Compounds

Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		39.61	n/a	633.21017	

MW: 633.21017
File: 211103-518021-60-PND4.raw (F21) FTMS (-) MS1
MW: 633.21017
File: 211103-518021-60-PND4.raw (F21) FTMS (+) MS1
MW: 633.21017
File: 211103-518027-19-PND3.raw (F27) FTMS (+) MS1

211103-518037-234-P3 (F37) #13054, RT=39.619 min, MS1, FTMS (-)
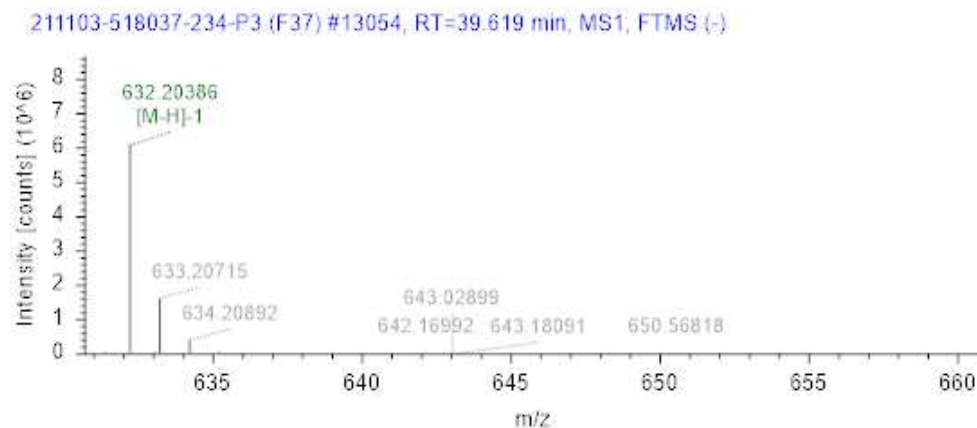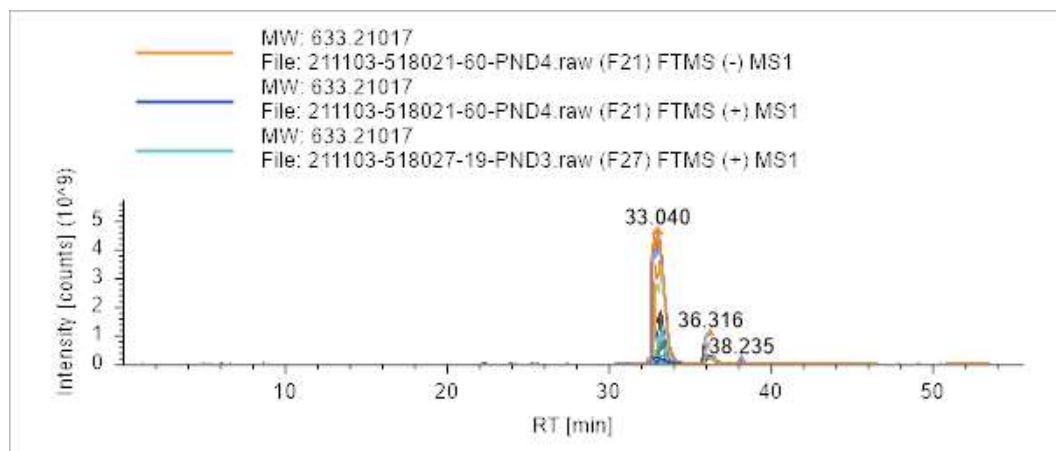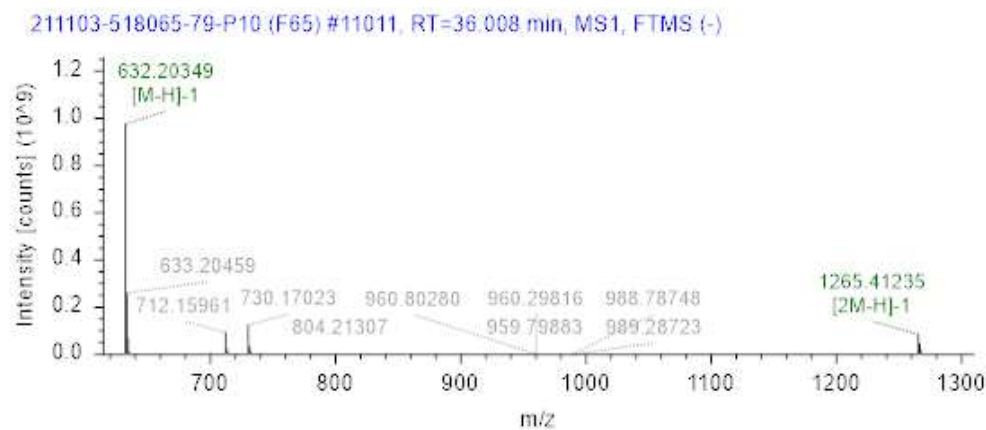

211103-518037-234-P3 (F37) #13032, RT=39.561 min, MS2, FTMS (-), (HCD, DDA, 632.2043@30, -1)

1

Compounds
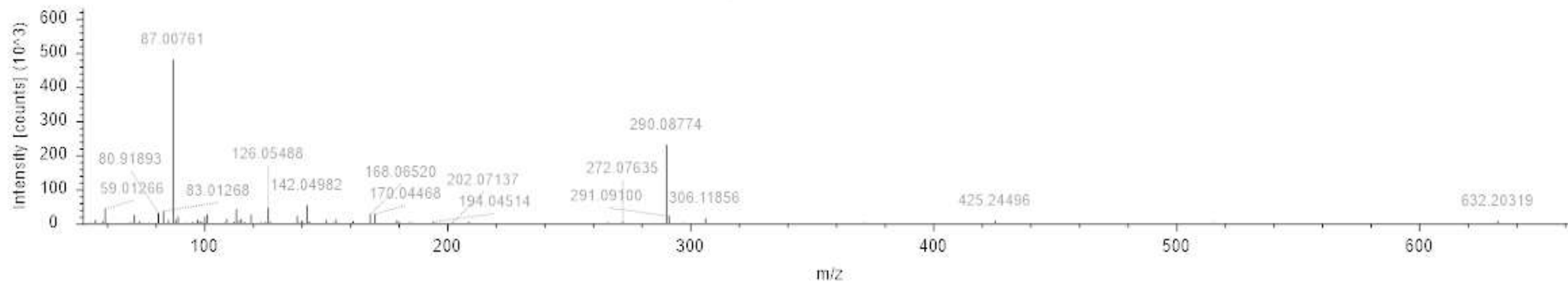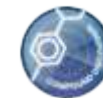
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		36.03	n/a	633.21056	

MW: 633.21056
File: 211103-518027-19-PND3.raw (F27) FTMS (-) MS1
MW: 633.21056
File: 211103-518027-19-PND3.raw (F27) FTMS (+) MS1
MW: 633.21056
File: 211103-518028-36-PND3.raw (F28) FTMS (-) MS1

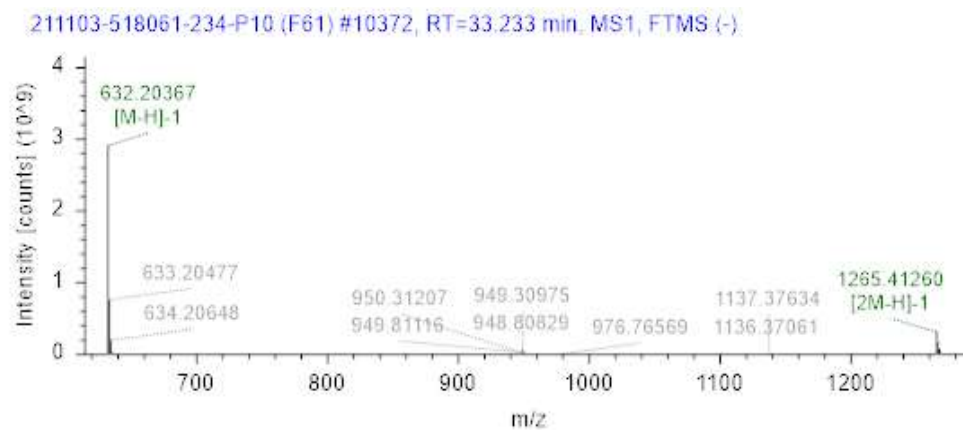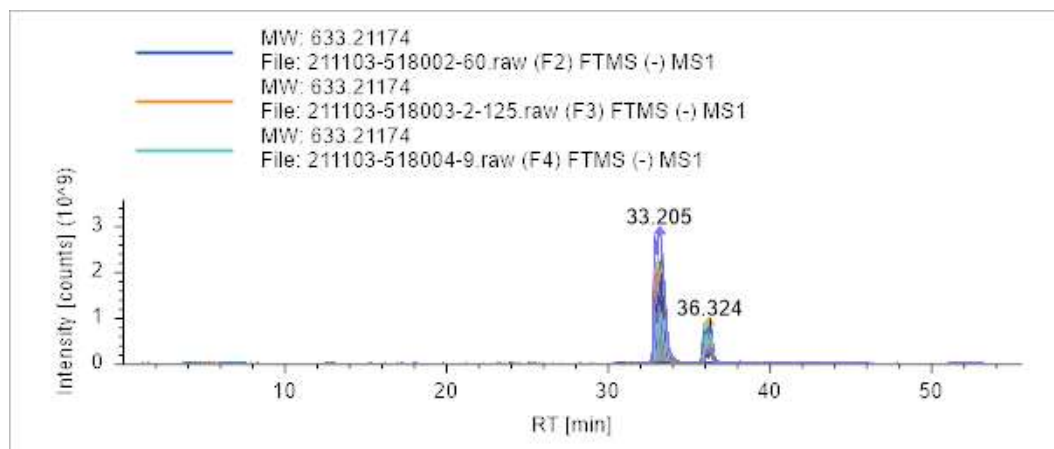211103-518065-79-P10 (F65) #11011, RT=36.008 min, MS1, FTMS (-)
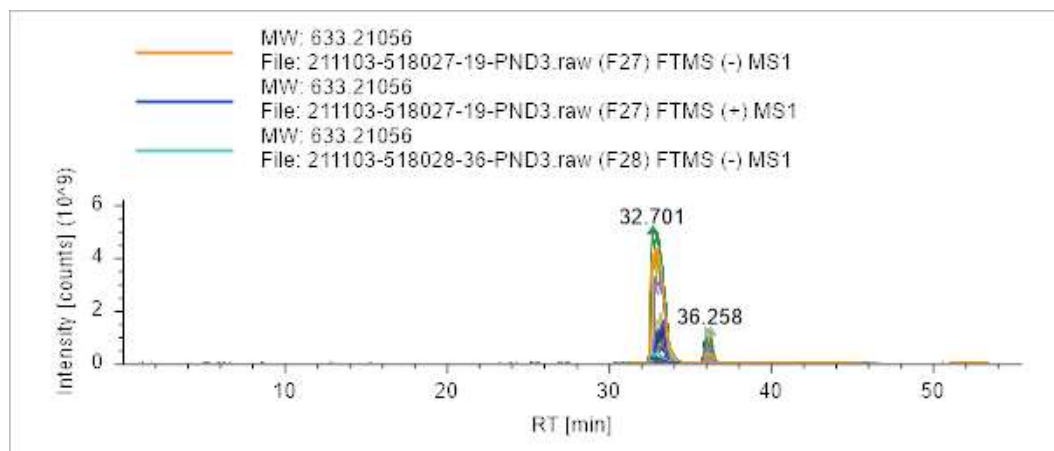
211103-518065-79-P10 (F65) #11036, RT=36.066 min, MS2, FTMS (-), (HCD, DDA, 632.2035@30, -1)

Compounds
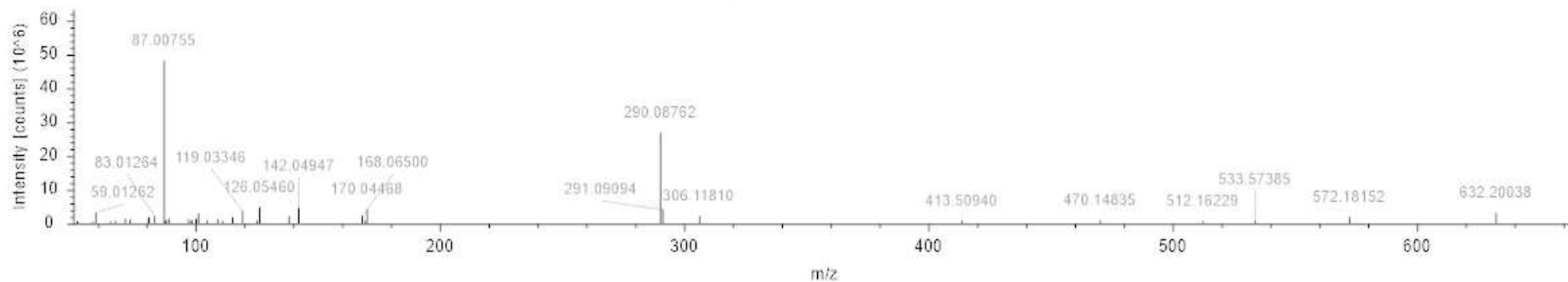
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		33.28	n/a	633.21174	

MW: 633.21174
File: 211103-518002-60.raw (F2) FTMS (-) MS1
MW: 633.21174
File: 211103-518003-2-125.raw (F3) FTMS (-) MS1
MW: 633.21174
File: 211103-518004-9.raw (F4) FTMS (-) MS1

33.205
36.324

211103-518061-234-P10 (F61) #10372, RT=33.233 min, MS1, FTMS (-)

632.20367
[M-H]-1
633.20477
634.20648
950.31207   949.30975
949.81116   948.60829   976.76569   1136.37061   1137.37634
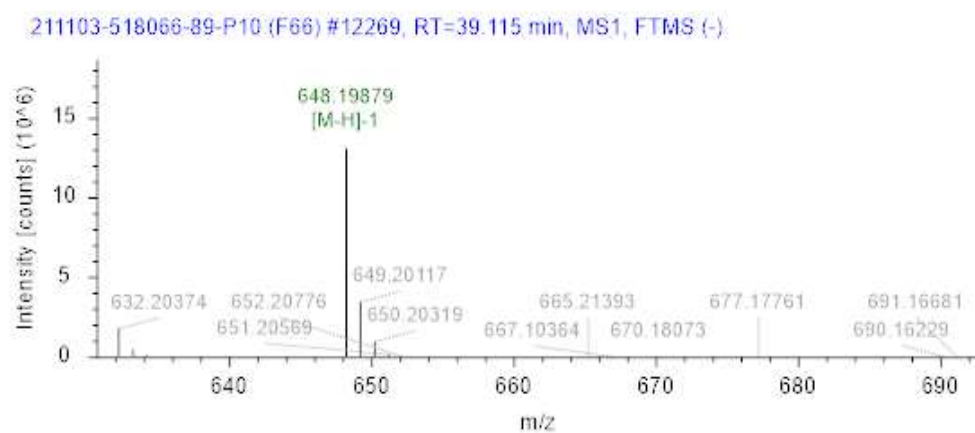1265.41260
[2M-H]-1

211103-518061-234-P10 (F61) #10373, RT=33.235 min, MS2, FTMS (-), (HCD, DDA, 632.7025@30, -1)

290.08740
113.02315   168.06526
170.04477   302.82162   364.91797
291.09058   408.15015   468.17126   632.20239   707.96552
633.20740   695.28094   1120.11243

Compounds
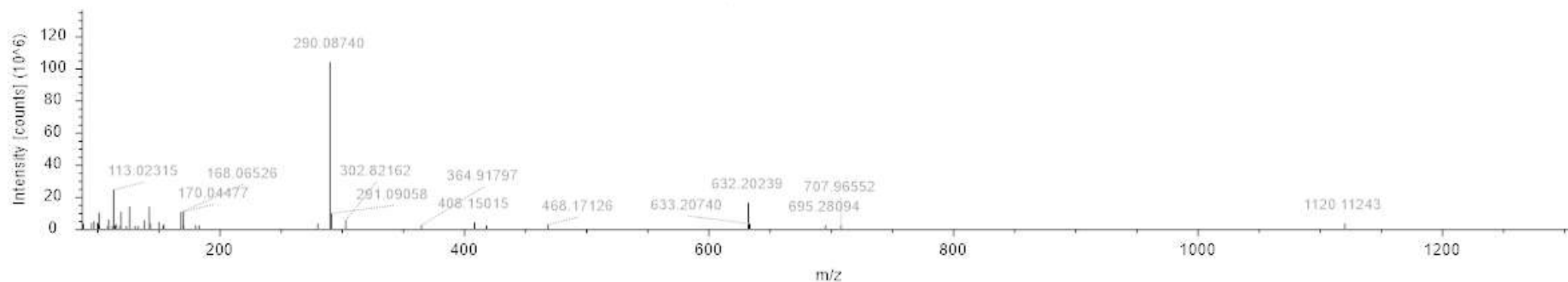
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		39.09	n/a	649.20553	
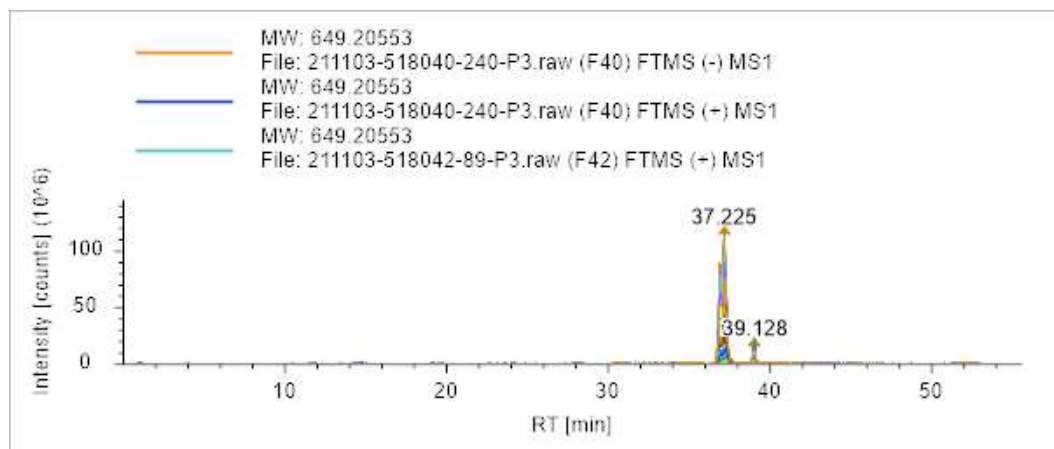
Compounds
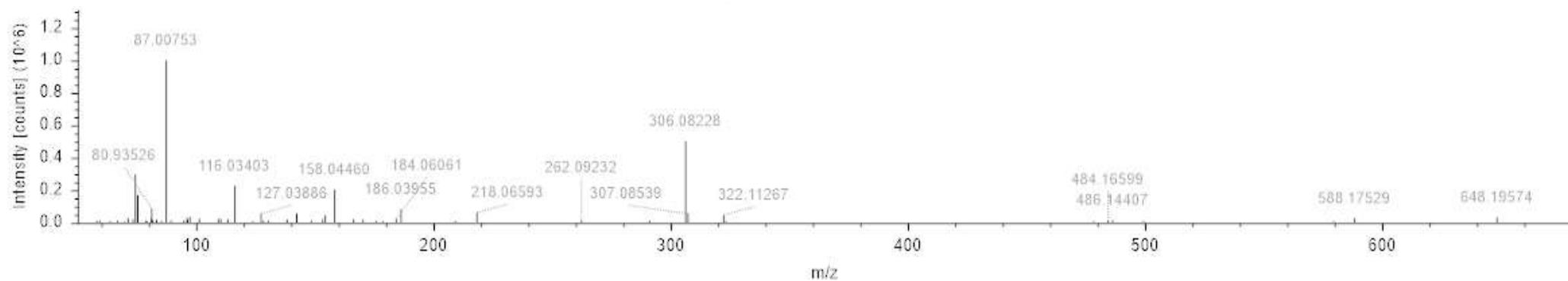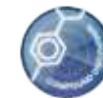
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		36.96	n/a	649.20665	

MW: 649.20665
File: 211103-518027-19-PND3.raw (F27) FTMS (-) MS1
MW: 649.20665
File: 211103-518052-36-10.raw (F52) FTMS (-) MS1
MW: 649.20665
File: 211103-518062-235-P10.raw (F62) FTMS (-) MS1

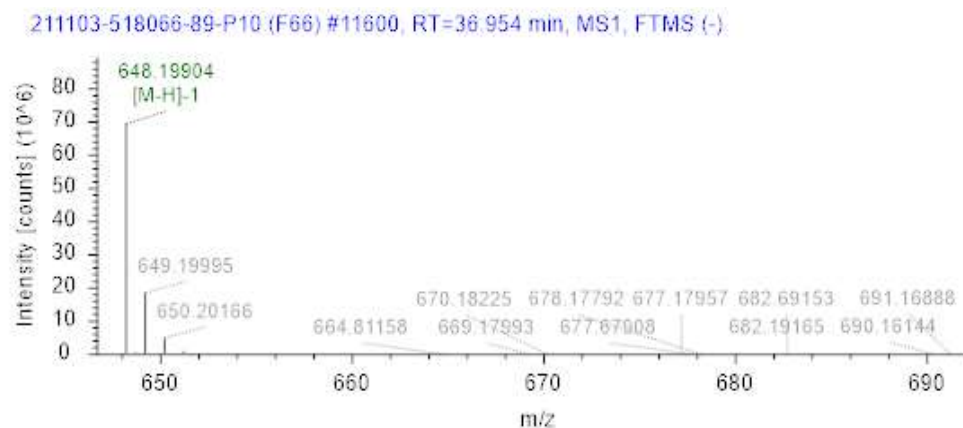211103-518066-89-P10 (F66) #11600, RT=36.954 min, MS1, FTMS (-)
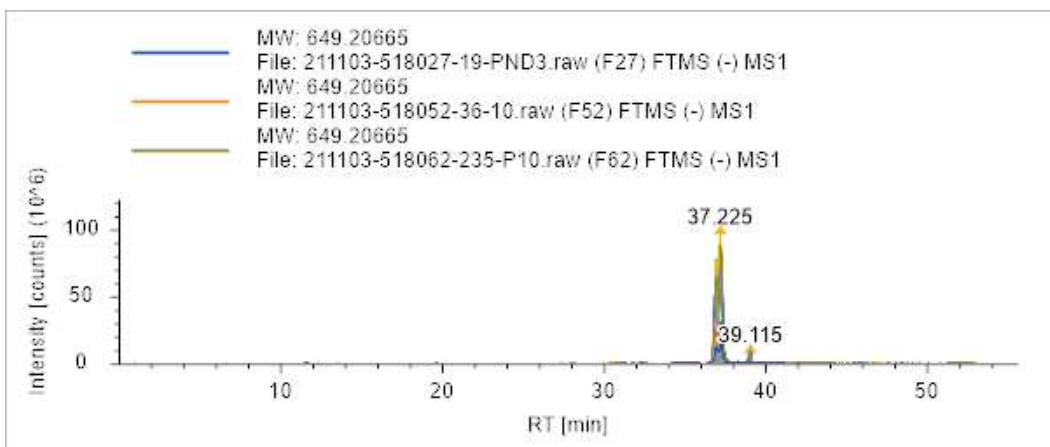
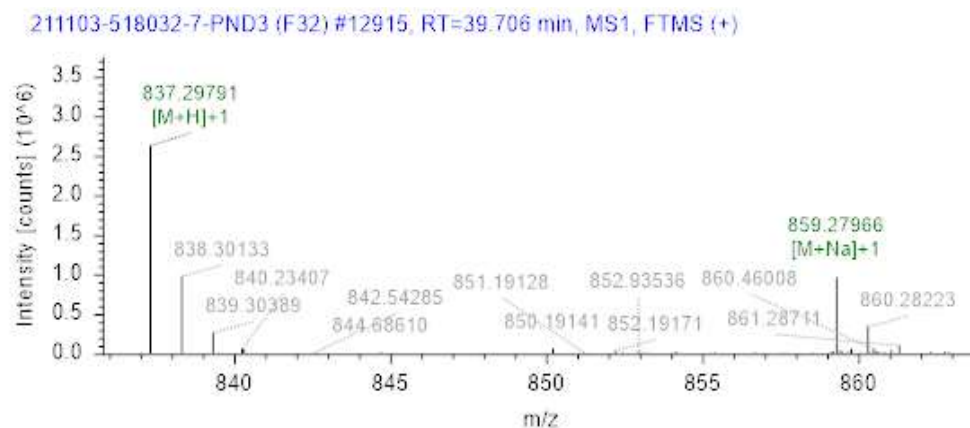211103-518066-89-P10 (F66) #11637, RT=37.037 min, MS2, FTMS (-), (HCD, DDA, 648.1992@30, -1)

© Reported with Compound Discoverer 3.3

Compounds
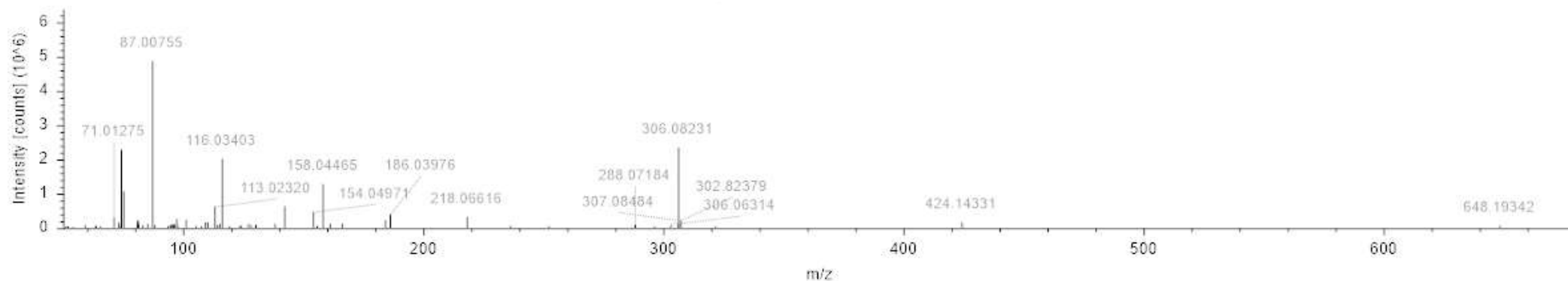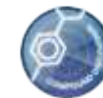
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		39.73	n/a	836.28940	

MW: 836.28940
File: 211103-518022-15-1-PND3.raw (F22) FTMS (+) MS1
MW: 836.28940
File: 211103-518027-19-PND3.raw (F27) FTMS (+) MS1
MW: 836.28940
File: 211103-518029-3-PND3.raw (F29) FTMS (+) MS1

211103-518032-7-PND3 (F32) #12915, RT=39.706 min, MS1, FTMS (+)

837.29791
[M+H]+1

838.30133
840.23407
839.30389
842.54285
844.68610
851.19128
850.19141 852.19171
852.93536 860.46008
861.28711
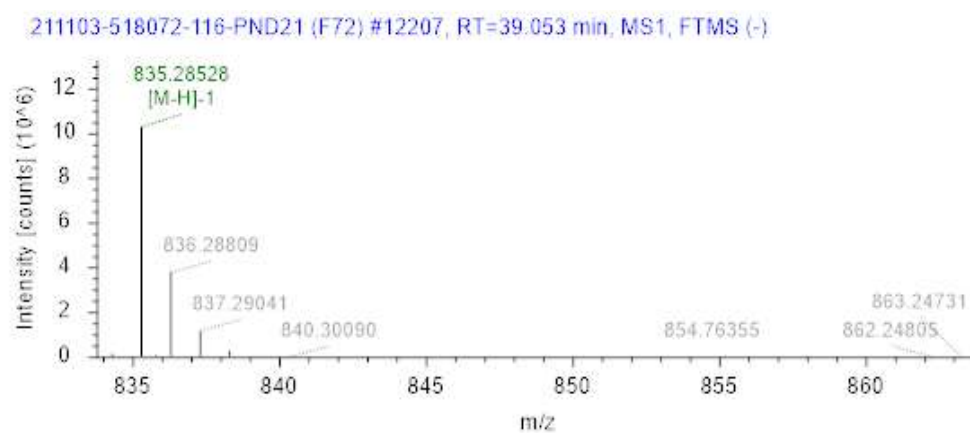859.27966
[M+Na]+1
860.28223
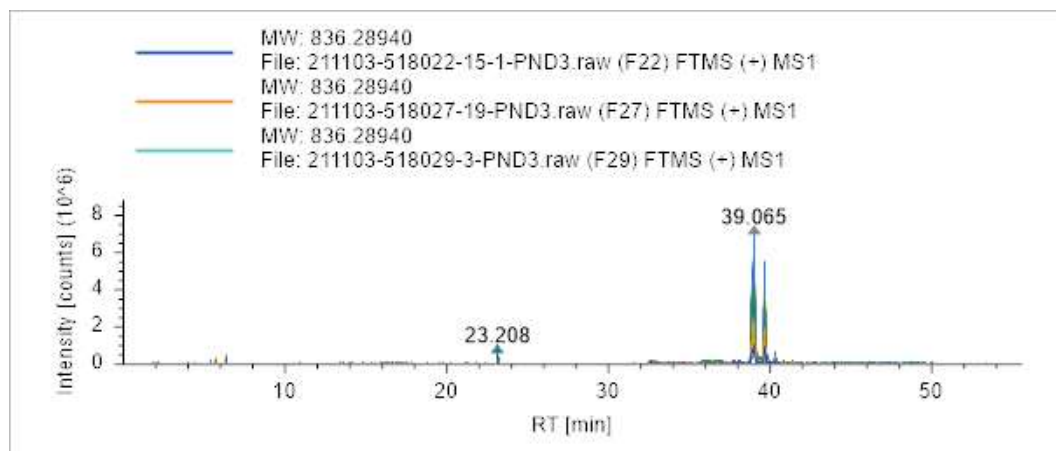
211103-518032-7-PND3 (F32) #12888, RT=39.631 min, MS2, FTMS (+), (HCD, DDA, 837.2964@30, +1)

60.04531
121.02849
126.05530
144.06577
186.07645
204.08698
197.04475
256.08112
274.09222
292.10287
304.73364
365.10504
374.94876
424.08420
459.87042

Compounds
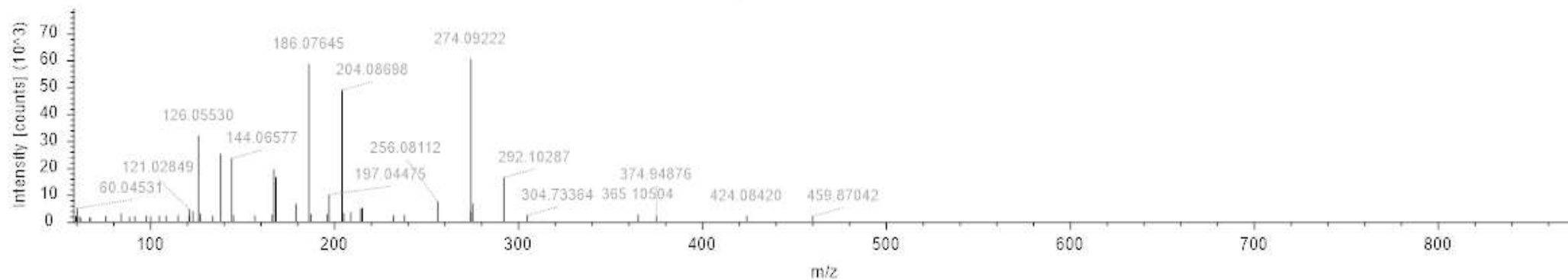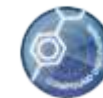
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		39.04	n/a	836.29114	

MW: 836.29114
File: 211103-518021-60-PND4.raw (F21) FTMS (-) MS1
MW: 836.29114
File: 211103-518021-60-PND4.raw (F21) FTMS (+) MS1
MW: 836.29114
File: 211103-518022-15-1-PND3.raw (F22) FTMS (-) MS1

211103-518072-116-PND21 (F72) #12207, RT=39.053 min, MS1, FTMS (-)

835.28528 [M-H]-1
836.28809
837.29041
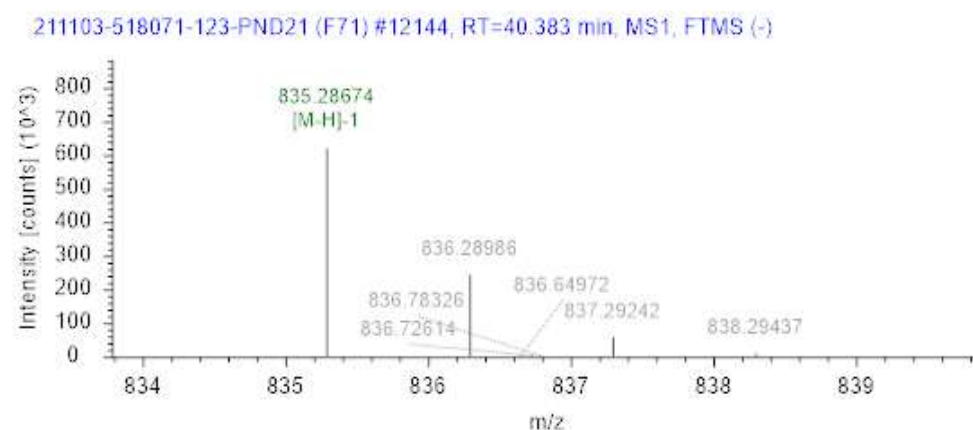840.30090
854.76355
862.24805
863.24731
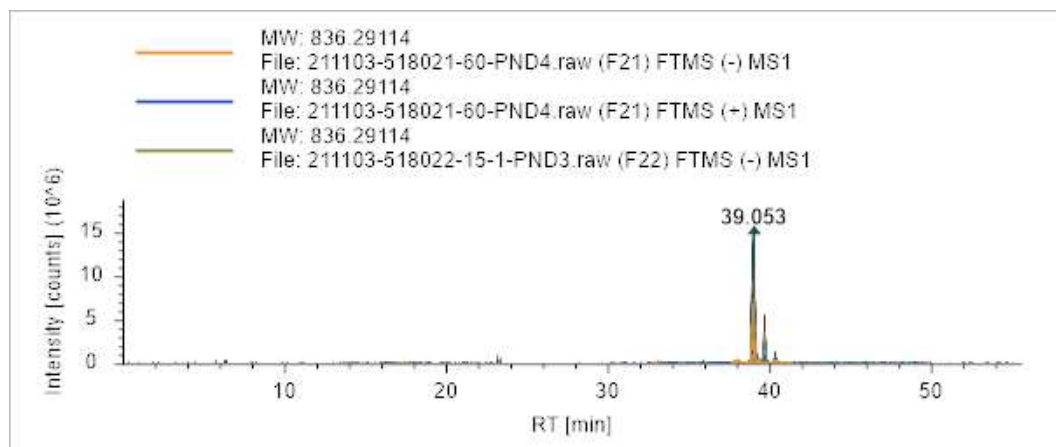
211103-518072-116-PND21 (F72) #12203, RT=39.033 min, MS2, FTMS (-), (HCD, DDA, 835.2853@30, -1)

87.00778
113.02345
126.05511
142.05016
168.06592
170.04520
221.06615
290.08832
291.09180
302.82227
333.58829
425.24286

Compounds
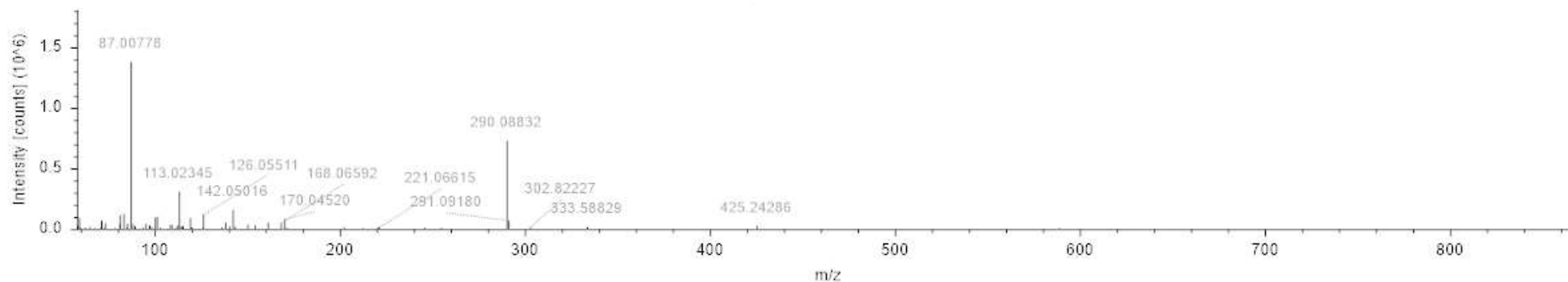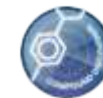
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		40.37	n/a	836.29285	
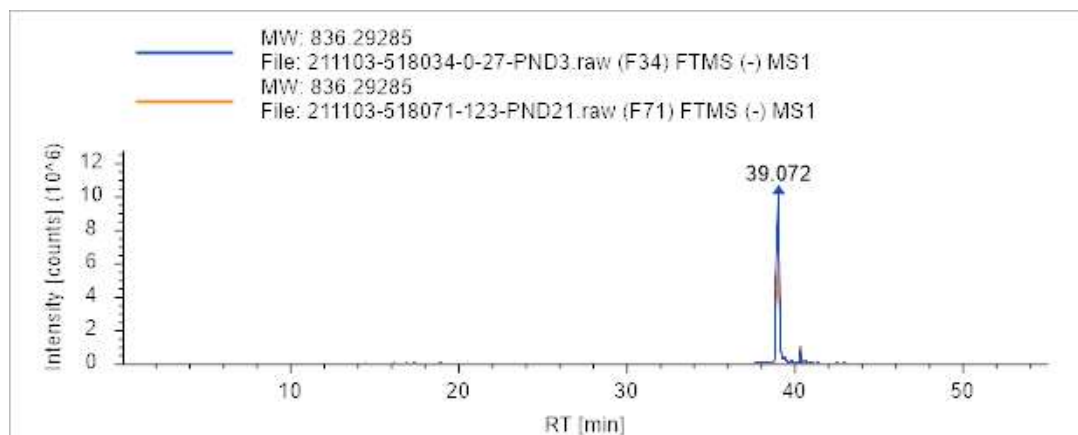
© Reported with Compound Discoverer 3.3

Compounds

Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		41.35	n/a	998.34169	

MW: 998.34169
File: 211103-518021-60-PND4.raw (F21) FTMS (-) MS1
MW: 998.34169
File: 211103-518021-60-PND4.raw (F21) FTMS (+) MS1
MW: 998.34169
File: 211103-518022-15-1-PND3.raw (F22) FTMS (-) MS1

211103-518055-12-PND10 (F55) #12974, RT=41.355 min, MS1, FTMS (-)

211103-518055-12-PND10 (F55) #12977, RT=41.360 min, MS2, FTMS (-), (HCD, DDA, 996.3340@30, -1)

Compounds
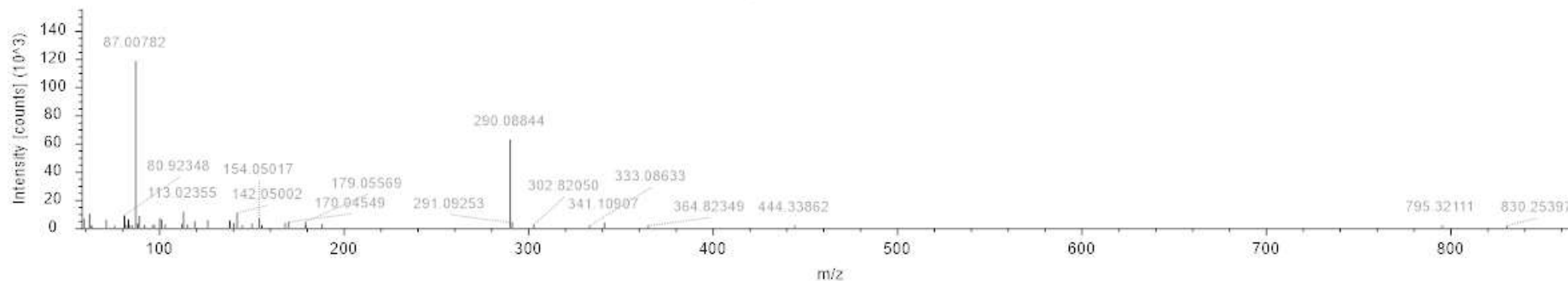
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		41.34	n/a	1127.38447	

MW: 1127.38447
File: 211103-518027-19-PND3.raw (F27) FTMS (-) MS1
MW: 1127.38447
File: 211103-518030-17-PND3.raw (F30) FTMS (-) MS1
MW: 1127.38447
File: 211103-518031-12-PND3.raw (F31) FTMS (-) MS1

211103-518072-116-PND21 (F72) #12649, RT=41.352 min, MS1, FTMS (-)
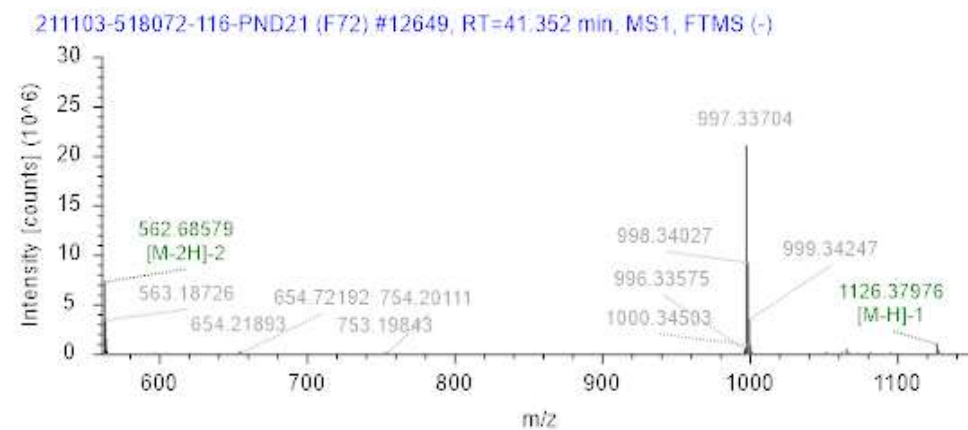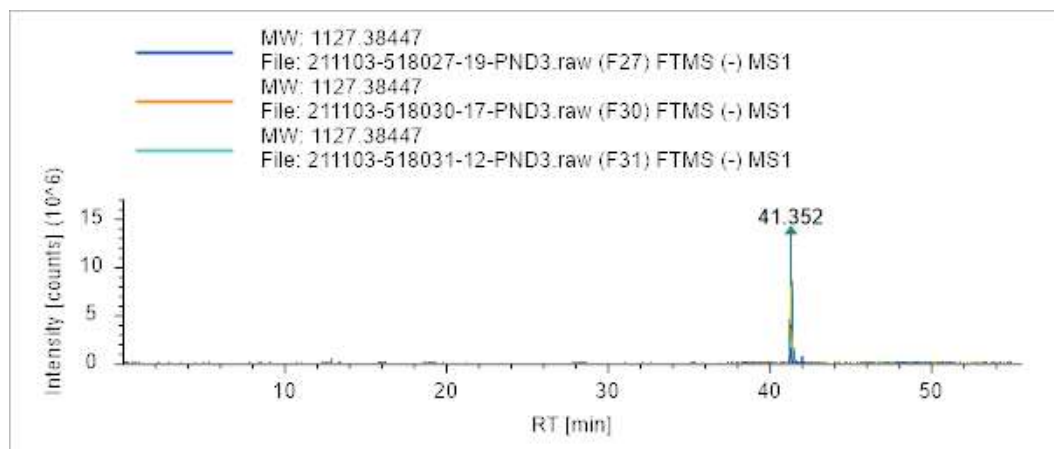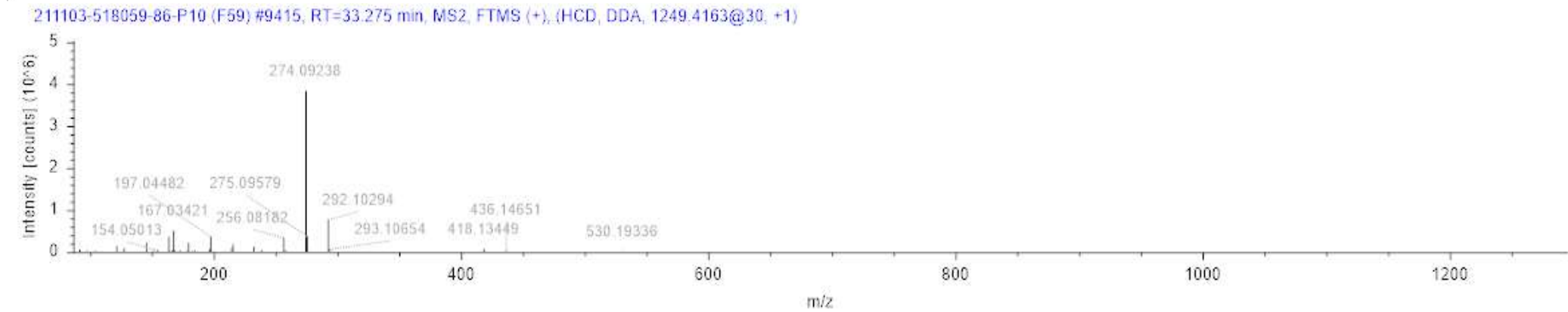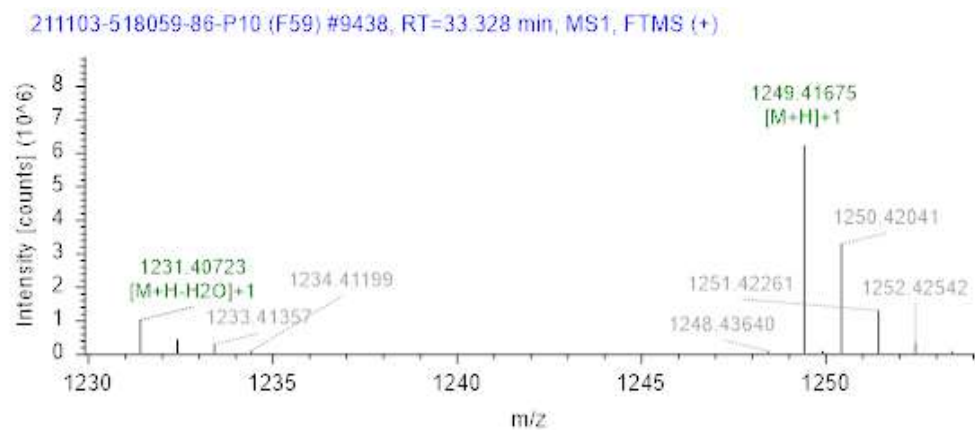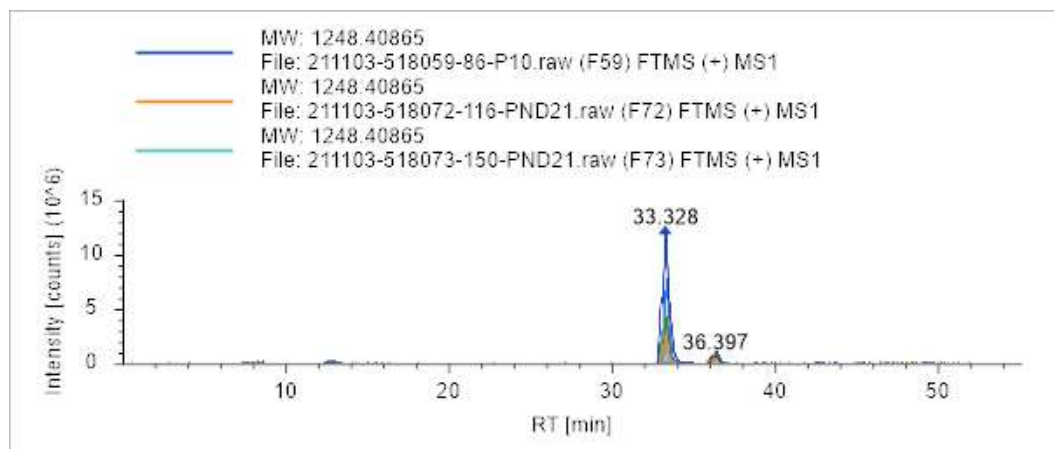
211103-518072-116-PND21 (F72) #12626, RT=41.289 min, MS2, FTMS (+), (HCD, DDA, 1128.3920@30, +1)

Compounds
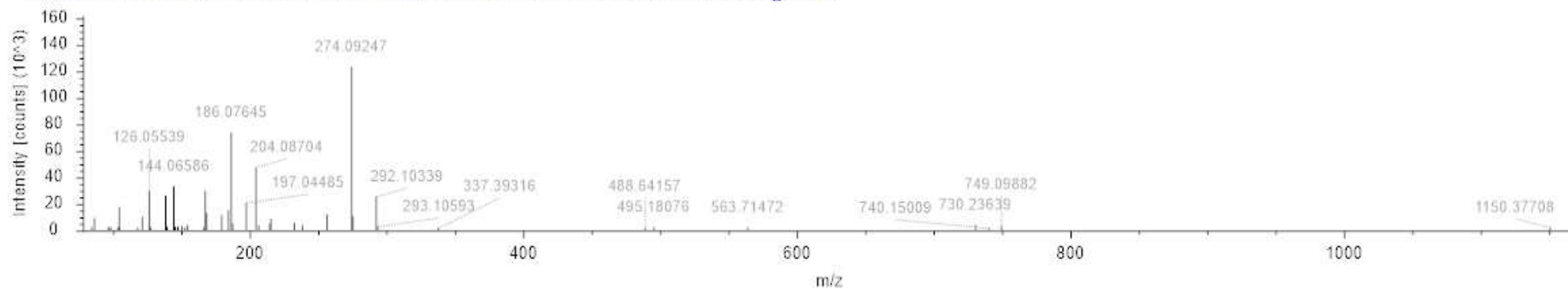
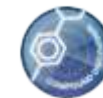| Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		33.36	n/a	1248.40865	

© Reported with Compound Discoverer 3.3

Compounds

Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		23.25	n/a	1596.53221	

MW: 1596.53221
File: 211103-518021-60-PND4.raw (F21) FTMS (+) MS1
MW: 1596.53221
File: 211103-518026-39-PND3.raw (F26) FTMS (+) MS1
MW: 1596.53221
File: 211103-518027-19-PND3.raw (F27) FTMS (+) MS1

211103-518072-116-PND21 (F72) #7204, RT=23.185 min, MS1, FTMS (+)

799.27411
[M+2H]+2 799.77454
798.77899

211103-518072-116-PND21 (F72) #7193, RT=23.160 min, MS2, FTMS (+), (HCD, DDA, 799.2733@30, +2)

258.11047
294.05820
259.11395
280.09232
416.13226
415.12949
466.03308
515.21399
583.14825
569.13324
634.71448
613.16016
781.88281
826.23645
827.23846
1209.00305
1426.07813

Compounds

Structure	Name	RT [min]	Formula	Calc. MW	Areas				
n/a		36.96	n/a	633.21110	3.32e8	8.33e8	6.47e9	4.92e8	

Compounds
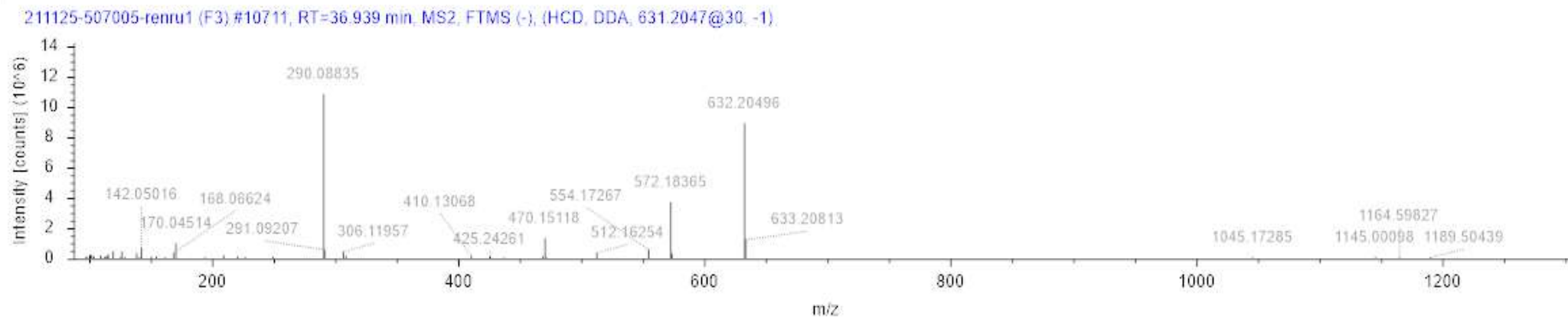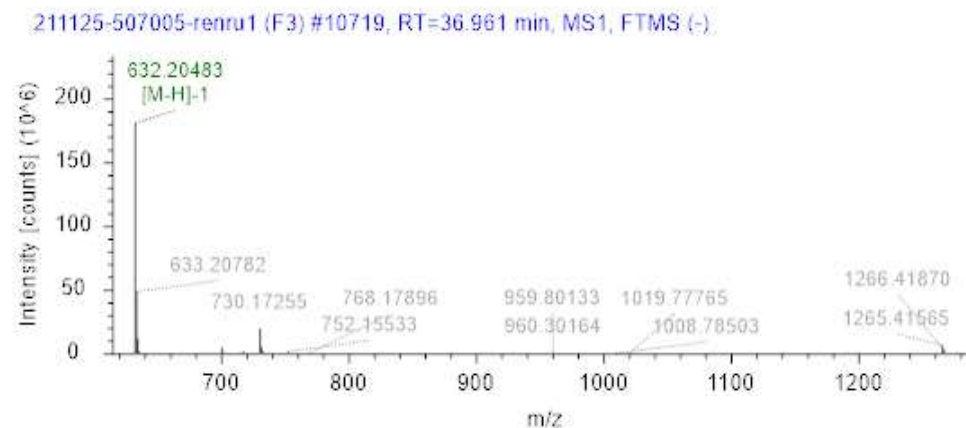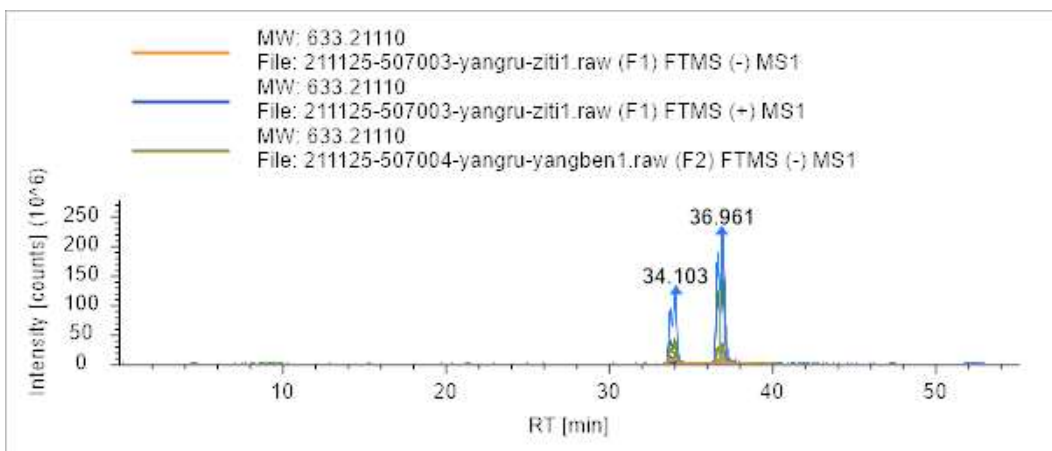
Structure	Name	RT [min]	Formula	Calc. MW	Areas					
n/a		34.05	n/a	633.21236	1.78e8	7.55e8	2.30e9	2.19e9		

MW: 633.21236
File: 211125-507003-yangru-ziti1.raw (F1) FTMS (-) MS1
MW: 633.21236
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (-) MS1
MW: 633.21236
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (+) MS1

211125-507005-renru1 (F3) #9993, RT=34.074 min, MS1, FTMS (-)

632.20490 [M-H]-1
633.20740
634.20905
717.18268
730.17285
975.32306 960.30365
974.32019 959.80212
1002.79163
1002.29041
1265.41553 [2M-H]-1
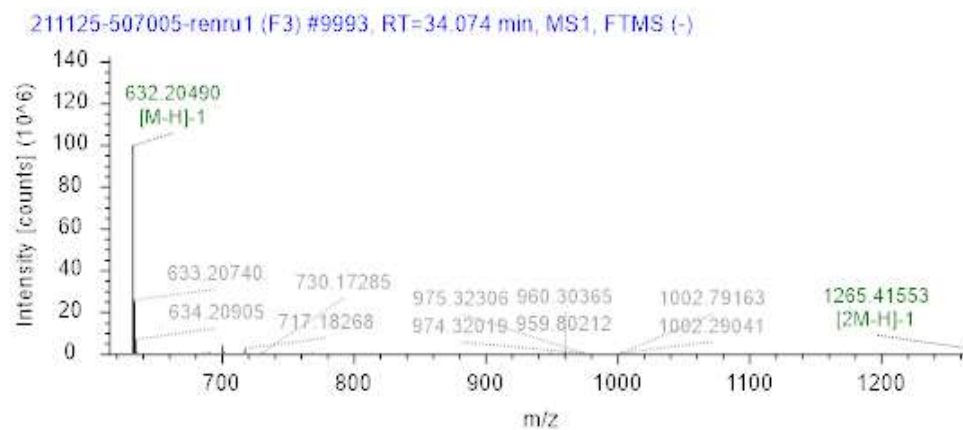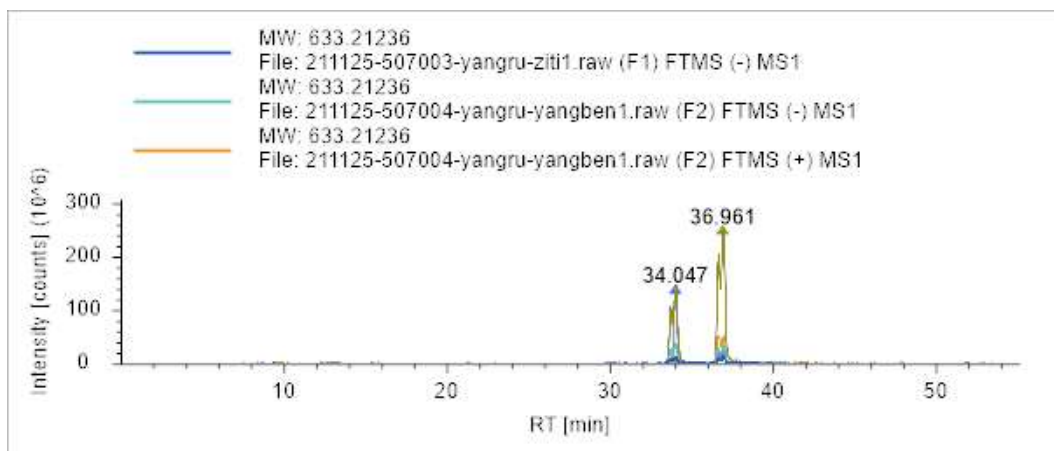
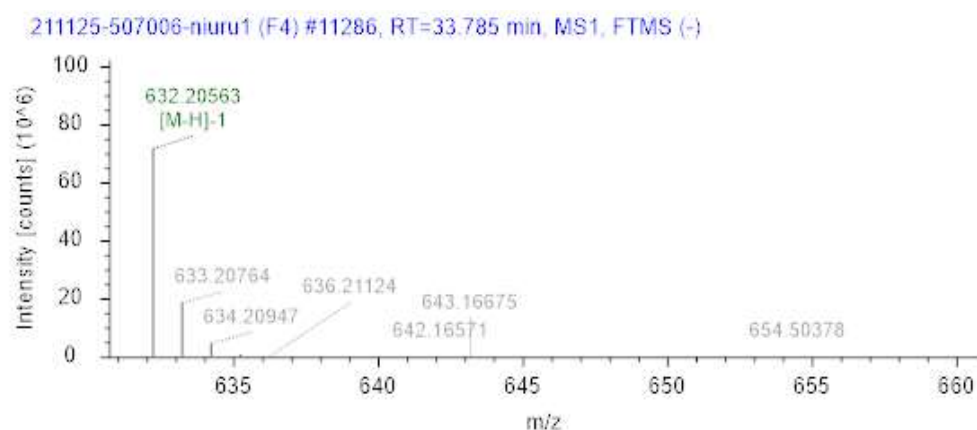211125-507005-renru1 (F3) #9994, RT=34.077 min, MS2, FTMS (-), (HCD, DDA, 632.2050@30, -1)

87.00781
80.93725
83.01287
113.02346
126.05517
142.05014
168.06572
202.07123
246.09770
272.07745
290.08826
291.09268
333.42538
408.15051
425.24603

© Reported with Compound Discoverer 3.3

Compounds
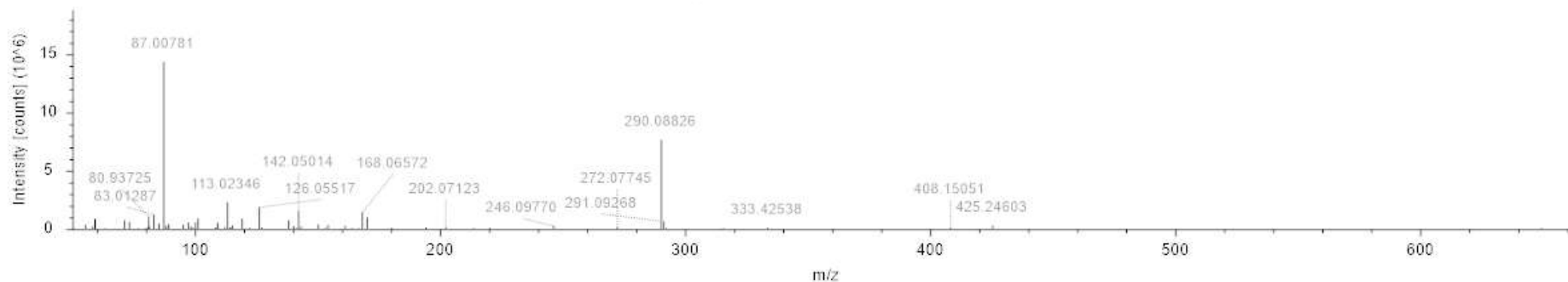
Structure	Name	RT [min]	Formula	Calc. MW	Areas			
n/a		33.78	n/a	633.21238	9.63e7	5.24e8	1.23e9	1.48e9

MW: 633.21238
File: 211125-507003-yangru-ziti1.raw (F1) FTMS (-) MS1
MW: 633.21238
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (-) MS1
MW: 633.21238
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (+) MS1

211125-507006-niuru1 (F4) #11286, RT=33.785 min, MS1, FTMS (-)

632.20563 [M-H]-1
633.20764
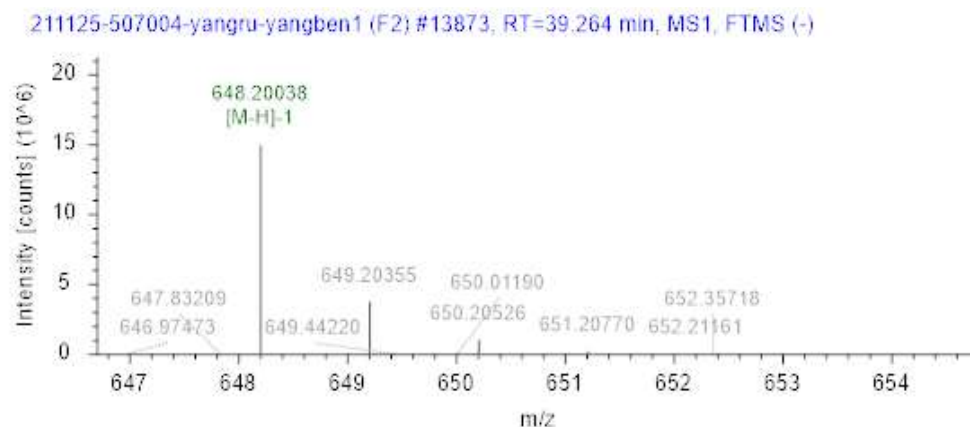634.20947
636.21124
643.16675
642.16571
654.50378
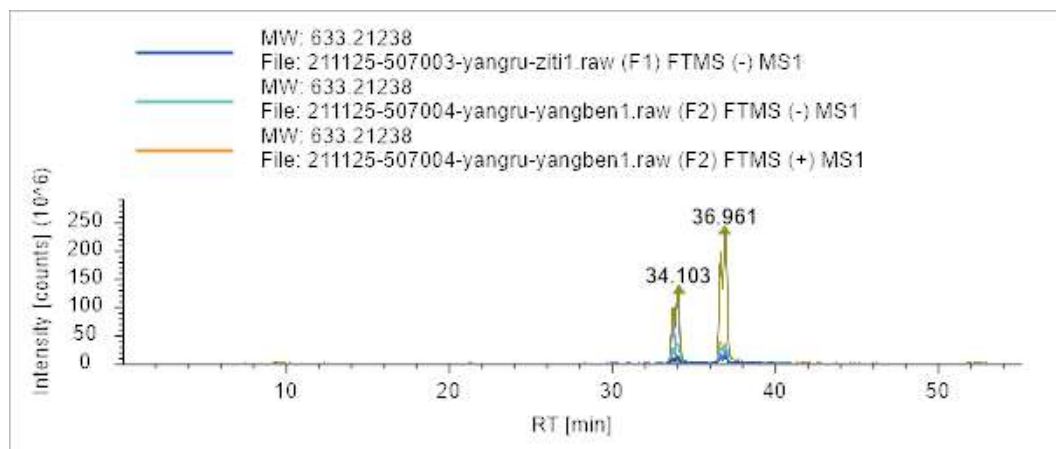
211125-507006-niuru1 (F4) #11323, RT=33.875 min, MS2, FTMS (-), (HCD, DDA, 632.2055@30, -1)

87.00785
59.01279
83.01287
113.02351
126.05523
142.05019
168.06602
194.04514
246.09874
252.95241
272.07776
291.09149
290.08850
358.15250
358.17569
425.23129
444.32312
632.20404

Compounds
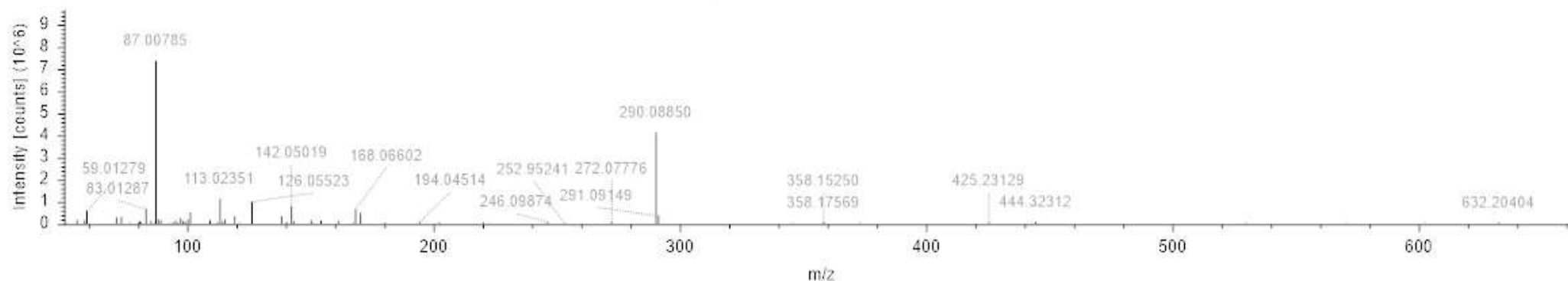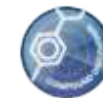
Structure	Name	RT [min]	Formula	Calc. MW	Areas				
n/a		39.26	n/a	649.20671	1.79e8	5.07e8			
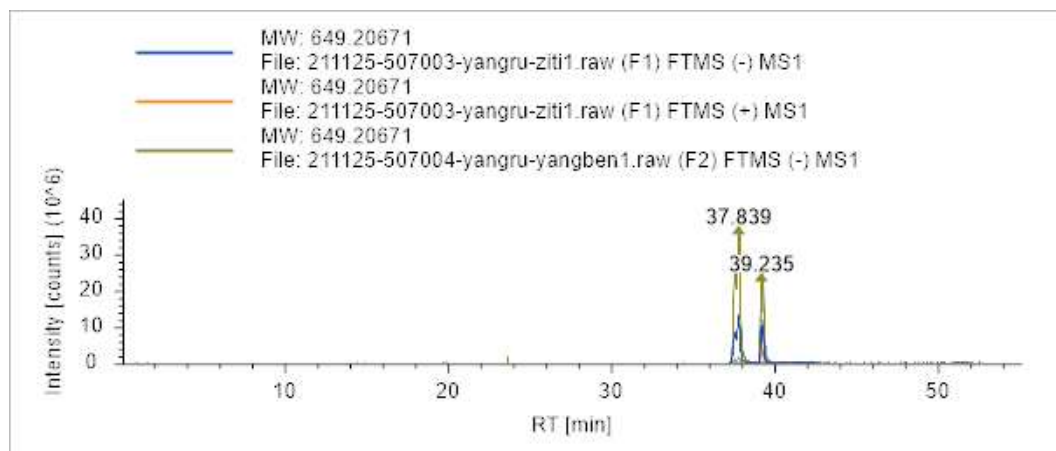
Compounds
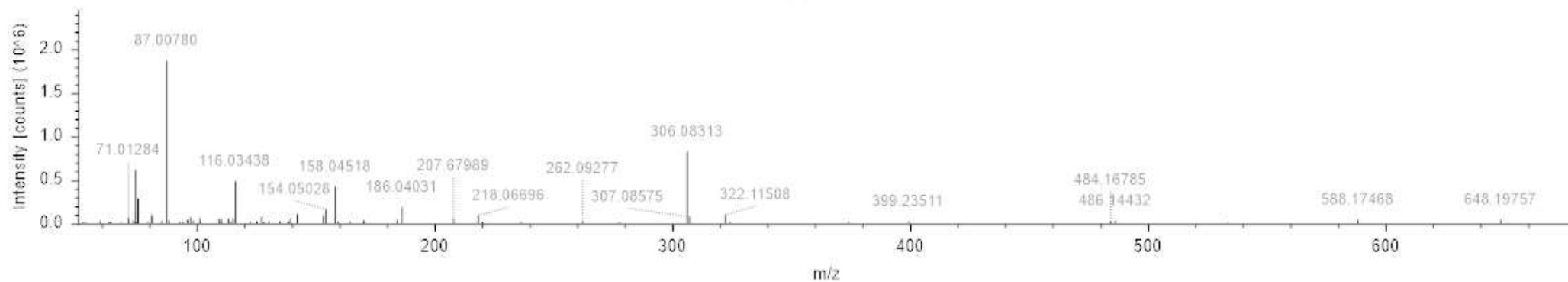
Structure	Name	RT [min]	Formula	Calc. MW	Areas				
n/a		37.78	n/a	649.20736	2.59e8	5.73e8			

MW: 649.20736
File: 211125-507003-yangru-ziti1.raw (F1) FTMS (-) MS1
MW: 649.20736
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (-) MS1
MW: 649.20736
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (+) MS1

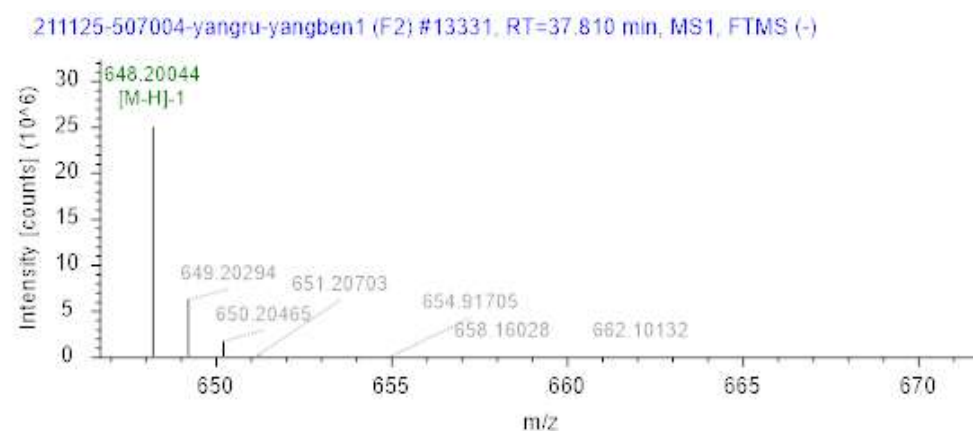211125-507004-yangru-yangben1 (F2) #13331, RT=37.810 min, MS1, FTMS (-)
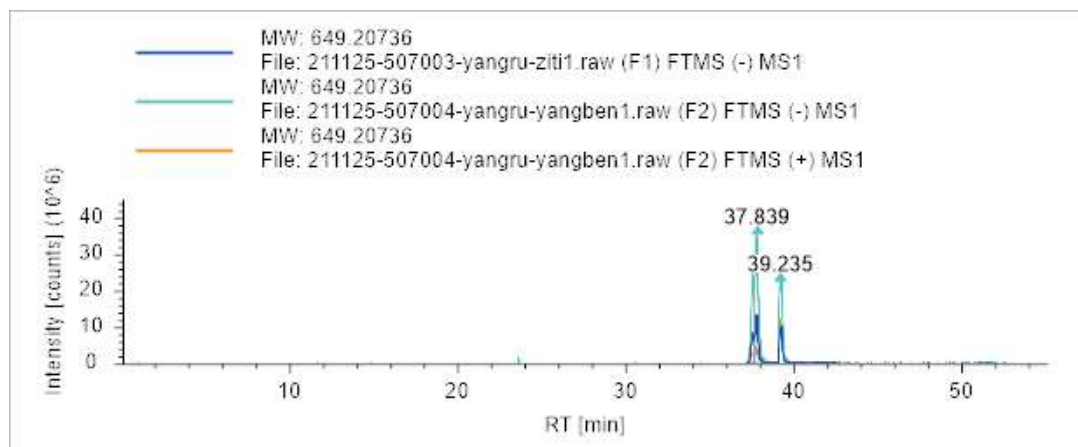
211125-507004-yangru-yangben1 (F2) #13368, RT=37.898 min, MS2, FTMS (-), (HCD, DDA, 648.2006@30, -1)

Compounds
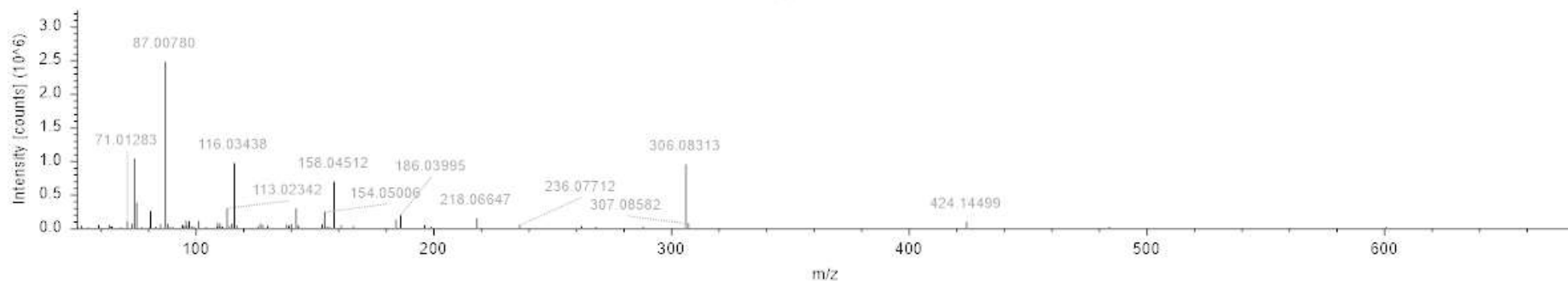
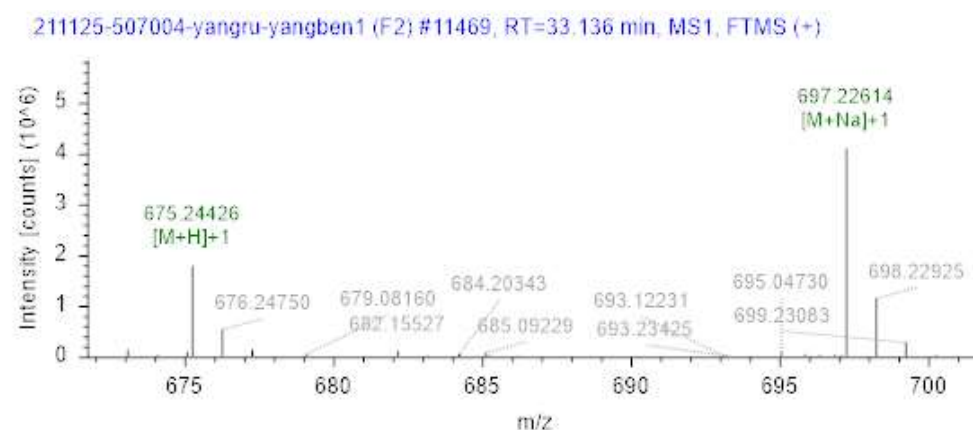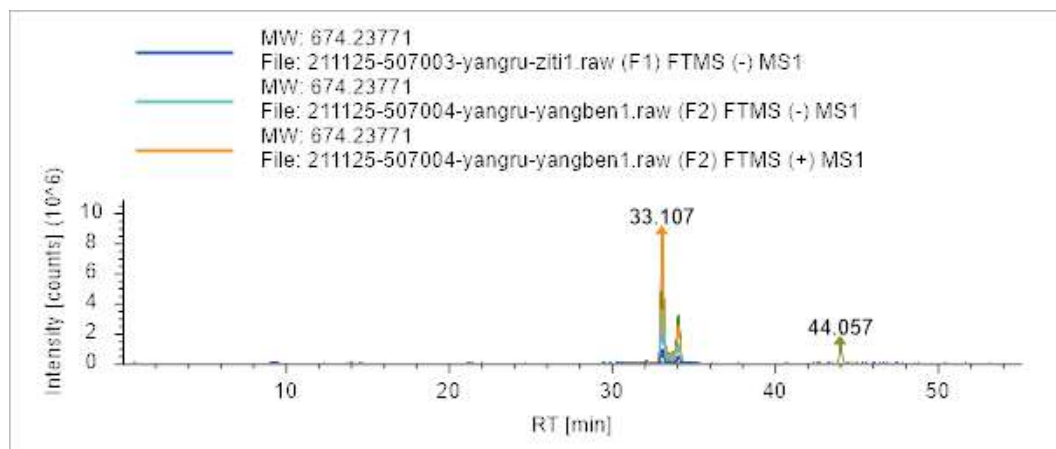| Structure	Name	RT [min]	Formula	Calc. MW	Areas				
n/a		33.12	n/a	674.23771	1.25e7	1.89e8	1.21e7	1.26e8	

Compounds

Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		34.11	n/a	674.23795	5.58e7 3.28e7

MW: 674.23795
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (-) MS1
MW: 674.23795
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (+) MS1
MW: 674.23795
File: 211125-507006-niuru1.raw (F4) FTMS (-) MS1

211125-507004-yangru-yangben1 (F2) #11877, RT=34.113 min, MS1, FTMS (+)

211125-507006-niuru1 (F4) #11431, RT=34.138 min, MS2, FTMS (-), (HCD, DDA, 673.2320@30, -1)

Compounds
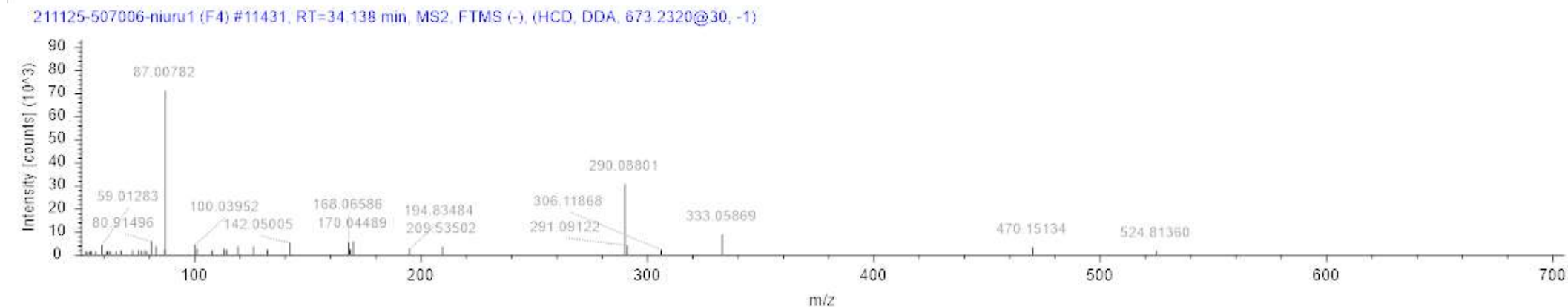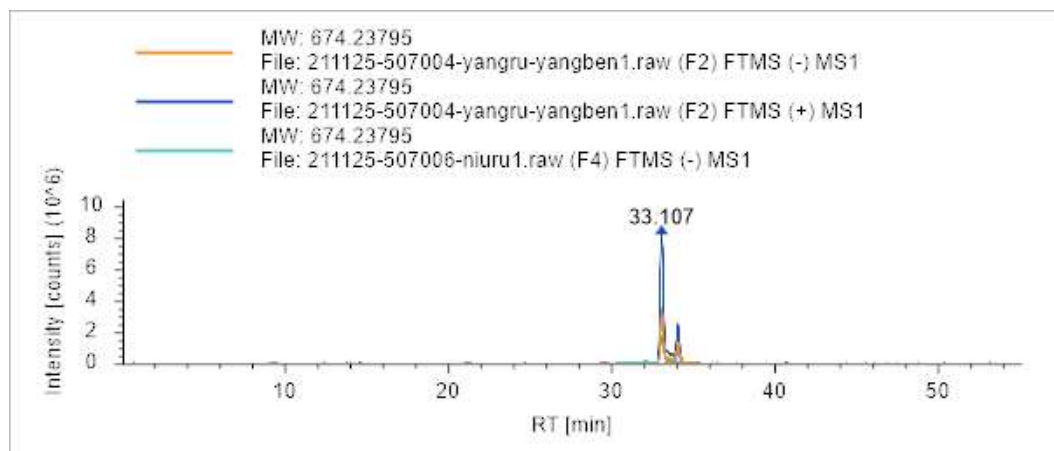
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		36.42	n/a	690.23344	2.69e7 1.18e8

Compounds

Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		37.50	n/a	690.23360	4.06e7

MW: 690.23360
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (-) MS1
MW: 690.23360
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (+) MS1

211125-507004-yangru-yangben1 (F2) #13211, RT=37.500 min, MS1, FTMS (-)

689.22736 [M-H]-1
690.23077
691.23254
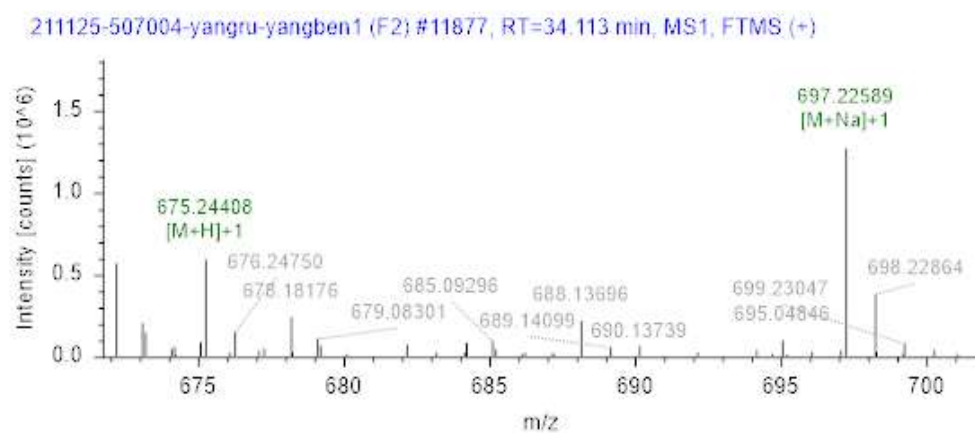692.15997
692.23401
694.97211
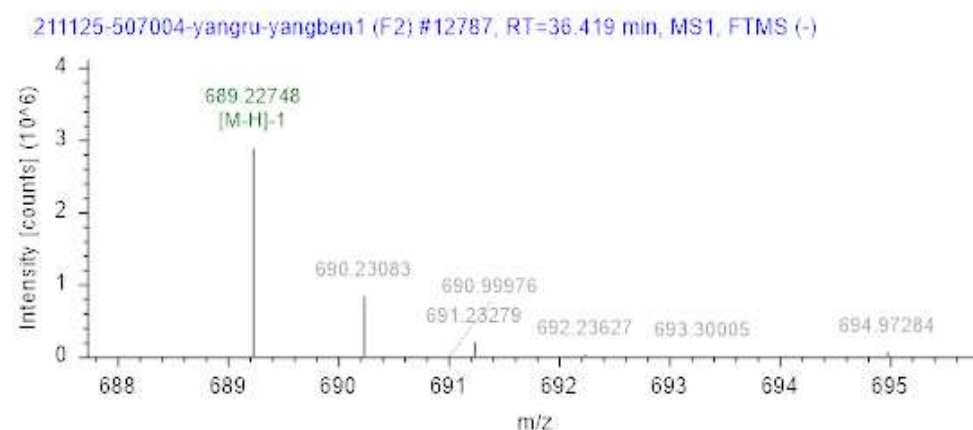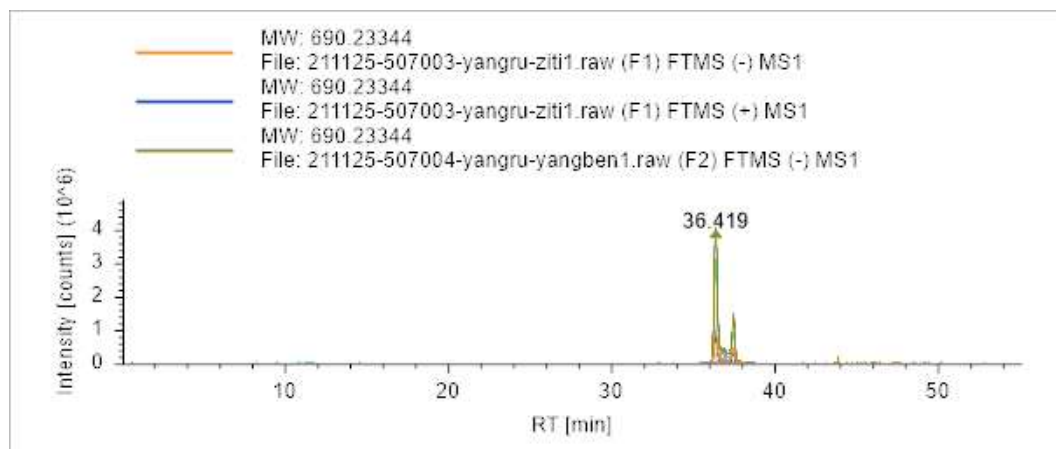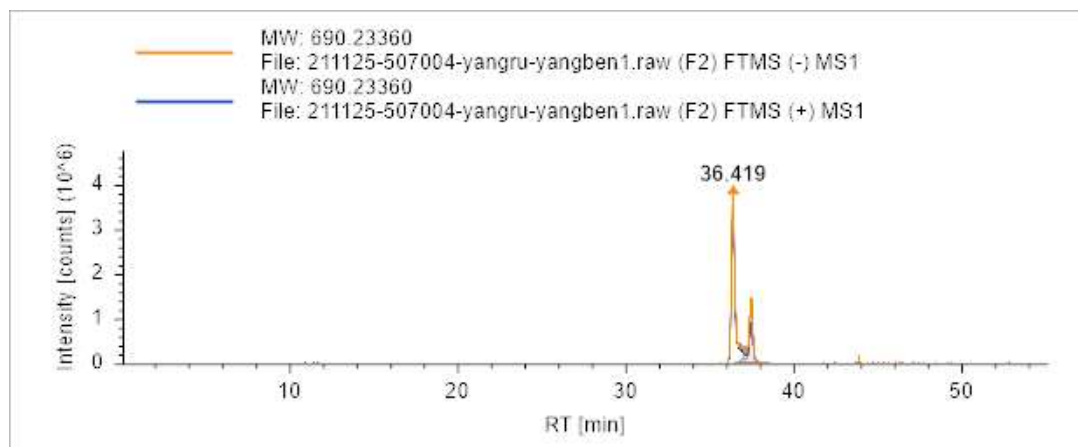
211125-507004-yangru-yangben1 (F2) #13188, RT=37.445 min, MS2, FTMS (-), (HCD, DDA, 689.2274@30, -1)

87.00779
80.93050
116.03446
154.04987
158.04507
184.06036
186.03984
218.06616
306.08307
307.08591
338.98187
408.55585
486.14651
528.15576
588.17596

9

Compounds

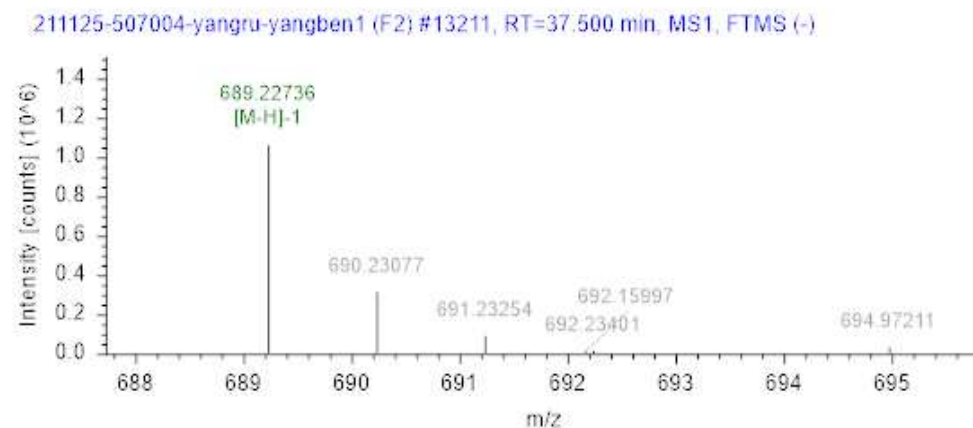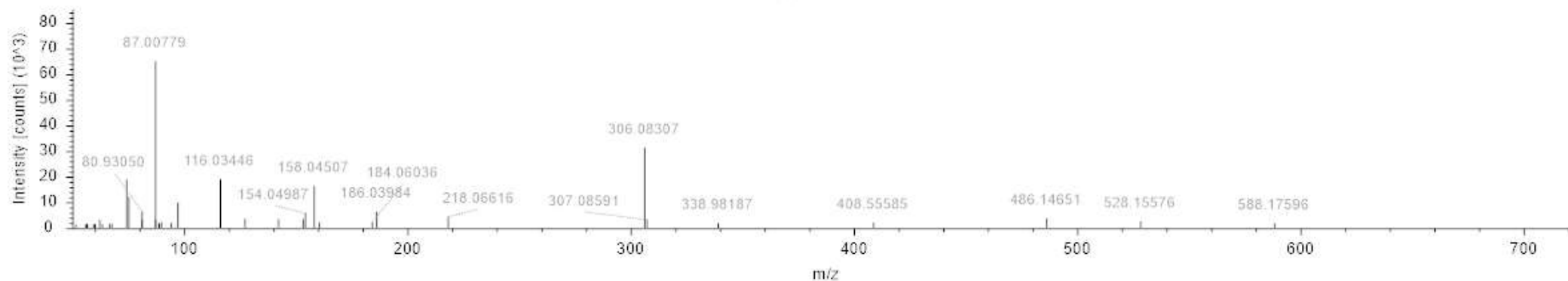| Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		38.99	n/a	779.27138	6.52e7

MW: 779.27138
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1

39.238

44.085

211125-507005-renru1 (F3) #11455, RT=38.979 min, MS1, FTMS (-)

778.26385
[M-H]-1

776.95868   779.26715   780.26910   781.27222   782.27496
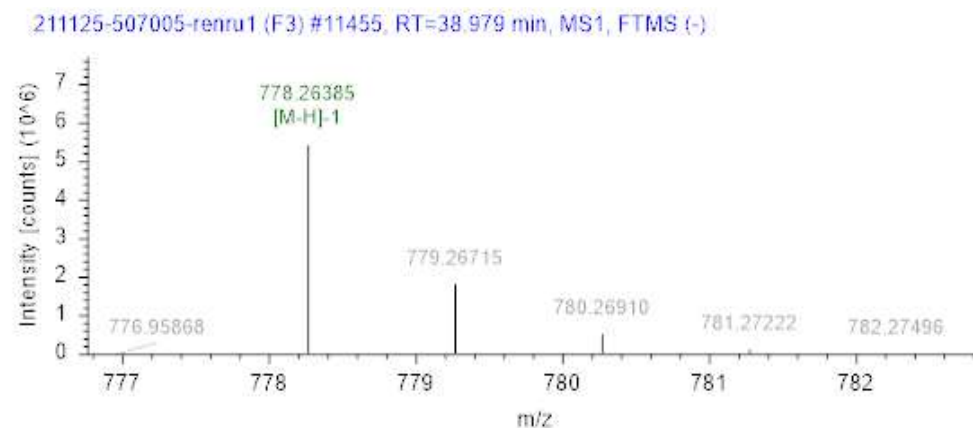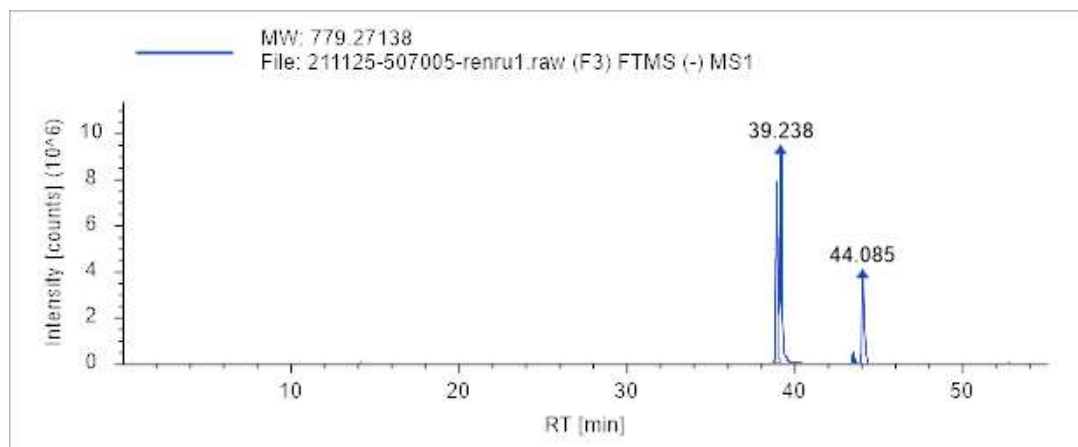
211125-507005-renru1 (F3) #11426, RT=38.899 min, MS2, FTMS (-), (HCD, DDA, 778.2632@30, -1)

87.00783

113.02349   126.05529
170.04526   178.82672
161.04514   290.08835
291.09128   308.09772   425.24673   507.62772

© Reported with Compound Discoverer 3.3

Compounds
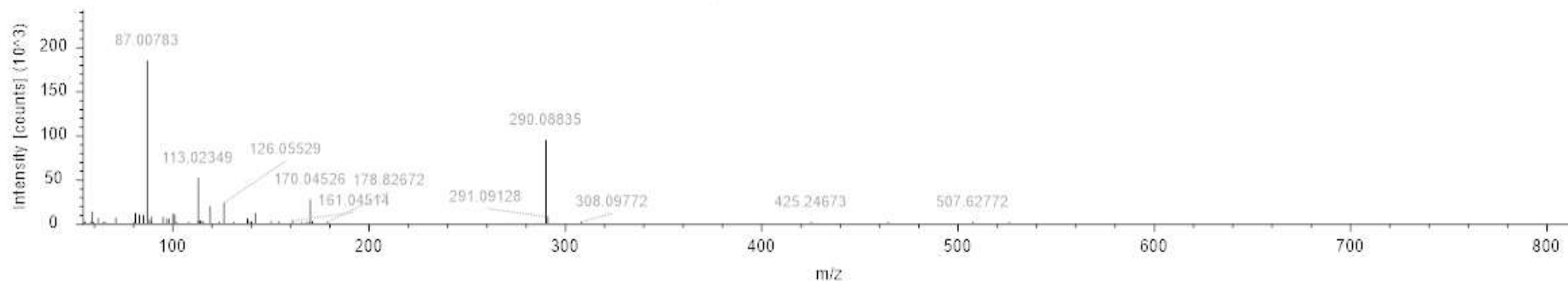
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		39.80	n/a	795.26640	1.68e7 4.02e7

MW: 795.26640
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (-) MS1
MW: 795.26640
File: 211125-507006-niuru1.raw (F4) FTMS (-) MS1

39.811

211125-507006-niuru1 (F4) #12968, RT=39.811 min, MS1, FTMS (-)

794.25885
[M-H]-1

793.26398   795.26208   796.26392   797.26660   798.27362
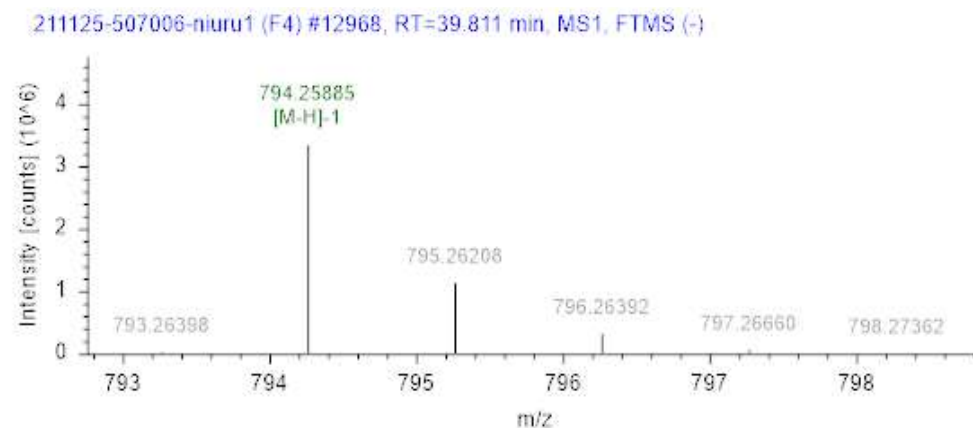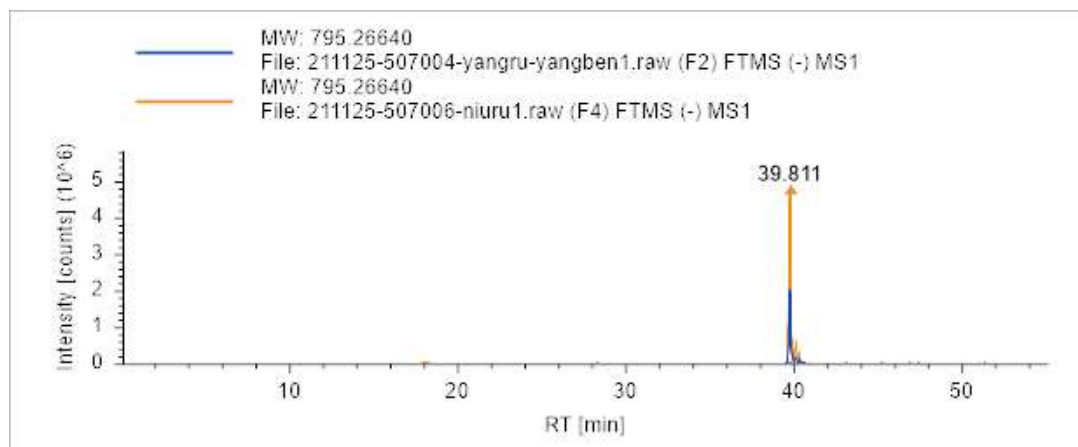
211125-507006-niuru1 (F4) #12993, RT=39.885 min, MS2, FTMS (-), (HCD, DDA, 794.2593@30, -1)

87.00780
113.02347
126.05511 168.06569
142.04991 170.04507
259.99075
290.08823
291.09088
286.83499 373.45370

Compounds
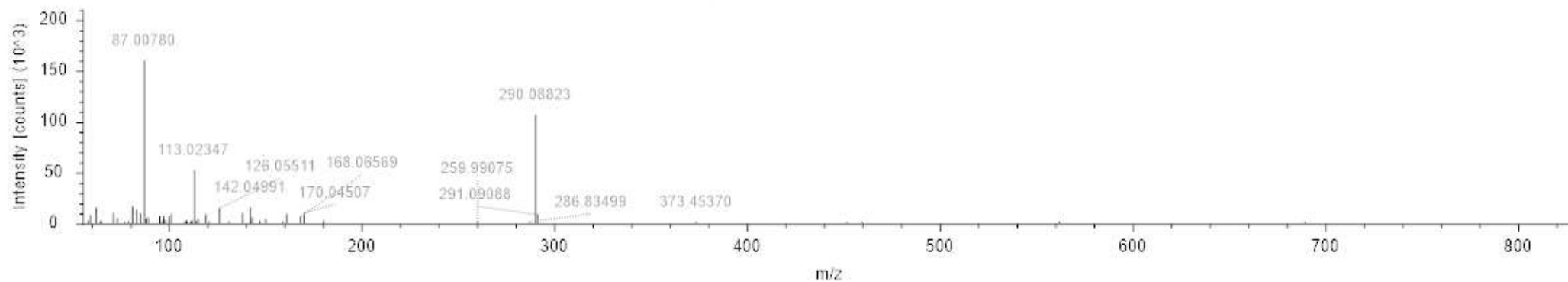
Structure	Name	RT [min]	Formula	Calc. MW	Areas					
n/a		40.76	n/a	811.26171	6.41e6	1.85e7				

MW: 811.26171
File: 211125-507003-yangru-ziti1.raw (F1) FTMS (-) MS1
MW: 811.26171
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (-) MS1

211125-507004-yangru-yangben1 (F2) #14322, RT=40.758 min, MS1, FTMS (-)

810.25452
[M-H]-1
811.25787
812.26007
813.26208
814.26495
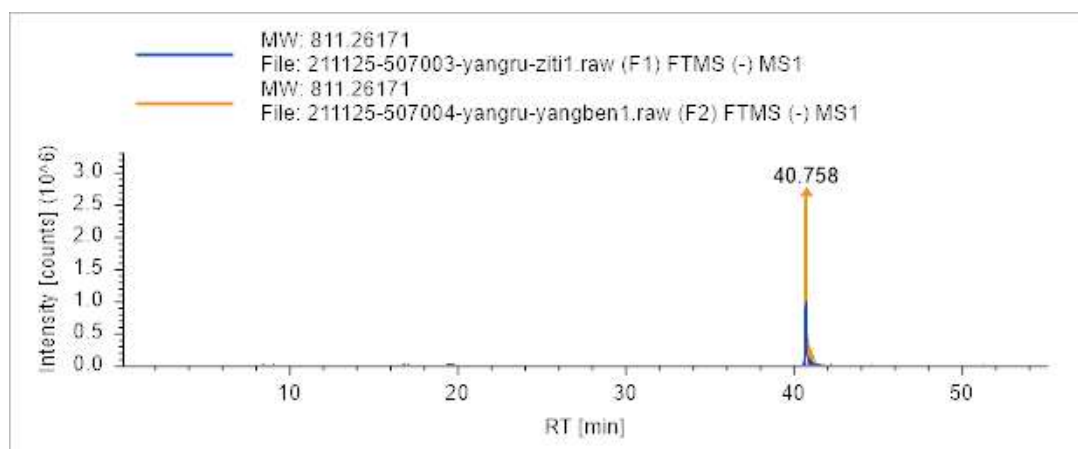
211125-507004-yangru-yangben1 (F2) #14305, RT=40.678 min, MS2, FTMS (-), (HCD, DDA, 810.2548@30, -1)

87.00781
116.03453
113.02353
158.04498
186.04015
218.06592
249.09334
306.08310
330.79794
397.29181

Compounds
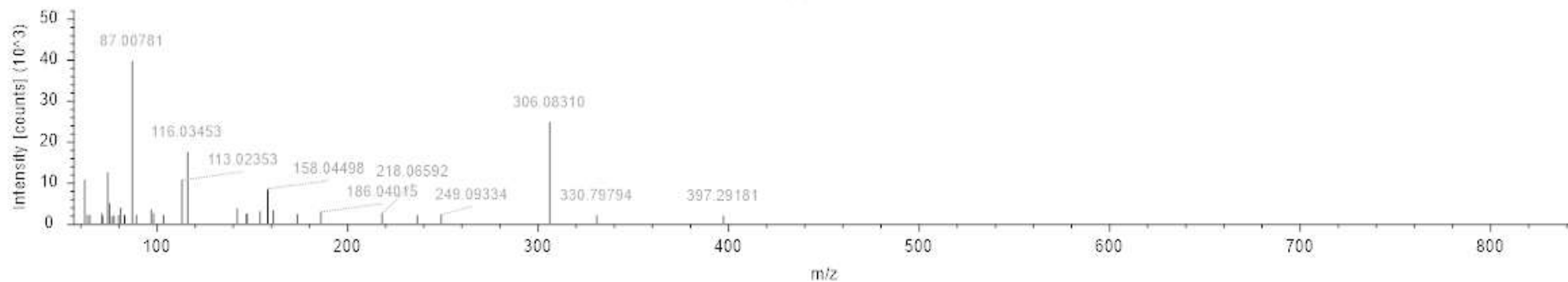
Structure	Name	RT [min]	Formula	Calc. MW	Areas			
n/a		39.29	n/a	924.30875	1.20e7	3.10e7	4.97e7	

MW: 924.30875
File: 211125-507003-yangru-ziti1.raw (F1) FTMS (-) MS1
MW: 924.30875
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (-) MS1
MW: 924.30875
File: 211125-507006-niuru1.raw (F4) FTMS (-) MS1

39.326

211125-507006-niuru1 (F4) #12816, RT=39.303 min, MS1, FTMS (-)

923.30121
[M-H]-1

924.30426

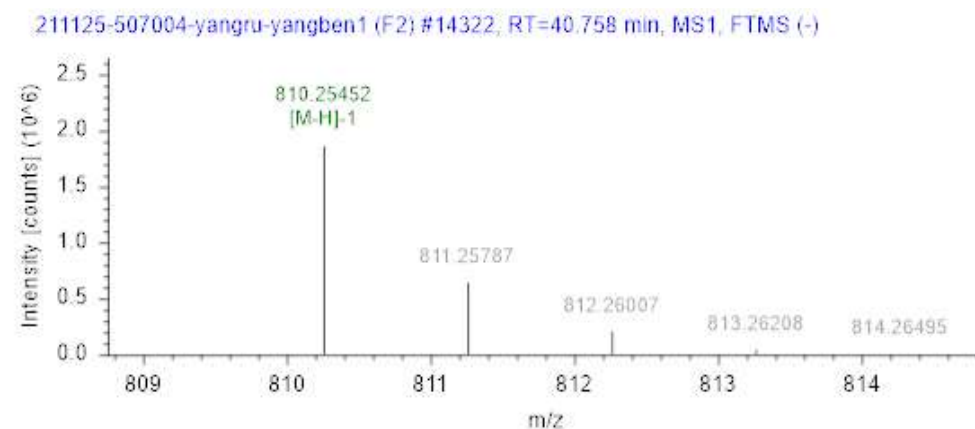923.79913
924.25122

925.30585

926.30865
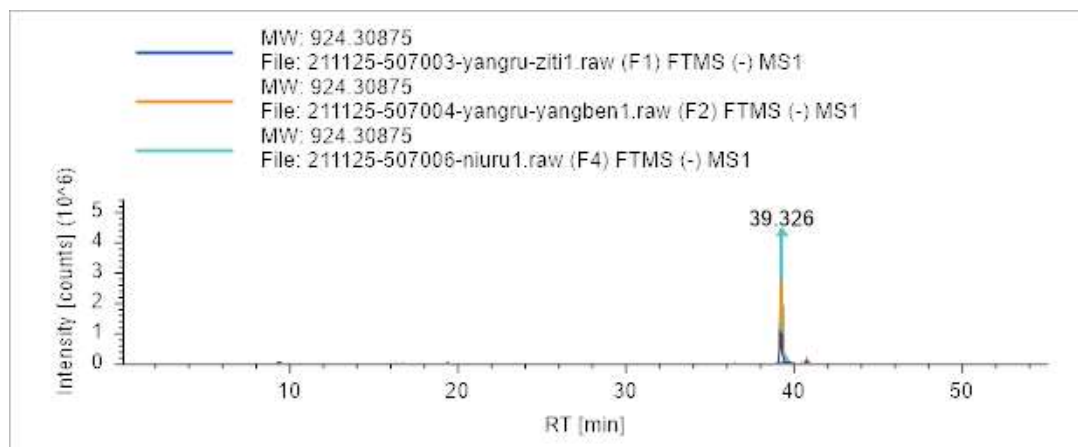
211125-507006-niuru1 (F4) #12847, RT=39.388 min, MS2, FTMS (-), (HCD, DDA, 923.3016@30, -1)

87.00784

290.08844

168.06599   158.97787
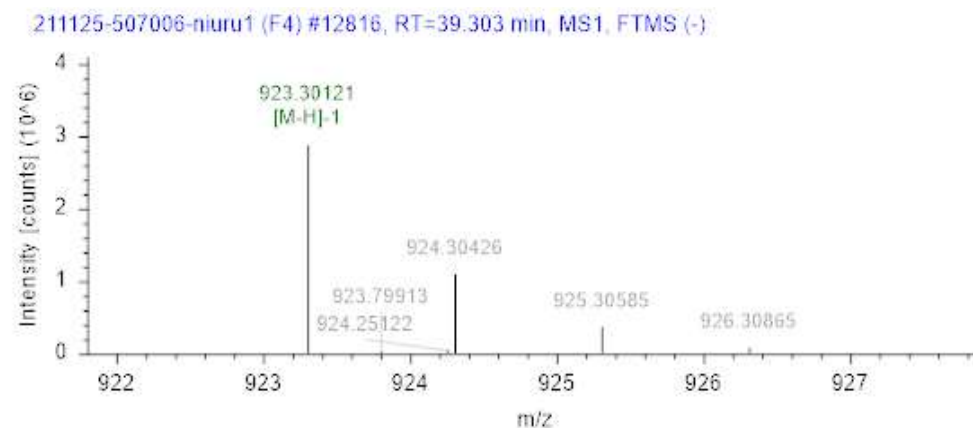142.05011   170.04514   180.06586

291.09201
308.09802
359.08307

408.15237
425.23062

632.20435

Compounds
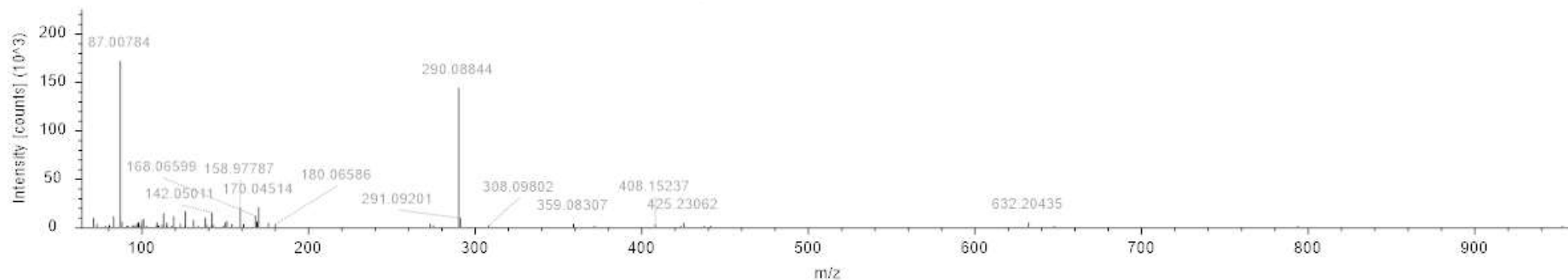
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		40.34	n/a	940.30444	8.78e6 · 2.57e7

MW: 940.30444
File: 211125-507003-yangru-ziti1.raw (F1) FTMS (-) MS1
MW: 940.30444
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (-) MS1

40.351

211125-507004-yangru-yangben1 (F2) #14235, RT=40.351 min, MS1, FTMS (-)

939.29718
[M-H]-1

940.30060

941.30176

942.30255 943.58423
943.30609

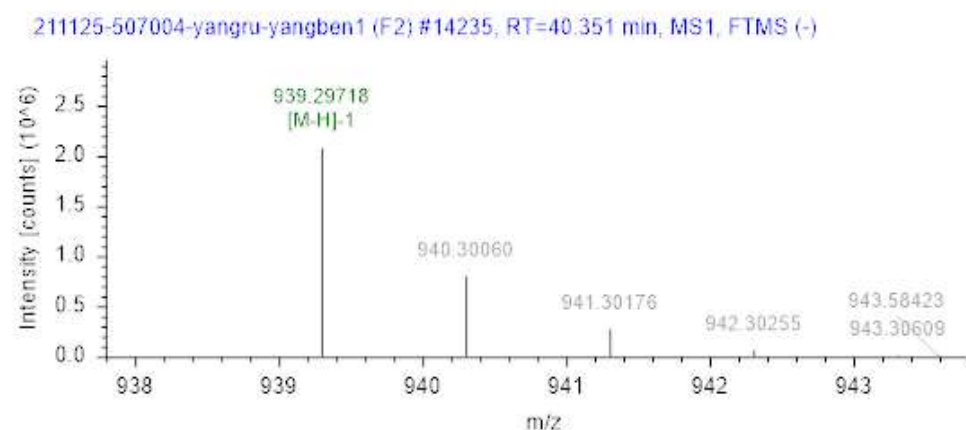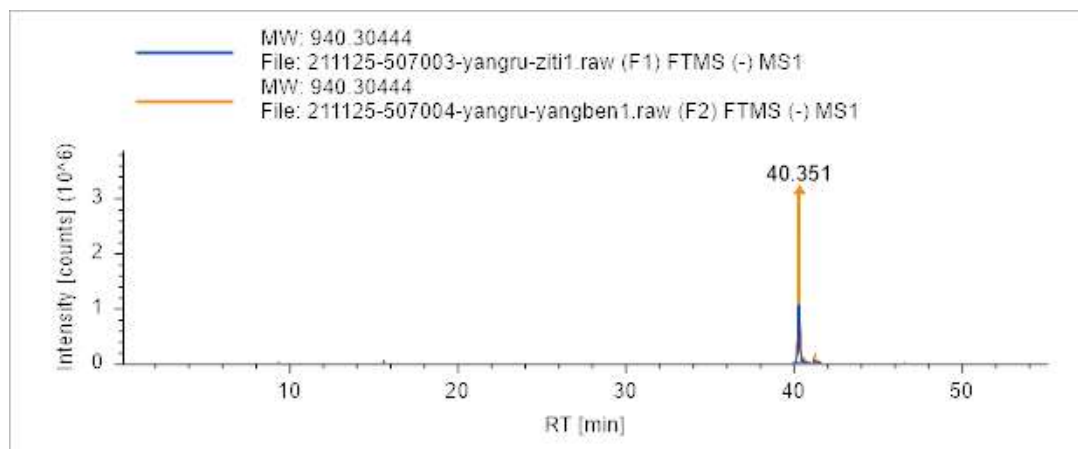211125-507004-yangru-yangben1 (F2) #14248, RT=40.399 min, MS2, FTMS (-), (HCD, DDA, 939.2975@30, -1)

87.00782

116.03442 142.05017 158.04503 207.57881 218.08621 290.08832 306.08325 307.08606 380.11911 424.14456 478.15762 648.19757

Compounds
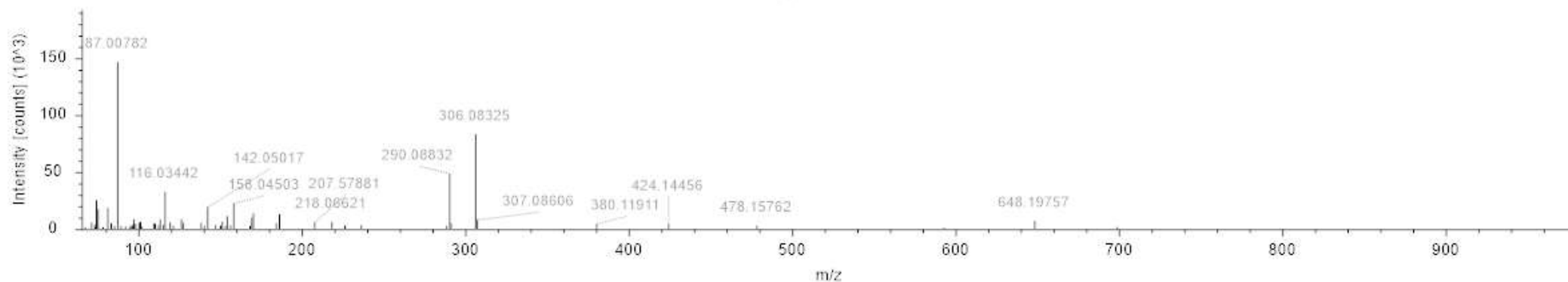
Structure	Name	RT [min]	Formula	Calc. MW	Areas	
n/a		41.14	n/a	956.29852	9.29e6	3.29e7

MW: 956.29852
File: 211125-507003-yangru-ziti1.raw (F1) FTMS (-) MS1
MW: 956.29852
File: 211125-507004-yangru-yangben1.raw (F2) FTMS (-) MS1
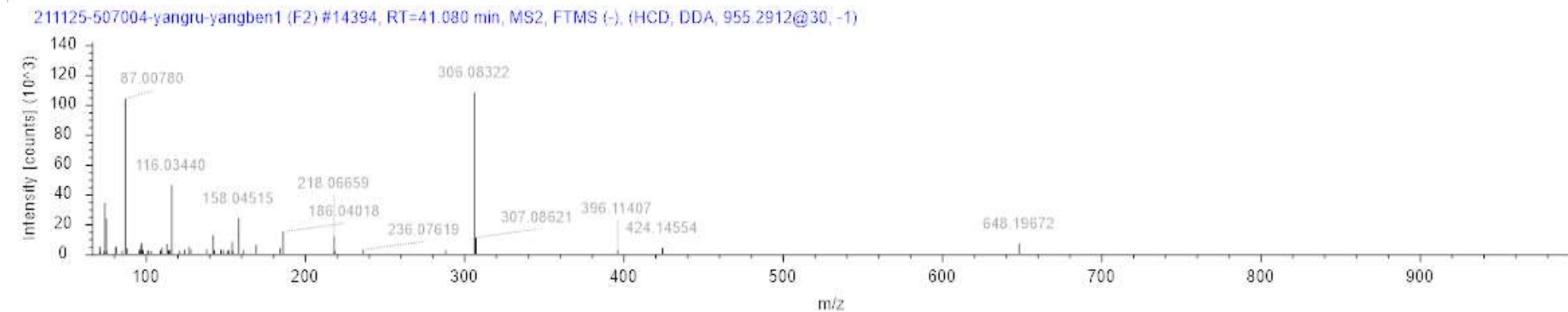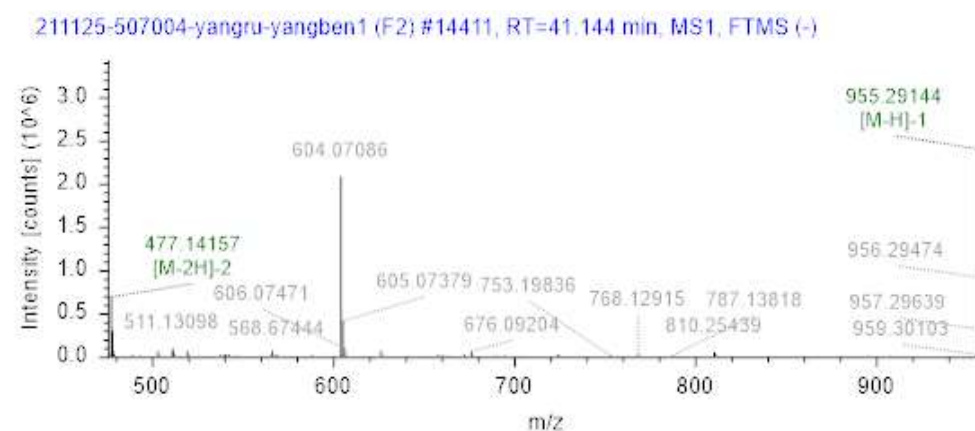
41.144

211125-507004-yangru-yangben1 (F2) #14411, RT=41.144 min, MS1, FTMS (-)

955.29144 [M-H]-1
604.07086
477.14157 [M-2H]-2
511.13098 568.67444 605.07379 753.19836 768.12915 787.13818 956.29474
606.07471 676.09204 810.25439 957.29639 959.30103

211125-507004-yangru-yangben1 (F2) #14394, RT=41.080 min, MS2, FTMS (-), (HCD, DDA, 955.2912@30, -1)

87.00780
306.08322
116.03440
158.04515
218.06659
186.04018
236.07619
307.08621
396.11407
424.14554
648.19672

Compounds

Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		44.20	n/a	998.34130	9.33e6

MW: 998.34130
File: 211125-507005-renru1.raw (F3) FTMS (+) MS1

41.555

211125-507005-renru1 (F3) #13395, RT=44.215 min, MS1, FTMS (+)

999.34851
[M+H]+1

998.09589
998.86810
1000.35114
1001.35284
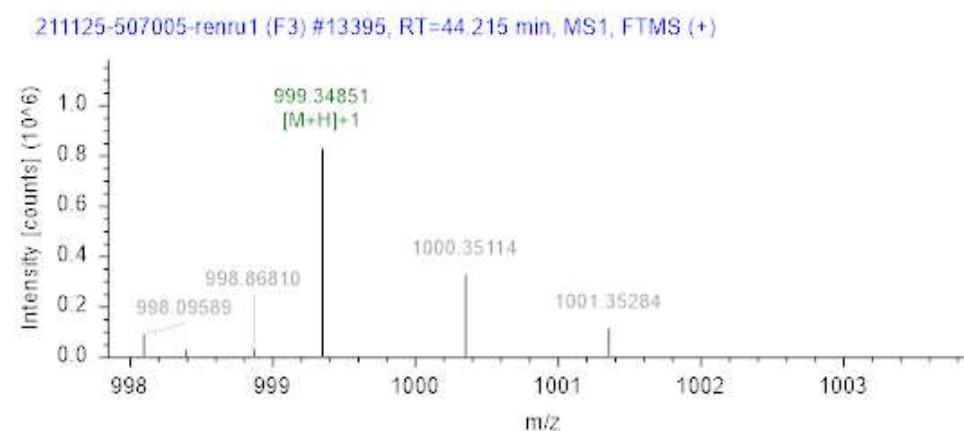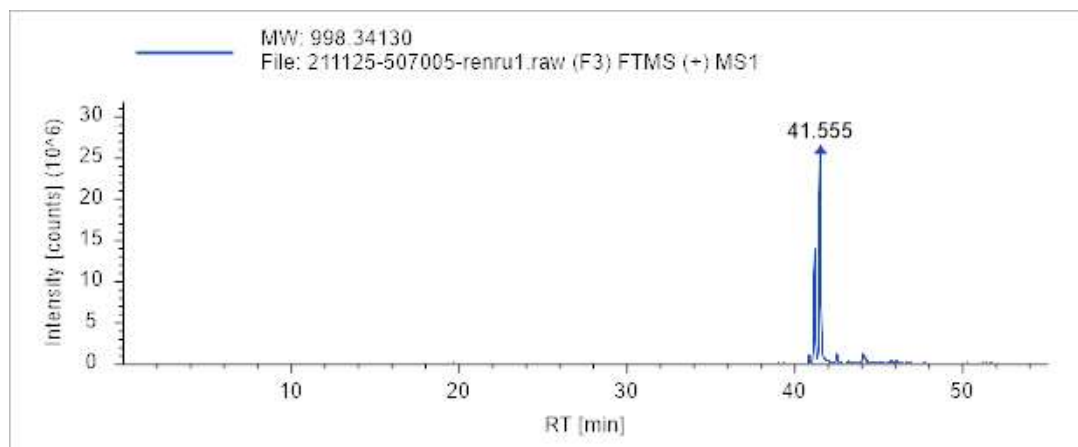
211125-507005-renru1 (F3) #13408, RT=44.246 min, MS2, FTMS (+), (HCD, DDA, 999.3485@30, +1)

115.08705
138.05521
168.06584
204.08704
70.06594
126.05532
197.04465
205.09024
274.09238
275.09564
292.10318
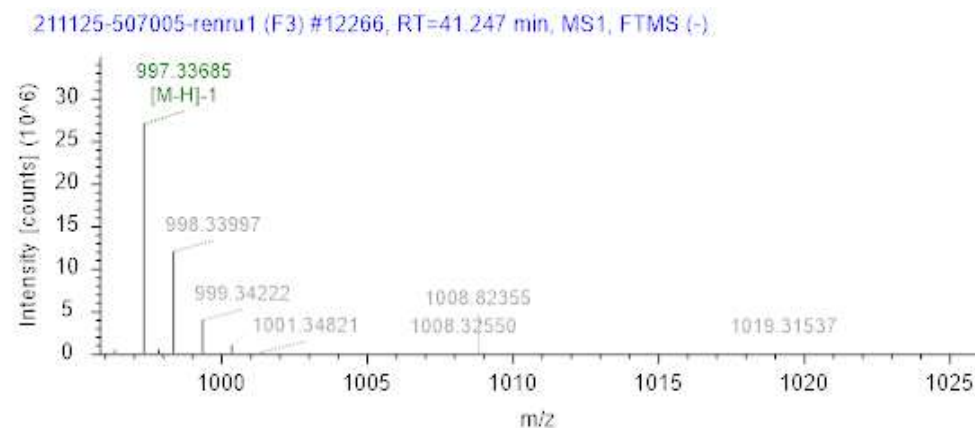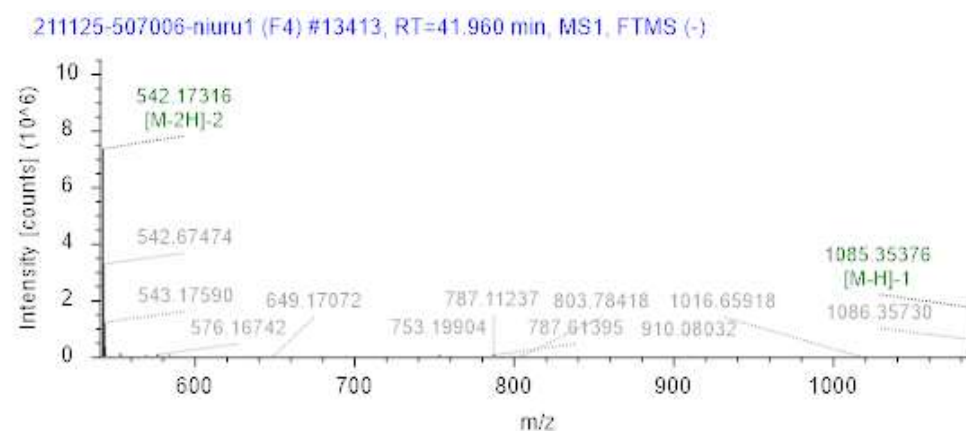366.14001
367.14243

Compounds
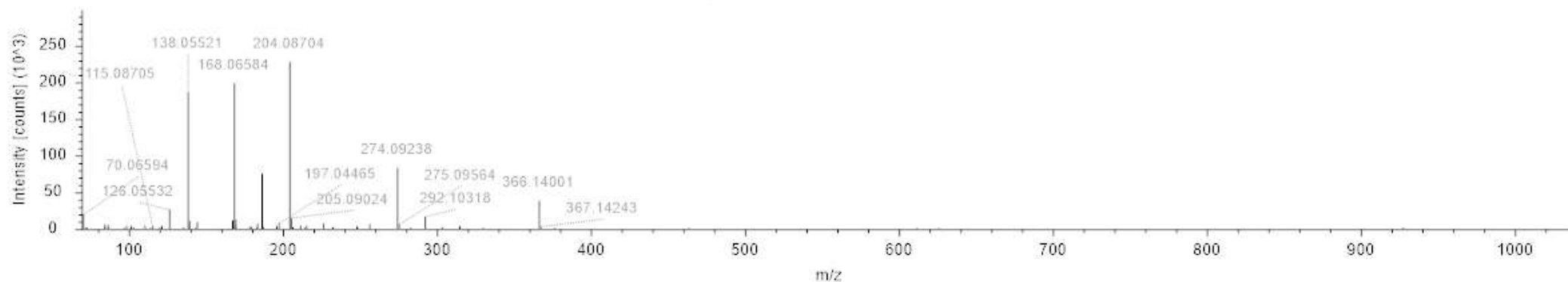
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		41.23	n/a	998.34363	5.24e8
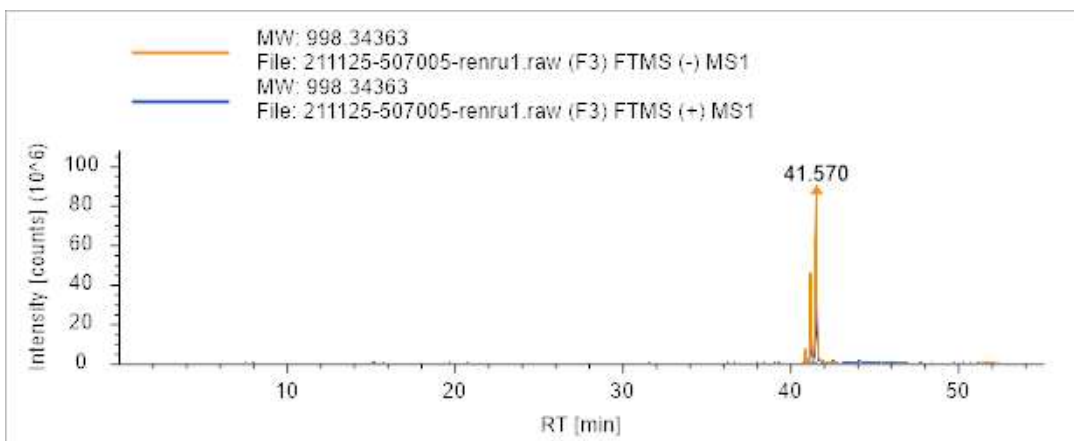
Compounds
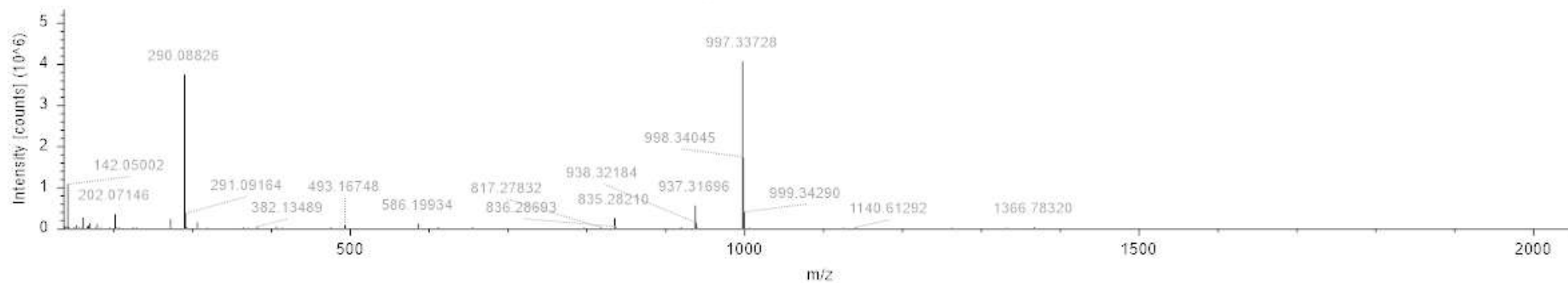
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		41.97	n/a	1086.36090	9.03e7

MW: 1086.36090
File: 211125-507006-niuru1.raw (F4) FTMS (-) MS1

211125-507006-niuru1 (F4) #13413, RT=41.960 min, MS1, FTMS (-)

542.17316 [M-2H]-2
542.67474
543.17590
576.16742
649.17072
753.19904
787.11237
787.61395
803.78418
910.08032
1016.65918
1085.35376 [M-H]-1
1086.35730
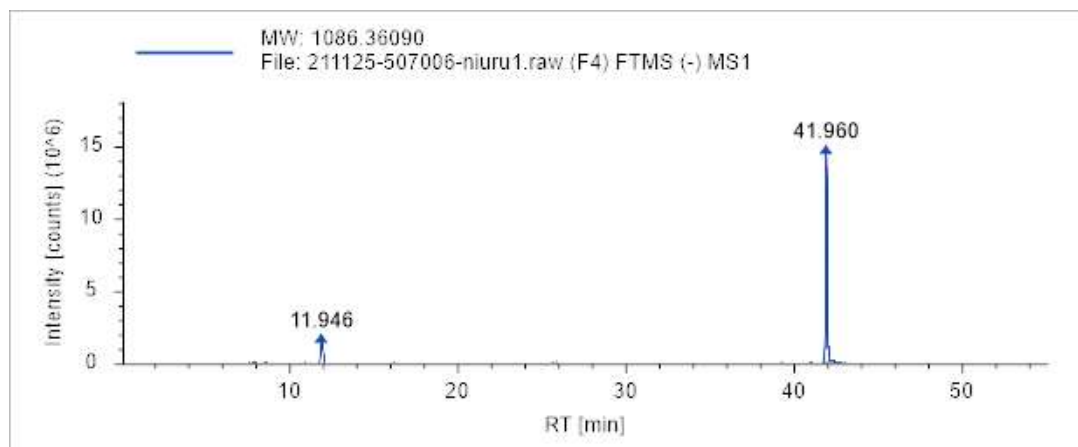
211125-507006-niuru1 (F4) #13399, RT=41.902 min, MS2, FTMS (-), (HCD, DDA, 1085.3539@30, -1)

87.00780
96.95912
113.02335
126.05499
170.04485
191.01913
291.09085
290.08841
348.18277
698.21423
795.26294
794.25494

Compounds
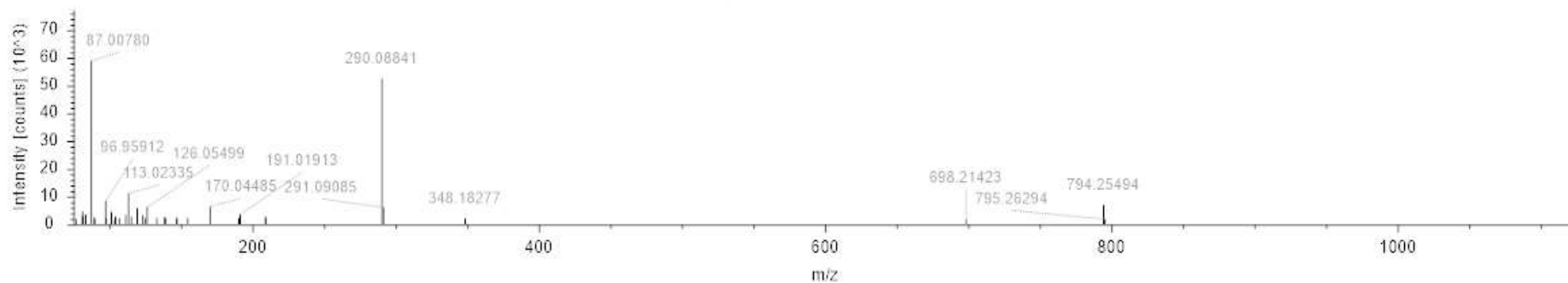
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		42.50	n/a	1144.40192	2.91e8

MW: 1144.40192
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1
MW: 1144.40192
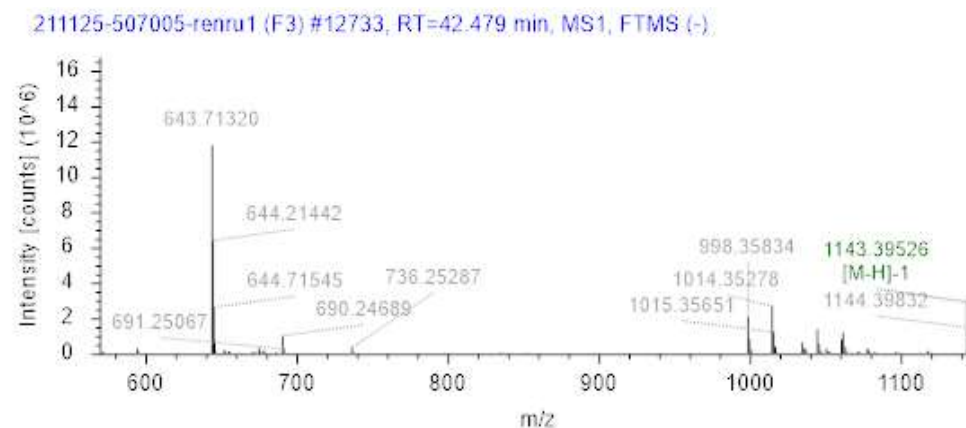File: 211125-507005-renru1.raw (F3) FTMS (+) MS1

42.392

211125-507005-renru1 (F3) #12733, RT=42.479 min, MS1, FTMS (-)

643.71320
644.21442
644.71545
691.25067
690.24689
736.25287
998.35834
1014.35278
1015.35651
1143.39526
[M-H]-1
1144.39832
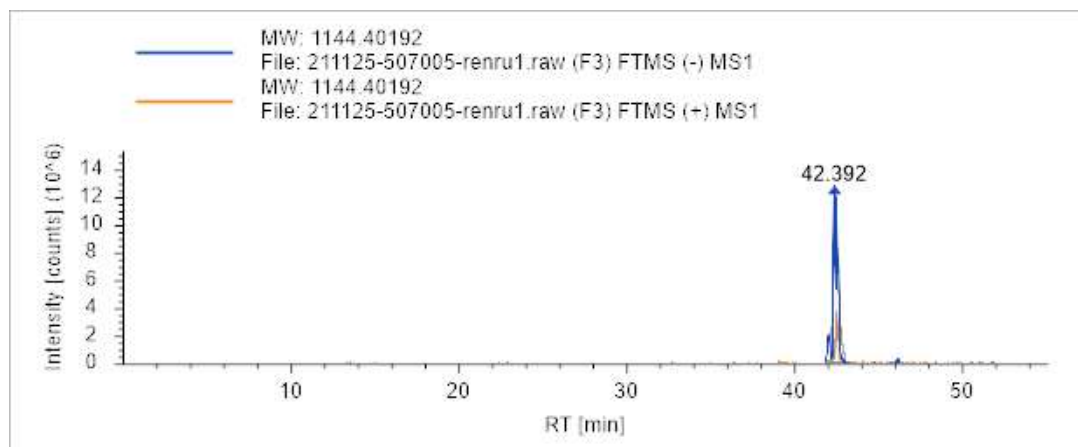
211125-507005-renru1 (F3) #12710, RT=42.423 min, MS2, FTMS (-), (HCD, DDA, 1143.3953@30, -1)

87.00784
113.02350
154.05022
170.04518
184.06096
290.08844
288.10901
291.09216
348.12985
358.11420
425.24606
510.18188

Compounds
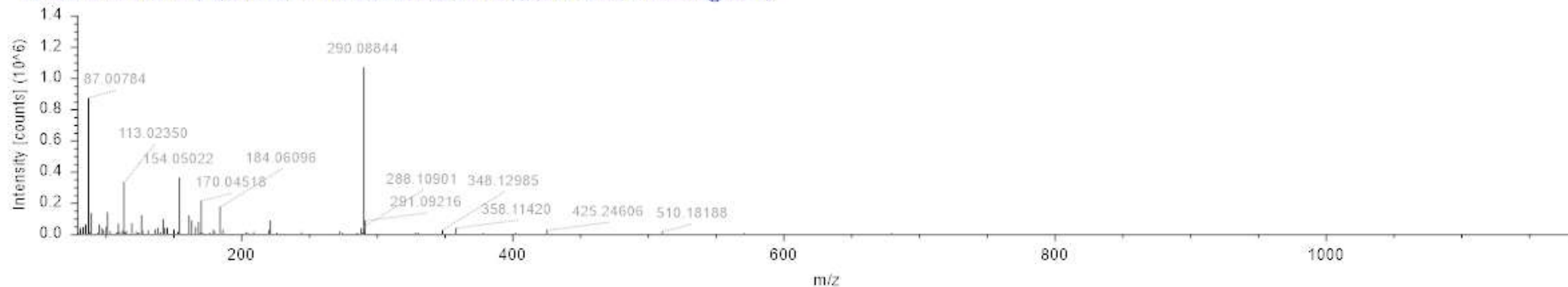
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		42.86	n/a	1160.39668	5.43e6

MW: 1160.39668
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1

211125-507005-renru1 (F3) #12872, RT=42.854 min, MS1, FTMS (-)
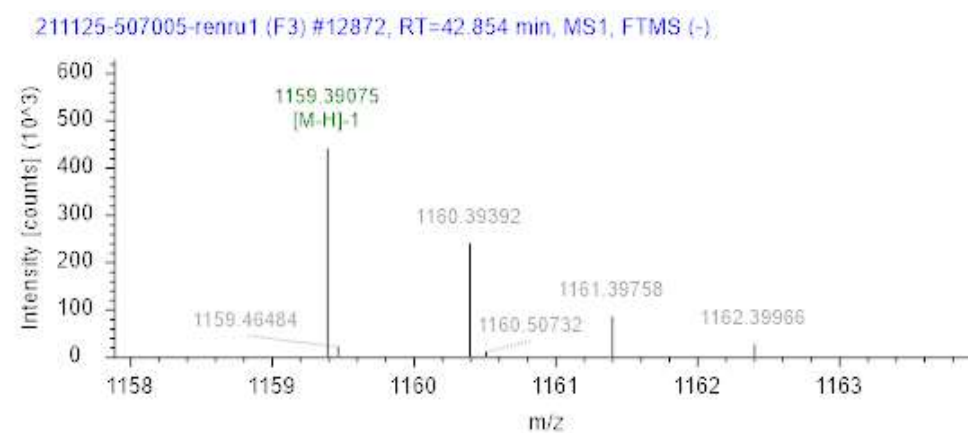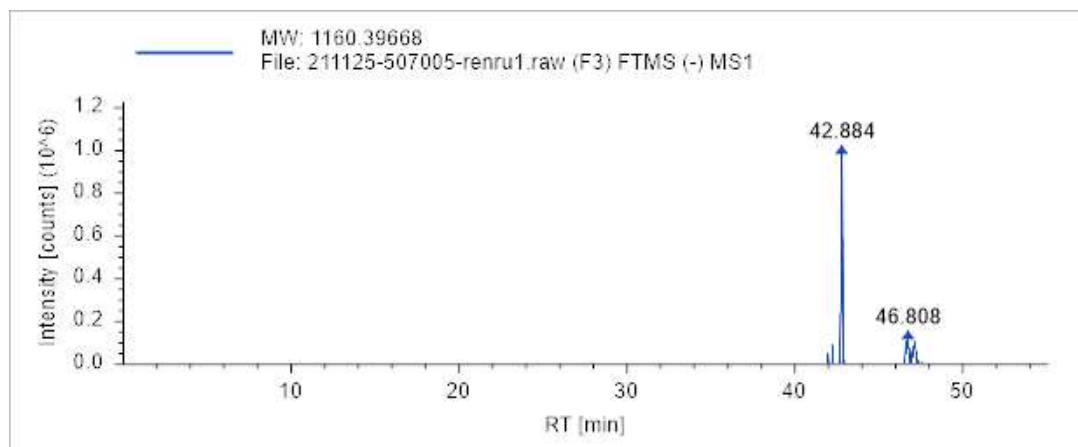

211125-507005-renru1 (F3) #12899, RT=42.918 min, MS2, FTMS (-), (HCD, DDA, 1157.4119@30, -1)

Compounds
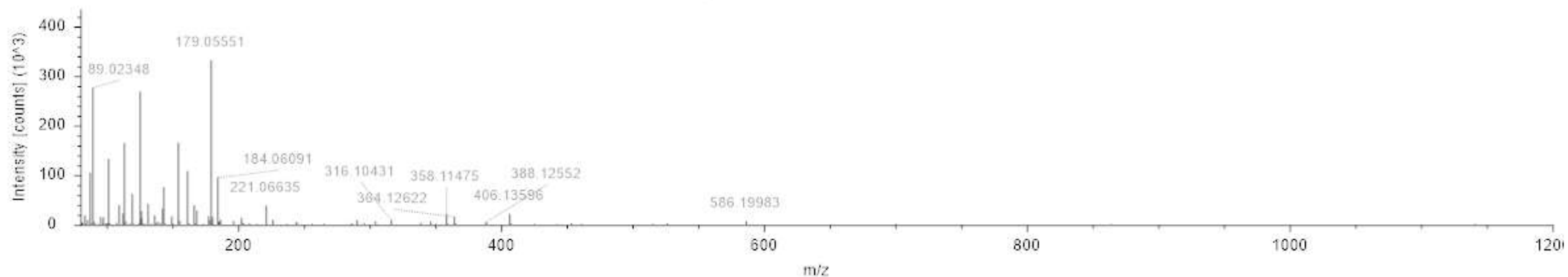
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		42.56	n/a	1289.43515	2.29e7

MW: 1289.43515
File: 211125-507005-renru1.raw (F3) FTMS (+) MS1

211125-507005-renru1 (F3) #12763, RT=42.554 min, MS1, FTMS (+)

645.72485
[M+2H]+2

644.69672
645.23242
646.22620
646.72748
647.22815
649.71149

42.554
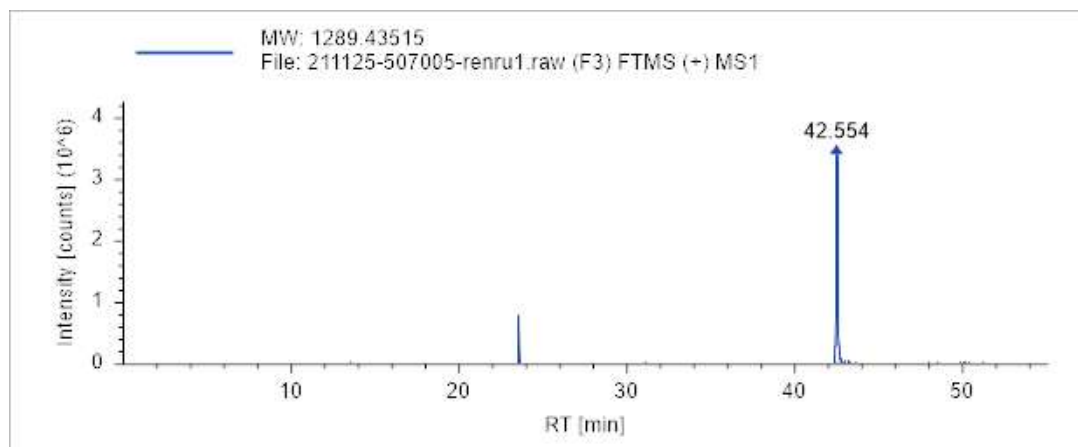
211125-507005-renru1 (F3) #12744, RT=42.503 min, MS2, FTMS (+), (HCD, DDA, 645.7255@30, +2)

274.09238
204.08701
167.03419
126.05530
186.07642
275.09576
292.10300
366.14020
444.79111
495.18155
682.02301
744.46857
745.58710

Compounds
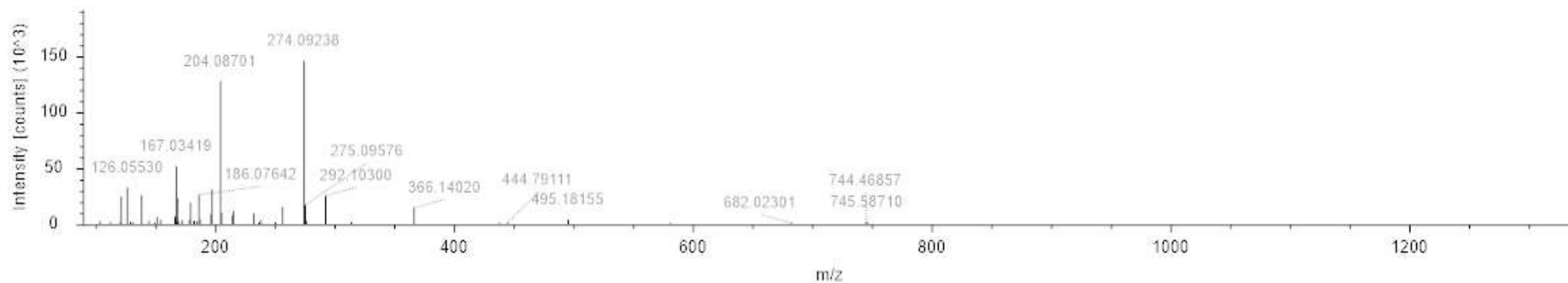
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		43.30	n/a	1363.47521	2.48e8

211125-507005-renru1 (F3) #13052, RT=43.285 min, MS1, FTMS (-)

MW: 1363.47521
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1
MW: 1363.47521
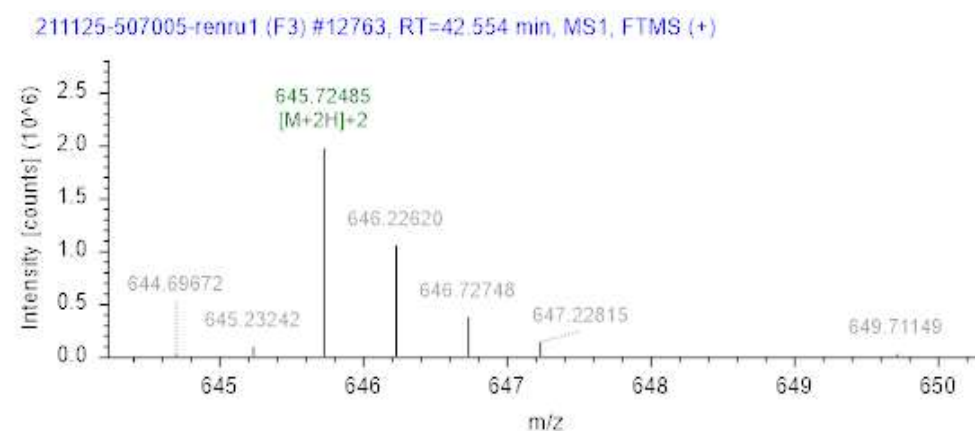File: 211125-507005-renru1.raw (F3) FTMS (+) MS1
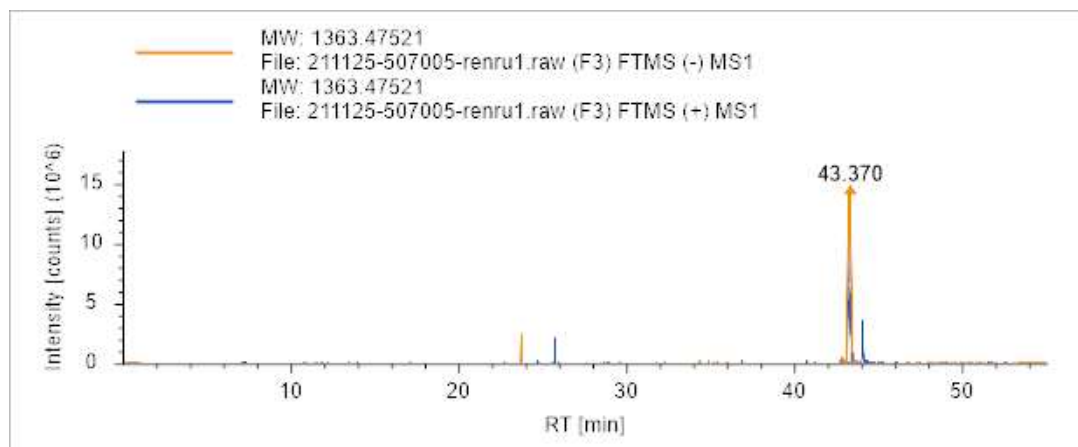
211125-507005-renru1 (F3) #13088, RT=43.374 min, MS2, FTMS (-), (HCD, DDA, 1362.4690@30, -1)

Compounds
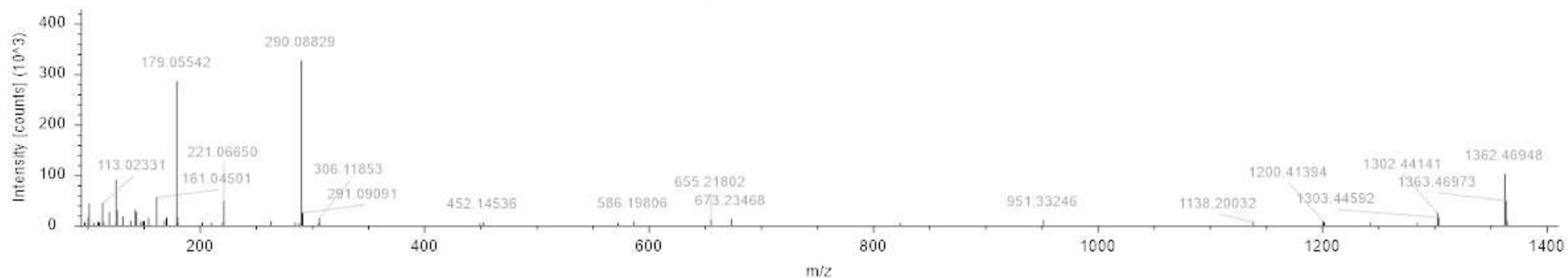
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		43.28	n/a	1435.49868	1.19e8

MW: 1435.49868
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1

43.285

211125-507005-renru1 (F3) #13052, RT=43.285 min, MS1, FTMS (-)

716.74207
[M-2H]-2
717.24353
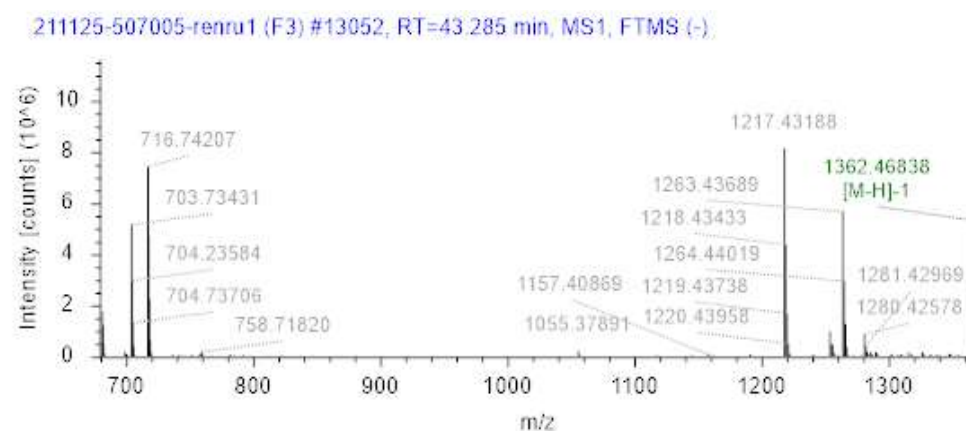717.74475
718.24609
718.74805 719.24847
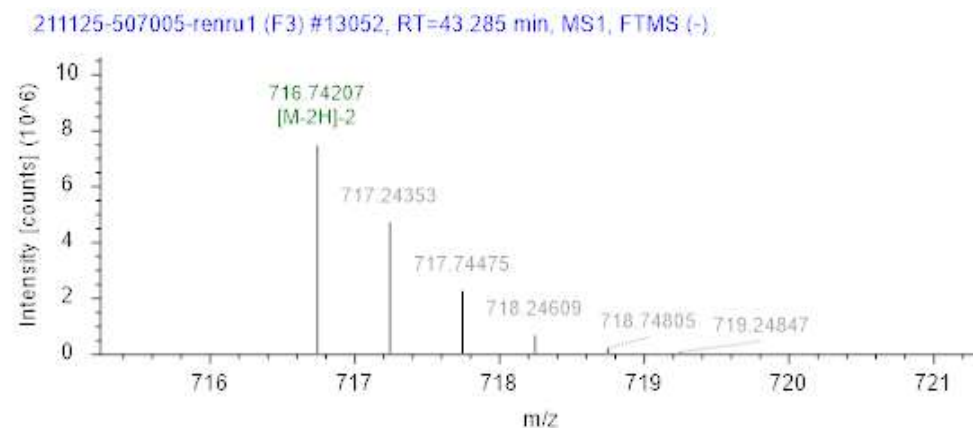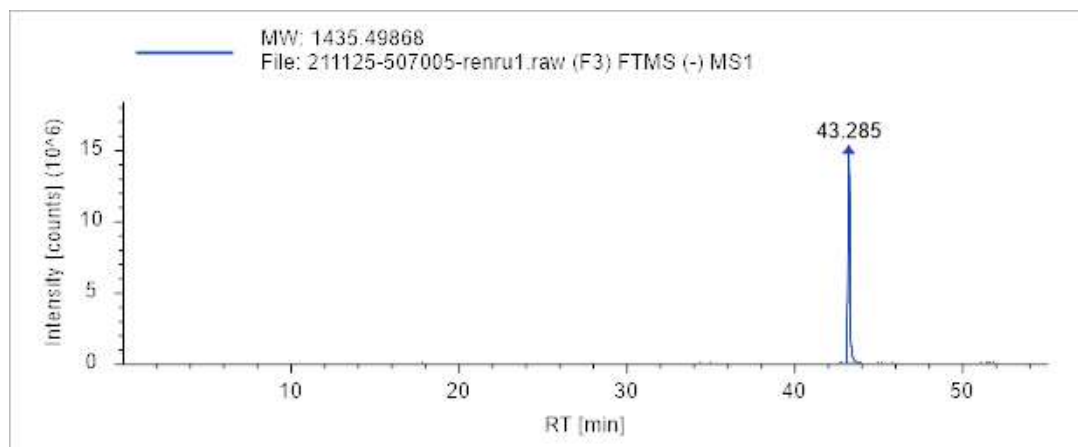
211125-507005-renru1 (F3) #13017, RT=43.201 min, MS2, FTMS (-), (HCD, DDA, 716.7418@30, -2)

113.02350
126.05502 170.04504
142.05005
290.08835
291.09164
350.10880
470.15195
493.16803
583.18933
562.68616
639.22699 836.28845
717.24323
835.28436
1023.35150
1144.40332
1143.39294

Compounds
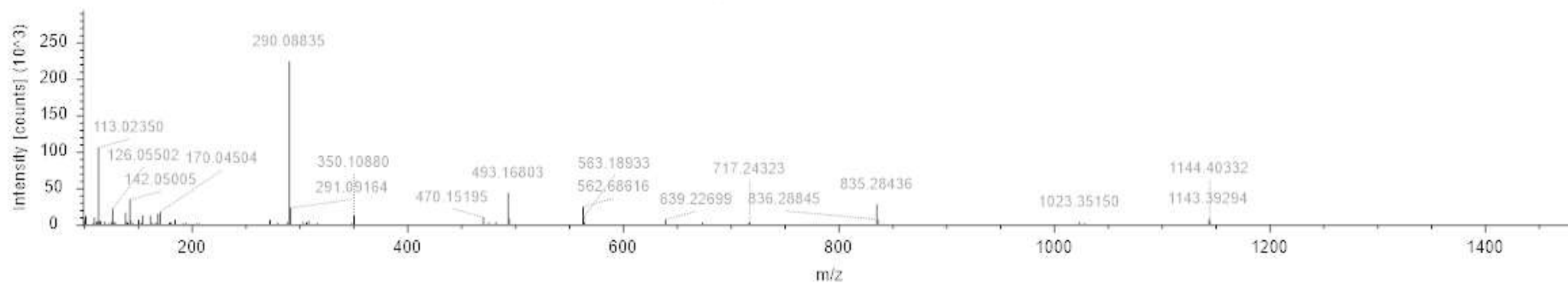
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		44.08	n/a	1509.53278	1.29e9

MW: 1509.53278
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1
MW: 1509.53278
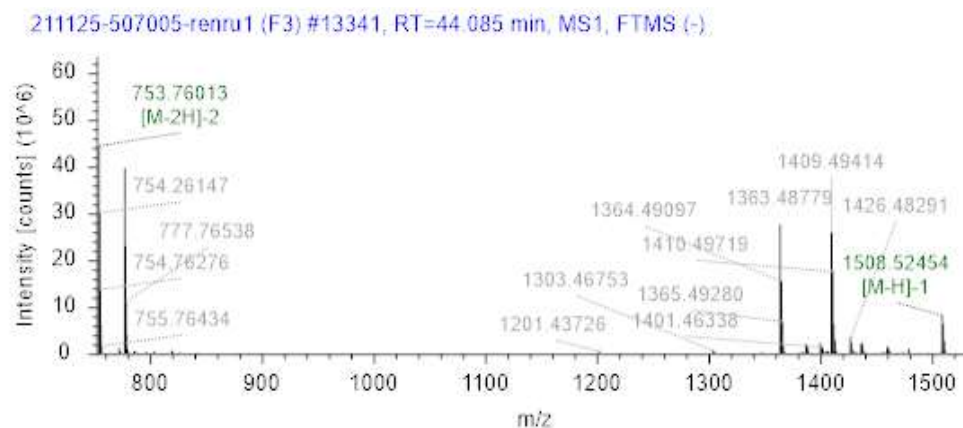File: 211125-507005-renru1.raw (F3) FTMS (+) MS1

211125-507005-renru1 (F3) #13341, RT=44.085 min, MS1, FTMS (-)

753.76013 [M-2H]-2
754.26147
777.76538
754.76276
755.76434
1201.43726
1303.46753
1364.49097
1365.49280
1401.46338
1409.49414
1410.49719
1363.48779
1426.48291
1508.52454 [M-H]-1
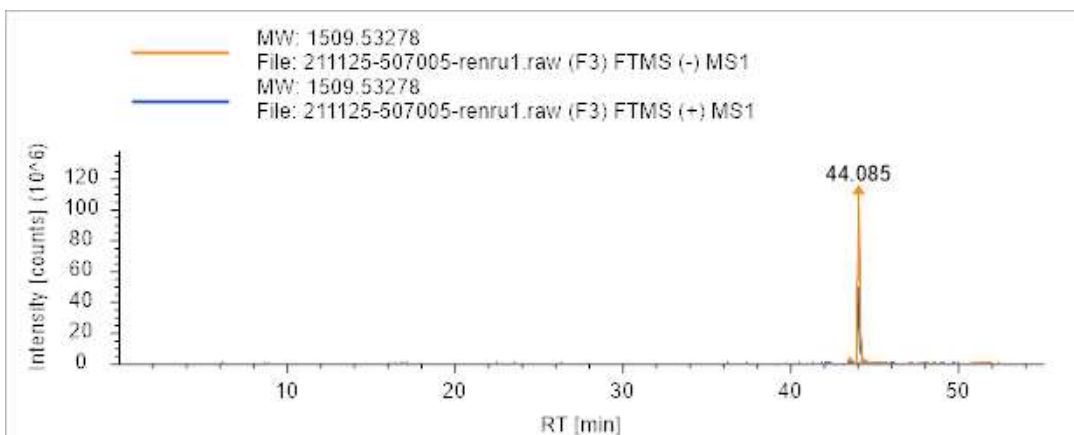
211125-507005-renru1 (F3) #13327, RT=44.049 min, MS2, FTMS (+), (HCD, DDA, 1510.5369@30, +1)

144.06572
204.08690
186.07631
274.09222
292.10287
366.13971
367.14325
454.27460
512.19812

Compounds
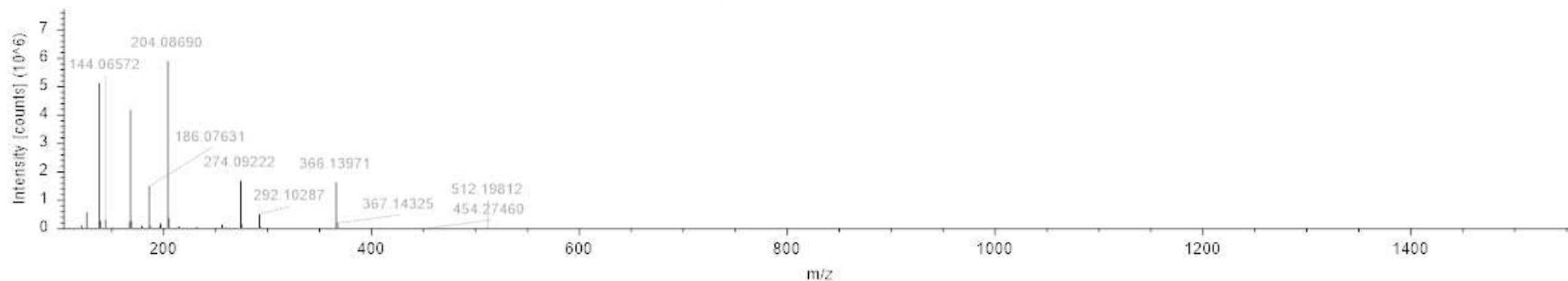
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		43.57	n/a	1509.53482	3.54e7

MW: 1509.53482
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1

44.085

211125-507005-renru1 (F3) #13159, RT=43.577 min, MS1, FTMS (-)

753.76086
[M-2H]-2

754.26282
754.76367
752.74554
753.28821
755.26532
755.76245
756.25891

211125-507005-renru1 (F3) #13197, RT=43.672 min, MS2, FTMS (-), (HCD, DDA, 753.7609@30, -2)

290.08826
179.05542
161.04483
184.06079
291.09143
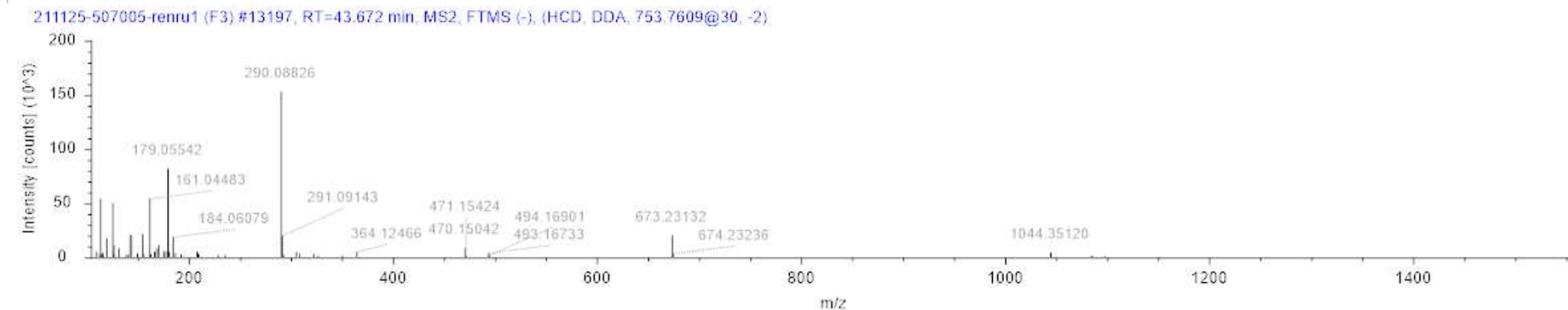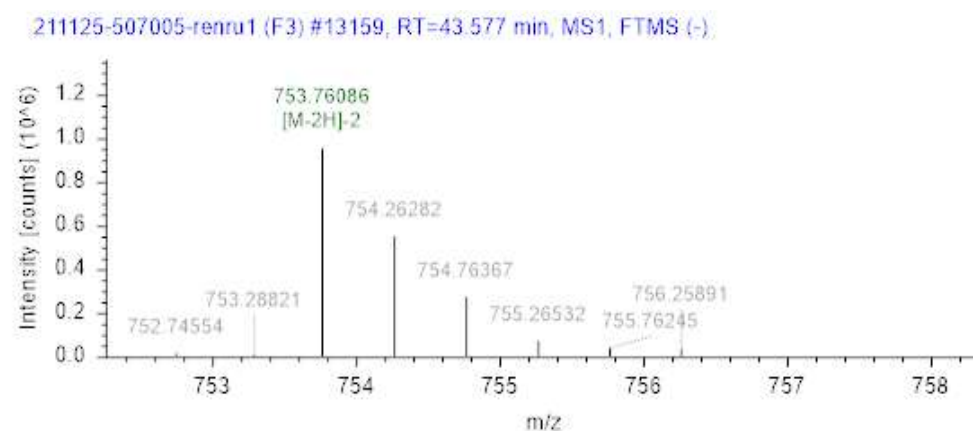364.12466
470.15042
471.15424
493.16733
494.16901
673.23132
674.23236
1044.35120

Compounds

Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		44.35	n/a	1654.57206	1.42e8

MW: 1654.57206
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1
MW: 1654.57206
File: 211125-507005-renru1.raw (F3) FTMS (+) MS1

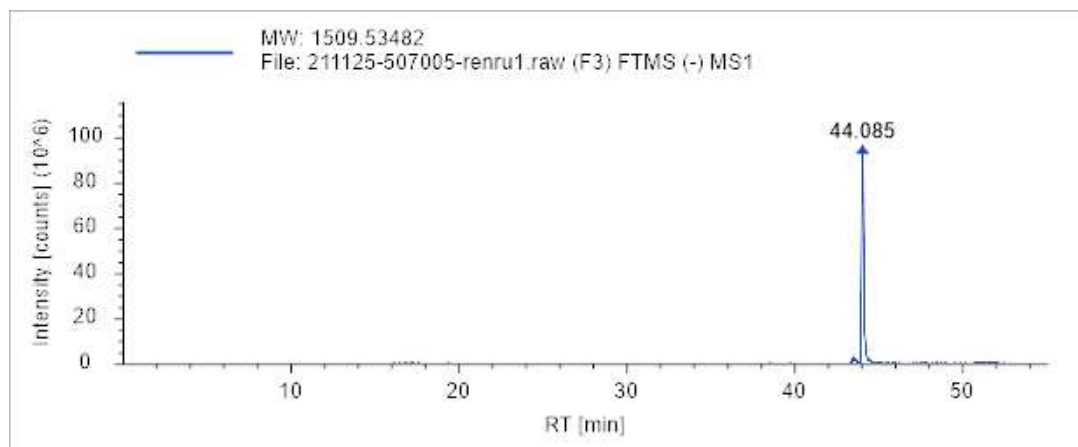211125-507005-renru1 (F3) #13449, RT=44.346 min, MS1, FTMS (-)
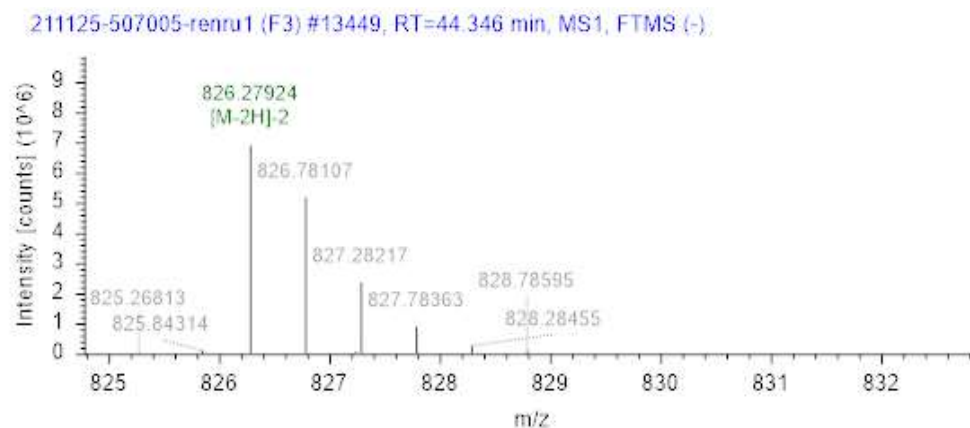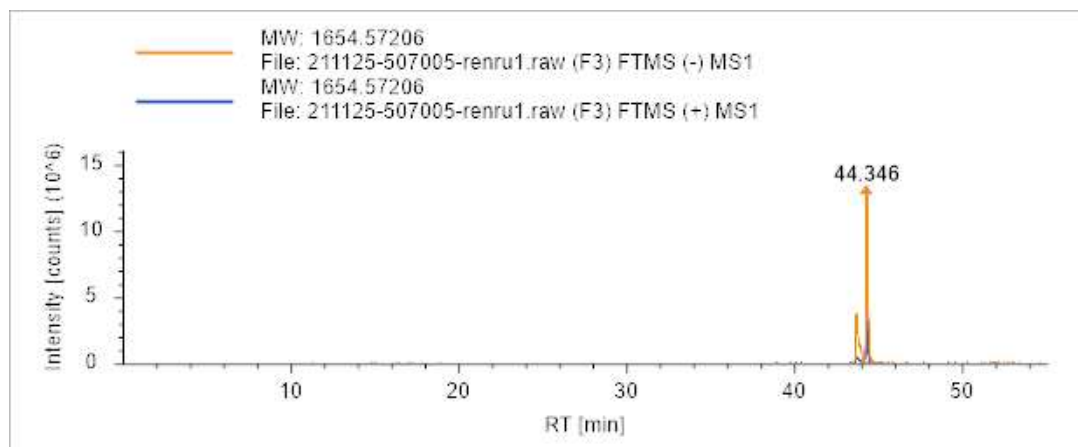
826.27924
[M-2H]-2

211125-507005-renru1 (F3) #13486, RT=44.439 min, MS2, FTMS (-), (HCD, DDA, 826.2795@30, -2)

Compounds
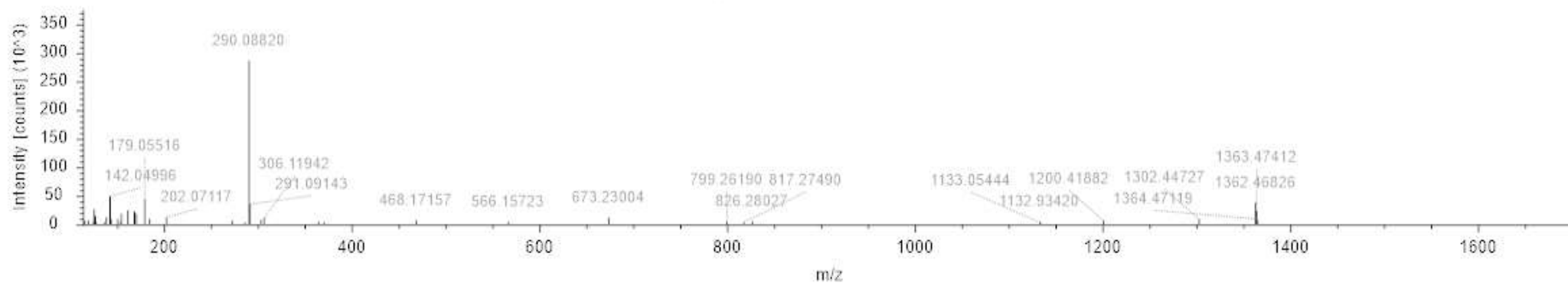
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		43.75	n/a	1654.57302	3.34e7

MW: 1654.57302
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1

211125-507005-renru1 (F3) #13218, RT=43.740 min, MS1, FTMS (-)

826.28027 [M-2H]-2
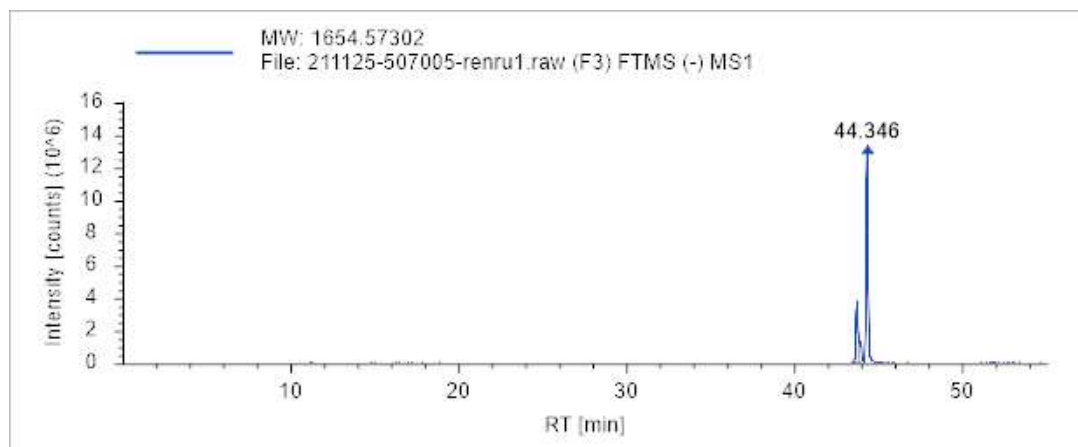
211125-507005-renru1 (F3) #13247, RT=43.838 min, MS2, FTMS (-), (HCD, DDA, 826.2805@30, -2)

Compounds
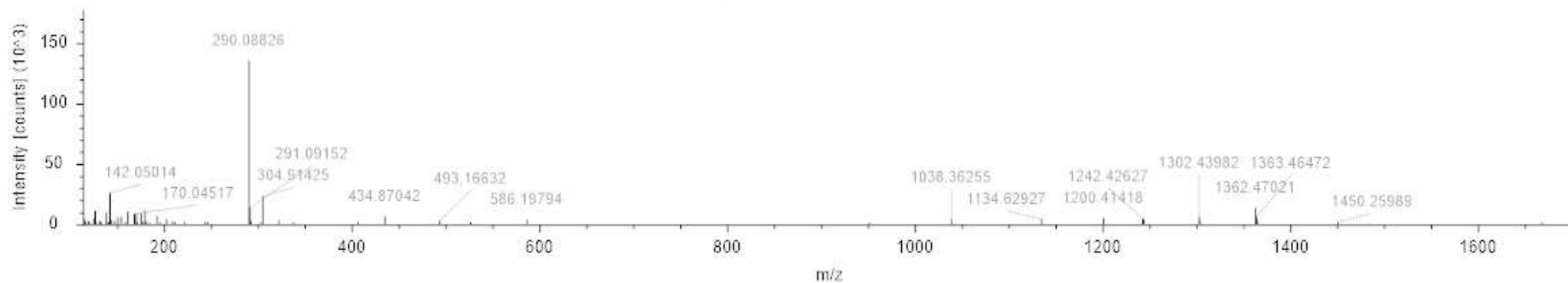
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		44.58	n/a	1728.61050	1.64e7

MW: 1728.61050
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1

44.586

211125-507005-renru1 (F3) #13542, RT=44.586 min, MS1, FTMS (-)

863.29797
[M-2H]-2
863.80011
862.23248
864.30115
864.80237
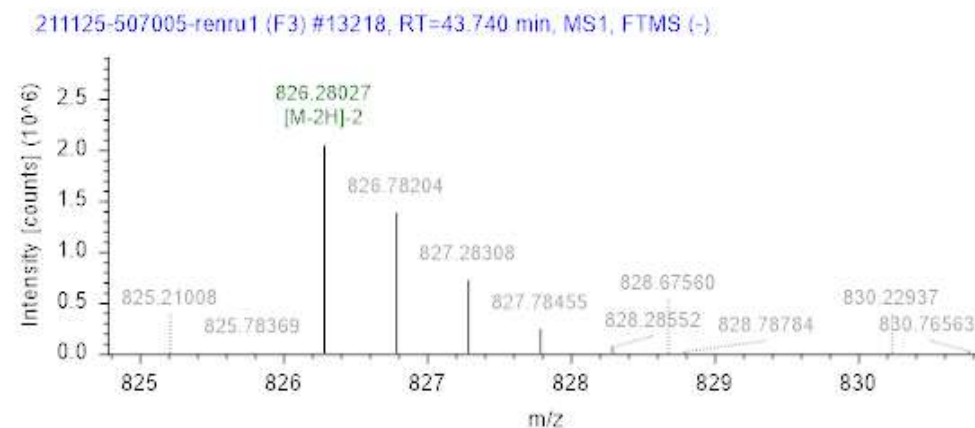865.80554
865.30438
866.76306
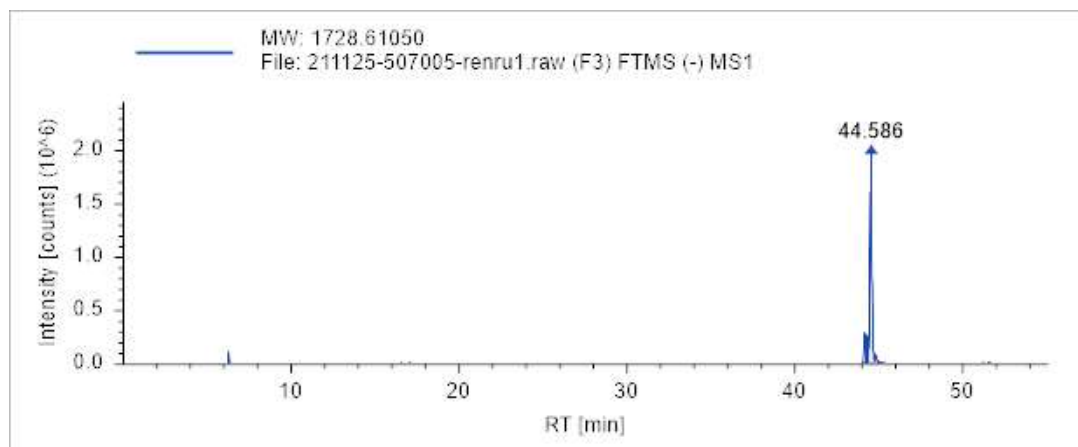
211125-507005-renru1 (F3) #13512, RT=44.503 min, MS2, FTMS (-), (HCD, DDA, 863.2968@30, -2)

161.04468
179.05530
290.08786
207.91638
304.91364
364.12622
572.18152
673.23077
785.13257
1141.20605
1141.05151
1200.41089
1238.41565
1385.45435
1404.50098
1403.48376
1565.54395

Compounds
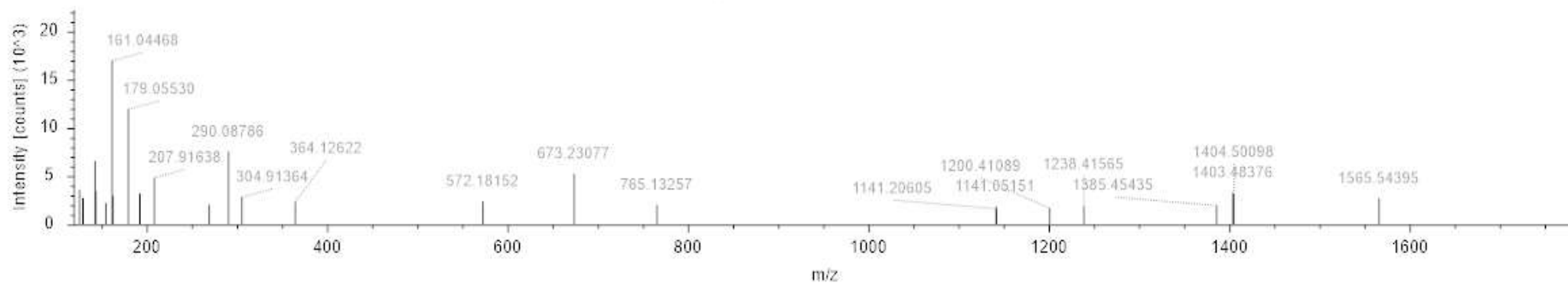
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		45.27	n/a	1874.66881	6.77e7

MW: 1874.66881
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1
MW: 1874.66881
File: 211125-507005-renru1.raw (F3) FTMS (+) MS1

45.266

211125-507005-renru1 (F3) #13777, RT=45.266 min, MS1, FTMS (-)

936.32794
[M-2H]-2

935.26135
936.86853
936.82922
937.33020
937.83209
938.83527
938.33374
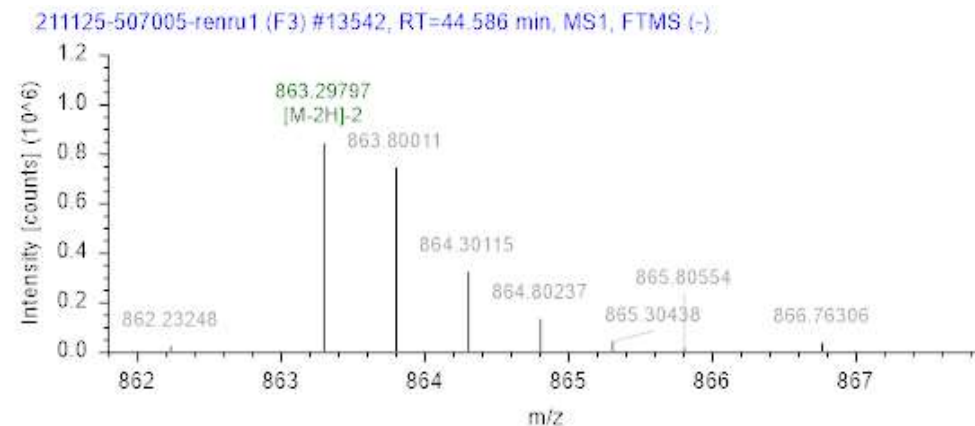939.77777
939.28503
942.27313
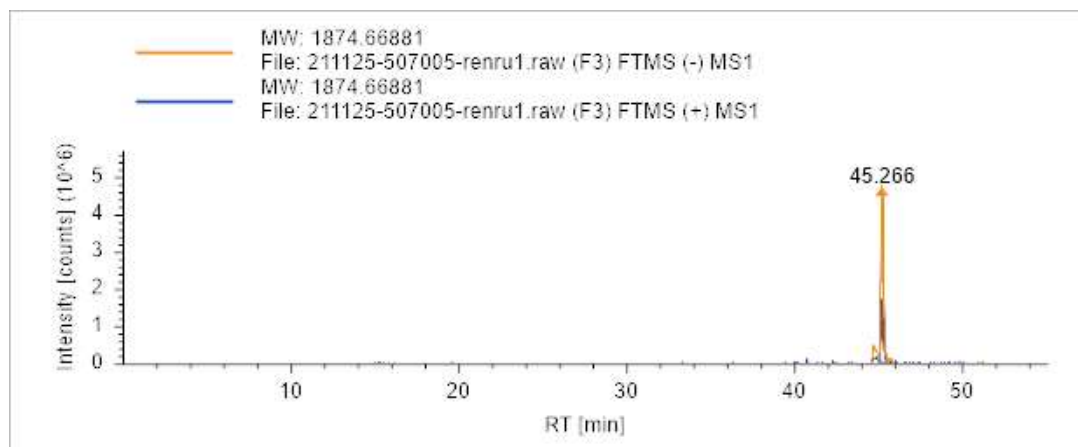
211125-507005-renru1 (F3) #13804, RT=45.334 min, MS2, FTMS (-), (HCD, DDA, 936.3269@30, -2)

179.05542
161.04482
154.05013
162.04831
290.08832
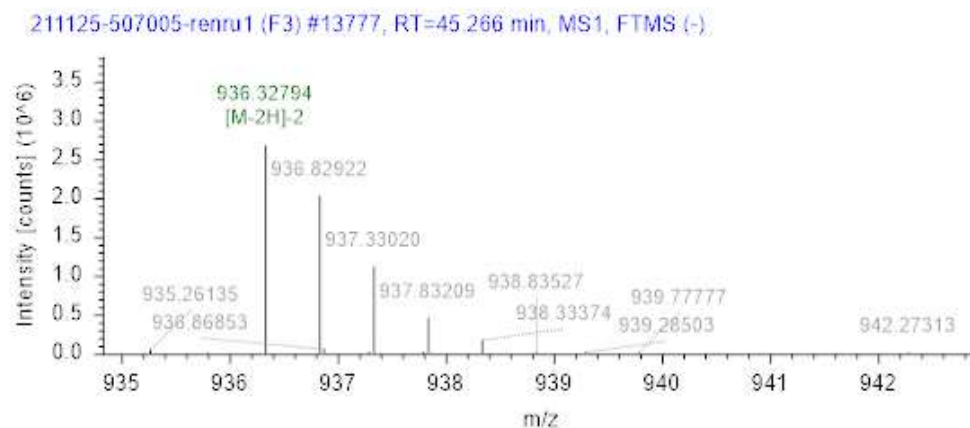263.07794
364.12500
470.15124
573.18286
572.18256
673.23230
674.23358
817.27179
835.28217
799.26105
957.99567
1020.35266
1129.22046
1310.45398
1329.45862
1328.46155
1550.54919
1549.55212
1531.54370
1712.60803
1711.61206
1714.61536
1713.59937

Compounds
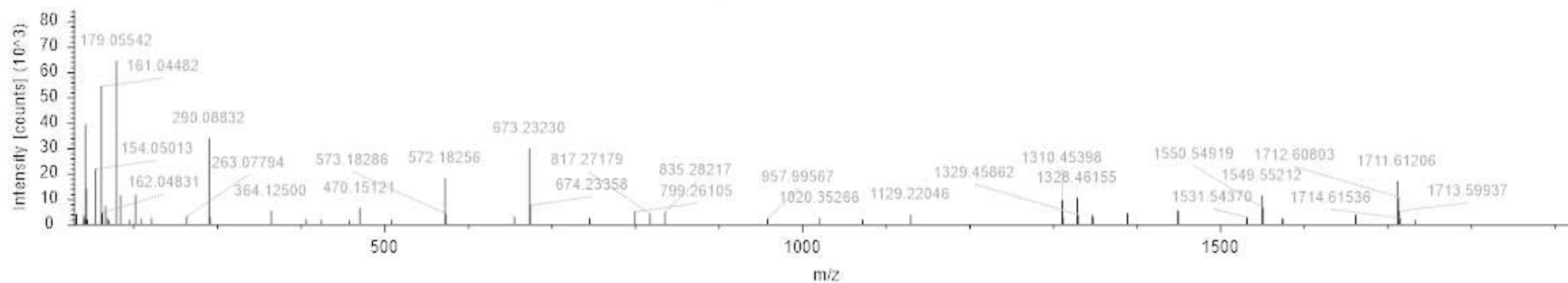
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		44.91	n/a	2019.70694	9.09e6

MW: 2019.70694
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1

44.922

211125-507005-renru1 (F3) #13669, RT=44.922 min, MS1, FTMS (-)

1008.84619 [M-2H]-2
1009.34729
1009.84882
1008.27997
1007.77643
1010.34943
1010.75201
1010.84875

211125-507005-renru1 (F3) #13682, RT=44.956 min, MS2, FTMS (-), (HCD, DDA, 1008.8462@30, -2)

290.08835
142.05016
179.05531
291.09183
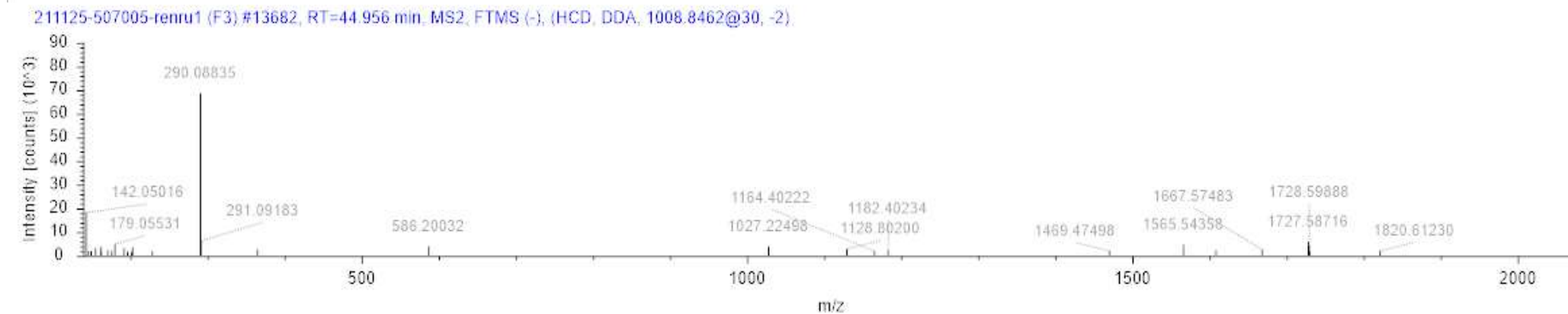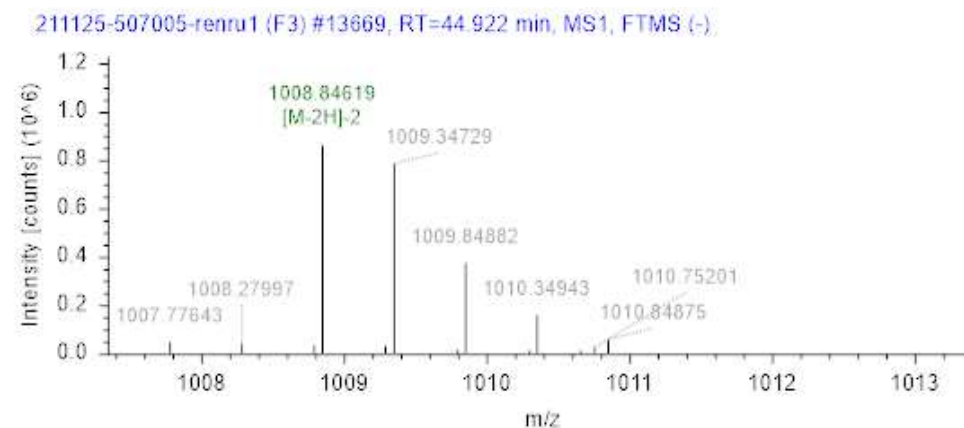586.20032
1027.22498
1164.40222
1128.80200
1182.40234
1469.47498
1565.54358
1667.57483
1727.58716
1728.59888
1820.61230

Compounds

Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		46.10	n/a	2020.72648	4.06e7

MW: 2020.72648
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1
MW: 2020.72648
File: 211125-507005-renru1.raw (F3) FTMS (+) MS1

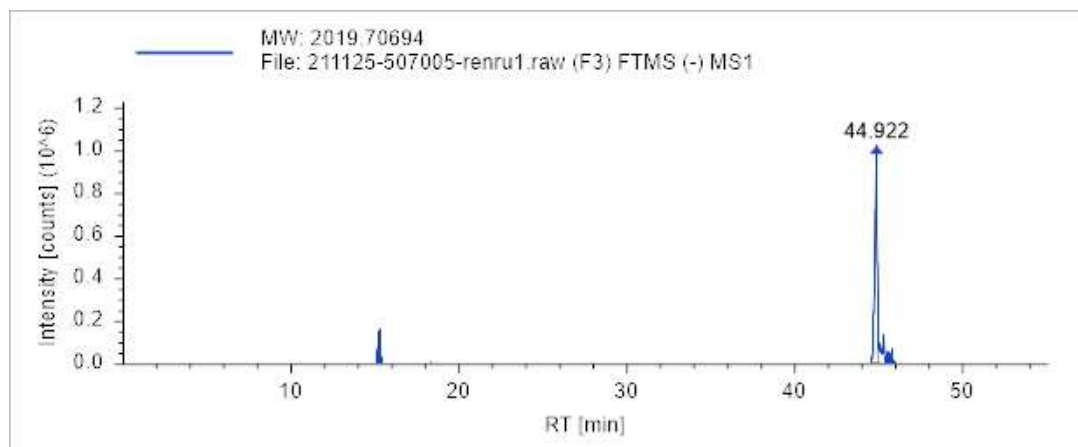211125-507005-renru1 (F3) #14071, RT=46.090 min, MS1, FTMS (-)
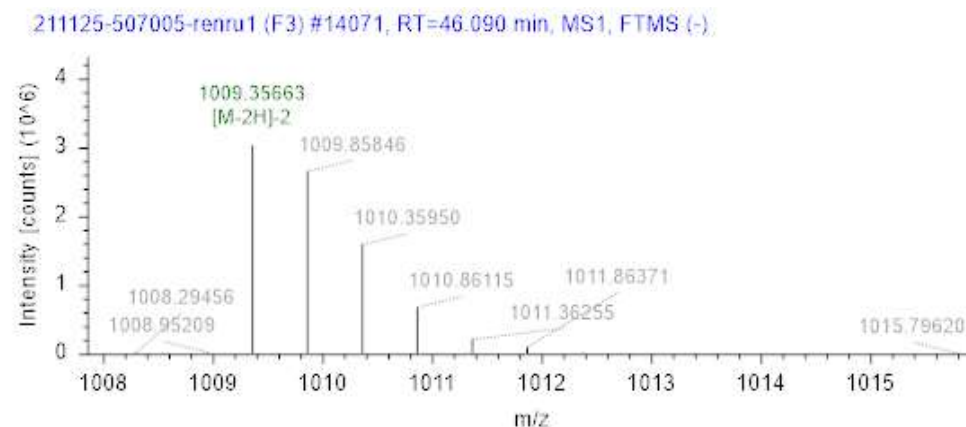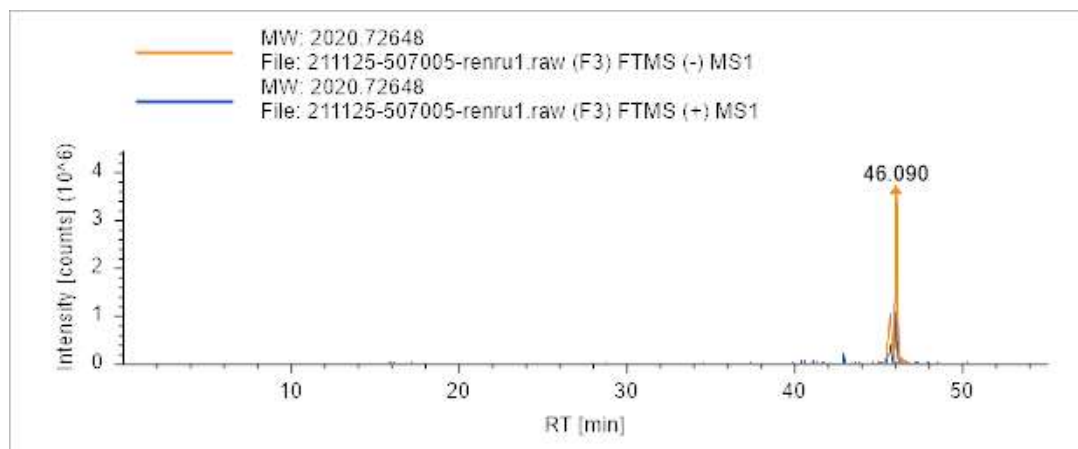
211125-507005-renru1 (F3) #14097, RT=46.162 min, MS2, FTMS (-), (HCD, DDA, 1009.3569@30, -2)

Compounds
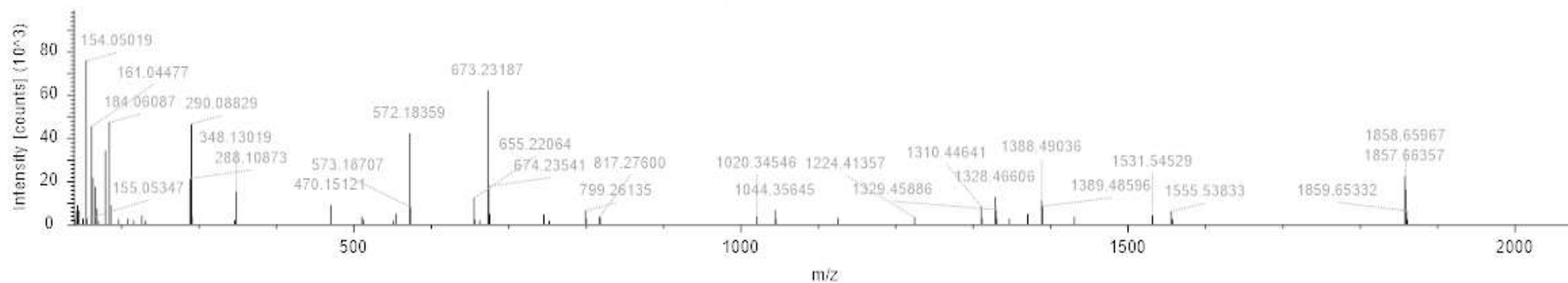
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		45.65	n/a	2093.74112	1.98e7

MW: 2093.74112
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1
MW: 2093.74112
File: 211125-507005-renru1.raw (F3) FTMS (+) MS1

211125-507005-renru1 (F3) #13919, RT=45.639 min, MS1, FTMS (-)

1045.86475 [M-2H]-2

211125-507005-renru1 (F3) #13888, RT=45.552 min, MS2, FTMS (-), (HCD, DDA, 1045.8647@30, -2)

Compounds

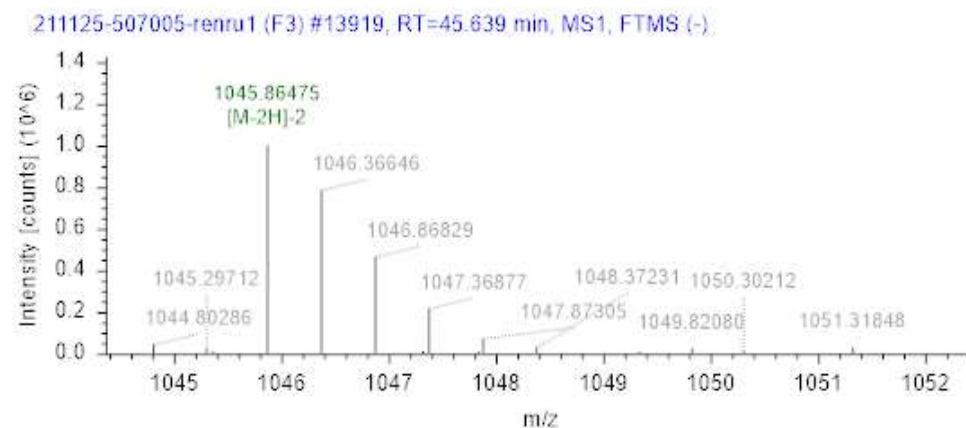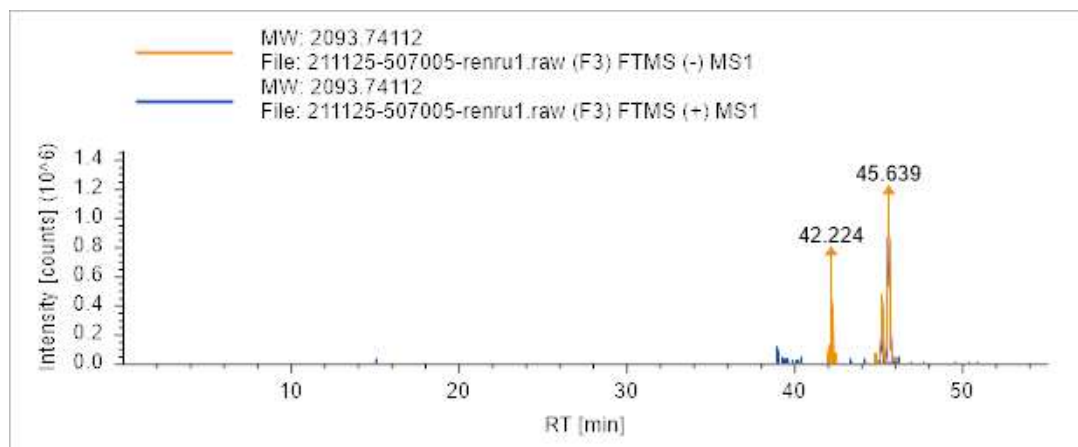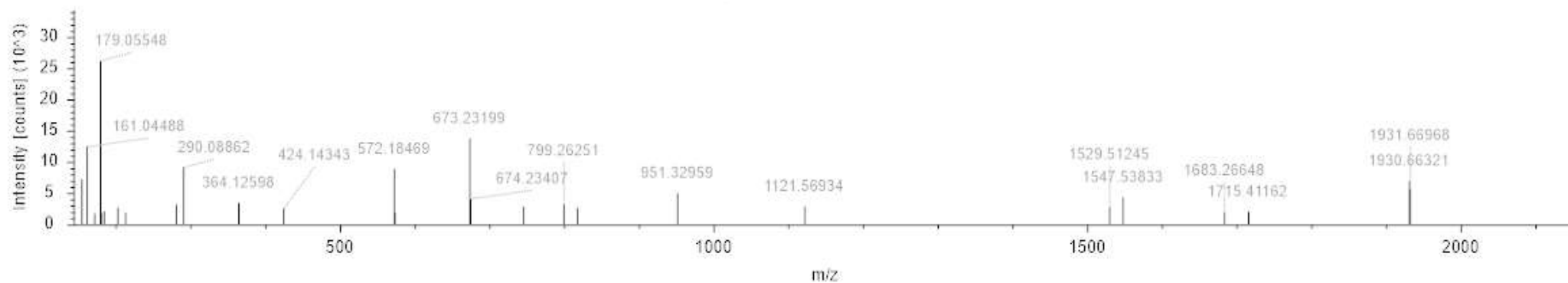| Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		45.34	n/a	2165.76309	4.78e7

MW: 2165.76309
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1

211125-507005-renru1 (F3) #13801, RT=45.328 min, MS1, FTMS (-)

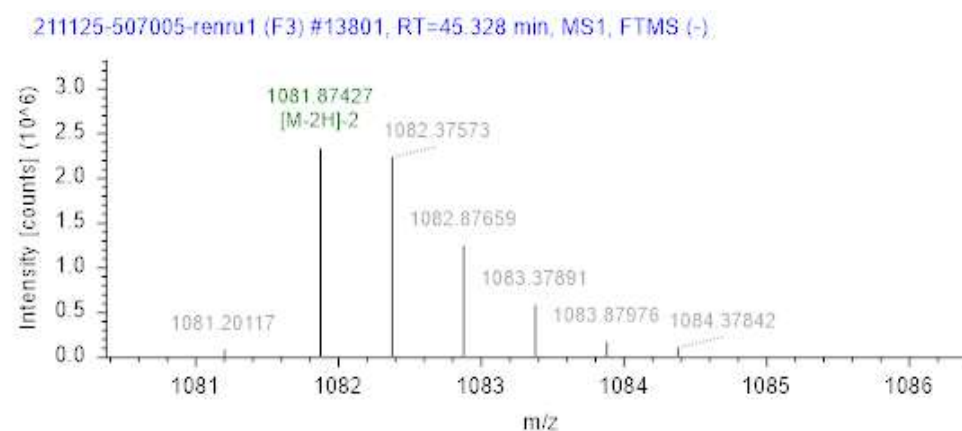1081.87427 [M-2H]-2
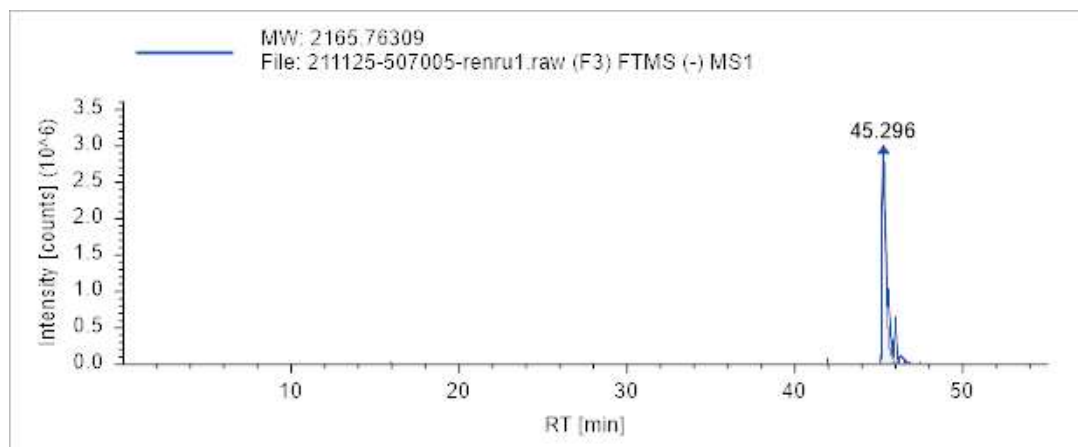
211125-507005-renru1 (F3) #13768, RT=45.241 min, MS2, FTMS (-), (HCD, DDA, 1081.8751@30, -2)

Compounds
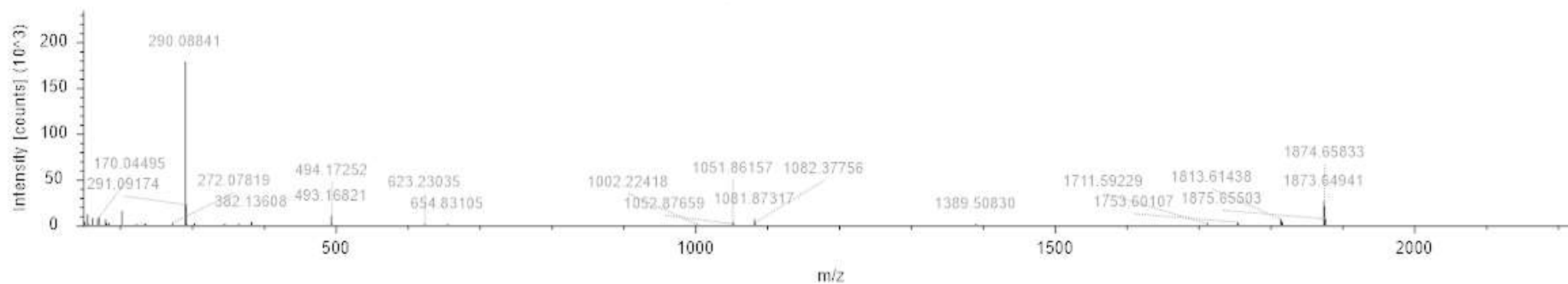
Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		46.32	n/a	2239.79769	5.06e7

MW: 2239.79769
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1
MW: 2239.79769
File: 211125-507005-renru1.raw (F3) FTMS (+) MS1

211125-507005-renru1 (F3) #14167, RT=46.354 min, MS1, FTMS (-)

1118.89331
[M-2H]-2

1119.39478

1118.84143
1118.33240
1119.89612
1120.40100
1122.84778
1124.33167
1122.31372
1123.32202

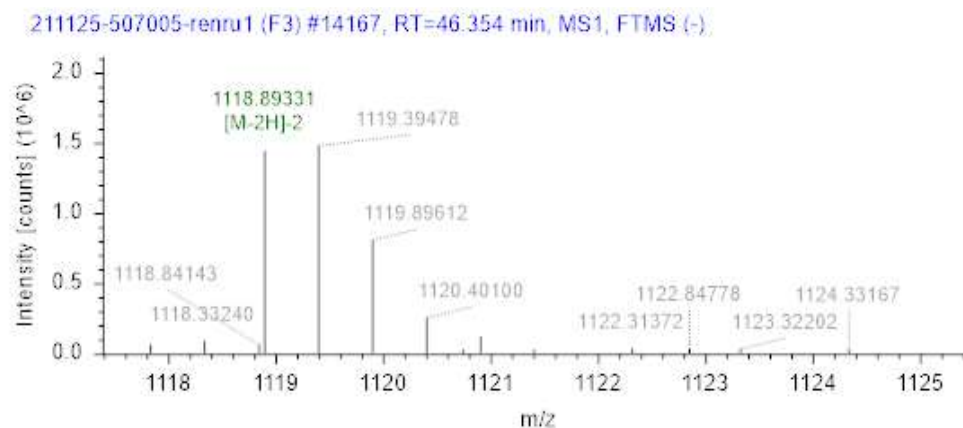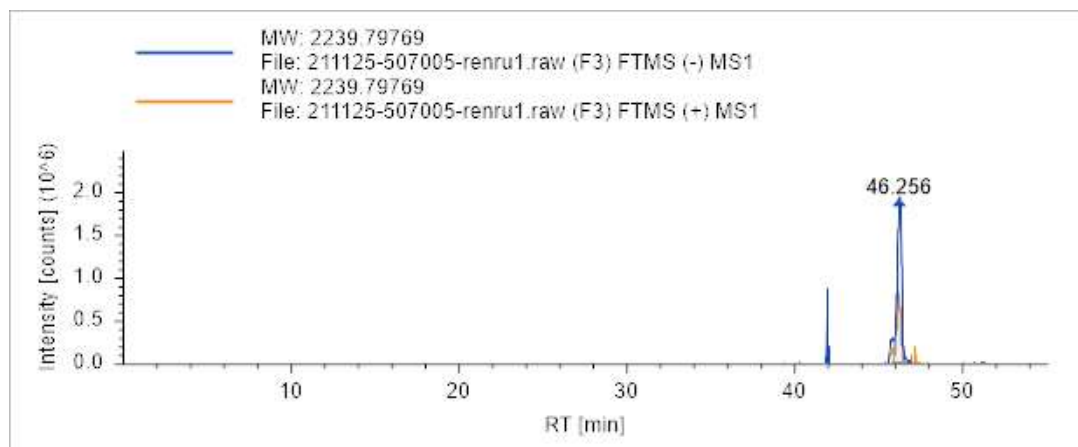211125-507005-renru1 (F3) #14181, RT=46.390 min, MS2, FTMS (-), (HCD, DDA, 1119.3948@30, -2)

179.05542
154.05016
161.04472
290.08817
572.18341
673.23218
655.21906
674.23431
799.26416
817.27472
1062.34949
1097.38562
1385.48120
1530.51929
1529.51318
1548.53955
1547.53979
1608.54956
1607.55530
2077.73535
2078.74316
2076.73340
2079.73291
263.07718
470.15167
586.19952

46.256

Compounds

Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		46.34	n/a	2240.80313	3.09e7

MW: 2240.80313
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1

46.320

211125-507005-renru1 (F3) #14167, RT=46.354 min, MS1, FTMS (-)

1119.39478
[M-2H]-2

1118.89331
1119.89612
1118.33240
1120.40100
1120.90283
1121.40295
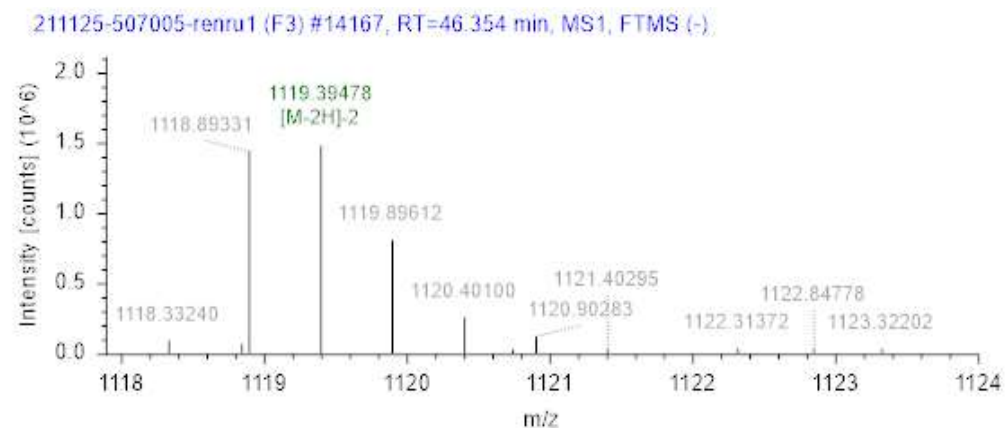1122.84778
1122.31372
1123.32202

211125-507005-renru1 (F3) #14181, RT=46.390 min, MS2, FTMS (-), (HCD, DDA, 1119.3948@30, -2)

179.05542
154.05016
161.04472
290.08817
572.18341
673.23218
655.21906
674.23431
799.26416
817.27472
1062.34949
1097.38562
586.19952
470.15167
263.07718
1385.48120
1529.51318
1530.51929
1547.53979
1548.53955
1607.55530
1608.54956
2078.74316
2076.73340
2077.73535
2079.73291

Compounds

Structure	Name	RT [min]	Formula	Calc. MW	Areas
n/a		47.18	n/a	2241.82583	4.63e7

MW: 2241.82583
File: 211125-507005-renru1.raw (F3) FTMS (-) MS1

47.194

211125-507005-renru1 (F3) #14417, RT=47.194 min, MS1, FTMS (-)

1119.40442
1119.90564 [M-2H]-2
1120.40698
1118.88696
1120.90857
1121.41003
1121.91040
1122.41162
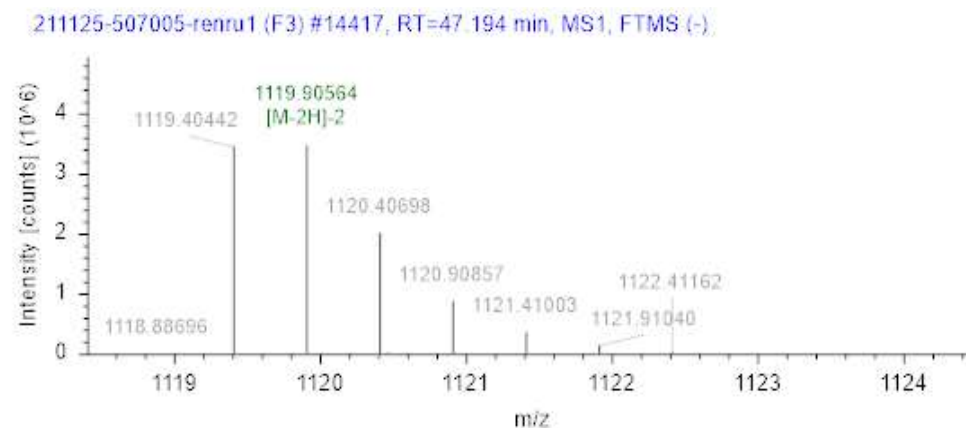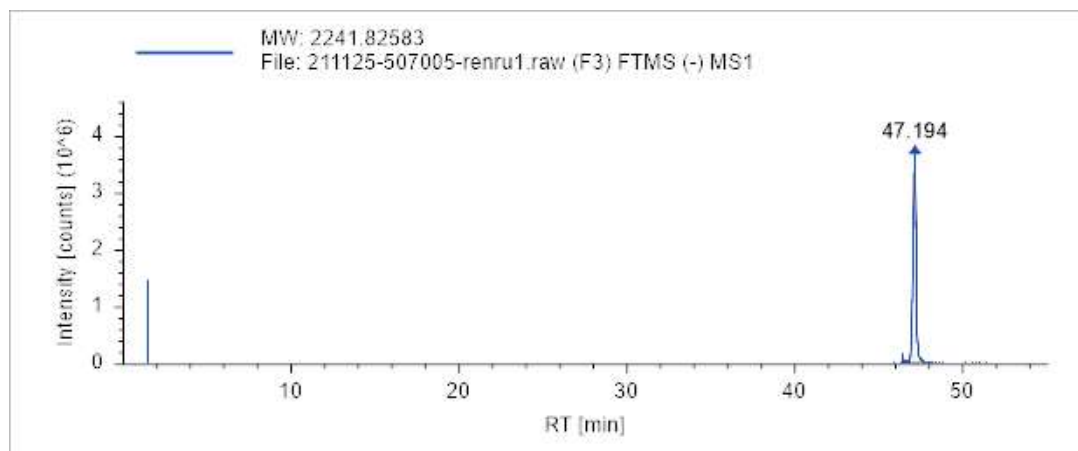
211125-507005-renru1 (F3) #14429, RT=47.231 min, MS2, FTMS (-), (HCD, DDA, 1119.9056@30, -2)

179.05544
154.05014
161.04475
348.13052
288.10904
364.12500
388.12625
510.18356
586.20081
672.23694
732.25824
870.30927
869.30579
1183.42407
1097.39026
1244.44934
1243.44482