Supporting Information For：

Design, synthesis and antifungal activity of psoralen derivatives

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Jiangsu Key Laboratory of Pesticide Science, Department of Chemistry, College of Sciences, Nanjing Agricultural University, Nanjing 210095, P.R. China

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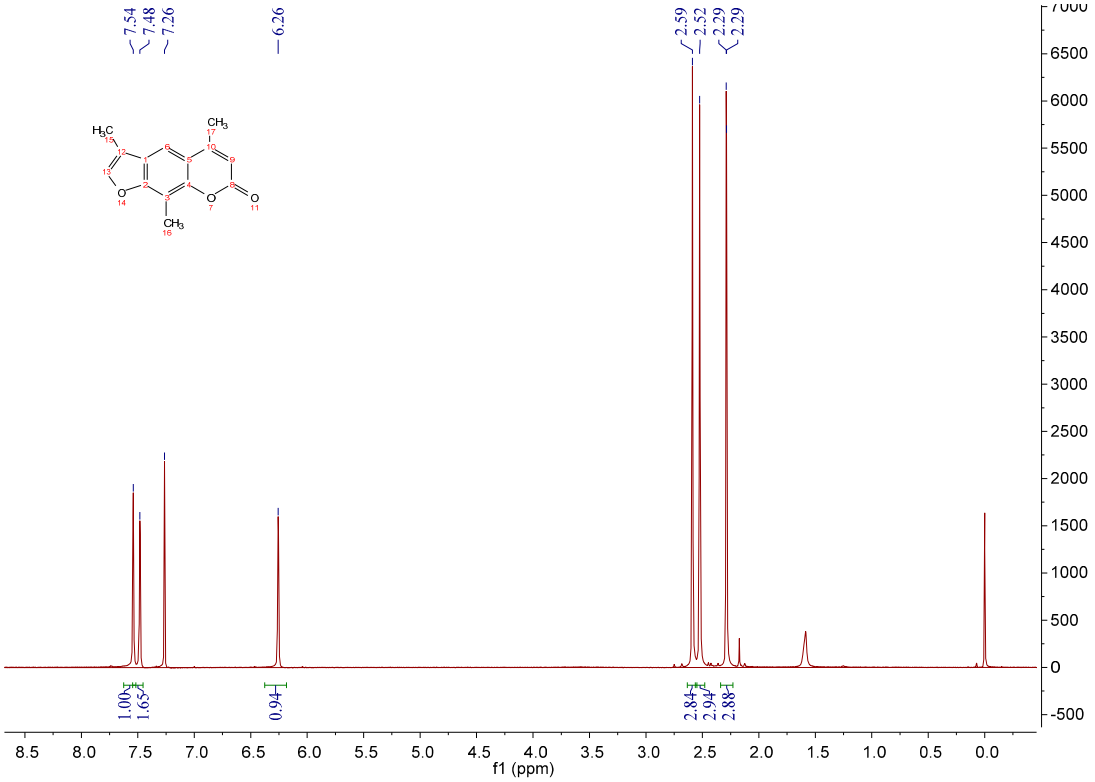
1. [1]HNMR and [13]CNMR Spectra of Products

[1]H-NMR

3a



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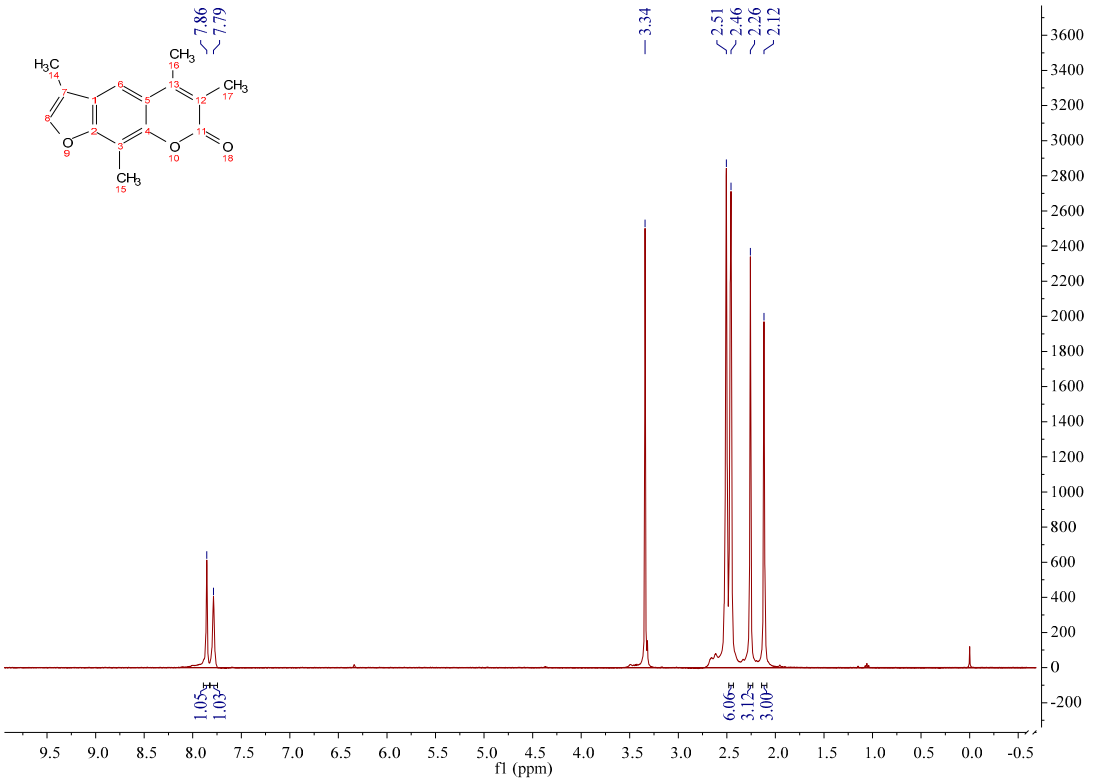

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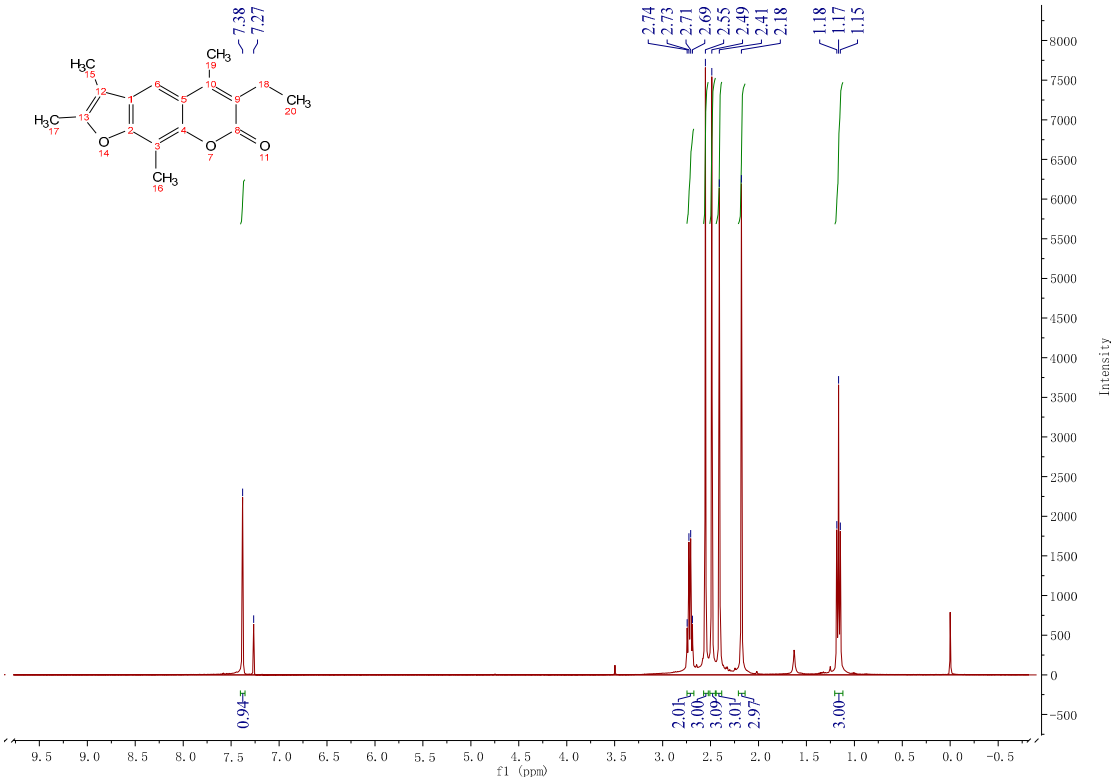
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2.18
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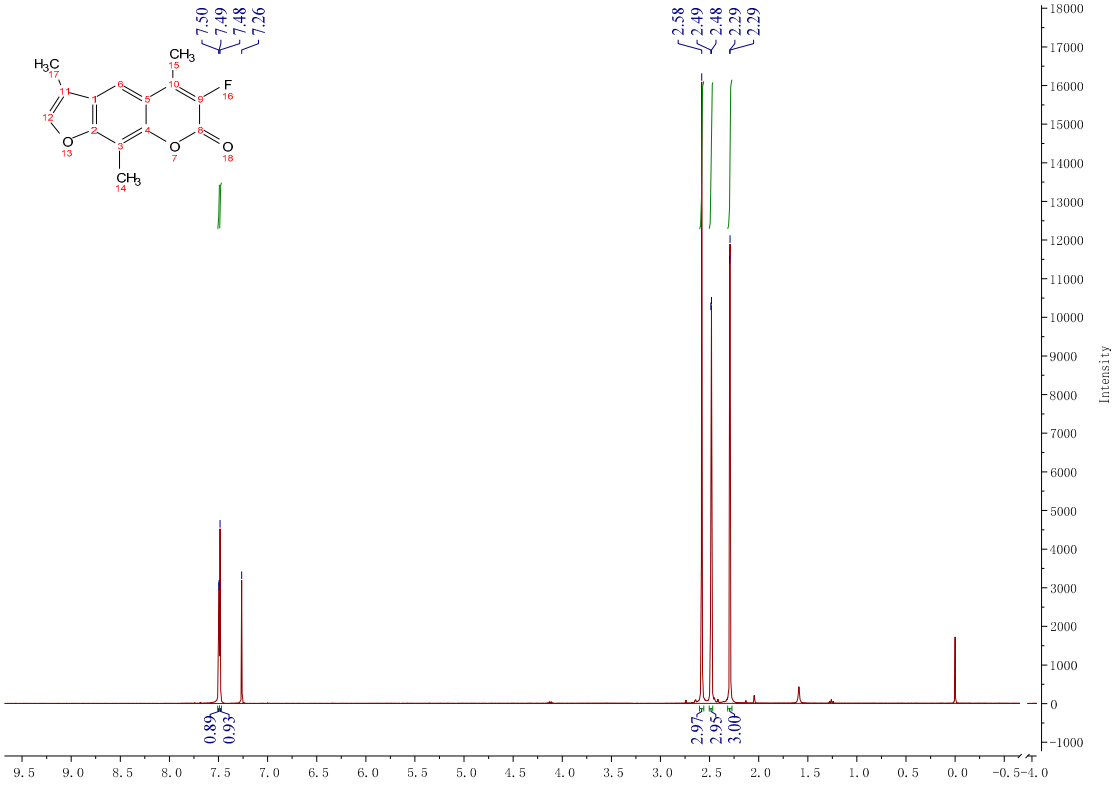
2.01
3.00
3.09
3.01
2.97
3.00
f1 (ppm)
Intensity

3d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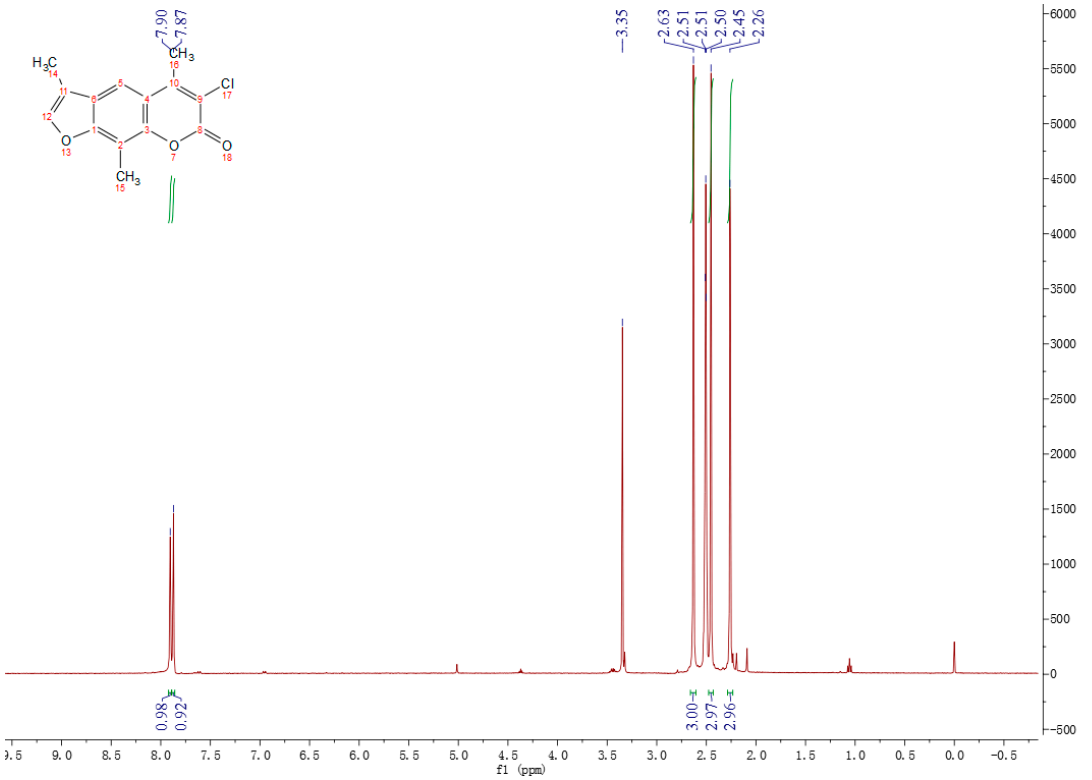
3.00
Intensity

3e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f1 (ppm)

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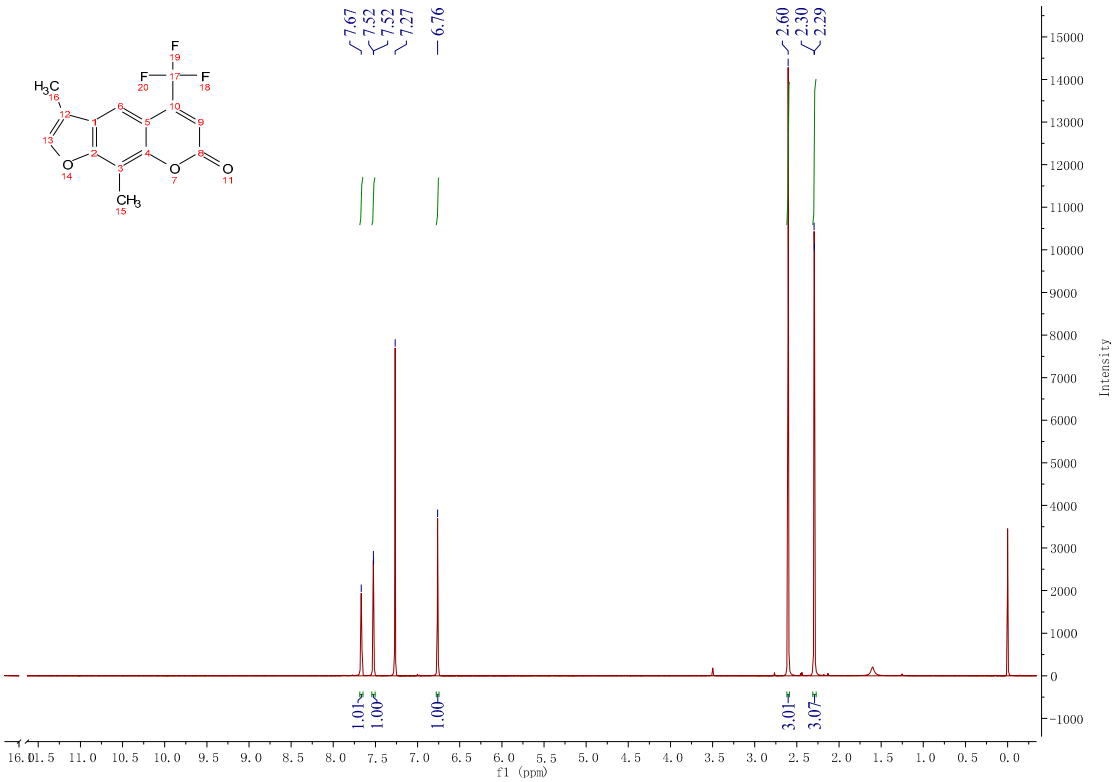
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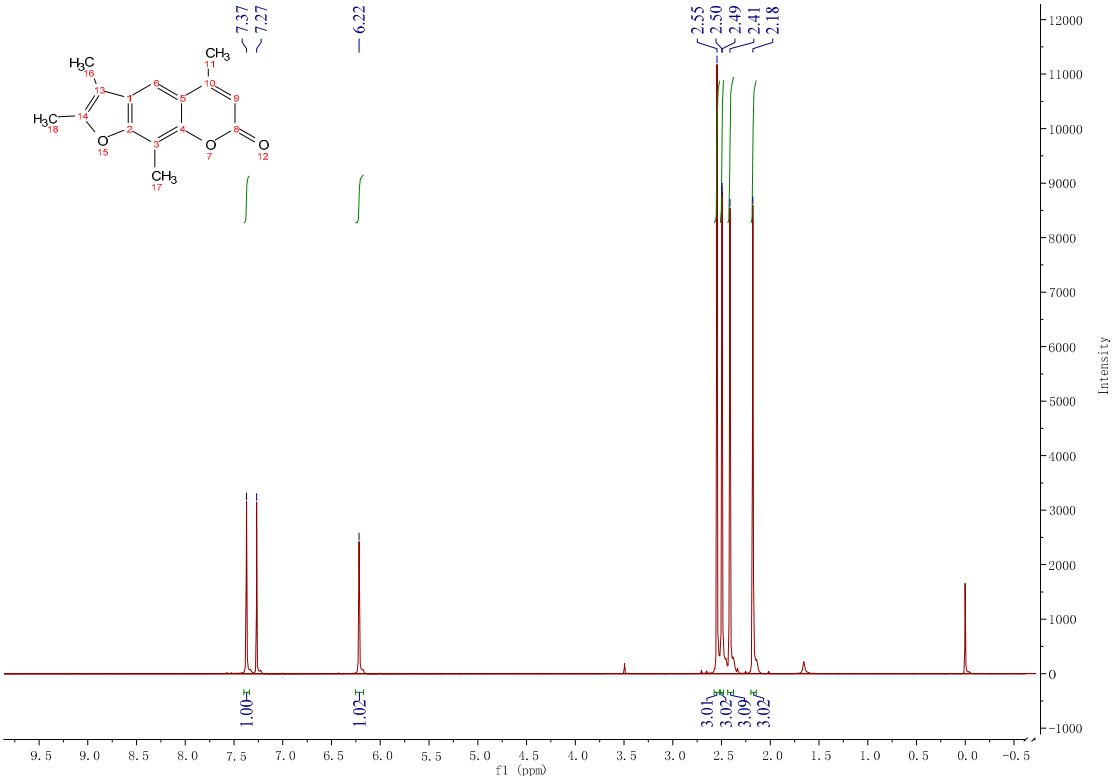
f1 (ppm)
Intensity

4a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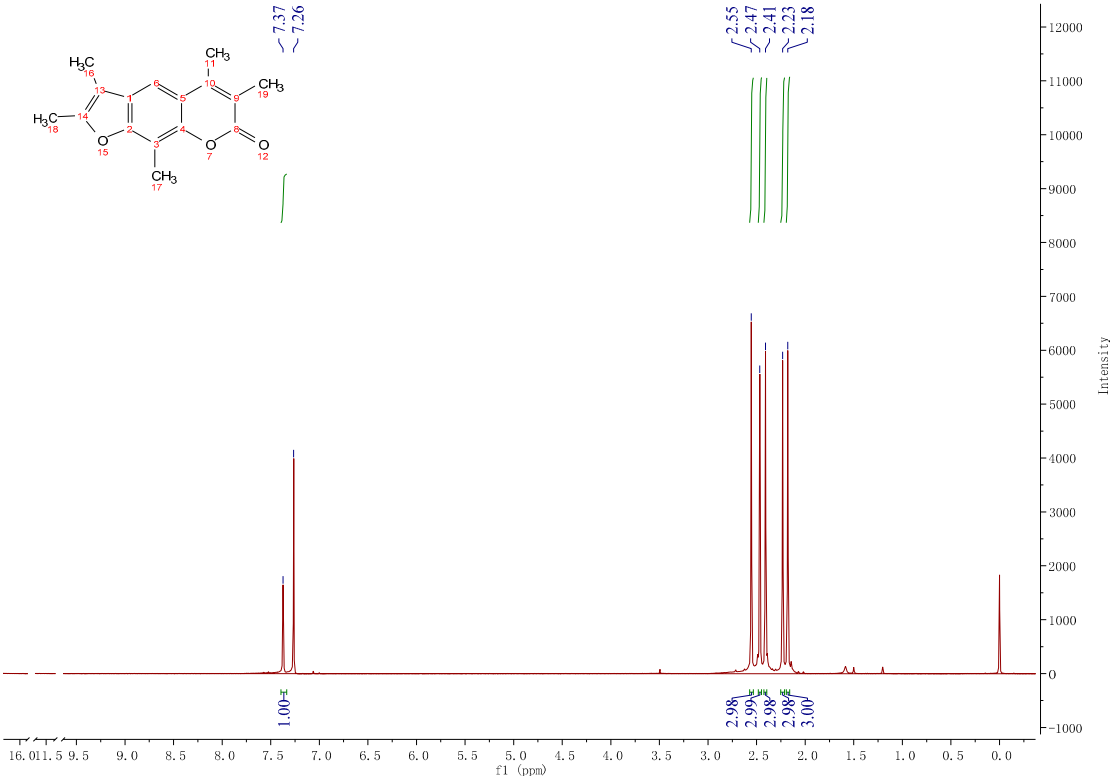
f1 (ppm)
Intensity

4b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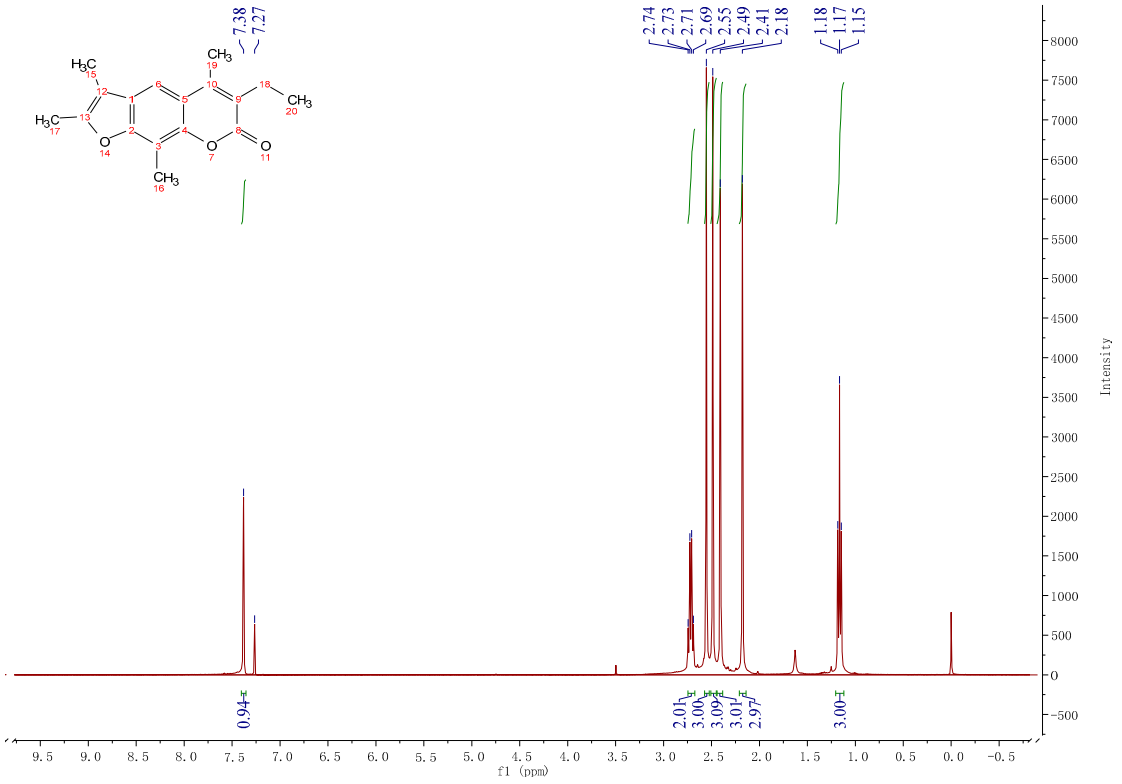
f1 (ppm)
Intensity

4c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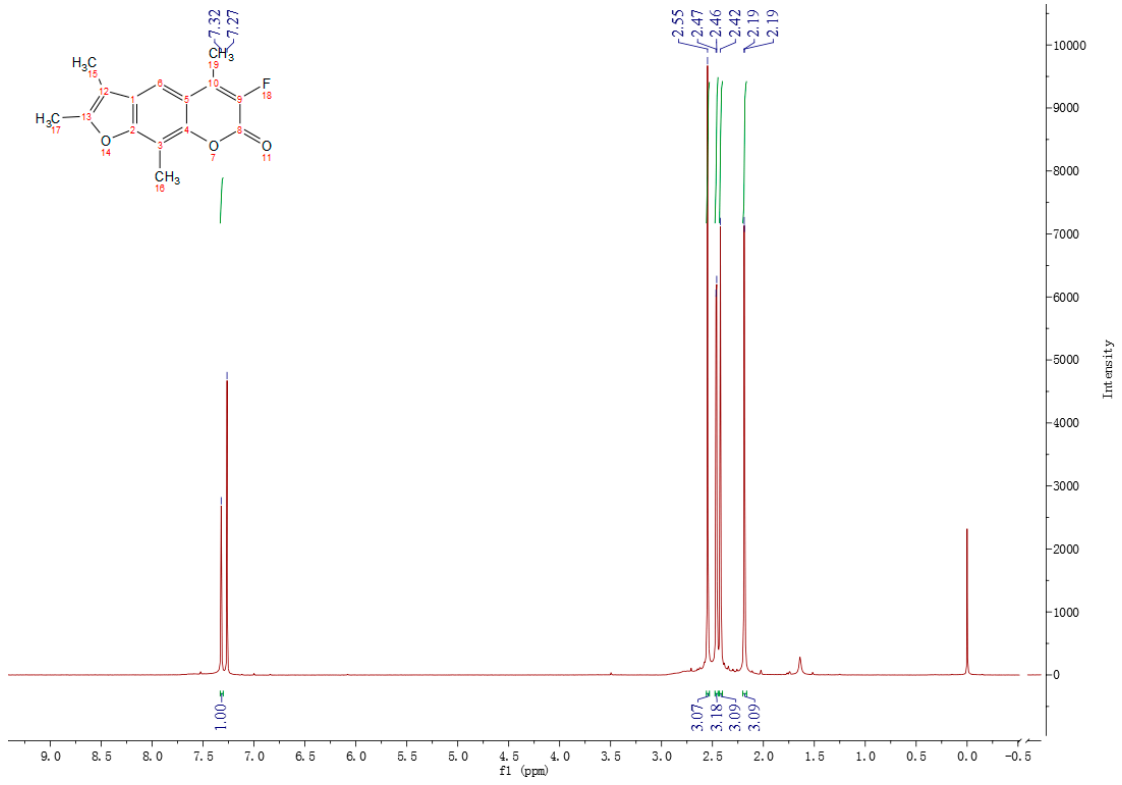
f1 (ppm)
Intensity

4d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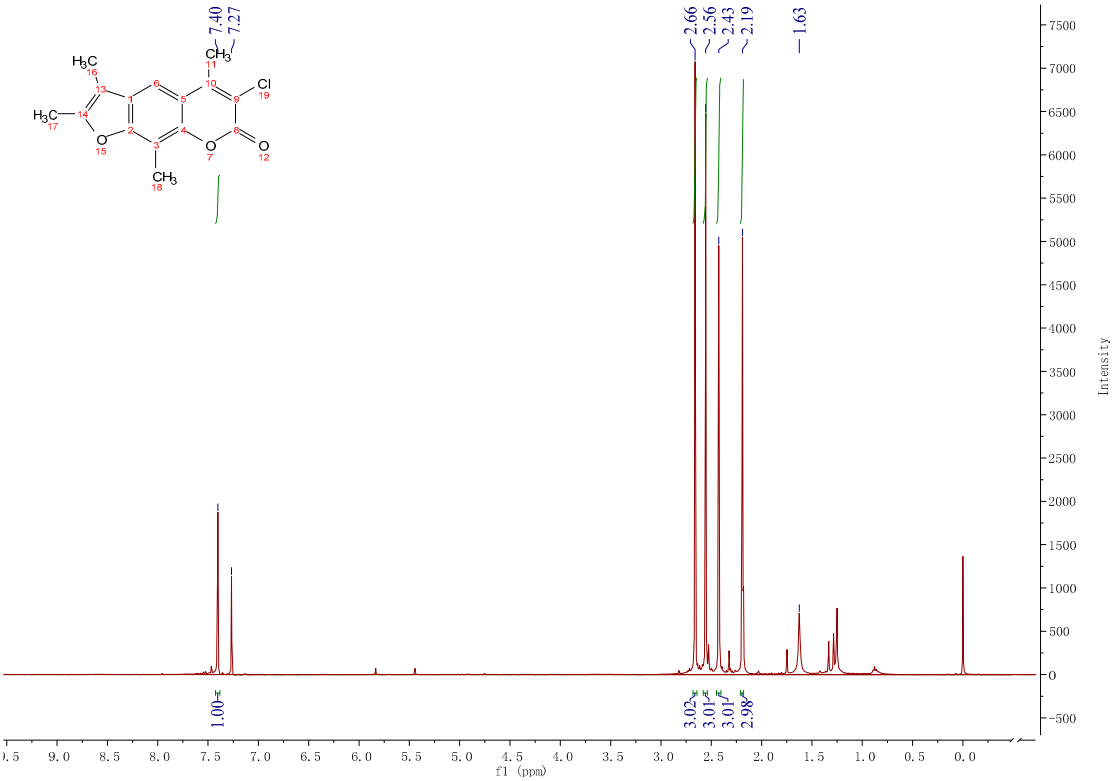
Intensity

4e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f1 (ppm)
Intensity

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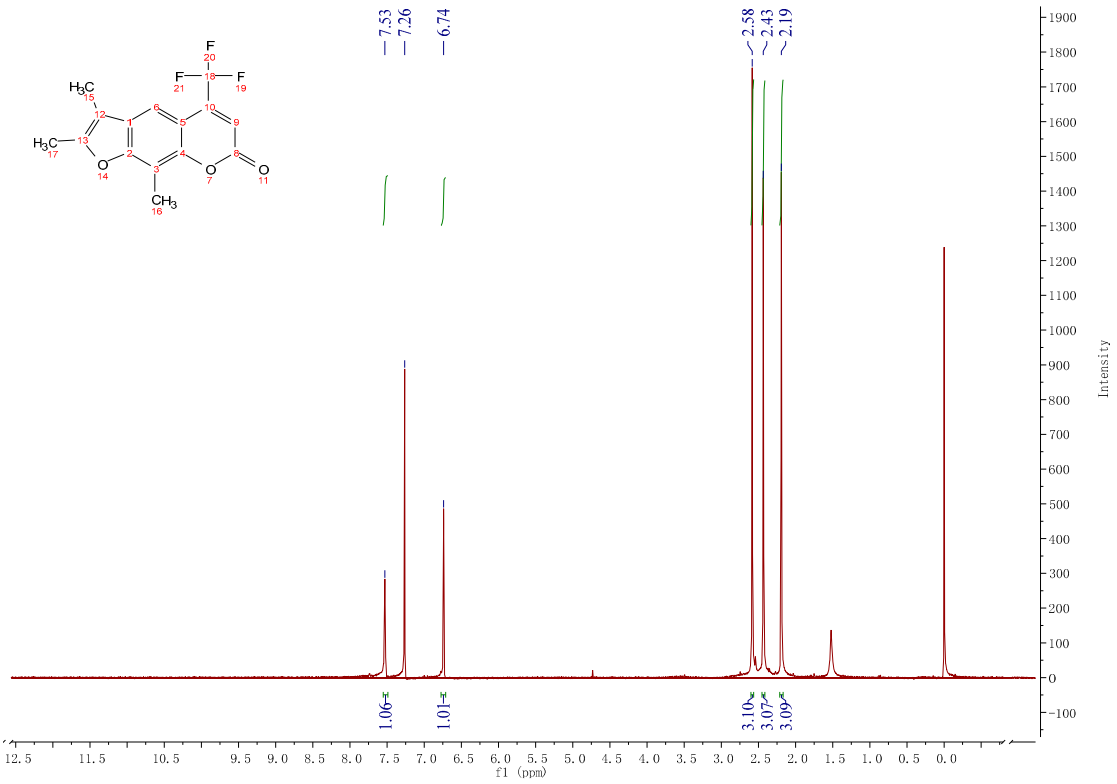
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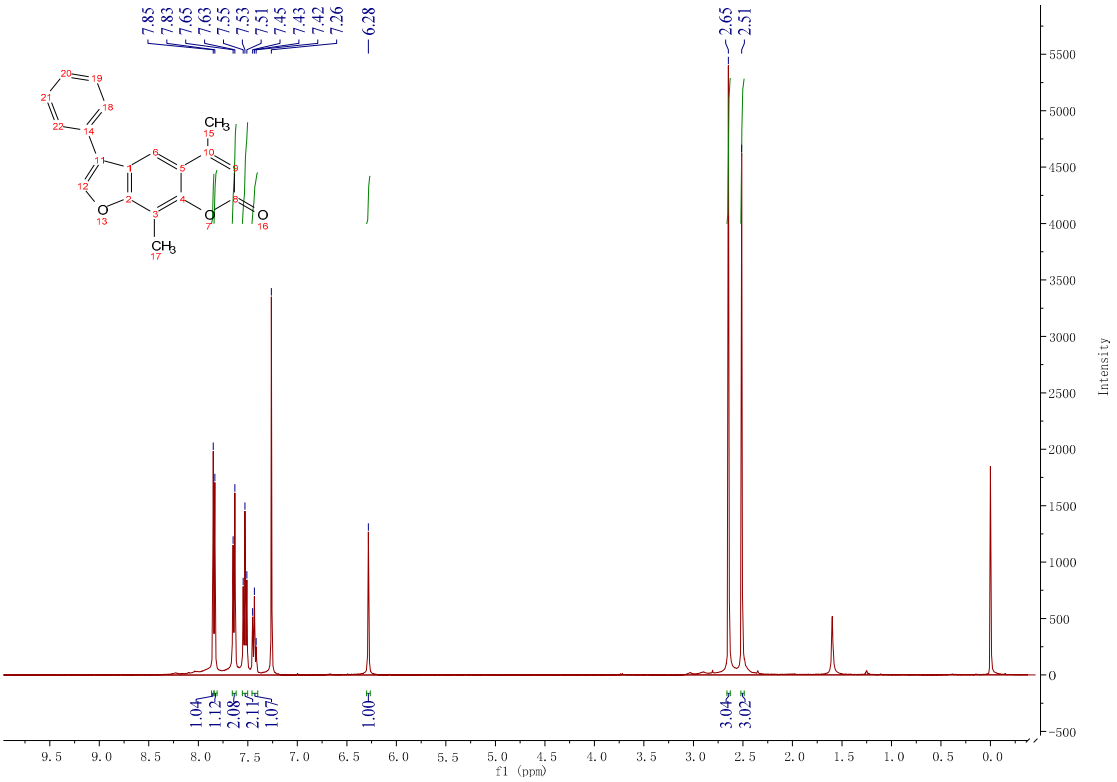
f1 (ppm)
Intensity

5a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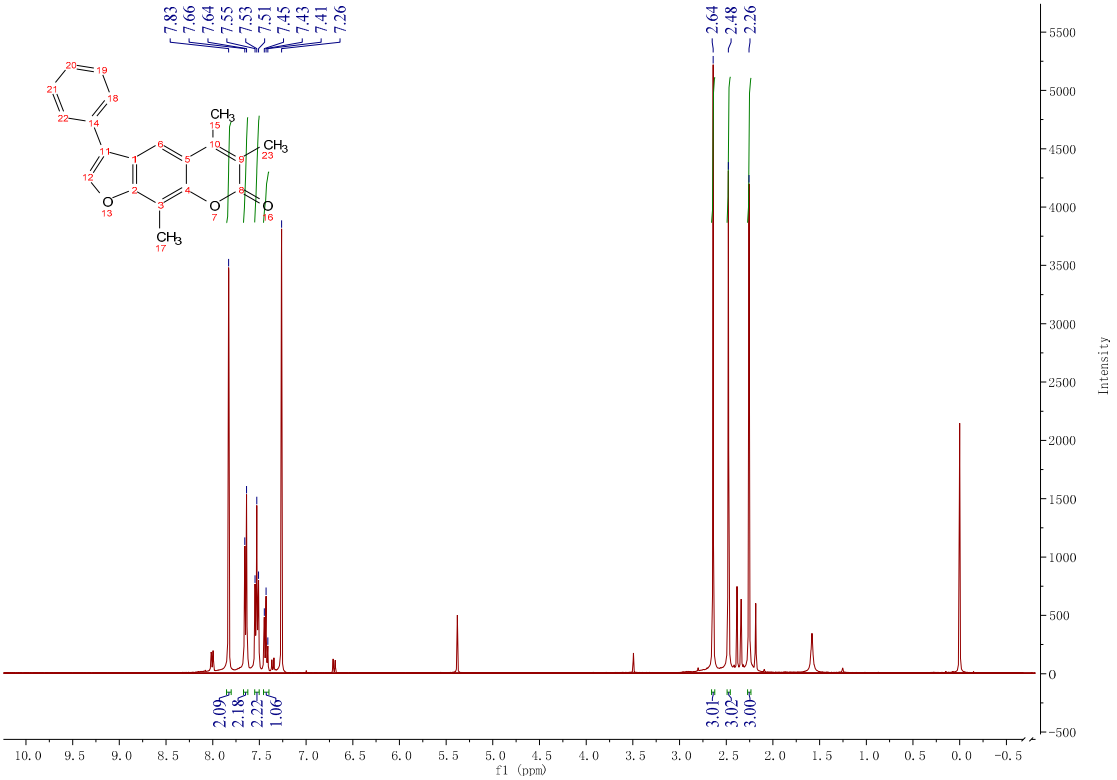
1.00
3.04
3.02
Intensity
f1 (ppm)

5b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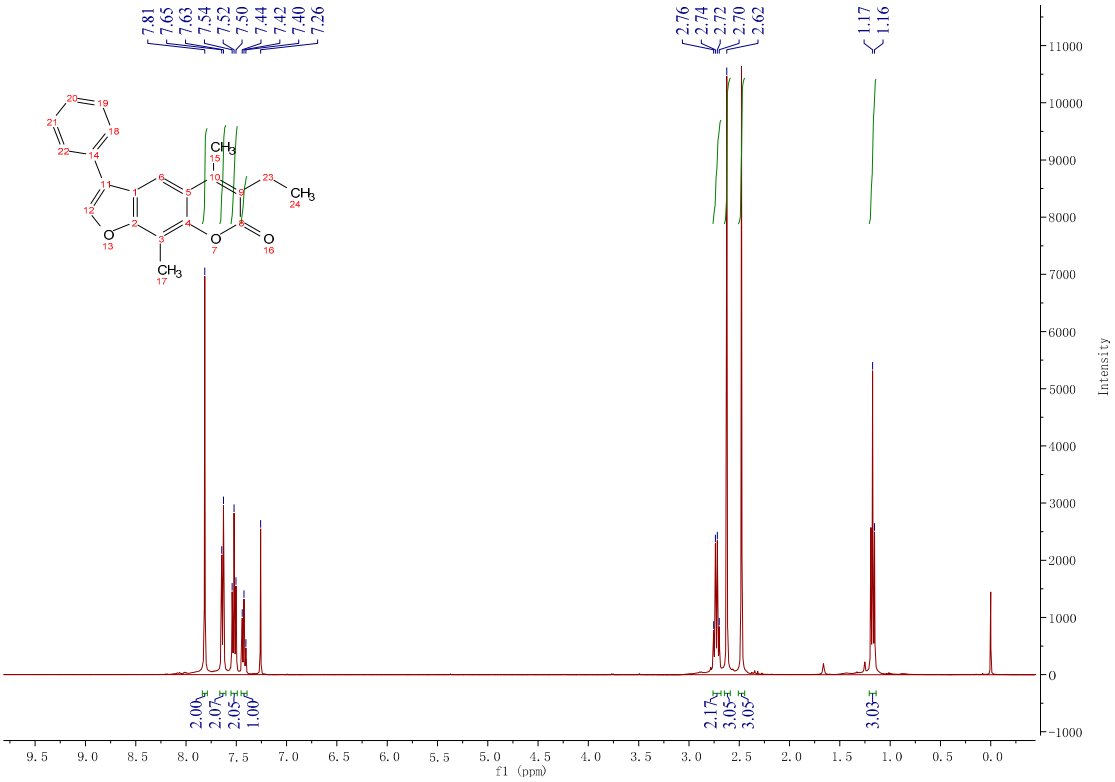
3.01
3.02
3.00
Intensity
f1 (ppm)

5c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1.17
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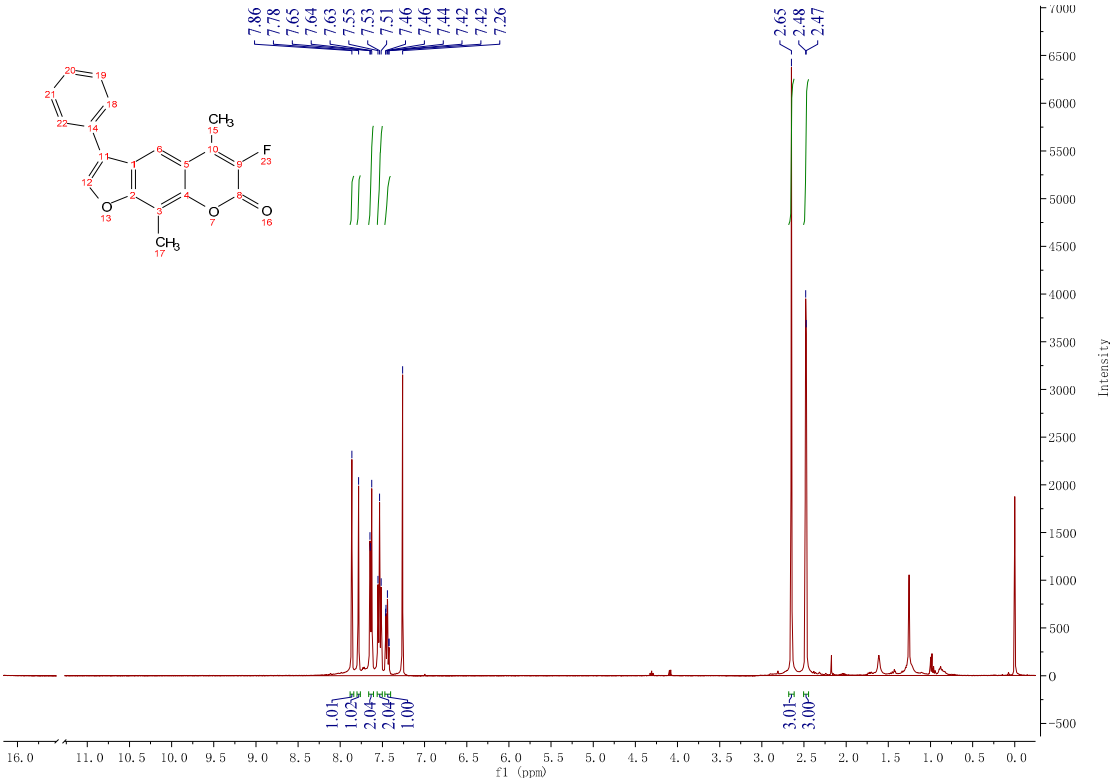
3.03
f1 (ppm)
Intensity

5d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2.65
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2.04
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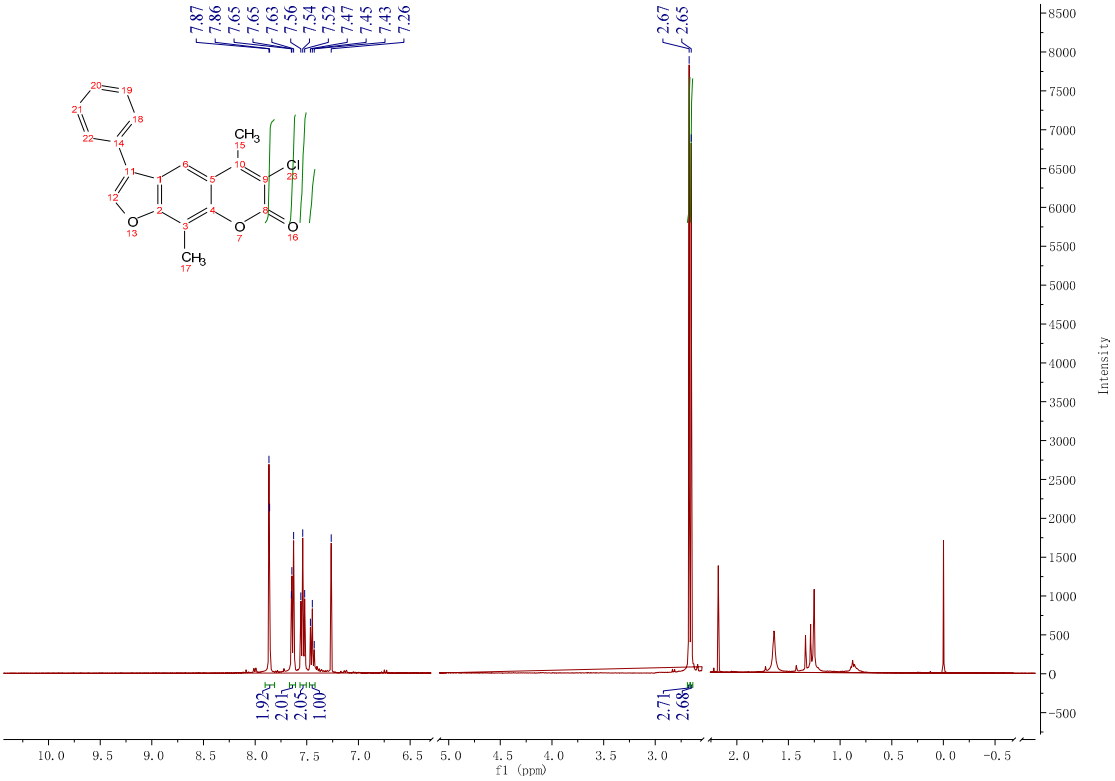
3.00
f1 (ppm)
Intensity

5e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CH3
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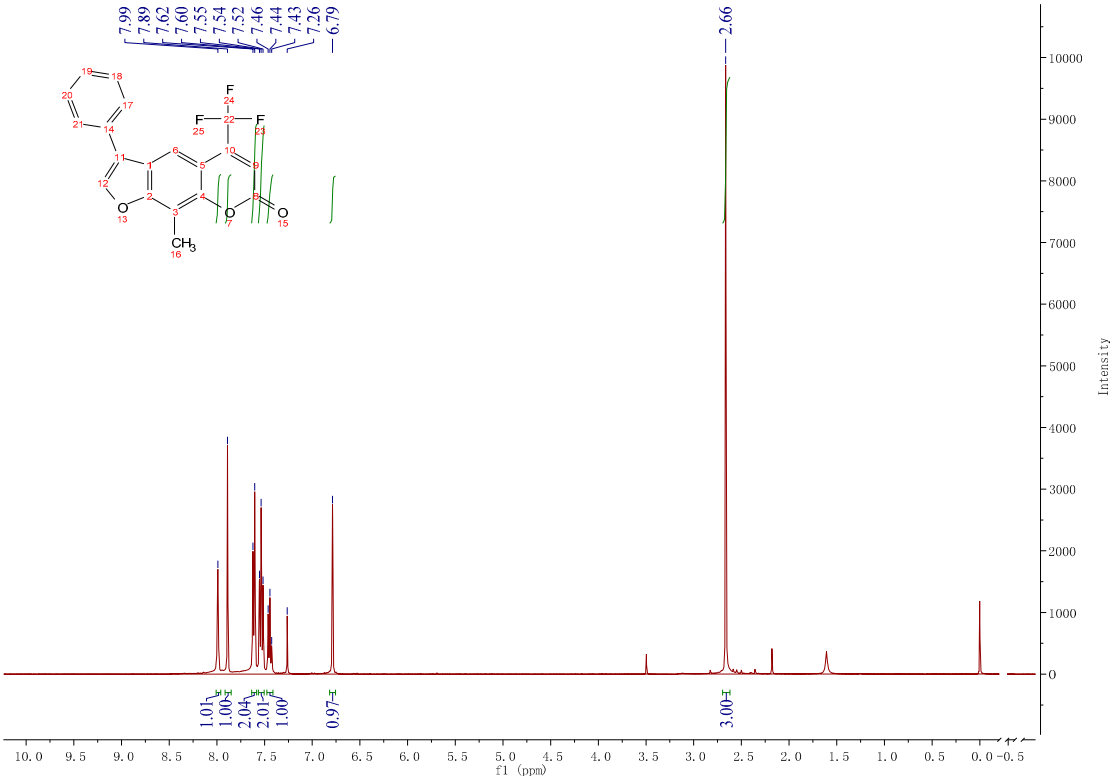
Intensity
f1 (ppm)

5f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F
F
F
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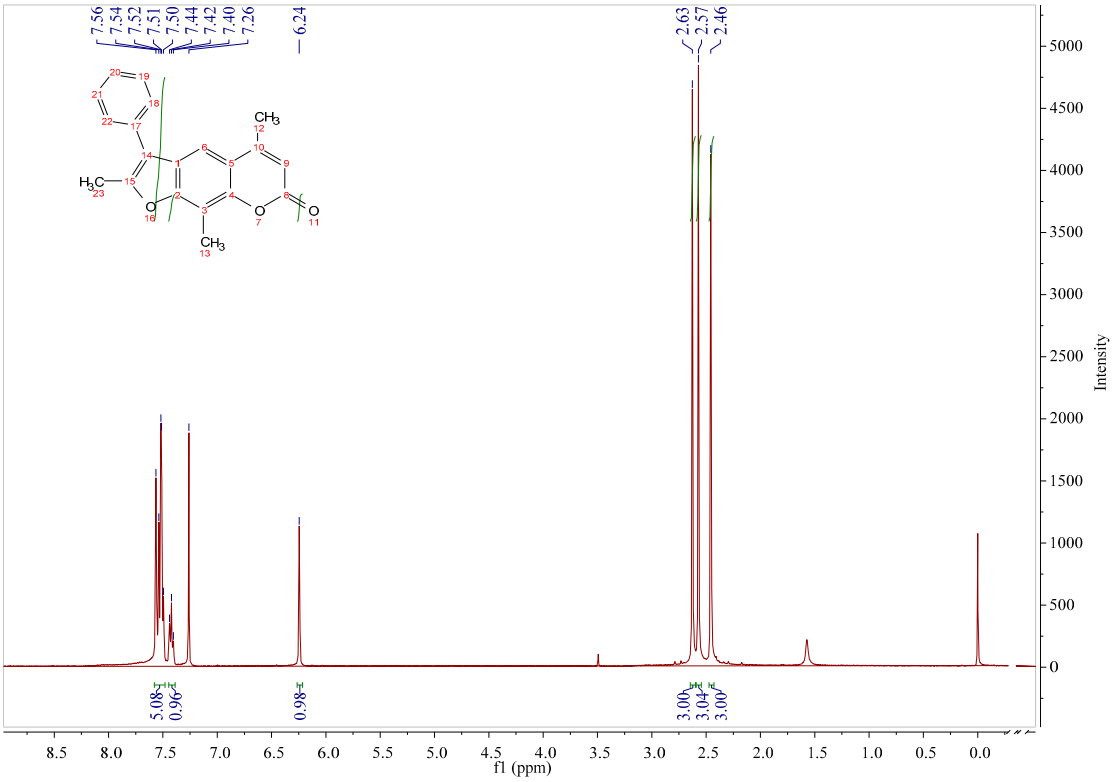
3.00
Intensity
f1 (ppm)

6a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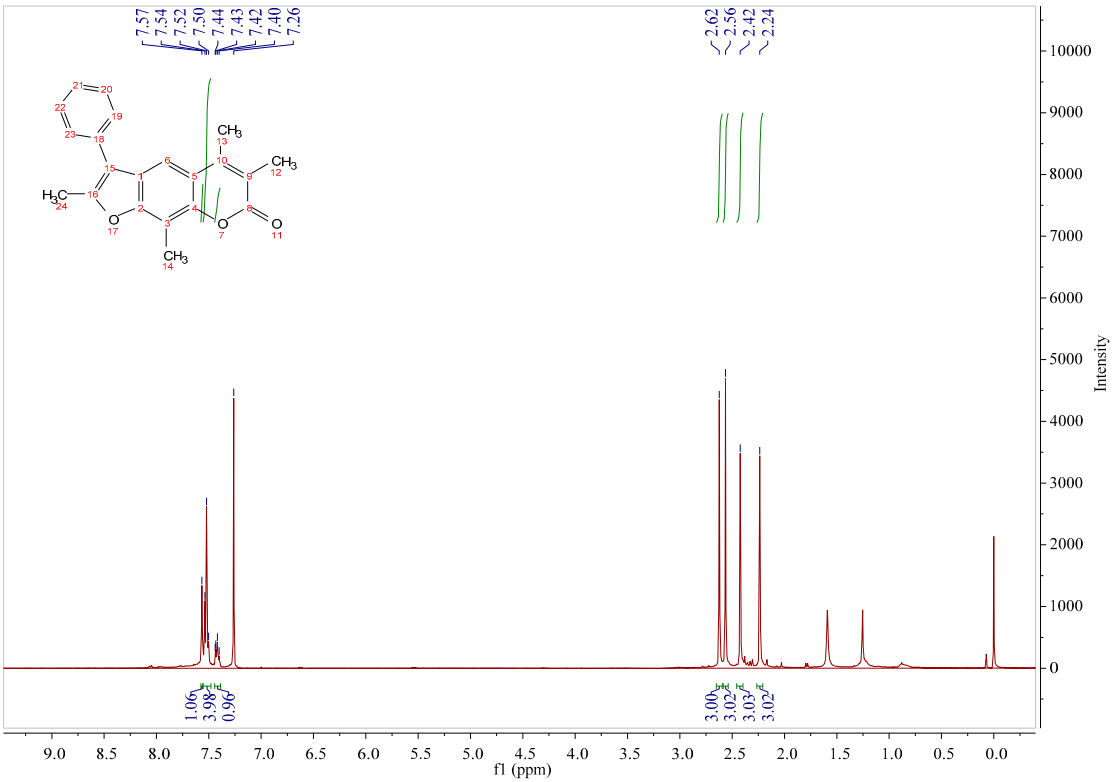
3.00
3.04
3.00
f1 (ppm)
Intensity

6b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7.26
2.62
2.56
2.42
2.24
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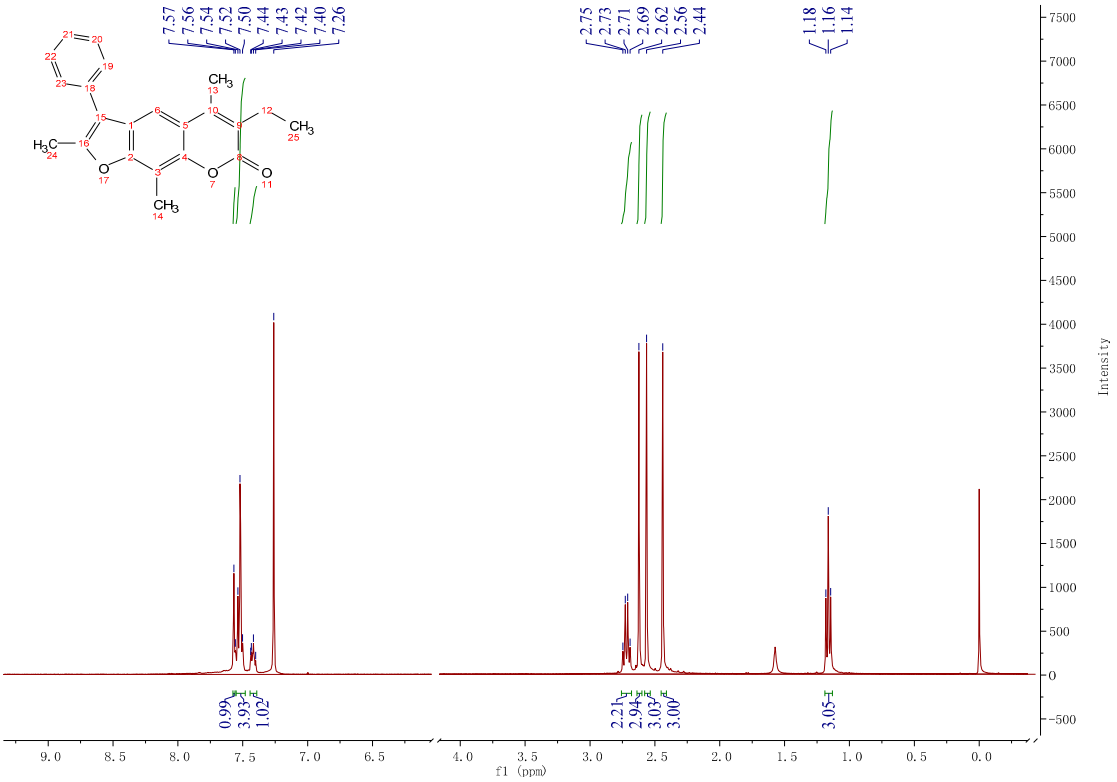
3.98
0.96
3.00
3.02
3.03
3.02
f1 (ppm)
Intensity

6c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2.71
2.69
2.62
2.56
2.44
1.18
1.16
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1.02
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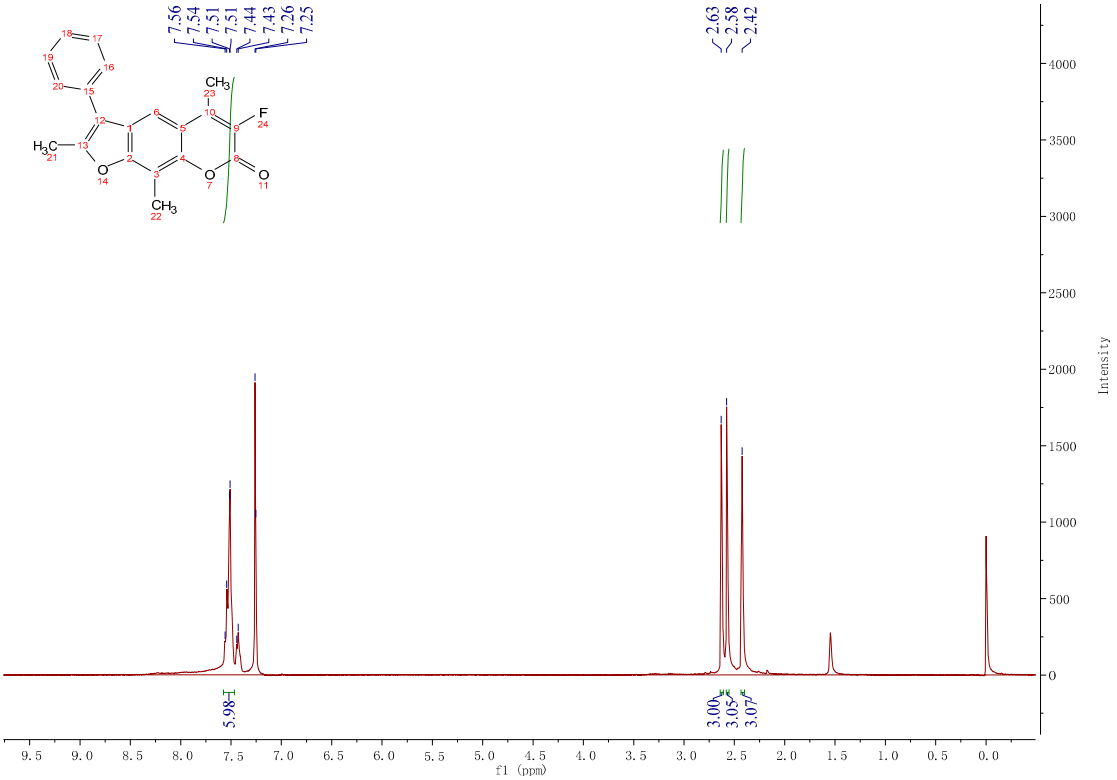
3.03
3.00
3.05
f1 (ppm)
Intensity

6d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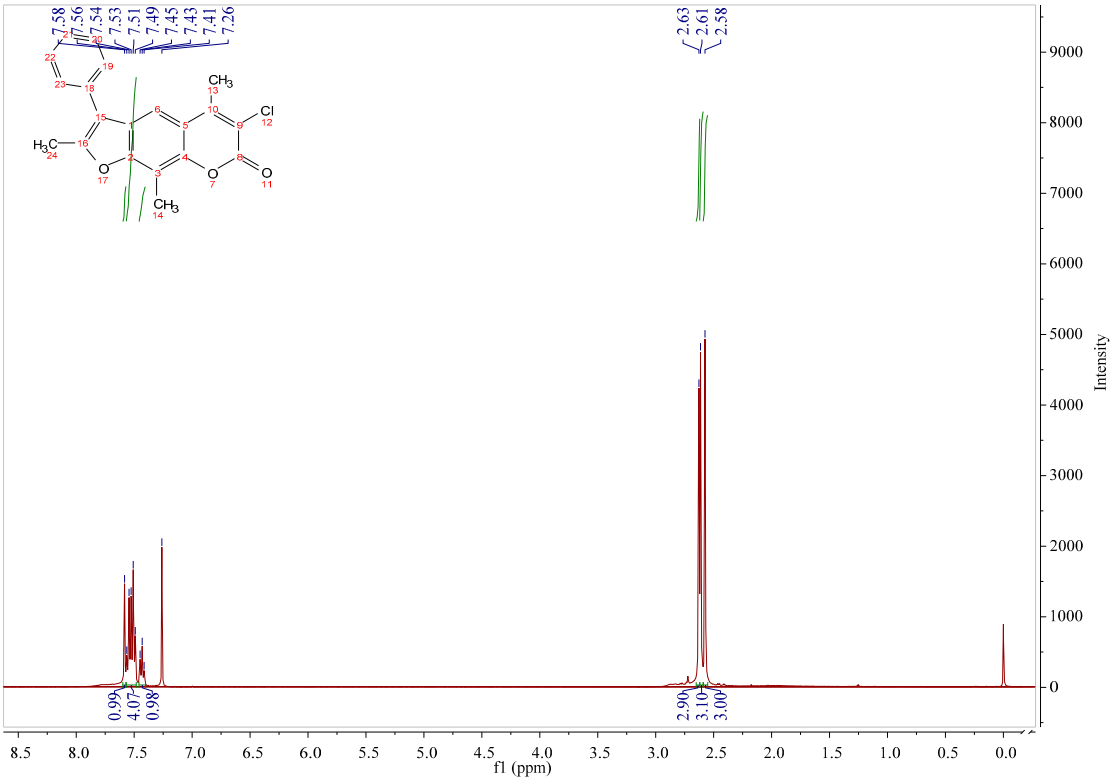
3.05
3.07
f1 (ppm)
Intensity

6e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2.61
2.58
Cl
CH3
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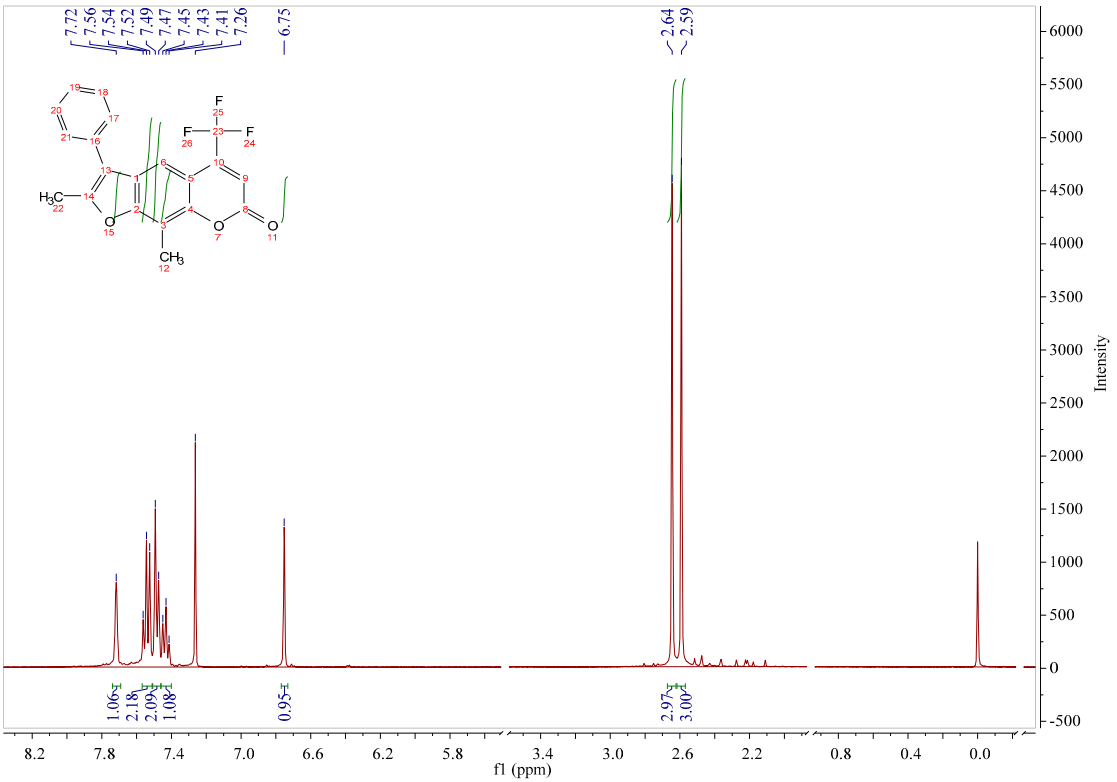
Intensity
f1 (ppm)

6f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2.59
F
F
F
H3C
O
O
O
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2.09
1.08
0.95
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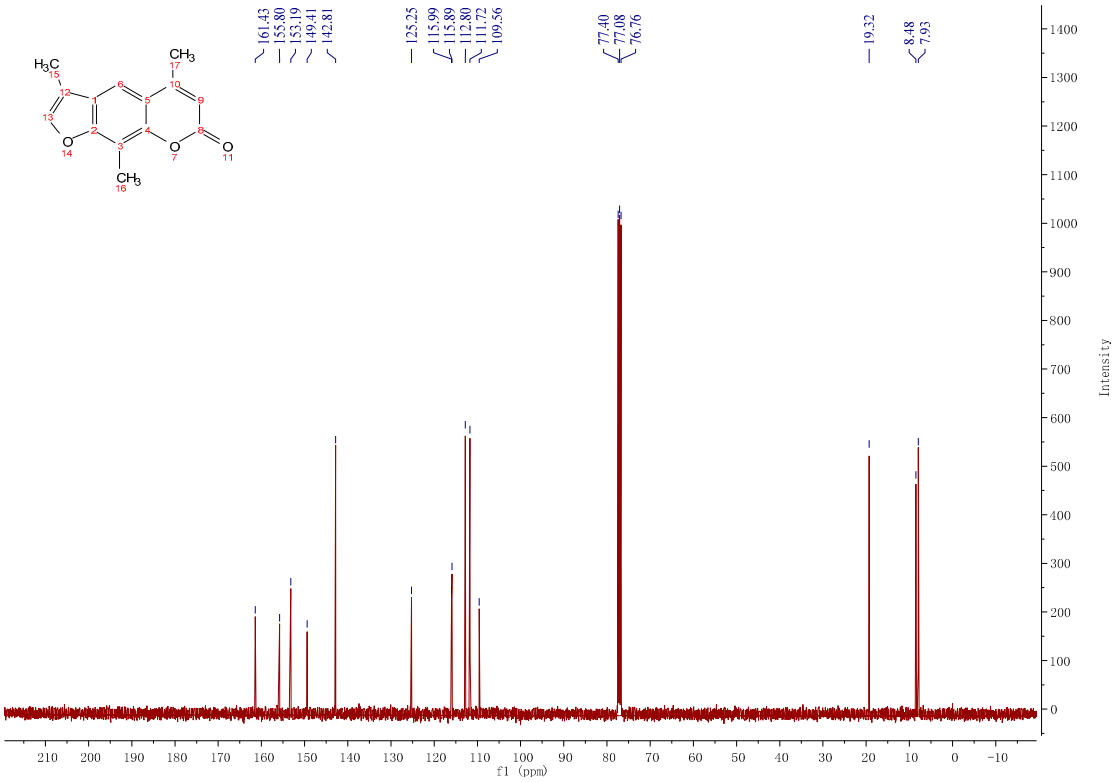
3.00
Intensity
f1 (ppm)

^{13}C-NMR

3a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115.89
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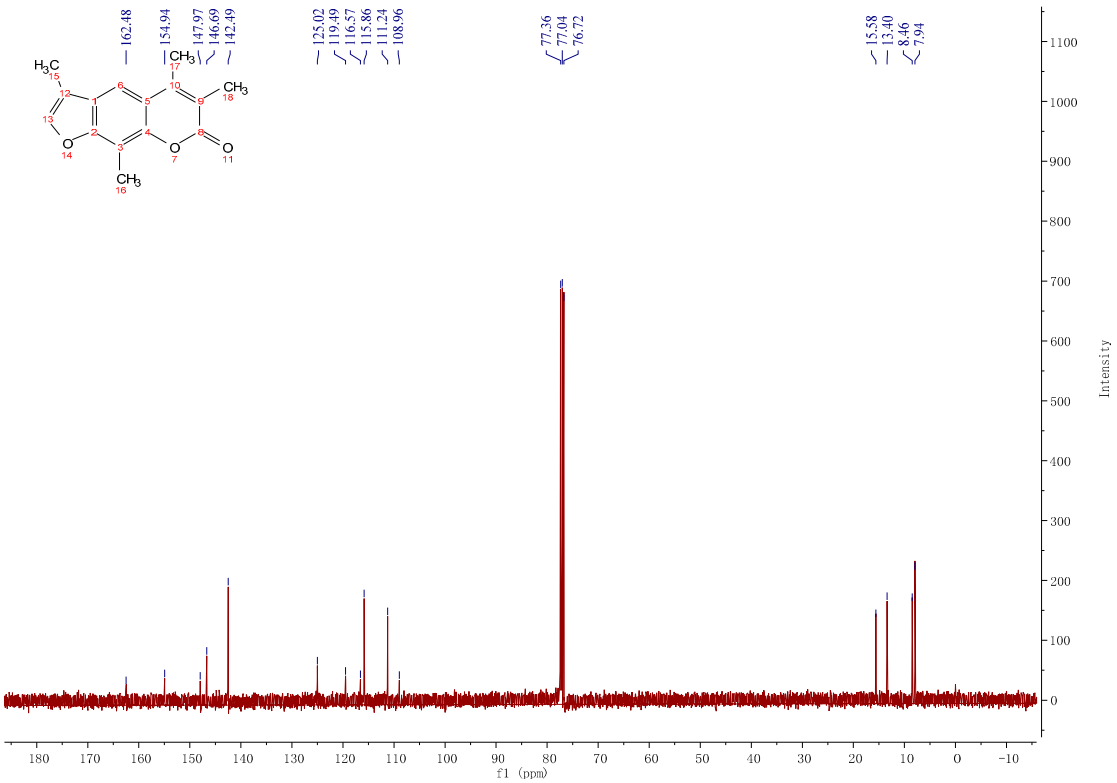
8.48
7.93
Intensity
f1 (ppm)

3b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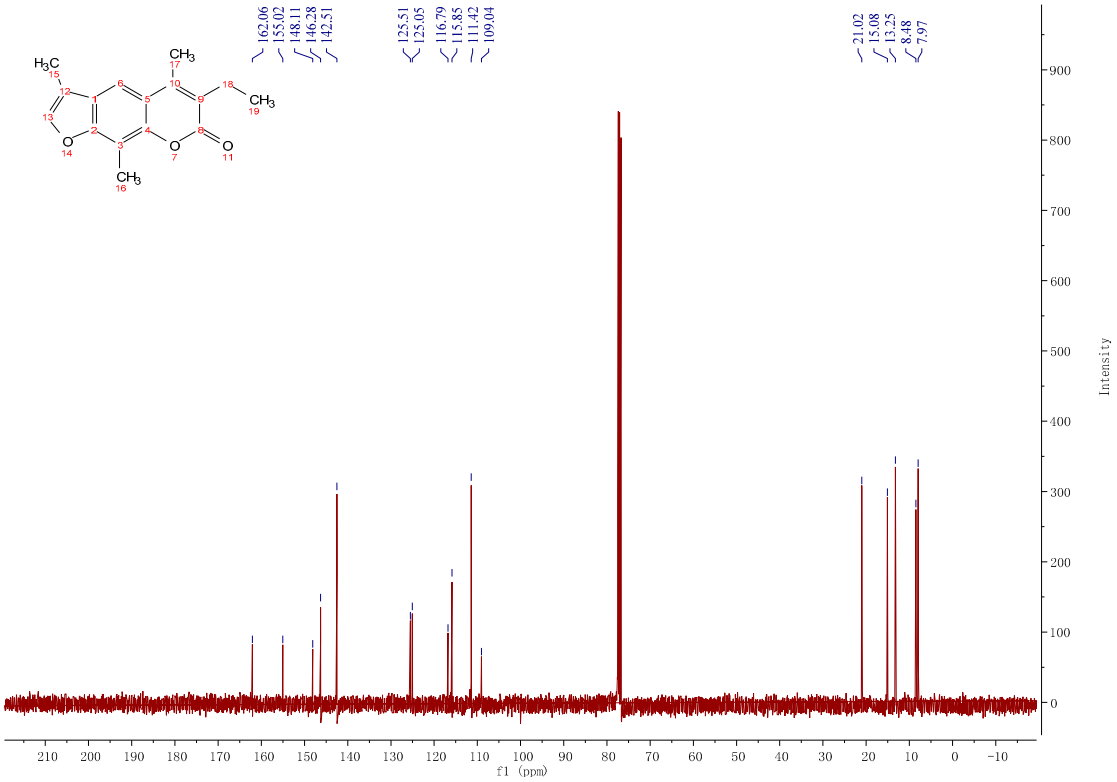
7.94
Intensity
f1 (ppm)

3c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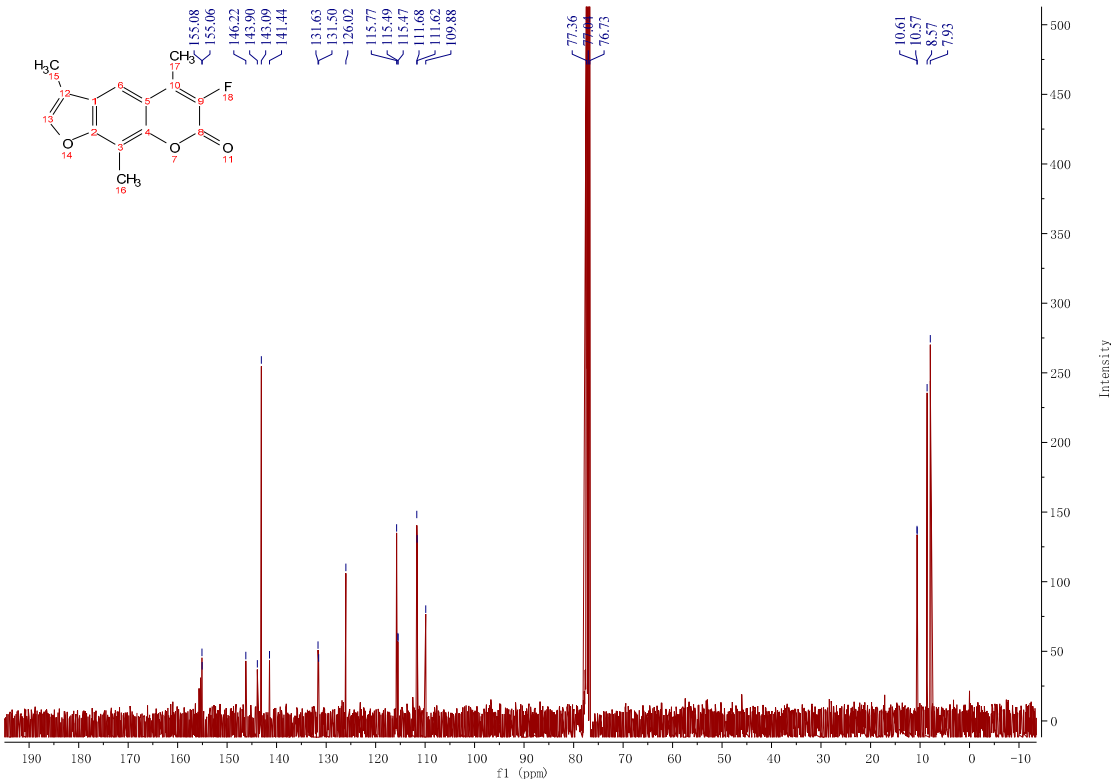
8.48
7.97
Intensity
f1 (ppm)

3d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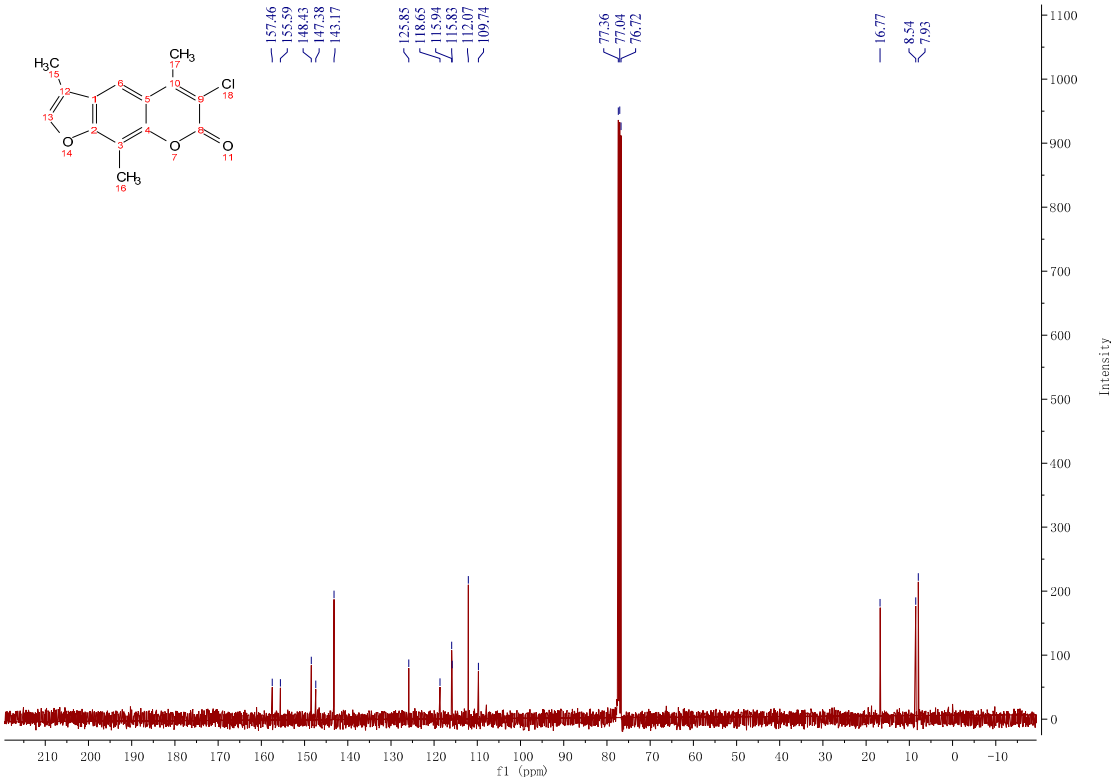
Intensity
f1 (ppm)

3e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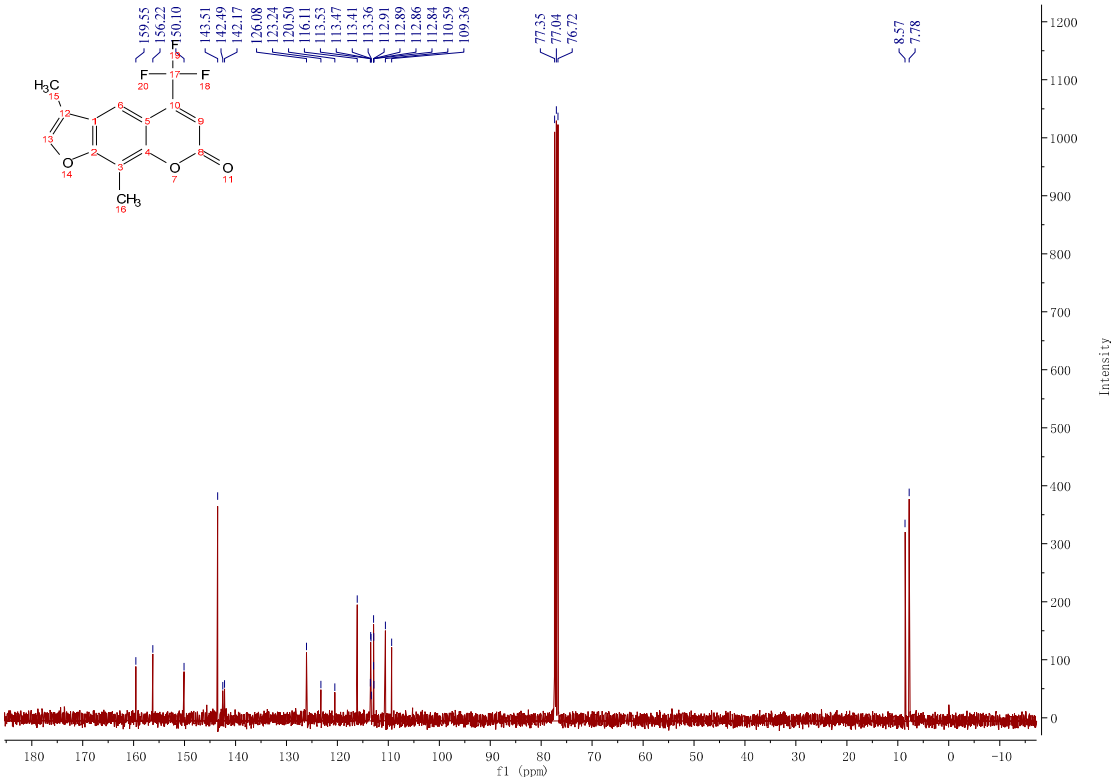
Intensity
f1 (ppm)

3f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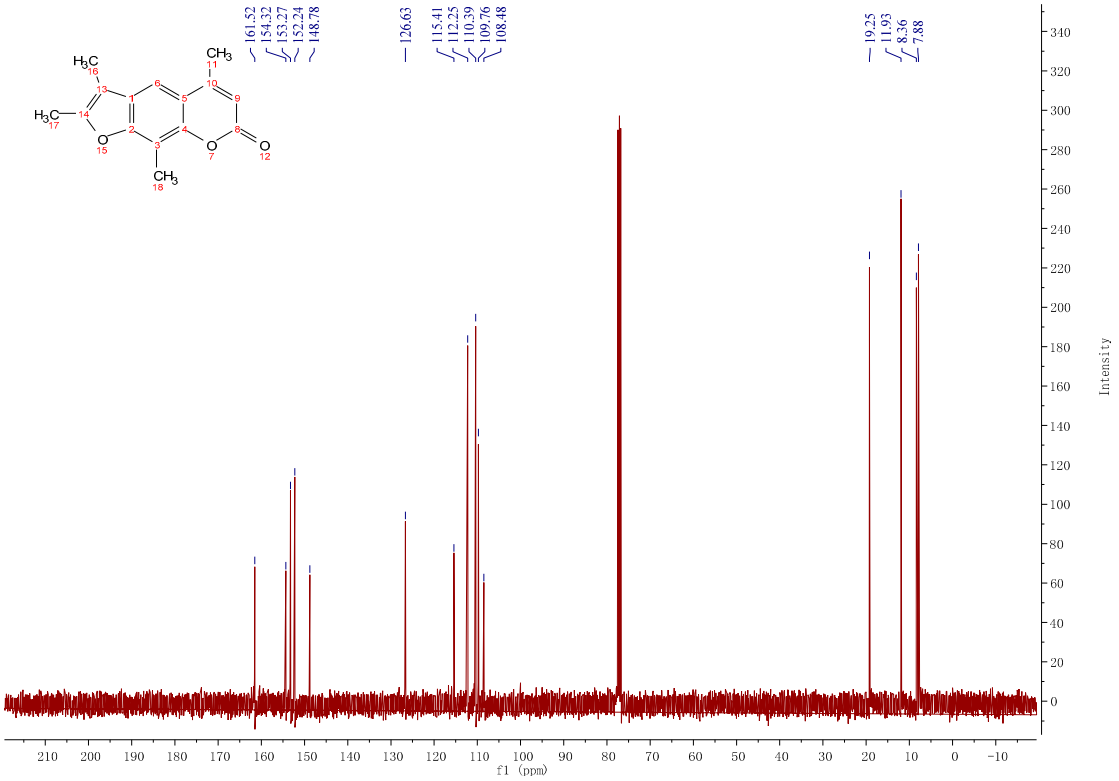
f1 (ppm)

4a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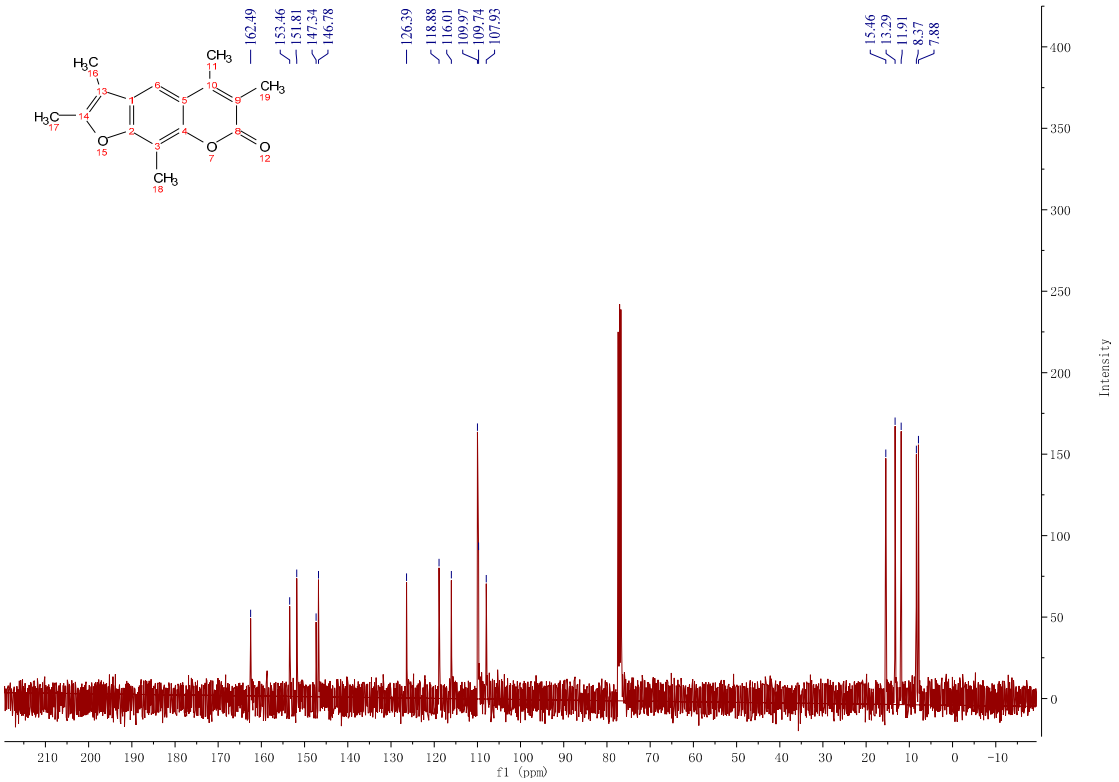
8.36
7.88
f1 (ppm)
Intensity

4b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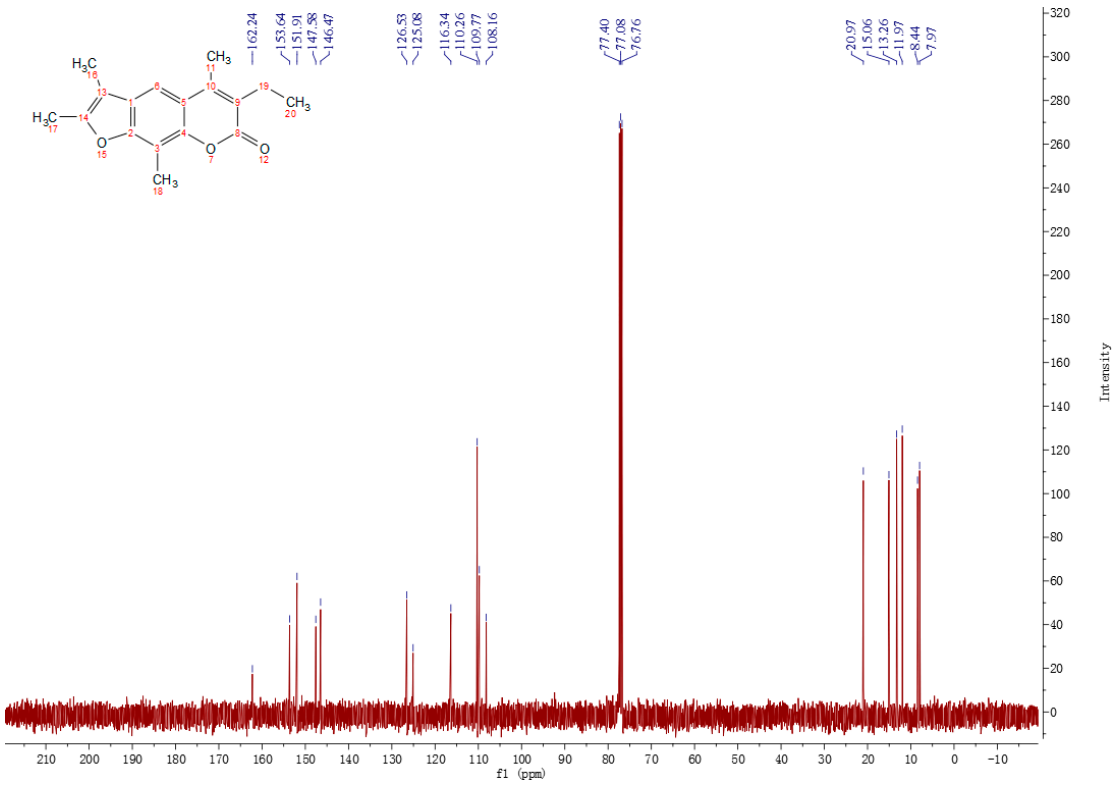
f1 (ppm)
Intensity

4c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15.06
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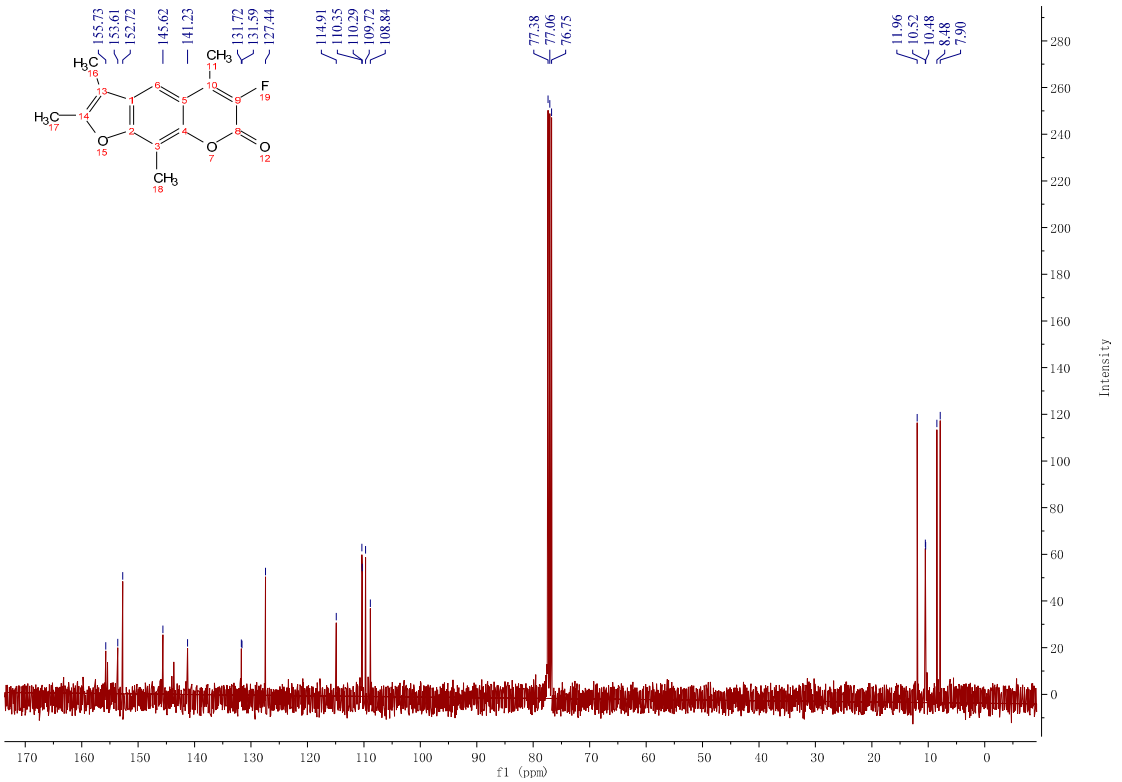
11.97
8.44
7.97
Intensity
f1 (ppm)

4d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110.29
109.72
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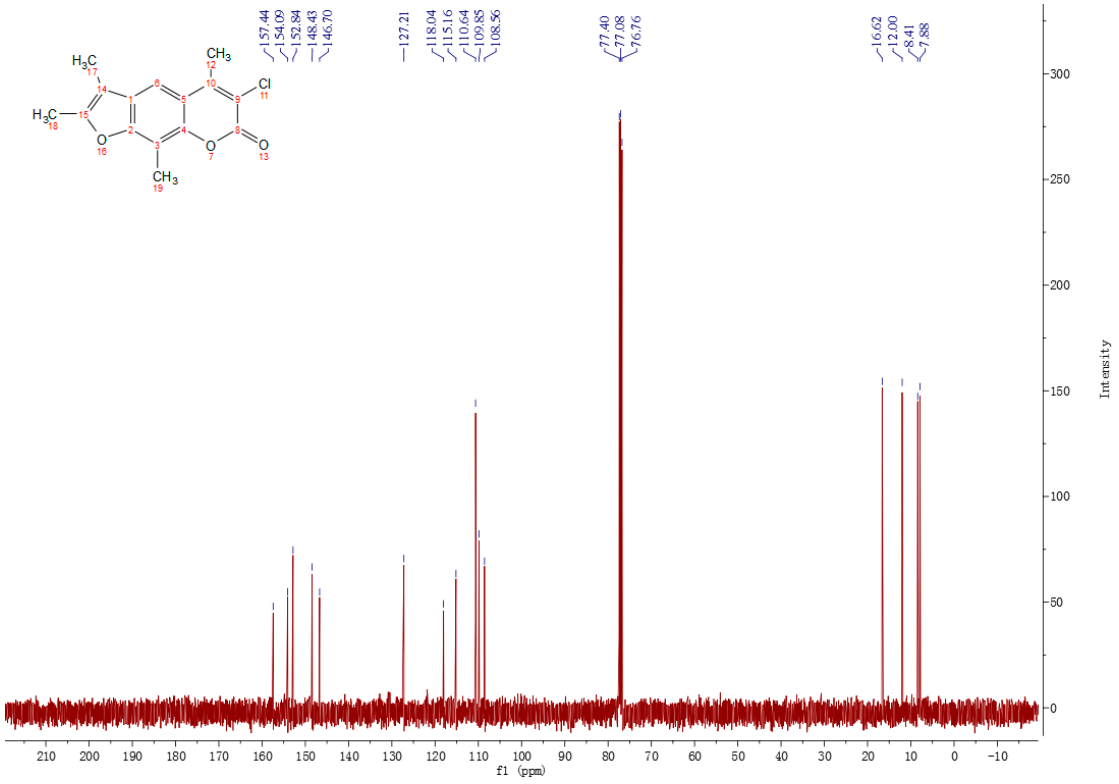
76.75
11.96
10.52
10.48
8.48
7.90
Intensity
f1 (ppm)

4e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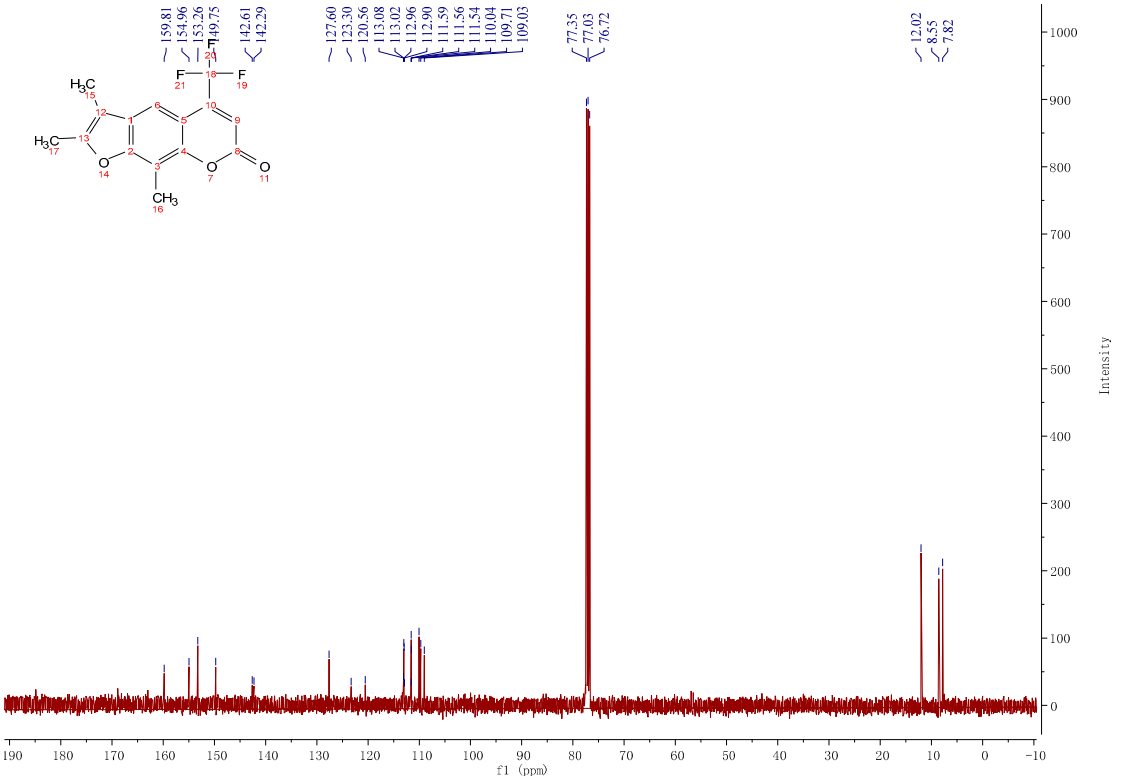
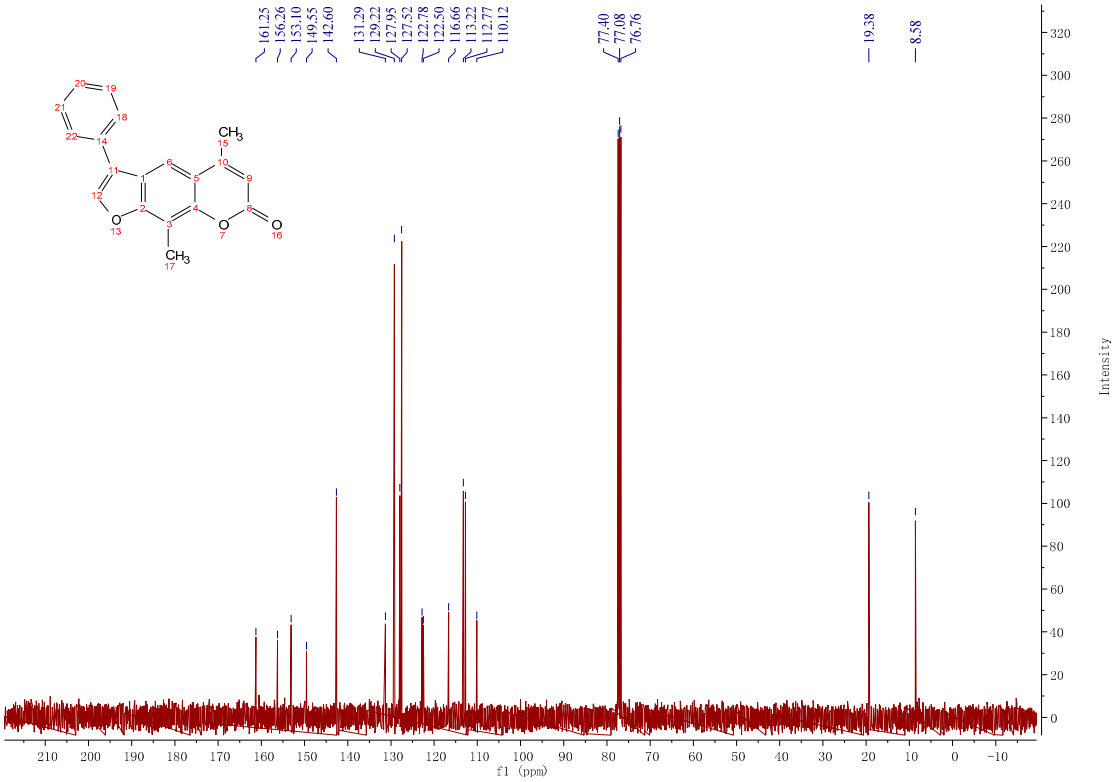
77.40
77.08
76.76
16.62
12.00
8.41
7.88
Intensity
f1 (ppm)

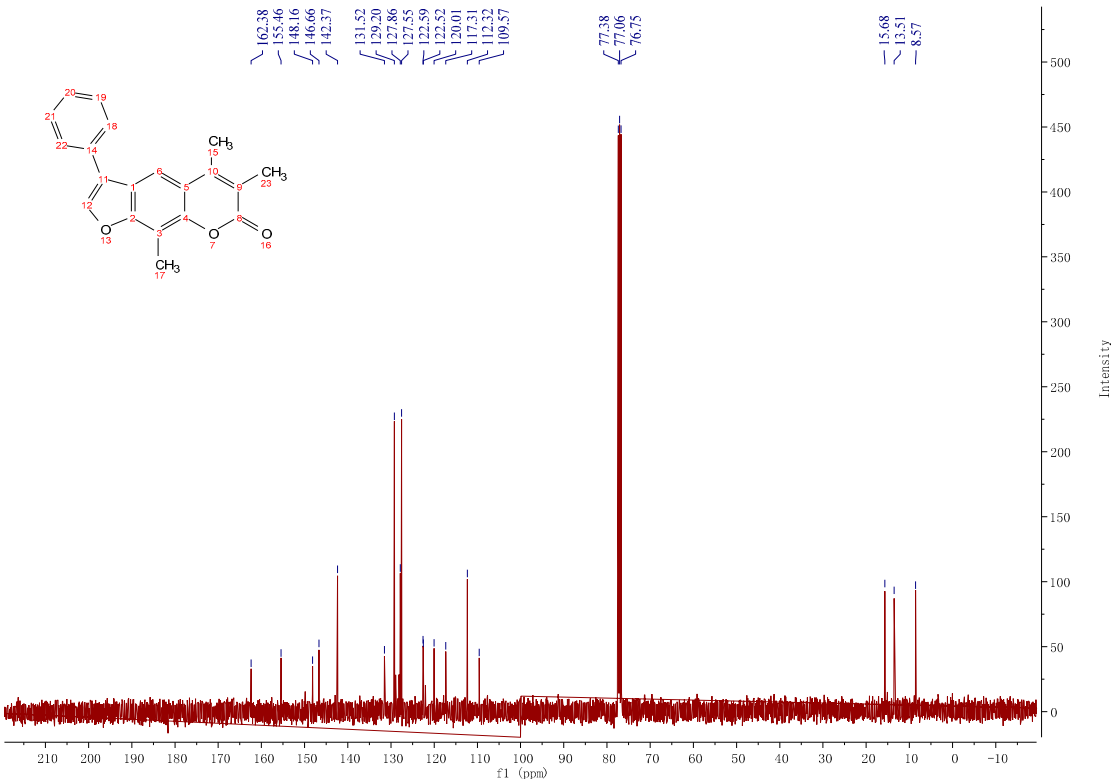
4f


159.81
154.96
153.26
149.75
142.61
142.29
127.60
123.30
120.56
113.08
113.02
112.96
112.90
111.59
111.56
111.54
110.04
109.71
109.03
77.35
77.03
76.72
12.02
8.55
7.82
Intensity
f1 (ppm)

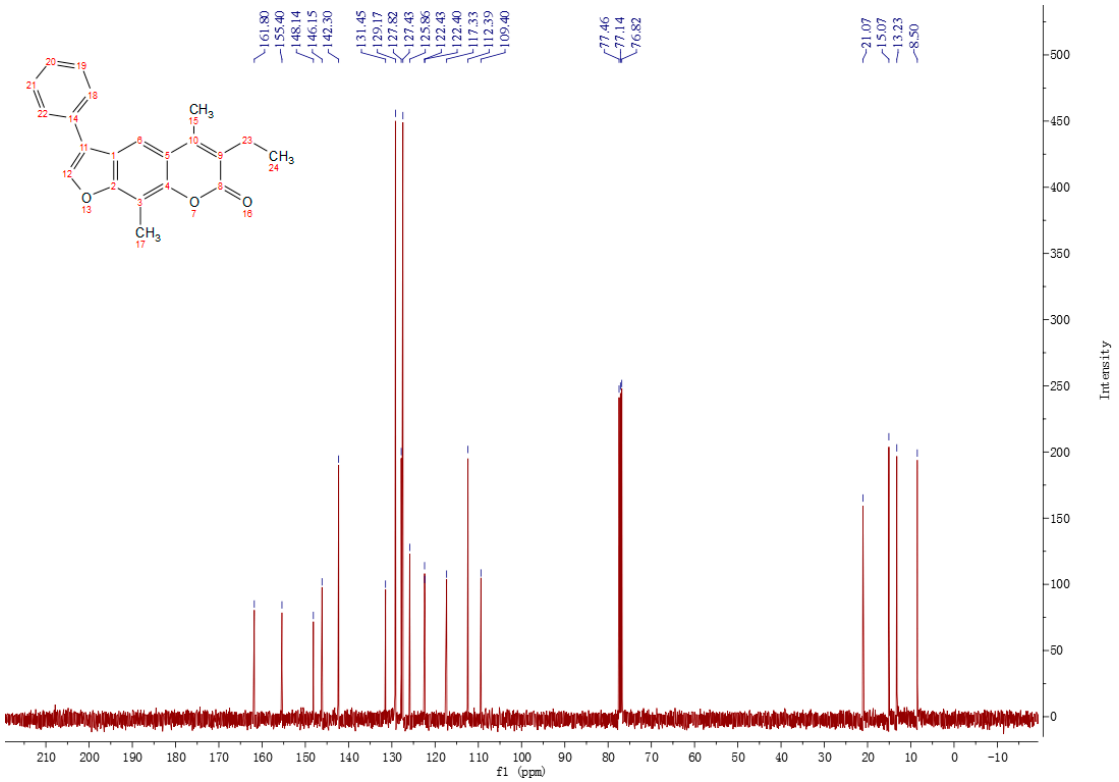
5a


161.25
156.26
153.10
149.55
142.60
131.29
129.22
127.95
127.52
122.78
122.50
116.66
113.22
112.77
110.12
77.40
77.08
76.76
19.38
8.58
Intensity
f1 (ppm)

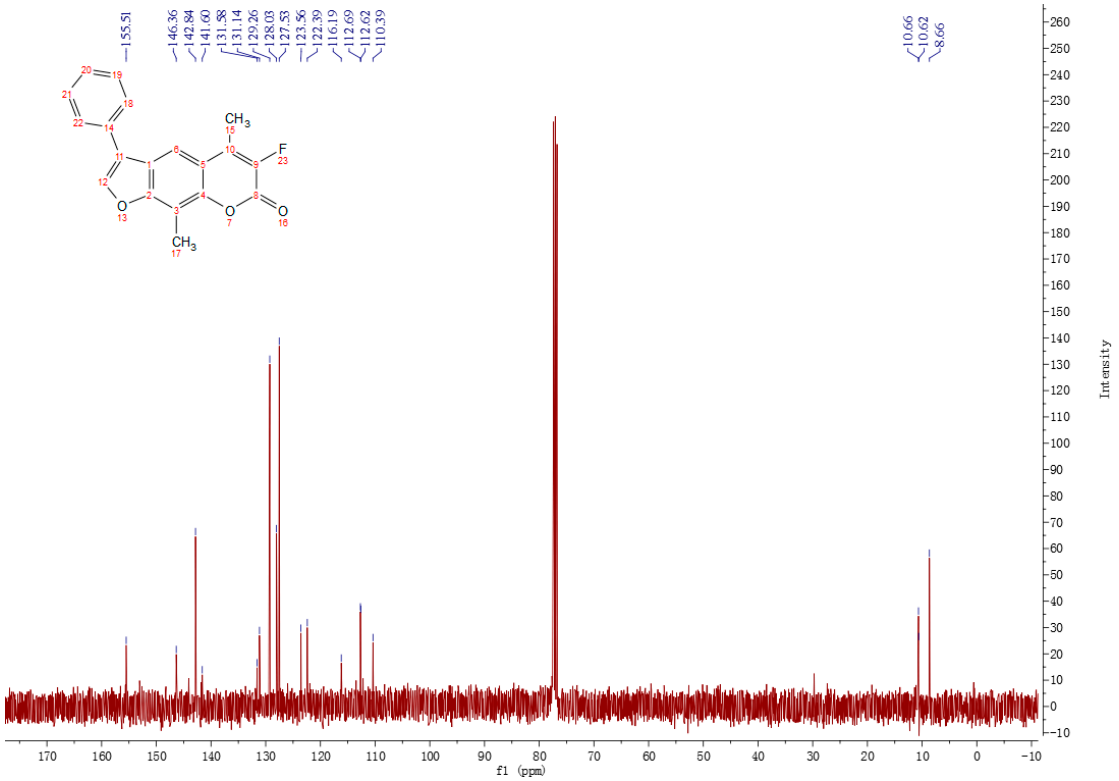
5b


162.38
155.46
148.16
146.66
142.37
131.52
129.20
127.86
127.55
122.59
122.52
120.01
117.31
112.32
109.57
77.38
77.06
76.75
15.68
13.51
8.57
Intensity
f1 (ppm)

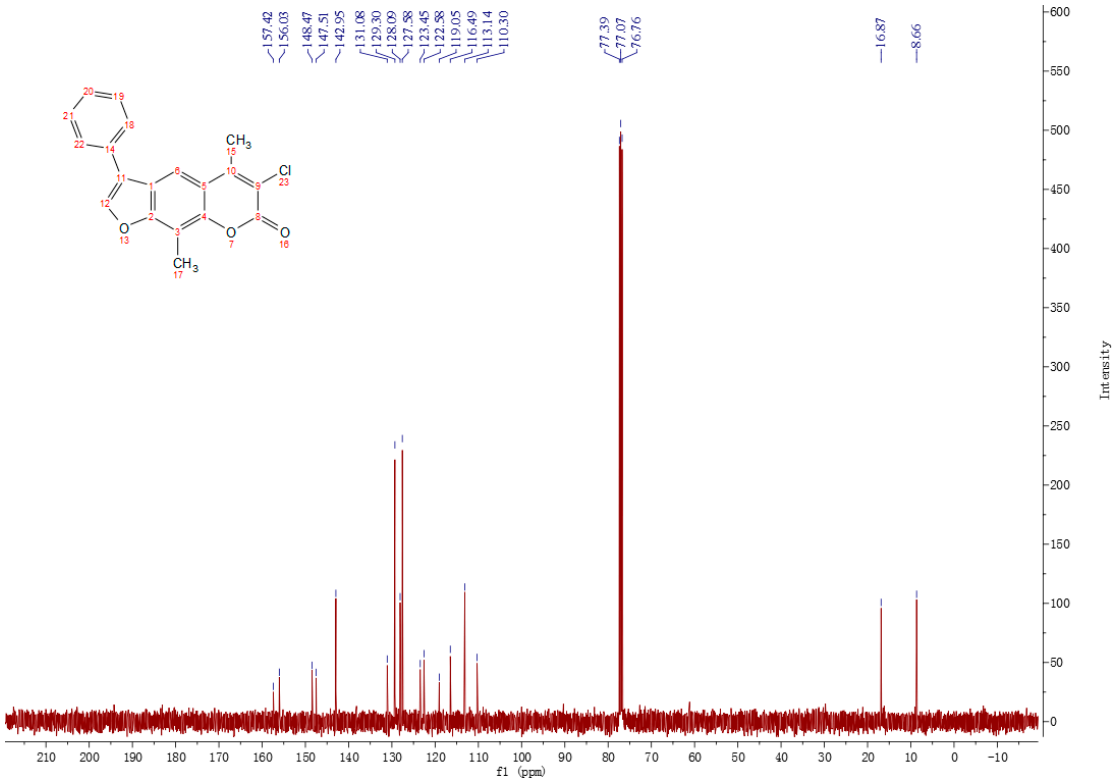
5c


161.80
155.40
148.14
146.15
142.30
131.45
129.17
127.82
127.43
125.86
122.43
122.40
117.33
112.39
109.40
77.46
77.14
76.82
21.07
15.07
13.23
8.50
Intensity
f1 (ppm)

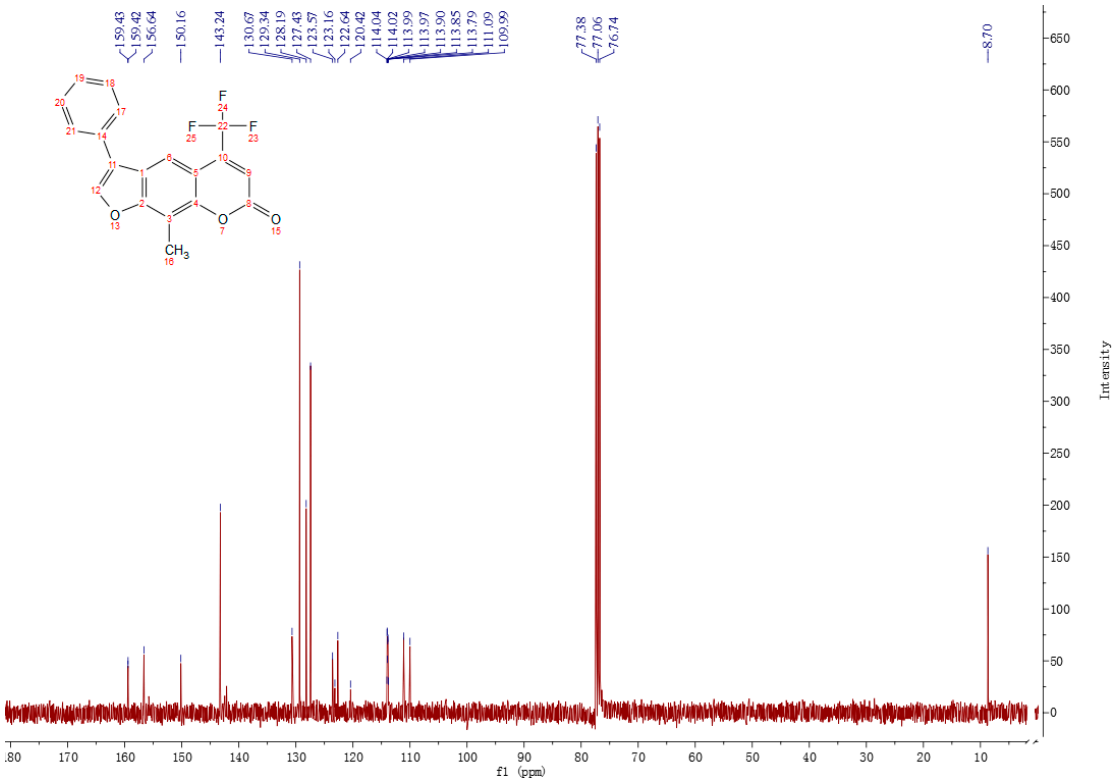
5d


155.51
146.36
142.84
141.60
131.58
131.14
129.26
128.03
127.53
123.56
122.39
116.19
112.69
112.62
110.39
10.66
10.62
8.66
Intensity
f1 (ppm)

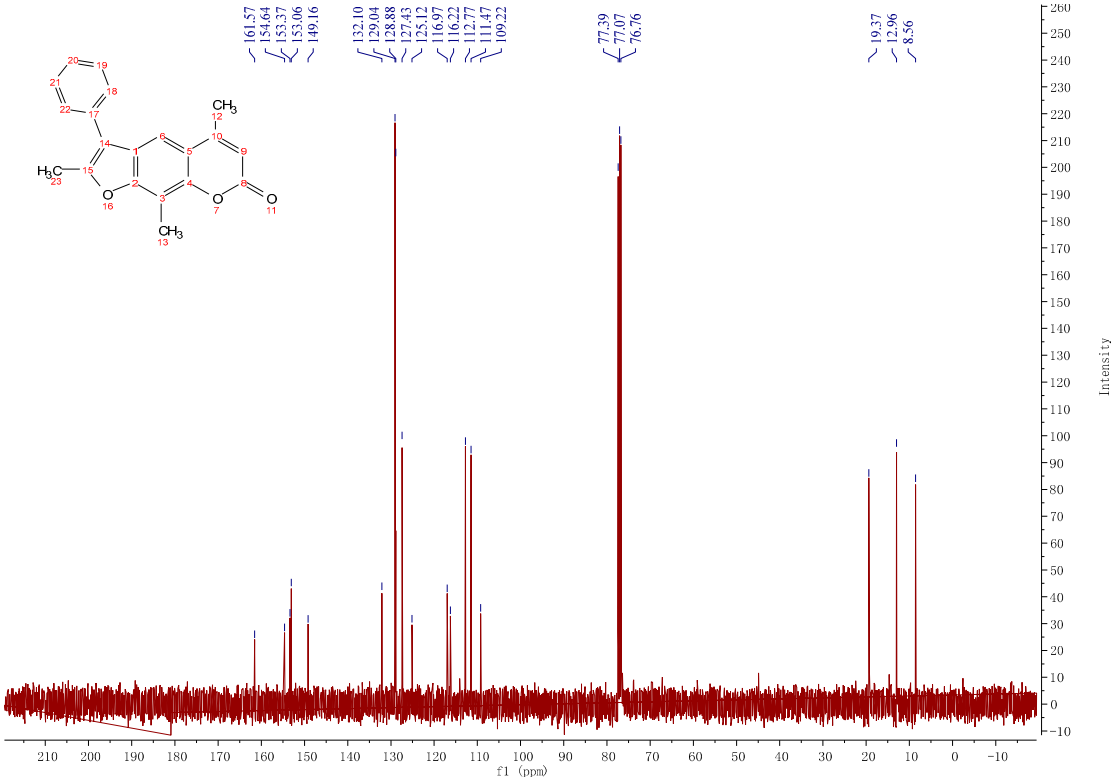
5e


157.42
156.03
148.47
147.51
142.95
131.08
129.30
128.09
127.58
123.45
122.58
119.05
116.49
113.14
110.30
77.39
77.07
76.76
16.87
8.66
Intensity
f1 (ppm)

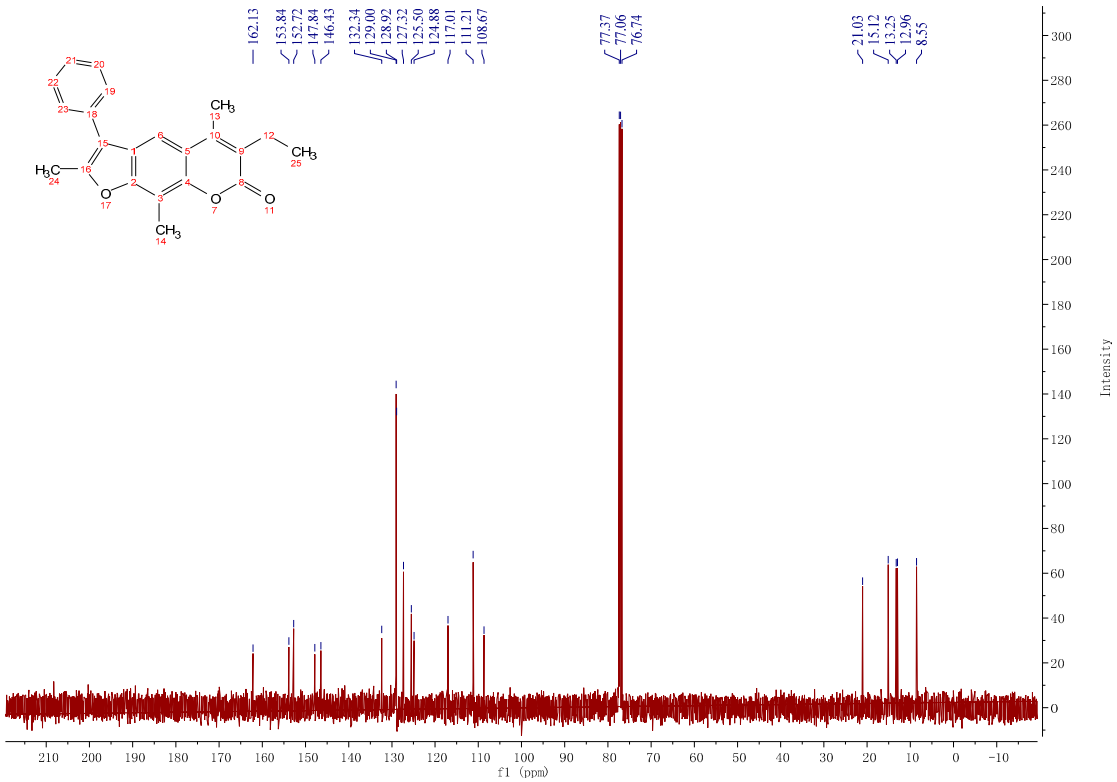
5f


159.43
159.42
156.64
150.16
143.24
130.67
129.34
128.19
127.43
123.57
123.16
122.64
120.42
114.04
114.02
113.99
113.97
113.90
113.85
113.79
111.09
109.99
77.38
77.06
76.74
8.70
Intensity
f1 (ppm)

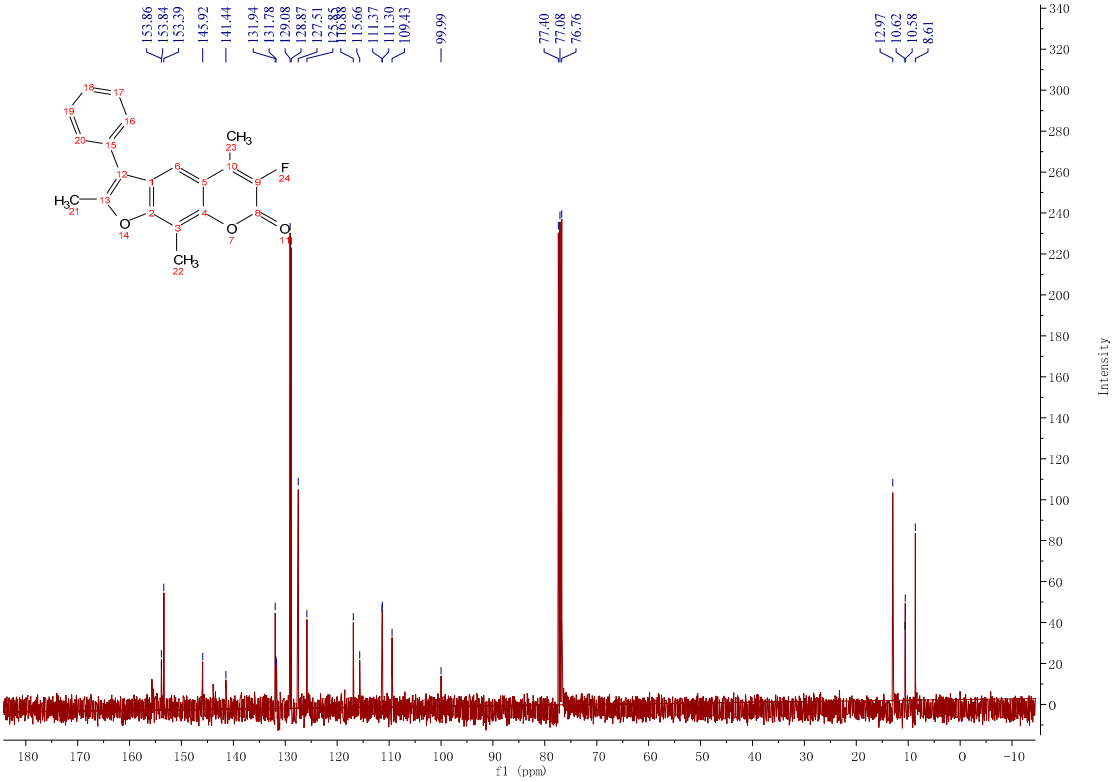
6a


161.57
154.64
153.37
153.06
149.16
132.10
129.04
128.88
127.43
125.12
116.97
116.22
112.77
111.47
109.22
77.39
77.07
76.76
19.37
12.96
8.56
f1 (ppm)
Intensity

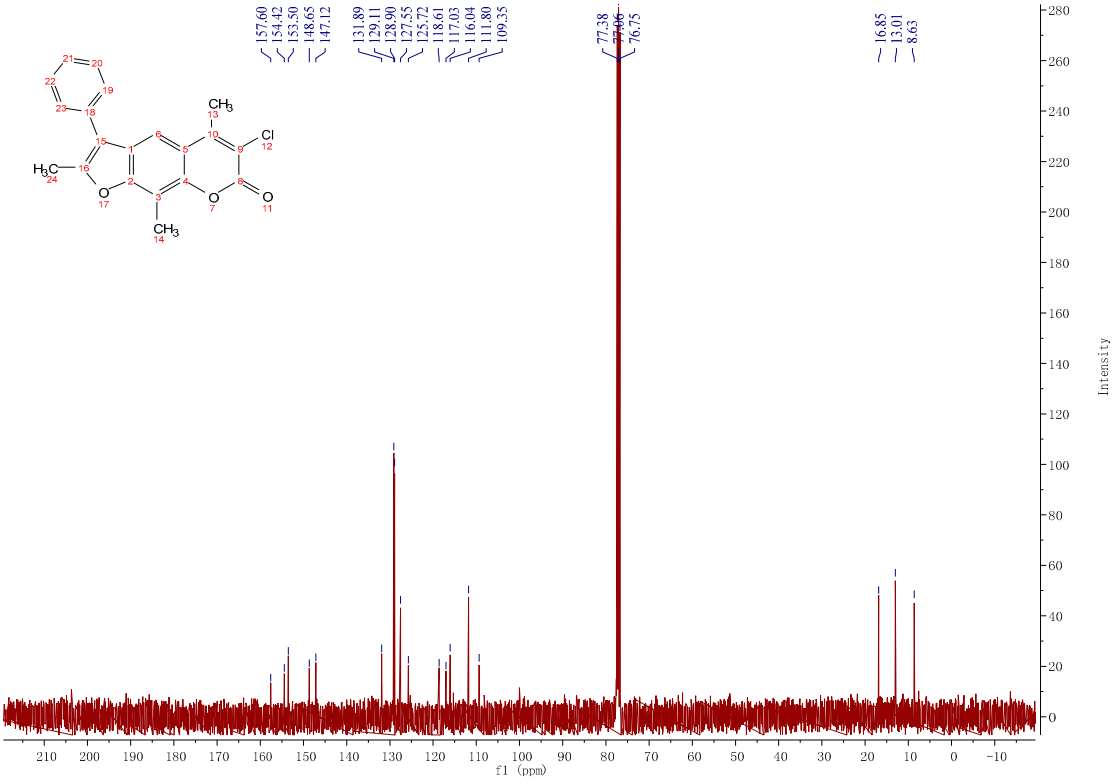
6c


162.13
153.84
152.72
147.84
146.43
132.34
129.00
128.92
127.32
125.50
124.88
117.01
111.21
108.67
77.37
77.06
76.74
21.03
15.12
13.25
12.96
8.55
f1 (ppm)
Intensity

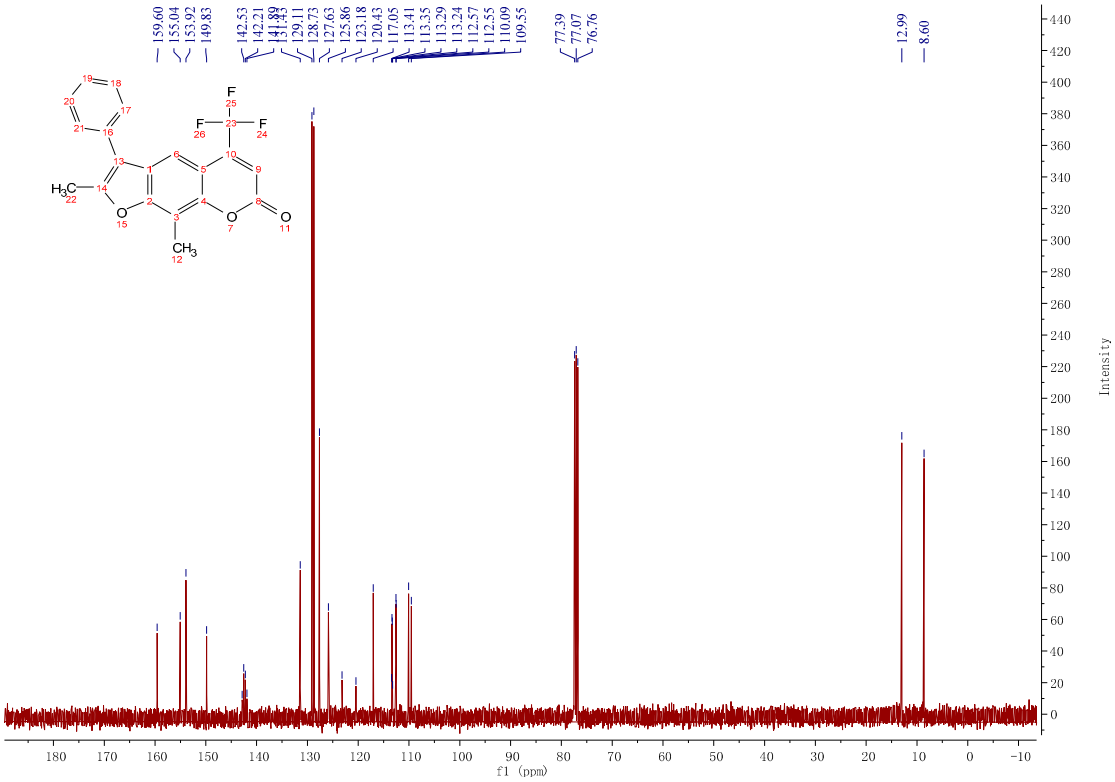
6d


153.86
153.84
153.39
145.92
141.44
131.94
131.78
129.08
128.87
127.51
125.85
116.88
115.66
111.37
111.30
109.43
99.99
77.40
77.08
76.76
12.97
10.62
10.58
8.61
CH3
F
H3C
O
O
O
CH3
Intensity
f1 (ppm)

6e

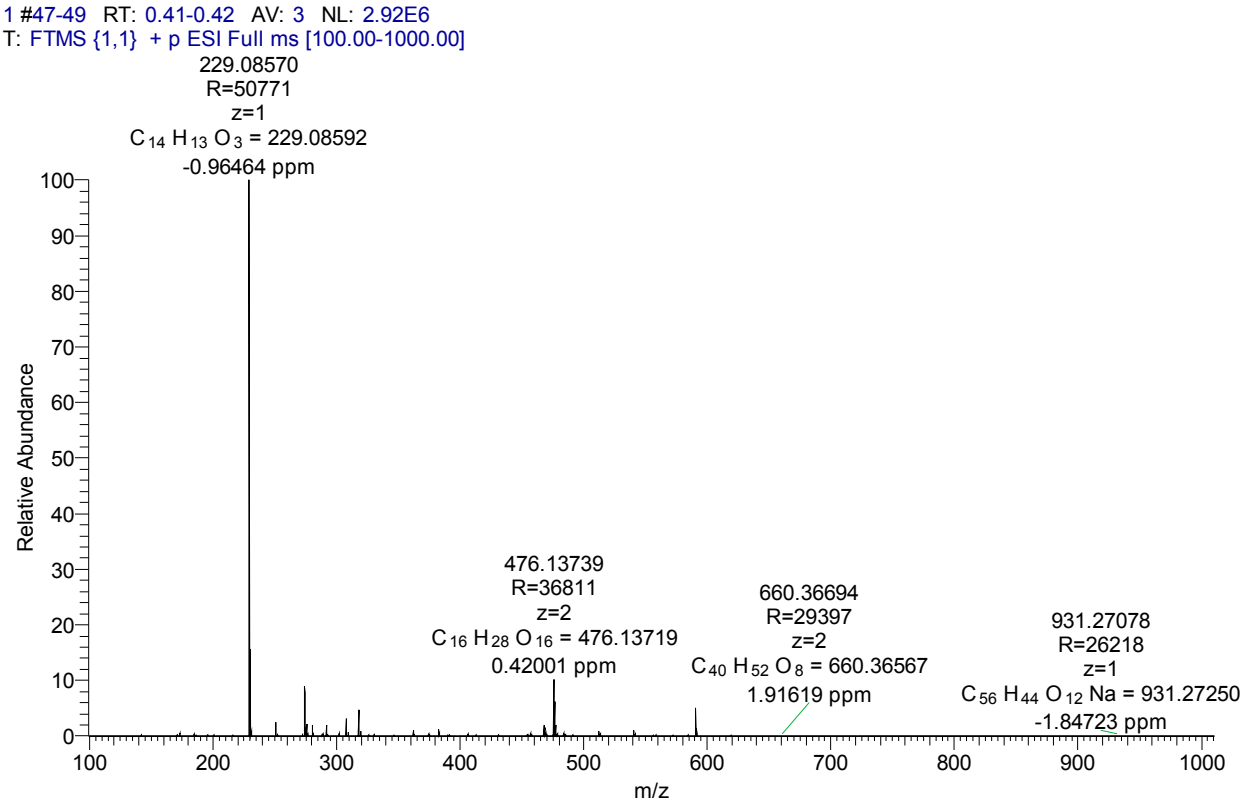

157.60
154.42
153.50
148.65
147.12
131.89
129.11
128.90
127.55
125.72
118.61
117.03
116.04
111.80
109.35
77.38
77.06
76.75
16.85
13.01
8.63
CH3
Cl
H3C
O
O
O
CH3
Intensity
f1 (ppm)

6f

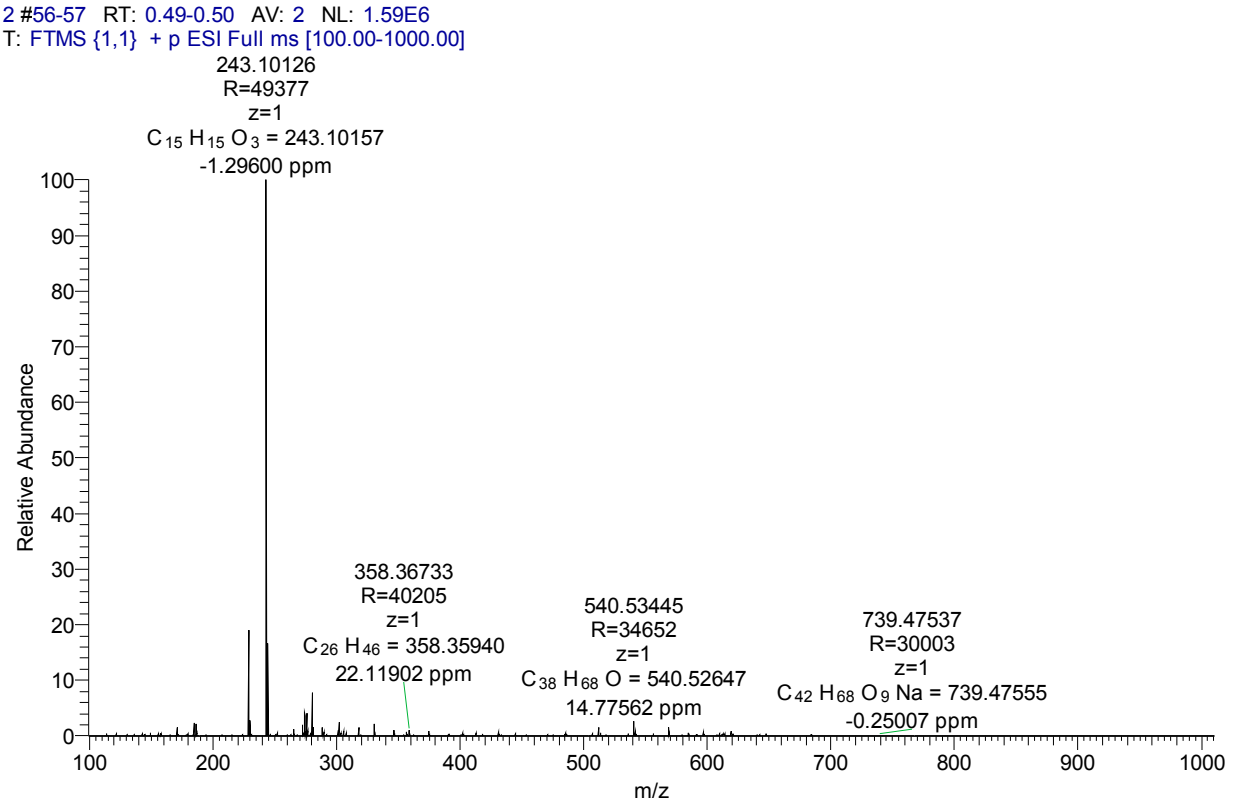

159.60
155.04
153.92
149.83
142.53
142.21
141.89
141.43
129.11
128.73
127.63
125.86
123.18
120.43
117.05
113.41
113.35
113.29
113.24
112.57
112.55
110.09
109.55
77.39
77.07
76.76
12.99
8.60
Intensity
f1 (ppm)

2. HRMS Spectra of New Compounds

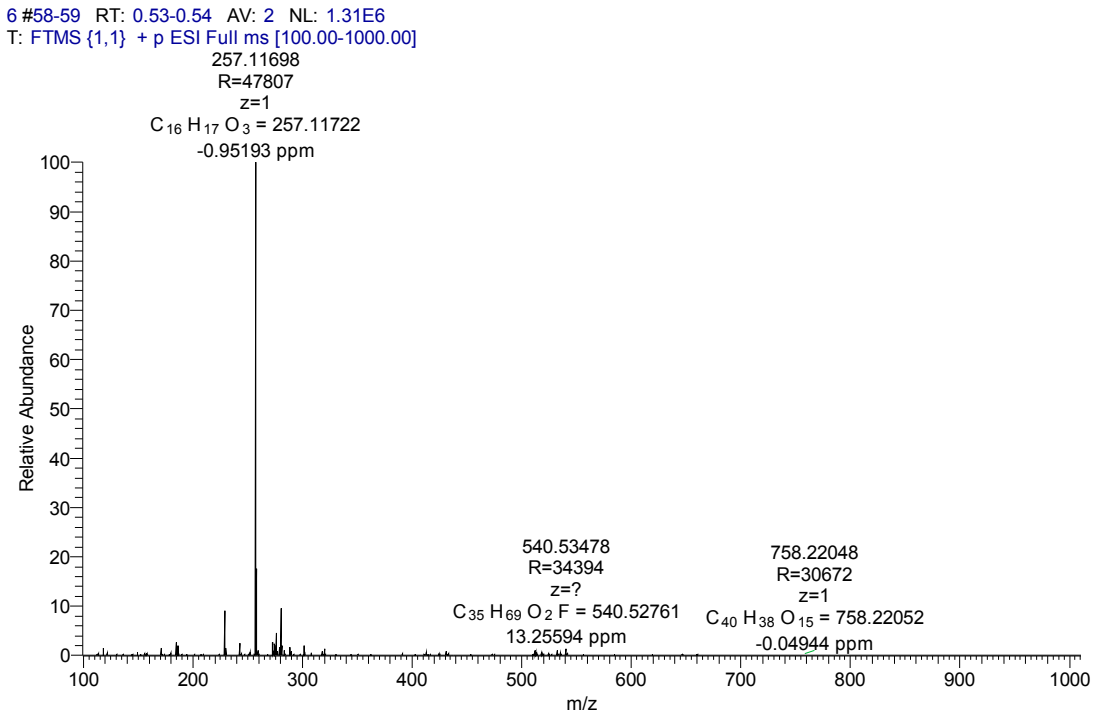
3a



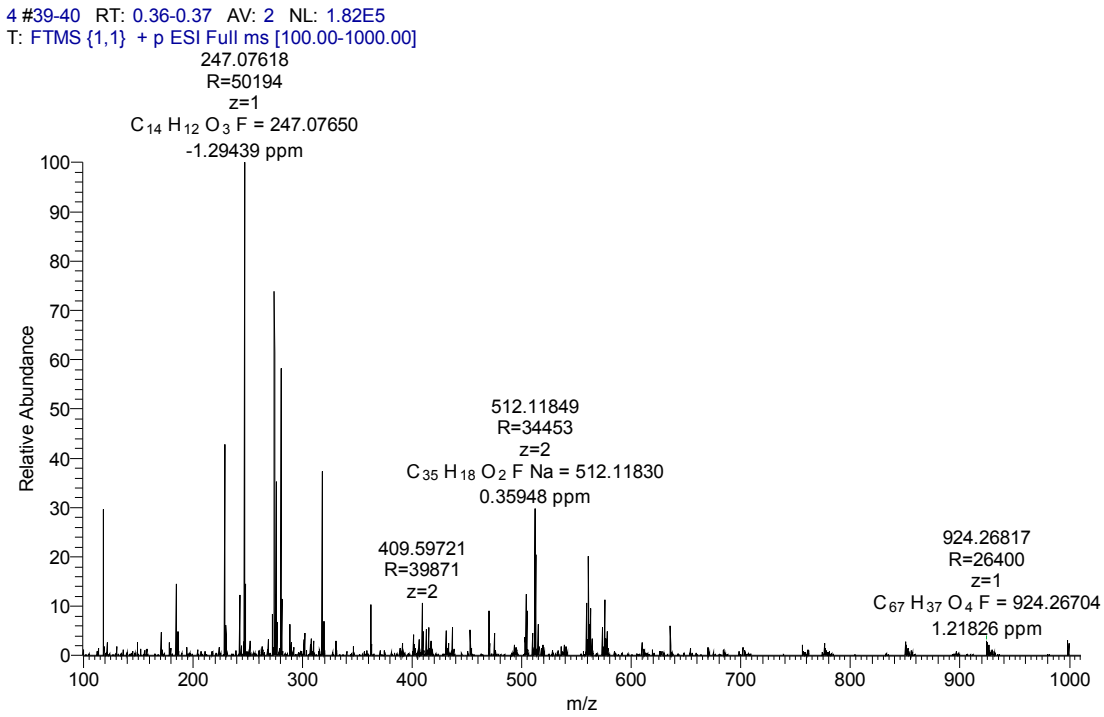
3b



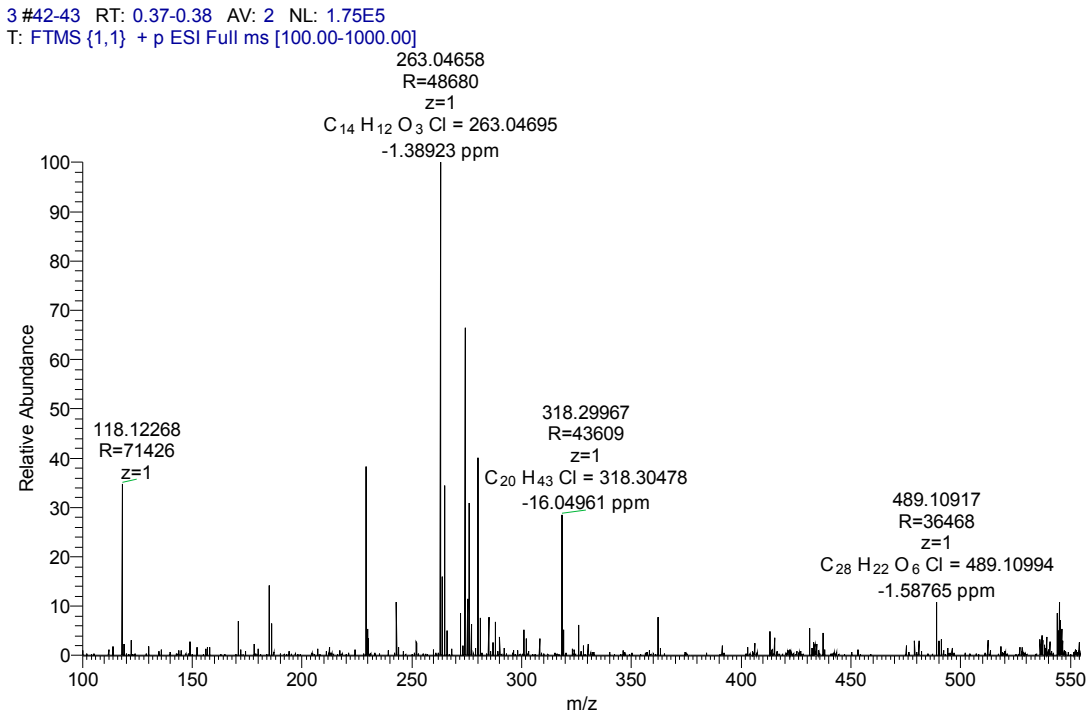
3c


6 #58-59 RT: 0.53-0.54 AV: 2 NL: 1.31E6
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]
257.11698
R=47807
z=1
C16 H17 O3 = 257.11722
-0.95193 ppm
540.53478
R=34394
z=?
C35 H69 O2 F = 540.52761
13.25594 ppm
758.22048
R=30672
z=1
C40 H38 O15 = 758.22052
-0.04944 ppm
Relative Abundance
m/z

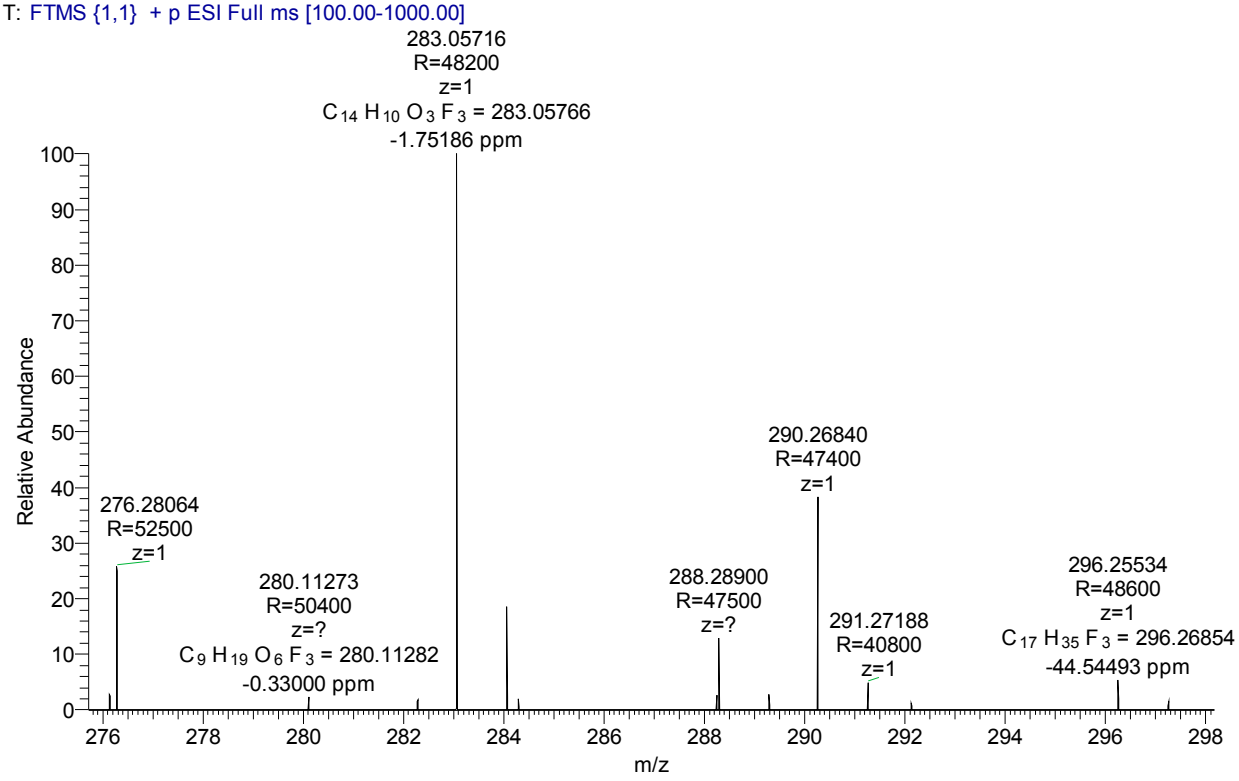
3d


4 #39-40 RT: 0.36-0.37 AV: 2 NL: 1.82E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]
247.07618
R=50194
z=1
C14 H12 O3 F = 247.07650
-1.29439 ppm
512.11849
R=34453
z=2
C35 H18 O2 F Na = 512.11830
0.35948 ppm
409.59721
R=39871
z=2
924.26817
R=26400
z=1
C67 H37 O4 F = 924.26704
1.21826 ppm
Relative Abundance
m/z

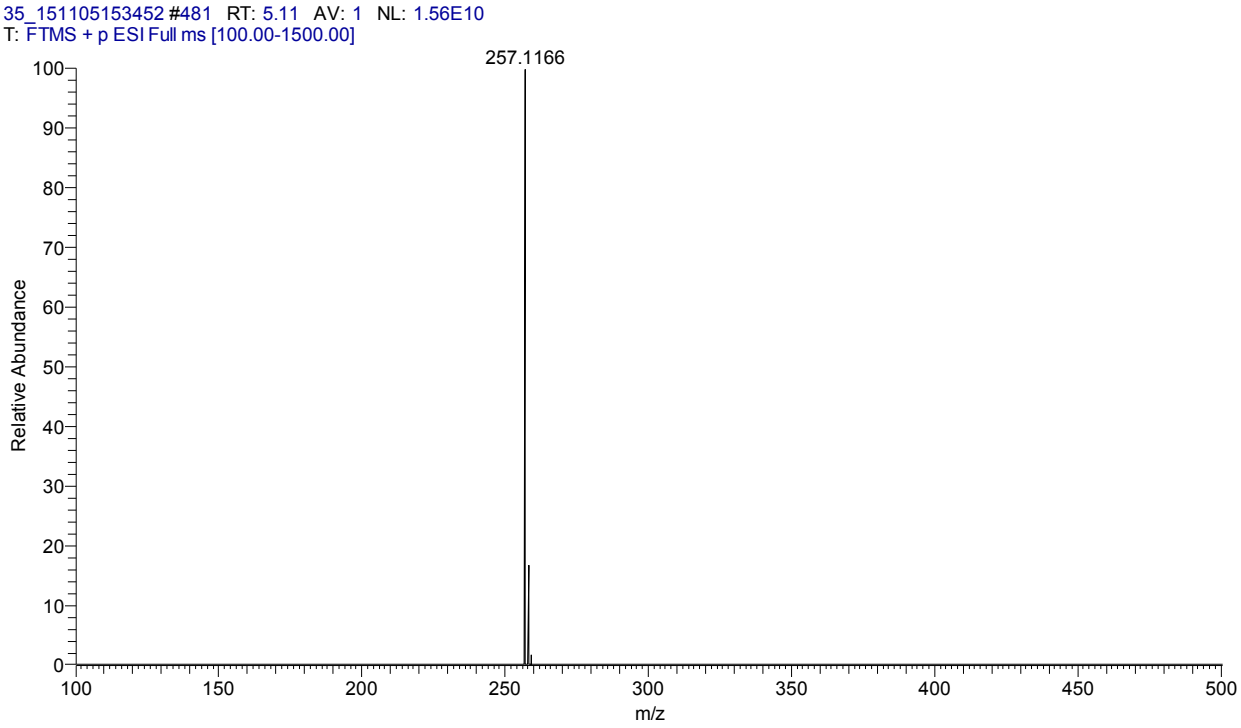
3e


3 #42-43 RT: 0.37-0.38 AV: 2 NL: 1.75E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]
263.04658
R=48680
z=1
C14 H12 O3 Cl = 263.04695
-1.38923 ppm
118.12268
R=71426
z=1
318.29967
R=43609
z=1
C20 H43 Cl = 318.30478
-16.04961 ppm
489.10917
R=36468
z=1
C28 H22 O6 Cl = 489.10994
-1.58765 ppm
Relative Abundance
m/z

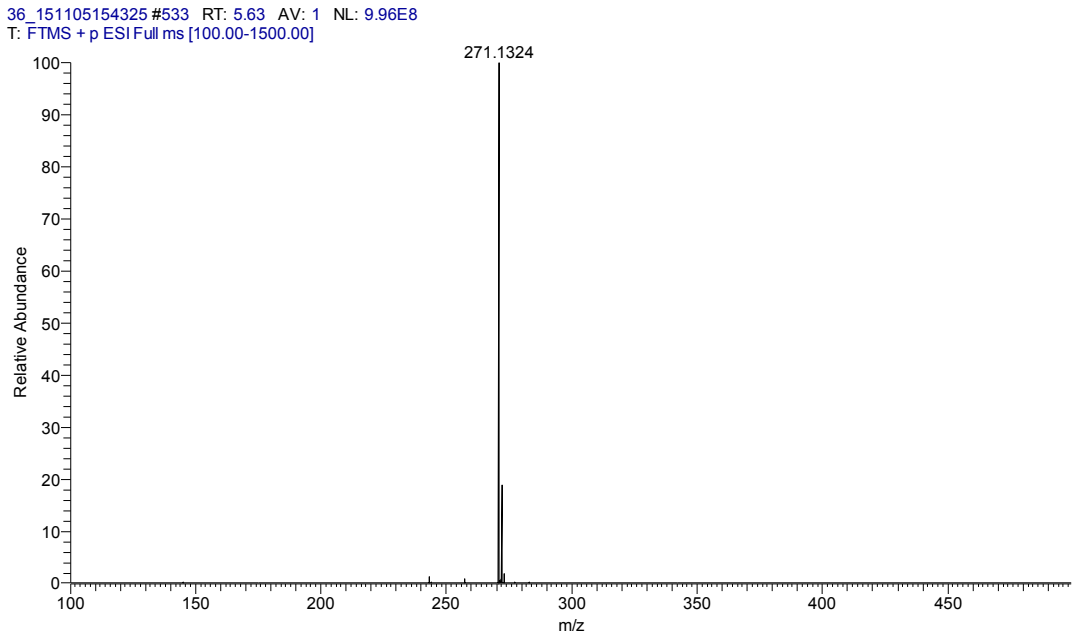
3f


5 #18 RT: 0.16 AV: 1 NL: 7.06E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]
283.05716
R=48200
z=1
C14 H10 O3 F3 = 283.05766
-1.75186 ppm
276.28064
R=52500
z=1
280.11273
R=50400
z=?
C9 H19 O6 F3 = 280.11282
-0.33000 ppm
288.28900
R=47500
z=?
290.26840
R=47400
z=1
291.27188
R=40800
z=1
296.25534
R=48600
z=1
C17 H35 F3 = 296.26854
-44.54493 ppm
Relative Abundance
m/z

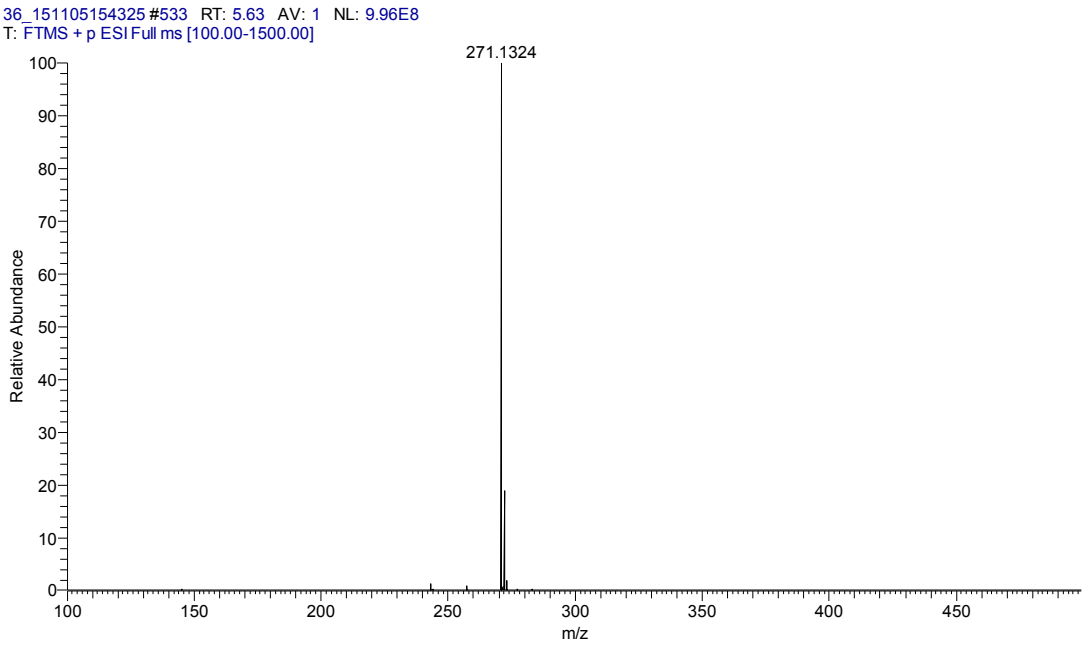
4a


35_151105153452 #481 RT: 5.11 AV: 1 NL: 1.56E10
T: FTMS + p ESI Full ms [100.00-1500.00]
257.1166
Relative Abundance
m/z

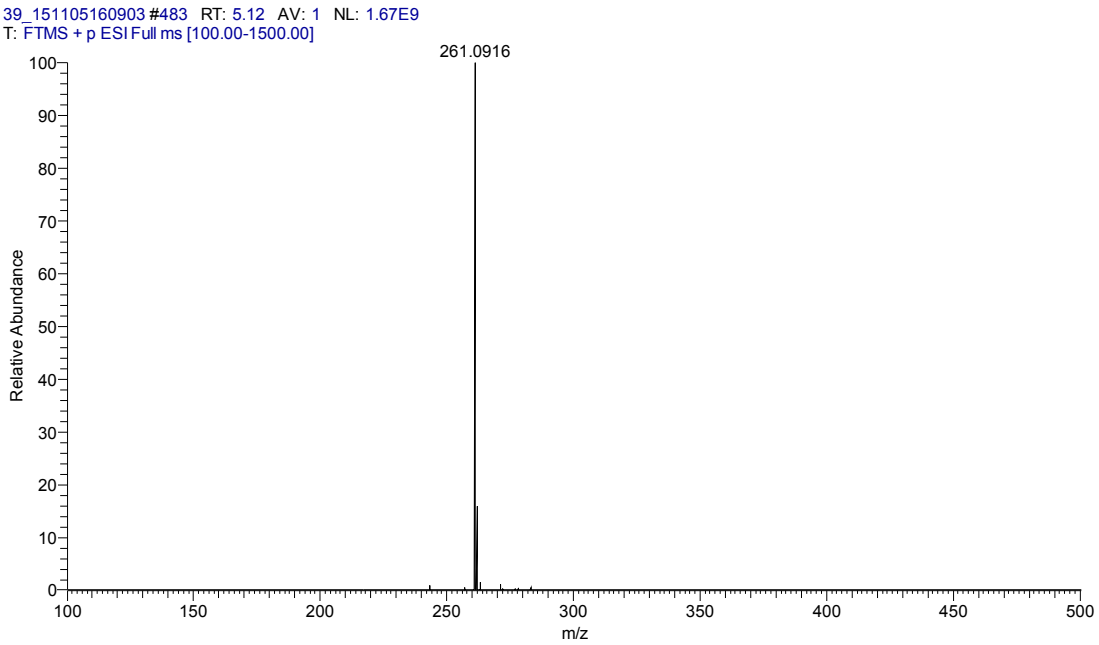
4b


36_151105154325 #533 RT: 5.63 AV: 1 NL: 9.96E8
T: FTMS + p ESI Full ms [100.00-1500.00]
271.1324
Relative Abundance
m/z

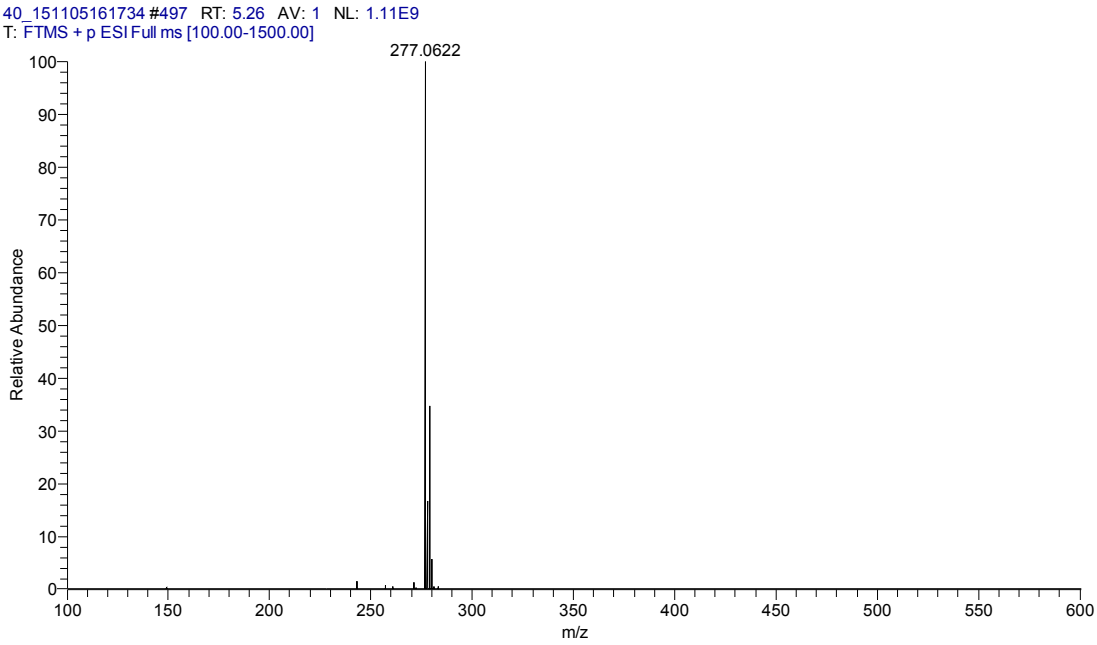
4c


36_151105154325 #533 RT: 5.63 AV: 1 NL: 9.96E8
T: FTMS + p ESI Full ms [100.00-1500.00]
271.1324
Relative Abundance
m/z

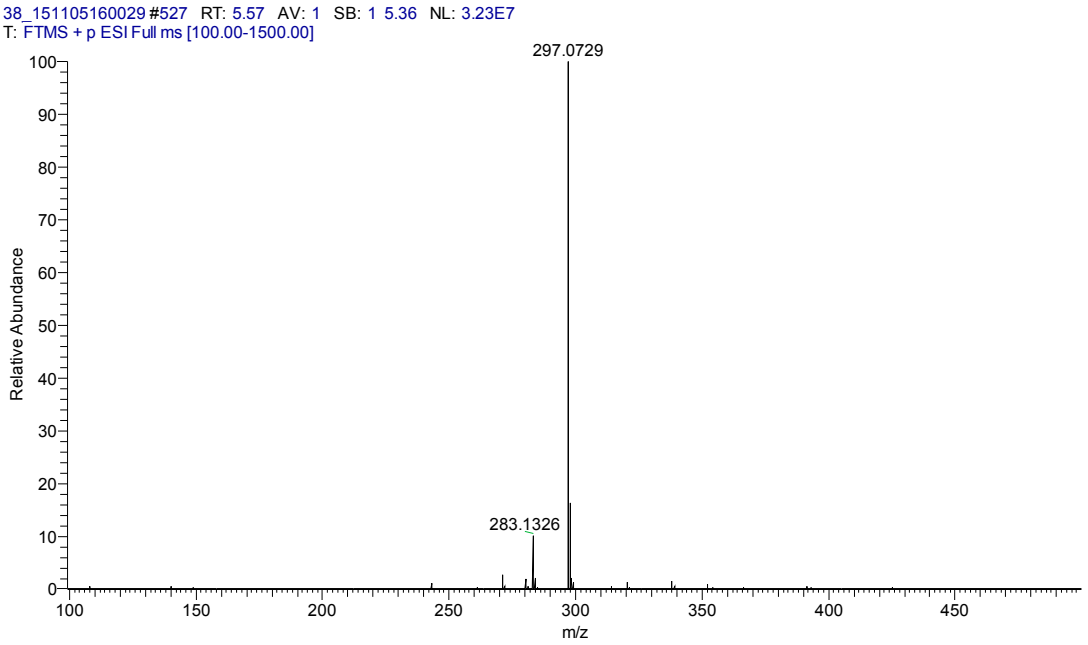
4d


39_151105160903 #483 RT: 5.12 AV: 1 NL: 1.67E9
T: FTMS + p ESI Full ms [100.00-1500.00]
261.0916
Relative Abundance
m/z

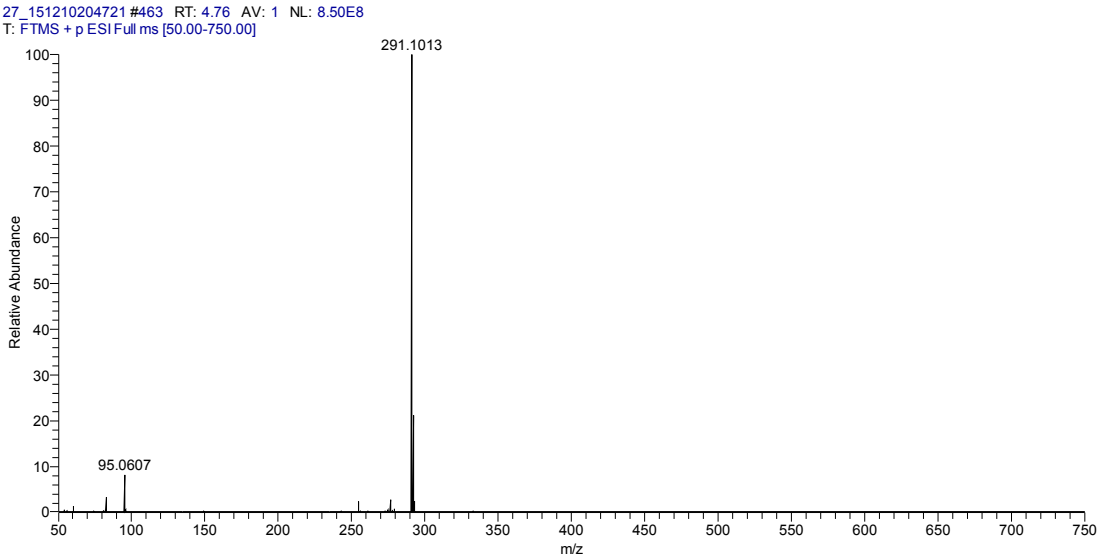
4e


40_151105161734 #497 RT: 5.26 AV: 1 NL: 1.11E9
T: FTMS + p ESI Full ms [100.00-1500.00]
277.0622
Relative Abundance
m/z

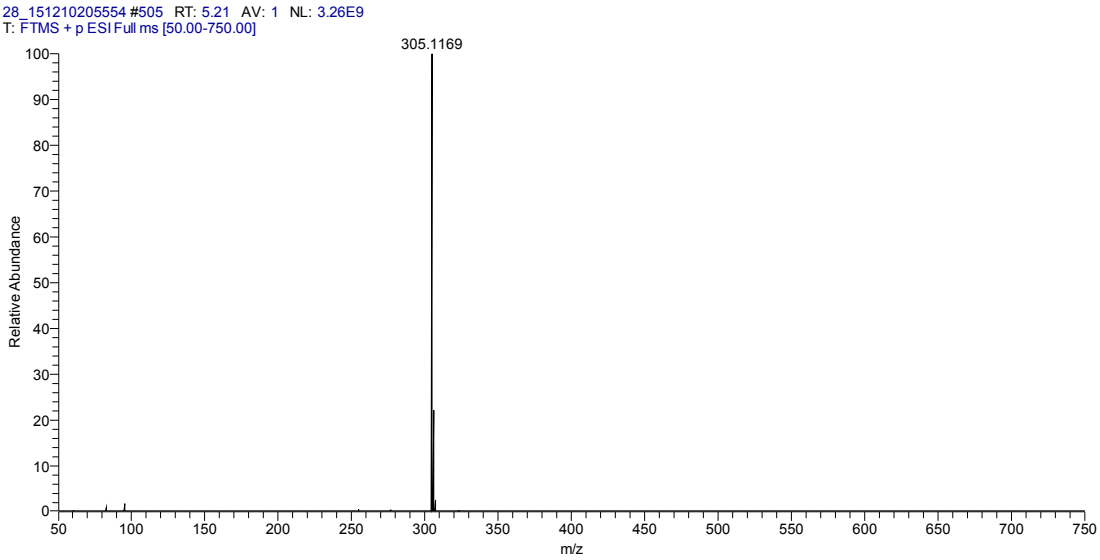
4f


38_151105160029 #527 RT: 5.57 AV: 1 SB: 1 5.36 NL: 3.23E7
T: FTMS + p ESI Full ms [100.00-1500.00]
297.0729
283.1326
Relative Abundance
m/z

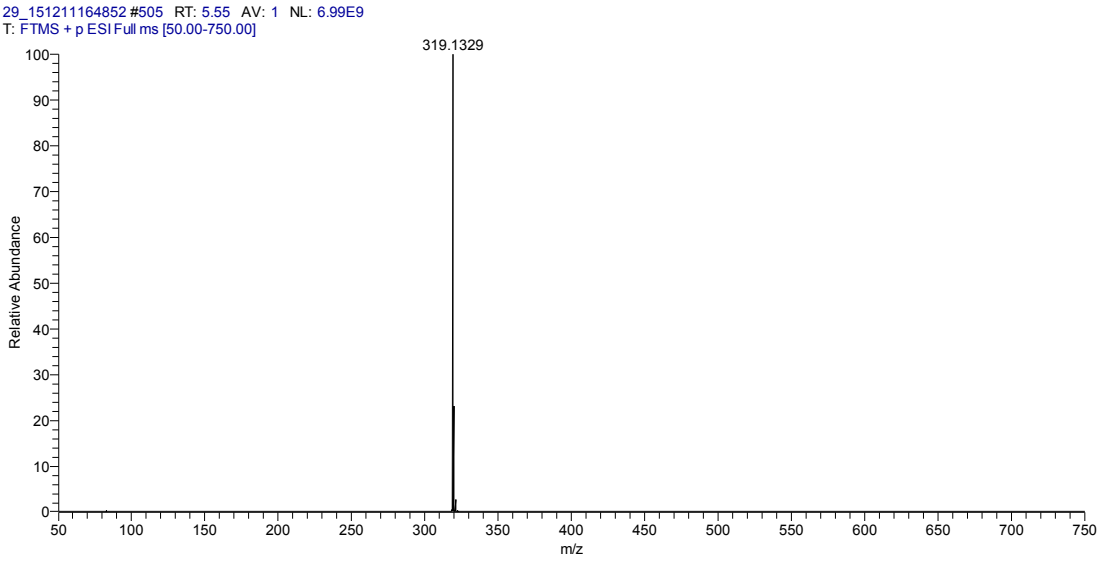
5a


27_151210204721 #463 RT: 4.76 AV: 1 NL: 8.50E8
T: FTMS + p ESI Full ms [50.00-750.00]
291.1013
95.0607
Relative Abundance
m/z

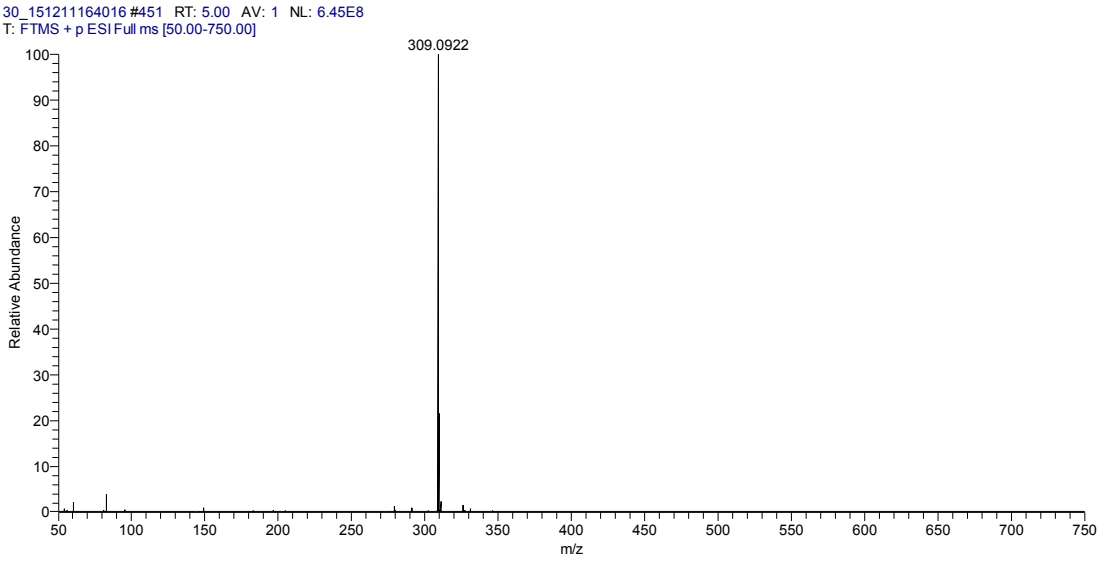
5b


28_151210205554 #505 RT: 5.21 AV: 1 NL: 3.26E9
T: FTMS + p ESI Full ms [50.00-750.00]
305.1169
Relative Abundance
m/z

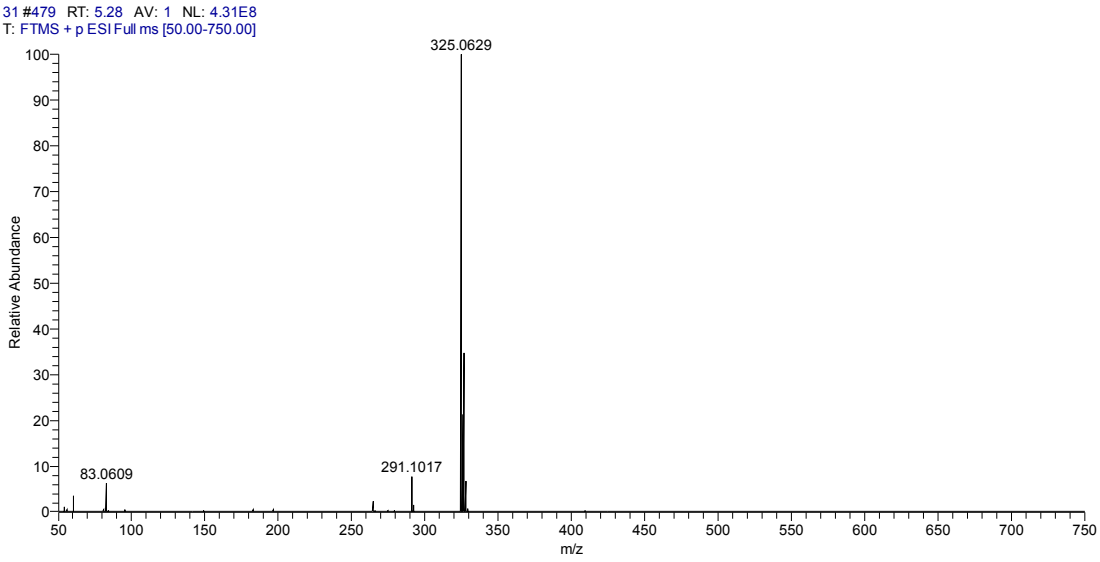
5c


29_151211164852 #505 RT: 5.55 AV: 1 NL: 6.99E9
T: FTMS + p ESI Full ms [50.00-750.00]
319.1329
Relative Abundance
m/z

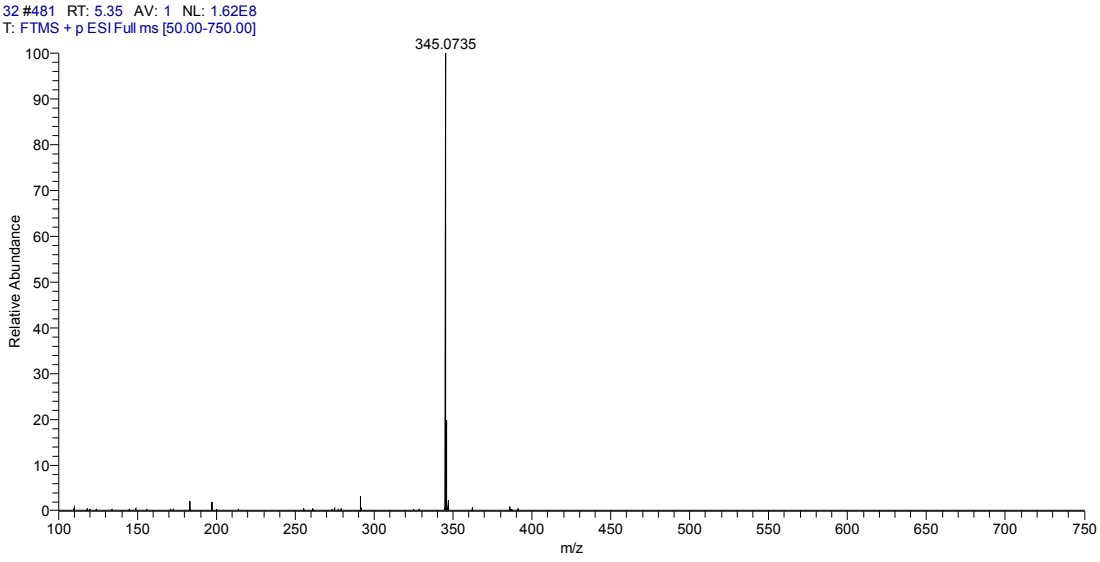
5d


30_151211164016 #451 RT: 5.00 AV: 1 NL: 6.45E8
T: FTMS + p ESI Full ms [50.00-750.00]
309.0922
Relative Abundance
m/z

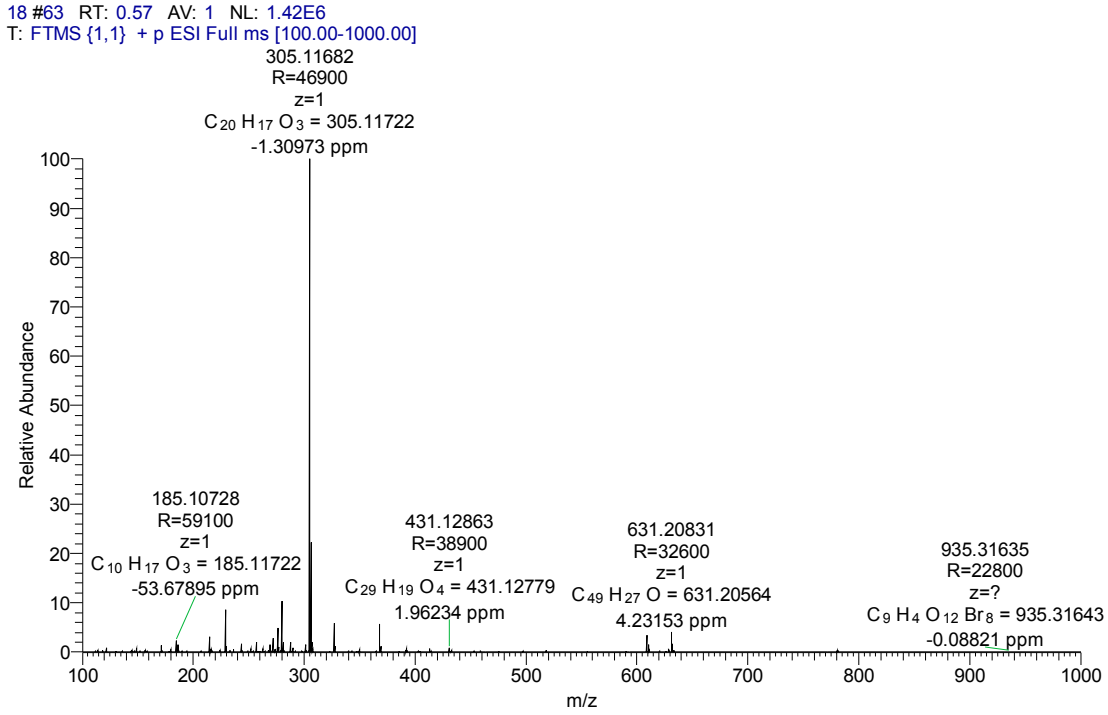
5e


31 #479 RT: 5.28 AV: 1 NL: 4.31E8
T: FTMS + p ESI Full ms [50.00-750.00]
325.0629
291.1017
83.0609
Relative Abundance
m/z

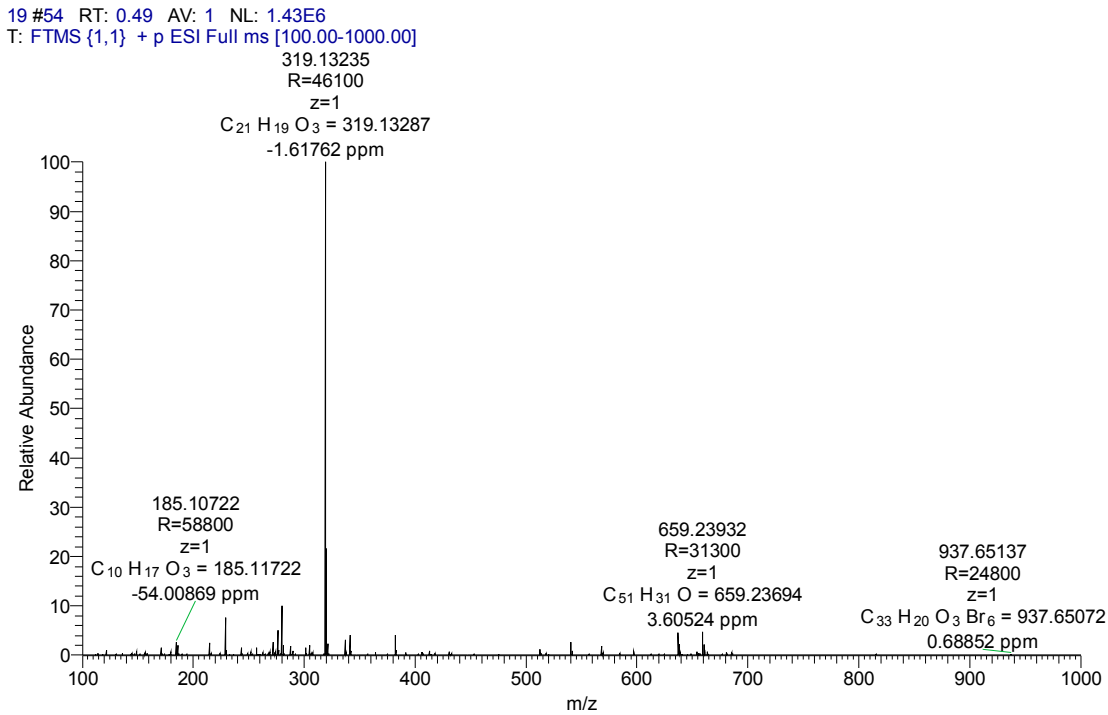
5f


32 #481 RT: 5.35 AV: 1 NL: 1.62E8
T: FTMS + p ESI Full ms [50.00-750.00]
345.0735
Relative Abundance
m/z

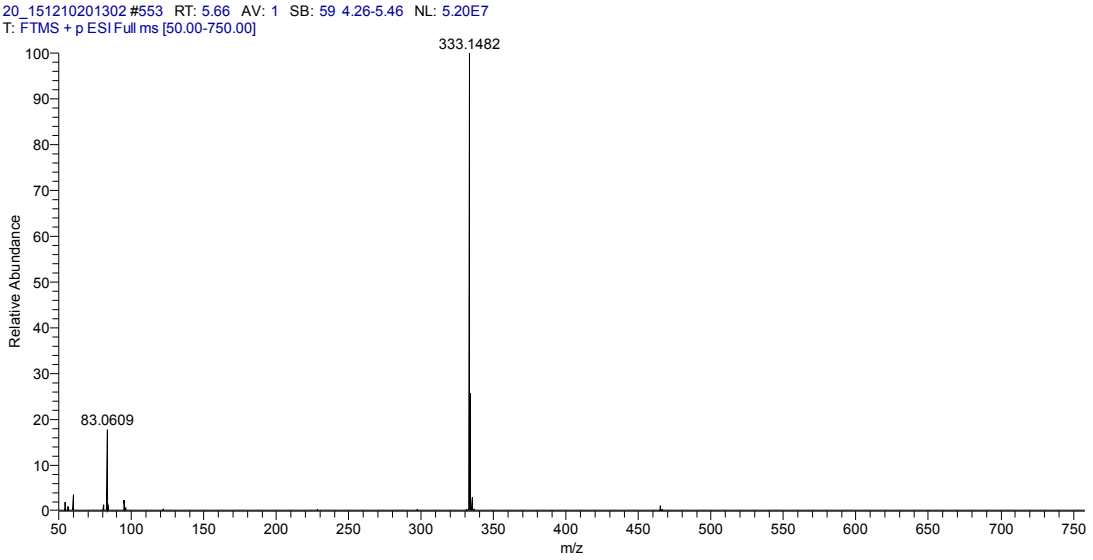
6a


18 #63 RT: 0.57 AV: 1 NL: 1.42E6
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]
305.11682
R=46900
z=1
C20 H17 O3 = 305.11722
-1.30973 ppm
185.10728
R=59100
z=1
C10 H17 O3 = 185.11722
-53.67895 ppm
431.12863
R=38900
z=1
C29 H19 O4 = 431.12779
1.96234 ppm
631.20831
R=32600
z=1
C49 H27 O = 631.20564
4.23153 ppm
935.31635
R=22800
z=?
C9 H4 O12 Br8 = 935.31643
-0.08821 ppm
Relative Abundance
m/z

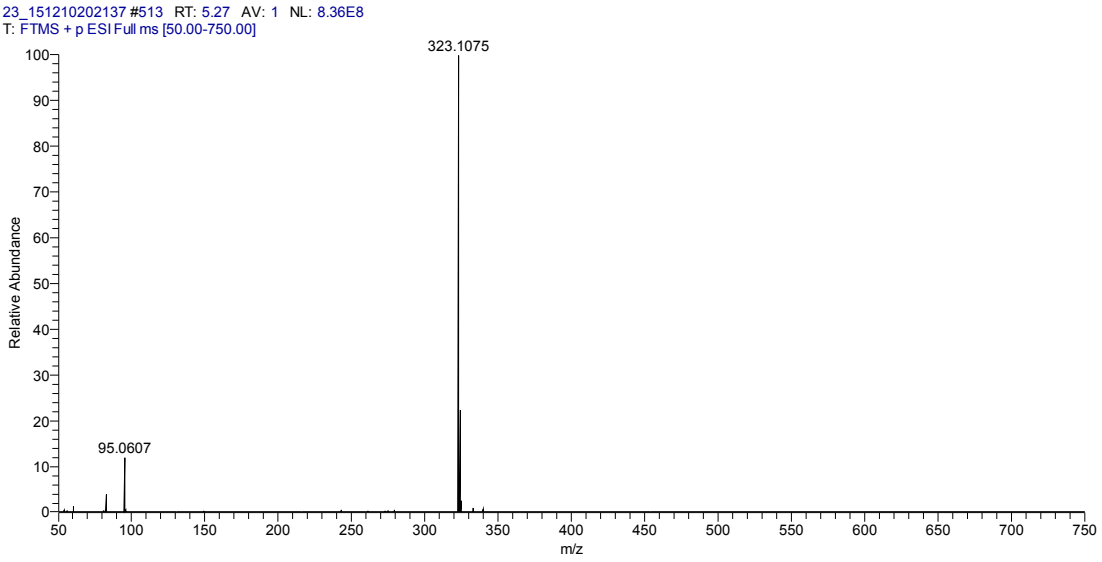
6b


19 #54 RT: 0.49 AV: 1 NL: 1.43E6
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]
319.13235
R=46100
z=1
C21 H19 O3 = 319.13287
-1.61762 ppm
185.10722
R=58800
z=1
C10 H17 O3 = 185.11722
-54.00869 ppm
659.23932
R=31300
z=1
C51 H31 O = 659.23694
3.60524 ppm
937.65137
R=24800
z=1
C33 H20 O3 Br6 = 937.65072
0.68852 ppm
Relative Abundance
m/z

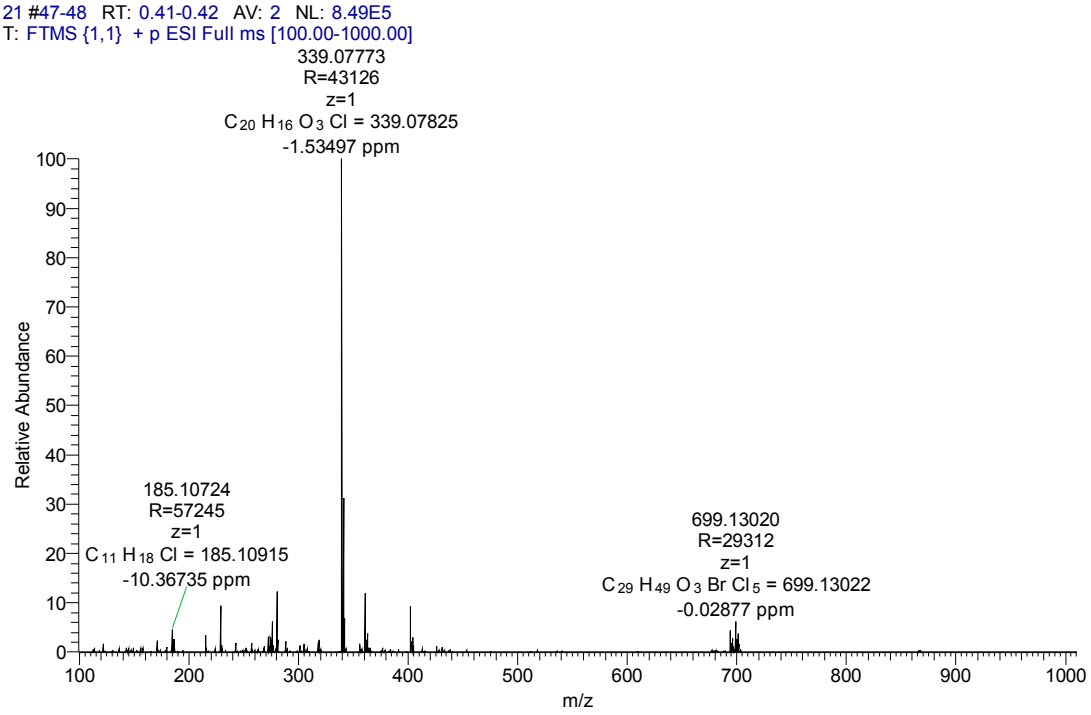
6c


20_151210201302 #553 RT: 5.66 AV: 1 SB: 59 4.26-5.46 NL: 5.20E7
T: FTMS + p ESI Full ms [50.00-750.00]
333.1482
83.0609
Relative Abundance
m/z

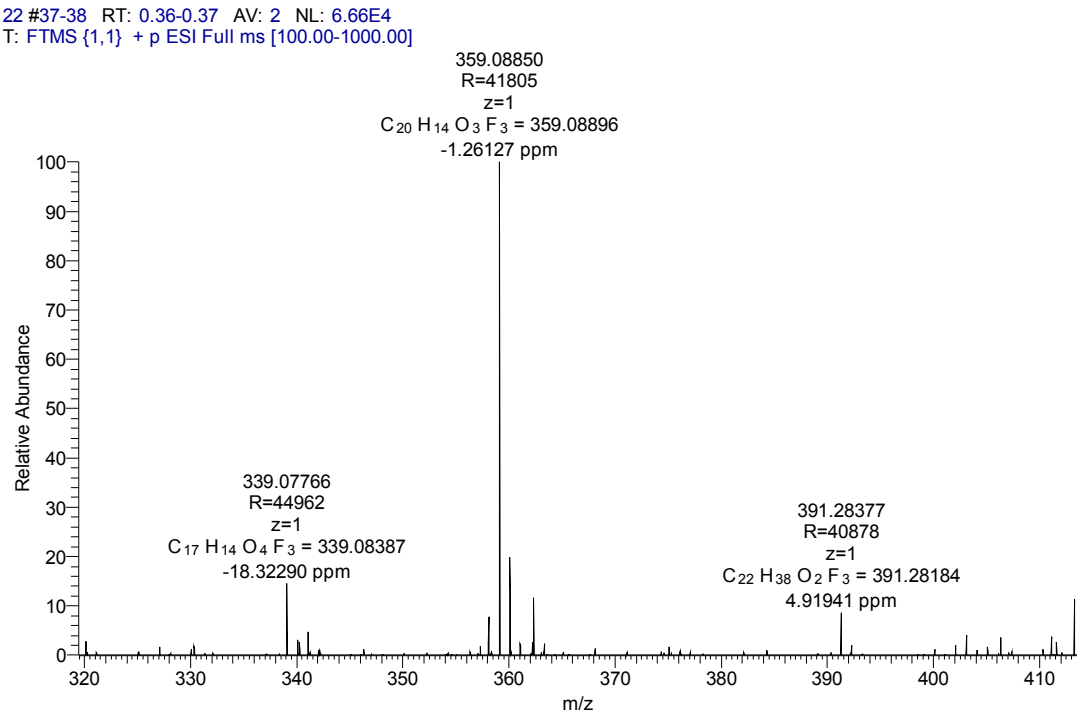
6d


23_151210202137 #513 RT: 5.27 AV: 1 NL: 8.36E8
T: FTMS + p ESI Full ms [50.00-750.00]
323.1075
95.0607
Relative Abundance
m/z

6e


21 #47-48 RT: 0.41-0.42 AV: 2 NL: 8.49E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]
339.07773
R=43126
z=1
C20 H16 O3 Cl = 339.07825
-1.53497 ppm
185.10724
R=57245
z=1
C11 H18 Cl = 185.10915
-10.36735 ppm
699.13020
R=29312
z=1
C29 H49 O3 Br Cl5 = 699.13022
-0.02877 ppm
Relative Abundance
m/z

6f


22 #37-38 RT: 0.36-0.37 AV: 2 NL: 6.66E4
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]
359.08850
R=41805
z=1
C20 H14 O3 F3 = 359.08896
-1.26127 ppm
339.07766
R=44962
z=1
C17 H14 O4 F3 = 339.08387
-18.32290 ppm
391.28377
R=40878
z=1
C22 H38 O2 F3 = 391.28184
4.91941 ppm
Relative Abundance
m/z