

	[M+H] ⁺ experimental	[M+H] ⁺ theoretical	Delta	RT, min	MS/MS fragments (Detected fragments are shown in bold)					
14:1_18:3 PC	726.5095	726.5074	0.0022	3.84	184.07	466.29	518.33	448.28	500.31	
14:1_18:2 PC	728.5222	728.5231	-0.0008	4.17	184.07	468.31	518.33	450.30	500.31	
14:0_18:2 PC	730.5400	730.5387	0.0014	4.49	184.07	466.29	520.34	448.28	502.32	
14:0_18:1 PC	732.5555	732.5543	0.0013	4.86	184.07	468.31	522.35	450.30	504.34	
15:0_18:3 PC	742.5394	742.5387	0.0008	4.43	184.07	482.32	518.33	464.31	500.31	
15:0_18:2 PC	744.5550	744.5543	0.0008	4.80	184.07	482.32	520.34	464.31	502.32	
15:0_18:1 PC	746.5714	746.5700	0.0015	5.14	184.07	482.32	522.35	464.31	504.35	
13:0_13:0 PC	650.4769	650.4761	0.0008	3.49	184.07	454.29	454.29	436.28	436.28	
34:5* PC	752.5252	752.5231	0.0022	3.96	184.07					
34:4 PC	754.5374	754.5387	-0.0012	4.31	184.07					
16:1_18:2	756.5557	756.5543	0.0014	4.72	184.07	494.32	520.34	476.31	502.32	
16:0_18:2	758.5701	758.5700	0.0002	5.07	184.07	496.34	520.34	478.32	502.32	
16:0_18:1 PC	760.5884	760.5856	0.0028	5.44	184.07	496.34	522.35	478.32	504.34	
35:4 PC	768.5555	768.5544	0.0012	4.59	184.07					
18:3_18:3 PC	778.5386	778.5387	0.0000	4.17	184.07	518.32	518.33	500.31	500.31	
18:2_18:3 PC	780.5543	780.5543	0.0000	4.52	184.07	520.34	518.33	502.32	500.31	
18:2_18:2 PC	782.5707	782.5700	0.0007	4.88	184.07	520.34	520.34	502.32	502.32	
18:1_18:2 PC	784.5854	784.5856	-0.0001	5.23	184.07	522.35	520.34	504.34	502.32	
18:0_18:2 PC	786.6010	786.6013	-0.0002	5.67	184.07	524.37	520.34	506.36	502.32	
18:0_18:1 PC	788.6149	788.6169	-0.0019	6.03	184.07	524.37	522.35	506.36	504.34	
37:4 PC	796.5864	796.5857	0.0008	5.02	184.07					
20:2_18:2 PC	810.6038	810.6013	0.0026	5.41	184.07	520.34	548.37	502.32	530.36	
38:3 PC	812.6195	812.6169	0.0027	5.78	184.07					
38:2 PC	814.6335	814.6326	0.0010	6.22	184.07					
19:0_19:0 PC	818.6642	818.6633	0.0009	6.87	184.07	538.39	538.39	520.37	520.37	
38:1 PC	816.6517	816.6482	0.0035	6.54	184.07					
40:3 PC	840.6457	840.6482	-0.0025	6.45	184.07					
40:2 PC	842.6653	842.6639	0.0015	6.75	184.07					
40:1 PC	844.6780	844.6796	-0.0015	7.04	184.07					
42:2 PC	870.6954	870.6952	0.0003	7.24	184.07					
42:1 PC	872.7139	872.7109	0.0031	7.51	184.07					
12:0_18:2 PE	660.4597	660.4604	-0.0007	4.02	519.44	142.03	257.21	337.27	183.17	263.24
15:0_15:0 PE	664.4940	664.4917	0.0023	4.83	523.4726	142.03	440.28	440.28	422.27	422.27
14:0_18:2 PE	688.4962	688.4917	0.0045	4.619	547.4726	142.03	285.24	337.27	211.21	263.24
14:0_18:1 PE	690.5040	690.5074	-0.0034	4.99	549.49	142.03	285.24	339.29	211.21	265.25
33:3 PE	700.4940	700.4934	0.0006	4.52	559.47	142.03	299.26	335.26	225.22	261.22
15:0_18:2 PE	702.4996	702.5074	-0.0078	4.91	561.49	142.03	299.26	337.27	225.22	263.24
34:4 PE	712.4954	712.4917	0.0037	4.41	571.47	142.03				
16:1_18:2 PE	714.5063	714.5074	-0.0011	4.81	573.49	142.03	311.26	337.27	237.22	263.24
16:0_18:2 PE	716.5256	716.5230	0.0026	5.20	575.50	142.03	313.27	337.27	239.24	263.24
16:0_18:1 PE	718.5395	718.5387	0.0008	5.57	577.52	142.03	313.27	339.29	239.24	265.25
18:3_18:3 PE	736.4929	736.5074	-0.0145	4.30	595.49	142.03	335.26	335.26		
18:2_18:3 PE	738.5099	738.5074	0.0025	4.65	597.49	142.03	337.27	335.26	263.24	261.22
18:2_18:2 PE	740.5245	740.5230	0.0015	4.99	599.50	142.03	337.27	337.27	263.24	263.24
18:1_18:2 PE	742.5401	742.5387	0.0014	5.35	601.52	142.03	337.27	339.29	263.24	265.25
36:2 PE	744.5543	744.5543	0.0000	5.77	603.54	142.03				

* For lipid species without detected fragments the number of carbon atoms and double bonds in the fatty acid side chains listed