

1 Supplemental Table 1: Listing of lipids in all empirically-derived sets from Barupal et al. 2019

Lipid Set	Lipid Class	Lipid ID	Network Label	FullName	AcylChainInformation	Adduct	RT	MZ
Set -1	Triacylglycerol	UCD.Lipid.173	TG 42:0	TG (42:0)	TG (14:0_14:0_14:0)	[M+N H4] ⁺	9.4 3	740.6 763
Set -1	Triacylglycerol	UCD.Lipid.174	TG 40:0	TG (40:0)	TG(12:0_12:0_16:0)	[M+N H4] ⁺	9.1	712.6 419
Set -1	Triacylglycerol	UCD.Lipid.177	TG 42:2	TG (42:2)	TG(12:0_12:0_18:2)	[M+N H4] ⁺	8.4 67	736.6 446
Set -1	Triacylglycerol	UCD.Lipid.179	TG 44:0	TG (44:0)	TG(14:0_14:0_16:0)	[M+N H4] ⁺	10. 13	768.7 037
Set -1	Triacylglycerol	UCD.Lipid.180	TG 44:1	TG (44:1)	TG(12:0_14:0_18:1)	[M+N H4] ⁺	9.4 55	766.7 919
Set -1	Triacylglycerol	UCD.Lipid.181	TG 44:2	TG (44:2)		[M+Na] ⁺	9.0 33	769.6 316
Set -1	Triacylglycerol	UCD.Lipid.182	TG 46:0	TG (46:0)	TG(14:0_16:0_16:0)	[M+N H4] ⁺	10. 38	796.7 389
Set -1	Triacylglycerol	UCD.Lipid.183	TG 46:1	TG (46:1)	TG(12:0_16:0_18:1)	[M+N H4] ⁺	9.9 44	794.7 232
Set -1	Triacylglycerol	UCD.Lipid.184	TG 46:2	TG (46:2)	TG(12:0_16:1_18:1)	[M+Na] ⁺	9.5 12	797.6 63
Set -1	Triacylglycerol	UCD.Lipid.185	TG 46:3	TG (46:3)	TG(12:0_16:1_18:2)	[M+Na] ⁺	9.0 65	795.6 473
Set -1	Triacylglycerol	UCD.Lipid.186	TG 46:4 A	TG (46:4) A		[M+Na] ⁺	8.8	793.6 322
Set -1	Triacylglycerol	UCD.Lipid.187	TG 48:0	TG (48:0)	TG(16:0_16:0_16:0)	[M+N H4] ⁺	10. 81	824.7 702
Set -1	Triacylglycerol	UCD.Lipid.188	TG 48:1	TG (48:1)	TG(14:0_16:0_18:1)	[M+N H4] ⁺	10. 4	822.7 545
Set -1	Triacylglycerol	UCD.Lipid.189	TG 48:2	TG (48:2)	TG(14:0_16:0_18:2)	[M+N H4] ⁺	9.9 93	820.7 389
Set -1	Triacylglycerol	UCD.Lipid.192	TG 49:0	TG (49:0)	TG(16:0_16:0_17:0)	[M+N H4] ⁺	10. 94	838.7 858
Set -1	Triacylglycerol	UCD.Lipid.193	TG 49:1	TG (49:1)	TG(15:0_16:0_18:1)	[M+N H4] ⁺	10. 6	836.7 702
Set -1	Triacylglycerol	UCD.Lipid.194	TG 49:2	TG (49:2)	TG(15:0_16:0_18:2)	[M+N H4] ⁺	10. 18	834.7 545
Set -1	Triacylglycerol	UCD.Lipid.196	TG 50:0	TG (50:0)	TG(16:0_16:0_18:0)	[M+N H4] ⁺	11. 21	852.8 015
Set -1	Triacylglycerol	UCD.Lipid.197	TG 50:1	TG (50:1)	TG(16:0_16:0_18:1)	[M+N H4] ⁺	10. 82	850.7 858
Set -1	Triacylglycerol	UCD.Lipid.198	TG 50:2	TG (50:2)	TG(16:0_16:1_18:1)	[M+N H4] ⁺	10. 42	848.7 702
Set -1	Triacylglycerol	UCD.Lipid.202	TG 50:6	TG (50:6)	TG(14:0_16:1_20:5)	[M+Na] ⁺	9.1 8	845.6 599
Set -1	Triacylglycerol	UCD.Lipid.203	TG 51:1	TG (51:1)	TG(16:0_17:0_18:1)	[M+N H4] ⁺	10. 96	864.8 015
Set -1	Triacylglycerol	UCD.Lipid.208	TG 52:0	TG (52:0)	TG(16:0_18:0_18:0)	[M+N H4] ⁺	11. 58	880.8 328
Set -1	Triacylglycerol	UCD.Lipid.209	TG 52:1	TG (52:1)	TG(16:0_18:0_18:1)	[M+N H4] ⁺	11. 22	878.8 171
Set -1	Triacylglycerol	UCD.Lipid.215	TG 53:1	TG (53:1)	TG(17:0_18:0_18:1)	[M+N H4] ⁺	11. 35	892.8 328
Set -1	Triacylglycerol	UCD.Lipid.220	TG 54:0	TG (54:0)	TG(18:0_18:0_18:0)	[M+N H4] ⁺	11. 92	908.8 576
Set -1	Triacylglycerol	UCD.Lipid.221	TG 54:1	TG (54:1)	TG(18:0_18:0_18:1)	[M+N H4] ⁺	11. 58	906.8 484
Set -1	Triacylglycerol	UCD.Lipid.229	TG 56:2	TG (56:2)	TG(18:1_18:1_20:0)	[M+N H4] ⁺	11. 58	932.8 641
Set -2	Cholesteryl ester	UCD.Lipid.10	CE 16:1	CE (16:1)	16:1 Cholesteryl ester	[M+Na] ⁺	10. 33	645.5 581
Set -2	Lysophosphatidylcholine	UCD.Lipid.119	LPC 14:0	LPC (14:0)	LysoPC 14:0	[M+H] ⁺	0.9 81	468.3 089
Set -2	Phosphatidylcholine	UCD.Lipid.133	PC 28:0	PC (28:0)		[M+H] ⁺	4.2 39	678.5 065

Set -2	Phosphatidylcholine	UCD.Lipi d.134	PC 30:0	PC (30:0)	PC(14:0_16:0)	[M+H] +	4.8 11	706.5 378
Set -2	Phosphatidylcholine	UCD.Lipi d.135	PC 30:1	PC (30:1)		[M+H] +	4.3 22	704.5 225
Set -2	Phosphatidylcholine	UCD.Lipi d.136	PC 31:0	PC (31:0)		[M+H] +	5.1 1	720.5 538
Set -2	Phosphatidylcholine	UCD.Lipi d.137	PC 31:1	PC (31:1)		[M+H] +	4.8 2	718.5 345
Set -2	Phosphatidylcholine	UCD.Lipi d.138	PC 32:3	PC (32:3)		[M+H] +	4.8 11	728.5 222
Set -2	Phosphatidylcholine	UCD.Lipi d.139	PC 33:0	PC (33:0)		[M+H] +	5.6 4	748.5 851
Set -2	Phosphatidylcholine	UCD.Lipi d.383	PC 32:1	PC (32:1)	PC(16:0_16:1)	[M+Ac -H]-	5.0 33	790.5 6
Set -2	Phosphatidylcholine	UCD.Lipi d.384	PC 32:2	PC (32:2)	PC(14:0_18:2)	[M+Ac -H]-	4.5 67	788.5 4
Set -2	Phosphatidylcholine	UCD.Lipi d.385	PC 33:1	PC (33:1)	PC(15:0_18:1)	[M+Ac -H]-	5.3 4	804.5 8
Set -2	Phosphatidylcholine	UCD.Lipi d.388	PC 34:1	PC (34:1)	PC(16:0_18:1)	[M+Ac -H]-	5.6 48	818.5 9
Set -2	Phosphatidylcholine	UCD.Lipi d.390	PC 34:3	PC (34:3)	PC(16:0_18:3)	[M+Ac -H]-	4.7 5	814.5 6
Set -2	Phosphatidylcholine	UCD.Lipi d.391	PC 34:4	PC (34:4)	PC(14:0_20:4)	[M+Ac -H]-	4.4 92	812.5 4
Set -2	Phosphatidylcholine	UCD.Lipi d.392	PC 35:1	PC (35:1)	PC(17:0_18:1)	[M+Ac -H]-	5.9 73	832.6 1
Set -2	Phosphatidylcholine	UCD.Lipi d.395	PC 36:1	PC (36:1)	PC(18:0_18:1)	[M+Ac -H]-	6.3 14	846.6 2
Set -2	Phosphatidylethanolamine	UCD.Lipi d.431	PE 36:1	PE (36:1)	PE(18:0_18:1)	[M- H]-	5.6 48	744.5 5
Set -2	Phosphatidylethanolamine	UCD.Lipi d.437	PE 40:6	PE (40:6)	PE(18:0_22:6)	[M- H]-	4.9 08	790.5 4
Set -2	Phosphatidylinositol	UCD.Lipi d.452	PI 32:1	PI (32:1)	PI(16:0_16:1)	[M- H]-	4.0 25	807.5
Set -2	Phosphatidylinositol	UCD.Lipi d.458	PI 36:4	PI (36:4)	PI(16:0_20:4)	[M- H]-	4.0 92	857.5 2
Set -3	Sphingomyelin	UCD.Lipi d.169	SM d30:1	SM (d30:1)	SM (d18:1_12:0)	[M+H] +	3.6 34	647.5 123
Set -3	Ceramide	UCD.Lipi d.257	Cer d32:1	Ceramide (d32:1)	Cer[NS](d16:1_16:0)	[M+Ac -H]-	5.0 91	568.4 9
Set -3	Ceramide	UCD.Lipi d.258	Cer d33:1	Ceramide (d33:1)	Cer[NS](d17:1_16:0)	[M+Cl] -	5.4 15	558.4 7
Set -3	Ceramide	UCD.Lipi d.260	Cer d34:1	Ceramide (d34:1)	Cer[NS](d18:1_16:0)	[M+Ac -H]-	5.7 48	596.5 3
Set -3	Ceramide	UCD.Lipi d.261	Cer d34:2	Ceramide (d34:2)		[M+Ac -H]-	5.1 82	594.5 1
Set -3	Ceramide	UCD.Lipi d.262	Cer d36:1	Ceramide (d36:1)	Cer[NS](d18:1_18:0)	[M+Cl] -	6.4 55	600.5 1
Set -3	Ceramide	UCD.Lipi d.272	Cer d43:1	Ceramide (d43:1)	Cer[NS](d19:1_24:0)	[M+Cl] -	8.6 82	698.6 2
Set -3	Sphingomyelin	UCD.Lipi d.463	SM d32:0	SM (d32:0)		[M+Ac -H]-	4.4 67	735.5 6
Set -3	Sphingomyelin	UCD.Lipi d.464	SM d32:1	SM (d32:1)	SM(d18:1_14:0)	[M+Ac -H]-	4.2 67	733.5 5
Set -3	Sphingomyelin	UCD.Lipi d.465	SM d32:2	SM (d32:2)		[M+Ac -H]-	3.8 18	731.5 3
Set -3	Sphingomyelin	UCD.Lipi d.466	SM d33:1	SM (d33:1)	SM(d17:1_16:0)	[M+Ac -H]-	4.5 58	747.5 7
Set -3	Sphingomyelin	UCD.Lipi d.469	SM d36:0	SM (d36:0)		[M+Ac -H]-	5.7 65	791.6 3
Set -3	Sphingomyelin	UCD.Lipi d.470	SM d36:1	SM (d36:1)	SM(d18:1_18:0)	[M+Ac -H]-	5.5 23	789.6 1
Set -3	Sphingomyelin	UCD.Lipi d.473	SM d37:1	SM (d37:1)		[M+Ac -H]-	5.8 73	803.6 3
Set -3	Sphingomyelin	UCD.Lipi d.474	SM d38:0	SM (d38:0)	SM(d18:0_20:0)	[M+Ac -H]-	6.4 55	819.6 6
Set -3	Sphingomyelin	UCD.Lipi d.475	SM d38:1	SM (d38:1)	SM(d18:1_20:0)	[M+Ac -H]-	6.2 14	817.6 4

Set -3	Sphingomyelin	UCD.Lipi d.477	SM d39:1	SM (d39:1)	SM(d16:1_23:0)	[M+Ac -H]-	6.5 55	831.6 6
Set -3	Sphingomyelin	UCD.Lipi d.490	SM d43:1	SM (d43:1)		[M+Ac -H]-	7.7 7	887.7 2
Set -3	Sphingomyelin	UCD.Lipi d.491	SM d43:2	SM (d43:2)		[M+Ac -H]-	7.0 79	885.7 1
Set -4	Lysophosphatidylcholine	UCD.Lipi d.126	LPC 20:5	LPC (20:5)	LysoPC 20:5	[M+H] +	0.9 64	542.3 239
Set -4	Lysophosphatidylcholine	UCD.Lipi d.128	LPC 22:6	LPC (22:6)	LysoPC 22:6	[M+H] +	1.1 55	568.3 404
Set -4	Phosphatidylcholine	UCD.Lipi d.143	PC 36:6	PC (36:6)		[M+H] +	4.2 31	778.5 378
Set -4	Phosphatidylcholine	UCD.Lipi d.145	PC 37:6	PC (37:6)		[M+H] +	4.4 96	792.5 538
Set -4	Phosphatidylcholine	UCD.Lipi d.148	PC 38:6 A	PC (38:6) A	PC(16:0_22:6)	[M+H] +	4.7 78	806.5 691
Set -4	Phosphatidylcholine	UCD.Lipi d.149	PC 38:7	PC (38:7)		[M+H] +	4.3 14	804.5 538
Set -4	Phosphatidylcholine	UCD.Lipi d.150	PC 39:6	PC (39:6)		[M+H] +	5.0 27	820.5 851
Set -4	Cholesteroyl ester	UCD.Lipi d.16	CE 20:5	CE (20:5)	20:5 Cholesteroyl ester	[M+Na]+	9.7 11	693.5 581
Set -4	Cholesteroyl ester	UCD.Lipi d.17	CE 22:6	CE (22:6)	22:6 Cholesteroyl ester	[M+Na]+	9.8 94	719.5 738
Set -4	Lysophosphatidylethanolamine	UCD.Lipi d.381	LPE 22:6	LPE (22:6)	LysoPC 22:6	[M-H]-	1.2 63	524.2 8
Set -4	Phosphatidylcholine	UCD.Lipi d.399	PC 36:5 B	PC (36:5) B	PC(16:1_20:4)	[M+Ac -H]-	4.6 83	838.5 6
Set -4	Phosphatidylcholine	UCD.Lipi d.406	PC 38:6	PC (38:6)	PC(18:1_20:5)_PC(18:2_20:4)	[M+Ac -H]-	4.9 08	864.5 8
Set -4	Phosphatidylcholine	UCD.Lipi d.409	PC 40:6 B	PC (40:6) B	PC(18:0_22:6)	[M+Ac -H]-	5.5 32	892.6 1
Set -4	Phosphatidylcholine	UCD.Lipi d.410	PC 40:7	PC (40:7)	PC(18:1_22:6)	[M+Ac -H]-	4.9 83	890.5 9
Set -4	Phosphatidylethanolamine	UCD.Lipi d.442	PE p-36:5	PE (p-36:5) or PE (o-36:6)	PE(P-16:0_20:5)	[M-H]-	5.0 99	720.5
Set -4	Phosphatidylinositol	UCD.Lipi d.462	PI 40:6	PI (40:6)	PI(18:0_22:6)	[M-H]-	4.5 08	909.5 5
Set -4	Fatty acid	UCD.Lipi d.513	FA 20:5	FA (20:5)	FA (20:5)	[M-H]-	1.5 3	301.2 2
Set -4	Fatty acid	UCD.Lipi d.517	FA 22:6	FA (22:6)	FA (22:6)	[M-H]-	1.7 2	327.2 3
Set -5	Diacylglycerol	UCD.Lipi d.104	DG 32:1	DG (32:1)	DG(16:0_16:1)	[M+Na]+	6.1 43	589.4 812
Set -5	Diacylglycerol	UCD.Lipi d.105	DG 34:1	DG (34:1)	DG(16:0_18:1)	[M+Na]+	6.8 92	617.5 116
Set -5	Diacylglycerol	UCD.Lipi d.106	DG 34:2	DG (34:2)	DG(16:0_18:2)	[M+Na]+	6.2 7	615.4 965
Set -5	Diacylglycerol	UCD.Lipi d.107	DG 34:3	DG (34:3)	DG(16:1_18:2)	[M+N H4] +	5.6 86	608.5 246
Set -5	Diacylglycerol	UCD.Lipi d.109	DG 36:2	DG (36:2)	DG(18:1_18:1)	[M+N H4] +	6.9 5	638.5 718
Set -5	Diacylglycerol	UCD.Lipi d.110	DG 36:3	DG (36:3)	DG(18:1_18:2)	[M+N H4] +	6.4 2	636.5 562
Set -5	Triacylglycerol	UCD.Lipi d.190	TG 48:3	TG (48:3)	TG(12:0_18:1_18:2)	[M+Na]+	9.5 46	823.6 789
Set -5	Triacylglycerol	UCD.Lipi d.191	TG 48:4	TG (48:4)	TG(12:0_18:2_18:2)	[M+Na]+	9.3 4	821.6 597
Set -5	Triacylglycerol	UCD.Lipi d.195	TG 49:3	TG (49:3)	TG(15:0_16:1_18:2)	[M+N H4] +	9.7 94	832.7 389
Set -5	Triacylglycerol	UCD.Lipi d.199	TG 50:3	TG (50:3)	TG(16:1_16:1_18:1)	[M+N H4] +	10. 02	846.7 545
Set -5	Triacylglycerol	UCD.Lipi d.200	TG 50:4	TG (50:4)	TG(16:1_16:1_18:2)	[M+Na]+	9.6 29	849.6 943
Set -5	Triacylglycerol	UCD.Lipi d.201	TG 50:5	TG (50:5)	TG(14:0_18:2_18:3)	[M+Na]+	9.2 4	847.6 786
Set -5	Triacylglycerol	UCD.Lipi d.204	TG 51:2	TG (51:2)	TG(16:0_17:0_18:2)	[M+N H4] +	10. 62	862.7 858

Set -5	Triacylglycerol	UCD.Lipid.205	TG 51:3	TG (51:3)	TG(15:0_18:1_18:2)	[M+N H4] ⁺	10.25	860.7702
Set -5	Triacylglycerol	UCD.Lipid.210	TG 52:2	TG (52:2)	TG(16:0_18:1_18:1)	[M+N H4] ⁺	10.83	876.8015
Set -5	Triacylglycerol	UCD.Lipid.211	TG 52:3	TG (52:3)	TG(16:0_18:1_18:2)	[M+N H4] ⁺	10.47	874.7858
Set -5	Triacylglycerol	UCD.Lipid.216	TG 53:2	TG (53:2)	TG(17:0_18:1_18:1)	[M+N H4] ⁺	11.01	890.8171
Set -5	Triacylglycerol	UCD.Lipid.217	TG 53:3	TG (53:3)	TG(17:0_18:1_18:2)	[M+N H4] ⁺	10.65	888.8015
Set -6	Diacylglycerol	UCD.Lipid.108	DG 36:1	DG (36:1)	DG(18:0_18:1)	[M+N H4] ⁺	7.47	640.588
Set -6	Diacylglycerol	UCD.Lipid.113	DG 38:0	DG (38:0)		[M+N H4] ⁺	7.94	670.6086
Set -6	Diacylglycerol	UCD.Lipid.114	DG 38:3	DG (38:3)	DG(20:1_18:2)	[M+Na] ⁺	6.974	669.5653
Set -6	Diacylglycerol	UCD.Lipid.116	DG 38:6	DG (38:6)	DG(18:2_20:4)	[M+Na] ⁺	5.732	663.4959
Set -6	Lysophosphatidylcholine	UCD.Lipid.127	LPC 22:4	LPC (22:4)	LysoPC 22:4	[M+H] ⁺	1.661	572.3711
Set -6	Lysophosphatidylcholine	UCD.Lipid.129	LPC o-16:0	LPC (o-16:0)	LPC (o-16:0)	[M+H] ⁺	1.752	482.3606
Set -6	Lysophosphatidylcholine	UCD.Lipid.130	LPC p-16:0	LPC (p-16:0) or LPC (o-16:1)	LPC (o-16:1)	[M+H] ⁺	1.694	480.3448
Set -6	Lysophosphatidylcholine	UCD.Lipid.131	LPC p-18:0	LPC (p-18:0) or LPC (o-18:1)	LPC (o-18:1)	[M+H] ⁺	1.909	508.3762
Set -6	Triacylglycerol	UCD.Lipid.175	TG 40:1	TG (40:1)		[M+N H4] ⁺	8.384	710.6298
Set -6	Triacylglycerol	UCD.Lipid.178	TG 42:3	TG (42:3)		[M+N H4] ⁺	8.24	734.6265
Set -6	Ceramide	UCD.Lipid.19	Cer d42:2	Ceramide (d42:2)	Cer[NS](d18:2_24:0)	[M+H] ⁺	7.615	648.6289
Set -6	Triacylglycerol	UCD.Lipid.253	TG 60:6	TG (60:6)		[M+Na] ⁺	11.27	985.8105
Set -6	Ceramide	UCD.Lipid.259	Cer d34:0	Ceramide (d34:0)	Cer[NDS](d18:0_16:0)	[M+Ac -H] ⁻	5.998	598.54
Set -6	Phosphatidylethanolamine	UCD.Lipid.439	PE p-36:1	PE (p-36:1) or PE (o-36:2)	PE(P-18:0_18:1)	[M-H] ⁻	6.838	728.56
Set -6	Fatty acid	UCD.Lipid.511	FA 20:3	FA (20:3)	FA (20:3)	[M-H] ⁻	2.5	305.25
Set -6	Fatty acid	UCD.Lipid.512	FA 20:4	FA (20:4)	FA (20:4)	[M-H] ⁻	1.93	303.23
Set -6	Fatty acid	UCD.Lipid.515	FA 22:1	FA (22:1)	FA (22:1)	[M-H] ⁻	3.9	337.31
Set -6	Acylcarnitine	UCD.Lipid.9	AC C18:3	Acylcarnitine C18:3	Acylcarnitine 18:3	[M+H] ⁺	1.13	422.3265
Set -7	Phosphatidylcholine	UCD.Lipid.142	PC 36:4 A	PC (36:4) A	PC(18:2_18:2)	[M+H] ⁺	4.637	782.5694
Set -7	Glucosylceramide	UCD.Lipid.368	GlcCer d24:1-2OH	GlcCer(d14:1(4E)/20:0(2OH))		[M+Cl] ⁻	4.966	750.53
Set -7	Phosphatidylcholine	UCD.Lipid.382	PC 32:0	PC (32:0)	PC(16:0_16:0)	[M+Ac -H] ⁻	5.573	792.58
Set -7	Phosphatidylcholine	UCD.Lipid.386	PC 33:2	PC (33:2)	PC(16:0_18:2)	[M+Ac -H] ⁻	4.858	802.56
Set -7	Phosphatidylcholine	UCD.Lipid.387	PC 34:0	PC (34:0)	PC(16:0_18:0)	[M+Ac -H] ⁻	6.239	820.61
Set -7	Phosphatidylcholine	UCD.Lipid.389	PC 34:2	PC (34:2)	PC(16:0_18:2)	[M+Ac -H] ⁻	5.166	816.58
Set -7	Phosphatidylcholine	UCD.Lipid.393	PC 35:2	PC (35:2)	PC(17:0_18:2)	[M+Ac -H] ⁻	5.48	830.59
Set -7	Phosphatidylcholine	UCD.Lipid.396	PC 36:2	PC (36:2)	PC(18:0_18:2)	[M+Ac -H] ⁻	5.806	844.61
Set -7	Phosphatidylcholine	UCD.Lipid.400	PC 37:2	PC (37:2)	PC(19:0_18:2)	[M+Ac -H] ⁻	6.14	858.62
Set -7	Phosphatidylethanolamine	UCD.Lipid.434	PE 38:2	PE (38:2)	PE(20:0_18:2)	[M-H] ⁻	5.806	770.57

Set -7	Phosphatidylethanolamine	UCD.Lipid.443	PE p-38:2	PE (p-38:2) or PE (o-38:3)		[M-H]-	6.98	754.58
Set -7	Phosphatidylethanolamine	UCD.Lipid.448	PE p-40:4	PE (p-40:4) or PE (o-40:5)	PE(P-20:0_20:4)	[M-H]-	6.87	778.58
Set -7	Phosphatidylinositol	UCD.Lipid.453	PI 34:1	PI (34:1)	PI(16:0_18:1)	[M-H]-	4.483	835.53
Set -7	Phosphatidylinositol	UCD.Lipid.454	PI 34:2	PI (34:2)	PI(16:0_18:2)	[M-H]-	4.158	833.52
Set -7	Phosphatidylinositol	UCD.Lipid.455	PI 36:1	PI (36:1)	PI(18:0_18:1)	[M-H]-	5.198	863.57
Set -7	Phosphatidylinositol	UCD.Lipid.456	PI 36:2	PI (36:2)	PI(18:0_18:2)	[M-H]-	4.732	861.55
Set -7	Phosphatidylinositol	UCD.Lipid.457	PI 36:3	PI (36:3)	PI(16:0_20:3)	[M-H]-	4.225	859.53
Set -8	Lysophosphatidylcholine	UCD.Lipid.120	LPC 15:0	LPC (15:0)	LysoPC 15:0	[M+H]+	1.206	482.3241
Set -8	Lysophosphatidylcholine	UCD.Lipid.121	LPC 17:1	LPC (17:1)	LysoPC 17:1	[M+H]+	1.345	508.3401
Set -8	Lysophosphatidylcholine	UCD.Lipid.122	LPC 18:0	LPC (18:0)	LysoPC 18:0	[M+H]+	2.258	524.3708
Set -8	Lysophosphatidylcholine	UCD.Lipid.123	LPC 18:3	LPC (18:3)	LysoPC 18:3	[M+H]+	0.981	518.3241
Set -8	Lysophosphatidylcholine	UCD.Lipid.124	LPC 20:0	LPC (20:0)	LysoPC 20:0	[M+H]+	3.062	552.4021
Set -8	Lysophosphatidylcholine	UCD.Lipid.369	LPC 16:0	LPC (16:0)	LysoPC 16:0	[M+Ac-H]-	1.563	554.35
Set -8	Lysophosphatidylcholine	UCD.Lipid.370	LPC 16:1	LPC (16:1)	LysoPC 16:1	[M+Ac-H]-	1.18	552.33
Set -8	Lysophosphatidylcholine	UCD.Lipid.371	LPC 18:0 A	LPC (18:0) A	LysoPC 18:0	[M+Ac-H]-	2.145	582.38
Set -8	Lysophosphatidylcholine	UCD.Lipid.372	LPC 18:1	LPC (18:1)	LysoPC 18:1	[M+Ac-H]-	1.713	580.36
Set -8	Lysophosphatidylcholine	UCD.Lipid.373	LPC 18:2	LPC (18:2)	LysoPC 18:2	[M+Ac-H]-	1.313	578.35
Set -8	Lysophosphatidylcholine	UCD.Lipid.374	LPC 20:1	LPC (20:1)	LysoPC 20:1	[M+Ac-H]-	2.47	608.39
Set -8	Lysophosphatidylcholine	UCD.Lipid.375	LPC 20:2	LPC (20:2)	LysoPC 20:2	[M+Ac-H]-	1.896	606.38
Set -8	Lysophosphatidylcholine	UCD.Lipid.376	LPC 20:3	LPC (20:3)	LysoPC 20:3	[M+Ac-H]-	1.505	604.36
Set -8	Lysophosphatidylcholine	UCD.Lipid.377	LPC 22:5	LPC (22:5)	LysoPC 22:5	[M+Ac-H]-	1.388	628.36
Set -8	Lysophosphatidylethanolamine	UCD.Lipid.378	LPE 16:0	LPE (16:0)	LysoPE 16:0	[M-H]-	1.596	452.28
Set -8	Lysophosphatidylethanolamine	UCD.Lipid.379	LPE 18:2	LPE (18:2)	LysoPE 18:2	[M-H]-	1.347	476.28
Set -9	Phosphatidylcholine	UCD.Lipid.132	PC 27:0-CHO	PC (16:0/9:0(CHO))	PC (16:0_9:0(CHO))	[M+H]+	2.374	650.4391
Set -9	Triacylglycerol	UCD.Lipid.176	TG 42:1	TG (42:1)	TG(12:0_12:0_18:1)	[M+Na]+	8.967	743.6162
Set -9	Fatty acid	UCD.Lipid.493	FA 11:0	FA (11:0)	FA (11:0)	[M-H]-	0.82	185.15
Set -9	Fatty acid	UCD.Lipid.494	FA 12:0	FA (12:0)	FA (12:0)	[M-H]-	1.06	199.17
Set -9	Fatty acid	UCD.Lipid.495	FA 13:0	FA (13:0)	FA (13:0)	[M-H]-	1.3	213.19
Set -9	Fatty acid	UCD.Lipid.496	FA 14:0	FA (14:0)	FA (14:0)	[M-H]-	1.63	227.2
Set -9	Fatty acid	UCD.Lipid.498	FA 15:0	FA (15:0)	FA (15:0)	[M-H]-	2.02	241.22
Set -9	Fatty acid	UCD.Lipid.499	FA 15:1	FA (15:1)	FA (15:1)	[M-H]-	1.5	239.2
Set -9	Fatty acid	UCD.Lipid.500	FA 16:0	FA (16:0)	FA (16:0)	[M-H]-	2.47	255.23
Set -9	Fatty acid	UCD.Lipid.502	FA 17:0	FA (17:0)	FA (17:0)	[M-H]-	2.96	269.25
Set -9	Fatty acid	UCD.Lipid.504	FA 18:0	FA (18:0)	FA (18:0)	[M-H]-	3.26	283.26

Set -9	Fatty acid	UCD.Lipi d.508	FA 20:0	FA (20:0)	FA (20:0)	[M-H]-	3.8 5	311.3
Set -9	Fatty acid	UCD.Lipi d.514	FA 22:0	FA (22:0)	FA (22:0)	[M-H]-	4.5	339.3 3
Set -9	Fatty acid	UCD.Lipi d.518	FA 24:0	FA (24:0)	FA (24:0)	[M-H]-	5.2 3	367.3 6
Set -9	Fatty acid	UCD.Lipi d.520	FA 26:0	FA (26:0)	FA (26:0)	[M-H]-	6.0 2	395.3 9
Set -9	Fatty acid	UCD.Lipi d.521	FA 28:0	FA (28:0)	FA (28:0)	[M-H]-	6.8 2	423.4 2
Set -10	Sphingomyelin	UCD.Lipi d.171	SM d40:2	SM (d40:2)		[M+H] +	6.0 38	785.6 531
Set -10	Phosphatidylinositol	UCD.Lipi d.461	PI 38:5	PI (38:5)	PI(18:1_20:4)	[M-H]-	4.1 42	883.5 3
Set -10	Sphingomyelin	UCD.Lipi d.468	SM d34:2	SM (d34:2)	SM(d18:2_16:0)	[M+Ac -H]-	4.3 59	759.5 7
Set -10	Sphingomyelin	UCD.Lipi d.471	SM d36:2	SM (d36:2)		[M+Ac -H]-	4.9 74	787.6
Set -10	Sphingomyelin	UCD.Lipi d.472	SM d36:3	SM (d36:3)		[M+Ac -H]-	4.5 08	785.5 8
Set -10	Sphingomyelin	UCD.Lipi d.476	SM d38:2	SM (d38:2)		[M+Ac -H]-	5.6 23	815.6 3
Set -10	Sphingomyelin	UCD.Lipi d.478	SM d39:2	SM (d39:2)		[M+Ac -H]-	5.9 88	829.6 4
Set -10	Sphingomyelin	UCD.Lipi d.479	SM d40:0	SM (d40:0)		[M+Ac -H]-	7.1 38	847.6 9
Set -10	Sphingomyelin	UCD.Lipi d.480	SM d40:1	SM (d40:1)	SM(d18:1_22:0)	[M+Ac -H]-	6.8 88	845.6 7
Set -10	Sphingomyelin	UCD.Lipi d.481	SM d40:2 A	SM (d40:2) A		[M+Ac -H]-	6.2 05	843.6 6
Set -10	Sphingomyelin	UCD.Lipi d.482	SM d40:2 B	SM (d40:2) B	SM(d18:2_22:0)	[M+Ac -H]-	6.3 06	843.6 6
Set -10	Sphingomyelin	UCD.Lipi d.483	SM d40:3	SM (d40:3)		[M+Ac -H]-	5.6 4	841.6 4
Set -10	Sphingomyelin	UCD.Lipi d.484	SM d41:1	SM (d41:1)	SM(d18:1_23:0)	[M+Ac -H]-	7.2 29	859.6 9
Set -10	Sphingomyelin	UCD.Lipi d.485	SM d41:2	SM (d41:2)	SM(d18:2_23:0)	[M+Ac -H]-	6.6 5	857.6 7
Set -10	Sphingomyelin	UCD.Lipi d.486	SM d42:0	SM (d42:0)		[M+Ac -H]-	7.7 94	875.7 2
Set -10	Sphingomyelin	UCD.Lipi d.487	SM d42:1	SM (d42:1)	SM(d18:1_24:0)	[M+Ac -H]-	7.5 62	873.7 1
Set -11	Glactoylceramide	UCD.Lipi d.117	LacCer d34:1	Gal-Gal-Cer(d18:1/16:0) or Lactosylceramide(d18:1/16:0)		[M+H] +	4.7 95	862.6 25
Set -11	Lactosylceramide	UCD.Lipi d.118	LacCer d32:2	Lactosylceramide (d18:1/24:1(15Z))		[M+H] +	6.6 85	972.7 346
Set -11	Cholesteryl ester	UCD.Lipi d.12	CE 18:2	CE (18:2)	18:2 Cholesteryl ester	[M+N H4]+	10. 4	666.6 184
Set -11	Phosphatidylcholine	UCD.Lipi d.155	PC o-34:0	PC (o-34:0)		[M+H] +	6.4 78	748.6 204
Set -11	Phosphatidylcholine	UCD.Lipi d.156	PC p-32:1	PC (p-32:1) or PC (o-32:2)		[M+H] +	4.9 1	716.5 626
Set -11	Phosphatidylcholine	UCD.Lipi d.157	PC p-34:1	PC (p-34:1) or PC (o-34:2) B	PC(P-16:0_18:1)	[M+H] +	5.7 9	744.5 908
Set -11	Phosphatidylcholine	UCD.Lipi d.160	PC p-40:1	PC (p-40:1) or PC (o-40:2)		[M+H] +	6.6 37	828.6 842
Set -11	Sphingomyelin	UCD.Lipi d.170	SM d34:0	SM (d34:0)		[M+H] +	4.9 6	705.5 905
Set -11	Glucosylceramide	UCD.Lipi d.363	GlcCer d38:1	GlcCer (d38:1)		[M+Ac -H]-	6.4 89	814.6 4
Set -11	Glucosylceramide	UCD.Lipi d.364	GlcCer d40:1	GlcCer (d40:1)	GlcCer[NS](d18:1_22:0)	[M+Ac -H]-	7.1 63	842.6 7
Set -11	Glucosylceramide	UCD.Lipi d.365	GlcCer d41:1	GlcCer (d41:1)		[M+Ac -H]-	7.4 95	856.6 9
Set -11	Glucosylceramide	UCD.Lipi d.366	GlcCer d42:1	GlcCer (d42:1)	GlcCer[NS](d18:1_24:0)	[M+Ac -H]-	7.8 2	870.7

Set -11	Glucosylceramide	UCD.Lipi d.367	GlcCer d42:2	GlcCer (d42:2)	GlcCer[NS](d18:1_24:1)	[M+Ac -H]-	7.1 38	868.6 9
Set -11	Phosphatidylcholine	UCD.Lipi d.412	PC o-32:0	PC (o-32:0)		[M+Ac -H]-	5.9 73	778.5 9
Set -11	Phosphatidylcholine	UCD.Lipi d.414	PC p-34:0	PC (p-34:0) or PC (o-34:1)	PC(P-18:0_16:0)	[M+Ac -H]-	6.0 39	804.6 1
Set -11	Sphingomyelin	UCD.Lipi d.467	SM d34:1	SM (d34:1)	SM(d18:1_16:0)	[M+Ac -H]-	4.8 66	761.5 8
Set -12	Diacylglycerol	UCD.Lipi d.111	DG 36:4	DG (36:4)	DG(18:2_18:2)	[M+N H4]+	5.8 15	634.5 404
Set -12	Diacylglycerol	UCD.Lipi d.112	DG 36:5	DG (36:5)	DG(18:2_18:3)	[M+N H4]+	5.6 5	632.5 248
Set -12	Triacylglycerol	UCD.Lipi d.206	TG 51:4	TG (51:4)	TG(15:0_18:2_18:2)	[M+Na]+	9.8 77	863.7 099
Set -12	Triacylglycerol	UCD.Lipi d.207	TG 51:5	TG (51:5)	TG(15:0_18:2_18:3)	[M+N H4]+	9.7 7	856.7 347
Set -12	Triacylglycerol	UCD.Lipi d.212	TG 52:4	TG (52:4)	TG(16:1_18:1_18:2)	[M+N H4]+	10. 1	872.7 702
Set -12	Triacylglycerol	UCD.Lipi d.213	TG 52:5	TG (52:5)	TG(16:0_18:2_18:3)	[M+N H4]+	9.7 28	870.7 545
Set -12	Triacylglycerol	UCD.Lipi d.214	TG 52:6	TG (52:6)	TG(16:1_18:2_18:3)	[M+Na]+	9.3 5	873.6 943
Set -12	Triacylglycerol	UCD.Lipi d.218	TG 53:4	TG (53:4)	TG(17:1_18:1_18:2)	[M+N H4]+	10. 32	886.7 858
Set -12	Triacylglycerol	UCD.Lipi d.219	TG 53:5	TG (53:5)	TG(17:1_18:2_18:2)	[M+N H4]+	9.9 02	884.7 702
Set -12	Triacylglycerol	UCD.Lipi d.223	TG 54:3	TG (54:3)	TG(18:0_18:1_18:2)	[M+N H4]+	10. 86	902.8 171
Set -12	Triacylglycerol	UCD.Lipi d.224	TG 54:4	TG (54:4)	TG(18:1_18:1_18:2)	[M+N H4]+	10. 49	900.8 015
Set -12	Triacylglycerol	UCD.Lipi d.225	TG 54:5	TG (54:5)	TG(18:1_18:2_18:2)	[M+Na]+	10. 12	903.7 412
Set -12	Triacylglycerol	UCD.Lipi d.226	TG 54:6	TG (54:6)	TG(18:1_18:2_18:3)	[M+Na]+	9.7 45	901.7 256
Set -12	Triacylglycerol	UCD.Lipi d.227	TG 54:8	TG (54:8)	TG(18:2_18:3_18:3)	[M+Na]+	8.9 4	897.6 943
Set -13	Triacylglycerol	UCD.Lipi d.228	TG 56:1	TG (56:1)	TG(18:0_18:1_20:0)	[M+N H4]+	11. 85	934.8 797
Set -13	Triacylglycerol	UCD.Lipi d.237	TG 57:1	TG (57:1)		[M+N H4]+	12	948.8 863
Set -13	Triacylglycerol	UCD.Lipi d.238	TG 57:2	TG (57:2)		[M+N H4]+	11. 88	946.8 718
Set -13	Triacylglycerol	UCD.Lipi d.239	TG 58:1	TG (58:1)	TG(18:0_18:1_22:0)	[M+N H4]+	11. 99	962.9 11
Set -13	Triacylglycerol	UCD.Lipi d.241	TG 58:2	TG (58:2)	TG(18:1_18:1_22:0)	[M+N H4]+	11. 85	960.8 954
Set -13	Triacylglycerol	UCD.Lipi d.242	TG 58:3	TG (58:3)	TG(18:1_20:1_20:1)	[M+N H4]+	11. 6	958.8 797
Set -13	Triacylglycerol	UCD.Lipi d.247	TG 59:2	TG (59:2)		[M+N H4]+	12	974.9 031
Set -13	Triacylglycerol	UCD.Lipi d.248	TG 59:3	TG (59:3)		[M+N H4]+	11. 89	972.8 871
Set -13	Triacylglycerol	UCD.Lipi d.250	TG 60:2	TG (60:2)	TG(18:1_20:1_22:0)	[M+N H4]+	11. 99	988.9 267
Set -13	Triacylglycerol	UCD.Lipi d.251	TG 60:3	TG (60:3)	TG(18:1_20:1_22:1)	[M+N H4]+	11. 95	986.9 034
Set -13	Triacylglycerol	UCD.Lipi d.252	TG 60:4	TG (60:4)	TG(18:1_20:2_22:1)	[M+N H4]+	11. 78	984.8 877
Set -13	Triacylglycerol	UCD.Lipi d.254	TG 62:3	TG (62:3)		[M+N H4]+	12. 04	1014. 934
Set -13	Triacylglycerol	UCD.Lipi d.255	TG 62:4	TG (62:4)		[M+N H4]+	11. 94	1012. 918
Set -13	Triacylglycerol	UCD.Lipi d.256	TG 64:4	TG (64:4)		[M+N H4]+	12. 04	1040. 949
Set -14	Ceramide	UCD.Lipi d.18	Cer d41:1	Ceramide (d18:1/23:0)	Cer[NS](d18:1_23:0)	[M+H]+	7.9 63	636.6 289
Set -14	Ceramide	UCD.Lipi d.263	Cer d38:1	Ceramide (d38:1)	Cer[NS](d18:1_20:0)	[M+Cl]-	7.1 63	628.5 4

Set -14	Ceramide	UCD.Lipi d.264	Cer d39:1	Ceramide (d39:1)	Cer[NS](d18:1_22:0)	[M+Cl] -	7.5 12	642.5 6
Set -14	Ceramide	UCD.Lipi d.265	Cer d40:0	Ceramide (d40:0)	Cer[NDS](d18:0_22:0)	[M+Ac -H]-	8.0 61	682.6 3
Set -14	Ceramide	UCD.Lipi d.266	Cer d40:1	Ceramide (d40:1)	Cer[NS](d18:1_22:0)	[M+Cl] -	7.8 36	656.5 8
Set -14	Ceramide	UCD.Lipi d.267	Cer d40:2	Ceramide (d40:2)	Cer[NS](d18:2_22:0)	[M+Cl] -	7.1 85	654.5 6
Set -14	Ceramide	UCD.Lipi d.268	Cer d41:1	Ceramide (d41:1)	Cer[NS](d18:1_23:0)	[M+Cl] -	8.1 61	670.5 9
Set -14	Ceramide	UCD.Lipi d.269	Cer d42:0	Ceramide (d42:0)	Cer[NDS](d18:0_24:0)	[M+Cl] -	8.6 85	686.6 2
Set -14	Ceramide	UCD.Lipi d.270	Cer d42:1	Ceramide (d42:1)	Cer[NS](d18:1_24:0)	[M+Ac -H]-	8.4 69	708.6 5
Set -14	Ceramide	UCD.Lipi d.271	Cer d42:2 A	Ceramide (d42:2) A	Cer[NS](d18:1_24:1)	[M+Cl] -	NA	NA
Set -14	Ceramide	UCD.Lipi d.273	Cer d44:1	Ceramide (d44:1)		[M+Cl] -	9.0 68	712.6 4
Set -15	Phosphatidylcholine	UCD.Lipi d.159	PC p-38:4	PC (p-38:4) or PC (o-38:5) B	PC(P-18:0_20:4)	[M+H] +	5.8 23	794.6 054
Set -15	Phosphatidylethanolamine	UCD.Lipi d.167	PE 38:4	PE (38:4)	PE(18:0_20:4)	[M+H] +	5.7 23	768.5 56
Set -15	Phosphatidylcholine	UCD.Lipi d.413	PC p-32:0	PC (p-32:0) or PC (o-32:1)	PC(P-16:0_16:0)	[M+Ac -H]-	5.8 81	776.5 8
Set -15	Phosphatidylcholine	UCD.Lipi d.415	PC p-34:1	PC (p-34:1) or PC (o-34:2) A	PC(P-16:0_18:1)	[M+Ac -H]-	5.5 4	802.6
Set -15	Phosphatidylcholine	UCD.Lipi d.416	PC p-34:2	PC (p-34:2) or PC (o-34:3)	PC(P-16:0_18:2)	[M+Ac -H]-	5.4 4	800.5 8
Set -15	Phosphatidylcholine	UCD.Lipi d.417	PC p-36:1	PC (p-36:1) or PC (o-36:2)	PC(P-18:0_18:1)	[M+Ac -H]-	6.2	830.6 3
Set -15	Phosphatidylcholine	UCD.Lipi d.418	PC p-36:2	PC (p-36:2) or PC (o-36:3)	PC(P-18:0_18:2)	[M+Ac -H]-	5.5 9	828.6 1
Set -15	Phosphatidylcholine	UCD.Lipi d.419	PC p-36:3	PC (p-36:3) or PC (o-36:4)	PC(P-16:0_20:3)	[M+Ac -H]-	5.4 4	826.6
Set -15	Phosphatidylcholine	UCD.Lipi d.420	PC p-36:4	PC (p-36:4) or PC (o-36:5)	PC(P-16:0_20:4)	[M+Ac -H]-	5.3 32	824.5 8
Set -15	Phosphatidylcholine	UCD.Lipi d.422	PC p-38:4	PC (p-38:4) or PC (o-38:5) A	PC(P-18:0_20:4)	[M+Ac -H]-	5.4 82	852.6 1
Set -15	Phosphatidylcholine	UCD.Lipi d.423	PC p-38:5	PC (p-38:5) or PC (o-38:6)	PC(P-18:0_20:5)	[M+Ac -H]-	5.2 57	850.6
Set -16	Acylcarnitine	UCD.Lipi d.1	AC C8:0	Acylcarnitine C8:0	Acylcarnitine 8:0	[M+H] +	0.5 5	288.2 169
Set -16	Acylcarnitine	UCD.Lipi d.2	AC C8:1	Acylcarnitine C8:1	Acylcarnitine 8:1	[M+H] +	0.5 2	286.2 013
Set -16	Cholesterol	UCD.Lipi d.20	Cholesterol	Cholesterol		[M- H2O+ H]+	4.8 61	369.3 516
Set -16	Acylcarnitine	UCD.Lipi d.3	AC C10:1	Acylcarnitine C10:1	Acylcarnitine 10:1	[M+H] +	0.5 9	314.2 326
Set -16	Acylcarnitine	UCD.Lipi d.4	AC C12:0	Acylcarnitine C12:0	Acylcarnitine 12:0	[M+H] +	0.7 4	344.2 801
Set -16	Acylcarnitine	UCD.Lipi d.5	AC C16:0	Acylcarnitine C16:0	Acylcarnitine 16:0	[M+H] +	1.5 86	400.3 42
Set -16	Fatty acid	UCD.Lipi d.519	FA 24:1	FA (24:1)	FA (24:1)	[M- H]-	4.5 2	365.3 4
Set -16	Acylcarnitine	UCD.Lipi d.6	AC C18:0	Acylcarnitine C18:0	Acylcarnitine 18:0	[M+H] +	2.3 4	428.3 727
Set -16	Acylcarnitine	UCD.Lipi d.7	AC C18:1	Acylcarnitine C18:1	Acylcarnitine 18:1	[M+H] +	1.7 43	426.3 578
Set -16	Acylcarnitine	UCD.Lipi d.8	AC C18:2	Acylcarnitine C18:2	Acylcarnitine 18:2	[M+H] +	1.3 29	424.3 425
Set -17	Fatty acid	UCD.Lipi d.497	FA 14:1	FA (14:1)	FA (14:1)	[M- H]-	1.2	225.1 9
Set -17	Fatty acid	UCD.Lipi d.501	FA 16:1	FA (16:1)	FA (16:1)	[M- H]-	1.8 2	253.2 2
Set -17	Fatty acid	UCD.Lipi d.503	FA 17:1	FA (17:1)	FA (17:1)	[M- H]-	2.2 2	267.2 3

Set -17	Fatty acid	UCD.Lipi d.505	FA 18:1	FA (18:1)	FA (18:1)	[M-H] ₋	2.7	281.25
Set -17	Fatty acid	UCD.Lipi d.506	FA 18:2	FA (18:2)	FA (18:2)	[M-H] ₋	2.05	279.23
Set -17	Fatty acid	UCD.Lipi d.507	FA 18:3	FA (18:3)	FA (18:3)	[M-H] ₋	1.623	277.22
Set -17	Fatty acid	UCD.Lipi d.509	FA 20:1	FA (20:1)	FA (20:1)	[M-H] ₋	3.35	309.28
Set -17	Fatty acid	UCD.Lipi d.510	FA 20:2	FA (20:2)	FA (20:2)	[M-H] ₋	2.91	307.26
Set -17	Fatty acid	UCD.Lipi d.516	FA 22:2	FA (22:2)	FA (22:2)	[M-H] ₋	3.47	335.3
Set -18	Diacylglycerol	UCD.Lipi d.115	DG 38:5	DG (38:5)	DG(18:1_20:4)	[M+N H4] ₊	6.246	660.5562
Set -18	Triacylglycerol	UCD.Lipi d.222	TG 54:2	TG (54:2)	TG(18:0_18:1_18:1)	[M+N H4] ₊	11.22	904.8328
Set -18	Triacylglycerol	UCD.Lipi d.230	TG 56:3	TG (56:3)	TG(18:0_18:1_20:2)	[M+N H4] ₊	11.22	930.8484
Set -18	Triacylglycerol	UCD.Lipi d.231	TG 56:4	TG (56:4)	TG(18:0_18:1_20:3)	[M+N H4] ₊	10.9	928.8328
Set -18	Triacylglycerol	UCD.Lipi d.232	TG 56:5	TG (56:5)	TG(18:0_18:1_20:4)	[M+N H4] ₊	10.78	926.8171
Set -18	Triacylglycerol	UCD.Lipi d.233	TG 56:6	TG (56:6)	TG(18:1_18:1_20:4)	[M+N H4] ₊	10.34	924.8015
Set -18	Triacylglycerol	UCD.Lipi d.234	TG 56:7	TG (56:7)	TG(18:1_18:2_20:4)	[M+N H4] ₊	9.968	922.7858
Set -18	Triacylglycerol	UCD.Lipi d.243	TG 58:4	TG (58:4)	TG(18:1_18:2_22:1)	[M+N H4] ₊	11.25	956.8641
Set -18	Triacylglycerol	UCD.Lipi d.244	TG 58:6	TG (58:6)	TG(18:0_18:1_22:5)	[M+N H4] ₊	10.67	952.8328
Set -19	Phosphatidylcholine	UCD.Lipi d.147	PC 38:5 B	PC (38:5) B	PC(16:0_22:5)	[M+H] ₊	5.168	808.5848
Set -19	Phosphatidylcholine	UCD.Lipi d.151	PC 40:5 B	PC (40:5) B	PC(18:0_22:5)	[M+H] ₊	5.806	836.6164
Set -19	Phosphatidylcholine	UCD.Lipi d.152	PC 40:6 A	PC (40:6) A	PC(18:0_22:6)	[M+H] ₊	5.151	834.6007
Set -19	Phosphatidylcholine	UCD.Lipi d.153	PC 42:5	PC (42:5)		[M+H] ₊	6.072	864.645
Set -19	Phosphatidylcholine	UCD.Lipi d.154	PC 42:6	PC (42:6)		[M+H] ₊	5.773	862.6311
Set -19	Phosphatidylcholine	UCD.Lipi d.405	PC 38:5 A	PC (38:5) A	PC(18:1_20:4)	[M+Ac -H] ₋	5.107	866.59
Set -19	Phosphatidylcholine	UCD.Lipi d.408	PC 40:5 A	PC (40:5) A	PC(18:0_22:5)	[M+Ac -H] ₋	5.74	894.62
Set -19	Phosphatidylcholine	UCD.Lipi d.411	PC 40:8	PC (40:8)	PC(18:2_22:6)	[M+Ac -H] ₋	4.533	888.58
Set -19	Phosphatidylinositol	UCD.Lipi d.460	PI 38:4	PI (38:4)	PI(18:0_20:4)	[M-H] ₋	4.606	885.55
Set -20	Phosphatidylcholine	UCD.Lipi d.158	PC p-38:2	PC (p-38:2) or PC (o-38:3)		[M+H] ₊	6.212	798.6359
Set -20	Phosphatidylcholine	UCD.Lipi d.165	PC p-42:3	PC (p-42:3) or PC (o-42:4)		[M+H] ₊	7.224	852.6859
Set -20	Phosphatidylcholine	UCD.Lipi d.421	PC p-38:3	PC (p-38:3) or PC (o-38:4)	PC(P-18:0_20:3)	[M+Ac -H] ₋	6.098	854.63
Set -20	Phosphatidylcholine	UCD.Lipi d.424	PC p-40:3	PC (p-40:3) or PC (o-40:4)		[M+Ac -H] ₋	6.763	882.66
Set -20	Phosphatidylcholine	UCD.Lipi d.425	PC p-40:4	PC (p-40:4) or PC (o-40:5)	PC(P-20:0_20:4)	[M+Ac -H] ₋	6.106	880.64
Set -20	Phosphatidylcholine	UCD.Lipi d.426	PC p-42:4	PC (p-42:4) or PC (o-42:5)	PC(P-22:0_20:4)	[M+Ac -H] ₋	6.747	908.67
Set -20	Phosphatidylcholine	UCD.Lipi d.427	PC p-42:5	PC (p-42:5) or PC (o-42:6)		[M+Ac -H] ₋	6.188	906.66
Set -20	Phosphatidylcholine	UCD.Lipi d.428	PC p-44:4	PC (p-44:4) or PC (o-44:5)		[M+Ac -H] ₋	7.387	936.71
Set -21	Lysophosphatidylcholine	UCD.Lipi d.125	LPC 20:4	LPC (20:4)	LysoPC 20:4	[M+H] ₊	1.205	544.3403
Set -21	Phosphatidylcholine	UCD.Lipi d.146	PC 38:4 B	PC (38:4) B		[M+H] ₊	6.146	810.6004

Set -21	Lysophosphatidylet hanolamine	UCD.Lipi d.380	LPE 20:4	LPE (20:4)	LysoPE 20:4	[M-H]-	1.3 13	500.2 8
Set -21	Phosphatidylcholine	UCD.Lipi d.394	PC 35:4	PC (35:4)	PC(15:0_20:4)	[M+Ac-H]-	4.7 65	826.5 6
Set -21	Phosphatidylcholine	UCD.Lipi d.398	PC 36:4 B	PC (36:4) B	PC(16:0_20:4)	[M+Ac-H]-	5.0 74	840.5 8
Set -21	Phosphatidylcholine	UCD.Lipi d.401	PC 37:4	PC (37:4)	PC(17:0_20:4)	[M+Ac-H]-	5.3 9	854.5 9
Set -21	Phosphatidylcholine	UCD.Lipi d.404	PC 38:4 A	PC (38:4) A	PC(18:0_20:4)	[M+Ac-H]-	5.7 06	868.6 1
Set -21	Phosphatidylcholine	UCD.Lipi d.407	PC 40:4	PC (40:4)	PC(18:0_22:4)	[M+Ac-H]-	6.1 72	896.6 4
Set -22	Phosphatidylethanol amine	UCD.Lipi d.168	PE p-34:1	PE (p-34:1) or PE (o-34:2)	PE(16:0_18:1)	[M+H] +	6.1 6	702.5 404
Set -22	Phosphatidylethanol amine	UCD.Lipi d.438	PE p-34:2	PE (p-34:2) or PE (o-34:3)	PE(P-16:0_18:2)	[M-H]-	5.6 4	698.5 1
Set -22	Phosphatidylethanol amine	UCD.Lipi d.440	PE p-36:2	PE (p-36:2) or PE (o-36:3)	PE(P-18:0_18:2)	[M-H]-	6.3 14	726.5 4
Set -22	Phosphatidylethanol amine	UCD.Lipi d.441	PE p-36:4	PE (p-36:4) or PE (o-36:5)	PE(P-16:0_20:4)	[M-H]-	5.5 23	722.5 1
Set -22	Phosphatidylethanol amine	UCD.Lipi d.444	PE p-38:3	PE (p-38:3) or PE (o-38:4)		[M-H]-	6.4 8	752.5 6
Set -22	Phosphatidylethanol amine	UCD.Lipi d.445	PE p-38:4	PE (p-38:4) or PE (o-38:5)	PE(P-18:0_20:4)	[M-H]-	6.1 89	750.5 4
Set -22	Phosphatidylethanol amine	UCD.Lipi d.446	PE p-38:5	PE (p-38:5) or PE (o-38:6)	PE(P-18:0_20:5)	[M-H]-	5.5 82	748.5 3
Set -22	Phosphatidylethanol amine	UCD.Lipi d.449	PE p-40:5	PE (p-40:5) or PE (o-40:6)	PE(P-18:0_22:5)	[M-H]-	6.2 14	776.5 6
Set -23	Phosphatidylcholine	UCD.Lipi d.161	PC p-40:5	PC (p-40:5) or PC (o-40:6)		[M+H] +	5.7 4	820.6 215
Set -23	Phosphatidylcholine	UCD.Lipi d.162	PC p-40:6	PC (p-40:6) or PC (o-40:7) A		[M+H] +	5.1 6	818.6 058
Set -23	Phosphatidylcholine	UCD.Lipi d.163	PC p-40:6	PC (p-40:6) or PC (o-40:7) B		[M+H] +	5.6 25	818.6 058
Set -23	Phosphatidylcholine	UCD.Lipi d.164	PC p-40:7	PC (p-40:7) or PC (o-40:8)		[M+H] +	5.0 85	816.5 902
Set -23	Phosphatidylethanol amine	UCD.Lipi d.447	PE p-38:6	PE (p-38:6) or PE (o-38:7)	PE(16:0_22:6)	[M-H]-	5.3 4	746.5 1
Set -23	Phosphatidylethanol amine	UCD.Lipi d.450	PE p-40:6	PE (p-40:6) or PE (o-40:7)	PE(P-18:0_22:6)	[M-H]-	5.9 98	774.5 4
Set -23	Phosphatidylethanol amine	UCD.Lipi d.451	PE p-40:7	PE (p-40:7) or PE (o-40:8)	PE(P-18:1_22:6)	[M-H]-	5.4 07	772.5 3
Set -24	Phosphatidylethanol amine	UCD.Lipi d.166	PE 36:4	PE (36:4)	PE(16:0_20:4)	[M+H] +	5.2 5	740.5 184
Set -24	Phosphatidylcholine	UCD.Lipi d.429	PE 34:1	PE (34:1)	PE(16:0_18:1)	[M-H]-	5.8 31	716.5 2
Set -24	Phosphatidylethanol amine	UCD.Lipi d.430	PE 34:2	PE (34:2)	PE(16:0_18:2)	[M-H]-	5.3 32	714.5 1
Set -24	Phosphatidylethanol amine	UCD.Lipi d.432	PE 36:2	PE (36:2)	PE(18:0_18:2)	[M-H]-	5.9 89	742.5 4
Set -24	Phosphatidylethanol amine	UCD.Lipi d.433	PE 36:3	PE (36:3)	PE(18:1_18:2)	[M-H]-	5.3 99	740.5 2
Set -24	Phosphatidylethanol amine	UCD.Lipi d.435	PE 38:4 B	PE (38:4) B	PE(18:0_20:4)	[M-H]-	5.8 81	766.5 4
Set -24	Phosphatidylethanol amine	UCD.Lipi d.436	PE 38:6	PE (38:6)	PE(16:0_22:6)	[M-H]-	5.0 74	762.5 1
Set -25	Phosphatidylcholine	UCD.Lipi d.140	PC 35:3	PC (35:3)		[M+H] +	4.8 61	770.5 694
Set -25	Phosphatidylcholine	UCD.Lipi d.141	PC 36:3 B	PC (36:3) B	PC(18:1_18:2)	[M+H] +	5.1 84	784.5 848
Set -25	Phosphatidylcholine	UCD.Lipi d.144	PC 37:3	PC (37:3)		[M+H] +	5.4 25	798.6 004
Set -25	Phosphatidylcholine	UCD.Lipi d.397	PC 36:3 A	PC (36:3) A	PC(18:1_18:2)	[M+Ac-H]-	5.2 3	842.5 9
Set -25	Phosphatidylcholine	UCD.Lipi d.402	PC 38:2	PC (38:2)	PC(20:0_18:2)	[M+Ac-H]-	6.3 89	872.6 4
Set -25	Phosphatidylcholine	UCD.Lipi d.403	PC 38:3	PC (38:3)	PC(18:0_20:3)	[M+Ac-H]-	5.9 81	870.6 2

Set -25	Phosphatidylinositol	UCD.Lipi d.459	PI 38:3	PI (38:3)	PI(18:0_20:3)	[M-H] ⁻	4.9	887.57
Set -26	Triacylglycerol	UCD.Lipi d.235	TG 56:8	TG (56:8)	TG(18:1_18:2_20:5)	[M+Na] ⁺	9.769	925.7256
Set -26	Triacylglycerol	UCD.Lipi d.236	TG 56:9	TG (56:9)	TG(18:2_18:2_20:5)	[M+Na] ⁺	9.48	923.7057
Set -26	Triacylglycerol	UCD.Lipi d.240	TG 58:10	TG (58:10)	TG(18:2_18:2_22:6)	[M+Na] ⁺	9.396	949.7256
Set -26	Triacylglycerol	UCD.Lipi d.245	TG 58:8	TG (58:8)	TG(18:1_18:2_22:5)	[M+N H4] ⁺	10.17	948.8015
Set -26	Triacylglycerol	UCD.Lipi d.246	TG 58:9	TG (58:9)	TG(18:2_18:2_22:5)	[M+Na] ⁺	9.794	951.7412
Set -26	Triacylglycerol	UCD.Lipi d.249	TG 60:11	TG (60:11)		[M+N H4] ⁺	9.645	970.7859
Set -27	Sphingomyelin	UCD.Lipi d.172	SM d42:2	SM (d42:2)	SM(d18:1_24:1)	[M+H] ⁺	6.685	813.6873
Set -27	Sphingomyelin	UCD.Lipi d.488	SM d42:2 A	SM (d42:2) A	SM(d18:1_24:1)	[M+Ac-H] ⁻	6.863	871.69
Set -27	Sphingomyelin	UCD.Lipi d.489	SM d42:3	SM (d42:3)	SM(d18:2_24:1)	[M+Ac-H] ⁻	6.289	869.68
Set -27	Sphingomyelin	UCD.Lipi d.492	SM d44:2	SM (d44:2)		[M+Ac-H] ⁻	7.528	899.72
Set -28	Cholesteroyl ester	UCD.Lipi d.11	CE 18:1	CE (18:1)	18:1 Cholesteryl ester	[M+Na] ⁺	10.88	673.5894
Set -28	Cholesteroyl ester	UCD.Lipi d.13	CE 18:3	CE (18:3)	18:3 Cholesteryl ester	[M+Na] ⁺	9.985	669.5581
Set -28	Cholesteroyl ester	UCD.Lipi d.14	CE 20:3	CE (20:3)	20:3 Cholesteryl ester	[M+N H4] ⁺	10.49	692.634
Set -28	Cholesteroyl ester	UCD.Lipi d.15	CE 20:4	CE (20:4)	20:4 Cholesteryl ester	[M+Na] ⁺	10.16	695.5738

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