Supplementary Information

Rational design for multicolor flavone-based fluorophores with Aggregation-induced emission enhancement characteristics and application for mitochondria-imaging

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Table of Contents

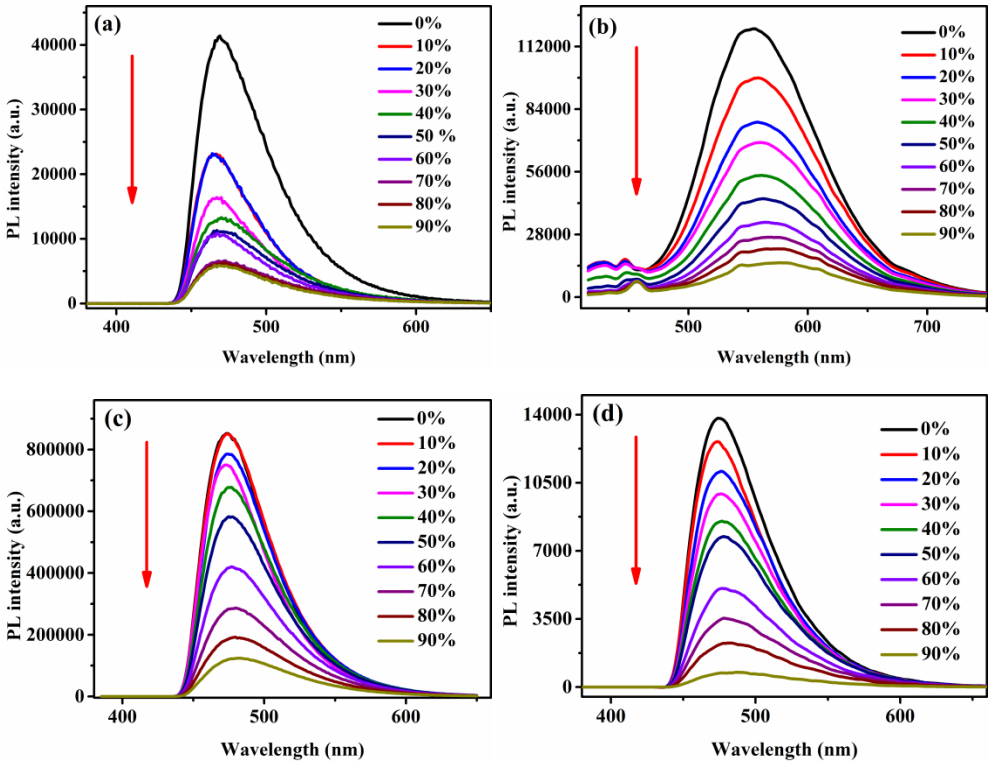


Figure S1. PL spectra of (a) **5g**, (b) **5h**, (c) **5i**, (d) **5j** (c = 2.09 × 10^{-5} M) in CH_3OH/H_2O mixtures with different water fractions (0-90 vol%)**.**

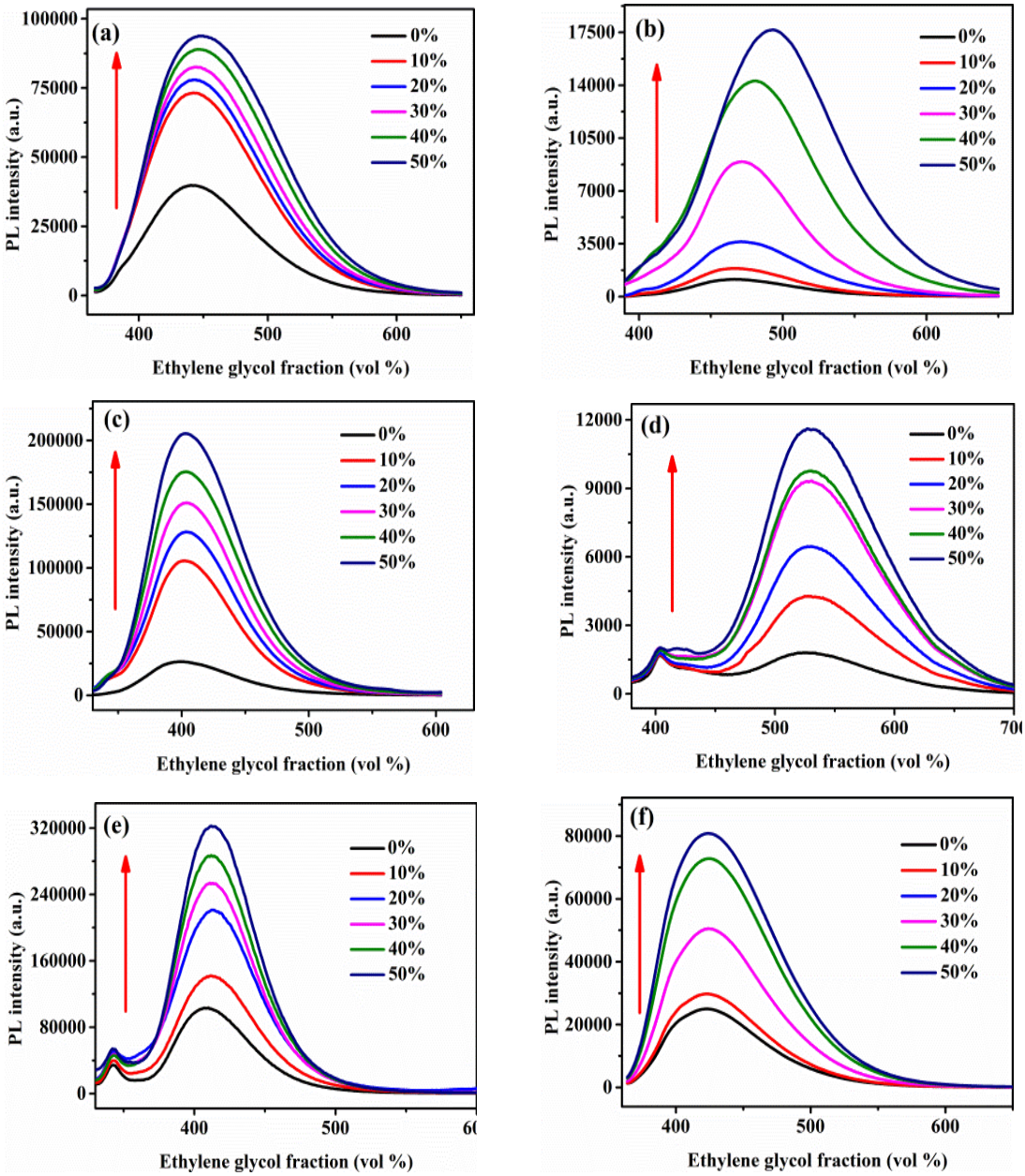


Figure S2. PL spectra of (a) **5a**, (b) **5b**, (c) **5c**, (d) **5d**, (e) **5e**, (f) **5f**. (c = 2.09 × 10^{-5} M) in CH_3OH/ ethylene glycol mixtures with different ethylene glycol fractions (0-50 vol%).

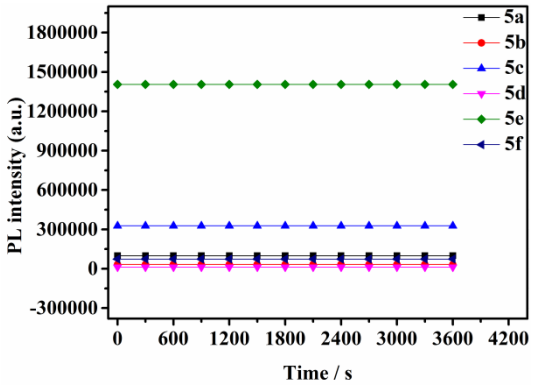


Figure S3. Time-dependent fluorescence spectra of **5a** (3: 7 v: v), **5b** (1: 9 v: v), **5c** (1: 9 v: v) , **5d** (5: 5 v: v), **5e** (1: 9 v: v) and **5f** (4: 6 v: v) in CH_3OH/H_2O (v: v) mixtures (c = 2.09×10^{-5} M).

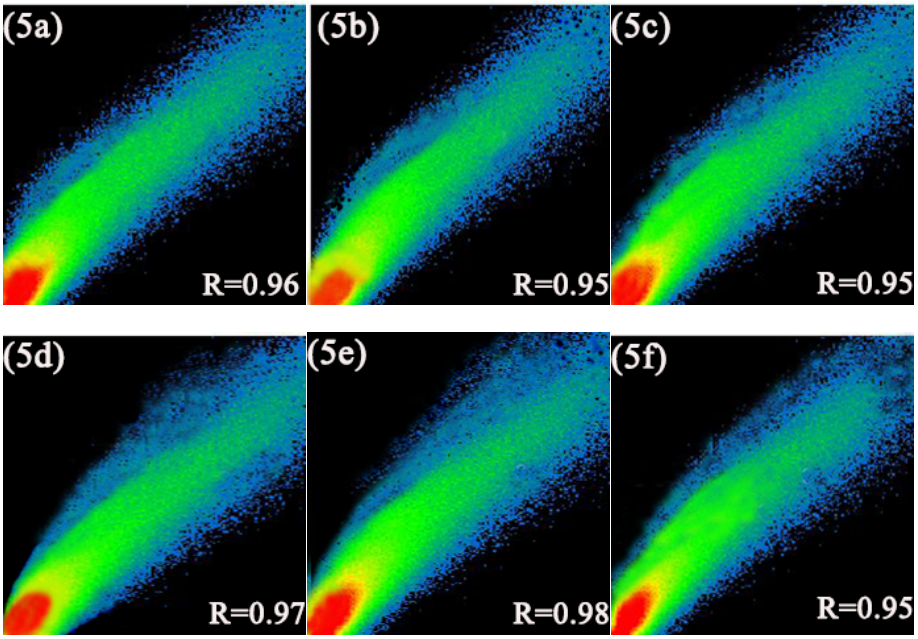
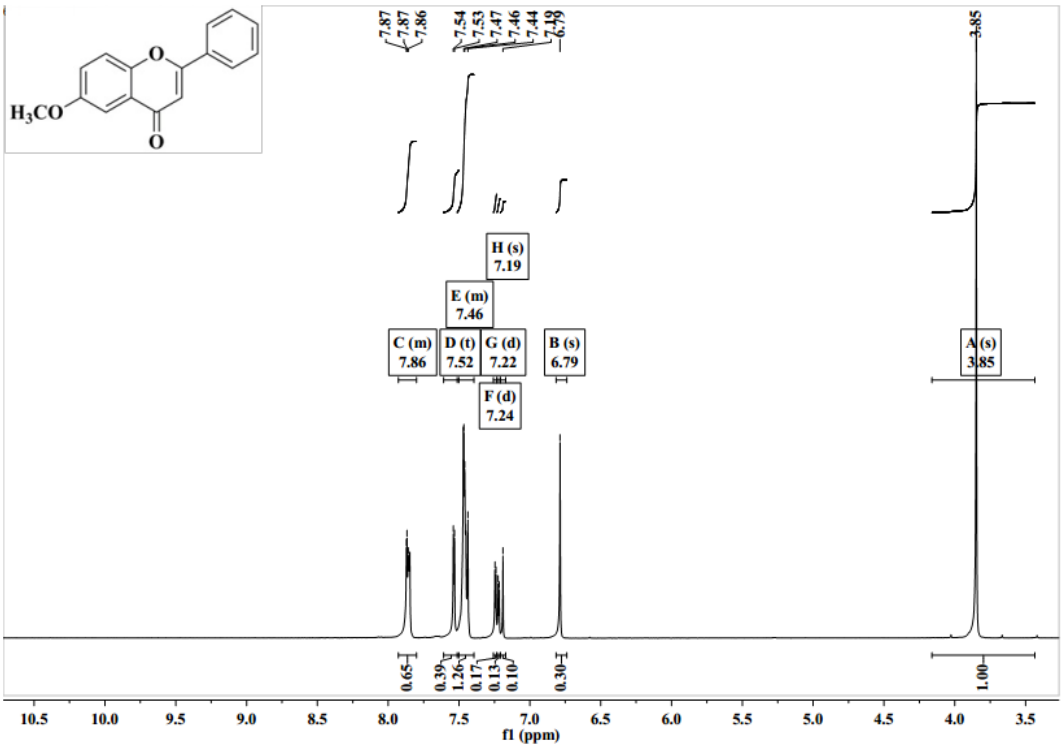
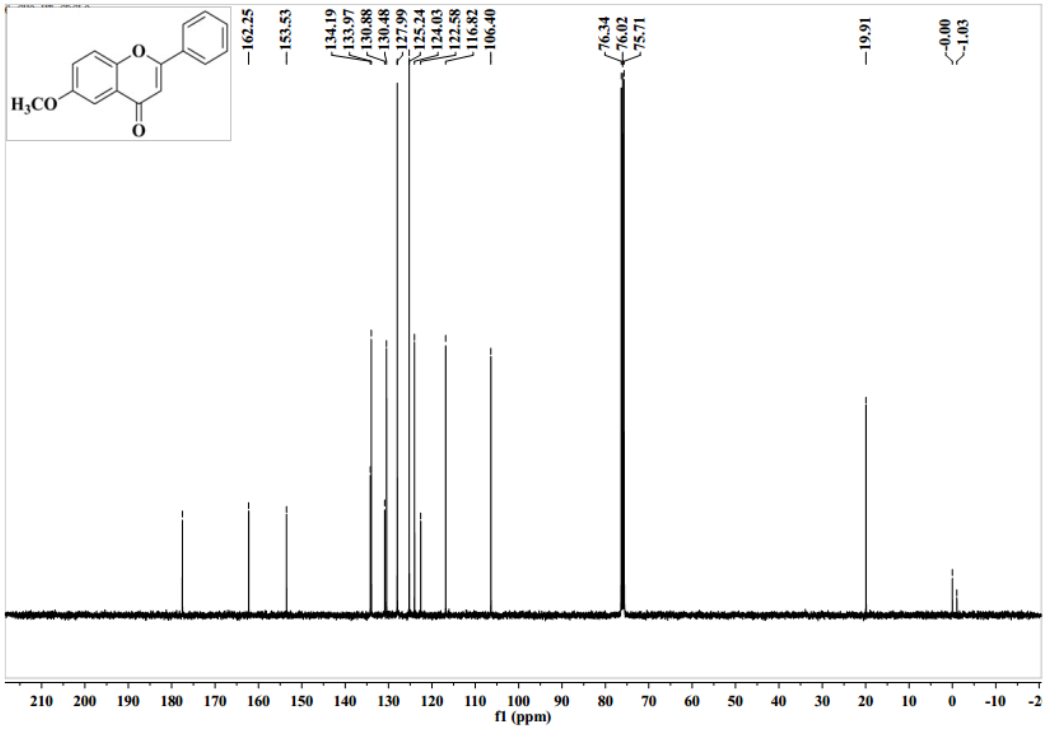


Figure S4.Pearson's correlation coefficient of **5a**, **5b**, **5c**, **5d**, **5e**, **5f** in A549 cells.


H3CO
O
O
7.87
7.87
7.86
7.54
7.53
7.47
7.46
7.44
7.19
6.79
3.85
H (s)
7.19
E (m)
7.46
C (m)
7.86
D (t)
7.52
G (d)
7.22
B (s)
6.79
A (s)
3.85
F (d)
7.24
0.65
0.39
1.26
0.17
0.13
0.10
0.30
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
f1 (ppm)


H3CO
O
O
162.25
153.53
134.19
133.97
130.88
130.48
127.99
125.24
124.03
122.58
116.82
106.40
76.34
76.02
75.71
19.91
0.00
-1.03
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-2
f1 (ppm)

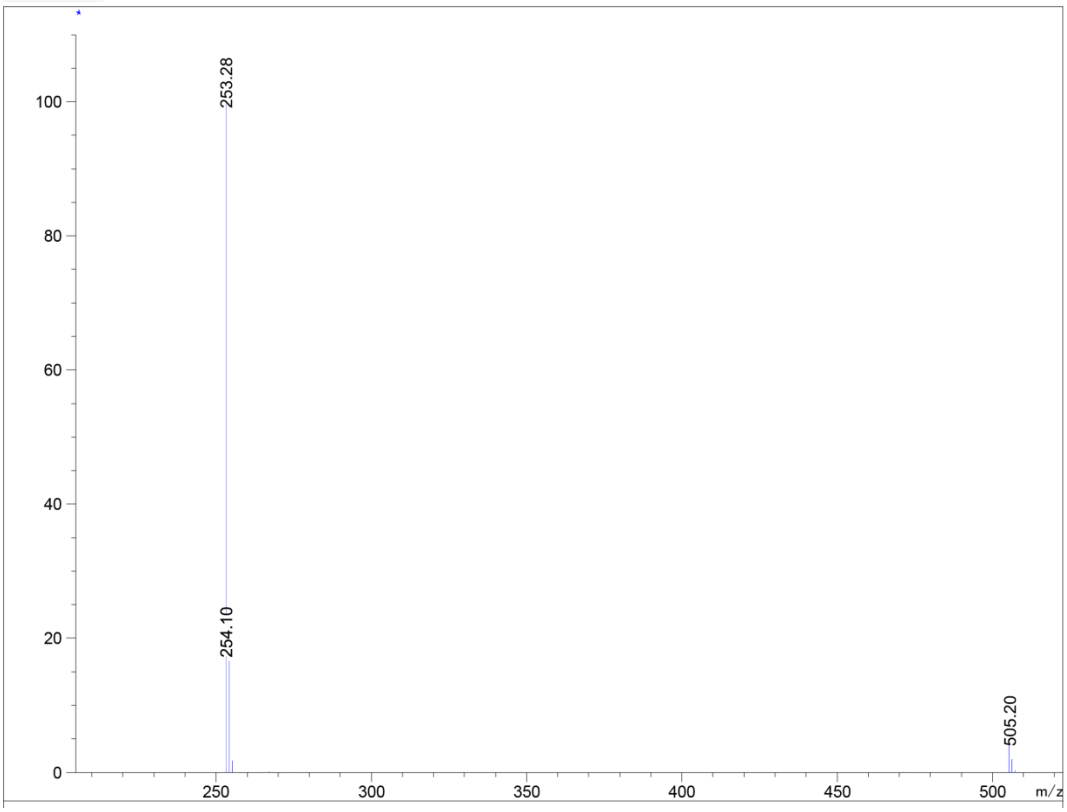
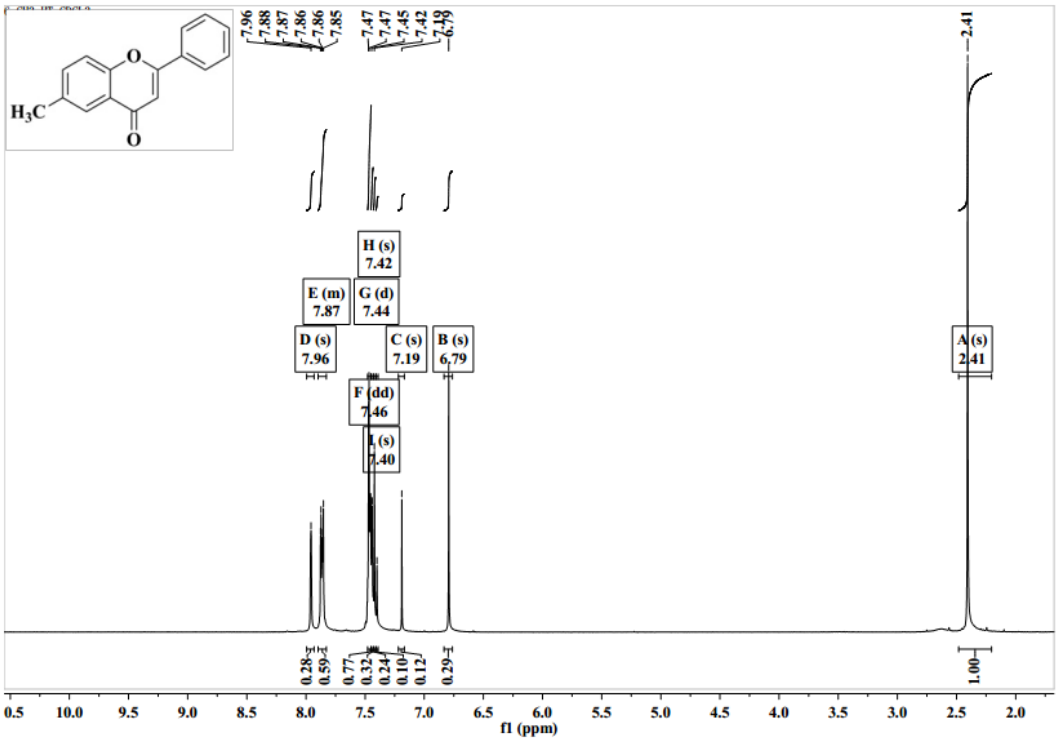
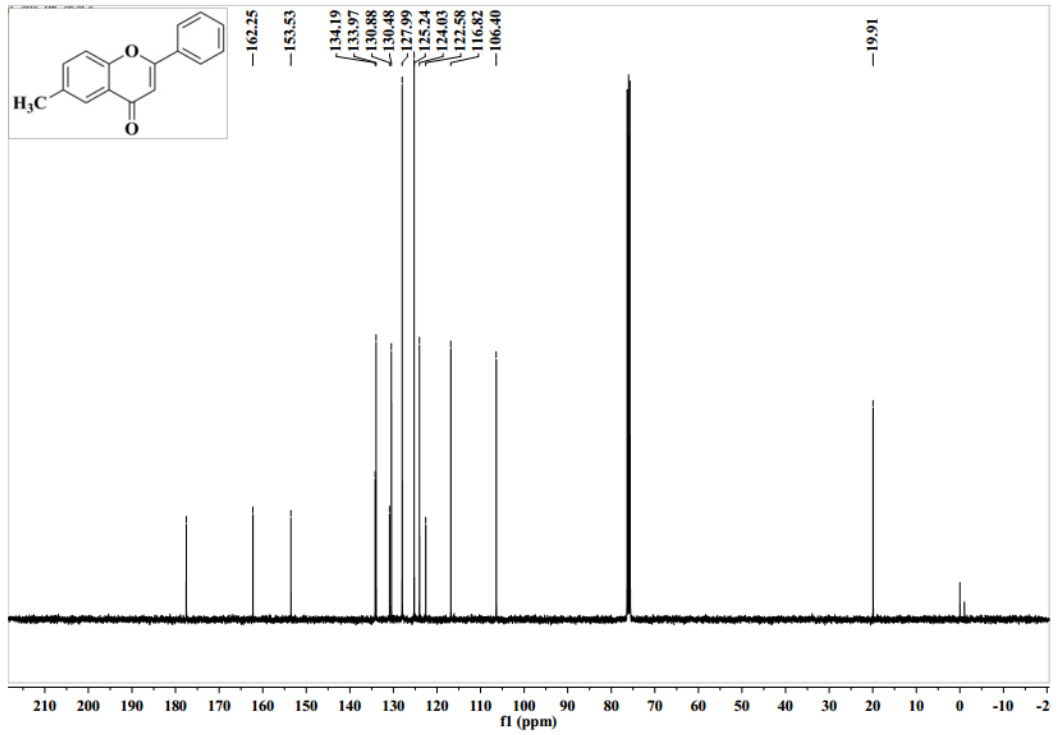


Figure S5. ^{1}H, ^{13}C NMR spectra and ESI-MS analysis for compound **5a.**


H (s)
7.42
E (m)
7.87
G (d)
7.44
D (s)
7.96
C (s)
7.19
B (s)
6.79
F (dd)
7.46
A (s)
2.41
f1 (ppm)


f1 (ppm)

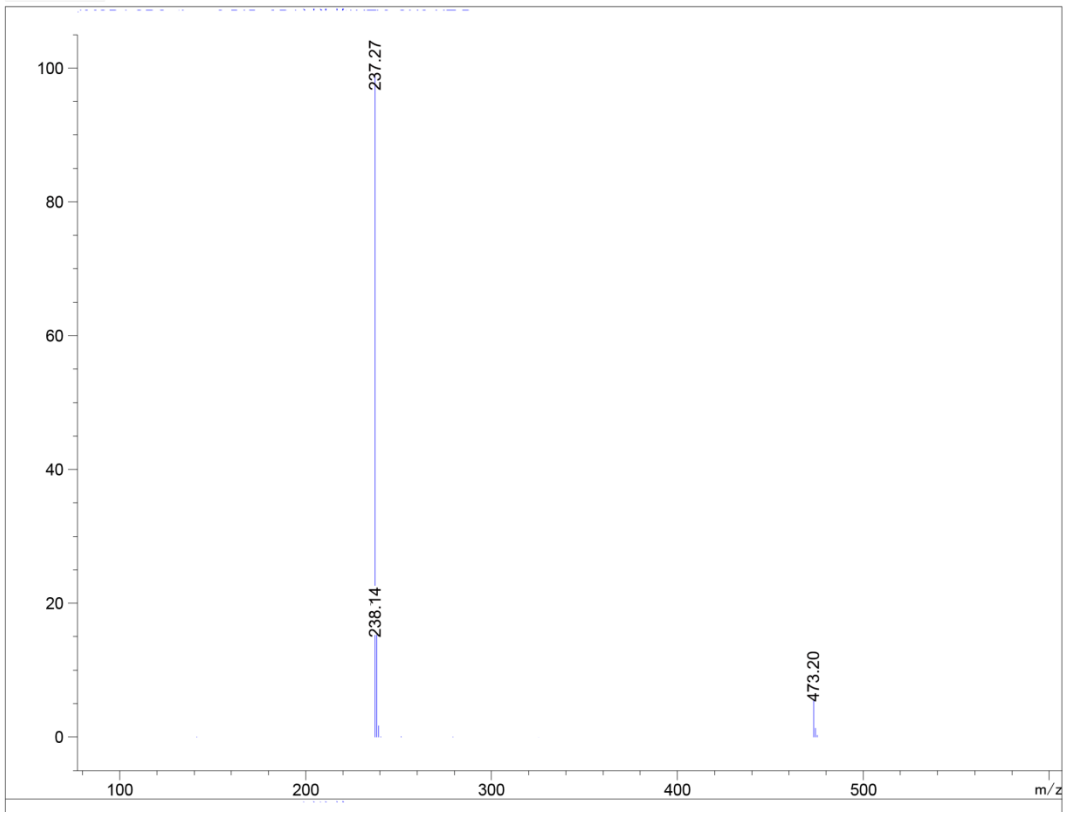
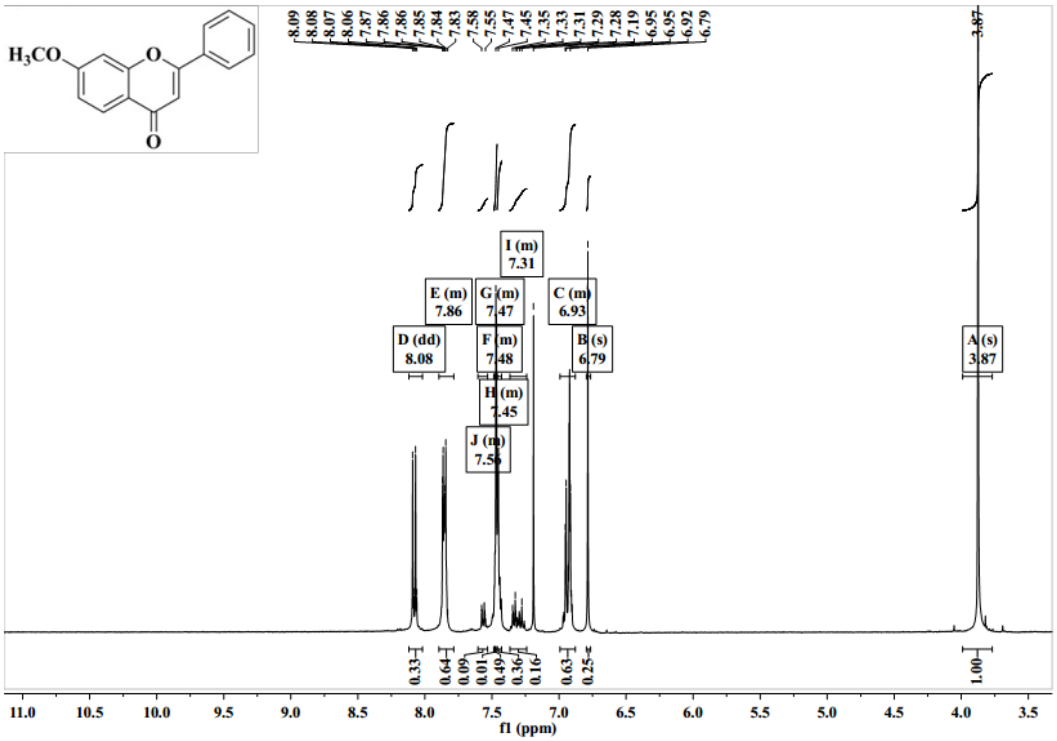
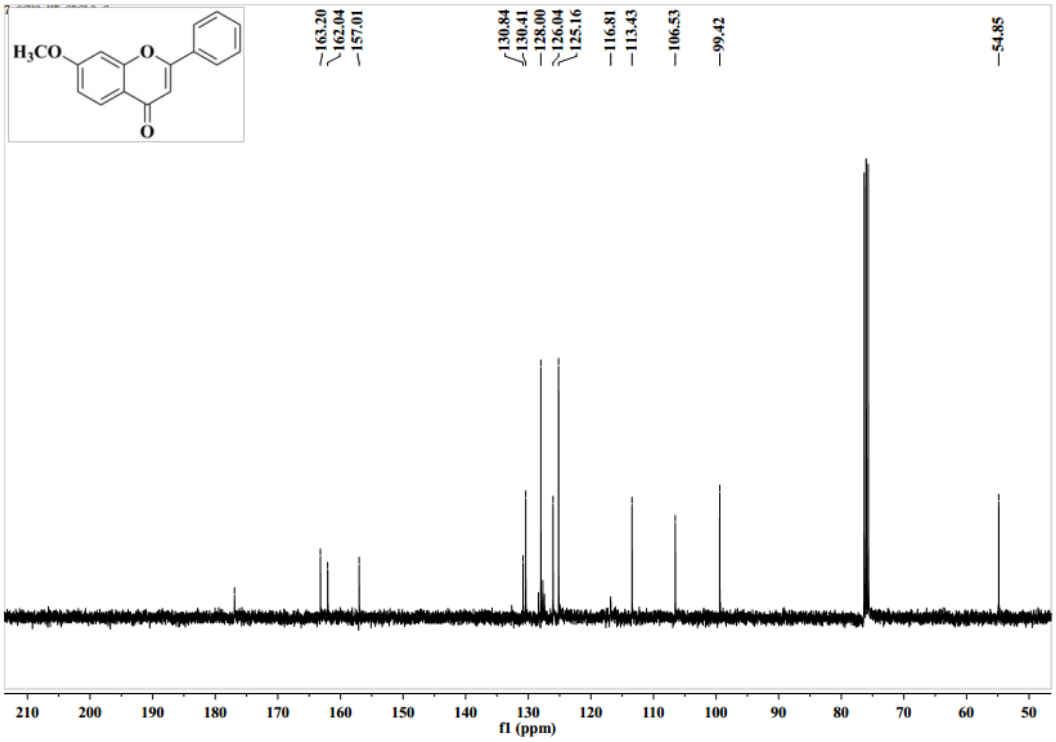


Figure S6. ^{1}H, ^{13}C NMR spectra and ESI-MSanalysis for compound **5b.**


H3CO
O
O
8.09
8.08
8.07
8.06
7.87
7.86
7.86
7.85
7.84
7.83
7.58
7.55
7.47
7.45
7.35
7.33
7.31
7.29
7.28
7.19
6.95
6.92
6.79
3.87
I (m) 7.31
E (m) 7.86
G (m) 7.47
C (m) 6.93
D (dd) 8.08
F (m) 7.48
B (s) 6.79
A (s) 3.87
H (m) 7.45
J (m) 7.56
0.33
0.64
0.09
0.01
0.49
0.36
0.16
0.63
0.25
1.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
f1 (ppm)


H3CO
O
O
163.20
162.04
157.01
130.84
130.41
128.00
126.04
125.16
116.81
113.43
106.53
99.42
54.85
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
f1 (ppm)

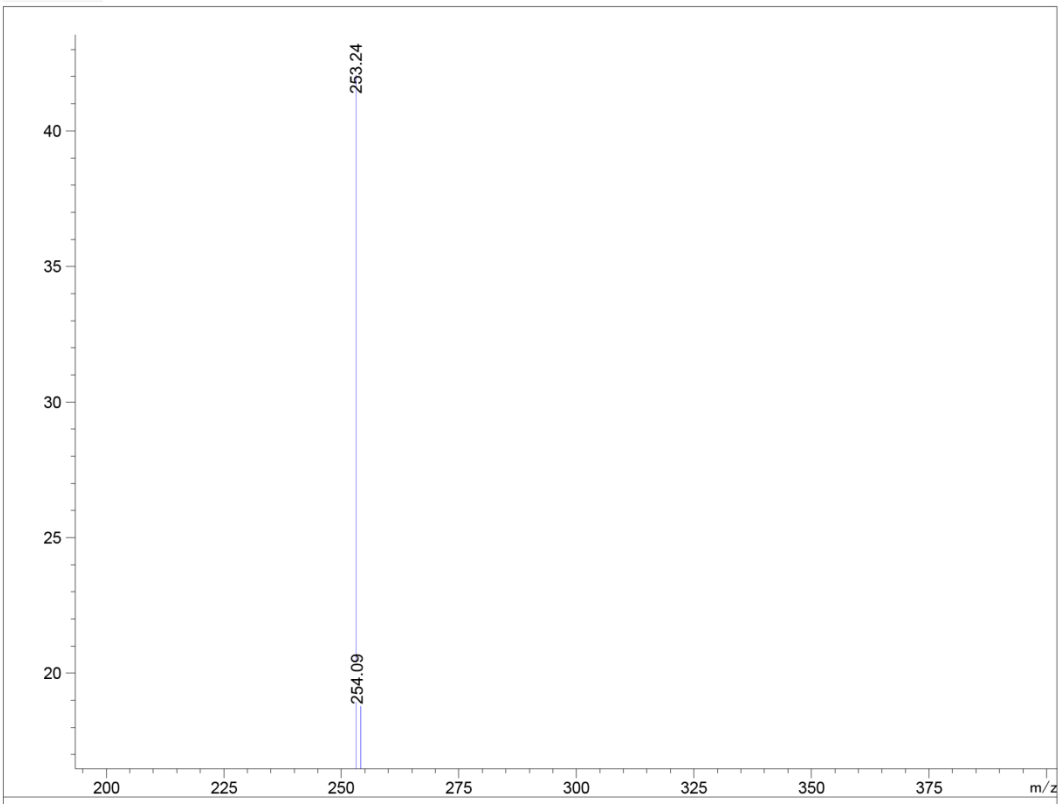
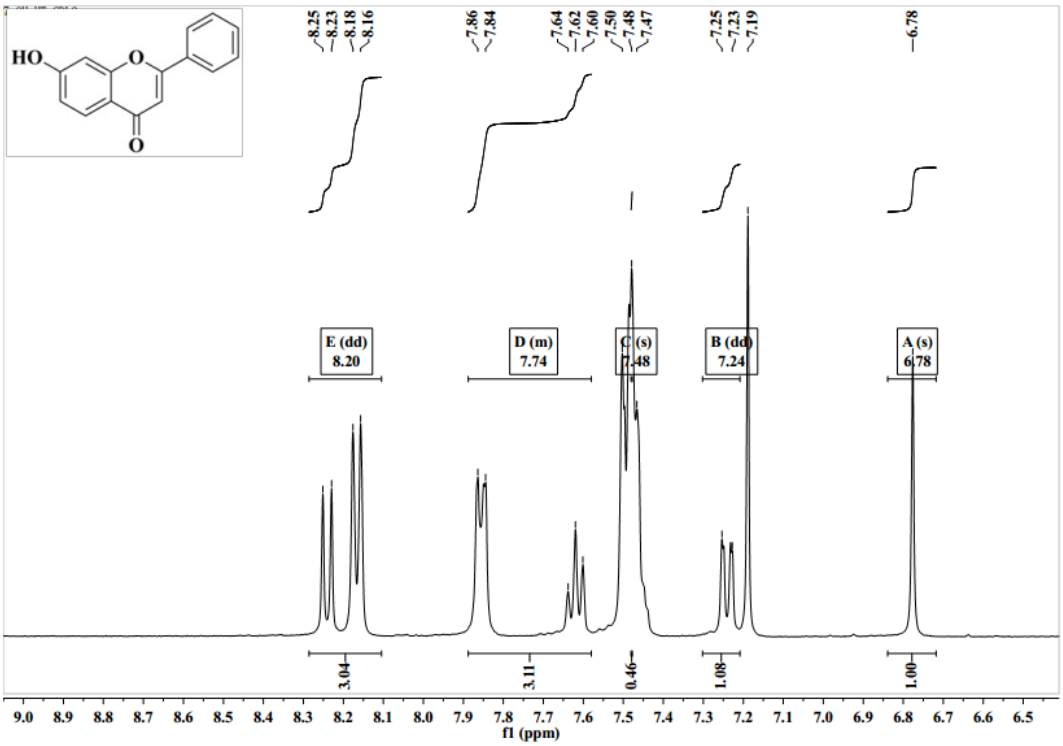
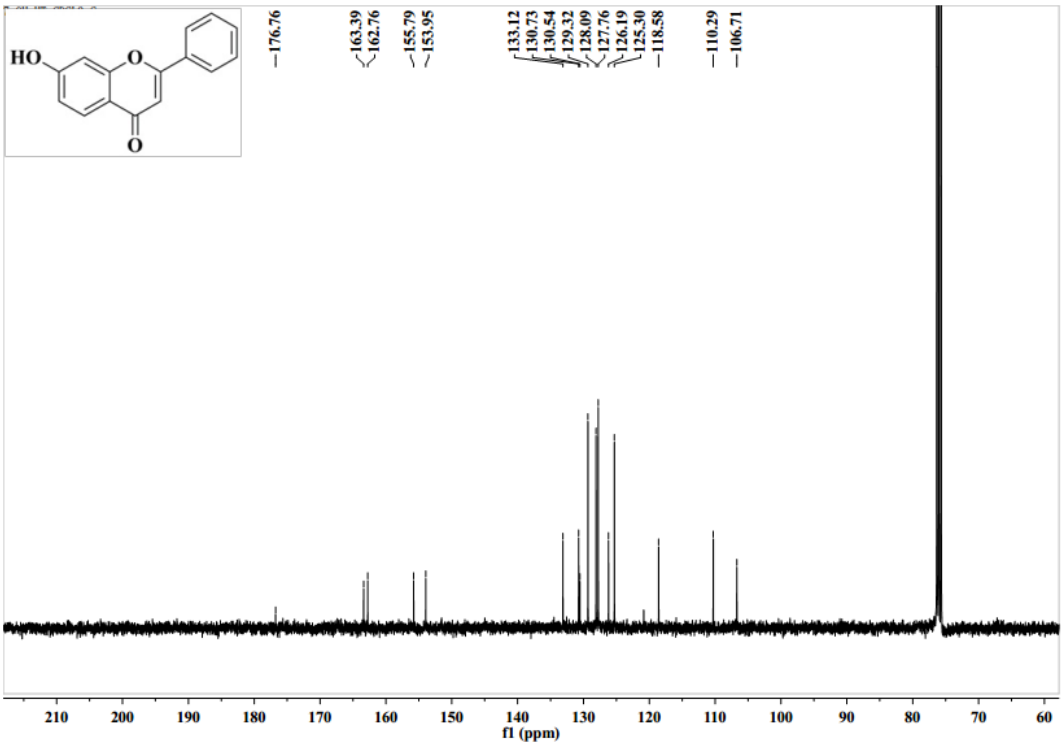


Figure S7. ^{1}H, ^{13}C NMR spectra and ESI-MSanalysis for compound **5c.**


HO
O
O
8.25
8.23
8.18
8.16
7.86
7.84
7.64
7.62
7.60
7.50
7.48
7.47
7.25
7.23
7.19
6.78
E (dd)
8.20
D (m)
7.74
C (s)
7.48
B (dd)
7.24
A (s)
6.78
3.04
3.11
0.46
1.08
1.00
9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5
f1 (ppm)


HO
O
O
176.76
163.39
162.76
155.79
153.95
133.12
130.73
130.54
129.32
128.09
127.76
126.19
125.30
118.58
110.29
106.71
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60
f1 (ppm)

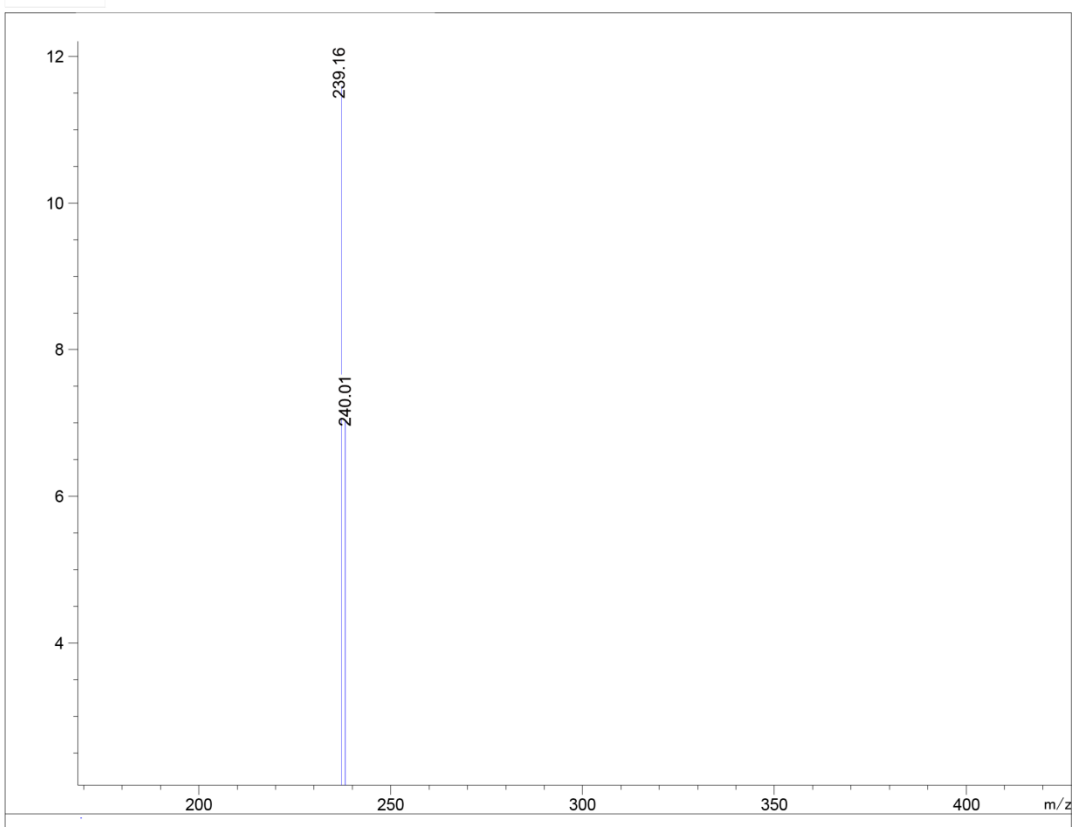
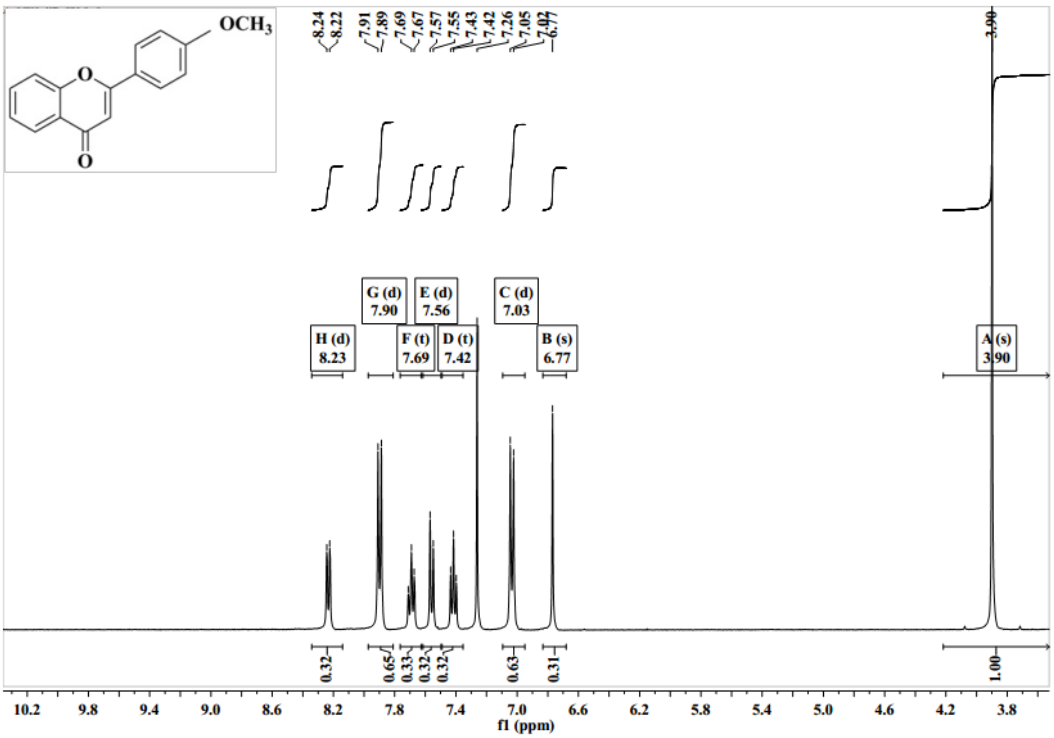
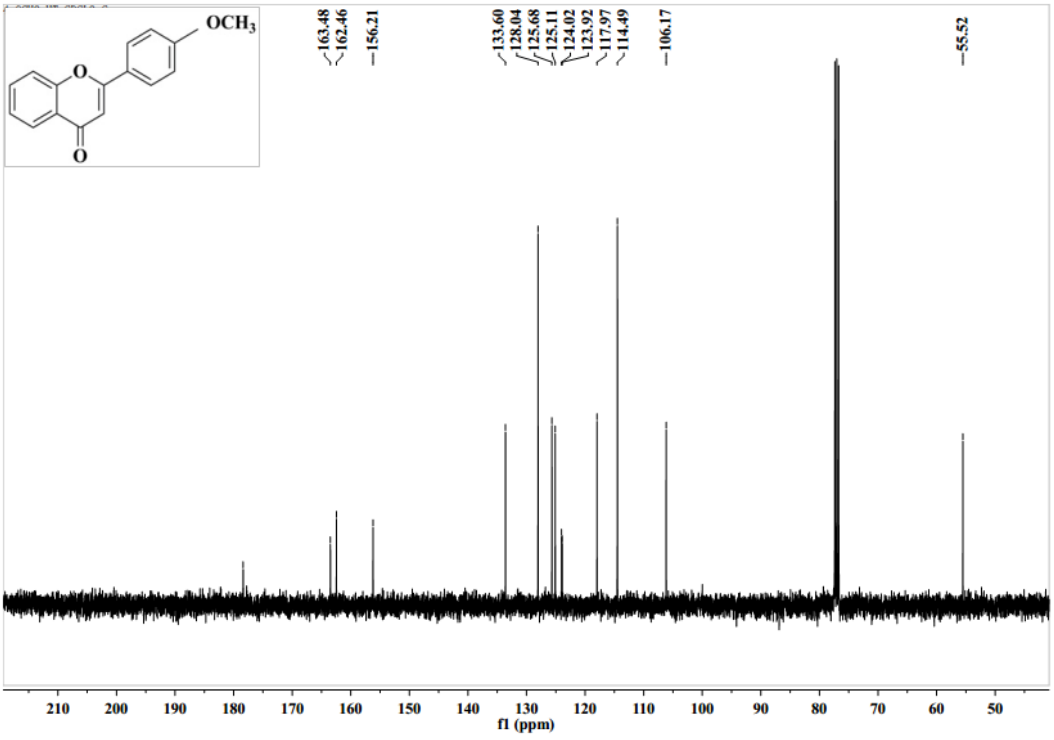


Figure S8. ^{1}H, ^{13}C NMR spectra and ESI-MS analysis for compound **5d.**


OCH3
O
O
8.24
8.22
7.91
7.89
7.69
7.67
7.57
7.55
7.43
7.42
7.26
7.05
7.02
6.77
3.90
G (d)
7.90
E (d)
7.56
C (d)
7.03
H (d)
8.23
F (t)
7.69
D (t)
7.42
B (s)
6.77
A (s)
3.90
0.32
0.65
0.33
0.32
0.32
0.63
0.31
1.00
10.2
9.8
9.4
9.0
8.6
8.2
7.8
7.4
7.0
6.6
6.2
5.8
5.4
5.0
4.6
4.2
3.8
f1 (ppm)


OCH3
O
O
163.48
162.46
156.21
133.60
128.04
125.68
125.11
124.02
123.92
117.97
114.49
106.17
55.52
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
f1 (ppm)

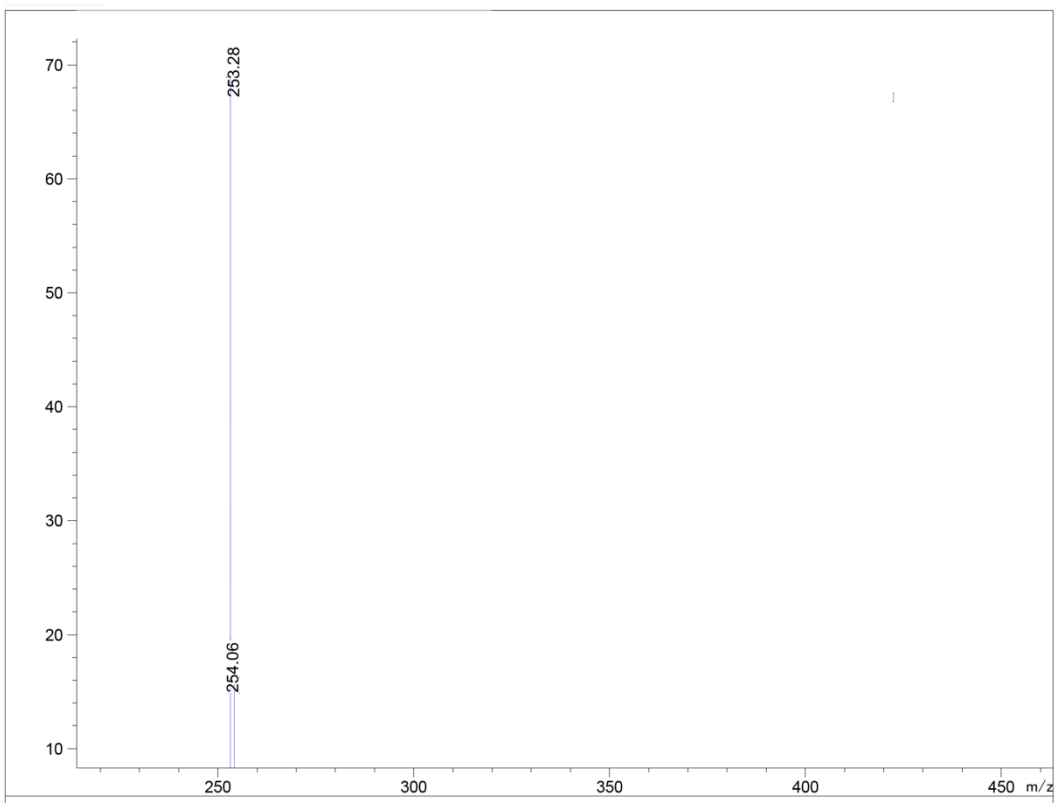
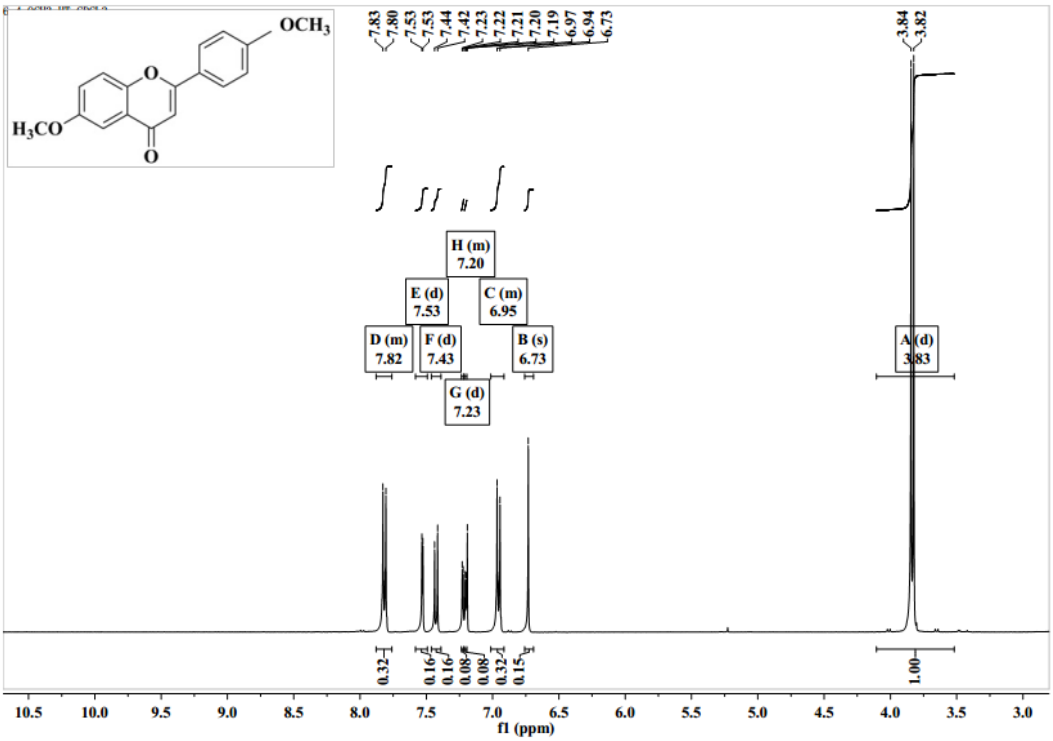
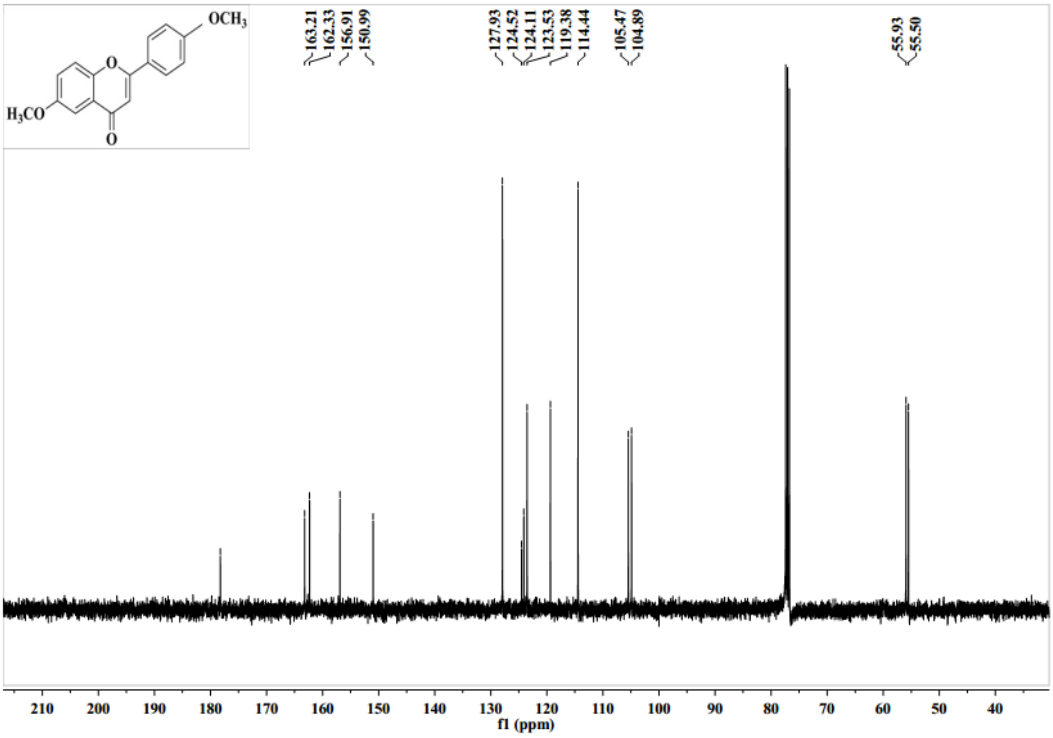


Figure S9. ^{1}H, ^{13}C NMR spectra and ESI-MS analysis for compound **5e.**


OCH3
H3CO
O
7.83
7.80
7.53
7.53
7.44
7.42
7.23
7.22
7.21
7.20
7.19
6.97
6.94
6.73
3.84
3.82
H (m) 7.20
E (d) 7.53
C (m) 6.95
D (m) 7.82
F (d) 7.43
B (s) 6.73
G (d) 7.23
A (d) 3.83
0.32
0.16
0.16
0.08
0.09
0.32
0.15
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0
f1 (ppm)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H3CO
O
163.21
162.33
156.91
150.99
127.93
124.52
124.11
123.53
119.38
114.44
105.47
104.89
55.93
55.50
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40
f1 (ppm)

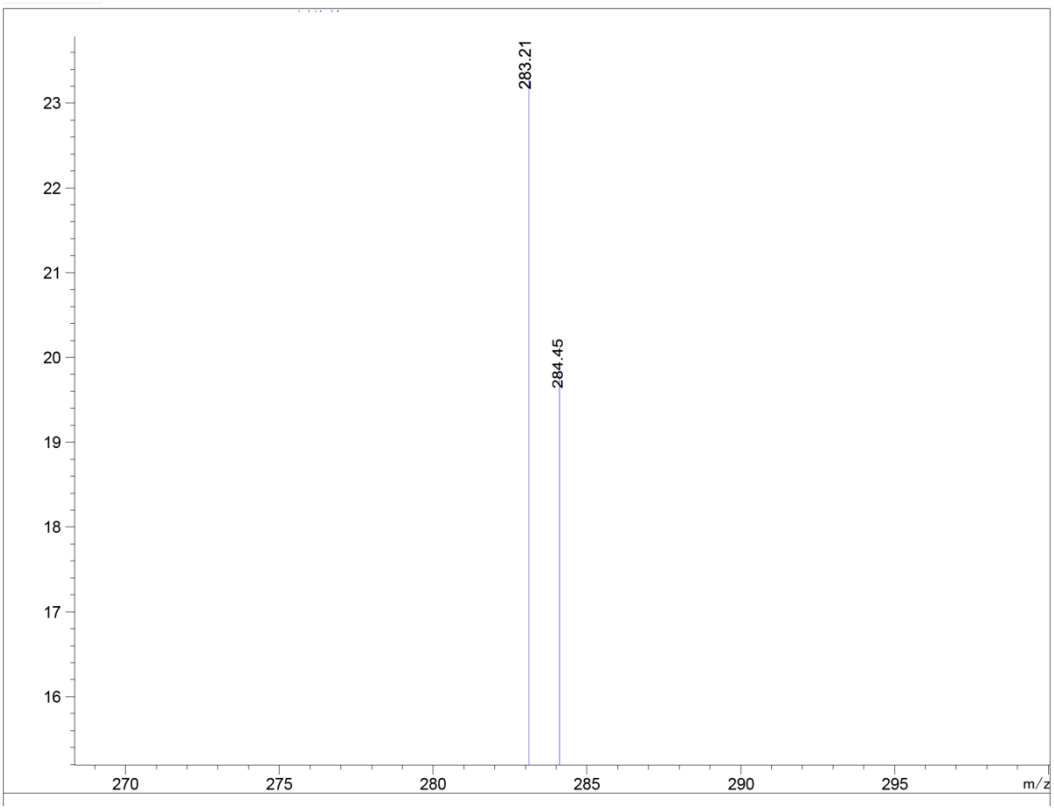
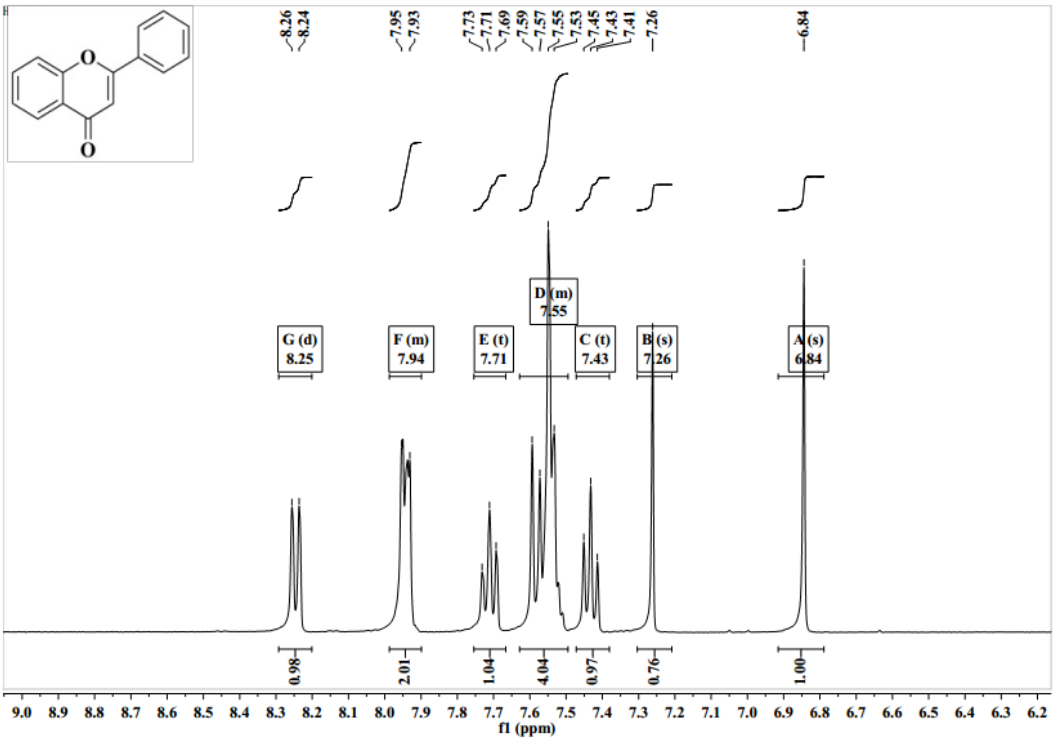
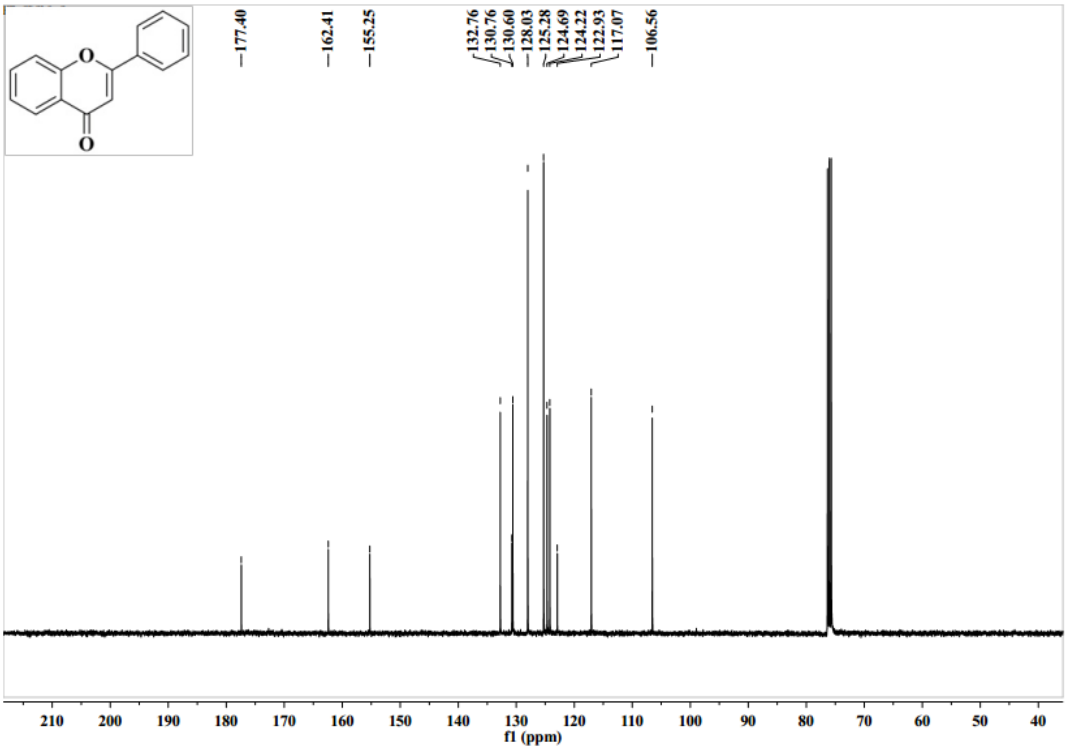


Figure S10. ^{1}H, ^{13}C NMR spectra and ESI-MS analysis for compound **5f.**


8.26
8.24
7.95
7.93
7.73
7.71
7.69
7.59
7.57
7.55
7.53
7.45
7.43
7.41
7.26
6.84
G (d)
8.25
F (m)
7.94
E (t)
7.71
D (m)
7.55
C (t)
7.43
B (s)
7.26
A (s)
6.84
0.98
2.01
1.04
4.04
0.97
0.76
1.00
fl (ppm)


177.40
162.41
155.25
132.76
130.76
130.60
128.03
125.28
124.69
124.22
122.93
117.07
106.56
fl (ppm)

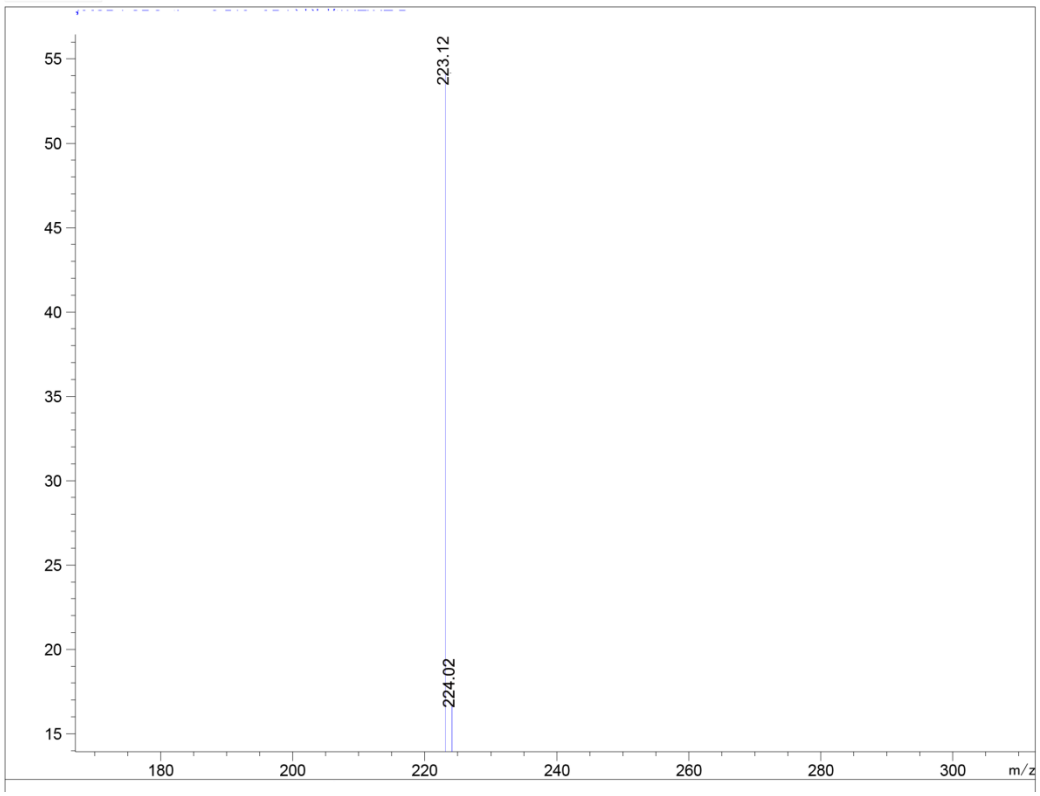
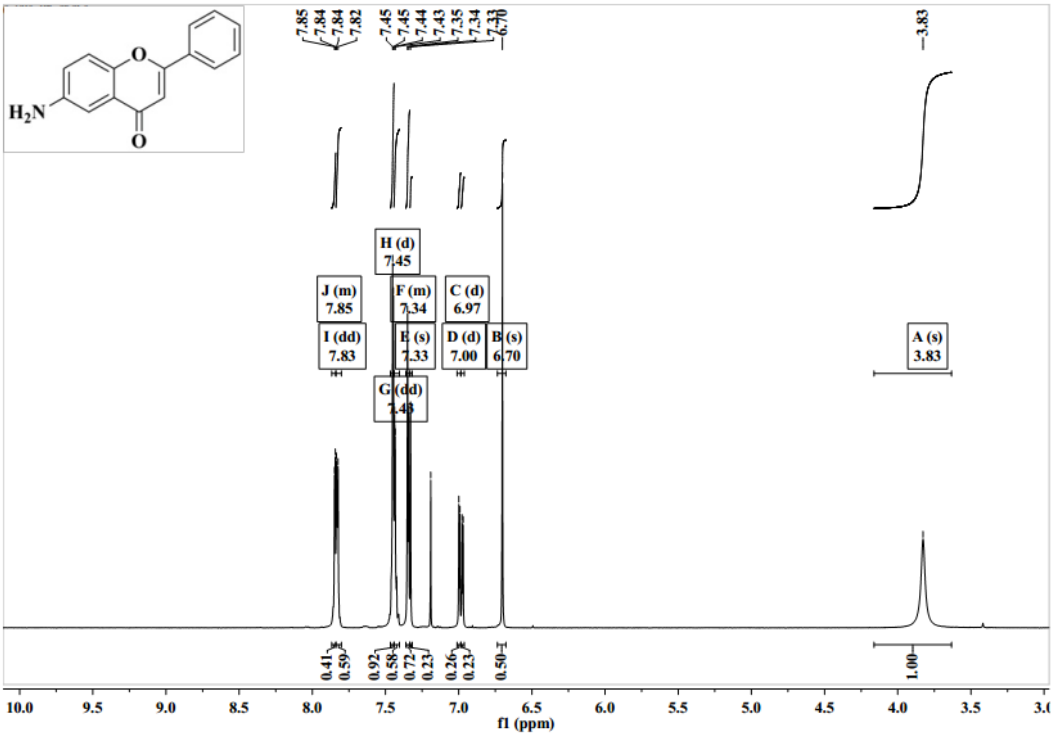
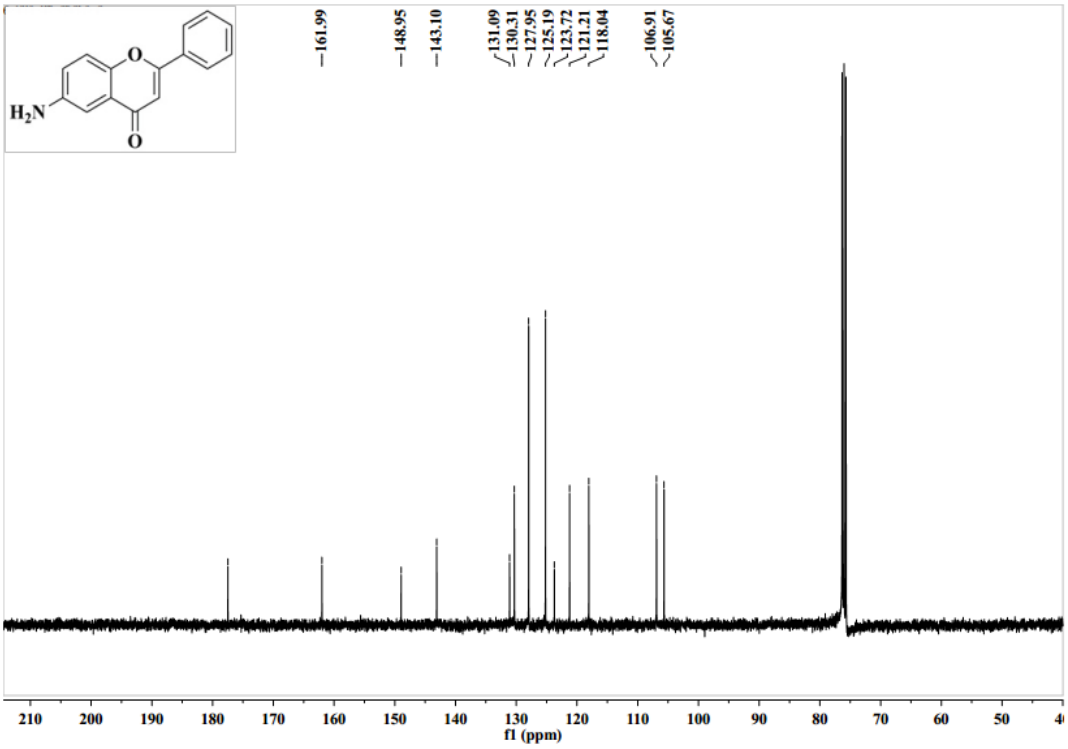


Figure S11. ^{1}H, ^{13}C NMR spectra and ESI-MS analysis for compound **5g.**


7.85
7.84
7.84
7.82
7.45
7.45
7.44
7.43
7.35
7.34
7.33
6.70
3.83
H (d) 7.45
J (m) 7.85
F (m) 7.34
C (d) 6.97
I (dd) 7.83
E (s) 7.33
D (d) 7.00
B (s) 6.70
G (dd) 7.48
A (s) 3.83
0.41
0.59
0.92
0.58
0.72
0.23
0.26
0.23
0.50
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
f1 (ppm)


161.99
148.95
143.10
131.09
130.31
127.95
125.19
123.72
121.21
118.04
106.91
105.67
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
f1 (ppm)

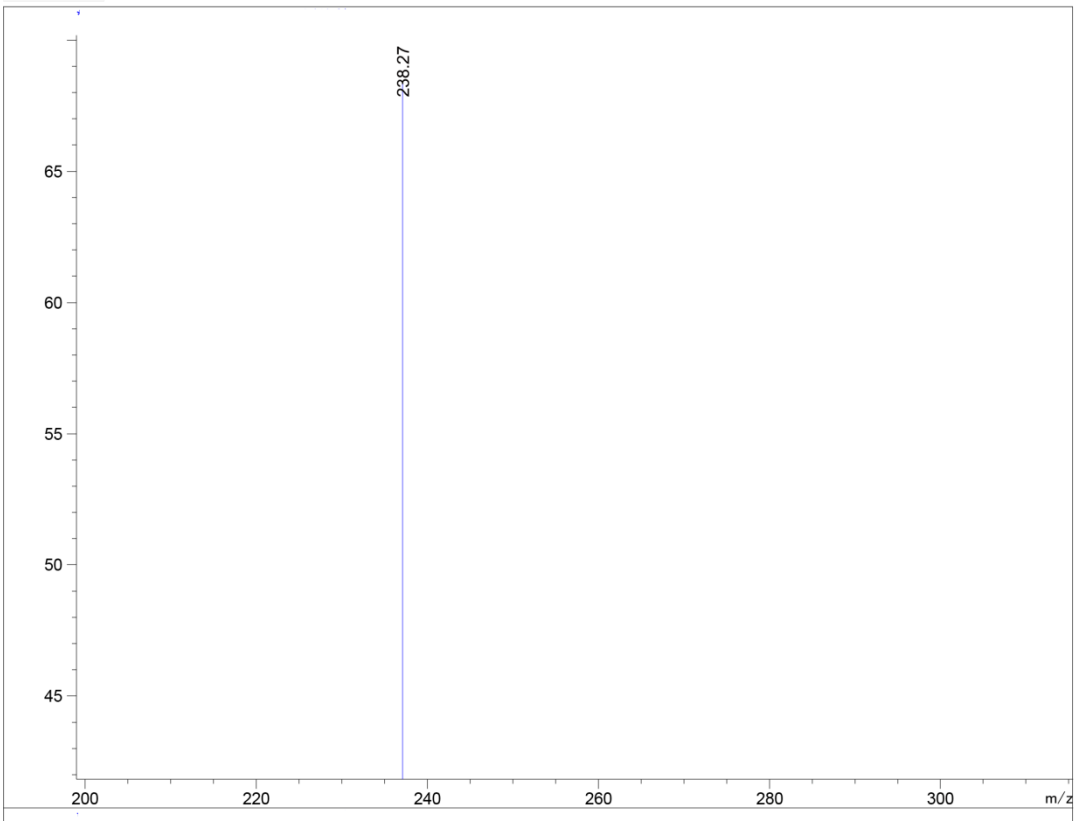
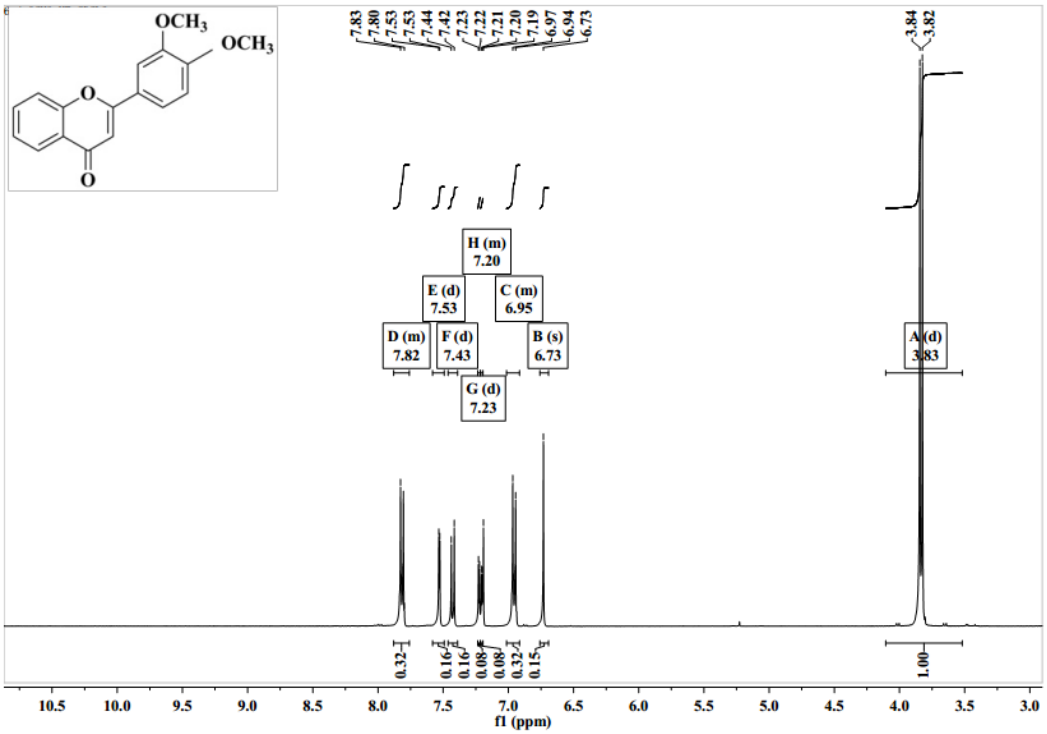
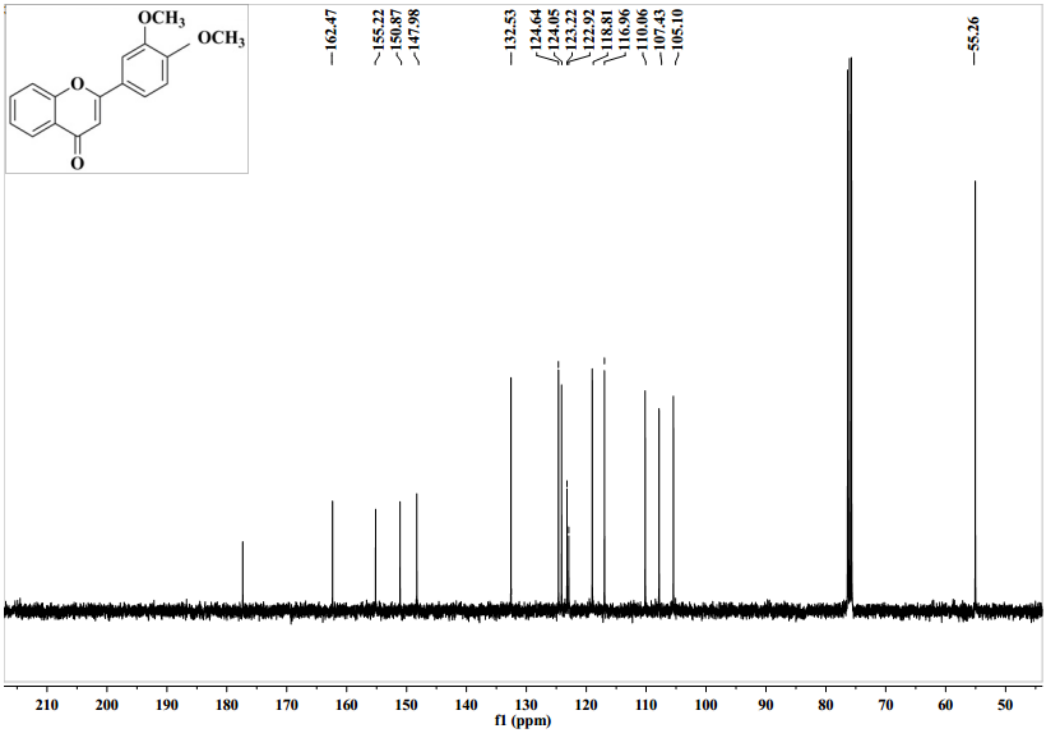


Figure S12. ^{1}H, ^{13}C NMR spectra and ESI-MS analysis for compound **5h.**


OCH3
OCH3
O
O
7.83
7.80
7.53
7.53
7.44
7.42
7.23
7.22
7.21
7.20
7.19
6.97
6.94
6.73
3.84
3.82
H (m)
7.20
E (d)
7.53
C (m)
6.95
D (m)
7.82
F (d)
7.43
B (s)
6.73
G (d)
7.23
A (d)
3.83
0.32
0.16
0.16
0.08
0.08
0.32
0.15
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
f1 (ppm)


OCH3
OCH3
O
O
162.47
155.22
150.87
147.98
132.53
124.64
124.05
123.22
122.92
118.81
116.96
110.06
107.43
105.10
55.26
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
f1 (ppm)

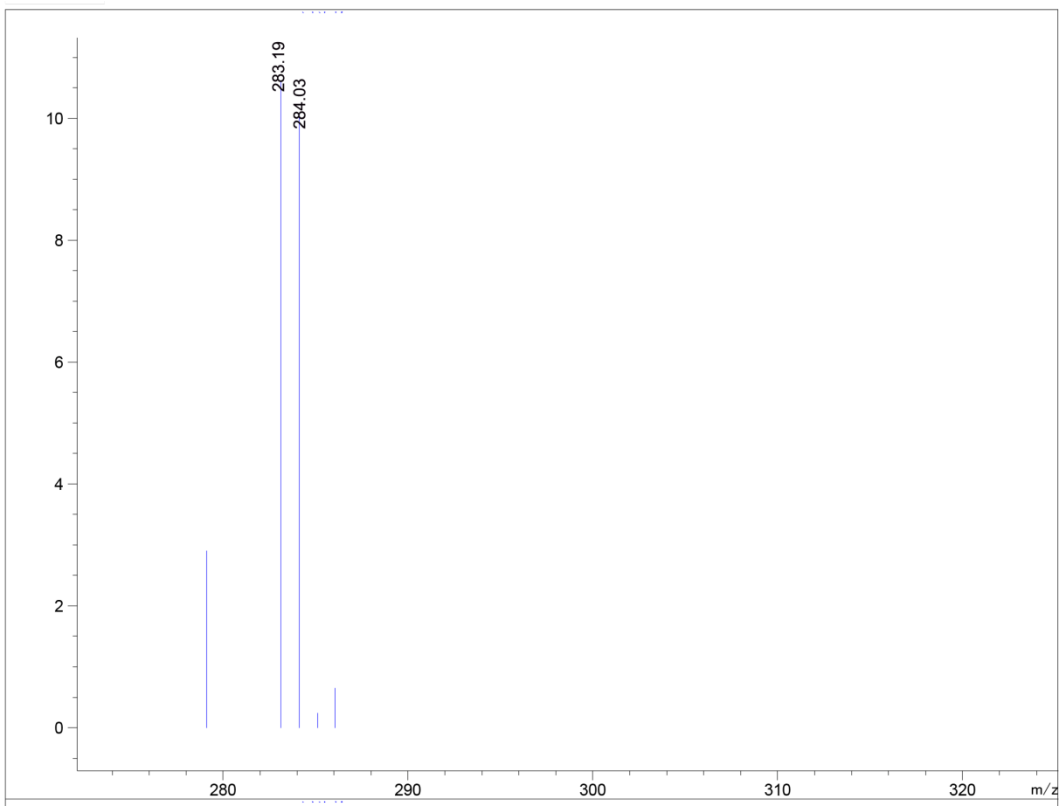
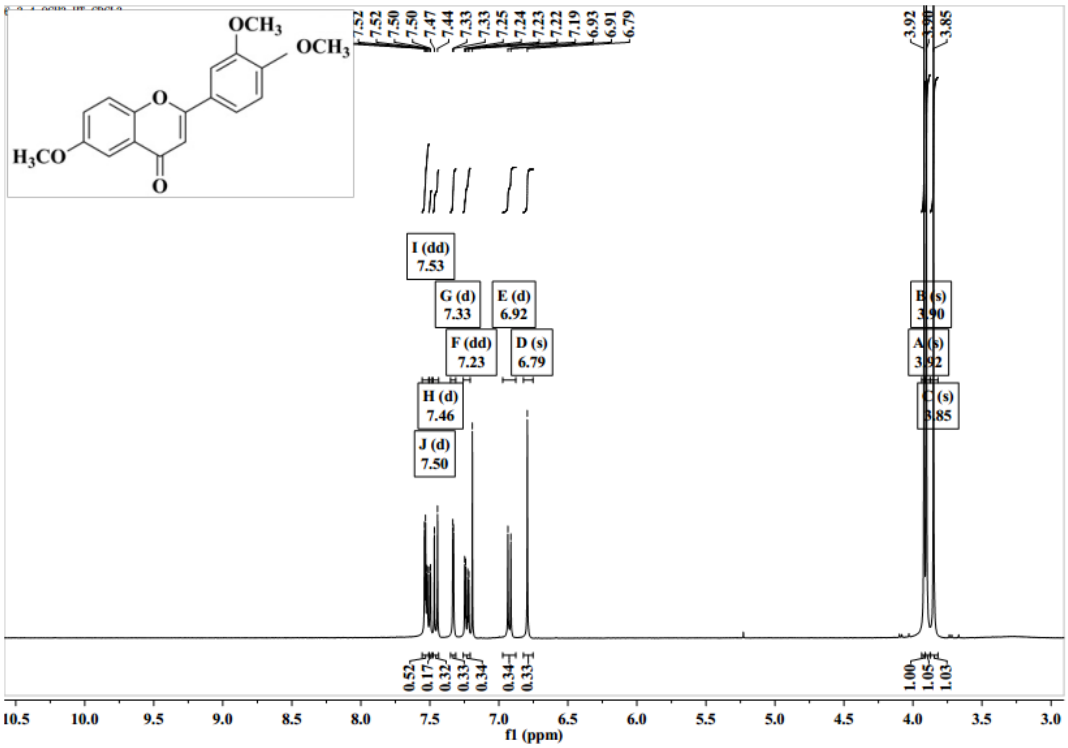
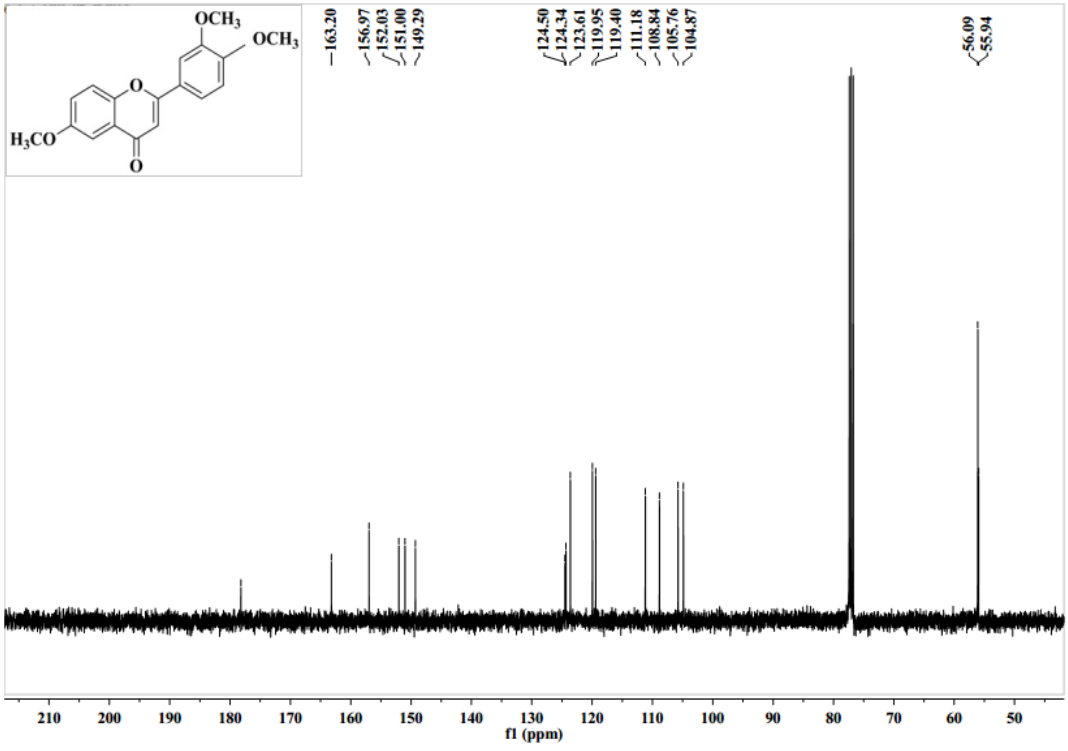


Figure S13. ^{1}H, ^{13}C NMR spectra and ESI-MS analysis for compound **5i.**


OCH3
OCH3
H3CO
O
O
I (dd) 7.53
G (d) 7.33
E (d) 6.92
F (dd) 7.23
D (s) 6.79
H (d) 7.46
J (d) 7.50
B (s) 3.90
A (s) 3.92
C (s) 3.85
fl (ppm)


OCH3
OCH3
H3CO
O
O
163.20
156.97
152.03
151.00
149.29
124.50
124.34
123.61
119.95
119.40
111.18
108.84
105.76
104.87
56.09
55.94
fl (ppm)

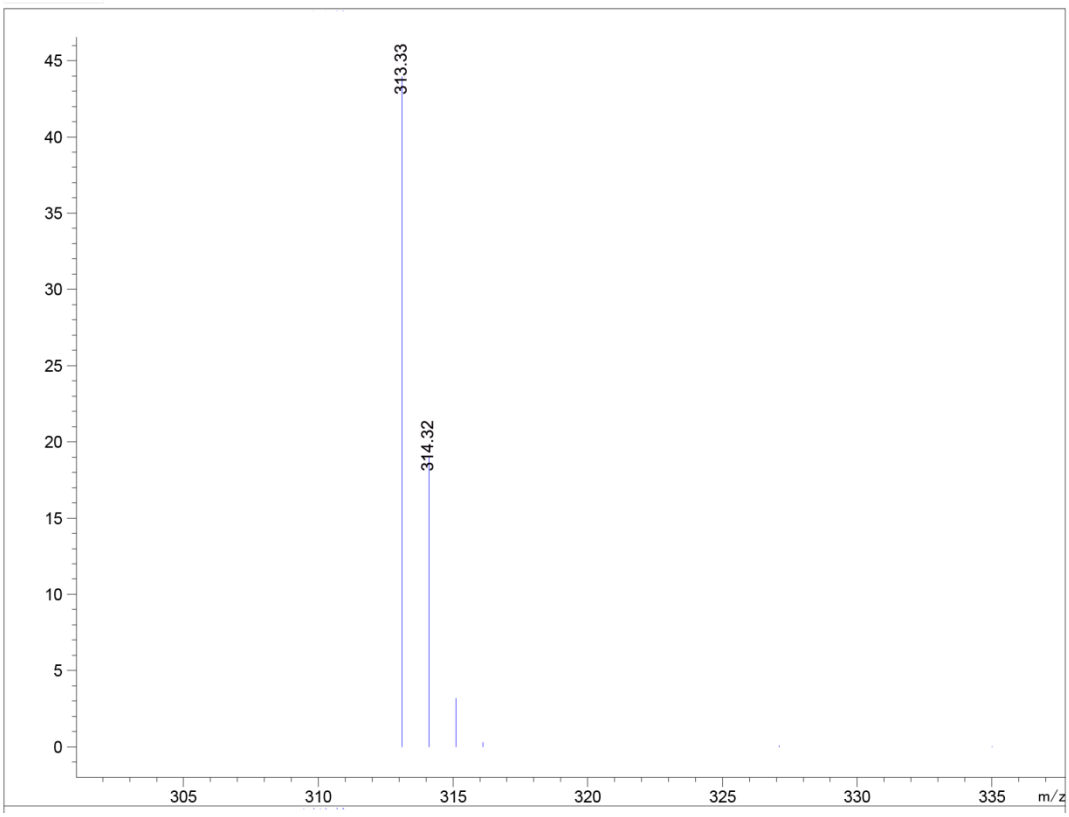


Figure S14. ^{1}H, ^{13}C NMR spectra and ESI-MS analysis for compound **5j.**