Synthesis and discovery of asiatic acid based 1,2,3-triazoles derivatives as antitumor agents blocking NF-κB activation and cell migration

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[1] Co-first author: These authors contributed equally to this work.

Table S1. Docking scores (kcal/mol) for all studied compounds

Comd.	Total score	Crash	Polar	D_score	PMF_score	G_score	Chem score	Cscore
5a	8.29	-20.84	0.57	-179.86	-81.73	-60.20	-5.48	3
5b	8.07	-28.64	0.21	-221.16	-92.19	-418.81	-24.65	2
5c	8.94	-23.95	0.55	-243.66	-133.28	-443.34	-40.06	3
5d	7.53	-21.54	2.33	-294.90	-97.15	-528.96	-46.25	5
5e	7.00	-24.01	0.82	-272.06	-146.81	-504.74	-37.39	4
5f	8.60	-29.61	0.31	-352.11	-35.83	-546.92	-42.16	4
5g	9.02	-29.03	1.10	-267.71	-113.76	-512.64	-34.25	5
5h	8.64	-23.93	0.16	-238.09	-98.21	-440.74	-30.99	3
6a	8.16	-17.65	2.45	-227.82	-58.56	-362.49	-41.78	2
6b	9.67	-38.19	1.29	-282.66	-62.68	-516.16	-40.42	4
6c	5.11	-15.67	2.45	-175.22	-67.91	-368.97	-30.06	2
6d	7.92	-23.05	1.20	-244.23	-138.36	-498.41	-37.53	3
6e	7.13	-21.13	0.15	-179.91	-30.43	-336.73	-25.32	4
6f	9.25	-15.52	3.22	-180.76	-68.64	-386.59	-35.75	3
6g	6.56	-30.26	1.07	-185.38	-22.30	-318.31	-30.93	2
6h	9.43	-37.56	1.45	-181.09	-48.65	-287.17	-26.19	4
6i	9.38	-14.94	2.02	-197.39	-38.91	-397.39	32.94	2
6j	10.75	-12.44	2.23	-216.12	-29.10	-374.00	-31.94	2
6k	10.08	-25.76	1.07	-266.97	-88.19	-508.92	-47.95	4
6l	8.21	-19.08	-0.69	-273.98	-113.34	-535.35	-40.53	3

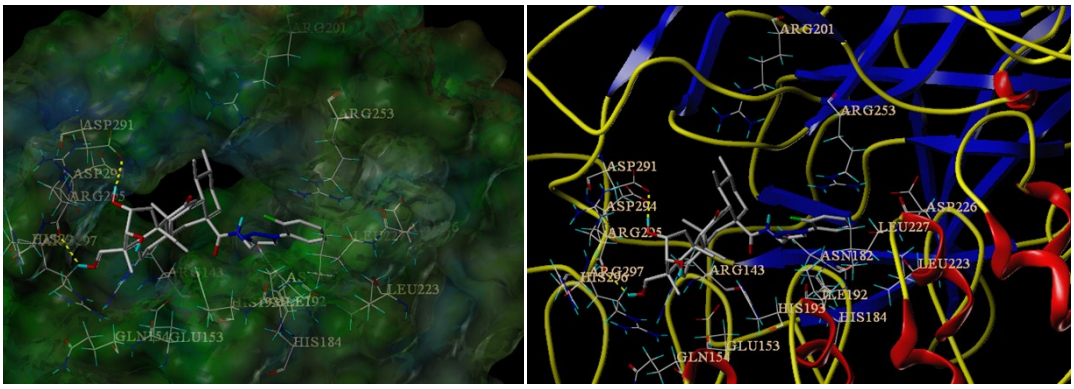
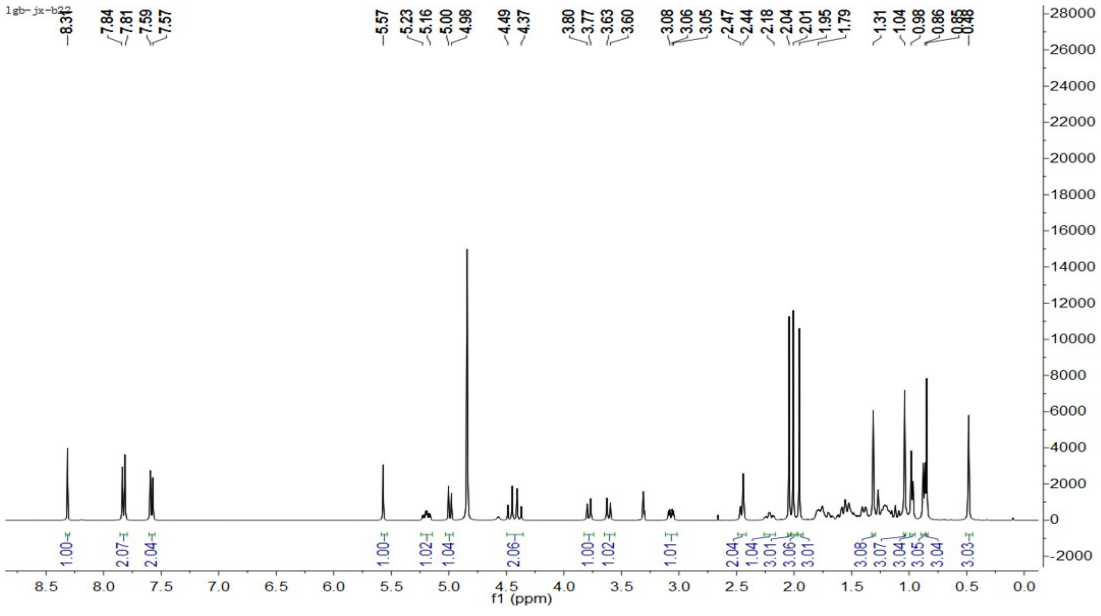
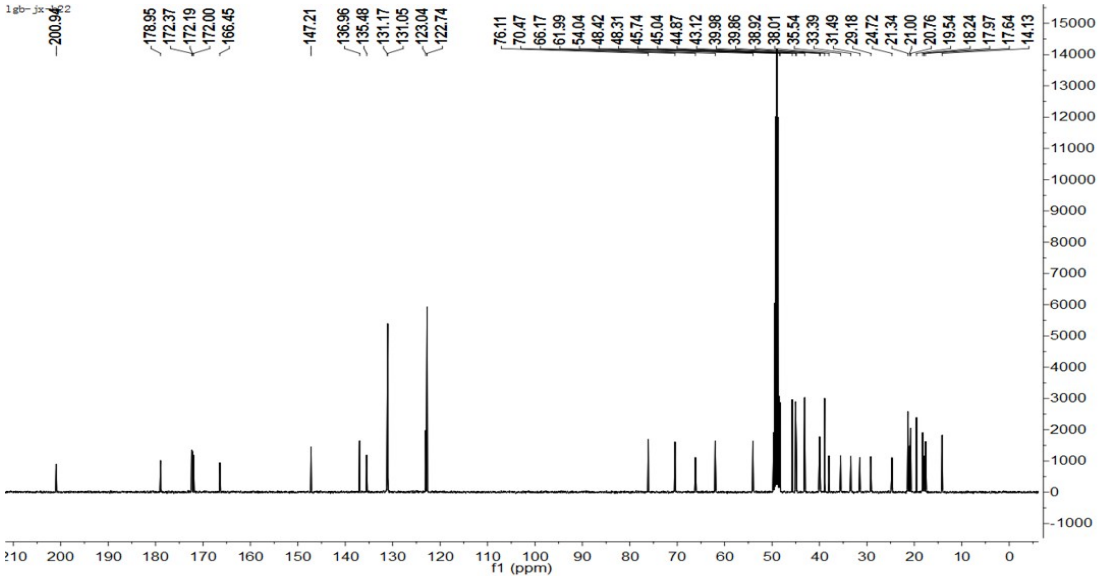


Fig. S1 Binding modes of compound **6k** in the active site of NF-κB (PDB: 1IKN). Ligands and the important residues for binding interactions are represented by stick and line models. The hydrogen bonds are shown as yellow dotted lines (color figure online).

^{1}H NMR, ^{13}C NMR and HR-MS of compounds **5a−5h** and **6a-6l**:

5a

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178.95
172.37
172.19
172.00
166.45
147.21
136.96
135.48
131.17
131.05
123.04
122.74
76.11
70.47
66.17
61.99
54.04
48.42
48.31
45.74
45.04
44.87
43.12
39.98
39.86
38.92
38.01
35.54
33.39
31.49
29.18
24.72
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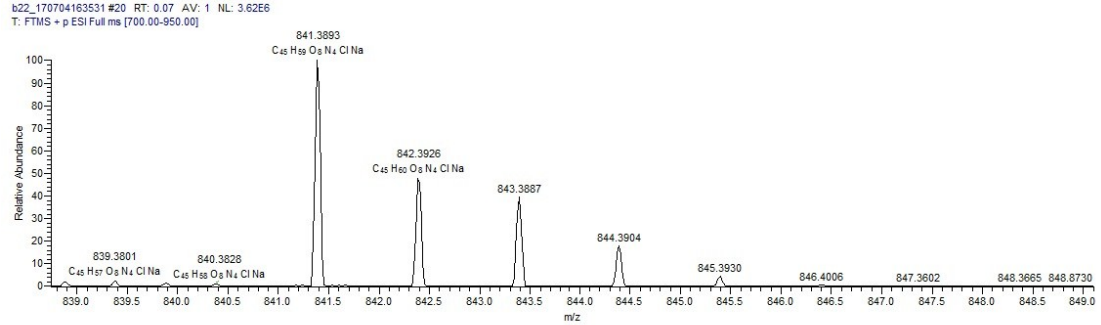
18.24
17.97
17.64
14.13
f1 (ppm)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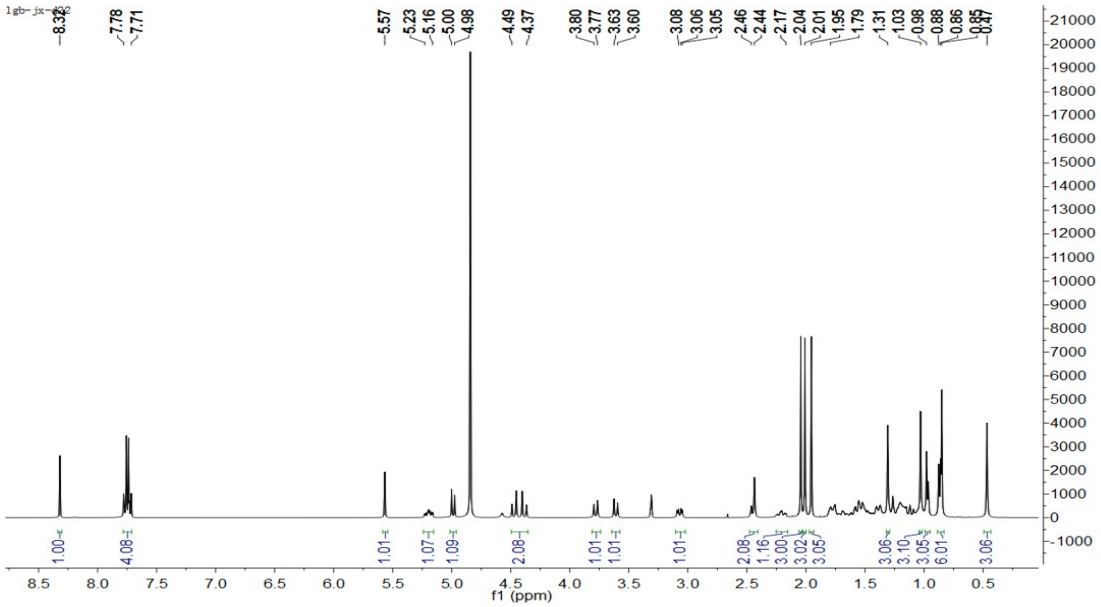
T: FTMS + p ESI Full ms [700.00-950.00]
841.3893
C45 H59 O8 N4 Cl Na
842.3926
C45 H60 O8 N4 Cl Na
843.3887
844.3904
845.3930
846.4006
847.3602
848.3665
848.8730
839.3801
C45 H57 O8 N4 Cl Na
840.3828
C45 H58 O8 N4 Cl Na
Relative Abundance
m/z

5b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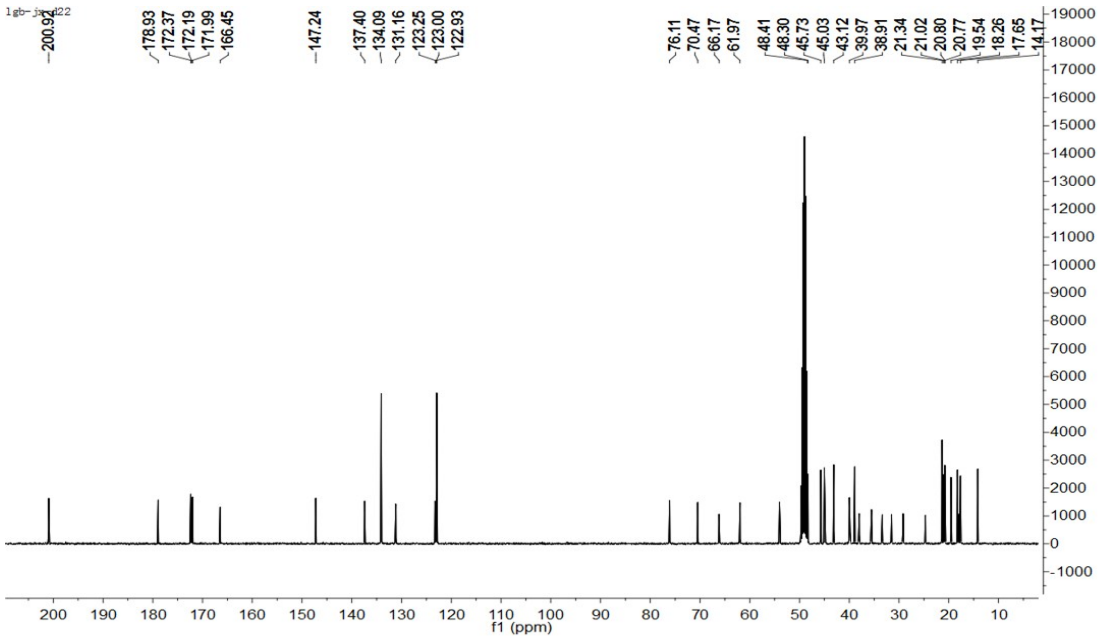
7.78
7.71
5.57
5.23
5.16
5.00
4.98
4.49
4.37
3.80
3.77
3.63
3.60
3.08
3.06
3.05
2.46
2.44
2.17
2.04
2.01
1.95
1.79
1.31
1.03
0.98
0.88
0.86
0.85
0.47
1.00
4.08
1.01
1.07
1.09
2.08
1.01
1.01
1.01
2.08
1.16
3.00
3.02
3.05
3.06
3.10
3.05
6.01
3.06
f1 (ppm)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178.93
172.37
172.19
171.99
166.45
147.24
137.40
134.09
131.16
123.25
123.00
122.93
76.11
70.47
66.17
61.97
48.41
48.30
45.73
45.03
43.12
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21.34
21.02
20.80
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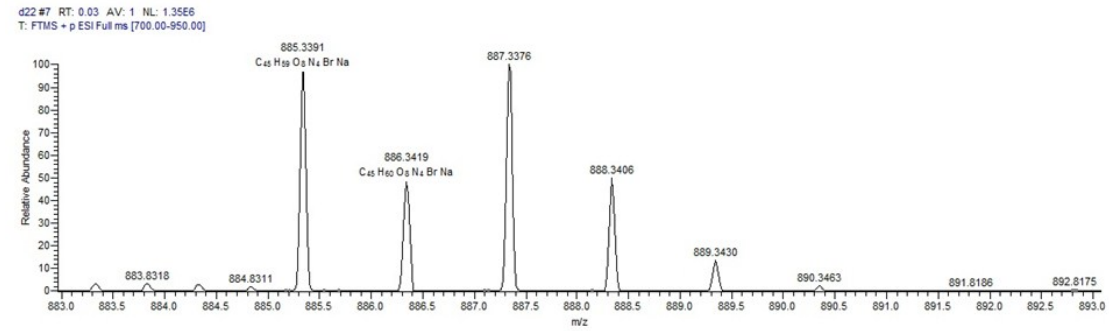
19.54
18.26
17.65
14.17
f1 (ppm)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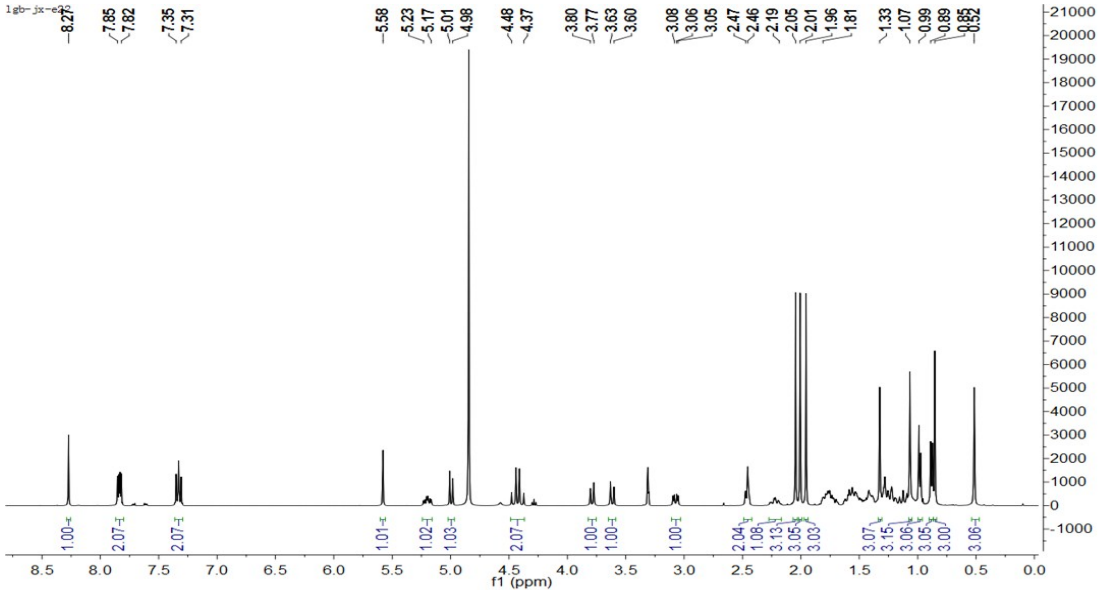
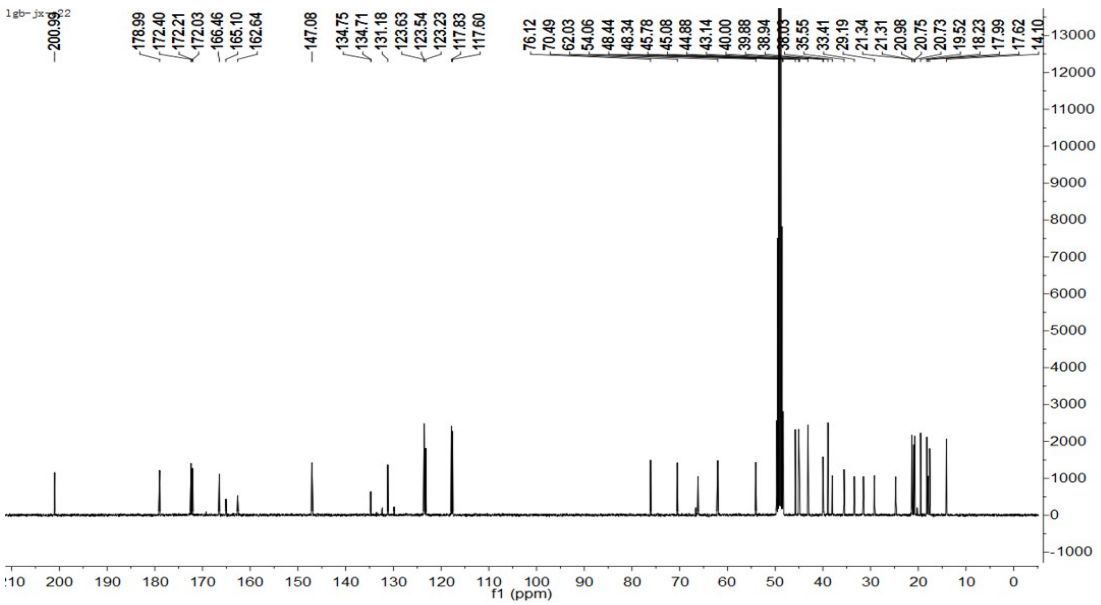
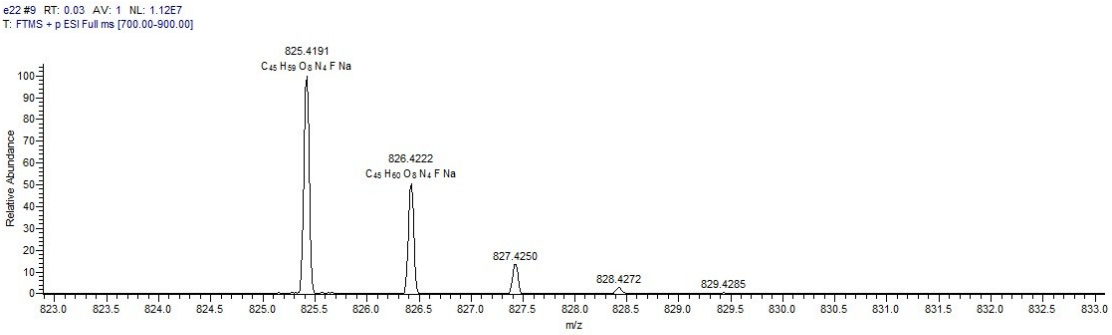
T: FTMS + p ESI Full ms [700.00-950.00]
885.3391
C45 H59 O8 N4 Br Na
887.3376
886.3419
C45 H60 O8 N4 Br Na
888.3406
889.3430
883.8318
884.8311
890.3463
891.8186
892.8175
Relative Abundance
m/z

5c


8.27
7.85
7.82
7.35
7.31
5.58
5.23
5.17
5.01
4.98
4.48
4.37
3.80
3.77
3.63
3.60
3.08
3.06
3.05
2.47
2.46
2.19
2.05
2.01
1.96
1.81
1.33
1.07
0.99
0.89
0.85
0.82
f1 (ppm)


200.99
178.99
172.40
172.21
172.03
166.46
165.10
162.64
147.08
134.75
134.71
131.18
123.63
123.54
123.23
117.83
117.60
76.12
70.49
62.03
54.06
48.44
48.34
45.78
45.08
44.88
43.14
40.00
39.88
38.94
38.03
35.55
33.41
29.19
21.34
21.31
20.98
20.75
20.73
19.52
18.23
17.99
17.62
14.10
f1 (ppm)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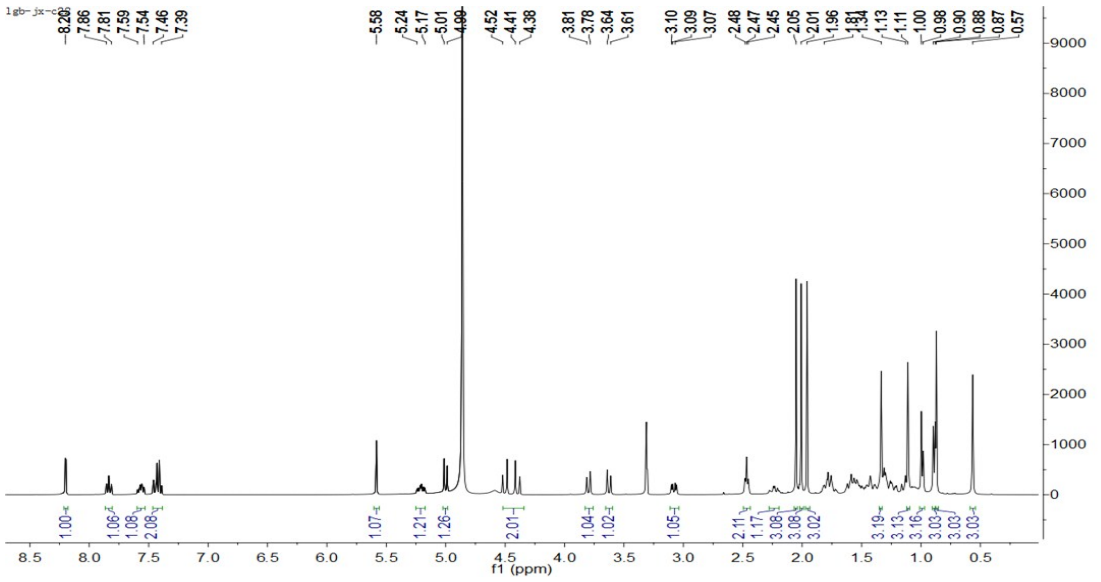
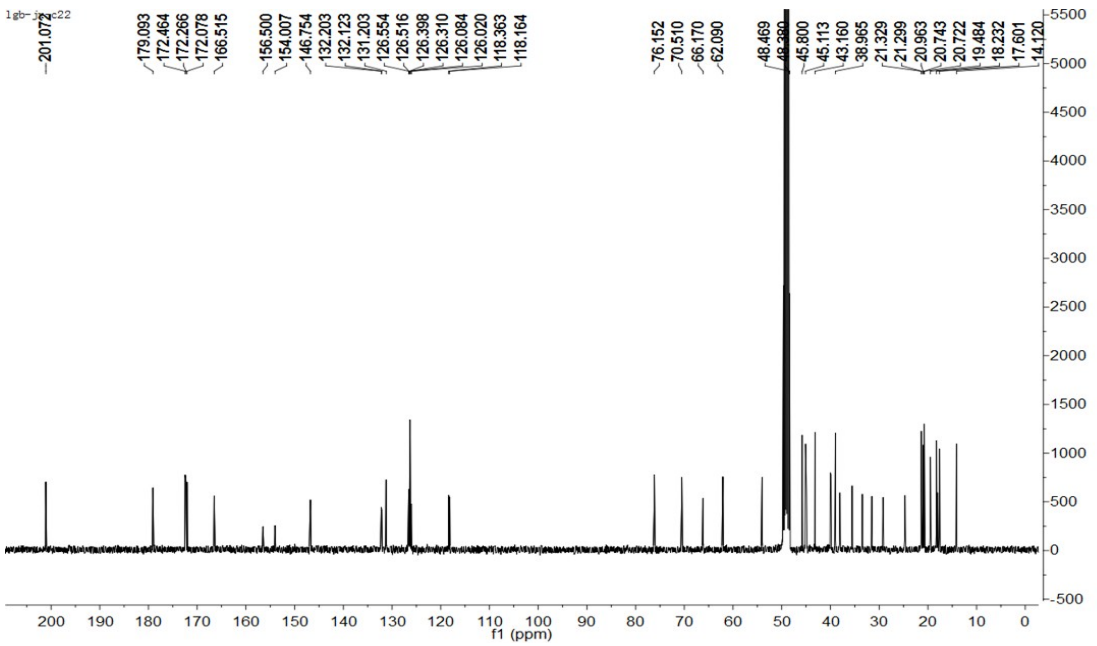
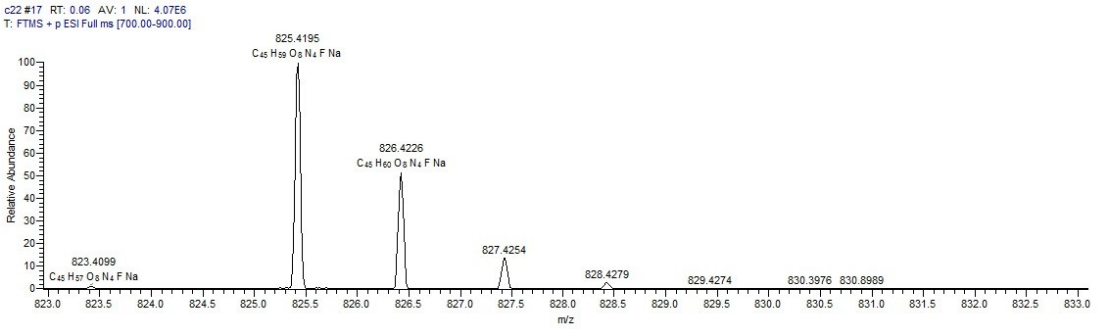
T: FTMS + p ESI Full ms [700.00-900.00]
825.4191
C45 H59 O8 N4 F Na
826.4222
C45 H60 O8 N4 F Na
827.4250
828.4272
829.4285
Relative Abundance
m/z

5d


8.20
7.86
7.81
7.59
7.54
7.46
7.39
5.58
5.24
5.17
5.01
4.99
4.52
4.41
4.38
3.81
3.78
3.64
3.61
3.10
3.09
3.07
2.48
2.47
2.45
2.05
2.01
1.96
1.81
1.34
1.13
1.11
1.00
0.98
0.90
0.88
0.87
0.57
1.00
1.06
1.08
2.08
1.07
1.21
1.26
2.01
1.04
1.02
1.05
2.11
1.17
3.08
3.08
3.02
3.19
3.13
3.16
3.03
3.03
3.03
f1 (ppm)


201.072
179.093
172.464
172.266
172.078
166.515
156.500
154.007
146.754
132.203
132.123
131.203
126.554
126.516
126.398
126.310
126.084
126.020
118.363
118.164
76.152
70.510
66.170
62.090
48.469
45.800
45.113
43.160
38.965
21.329
21.299
20.963
20.743
20.722
19.484
18.232
17.601
14.120
f1 (ppm)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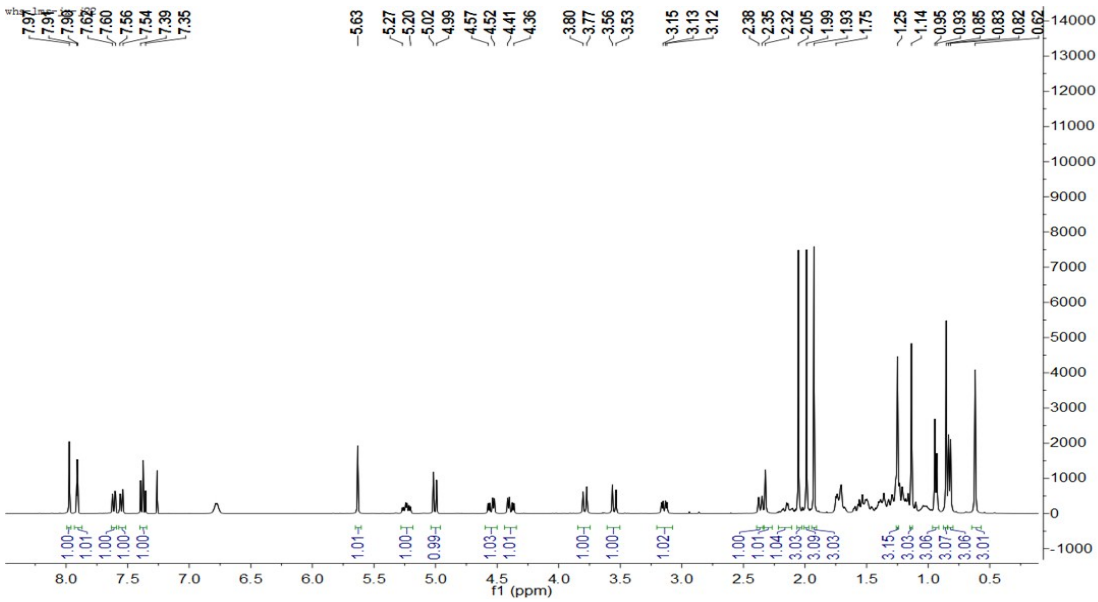
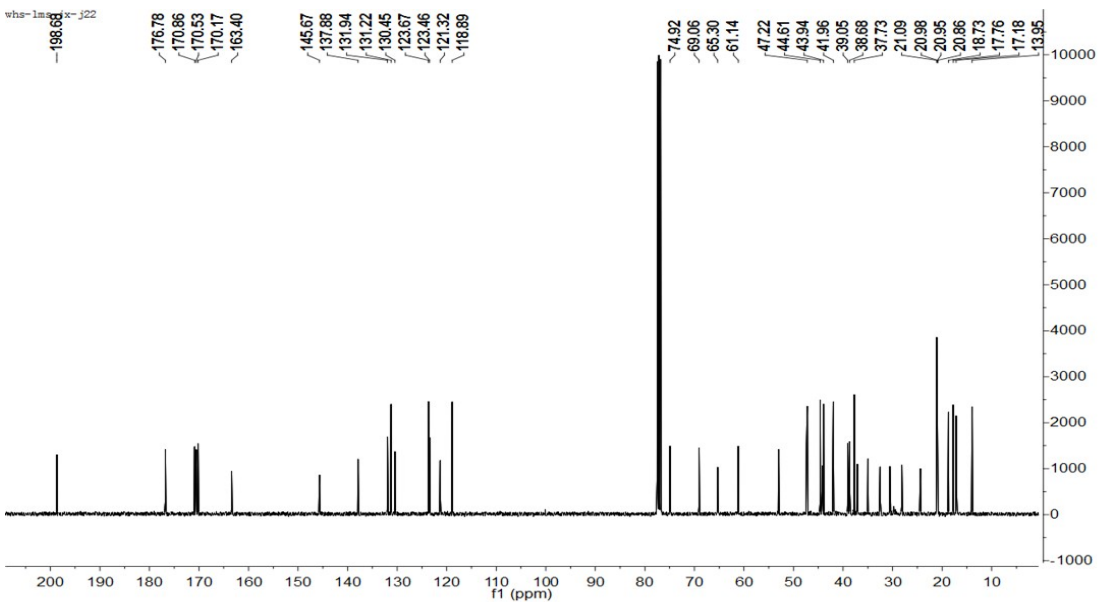
T: FTMS + p ESI Full ms [700.00-900.00]
825.4195
C45 H59 O8 N4 F Na
826.4226
C45 H60 O8 N4 F Na
823.4099
C45 H57 O8 N4 F Na
827.4254
828.4279
829.4274
830.3976
830.8989
Relative Abundance
m/z

5e


7.97
7.94
7.93
7.62
7.60
7.56
7.54
7.39
7.35
5.63
5.27
5.20
5.02
4.99
4.57
4.52
4.41
4.36
3.80
3.77
3.56
3.53
3.15
3.13
3.12
2.38
2.35
2.32
2.05
1.99
1.93
1.75
1.25
1.14
0.95
0.93
0.85
0.83
0.82
0.62
f1 (ppm)


whs-lmsd-jx-j22
198.68
176.78
170.86
170.53
170.17
163.40
145.67
137.88
131.94
131.22
130.45
123.67
123.46
121.32
118.89
74.92
69.06
65.30
61.14
47.22
44.61
43.94
41.96
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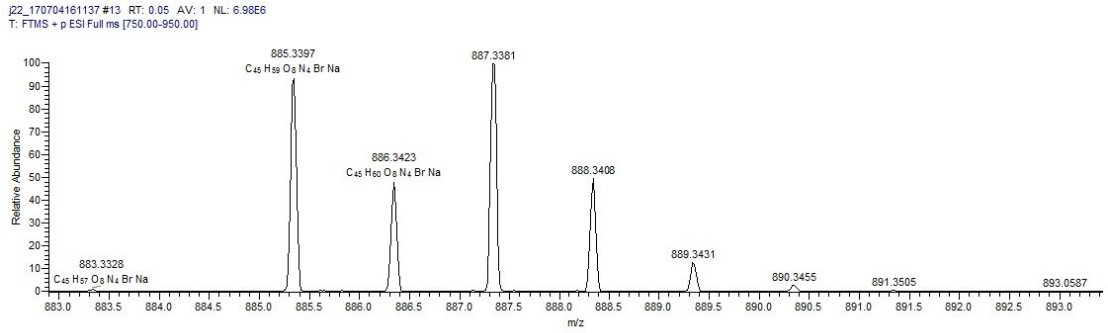
18.73
17.76
17.18
13.95
f1 (ppm)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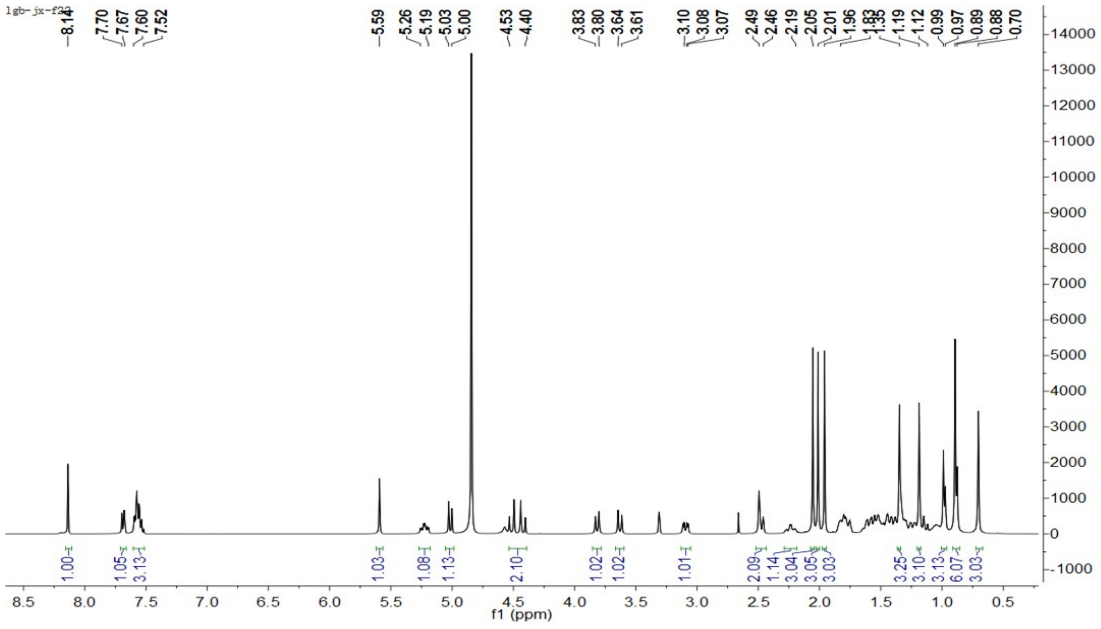
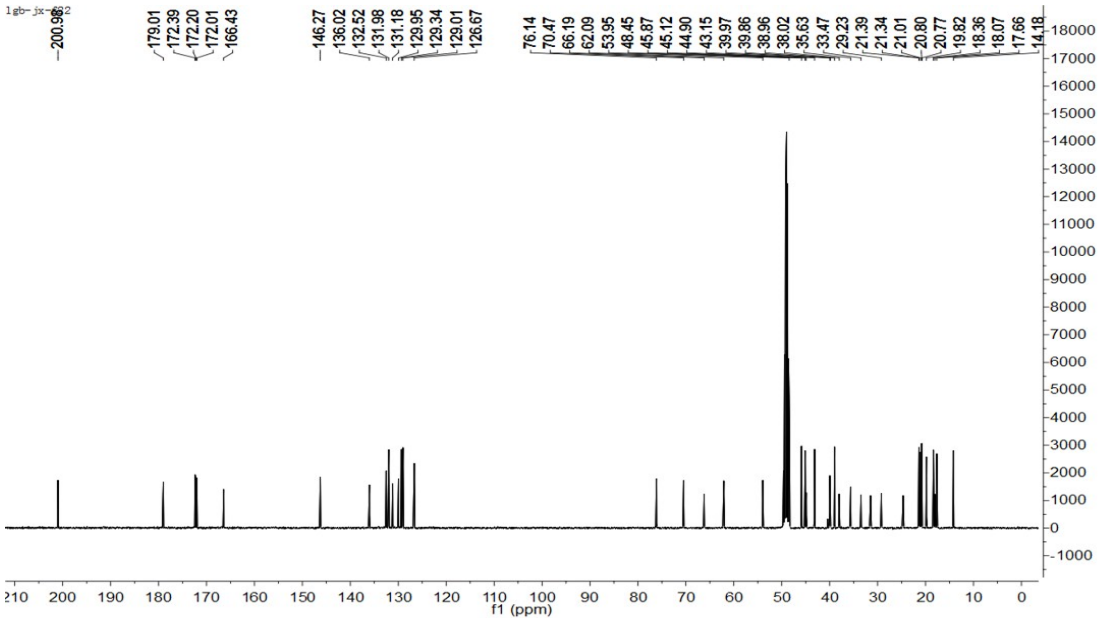
T: FTMS + p ESI Full ms [750.00-950.00]
885.3397
C45 H59 O8 N4 Br Na
887.3381
886.3423
C45 H60 O8 N4 Br Na
888.3408
889.3431
883.3328
C45 H57 O8 N4 Br Na
890.3455
891.3505
893.0587
Relative Abundance
m/z

5f


lgb-jx-f30
8.14
7.70
7.67
7.60
7.52
5.59
5.26
5.19
5.03
5.00
4.53
4.40
3.83
3.80
3.64
3.61
3.10
3.08
3.07
2.49
2.46
2.19
2.05
2.01
1.96
1.19
1.12
0.99
0.97
0.89
0.88
0.70
f1 (ppm)


1gb-jx-g22
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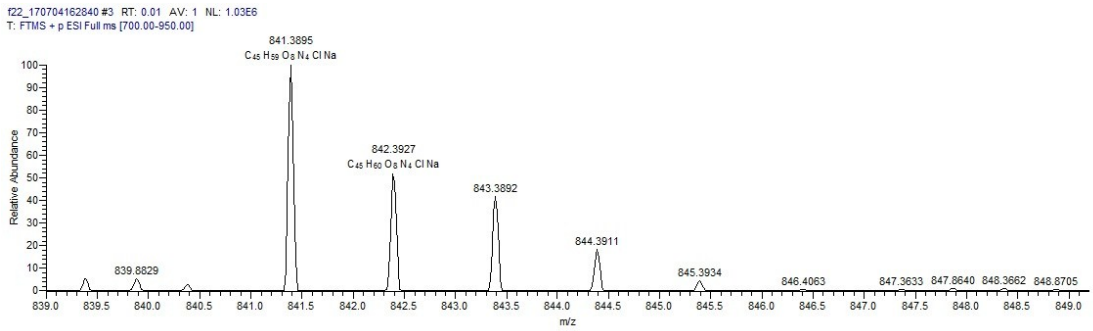
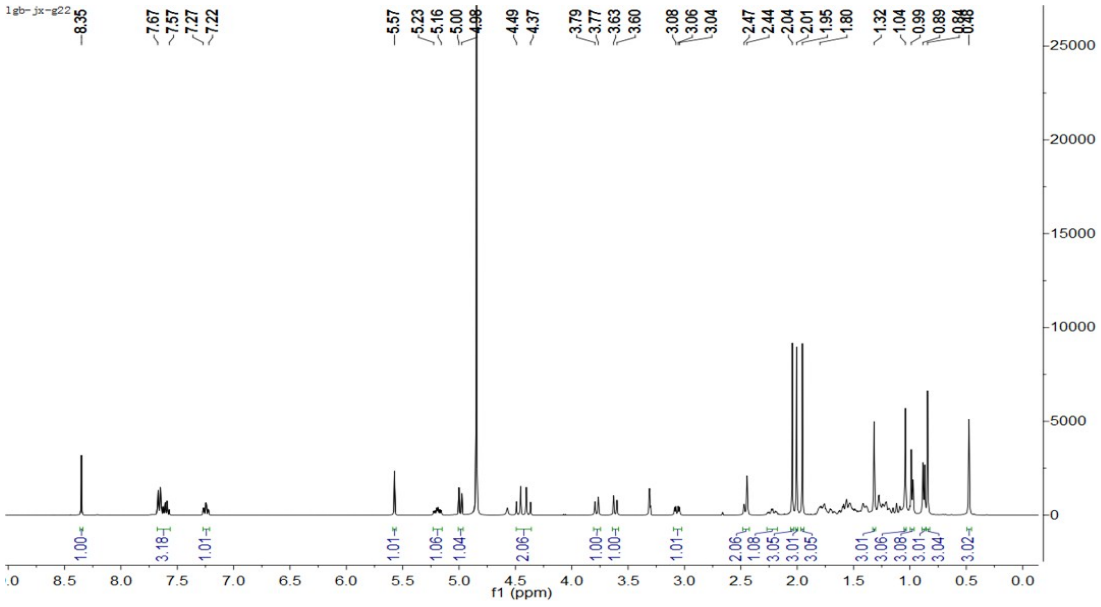
179.01
172.39
172.20
172.01
166.43
146.27
136.02
132.52
131.98
131.18
129.95
129.34
129.01
126.67
76.14
70.47
66.19
62.09
53.95
48.45
45.87
45.12
44.90
43.15
39.97
39.86
38.96
38.02
35.63
33.47
29.23
21.39
21.34
21.01
20.80
20.77
19.82
18.36
18.07
17.66
14.18
f1 (ppm)


f22_170704162840 #3 RT: 0.01 AV: 1 NL: 1.03E6
T: FTMS + p ESI Full ms [700.00-950.00]
841.3895
C45 H59 O8 N4 Cl Na
842.3927
C45 H60 O8 N4 Cl Na
843.3892
844.3911
839.8829
845.3934
846.4063
847.3633
847.8640
848.3662
848.8705
Relative Abundance
m/z

5g


1gb-jx-g22
8.35
7.67
7.57
7.27
7.22
5.57
5.23
5.16
5.00
4.98
4.49
4.37
3.79
3.77
3.63
3.60
3.08
3.06
3.04
2.47
2.44
2.04
2.01
1.95
1.80
1.32
1.04
0.99
0.89
0.84
0.48
1.00
3.18
1.01
1.01
1.06
1.04
2.06
1.00
1.00
1.01
2.06
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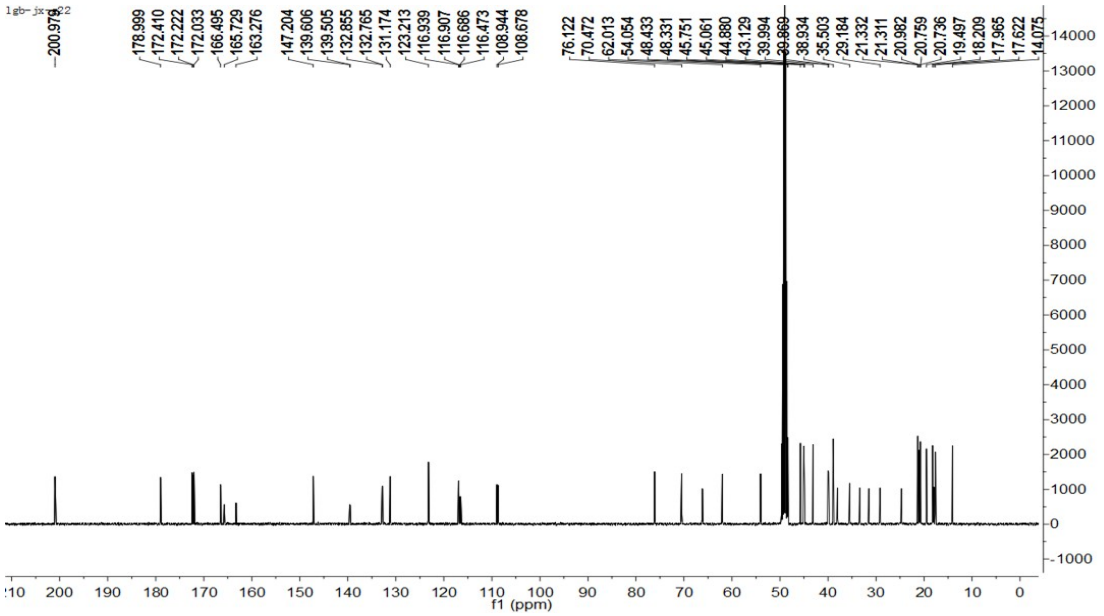
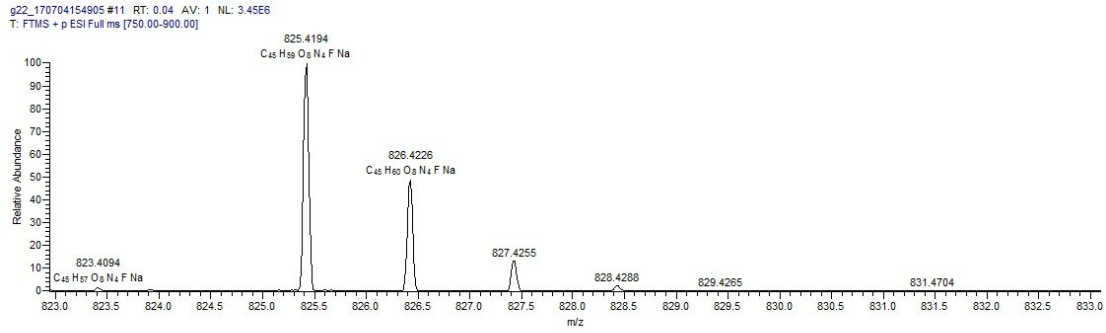
3.08
3.01
3.04
3.02
f1 (ppm)


200.9764
178.999
172.410
172.222
172.033
166.495
165.729
163.276
147.204
139.606
139.505
132.855
132.765
131.174
123.213
116.939
116.907
116.686
116.473
108.944
108.678
76.122
70.472
62.013
54.054
48.433
48.331
45.751
45.061
44.880
43.129
39.994
39.869
38.934
35.503
29.184
21.332
21.311
20.982
20.759
20.736
19.497
18.209
17.965
17.622
14.075
f1 (ppm)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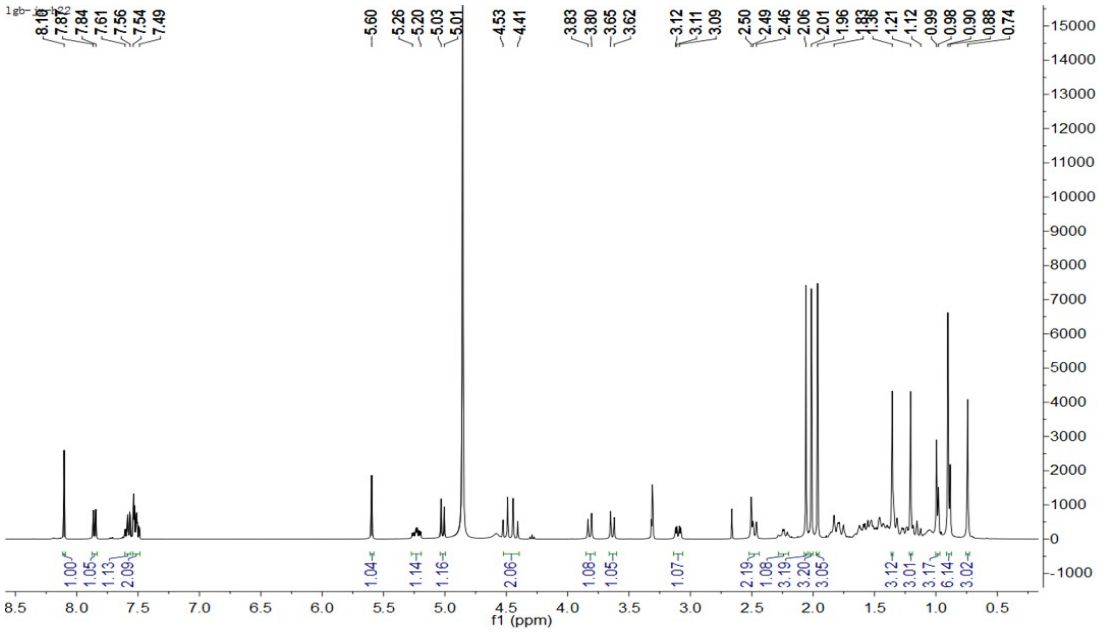
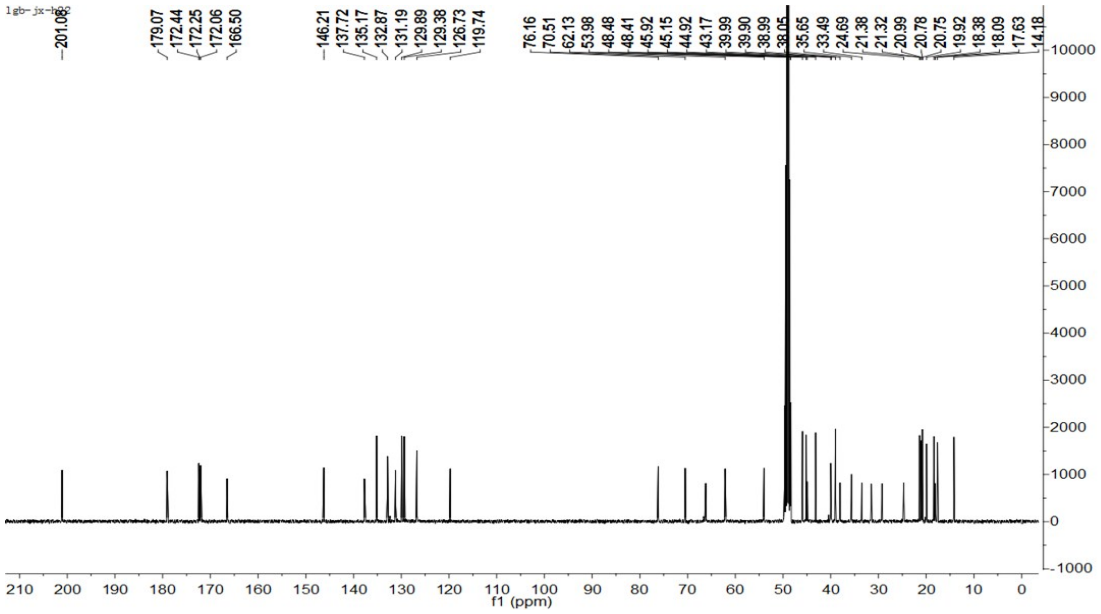
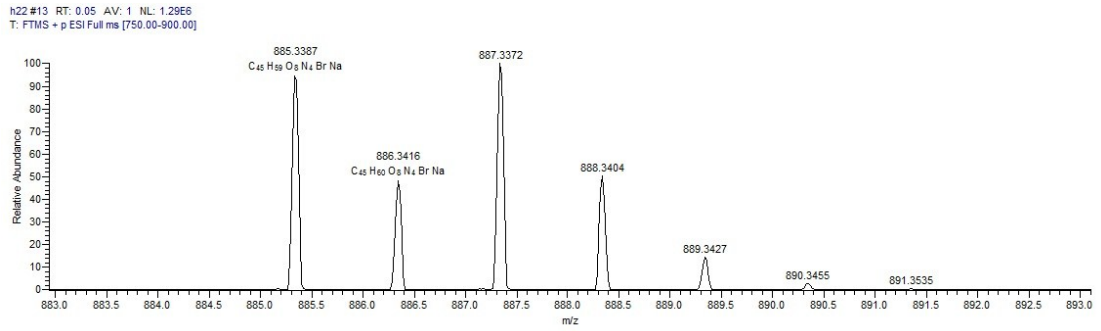
T: FTMS + p ESI Full ms [750.00-900.00]
825.4194
C45 H59 O8 N4 F Na
826.4226
C45 H60 O8 N4 F Na
823.4094
C45 H57 O8 N4 F Na
827.4255
828.4288
829.4265
831.4704
Relative Abundance
m/z

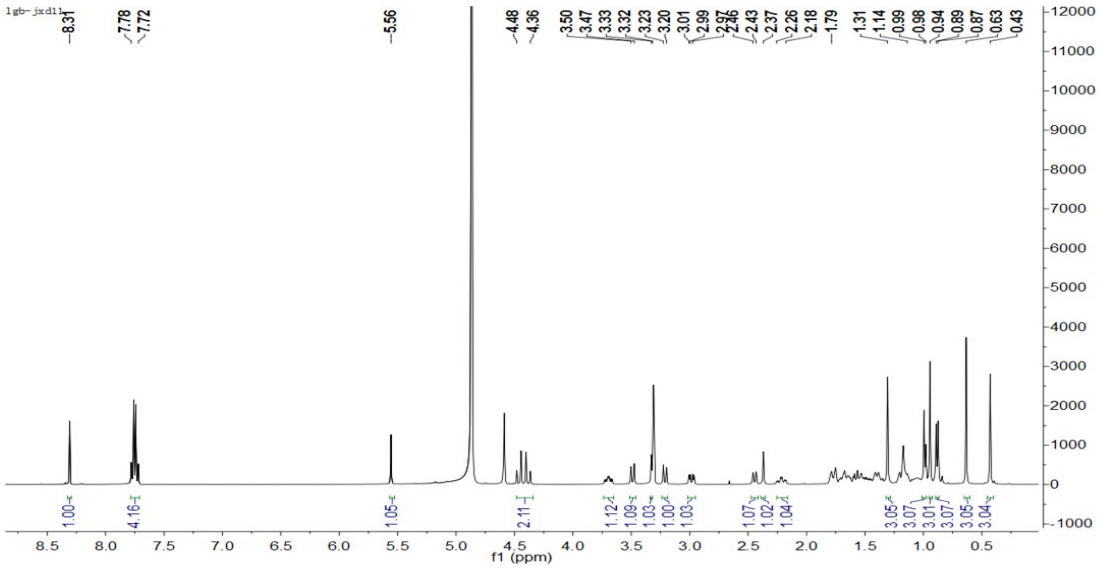
5h

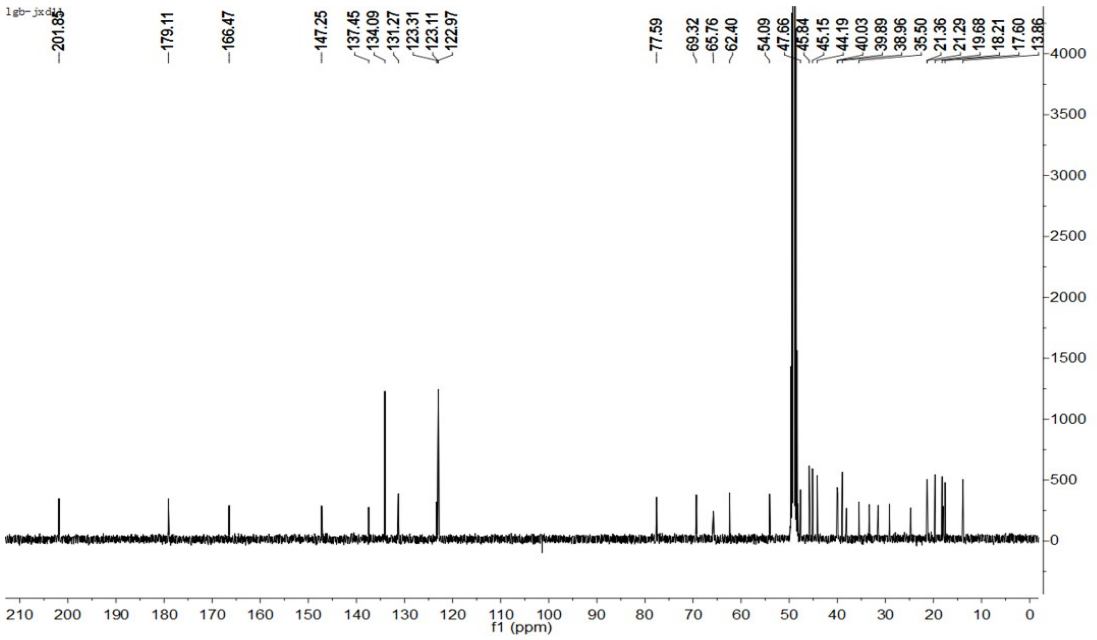

8.10
7.87
7.84
7.61
7.56
7.54
7.49
5.60
5.26
5.20
5.03
5.01
4.53
4.41
3.83
3.80
3.65
3.62
3.12
3.11
3.09
2.50
2.49
2.46
2.06
2.01
1.96
1.83
1.36
1.21
1.12
0.99
0.98
0.90
0.88
0.74
1.00
1.05
1.13
2.09
1.04
1.14
1.16
2.06
1.08
1.05
1.07
2.19
1.08
3.19
3.20
3.05
3.12
3.01
3.17
6.14
3.02
f1 (ppm)

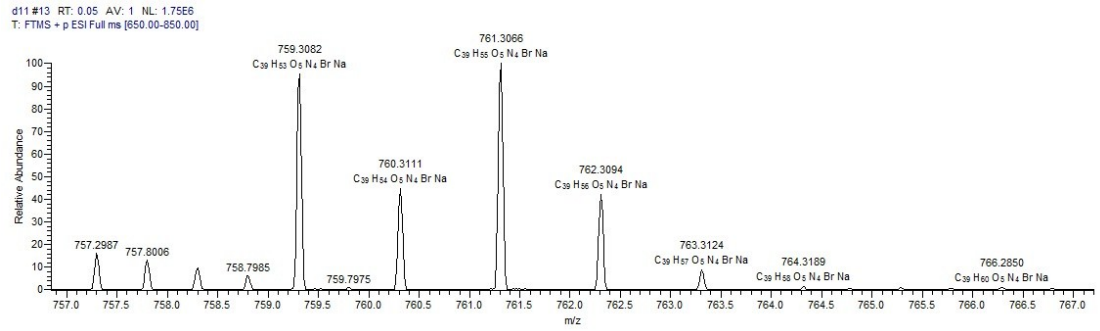

201.08
179.07
172.44
172.25
172.06
166.50
146.21
137.72
135.17
132.87
131.19
129.89
129.38
126.73
119.74
76.16
70.51
62.13
53.98
48.48
48.41
45.92
45.15
44.92
43.17
39.99
39.90
38.99
38.05
35.65
33.49
24.69
21.38
21.32
20.99
20.78
20.75
19.92
18.38
18.09
17.63
14.18
f1 (ppm)


h22 #13 RT: 0.05 AV: 1 NL: 1.29E6
T: FTMS + p ESI Full ms [750.00-900.00]
885.3387
C45 H59 O8 N4 Br Na
886.3416
C45 H60 O8 N4 Br Na
887.3372
888.3404
889.3427
890.3455
891.3535
Relative Abundance
m/z

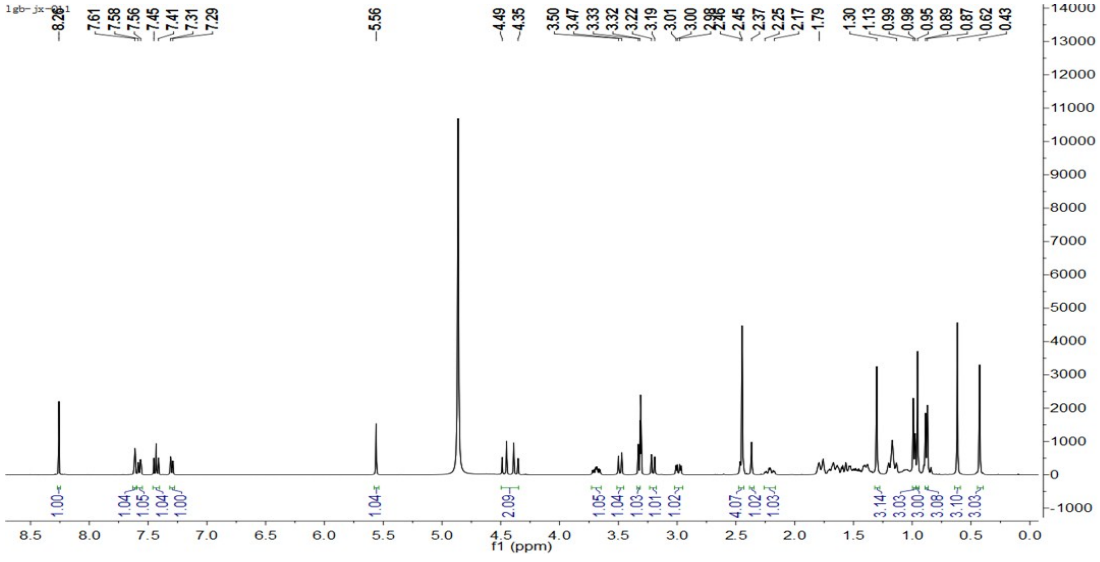
6a

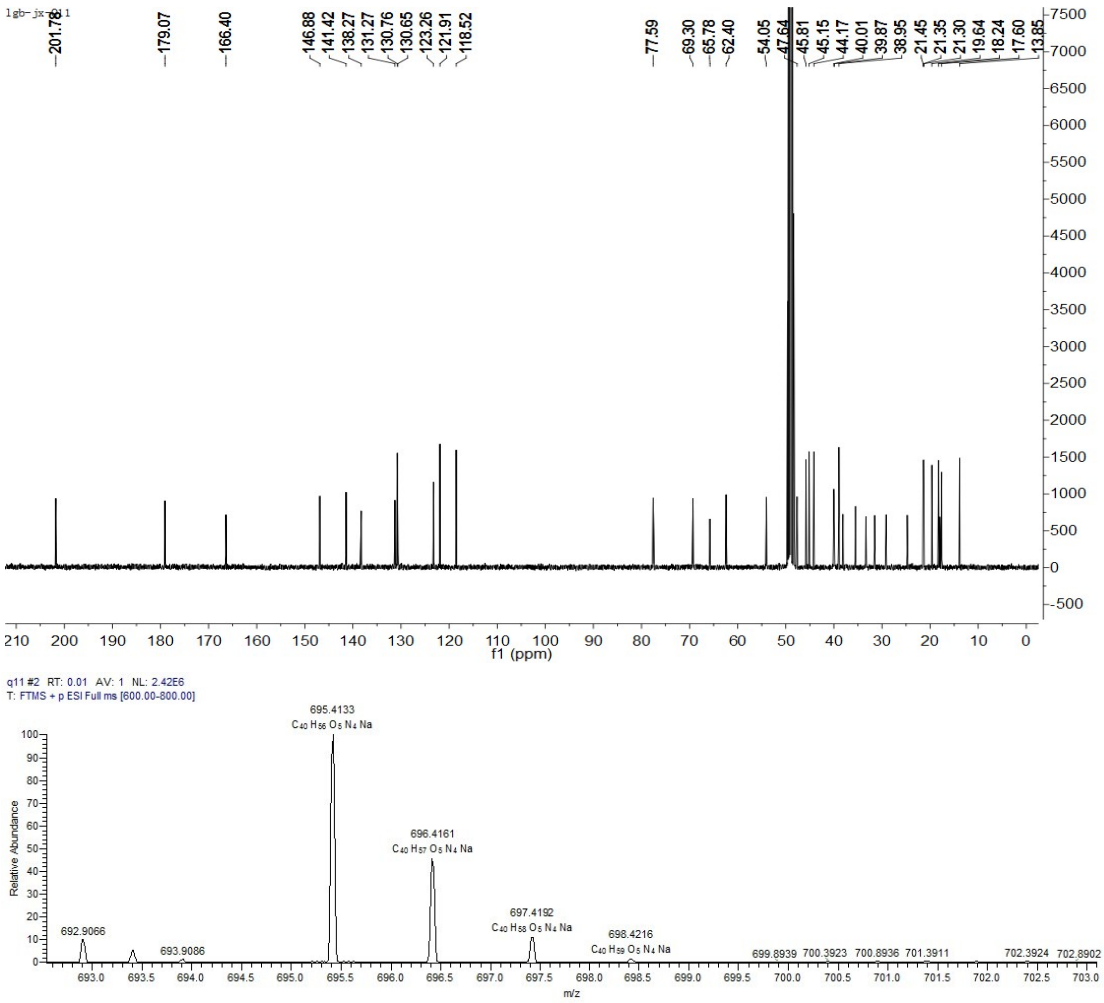

8.31
7.78
7.72
5.56
4.48
4.36
3.50
3.47
3.33
3.32
3.23
3.20
3.01
2.99
2.97
2.46
2.43
2.37
2.26
2.18
1.79
1.31
1.14
0.99
0.98
0.94
0.89
0.87
0.63
0.43
1.00
4.16
1.05
2.11
1.12
1.09
1.03
1.00
1.03
1.07
1.02
1.04
3.05
3.07
3.01
3.07
3.05
3.04
f1 (ppm)


201.85
179.11
166.47
147.25
137.45
134.09
131.27
123.31
123.11
122.97
77.59
69.32
65.76
62.40
54.09
47.66
45.84
45.15
44.19
40.03
39.89
38.96
35.50
21.36
21.29
19.68
18.21
17.60
13.86
f1 (ppm)

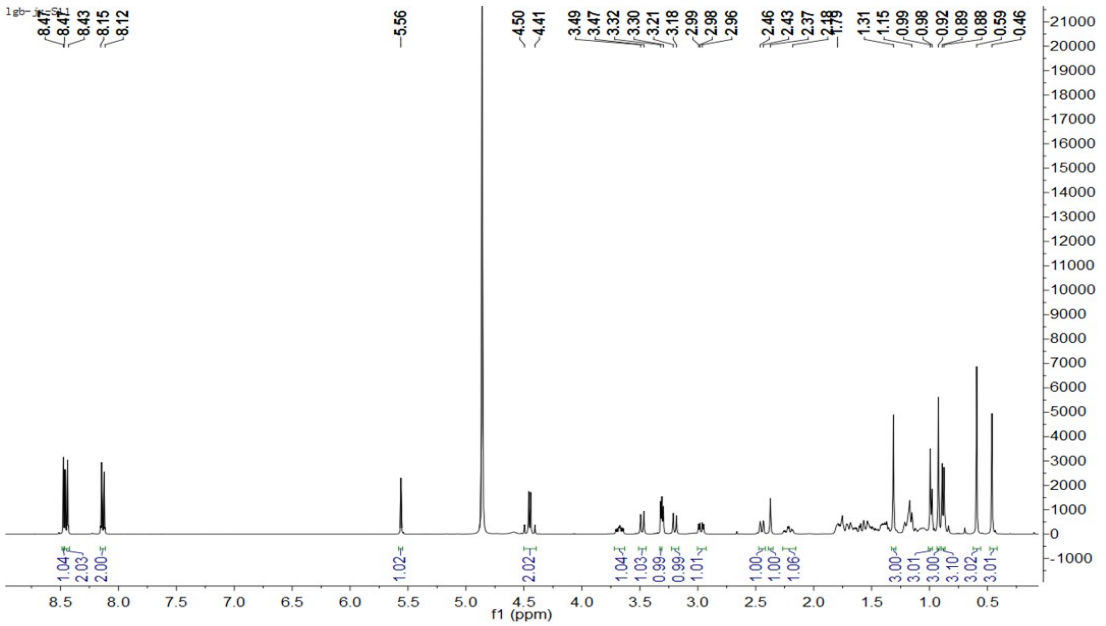

d11 #13 RT: 0.05 AV: 1 NL: 1.75E6
T: FTMS + p ESI Full ms [650.00-850.00]
759.3082
C39 H53 O5 N4 Br Na
761.3066
C39 H55 O5 N4 Br Na
760.3111
C39 H54 O5 N4 Br Na
762.3094
C39 H56 O5 N4 Br Na
763.3124
C39 H57 O5 N4 Br Na
764.3189
C39 H58 O5 N4 Br Na
766.2850
C39 H60 O5 N4 Br Na
757.2987
757.8006
758.7985
759.7975
Relative Abundance
m/z

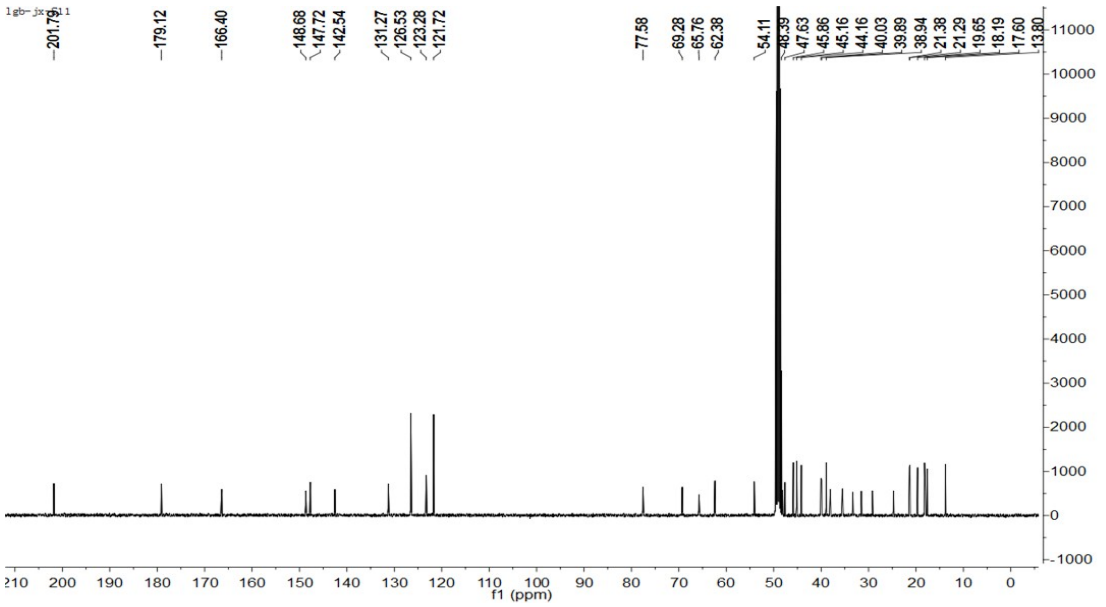
6b

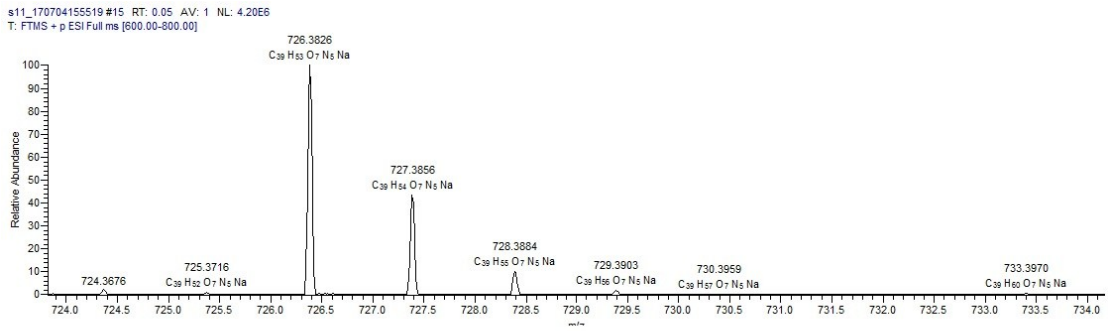

8.26
7.61
7.58
7.56
7.45
7.41
7.31
7.29
5.56
4.49
4.35
3.50
3.47
3.33
3.32
3.22
3.19
3.01
3.00
2.45
2.37
2.25
2.17
1.79
1.30
1.13
0.99
0.98
0.95
0.89
0.87
0.62
0.43
f1 (ppm)


201.78
179.07
166.40
146.88
141.42
138.27
131.27
130.76
130.65
123.26
121.91
118.52
77.59
69.30
65.78
62.40
54.05
47.64
45.81
45.15
44.17
40.01
39.87
38.95
21.45
21.35
21.30
19.64
18.24
17.60
13.85
f1 (ppm)
q11 #2 RT: 0.01 AV: 1 NL: 2.42E6
T: FTMS + p ESI Full ms [600.00-800.00]
695.4133
C40 H56 O5 N4 Na
696.4161
C40 H57 O5 N4 Na
697.4192
C40 H58 O5 N4 Na
698.4216
C40 H59 O5 N4 Na
692.9066
693.9086
699.8939
700.3923
700.8936
701.3911
702.3924
702.8902
Relative Abundance
m/z

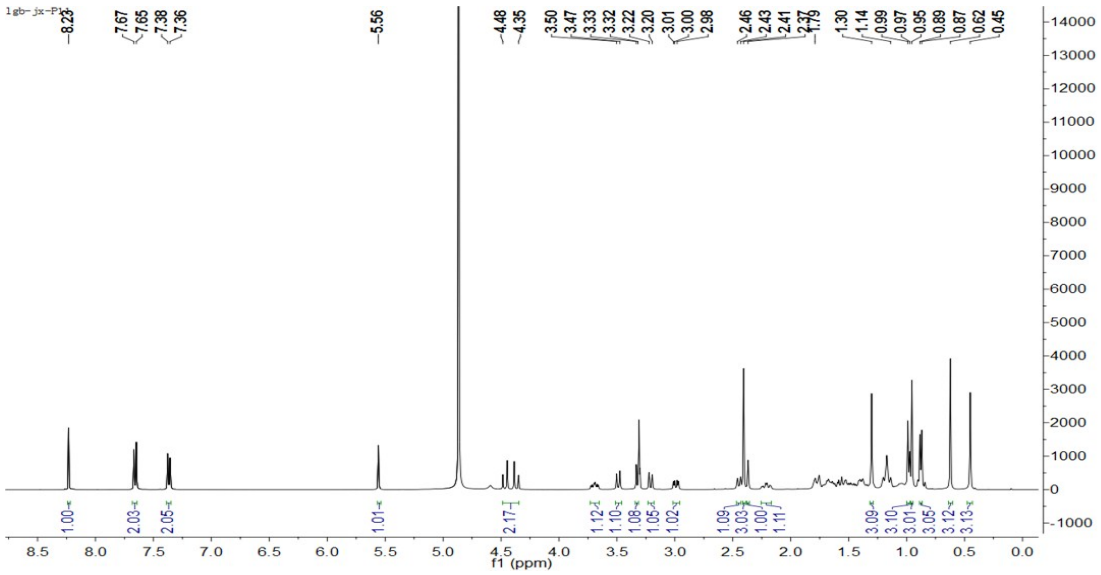
6c

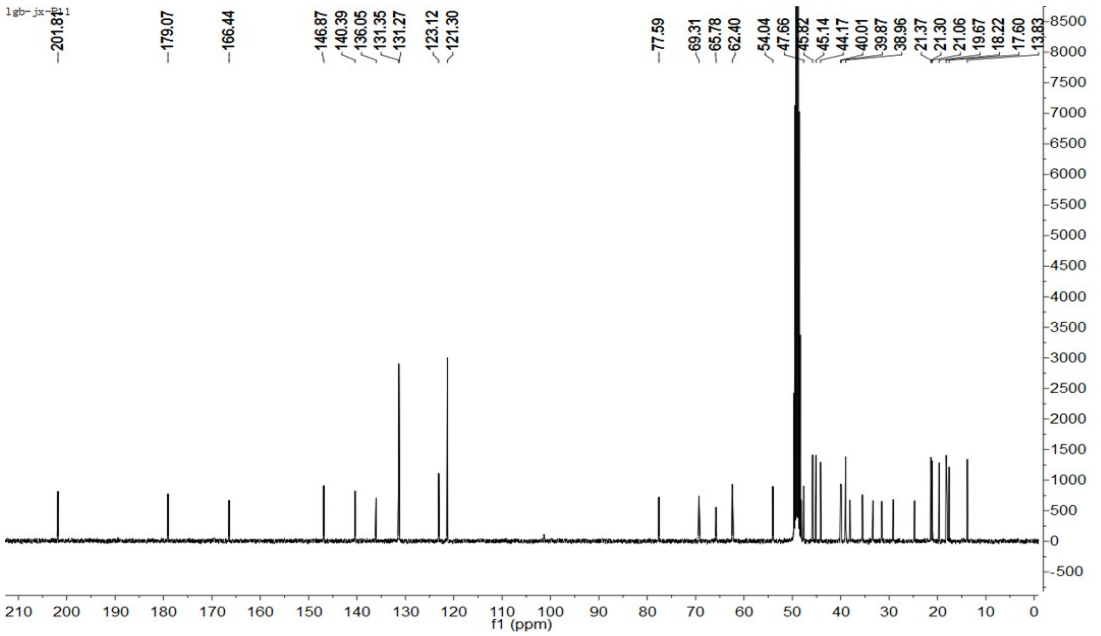

8.47
8.43
8.15
8.12
5.56
4.50
4.41
3.49
3.47
3.32
3.30
3.21
3.18
2.99
2.98
2.96
2.46
2.43
2.37
1.31
1.15
0.99
0.98
0.92
0.89
0.88
0.59
0.46
1.04
2.03
2.00
1.02
2.02
1.04
1.03
0.99
0.99
1.01
1.00
1.00
1.06
3.00
3.01
3.00
3.10
3.02
3.01
f1 (ppm)

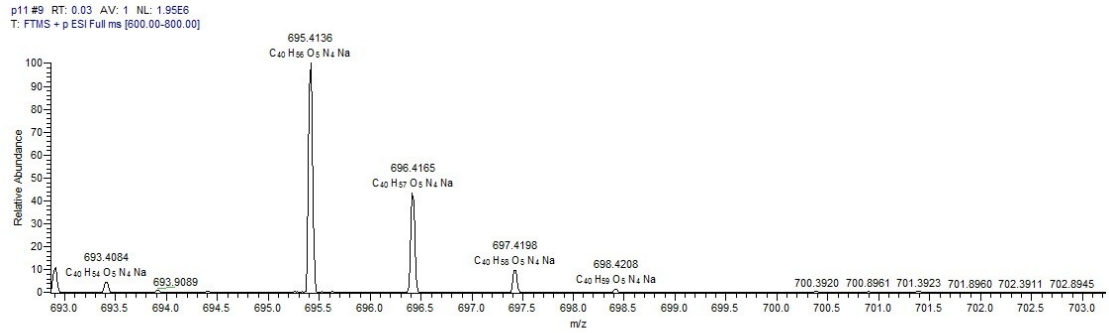

201.76
179.12
166.40
148.68
147.72
142.54
131.27
126.53
123.28
121.72
77.58
69.28
65.76
62.38
54.11
48.39
47.63
45.86
45.16
44.16
40.03
39.89
38.94
21.38
21.29
19.65
18.19
17.60
13.80
f1 (ppm)


s11_170704155519 #15 RT: 0.05 AV: 1 NL: 4.20E6
T: FTMS + p ESI Full ms [600.00-800.00]
726.3826
C39 H53 O7 N5 Na
727.3856
C39 H54 O7 N5 Na
728.3884
C39 H55 O7 N5 Na
724.3676
725.3716
C39 H52 O7 N5 Na
729.3903
C39 H56 O7 N5 Na
730.3959
C39 H57 O7 N5 Na
733.3970
C39 H60 O7 N5 Na
Relative Abundance
m/z

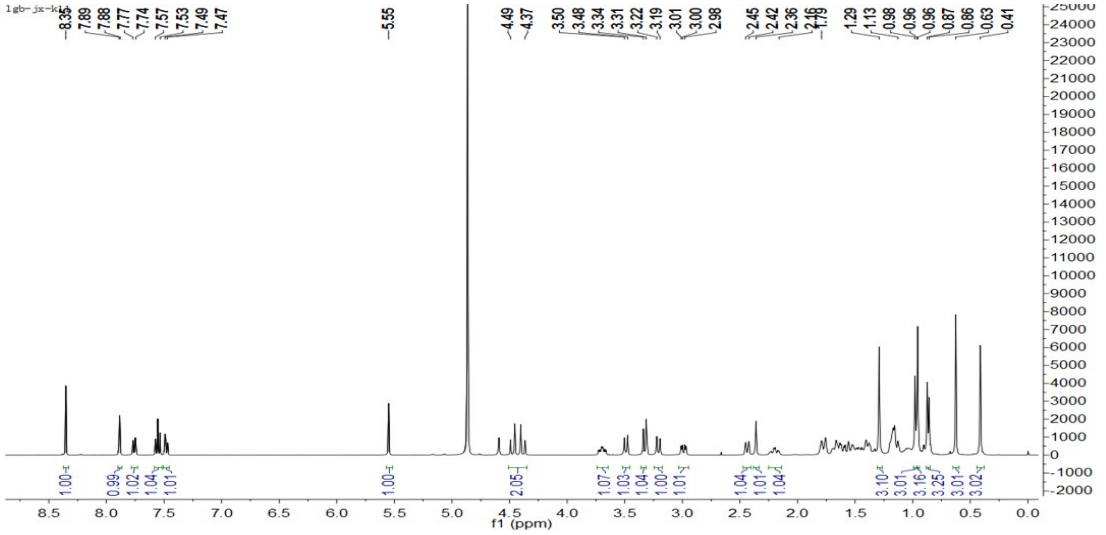
6d

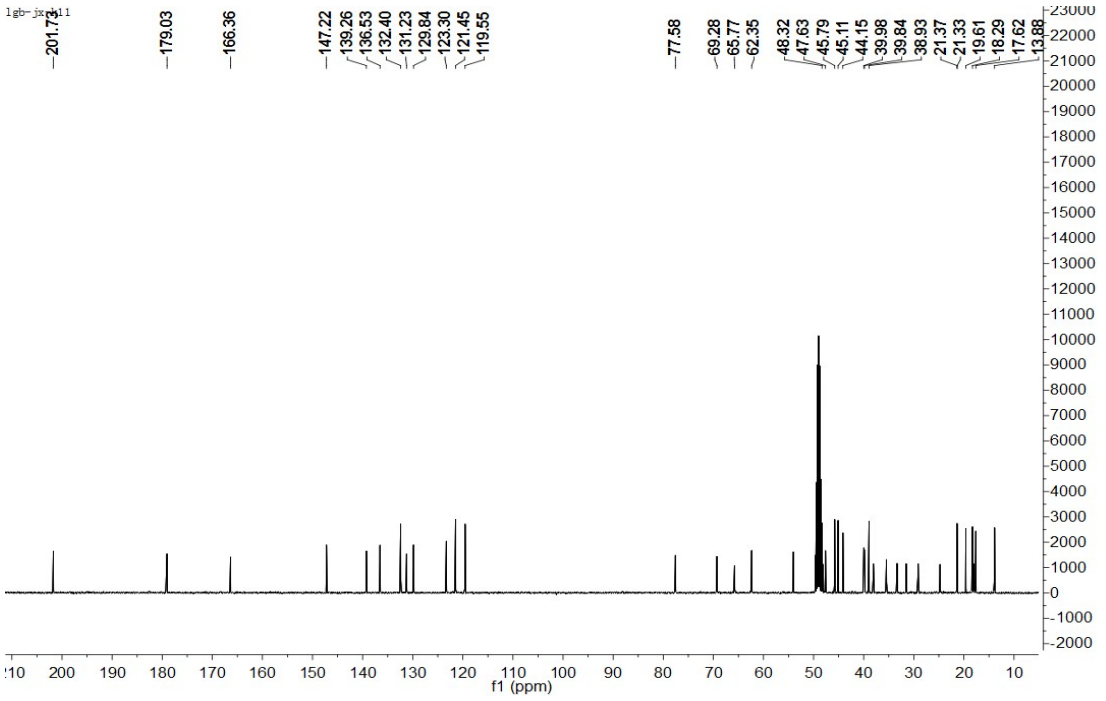

8.23
7.67
7.65
7.38
7.36
5.56
4.48
4.35
3.50
3.47
3.33
3.32
3.22
3.20
3.01
3.00
2.98
2.46
2.43
2.41
2.37
1.79
1.30
1.14
0.99
0.97
0.95
0.89
0.87
0.62
0.45
1.00
2.03
2.05
1.01
2.17
1.12
1.10
1.08
1.05
1.02
1.09
3.03
1.00
1.11
3.09
3.10
3.01
3.05
3.12
3.13
f1 (ppm)

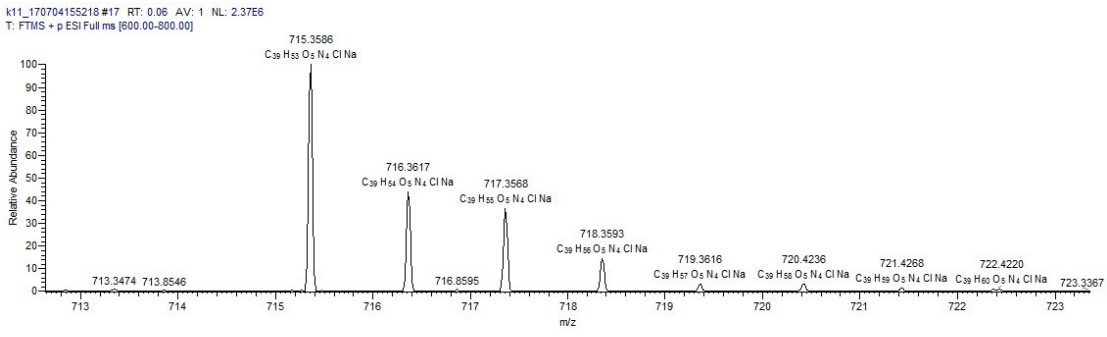

201.81
179.07
166.44
146.87
140.39
136.05
131.35
131.27
123.12
121.30
77.59
69.31
65.78
62.40
54.04
47.66
45.82
45.14
44.17
40.01
39.87
38.96
21.37
21.30
21.06
19.67
18.22
17.60
13.83
f1 (ppm)


p11 #9 RT: 0.03 AV: 1 NL: 1.95E6
T: FTMS + p ESI Full ms [600.00-800.00]
695.4136
C40 H56 O5 N4 Na
696.4165
C40 H57 O5 N4 Na
693.4084
C40 H54 O5 N4 Na
693.9089
697.4198
C40 H58 O5 N4 Na
698.4208
C40 H59 O5 N4 Na
700.3920 700.8961 701.3923 701.8960 702.3911 702.8945
Relative Abundance
m/z

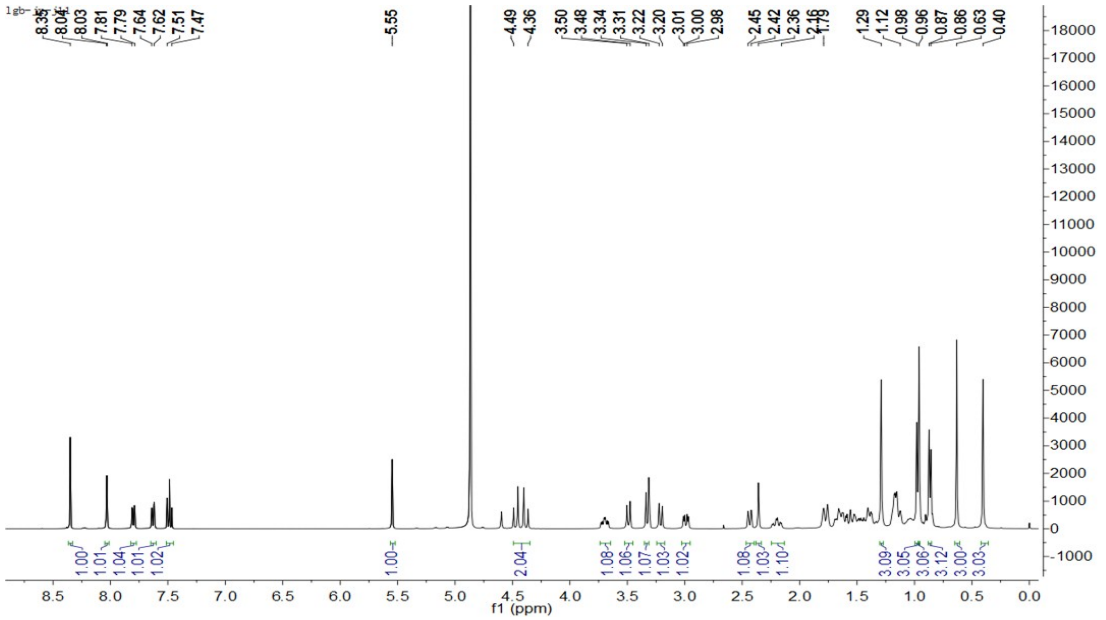
6e

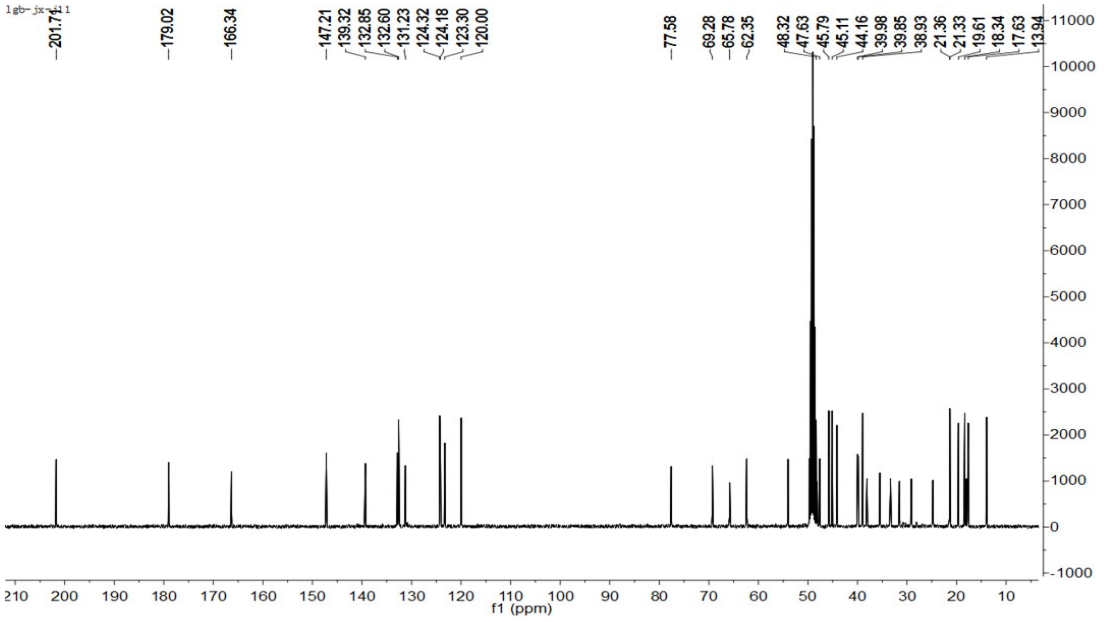


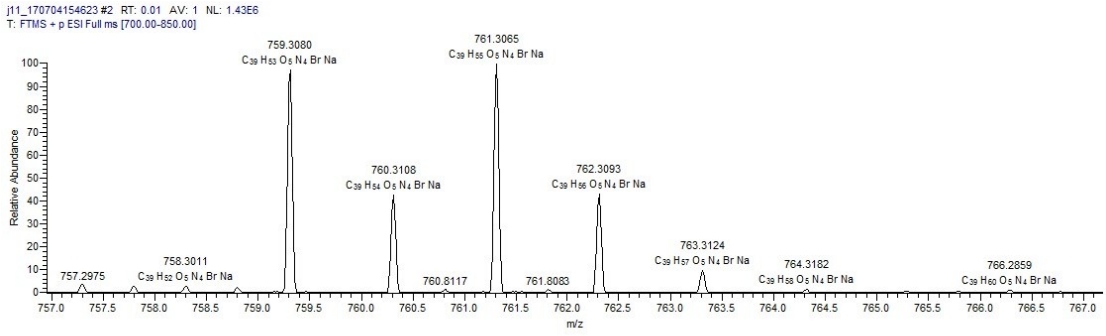



k11_170704155218 #17 RT: 0.06 AV: 1 NL: 2.37E6
T: FTMS + p ESI Full ms [600.00-800.00]
715.3586
C39 H53 O5 N4 Cl Na
716.3617
C39 H54 O5 N4 Cl Na
717.3568
C39 H55 O5 N4 Cl Na
718.3593
C39 H56 O5 N4 Cl Na
719.3616
C39 H57 O5 N4 Cl Na
720.4236
C39 H58 O5 N4 Cl Na
721.4268
C39 H59 O5 N4 Cl Na
722.4220
C39 H60 O5 N4 Cl Na
713.3474
713.8546
716.8595
723.3367
Relative Abundance
m/z

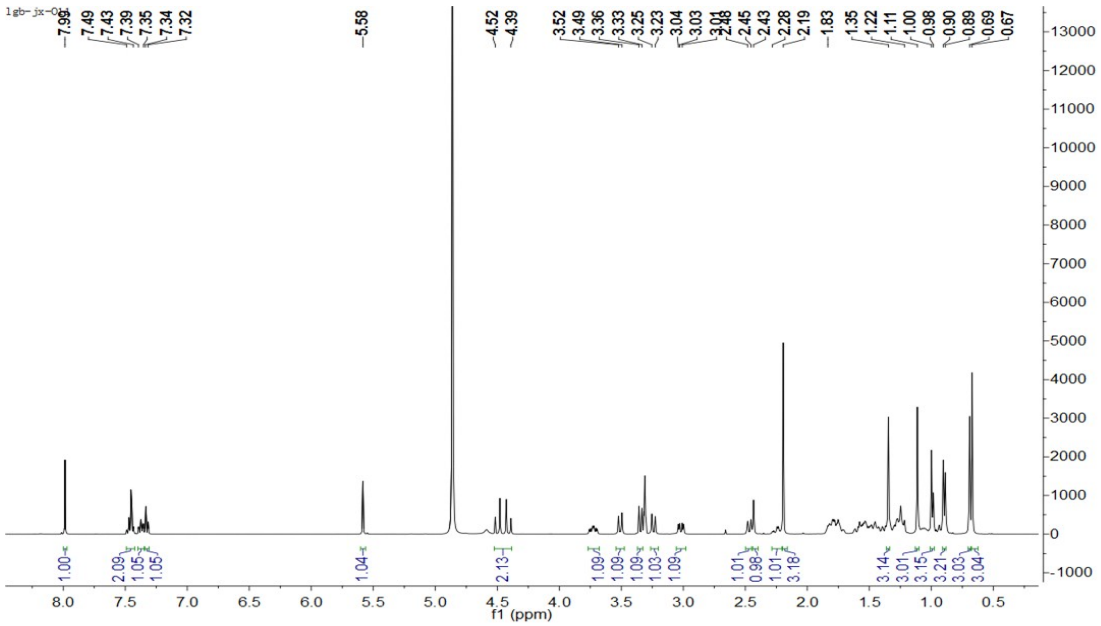
6f

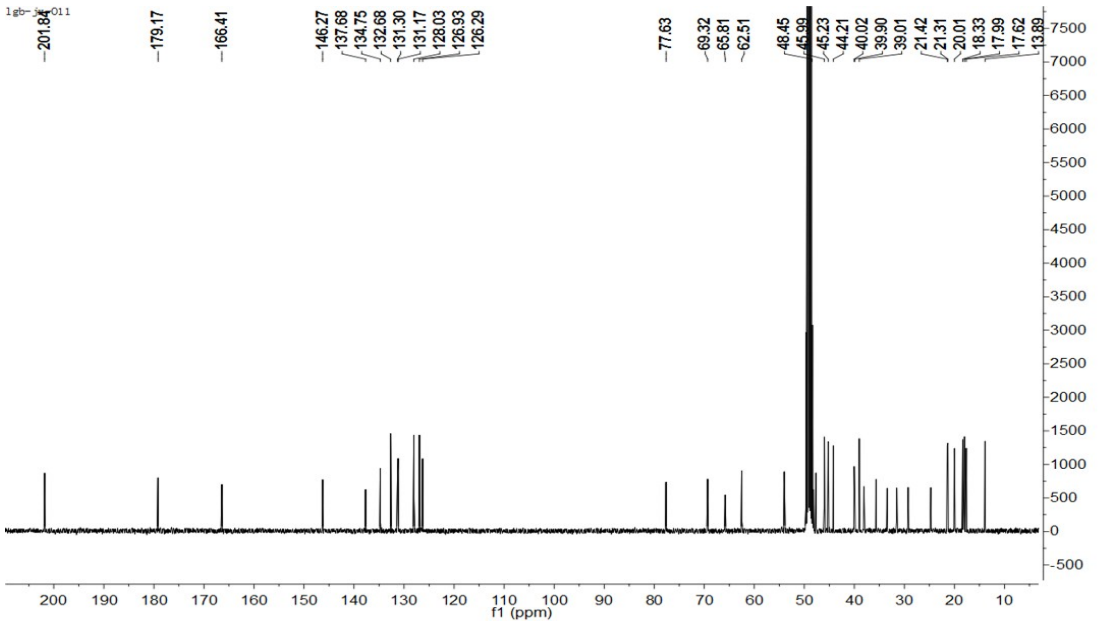

8.35
8.04
8.03
7.81
7.79
7.64
7.62
7.51
7.47
5.55
4.49
4.36
3.50
3.48
3.34
3.31
3.22
3.20
3.01
3.00
2.98
2.45
2.42
2.36
1.29
1.12
0.98
0.96
0.87
0.86
0.63
0.40
f1 (ppm)

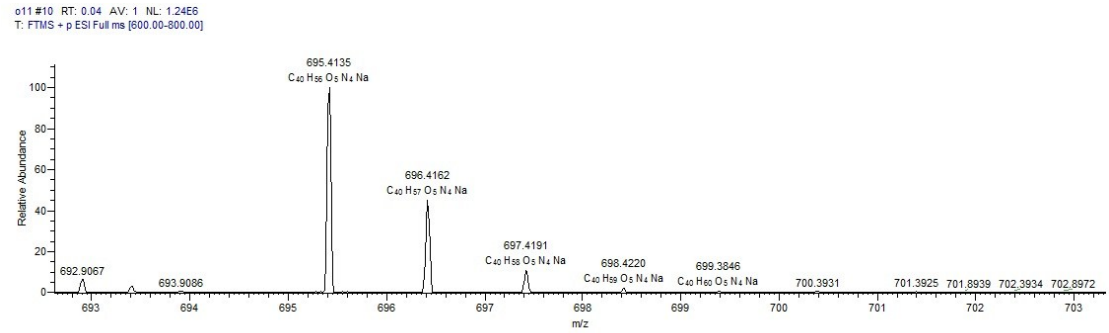

201.74
179.02
166.34
147.21
139.32
132.85
132.60
131.23
124.32
124.18
123.30
120.00
77.58
69.28
65.78
62.35
48.32
47.63
45.79
45.11
44.16
39.98
39.85
38.93
21.36
21.33
19.61
18.34
17.63
13.94
f1 (ppm)


j11_170704154623 #2 RT: 0.01 AV: 1 NL: 1.43E6
T: FTMS + p ESI Full ms [700.00-850.00]
759.3080
C39 H53 O5 N4 Br Na
761.3065
C39 H55 O5 N4 Br Na
760.3108
C39 H54 O5 N4 Br Na
762.3093
C39 H56 O5 N4 Br Na
758.3011
C39 H52 O5 N4 Br Na
757.2975
763.3124
C39 H57 O5 N4 Br Na
764.3182
C39 H58 O5 N4 Br Na
766.2859
C39 H60 O5 N4 Br Na
760.8117
761.8083
Relative Abundance
m/z

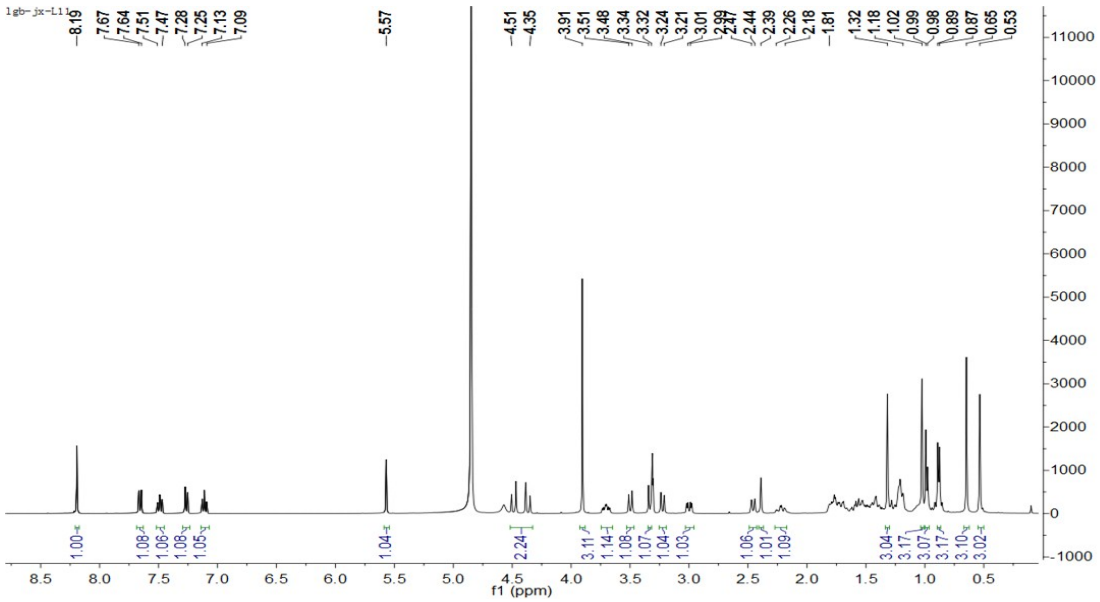
6g

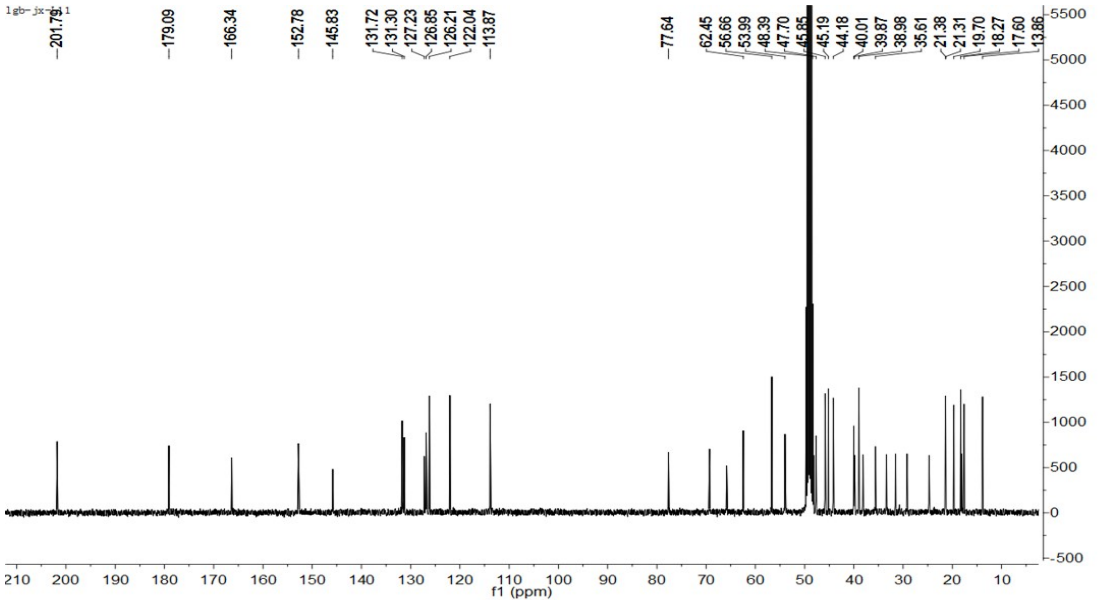

7.99
7.49
7.43
7.39
7.35
7.34
7.32
5.58
4.52
4.39
3.52
3.49
3.36
3.33
3.25
3.23
3.04
3.03
2.48
2.45
2.43
2.28
2.19
1.83
1.35
1.22
1.11
1.00
0.98
0.90
0.89
0.69
0.67
1.00
2.09
1.05
1.05
1.04
2.13
1.09
1.09
1.09
1.03
1.09
1.01
0.98
1.01
3.18
3.14
3.01
3.15
3.21
3.03
3.04
f1 (ppm)

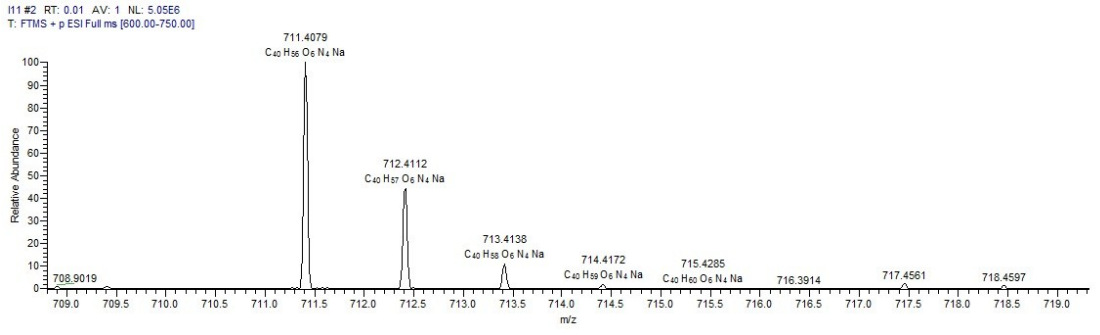

201.84
179.17
166.41
146.27
137.68
134.75
132.68
131.30
131.17
128.03
126.93
126.29
77.63
69.32
65.81
62.51
48.45
45.99
45.23
44.21
40.02
39.90
39.01
21.42
21.31
20.01
18.33
17.99
17.62
13.89
f1 (ppm)


o11 #10 RT: 0.04 AV: 1 NL: 1.24E6
T: FTMS + p ESI Full ms [600.00-800.00]
695.4135
C40 H56 O5 N4 Na
696.4162
C40 H57 O5 N4 Na
697.4191
C40 H58 O5 N4 Na
698.4220
C40 H59 O5 N4 Na
699.3846
C40 H60 O5 N4 Na
692.9067
693.9086
700.3931
701.3925
701.8939
702.3934
702.8972
Relative Abundance
m/z

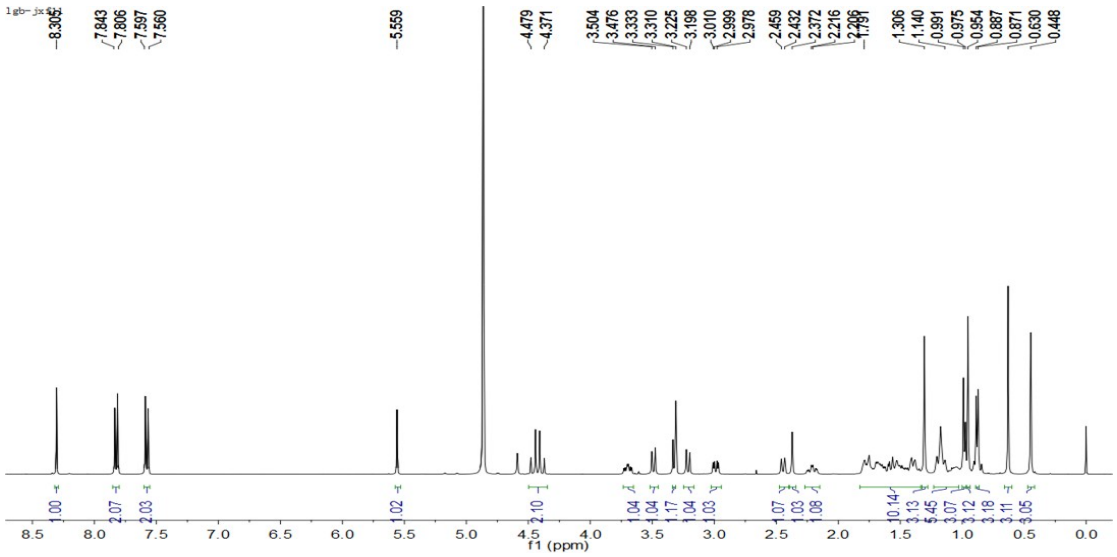
6h

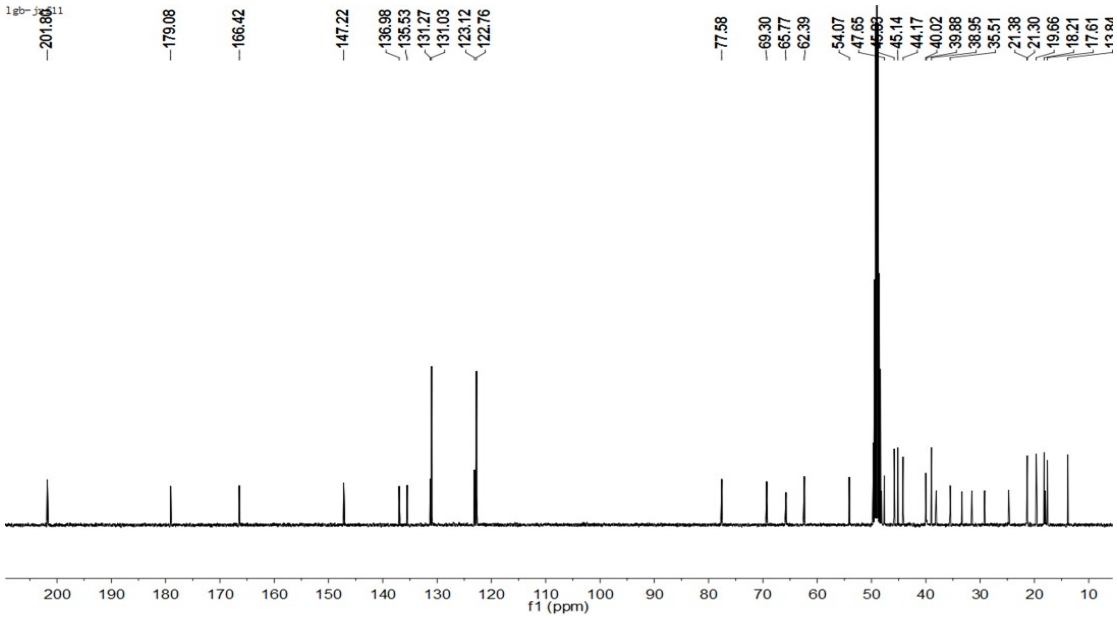

lgb-jx-L11
8.19
7.67
7.64
7.51
7.47
7.28
7.25
7.13
7.09
5.57
4.51
4.35
3.91
3.51
3.48
3.34
3.32
3.24
3.21
3.01
2.99
2.47
2.44
2.39
2.26
2.18
1.81
1.32
1.18
1.02
0.99
0.98
0.89
0.87
0.65
0.53
f1 (ppm)

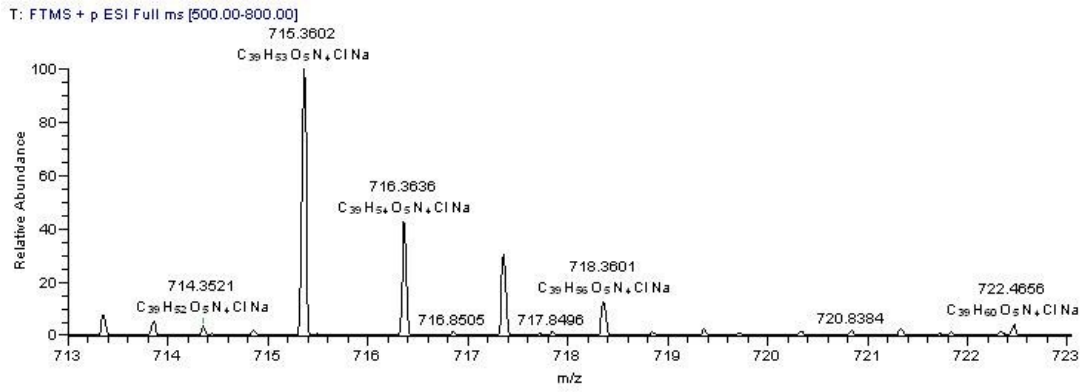

lgb-jx-L11
201.79
179.09
166.34
152.78
145.83
131.72
131.30
127.23
126.85
126.21
122.04
113.87
77.64
62.45
56.66
53.99
48.39
47.70
45.85
45.19
44.18
40.01
39.87
38.98
35.61
21.38
21.31
19.70
18.27
17.60
13.86
f1 (ppm)


I11 #2 RT: 0.01 AV: 1 NL: 5.05E6
T: FTMS + p ESI Full ms [600.00-750.00]
711.4079
C40 H56 O6 N4 Na
712.4112
C40 H57 O6 N4 Na
713.4138
C40 H58 O6 N4 Na
714.4172
C40 H59 O6 N4 Na
715.4285
C40 H60 O6 N4 Na
708.9019
716.3914
717.4561
718.4597
Relative Abundance
m/z

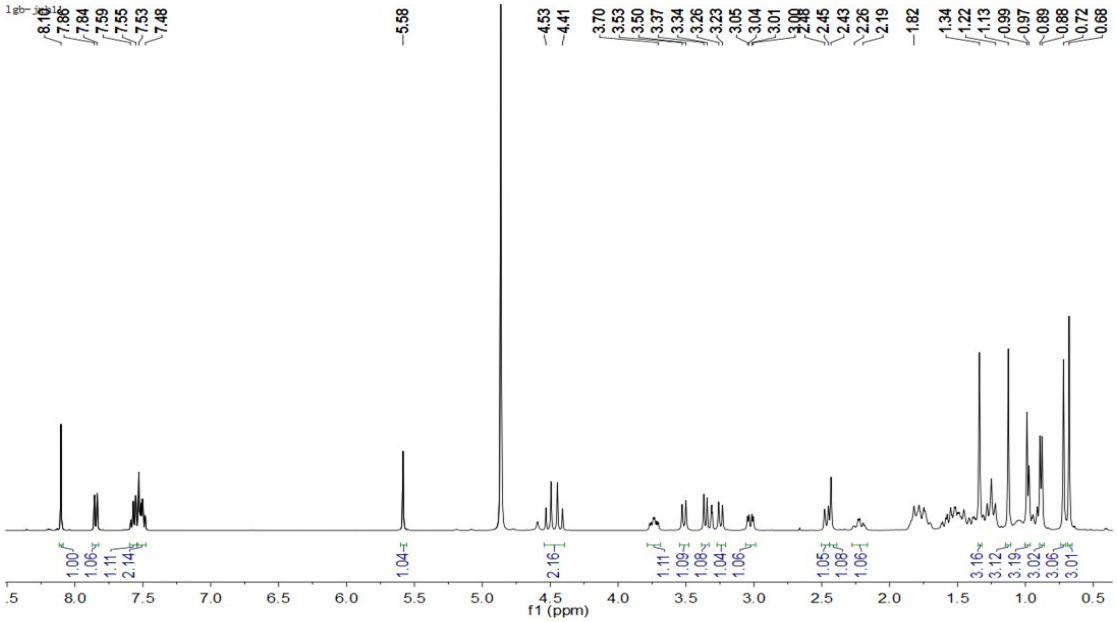
6i

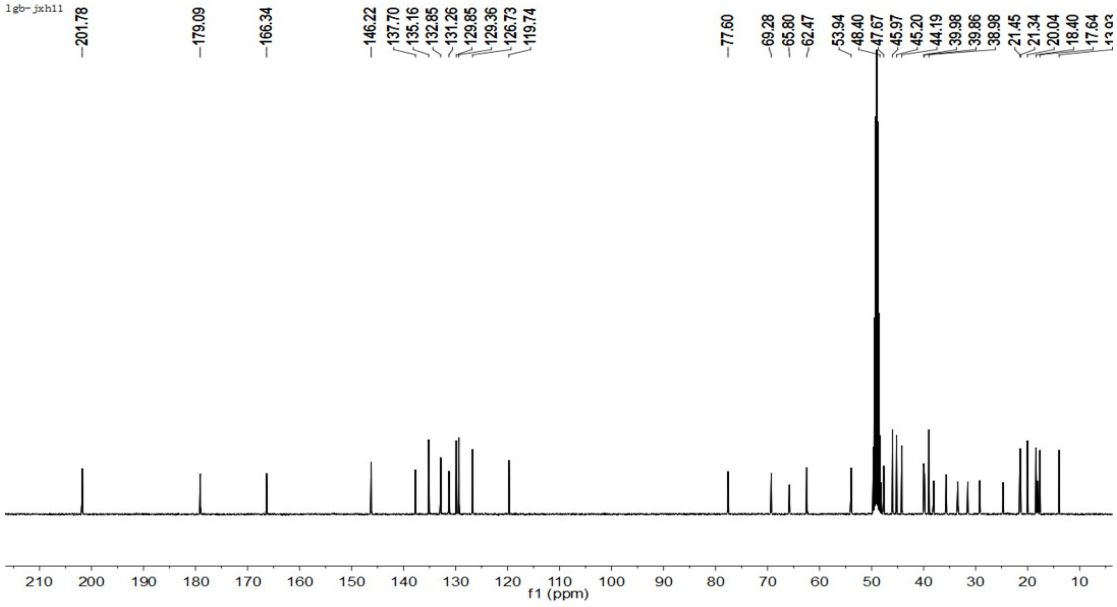

8.305
7.843
7.806
7.597
7.560
5.559
4.479
4.371
3.504
3.476
3.333
3.310
3.225
3.198
3.010
2.999
2.978
2.459
2.432
2.372
2.216
1.306
1.140
0.991
0.975
0.954
0.887
0.871
0.630
0.448
1.00
2.07
2.03
1.02
2.10
1.04
1.04
1.17
1.04
1.03
1.07
1.03
1.08
10.14
3.13
5.45
3.07
3.12
3.18
3.11
9.05
f1 (ppm)

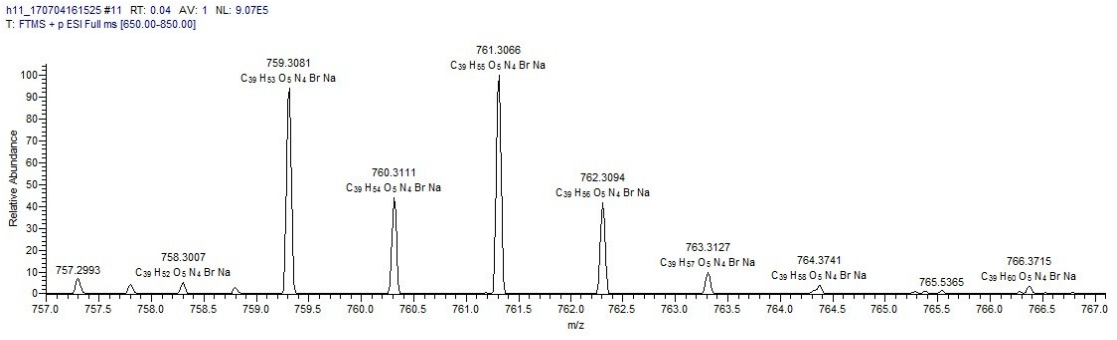

201.86
179.08
166.42
147.22
136.98
135.53
131.27
131.03
123.12
122.76
77.58
69.30
65.77
62.39
54.07
47.65
45.14
44.17
40.02
39.88
38.95
35.51
21.38
21.30
19.66
18.21
17.61
f1 (ppm)


T: FTMS + p ESI Full ms [500.00-800.00]
715.3602
C39H53O5N4ClNa
716.3636
C39H54O5N4ClNa
714.3521
C39H52O5N4ClNa
716.8505
717.8496
718.3601
C39H56O5N4ClNa
720.8384
722.4656
C39H60O5N4ClNa
Relative Abundance
m/z

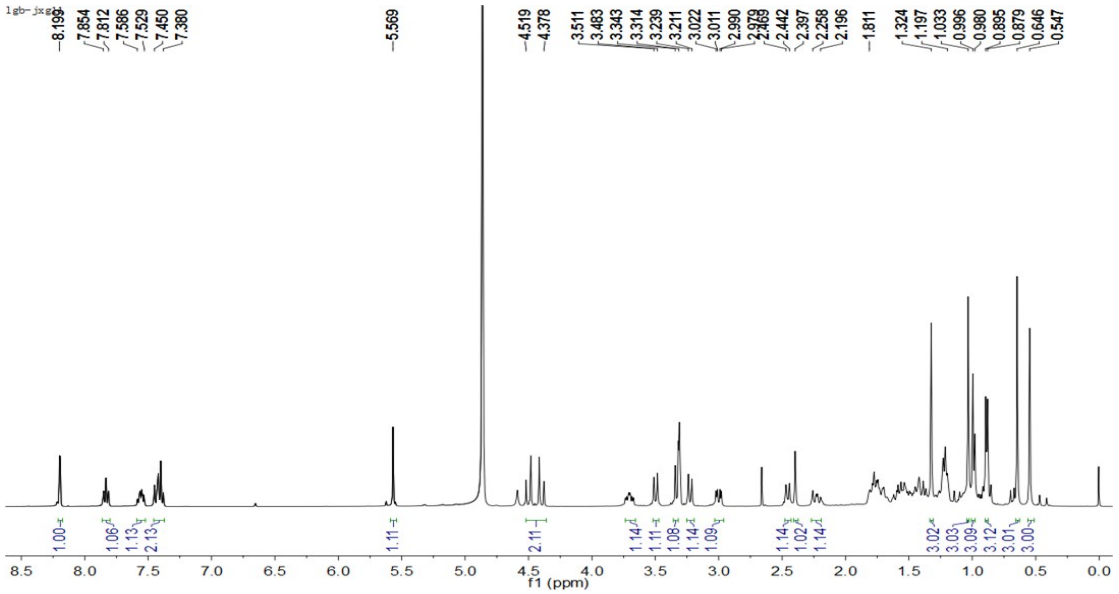
6j

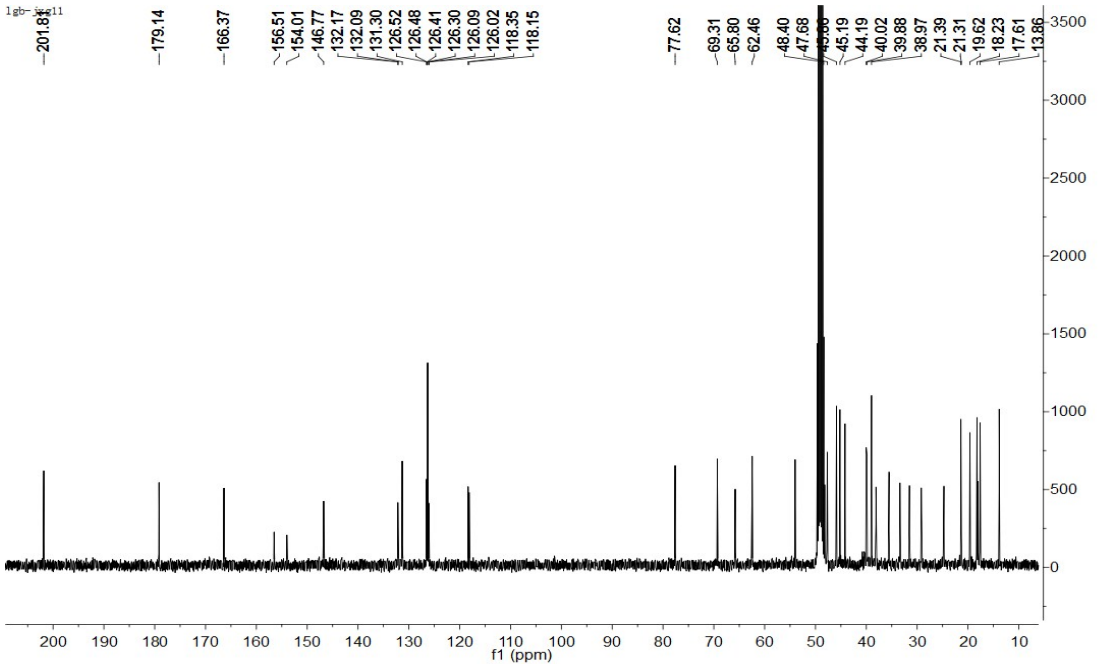

8.10
7.86
7.84
7.59
7.55
7.53
7.48
5.58
4.53
4.41
3.70
3.53
3.50
3.37
3.34
3.26
3.23
3.05
3.04
3.01
2.45
2.43
2.26
2.19
1.82
1.34
1.22
1.13
0.99
0.97
0.89
0.88
0.72
0.68
1.00
1.06
1.11
2.14
1.04
2.16
1.11
1.09
1.08
1.04
1.06
1.05
1.08
1.06
3.16
3.12
3.19
3.02
3.06
3.01
f1 (ppm)

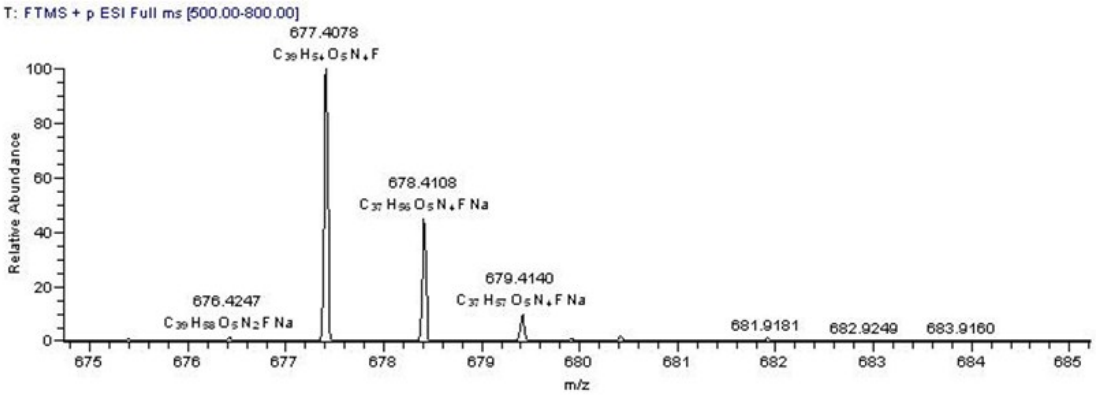

lgb-jxh11
201.78
179.09
166.34
146.22
137.70
135.16
132.85
131.26
129.85
129.36
126.73
119.74
77.60
69.28
65.80
62.47
53.94
48.40
47.67
45.97
45.20
44.19
39.98
39.86
38.98
21.45
21.34
20.04
18.40
17.64
f1 (ppm)


h11_170704161525 #11 RT: 0.04 AV: 1 NL: 9.07E5
T: FTMS + p ESI Full ms [650.00-850.00]
759.3081
C39 H53 O5 N4 Br Na
761.3066
C39 H55 O5 N4 Br Na
760.3111
C39 H54 O5 N4 Br Na
762.3094
C39 H56 O5 N4 Br Na
758.3007
C39 H52 O5 N4 Br Na
757.2993
763.3127
C39 H57 O5 N4 Br Na
764.3741
C39 H58 O5 N4 Br Na
765.5365
766.3715
C39 H60 O5 N4 Br Na
Relative Abundance
m/z

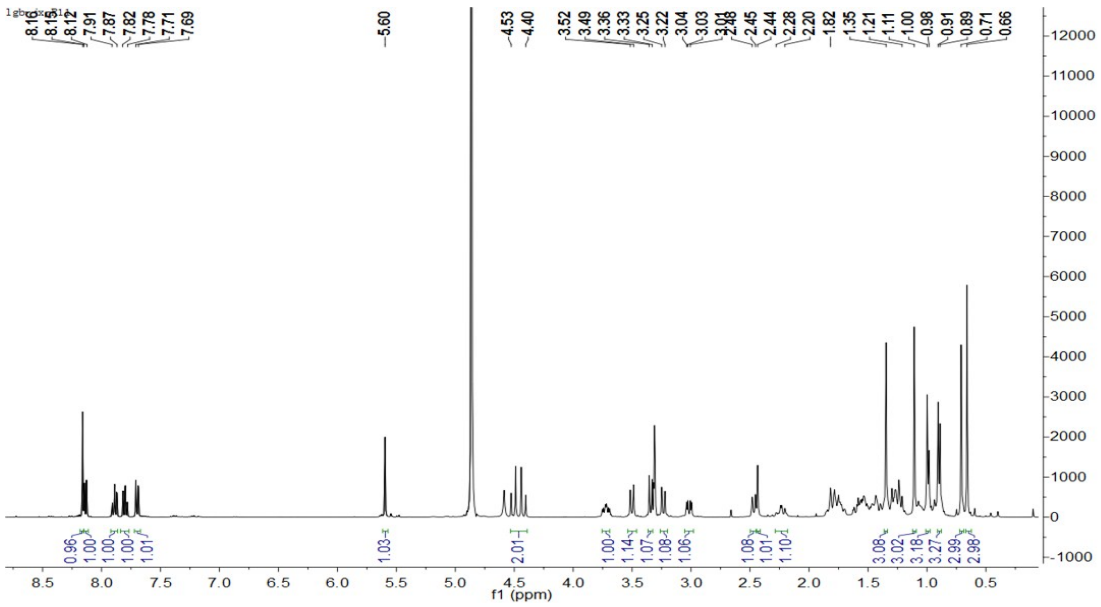
6k

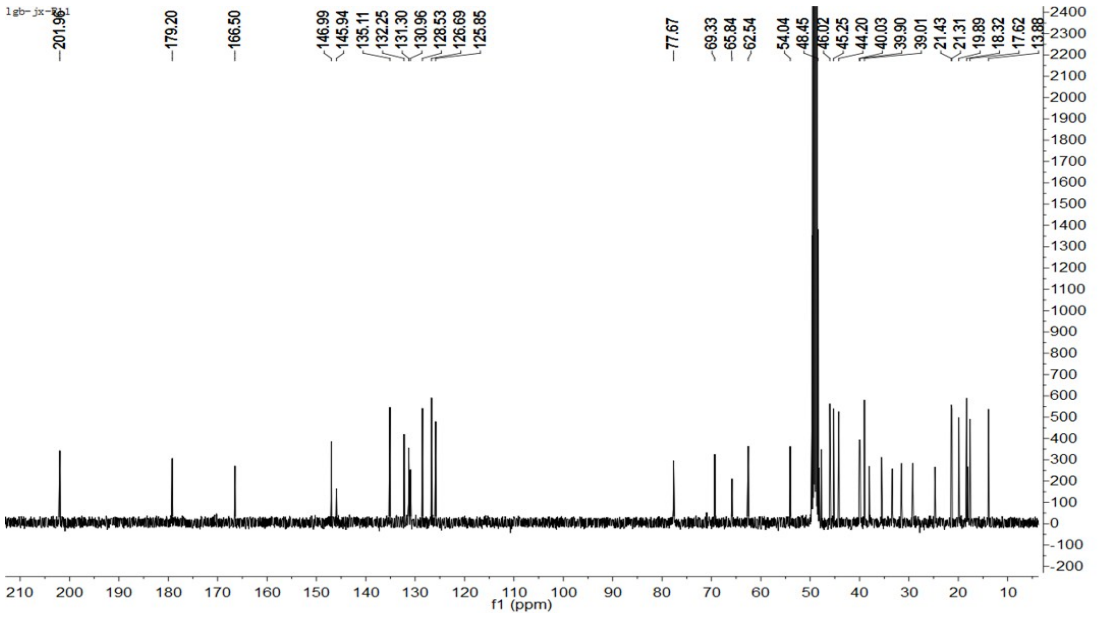

8.199
7.854
7.812
7.586
7.529
7.450
7.380
5.569
4.519
4.378
1.811
f1 (ppm)

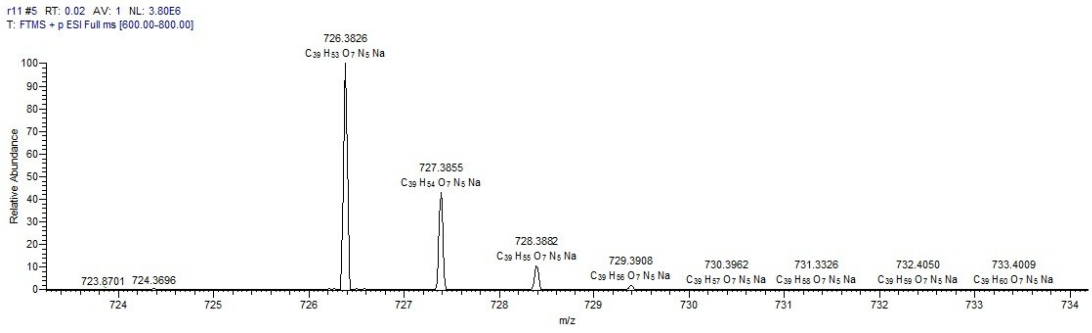

201.83
179.14
166.37
156.51
154.01
146.77
132.17
132.09
131.30
126.52
126.48
126.41
126.30
126.09
126.02
118.35
118.15
77.62
69.31
65.80
62.46
48.40
47.68
45.19
44.19
40.02
39.88
38.97
21.39
21.31
19.62
18.23
17.61
13.86
f1 (ppm)


T: FTMS + p ESI Full ms [500.00-800.00]
677.4078
C39H54O5N4F
678.4108
C37H56O5N4FNa
679.4140
C37H57O5N4FNa
676.4247
C39H58O5N2FNa
681.9181
682.9249
683.9160
Relative Abundance
m/z

6l


8.16
8.15
8.12
7.91
7.87
7.82
7.78
7.71
7.69
5.60
4.53
4.40
3.52
3.49
3.36
3.33
3.25
3.22
3.04
3.03
3.01
2.48
2.45
2.44
2.28
2.20
1.82
1.35
1.21
1.11
1.00
0.98
0.91
0.89
0.71
0.66
0.96
1.00
1.00
1.00
1.01
1.03
2.01
1.00
1.14
1.07
1.08
1.06
1.08
1.01
1.10
3.08
3.02
3.18
3.27
2.99
2.98
f1 (ppm)


201.96
179.20
166.50
146.99
145.94
135.11
132.25
131.30
130.96
128.53
126.69
125.85
77.67
69.33
65.84
62.54
54.04
48.45
46.02
45.25
44.20
40.03
39.90
39.01
21.43
21.31
19.89
18.32
17.62
13.88
f1 (ppm)


r11 #5 RT: 0.02 AV: 1 NL: 3.80E6
T: FTMS + p ESI Full ms [600.00-800.00]
726.3826
C39 H53 O7 N5 Na
727.3855
C39 H54 O7 N5 Na
728.3882
C39 H55 O7 N5 Na
729.3908
C39 H56 O7 N5 Na
730.3962
C39 H57 O7 N5 Na
731.3326
C39 H58 O7 N5 Na
732.4050
C39 H59 O7 N5 Na
733.4009
C39 H60 O7 N5 Na
723.8701
724.3696
Relative Abundance
m/z