+NH4	38
898.8	551.503	2.2	TAG(54:5/FA22:5)+NH4	38
896.8	623.5	2.2	TAG(54:6/FA16:0)+NH4	38
896.8	625.5	2.2	TAG(54:6/FA16:1)+NH4	38
896.8	597.5	2.2	TAG(54:6/FA18:1)+NH4	38
896.8	599.5	2.2	TAG(54:6/FA18:2)+NH4	38
896.8	601.5	2.2	TAG(54:6/FA18:3)+NH4	38
896.8	573.5	2.2	TAG(54:6/FA20:3)+NH4	38
896.8	575.5	2.2	TAG(54:6/FA20:4)+NH4	38
896.8	577.5	2.2	TAG(54:6/FA20:5)+NH4	38
896.8	549.5	2.2	TAG(54:6/FA22:5)+NH4	38
896.8	551.503	2.2	TAG(54:6/FA22:6)+NH4	38
894.8	623.5	2.2	TAG(54:7/FA16:1)+NH4	38
894.8	595.5	2.2	TAG(54:7/FA18:1)+NH4	38
894.8	597.5	2.2	TAG(54:7/FA18:2)+NH4	38
894.8	599.5	2.2	TAG(54:7/FA18:3)+NH4	38
894.8	573.5	2.2	TAG(54:7/FA20:4)+NH4	38
894.8	575.5	2.2	TAG(54:7/FA20:5)+NH4	38
894.8	547.5	2.2	TAG(54:7/FA22:5)+NH4	38
894.8	549.5	2.2	TAG(54:7/FA22:6)+NH4	38
892.8	595.5	2.2	TAG(54:8/FA18:2)+NH4	38
892.8	597.5	2.2	TAG(54:8/FA18:3)+NH4	38
892.8	571.5	2.2	TAG(54:8/FA20:4)+NH4	38
892.8	573.5	2.2	TAG(54:8/FA20:5)+NH4	38
892.8	547.5	2.2	TAG(54:8/FA22:6)+NH4	38
920.9	647.6	2.2	TAG(55:1/FA16:0)+NH4	38
920.9	621.6	2.2	TAG(55:1/FA18:1)+NH4	38
918.8	619.5	2.2	TAG(55:2/FA18:1)+NH4	38
918.8	621.5	2.2	TAG(55:2/FA18:2)+NH4	38
916.8	617.5	2.2	TAG(55:3/FA18:1)+NH4	38
916.8	619.5	2.2	TAG(55:3/FA18:2)+NH4	38
914.8	615.5	2.2	TAG(55:4/FA18:1)+NH4	38
914.8	617.5	2.2	TAG(55:4/FA18:2)+NH4	38
912.8	613.5	2.2	TAG(55:5/FA18:1)+NH4	38
912.8	615.5	2.2	TAG(55:5/FA18:2)+NH4	38

912.8	591.5	2.2	TAG(55:5/FA20:4)+NH4	38
908.8	563.5	2.2	TAG(55:7/FA22:6)+NH4	38
916.7	619.4	2.2	TAG(56:10/FA18:2)+NH4	38
934.9	661.6	2.2	TAG(56:1/FA16:0)+NH4	38
934.9	635.6	2.2	TAG(56:1/FA18:1)+NH4	38
932.9	659.6	2.2	TAG(56:2/FA16:0)+NH4	38
932.9	631.6	2.2	TAG(56:2/FA18:0)+NH4	38
932.9	603.6	2.2	TAG(56:2/FA20:0)+NH4	38
932.9	605.6	2.2	TAG(56:2/FA20:1)+NH4	38
930.8	657.5	2.2	TAG(56:3/FA16:0)+NH4	38
930.8	629.5	2.2	TAG(56:3/FA18:0)+NH4	38
930.8	631.5	2.2	TAG(56:3/FA18:1)+NH4	38
930.8	633.5	2.2	TAG(56:3/FA18:2)+NH4	38
930.8	601.5	2.2	TAG(56:3/FA20:0)+NH4	38
930.8	603.5	2.2	TAG(56:3/FA20:1)+NH4	38
930.8	605.5	2.2	TAG(56:3/FA20:2)+NH4	38
928.8	655.5	2.2	TAG(56:4/FA16:0)+NH4	38
928.8	627.5	2.2	TAG(56:4/FA18:0)+NH4	38
928.8	629.5	2.2	TAG(56:4/FA18:1)+NH4	38
928.8	631.5	2.2	TAG(56:4/FA18:2)+NH4	38
928.8	601.5	2.2	TAG(56:4/FA20:1)+NH4	38
928.8	603.5	2.2	TAG(56:4/FA20:2)+NH4	38
928.8	605.5	2.2	TAG(56:4/FA20:3)+NH4	38
928.8	607.5	2.2	TAG(56:4/FA20:4)+NH4	38
928.8	579.5	2.2	TAG(56:4/FA22:4)+NH4	38
926.8	653.5	2.2	TAG(56:5/FA16:0)+NH4	38
926.8	625.5	2.2	TAG(56:5/FA18:0)+NH4	38
926.8	627.5	2.2	TAG(56:5/FA18:1)+NH4	38
926.8	629.5	2.2	TAG(56:5/FA18:2)+NH4	38
926.8	599.5	2.2	TAG(56:5/FA20:1)+NH4	38
926.8	601.5	2.2	TAG(56:5/FA20:2)+NH4	38
926.8	603.5	2.2	TAG(56:5/FA20:3)+NH4	38
926.8	605.5	2.2	TAG(56:5/FA20:4)+NH4	38
926.8	577.5	2.2	TAG(56:5/FA22:4)+NH4	38
926.8	579.5	2.2	TAG(56:5/FA22:5)+NH4	38
924.8	651.5	2.2	TAG(56:6/FA16:0)+NH4	38
924.8	623.5	2.2	TAG(56:6/FA18:0)+NH4	38
924.8	625.5	2.2	TAG(56:6/FA18:1)+NH4	38
924.8	627.5	2.2	TAG(56:6/FA18:2)+NH4	38
924.8	629.5	2.2	TAG(56:6/FA18:3)+NH4	38
924.8	599.5	2.2	TAG(56:6/FA20:2)+NH4	38
924.8	601.5	2.2	TAG(56:6/FA20:3)+NH4	38
924.8	603.5	2.2	TAG(56:6/FA20:4)+NH4	38
924.8	605.5	2.2	TAG(56:6/FA20:5)+NH4	38

924.8	575.5	2.2	TAG(56:6/FA22:4)+NH4	38
924.8	577.5	2.2	TAG(56:6/FA22:5)+NH4	38
924.8	579.5	2.2	TAG(56:6/FA22:6)+NH4	38
922.8	649.5	2.2	TAG(56:7/FA16:0)+NH4	38
922.8	651.5	2.2	TAG(56:7/FA16:1)+NH4	38
922.8	621.5	2.2	TAG(56:7/FA18:0)+NH4	38
922.8	623.5	2.2	TAG(56:7/FA18:1)+NH4	38
922.8	625.5	2.2	TAG(56:7/FA18:2)+NH4	38
922.8	627.5	2.2	TAG(56:7/FA18:3)+NH4	38
922.8	599.5	2.2	TAG(56:7/FA20:3)+NH4	38
922.8	601.5	2.2	TAG(56:7/FA20:4)+NH4	38
922.8	603.5	2.2	TAG(56:7/FA20:5)+NH4	38
922.8	573.5	2.2	TAG(56:7/FA22:4)+NH4	38
922.8	575.5	2.2	TAG(56:7/FA22:5)+NH4	38
922.8	577.5	2.2	TAG(56:7/FA22:6)+NH4	38
920.8	647.5	2.2	TAG(56:8/FA16:0)+NH4	38
920.8	649.5	2.2	TAG(56:8/FA16:1)+NH4	38
920.8	621.5	2.2	TAG(56:8/FA18:1)+NH4	38
920.8	623.5	2.2	TAG(56:8/FA18:2)+NH4	38
920.8	625.5	2.2	TAG(56:8/FA18:3)+NH4	38
920.8	599.5	2.2	TAG(56:8/FA20:4)+NH4	38
920.8	601.5	2.2	TAG(56:8/FA20:5)+NH4	38
920.8	573.5	2.2	TAG(56:8/FA22:5)+NH4	38
920.8	575.5	2.2	TAG(56:8/FA22:6)+NH4	38
918.8	623.5	2.2	TAG(56:9/FA18:3)+NH4	38
918.8	597.5	2.2	TAG(56:9/FA20:4)+NH4	38
918.8	599.5	2.2	TAG(56:9/FA20:5)+NH4	38
918.8	573.5	2.2	TAG(56:9/FA22:6)+NH4	38
928.7	583.4	2.2	TAG(57:10/FA22:6)+NH4	38
946.9	647.6	2.2	TAG(57:2/FA18:1)+NH4	38
944.9	647.6	2.2	TAG(57:3/FA18:2)+NH4	38
944.8	647.5	2.2	TAG(58:10/FA18:2)+NH4	38
944.8	623.5	2.2	TAG(58:10/FA20:4)+NH4	38
944.8	625.5	2.2	TAG(58:10/FA20:5)+NH4	38
944.8	597.5	2.2	TAG(58:10/FA22:5)+NH4	38
944.8	599.5	2.2	TAG(58:10/FA22:6)+NH4	38
960.9	661.6	2.2	TAG(58:2/FA18:1)+NH4	38
958.9	659.6	2.2	TAG(58:3/FA18:1)+NH4	38
954.9	655.6	2.2	TAG(58:5/FA18:1)+NH4	38
952.8	679.5	2.2	TAG(58:6/FA16:0)+NH4	38
952.8	651.5	2.2	TAG(58:6/FA18:0)+NH4	38
952.8	653.5	2.2	TAG(58:6/FA18:1)+NH4	38
952.8	631.5	2.2	TAG(58:6/FA20:4)+NH4	38
952.8	603.5	2.2	TAG(58:6/FA22:4)+NH4	38

952.8	605.5	2.2	TAG(58:6/FA22:5)+NH4	38
950.8	677.5	2.2	TAG(58:7/FA16:0)+NH4	38
950.8	649.5	2.2	TAG(58:7/FA18:0)+NH4	38
950.8	651.5	2.2	TAG(58:7/FA18:1)+NH4	38
950.8	653.5	2.2	TAG(58:7/FA18:2)+NH4	38
950.8	629.5	2.2	TAG(58:7/FA20:4)+NH4	38
950.8	601.5	2.2	TAG(58:7/FA22:4)+NH4	38
950.8	603.5	2.2	TAG(58:7/FA22:5)+NH4	38
950.8	605.5	2.2	TAG(58:7/FA22:6)+NH4	38
948.8	649.5	2.2	TAG(58:8/FA18:1)+NH4	38
948.8	651.5	2.2	TAG(58:8/FA18:2)+NH4	38
948.8	625.5	2.2	TAG(58:8/FA20:3)+NH4	38
948.8	627.5	2.2	TAG(58:8/FA20:4)+NH4	38
948.8	601.5	2.2	TAG(58:8/FA22:5)+NH4	38
948.8	603.5	2.2	TAG(58:8/FA22:6)+NH4	38
946.8	647.5	2.2	TAG(58:9/FA18:1)+NH4	38
946.8	649.5	2.2	TAG(58:9/FA18:2)+NH4	38
946.8	625.5	2.2	TAG(58:9/FA20:4)+NH4	38
946.8	599.5	2.2	TAG(58:9/FA22:5)+NH4	38
946.8	601.5	2.2	TAG(58:9/FA22:6)+NH4	38
972.8	625.5	2.2	TAG(60:10/FA22:5)+NH4	38
972.8	627.5	2.2	TAG(60:10/FA22:6)+NH4	38
970.8	623.5	2.2	TAG(60:11/FA22:5)+NH4	38
970.8	625.5	2.2	TAG(60:11/FA22:6)+NH4	38
968.8	623.5	2.2	TAG(60:12/FA22:6)+NH4	26
605.5	306.307	2.2	DAG(15:0/18:1)+NH4d7_SPLASH.IS	26
530.4	285.2	2.2	DAG(14:0/14:0)+NH4	26
556.5	285.2	2.2	DAG(14:0/16:1)+NH4	26
586.5	313.3	2.2	DAG(16:0/16:0)+NH4	26
584.4	313.2	2.2	DAG(16:0/16:1)+NH4	26
584.4	285.2	2.2	DAG(14:0/18:1)+NH4	26
582.4	311.2	2.2	DAG(16:1/16:1)+NH4	26
582.4	285.2	2.2	DAG(14:0/18:2)+NH4	26
580.4	285.2	2.2	DAG(14:0/18:3)+NH4	26
614.6	285.2	2.2	DAG(14:0/20:0)+NH4	26
614.4	313.2	2.2	DAG(16:0/18:0)+NH4	26
612.6	311.3	2.2	DAG(16:1/18:0)+NH4	26
612.6	313.2	2.2	DAG(16:0/18:1)+NH4	26
610.4	311.2	2.2	DAG(16:1/18:1)+NH4	26
610.4	313.2	2.2	DAG(16:0/18:2)+NH4	26
608.5	311.2	2.2	DAG(16:1/18:2)+NH4	26
608.5	313.2	2.2	DAG(16:0/18:3)+NH4	26
606.4	311.2	2.2	DAG(16:1/18:3)+NH4	26
606.4	285.2	2.2	DAG(14:0/20:4)+NH4	26

640.6	283.2	2.2	DAG(16:1/20:0)+NH4	26
640.4	341.3	2.2	DAG(18:0/18:1)+NH4	26
638.4	339.3	2.2	DAG(18:1/18:1)+NH4	26
638.4	341.3	2.2	DAG(18:0/18:2)+NH4	26
636.5	339.3	2.2	DAG(18:1/18:2)+NH4	26
636.5	341.3	2.2	DAG(18:0/18:3)+NH4	26
636.6	311.3	2.2	DAG(16:1/20:2)+NH4	26
636.5	313.3	2.2	DAG(16:0/20:3)+NH4	26
634.5	313.3	2.2	DAG(16:0/20:4)+NH4	26
632.4	337.3	2.2	DAG(18:2/18:3)+NH4	26
632.4	311.3	2.2	DAG(16:1/20:4)+NH4	26
632.4	313.3	2.2	DAG(16:0/20:5)+NH4	26
630.5	285.3	2.2	DAG(14:0/22:6)+NH4	26
666.6	339.3	2.2	DAG(18:1/20:1)+NH4	26
664.6	339.3	2.2	DAG(18:1/20:2)+NH4	26
662.6	339.3	2.2	DAG(18:1/20:3)+NH4	26
660.5	337.3	2.2	DAG(18:2/20:3)+NH4	26
660.5	339.3	2.2	DAG(18:1/20:4)+NH4	26
660.5	313.3	2.2	DAG(16:0/22:5)+NH4	26
658.5	337.3	2.2	DAG(18:2/20:4)+NH4	26
658.5	339.3	2.2	DAG(18:1/20:5)+NH4	26
658.5	313.3	2.2	DAG(16:0/22:6)+NH4	26
656.5	337.3	2.2	DAG(18:2/20:5)+NH4	26
656.5	311.3	2.2	DAG(16:1/22:6)+NH4	26
698.6	369.3	2.2	DAG(20:0/20:0)+NH4	26
688.6	339.3	2.2	DAG(18:1/22:4)+NH4	26
686.6	337.3	2.2	DAG(18:2/22:4)+NH4	26
686.6	339.3	2.2	DAG(18:1/22:5)+NH4	26
686.6	341.3	2.2	DAG(18:0/22:6)+NH4	26
684.6	337.3	2.2	DAG(18:2/22:5)+NH4	26
684.6	339.3	2.2	DAG(18:1/22:6)+NH4	26
682.5	337.3	2.2	DAG(18:2/22:6)+NH4	26
381.3	288.298	2	MAG(18:1)+NH4d7_SPLASH.IS	26
313.2	239.2	2	MAG(16:0)+NH4	25
311.2	237.2	2	MAG(16:1)+NH4	25
341.2	267.2	2	MAG(18:0)+NH4	25
339.2	265.2	2	MAG(18:1)+NH4	25
337.2	263.2	2	MAG(18:2)+NH4	25
369.2	295.2	2	MAG(20:0)+NH4	25
367.2	293.2	2	MAG(20:1)+NH4	25
365.2	291.2	2	MAG(20:2)+NH4	25
363.2	289.2	2	MAG(20:3)+NH4	25
361.2	287.2	2	MAG(20:4)+NH4	25
397.2	323.2	2	MAG(22:0)+NH4	25

395.2	321.2	2	MAG(22:1)+NH4	25
393.2	319.2	2	MAG(22:2)+NH4	25
391.2	317.2	2	MAG(22:3)+NH4	25
389.2	315.2	2	MAG(22:4)+NH4	25
387.2	313.2	2	MAG(22:5)+NH4	25
385.2	311.2	2	MAG(22:6)+NH4	25

Supplementary Table 4. Scan information for lipids in negative ion mode. Declustering potential = -80V, entrance potential = -10V, and collision exit potential = -15V for all lipids in negative mode.

Negative mode (-)				
Q1 (m/z)	Q3 (m/z)	Retention Time (min)	Lipid ID	Collision Energy (V)
587.409	288.296	12.2	LPC(18:1)+AcOd7_SPLASH.IS	-50
526.317	227.202	12.2	LPC(14:0)+AcO	-50
554.346	255.233	12.2	LPC(16:0)+AcO	-50
552.331	253.217	12.2	LPC(16:1)+AcO	-50
582.378	283.264	12.2	LPC(18:0)+AcO	-50
580.362	281.249	12.2	LPC(18:1)+AcO	-50
578.346	279.233	12.2	LPC(18:2)+AcO	-50
576.331	277.217	12.2	LPC(18:3)+AcO	-50
610.409	311.3	12.2	LPC(20:0)+AcO	-50
608.393	309.28	12.2	LPC(20:1)+AcO	-50
606.378	307.264	12.2	LPC(20:2)+AcO	-50
604.362	305.249	12.2	LPC(20:3)+AcO	-50
602.346	303.233	12.2	LPC(20:4)+AcO	-50
600.331	301.217	12.2	LPC(20:5)+AcO	-50
630.364	331.264	12.2	LPC(22:4)+AcO	-50
628.362	329.249	12.2	LPC(22:5)+AcO	-50
626.346	327.233	12.2	LPC(22:6)+AcO	-50
811.625	288.298	10.2	PC(15:0/18:1)+AcOd7_SPLASH.IS	-50
736.513	227.202	10.2	PC(14:0/14:0)+AcO	-50
790.56	281.249	10.2	PC(14:0/18:1)+AcO	-50
788.545	279.233	10.2	PC(14:0/18:2)+AcO	-50
786.529	277.217	10.2	PC(14:0/18:3)+AcO	-50
818.592	309.28	10.2	PC(14:0/20:1)+AcO	-50
816.576	307.264	10.2	PC(14:0/20:2)+AcO	-50
814.56	305.249	10.2	PC(14:0/20:3)+AcO	-50
812.545	303.233	10.2	PC(14:0/20:4)+AcO	-50
810.529	301.217	10.2	PC(14:0/20:5)+AcO	-50
840.576	331.264	10.2	PC(14:0/22:4)+AcO	-50
838.56	329.249	10.2	PC(14:0/22:5)+AcO	-50

836.545	327.233	10.2	PC(14:0/22:6)+AcO	-50
732.5	225.2	10.2	PC(14:1/14:1)+AcO	-50
764.545	227.202	10.2	PC(16:0/14:0)+AcO	-50
792.576	255.233	10.2	PC(16:0/16:0)+AcO	-50
790.56	253.217	10.2	PC(16:0/16:1)+AcO	-50
820.607	283.264	10.2	PC(16:0/18:0)+AcO	-50
818.592	281.249	10.2	PC(16:0/18:1)+AcO	-50
816.576	279.233	10.2	PC(16:0/18:2)+AcO	-50
814.56	277.217	10.2	PC(16:0/18:3)+AcO	-50
846.623	309.28	10.2	PC(16:0/20:1)+AcO	-50
844.607	307.264	10.2	PC(16:0/20:2)+AcO	-50
842.592	305.249	10.2	PC(16:0/20:3)+AcO	-50
840.576	303.233	10.2	PC(16:0/20:4)+AcO	-50
838.56	301.217	10.2	PC(16:0/20:5)+AcO	-50
868.607	331.264	10.2	PC(16:0/22:4)+AcO	-50
866.592	329.249	10.2	PC(16:0/22:5)+AcO	-50
816.576	281.249	10.2	PC(16:1/18:1)+AcO	-50
814.56	253.217	10.2	PC(16:1/18:2)+AcO	-50
864.576	327.233	10.2	PC(16:0/22:6)+AcO	-50
792.576	227.202	10.2	PC(18:0/14:0)+AcO	-50
818.592	253.217	10.2	PC(18:0/16:1)+AcO	-50
848.639	283.264	10.2	PC(18:0/18:0)+AcO	-50
846.623	281.249	10.2	PC(18:0/18:1)+AcO	-50
844.607	279.233	10.2	PC(18:0/18:2)+AcO	-50
842.592	277.217	10.2	PC(18:0/18:3)+AcO	-50
876.67	283.264	10.2	PC(18:0/20:0)+AcO	-50
874.654	309.28	10.2	PC(18:0/20:1)+AcO	-50
872.639	307.264	10.2	PC(18:0/20:2)+AcO	-50
870.623	305.249	10.2	PC(18:0/20:3)+AcO	-50
868.607	303.233	10.2	PC(18:0/20:4)+AcO	-50
866.592	301.217	10.2	PC(18:0/20:5)+AcO	-50
896.639	331.264	10.2	PC(18:0/22:4)+AcO	-50
894.623	329.249	10.2	PC(18:0/22:5)+AcO	-50
892.607	327.233	10.2	PC(18:0/22:6)+AcO	-50
816.576	281.249	10.2	PC(18:1/16:1)+AcO	-50
844.607	281.249	10.2	PC(18:1/18:1)+AcO	-50
842.592	279.233	10.2	PC(18:1/18:2)+AcO	-50
840.576	277.217	10.2	PC(18:1/18:3)+AcO	-50
872.639	309.28	10.2	PC(18:1/20:1)+AcO	-50
870.623	307.264	10.2	PC(18:1/20:2)+AcO	-50
868.607	305.249	10.2	PC(18:1/20:3)+AcO	-50
866.592	303.233	10.2	PC(18:1/20:4)+AcO	-50
864.576	301.217	10.2	PC(18:1/20:5)+AcO	-50
894.623	331.264	10.2	PC(18:1/22:4)+AcO	-50

892.607	329.249	10.2	PC(18:1/22:5)+AcO	-50
890.592	327.233	10.2	PC(18:1/22:6)+AcO	-50
814.56	279.233	10.2	PC(18:2/16:1)+AcO	-50
840.576	279.233	10.2	PC(18:2/18:2)+AcO	-50
838.56	277.217	10.2	PC(18:2/18:3)+AcO	-50
870.623	309.28	10.2	PC(18:2/20:1)+AcO	-50
868.607	307.264	10.2	PC(18:2/20:2)+AcO	-50
866.592	305.249	10.2	PC(18:2/20:3)+AcO	-50
864.576	303.233	10.2	PC(18:2/20:4)+AcO	-50
862.56	301.217	10.2	PC(18:2/20:5)+AcO	-50
892.607	331.264	10.2	PC(18:2/22:4)+AcO	-50
890.592	329.249	10.2	PC(18:2/22:5)+AcO	-50
888.576	327.233	10.2	PC(18:2/22:6)+AcO	-50
846.623	253.217	10.2	PC(20:0/16:1)+AcO	-50
874.654	281.249	10.2	PC(20:0/18:1)+AcO	-50
870.623	277.217	10.2	PC(20:0/18:3)+AcO	-50
902.685	309.28	10.2	PC(20:0/20:1)+AcO	-50
900.67	307.264	10.2	PC(20:0/20:2)+AcO	-50
898.654	305.249	10.2	PC(20:0/20:3)+AcO	-50
896.639	303.233	10.2	PC(20:0/20:4)+AcO	-50
894.623	301.217	10.2	PC(20:0/20:5)+AcO	-50
924.67	331.264	10.2	PC(20:0/22:4)+AcO	-50
922.654	329.249	10.2	PC(20:0/22:5)+AcO	-50
920.639	327.233	10.2	PC(20:0/22:6)+AcO	-50
485.343	288.298	12.3	LPE(18:1)-Hd7_SPLASH.IS	-50
424.247	227.202	12.3	LPE(14:0)-H	-50
452.278	255.233	12.3	LPE(16:0)-H	-40
450.263	253.217	12.3	LPE(16:1)-H	-40
480.31	283.264	12.3	LPE(18:0)-H	-40
478.293	281.249	12.3	LPE(18:1)-H	-40
476.278	279.233	12.3	LPE(18:2)-H	-40
474.263	277.217	12.3	LPE(18:3)-H	-40
508.341	311.3	12.3	LPE(20:0)-H	-40
506.325	309.28	12.3	LPE(20:1)-H	-40
504.31	307.264	12.3	LPE(20:2)-H	-40
502.294	305.249	12.3	LPE(20:3)-H	-40
500.278	303.233	12.3	LPE(20:4)-H	-40
498.263	301.217	12.3	LPE(20:5)-H	-40
528.31	331.264	12.3	LPE(22:4)-H	-40
526.294	329.249	12.3	LPE(22:5)-H	-40
524.278	327.233	12.3	LPE(22:6)-H	-40
709.557	288.298	10.3	PE(15:0/18:1)-Hd7_SPLASH.IS	-50
634.445	227.202	10.3	PE(14:0/14:0)-H	-43
660.461	253.217	10.3	PE(14:0/16:1)-H	-43

688.492	281.249	10.3	PE(14:0/18:1)-H	-43
686.477	279.233	10.3	PE(14:0/18:2)-H	-50
684.461	277.217	10.3	PE(14:0/18:3)-H	-50
716.524	309.28	10.3	PE(14:0/20:1)-H	-50
714.508	307.264	10.3	PE(14:0/20:2)-H	-50
712.492	305.249	10.3	PE(14:0/20:3)-H	-50
710.477	303.233	10.3	PE(14:0/20:4)-H	-50
708.461	301.217	10.3	PE(14:0/20:5)-H	-50
738.508	331.264	10.3	PE(14:0/22:4)-H	-50
736.492	329.249	10.3	PE(14:0/22:5)-H	-50
734.477	327.233	10.3	PE(14:0/22:6)-H	-50
630.4	225.2	10.3	PE(14:1/14:1)-H	-50
662.477	255.233	10.3	PE(16:0/14:0)-H	-50
690.508	255.233	10.3	PE(16:0/16:0)-H	-50
688.492	253.217	10.3	PE(16:0/16:1)-H	-50
716.524	281.249	10.3	PE(16:0/18:1)-H	-50
714.508	279.233	10.3	PE(16:0/18:2)-H	-50
712.492	277.217	10.3	PE(16:0/18:3)-H	-50
744.555	309.28	10.3	PE(16:0/20:1)-H	-50
742.539	307.264	10.3	PE(16:0/20:2)-H	-50
740.524	305.249	10.3	PE(16:0/20:3)-H	-50
738.508	303.233	10.3	PE(16:0/20:4)-H	-50
736.492	301.217	10.3	PE(16:0/20:5)-H	-50
766.539	331.264	10.3	PE(16:0/22:4)-H	-50
764.524	329.249	10.3	PE(16:0/22:5)-H	-50
762.508	327.233	10.3	PE(16:0/22:6)-H	-50
690.508	283.264	10.3	PE(18:0/14:0)-H	-50
718.539	283.264	10.3	PE(18:0/16:0)-H	-50
716.524	283.264	10.3	PE(18:0/16:1)-H	-50
746.57	283.264	10.3	PE(18:0/18:0)-H	-50
744.555	281.249	10.3	PE(18:0/18:1)-H	-50
742.539	279.233	10.3	PE(18:0/18:2)-H	-50
740.524	277.217	10.3	PE(18:0/18:3)-H	-50
772.586	309.28	10.3	PE(18:0/20:1)-H	-50
770.57	307.264	10.3	PE(18:0/20:2)-H	-50
768.555	305.249	10.3	PE(18:0/20:3)-H	-50
766.539	303.233	10.3	PE(18:0/20:4)-H	-50
764.524	301.217	10.3	PE(18:0/20:5)-H	-50
794.57	331.264	10.3	PE(18:0/22:4)-H	-50
792.555	329.249	10.3	PE(18:0/22:5)-H	-50
790.539	327.233	10.3	PE(18:0/22:6)-H	-50
714.508	281.249	10.3	PE(18:1/16:1)-H	-50
742.539	281.249	10.3	PE(18:1/18:1)-H	-50
740.524	279.233	10.3	PE(18:1/18:2)-H	-50

738.508	277.217	10.3	PE(18:1/18:3)-H	-50
770.57	309.28	10.3	PE(18:1/20:1)-H	-50
768.555	307.264	10.3	PE(18:1/20:2)-H	-50
766.539	305.249	10.3	PE(18:1/20:3)-H	-50
764.524	303.233	10.3	PE(18:1/20:4)-H	-50
762.508	301.217	10.3	PE(18:1/20:5)-H	-50
792.555	331.264	10.3	PE(18:1/22:4)-H	-50
790.539	329.249	10.3	PE(18:1/22:5)-H	-50
788.524	327.233	10.3	PE(18:1/22:6)-H	-50
712.492	279.233	10.3	PE(18:2/16:1)-H	-50
738.508	279.233	10.3	PE(18:2/18:2)-H	-50
736.492	277.217	10.3	PE(18:2/18:3)-H	-50
768.555	309.28	10.3	PE(18:2/20:1)-H	-50
766.539	307.264	10.3	PE(18:2/20:2)-H	-50
764.524	305.249	10.3	PE(18:2/20:3)-H	-50
762.508	303.233	10.3	PE(18:2/20:4)-H	-50
760.492	301.217	10.3	PE(18:2/20:5)-H	-50
790.539	331.264	10.3	PE(18:2/22:4)-H	-50
788.524	329.249	10.3	PE(18:2/22:5)-H	-50
786.508	327.233	10.3	PE(18:2/22:6)-H	-50
676.529	255.233	10.3	PE(O-16:0/16:0)-H	-50
674.513	253.217	10.3	PE(O-16:0/16:1)-H	-50
704.56	283.264	10.3	PE(O-16:0/18:0)-H	-50
702.544	281.249	10.3	PE(O-16:0/18:1)-H	-50
700.529	279.233	10.3	PE(O-16:0/18:2)-H	-50
698.513	277.217	10.3	PE(O-16:0/18:3)-H	-50
730.576	309.28	10.3	PE(O-16:0/20:1)-H	-50
728.56	307.264	10.3	PE(O-16:0/20:2)-H	-50
726.544	305.249	10.3	PE(O-16:0/20:3)-H	-50
724.529	303.233	10.3	PE(O-16:0/20:4)-H	-50
722.513	301.217	10.3	PE(O-16:0/20:5)-H	-50
752.56	331.264	10.3	PE(O-16:0/22:4)-H	-50
750.544	329.249	10.3	PE(O-16:0/22:5)-H	-50
748.529	327.233	10.3	PE(O-16:0/22:6)-H	-50
704.56	255.233	10.3	PE(O-18:0/16:0)-H	-50
702.544	253.217	10.3	PE(O-18:0/16:1)-H	-50
732.591	283.264	10.3	PE(O-18:0/18:0)-H	-50
730.576	281.249	10.3	PE(O-18:0/18:1)-H	-50
728.56	279.233	10.3	PE(O-18:0/18:2)-H	-50
726.544	277.217	10.3	PE(O-18:0/18:3)-H	-50
758.607	309.28	10.3	PE(O-18:0/20:1)-H	-50
756.591	307.264	10.3	PE(O-18:0/20:2)-H	-50
754.576	305.249	10.3	PE(O-18:0/20:3)-H	-50
752.56	303.233	10.3	PE(O-18:0/20:4)-H	-50

750.544	301.217	10.3	PE(O-18:0/20:5)-H	-50
780.591	331.264	10.3	PE(O-18:0/22:4)-H	-50
778.576	329.249	10.3	PE(O-18:0/22:5)-H	-50
776.56	327.233	10.3	PE(O-18:0/22:6)-H	-50
674.5	283.264	9.2	PE(P-14:0/18:0)-H	-50
672.5	281.249	9.2	PE(P-14:0/18:1)-H	-50
674.5	255.233	9.2	PE(P-16:0/16:0)-H	-50
672.5	253.217	9.2	PE(P-16:0/16:1)-H	-50
702.5	283.264	9.2	PE(P-16:0/18:0)-H	-50
700.5	281.249	9.2	PE(P-16:0/18:1)-H	-50
698.5	279.233	9.2	PE(P-16:0/18:2)-H	-50
696.5	277.217	9.2	PE(P-16:0/18:3)-H	-50
728.6	309.28	9.2	PE(P-16:0/20:1)-H	-50
726.5	307.264	9.2	PE(P-16:0/20:2)-H	-50
724.5	305.249	9.2	PE(P-16:0/20:3)-H	-50
722.5	303.233	9.2	PE(P-16:0/20:4)-H	-50
720.5	301.217	9.2	PE(P-16:0/20:5)-H	-50
750.5	331.264	9.2	PE(P-16:0/22:4)-H	-50
748.5	329.249	9.2	PE(P-16:0/22:5)-H	-50
746.5	327.233	9.2	PE(P-16:0/22:6)-H	-50
698.5	281.249	9.2	PE(P-16:1/18:1)-H	-50
702.5	255.233	9.2	PE(P-18:0/16:0)-H	-50
700.5	253.217	9.2	PE(P-18:0/16:1)-H	-50
730.6	283.264	9.2	PE(P-18:0/18:0)-H	-50
728.6	281.249	9.2	PE(P-18:0/18:1)-H	-50
726.5	279.233	9.2	PE(P-18:0/18:2)-H	-50
724.5	277.217	9.2	PE(P-18:0/18:3)-H	-50
756.6	309.28	9.2	PE(P-18:0/20:1)-H	-50
754.6	307.264	9.2	PE(P-18:0/20:2)-H	-50
752.6	305.249	9.2	PE(P-18:0/20:3)-H	-50
750.5	303.233	9.2	PE(P-18:0/20:4)-H	-50
748.5	301.217	9.2	PE(P-18:0/20:5)-H	-50
778.6	331.264	9.2	PE(P-18:0/22:4)-H	-50
776.6	329.249	9.2	PE(P-18:0/22:5)-H	-50
774.5	327.233	9.2	PE(P-18:0/22:6)-H	-50
700.5	255.233	9.2	PE(P-18:1/16:0)-H	-50
698.5	253.217	9.2	PE(P-18:1/16:1)-H	-50
728.6	283.2	9.2	PE(P-18:1/18:0)-H	-50
726.5	281.249	9.2	PE(P-18:1/18:1)-H	-50
724.5	279.233	9.2	PE(P-18:1/18:2)-H	-50
722.5	277.217	9.2	PE(P-18:1/18:3)-H	-50
754.6	309.28	9.2	PE(P-18:1/20:1)-H	-50
752.6	307.264	9.2	PE(P-18:1/20:2)-H	-50
750.5	305.249	9.2	PE(P-18:1/20:3)-H	-50

748.5	303.233	9.2	PE(P-18:1/20:4)-H	-50
746.5	301.217	9.2	PE(P-18:1/20:5)-H	-50
776.6	331.264	9.2	PE(P-18:1/22:4)-H	-50
774.5	329.249	9.2	PE(P-18:1/22:5)-H	-50
772.5	327.233	9.2	PE(P-18:1/22:6)-H	-50
722.5	279.233	9.2	PE(P-18:2/18:2)-H	-50
746.5	303.233	9.2	PE(P-18:2/20:4)-H	-50
770.5	327.233	9.2	PE(P-18:2/22:6)-H	-50
495.272	267.233	8.5	LPG(17:1)-Hstd.IS	-50
455.241	227.202	8.5	LPG(14:0)-H	-50
483.273	255.233	8.5	LPG(16:0)-H	-50
481.257	253.217	8.5	LPG(16:1)-H	-50
511.304	283.264	8.5	LPG(18:0)-H	-50
509.289	281.249	8.5	LPG(18:1)-H	-50
507.273	279.233	8.5	LPG(18:2)-H	-50
505.257	277.217	8.5	LPG(18:3)-H	-50
539.335	311.3	8.5	LPG(20:0)-H	-50
537.32	309.28	8.5	LPG(20:1)-H	-50
535.304	307.264	8.5	LPG(20:2)-H	-50
533.289	305.249	8.5	LPG(20:3)-H	-50
531.273	303.233	8.5	LPG(20:4)-H	-50
529.257	301.217	8.5	LPG(20:5)-H	-50
559.304	331.264	8.5	LPG(22:4)-H	-50
557.289	329.249	8.5	LPG(22:5)-H	-50
555.273	327.233	8.5	LPG(22:6)-H	-50
740.552	288.298	4	PG(15:0/18:1)-Hd7_SPLASH.IS	-50
665.44	227.202	4	PG(14:0/14:0)-H	-50
661.4	225.2	4	PG(14:1/14:1)-H	-50
719.487	281.249	4	PG(14:0/18:1)-H	-50
717.471	279.233	4	PG(14:0/18:2)-H	-50
715.456	277.217	4	PG(14:0/18:3)-H	-50
747.518	309.28	4	PG(14:0/20:1)-H	-50
745.503	307.264	4	PG(14:0/20:2)-H	-50
743.487	305.249	4	PG(14:0/20:3)-H	-50
741.471	303.233	4	PG(14:0/20:4)-H	-50
739.456	301.217	4	PG(14:0/20:5)-H	-50
769.503	331.264	4	PG(14:0/22:4)-H	-50
767.487	329.249	4	PG(14:0/22:5)-H	-50
765.471	327.233	4	PG(14:0/22:6)-H	-50
693.471	227.202	4	PG(16:0/14:0)-H	-50
721.503	255.233	4	PG(16:0/16:0)-H	-50
719.487	253.217	4	PG(16:0/16:1)-H	-50
749.534	283.264	4	PG(16:0/18:0)-H	-50
747.518	281.249	4	PG(16:0/18:1)-H	-50

745.503	279.233	4	PG(16:0/18:2)-H	-50
743.487	277.217	4	PG(16:0/18:3)-H	-50
775.549	309.28	4	PG(16:0/20:1)-H	-50
773.534	307.264	4	PG(16:0/20:2)-H	-50
771.518	305.249	4	PG(16:0/20:3)-H	-50
769.503	303.233	4	PG(16:0/20:4)-H	-50
767.487	301.217	4	PG(16:0/20:5)-H	-50
797.534	331.264	4	PG(16:0/22:4)-H	-50
795.518	329.249	4	PG(16:0/22:5)-H	-50
793.503	327.233	4	PG(16:0/22:6)-H	-50
721.503	227.202	4	PG(18:0/14:0)-H	-50
747.518	253.217	4	PG(18:0/16:1)-H	-50
777.565	283.264	4	PG(18:0/18:0)-H	-50
775.549	281.249	4	PG(18:0/18:1)-H	-50
773.534	279.233	4	PG(18:0/18:2)-H	-50
771.518	277.217	4	PG(18:0/18:3)-H	-50
805.596	283.264	4	PG(18:0/20:0)-H	-50
803.581	309.28	4	PG(18:0/20:1)-H	-50
801.565	307.264	4	PG(18:0/20:2)-H	-50
799.549	305.249	4	PG(18:0/20:3)-H	-50
797.534	303.233	4	PG(18:0/20:4)-H	-50
795.518	301.217	4	PG(18:0/20:5)-H	-50
825.565	331.264	4	PG(18:0/22:4)-H	-50
823.549	329.249	4	PG(18:0/22:5)-H	-50
821.534	327.233	4	PG(18:0/22:6)-H	-50
745.503	281.249	4	PG(18:1/16:1)-H	-50
773.534	281.249	4	PG(18:1/18:1)-H	-50
771.518	279.233	4	PG(18:1/18:2)-H	-50
769.503	277.217	4	PG(18:1/18:3)-H	-50
801.565	309.28	4	PG(18:1/20:1)-H	-50
799.549	307.264	4	PG(18:1/20:2)-H	-50
797.534	305.249	4	PG(18:1/20:3)-H	-50
795.518	303.233	4	PG(18:1/20:4)-H	-50
793.503	301.217	4	PG(18:1/20:5)-H	-50
823.549	331.264	4	PG(18:1/22:4)-H	-50
821.534	329.249	4	PG(18:1/22:5)-H	-50
819.518	327.233	4	PG(18:1/22:6)-H	-50
743.487	279.233	4	PG(18:2/16:1)-H	-50
769.503	279.233	4	PG(18:2/18:2)-H	-50
767.487	277.217	4	PG(18:2/18:3)-H	-50
799.549	309.28	4	PG(18:2/20:1)-H	-50
797.534	307.264	4	PG(18:2/20:2)-H	-50
795.518	305.249	4	PG(18:2/20:3)-H	-50
793.503	303.233	4	PG(18:2/20:4)-H	-50

791.487	301.217	4	PG(18:2/20:5)-H	-50
821.534	331.264	4	PG(18:2/22:4)-H	-50
819.518	329.249	4	PG(18:2/22:5)-H	-50
817.503	327.233	4	PG(18:2/22:6)-H	-50
775.549	253.217	4	PG(20:0/16:1)-H	-50
803.581	281.249	4	PG(20:0/18:1)-H	-50
801.565	279.233	4	PG(20:0/18:2)-H	-50
799.549	277.217	4	PG(20:0/18:3)-H	-50
831.612	309.28	4	PG(20:0/20:1)-H	-50
829.596	307.264	4	PG(20:0/20:2)-H	-50
827.581	305.249	4	PG(20:0/20:3)-H	-50
825.565	303.233	4	PG(20:0/20:4)-H	-50
823.549	301.217	4	PG(20:0/20:5)-H	-50
853.596	331.264	4	PG(20:0/22:4)-H	-50
851.581	329.249	4	PG(20:0/22:5)-H	-50
849.565	327.233	4	PG(20:0/22:6)-H	-50
583.289	267.233	11.6	LPI(17:1)-Hd7_Lyso.IS	-51
543.258	227.202	11.6	LPI(14:0)-H	-50
571.289	255.233	11.6	LPI(16:0)-H	-50
569.273	253.217	11.6	LPI(16:1)-H	-50
599.32	283.264	11.6	LPI(18:0)-H	-50
597.305	281.249	11.6	LPI(18:1)-H	-50
595.289	279.233	11.6	LPI(18:2)-H	-50
593.273	277.217	11.6	LPI(18:3)-H	-50
627.352	311.3	11.6	LPI(20:0)-H	-50
625.336	309.28	11.6	LPI(20:1)-H	-50
623.32	307.264	11.6	LPI(20:2)-H	-50
621.305	305.249	11.6	LPI(20:3)-H	-50
619.289	303.233	11.6	LPI(20:4)-H	-50
617.273	301.217	11.6	LPI(20:5)-H	-50
647.32	331.264	11.6	LPI(22:4)-H	-50
645.305	329.249	11.6	LPI(22:5)-H	-50
643.289	327.233	11.6	LPI(22:6)-H	-50
828.56	288.298	11.4	PI(15:0/18:1)-Hd7_SPLASH.IS	-50
749.4	225.2	11.4	PI(14:1/14:1)-H	-61
753.456	227.202	11.4	PI(14:0/14:0)-H	-60
807.503	281.249	11.4	PI(14:0/18:1)-H	-60
805.487	279.233	11.4	PI(14:0/18:2)-H	-60
803.472	277.217	11.4	PI(14:0/18:3)-H	-60
835.534	309.28	11.4	PI(14:0/20:1)-H	-60
833.518	307.264	11.4	PI(14:0/20:2)-H	-60
831.503	305.249	11.4	PI(14:0/20:3)-H	-60
829.487	303.233	11.4	PI(14:0/20:4)-H	-60
827.472	301.217	11.4	PI(14:0/20:5)-H	-60

857.518	331.264	11.4	PI(14:0/22:4)-H	-60
855.503	329.249	11.4	PI(14:0/22:5)-H	-60
853.487	327.233	11.4	PI(14:0/22:6)-H	-60
781.487	227.202	11.4	PI(16:0/14:0)-H	-60
809.518	255.233	11.4	PI(16:0/16:0)-H	-60
807.503	253.217	11.4	PI(16:0/16:1)-H	-60
837.55	283.264	11.4	PI(16:0/18:0)-H	-60
835.534	281.249	11.4	PI(16:0/18:1)-H	-60
833.518	279.233	11.4	PI(16:0/18:2)-H	-60
814.561	277.218	11.4	PI(16:0/18:3)-H	-60
863.565	309.28	11.4	PI(16:0/20:1)-H	-60
861.55	307.264	11.4	PI(16:0/20:2)-H	-60
859.534	305.249	11.4	PI(16:0/20:3)-H	-60
857.518	303.233	11.4	PI(16:0/20:4)-H	-60
855.503	301.217	11.4	PI(16:0/20:5)-H	-60
885.55	331.264	11.4	PI(16:0/22:4)-H	-60
883.534	329.249	11.4	PI(16:0/22:5)-H	-60
881.518	327.233	11.4	PI(16:0/22:6)-H	-60
809.518	227.202	11.4	PI(18:0/14:0)-H	-60
835.534	253.217	11.4	PI(18:0/16:1)-H	-60
865.581	283.264	11.4	PI(18:0/18:0)-H	-60
863.565	281.249	11.4	PI(18:0/18:1)-H	-60
861.55	279.233	11.4	PI(18:0/18:2)-H	-60
859.534	277.217	11.4	PI(18:0/18:3)-H	-60
893.612	283.264	11.4	PI(18:0/20:0)-H	-60
891.597	309.28	11.4	PI(18:0/20:1)-H	-60
889.581	307.264	11.4	PI(18:0/20:2)-H	-60
887.565	305.249	11.4	PI(18:0/20:3)-H	-60
885.55	283.3	11.4	PI(18:0/20:4)-H	-60
883.534	301.217	11.4	PI(18:0/20:5)-H	-60
913.581	331.264	11.4	PI(18:0/22:4)-H	-60
911.565	329.249	11.4	PI(18:0/22:5)-H	-60
909.55	327.233	11.4	PI(18:0/22:6)-H	-60
833.518	281.249	11.4	PI(18:1/16:1)-H	-60
861.55	281.249	11.4	PI(18:1/18:1)-H	-60
859.534	279.233	11.4	PI(18:1/18:2)-H	-60
857.518	277.217	11.4	PI(18:1/18:3)-H	-60
889.581	309.28	11.4	PI(18:1/20:1)-H	-60
887.565	307.264	11.4	PI(18:1/20:2)-H	-60
885.55	305.249	11.4	PI(18:1/20:3)-H	-60
883.534	303.233	11.4	PI(18:1/20:4)-H	-60
881.518	301.217	11.4	PI(18:1/20:5)-H	-60
911.565	331.264	11.4	PI(18:1/22:4)-H	-60
909.55	329.249	11.4	PI(18:1/22:5)-H	-60

907.534	327.233	11.4	PI(18:1/22:6)-H	-60
831.503	279.233	11.4	PI(18:2/16:1)-H	-60
857.518	279.233	11.4	PI(18:2/18:2)-H	-60
855.503	277.217	11.4	PI(18:2/18:3)-H	-60
887.565	309.28	11.4	PI(18:2/20:1)-H	-60
885.55	307.264	11.4	PI(18:2/20:2)-H	-60
883.534	305.249	11.4	PI(18:2/20:3)-H	-60
881.518	303.233	11.4	PI(18:2/20:4)-H	-60
879.503	301.217	11.4	PI(18:2/20:5)-H	-60
909.55	331.264	11.4	PI(18:2/22:4)-H	-60
907.534	329.249	11.4	PI(18:2/22:5)-H	-60
905.518	327.233	11.4	PI(18:2/22:6)-H	-60
863.565	253.217	11.4	PI(20:0/16:1)-H	-60
891.597	281.249	11.4	PI(20:0/18:1)-H	-60
889.581	279.233	11.4	PI(20:0/18:2)-H	-60
887.565	277.217	11.4	PI(20:0/18:3)-H	-60
919.628	309.28	11.4	PI(20:0/20:1)-H	-60
917.612	307.264	11.4	PI(20:0/20:2)-H	-60
915.597	305.249	11.4	PI(20:0/20:3)-H	-60
913.581	303.233	11.4	PI(20:0/20:4)-H	-60
911.565	301.217	11.4	PI(20:0/20:5)-H	-60
939.597	329.249	11.4	PI(20:0/22:5)-H	-60
937.581	327.233	11.4	PI(20:0/22:6)-H	-60
508.268	267.233	12	LPS(17:1)-Hd7_Lyso.IS	-50
468.233	227.202	12	LPS(14:0)-H	-50
496.268	255.233	12	LPS(16:0)-H	-50
494.252	253.217	12	LPS(16:1)-H	-50
524.299	283.264	12	LPS(18:0)-H	-50
522.284	281.249	12	LPS(18:1)-H	-50
520.268	279.233	12	LPS(18:2)-H	-50
518.252	277.217	12	LPS(18:3)-H	-50
552.331	311.3	12	LPS(20:0)-H	-50
550.315	309.28	12	LPS(20:1)-H	-50
548.299	307.264	12	LPS(20:2)-H	-50
546.284	305.249	12	LPS(20:3)-H	-50
544.268	303.233	12	LPS(20:4)-H	-50
542.252	301.217	12	LPS(20:5)-H	-50
572.299	331.264	12	LPS(22:4)-H	-50
570.284	329.249	12	LPS(22:5)-H	-50
568.268	327.233	12	LPS(22:6)-H	-50
753.547	288.298	9.6	PS(15:0/18:1)-Hd7_SPLASH.IS	-50
674.4	225.2	9.2	PS(14:1/14:1)	-51
678.435	227.202	9.2	PS(14:0/14:0)-H	-50
732.482	281.249	9.2	PS(14:0/18:1)-H	-50

730.466	279.233	9.2	PS(14:0/18:2)-H	-50
728.451	277.217	9.2	PS(14:0/18:3)-H	-50
760.513	309.28	9.2	PS(14:0/20:1)-H	-50
758.498	307.264	9.2	PS(14:0/20:2)-H	-50
756.482	305.249	9.2	PS(14:0/20:3)-H	-50
754.466	303.233	9.2	PS(14:0/20:4)-H	-50
752.451	301.217	9.2	PS(14:0/20:5)-H	-50
782.498	331.264	9.2	PS(14:0/22:4)-H	-50
780.482	329.249	9.2	PS(14:0/22:5)-H	-50
778.466	327.233	9.2	PS(14:0/22:6)-H	-50
706.466	227.202	9.2	PS(16:0/14:0)-H	-50
734.498	255.233	9.2	PS(16:0/16:0)-H	-50
732.482	253.217	9.2	PS(16:0/16:1)-H	-50
760.513	283.264	9.2	PS(16:0/18:0)-H	-50
760.513	281.249	9.2	PS(16:0/18:1)-H	-50
758.498	279.233	9.2	PS(16:0/18:2)-H	-50
756.482	277.217	9.2	PS(16:0/18:3)-H	-50
788.545	309.28	9.2	PS(16:0/20:1)-H	-50
786.529	307.264	9.2	PS(16:0/20:2)-H	-50
784.513	305.249	9.2	PS(16:0/20:3)-H	-50
782.498	303.233	9.2	PS(16:0/20:4)-H	-50
780.482	301.217	9.2	PS(16:0/20:5)-H	-50
810.529	331.264	9.2	PS(16:0/22:4)-H	-50
808.513	329.249	9.2	PS(16:0/22:5)-H	-50
806.498	327.233	9.2	PS(16:0/22:6)-H	-50
734.498	227.202	9.2	PS(18:0/14:0)-H	-50
760.513	253.217	9.2	PS(18:0/16:1)-H	-50
790.56	283.264	9.2	PS(18:0/18:0)-H	-50
788.545	281.249	9.2	PS(18:0/18:1)-H	-50
786.529	279.233	9.2	PS(18:0/18:2)-H	-50
784.513	277.217	9.2	PS(18:0/18:3)-H	-50
818.592	283.264	9.2	PS(18:0/20:0)-H	-50
816.576	309.28	9.2	PS(18:0/20:1)-H	-50
814.56	307.264	9.2	PS(18:0/20:2)-H	-50
812.545	305.249	9.2	PS(18:0/20:3)-H	-50
810.529	303.233	9.2	PS(18:0/20:4)-H	-50
808.513	301.217	9.2	PS(18:0/20:5)-H	-50
838.56	331.264	9.2	PS(18:0/22:4)-H	-50
836.545	329.249	9.2	PS(18:0/22:5)-H	-50
834.529	327.233	9.2	PS(18:0/22:6)-H	-50
758.498	281.249	9.2	PS(18:1/16:1)-H	-50
786.529	281.249	9.2	PS(18:1/18:1)-H	-50
784.513	279.233	9.2	PS(18:1/18:2)-H	-50
782.498	277.217	9.2	PS(18:1/18:3)-H	-50

814.56	309.28	9.2	PS(18:1/20:1)-H	-50
812.545	307.264	9.2	PS(18:1/20:2)-H	-50
810.529	305.249	9.2	PS(18:1/20:3)-H	-50
808.513	303.233	9.2	PS(18:1/20:4)-H	-50
806.498	301.217	9.2	PS(18:1/20:5)-H	-50
836.545	331.264	9.2	PS(18:1/22:4)-H	-50
834.529	329.249	9.2	PS(18:1/22:5)-H	-50
832.513	327.233	9.2	PS(18:1/22:6)-H	-50
756.482	279.233	9.2	PS(18:2/16:1)-H	-50
782.498	279.233	9.2	PS(18:2/18:2)-H	-50
780.482	277.217	9.2	PS(18:2/18:3)-H	-50
812.545	309.28	9.2	PS(18:2/20:1)-H	-50
810.529	307.264	9.2	PS(18:2/20:2)-H	-50
808.513	305.249	9.2	PS(18:2/20:3)-H	-50
806.498	303.233	9.2	PS(18:2/20:4)-H	-50
804.482	301.217	9.2	PS(18:2/20:5)-H	-50
834.529	331.264	9.2	PS(18:2/22:4)-H	-50
832.513	329.249	9.2	PS(18:2/22:5)-H	-50
830.498	327.233	9.2	PS(18:2/22:6)-H	-50
788.545	253.217	9.2	PS(20:0/16:1)-H	-50
814.56	281.249	9.2	PS(20:0/18:1)-H	-50
814.561	279.234	9.2	PS(20:0/18:2)-H	-50
812.545	277.217	9.2	PS(20:0/18:3)-H	-50
844.607	309.28	9.2	PS(20:0/20:1)-H	-50
842.592	307.264	9.2	PS(20:0/20:2)-H	-50
840.576	305.249	9.2	PS(20:0/20:3)-H	-50
838.56	303.233	9.2	PS(20:0/20:4)-H	-50
836.545	301.217	9.2	PS(20:0/20:5)-H	-50
866.592	331.264	9.2	PS(20:0/22:4)-H	-50
864.576	329.249	9.2	PS(20:0/22:5)-H	-50
862.56	327.233	9.2	PS(20:0/22:6)-H	-50