Supplementary Information

Design, synthesis, crystal structure, and herbicidal activity of Novel pyrrolidine-2,4-dione derivatives incorporating an alkyl ether pharmacophore with natural tetramic acids as lead compounds

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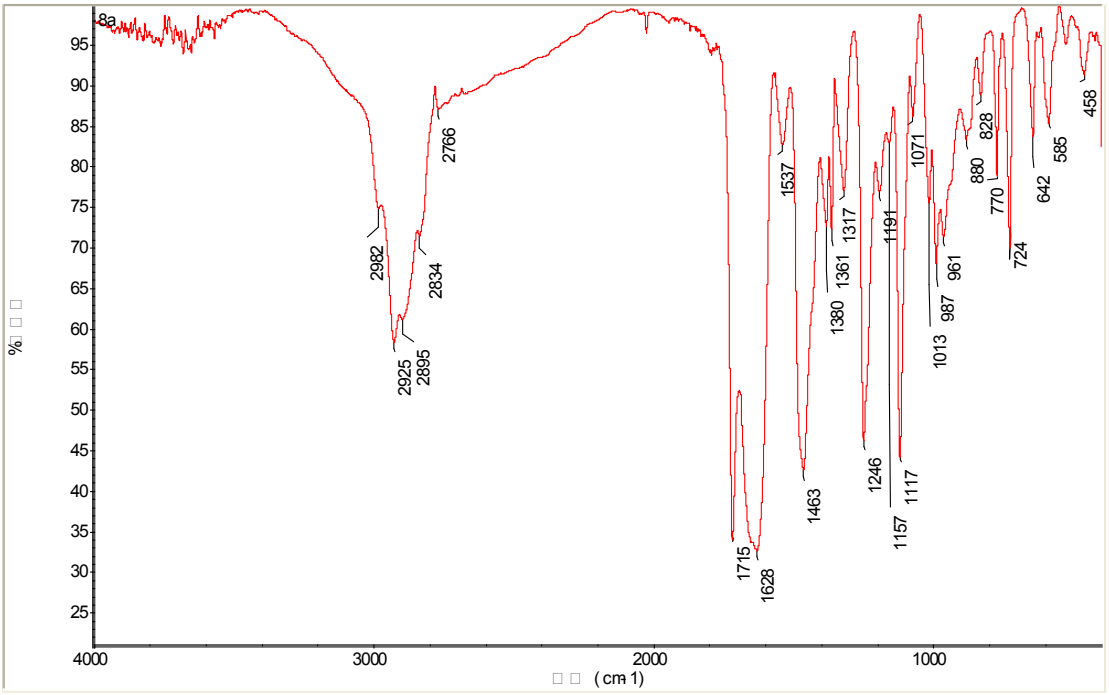
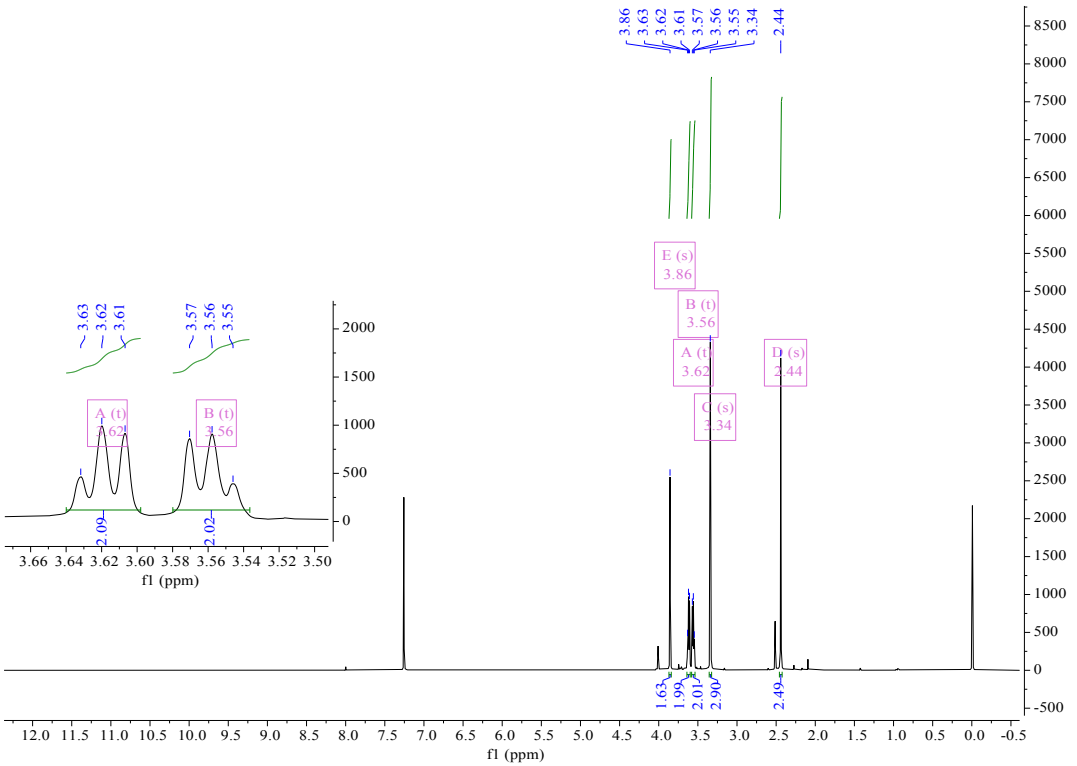
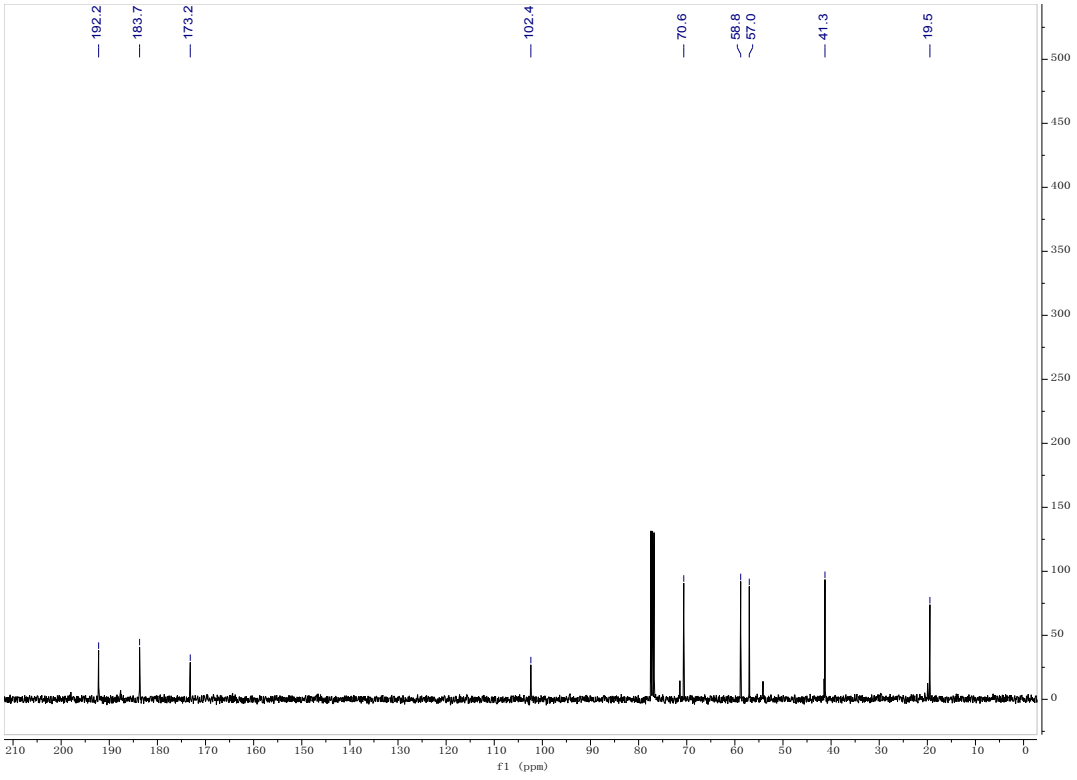
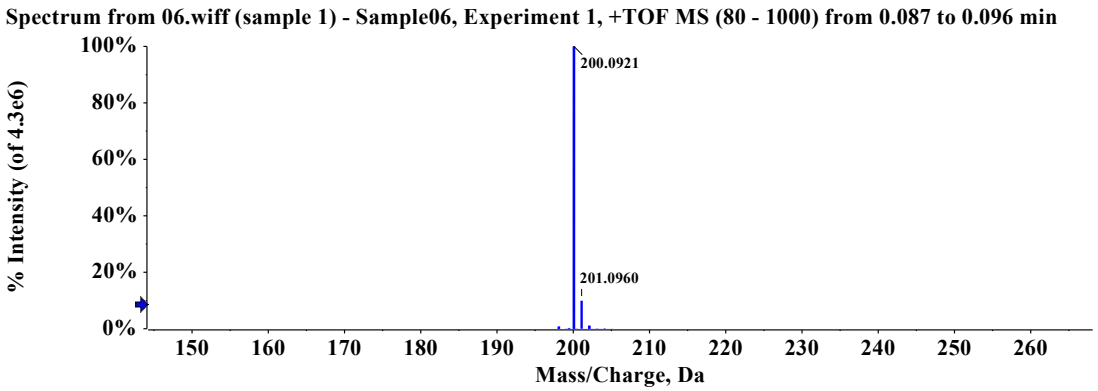
1. Spectrograms of title compounds

Compound 4a:

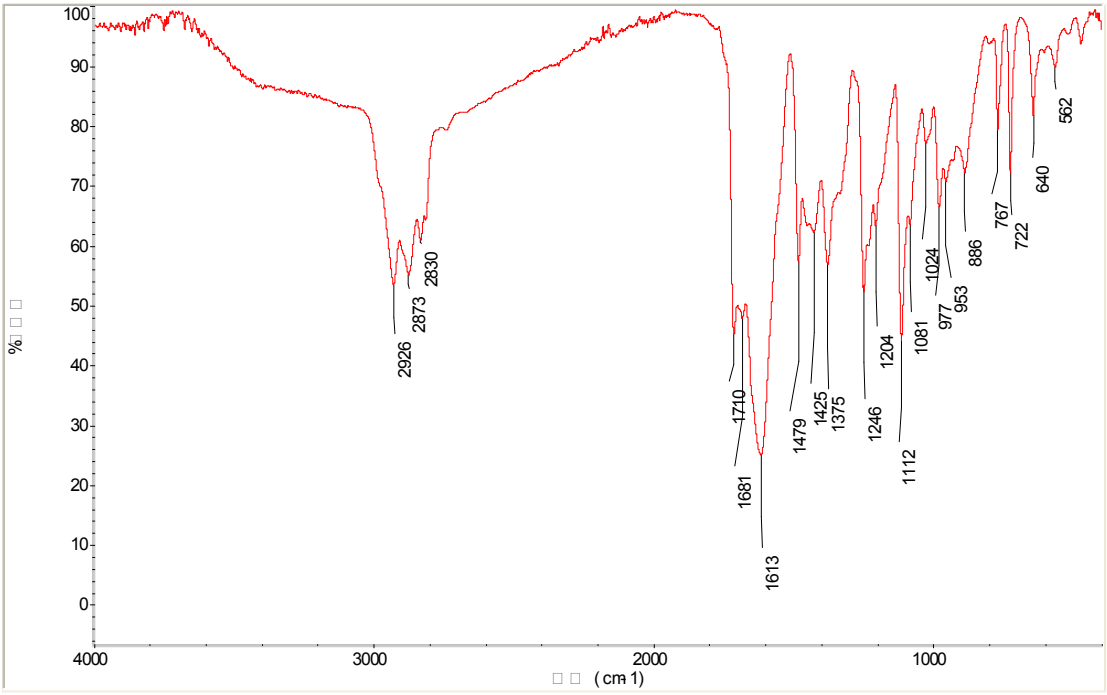


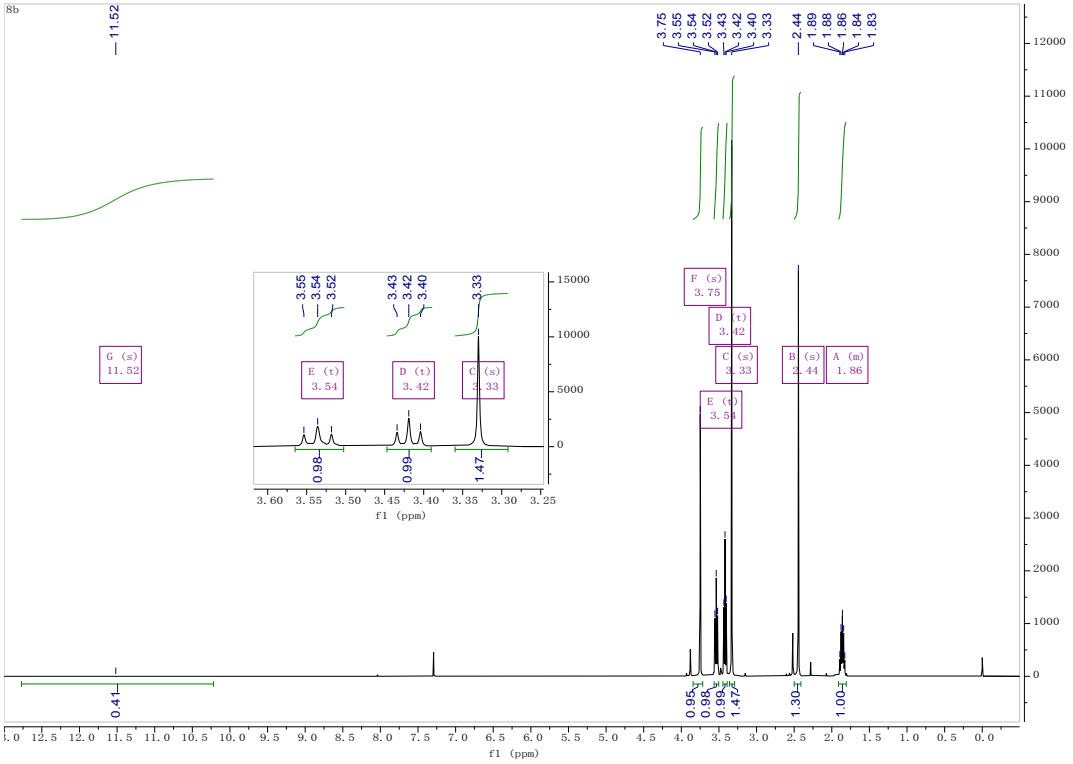

3.86
3.63
3.62
3.61
3.57
3.56
3.55
3.34
2.44
E (s)
3.86
B (t)
3.56
A (t)
3.62
D (s)
2.44
C (s)
3.34
1.63
1.99
2.01
2.90
2.49
f1 (ppm)

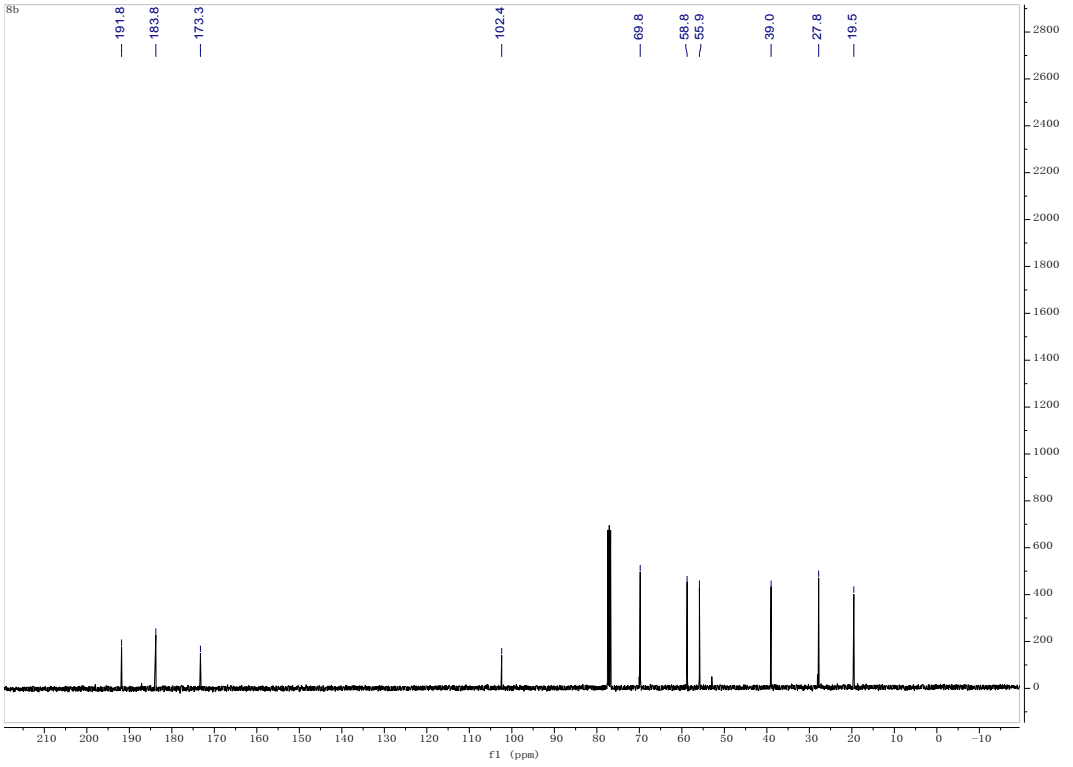

192.2
183.7
173.2
102.4
70.6
58.8
57.0
41.3
19.5
f1 (ppm)

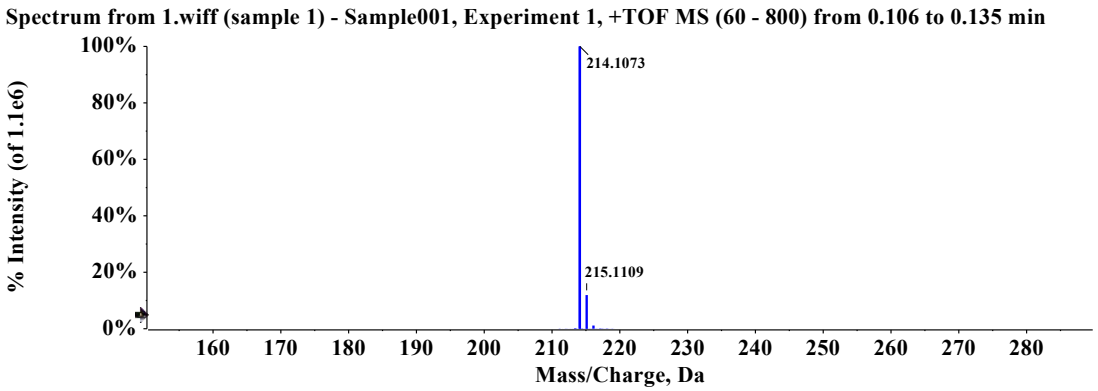

Spectrum from 06.wiff (sample 1) - Sample06, Experiment 1, +TOF MS (80 - 1000) from 0.087 to 0.096 min
% Intensity (of 4.3e6)
100%
80%
60%
40%
20%
0%
200.0921
201.0960
150
160
170
180
190
200
210
220
230
240
250
260
Mass/Charge, Da

Compound 4b：

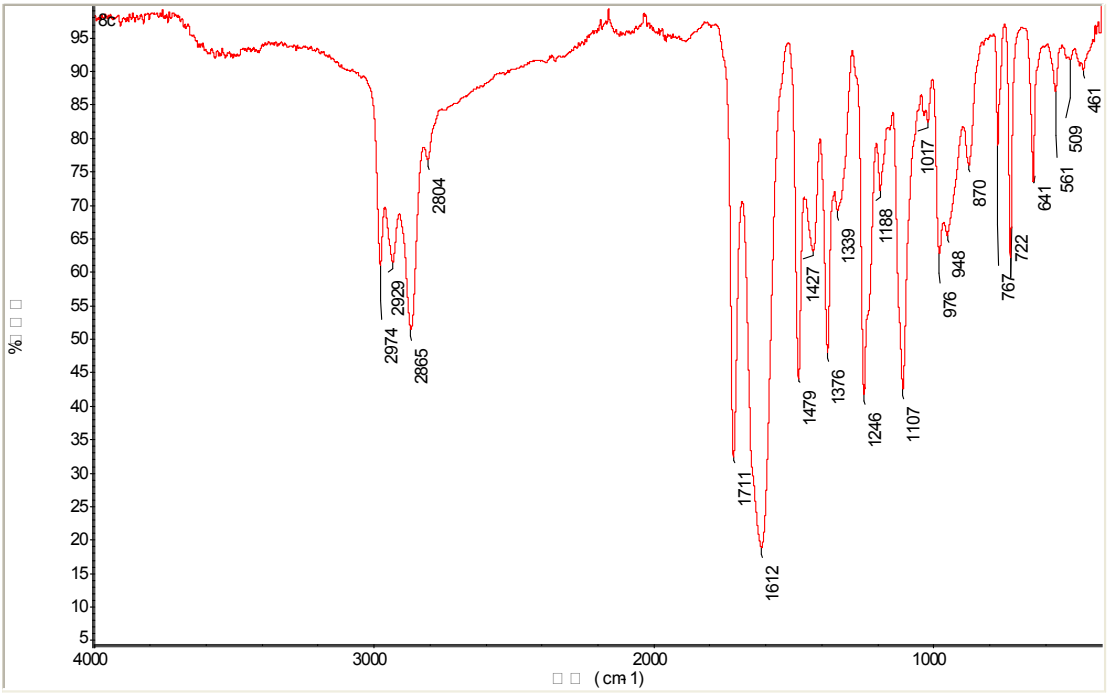

100
90
80
70
60
50
40
30
20
10
0
%
2926
2873
2830
1710
1681
1613
1479
1425
1375
1246
1204
1112
1081
1024
977
953
886
767
722
640
562
4000
3000
2000
1000
(cm-1)

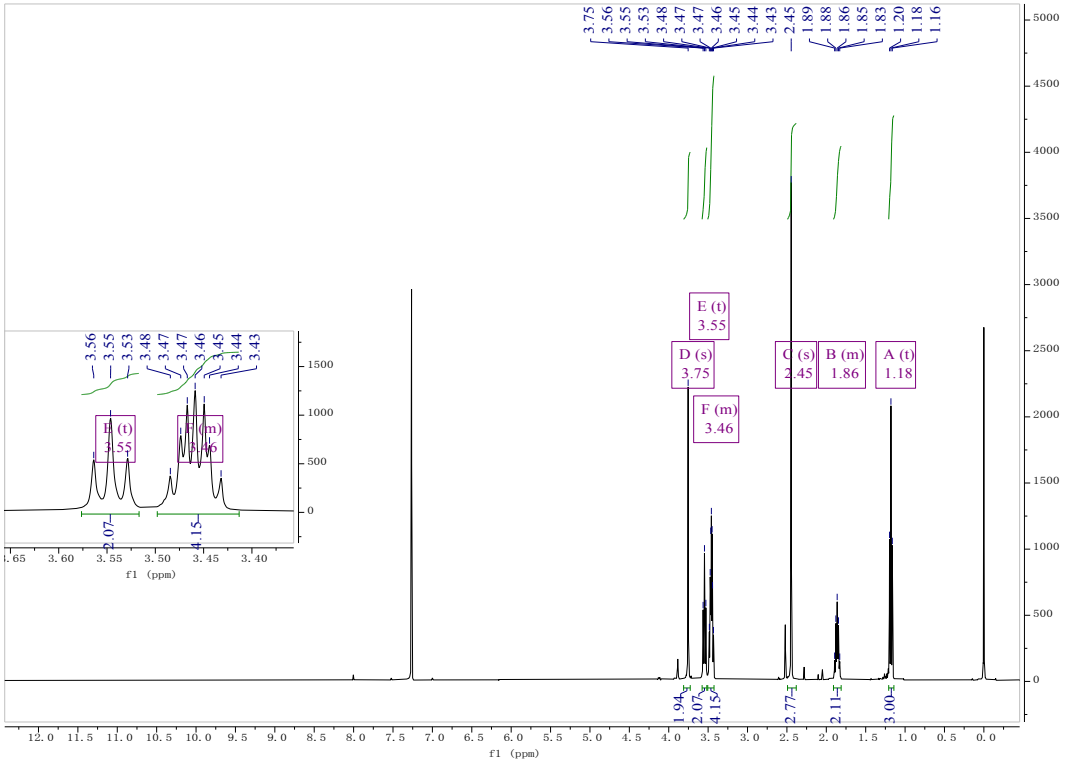

8b
11.52
3.75
3.55
3.54
3.52
3.43
3.42
3.40
3.33
2.44
1.89
1.88
1.86
1.84
1.83
G (s) 11.52
E (t) 3.54
D (t) 3.42
C (s) 3.33
F (s) 3.75
B (s) 2.44
A (m) 1.86
0.41
0.98
0.99
1.47
0.95
1.30
1.00
f1 (ppm)

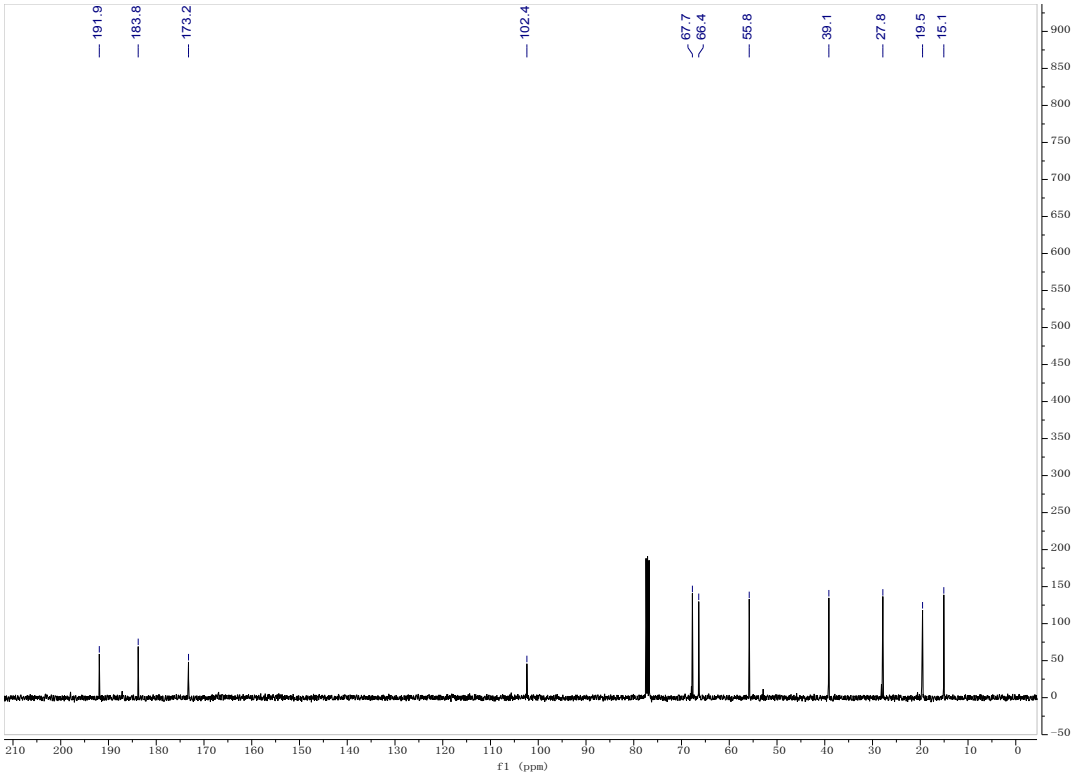

8b
191.8
183.8
173.3
102.4
69.8
58.8
55.9
39.0
27.8
19.5
f1 (ppm)

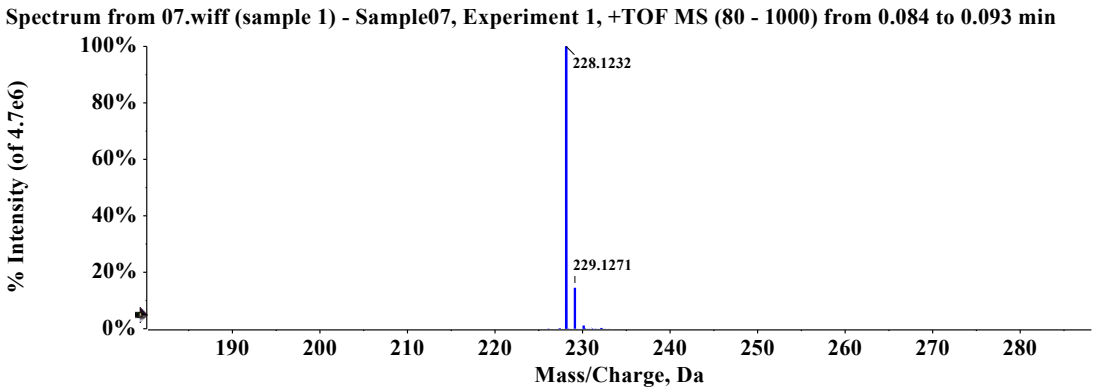

Spectrum from 1.wiff (sample 1) - Sample001, Experiment 1, +TOF MS (60 - 800) from 0.106 to 0.135 min
% Intensity (of 1.1e6)
100%
80%
60%
40%
20%
0%
214.1073
215.1109
160
170
180
190
200
210
220
230
240
250
260
270
280
Mass/Charge, Da

Compound 4c：

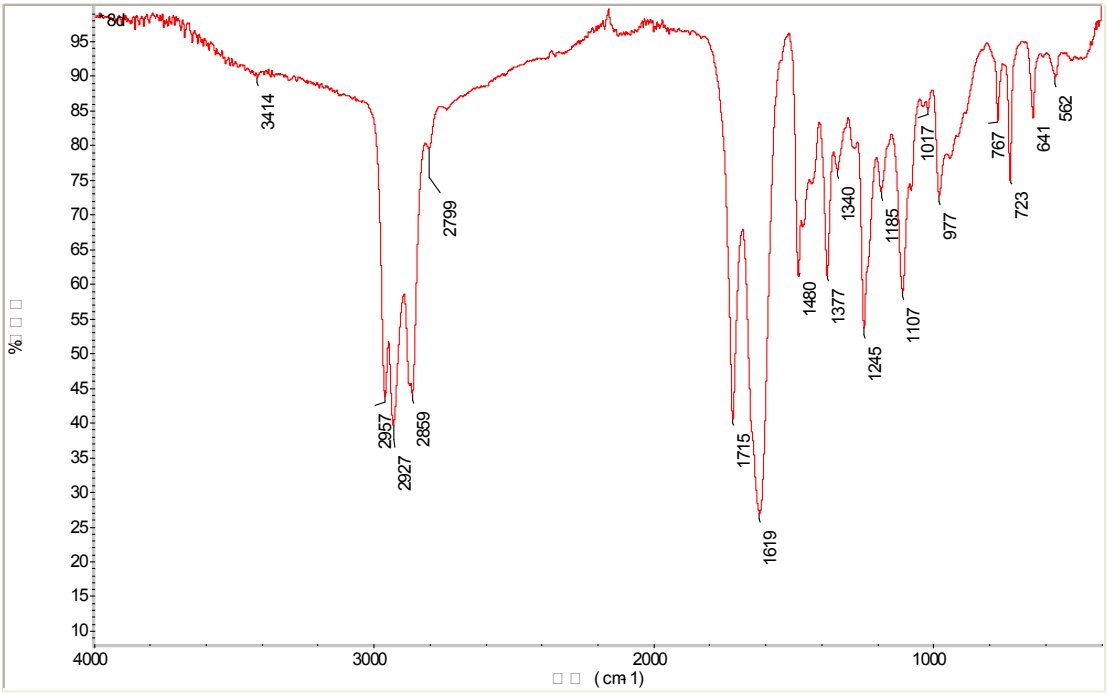

4c
%
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
2974
2929
2865
2804
1711
1612
1479
1427
1376
1339
1246
1188
1107
1017
976
948
870
767
722
641
561
509
461
4000
3000
2000
1000
(cm-1)

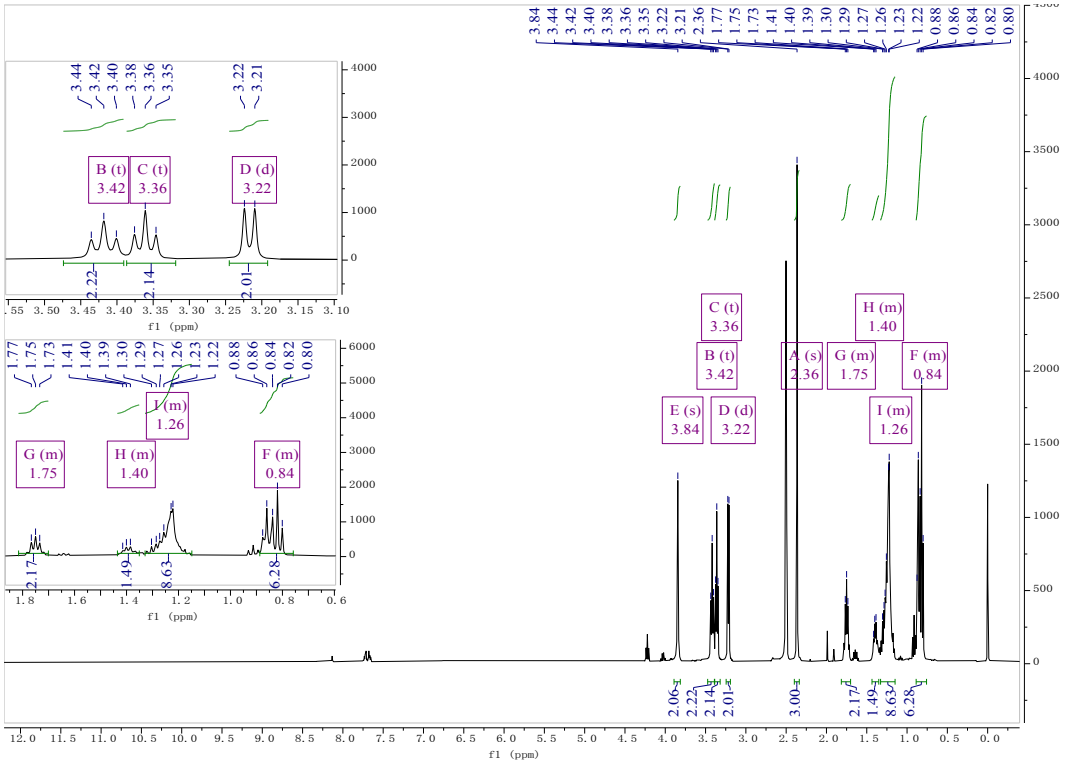

E (t)
3.55
D (s)
3.75
F (m)
3.46
C (s)
2.45
B (m)
1.86
A (t)
1.18
f1 (ppm)

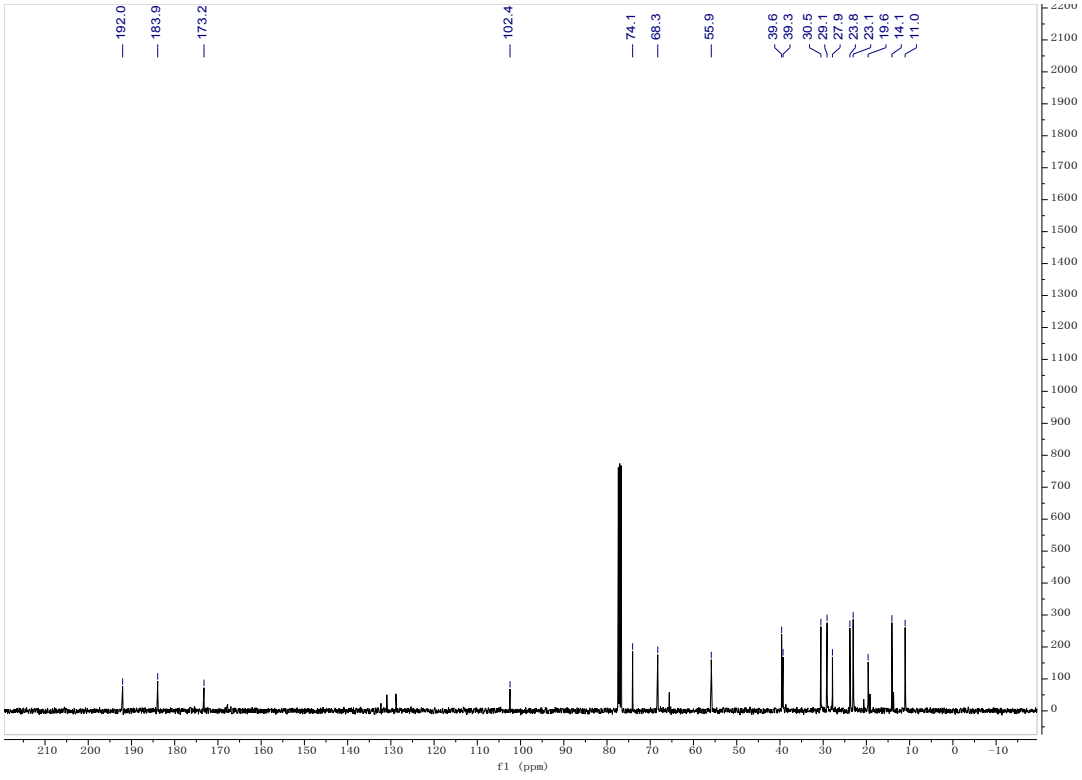

191.9
183.8
173.2
102.4
67.7
66.4
55.8
39.1
27.8
19.5
15.1
f1 (ppm)

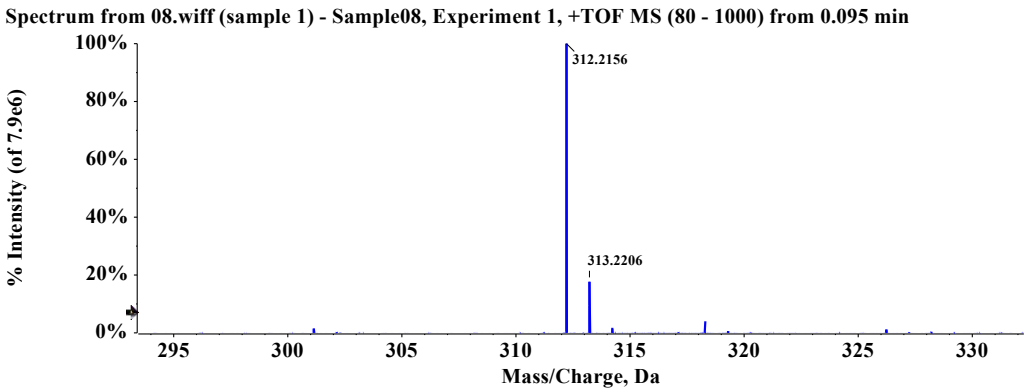

Spectrum from 07.wiff (sample 1) - Sample07, Experiment 1, +TOF MS (80 - 1000) from 0.084 to 0.093 min
% Intensity (of 4.7e6)
100%
80%
60%
40%
20%
0%
228.1232
229.1271
190
200
210
220
230
240
250
260
270
280
Mass/Charge, Da

Compound 4d:

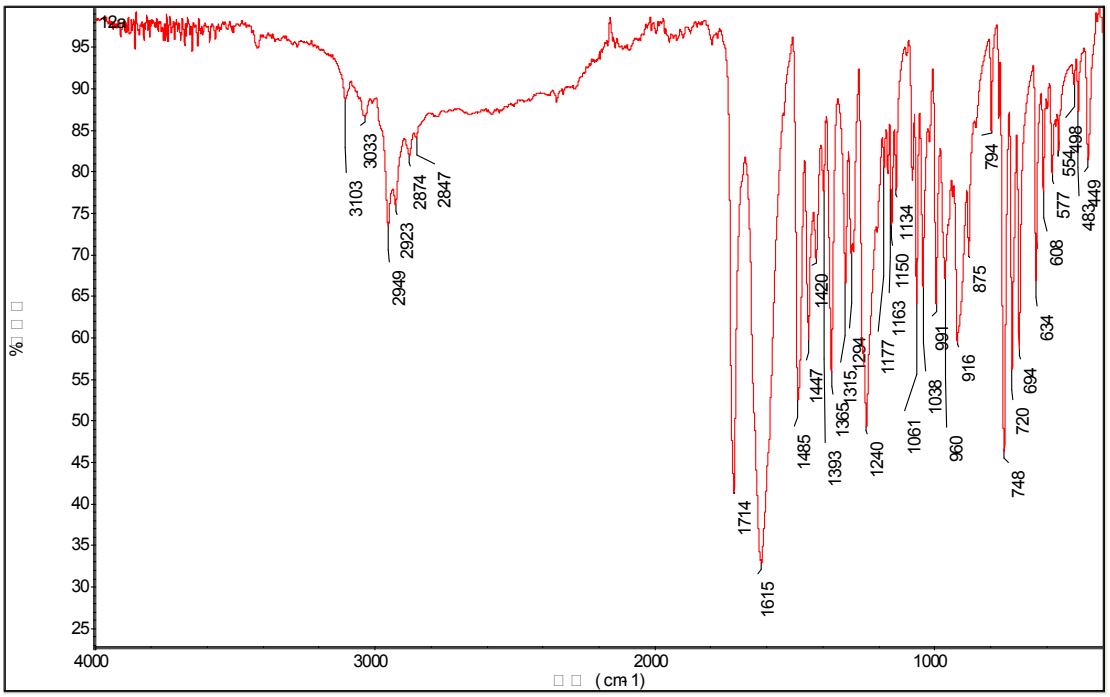

8d
%
3414
2957
2927
2859
2799
1715
1619
1480
1377
1340
1245
1185
1107
1017
977
767
723
641
562
4000
3000
2000
1000
(cm-1)

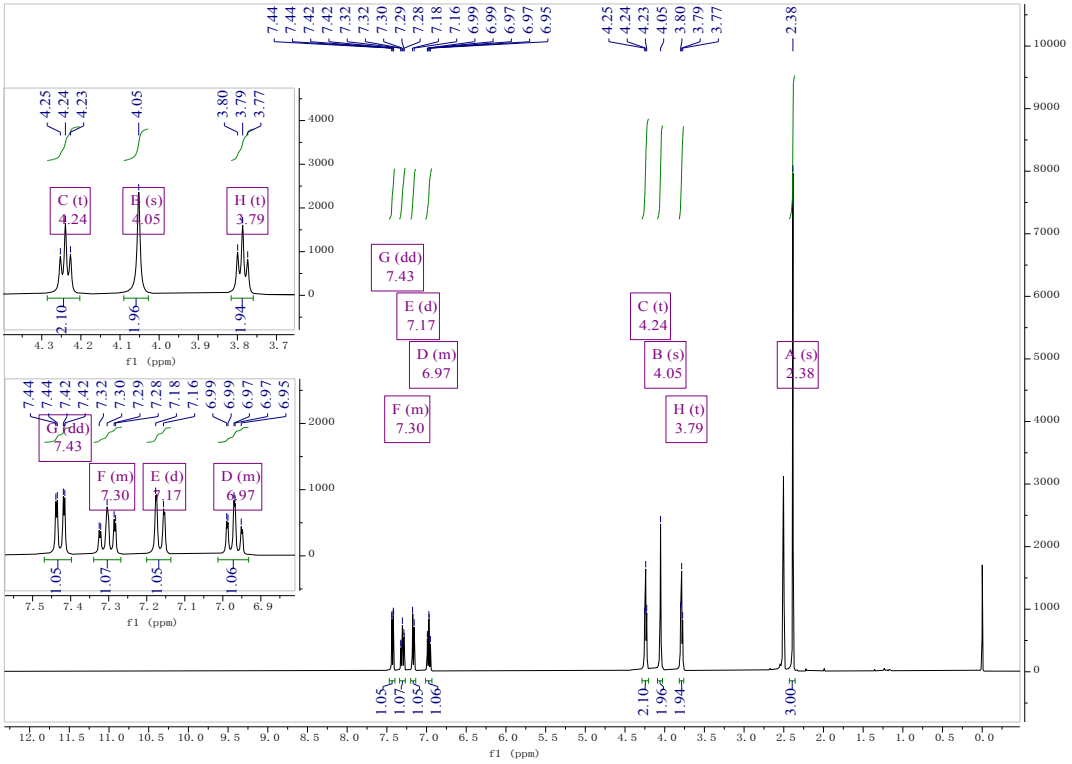

B (t) 3.42
C (t) 3.36
D (d) 3.22
I (m) 1.26
G (m) 1.75
H (m) 1.40
F (m) 0.84
E (s) 3.84
A (s) 2.36
f1 (ppm)

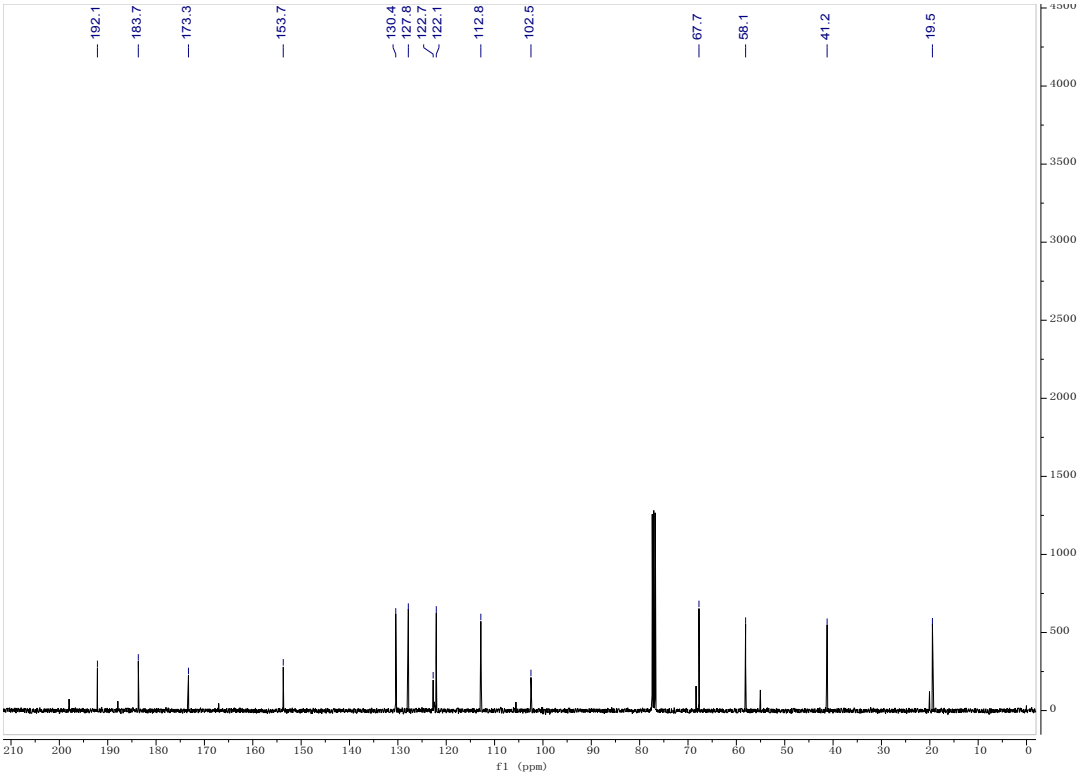

192.0
183.9
173.2
102.4
74.1
68.3
55.9
39.6
39.3
30.5
29.1
27.9
23.8
23.1
19.6
14.1
11.0
f1 (ppm)

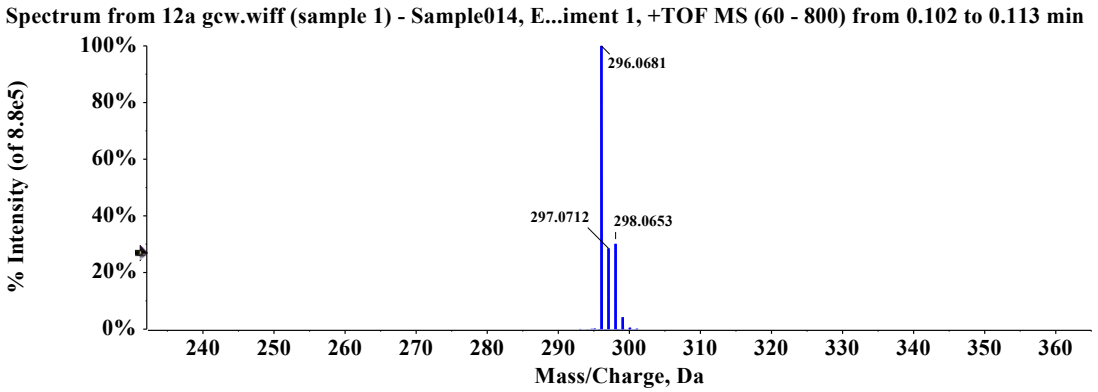


Compound 10a：

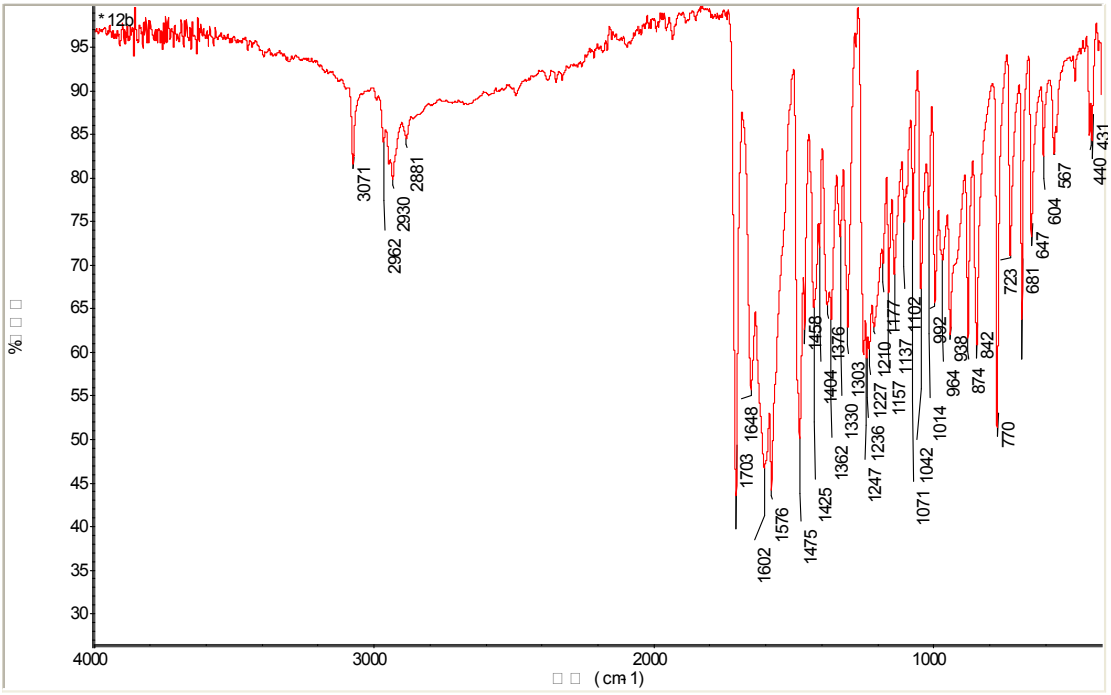


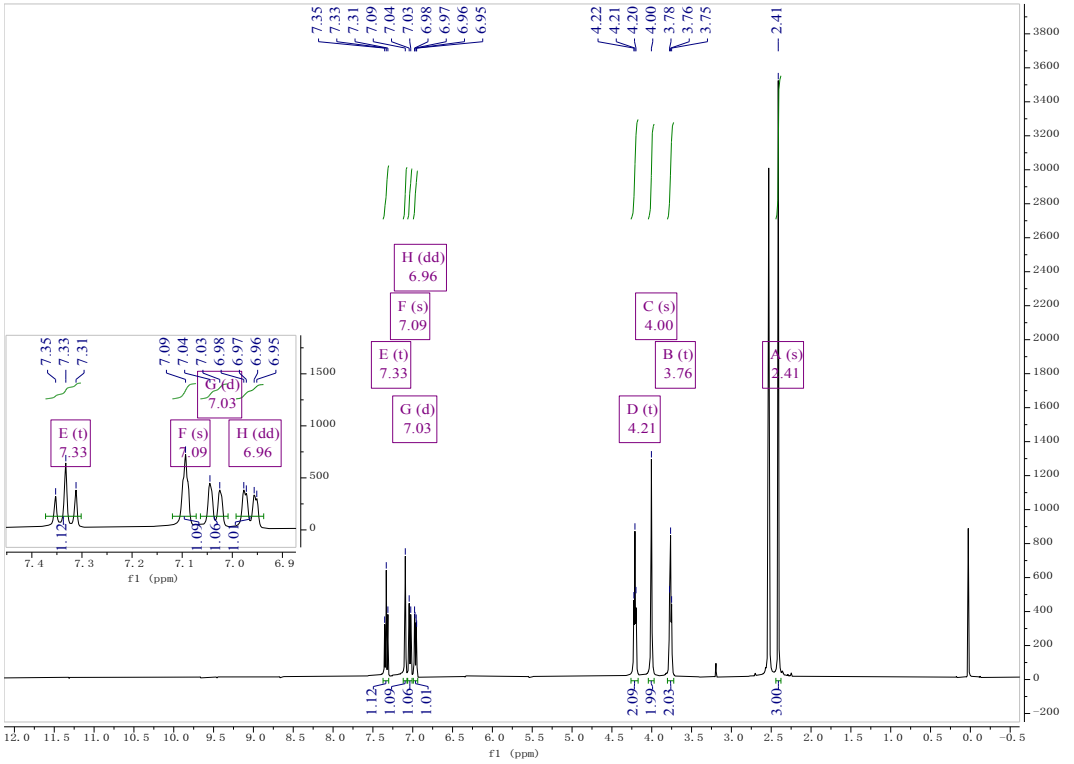

G (dd) 7.43
E (d) 7.17
D (m) 6.97
F (m) 7.30
C (t) 4.24
B (s) 4.05
H (t) 3.79
A (s) 2.38
f1 (ppm)

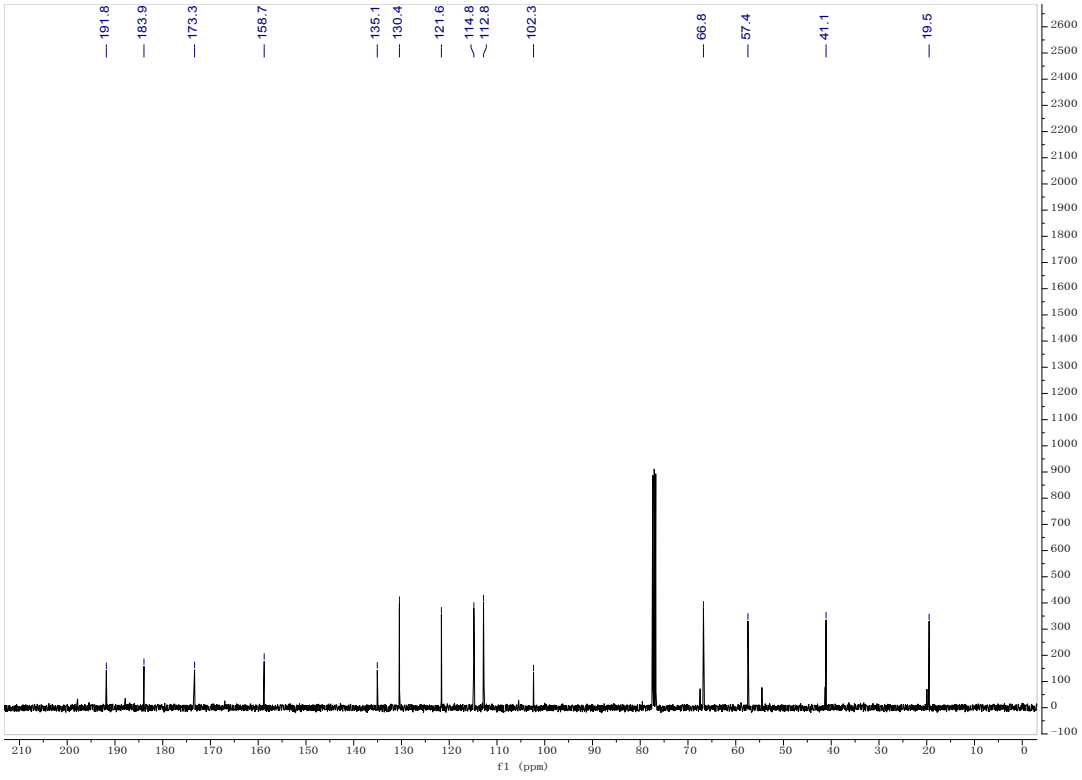

192.1
183.7
173.3
153.7
130.4
127.8
122.7
122.1
112.8
102.5
67.7
58.1
41.2
19.5
f1 (ppm)

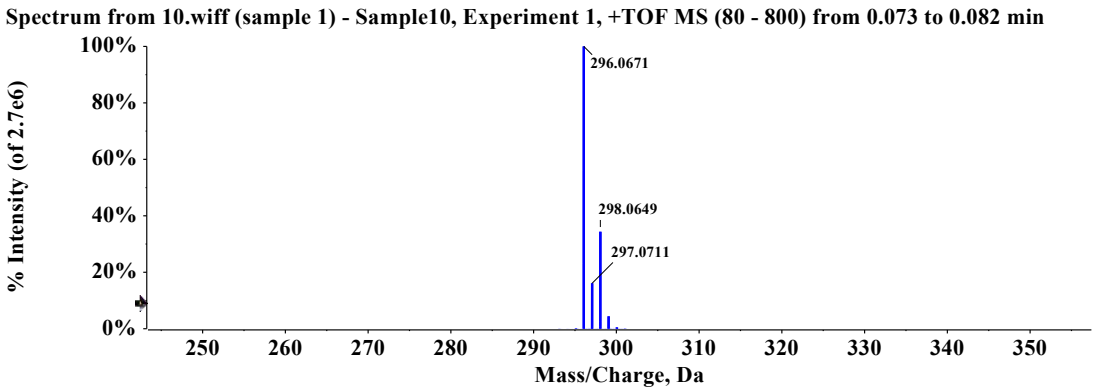


Compound 10b：

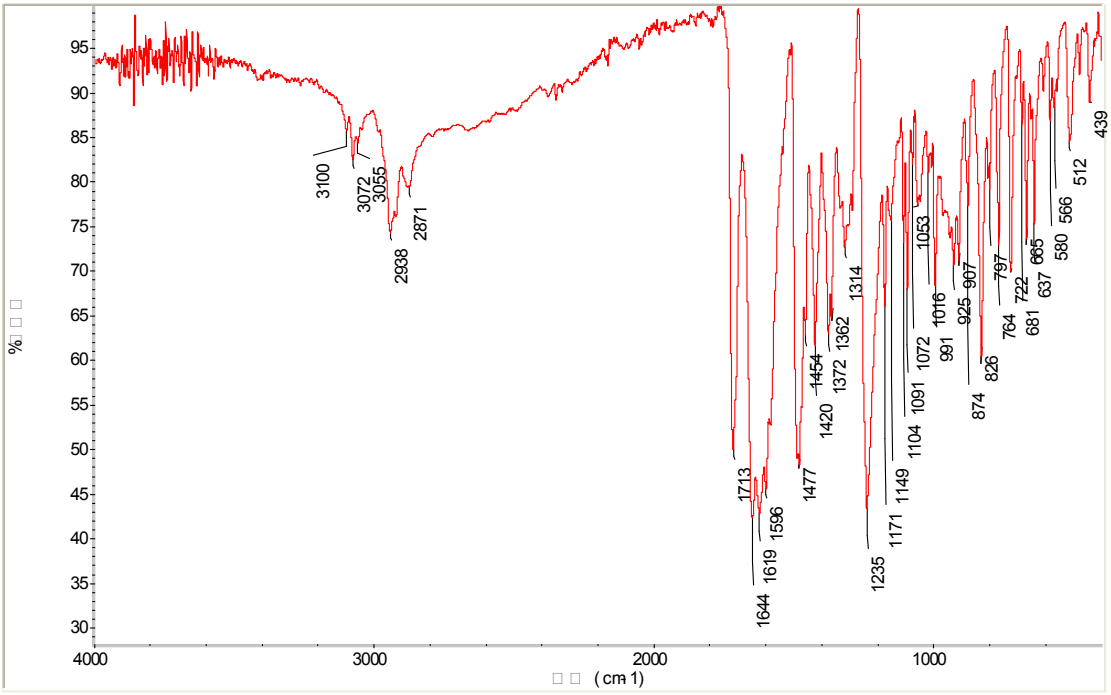


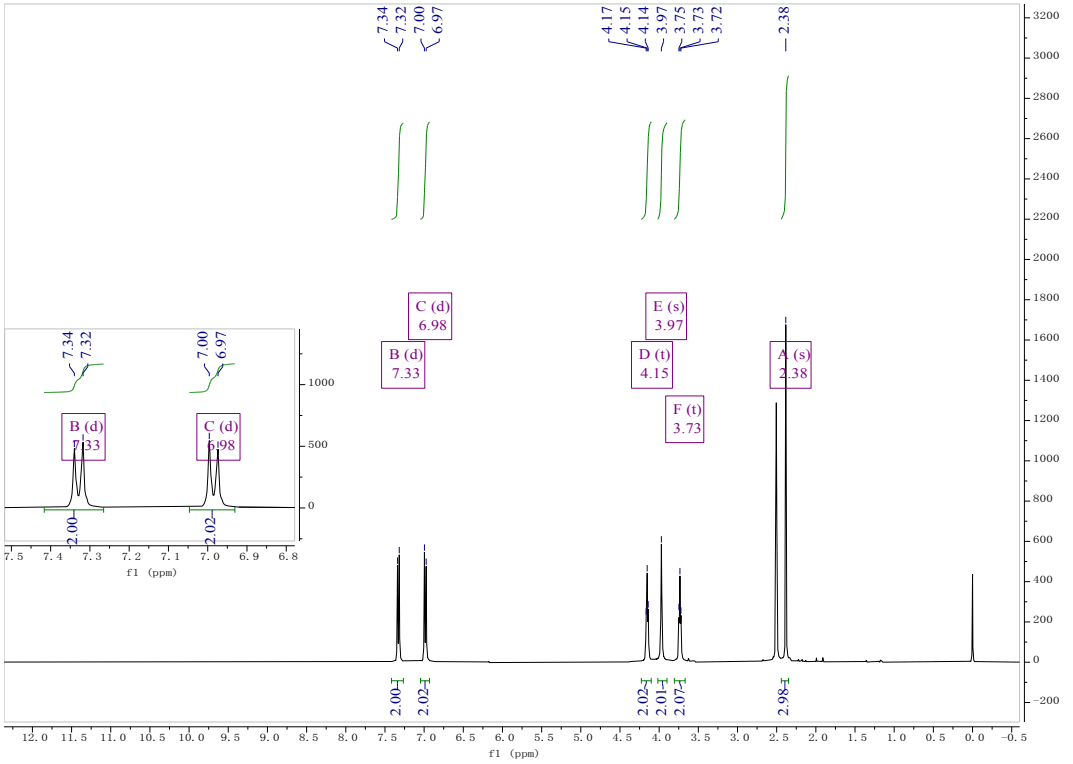

7.35
7.33
7.31
7.09
7.04
7.03
6.98
6.97
6.96
6.95
4.22
4.21
4.20
4.00
3.78
3.76
3.75
2.41
H (dd) 6.96
F (s) 7.09
E (t) 7.33
G (d) 7.03
C (s) 4.00
B (t) 3.76
A (s) 2.41
D (t) 4.21
1.12
1.09
1.06
1.01
2.09
1.99
2.03
3.00
f1 (ppm)

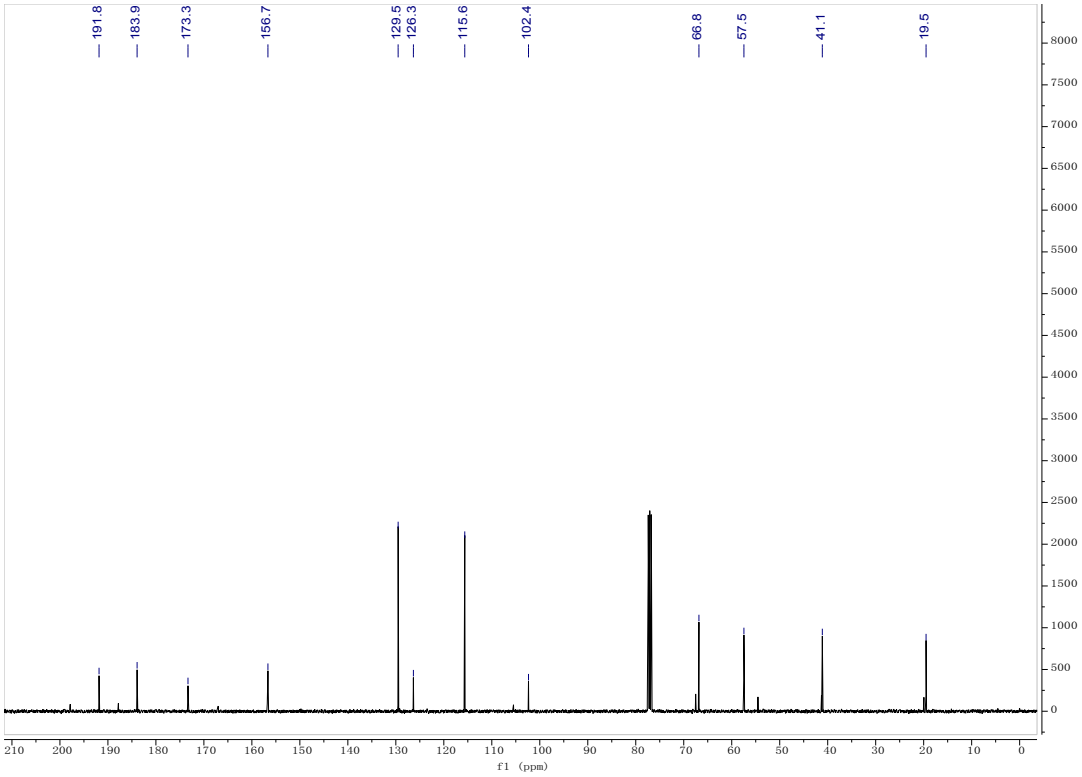

191.8
183.9
173.3
158.7
135.1
130.4
121.6
114.8
112.8
102.3
66.8
57.4
41.1
19.5
f1 (ppm)

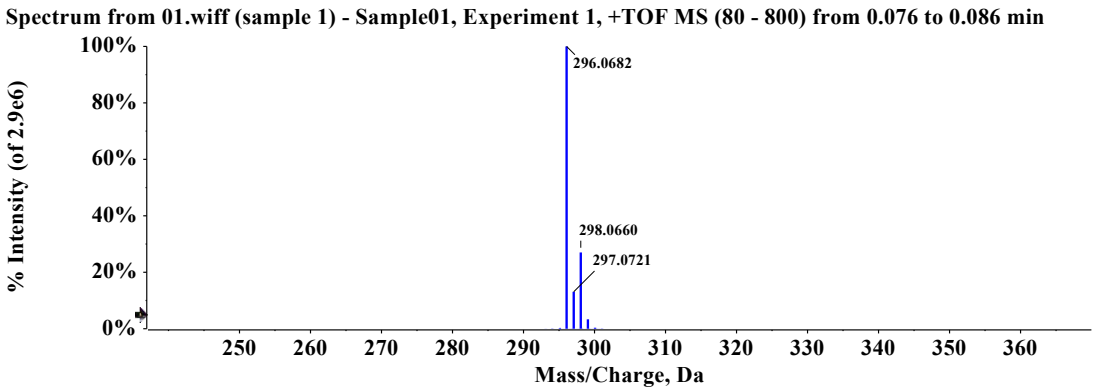


Compound 10c：

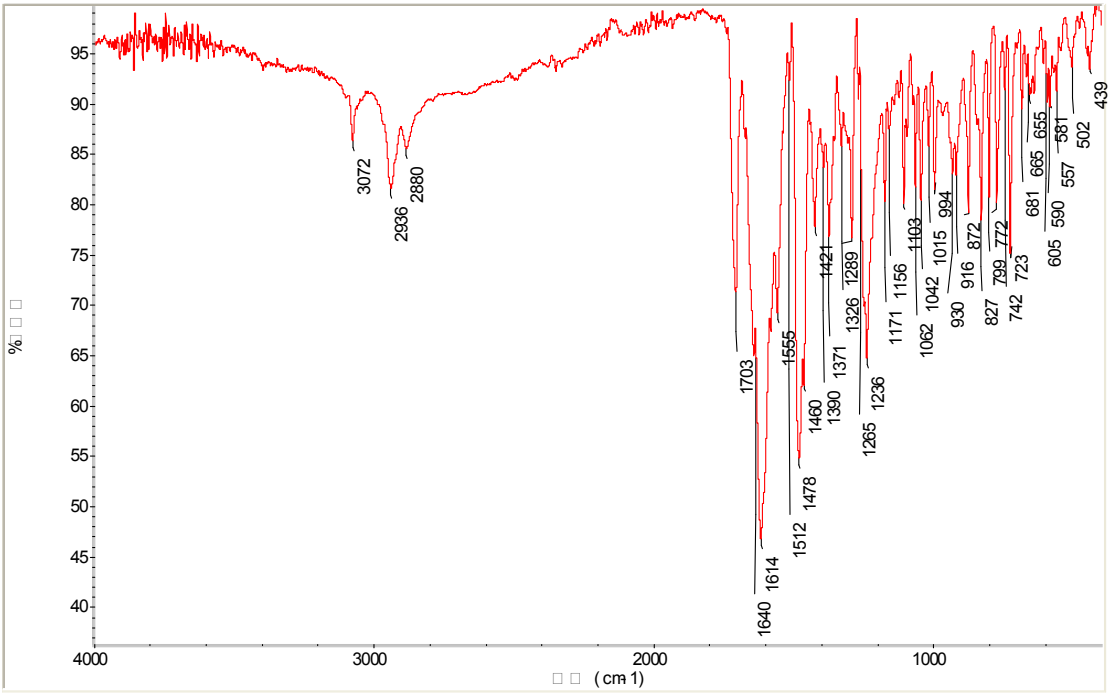


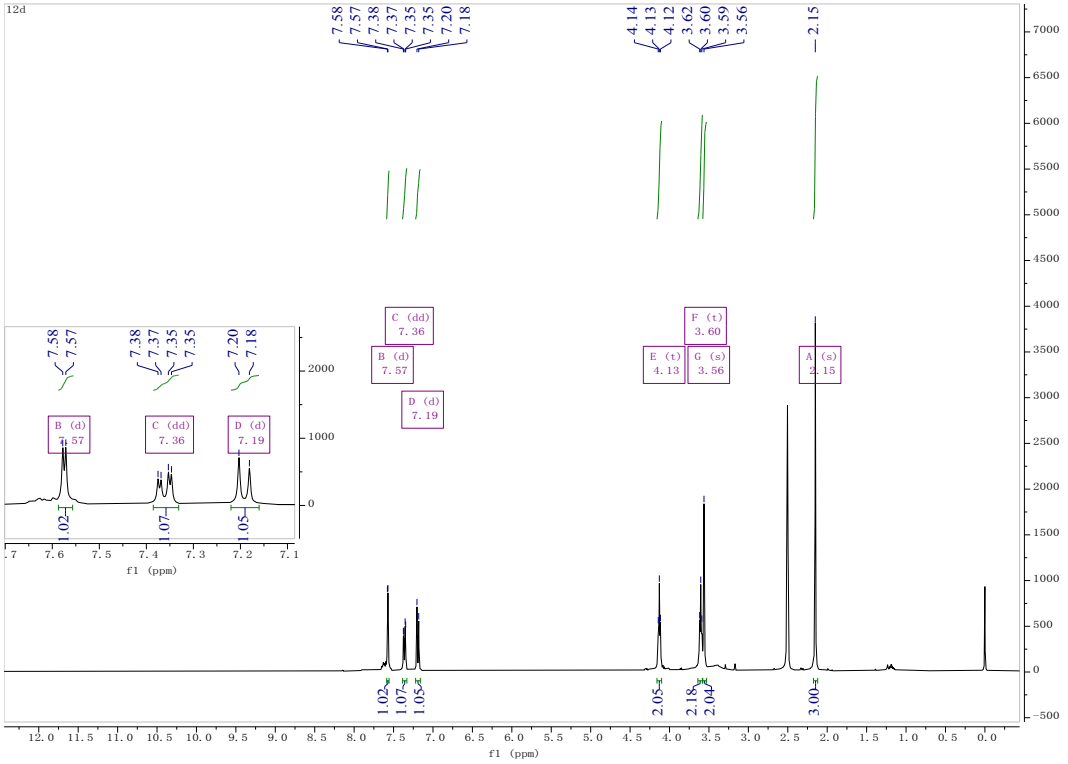

7.34
7.32
7.00
6.97
4.17
4.15
4.14
3.97
3.75
3.73
3.72
2.38
C (d)
6.98
B (d)
7.33
E (s)
3.97
D (t)
4.15
F (t)
3.73
A (s)
2.38
2.00
2.02
2.00
2.02
2.01
2.07
2.98
f1 (ppm)

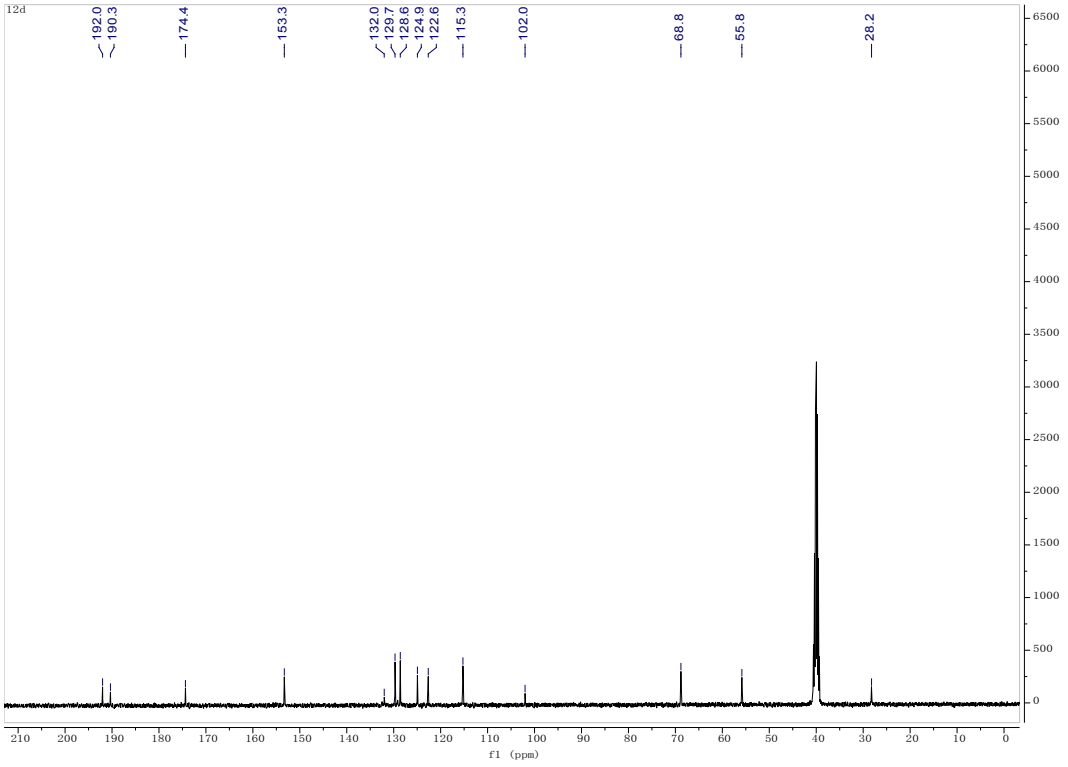

191.8
183.9
173.3
156.7
129.5
126.3
115.6
102.4
66.8
57.5
41.1
19.5
f1 (ppm)

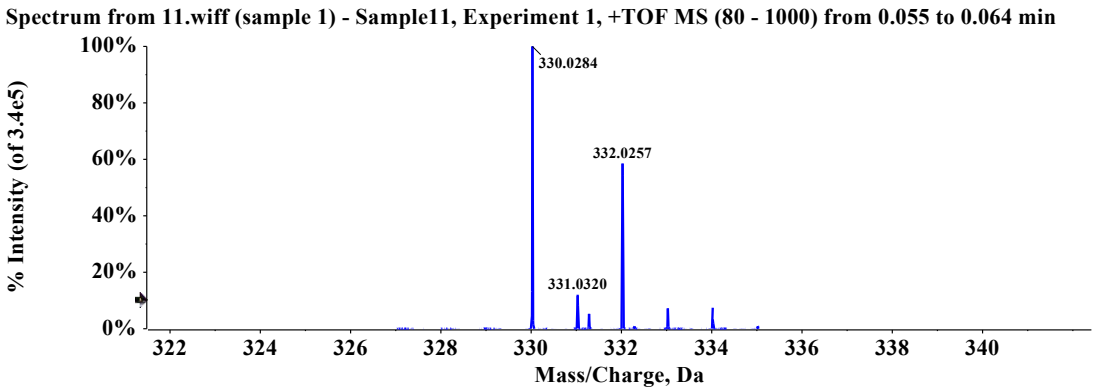


Compound 10d：

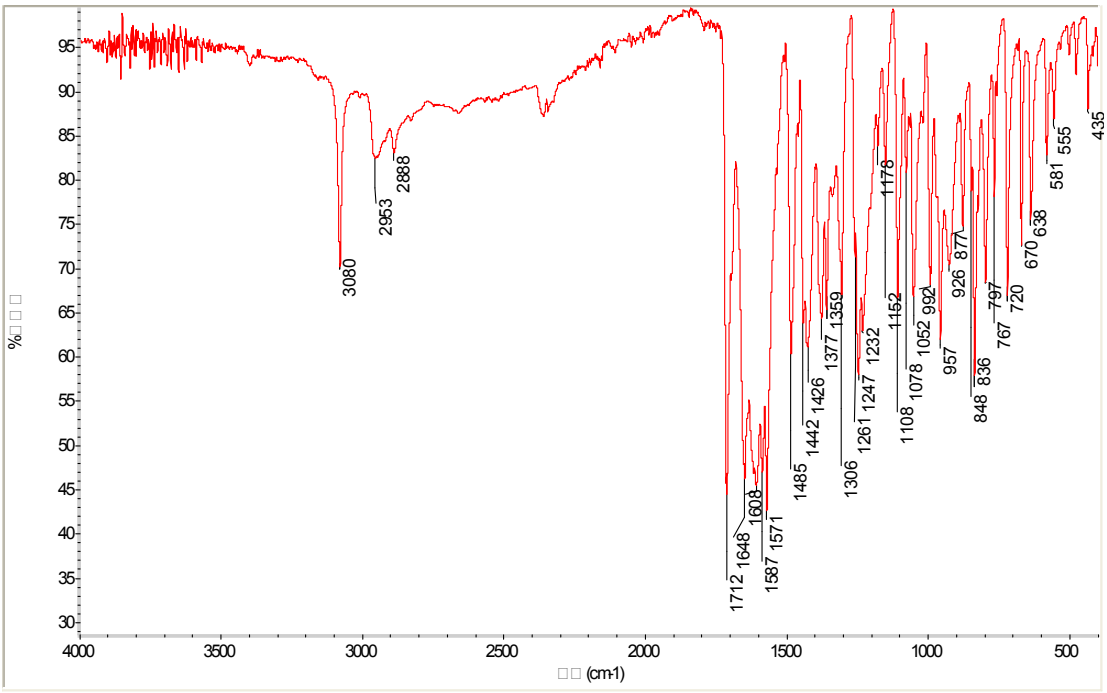


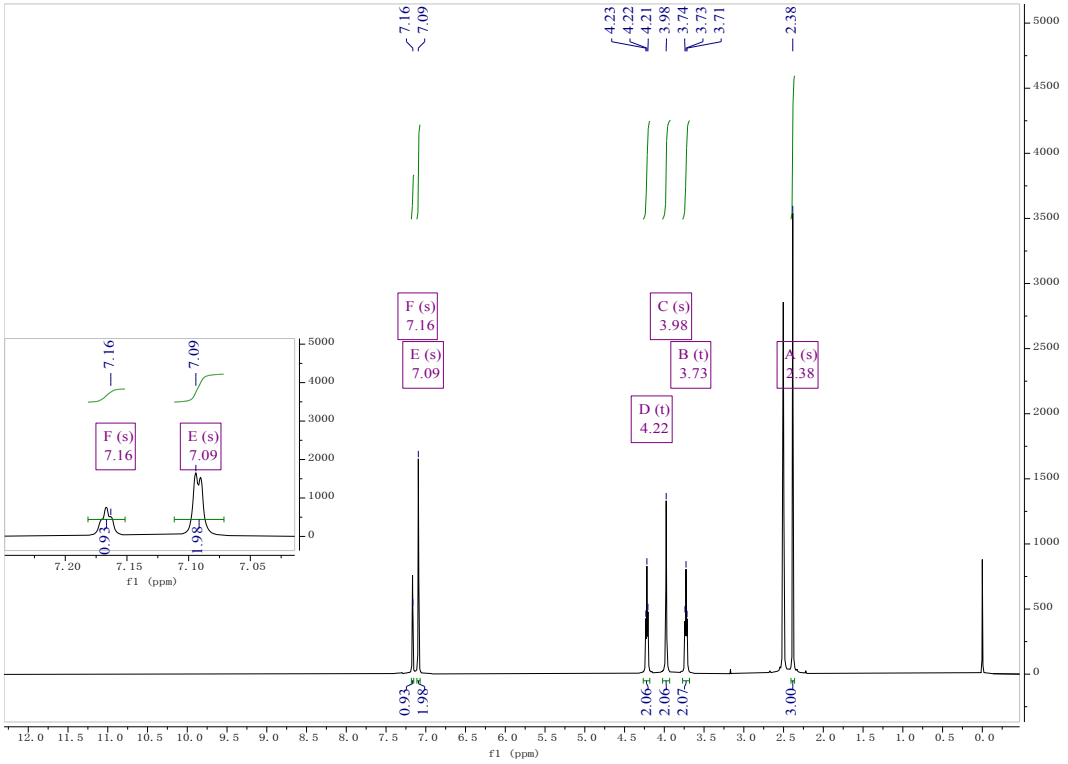

12d
7.58
7.57
7.38
7.37
7.35
7.35
7.20
7.18
4.14
4.13
4.12
3.62
3.60
3.59
3.56
2.15
C (dd) 7.36
B (d) 7.57
D (d) 7.19
F (t) 3.60
E (t) 4.13
G (s) 3.56
A (s) 2.15
1.02
1.07
1.05
2.05
2.18
2.04
3.00
f1 (ppm)

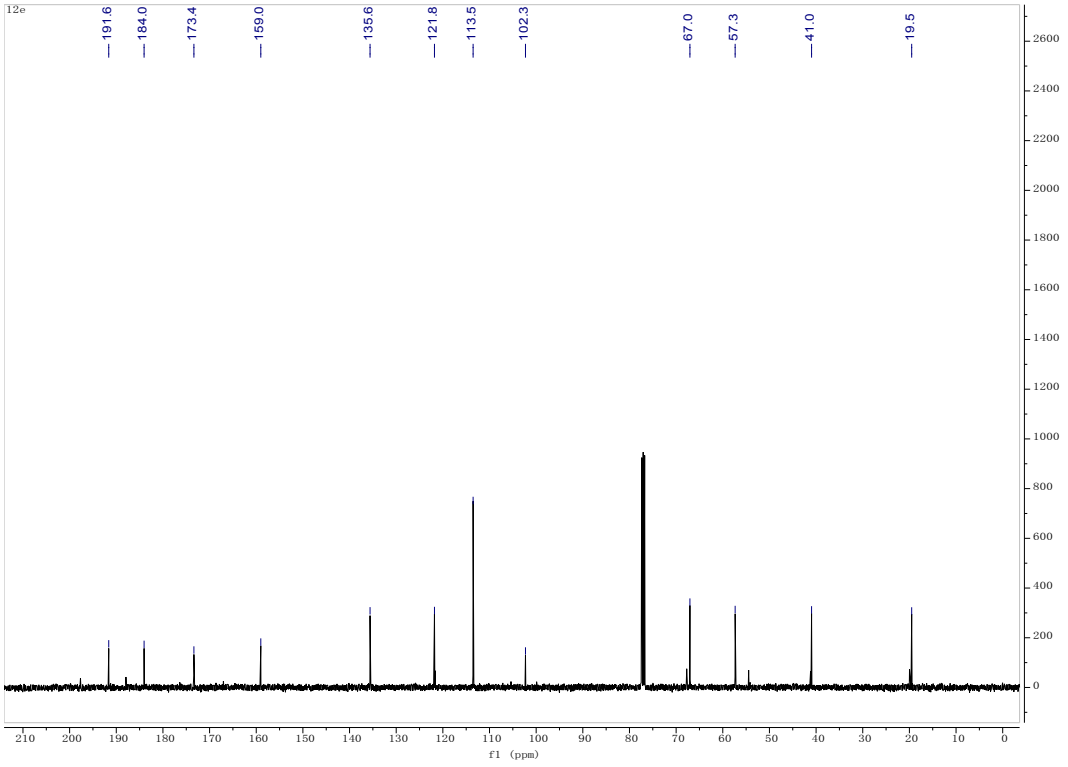

12d
192.0
190.3
174.4
153.3
132.0
129.7
128.6
124.9
122.6
115.3
102.0
68.8
55.8
28.2
f1 (ppm)

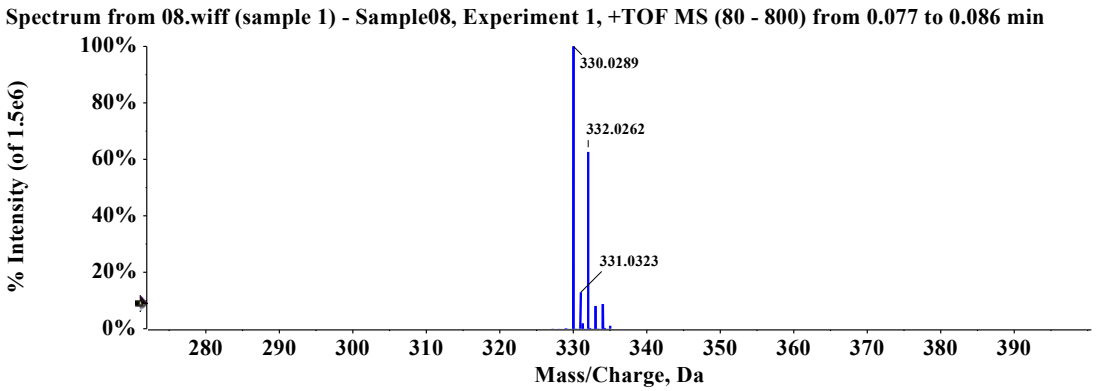


Compound 10e:




7.16
7.09
4.23
4.22
4.21
3.98
3.74
3.73
3.71
2.38
F (s)
7.16
E (s)
7.09
C (s)
3.98
B (t)
3.73
A (s)
2.38
D (t)
4.22
0.93
1.98
2.06
2.06
2.07
3.00
f1 (ppm)


12e
191.6
184.0
173.4
159.0
135.6
121.8
113.5
102.3
67.0
57.3
41.0
19.5
f1 (ppm)



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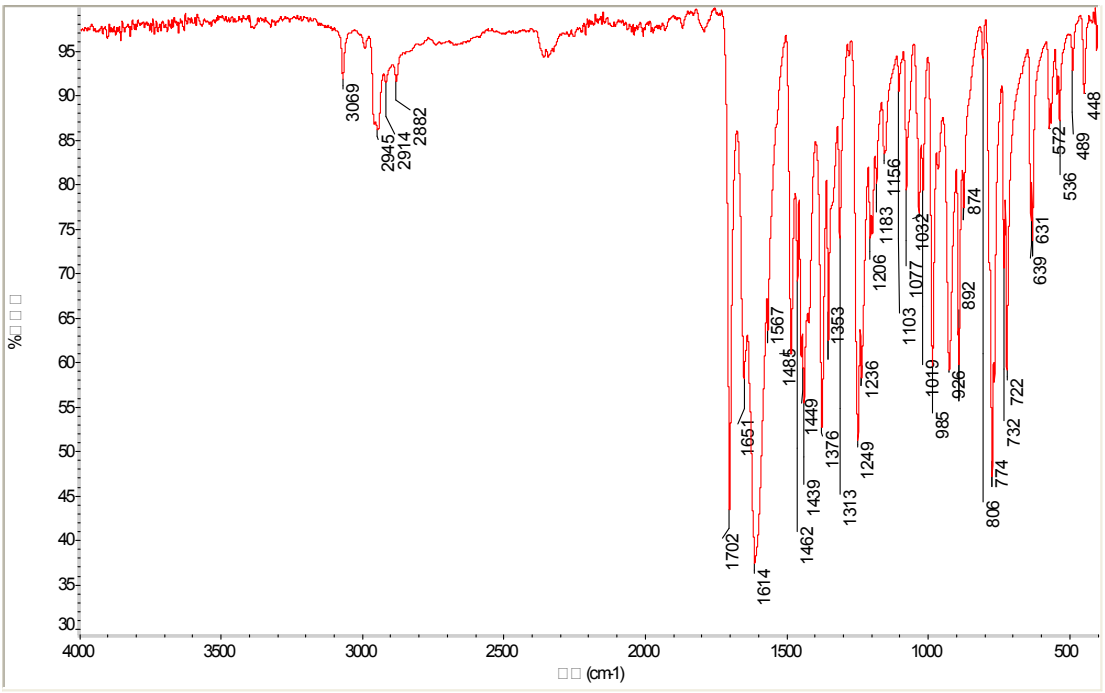
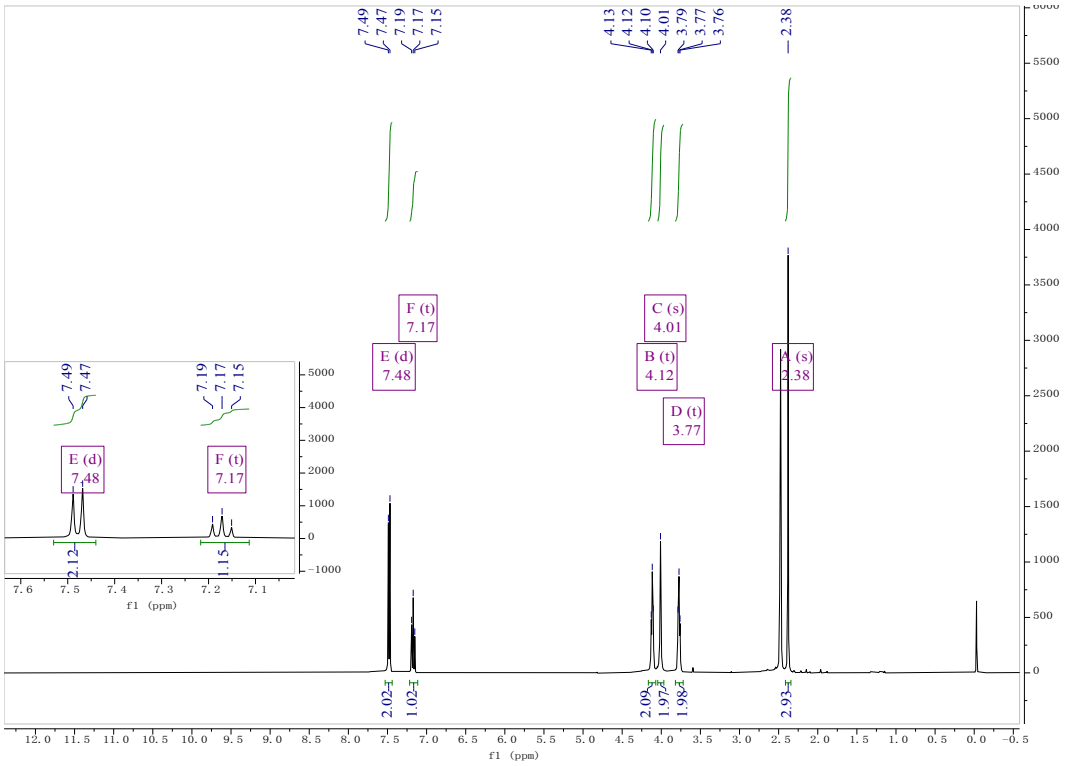
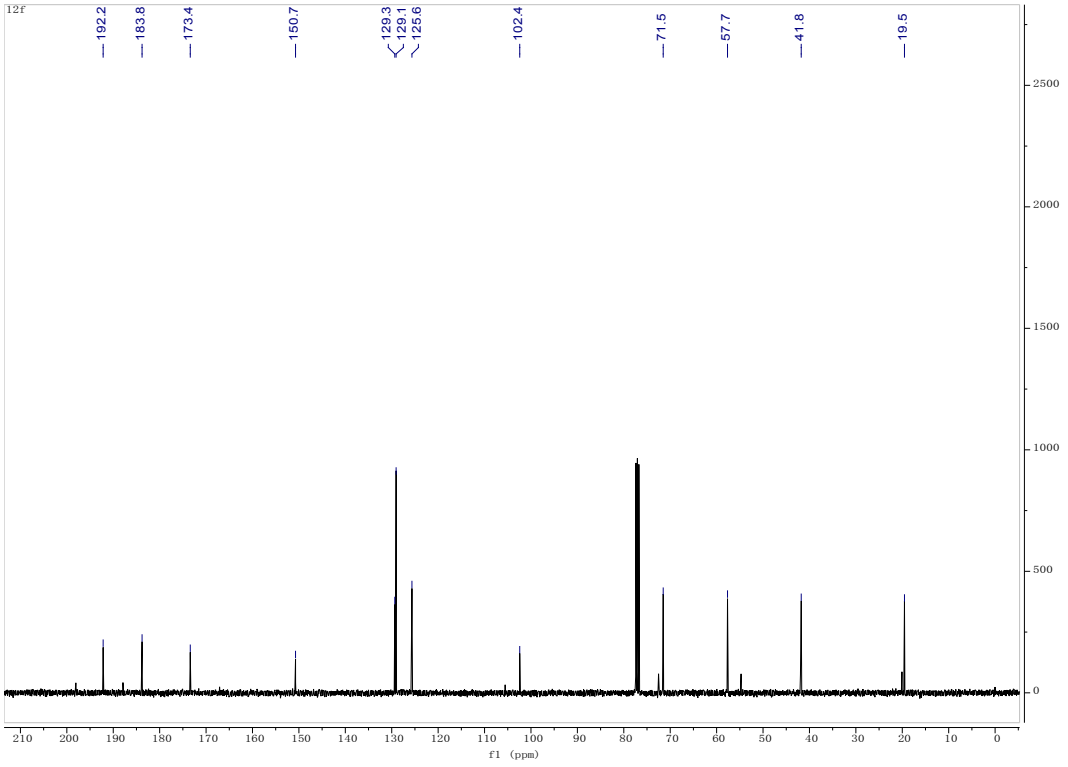
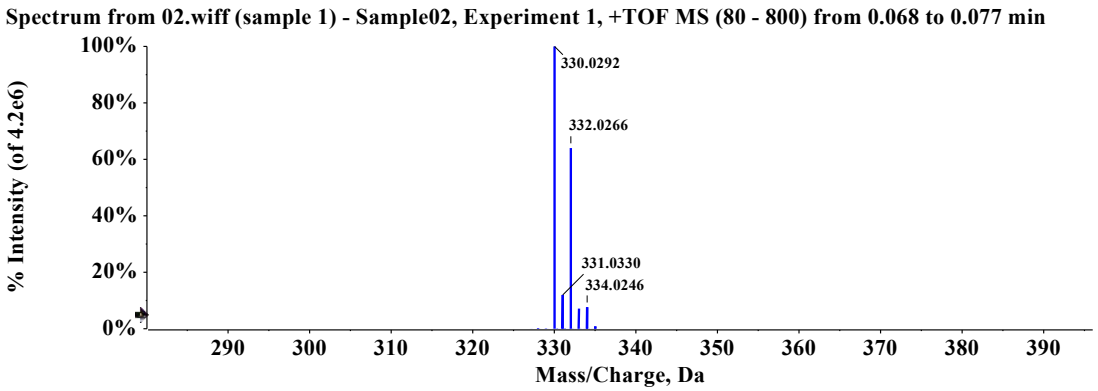
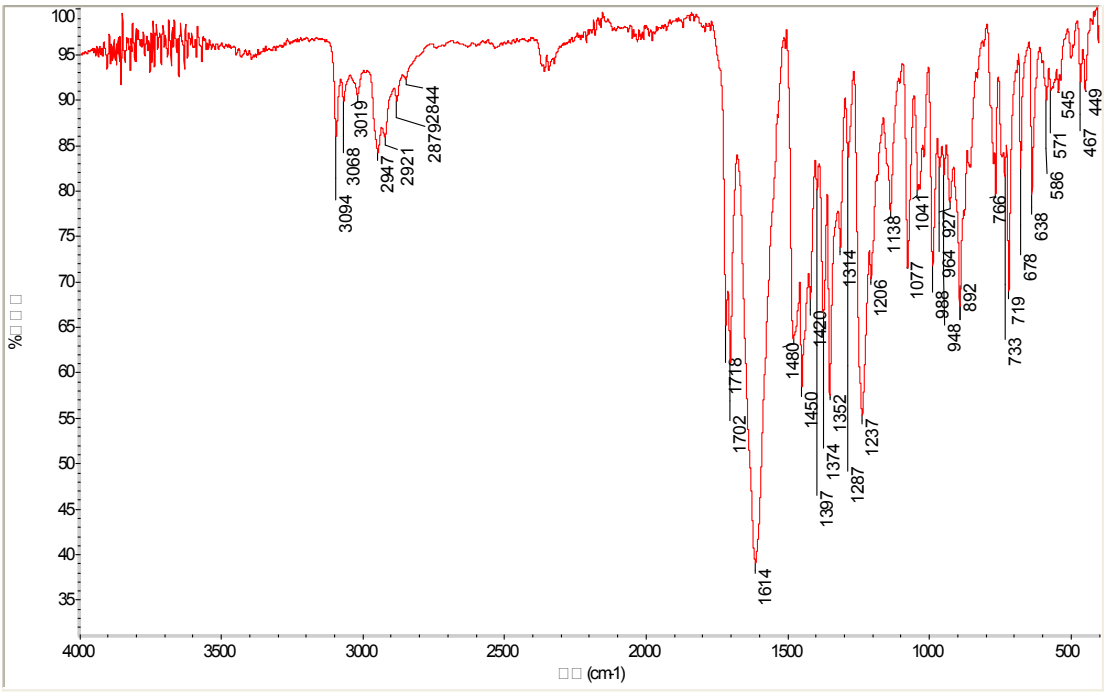


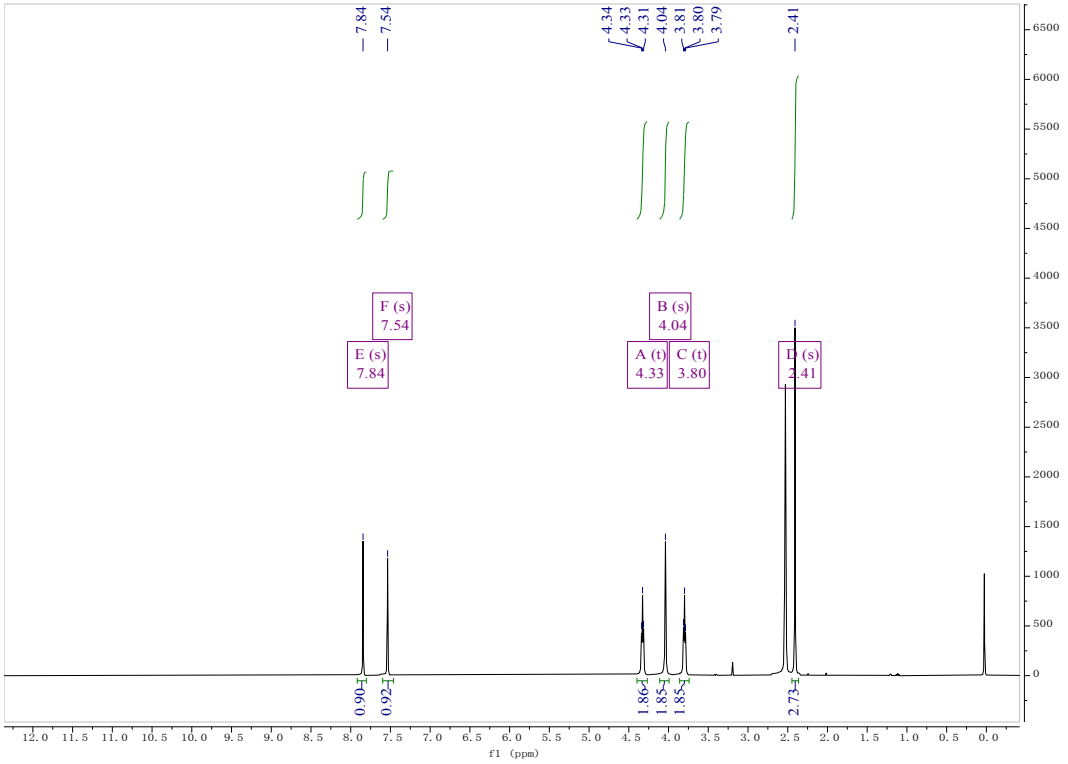

7.49
7.47
7.19
7.17
7.15
4.13
4.12
4.10
4.01
3.79
3.77
3.76
2.38
F (t)
7.17
E (d)
7.48
C (s)
4.01
B (t)
4.12
A (s)
2.38
D (t)
3.77
2.02
1.02
2.09
1.97
1.98
2.93
2.12
1.15
f1 (ppm)

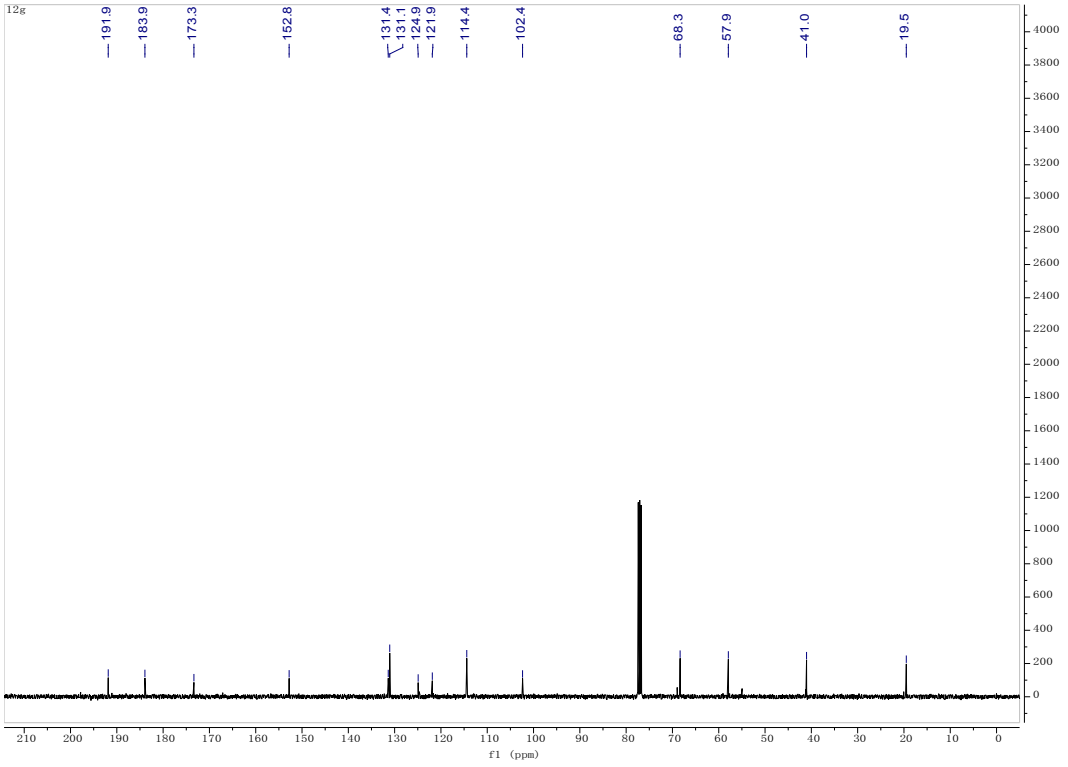

12f
192.2
183.8
173.4
150.7
129.3
129.1
125.6
102.4
71.5
57.7
41.8
19.5
f1 (ppm)

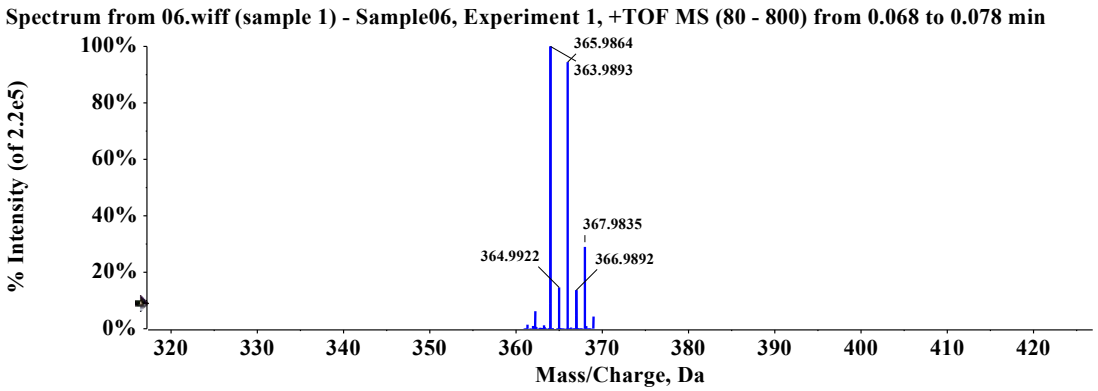


Compound 10g:

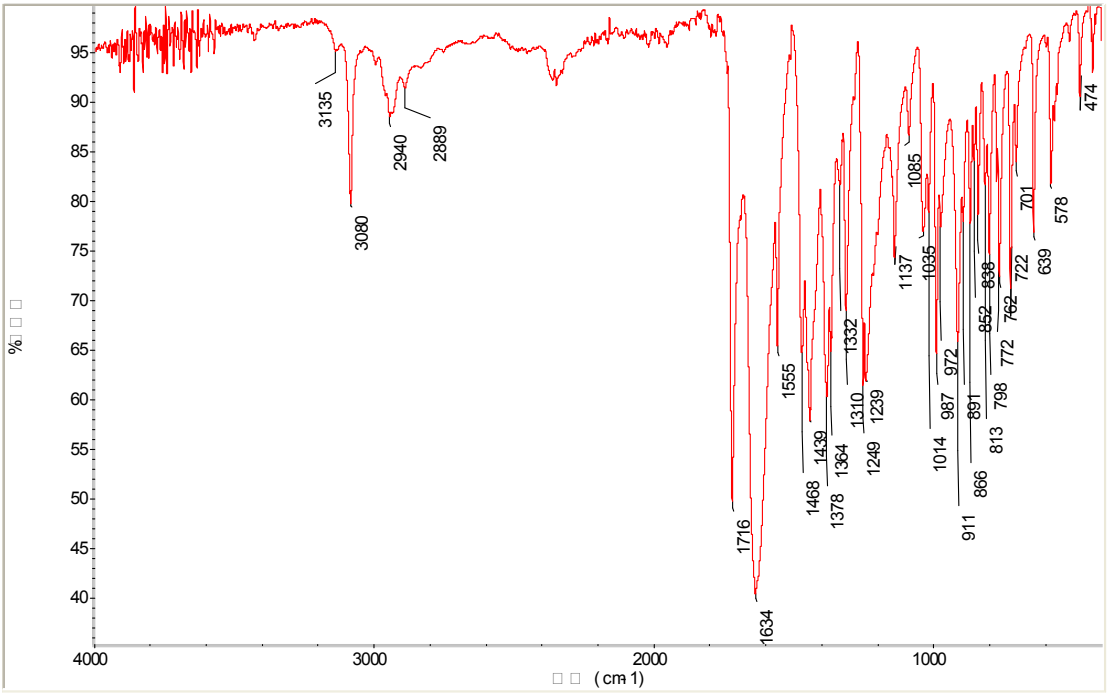


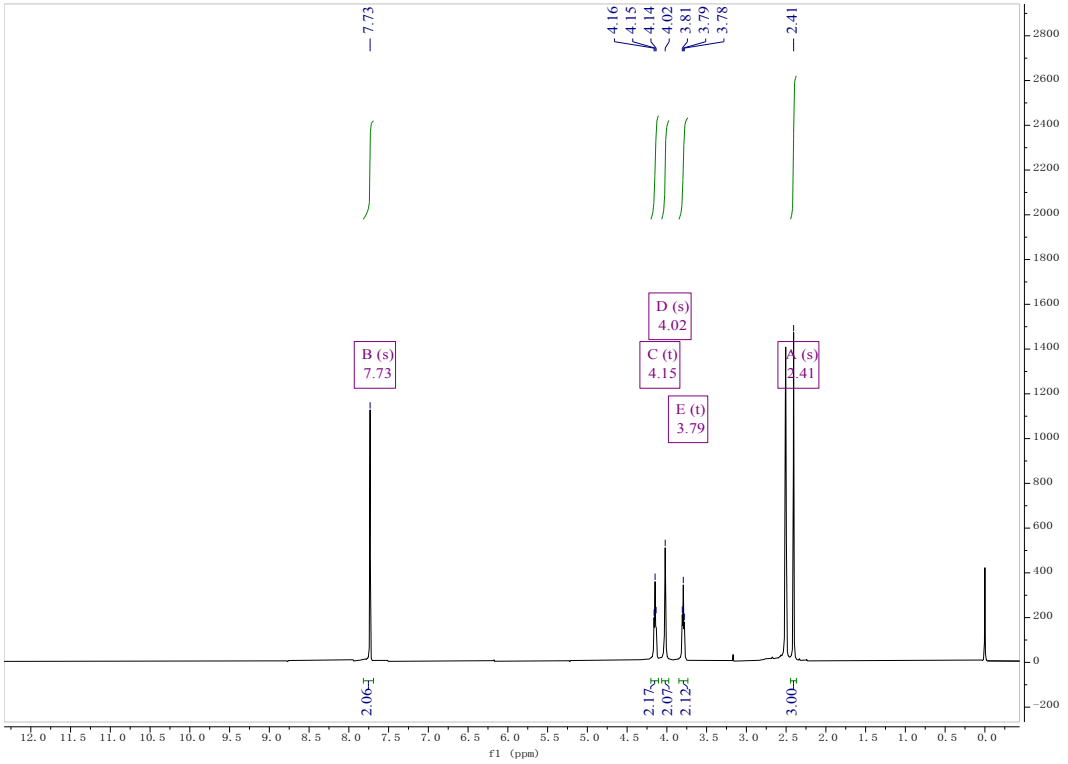

7.84
7.54
4.34
4.33
4.31
4.04
3.81
3.80
3.79
2.41
F (s) 7.54
E (s) 7.84
B (s) 4.04
A (t) 4.33
C (t) 3.80
D (s) 2.41
0.90
0.92
1.86
1.85
1.85
2.73
f1 (ppm)

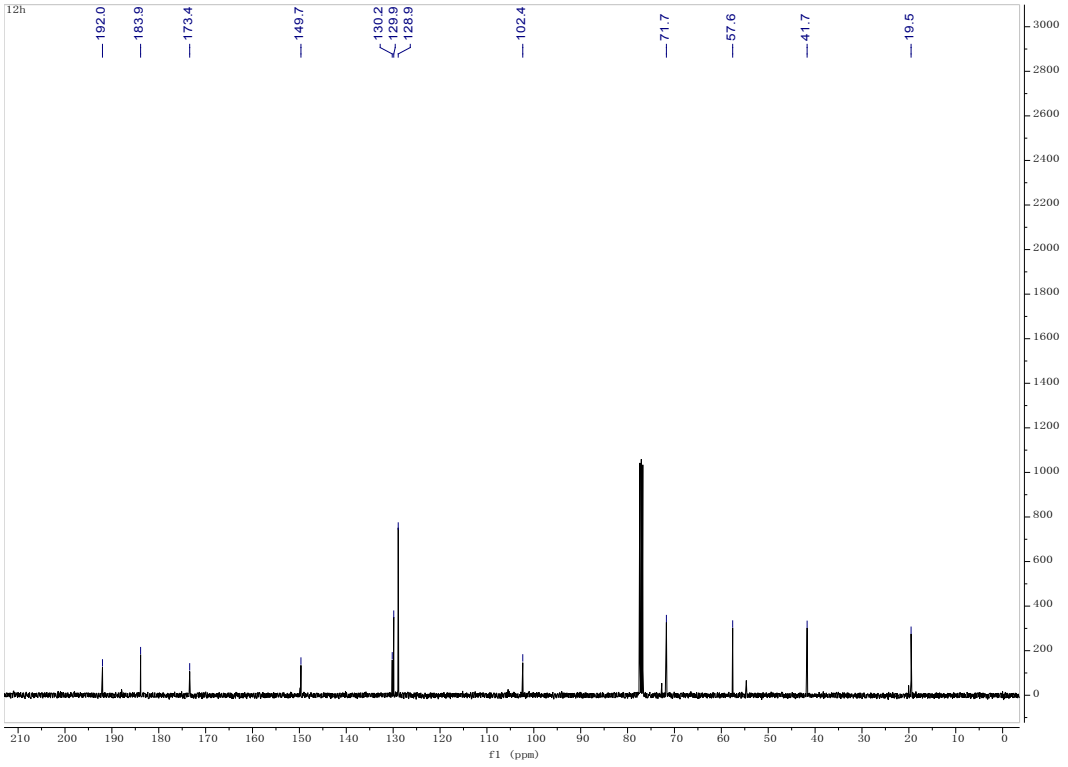

12g
191.9
183.9
173.3
152.8
131.4
131.1
124.9
121.9
114.4
102.4
68.3
57.9
41.0
19.5
f1 (ppm)

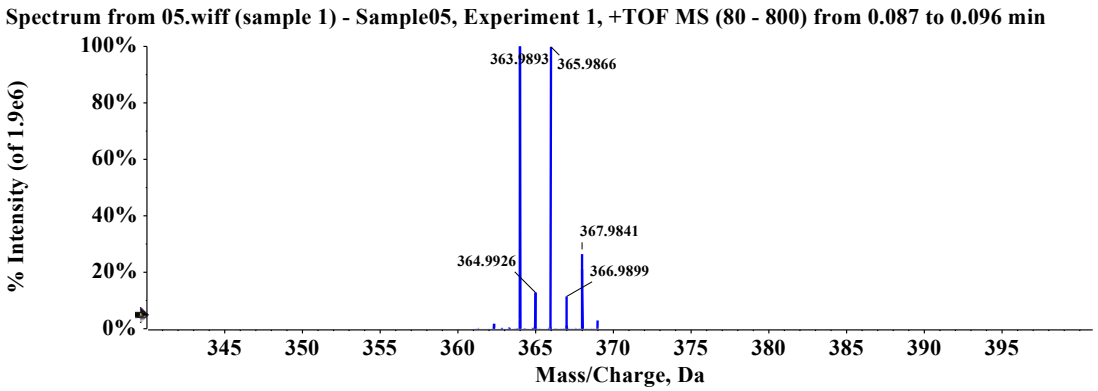


Compound 10h：

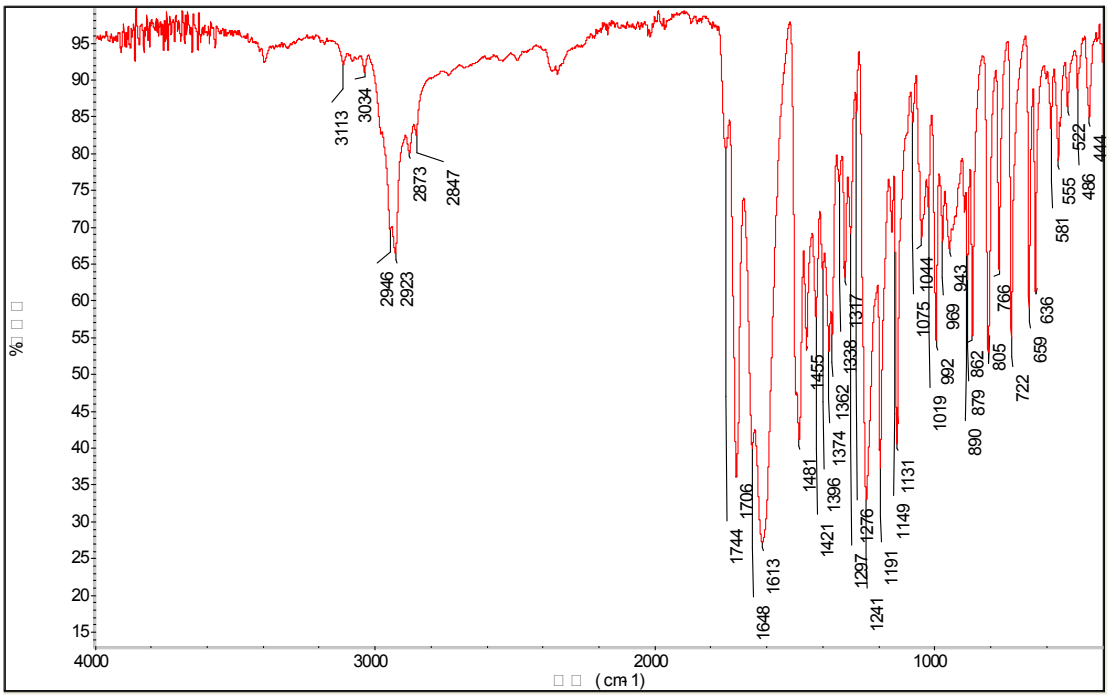


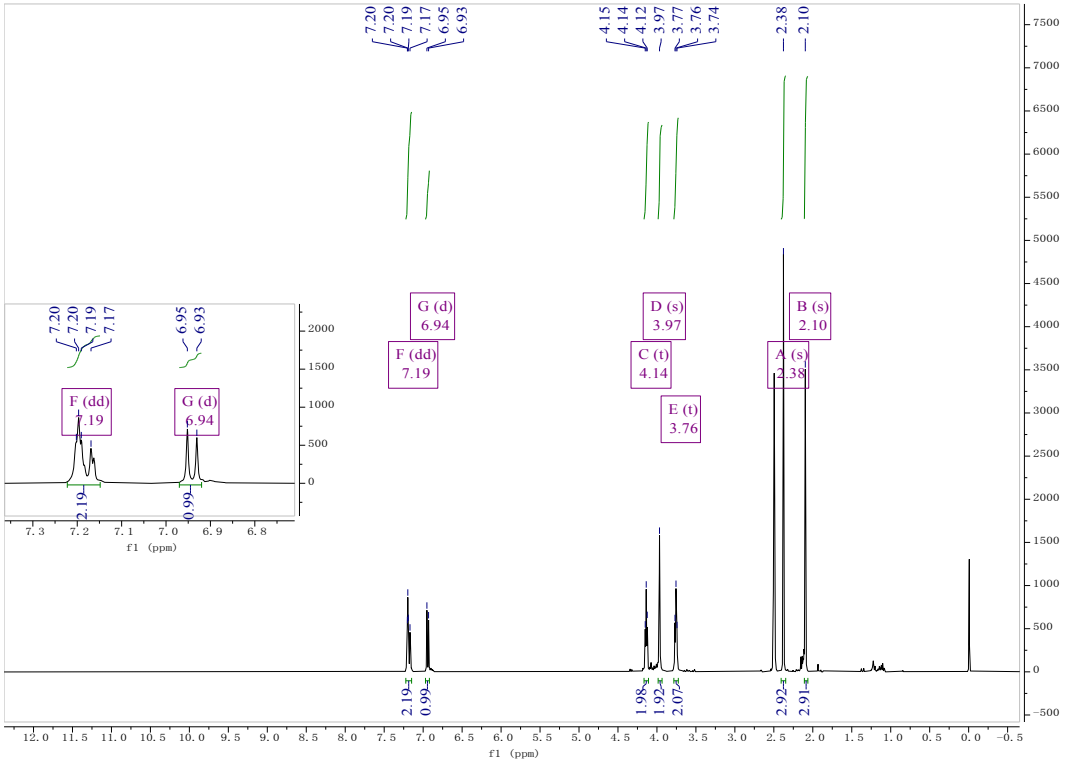

7.73
4.16
4.15
4.14
4.02
3.81
3.79
3.78
2.41
D (s)
4.02
B (s)
7.73
C (t)
4.15
A (s)
2.41
E (t)
3.79
2.06
2.17
2.07
2.12
3.00
f1 (ppm)

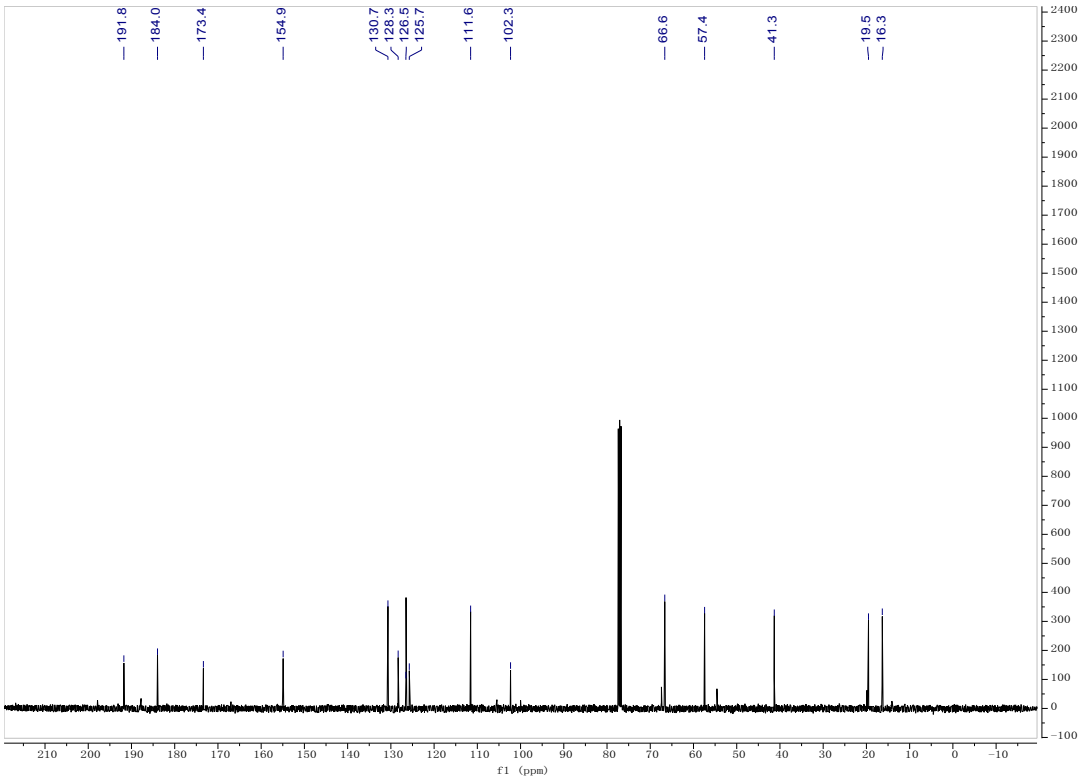

12h
192.0
183.9
173.4
149.7
130.2
129.9
128.9
102.4
71.7
57.6
41.7
19.5
f1 (ppm)

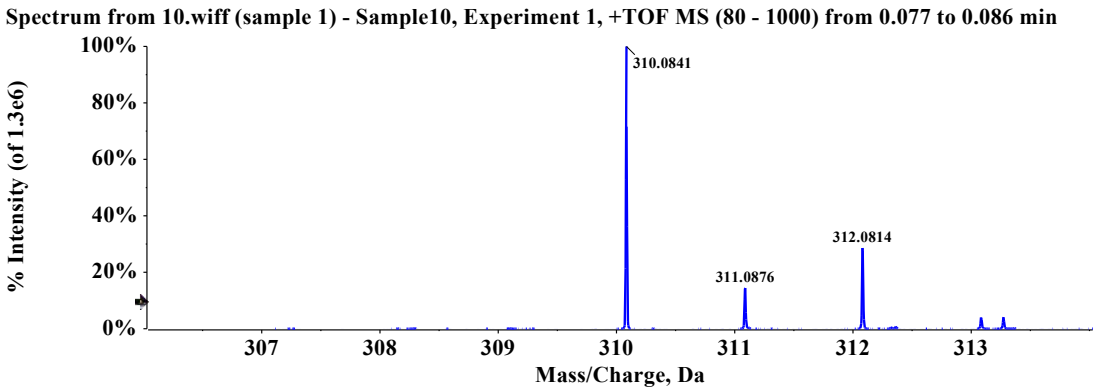


Compound 10i：

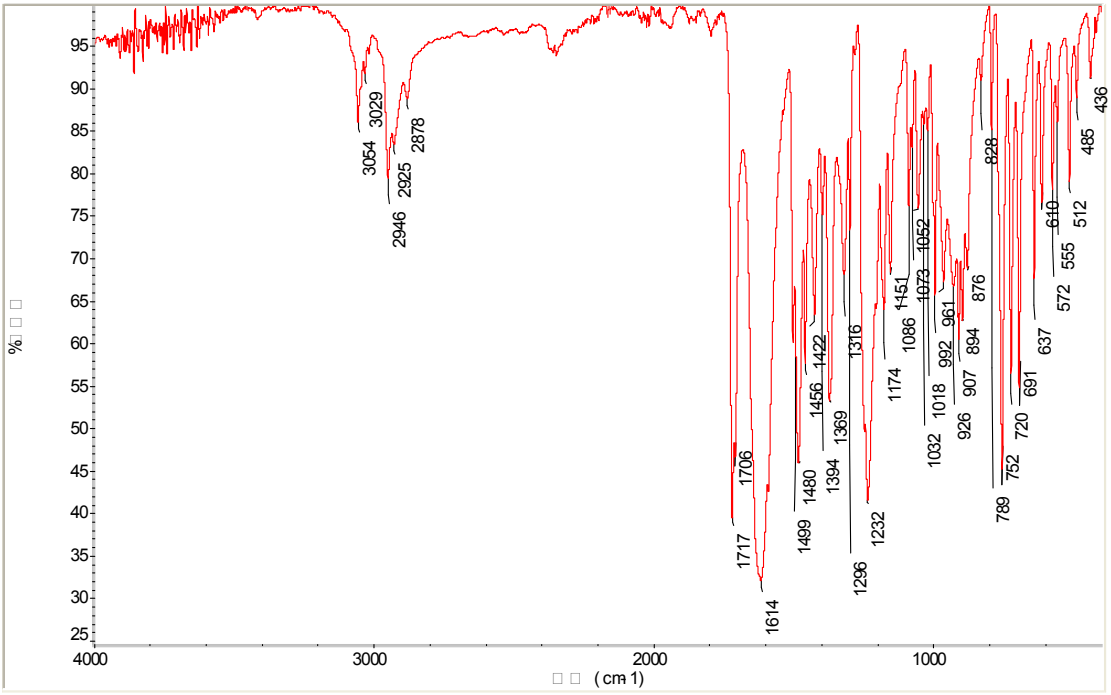


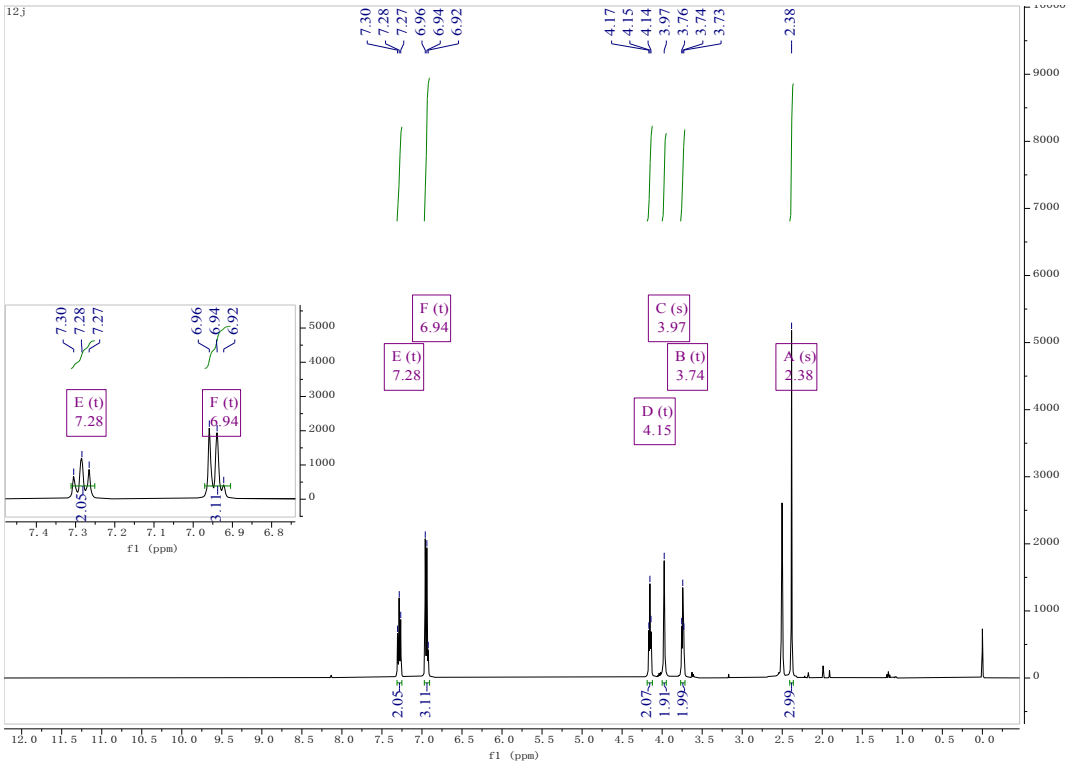

7.20
7.20
7.19
7.17
6.95
6.93
4.15
4.14
4.12
3.97
3.77
3.76
3.74
2.38
2.10
G (d)
6.94
F (dd)
7.19
D (s)
3.97
C (t)
4.14
E (t)
3.76
B (s)
2.10
A (s)
2.38
2.19
0.99
1.98
1.92
2.07
2.92
2.91
f1 (ppm)

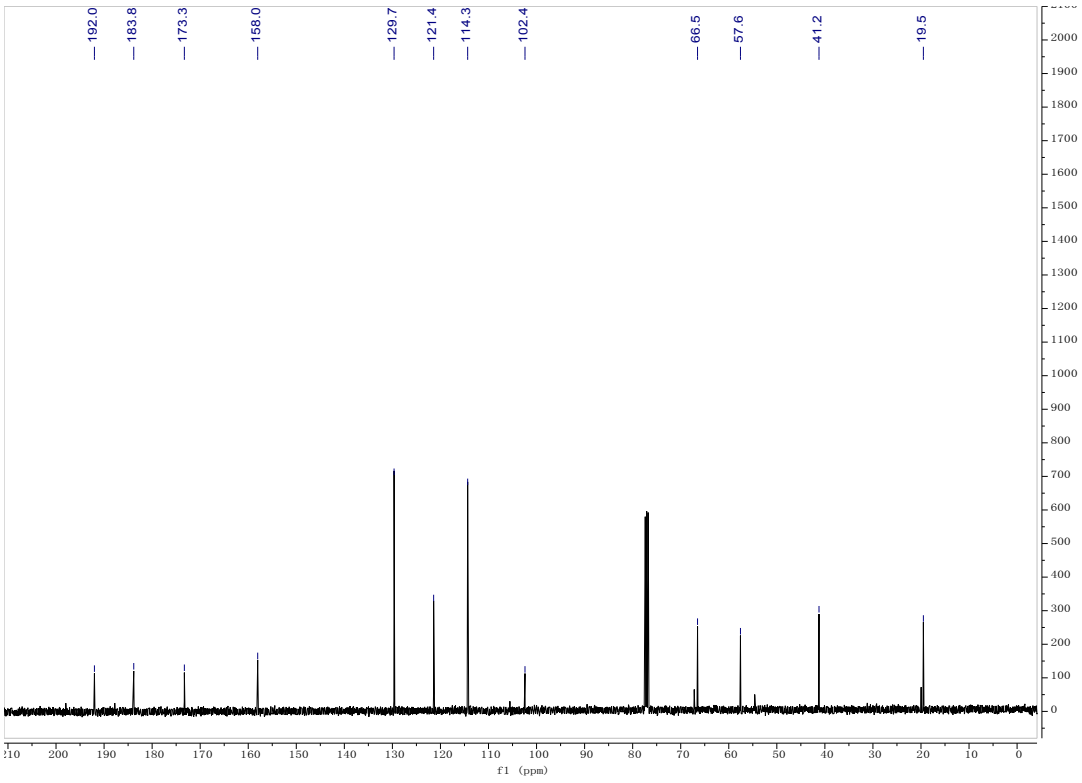

191.8
184.0
173.4
154.9
130.7
128.3
126.5
125.7
111.6
102.3
66.6
57.4
41.3
19.5
16.3
f1 (ppm)

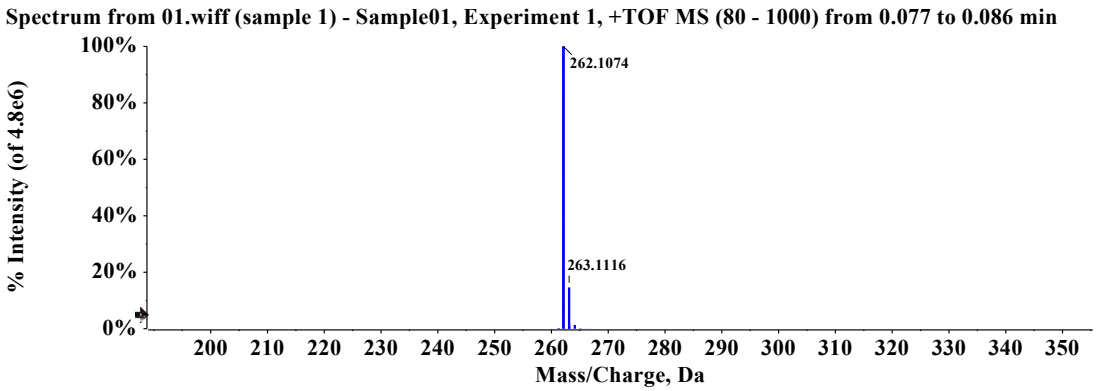


Compound 10j：

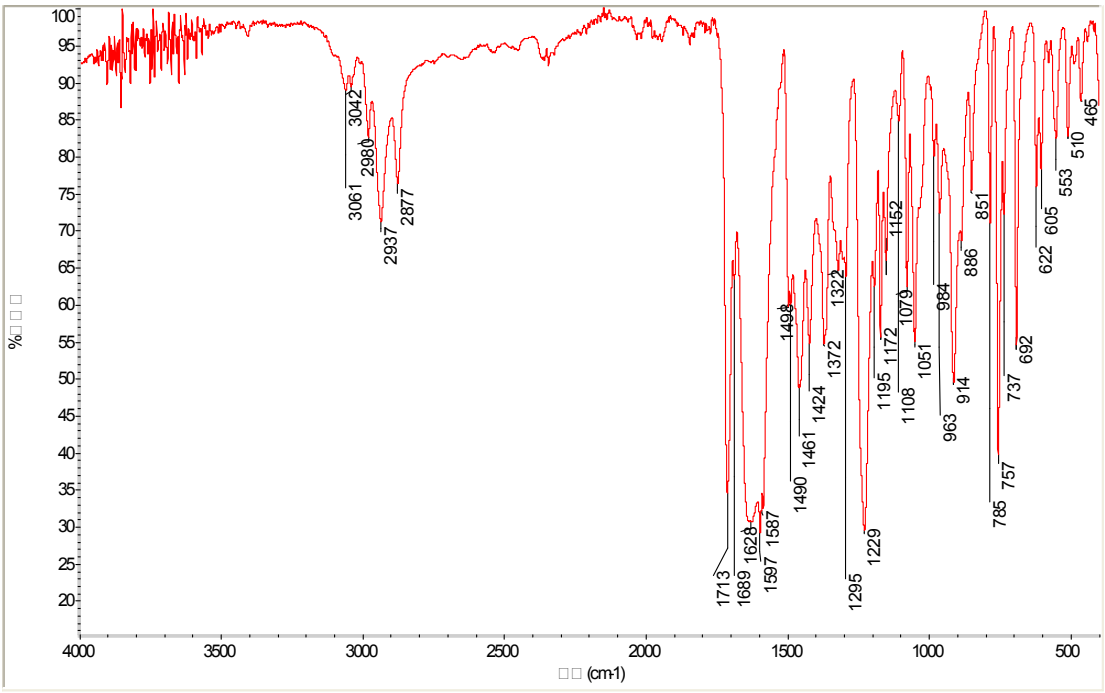


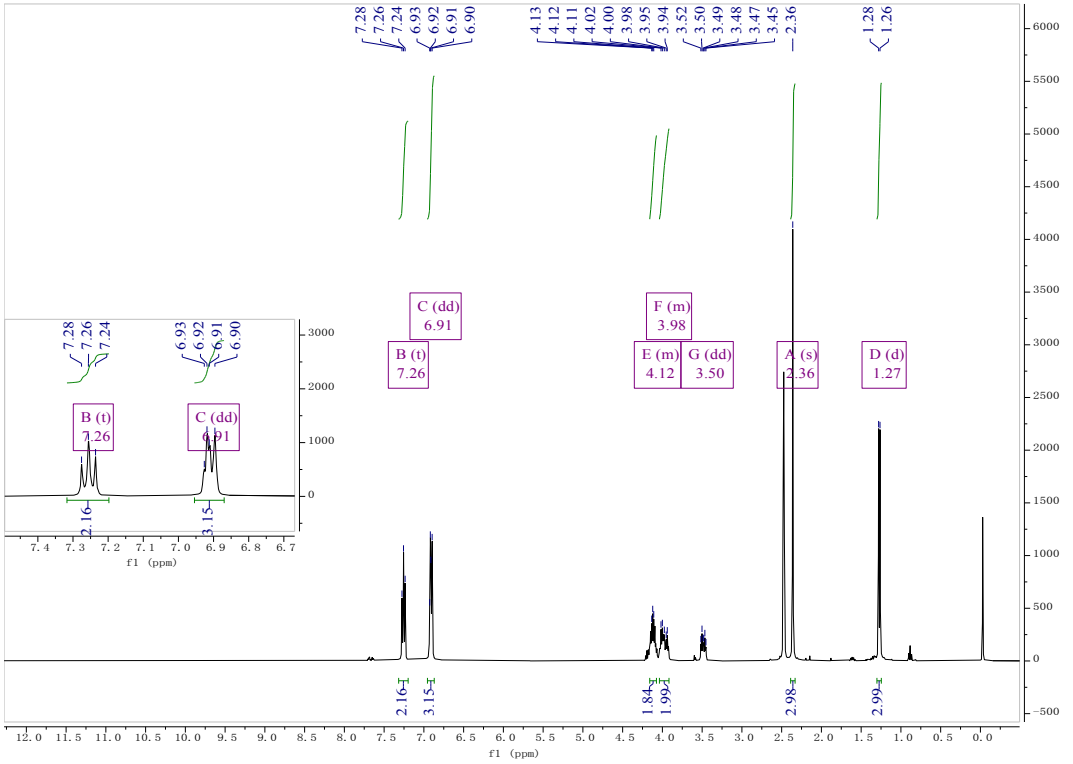

12j
7.30
7.28
7.27
6.96
6.94
6.92
4.17
4.15
4.14
3.97
3.76
3.74
3.73
2.38
F (t)
6.94
E (t)
7.28
C (s)
3.97
B (t)
3.74
A (s)
2.38
D (t)
4.15
2.05
3.11
2.07
1.91
1.99
2.99
f1 (ppm)

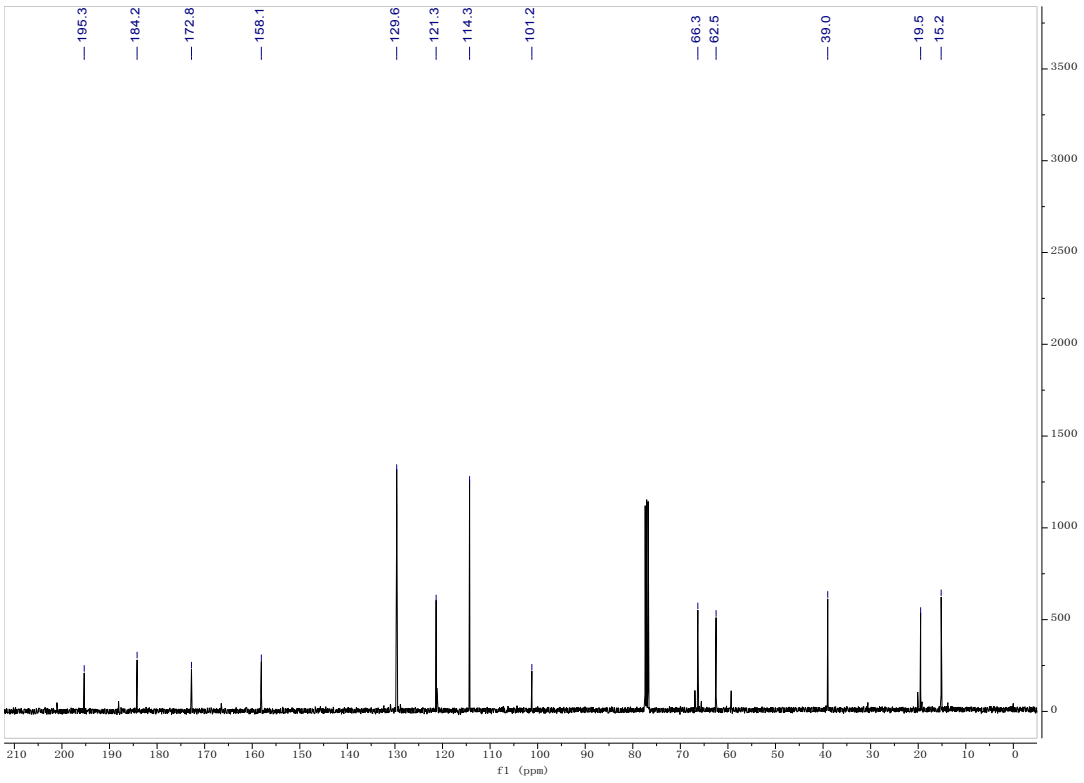

192.0
183.8
173.3
158.0
129.7
121.4
114.3
102.4
66.5
57.6
41.2
19.5
f1 (ppm)

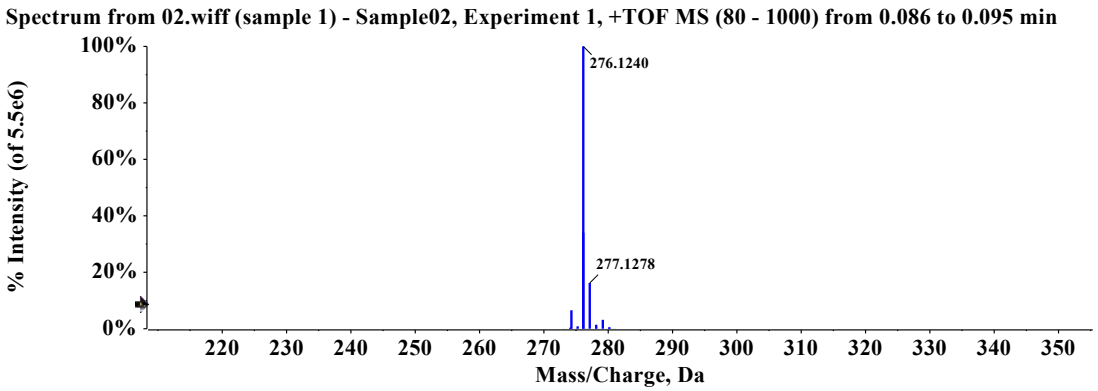


Compound 10k：

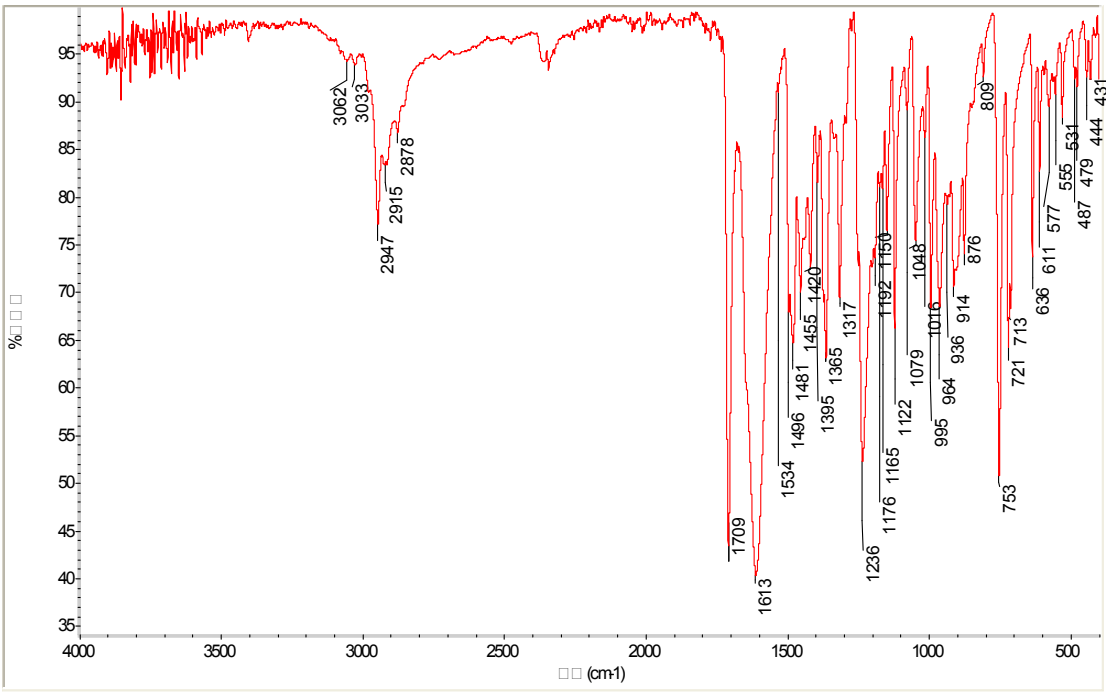


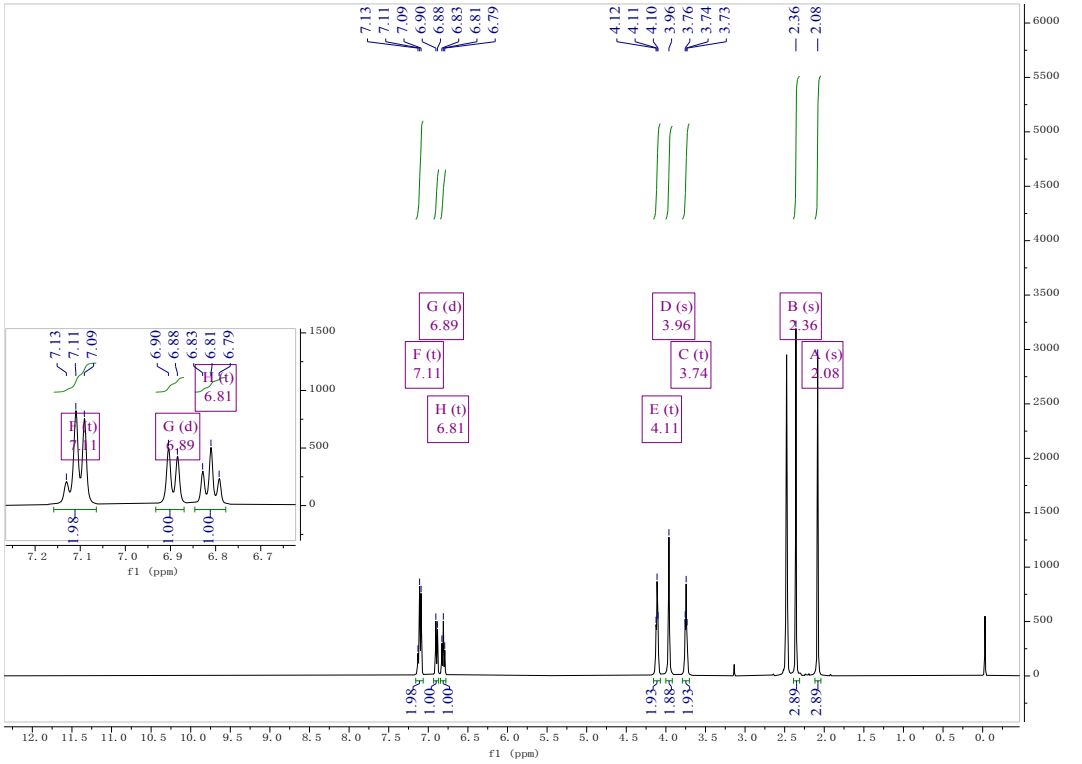

7.28
7.26
7.24
6.93
6.92
6.91
6.90
4.13
4.12
4.11
4.02
4.00
3.98
3.95
3.94
3.52
3.50
3.49
3.48
3.47
3.45
2.36
1.28
1.26
C (dd)
6.91
B (t)
7.26
F (m)
3.98
E (m)
4.12
G (dd)
3.50
A (s)
2.36
D (d)
1.27
2.16
3.15
1.84
1.99
2.98
2.99
f1 (ppm)

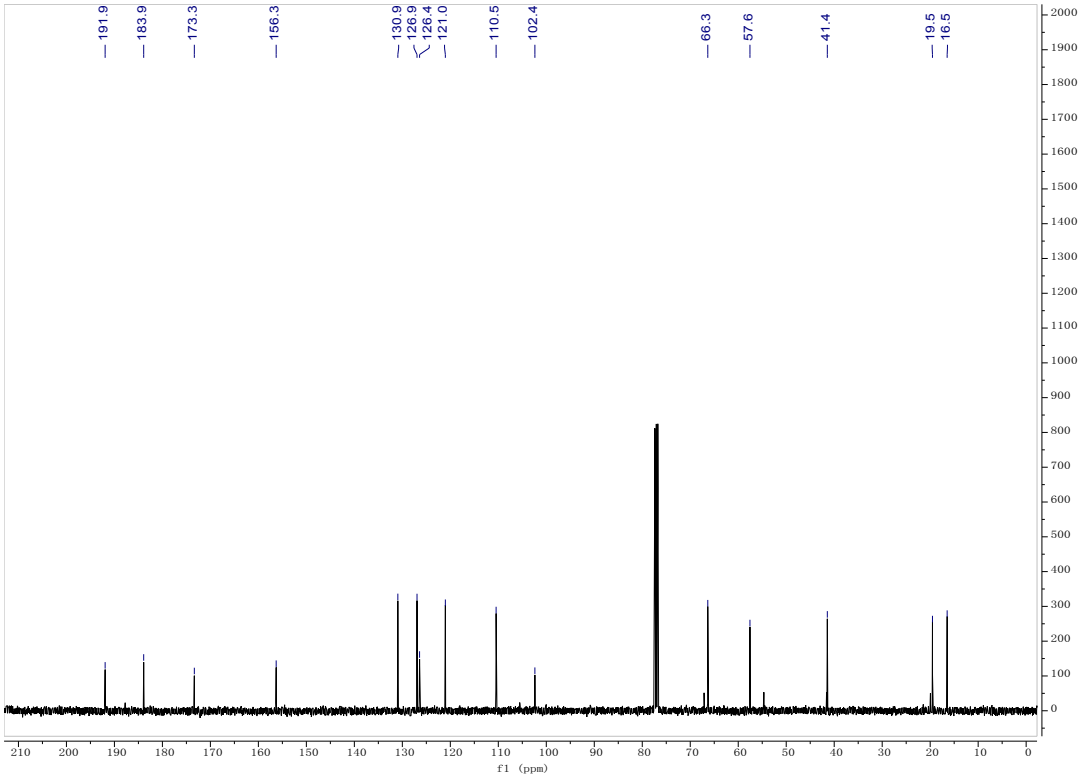

195.3
184.2
172.8
158.1
129.6
121.3
114.3
101.2
66.3
62.5
39.0
19.5
15.2
f1 (ppm)

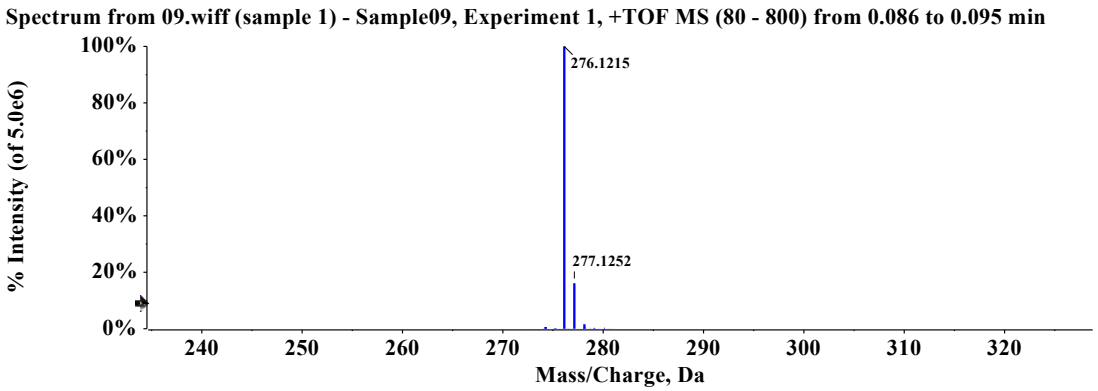


Compound 10l:

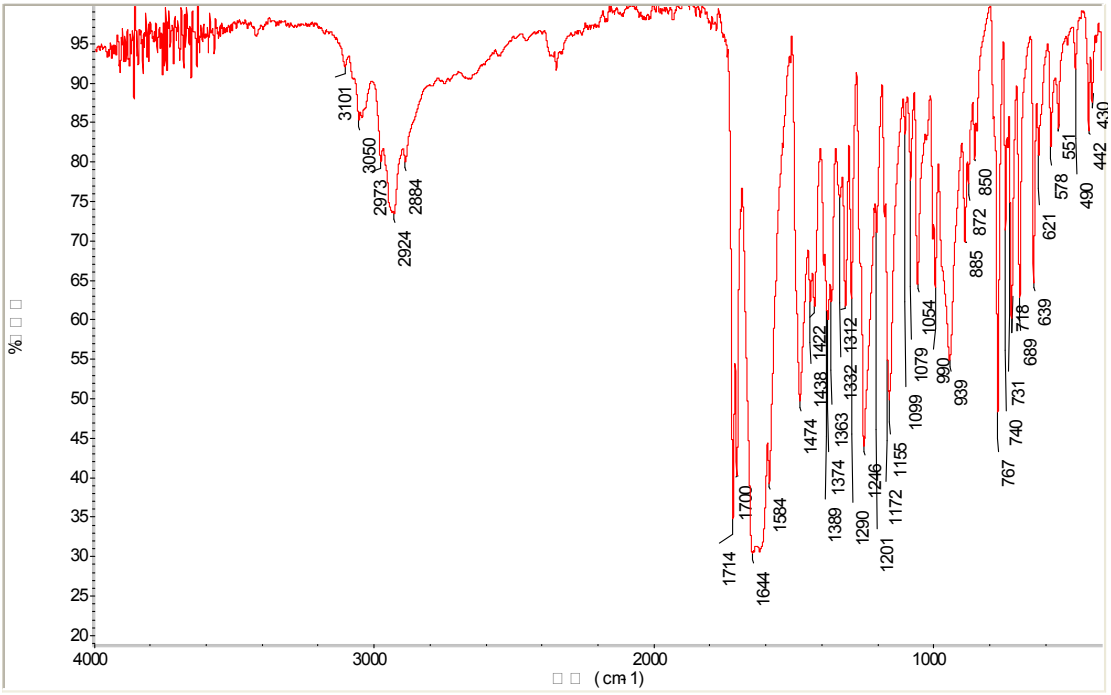


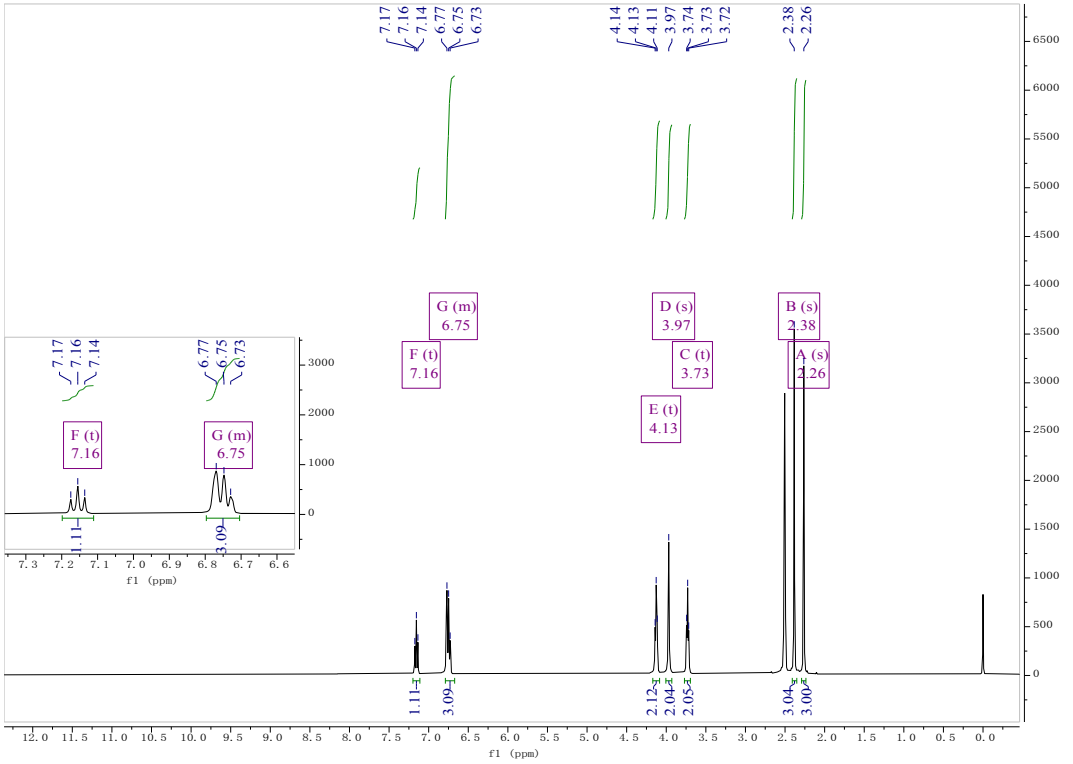

7.13
7.11
7.09
6.90
6.88
6.83
6.81
6.79
4.12
4.11
4.10
3.96
3.76
3.74
3.73
2.36
2.08
G (d) 6.89
F (t) 7.11
H (t) 6.81
D (s) 3.96
C (t) 3.74
E (t) 4.11
B (s) 2.36
A (s) 2.08
1.98
1.00
1.00
1.93
1.88
1.93
2.89
2.89
f1 (ppm)

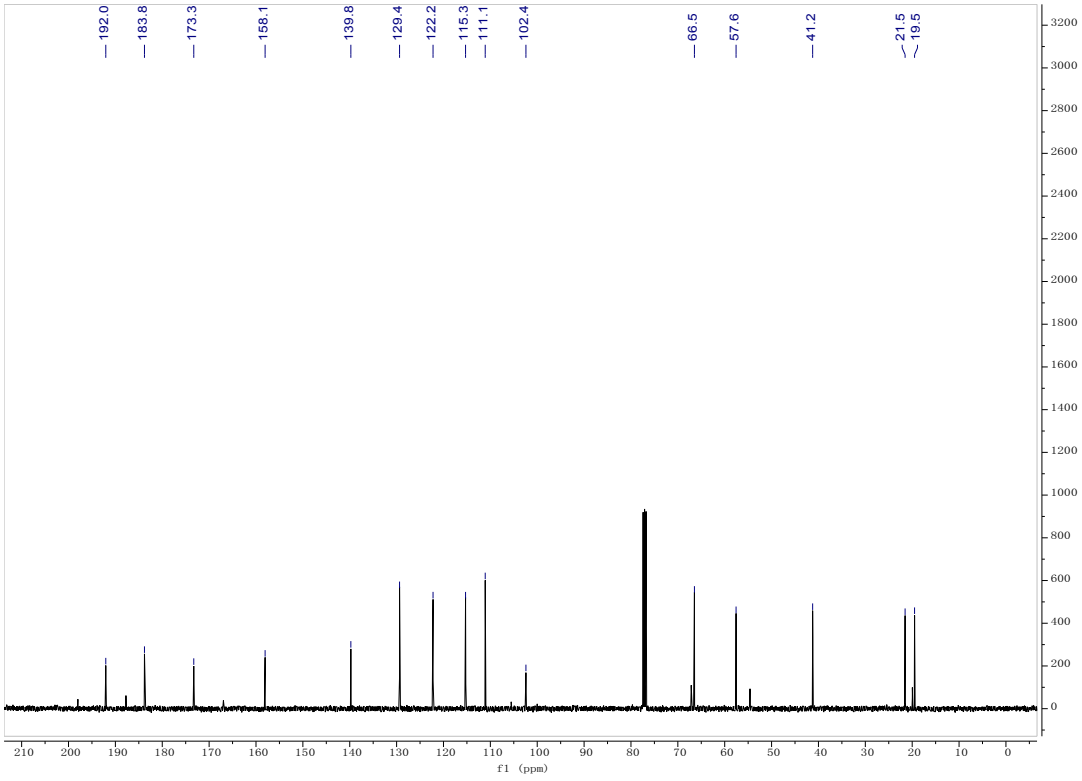

191.9
183.9
173.3
156.3
130.9
126.9
126.4
121.0
110.5
102.4
66.3
57.6
41.4
19.5
16.5
f1 (ppm)

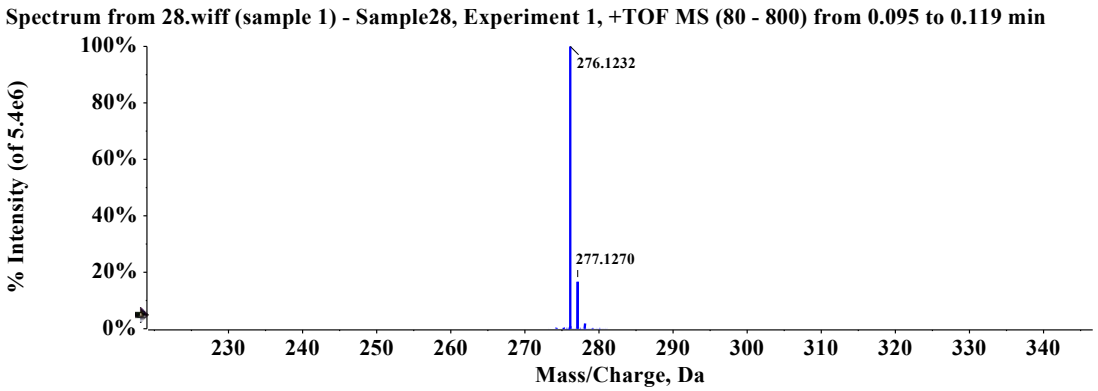


Compound 10m：

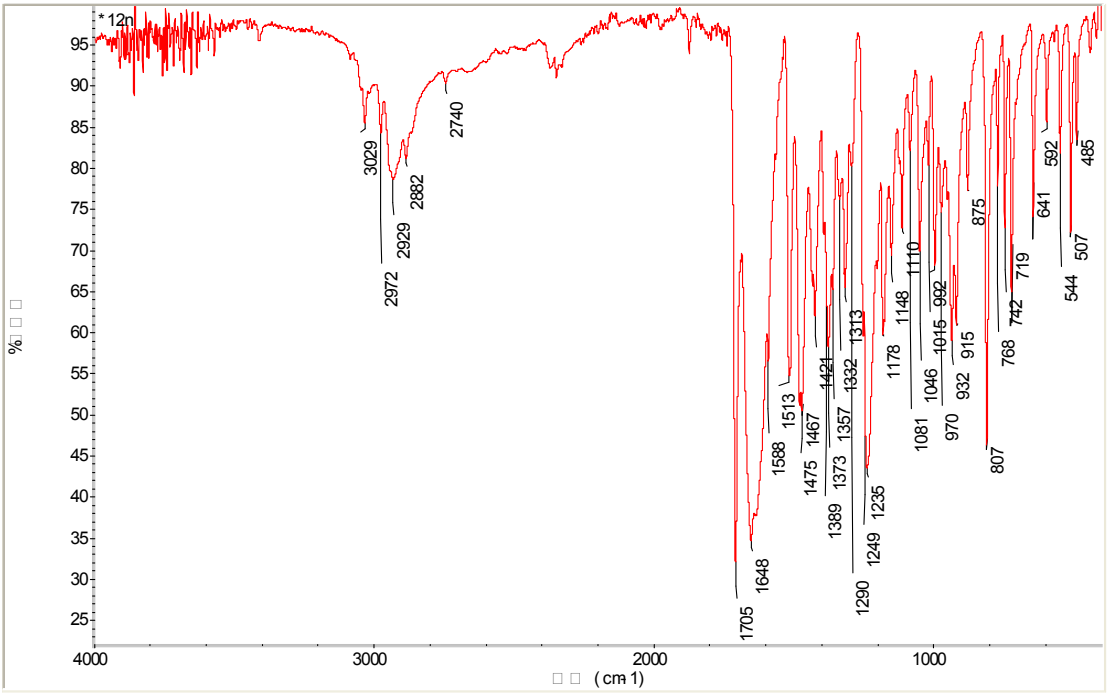


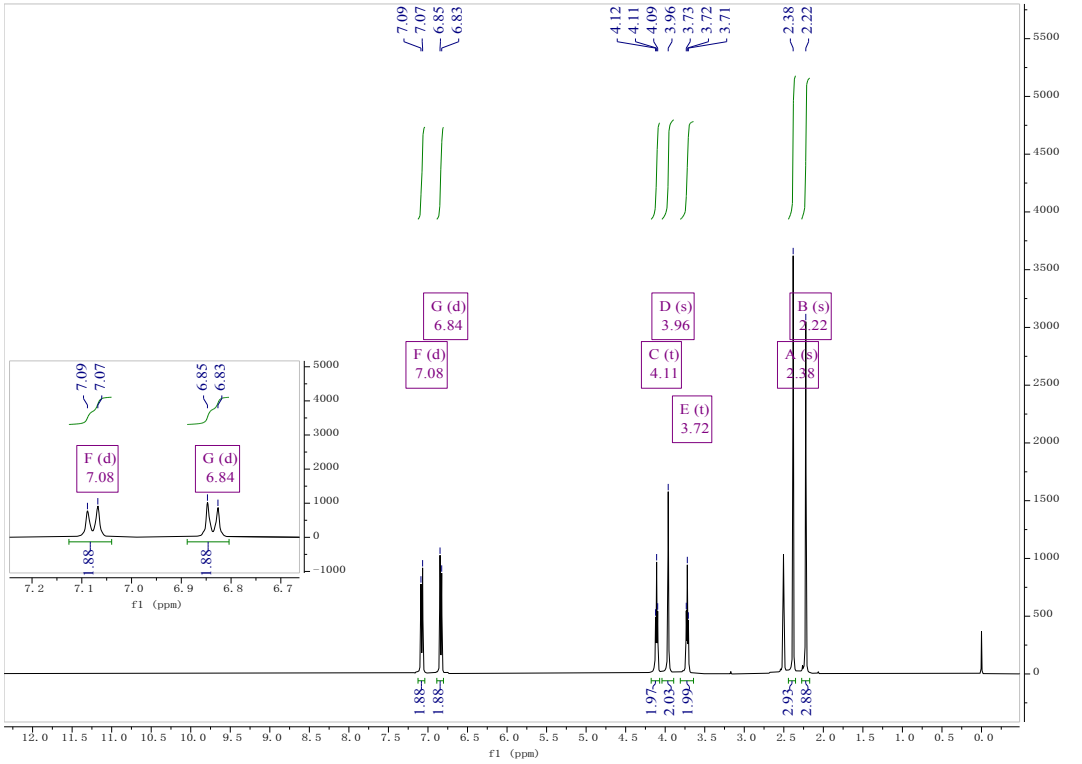

7.17
7.16
7.14
6.77
6.75
6.73
4.14
4.13
4.11
3.97
3.74
3.73
3.72
2.38
2.26
G (m)
6.75
F (t)
7.16
D (s)
3.97
C (t)
3.73
E (t)
4.13
B (s)
2.38
A (s)
2.26
1.11
3.09
2.12
2.04
2.05
3.04
3.00
f1 (ppm)

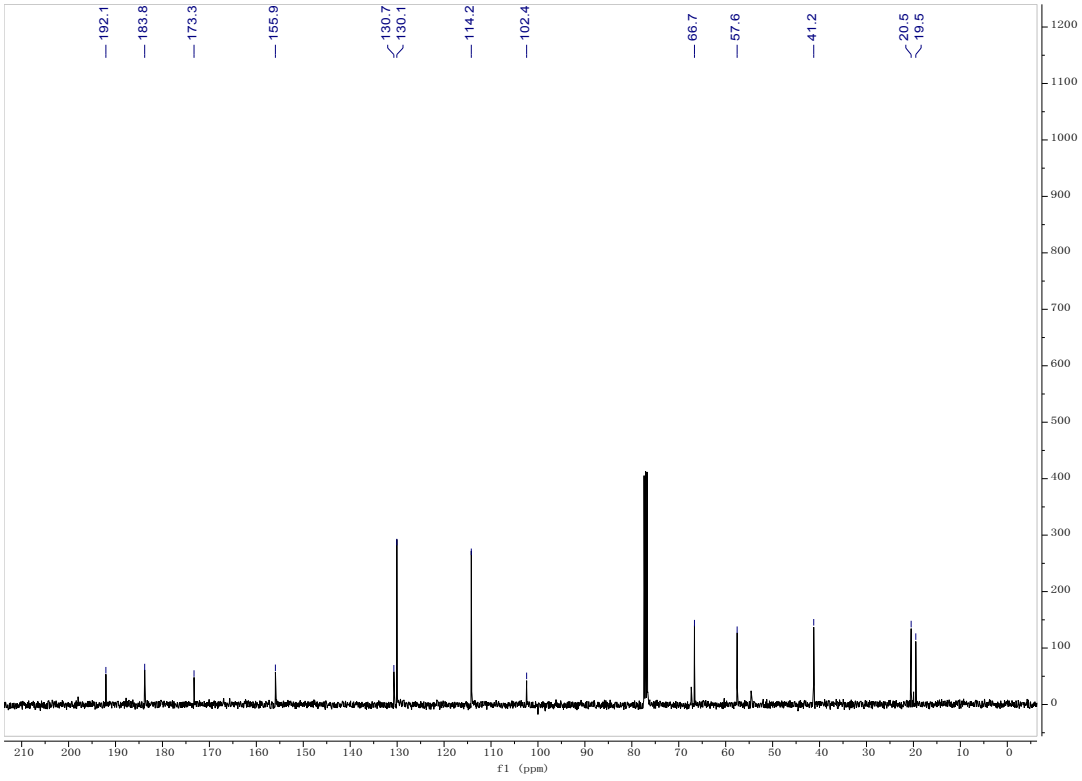

192.0
183.8
173.3
158.1
139.8
129.4
122.2
115.3
111.1
102.4
66.5
57.6
41.2
21.5
19.5
f1 (ppm)

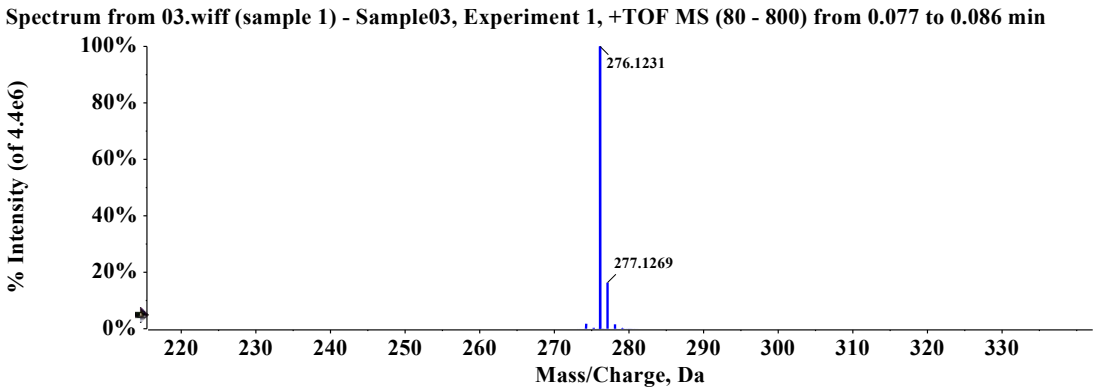


Compound 10n：

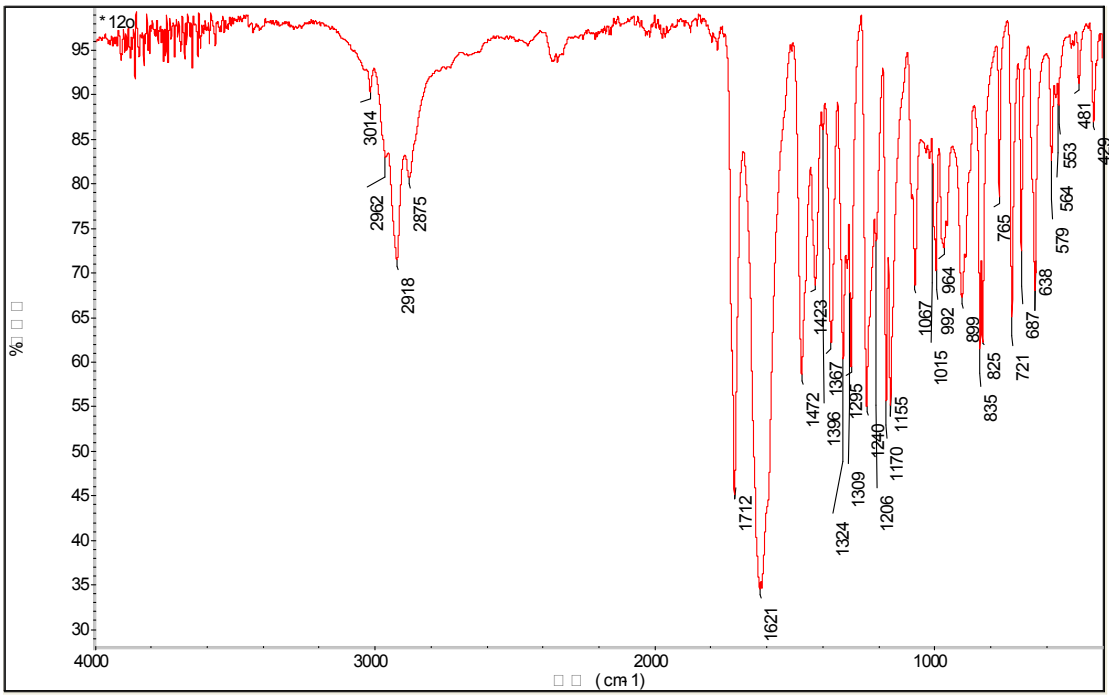


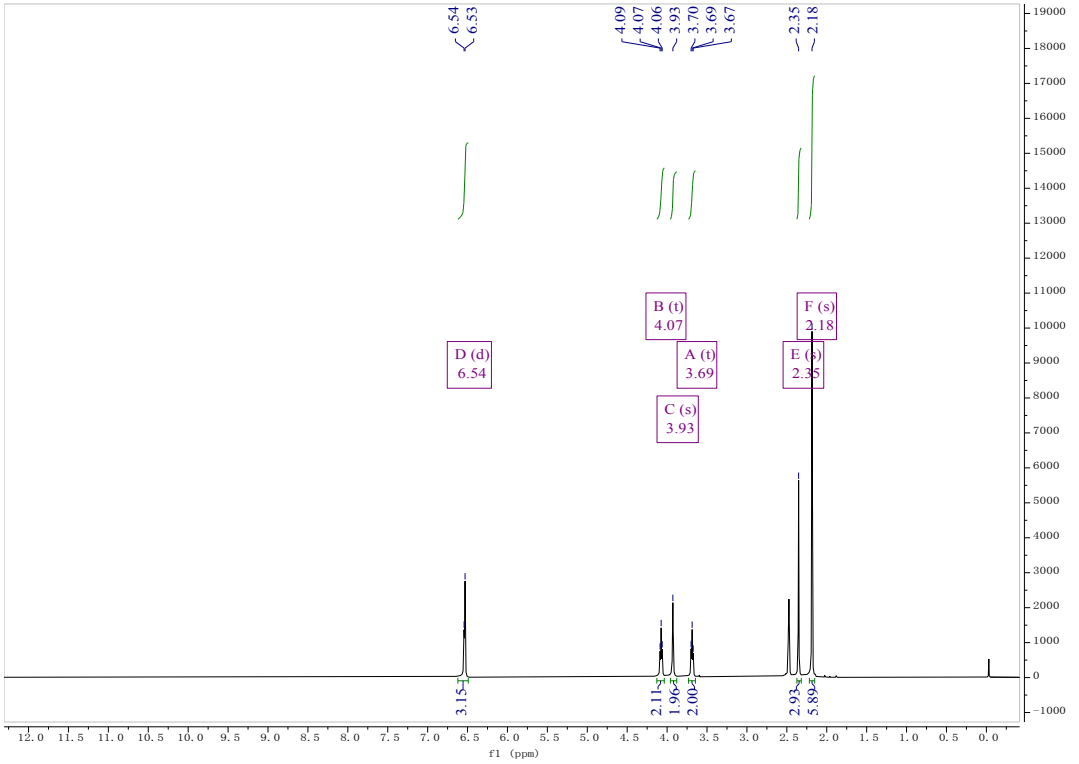

7.09
7.07
6.85
6.83
4.12
4.11
4.09
3.96
3.73
3.72
3.71
2.38
2.22
G (d)
6.84
F (d)
7.08
D (s)
3.96
C (t)
4.11
E (t)
3.72
B (s)
2.22
A (s)
2.38
1.88
1.88
1.88
1.97
2.03
1.99
2.93
2.88
f1 (ppm)

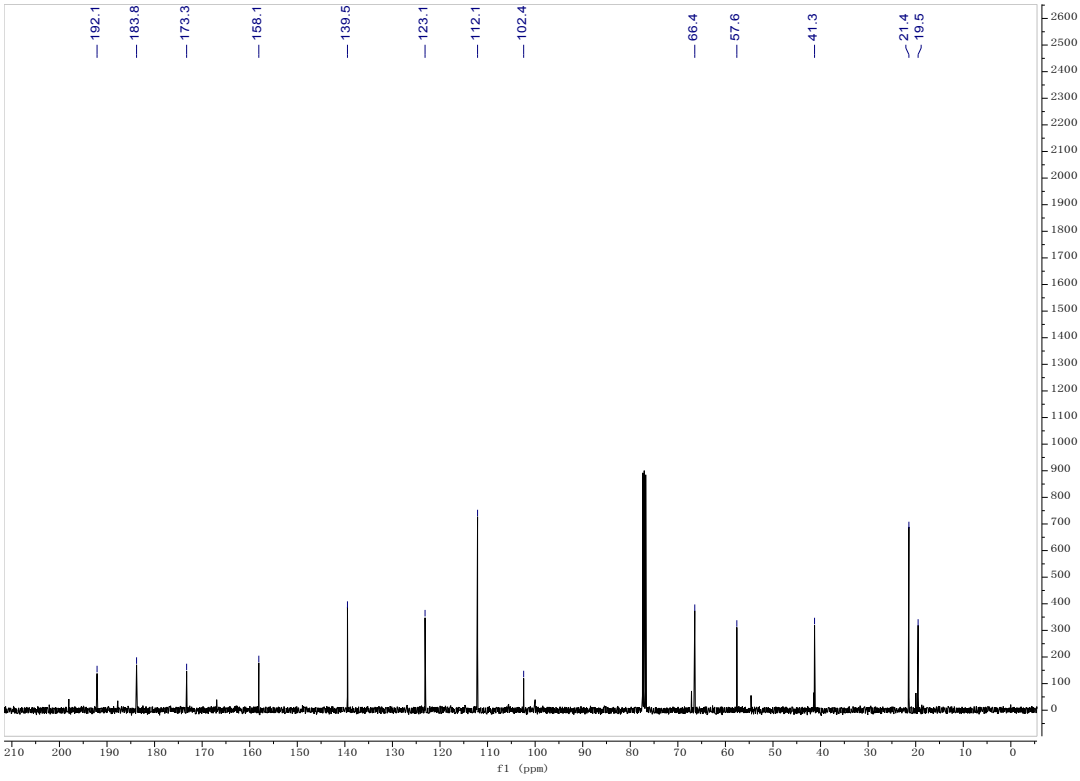

192.1
183.8
173.3
155.9
130.7
130.1
114.2
102.4
66.7
57.6
41.2
20.5
19.5
f1 (ppm)

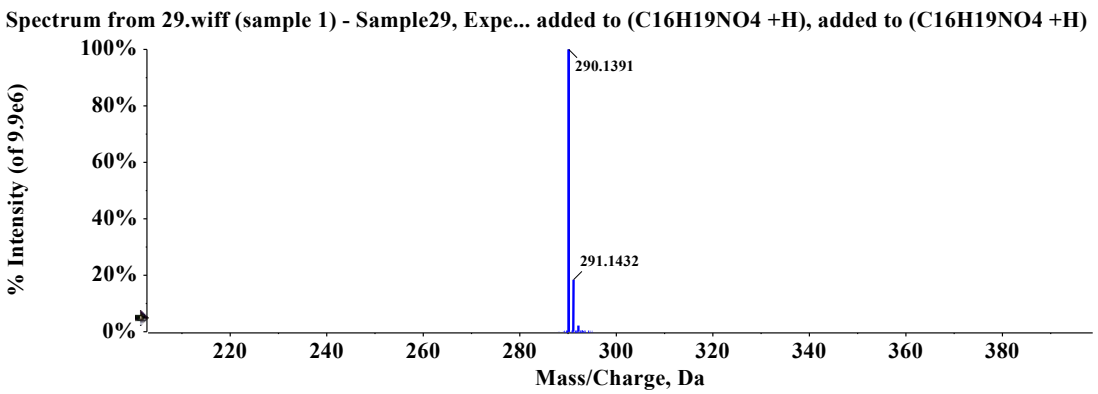


Compound 10o：

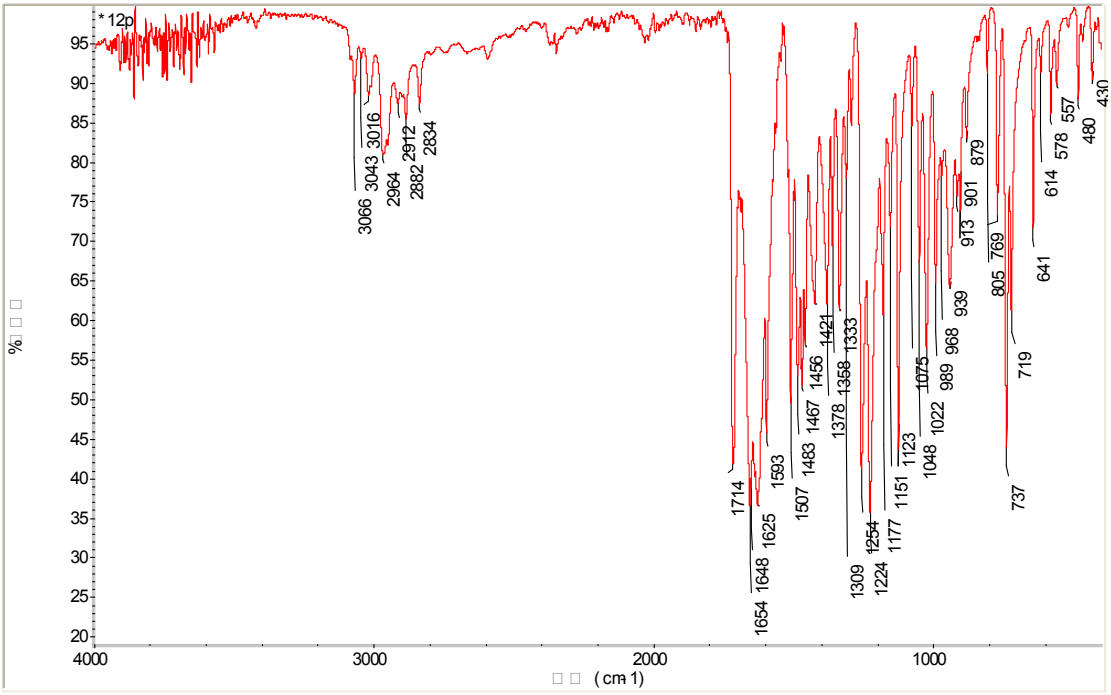


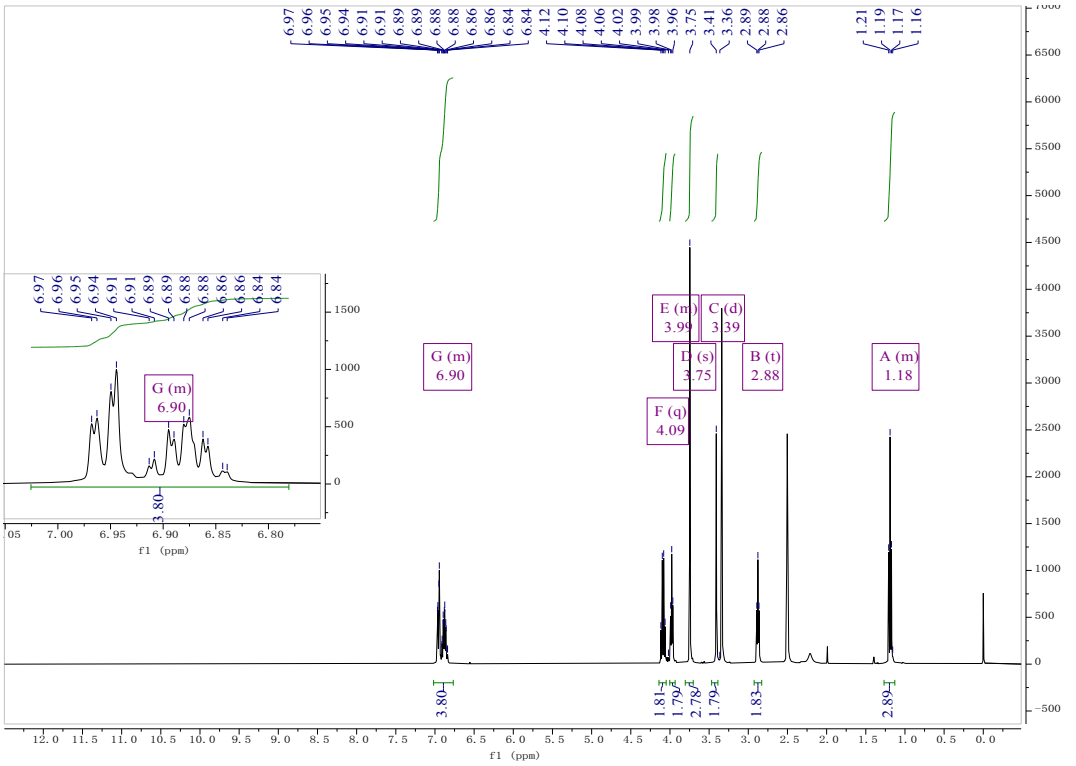

6.54
6.53
4.09
4.07
4.06
3.93
3.70
3.69
3.67
2.35
2.18
B (t)
4.07
F (s)
2.18
D (d)
6.54
A (t)
3.69
E (s)
2.35
C (s)
3.93
3.15
2.11
1.96
2.00
2.93
5.89
f1 (ppm)

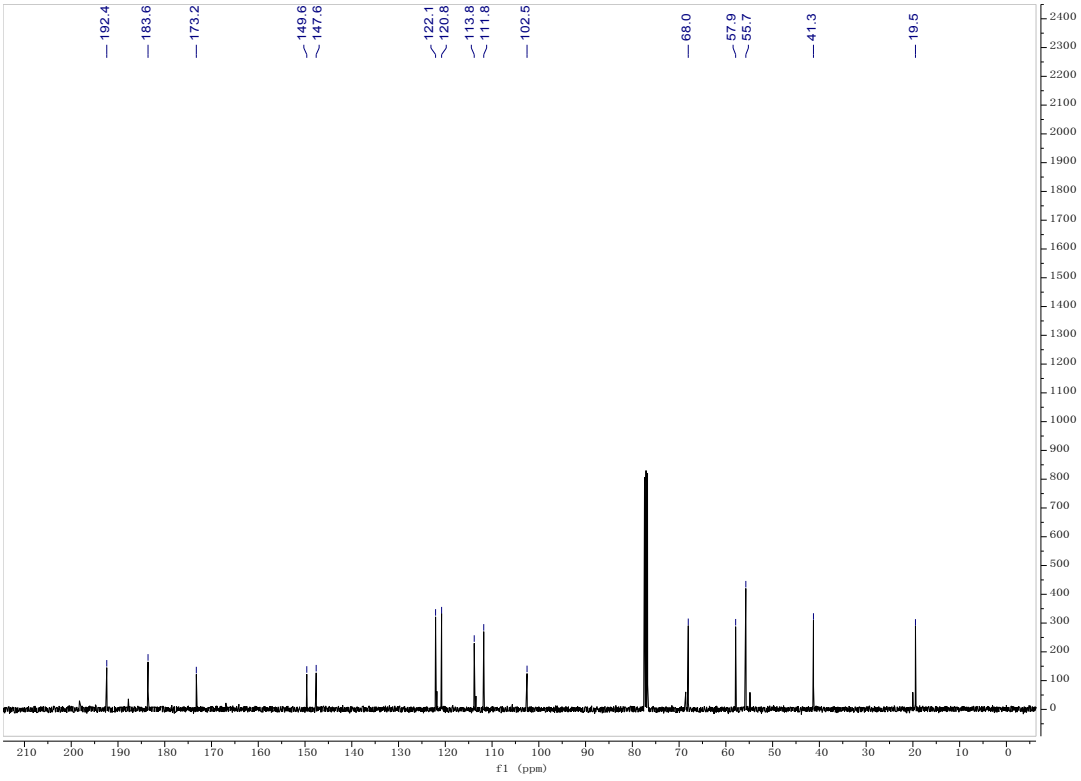

192.1
183.8
173.3
158.1
139.5
123.1
112.1
102.4
66.4
57.6
41.3
21.4
19.5
f1 (ppm)

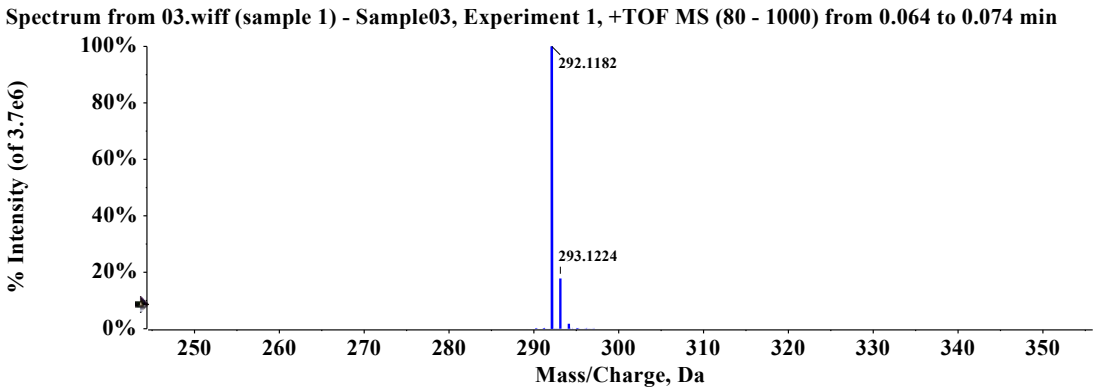


Compound 10p：

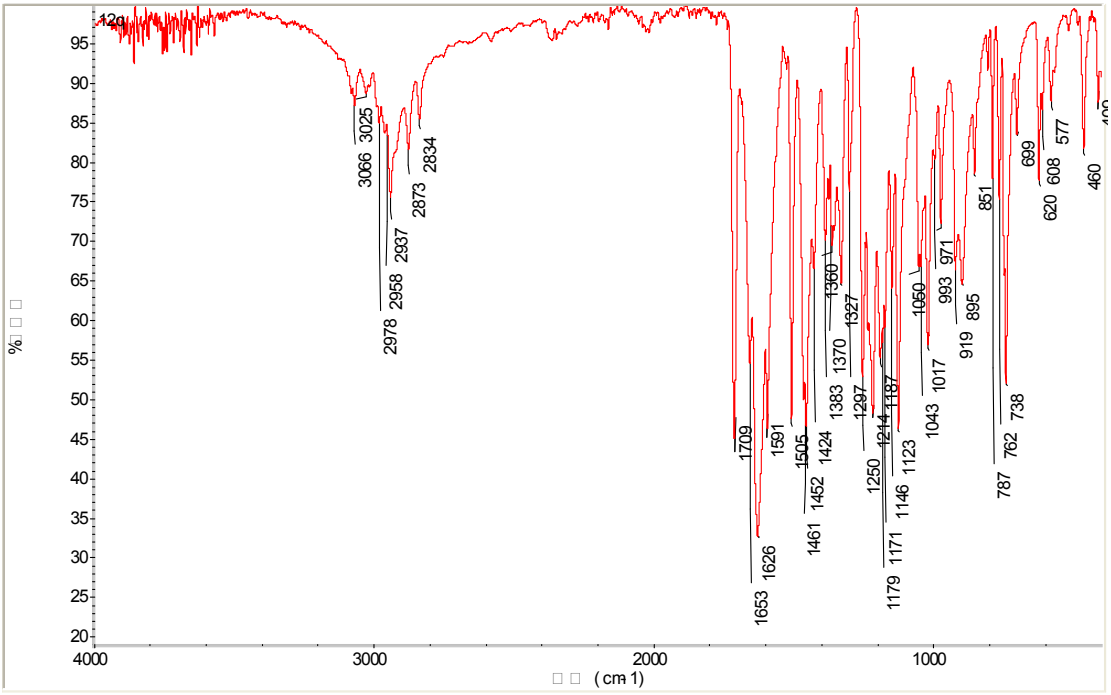


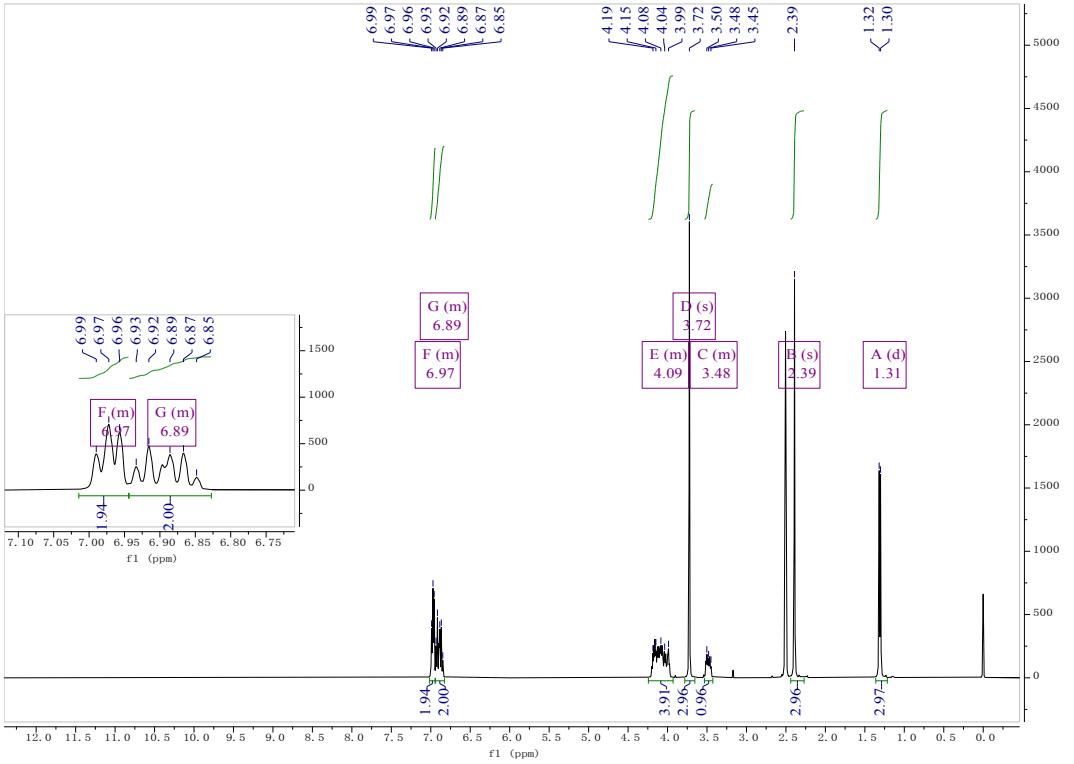

G (m)
6.90
E (m)
3.99
C (d)
3.39
D (s)
3.75
B (t)
2.88
F (q)
4.09
A (m)
1.18
f1 (ppm)

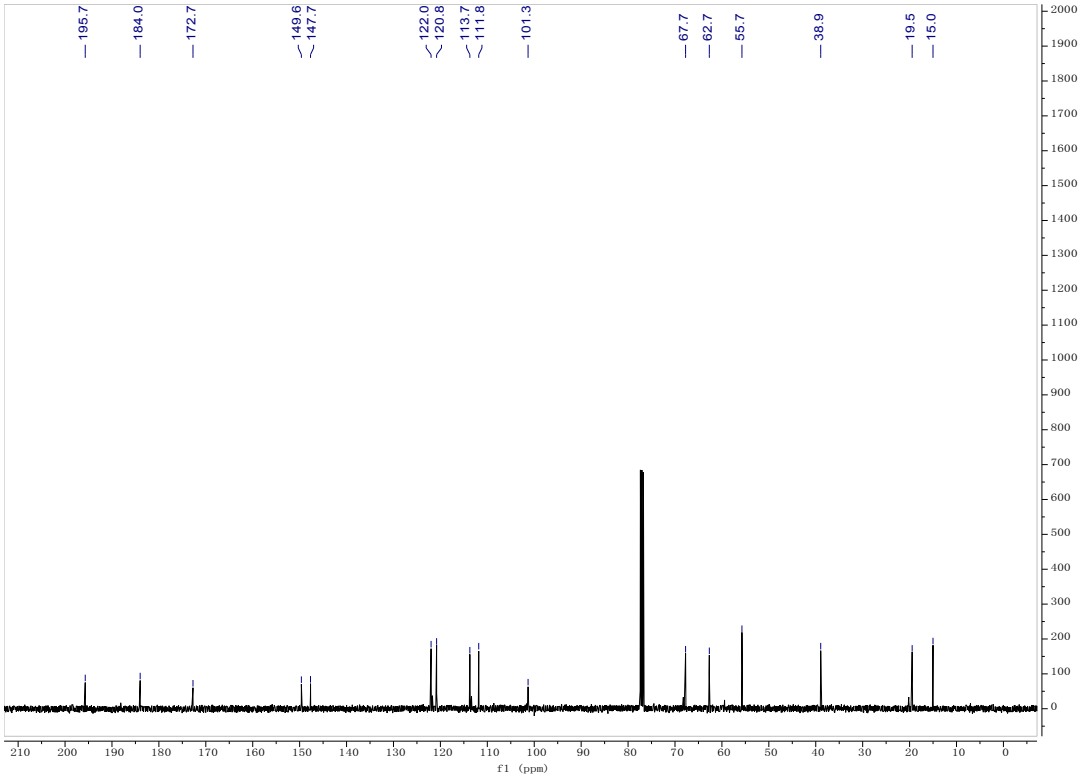

192.4
183.6
173.2
149.6
147.6
122.1
120.8
113.8
111.8
102.5
68.0
57.9
55.7
41.3
19.5
f1 (ppm)



Compound 10q:




6.99
6.97
6.96
6.93
6.92
6.89
6.87
6.85
4.19
4.15
4.08
4.04
3.99
3.72
3.50
3.48
3.45
2.39
1.32
1.30
G (m)
6.89
F (m)
6.97
D (s)
3.72
E (m)
4.09
C (m)
3.48
B (s)
2.39
A (d)
1.31
1.94
2.00
3.91
2.96
0.96
2.96
2.97
f1 (ppm)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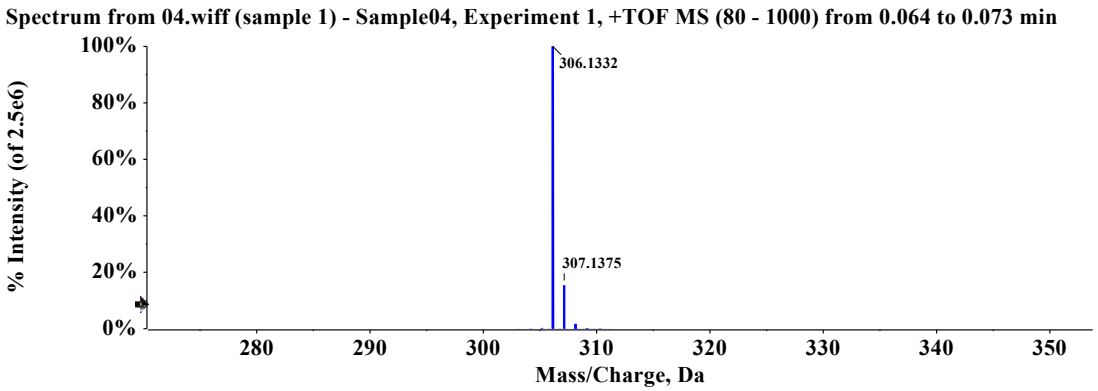
184.0
172.7
149.6
147.7
122.0
120.8
113.7
111.8
101.3
67.7
62.7
55.7
38.9
19.5
15.0
f1 (ppm)



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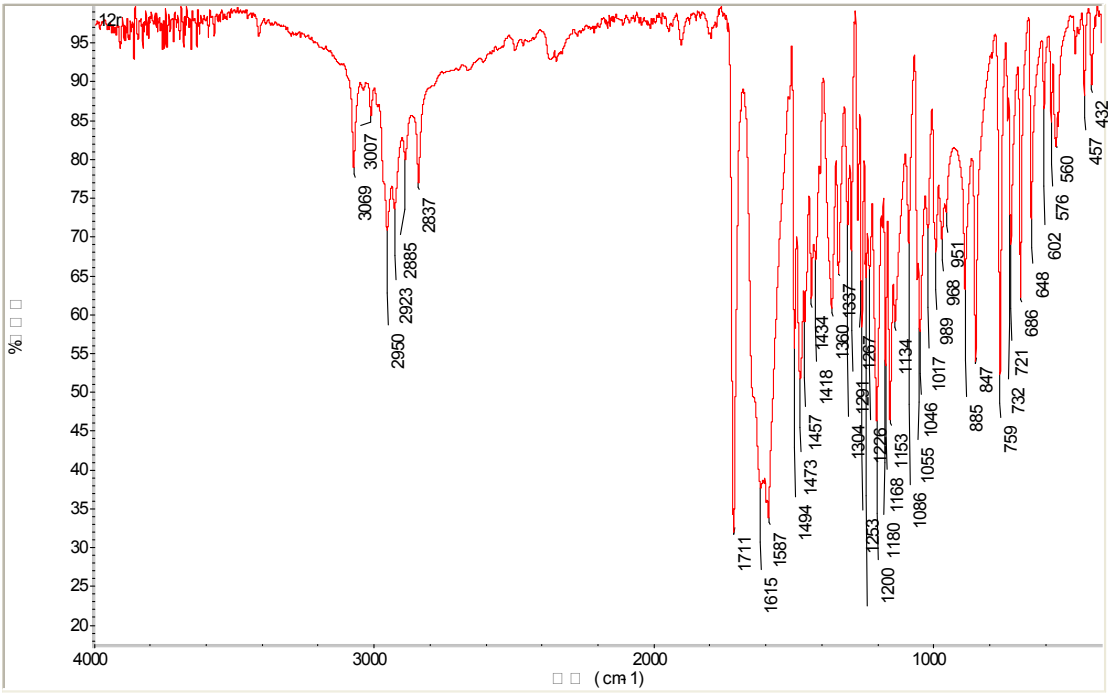
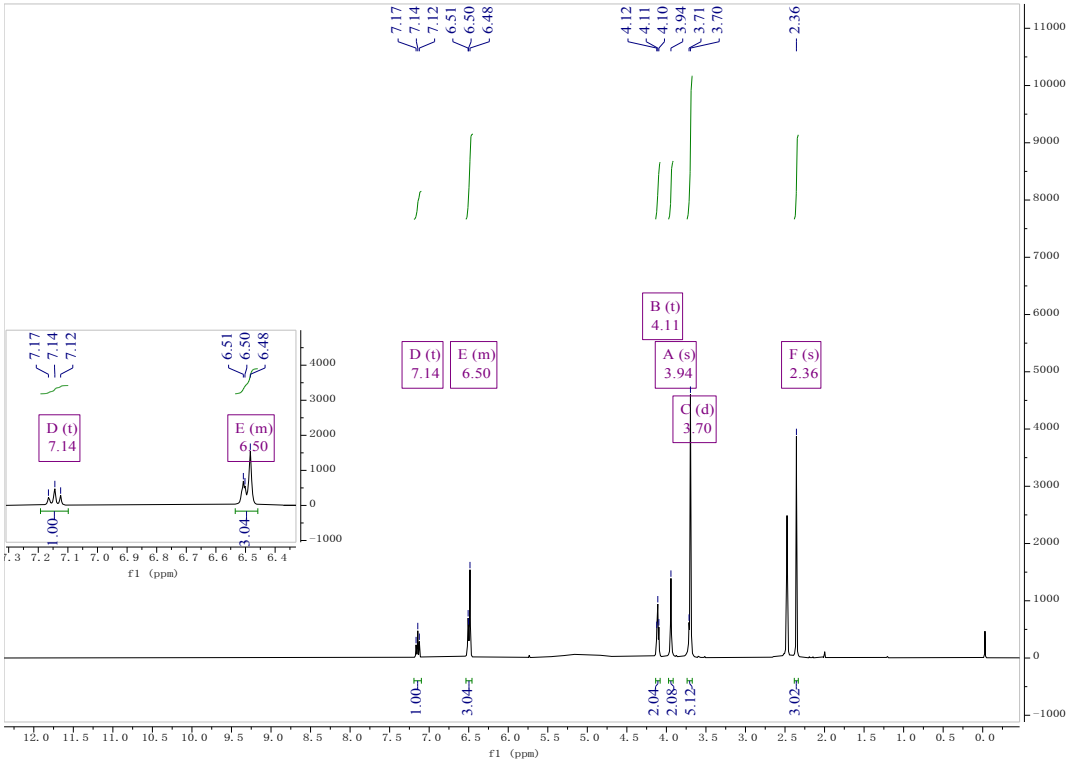
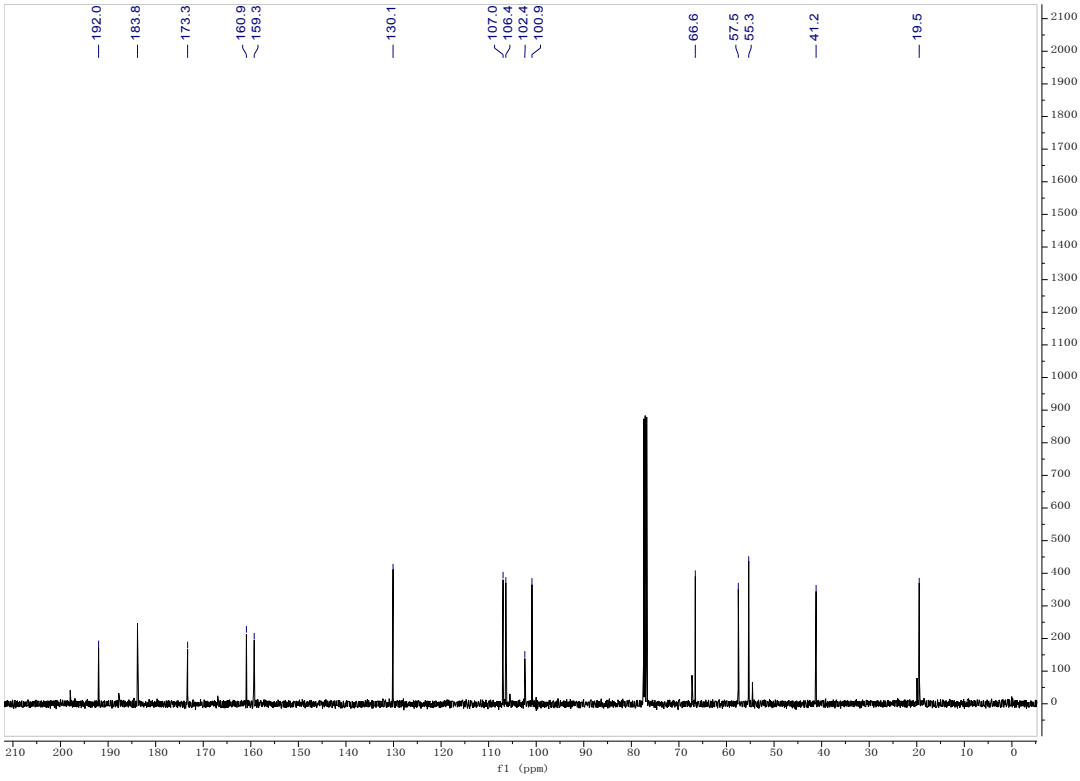
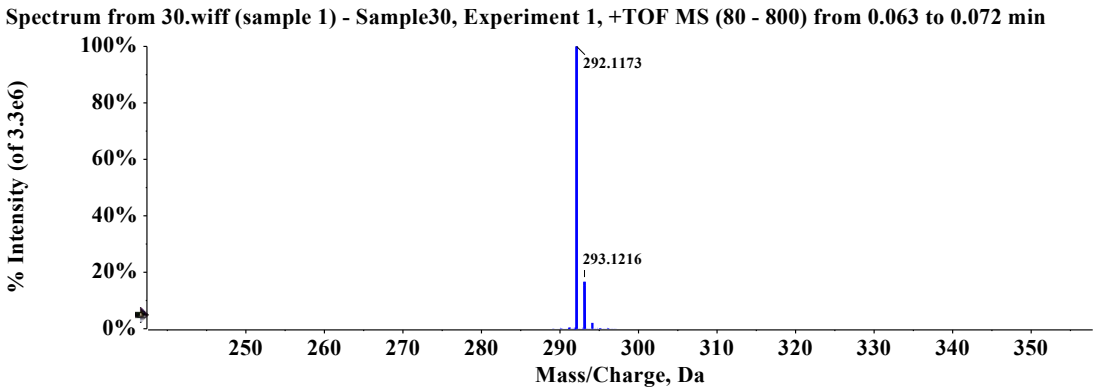
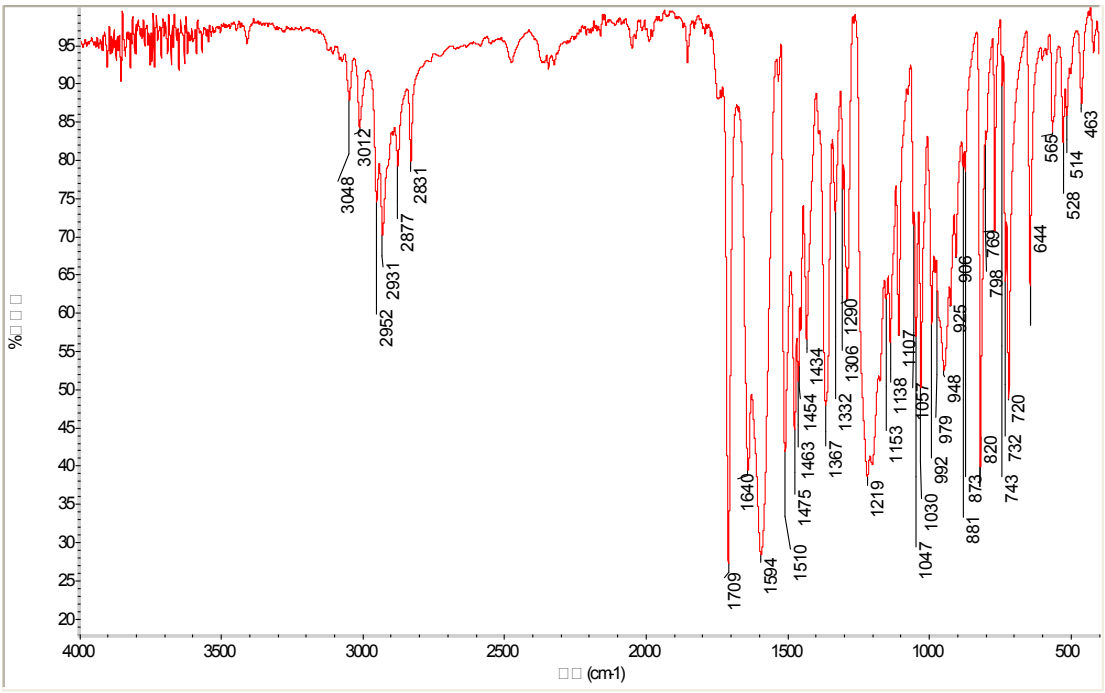


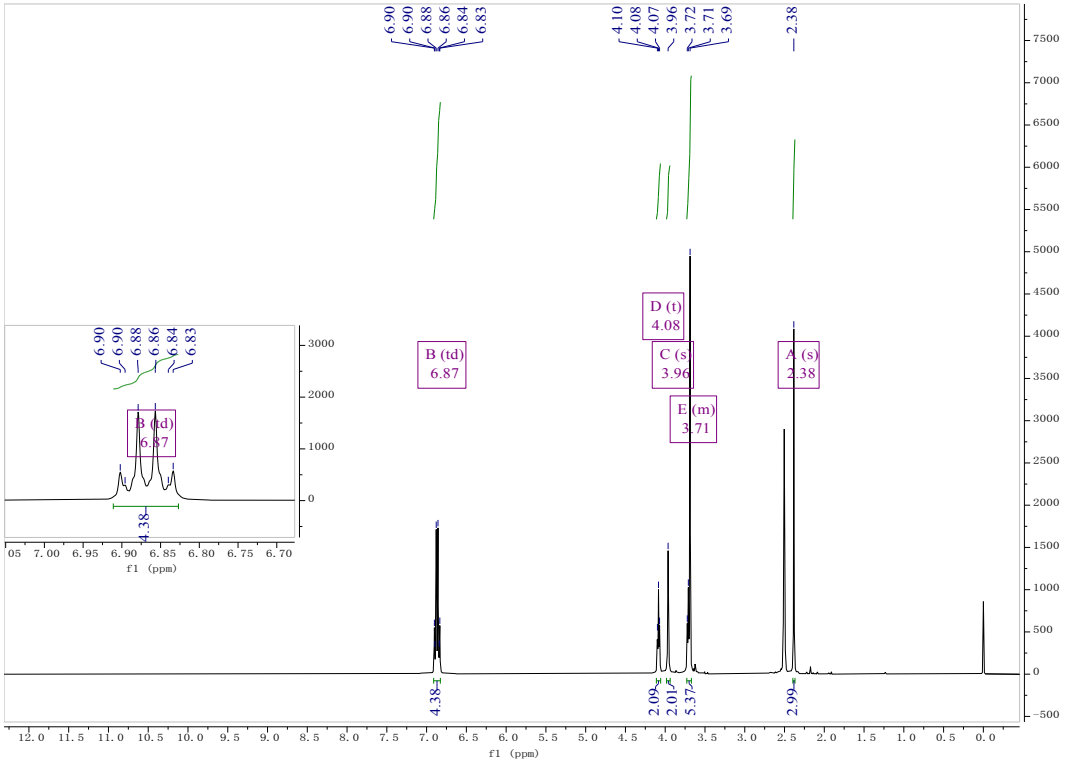

7.17
7.14
7.12
6.51
6.50
6.48
4.12
4.11
4.10
3.94
3.71
3.70
2.36
B (t)
4.11
D (t)
7.14
E (m)
6.50
A (s)
3.94
F (s)
2.36
C (d)
3.70
1.00
3.04
2.04
2.08
5.12
3.02
f1 (ppm)


192.0
183.8
173.3
160.9
159.3
130.1
107.0
106.4
102.4
100.9
66.6
57.5
55.3
41.2
19.5
f1 (ppm)



Compound 10s:

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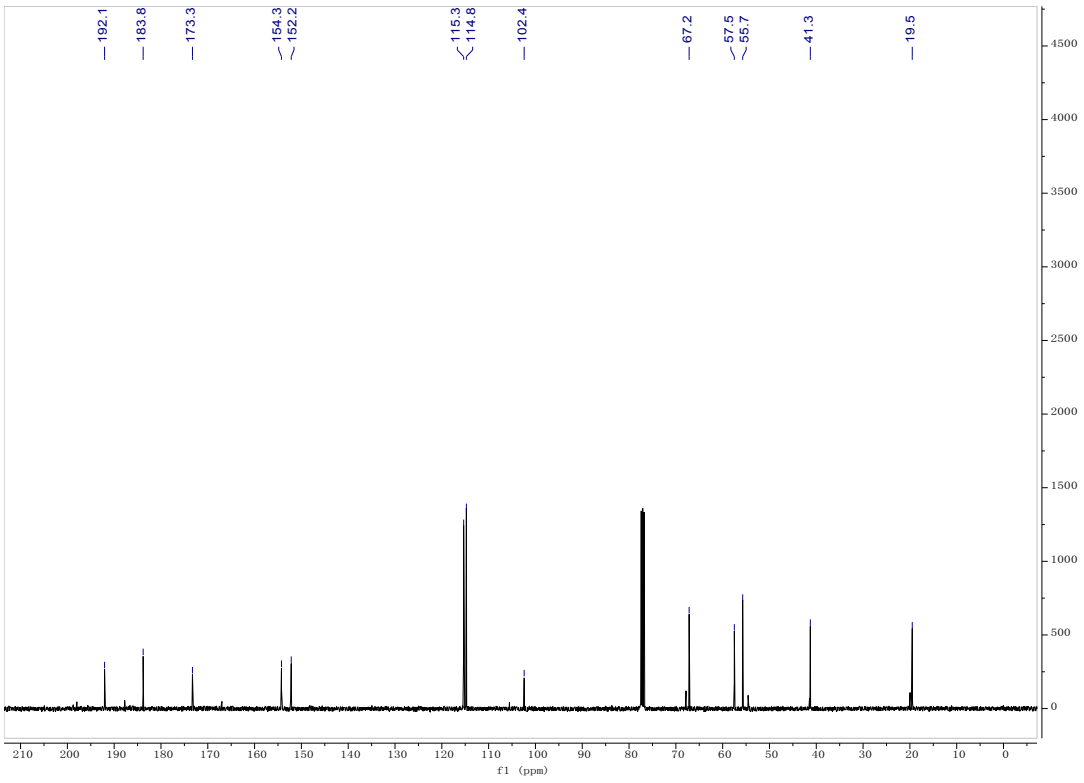
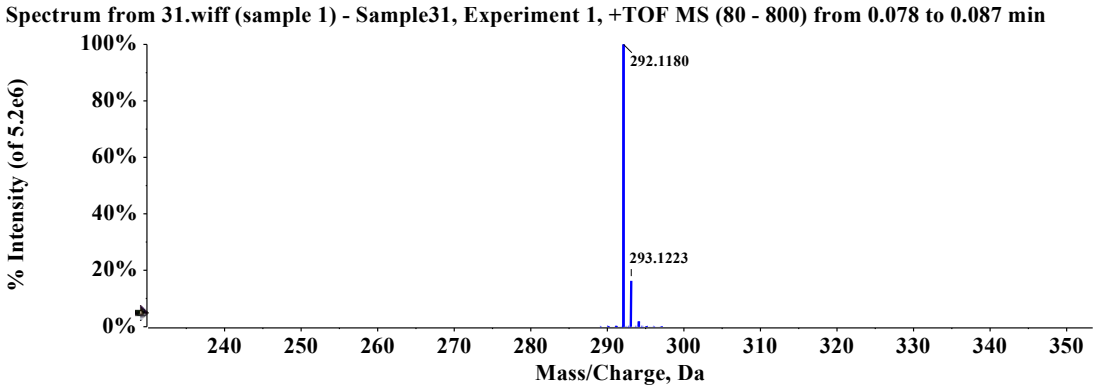
6.90
6.88
6.86
6.84
6.83
4.10
4.08
4.07
3.96
3.72
3.71
3.69
2.38
B (td)
6.87
D (t)
4.08
C (s)
3.96
E (m)
3.71
A (s)
2.38
4.38
2.09
2.01
5.37
2.99
f1 (ppm)


192.1
183.8
173.3
154.3
152.2
115.3
114.8
102.4
67.2
57.5
55.7
41.3
19.5
f1 (ppm)



2. Crystallographic data of compound **10a**

Table S1 Selected bond distances of crystal 10a

Molecule A		Molecule B	
Bond	Distance (Å)	Bond	Distance (Å)
Cl1–C10	1.731(2)	Cl2–C24	1.731(2)
O1–C1	1.244(2)	O5–C15	1.247(3)
O2–C5	1.322(3)	O6–C19	1.335(3)
O3–C3	1.219(3)	O7–C17	1.217(3)
O4–C8	1.437(2)	O8–C22	1.432(3)
O4–C9	1.363(3)	O8–C23	1.359(3)
N1–C1	1.345(3)	N2–C15	1.335(3)
N1–C4	1.455(3)	N2–C18	1.463(3)
N1–C7	1.451(3)	N2–C21	1.450(3)
C1–C2	1.450(3)	C15–C16	1.458(3)
C2–C3	1.451(3)	C16–C17	1.452(3)
C2–C5	1.358(3)	C16–C19	1.355(3)
C3–C4	1.522(3)	C17–C18	1.518(3)
C5–C6	1.477(4)	C19–C20	1.466(4)
C7–C8	1.505(3)	C21–C22	1.504(3)
C9–C10	1.395(3)	C23–C28	1.383(3)
C9–C14	1.386(3)	C23–C24	1.398(3)
C10–C11	1.375(4)	C24–C25	1.377(4)
C11–C12	1.380(4)	C25–C26	1.382(4)
C12–C13	1.373(4)	C26–C27	1.366(4)
C13–C14	1.387(3)	C27–C28	1.393(3)

Table S2 Selected bond angles of crystal 10a

Molecule A		Molecule B	
Bond angle	Degree (°)	Bond angle	Degree (°)
C1–N1–C4	112.33(17)	C15–N2 –C18	112.42(18)
C1–N1–C7	122.81(17)	C15–N2 –C21	123.58(18)
C4–N1–C7	124.24(18)	C18–N2 –C21	123.94(18)
O1–C1–C2	125.4(2)	O5–C15–C16	125.0(2)
N1–C1–C2	109.31(17)	N2–C15–C16	109.62(18)
O1–C1–N1	125.3(2)	O5–C15–N2	125.4(2)
C1–C2–C5	121.09(19)	C15–C16–C19	121.75(19)
C3–C2–C5	130.7(2)	C17–C16–C19	130.8(2)
C1–C2–C3	108.04(19)	C15–C16–C17	107.47(19)
O3–C3–C2	129.9(2)	O7–C17–C16	129.3(2)
C2–C3–C4	106.22(18)	C16–C17–C18	106.67(17)
O3–C3–C4	123.9(2)	O7–C17–C18	124.0(2)
N1–C4–C3	104.04(18)	N2–C18–C17	103.80(17)
O2–C5–C6	114.7(2)	O6–C19–C20	114.7(2)
C2–C5–C6	124.9(2)	C16–C19–C20	125.4(2)
O2–C5–C2	120.5(2)	O6–C19–C16	119.9(2)
N1–C7–C8	113.8(2)	N2–C21–C22	113.6(2)
O4–C8–C7	106.26(16)	O8–C22–C21	106.53(16)
C8–O4–C9	117.72(15)	C22–O8–C23	118.03(15)
O4–C9–C14	124.58(18)	O8–C23–C28	124.85(19)
O4–C9–C10	116.04(18)	O8–C23–C24	116.18(18)
C10–C9–C14	119.4(2)	C24–C23–C28	119.0(2)
Cl1–C10–C11	120.97(18)	Cl2–C24–C25	120.58(18)
Cl1–C10–C9	118.59(17)	Cl2–C24–C23	118.50(18)
C9–C10–C11	120.4(2)	C23–C24–C25	120.9(2)
C10–C11–C12	119.9(2)	C24–C25–C26	119.5(2)
C11–C12–C13	120.1(2)	C25–C26–C27	120.2(2)
C12–C13–C14	120.6(2)	C26–C27–C28	120.9(2)
C9–C14–C13	119.6(2)	C23–C28–C27	119.6(2)