Supporting Information

Integrated lipidomics and transcriptomics characterization upon aging related changes of bone marrow mesenchymal stem cells

Xin Lu[1,‡], Yue Chen[2,‡], Huiyu Wang[3], Yunfan Bai[2], Jianxiang Zhao[2], Xiaohan Zhang[2], Li Liang[1], Yang Chen[1], Chenfei Ye[1], Yiqun Li[2], Yi Zhang[4], Yu Li[2,*] and Ting Ma[1,*]

[*]Correspondence to:

Ting Ma

School of Electronic and Information Engineering, Harbin Institute of Technology, Shenzhen

HIT campus of University Town of Shenzhen, Shenzhen, 518055, China

Fax/Tel: (+86)-755-26033608

E-mail: tmahit@outlook.com

Yu Li

School of Life Science of Technology, Harbin Institute of Technology

No. 2, Yikuang Street, Harbin 150081, China

Fax/Tel: (+86)-451-86402690

E-mail: liyugene@hit.edu.cn

Affiliations:

[1]School of Electronic and Information Engineering, Harbin Institute of Technology, Shenzhen

[2]School of Life Science and Technology, Harbin Institute of Technology, Harbin, China

[3]School of Pharmacy, Qiqihar Medical University, Qiqihar, China

[4]Tian Qing Stem Cell Co. Ltd., Harbin, China

[‡]These authors contributed equally to this work.

Figure Legend

Figure S1. The expressions of surface antigens in p7-BMSCs

Figure S2. The typical MS/MS spectra of a portion of lipids identified

Figure S3. Metabolic trend plots of various categories of lipids in BMSCs of D1 and D2 during BMSC aging

Figure S4. HCA-heatmap diagram showing the metabolic similarities of lipidomics patterns between BMSCs from D1 and D2 during passaging

Figure S5. Univariate characterizations of alterations of lipid species between BMSCs of p7/p13 and p9/p11. (A) –log(*p*) values of lipids in Student t-test between BMSCs of p7/p13 and p9/p11. (B) The fold-change values of lipid species in BMSCs of p7/p13 relative to those of p9/p11

Figure S6. DVC plots of LyPCs, LyPEs, diacyl-PCs, diacyl-PEs, PC-Os and PE-Os showing fold-change alterations in BMSCs of p13 relative to those of p7

Figure S7. Fold-change values (p13 to p7) of TGs with CN of 54 and DBE of 2 compared with those at other coordinates. The data were represented as mean +/- SEM

Figure S8. Changing trends of PAs, PSs and PIs in subnet-a and subnet-b at sequential passages. The data were represented as mean +/- SEM.

Figure S9. Correlation networks constructed with SPs of different categories based on |Pearson CC| larger than 0.9.

Figure S10. Relative mRNA expressions of enzymes anchored in pathway analysis in p7- and p13-BMSCs. The data were represented as mean +/- SEM.

Table Legend

Table S1. Detailed methods and parameters for feature selection

Table S2. The primer sequences of genes anchored in pathway analysis

Table S3. The characterization information of lipid species identified in BMSC lipidomics profiles

Table S4. The enzymes in glycerophospholipid and sphingolipid metabolism pathways with mRNA significantly altered between p7- and p13-BMSCs

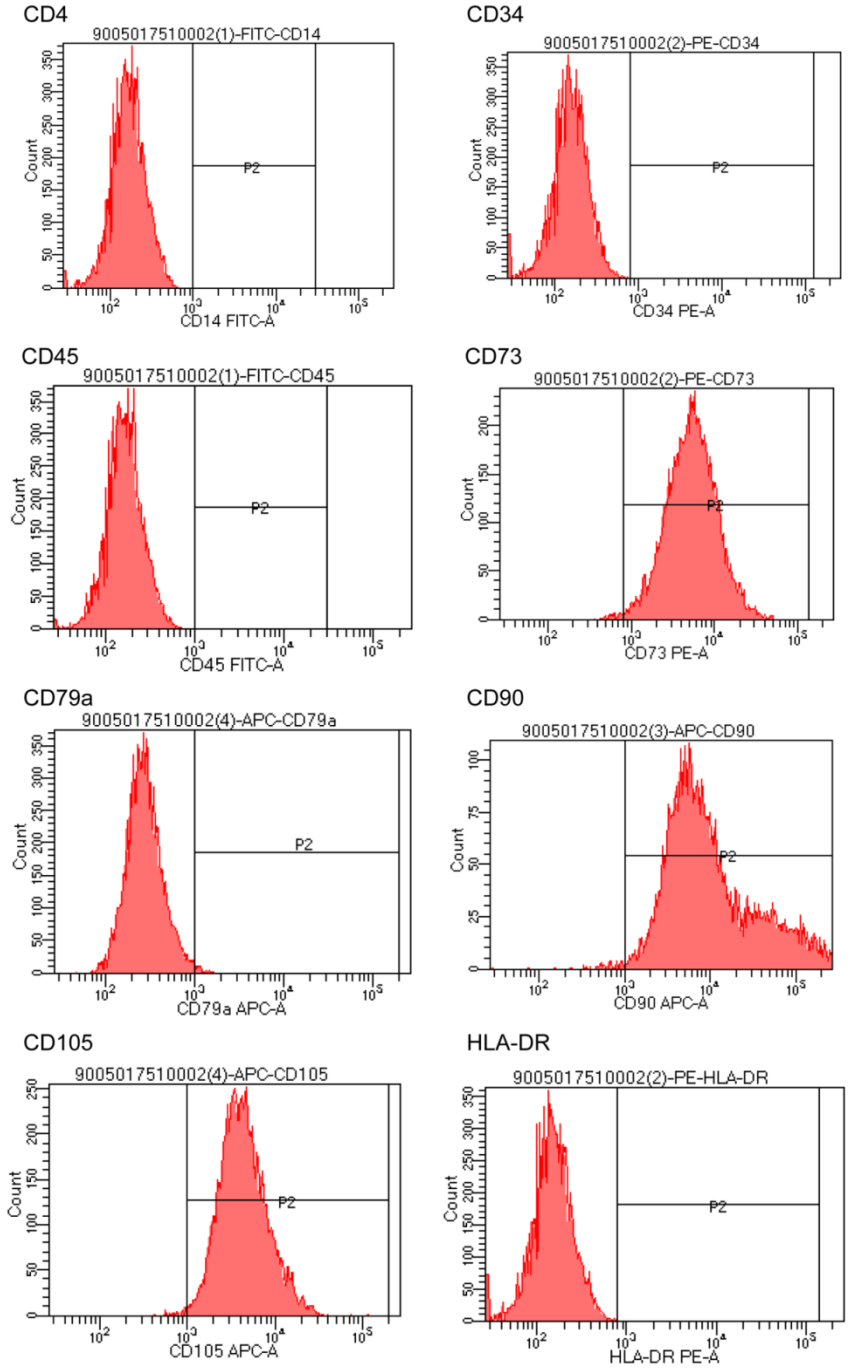
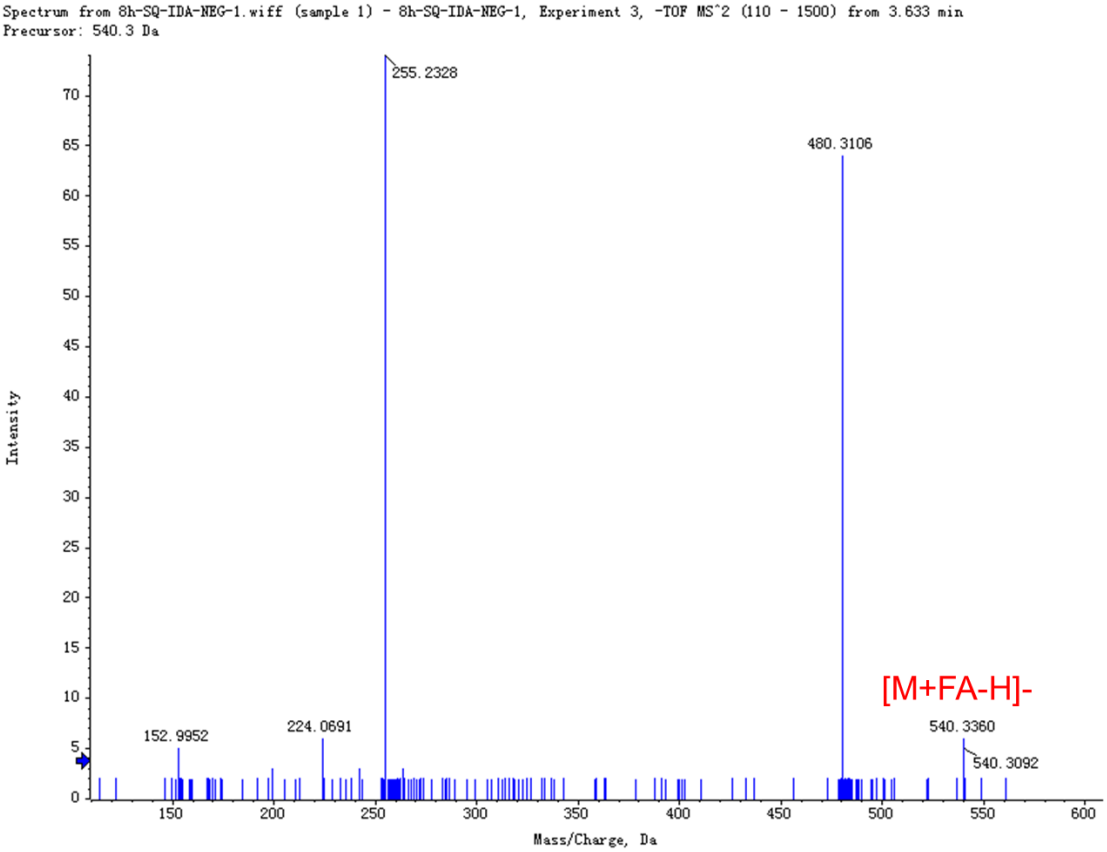
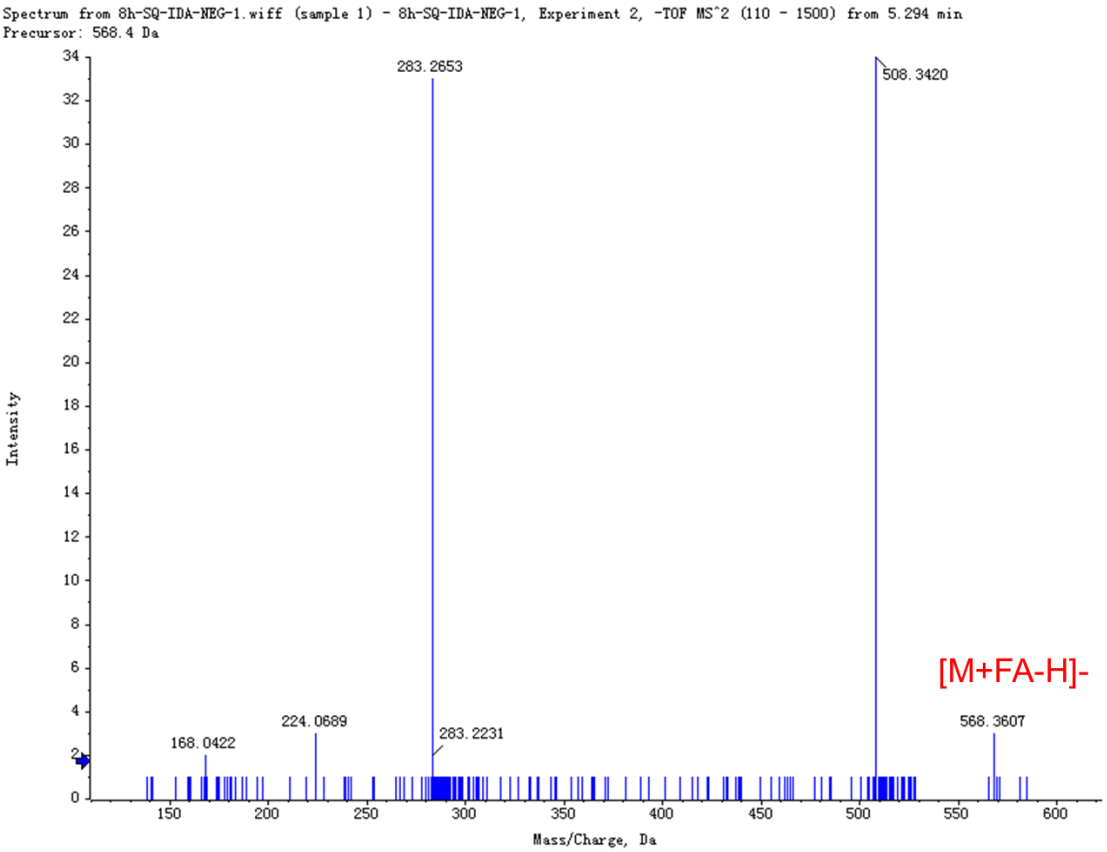


Figure S1. The expressions of surface antigens in p7-BMSCs

LyPC(16:0):

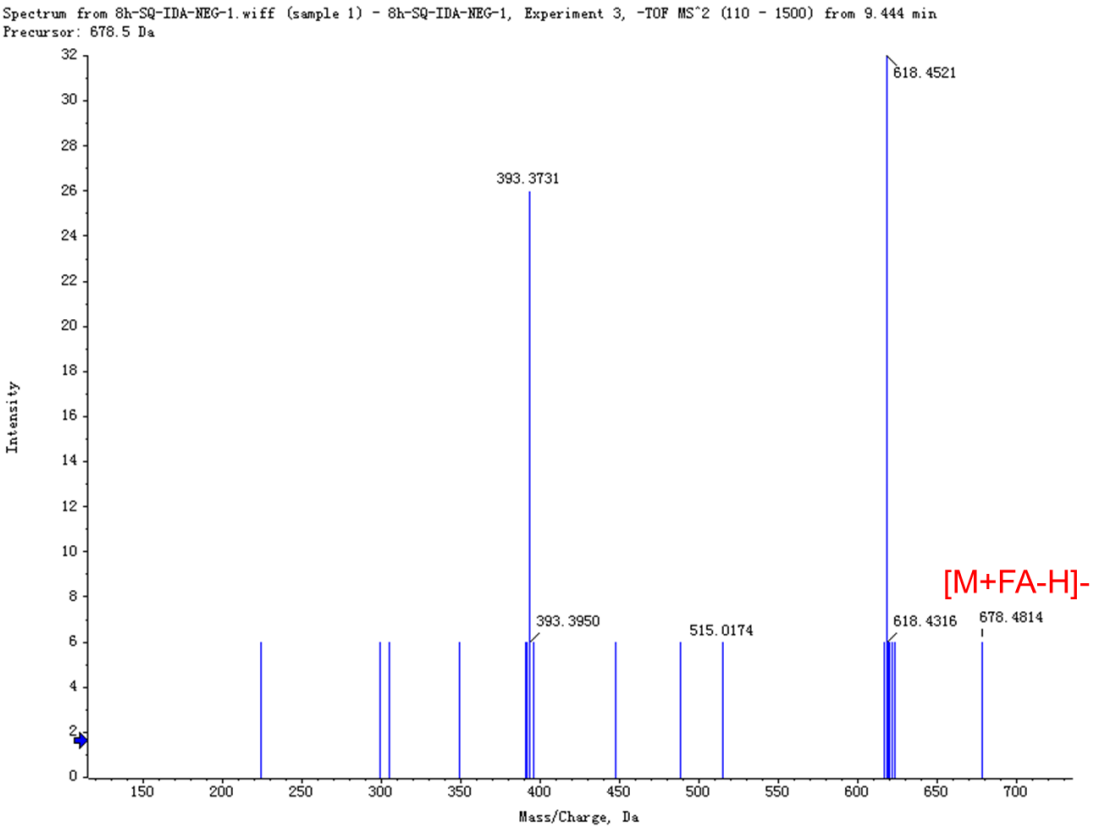


LyPC(18:0):



LyPC(18:1):

LyPC(26:1):



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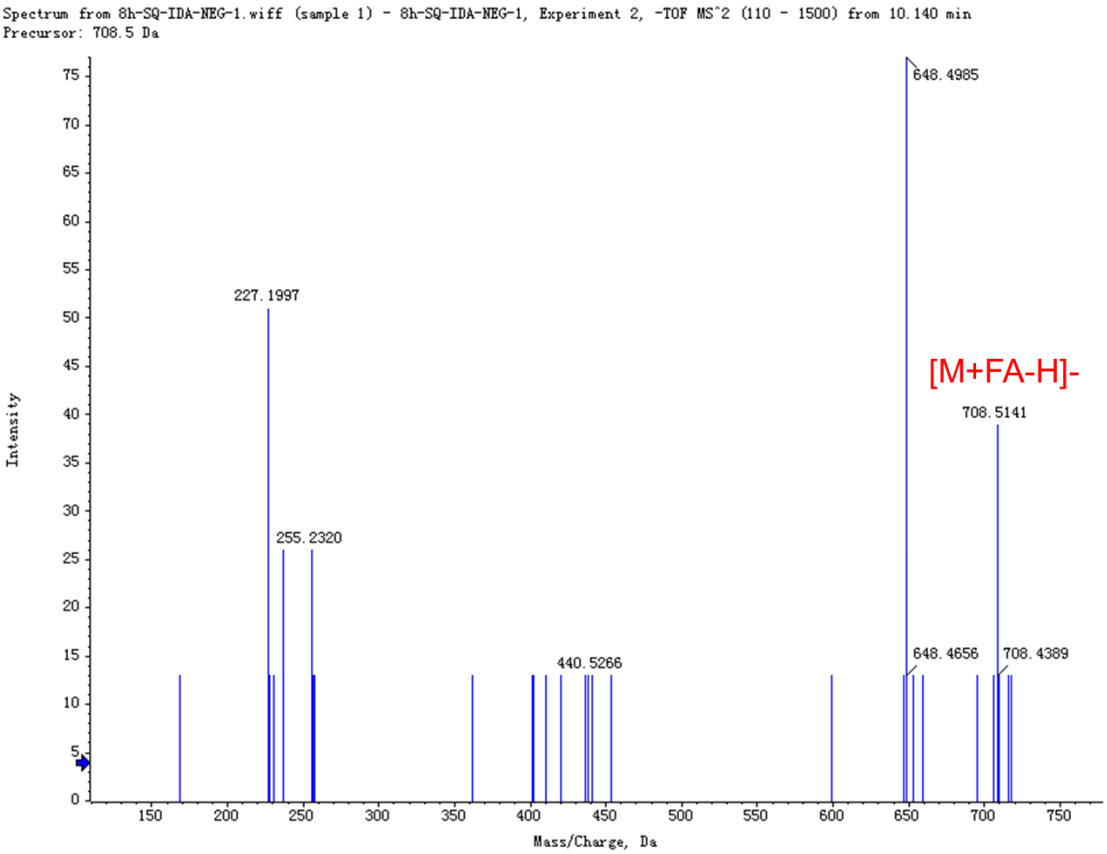

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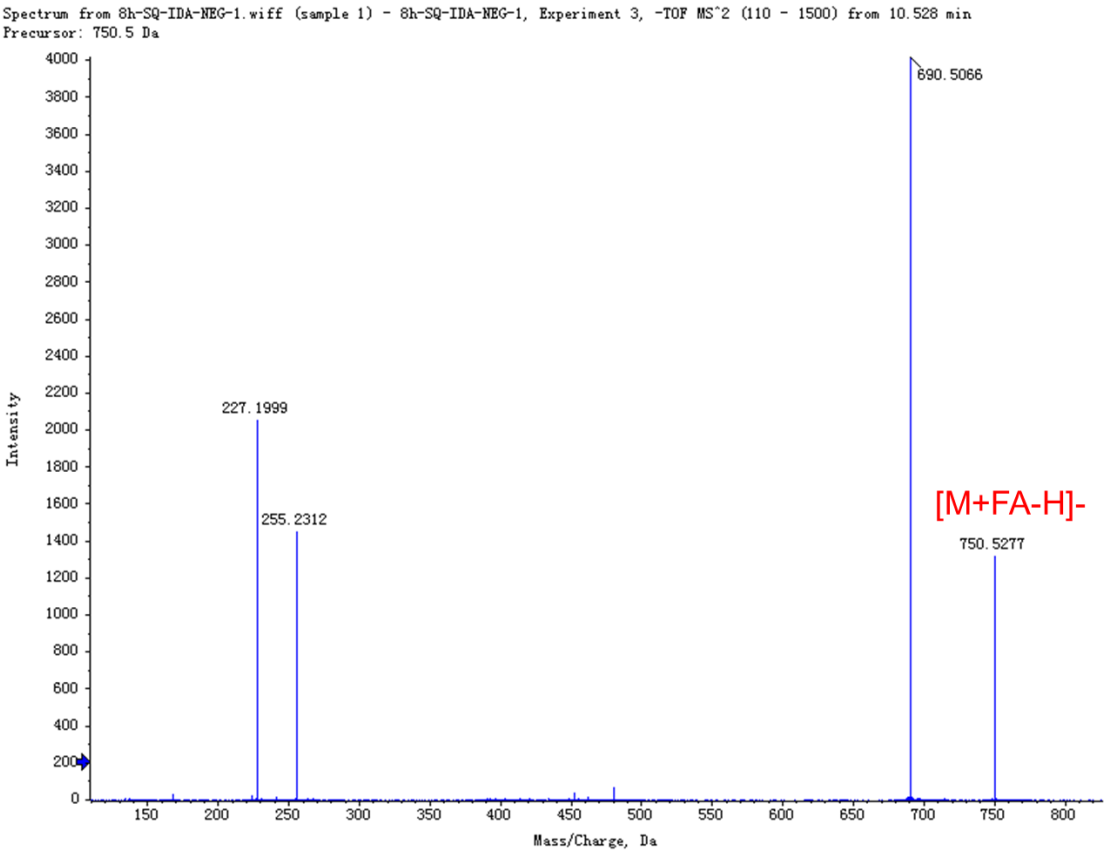
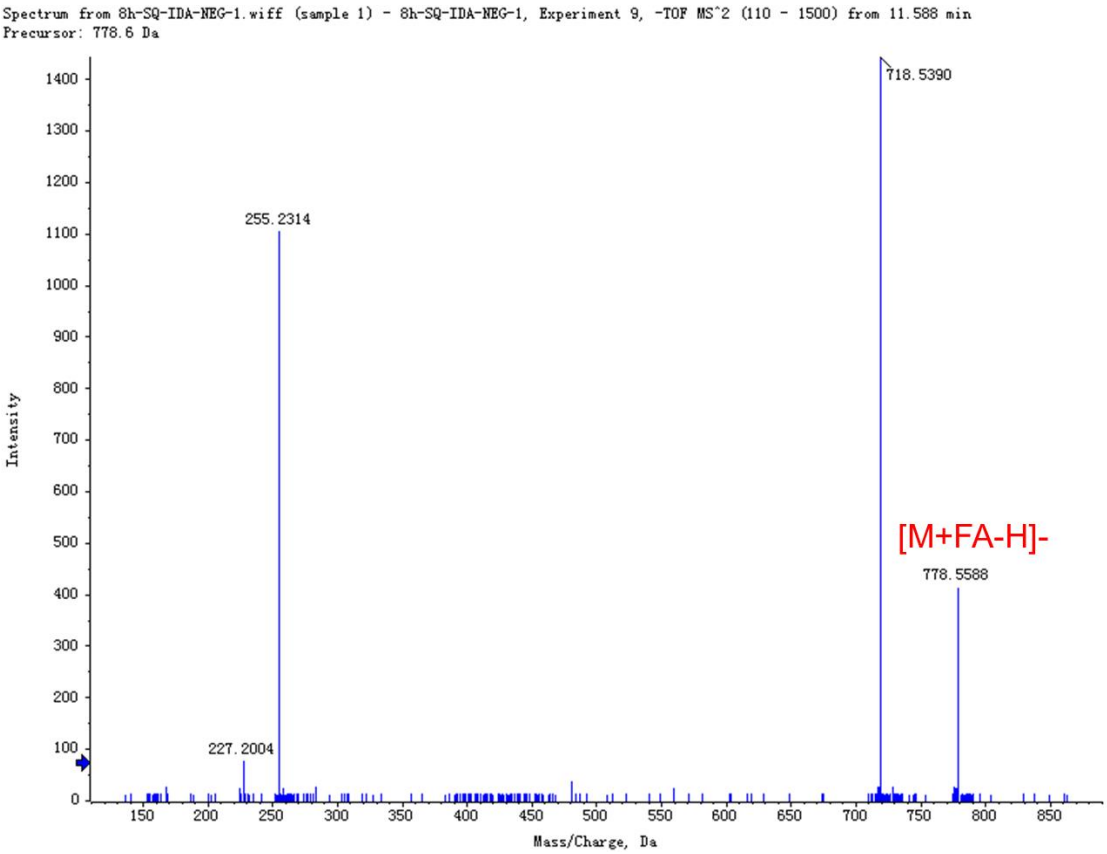
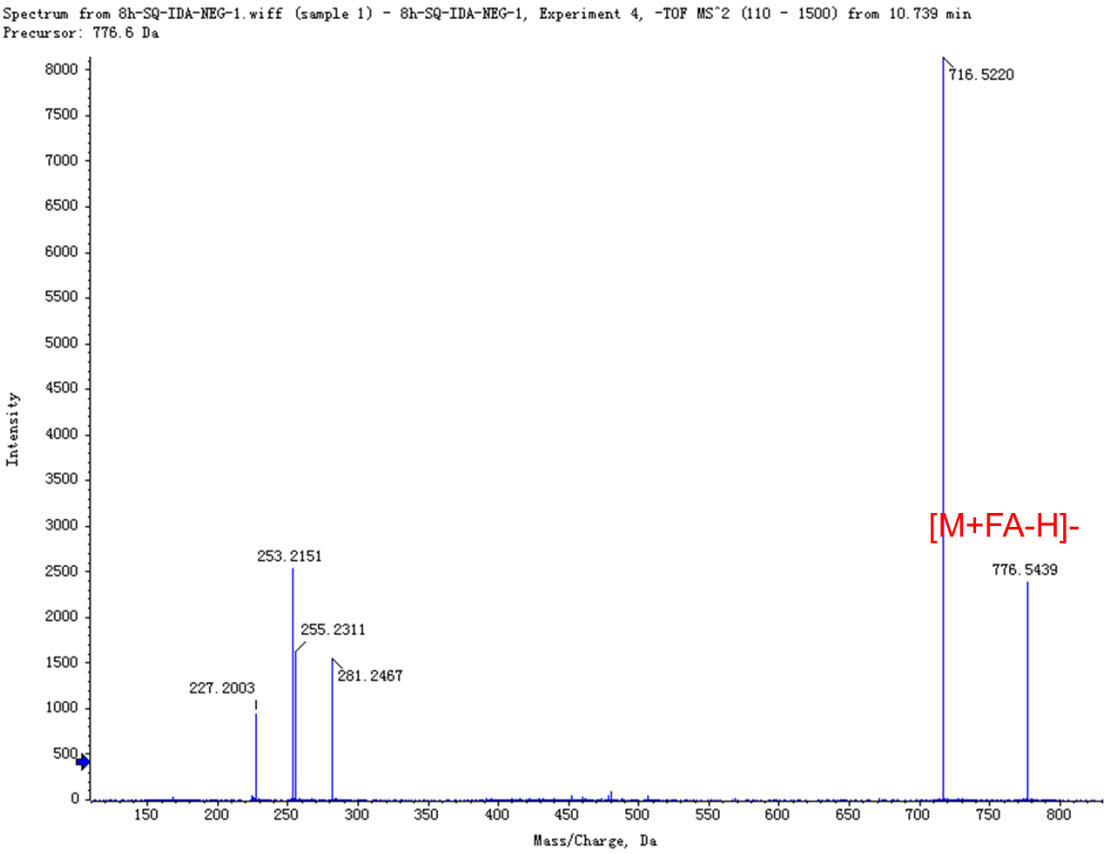


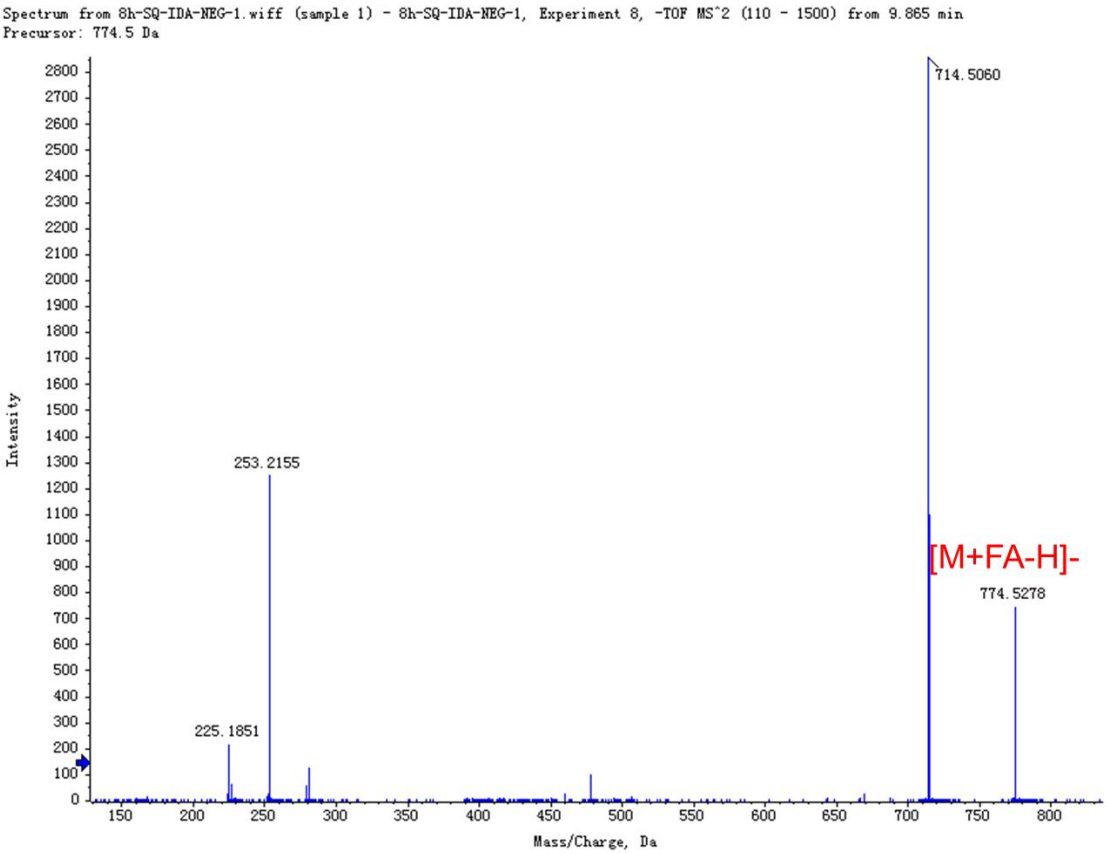
PC(32:0):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 9, -TOF MS^2 (110 - 1500) from 11.588 min
Precursor: 778.6 Da
718.5390
255.2314
[M+FA-H]-
778.5588
227.2004
Intensity
Mass/Charge, Da

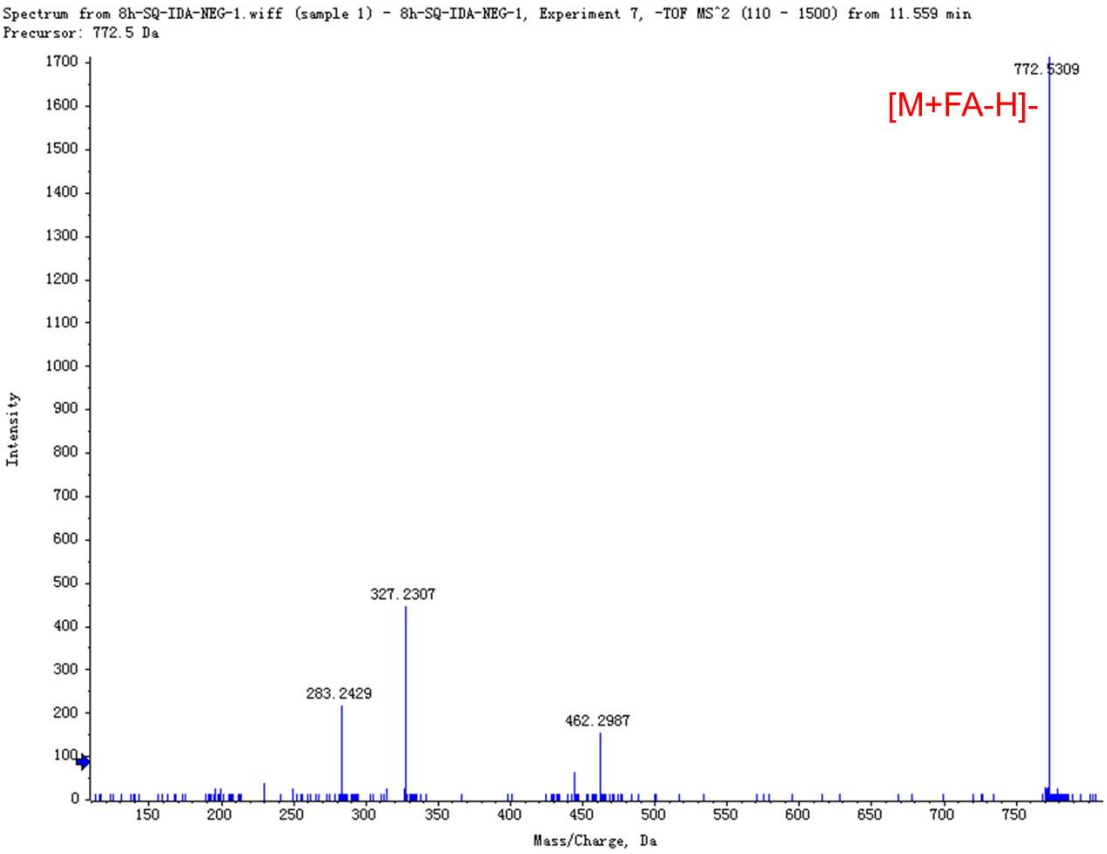
PC(32:1):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 4, -TOF MS^2 (110 - 1500) from 10.739 min
Precursor: 776.6 Da
716.5220
[M+FA-H]-
776.5439
253.2151
255.2311
281.2467
227.2003
Intensity
Mass/Charge, Da

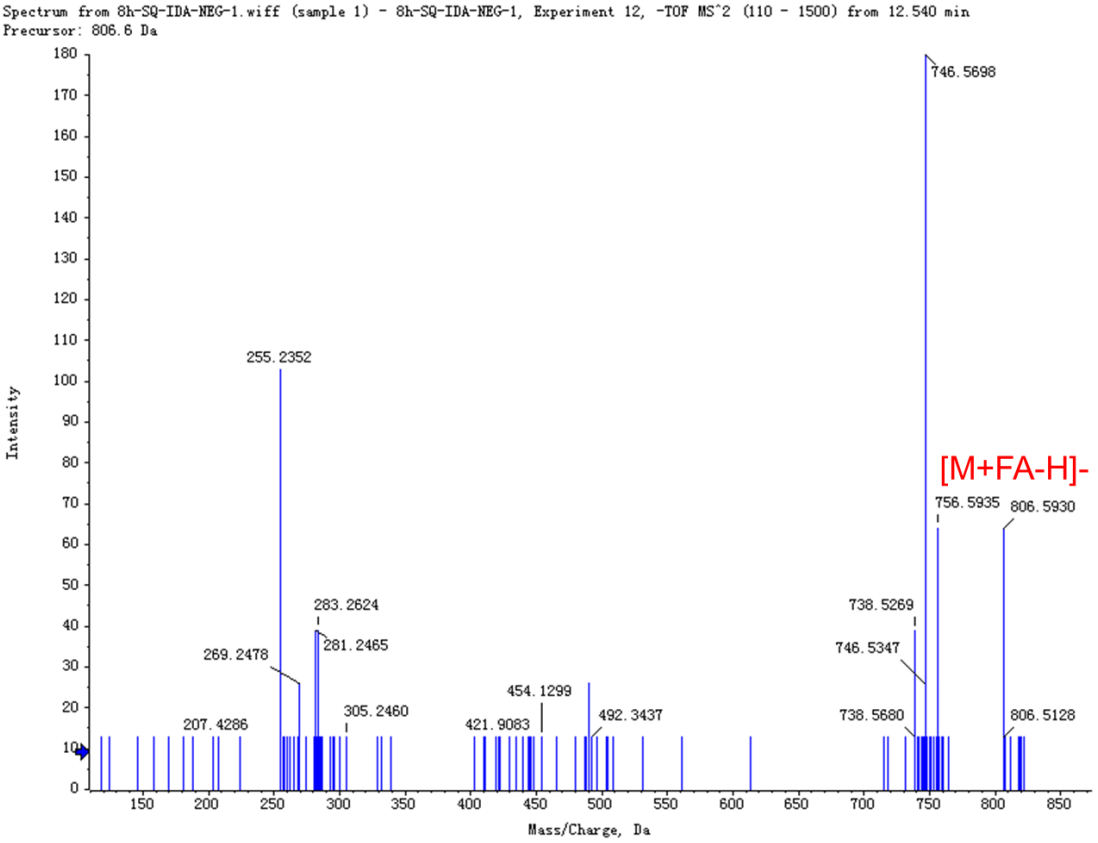
PC(32:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 8, -TOF MS^2 (110 - 1500) from 9.865 min
Precursor: 774.5 Da
714.5060
253.2155
[M+FA-H]-
774.5278
225.1851
Intensity
Mass/Charge, Da

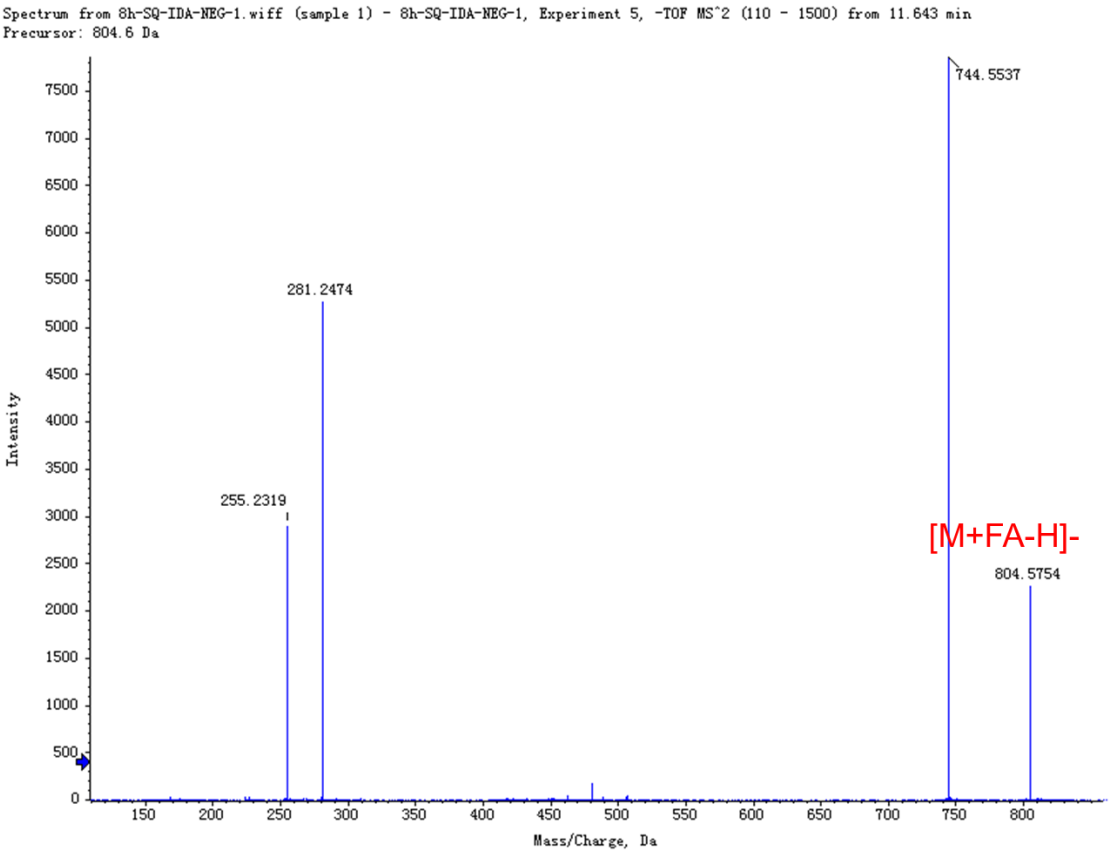
PC(32:3):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 7, -TOF MS^2 (110 - 1500) from 11.559 min
Precursor: 772.5 Da
772.5309
[M+FA-H]-
327.2307
283.2429
462.2987
Intensity
Mass/Charge, Da

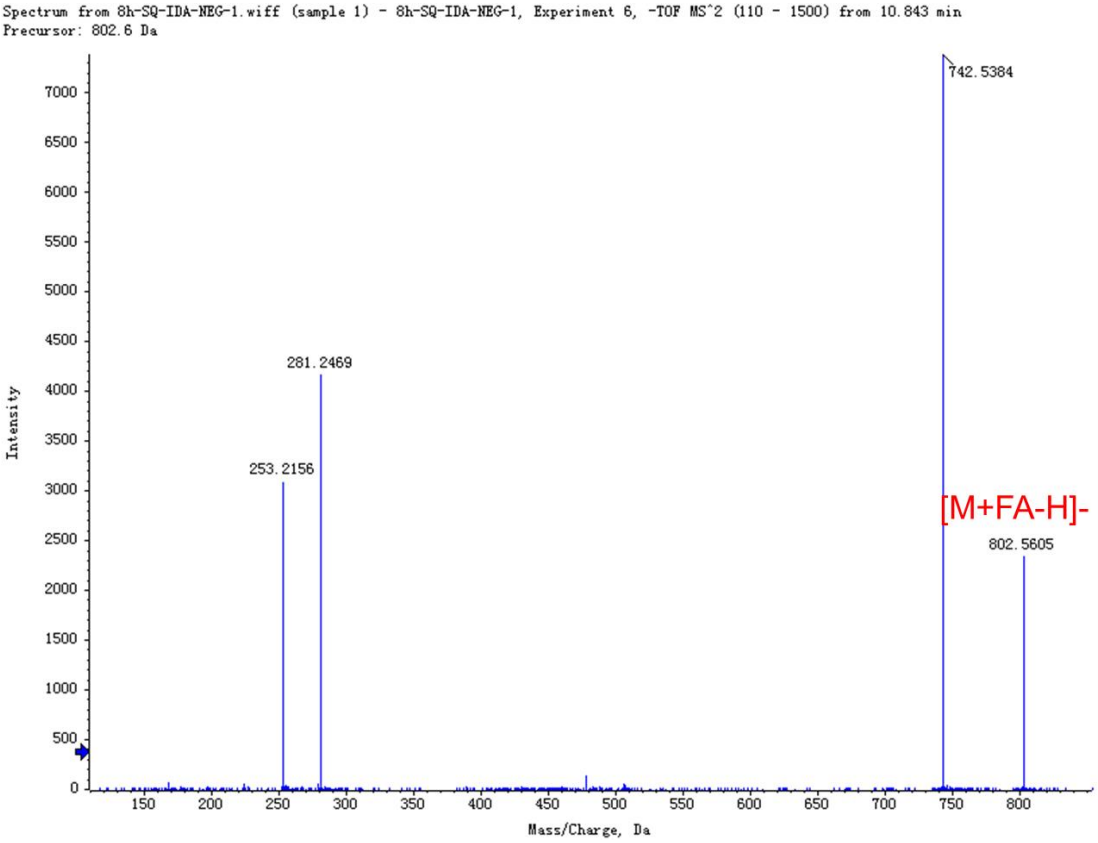
PC(34:0):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 12, -TOF MS^2 (110 - 1500) from 12.540 min
Precursor: 806.6 Da
Intensity
Mass/Charge, Da
746.5698
255.2352
[M+FA-H]-
756.5935
806.5930
283.2624
281.2465
738.5269
746.5347
269.2478
454.1299
305.2460
492.3437
207.4286
421.9083
738.5680
806.5128

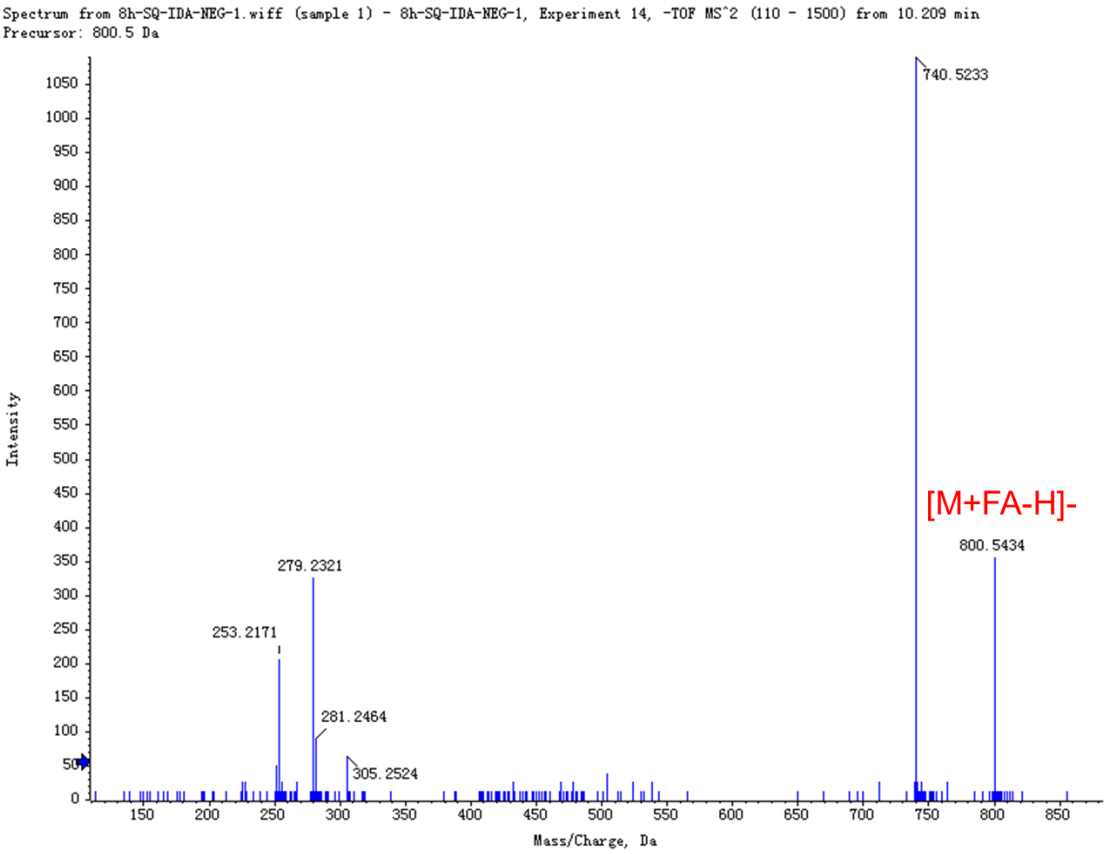
PC(34:1):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 5, -TOF MS^2 (110 - 1500) from 11.643 min
Precursor: 804.6 Da
Intensity
Mass/Charge, Da
744.5537
281.2474
255.2319
[M+FA-H]-
804.5754

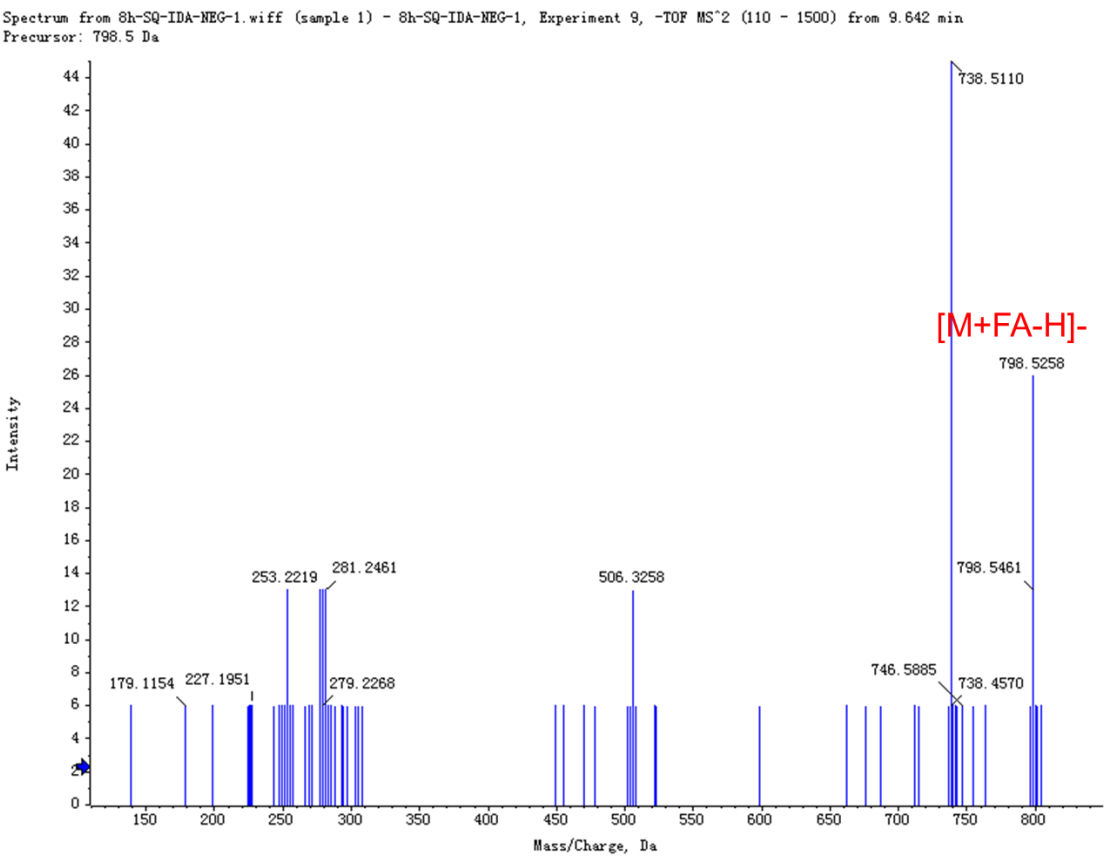
PC(34:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 6, -TOF MS^2 (110 - 1500) from 10.843 min
Precursor: 802.6 Da
742.5384
281.2469
253.2156
[M+FA-H]-
802.5605
Intensity
Mass/Charge, Da

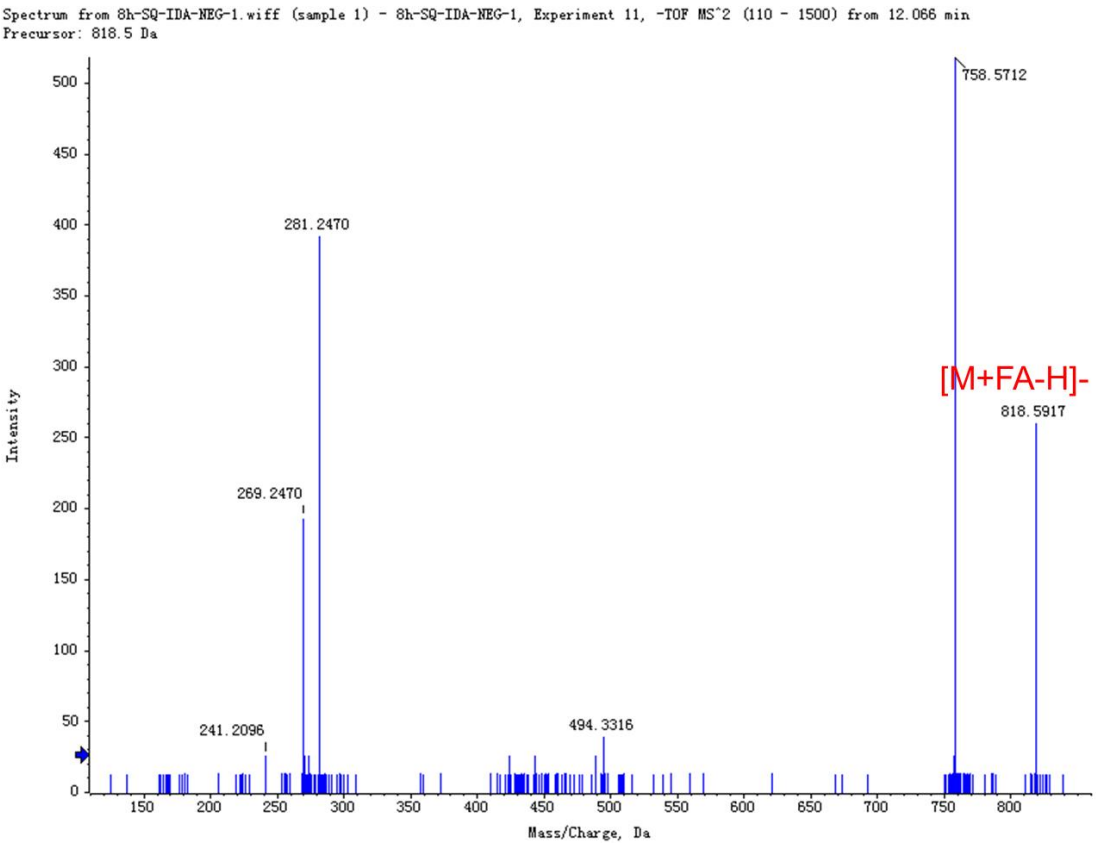
PC(34:3):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 14, -TOF MS^2 (110 - 1500) from 10.209 min
Precursor: 800.5 Da
740.5233
[M+FA-H]-
800.5434
279.2321
253.2171
281.2464
305.2524
Intensity
Mass/Charge, Da

PC(34:4):

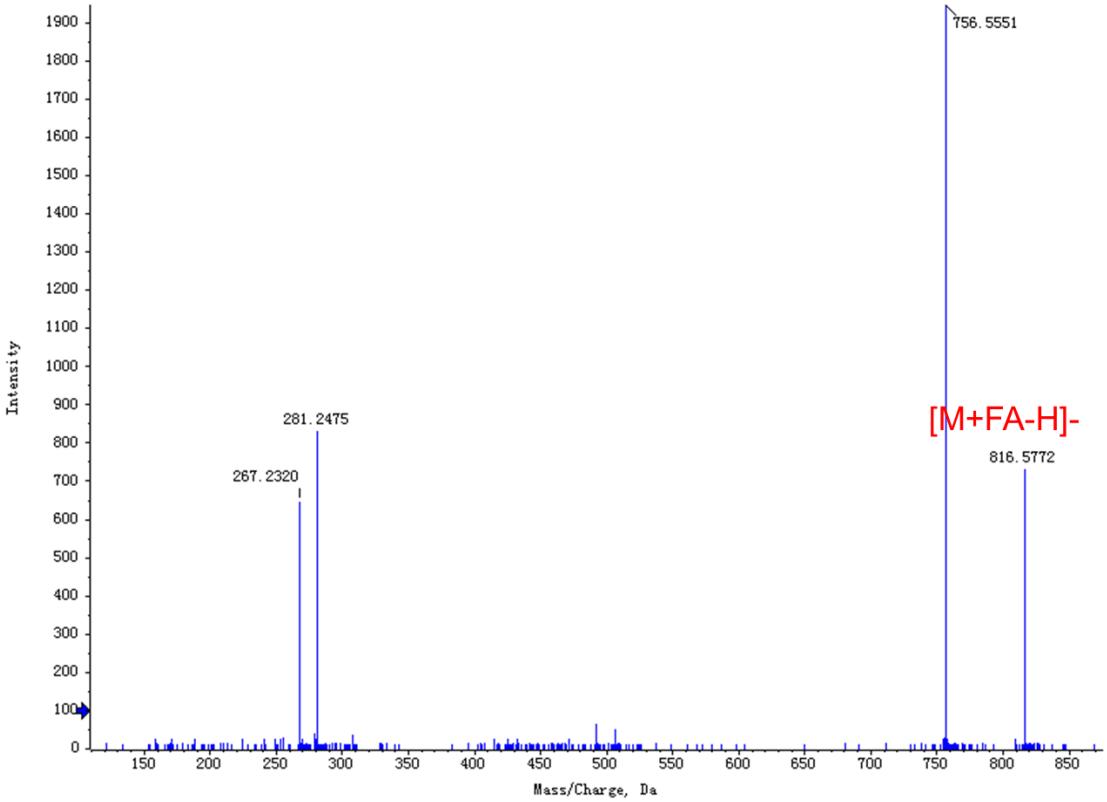

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 9, -TOF MS^2 (110 - 1500) from 9.642 min
Precursor: 798.5 Da
Intensity
Mass/Charge, Da
738.5110
[M+FA-H]-
798.5258
798.5461
253.2219
281.2461
506.3258
179.1154
227.1951
279.2268
746.5885
738.4570

PC(35:1):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 11, -TOF MS^2 (110 - 1500) from 12.066 min
Precursor: 818.5 Da
Intensity
Mass/Charge, Da
758.5712
281.2470
[M+FA-H]-
818.5917
269.2470
241.2096
494.3316

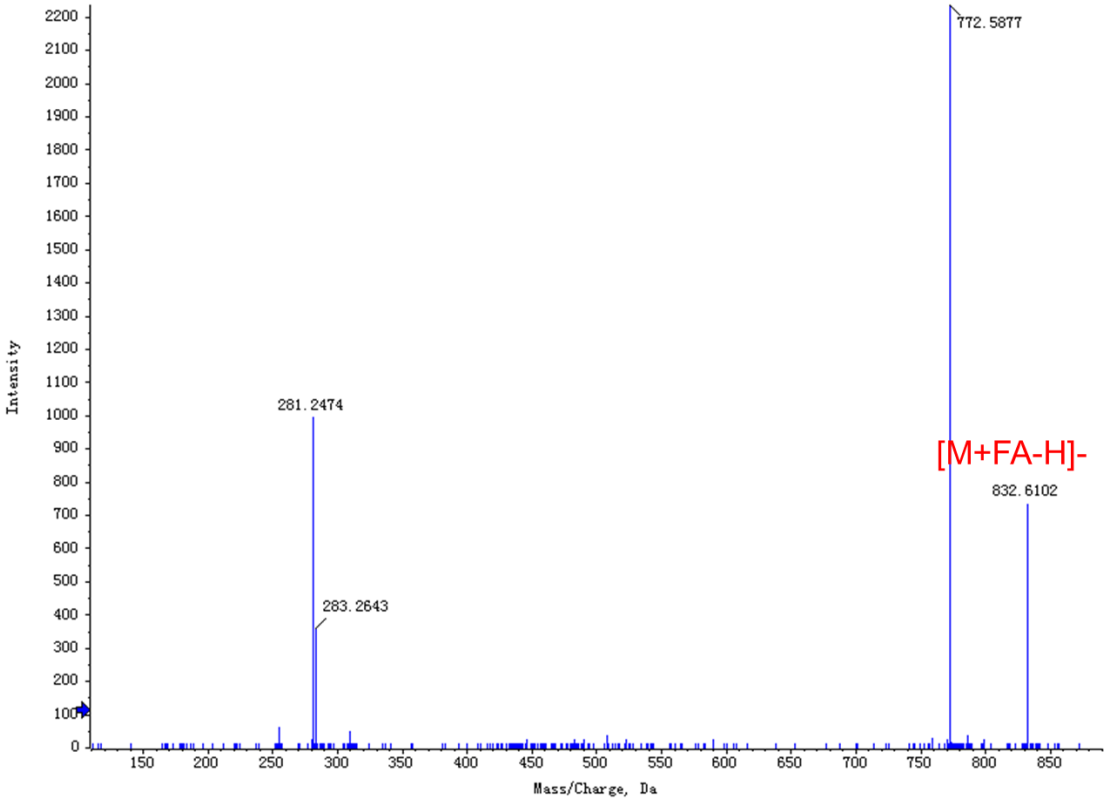
PC(35:2):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 10, -TOF MS^2 (110 - 1500) from 11.325 min
Precursor: 816.6 Da

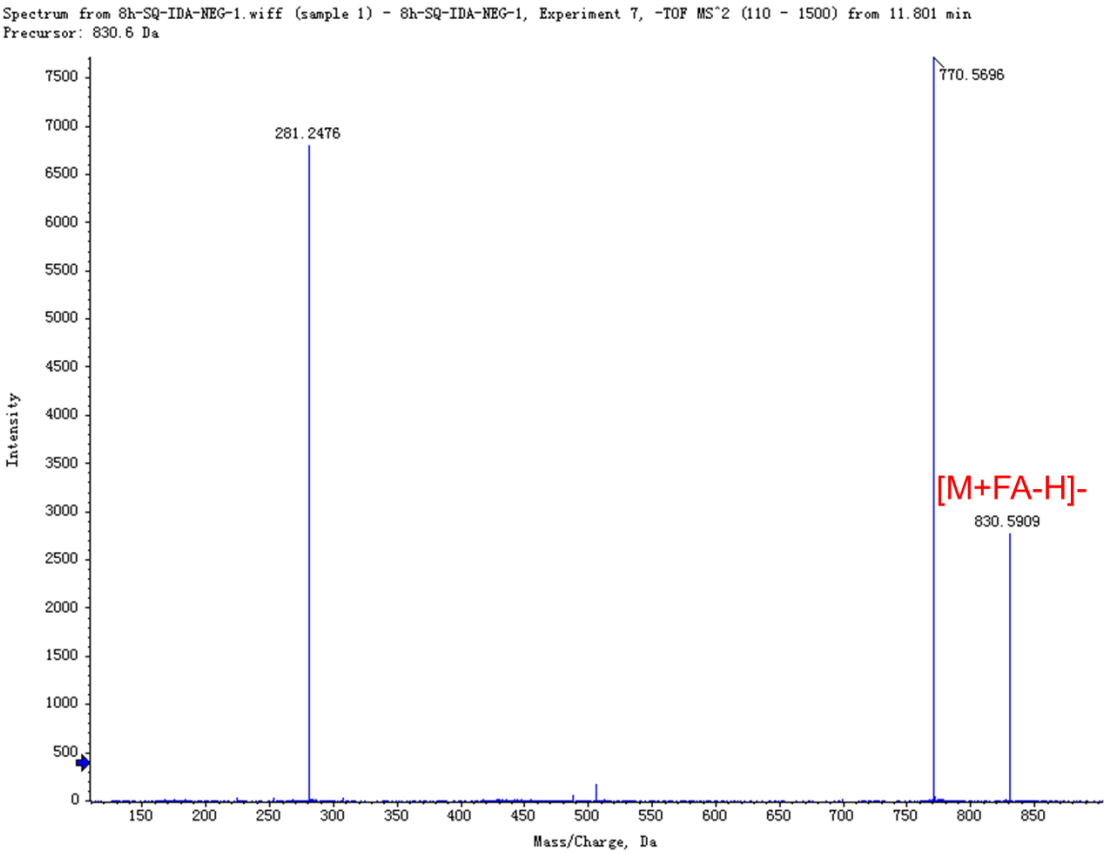


PC(36:1):

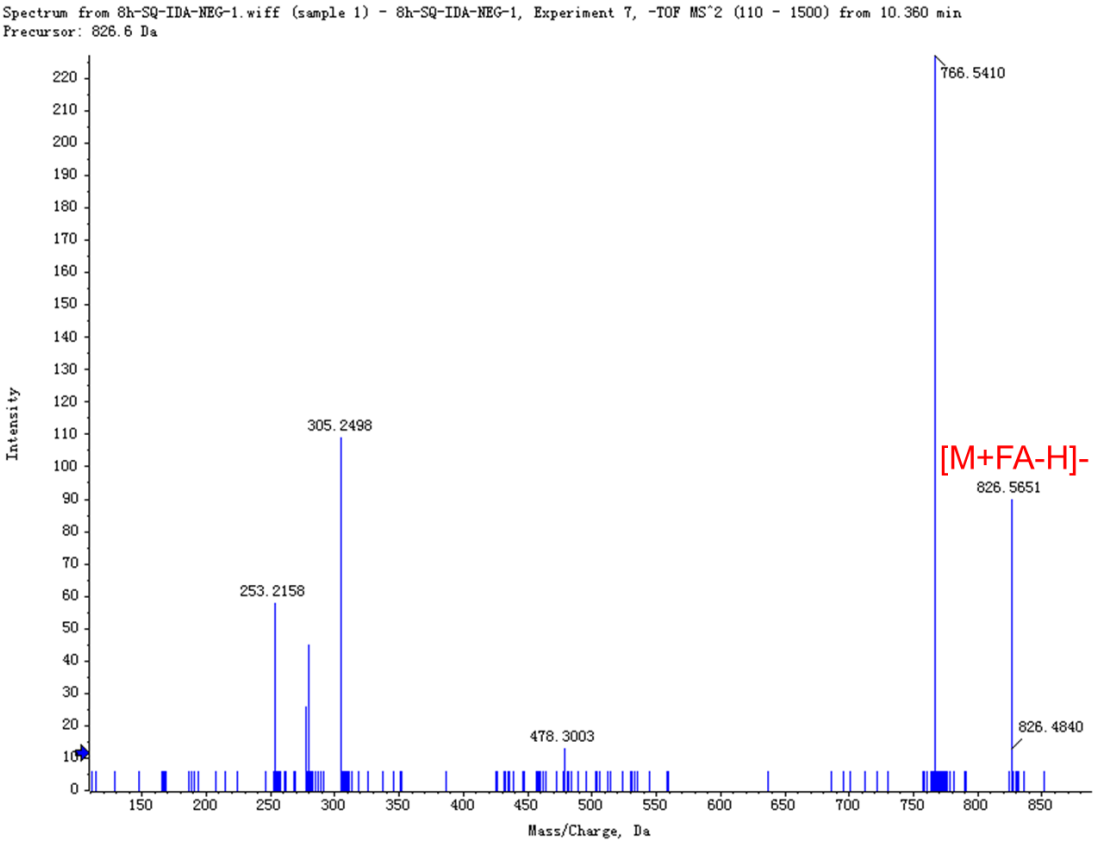
Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 8, -TOF MS^2 (110 - 1500) from 12.694 min
Precursor: 832.6 Da



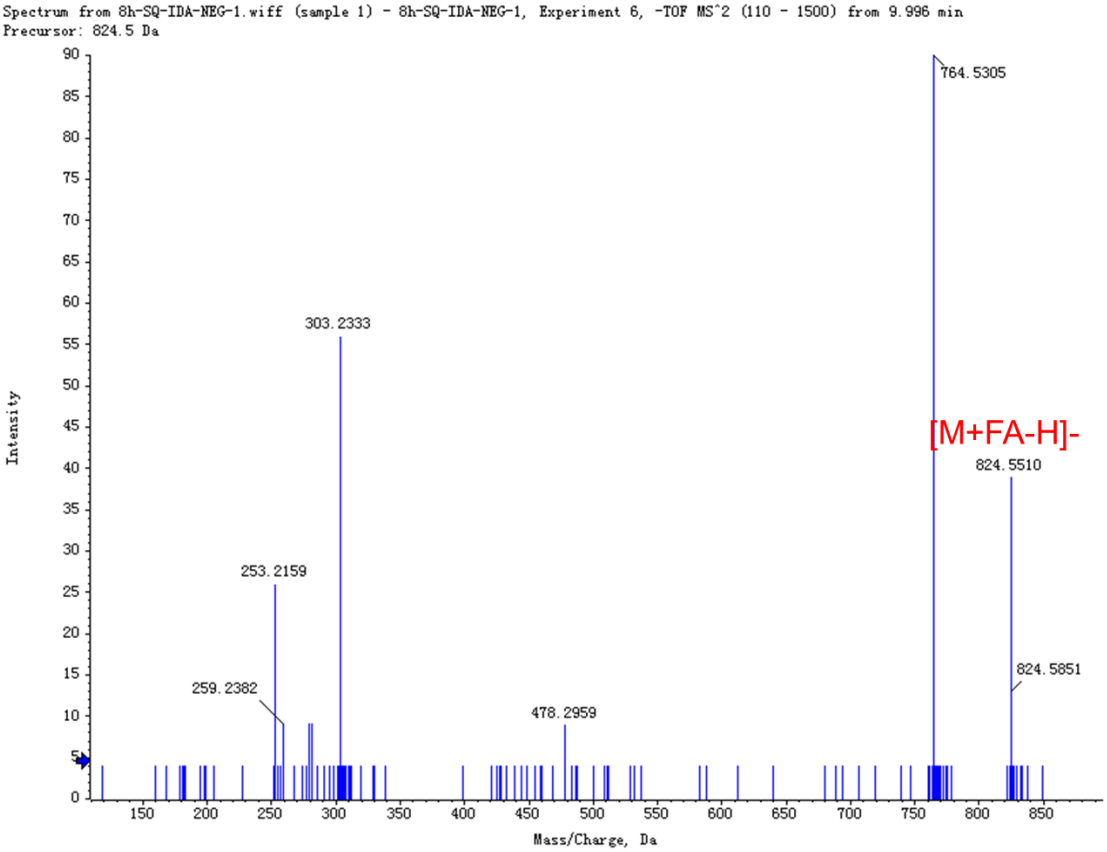
PC(36:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 7, -TOF MS^2 (110 - 1500) from 11.801 min
Precursor: 830.6 Da
Intensity
Mass/Charge, Da
281.2476
770.5696
[M+FA-H]-
830.5909

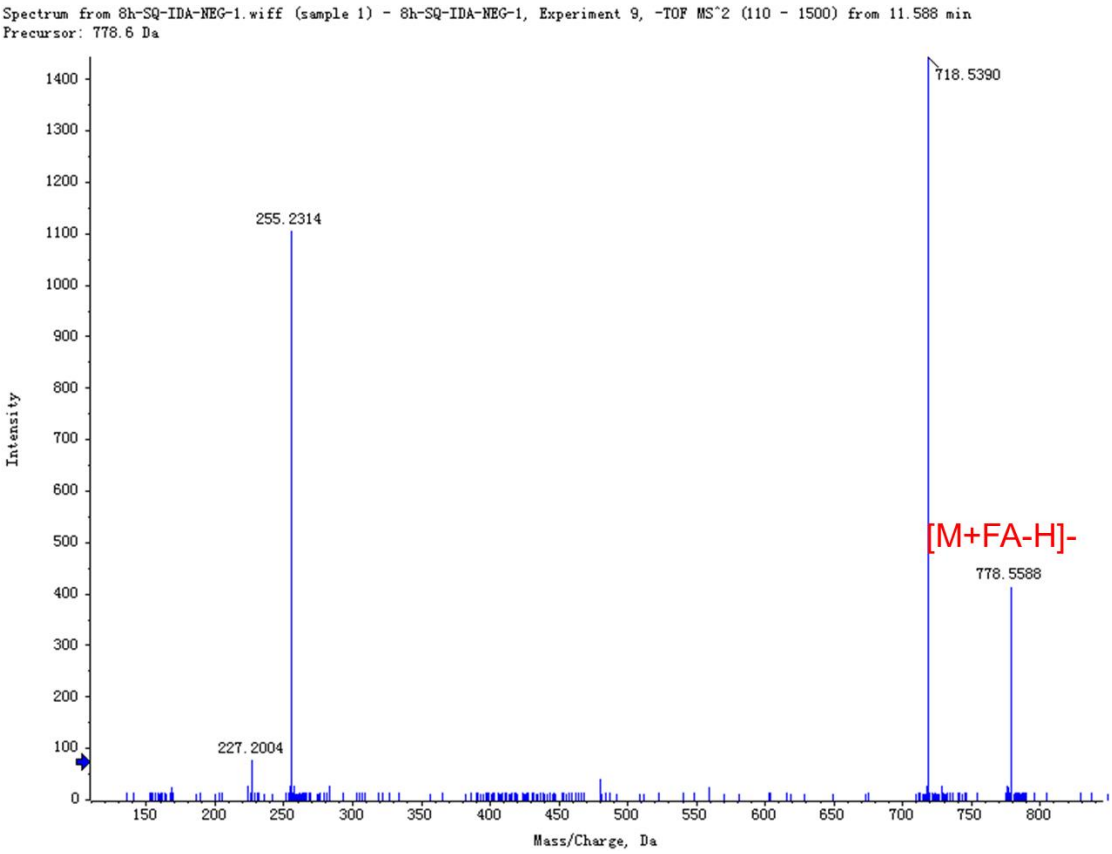
PC(36:4):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 7, -TOF MS^2 (110 - 1500) from 10.360 min
Precursor: 826.6 Da
Intensity
Mass/Charge, Da
766.5410
305.2498
[M+FA-H]-
826.5651
253.2158
478.3003
826.4840

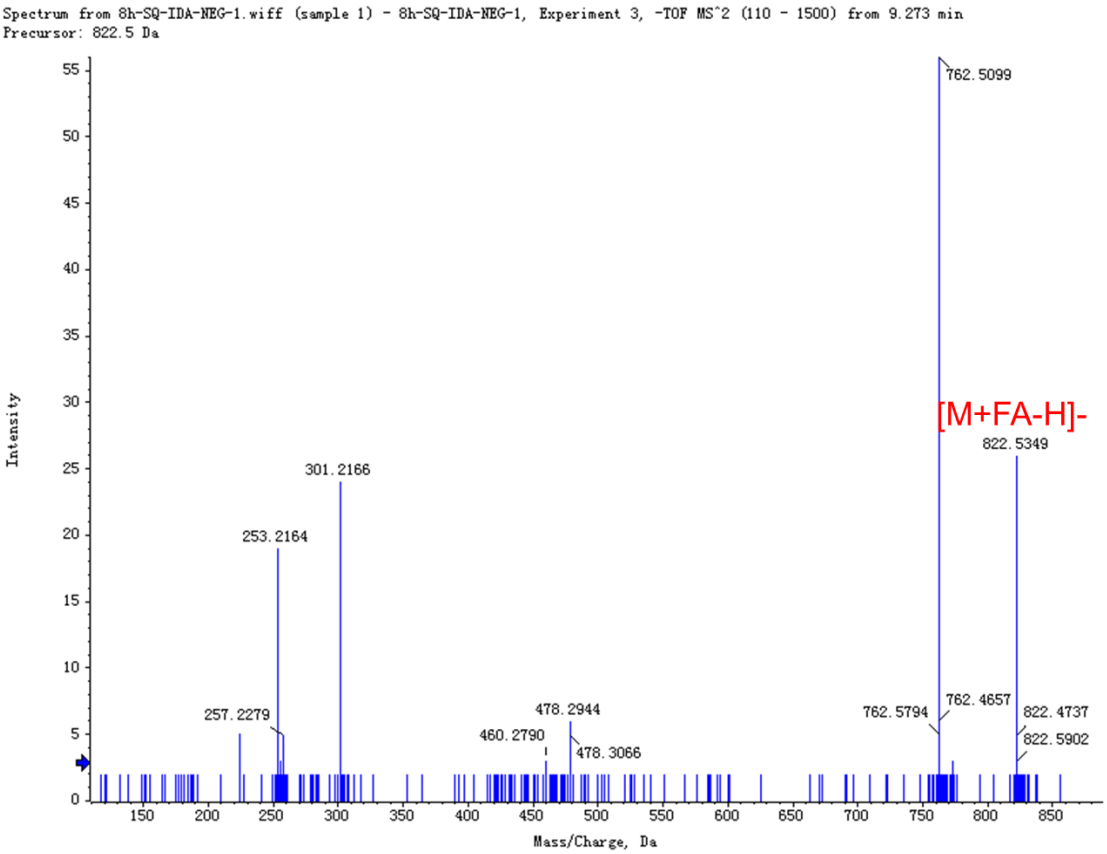
PC(36:5):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 6, -TOF MS^2 (110 - 1500) from 9.996 min
Precursor: 824.5 Da
764.5305
303.2333
[M+FA-H]-
824.5510
253.2159
824.5851
259.2382
478.2959
Intensity
Mass/Charge, Da

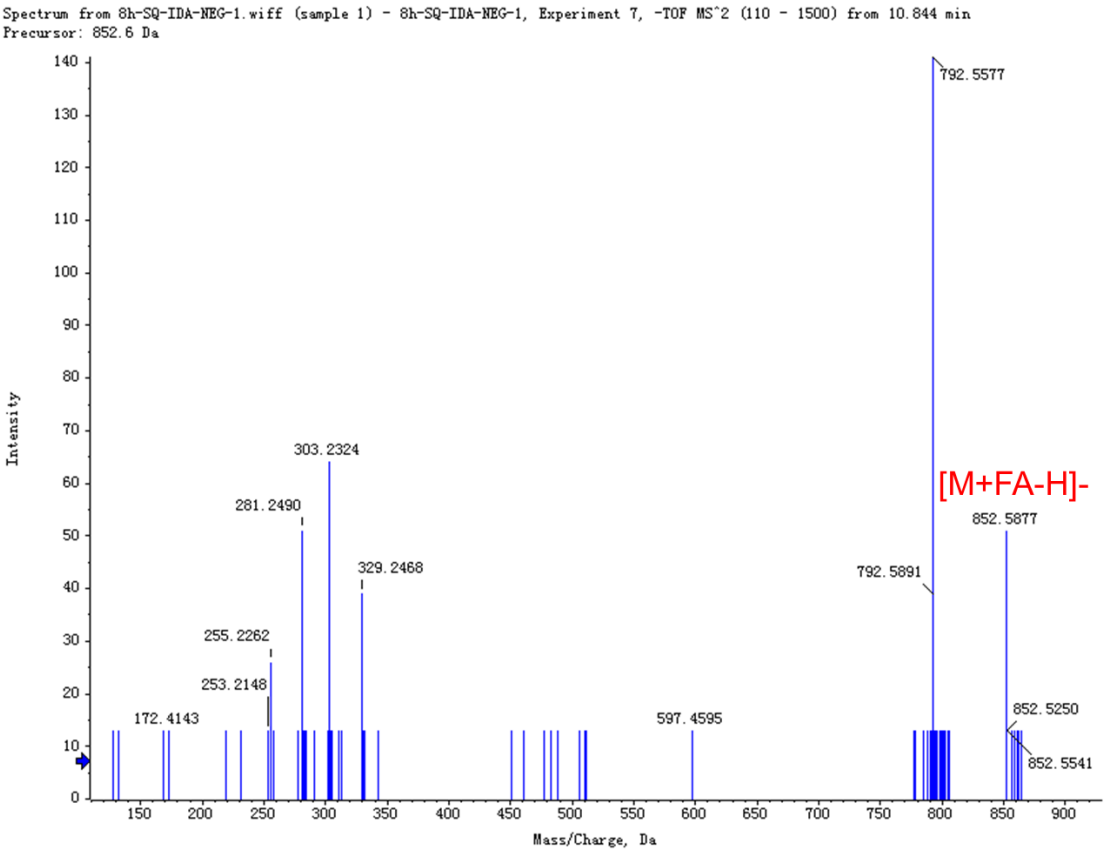
PC(36:5):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 9, -TOF MS^2 (110 - 1500) from 11.588 min
Precursor: 778.6 Da
718.5390
255.2314
[M+FA-H]-
778.5588
227.2004
Intensity
Mass/Charge, Da

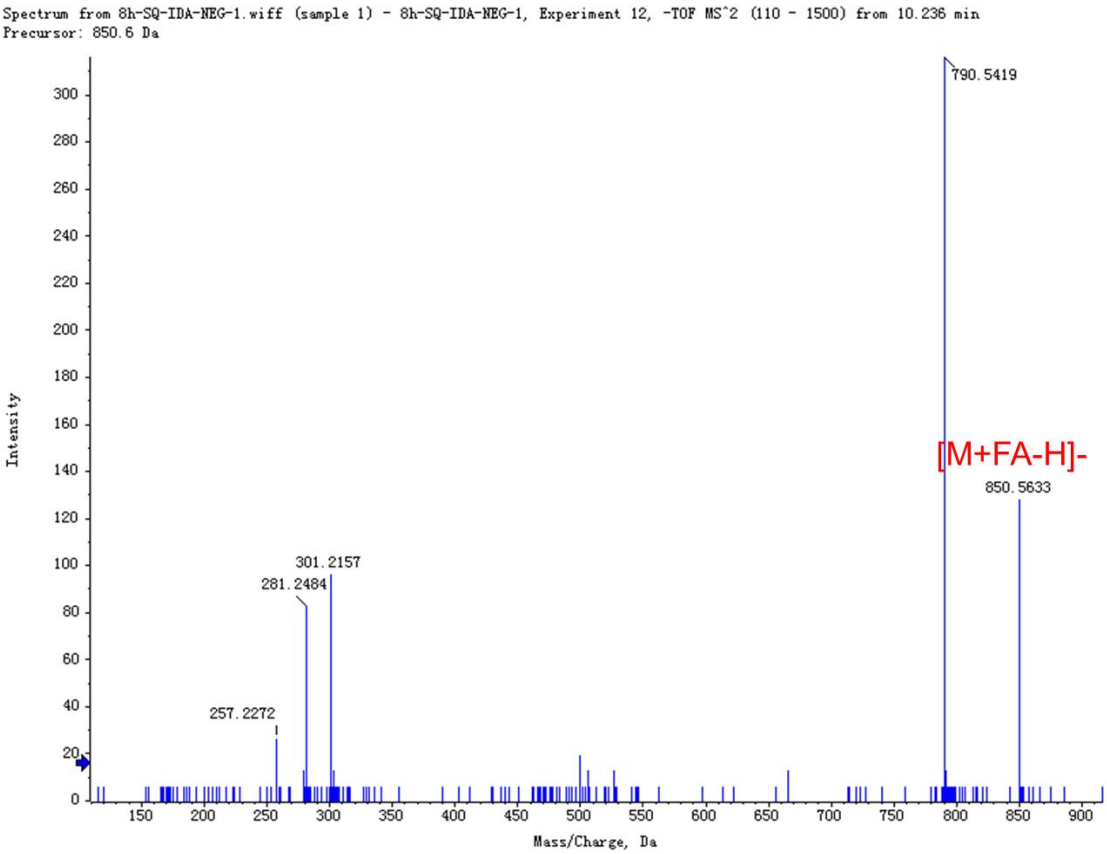
PC(36:6):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 3, -TOF MS^2 (110 - 1500) from 9.273 min
Precursor: 822.5 Da
Intensity
Mass/Charge, Da
762.5099
[M+FA-H]-
822.5349
301.2166
253.2164
257.2279
478.2944
460.2790
478.3066
762.5794
762.4657
822.4737
822.5902

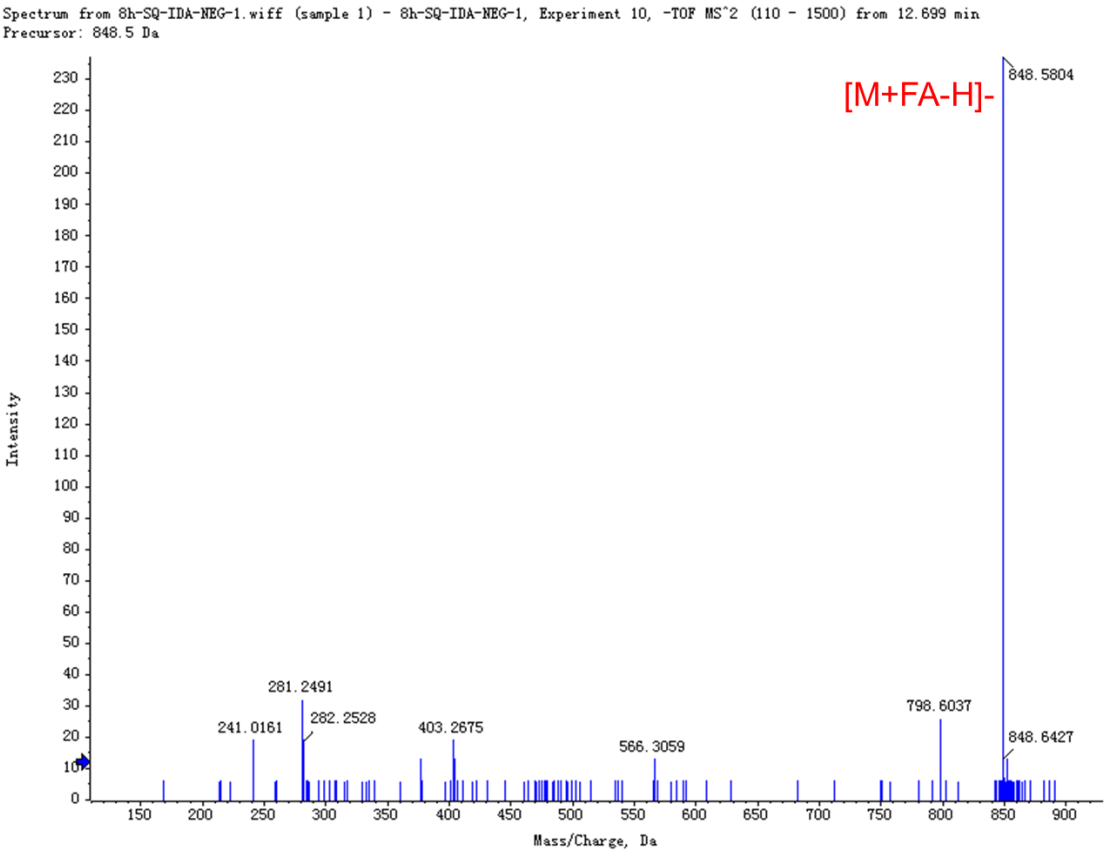
PC(38:5):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 7, -TOF MS^2 (110 - 1500) from 10.844 min
Precursor: 852.6 Da
Intensity
Mass/Charge, Da
792.5577
[M+FA-H]-
852.5877
303.2324
281.2490
329.2468
792.5891
255.2262
253.2148
172.4143
597.4595
852.5250
852.5541

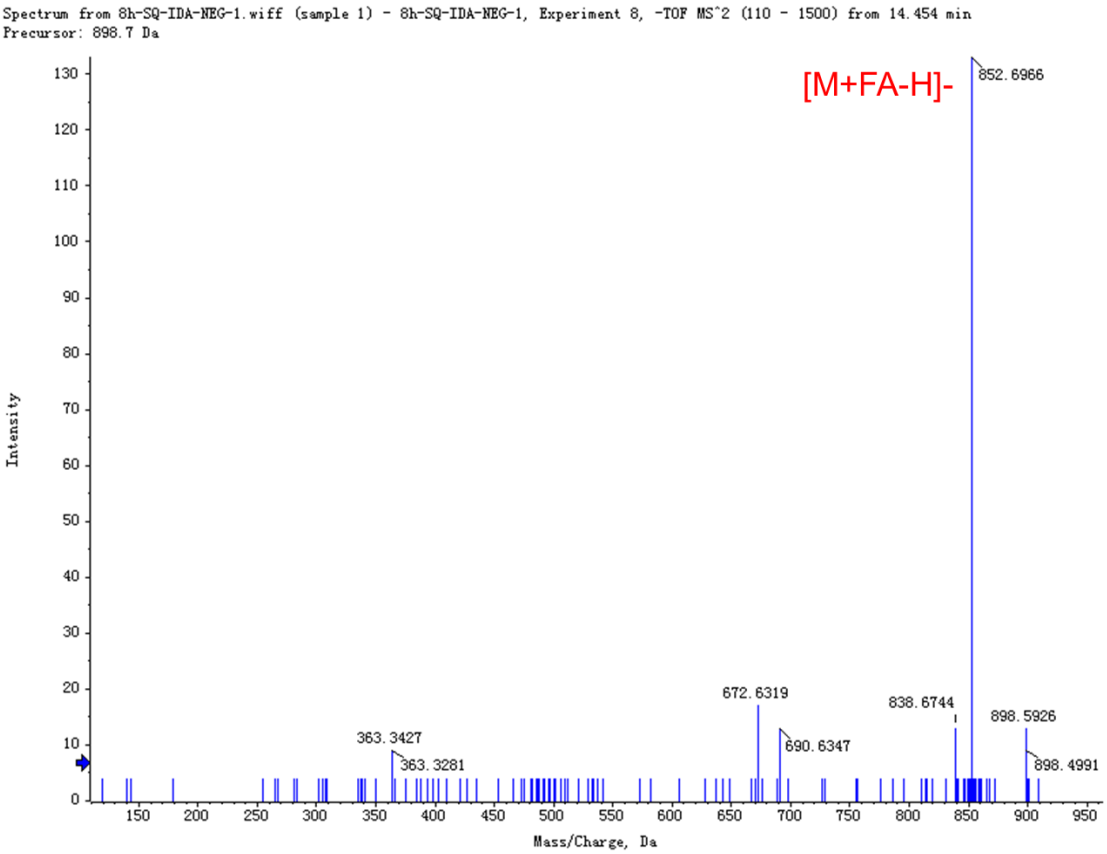
PC(38:6):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 12, -TOF MS^2 (110 - 1500) from 10.236 min
Precursor: 850.6 Da
790.5419
[M+FA-H]-
850.5633
301.2157
281.2484
257.2272
Intensity
Mass/Charge, Da

PC(38:7):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 10, -TOF MS^2 (110 - 1500) from 12.699 min
Precursor: 848.5 Da
848.5804
[M+FA-H]-
281.2491
282.2528
241.0161
403.2675
566.3059
798.6037
848.6427
Intensity
Mass/Charge, Da

PC(42:10):



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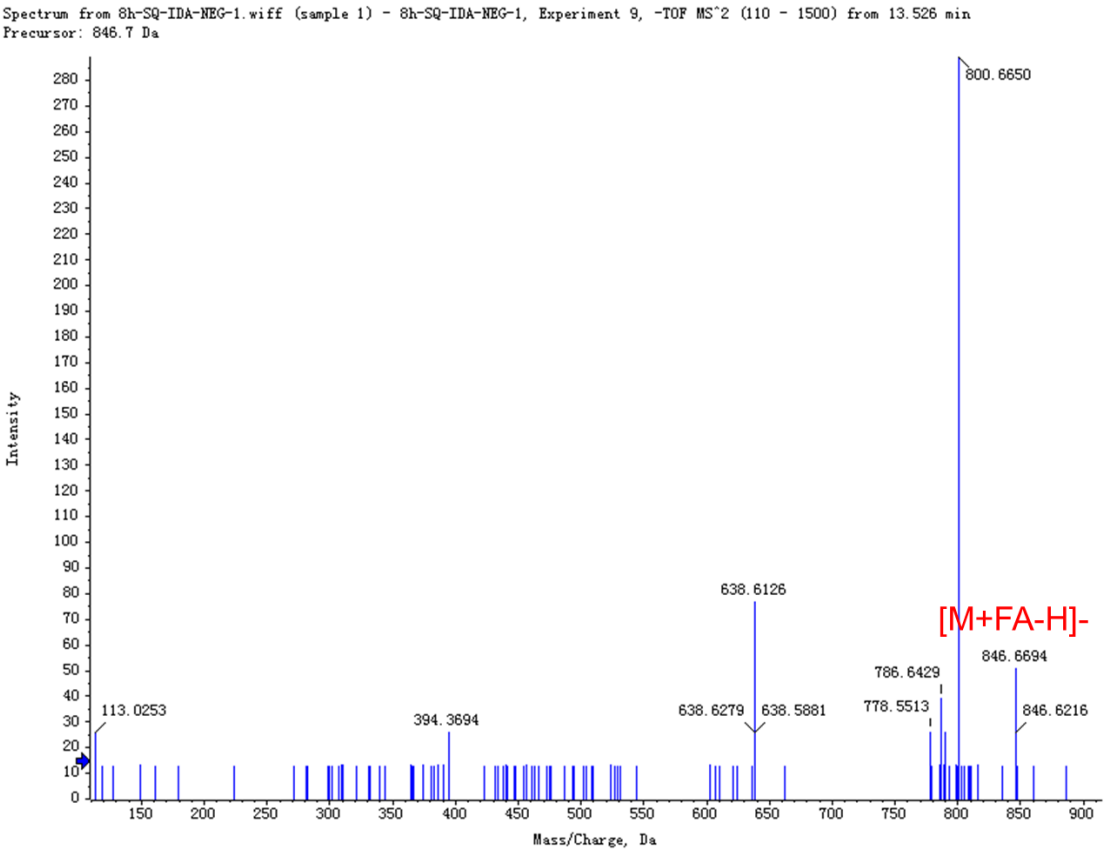
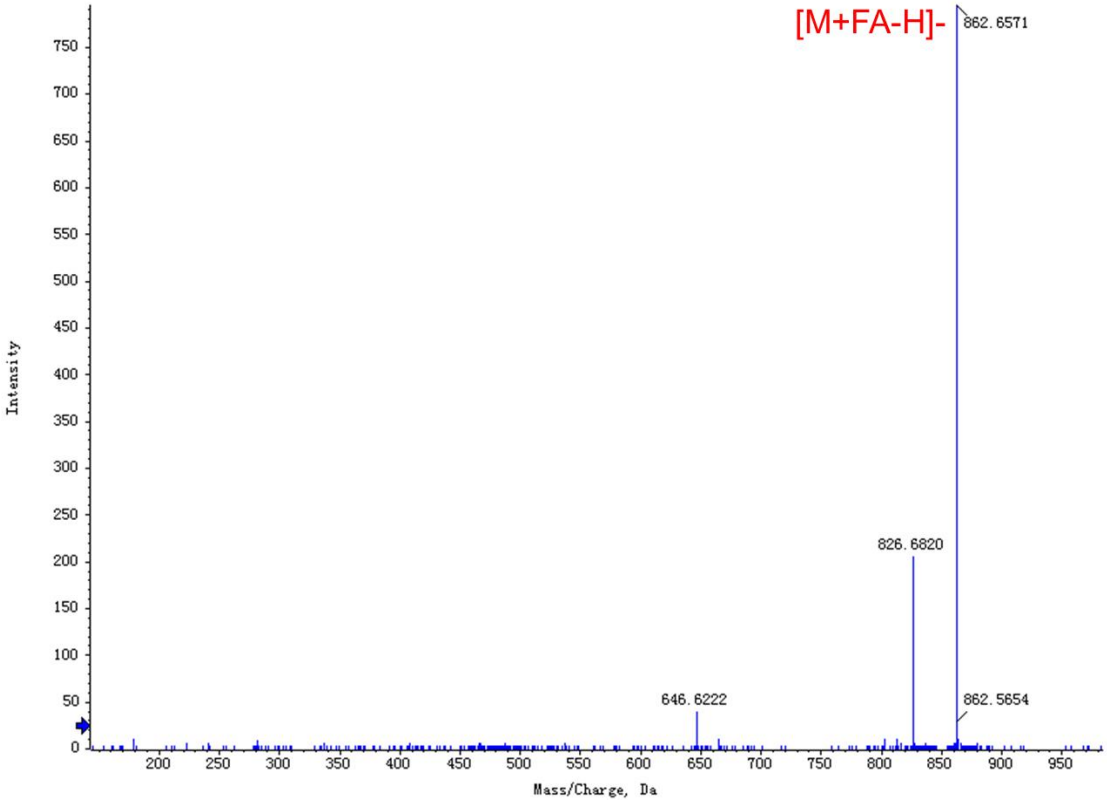


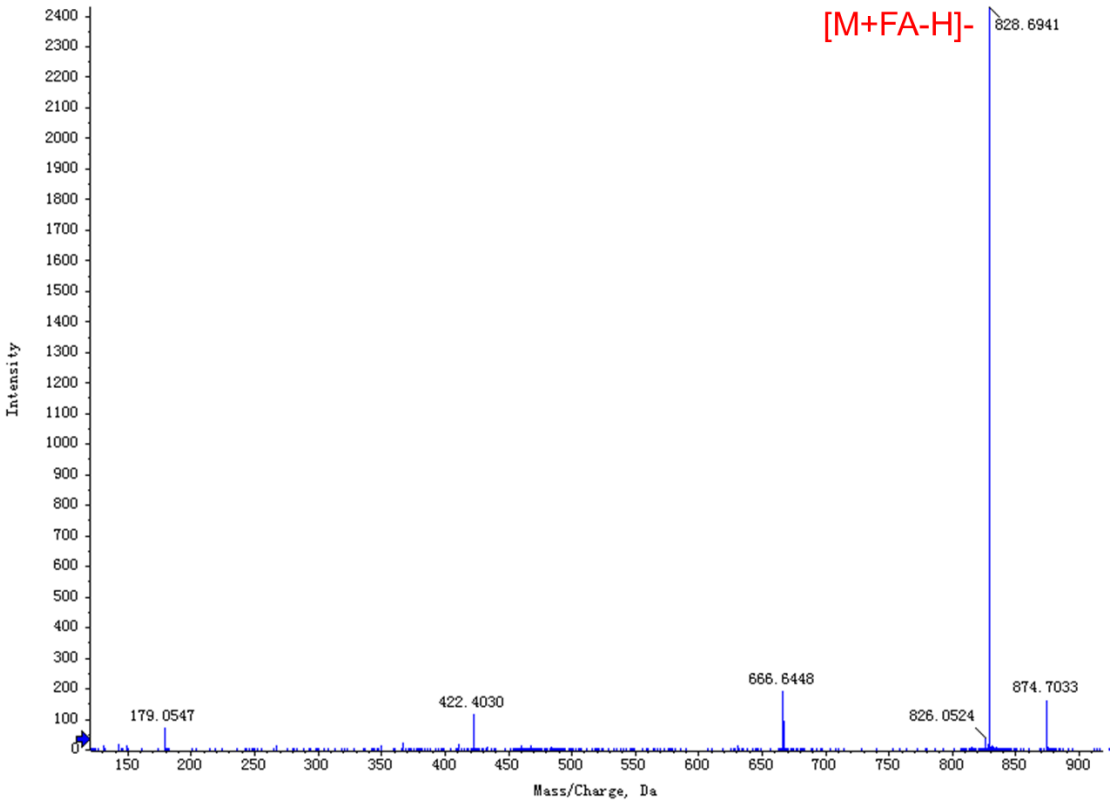
PC(O-39:0):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 4, -TOF MS^2 (110 - 1500) from 14.528 min
Precursor: 862.7 Da

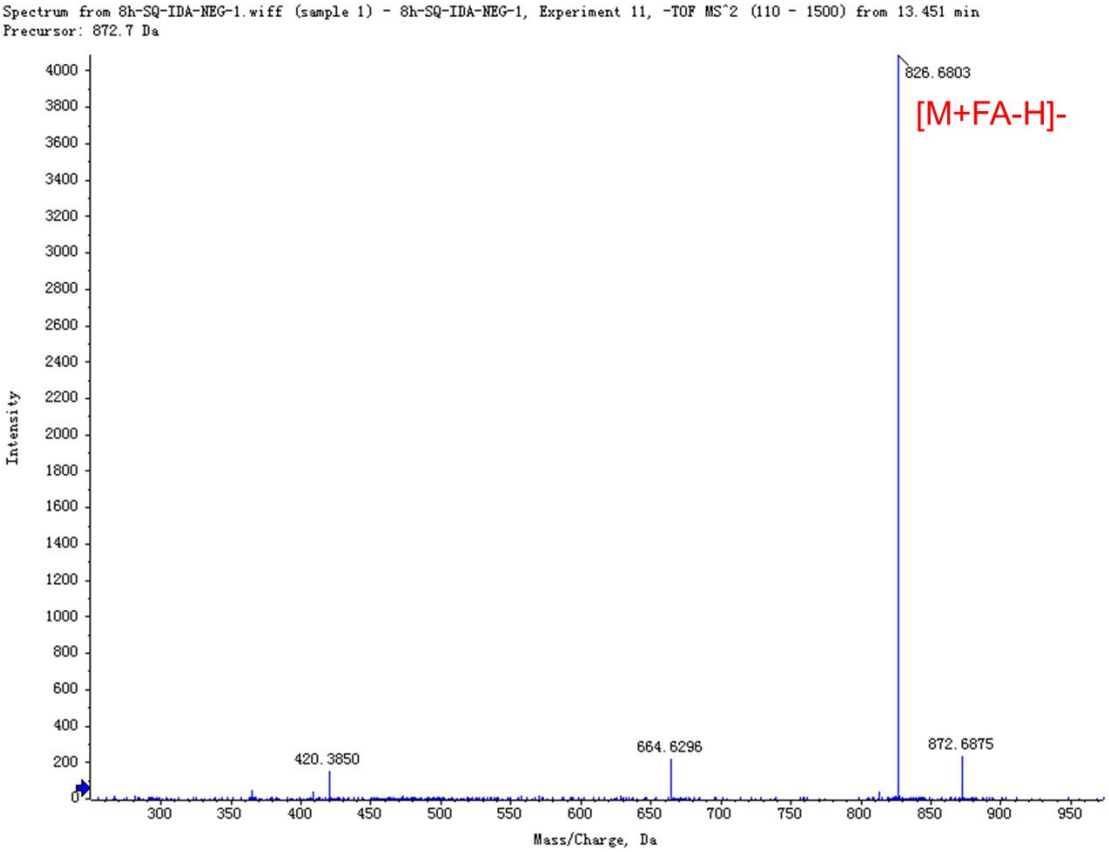


PC(O-40:1):

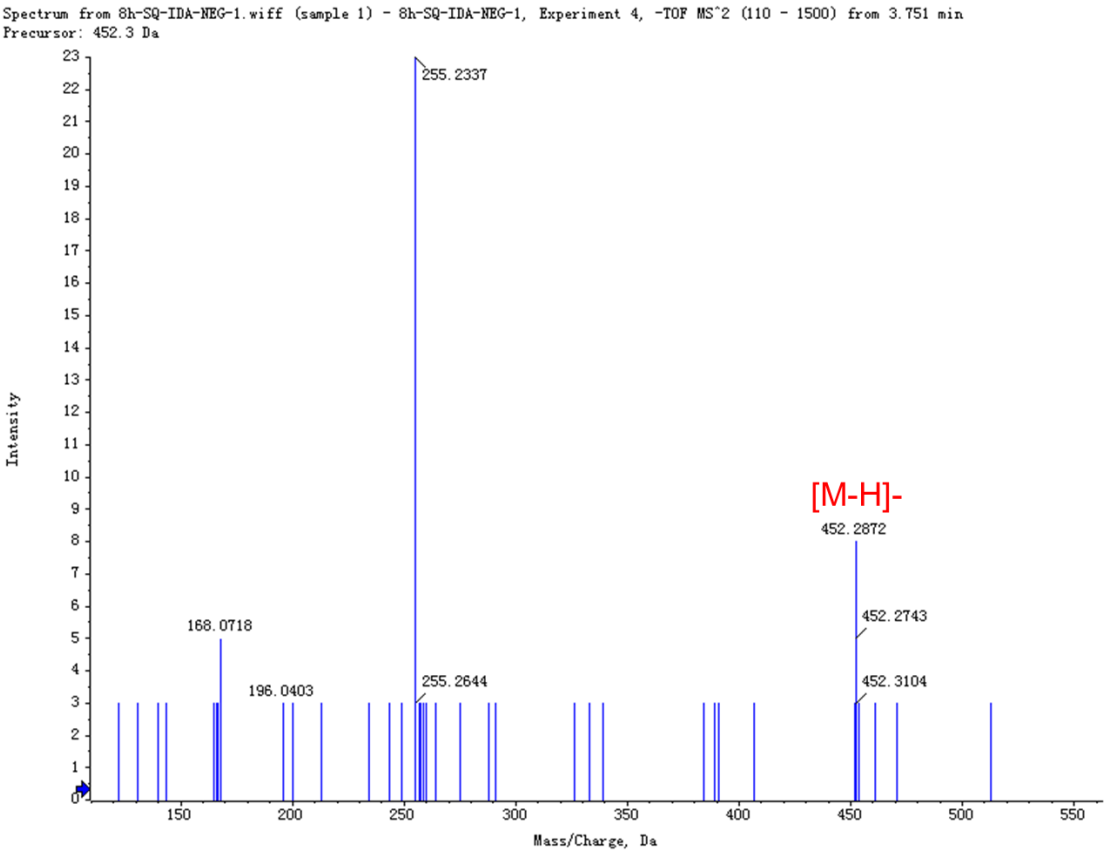
Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 7, -TOF MS^2 (110 - 1500) from 14.379 min
Precursor: 874.7 Da



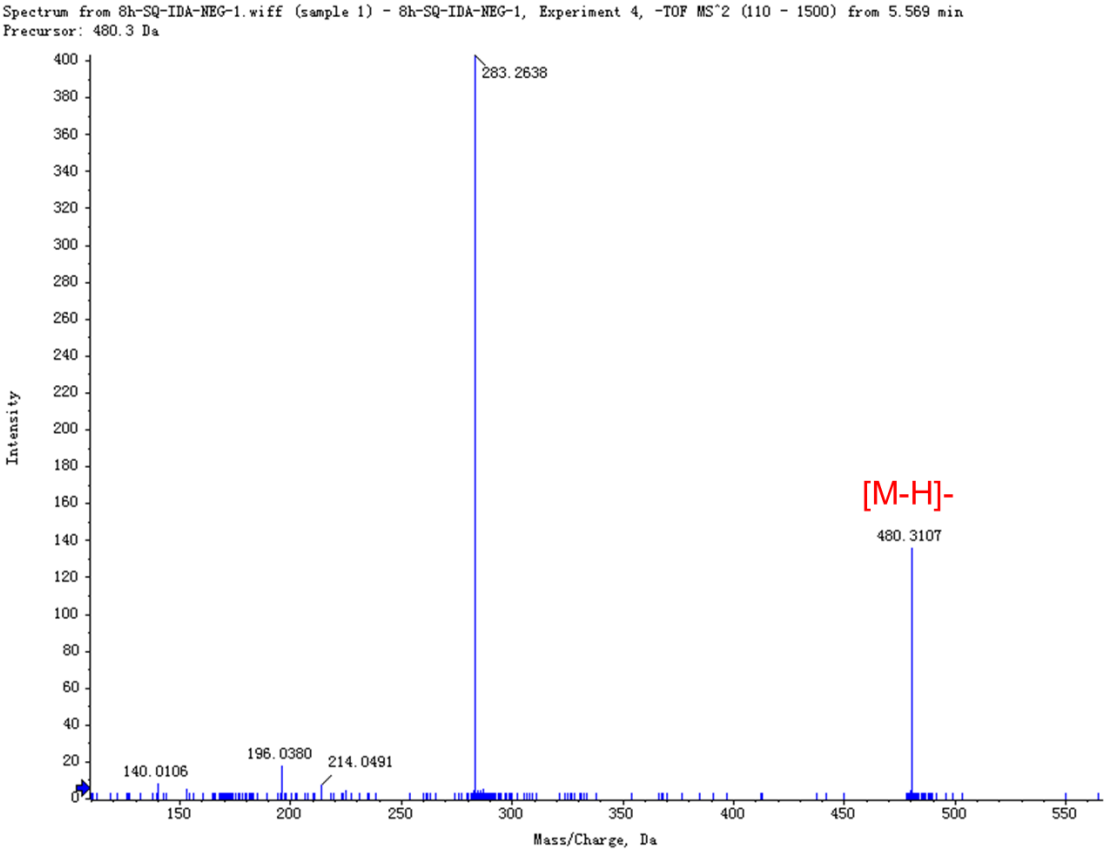
PC(O-40:2):



LyPE(16:0):

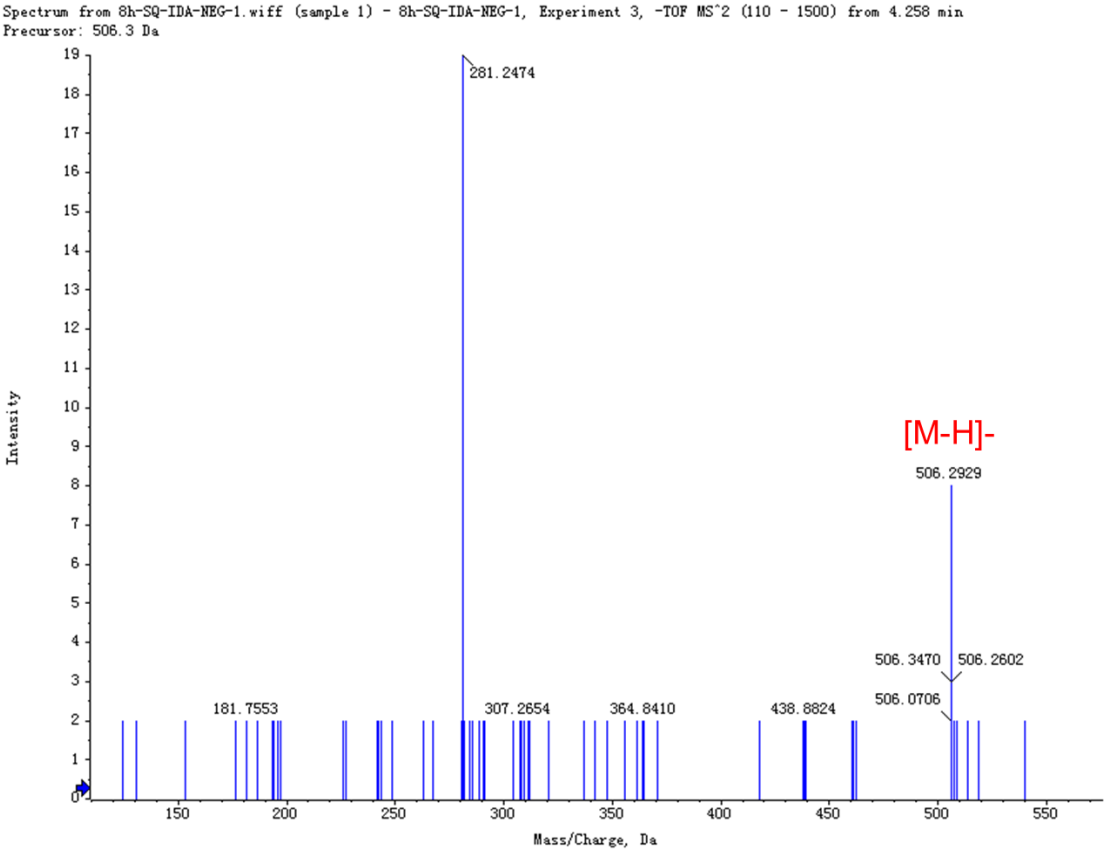


LyPE(18:0):

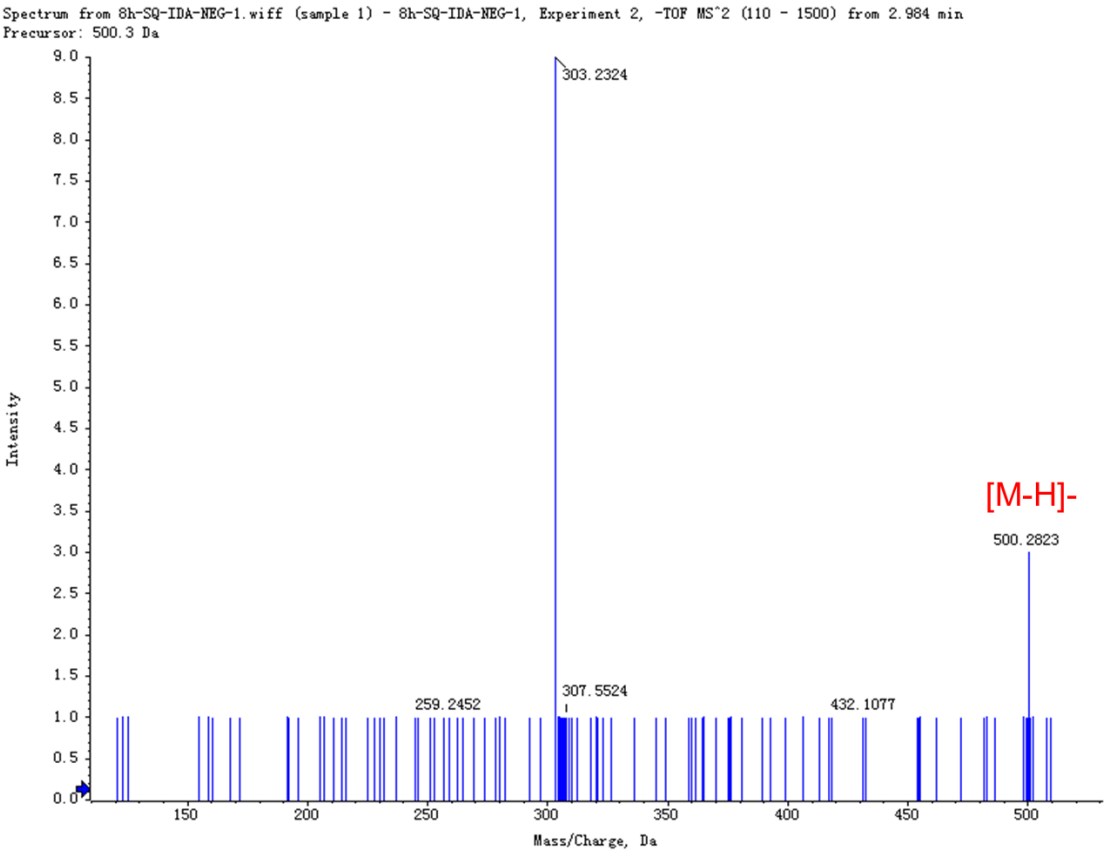


LyPE(18:1):

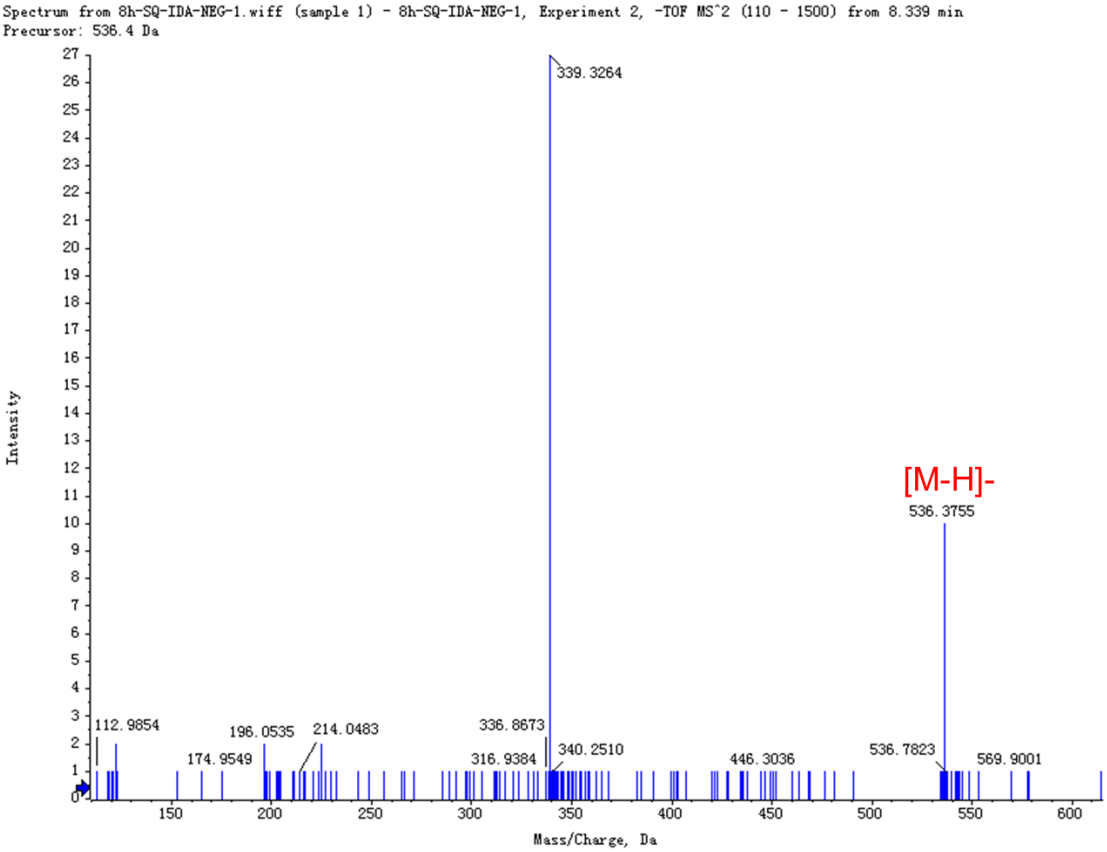
LyPE(20:1):



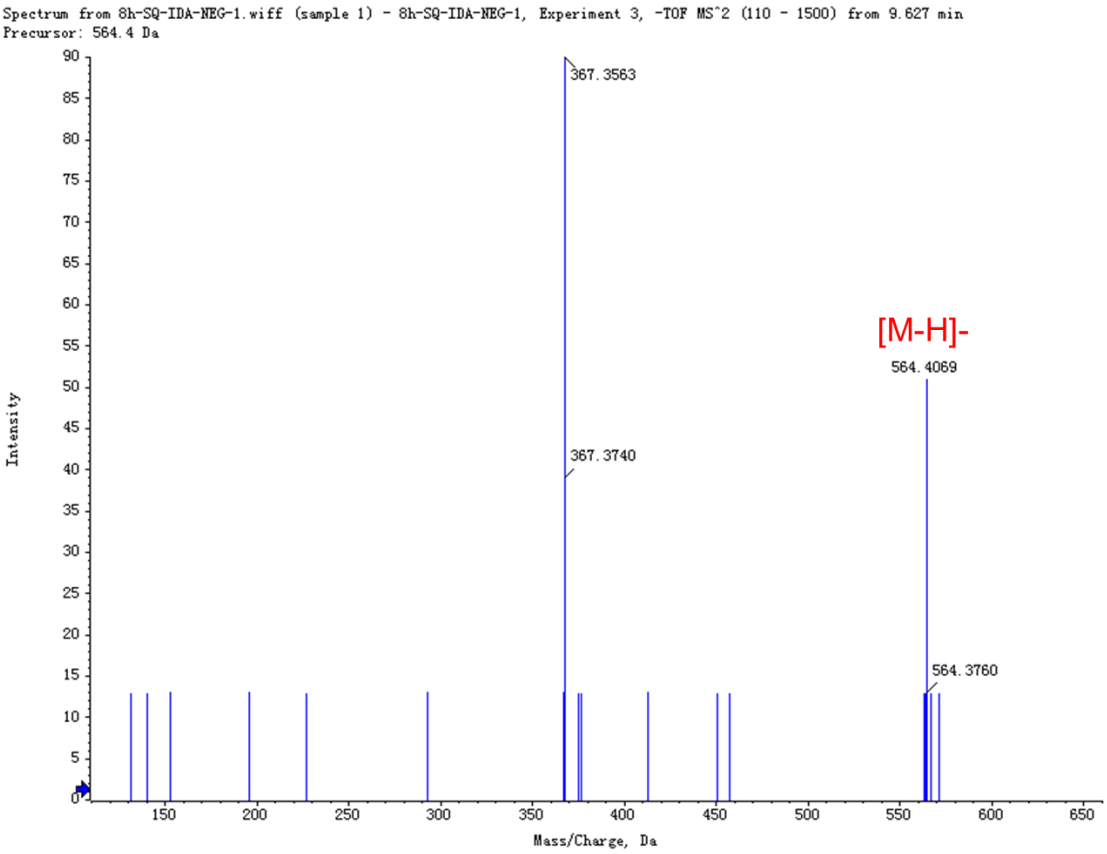
LyPE(20:4):



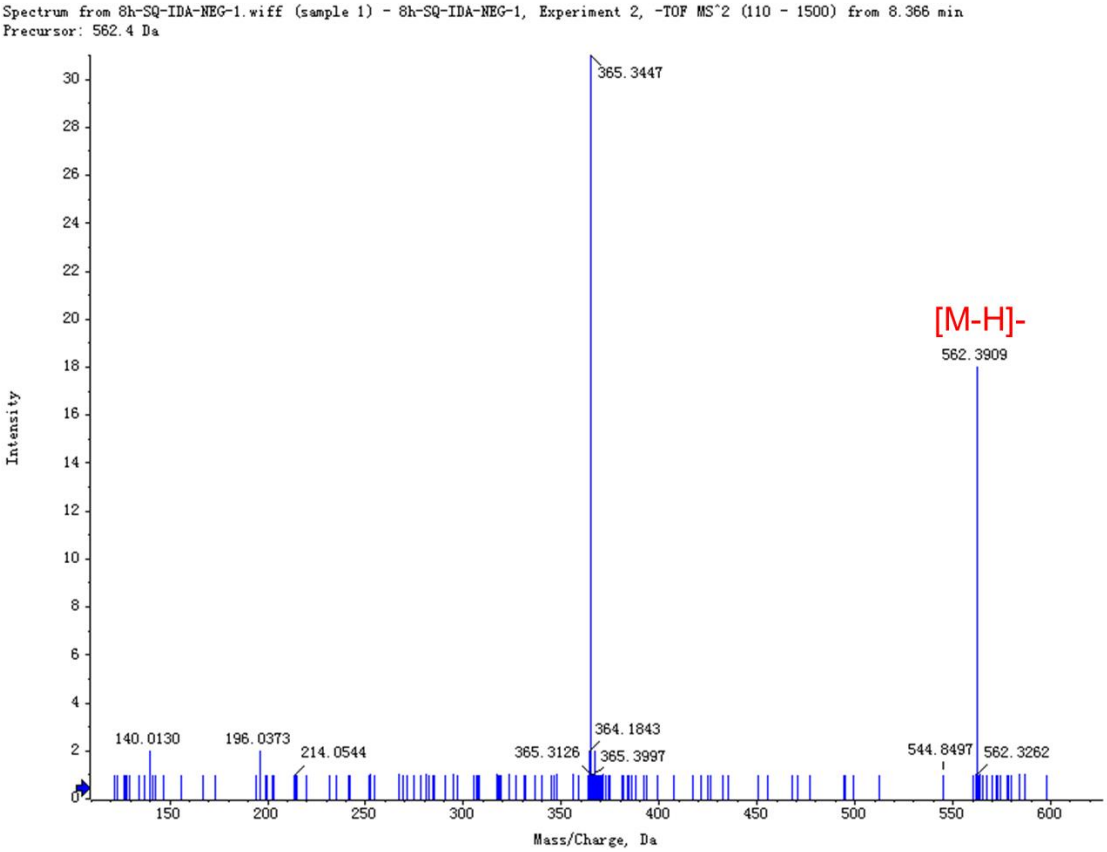
LyPE(22:0):



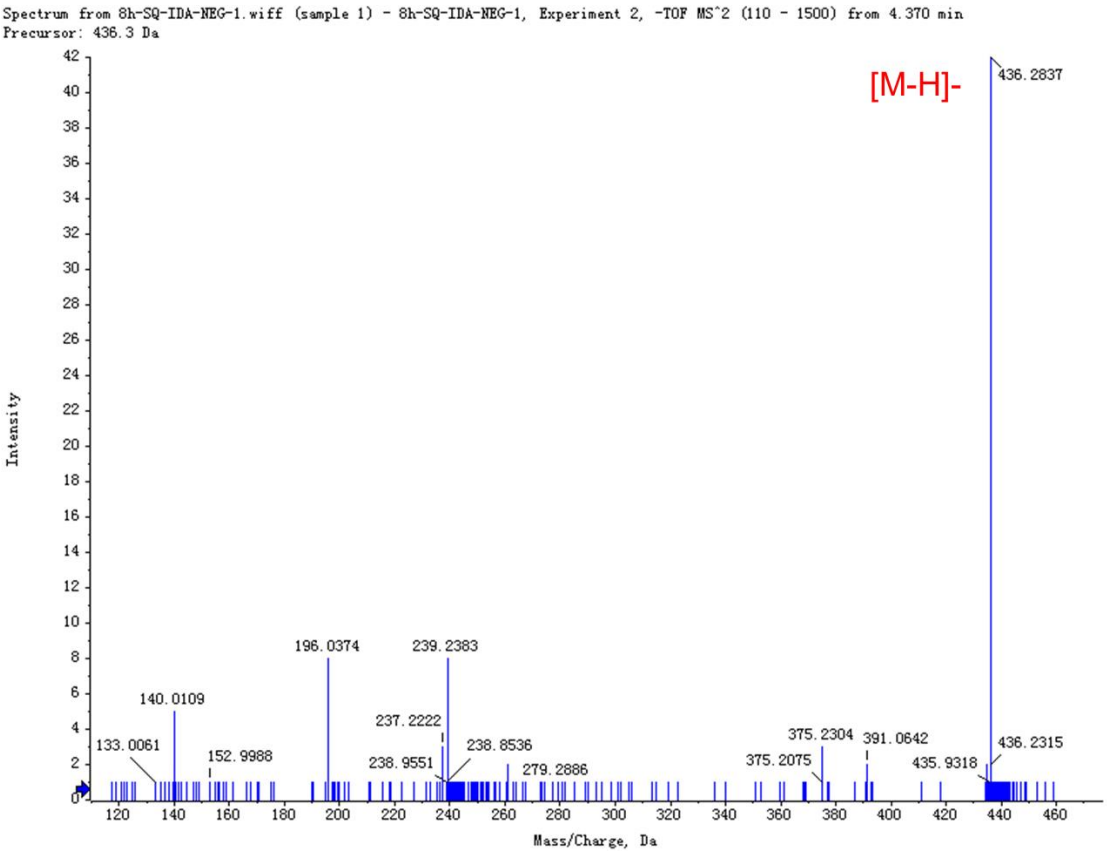
LyPE(24:0):



LyPE(24:1):

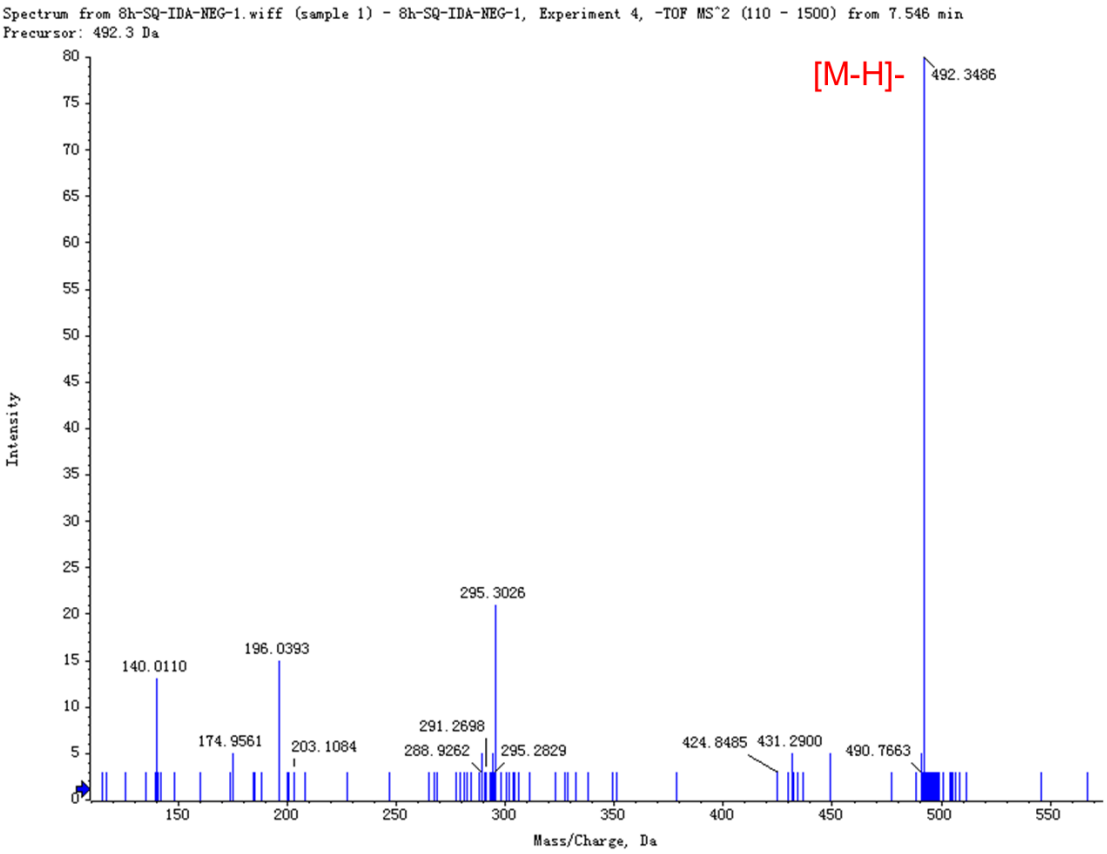


LyPE(P-16:0):

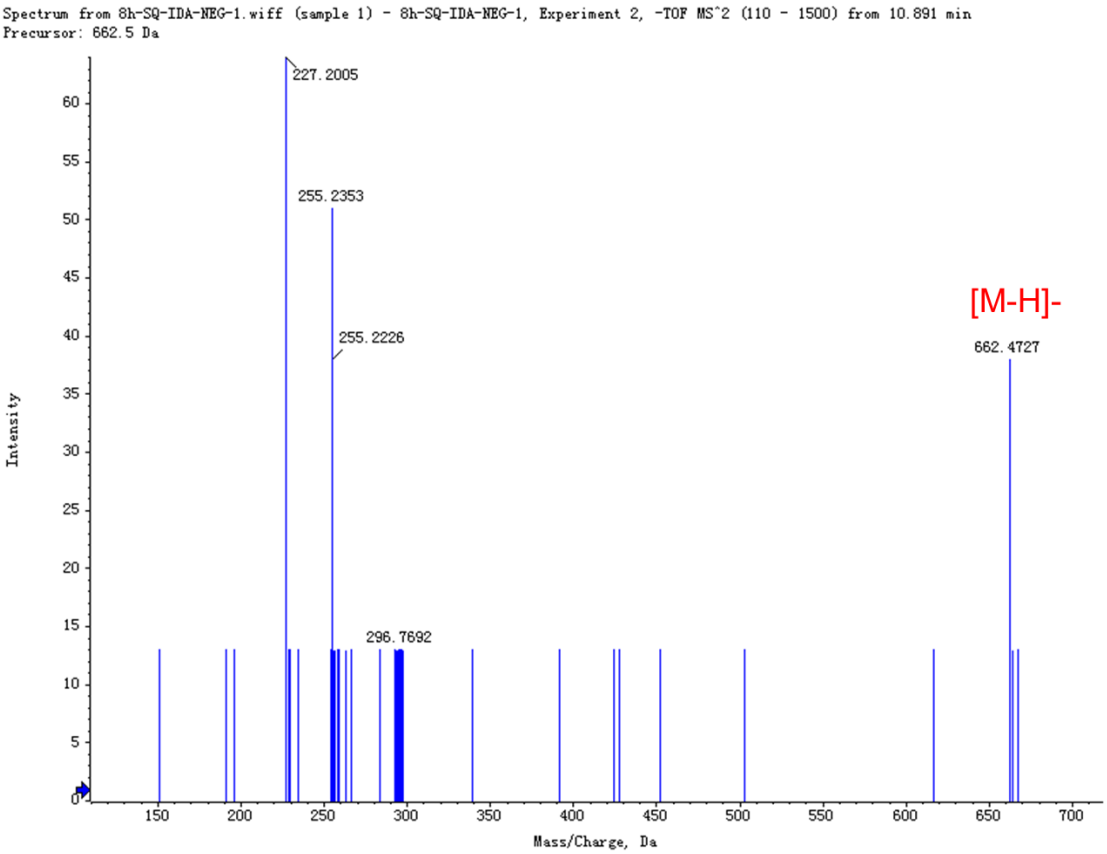


LyPE(P-18:0):

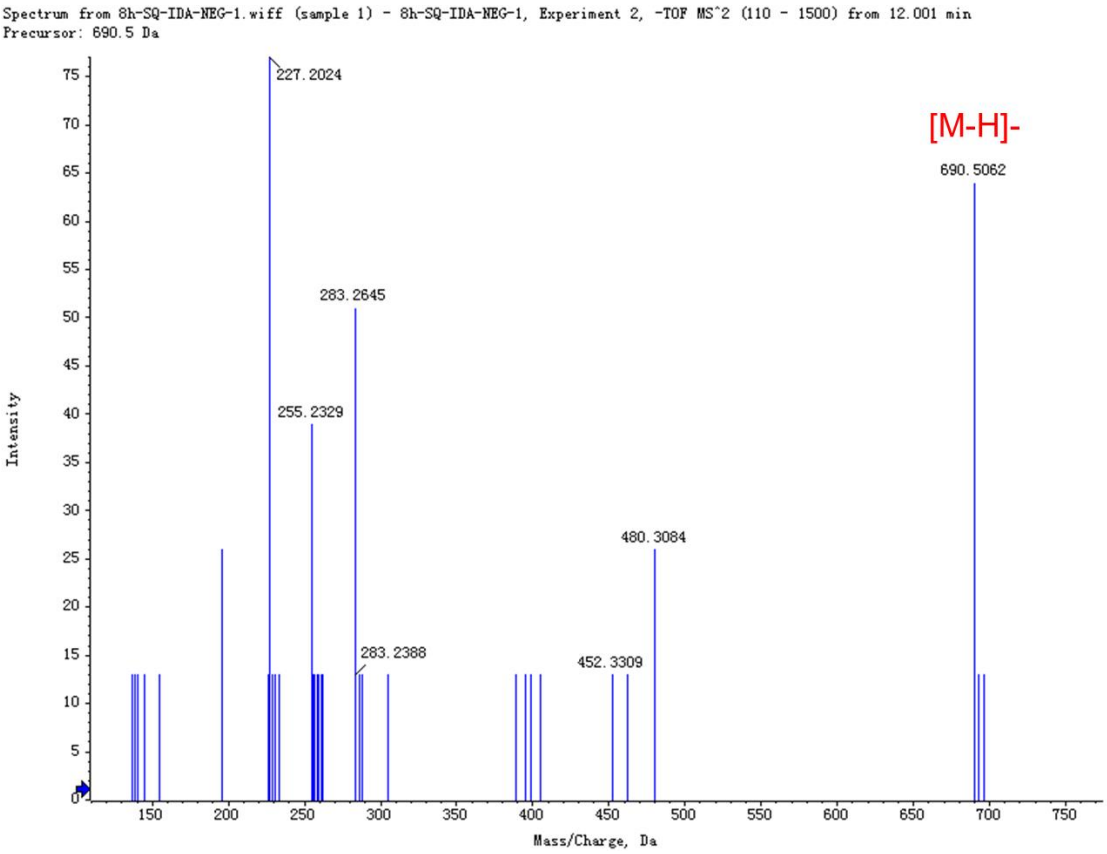
LyPE(P-20:0):



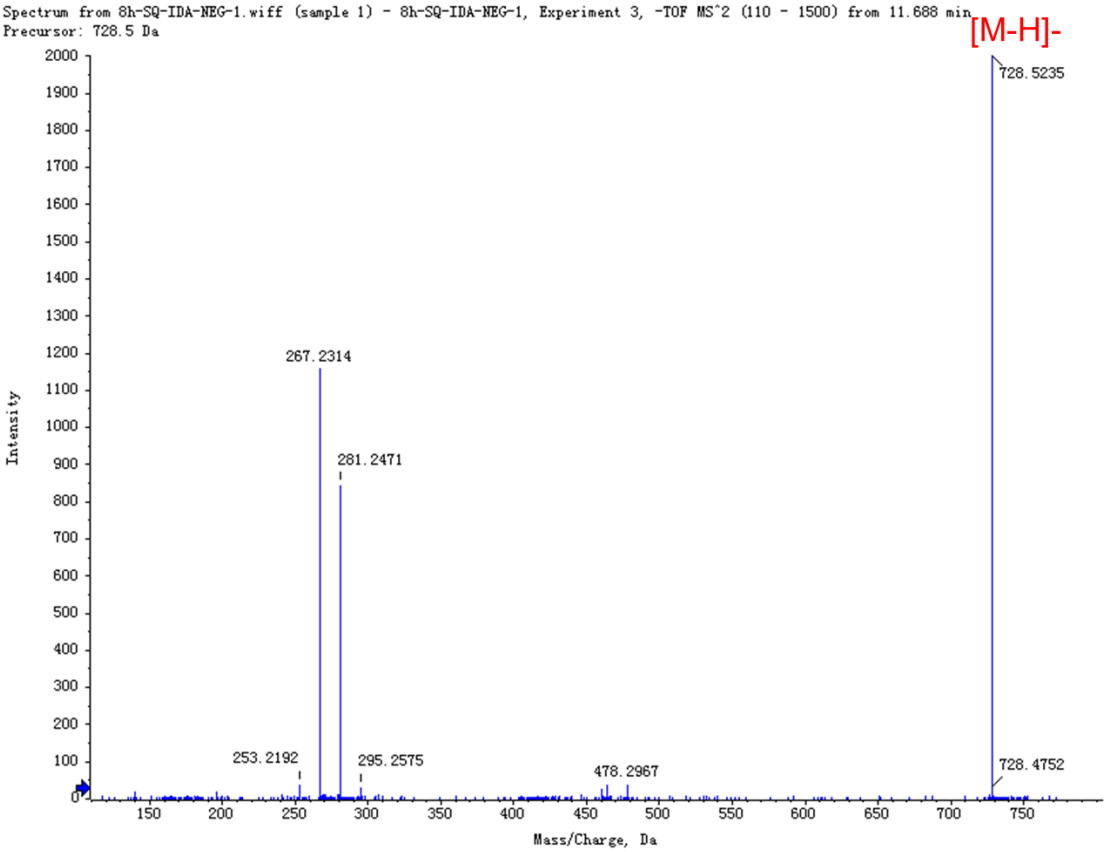
PE(30:0):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 2, -TOF MS^2 (110 - 1500) from 10.891 min
Precursor: 662.5 Da
227.2005
255.2353
255.2226
296.7692
[M-H]-
662.4727
Intensity
Mass/Charge, Da

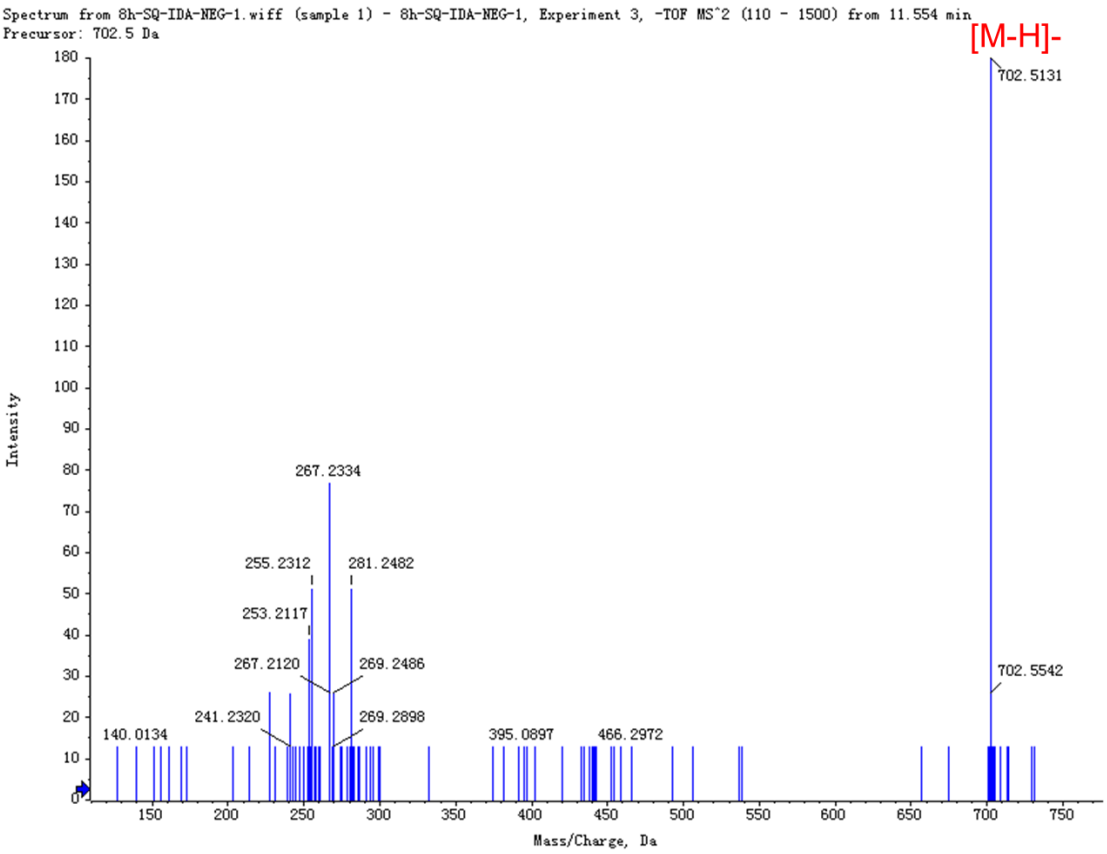
PE(32:0):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 2, -TOF MS^2 (110 - 1500) from 12.001 min
Precursor: 690.5 Da
227.2024
[M-H]-
690.5062
283.2645
255.2329
480.3084
283.2388
452.3309
Intensity
Mass/Charge, Da

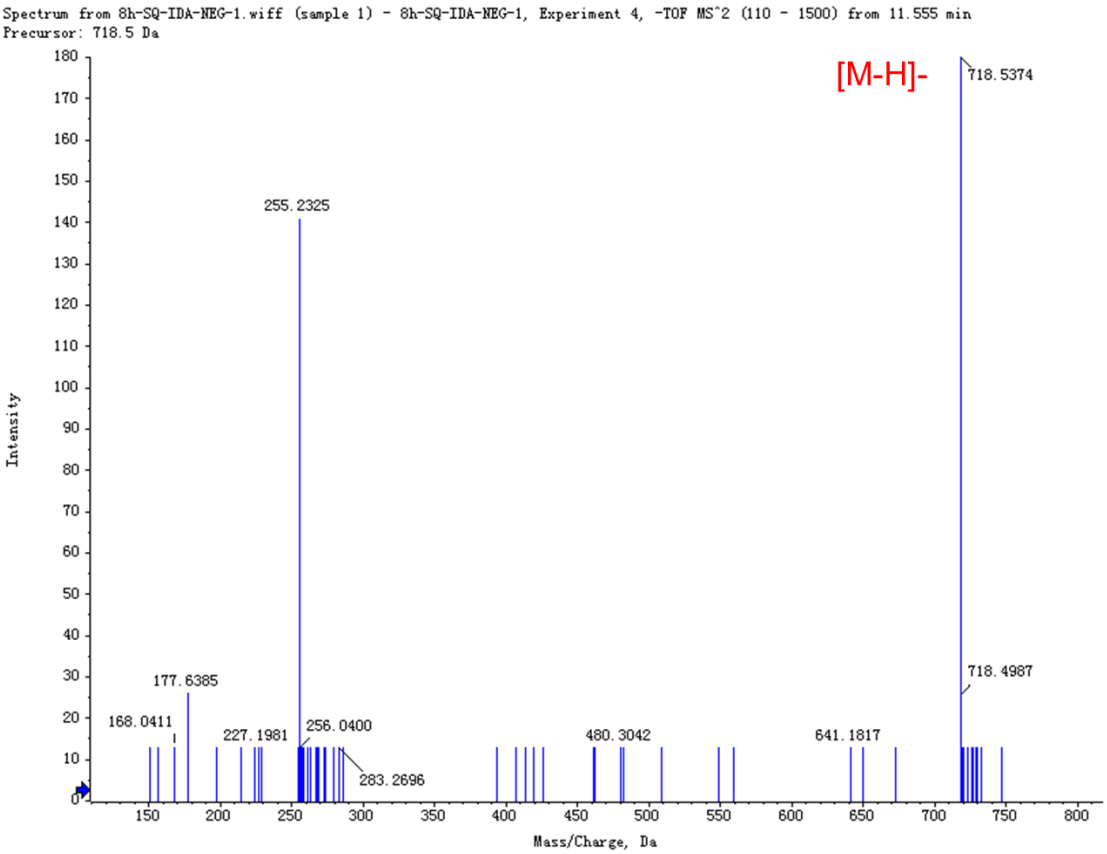
PE(35:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 3, -TOF MS^2 (110 - 1500) from 11.688 min
Precursor: 728.5 Da
[M-H]-
728.5235
267.2314
281.2471
253.2192
295.2575
478.2967
728.4752
Intensity
Mass/Charge, Da

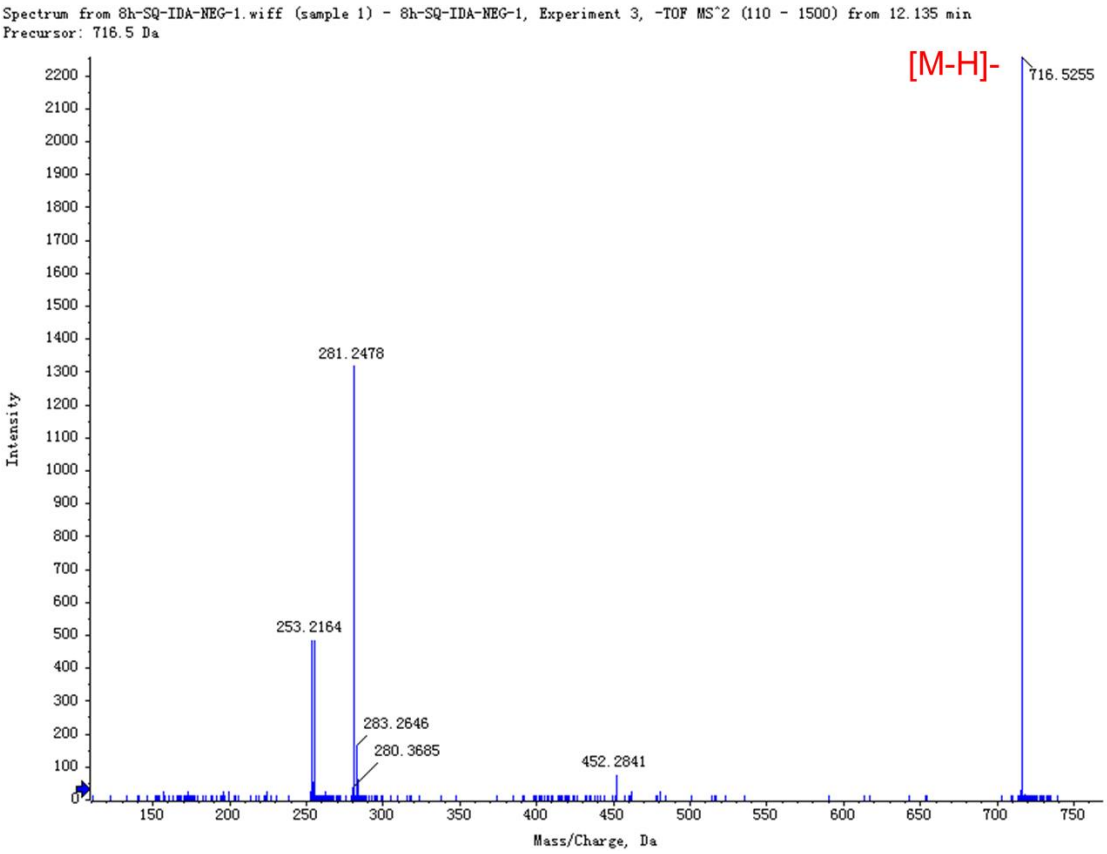
PE(33:1):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 3, -TOF MS^2 (110 - 1500) from 11.554 min
Precursor: 702.5 Da
[M-H]-
702.5131
267.2334
255.2312
281.2482
253.2117
267.2120
269.2486
241.2320
269.2898
140.0134
395.0897
466.2972
702.5542
Intensity
Mass/Charge, Da

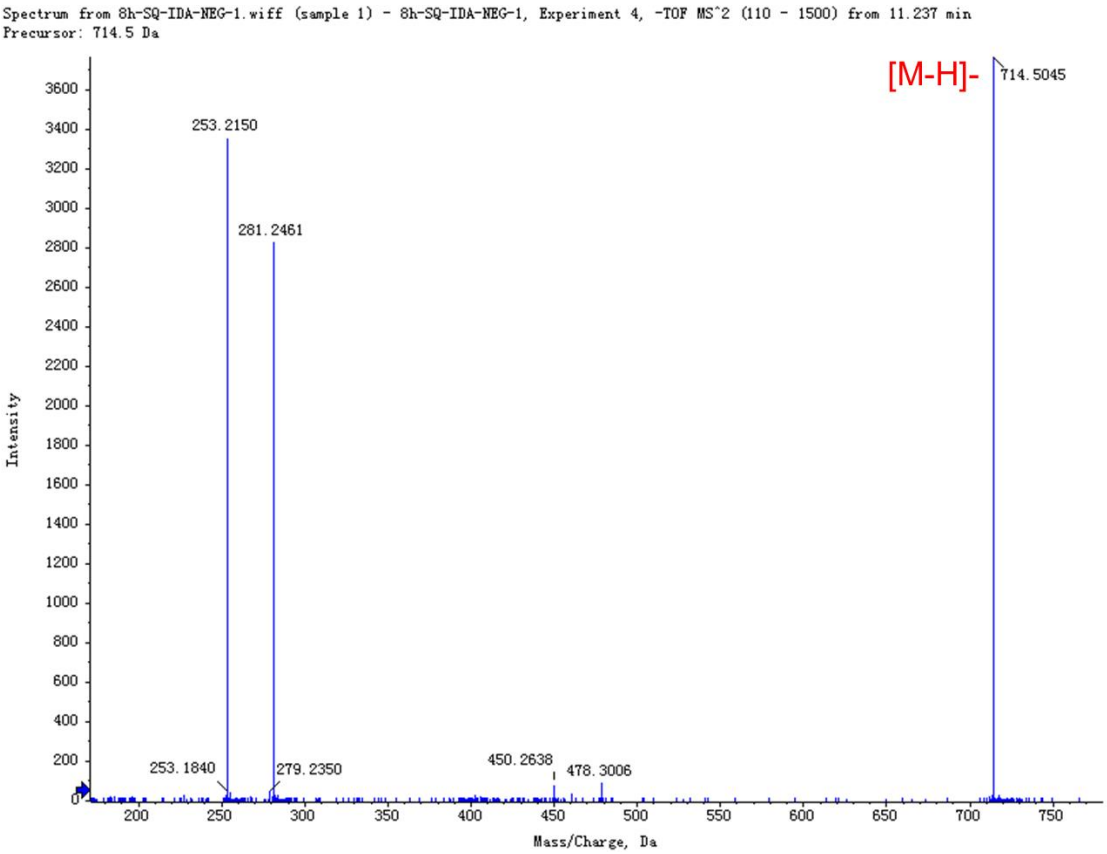
PE(34:0):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 4, -TOF MS^2 (110 - 1500) from 11.555 min
Precursor: 718.5 Da
[M-H]-
718.5374
255.2325
177.6385
168.0411
227.1981
256.0400
283.2696
480.3042
641.1817
718.4987
Intensity
Mass/Charge, Da

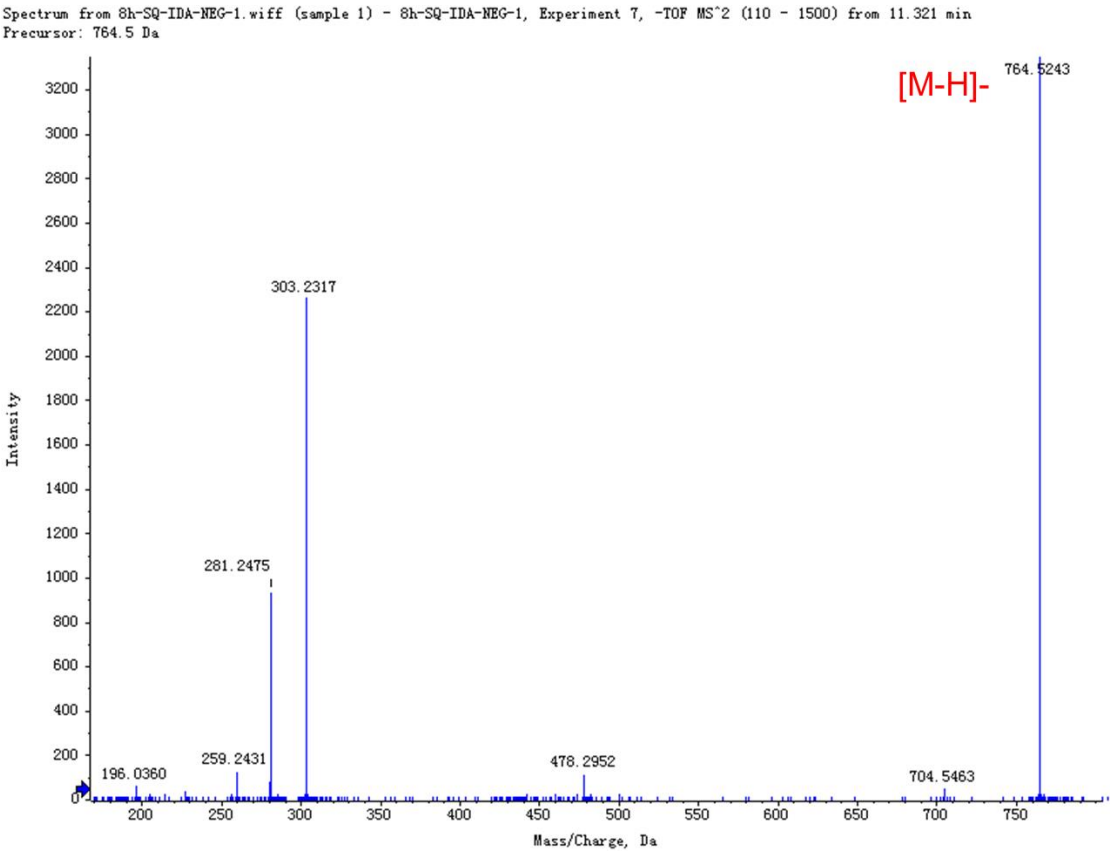
PE(34:1):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 3, -TOF MS^2 (110 - 1500) from 12.135 min
Precursor: 716.5 Da
[M-H]-
716.5255
281.2478
253.2164
283.2646
280.3685
452.2841
Intensity
Mass/Charge, Da

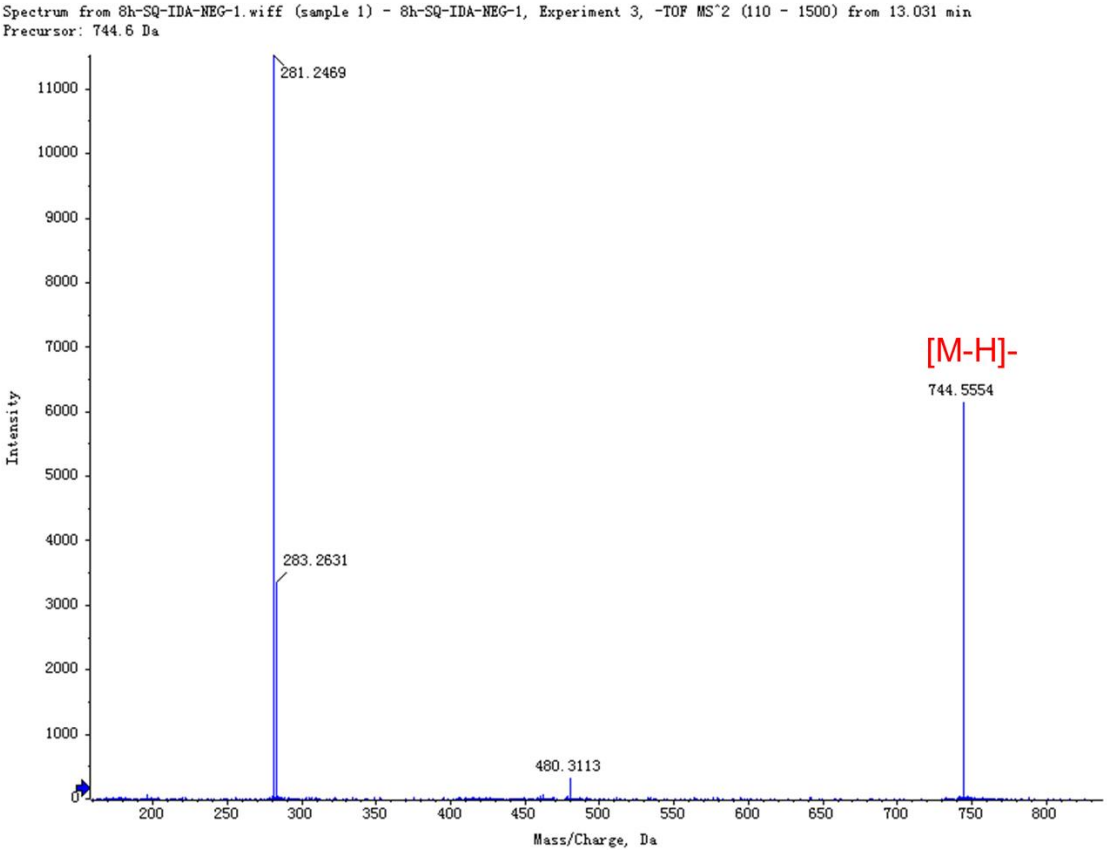
PE(34:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 4, -TOF MS^2 (110 - 1500) from 11.237 min
Precursor: 714.5 Da
[M-H]-
714.5045
253.2150
281.2461
253.1840
279.2350
450.2638
478.3006
Intensity
Mass/Charge, Da

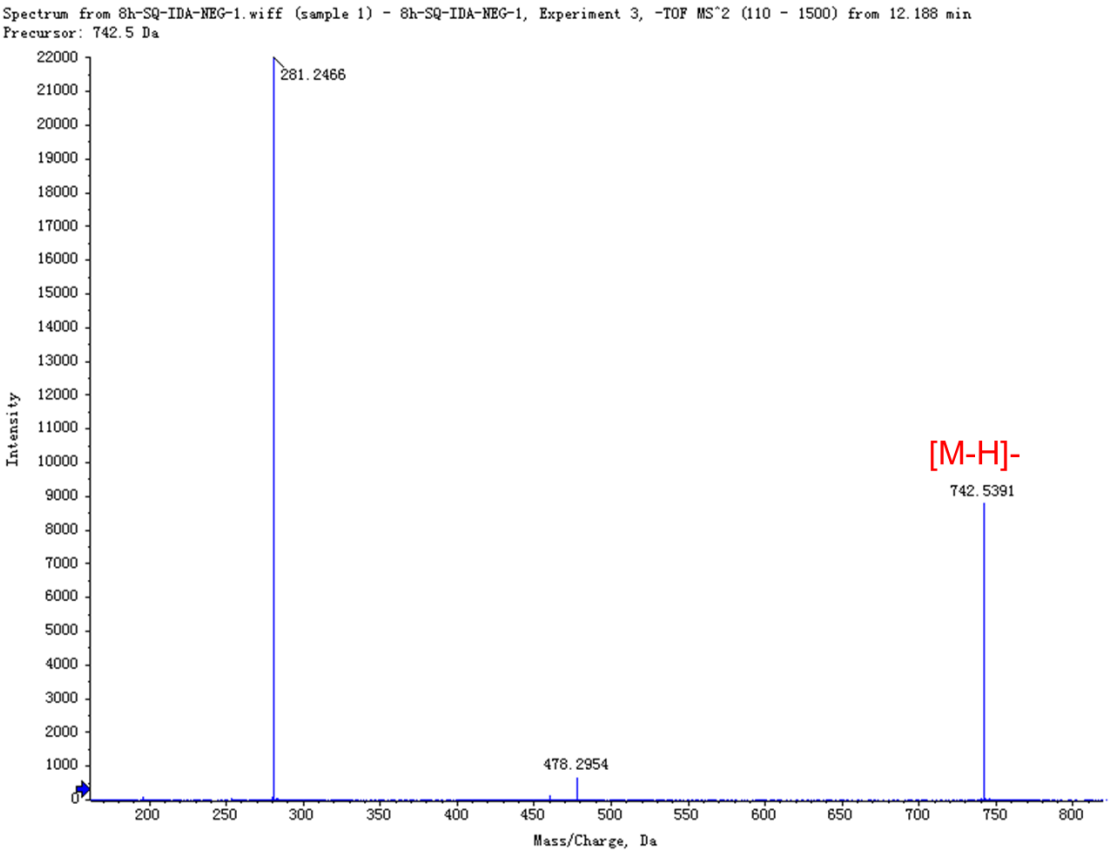
PE(38:5):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 7, -TOF MS^2 (110 - 1500) from 11.321 min
Precursor: 764.5 Da
[M-H]-
764.5243
303.2317
281.2475
196.0360
259.2431
478.2952
704.5463
Intensity
Mass/Charge, Da

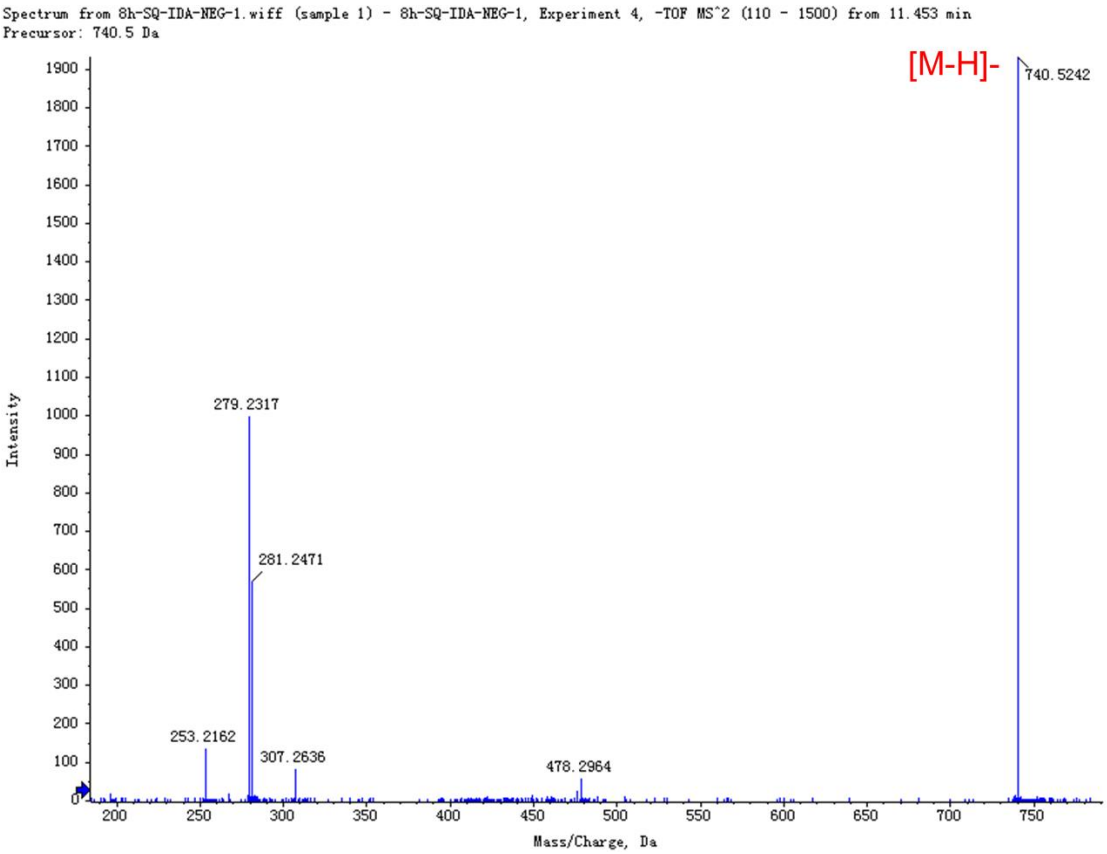
PE(36:1):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 3, -TOF MS^2 (110 - 1500) from 13.031 min
Precursor: 744.6 Da
281.2469
283.2631
480.3113
[M-H]-
744.5554
Intensity
Mass/Charge, Da

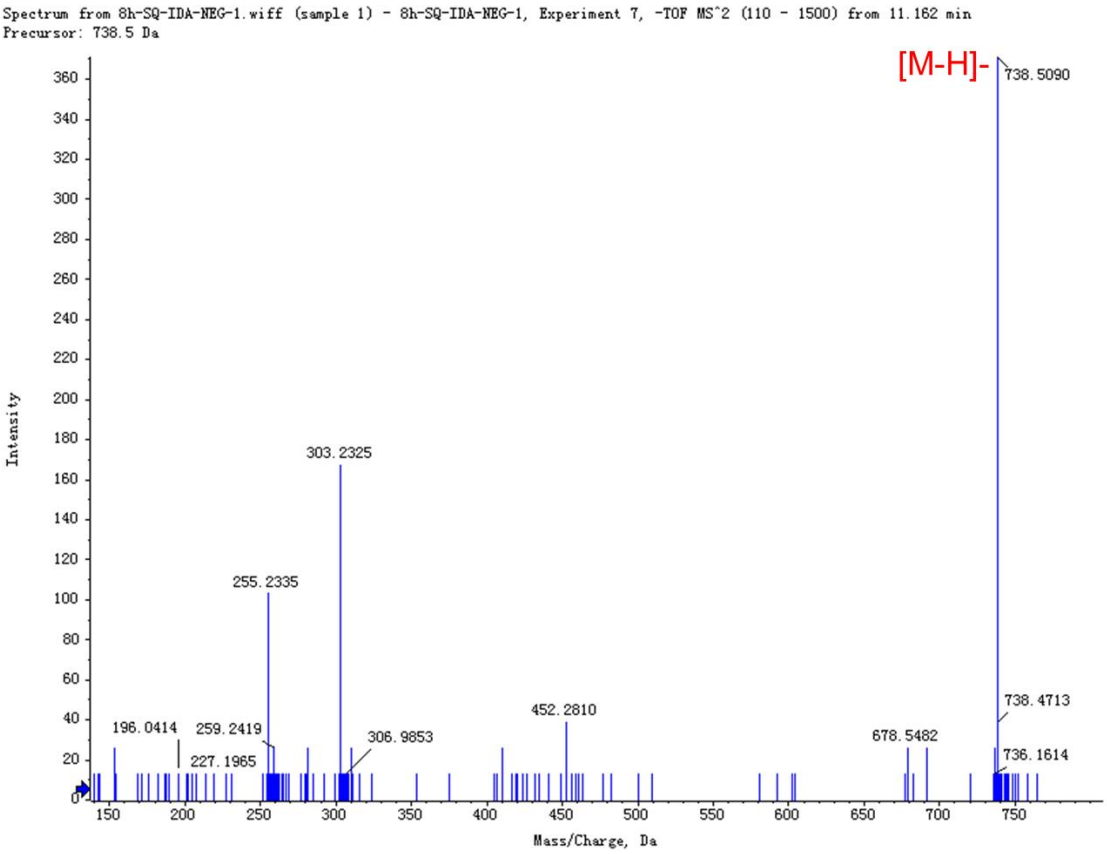
PE(36:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 3, -TOF MS^2 (110 - 1500) from 12.188 min
Precursor: 742.5 Da
281.2466
478.2954
[M-H]-
742.5391
Intensity
Mass/Charge, Da

PE(36:3):

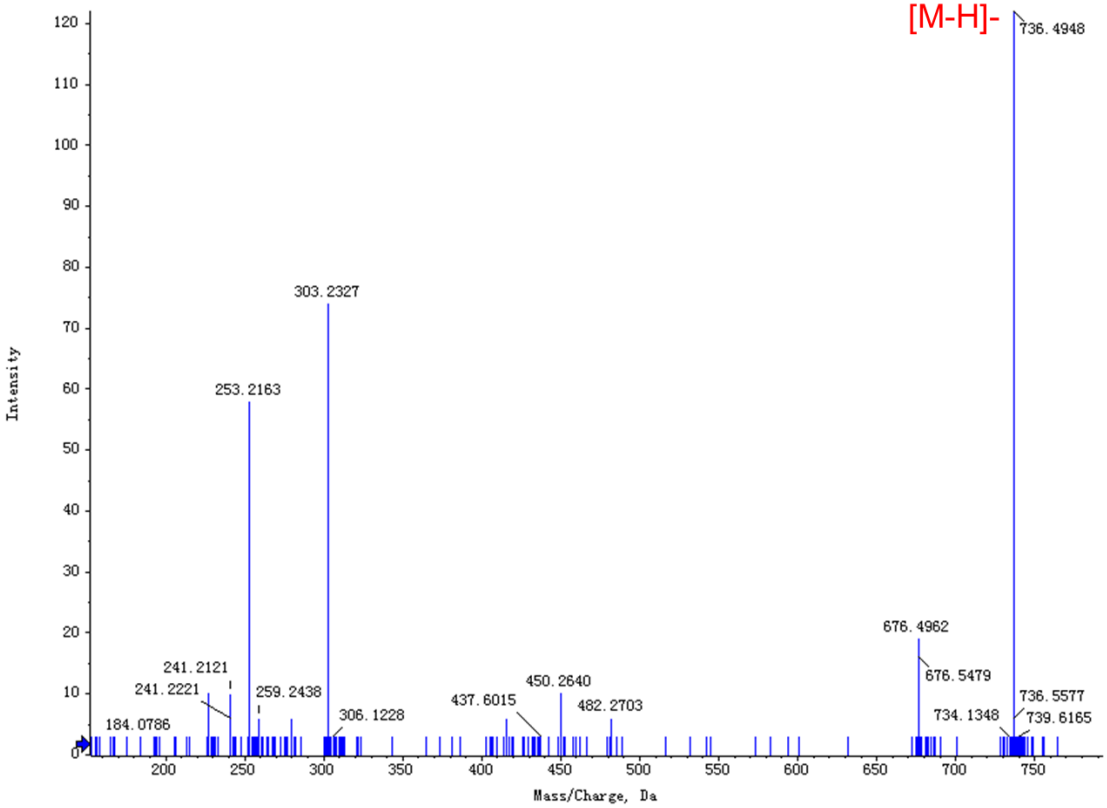

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 4, -TOF MS^2 (110 - 1500) from 11.453 min
Precursor: 740.5 Da
[M-H]-
740.5242
279.2317
281.2471
253.2162
307.2636
478.2964
Intensity
Mass/Charge, Da

PE(36:4):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 7, -TOF MS^2 (110 - 1500) from 11.162 min
Precursor: 738.5 Da
[M-H]-
738.5090
303.2325
255.2335
196.0414
259.2419
227.1965
306.9853
452.2810
678.5482
738.4713
736.1614
Intensity
Mass/Charge, Da

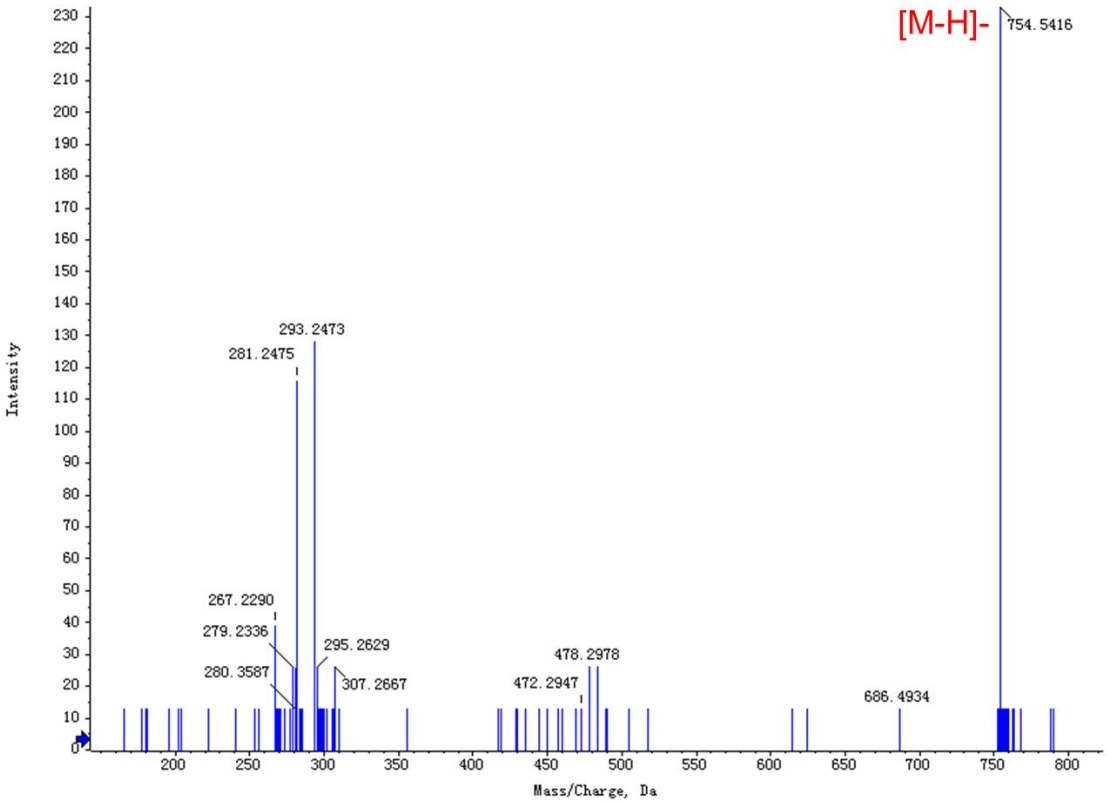
PE(36:5):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 3, -TOF MS^2 (110 - 1500) from 10.281 min
Precursor: 736.5 Da



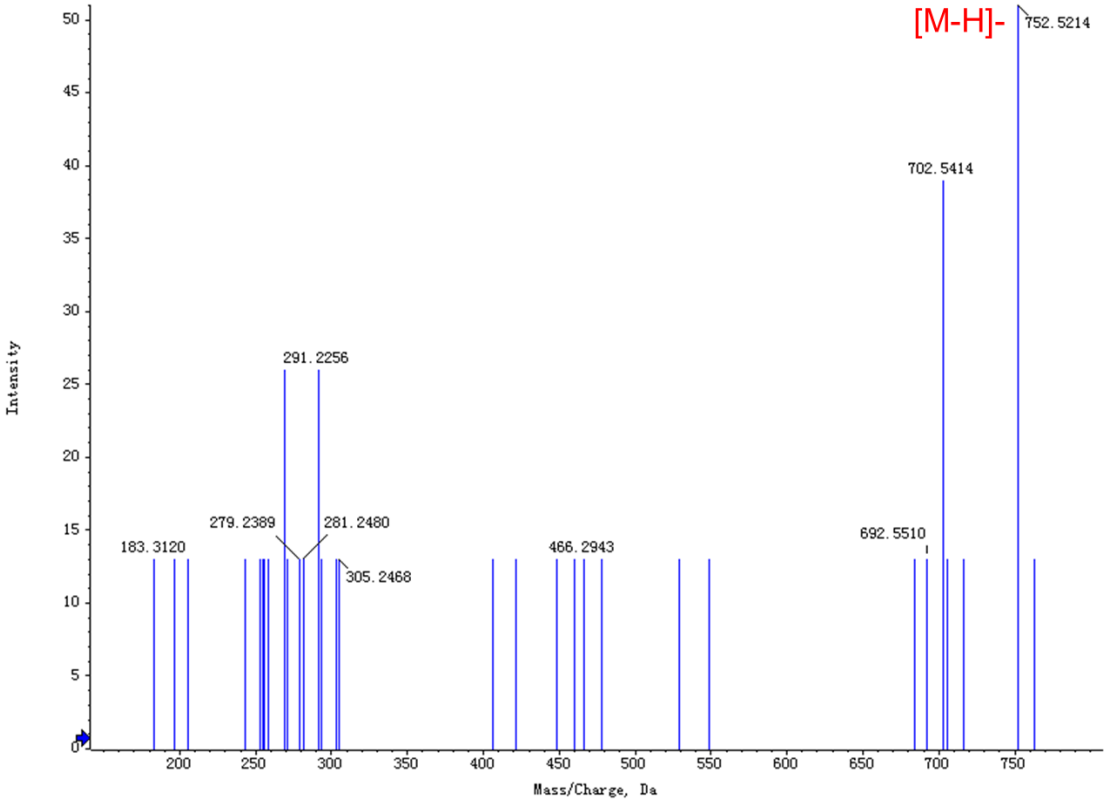
PE(37:3):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 8, -TOF MS^2 (110 - 1500) from 11.930 min
Precursor: 754.5 Da



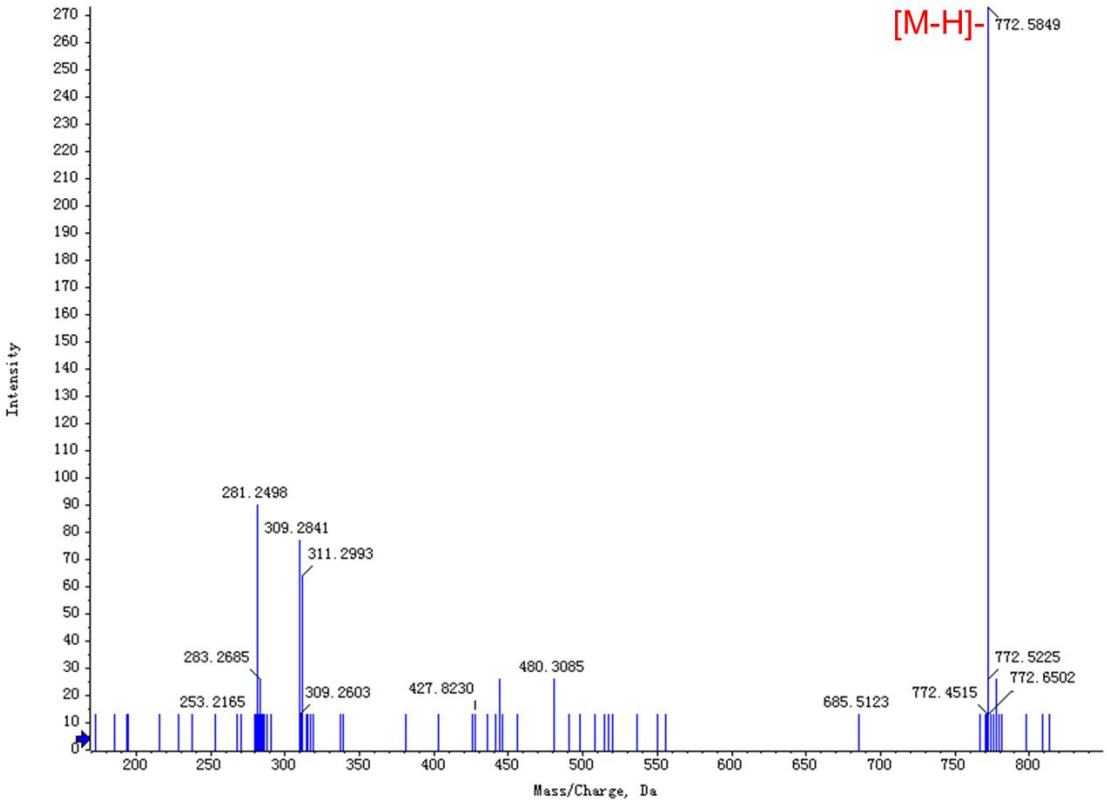
PE(37:4):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 5, -TOF MS^2 (110 - 1500) from 11.530 min
Precursor: 752.5 Da

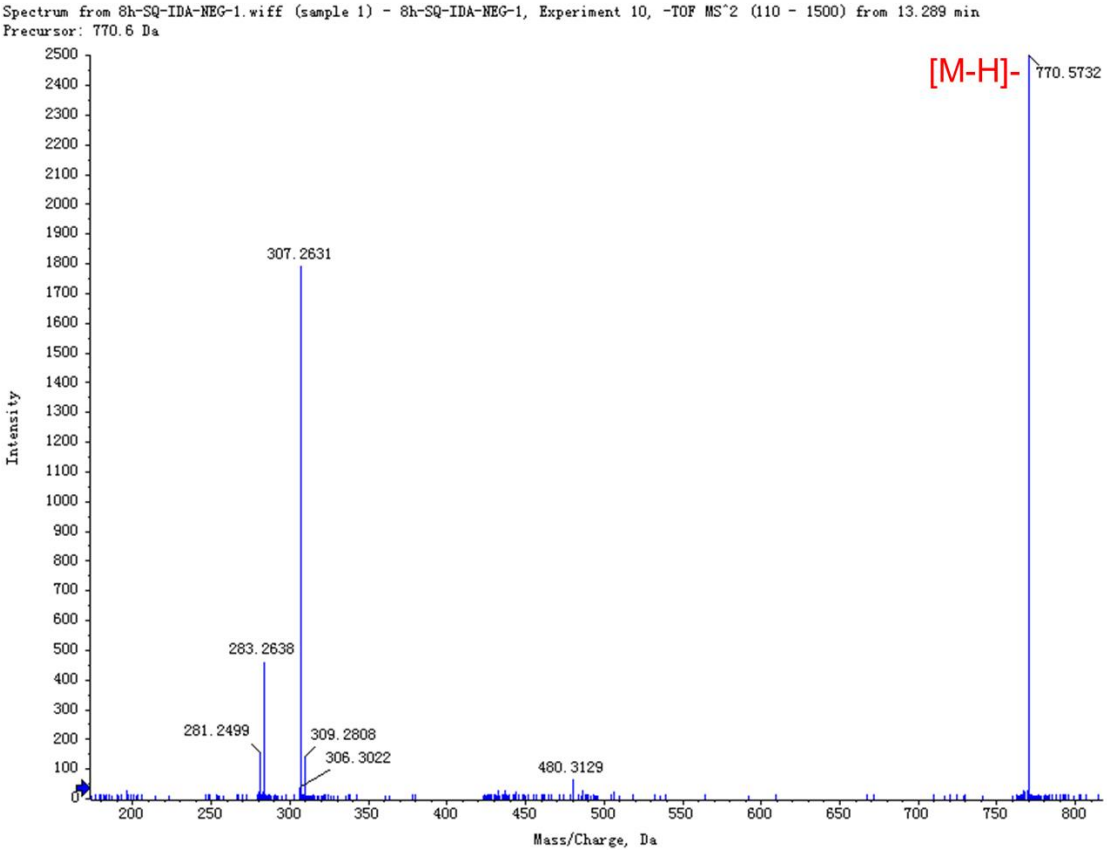


PE(38:1):

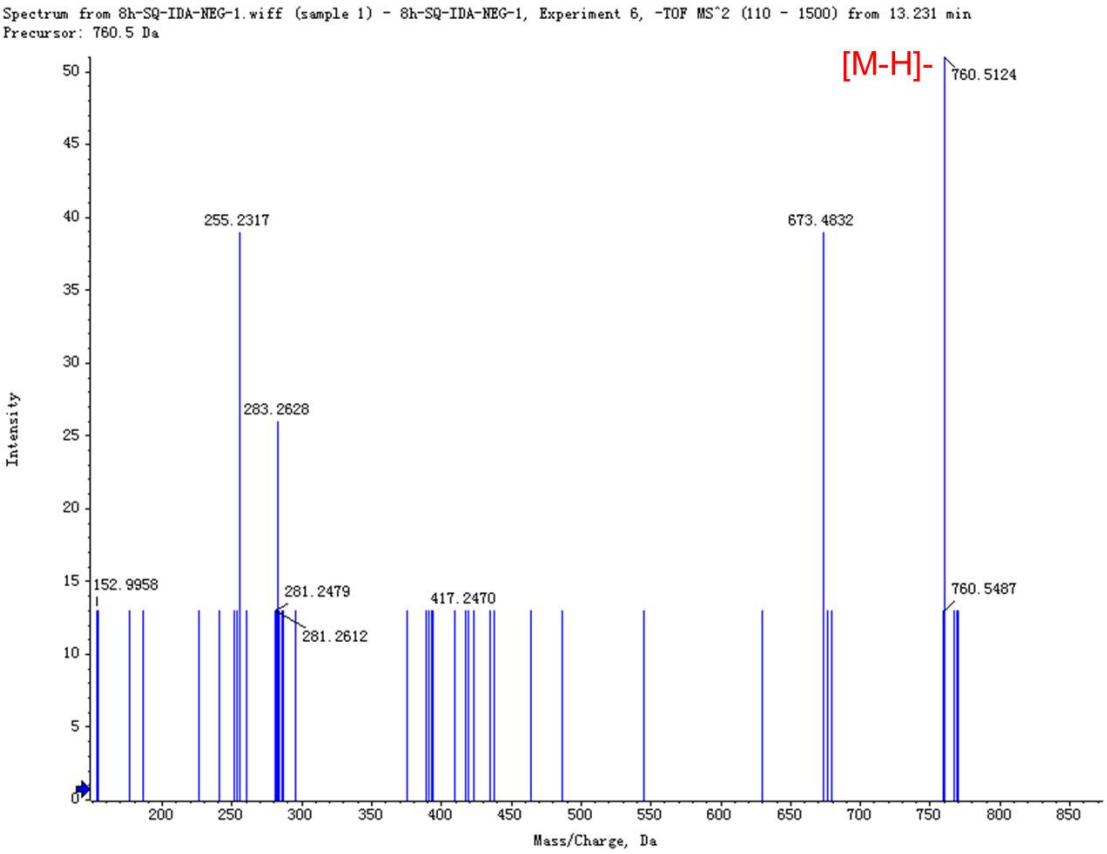
Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 7, -TOF MS^2 (110 - 1500) from 14.032 min
Precursor: 772.6 Da



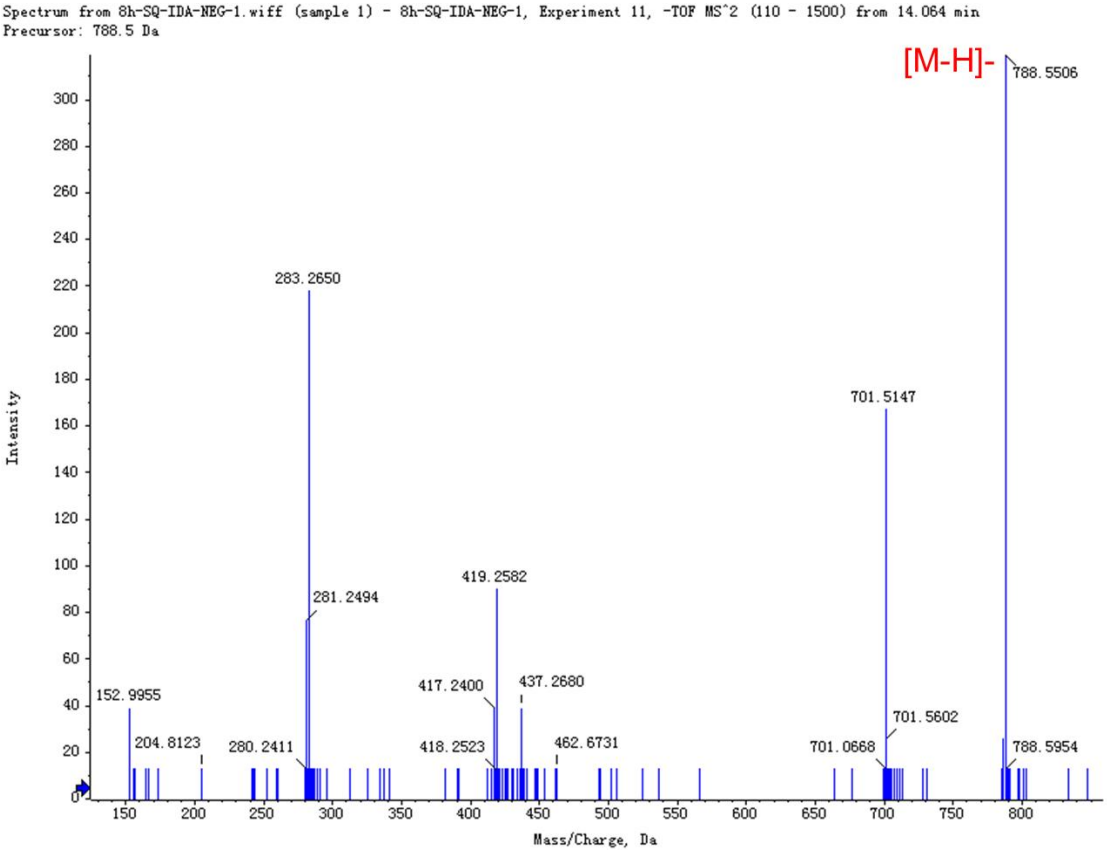
PE(38:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 10, -TOF MS^2 (110 - 1500) from 13.289 min
Precursor: 770.6 Da
[M-H]-
770.5732
307.2631
283.2638
281.2499
309.2808
306.3022
480.3129
Intensity
Mass/Charge, Da

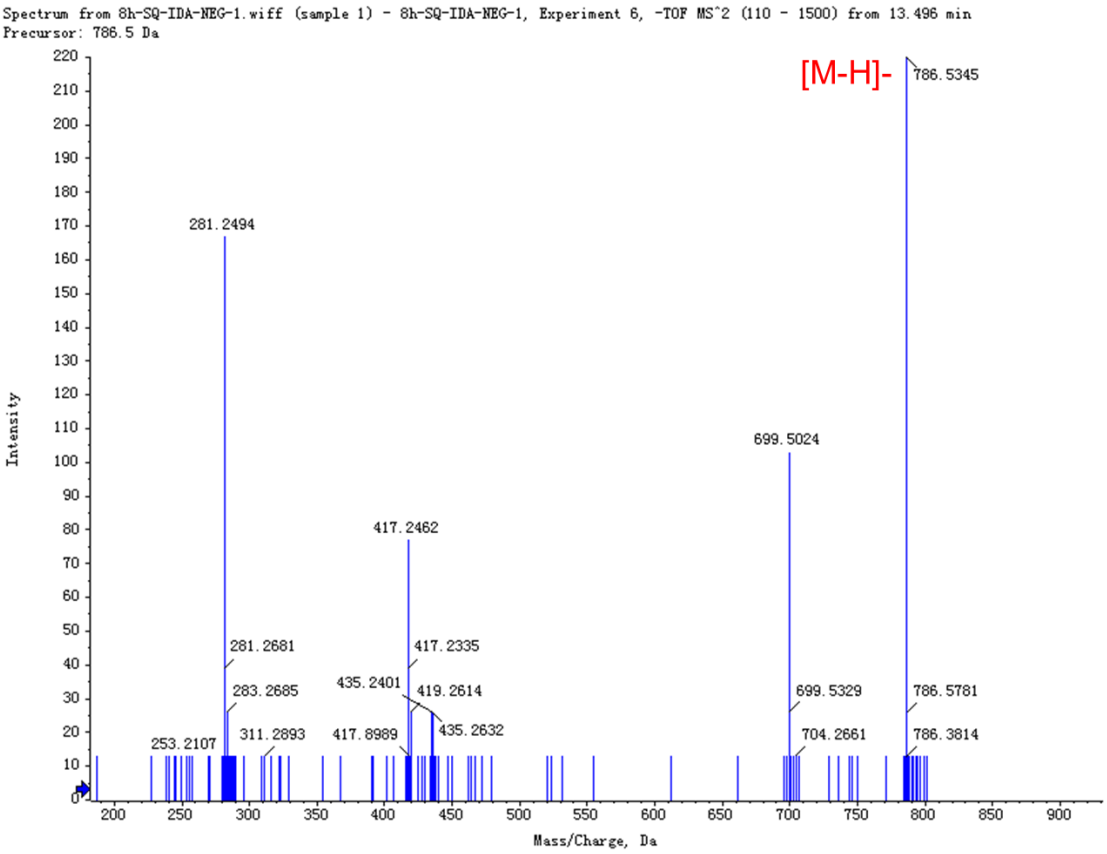
PE(38:7):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 6, -TOF MS^2 (110 - 1500) from 13.231 min
Precursor: 760.5 Da
[M-H]-
760.5124
255.2317
673.4832
283.2628
152.9958
281.2479
281.2612
417.2470
760.5487
Intensity
Mass/Charge, Da

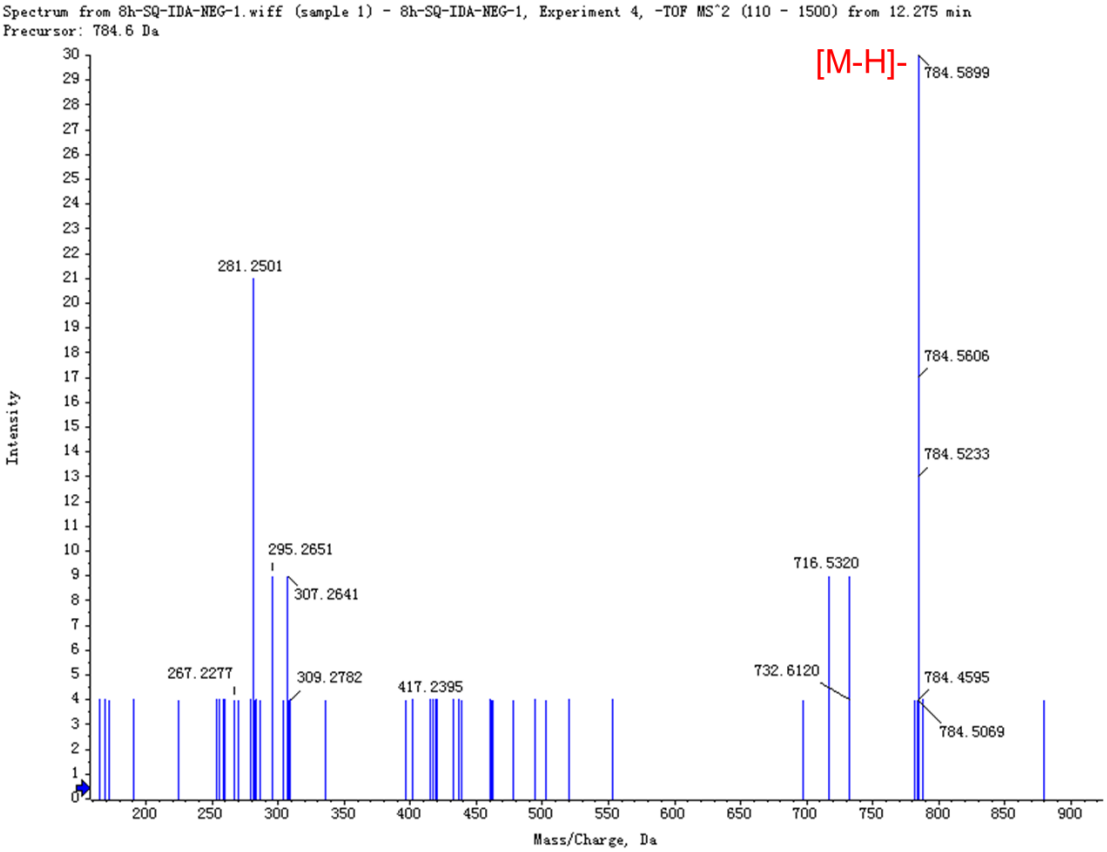
PE(40:7):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 11, -TOF MS^2 (110 - 1500) from 14.064 min
Precursor: 788.5 Da
[M-H]-
788.5506
283.2650
701.5147
419.2582
281.2494
417.2400
437.2680
152.9955
701.5602
204.8123
280.2411
418.2523
462.6731
701.0668
788.5954
Intensity
Mass/Charge, Da

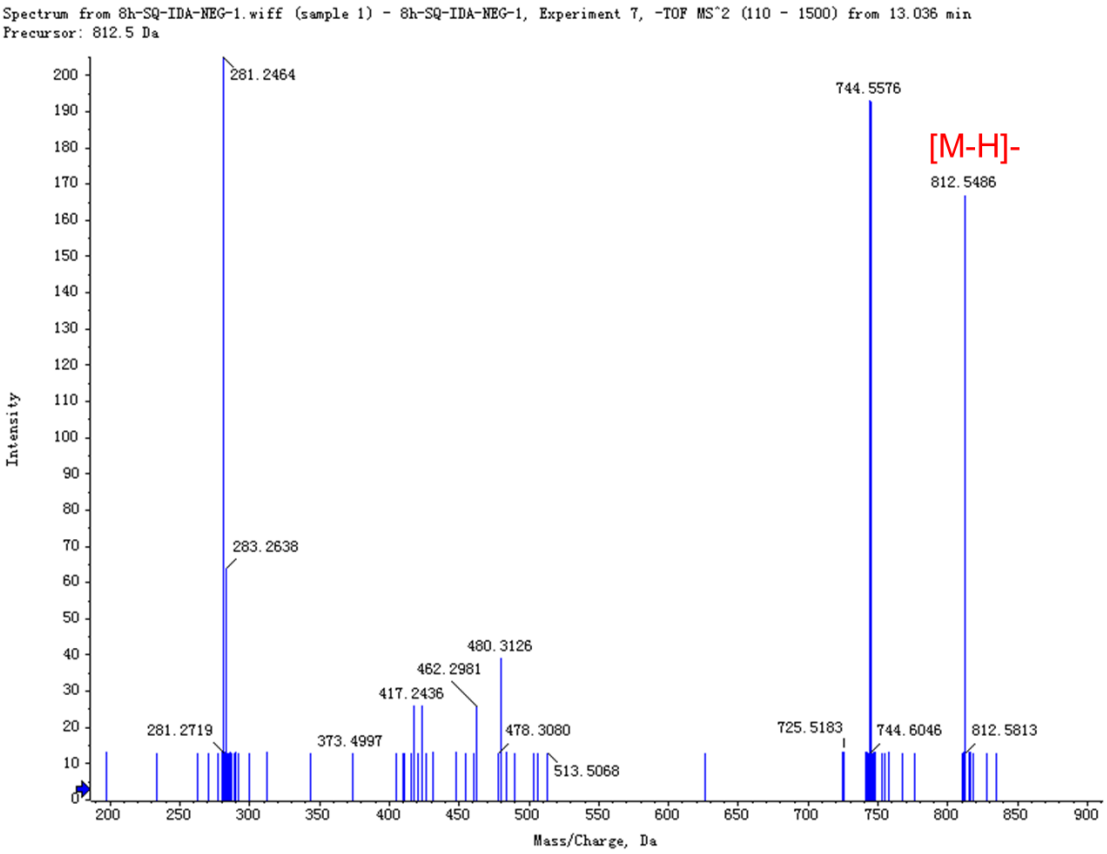
PS(36:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 6, -TOF MS^2 (110 - 1500) from 13.496 min
Precursor: 786.5 Da
[M-H]-
786.5345
281.2494
699.5024
417.2462
281.2681
417.2335
283.2685
435.2401
419.2614
699.5329
786.5781
253.2107
311.2893
417.8989
435.2632
704.2661
786.3814
Intensity
Mass/Charge, Da

PS(36:3):

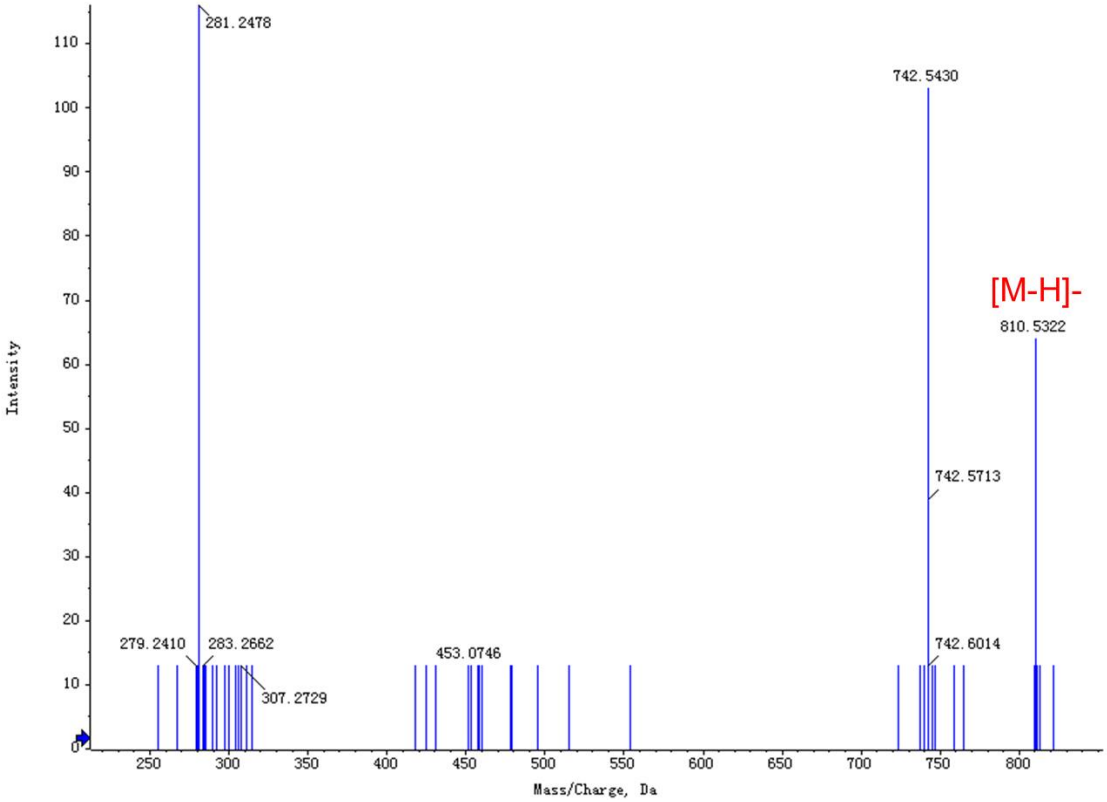

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 4, -TOF MS^2 (110 - 1500) from 12.275 min
Precursor: 784.6 Da
[M-H]-
784.5899
281.2501
784.5606
784.5233
295.2651
307.2641
716.5320
267.2277
309.2782
417.2395
732.6120
784.4595
784.5069
Intensity
Mass/Charge, Da

PS(38:3):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 7, -TOF MS^2 (110 - 1500) from 13.036 min
Precursor: 812.5 Da
281.2464
744.5576
[M-H]-
812.5486
283.2638
480.3126
462.2981
417.2436
281.2719
373.4997
478.3080
725.5183
744.6046
812.5813
513.5068
Intensity
Mass/Charge, Da

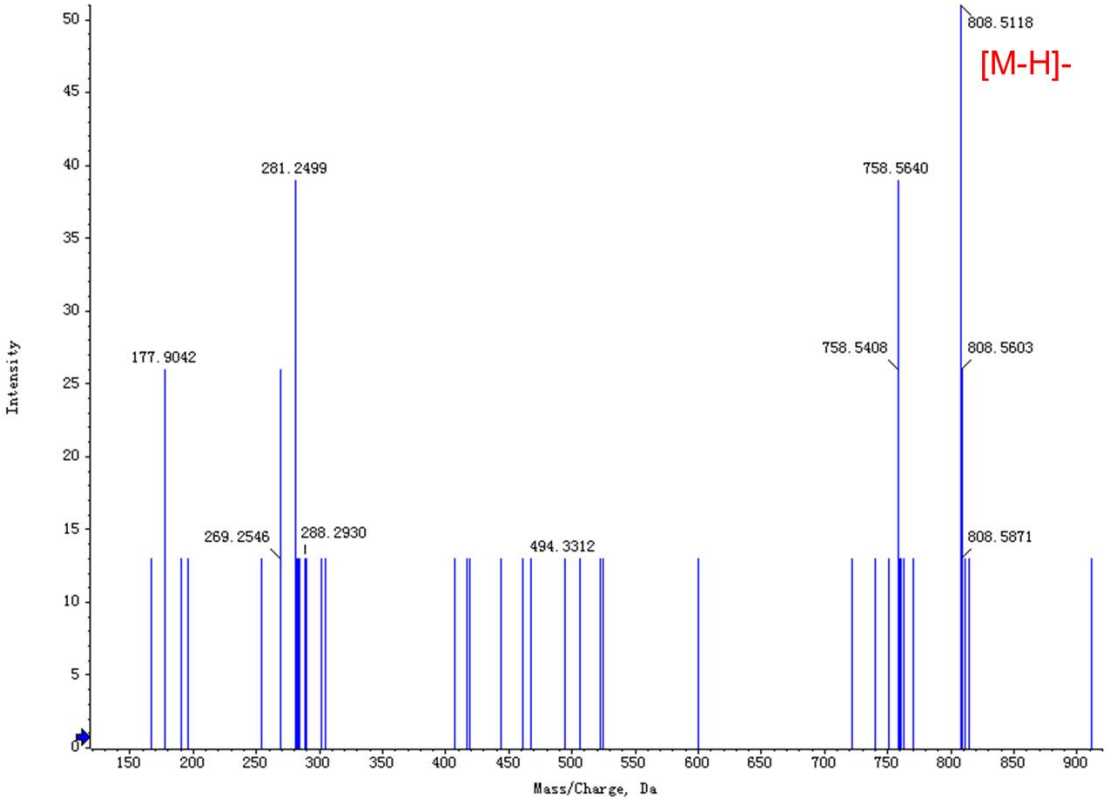
PS(38:4):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 13, -TOF MS^2 (110 - 1500) from 12.384 min
Precursor: 810.5 Da



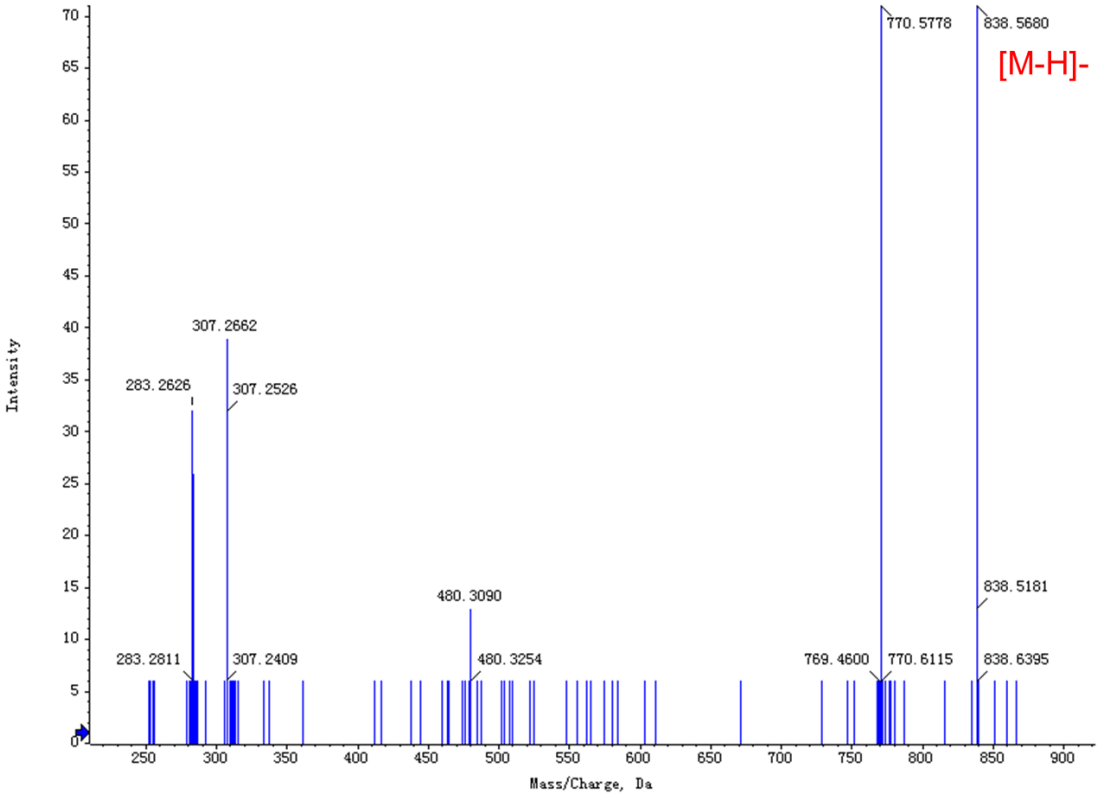
PS(38:5):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 10, -TOF MS^2 (110 - 1500) from 12.012 min
Precursor: 808.6 Da



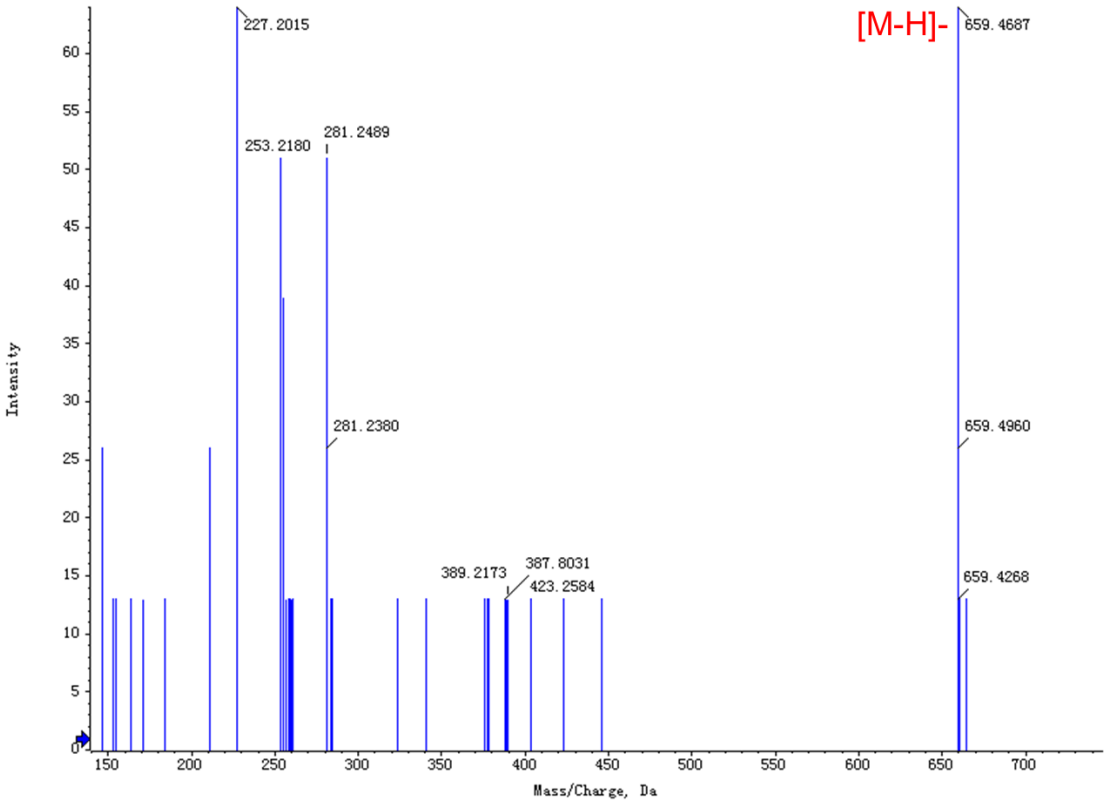
PS(40:4):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 9, -TOF MS^2 (110 - 1500) from 13.342 min
Precursor: 838.6 Da

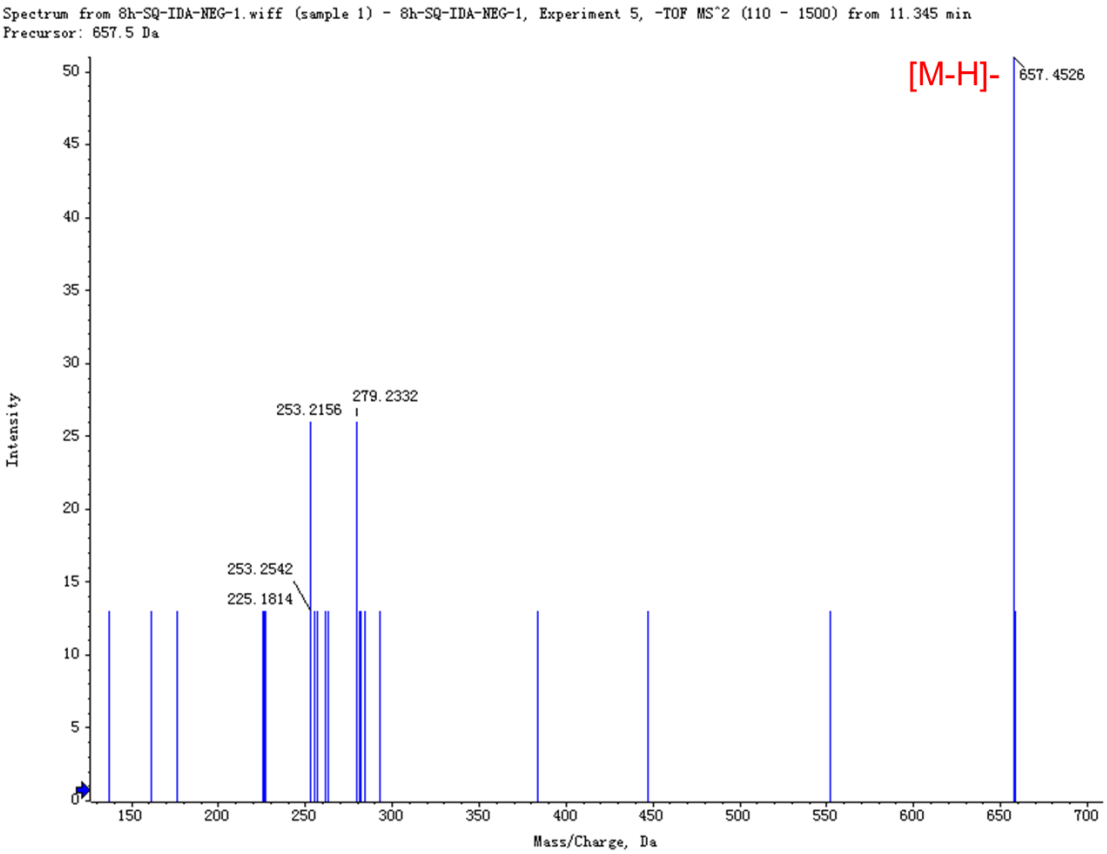


PA(33:1):

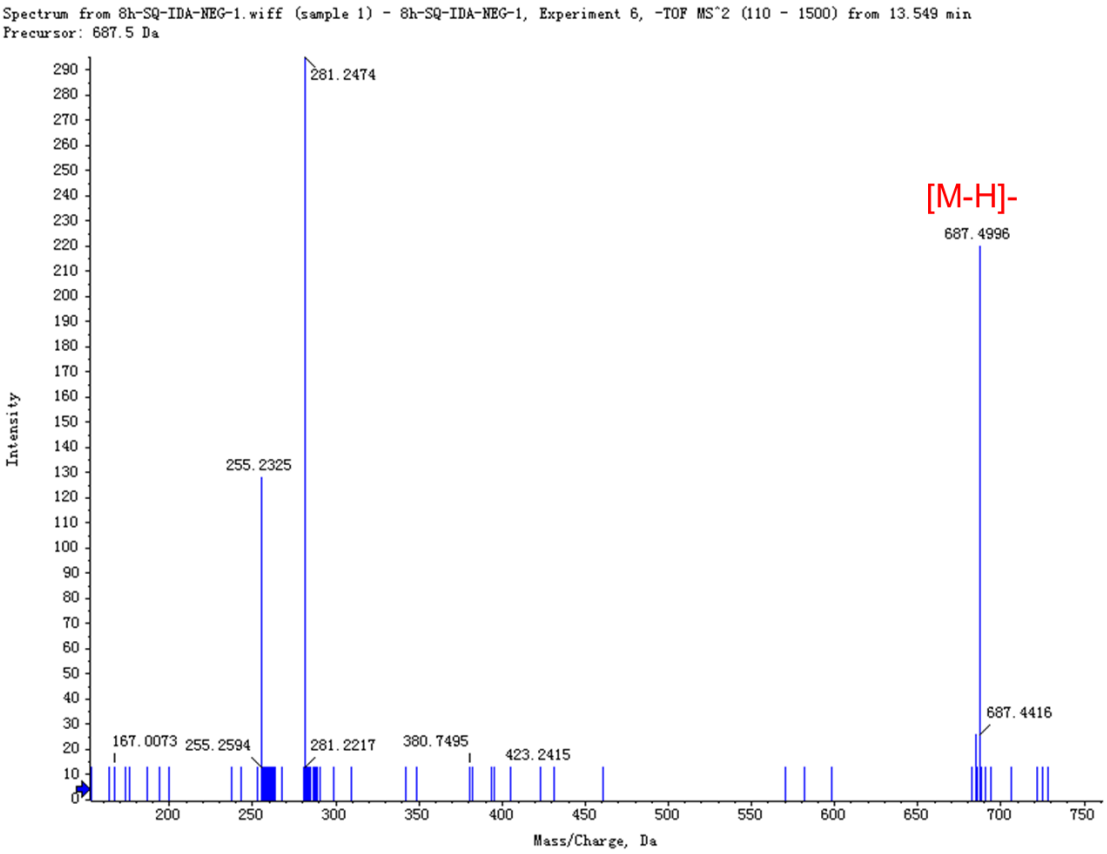
Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 7, -TOF MS^2 (110 - 1500) from 12.428 min
Precursor: 659.5 Da



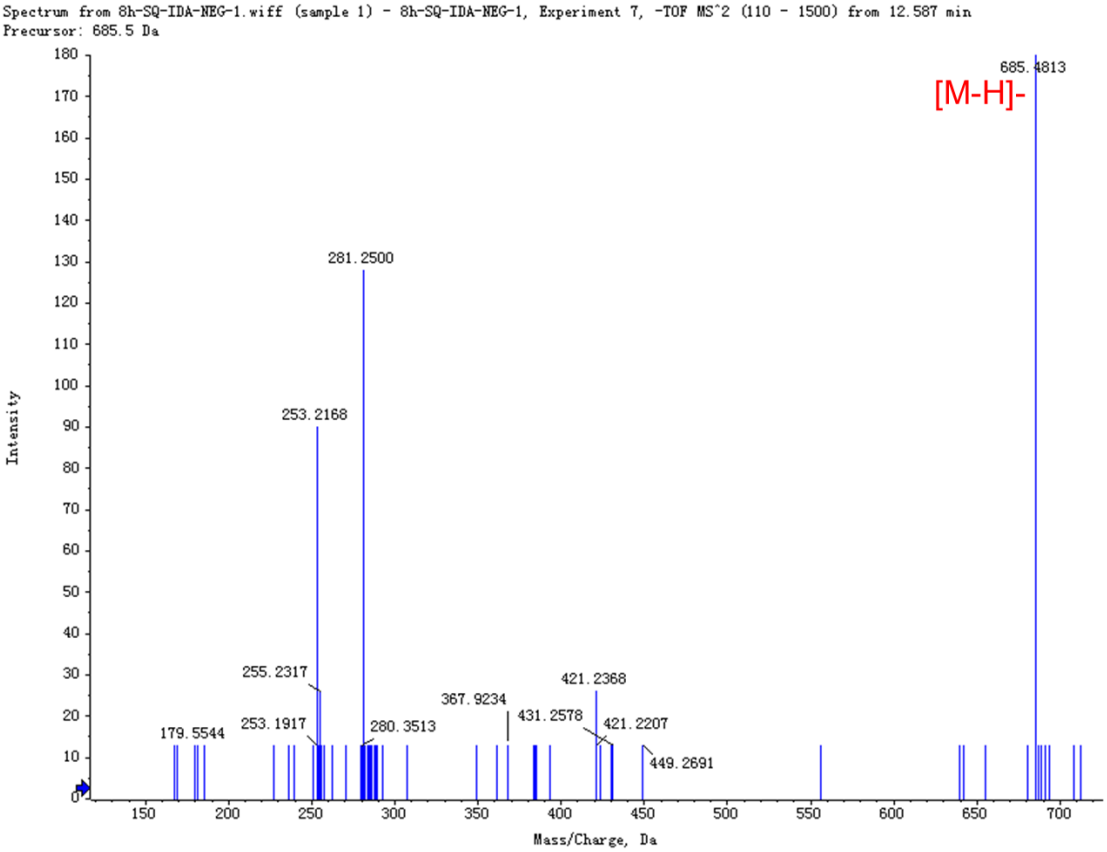
PA(33:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 5, -TOF MS^2 (110 - 1500) from 11.345 min
Precursor: 657.5 Da
[M-H]-
657.4526
253.2156
279.2332
253.2542
225.1814
Intensity
Mass/Charge, Da

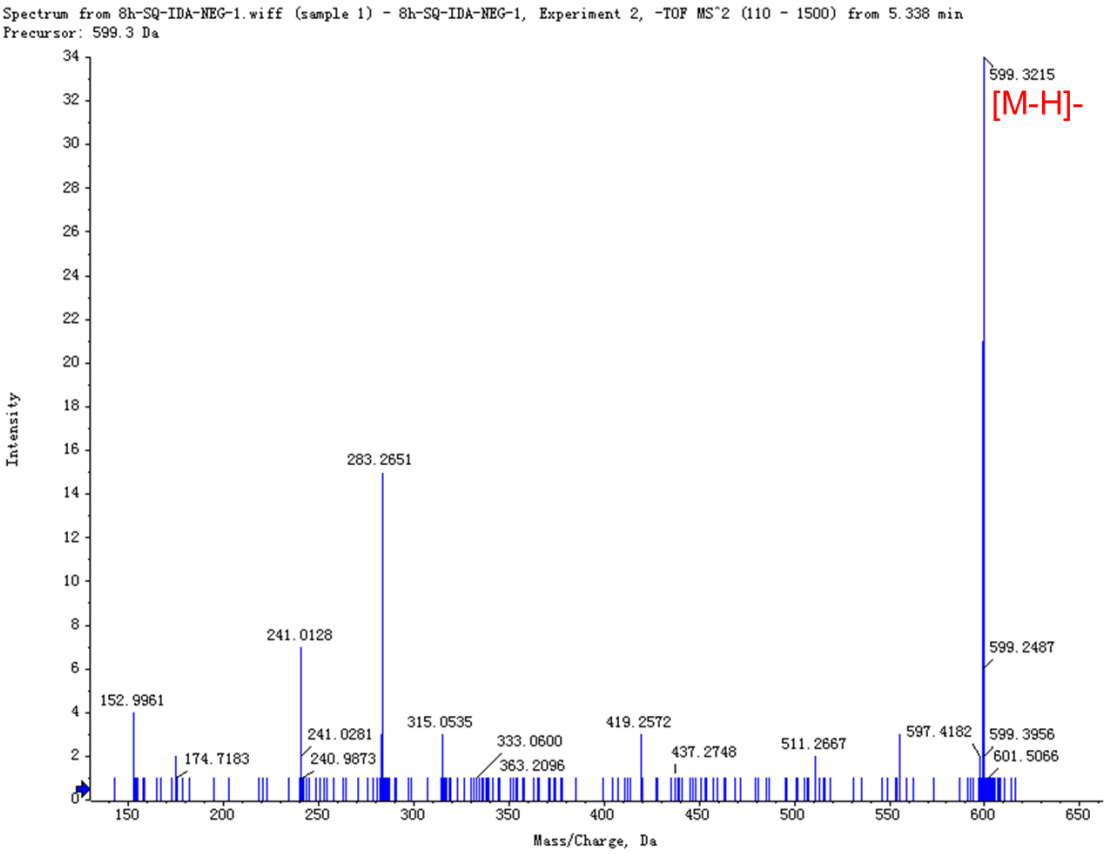
PA(35:1):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 6, -TOF MS^2 (110 - 1500) from 13.549 min
Precursor: 687.5 Da
281.2474
[M-H]-
687.4996
255.2325
687.4416
167.0073
255.2594
281.2217
380.7495
423.2415
Intensity
Mass/Charge, Da

PA(35:2):

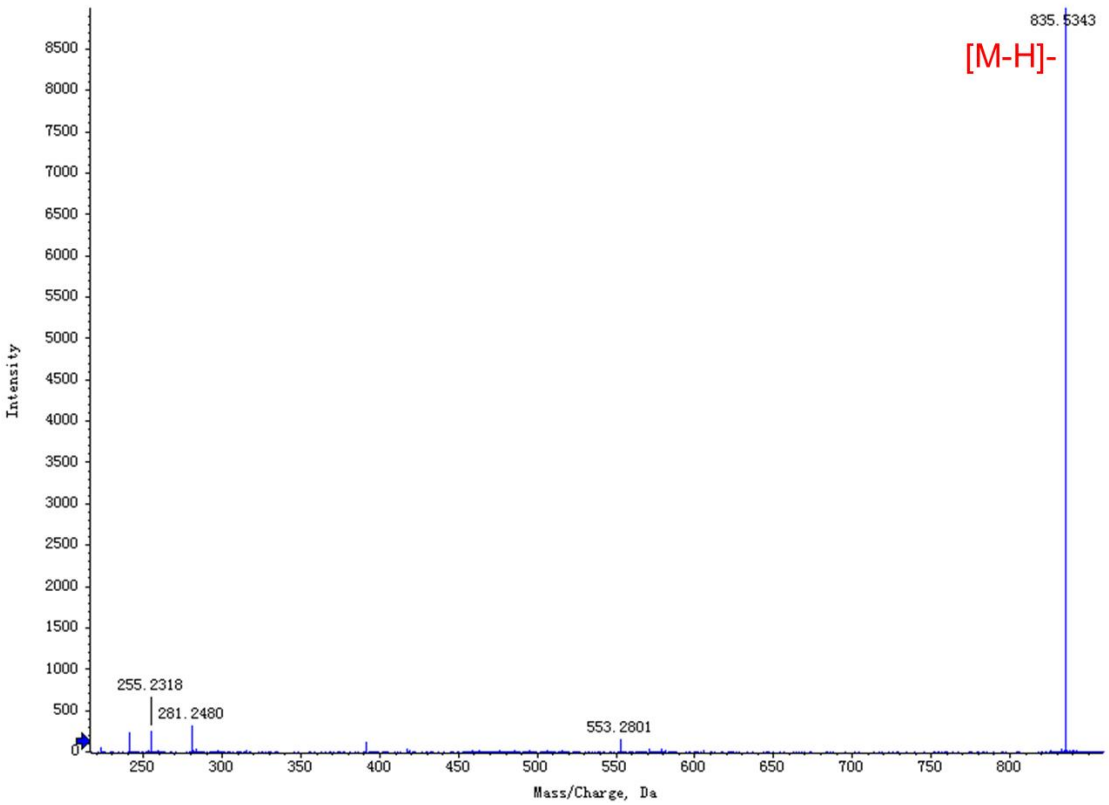


LyPI(18:0):



PI(34:1):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 9, -TOF MS^2 (110 - 1500) from 11.563 min
Precursor: 835.5 Da

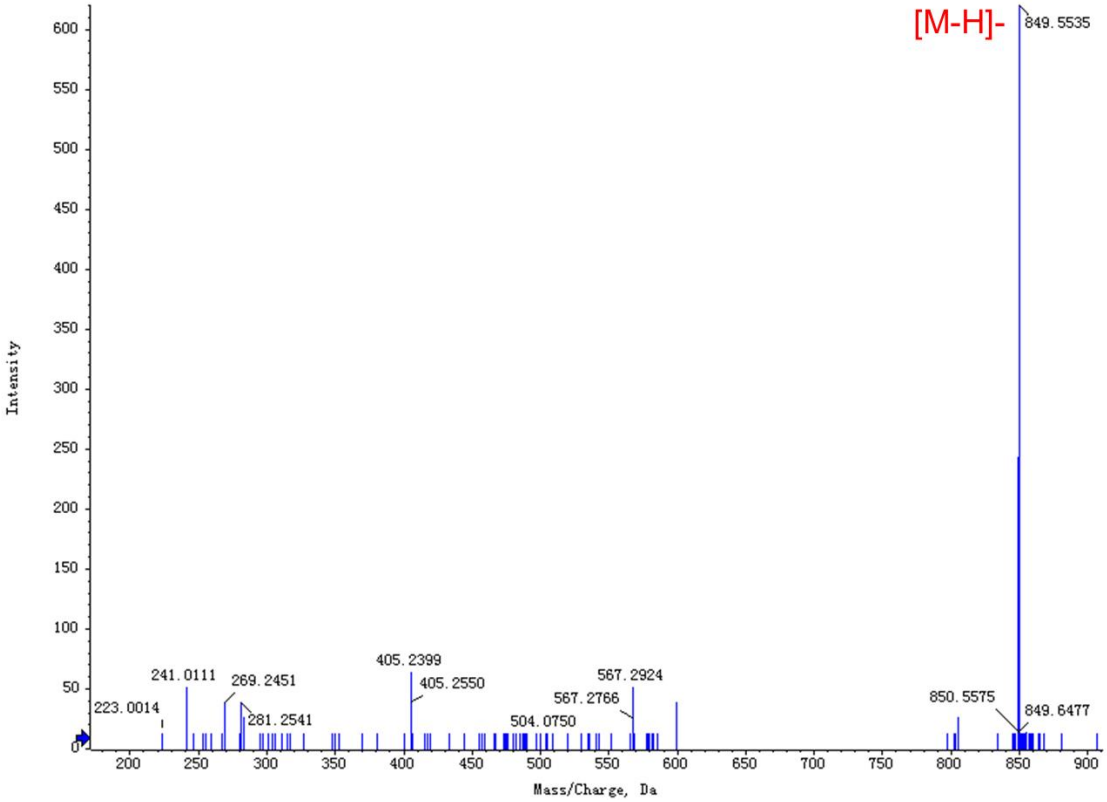


PI(34:2):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 13, -TOF MS^2 (110 - 1500) from 10.958 min
Precursor: 833.5 Da

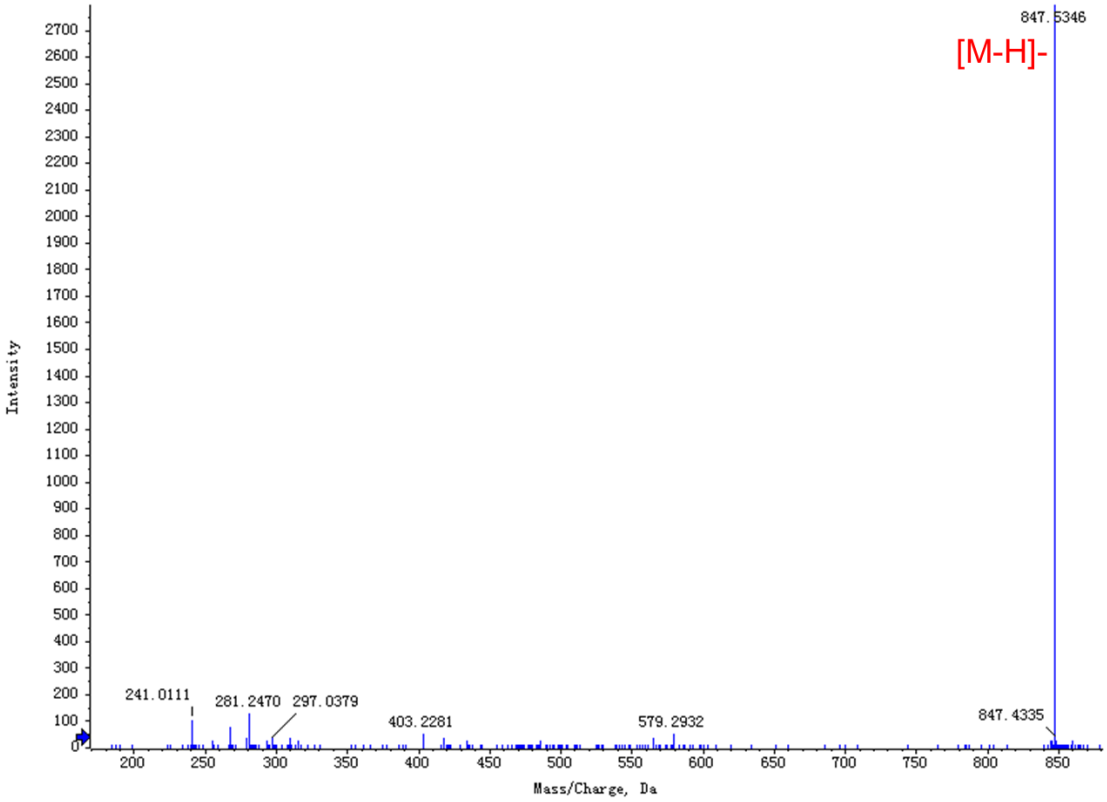
PI(35:1):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 13, -TOF MS^2 (110 - 1500) from 12.410 min
Precursor: 849.6 Da



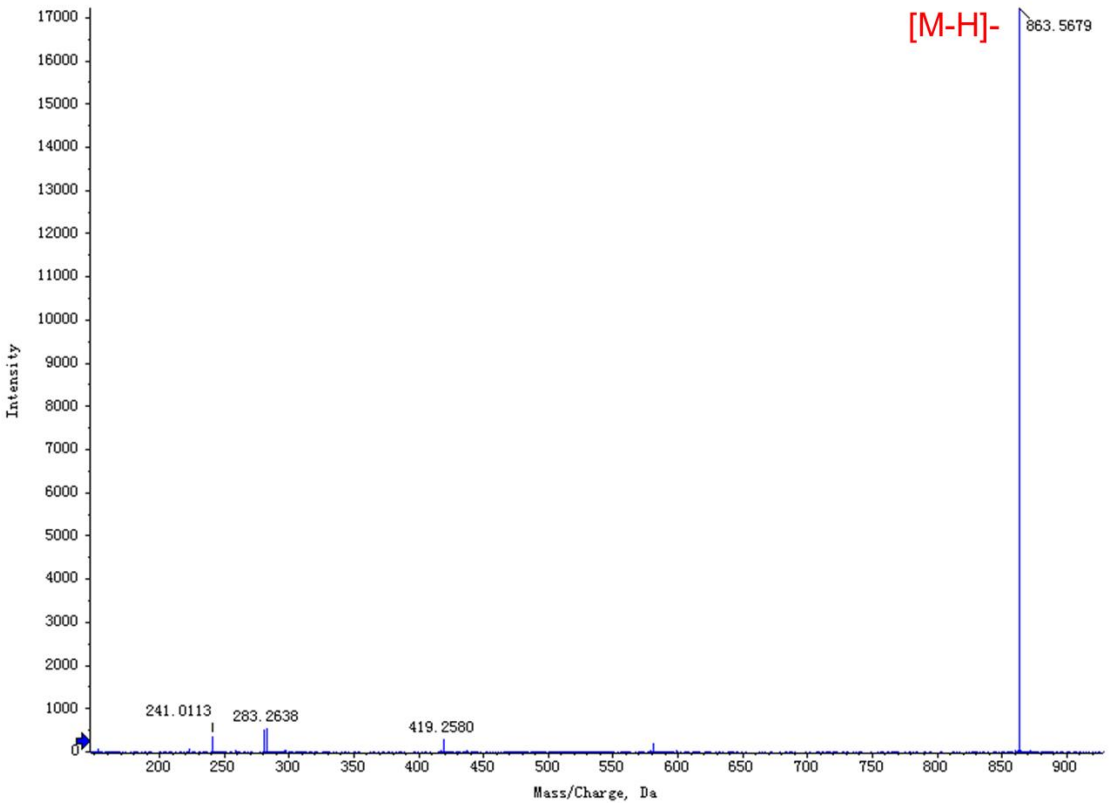
PI(35:2):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 12, -TOF MS^2 (110 - 1500) from 11.407 min
Precursor: 847.5 Da



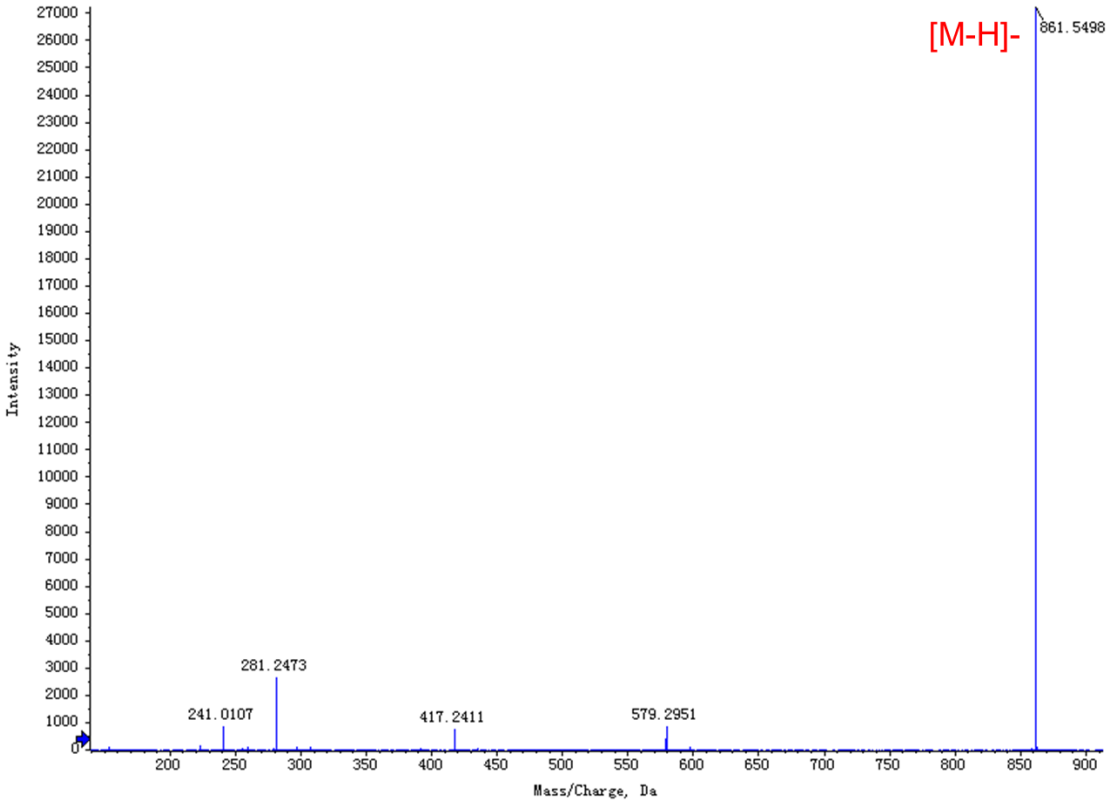
PI(36:1):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 9, -TOF MS^2 (110 - 1500) from 12.988 min
Precursor: 863.6 Da

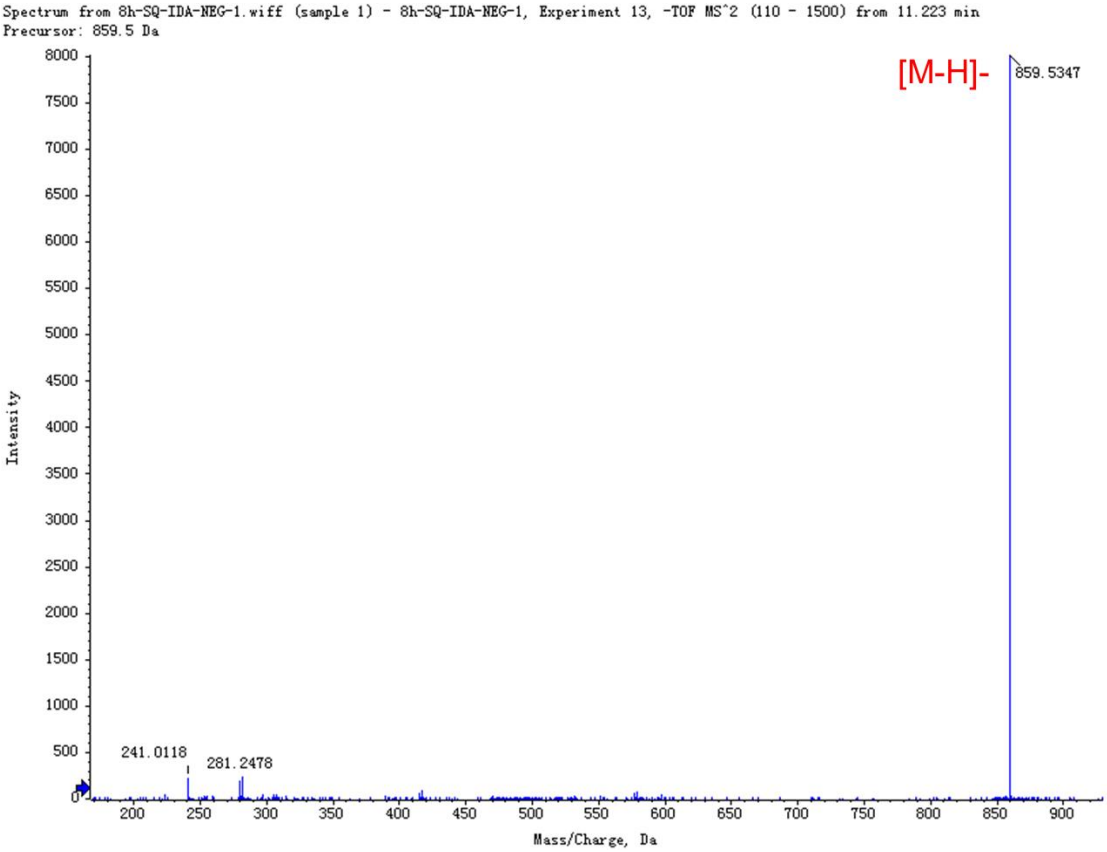


PI(36:2):

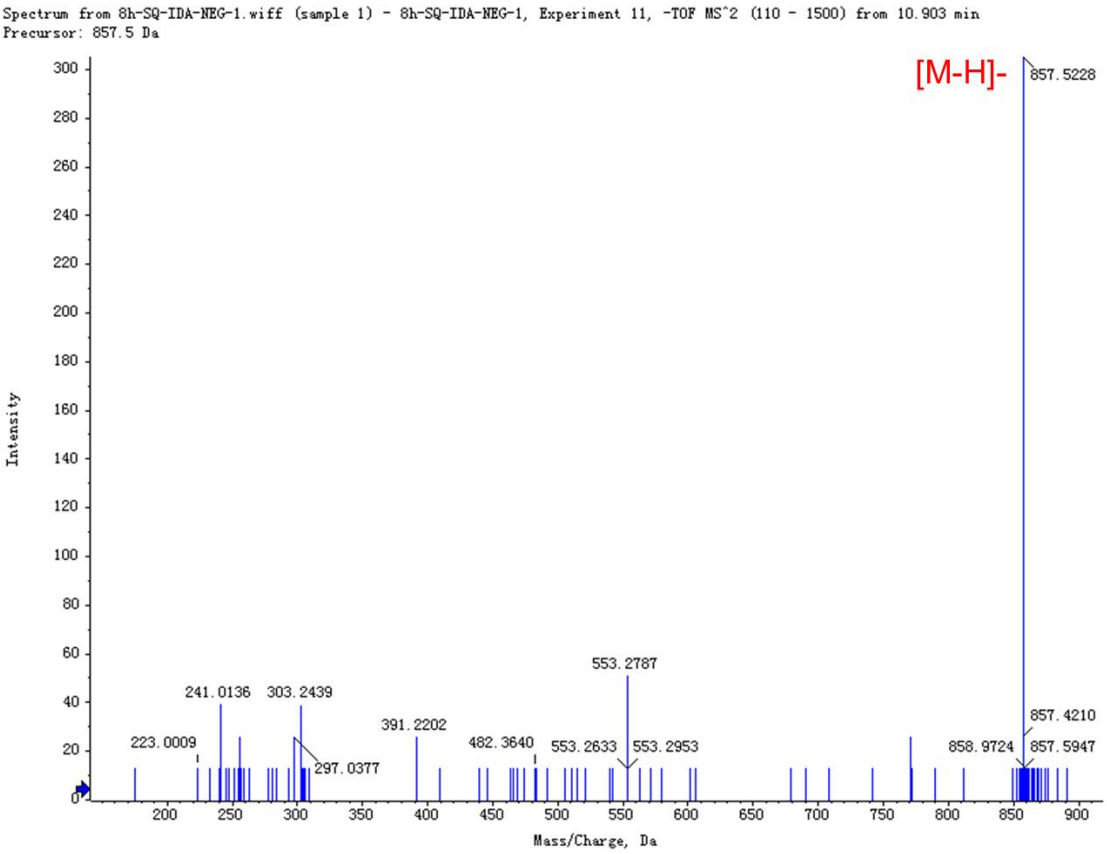
Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 7, -TOF MS^2 (110 - 1500) from 11.884 min
Precursor: 861.6 Da



PI(36:3):

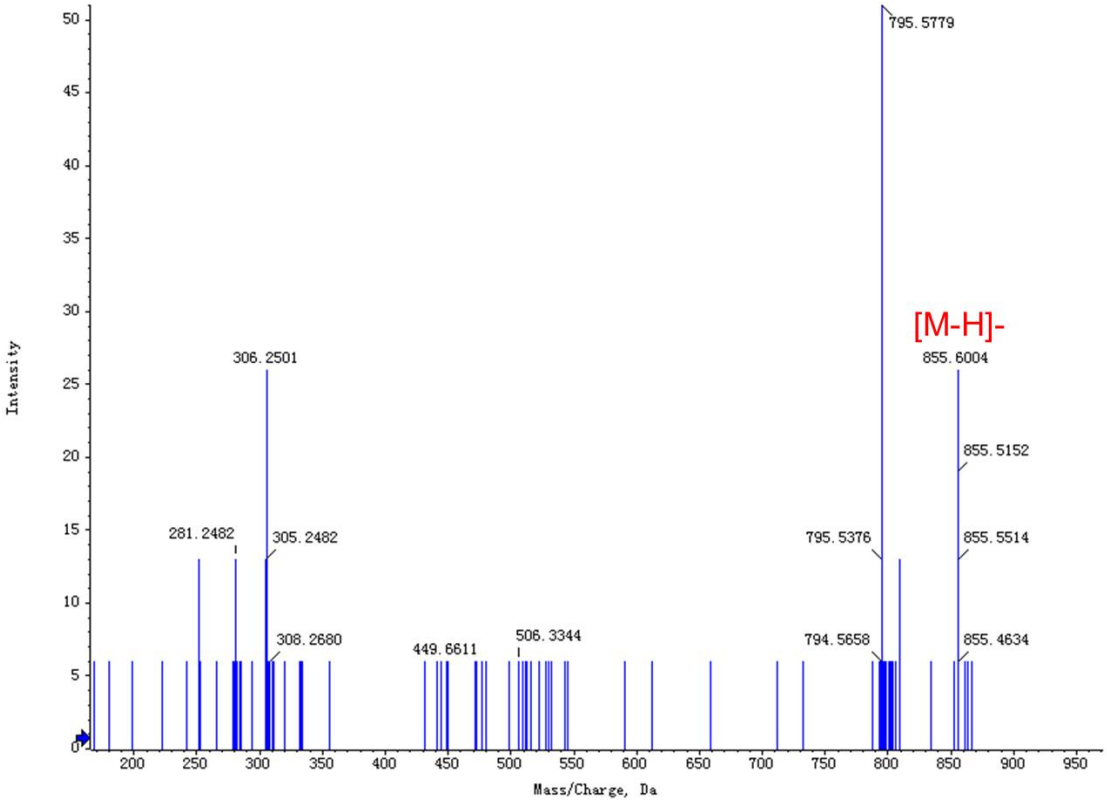

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 13, -TOF MS^2 (110 - 1500) from 11.223 min
Precursor: 859.5 Da
[M-H]-
859.5347
241.0118
281.2478
Intensity
Mass/Charge, Da

PI(36:4):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 11, -TOF MS^2 (110 - 1500) from 10.903 min
Precursor: 857.5 Da
[M-H]-
857.5228
553.2787
241.0136
303.2439
391.2202
223.0009
297.0377
482.3640
553.2633
553.2953
858.9724
857.4210
857.5947
Intensity
Mass/Charge, Da

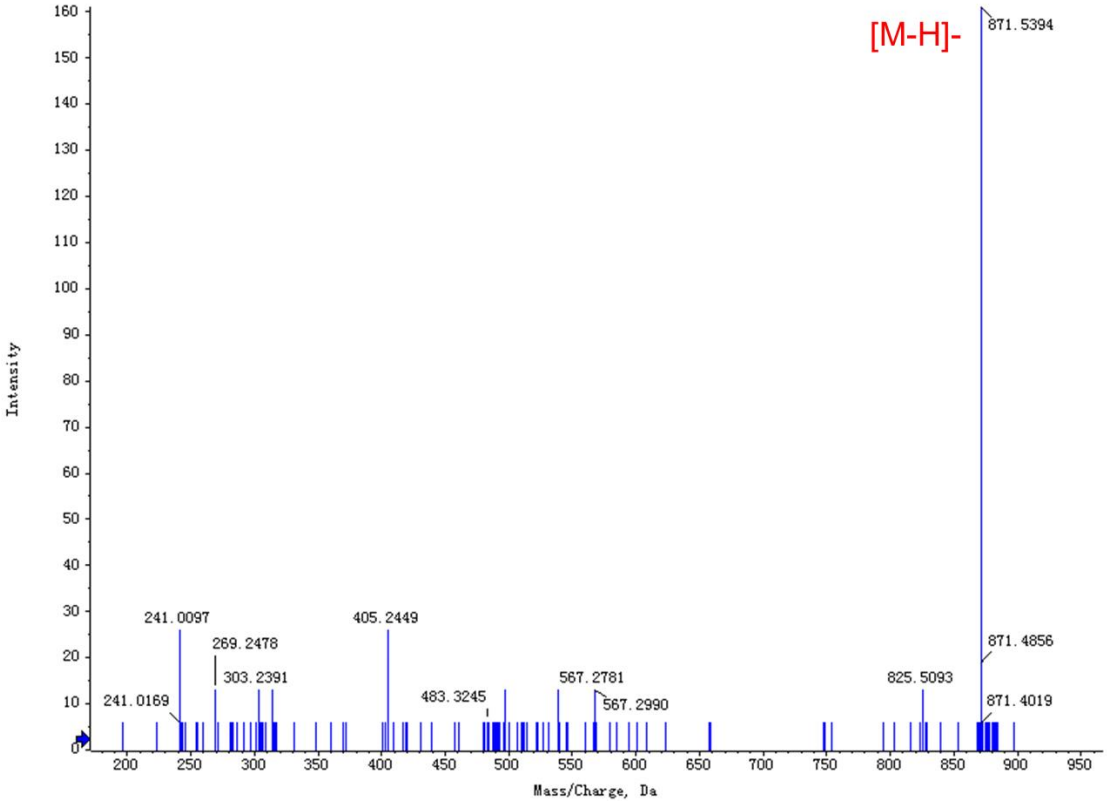
PI(36:5):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 11, -TOF MS^2 (110 - 1500) from 11.248 min
Precursor: 855.6 Da

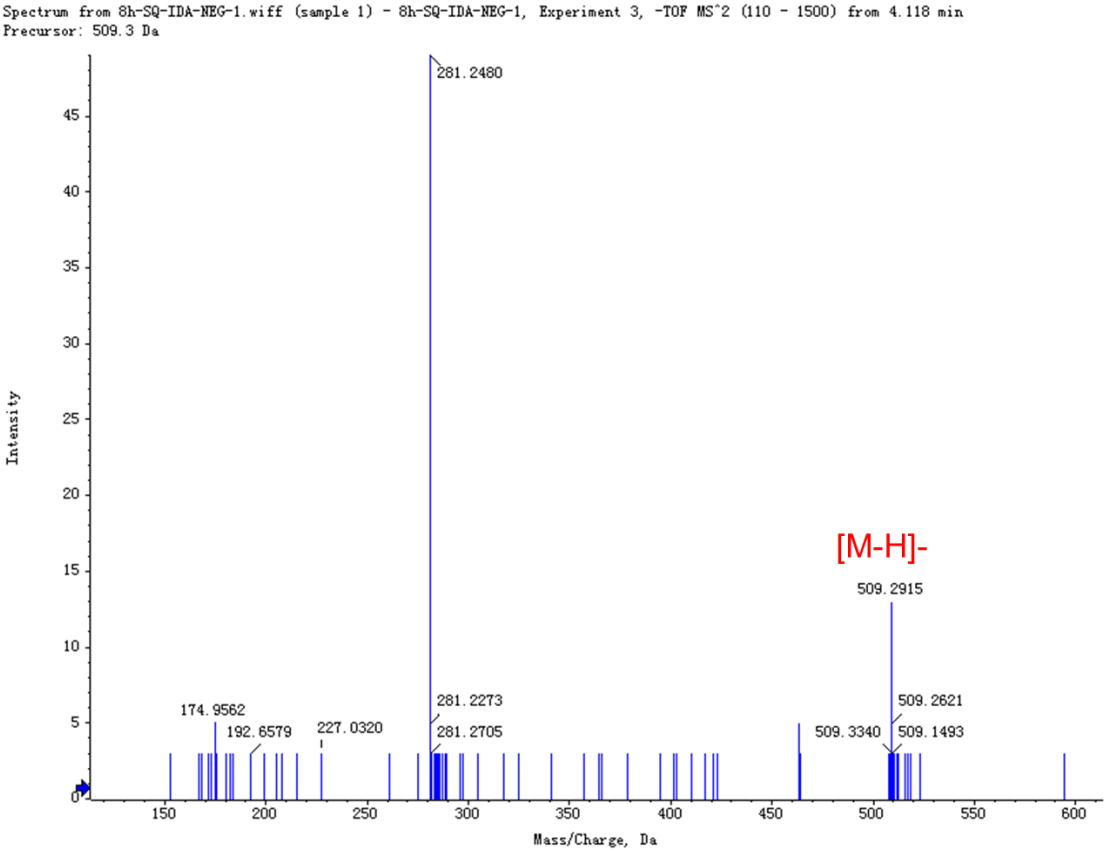


PI(37:4):

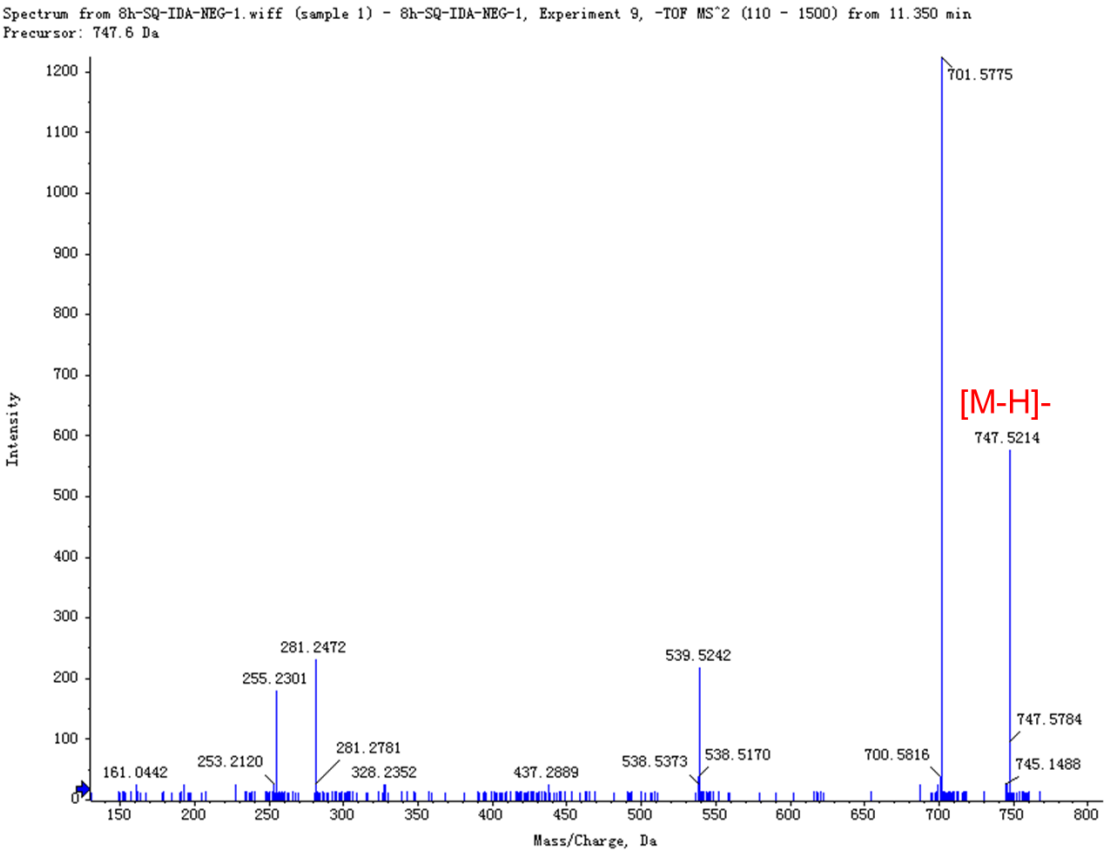
Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 11, -TOF MS^2 (110 - 1500) from 11.381 min
Precursor: 871.5 Da



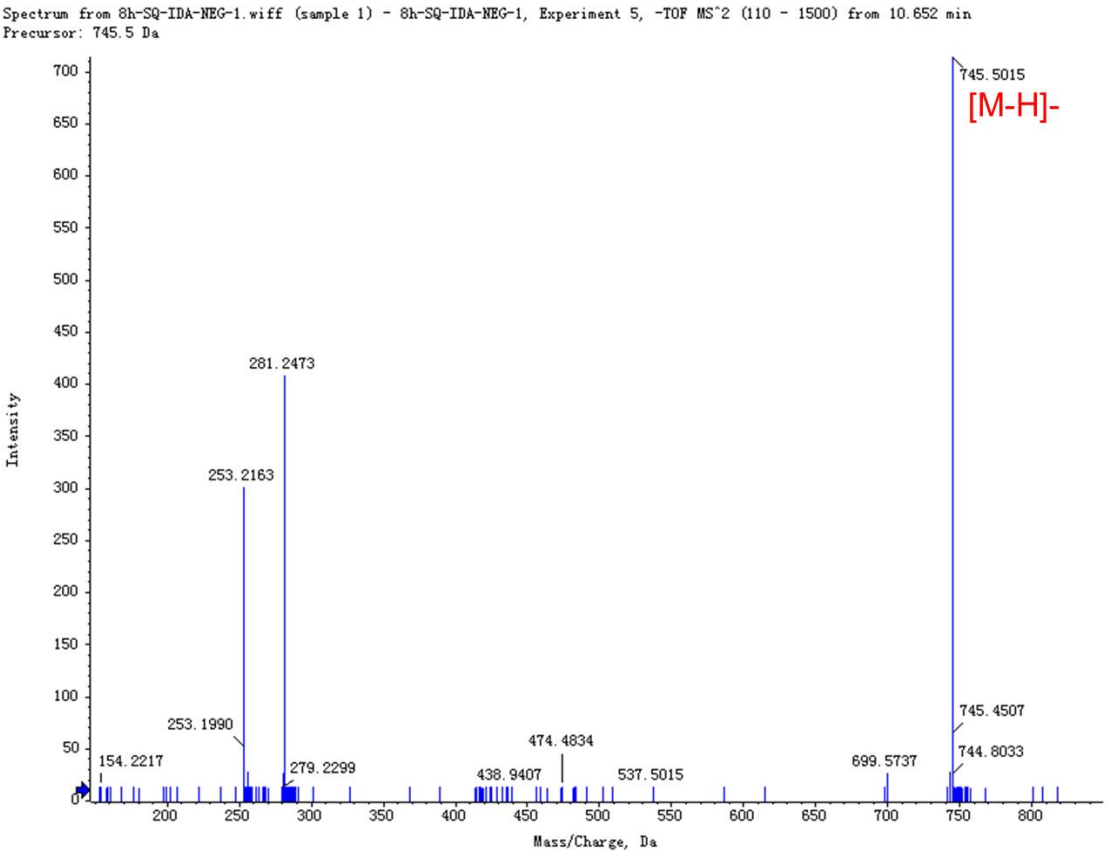
LyPG(18:1):



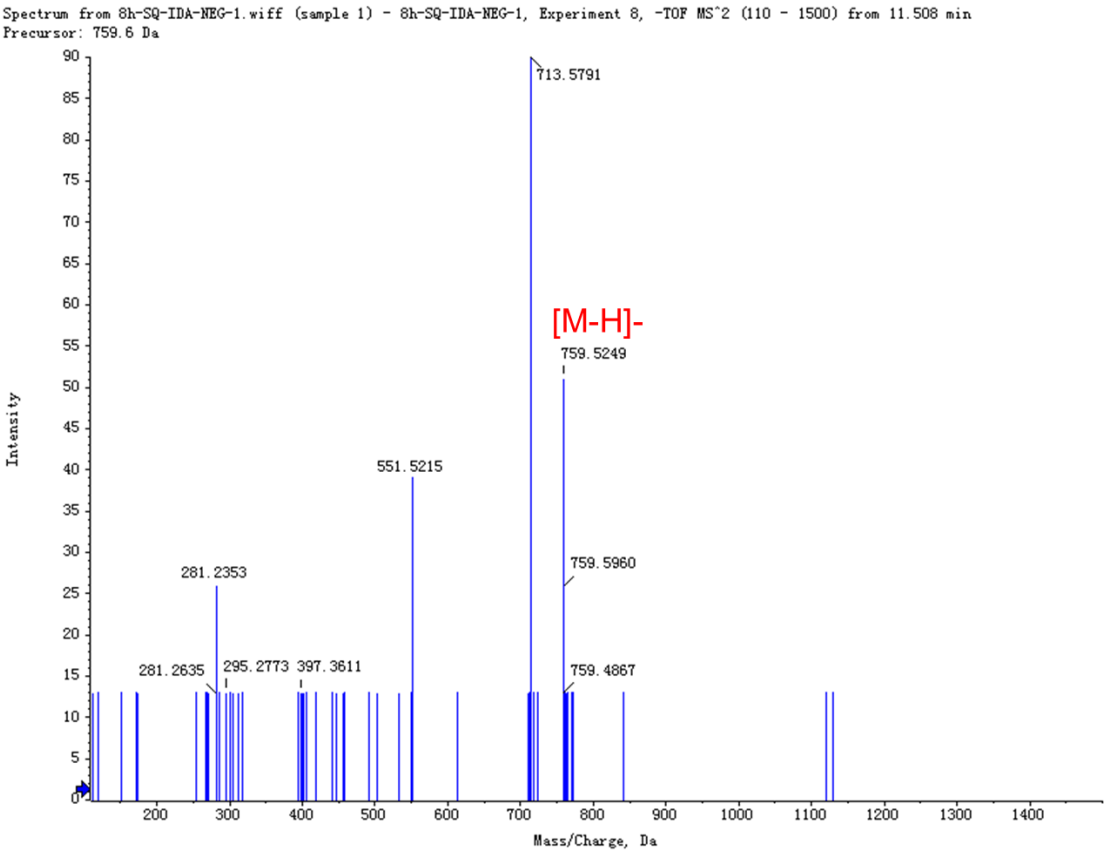
PG(34:1):



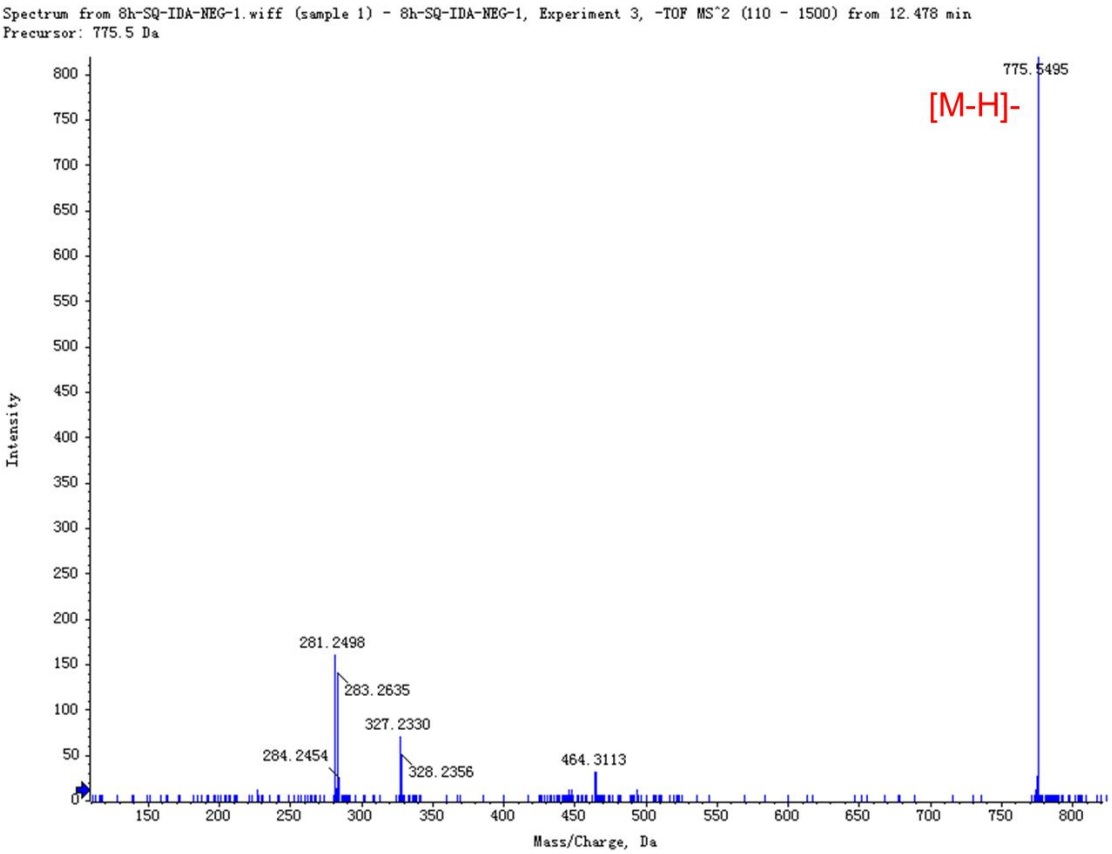
PG(34:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 5, -TOF MS^2 (110 - 1500) from 10.652 min
Precursor: 745.5 Da
745.5015
[M-H]-
281.2473
253.2163
253.1990
154.2217
279.2299
474.4834
438.9407
537.5015
699.5737
745.4507
744.8033
Intensity
Mass/Charge, Da

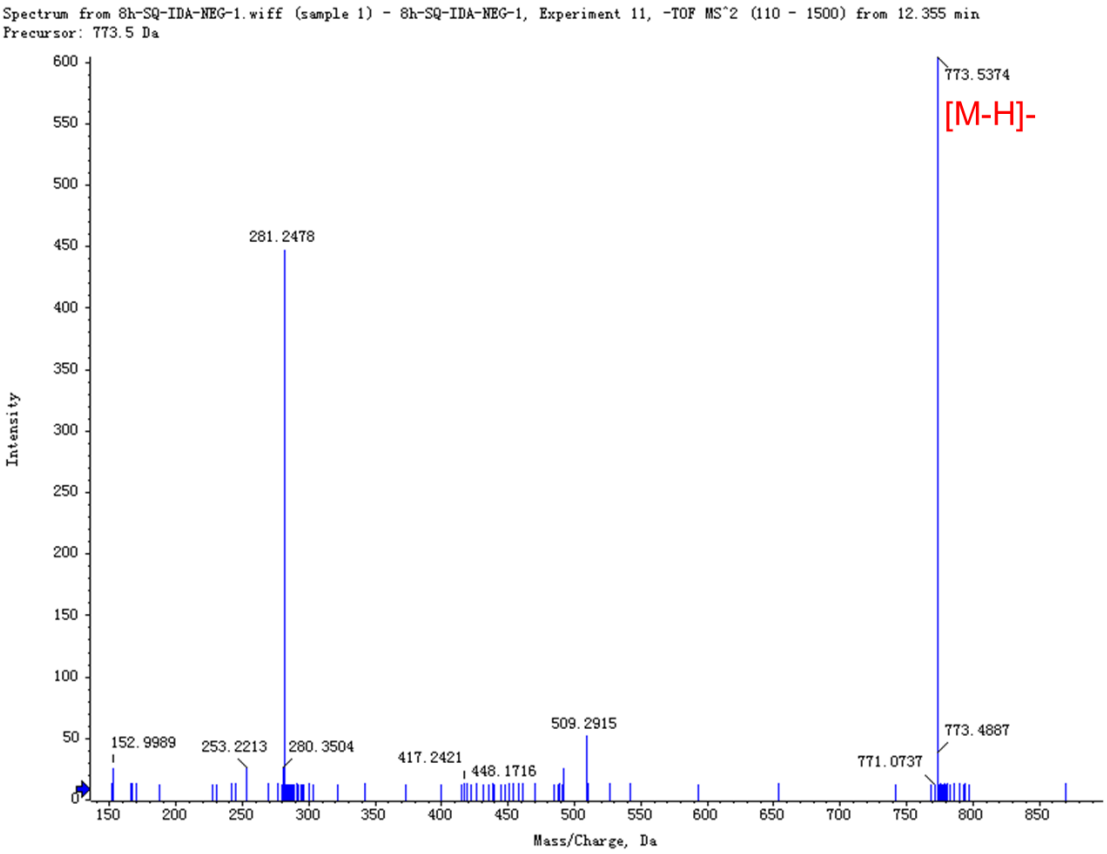
PG(35:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 8, -TOF MS^2 (110 - 1500) from 11.508 min
Precursor: 759.6 Da
713.5791
[M-H]-
759.5249
551.5215
759.5960
281.2353
281.2635
295.2773
397.3611
759.4867
Intensity
Mass/Charge, Da

PG(36:1):

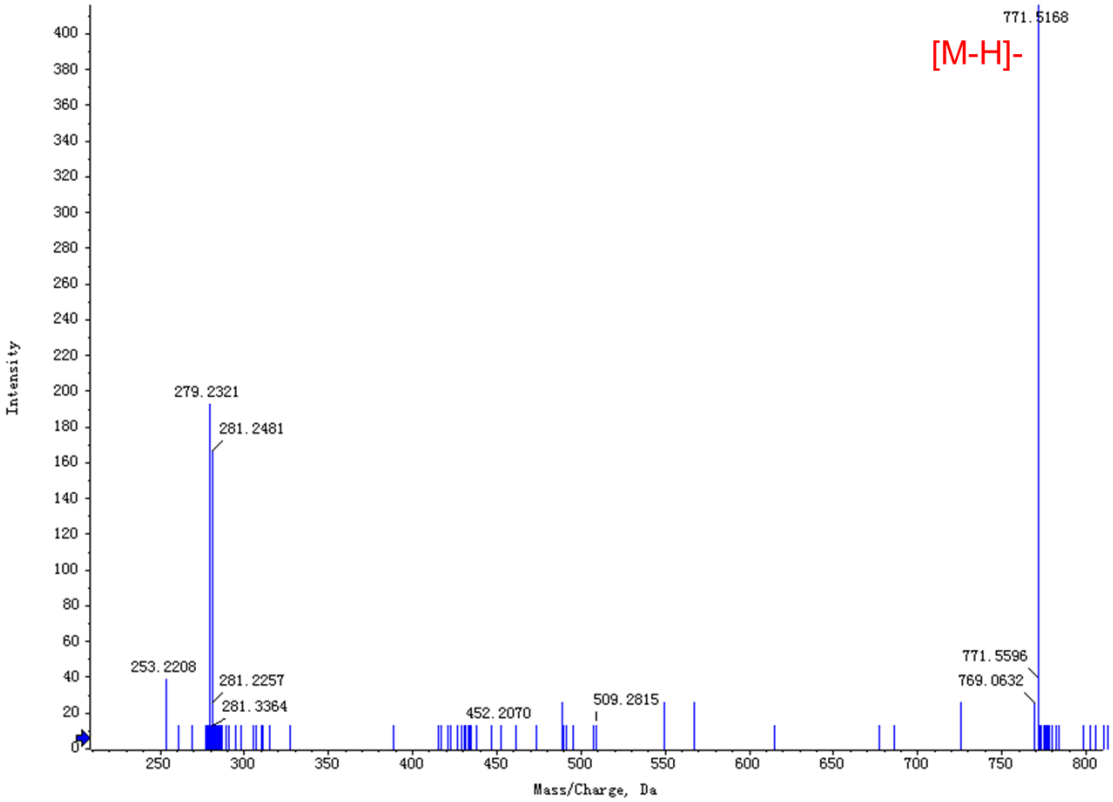

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 3, -TOF MS^2 (110 - 1500) from 12.478 min
Precursor: 775.5 Da
775.5495
[M-H]-
281.2498
283.2635
327.2330
284.2454
328.2356
464.3113
Intensity
Mass/Charge, Da

PG(36:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 11, -TOF MS^2 (110 - 1500) from 12.355 min
Precursor: 773.5 Da
773.5374
[M-H]-
281.2478
509.2915
773.4887
152.9989
253.2213
280.3504
417.2421
448.1716
771.0737
Intensity
Mass/Charge, Da

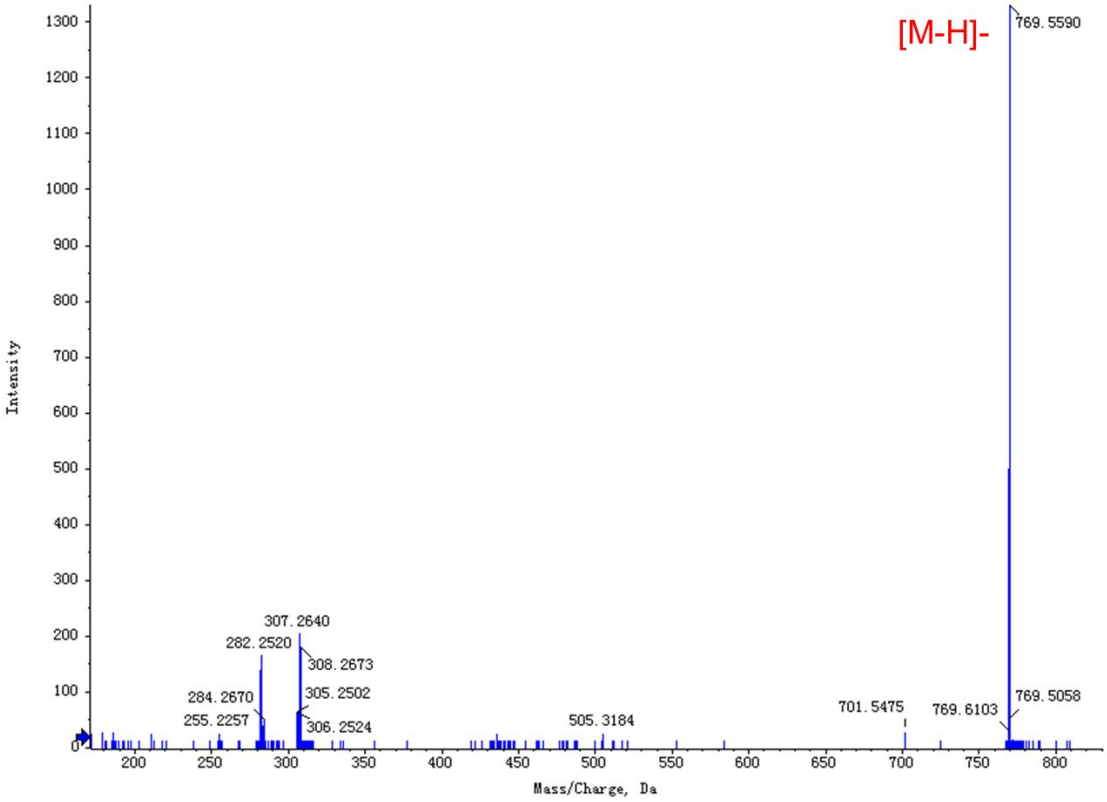
PG(36:3):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 10, -TOF MS^2 (110 - 1500) from 10.928 min
Precursor: 771.5 Da

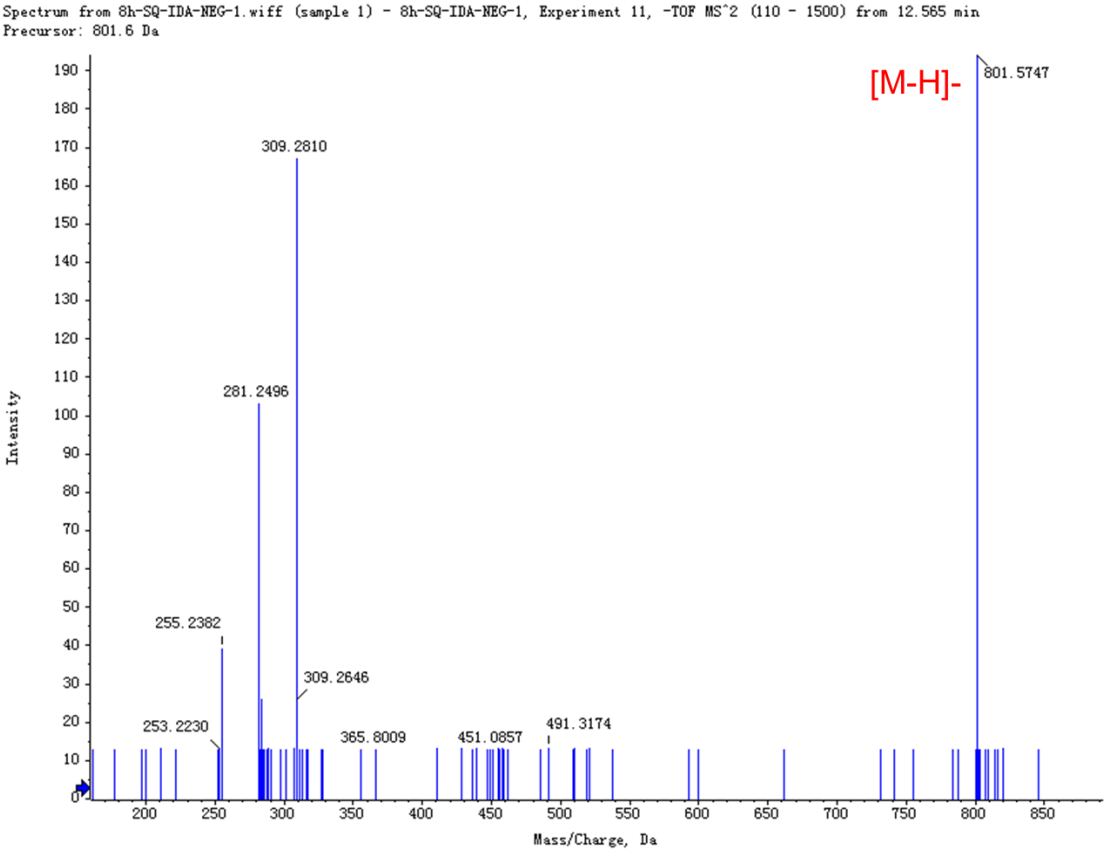


PG(36:4):

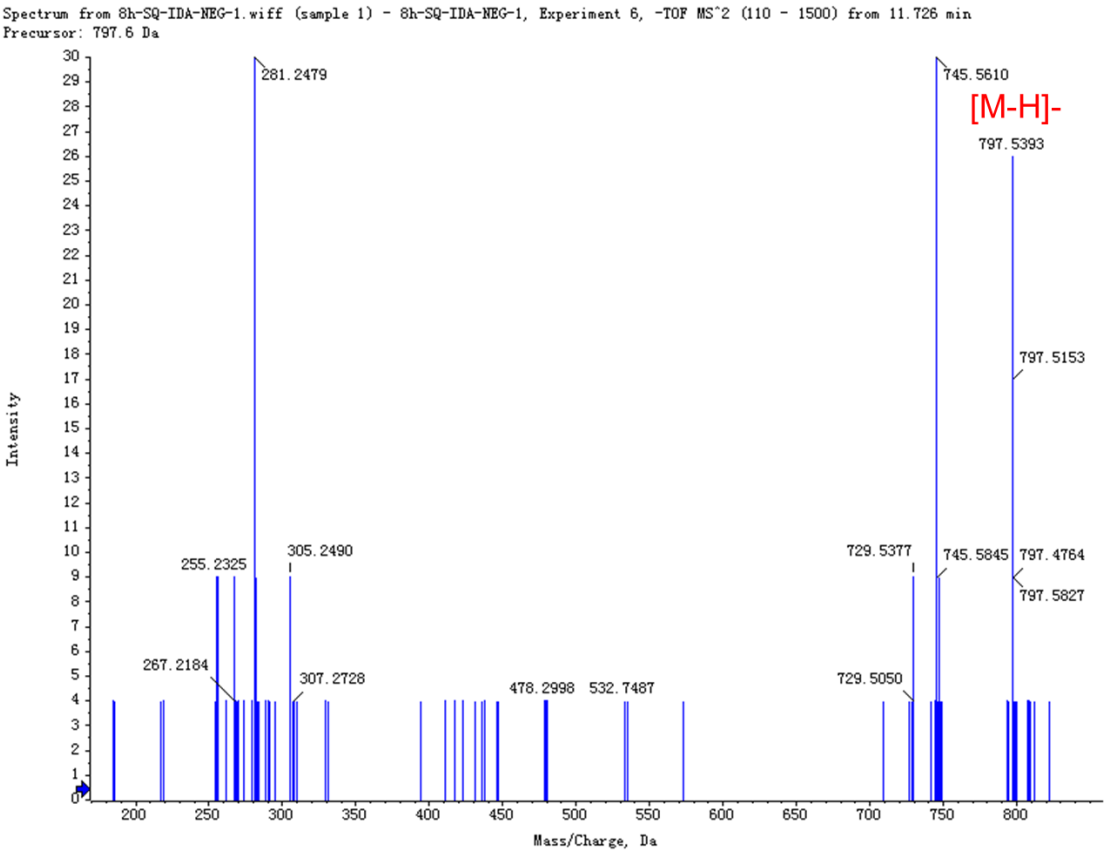
Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 8, -TOF MS^2 (110 - 1500) from 12.535 min
Precursor: 769.6 Da



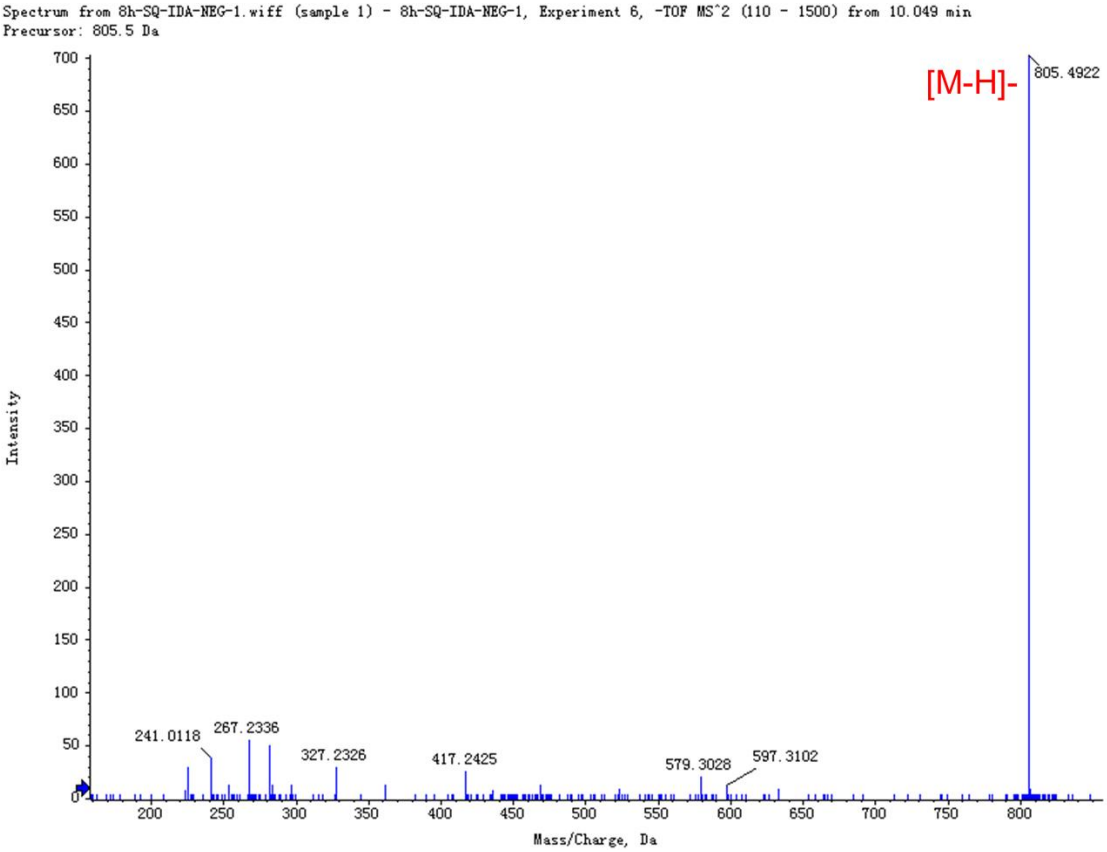
PG(38:2):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 11, -TOF MS^2 (110 - 1500) from 12.565 min
Precursor: 801.6 Da
[M-H]-
801.5747
309.2810
281.2496
255.2382
309.2646
253.2230
365.8009
451.0857
491.3174
Intensity
Mass/Charge, Da

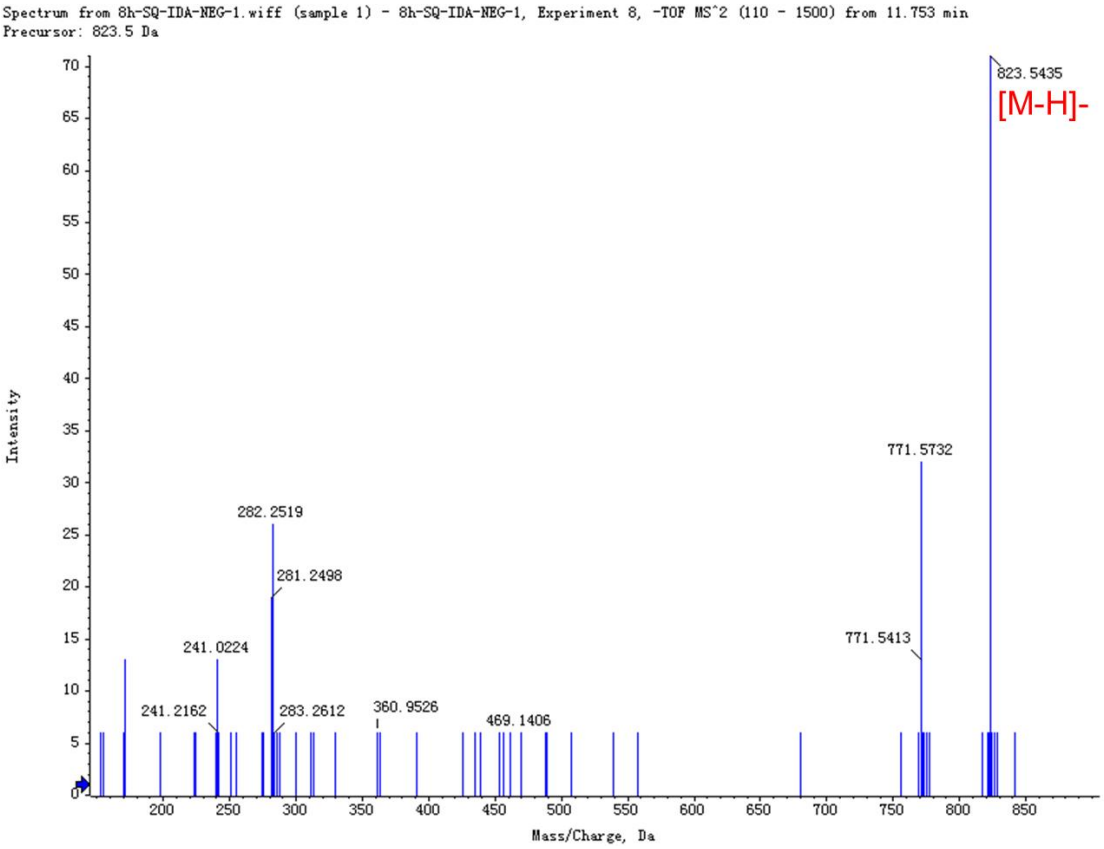
PG(38:4):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 6, -TOF MS^2 (110 - 1500) from 11.726 min
Precursor: 797.6 Da
281.2479
745.5610
[M-H]-
797.5393
797.5153
255.2325
305.2490
729.5377
745.5845
797.4764
797.5827
267.2184
307.2728
478.2998
532.7487
729.5050
Intensity
Mass/Charge, Da

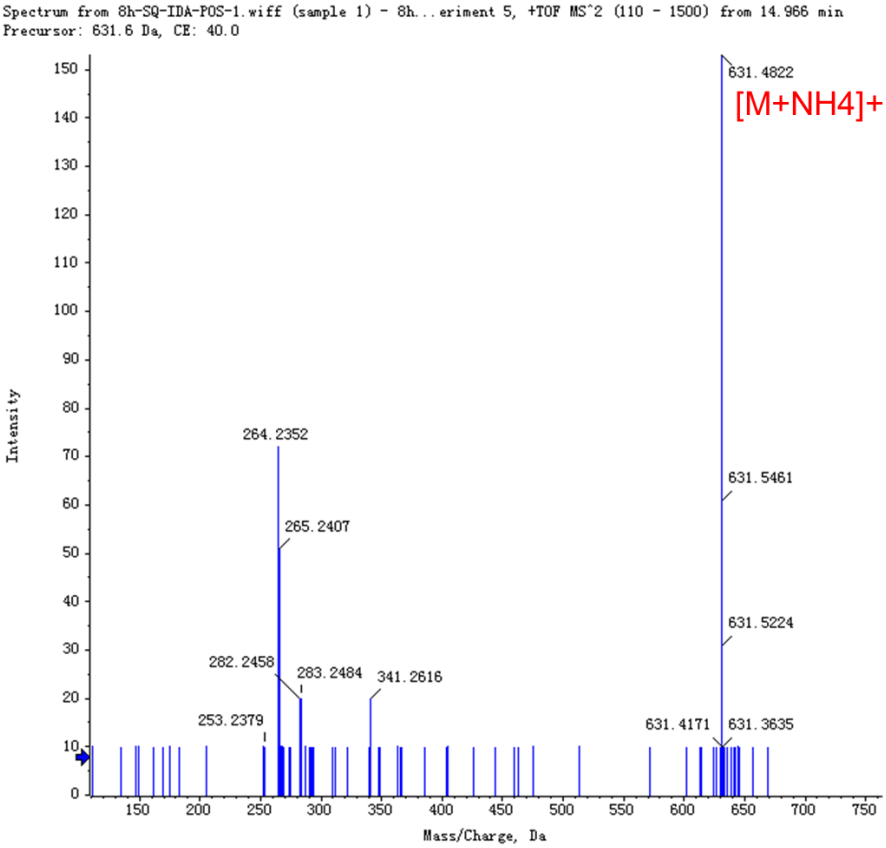
PG(39:7):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 6, -TOF MS^2 (110 - 1500) from 10.049 min
Precursor: 805.5 Da
[M-H]-
805.4922
241.0118
267.2336
327.2326
417.2425
579.3028
597.3102
Intensity
Mass/Charge, Da

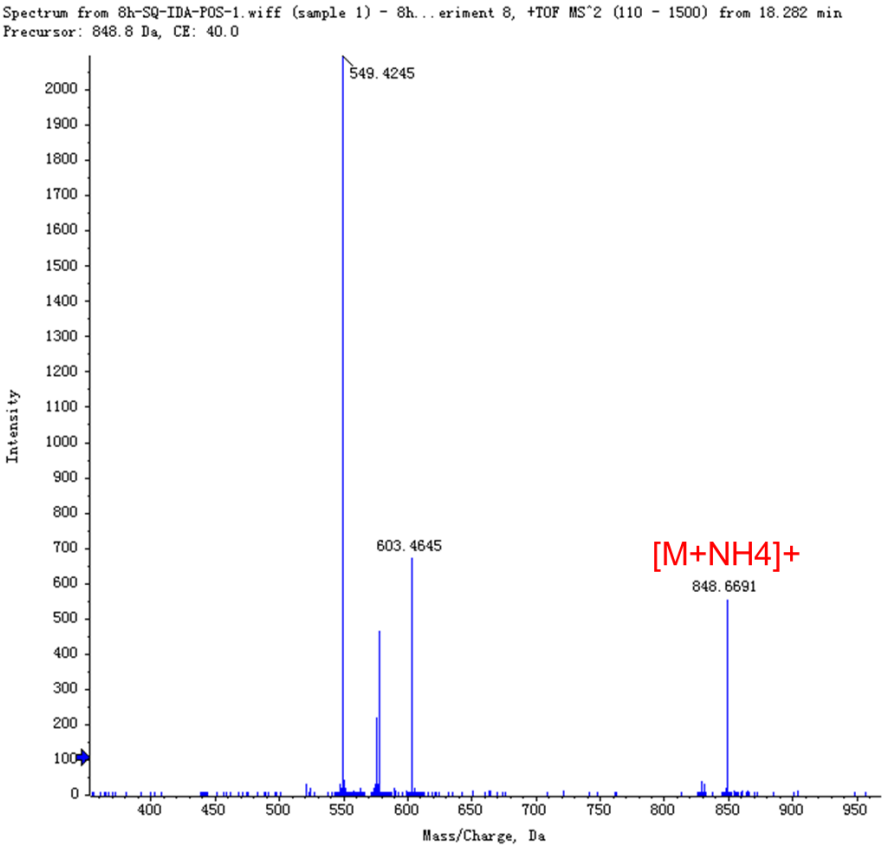
PG(40:5):


Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h-SQ-IDA-NEG-1, Experiment 8, -TOF MS^2 (110 - 1500) from 11.753 min
Precursor: 823.5 Da
823.5435
[M-H]-
771.5732
282.2519
281.2498
241.0224
771.5413
241.2162
283.2612
360.9526
469.1406
Intensity
Mass/Charge, Da

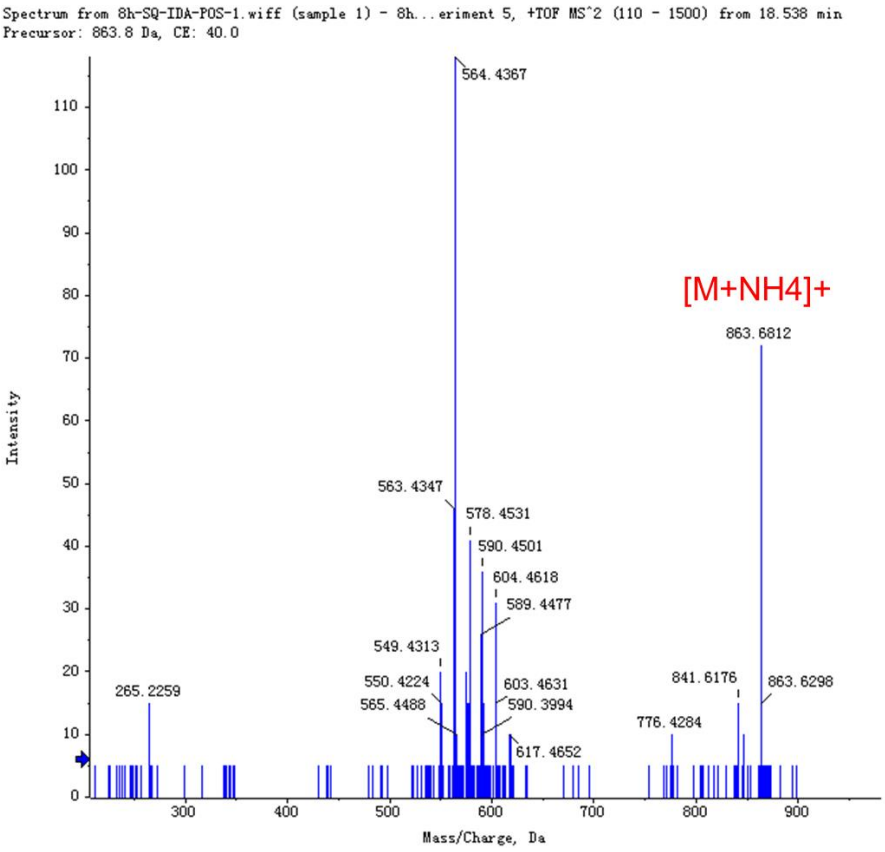
DG(36:6):


Spectrum from 8h-SQ-IDA-POS-1.wiff (sample 1) - 8h...eriment 5, +TOF MS^2 (110 - 1500) from 14.966 min
Precursor: 631.6 Da, CE: 40.0
631.4822
[M+NH4]+
264.2352
631.5461
265.2407
631.5224
282.2458
283.2484
341.2616
253.2379
631.4171
631.3635
Intensity
Mass/Charge, Da

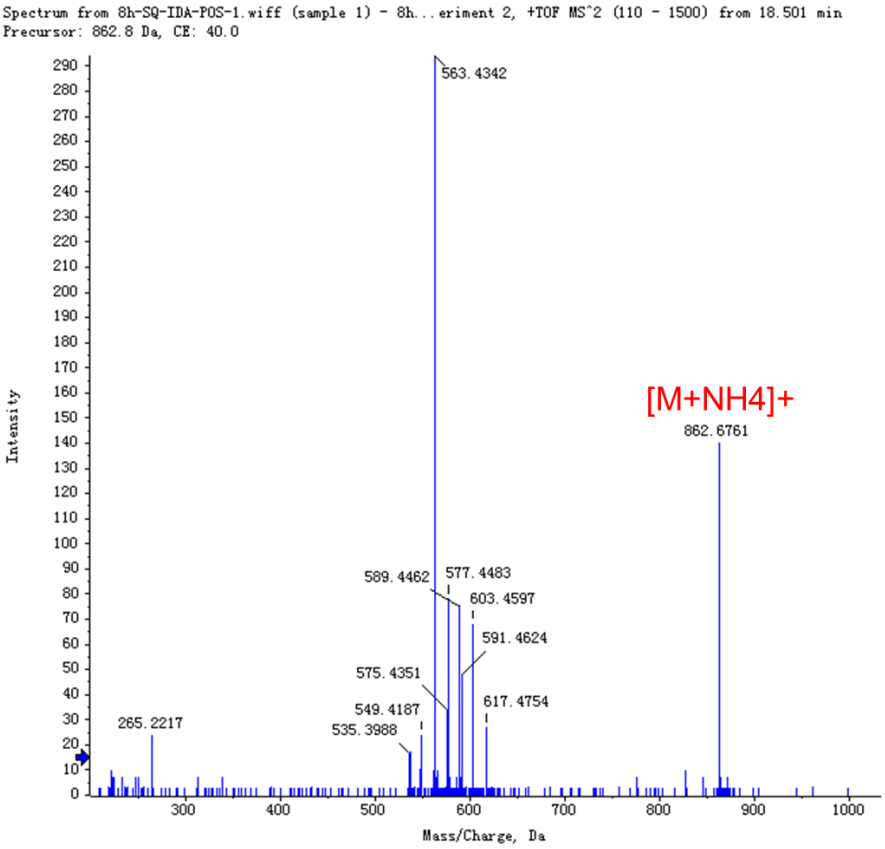
TG(50:2):


Spectrum from 8h-SQ-IDA-POS-1.wiff (sample 1) - 8h...eriment 8, +TOF MS^2 (110 - 1500) from 18.282 min
Precursor: 848.8 Da, CE: 40.0
549.4245
603.4645
[M+NH4]+
848.6691
Intensity
Mass/Charge, Da

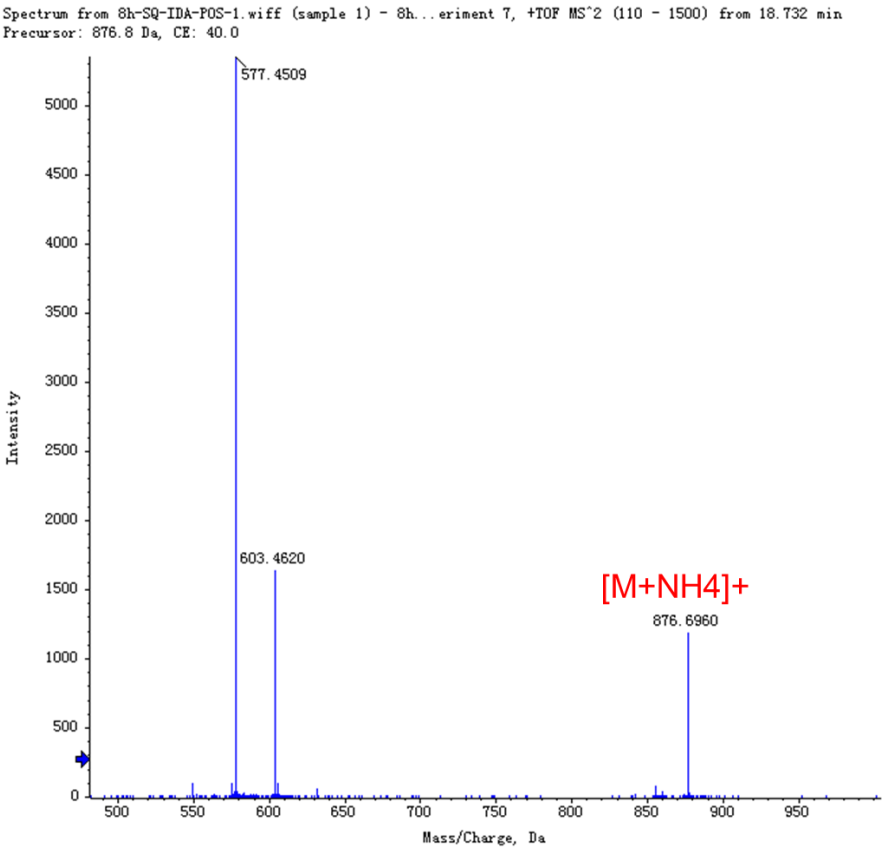
TG(51:1)


Spectrum from 8h-SQ-IDA-POS-1.wiff (sample 1) - 8h...eriment 5, +TOF MS^2 (110 - 1500) from 18.538 min
Precursor: 863.8 Da, CE: 40.0
[M+NH4]+
863.6812
564.4367
563.4347
578.4531
590.4501
604.4618
589.4477
549.4313
550.4224
565.4488
603.4631
590.3994
617.4652
265.2259
841.6176
863.6298
776.4284
Intensity
Mass/Charge, Da

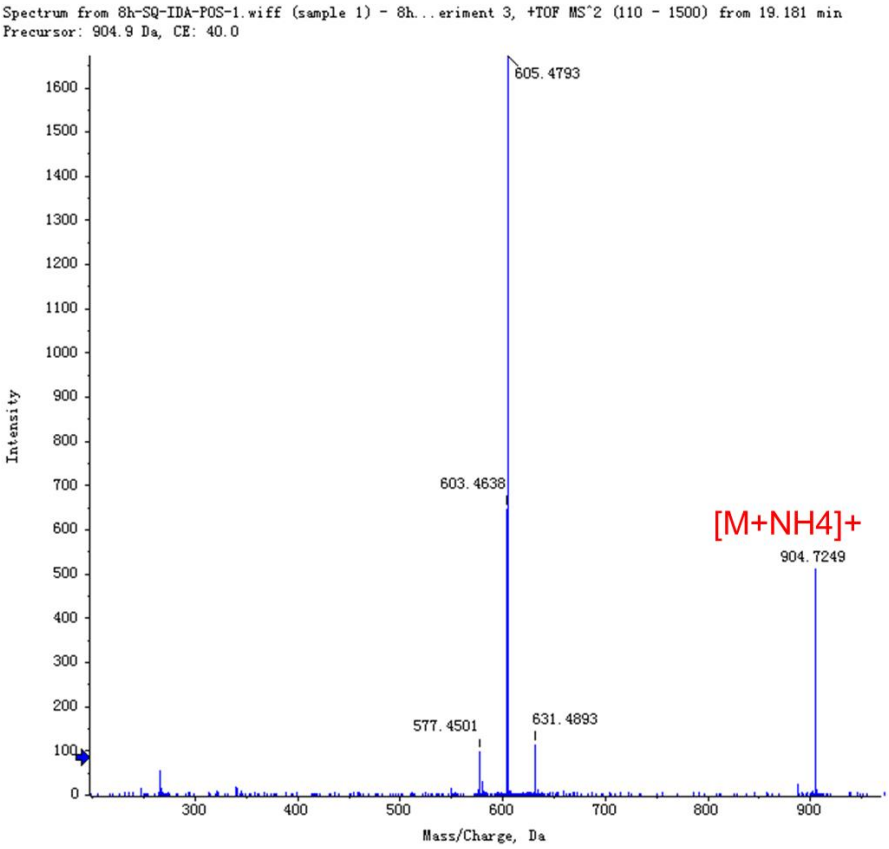
TG(51:2):


Spectrum from 8h-SQ-IDA-POS-1.wiff (sample 1) - 8h...eriment 2, +TOF MS^2 (110 - 1500) from 18.501 min
Precursor: 862.8 Da, CE: 40.0
[M+NH4]+
862.6761
563.4342
589.4462
577.4483
603.4597
591.4624
575.4351
549.4187
535.3988
617.4754
265.2217
Intensity
Mass/Charge, Da

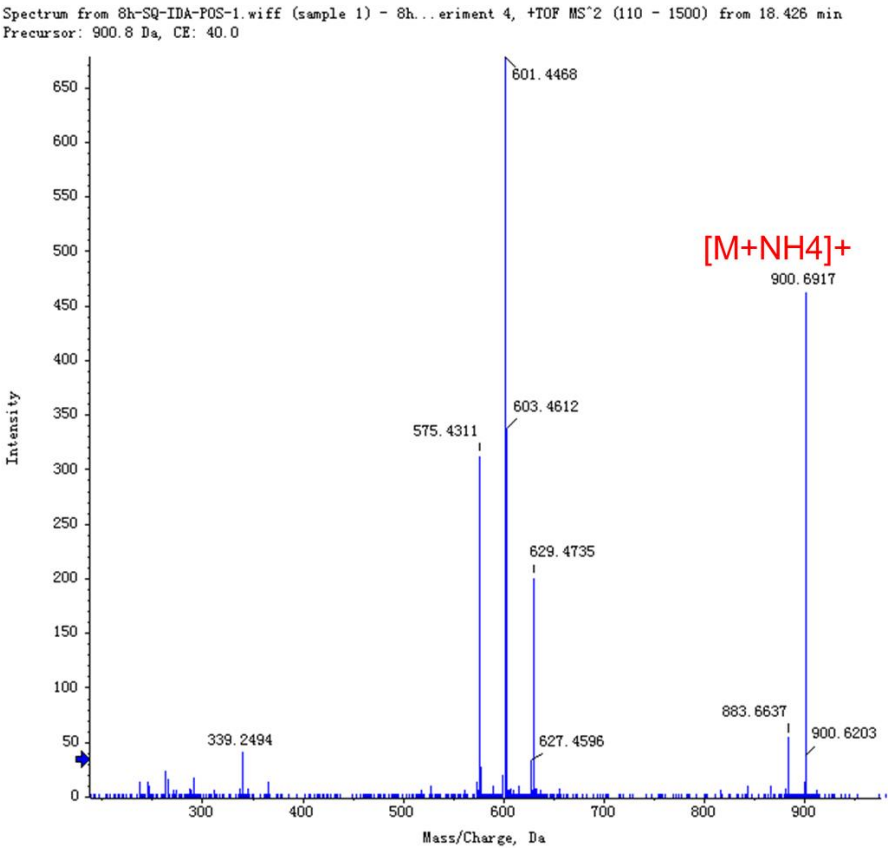
TG(52:2):


Spectrum from 8h-SQ-IDA-POS-1.wiff (sample 1) - 8h...eriment 7, +TOF MS^2 (110 - 1500) from 18.732 min
Precursor: 876.8 Da, CE: 40.0
577.4509
603.4620
[M+NH4]+
876.6960
Intensity
Mass/Charge, Da

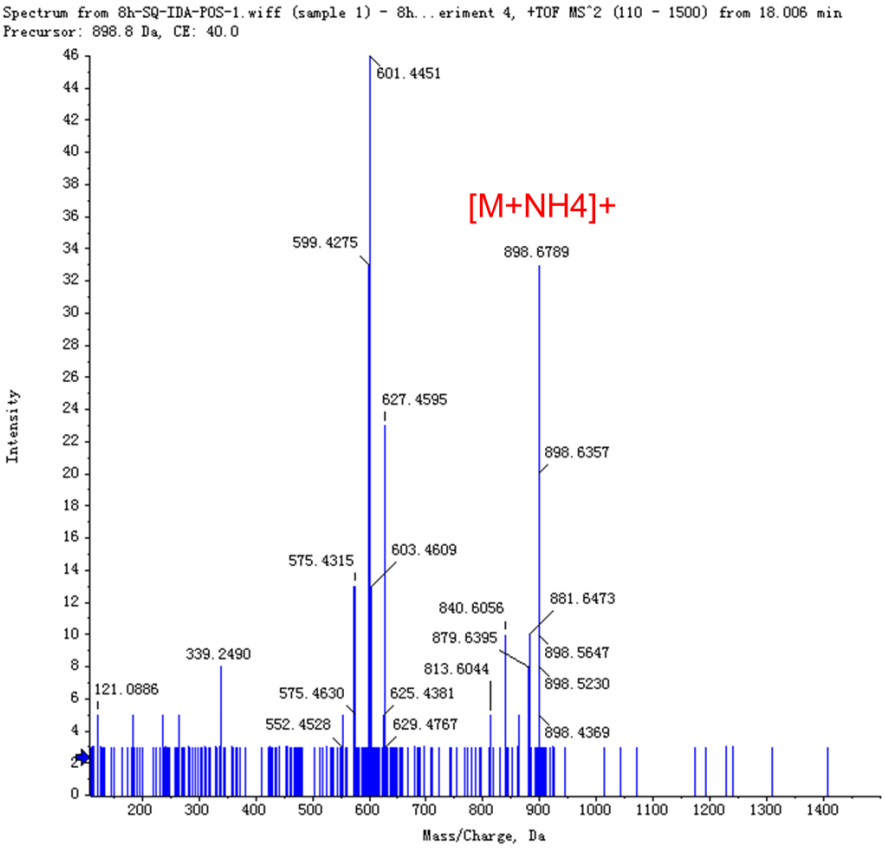
TG(54:2):


Spectrum from 8h-SQ-IDA-POS-1.wiff (sample 1) - 8h...eriment 3, +TOF MS^2 (110 - 1500) from 19.181 min
Precursor: 904.9 Da, CE: 40.0
605.4793
603.4638
[M+NH4]+
904.7249
577.4501
631.4893
Intensity
Mass/Charge, Da

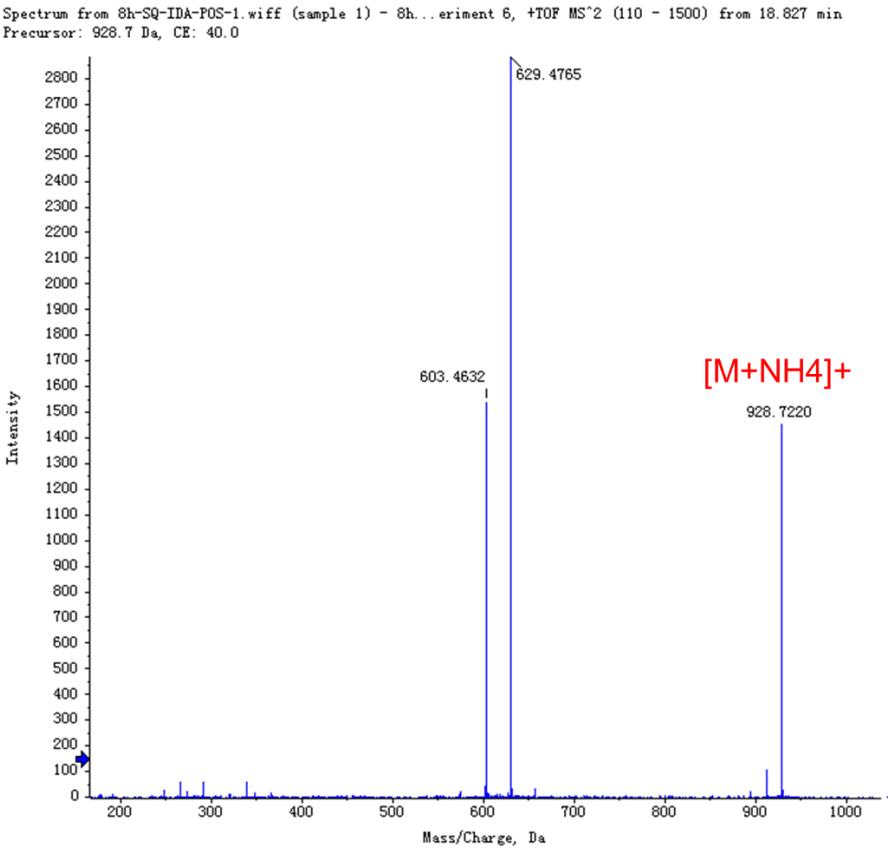
TG(54:4):


Spectrum from 8h-SQ-IDA-POS-1.wiff (sample 1) - 8h...eriment 4, +TOF MS^2 (110 - 1500) from 18.426 min
Precursor: 900.8 Da, CE: 40.0
[M+NH4]+
601.4468
900.6917
603.4612
575.4311
629.4735
883.6637
900.6203
339.2494
627.4596
Intensity
Mass/Charge, Da

TG(54:5):


Spectrum from 8h-SQ-IDA-POS-1.wiff (sample 1) - 8h...eriment 4, +TOF MS^2 (110 - 1500) from 18.006 min
Precursor: 898.8 Da, CE: 40.0
[M+NH4]+
601.4451
599.4275
898.6789
627.4595
898.6357
603.4609
575.4315
881.6473
840.6056
879.6395
898.5647
339.2490
813.6044
898.5230
121.0886
575.4630
625.4381
552.4528
629.4767
898.4369
Intensity
Mass/Charge, Da

TG(56:4):



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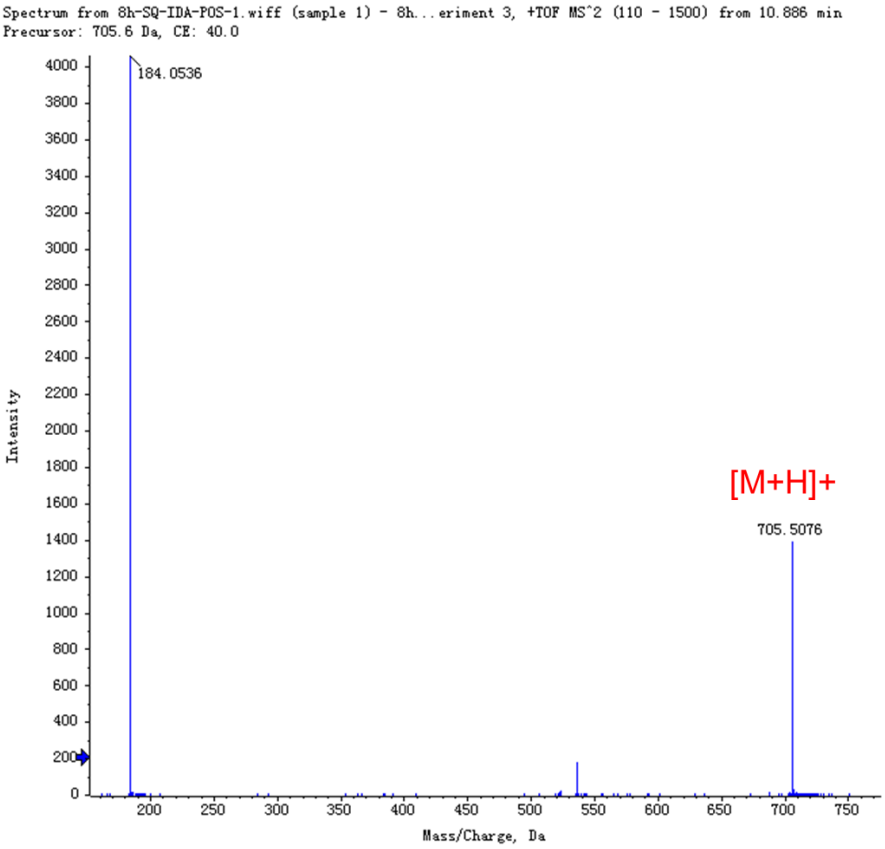
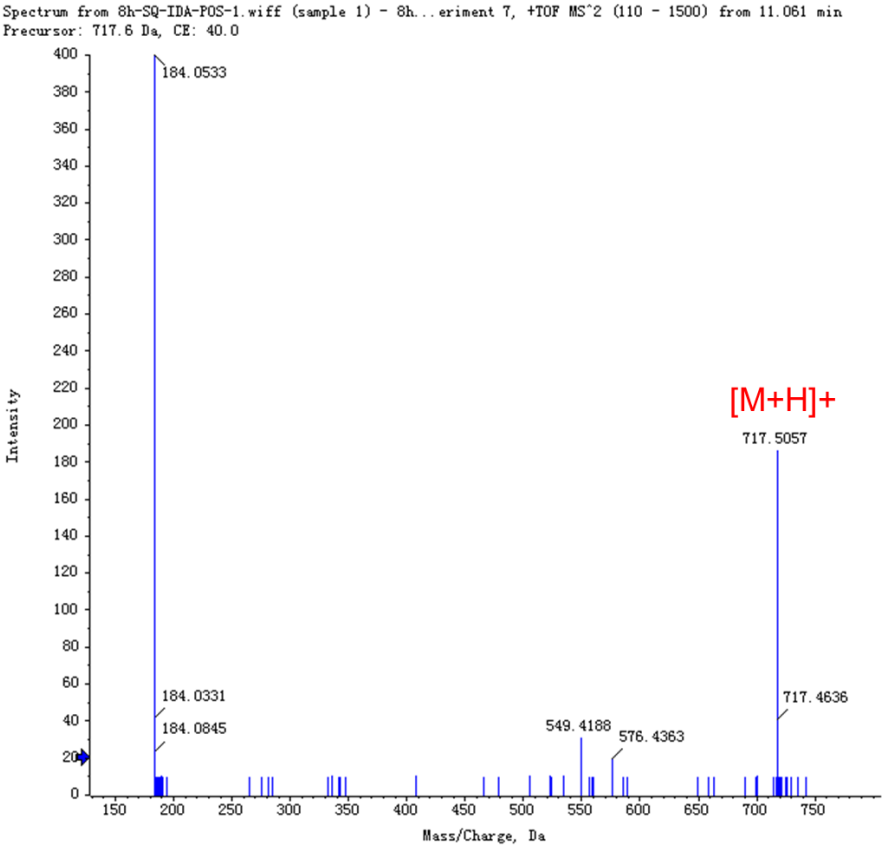
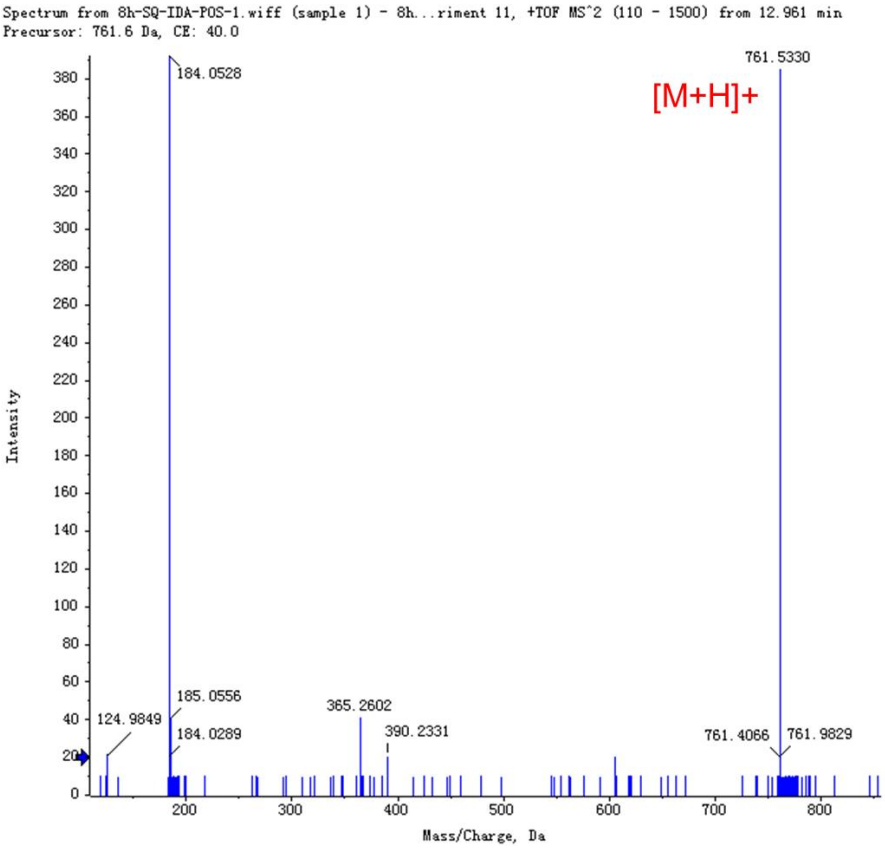


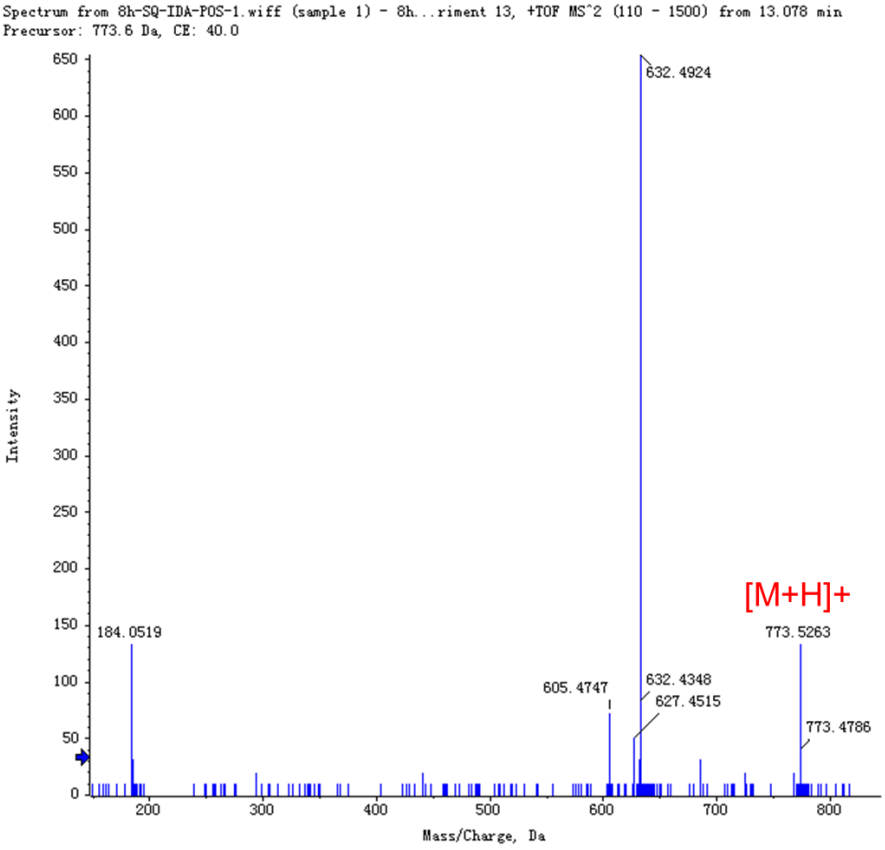
SM(d35:1):



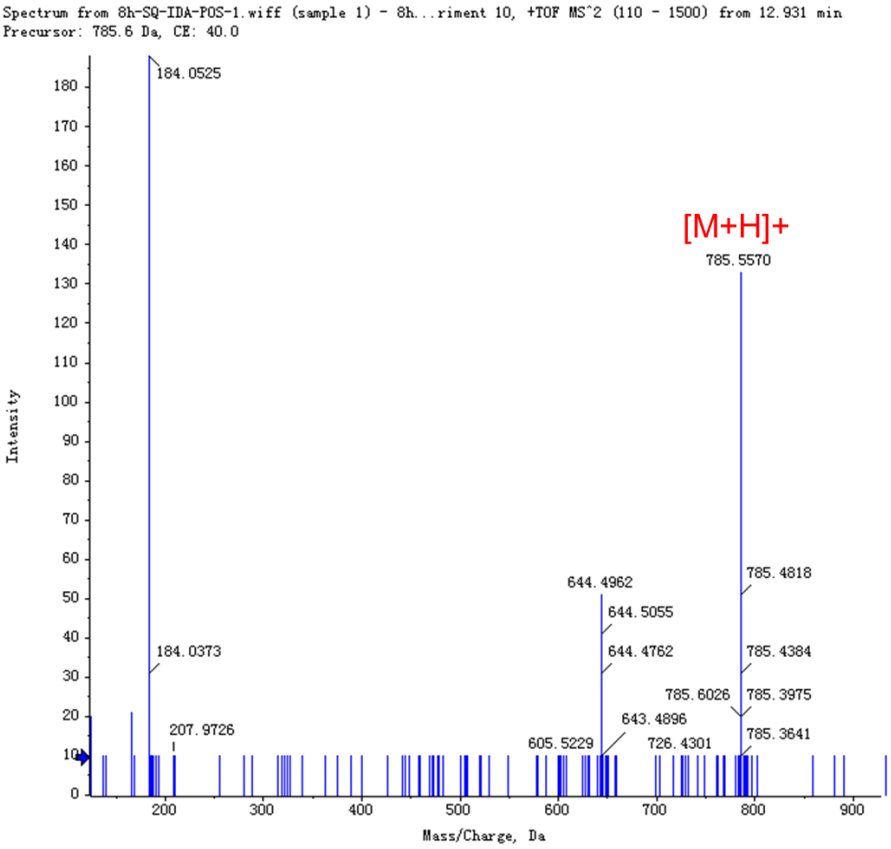
SM(d38:0):



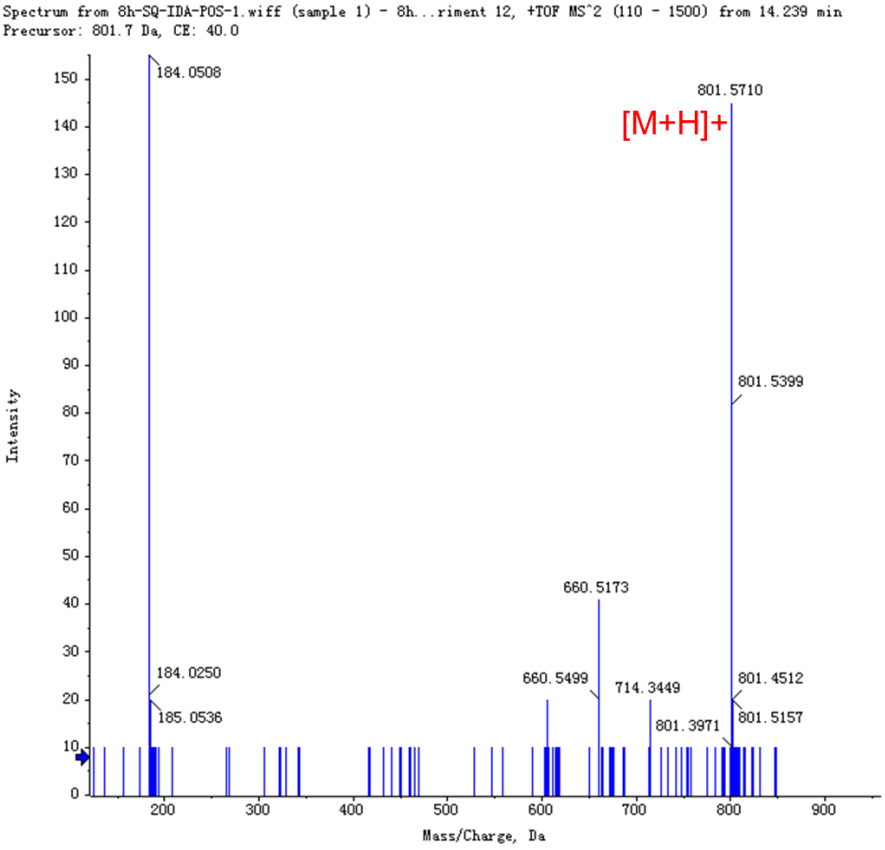
SM(d39:1):



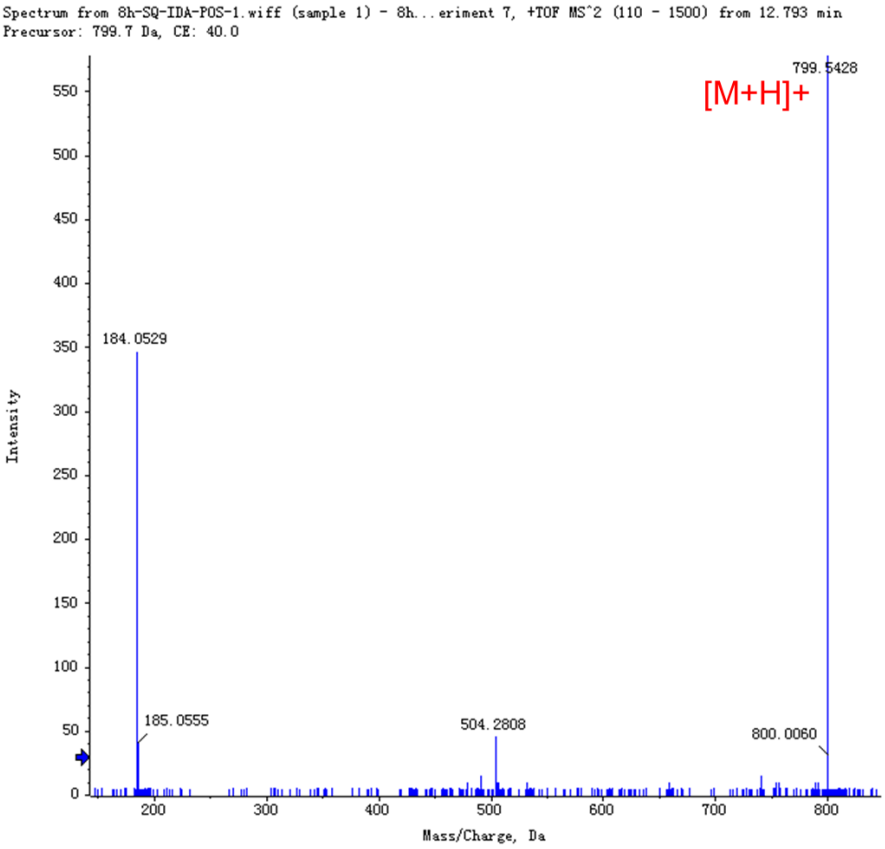
SM(d40:2):



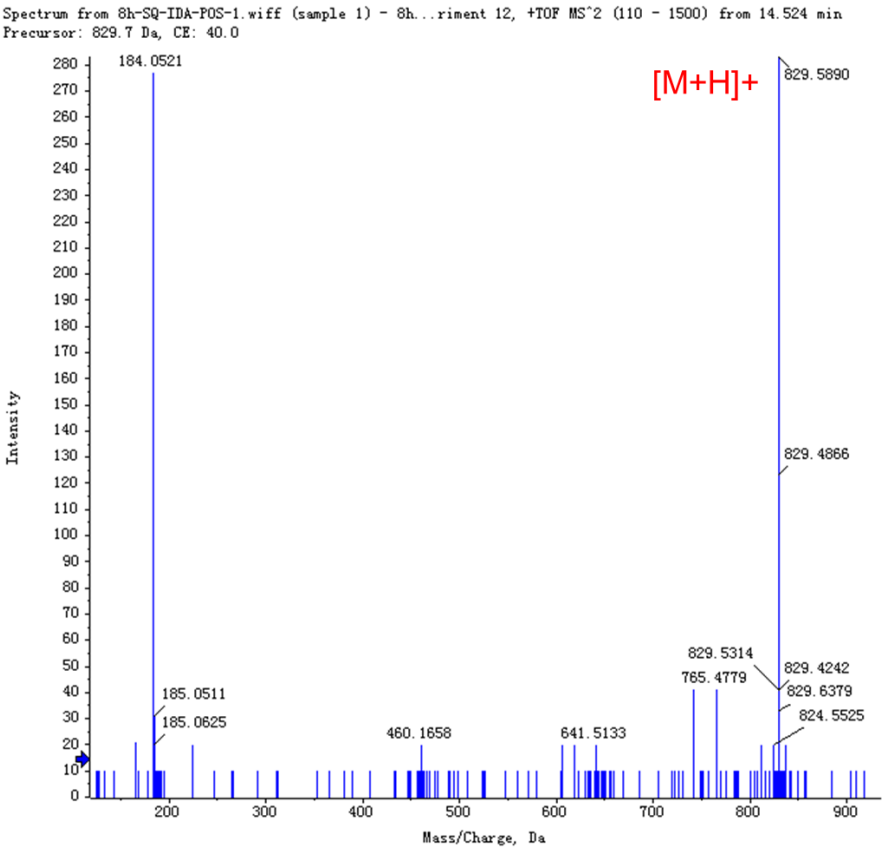
SM(d41:1):



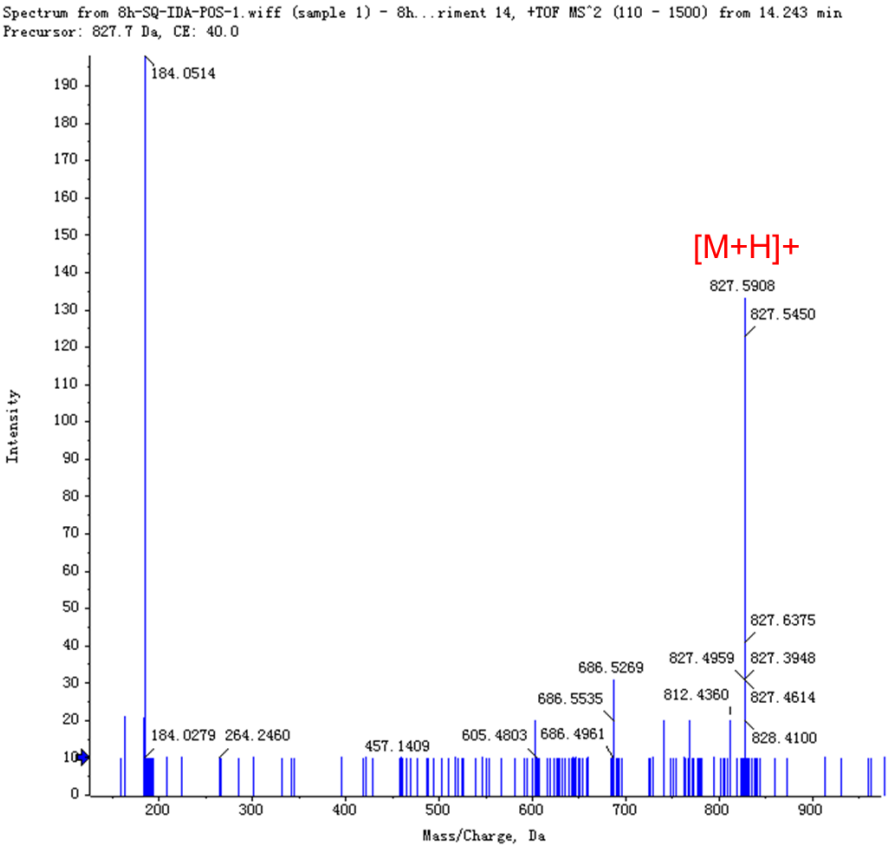
SM(d41:2):



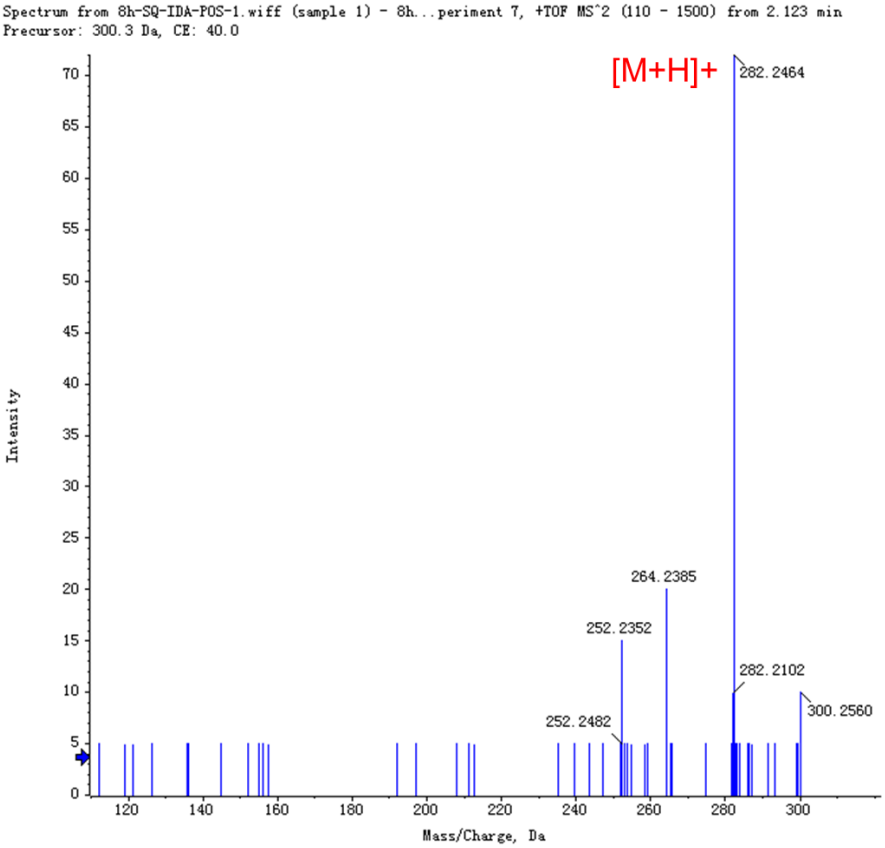
SM(d43:1):



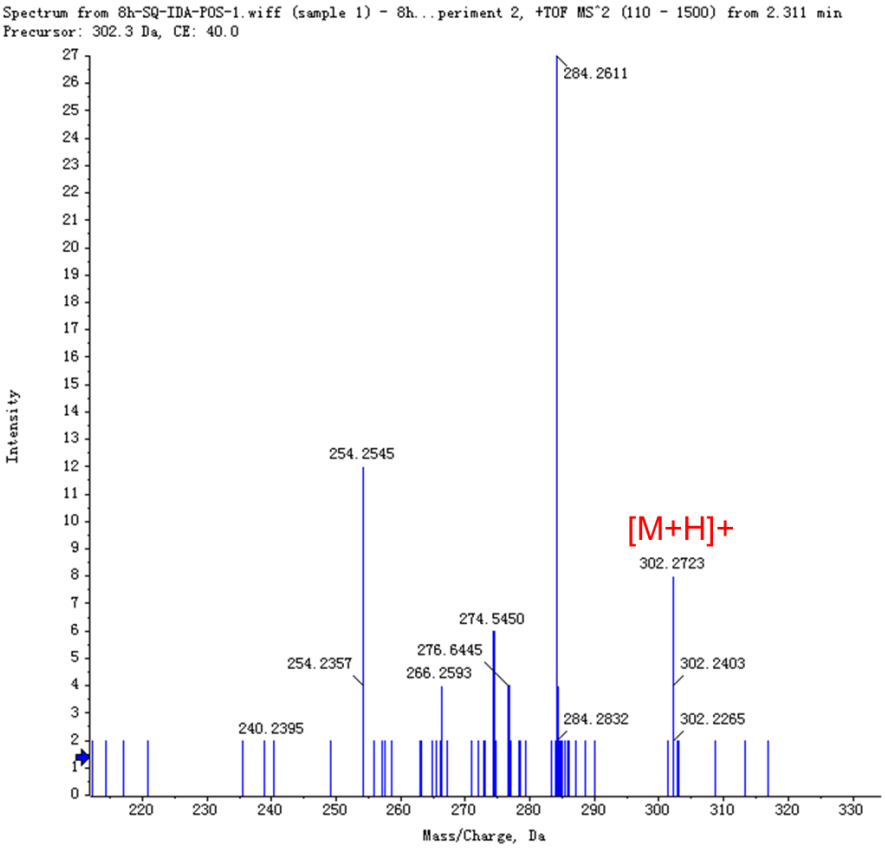
SM(d43:2):



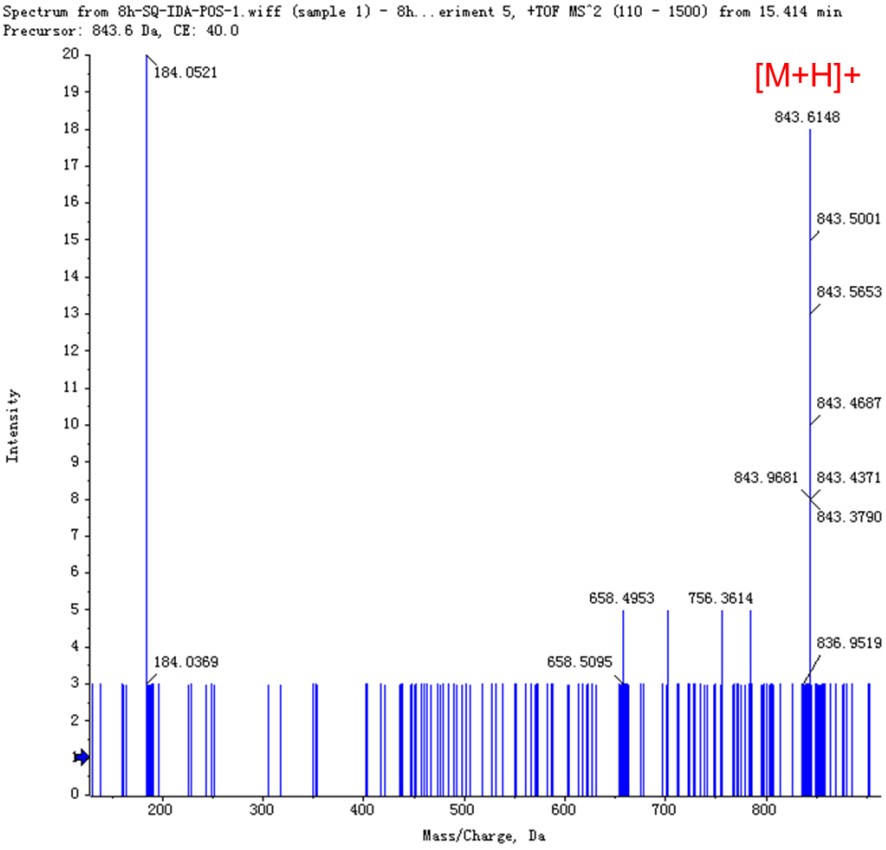
Sphingosine:



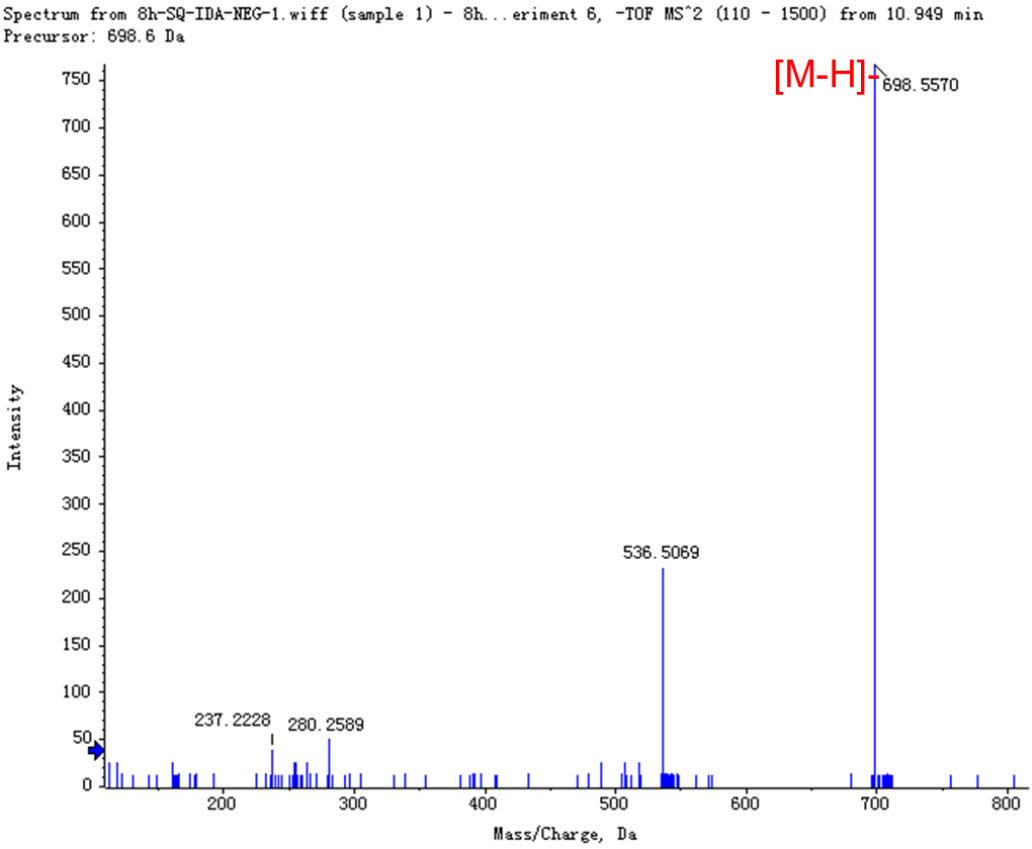
Sphinganine:



SM(d44:1):

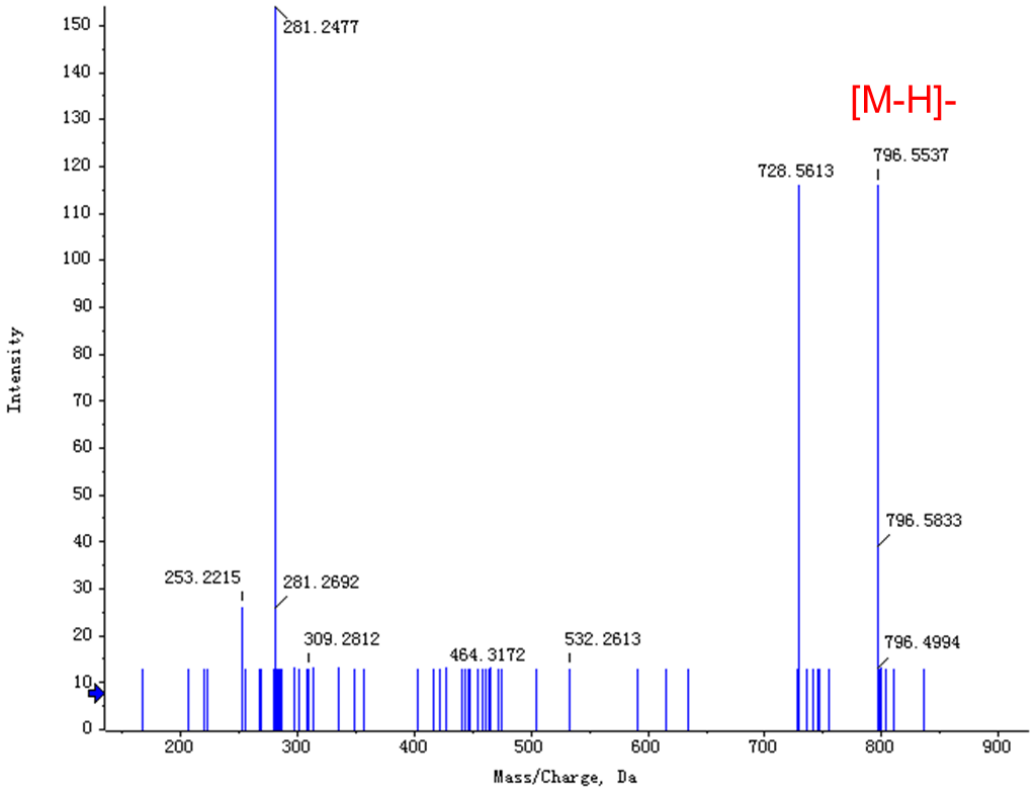


GlcCer(d34:1):



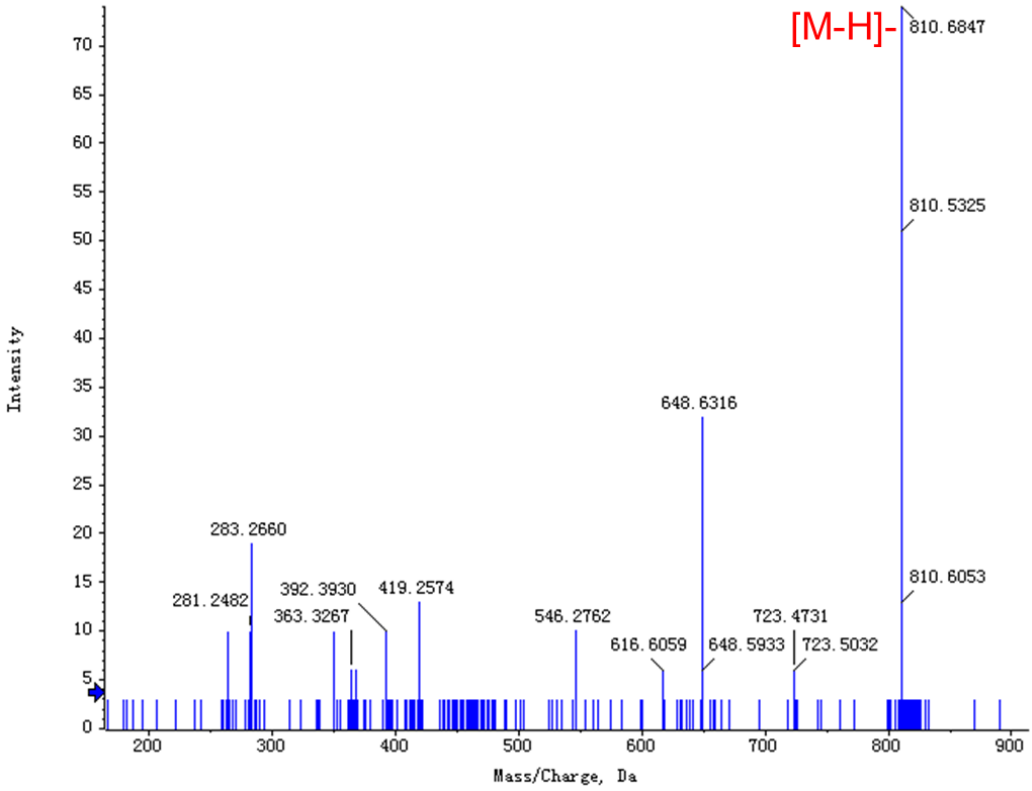
GlcCer(d41:1):

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h...riment 10, -TOF MS^2 (110 - 1500) from 13.745 min
Precursor: 796.5 Da

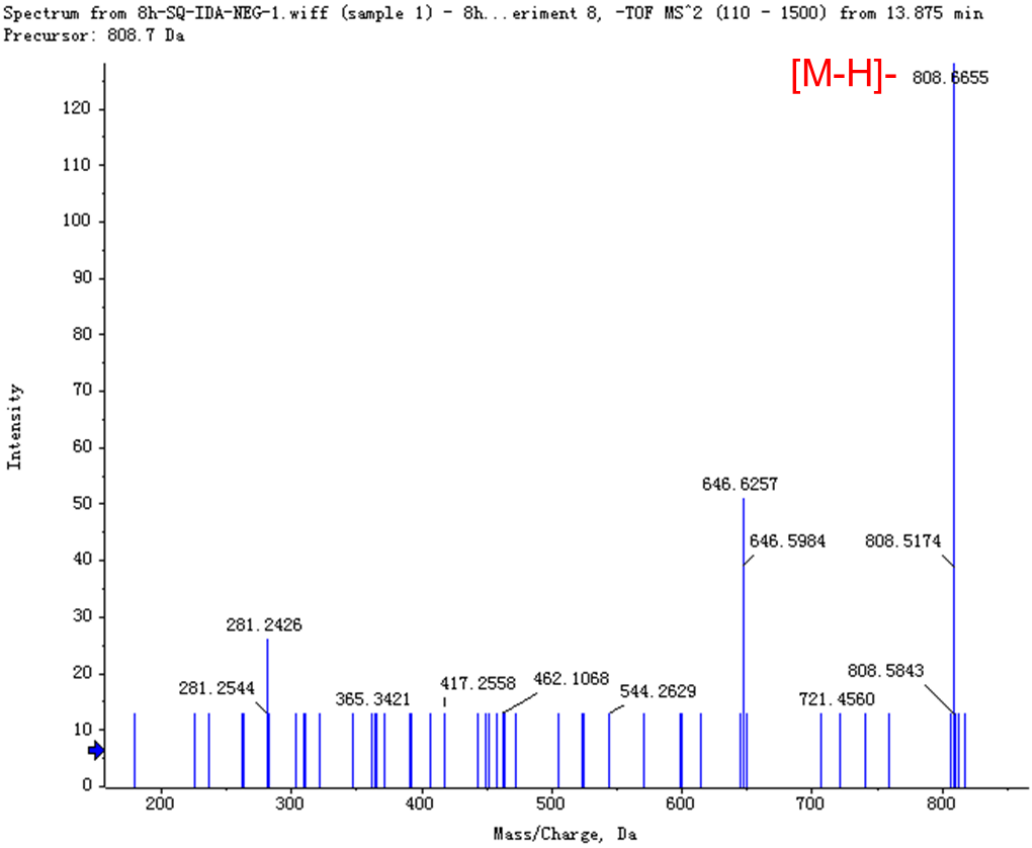


GlcCer(d42:1):

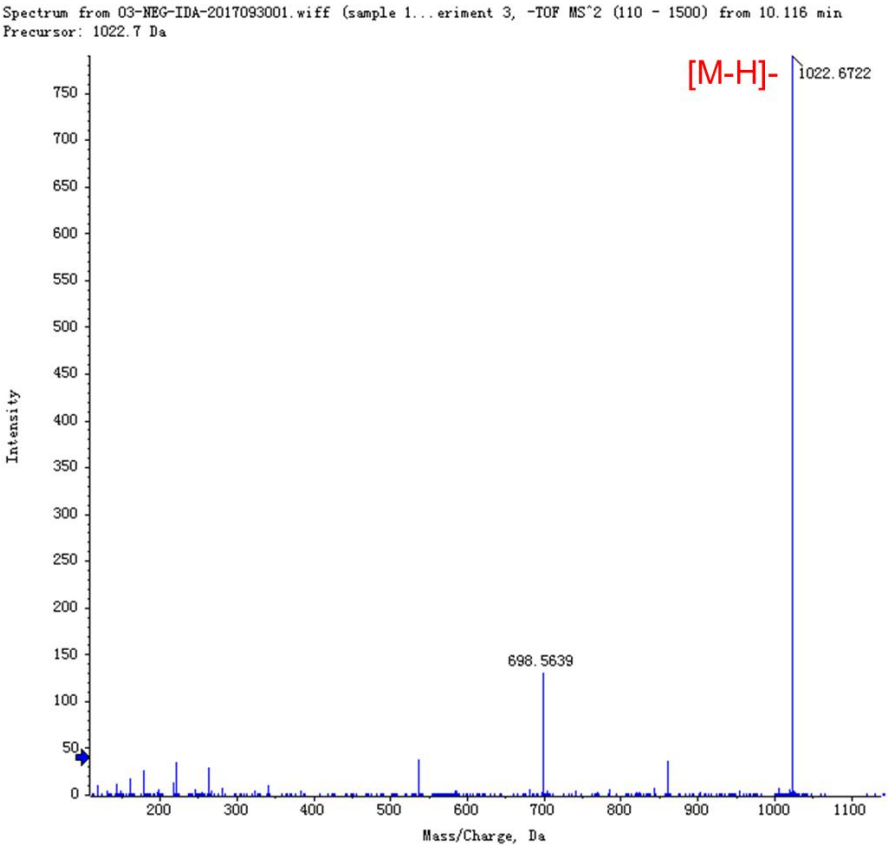
Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h...eriment 3, -TOF MS^2 (110 - 1500) from 14.787 min
Precursor: 810.7 Da



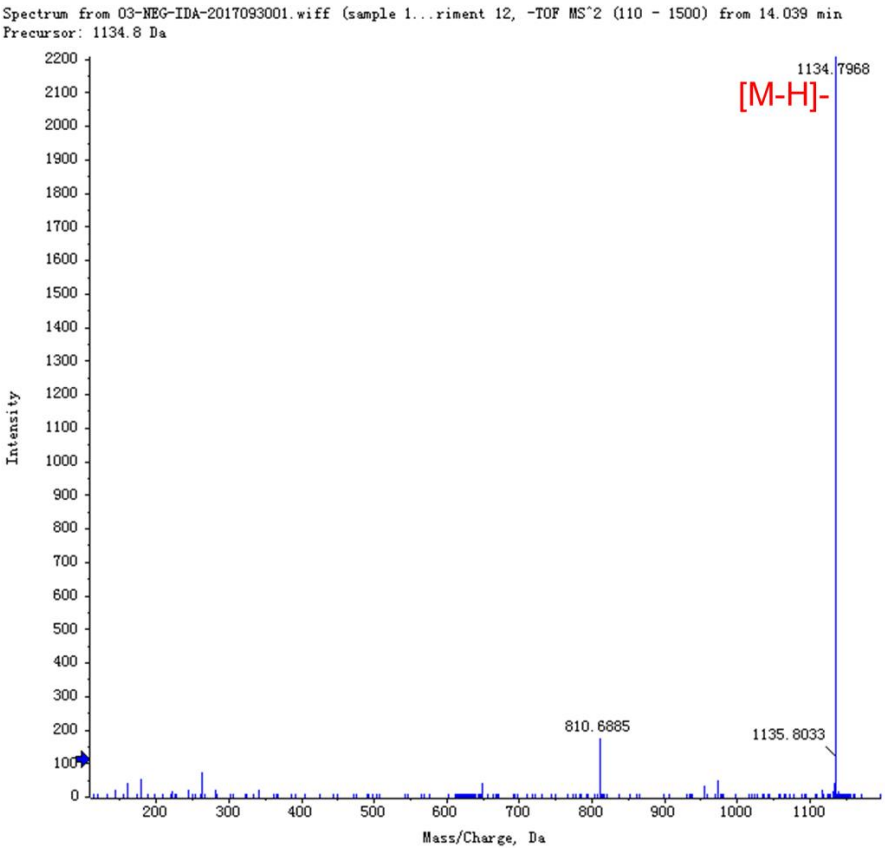
GlcCer(d42:2):



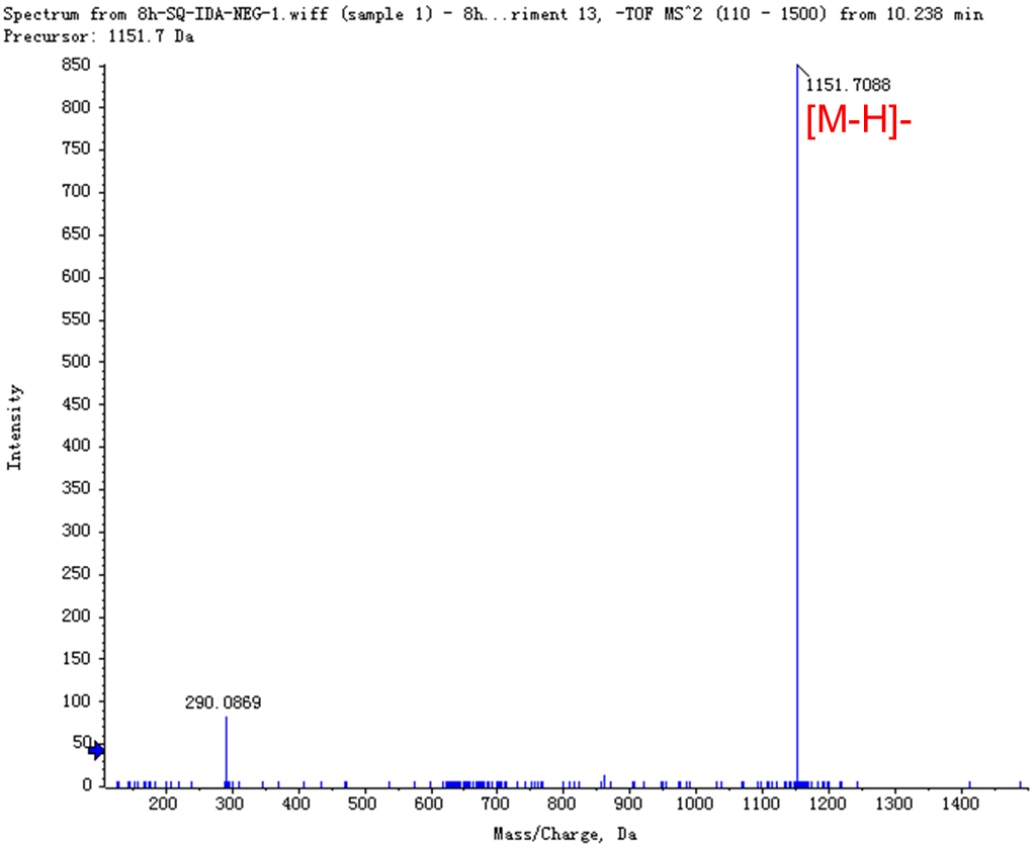
TrihexosylCer(d34:1):



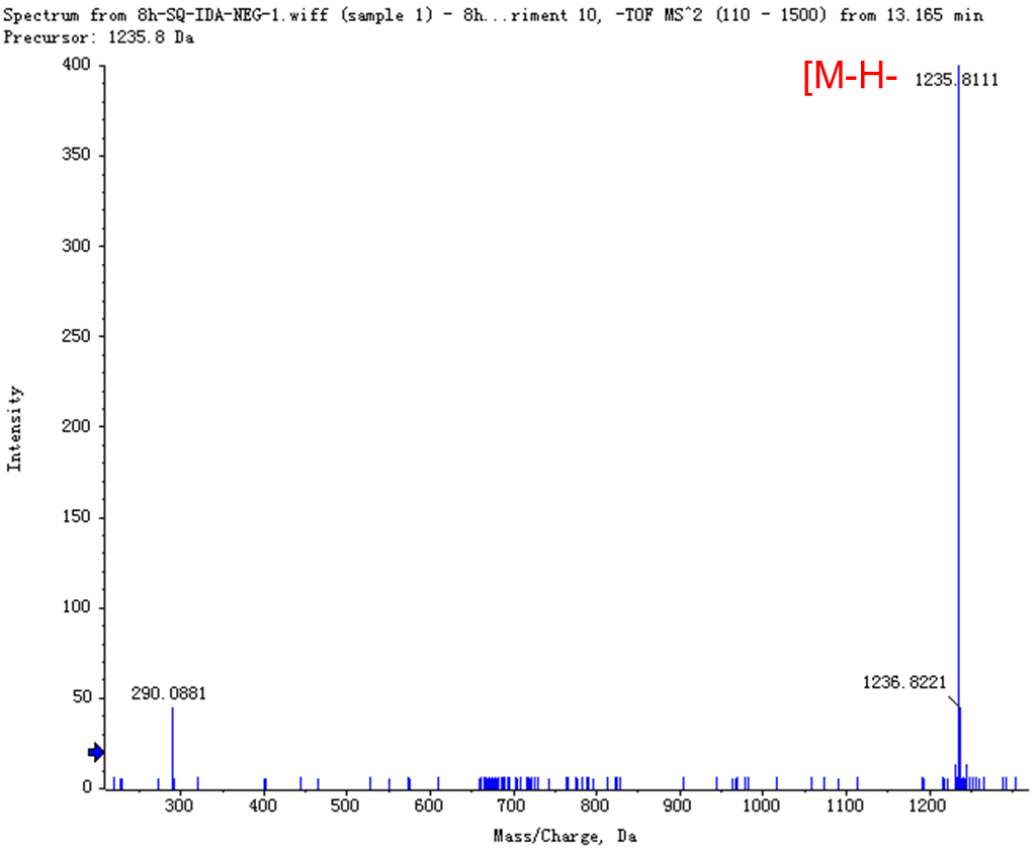
TrihexosylCer(d42:1):



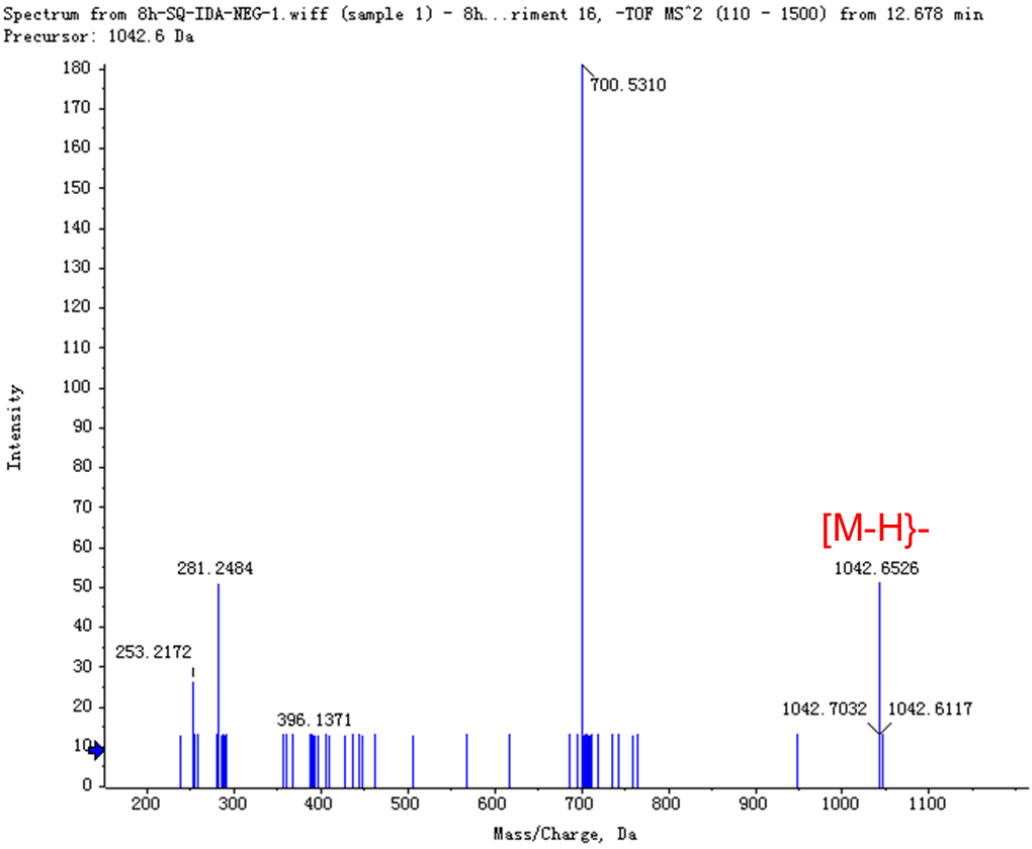
Ganglioside GM3(d34:1):



Ganglioside GM3(d40:1):

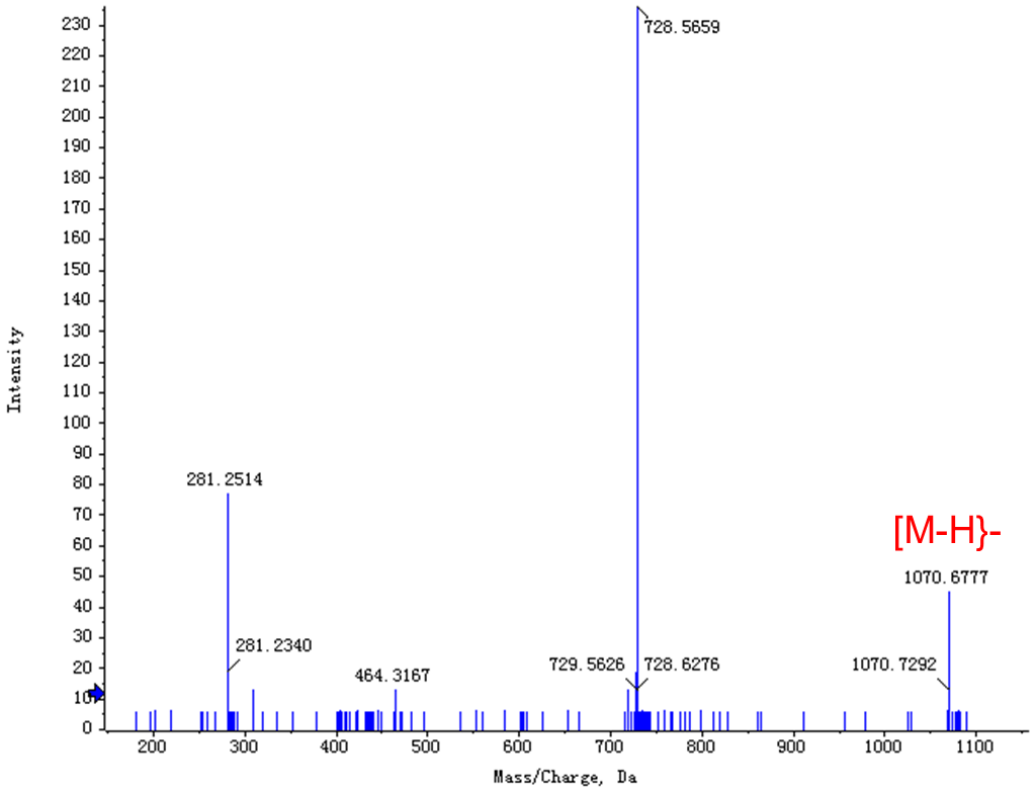


MIPC(t40:0)



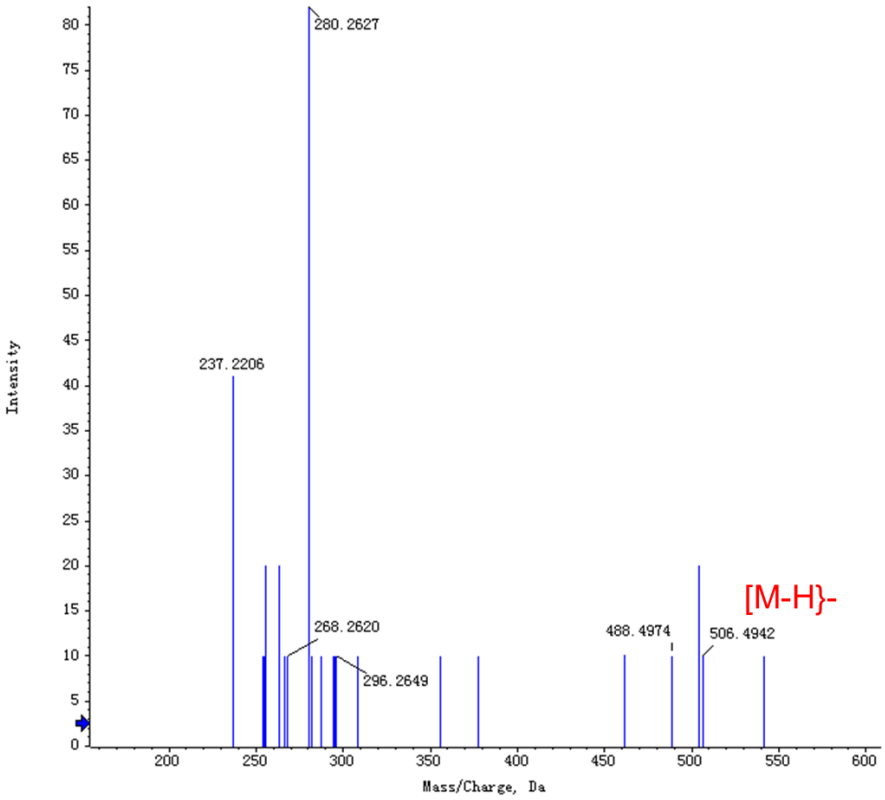
MIPC(t42:0)

Spectrum from 8h-SQ-IDA-NEG-1.wiff (sample 1) - 8h...riment 11, -TOF MS^2 (110 - 1500) from 13.647 min
Precursor: 1070.7 Da

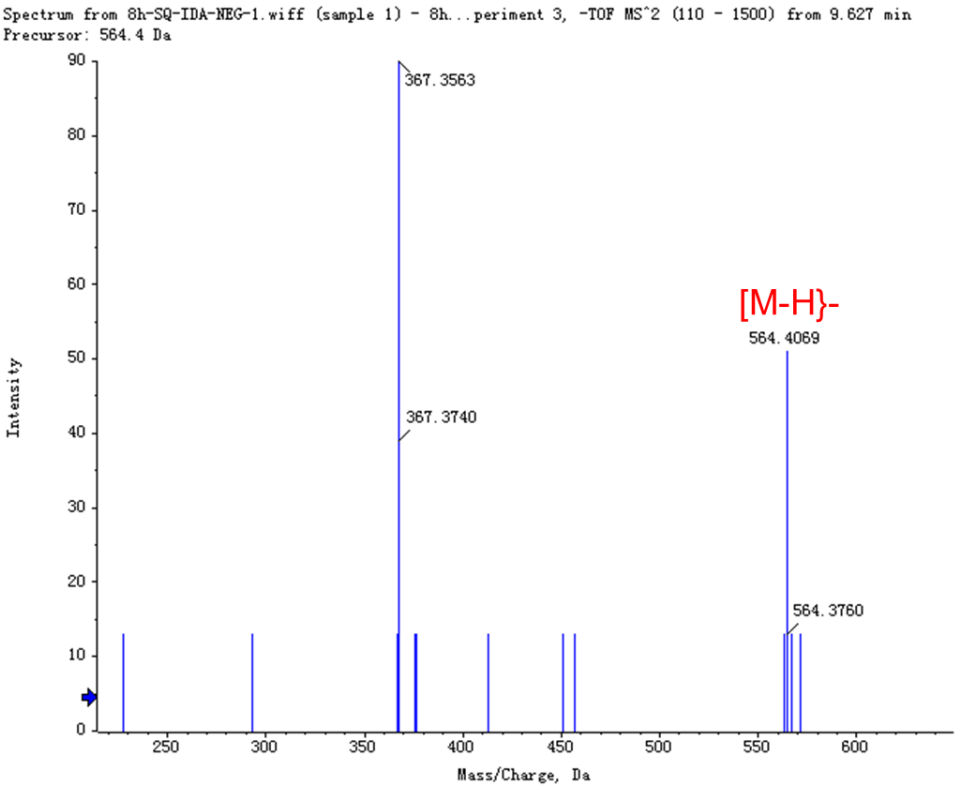


Cer(d34:1):

Spectrum from 03-NEG-IDA-2017093001.wiff (sample 1...eriment 2, -TOF MS^2 (110 - 1500) from 12.044 min
Precursor: 536.5 Da



Cer(d36:1):



Cer(d40:2):

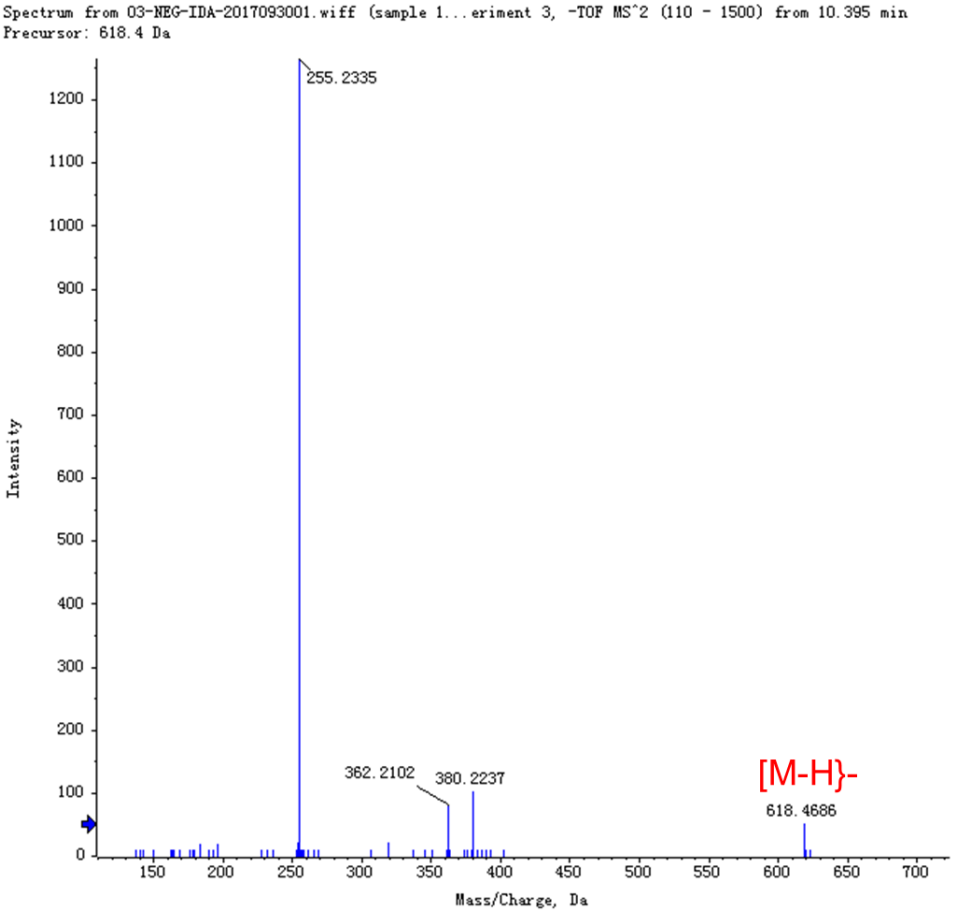


Figure S2. The typical MS/MS spectra of a portion of lipids identified

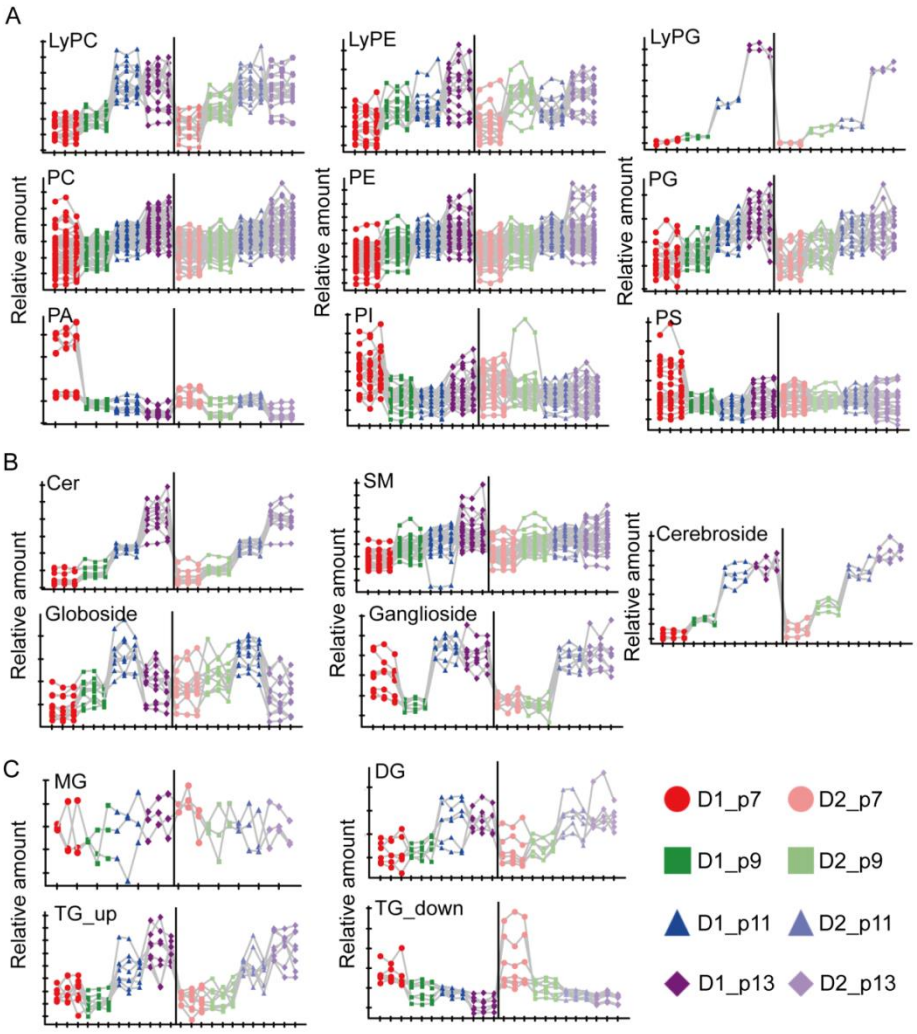


Figure S3. Metabolic trend plots of various categories of lipids in BMSCs of D1 and D2 during BMSC aging

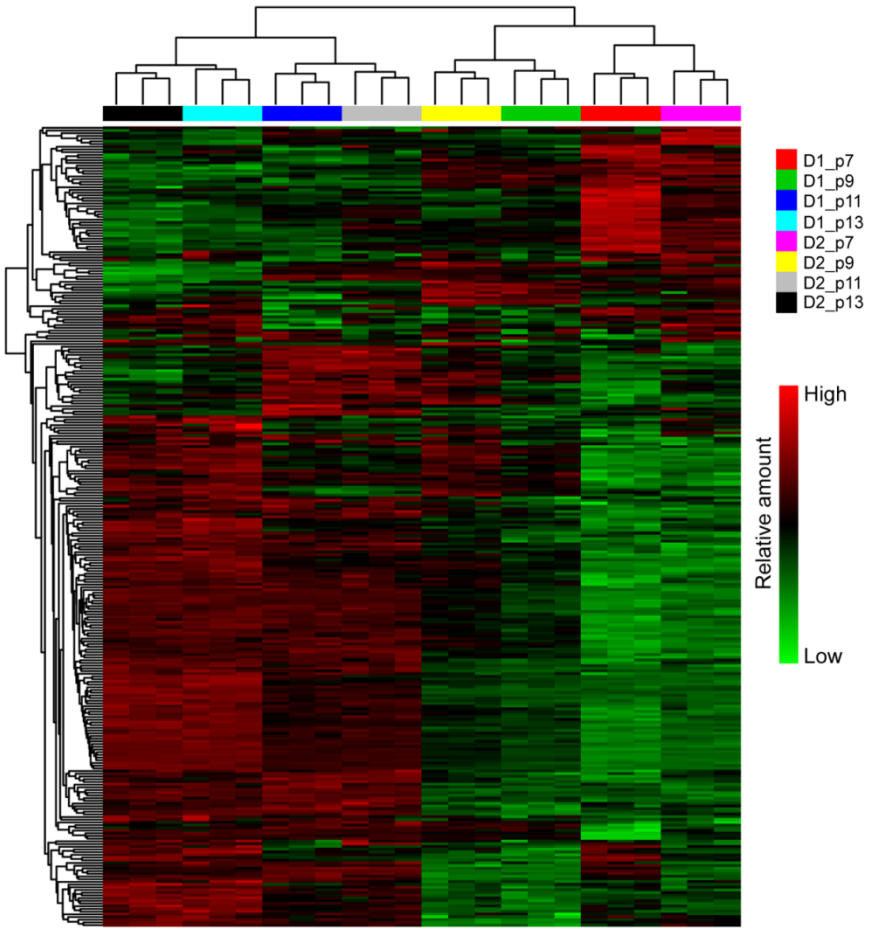


Figure S4. HCA-heatmap diagram showing the metabolic similarities of lipidomics patterns between BMSCs from D1 and D2 during passaging

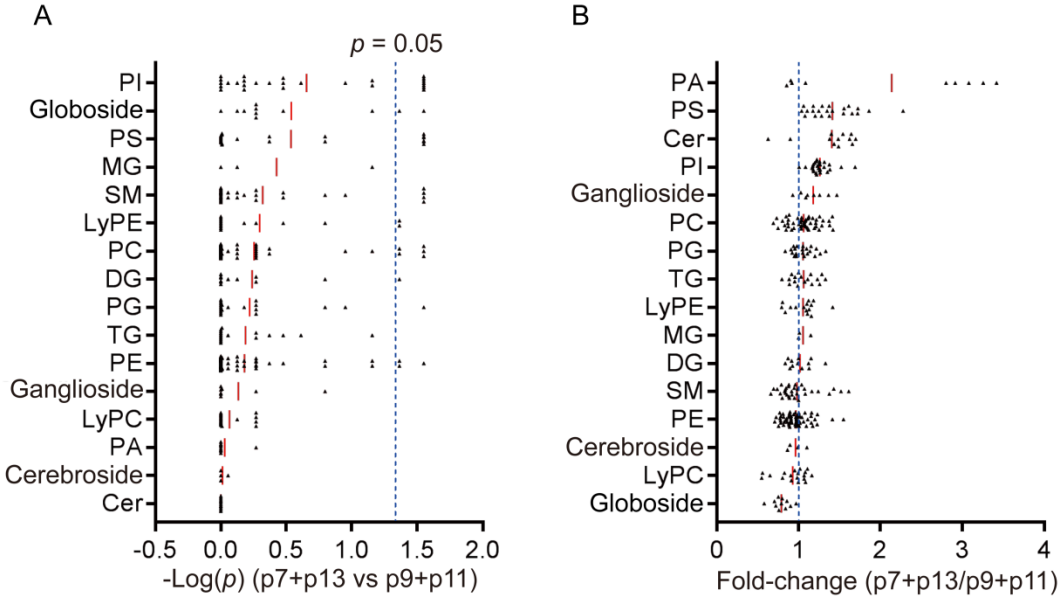


Figure S5. Univariate characterizations of alterations of lipid species between BMSCs of p7/p13 and p9/p11. (A) –log(*p*) values of lipids in Student t-test between BMSCs of p7/p13 and p9/p11. (B) The fold-change values of lipid species in BMSCs of p7/p13 relative to those of p9/p11

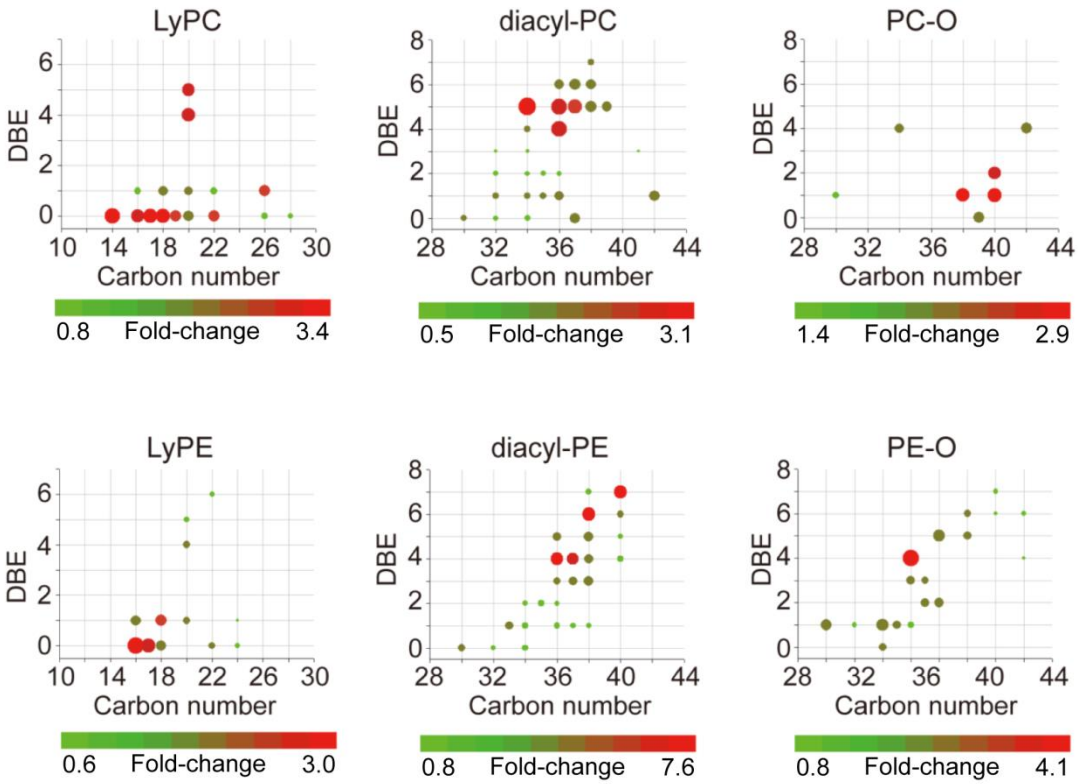


Figure S6. DVC plots of LyPCs, LyPEs, diacyl-PCs, diacyl-PEs, PC-Os and PE-Os showing fold-change alterations in BMSCs of p13 relative to those of p7

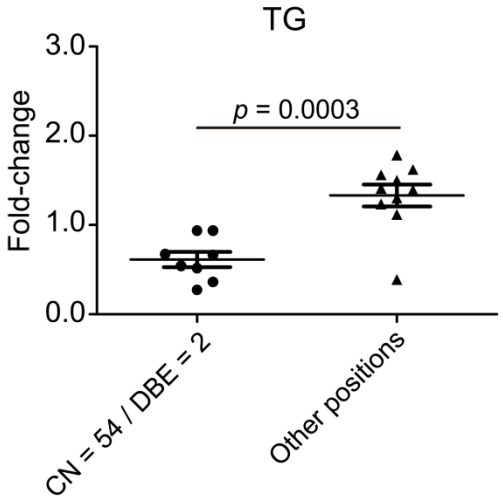


Figure S7. Fold-change values (p13 to p7) of TGs with CN of 54 and DBE of 2 compared with those at other coordinates. The data were represented as mean +/- SEM

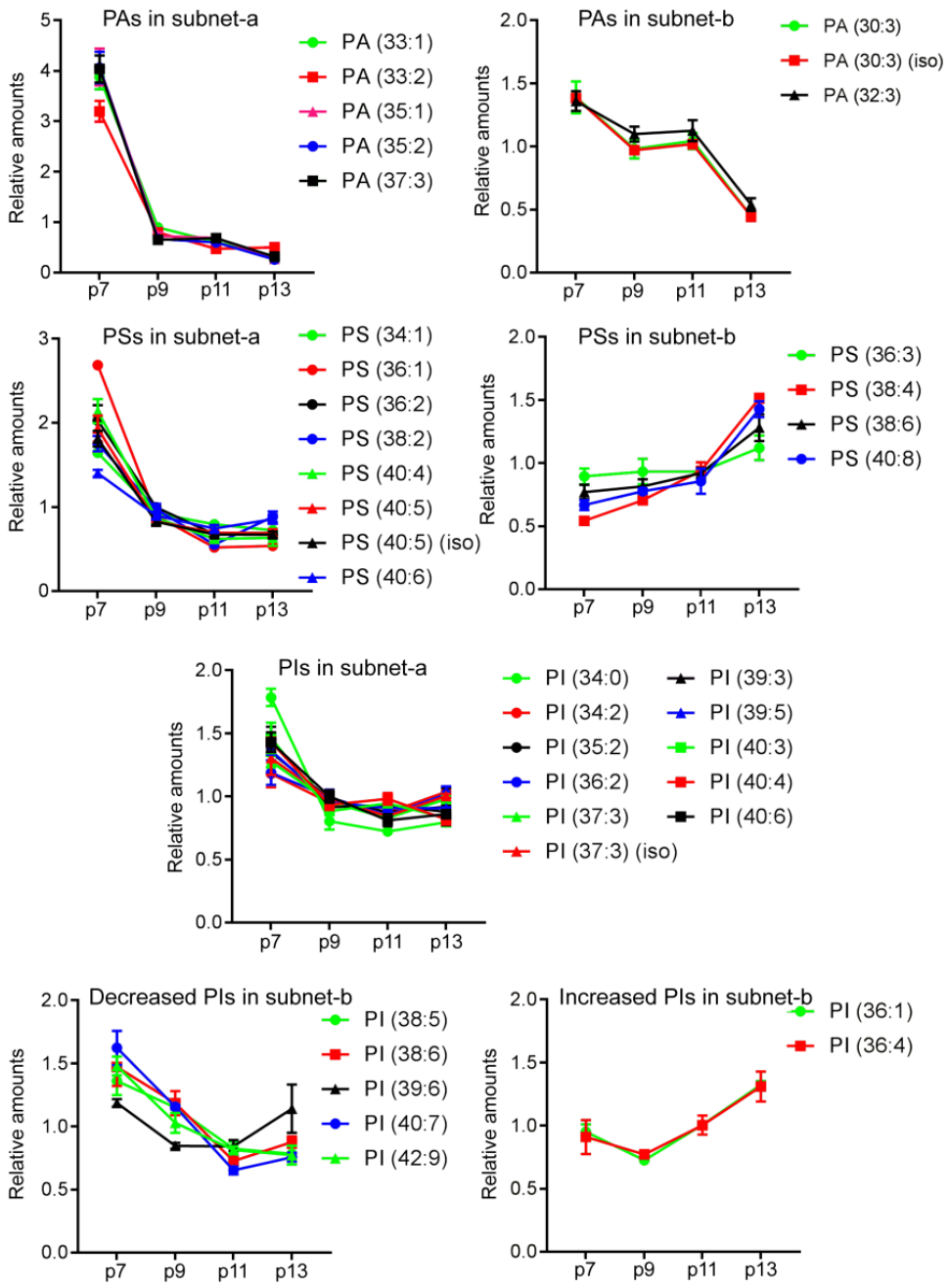


Figure S8. Changing trends of PAs, PSs and PIs in subnet-a and subnet-b at sequential passages. The data were represented as mean +/- SEM

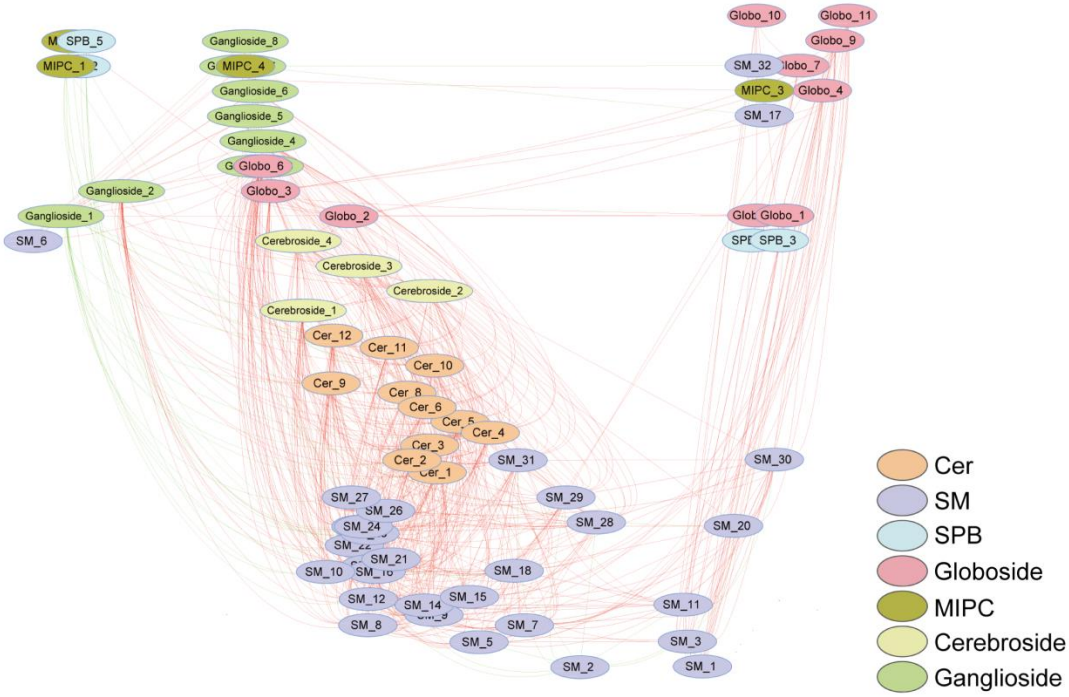


Figure S9. Correlation networks constructed with SPs of different categories based on |Pearson CC| larger than 0.9

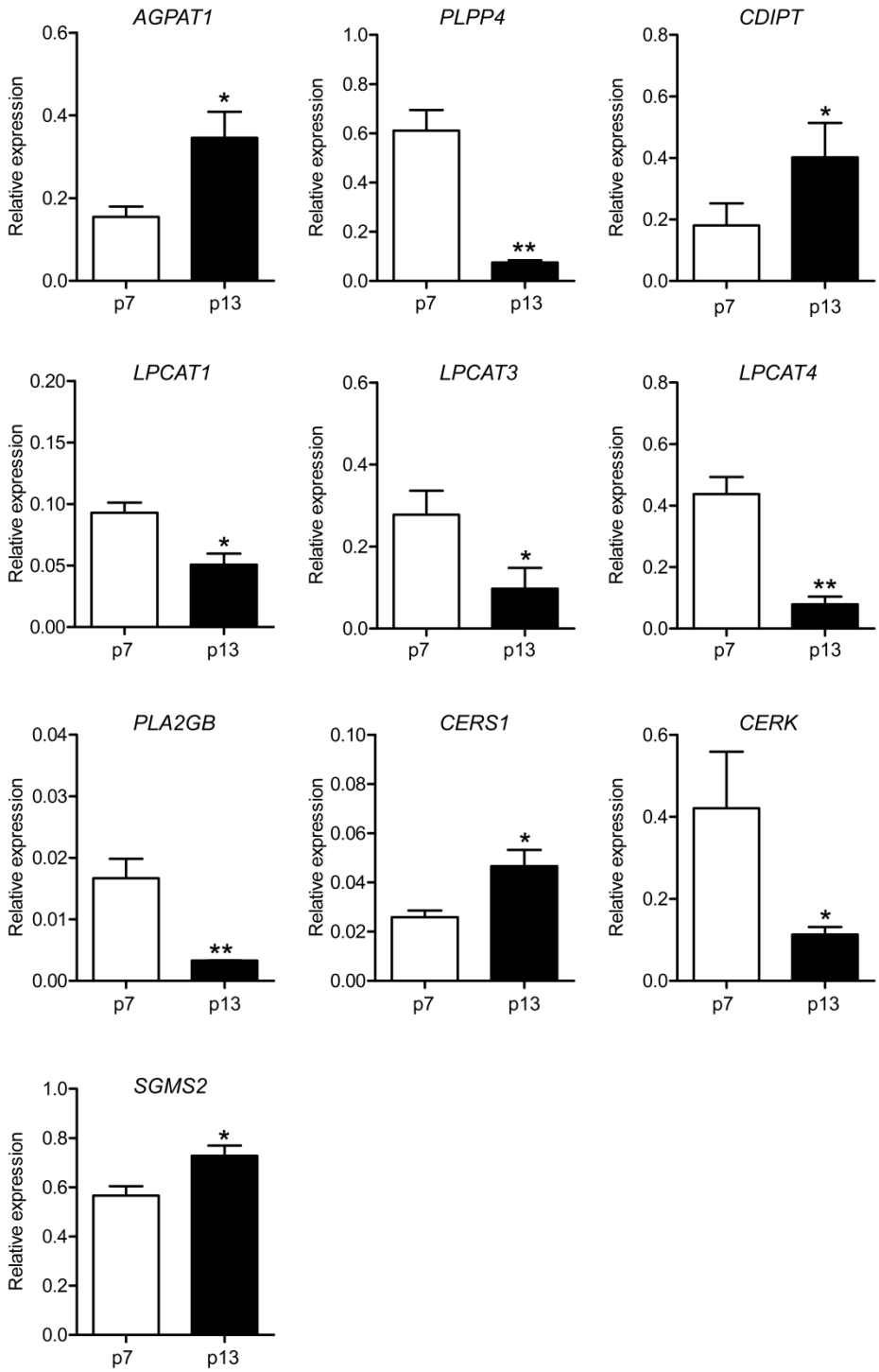


Figure S10. Relative mRNA expressions of enzymes anchored in pathway analysis in p7- and p13-BMSCs. The data were represented as mean +/- SEM

Table S1. Detailed methods and parameters for feature selection

Option	Method/Value
Retention time format	minute
Feature detection method	centWave
Maximal m/z deviation in consecutive scans (ppm)	10
Minimum chromatographic peak width (sec)	5
Maximum chromatographic peak width (sec)	20
Signal/Noise threshold	30
Minimum m/z difference for peaks with overlapping retention times	0.005
Integration method for feature detection	1
Prefilter peaks	3
Prefilter intensity	500
Intensity threshold for noise filter	100
Retention time correction method	obiwarp
Width of overlapping m/z for alignment	0.015
Band width (sec)	10
Minimum fraction for alignment	0.5
Minimum number of samples necessary in one group	1
Maximum number of groups in a single m/z slice	100
Annotation searching feature	Isotopes+adducts
ppm error for annotation	5
m/z absolute error for annotation	0.005
Signal for quantification	peak area

Table S2. The primer sequences of genes anchored in pathway analysis

Gene name	Sequence
AGPAT1	forward, 5′ -AGGACGCAACGTCGAGAAC-3′ ;
	reverse, 5′ - GCAGTACCTCCATCATCCCAAG-3′
CDS1	forward, 5′ -AGTTCCTCATTCGCTACCATAGA-3′
	reverse, 5′ - GGTGTGACTGAGTGACAGTTATC-3′
CDIPT	forward, 5′ - GTGCCCAACCTCATCGGTTAT-3′
	reverse, 5′ - TGTCCATCGAAAGCGTCCAG-3′
SGPP2	forward, 5′ - ACTGGAAAAGAGACTGATCGCT-3′
	reverse, 5′ - CCTGCTGAGACACACCAAGG-3′
CERS1	forward, 5′ - TACAGTGCCTACCTGCTGTTT-3′
	reverse, 5′ - TAGCGTAGCGTAGATGGAGTG-3′
SGMS2	forward, 5′ - TCCTACGAACACTTATGCAAGAC-3′
	reverse, 5′ - CCGGGTACTTTTTGGTGCCT-3′
CERK	forward, 5′ - TGTGCCTGTATCTGAGATCATCG-3′
	reverse, 5′ - TGCCGTCGTGCTCTCTTTAC-3′
PLPP4	forward, 5′ - CCCTGCTCTTCGGAGTCTTC-3′
	reverse, 5′ - AGGCGGGTAGGTATGTTATCTG-3′
CEPT1	forward, 5′ - ATGTGGAGATTCTCACCCGGA-3′
	reverse, 5′ - TCTTCTAGCCGCTTTAGTTGGT-3′
PLA2G4B	forward, 5′ - CAACCTCCAGGACAGCTTATAC-3′
	reverse, 5′ - CTGTTGAGGGTGGTTCTTCTATC-3′
LPCAT1	forward, 5′ - CGCCTCACTCGTCCTACTTC-3′
	reverse, 5′ - TTCCCCAGATCGGGATGTCTC-3′
LPCAT3	forward, 5′ - GGAGCTGAGCCTTAACAAGTT-3′
	reverse, 5′ - CAAAGCAAAGGGGTAACCCAG-3′
LPCAT4	forward, 5′ - TCTCGCCTCCAGAGGGTTAAG-3′
	reverse, 5′ - AAGAGGACGATAAAGGCCAGA-3′

Table S3. The characterization information of lipid species identified in BMSC lipidomics profiles

ID	Name	Formula	RT (min)	*m/z* (Da)	Adduct	Student *p*-value	Pearson CC	Fold-change O4/O1
LyPC_1	LyPC(14:0)	C22H46NO7P	2.31	512.3003	M+FA-H	8.83E-03	0.999	3.39
LyPC_2	LyPC(16:0)	C24H50NO7P	3.43	540.3316	M+FA-H	4.63E-03	0.980	2.95
LyPC_3	LyPC(16:1)	C24H48NO7P	2.55	538.3146	M+FA-H	1.54E-03	0.950	1.69
LyPC_4	LyPC(17:0)	C25H52NO7P	4.33	554.3465	M+FA-H	8.18E-03	0.960	3.24
LyPC_5	LyPC(18:0)	C26H54NO7P	5.21	568.3630	M+FA-H	1.29E-02	0.981	3.21
LyPC_6	LyPC(18:1)	C26H52NO7P	3.68	566.3473	M+FA-H	1.04E-02	0.960	2.28
LyPC_7	LyPC(19:0)	C27H56NO7P	5.97	582.3783	M+FA-H	1.61E-03	0.882	2.63
LyPC_8	LyPC(20:0)	C28H58NO7P	6.73	596.3925	M+FA-H	8.83E-03	0.989	2.45
LyPC_9	LyPC(20:1)	C28H56NO7P	5.46	594.3780	M+FA-H	2.04E-02	0.988	2.03
LyPC_10	LyPC(20:4)	C28H50NO7P	2.65	588.3302	M+FA-H	1.40E-02	0.997	3.00
LyPC_11	LyPC(20:5)	C28H48NO7P	2.16	586.3160	M+FA-H	4.90E-03	0.977	2.87
LyPC_12	LyPC(22:0)	C30H62NO7P	8.02	624.4237	M+FA-H	4.50E-03	0.989	2.68
LyPC_13	LyPC(22:1)	C30H60NO7P	6.86	622.4093	M+FA-H	4.85E-02	0.865	1.70
LyPC_14	LyPC(26:0)	C34H70NO7P	8.94	680.4876	M+FA-H	3.17E-03	0.829	1.60
LyPC_15	LyPC(26:1)	C34H68NO7P	9.28	678.4706	M+FA-H	2.98E-03	0.812	2.62
LyPC_16	LyPC(28:0)	C36H74NO7P	10.00	708.5167	M+FA-H	2.72E-02	0.608	1.30
LyPC_17	LyPC(P-15:0)	C23H48NO6P	3.09	510.3187	M+FA-H	6.30E-02	0.184	0.84

LyPC_18	LyPC(O-16:0)	C24H52NO6P	4.18	526.3520	M+FA-H	2.51E-02	0.721	1.47
LyPC_19	LyPC(O-18:0)	C26H56NO6P	5.90	554.3832	M+FA-H	2.76E-03	0.898	1.77
LyPC_20	LyPC(O-18:1)	C26H54NO6P	4.44	552.3668	M+FA-H	4.84E-02	0.783	1.62
LyPC_21	LyPC(O-18:2)	C26H52NO6P	4.42	550.3527	M+FA-H	1.47E-02	0.466	1.35
LyPC_22	LyPC(O-20:0)	C28H60NO6P	7.38	582.4128	M+FA-H	1.01E-02	0.908	1.72
PC_1	PC(30:0)	C38H76NO8P	10.55	750.5290	M+FA-H	2.10E-01	0.856	1.16
PC_2	PC(32:0)	C40H80NO8P	11.53	778.5584	M+FA-H	4.87E-01	-0.343	0.97
PC_3	PC(32:1)	C40H78NO8P	10.70	776.5432	M+FA-H	4.14E-02	0.889	1.23
PC_4	PC(32:2)	C40H76NO8P	9.91	774.5292	M+FA-H	5.42E-01	-0.295	0.97
PC_5	PC(32:3)	C40H74NO8P	9.41	772.5121	M+FA-H	1.27E-02	-0.929	0.66
PC_6	PC(34:0)	C42H84NO8P	12.56	806.5924	M+FA-H	7.26E-01	0.742	1.07
PC_7	PC(34:1)	C42H82NO8P	11.66	804.5760	M+FA-H	2.44E-01	0.525	1.22
PC_8	PC(34:2)	C42H80NO8P	10.87	802.5598	M+FA-H	3.06E-01	-0.376	0.95
PC_9	PC(34:3)	C42H78NO8P	10.23	800.5446	M+FA-H	4.97E-03	-0.803	0.68
PC_10	PC(34:4)	C42H76NO8P	9.64	798.5302	M+FA-H	1.55E-02	0.759	1.18
PC_11	PC(34:5)	C42H74NO8P	9.00	796.5135	M+FA-H	2.76E-03	0.995	3.01
PC_12	PC(35:1)	C43H84NO8P	12.17	818.5934	M+FA-H	1.62E-02	0.783	1.27
PC_13	PC(35:2)	C43H82NO8P	11.33	816.5753	M+FA-H	7.34E-01	-0.246	0.98
PC_14	PC(36:1)	C44H86NO8P	12.66	832.6066	M+FA-H	4.97E-03	0.901	1.68
PC_15	PC(36:2)	C44H84NO8P	11.81	830.5905	M+FA-H	1.14E-02	-0.509	0.85

PC_16	PC(36:4)	C44H80NO8P	10.71	826.5611	M+FA-H	1.48E-03	0.990	2.59
PC_17	PC(36:5)	C44H78NO8P	10.03	824.5439	M+FA-H	4.55E-03	0.995	2.69
PC_18	PC(36:5)	C44H78NO8P	10.18	778.5398	M+FA-H	8.07E-03	0.901	1.50
PC_19	PC(36:6)	C44H76NO8P	9.24	822.5291	M+FA-H	8.83E-03	0.898	1.73
PC_20	PC(37:0)	C45H90NO8P	13.54	848.6385	M+FA-H	1.95E-02	0.891	1.76
PC_21	PC(37:5)	C45H80NO8P	10.39	838.5598	M+FA-H	1.20E-03	0.997	2.35
PC_22	PC(37:6)	C45H78NO8P	11.64	836.5455	M+FA-H	9.58E-03	0.926	1.97
PC_23	PC(38:5)	C46H82NO8P	10.90	852.5757	M+FA-H	1.90E-03	0.980	2.02
PC_24	PC(38:6)	C46H80NO8P	10.24	850.5584	M+FA-H	1.21E-02	0.989	1.73
PC_25	PC(38:7)	C46H78NO8P	9.58	848.5442	M+FA-H	8.41E-02	0.881	1.19
PC_26	PC(38:7)	C46H78NO8P	11.42	848.5445	M+FA-H	1.29E-02	-0.785	0.76
PC_27	PC(39:5)	C47H84NO8P	11.29	866.5906	M+FA-H	6.93E-03	0.939	1.76
PC_28	PC(41:3)	C49H92NO8P	14.10	898.6564	M+FA-H	2.19E-02	-0.813	0.54
PC_29	PC(42:1)	C50H98NO8P	15.33	916.6990	M+FA-H	3.32E-03	0.828	1.80
PC_30	PC(42:10)	C50H80NO8P	9.53	898.5615	M+FA-H	3.14E-03	0.943	1.74
PC_31	PC(44:12)	C52H80NO8P	9.42	922.5616	M+FA-H	1.23E-01	0.871	1.07
PC_32	PC(O-30:1)	C38H76NO7P	9.81	734.5359	M+FA-H	9.46E-03	0.851	1.47
PC_33	PC(O-34:5)	C42H76NO7P	9.33	782.5321	M+FA-H	1.62E-02	0.858	1.94
PC_34	PC(O-38:1)	C46H92NO7P	14.80	846.6590	M+FA-H	2.56E-03	0.887	2.74
PC_35	PC(O-39:0)	C47H96NO7P	14.48	862.6905	M+FA-H	1.06E-02	0.953	2.26

PC_36	PC(O-40:1)	C48H96NO7P	14.78	874.6904	M+FA-H	9.25E-03	0.881	2.85
PC_37	PC(O-40:2)	C48H94NO7P	13.93	872.6768	M+FA-H	3.32E-03	0.822	2.56
PC_38	PC(O-42:4)	C50H94NO7P	14.38	896.6763	M+FA-H	8.39E-03	0.935	2.26
LyPE_1	LyPE(13:0)	C18H38NO7P	3.24	410.2318	M-H	5.08E-03	0.042	0.80
LyPE_2	LyPE(16:0)	C21H44NO7P	3.68	452.2787	M-H	1.84E-02	0.961	3.00
LyPE_3	LyPE(16:1)	C21H42NO7P	2.67	450.2637	M-H	4.71E-03	0.863	1.86
LyPE_4	LyPE(17:0)	C22H46NO7P	4.54	466.2944	M-H	1.47E-02	0.910	2.55
LyPE_5	LyPE(18:0)	C23H48NO7P	5.47	480.3103	M-H	2.67E-03	0.859	1.98
LyPE_6	LyPE(18:1)	C23H46NO7P	3.99	478.2946	M-H	1.69E-03	0.798	2.13
LyPE_7	LyPE(20:1)	C25H50NO7P	5.72	506.3263	M-H	4.80E-02	0.285	1.43
LyPE_8	LyPE(20:4)	C25H44NO7P	2.81	500.2785	M-H	8.89E-03	0.828	1.38
LyPE_9	LyPE(20:5)	C25H42NO7P	2.29	498.2634	M-H	2.81E-02	0.463	1.15
LyPE_10	LyPE(22:0)	C27H56NO7P	8.33	536.3722	M-H	2.41E-03	0.844	1.38
LyPE_11	LyPE(22:6)	C27H44NO7P	2.68	524.2786	M-H	1.74E-01	0.307	1.10
LyPE_12	LyPE(24:0)	C29H60NO7P	9.69	564.4024	M-H	4.76E-02	-0.118	1.09
LyPE_13	LyPE(24:1)	C29H58NO7P	8.37	562.3873	M-H	4.71E-03	-0.689	0.66
LyPE_14	LyPE(P-16:0)	C21H44NO6P	4.36	436.2838	M-H	6.27E-03	0.890	2.98
LyPE_15	LyPE(P-18:0)	C23H48NO6P	6.11	464.3154	M-H	8.18E-03	0.795	1.85
LyPE_16	LyPE(P-20:0)	C25H52NO6P	7.54	492.3460	M-H	2.80E-01	0.518	1.19
PE_1	PE(30:0)	C35H70NO8P	10.93	662.4768	M-H	1.15E-02	0.482	1.26

PE_2	PE(32:0)	C37H74NO8P	12.06	690.5071	M-H	5.71E-02	-0.581	0.87
PE_3	PE(35:2)	C40H76NO8P	11.72	728.5241	M-H	7.59E-02	0.777	1.19
PE_4	PE(33:1)	C38H74NO8P	11.51	702.5091	M-H	9.16E-03	0.851	1.40
PE_5	PE(34:0)	C39H78NO8P	13.12	718.5387	M-H	4.44E-02	0.661	1.16
PE_6	PE(34:1)	C39H76NO8P	12.10	716.5239	M-H	8.07E-03	0.875	1.15
PE_7	PE(34:2)	C39H74NO8P	11.25	714.5071	M-H	6.97E-02	0.330	1.01
PE_8	PE(38:5)	C43H76NO8P	11.32	764.5235	M-H	3.17E-03	0.975	1.66
PE_9	PE(36:1)	C41H80NO8P	13.13	744.5548	M-H	4.71E-03	0.810	1.17
PE_10	PE(36:2)	C41H78NO8P	12.26	742.5392	M-H	5.50E-01	-0.597	0.95
PE_11	PE(36:3)	C41H76NO8P	11.44	740.5251	M-H	1.38E-01	0.950	1.30
PE_12	PE(36:4)	C41H74NO8P	11.13	738.5071	M-H	8.43E-03	0.859	2.11
PE_13	PE(36:5)	C41H72NO8P	10.38	736.4944	M-H	7.02E-02	0.946	1.47
PE_14	PE(37:3)	C42H78NO8P	12.09	754.5400	M-H	3.06E-03	0.937	1.46
PE_15	PE(37:4)	C42H76NO8P	11.62	752.5245	M-H	1.69E-03	0.968	2.04
PE_16	PE(38:1)	C43H84NO8P	14.10	772.5870	M-H	4.87E-01	0.269	1.01
PE_17	PE(38:2)	C43H82NO8P	13.23	770.5726	M-H	3.03E-02	0.487	1.08
PE_18	PE(38:3)	C43H80NO8P	12.55	768.5553	M-H	8.43E-03	0.963	1.70
PE_19	PE(38:4)	C43H78NO8P	12.21	766.5392	M-H	1.18E-02	0.922	1.62
PE_20	PE(38:6)	C43H74NO8P	10.82	762.5068	M-H	5.97E-03	0.974	2.24
PE_21	PE(38:7)	C43H72NO8P	9.98	760.4924	M-H	5.27E-01	0.067	1.06

PE_22	PE(40:4)	C45H82NO8P	12.92	794.5682	M-H	2.12E-02	0.682	1.14
PE_23	PE(40:5)	C45H80NO8P	12.21	792.5540	M-H	5.67E-01	0.268	0.98
PE_24	PE(40:6)	C45H78NO8P	11.17	790.5415	M-H	6.24E-02	0.841	1.23
PE_25	PE(40:7)	C45H76NO8P	11.02	788.5245	M-H	1.42E-02	0.873	2.20
PE_26	PE(42:0)	C47H94NO8P	13.98	830.6635	M-H	2.56E-03	0.963	7.53
PE_27	PE(O-28:1)	C33H66NO7P	10.45	618.4513	M-H	8.44E-03	0.967	2.52
PE_28	PE(O-30:0)	C35H72NO7P	10.10	648.4957	M-H	8.18E-03	0.626	1.23
PE_29	PE(O-30:0)	C35H70NO7P	11.51	646.4830	M-H	6.75E-03	0.936	3.38
PE_30	PE(O-30:1)	C35H68NO7P	10.59	644.4670	M-H	6.03E-03	0.945	4.03
PE_31	PE(O-32:1)	C37H74NO7P	12.60	674.5122	M-H	1.48E-03	0.843	1.80
PE_32	PE(O-32:2)	C37H72NO7P	11.68	672.4970	M-H	3.40E-03	0.973	2.72
PE_33	PE(O-33:2)	C38H74NO7P	12.17	686.5119	M-H	4.97E-03	0.960	1.98
PE_34	PE(O-34:1)	C39H78NO7P	13.67	702.5440	M-H	5.68E-03	0.746	1.55
PE_35	PE(O-34:2)	C39H76NO7P	12.68	700.5286	M-H	9.71E-03	0.977	2.17
PE_36	PE(O-34:3)	C39H74NO7P	11.89	698.5120	M-H	5.74E-03	0.996	1.96
PE_37	PE(O-34:4)	C39H72NO7P	9.25	696.4963	M-H	1.20E-03	0.926	3.74
PE_38	PE(O-34:5)	C39H70NO7P	10.62	694.4818	M-H	4.97E-03	0.967	2.13
PE_39	PE(O-35:2)	C40H78NO7P	13.19	714.5440	M-H	1.82E-02	0.984	2.02
PE_40	PE(O-35:3)	C40H76NO7P	12.38	712.5271	M-H	1.29E-02	0.997	1.76
PE_41	PE(O-36:1)	C41H82NO7P	13.72	730.5749	M-H	2.76E-03	0.992	2.09

PE_42	PE(O-36:2)	C41H80NO7P	13.72	728.5593	M-H	2.67E-03	0.999	2.72
PE_43	PE(O-36:3)	C41H78NO7P	12.81	726.5435	M-H	5.28E-03	0.998	2.23
PE_44	PE(O-36:5)	C41H74NO7P	11.70	722.5121	M-H	1.00E-03	0.984	2.62
PE_45	PE(O-36:6)	C41H72NO7P	11.02	720.4968	M-H	6.81E-04	0.915	3.81
PE_46	PE(O-38:5)	C43H78NO7P	12.74	750.5440	M-H	4.97E-03	0.966	1.92
PE_47	PE(O-38:6)	C43H76NO7P	11.85	748.5269	M-H	8.44E-03	0.945	1.71
PE_48	PE(O-38:7)	C43H74NO7P	11.30	746.5139	M-H	6.30E-03	0.951	1.75
PE_49	PE(O-40:5)	C45H82NO7P	13.59	778.5740	M-H	5.05E-01	0.315	1.04
PE_50	PE(O-40:6)	C45H80NO7P	12.75	776.5586	M-H	9.24E-02	0.704	1.15
PE_51	PE(O-40:7)	C45H78NO7P	12.46	774.5444	M-H	2.76E-03	0.950	1.44
PE_52	PE(O-40:8)	C45H76NO7P	11.50	772.5286	M-H	2.84E-02	0.988	1.28
PE_53	PE(O-42:5)	C47H86NO7P	14.56	806.6044	M-H	2.00E-01	-0.029	0.88
PE_54	PE(O-42:6)	C47H84NO7P	13.71	804.5894	M-H	3.95E-02	0.491	1.18
PE_55	PE(O-42:7)	C47H82NO7P	13.48	802.5743	M-H	7.56E-01	0.595	1.11
PS_1	PS(34:1)	C40H76NO10P	13.25	760.5117	M-H	1.48E-03	-0.882	0.43
PS_2	PS(36:1)	C42H80NO10P	13.98	788.5445	M-H	1.62E-02	-0.853	0.20
PS_3	PS(36:2)	C42H78NO10P	13.39	786.5272	M-H	1.15E-02	-0.883	0.33
PS_4	PS(36:3)	C42H76NO10P	12.13	784.5115	M-H	8.56E-02	0.860	1.25
PS_5	PS(38:2)	C44H82NO10P	13.32	814.5584	M-H	2.75E-03	-0.770	0.50
PS_6	PS(38:3)	C44H80NO10P	13.25	812.5464	M-H	7.19E-02	-0.474	0.79

PS_7	PS(38:4)	C44H78NO10P	13.06	810.5277	M-H	5.67E-01	0.059	1.01
PS_8	PS(38:5)	C44H76NO10P	12.50	808.5143	M-H	2.98E-03	0.960	1.32
PS_9	PS(40:4)	C46H82NO10P	13.54	838.5604	M-H	2.76E-03	-0.849	0.29
PS_10	PS(40:5)	C46H80NO10P	13.08	836.5426	M-H	8.05E-03	-0.830	0.35
PS_11	PS(40:6)	C46H78NO10P	12.61	834.5280	M-H	2.67E-03	-0.792	0.61
PS_12	PS(40:7)	C46H76NO10P	11.28	832.5099	M+H	2.03E-03	0.897	2.13
PS_13	PS(42:5)	C48H84NO10P	13.83	866.5897	M+H	1.39E-01	-0.461	0.92
PS_14	PS(42:8)	C48H78NO10P	12.07	860.5407	M+H	5.15E-01	-0.087	1.06
PS_15	PS(42:9)	C48H76NO10P	11.60	858.5260	M+H	1.40E-01	0.045	1.07
PA_1	PA(30:3)	C33H59O8P	9.22	613.3890	M-H	1.90E-03	-0.925	0.32
PA_2	PA(32:3)	C35H63O8P	10.43	641.4172	M-H	2.76E-03	-0.902	0.39
PA_3	PA(33:1)	C36H69O8P	12.38	659.4657	M-H	5.52E-03	-0.855	0.08
PA_4	PA(33:2)	C36H67O8P	11.42	657.4518	M-H	5.42E-03	-0.828	0.15
PA_5	PA(35:1)	C38H73O8P	13.46	687.4975	M-H	8.13E-03	-0.835	0.06
PA_6	PA(35:2)	C38H71O8P	12.52	685.4815	M-H	5.97E-03	-0.829	0.06
PA_7	PA(37:3)	C40H73O8P	12.77	711.4961	M-H	5.28E-03	-0.820	0.07
LyPI_1	LyPI(18:0)	C27H53O12P	5.35	599.3197	M-H	2.56E-03	0.570	1.69
LyPI_2	LyPI(20:4)	C29H49O12P	2.70	619.2896	M-H	1.07E-02	0.862	1.66
PI_1	PI(34:0)	C43H83O13P	13.06	837.5511	M-H	2.41E-03	-0.776	0.44
PI_2	PI(34:1)	C43H81O13P	11.64	835.5339	M-H	1.62E-02	0.528	1.32

PI_3	PI(34:2)	C43H79O13P	11.05	833.5185	M-H	1.64E-01	-0.504	0.87
PI_4	PI(35:1)	C44H83O13P	12.52	849.5485	M-H	4.44E-01	0.116	1.01
PI_5	PI(35:2)	C44H81O13P	11.47	847.5338	M-H	3.99E-02	-0.832	0.68
PI_6	PI(36:1)	C45H85O13P	13.15	863.5650	M-H	6.89E-03	0.732	1.39
PI_7	PI(36:2)	C45H83O13P	11.84	861.5488	M-H	8.83E-02	-0.613	0.85
PI_8	PI(36:3)	C45H81O13P	11.26	859.5323	M-H	9.16E-03	-0.414	0.82
PI_9	PI(36:4)	C45H79O13P	10.92	857.5189	M-H	1.25E-02	0.810	1.44
PI_10	PI(36:5)	C45H77O13P	10.16	855.5019	M-H	4.39E-03	-0.657	0.80
PI_11	PI(37:2)	C46H85O13P	12.67	875.5632	M-H	5.30E-02	-0.635	0.85
PI_12	PI(37:3)	C46H83O13P	11.49	873.5476	M-H	4.39E-03	-0.692	0.76
PI_13	PI(37:4)	C46H81O13P	11.42	871.5342	M-H	8.89E-03	-0.617	0.81
PI_14	PI(38:3)	C47H85O13P	12.58	887.5663	M-H	2.45E-01	-0.325	0.90
PI_15	PI(38:4)	C47H83O13P	11.81	885.5498	M-H	5.75E-02	0.925	1.11
PI_16	PI(38:5)	C47H81O13P	11.07	883.5345	M-H	1.95E-02	-0.965	0.57
PI_17	PI(38:6)	C47H79O13P	10.47	881.5186	M-H	3.53E-02	-0.872	0.59
PI_18	PI(39:3)	C48H87O13P	13.18	901.5803	M-H	1.29E-02	-0.807	0.60
PI_19	PI(39:5)	C48H83O13P	11.46	897.5499	M-H	3.17E-03	-0.826	0.66
PI_20	PI(39:6)	C48H81O13P	11.09	895.5363	M-H	6.55E-01	-0.097	0.96
PI_21	PI(40:3)	C49H89O13P	12.88	915.5960	M-H	1.03E-02	-0.811	0.56
PI_22	PI(40:4)	C49H87O13P	12.92	913.5804	M-H	1.20E-03	-0.860	0.57

PI_23	PI(40:5)	C49H85O13P	11.94	911.5643	M-H	3.22E-01	0.073	0.98
PI_24	PI(40:6)	C49H83O13P	11.37	909.5493	M-H	5.28E-03	-0.870	0.60
PI_25	PI(40:7)	C49H81O13P	10.75	907.5347	M-H	1.03E-02	-0.907	0.46
PI_26	PI(42:9)	C51H81O13P	10.22	931.5314	M-H	2.76E-03	-0.930	0.52
LyPG_1	LyPG(18:0)	C24H49O9P	5.65	511.3048	M-H	1.28E-03	0.955	4.13
LyPG_2	LyPG(18:1)	C24H47O9P	4.07	509.2887	M-H	4.97E-03	0.929	3.77
PG_1	PG(33:1)	C39H75O10P	10.87	733.5015	M-H	8.07E-03	0.999	2.60
PG_2	PG(34:1)	C40H77O10P	11.35	747.5166	M-H	8.68E-03	0.969	1.75
PG_3	PG(34:2)	C40H75O10P	10.66	745.5011	M-H	7.55E-02	0.836	1.44
PG_4	PG(35:2)	C41H77O10P	11.13	759.5174	M-H	2.06E-02	0.962	1.57
PG_5	PG(36:1)	C42H81O10P	13.41	775.5473	M-H	1.93E-03	-0.067	0.53
PG_6	PG(36:2)	C42H79O10P	11.53	773.5316	M-H	5.29E-02	0.944	1.35
PG_7	PG(36:3)	C42H77O10P	10.93	771.5180	M-H	4.54E-03	0.928	1.83
PG_8	PG(36:4)	C42H75O10P	10.29	769.5035	M-H	5.85E-02	0.609	1.28
PG_9	PG(38:2)	C44H83O10P	12.54	801.5641	M-H	1.08E-01	0.935	1.15
PG_10	PG(38:4)	C44H79O10P	11.14	797.5335	M-H	2.90E-02	0.916	1.60
PG_11	PG(38:5)	C44H77O10P	10.71	795.5157	M-H	7.72E-04	0.953	2.22
PG_12	PG(39:7)	C45H75O10P	10.09	805.5038	M-H	6.11E-01	-0.320	0.96
PG_13	PG(40:5)	C46H81O10P	11.32	823.5482	M-H	3.17E-03	0.983	1.95
PG_14	PG(40:6)	C46H79O10P	10.72	821.5316	M-H	5.91E-03	0.978	1.83

PG_15	PG(40:7)	C46H77O10P	10.52	819.5190	M-H	7.90E-03	0.943	1.28
PG_16	PG(40:8)	C46H75O10P	9.80	817.5013	M-H	1.58E-01	0.619	1.09
PG_17	PG(42:8)	C48H79O10P	10.67	845.5332	M-H	9.46E-03	0.909	1.28
PG_18	PG(42:9)	C48H77O10P	10.07	843.5156	M-H	3.35E-02	0.878	1.58
PG_19	PG(42:10)	C48H75O10P	9.58	841.5042	M-H	9.14E-03	0.873	1.59
PG_20	PG(42:11)	C48H73O10P	9.02	839.4879	M-H	1.87E-03	0.928	1.64
PG_21	PG(44:12)	C50H75O10P	9.40	865.5017	M-H	6.25E-01	0.289	1.03
MG_1	MG(16:0)	C19H38O4	6.09	331.2841	M+H	2.67E-01	0.104	1.04
MG_2	MG(18:0)	C21H42O4	7.45	359.3154	M+H	1.78E-01	0.566	1.03
DG_1	DG(34:3)	C37H66O5	11.46	608.5248	M+NH4	4.50E-03	0.930	1.57
DG_2	DG(35:4)	C38H66O5	11.92	620.5245	M+NH4	9.55E-02	-0.503	0.94
DG_3	DG(36:6)	C39H64O5	12.35	630.5089	M+NH4	4.27E-02	0.580	1.12
DG_4	DG(37:4)	C40H70O5	12.81	648.5567	M+NH4	5.82E-03	0.787	1.65
DG_5	DG(38:4)	C41H72O5	13.26	662.5719	M+NH4	5.71E-02	-0.593	0.87
DG_6	DG(38:7)	C41H66O5	12.55	656.5251	M+NH4	4.99E-02	0.946	1.25
DG_7	DG(39:6)	C42H70O5	13.19	672.5566	M+NH4	6.75E-03	0.837	1.27
DG_8	DG(42:3)	C45H82O5	14.59	720.6509	M+NH4	1.20E-03	0.975	2.45
DG_9	DG(42:8)	C45H72O5	13.8	710.5726	M+NH4	4.97E-03	0.764	1.53
DG_10	DG(44:10)	C47H72O5	14.28	734.5718	M+NH4	1.28E-02	0.946	1.67
TG_1	TG(50:1)	C53H100O6	18.93	850.7862	M+NH4	6.92E-02	0.585	1.11

TG_2	TG(50:2)	C53H98O6	18.53	848.7709	M+NH4	4.50E-03	-0.991	0.51
TG_3	TG(51:1)	C54H102O6	19.14	864.8021	M+NH4	1.38E-01	0.776	1.39
TG_4	TG(51:2)	C54H100O6	18.72	862.7857	M+NH4	2.32E-02	-0.998	0.67
TG_5	TG(52:0)	C55H106O6	19.72	880.8324	M+NH4	2.06E-02	0.760	1.40
TG_6	TG(52:2)	C55H102O6	18.95	876.8006	M+NH4	4.21E-03	-0.925	0.66
TG_7	TG(52:3)	C55H100O6	18.56	874.7871	M+NH4	6.93E-03	-0.995	0.38
TG_8	TG(52:5)	C55H96O6	14.96	870.7524	M+NH4	5.02E-02	0.836	1.30
TG_9	TG(53:5)	C56H98O6	15.29	884.7666	M+NH4	1.79E-01	0.947	1.23
TG_10	TG(54:2)	C57H106O6	19.38	904.8338	M+NH4	8.56E-02	-0.017	0.93
TG_11	TG(54:4)	C57H102O6	18.62	900.8015	M+NH4	1.54E-03	-0.798	0.36
TG_12	TG(54:5)	C57H100O6	18.21	898.7844	M+NH4	1.29E-02	-0.760	0.54
TG_13	TG(54:6)	C57H98O6	17.78	896.7713	M+NH4	6.26E-03	-0.821	0.27
TG_14	TG(56:4)	C59H106O6	19.07	928.8355	M+NH4	7.66E-03	0.928	1.56
SM_1	SM(d32:0)	C37H77N2O6P	9.74	721.5533	M+FA-H	6.12E-04	0.274	2.65
SM_2	SM(d32:1)	C37H75N2O6P	9.33	719.5343	M+FA-H	8.03E-03	0.494	1.17
SM_3	SM(d33:1)	C38H77N2O6P	9.90	733.5493	M+FA-H	2.67E-03	0.803	1.59
SM_4	SM(d34:0)	C39H81N2O6P	11.06	705.5897	M+H	8.52E-03	0.894	2.78
SM_5	SM(d34:1)	C39H79N2O6P	10.44	747.5667	M+FA-H	6.16E-03	0.993	1.54
SM_6	SM(d34:2)	C39H77N2O6P	9.55	745.5494	M+FA-H	4.61E-02	0.744	1.47
SM_7	SM(d35:1)	C40H81N2O6P	11.15	717.5872	M+H	2.67E-03	0.999	1.60

SM_8	SM(d36:1)	C41H83N2O6P	11.54	775.5966	M+FA-H	3.32E-03	0.863	2.74
SM_9	SM(d36:2)	C41H81N2O6P	10.66	773.5812	M+FA-H	6.27E-03	0.991	2.44
SM_10	SM(d36:3)	C41H79N2O6P	11.06	727.5713	M+H	9.08E-03	0.754	2.07
SM_11	SM(d38:0)	C43H89N2O6P	13.14	761.6543	M+H	7.98E-03	0.918	3.47
SM_12	SM(d39:1)	C44H89N2O6P	13.30	773.6521	M+H	3.10E-03	0.964	1.87
SM_13	SM(d40:1)	C45H91N2O6P	13.62	831.6590	M+FA-H	2.56E-03	0.988	2.30
SM_14	SM(d40:2)	C45H89N2O6P	12.92	785.6504	M+H	4.23E-03	0.952	1.34
SM_15	SM(d41:1)	C46H93N2O6P	14.20	801.6860	M+H	2.12E-02	0.962	1.64
SM_16	SM(d41:2)	C46H91N2O6P	13.26	799.6697	M+H	2.04E-02	0.763	1.34
SM_17	SM(d42:1)	C47H95N2O6P	14.52	859.6885	M+FA-H	2.97E-03	0.992	2.01
SM_18	SM(d42:2)	C47H93N2O6P	13.58	857.6739	M+FA-H	2.90E-02	0.866	1.46
SM_19	SM(d42:3)	C47H91N2O6P	12.73	855.6601	M+FA-H	2.02E-01	0.636	1.17
SM_20	SM(d43:1)	C48H97N2O6P	14.94	829.7167	M+H	3.33E-02	0.904	1.54
SM_21	SM(d43:2)	C48H95N2O6P	14.04	827.7006	M+H	2.36E-01	-0.084	0.96
SM_22	SM(d44:1)	C49H99N2O6P	15.45	843.7315	M+H	4.59E-03	0.969	1.71
SM_23	SM(d44:2)	C49H97N2O6P	14.46	885.7025	M+FA-H	1.93E-03	0.713	1.87
SPB_1	sphingosine	C18H37NO2	2.15	300.2894	M+H	7.65E-03	-0.260	0.74
SPB_2	sphinganine	C18H39NO2	1.72	302.3050	M+H	2.34E-01	-0.790	0.86
SPB_3	sphingosine-1-phosphate	C18H38NO5P	1.62	378.2426	M-H	1.54E-02	0.561	1.34
SPB_4	C17 sphinganine-1-phosphate	C17H38NO5P	5.92	366.2416	M-H	5.35E-01	0.330	1.07

SPB_5	C17 sphingosine-1-phosphocholine	C22H47N2O5P	5.39	449.3157	M-H	3.26E-03	-0.623	0.22
Cer_1	Cer(d33:1)	C33H65NO3	11.50	522.4916	M-H	1.14E-02	0.930	2.79
Cer_2	Cer(d34:1)	C34H67NO3	12.05	536.5025	M-H	6.75E-03	0.937	4.17
Cer_3	Cer(d36:1)	C36H71NO3	13.12	564.5370	M-H	8.44E-03	0.950	11.1
Cer_4	Cer(d38:1)	C38H75NO3	14.10	592.5676	M-H	1.93E-03	0.960	23.3
Cer_5	Cer(d39:1)	C39H77NO3	14.59	606.5804	M-H	8.18E-03	0.962	21.1
Cer_6	Cer(d40:1)	C40H79NO3	14.96	620.6006	M-H	8.18E-03	0.962	13.7
Cer_7	Cer(d40:2)	C40H77NO3	14.15	618.5839	M-H	4.55E-03	0.955	17.1
Cer_8	Cer(d41:1)	C41H81NO3	15.39	634.6173	M-H	5.95E-03	0.964	8.81
Cer_9	Cer(d42:1)	C42H83NO3	15.78	648.6299	M-H	8.44E-03	0.967	11.8
Cer_10	Cer(d42:2)	C42H81NO3	14.96	646.6124	M-H	8.07E-03	0.974	12.2
MIPC_1	MIPC(t40:0)	C52H102NO17P	13.47	1042.6777	M-H	2.41E-03	-0.704	0.45
MIPC_2	MIPC(t42:0)	C54H106NO17P	14.35	1070.7103	M-H	1.19E-02	-0.792	0.27
MIPC_3	MIPC(t44:0)	C56H110NO17P	15.16	1098.7448	M-H	6.86E-03	-0.547	0.43
MIPC_4	MIPC(d44:0)	C56H110NO16P	16.13	1082.7501	M-H	1.46E-01	-0.146	0.84
Cerebroside_1	GlcCer(d34:1)	C40H77NO8	10.91	698.5551	M-H	1.23E-04	0.979	3.56
Cerebroside_2	GlcCer(d41:1)	C47H91NO8	14.38	796.6685	M-H	8.17E-03	0.930	5.87
Cerebroside_3	GlcCer(d42:1)	C48H93NO8	14.77	810.6823	M-H	1.91E-02	0.957	4.34

Cerebroside_4	GlcCer(d42:2)	C48H91NO8	13.91	808.6709	M-H	8.07E-03	0.962	5.13
Globoside_1	TrihexosylCer(d34:1)	C52H97NO18	10.15	1022.6614	M-H	2.56E-03	0.664	1.35
Globoside_2	TrihexosylCer(d40:1)	C58H109NO18	13.18	1106.7542	M-H	2.56E-03	0.778	1.84
Globoside_3	TrihexosylCer(d42:1)	C60H113NO18	14.04	1134.7850	M-H	1.57E-02	0.851	1.86
Globoside_4	TrihexosylCer(d42:2)	C60H111NO18	13.17	1132.7723	M-H	2.64E-02	0.673	1.37
Globoside_5	TetrahexosylCer(d34:1)	C60H110N2O23	9.79	1225.7398	M-H	1.47E-02	-0.047	0.82
Globoside_6	TetrahexosylCer(d36:1)	C62H114N2O23	10.86	1253.7691	M-H	6.30E-03	0.990	1.54
Globoside_7	TetrahexosylCer(d40:1)	C66H122N2O23	12.83	1309.8352	M-H	1.30E-01	0.588	1.17
Globoside_8	TetrahexosylCer(d42:2)	C68H124N2O23	12.83	1335.8496	M-H	5.28E-03	-0.573	0.70
Globoside_9	TetrahexosylCer(d42:1)	C68H126N2O23	13.70	1337.8653	M-H	8.17E-03	0.697	1.54
Globoside_10	TetrahexosylCer(d44:1)	C70H130N2O23	14.49	1365.8951	M-H	3.26E-03	0.663	1.65
Globoside_11	TetrahexosylCer(d44:2)	C70H128N2O23	13.57	1363.8818	M-H	2.76E-03	0.284	1.18
Ganglioside_1	Ganglioside GM3(d34:1)	C57H104N2O21	10.21	1151.7027	M-H	1.87E-02	0.459	1.11
Ganglioside_2	Ganglioside GM3(d36:1)	C59H108N2O21	11.24	1179.7379	M-H	3.17E-03	0.856	1.96
Ganglioside_3	Ganglioside GM3(d38:1)	C61H112N2O21	12.33	1207.7666	M-H	8.17E-03	0.773	1.68
Ganglioside_4	Ganglioside GM3(d40:1)	C63H116N2O21	13.28	1235.7996	M-H	5.68E-03	0.801	1.64
Ganglioside_5	Ganglioside GM3(d42:1)	C65H120N2O21	14.20	1263.8285	M-H	7.98E-03	0.597	1.25
Ganglioside_6	Ganglioside GM3(d42:2)	C65H118N2O21	13.25	1261.8147	M-H	5.40E-01	0.502	1.13
Ganglioside_7	Ganglioside GM3(d44:1)	C67H124N2O21	15.05	1291.8605	M-H	6.81E-01	0.096	0.90
Ganglioside_8	Ganglioside GM3(d44:2)	C67H122N2O21	14.14	1289.8445	M-H	3.24E-01	-0.021	0.80

Table S4 The enzymes in glycerophospholipid and sphingolipid metabolism pathways with mRNA significantly altered between p7- and p13-BMSCs

Name	Symbol	Gene ID	FC (p13/p7)	Adjusted *p*-value	Pathway mapping
lysophosphatidate acyltransferase 1	AGPAT1	10554	1.81	8.58E-03	Glycerophospholipid metabolism
CDP-diacylglycerol--inositol 3-phosphatidyltransferase	CDIPT	10423	1.66	2.44 E-02	Glycerophospholipid metabolism
CDP-diacylglycerol synthase 1	CDS1	1040	2.63	2.56 E-04	Glycerophospholipid metabolism
choline kinase alpha	CHKA	1119	0.61	9.79 E-04	Glycerophospholipid metabolism
ethanolamine-phosphate phospholyase	ETNPPL	64850	1.81	2.89 E-07	Glycerophospholipid metabolism
glyceronephosphate O-acyltransferase	GNPAT	8443	0.51	1.74 E-03	Glycerophospholipid metabolism
glycerol-3-phosphate dehydrogenase 1 like	GPD1L	23171	0.62	5.64 E-03	Glycerophospholipid metabolism
lysophosphatidylcholine acyltransferase 1	LPCAT1	79888	0.66	2.44 E-02	Glycerophospholipid metabolism
lysophosphatidylcholine acyltransferase 3	LPCAT3	10162	0.63	1.90 E-03	Glycerophospholipid metabolism
lysophosphatidylcholine acyltransferase 4	LPCAT4	254531	0.53	9.65 E-04	Glycerophospholipid metabolism
lysophospholipase I	LYPLA1	10434	0.58	7.63 E-04	Glycerophospholipid metabolism

phosphate cytidylyltransferase 1, choline, alpha	PCYT1A	5130	1.52	2.79 E-04	Glycerophospholipid metabolism
phosphatidyl-N-methylethanolamine N-methyltransferase	PEMT	10400	0.64	5.08 E-03	Glycerophospholipid metabolism
phosphatidylglycerophosphate synthase 1	PGS1	9489	0.61	5.82 E-05	Glycerophospholipid metabolism
cytosolic phospholipase A2 beta	PLA2G4B	100137049	0.15	5.82 E-05	Glycerophospholipid metabolism
phospholipid phosphatase 4	PLPP4	196051	0.59	6.61 E-05	Glycerophospholipid metabolism
patatin like phospholipase domain containing 6	PNPLA6	10908	0.63	7.63 E-04	Glycerophospholipid metabolism
acid ceramidase	ASAH1	427	1.78	5.82 E-05	Sphingolipid metabolism
beta-1,3-N-acetylgalactosaminyltransferase 1	B3GALNT1	8706	0.33	7.63 E-04	Sphingolipid metabolism
ceramide kinase	CERK	64781	0.58	3.99 E-03	Sphingolipid metabolism
ceramide synthetase 1	CERS1	10715	1.68	7.98 E-04	Sphingolipid metabolism
galactosylceramide sulfotransferase	GAL3ST1	9514	3.24	1.13 E-05	Sphingolipid metabolism
galactosylceramidase	GALC	2581	0.55	9.46 E-03	Sphingolipid metabolism
alpha-galactosidase	GLA	2717	1.70	8.33 E-04	Sphingolipid metabolism
neuraminidase 3	NEU3	10825	0.58	7.33 E-04	Sphingolipid metabolism
phospholipid phosphatase 1	PLPP1	8611	0.52	2.24 E-05	Sphingolipid metabolism
sphingomyelin synthase 2	SGMS2	166929	1.59	5.82 E-05	Sphingolipid metabolism
sphingosine-1-phosphate lyase 1	SGPL1	8879	0.67	7.00 E-04	Sphingolipid metabolism
sphingosine-1-phosphate phosphotase 2	SGPP2	130367	3.25	2.16 E-05	Sphingolipid metabolism
sphingosine kinase 2	SPHK2	56848	0.63	3.99 E-03	Sphingolipid metabolism
ST3 beta-galactoside	ST3GAL5	8869	0.56	9.80 E-04	Sphingolipid metabolism

alpha-2,3-sialyltransferase 5