Supporting Information for:

Water-assisted metal-free catalyzed cyclization of 2-alkynylarylketones: a facile approach to indenones

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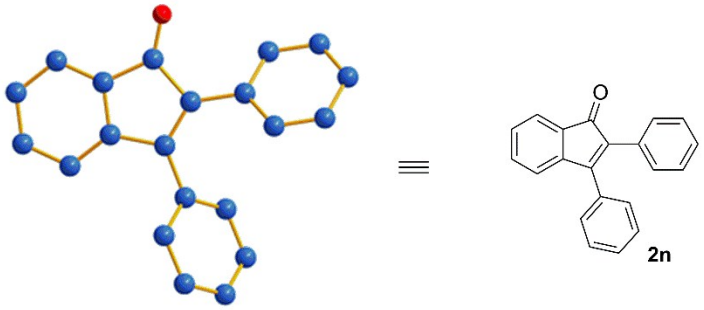
1. Crystallography of 2n

Single crystals of complex **2n** suitable for X-ray structural analysis were obtained from a CH_3CN/hexane solution. Diffraction datas were collected at 296 K ona Bruker SMART-CCD diffractometer using graphite-monochromated Mo Kα radiation (λ= 0.71073 Å). The structures were solved by direct method sand refined by full-matrix least squares on F^2. All nonhydrogenatoms were refined anisotropically, and the hydrogen atoms were included in idealized positions. All calculations were performed using the SHELXTL crystallographic software packages. CCDC-1510707 (**2n**) contain supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

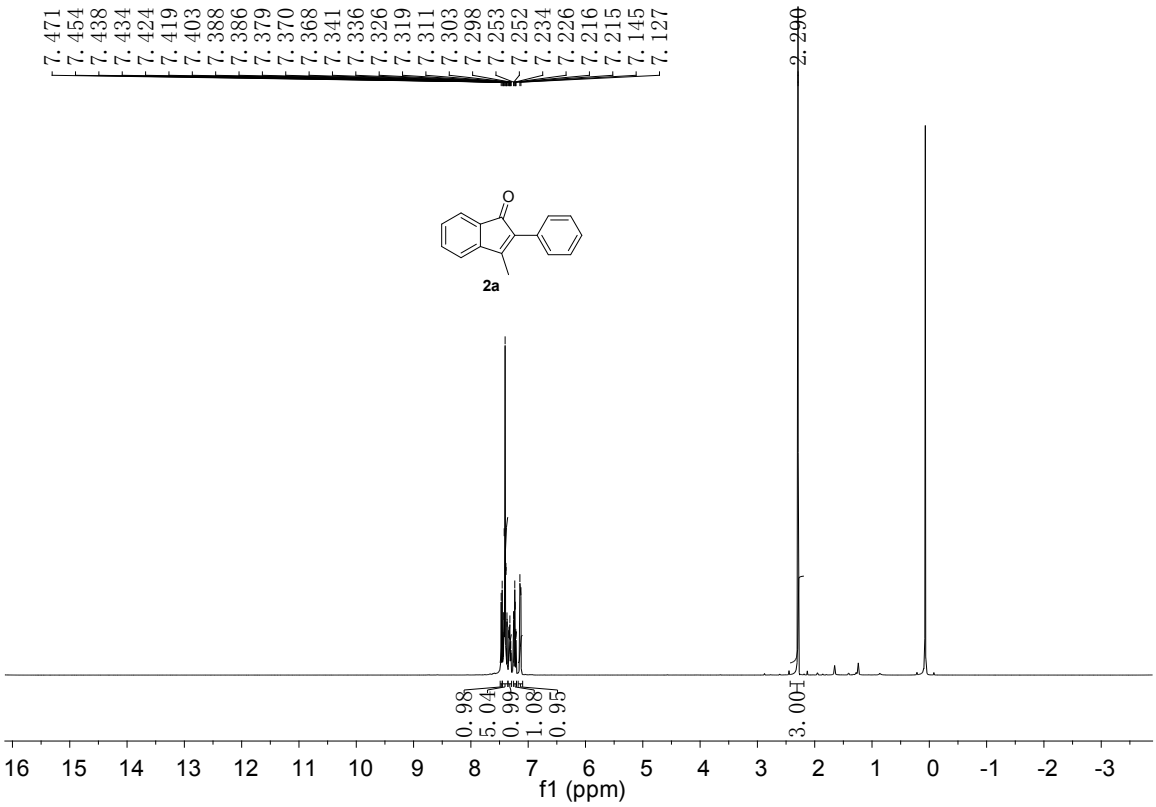


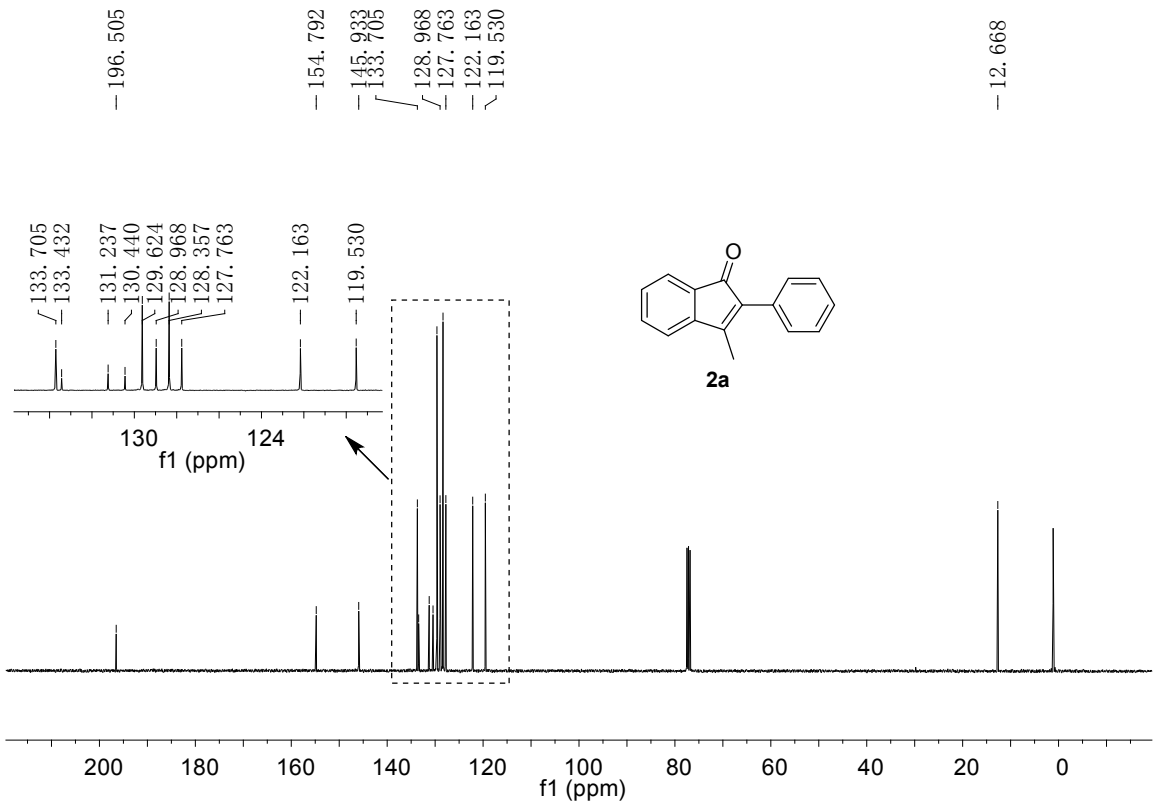
Crystal data and structural refinement details for complex **2n**

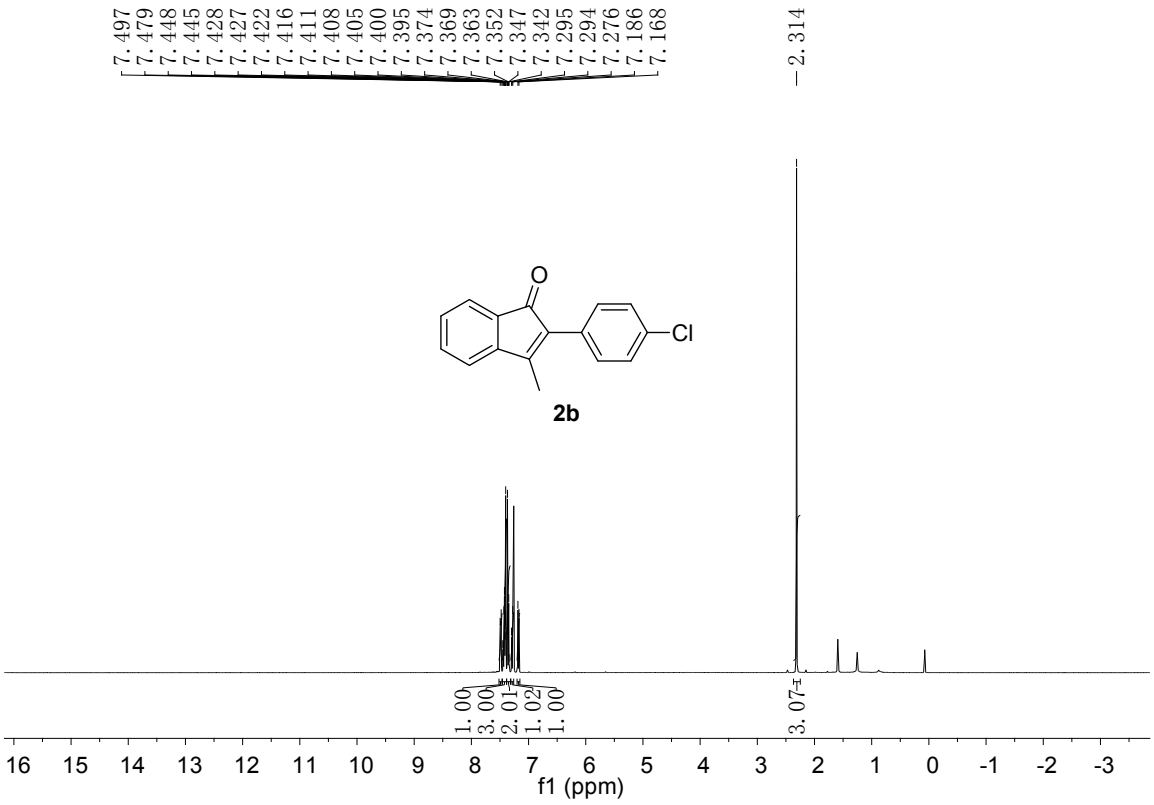
Empirical formula	C21 H14 O
Formula weight	282.32
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
space group	P2(1)/n
Unit cell dimensions	a = 9.567(5) Å α = 90 °

	b = 17.241(9) Å β = 110.813(8) °
	c = 9.945(5) Å γ = 90 °
Volume	1533.3(14) Å^3
Z	4
Calculated density	1.223 Mg/m^3
Absorption coefficient	0.074 mm^{-1}
F(000)	592
Crystal size	0.16 x 0.14 x 0.12 mm^3
Theta range for data collection	2.36 to 28.24 °
Limiting indices	-12<=h<=12, -9<=k<=22, -13<=l<=12
Reflections collected / unique	9431 / 3690 [R(int) = 0.0286]
Completeness to theta = 28.24	97.3 %
Absorption correction	Multi scan
Max. and min. transmission	1.0000 and 0.2000
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3690 / 0 / 199
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.0949
R indices (all data)	R1 = 0.0712, wR2 = 0.1089
Largest diff. peak and hole	0.131 and -0.141 e.Å^{-3}

2. ^{1}H NMR and ^{13}C NMR spectra of Products 2



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7.363
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7.347
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7.294
7.276
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Cl
2b
1.00
3.00
2.01
1.02
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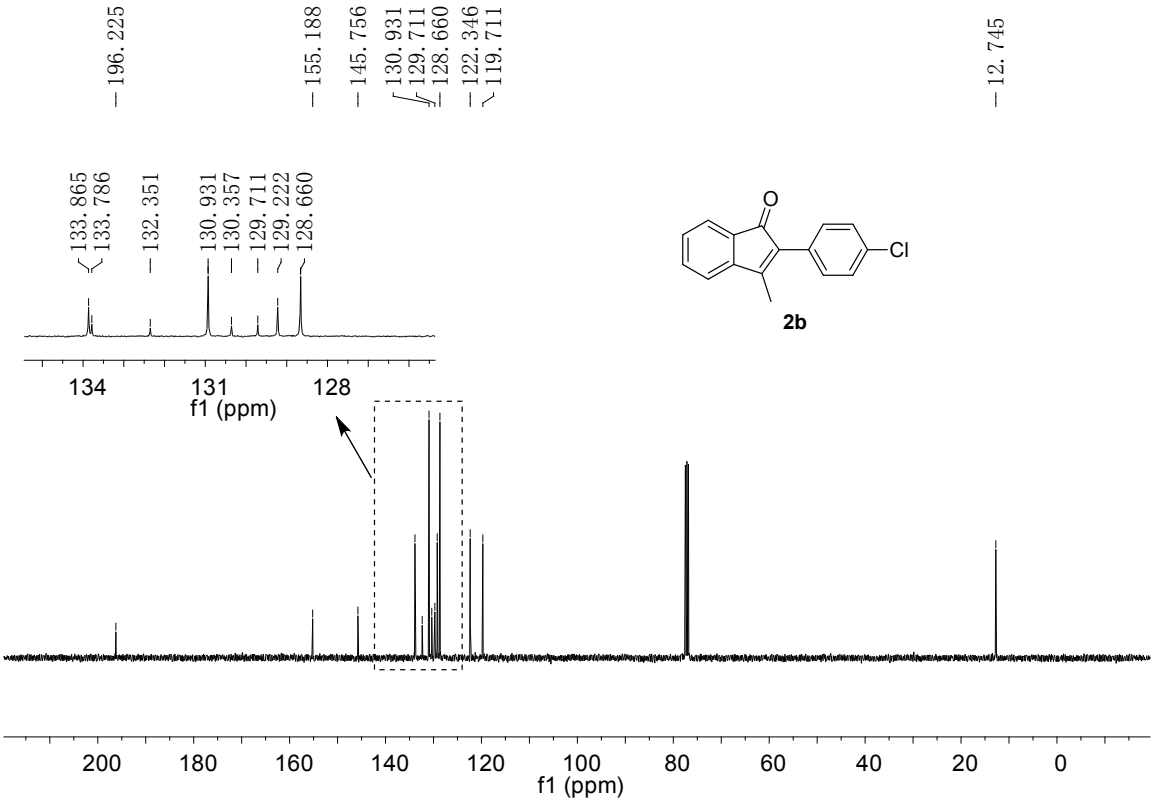
f1 (ppm)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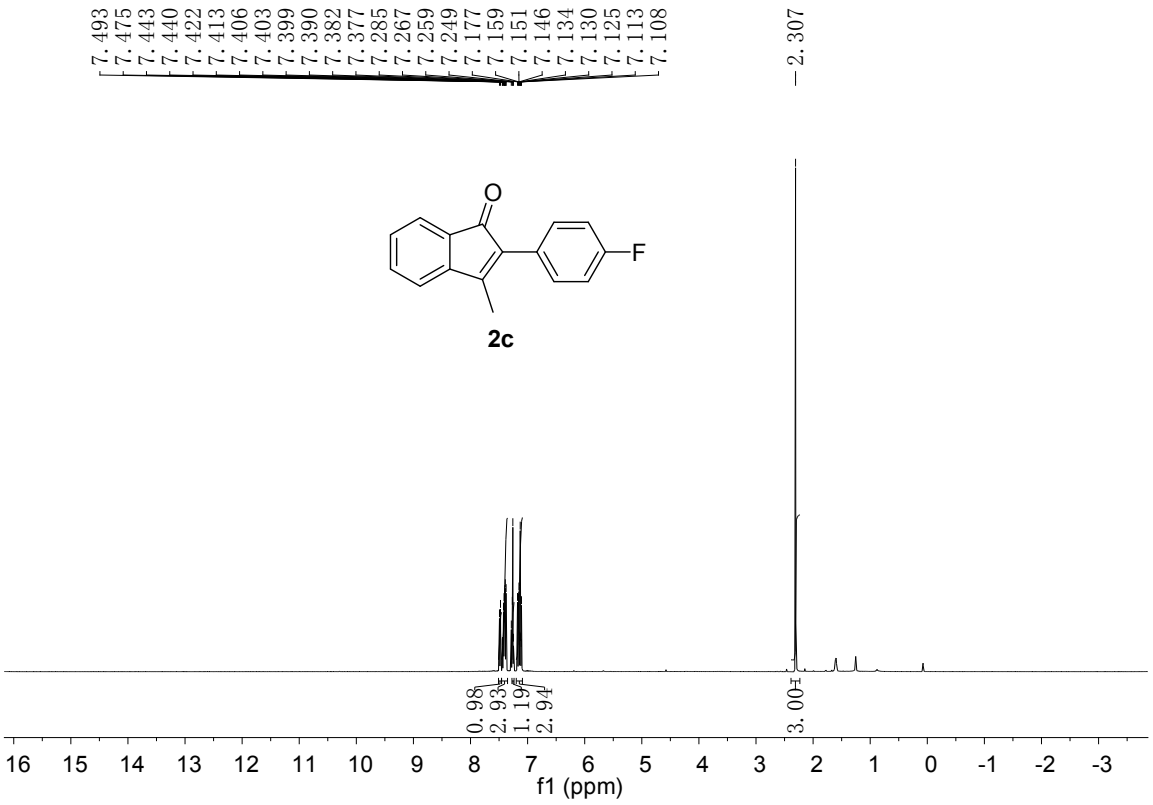
f1 (ppm)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7.259
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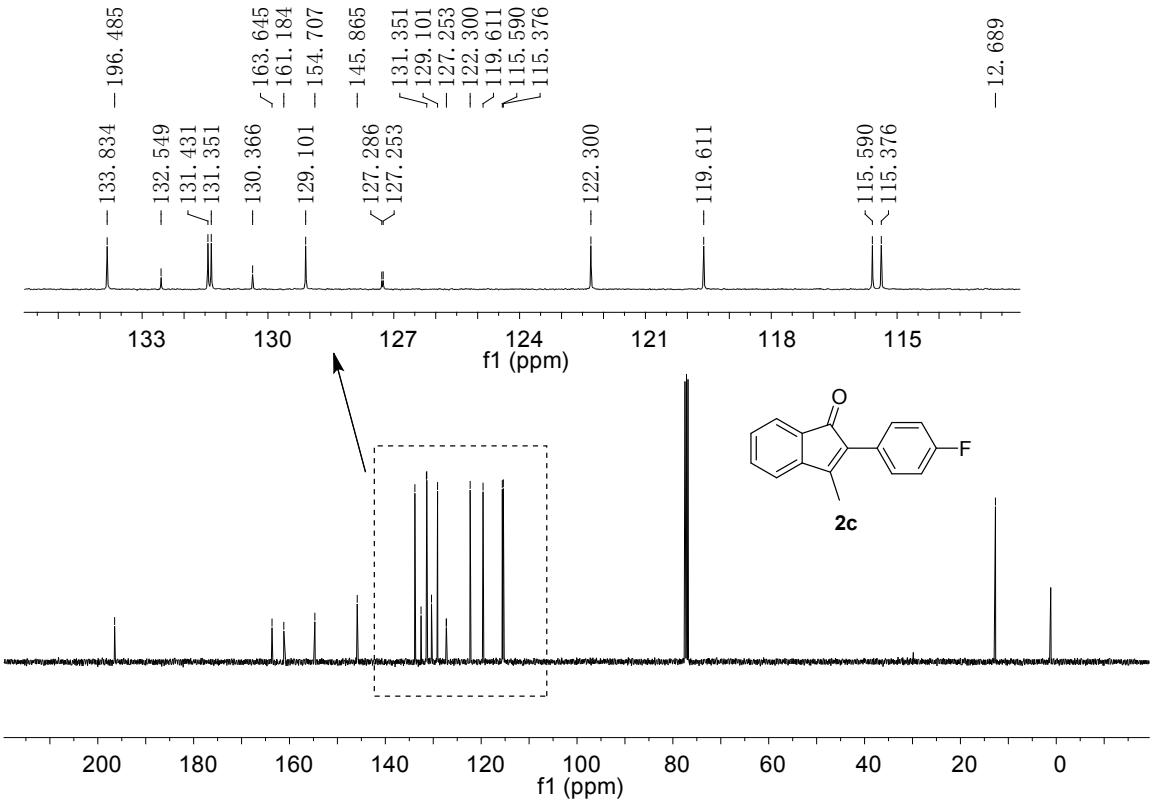
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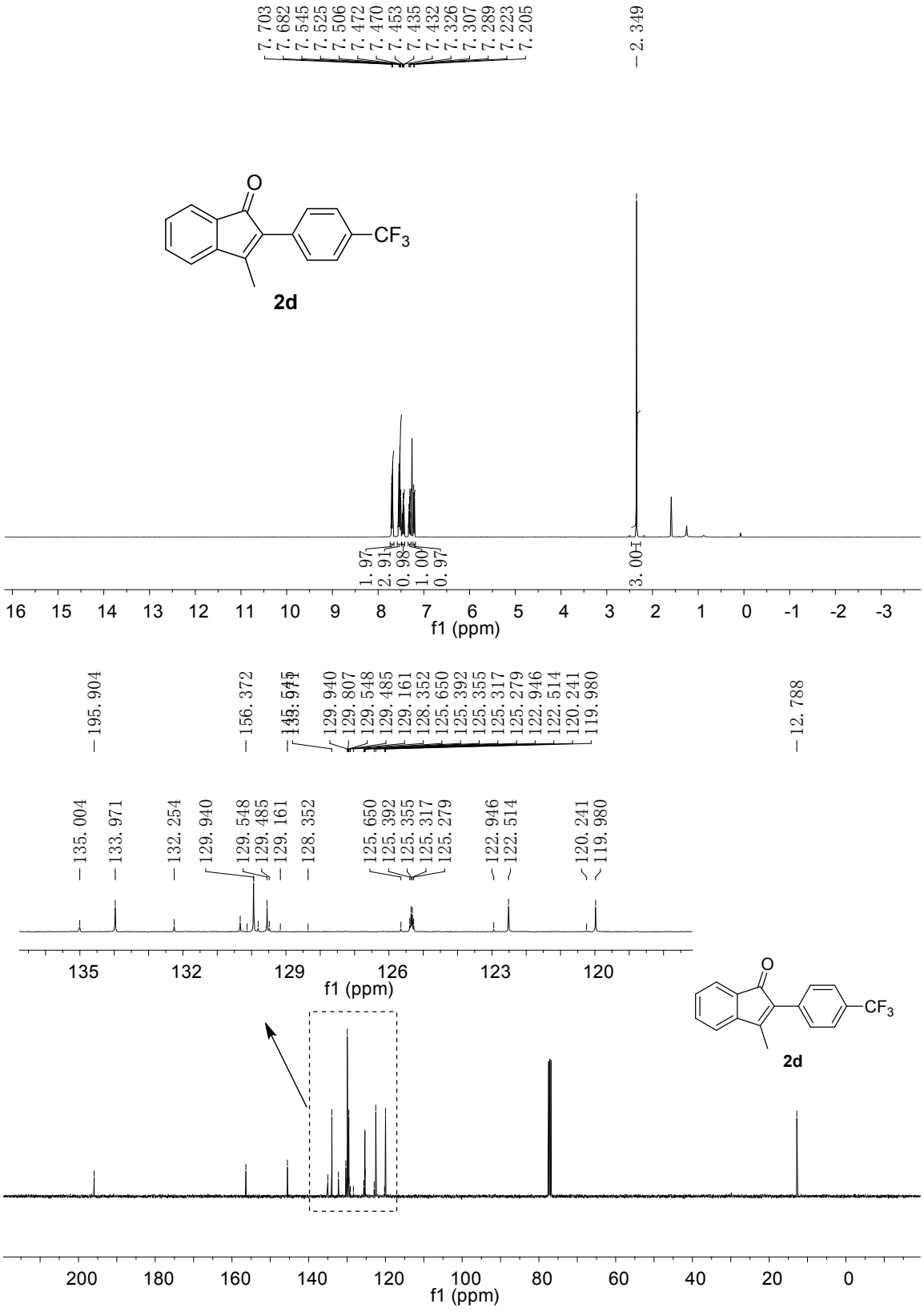
f1 (ppm)
O
F
2c
f1 (ppm)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7.205
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O
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0.97
3.00
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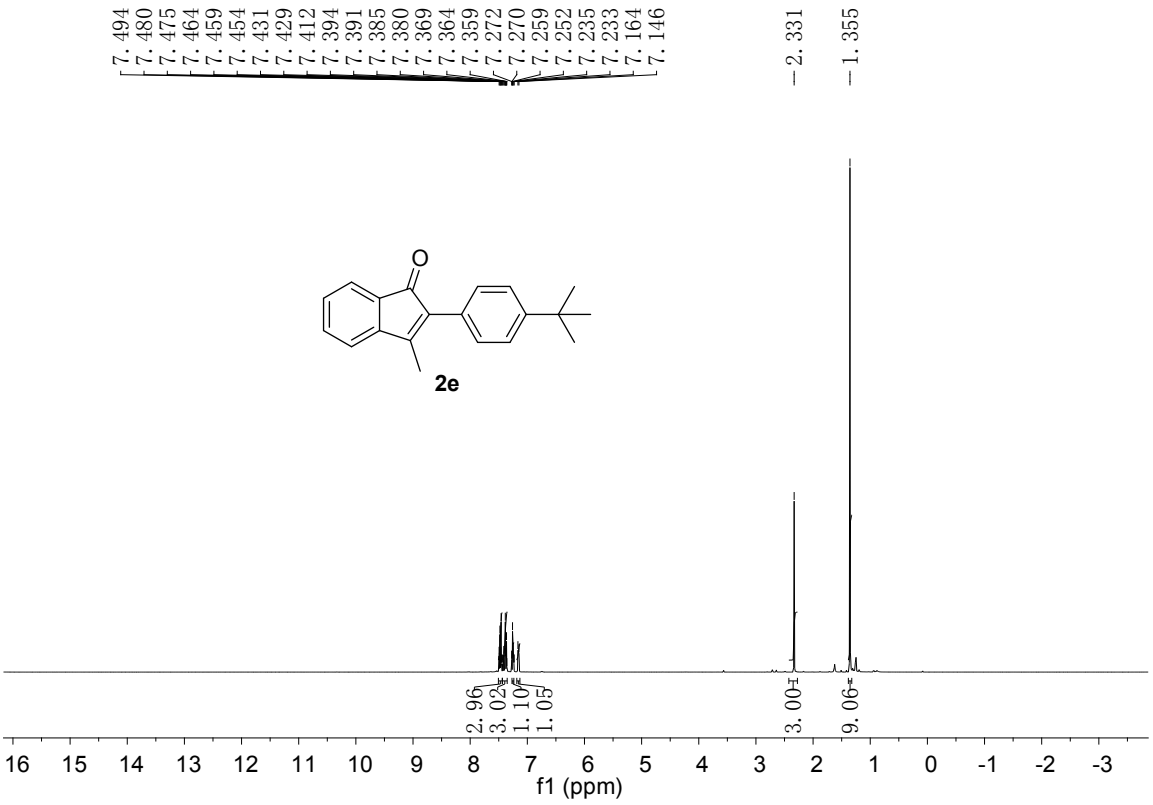
2d
f1 (ppm)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7.270
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7.233
7.164
7.146
2.331
1.355
O
2e
2.96
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1.05
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9.06
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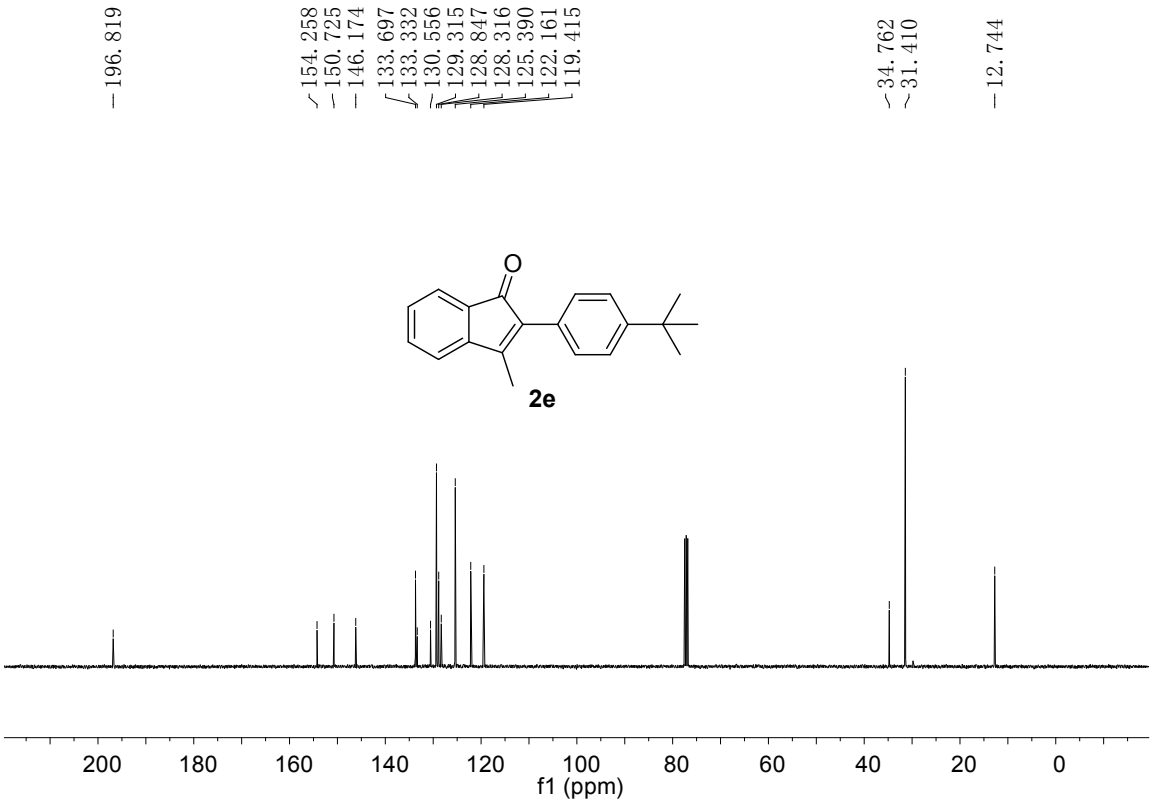
f1 (ppm)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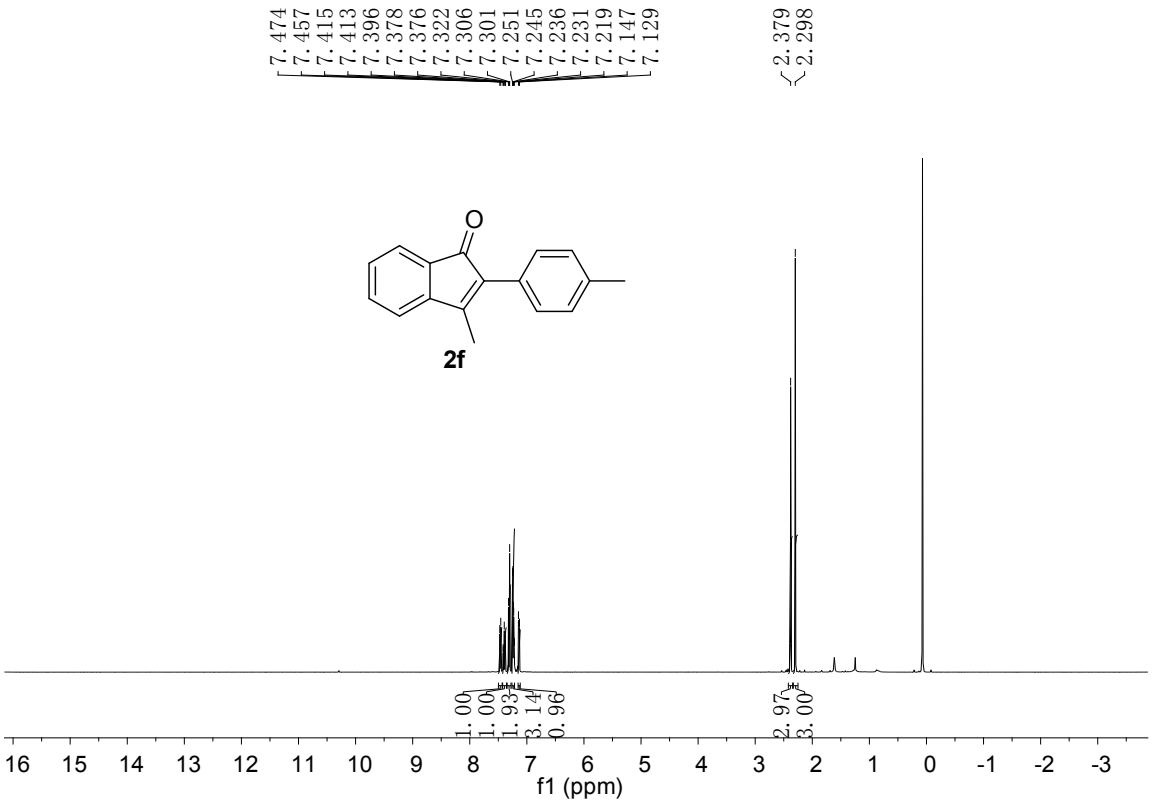
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7.231
7.219
7.147
7.129
2.379
2.298
O
2f
1.00
1.00
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0.96
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3.00
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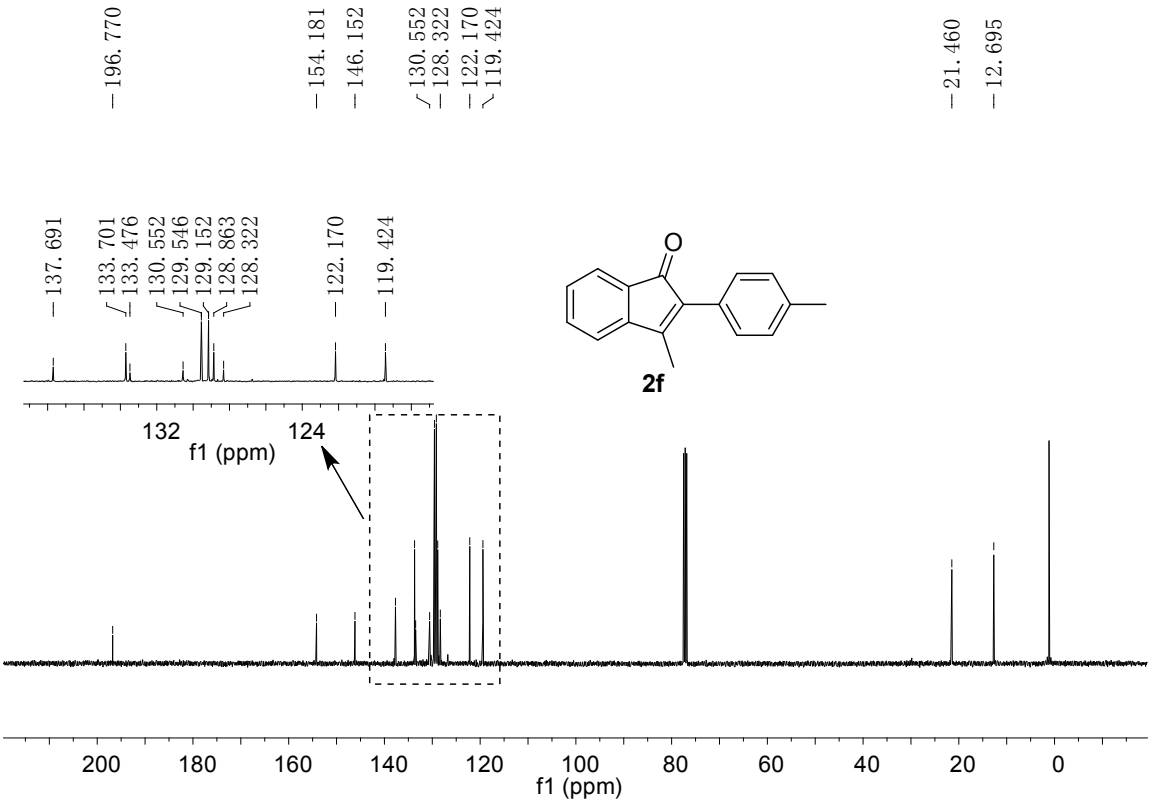
f1 (ppm)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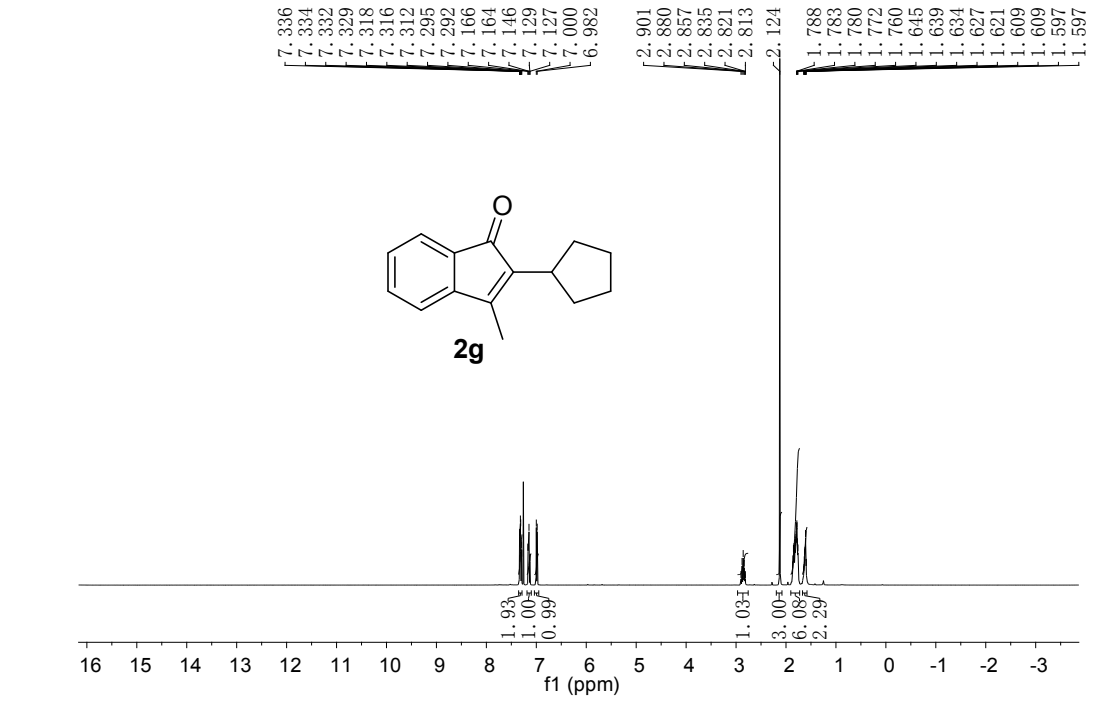
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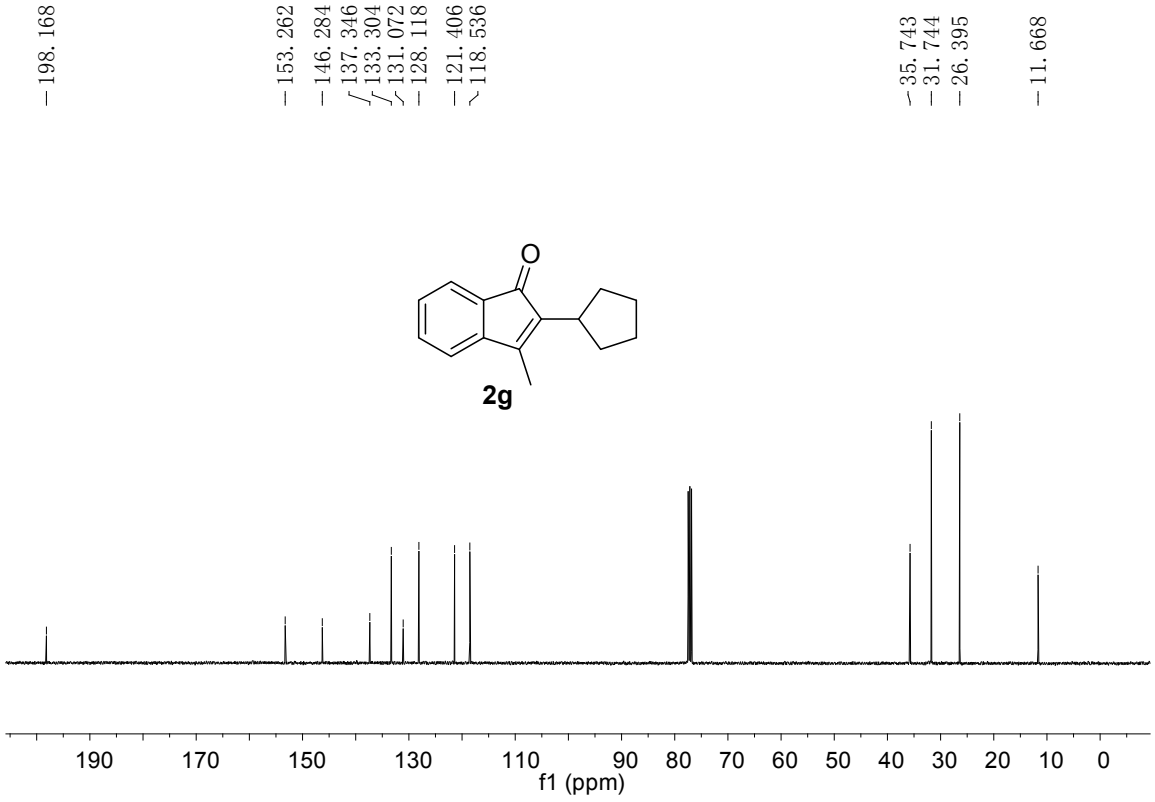
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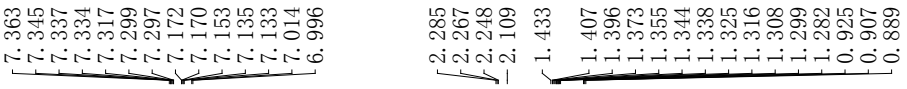
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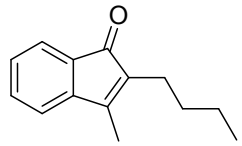
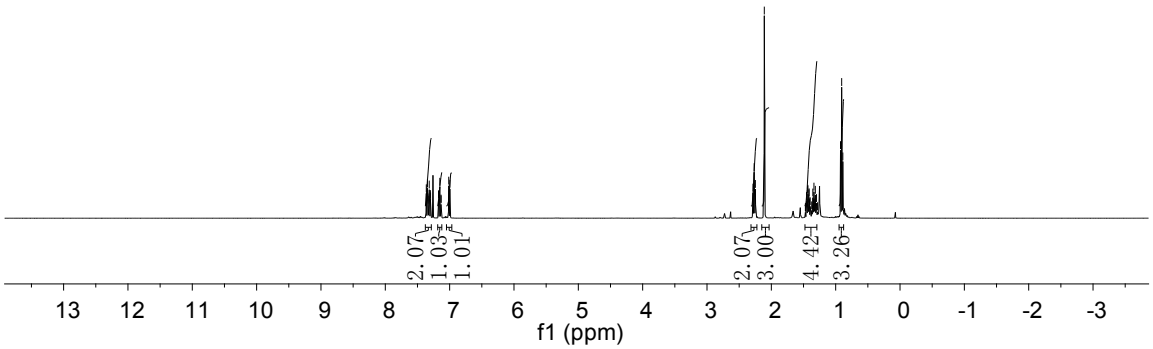

O

2h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f1 (ppm)


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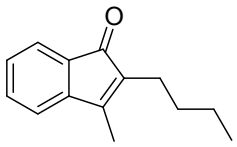
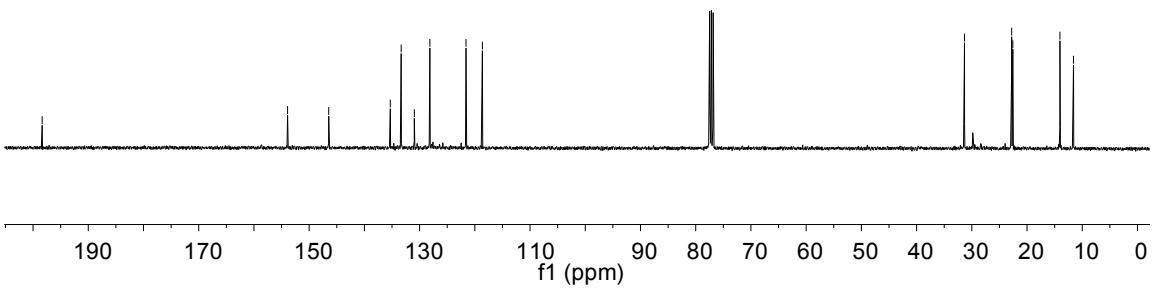
11.585


O

2h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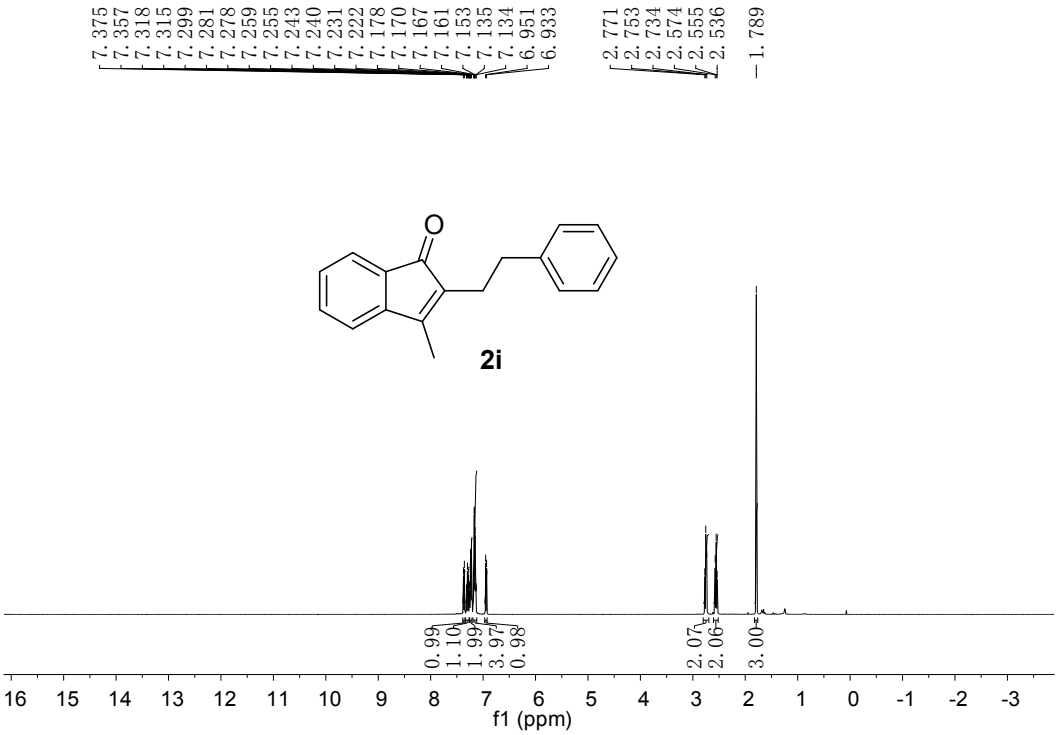
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2.734
2.574
2.555
2.536
1.789
O
2i
0.99
1.10
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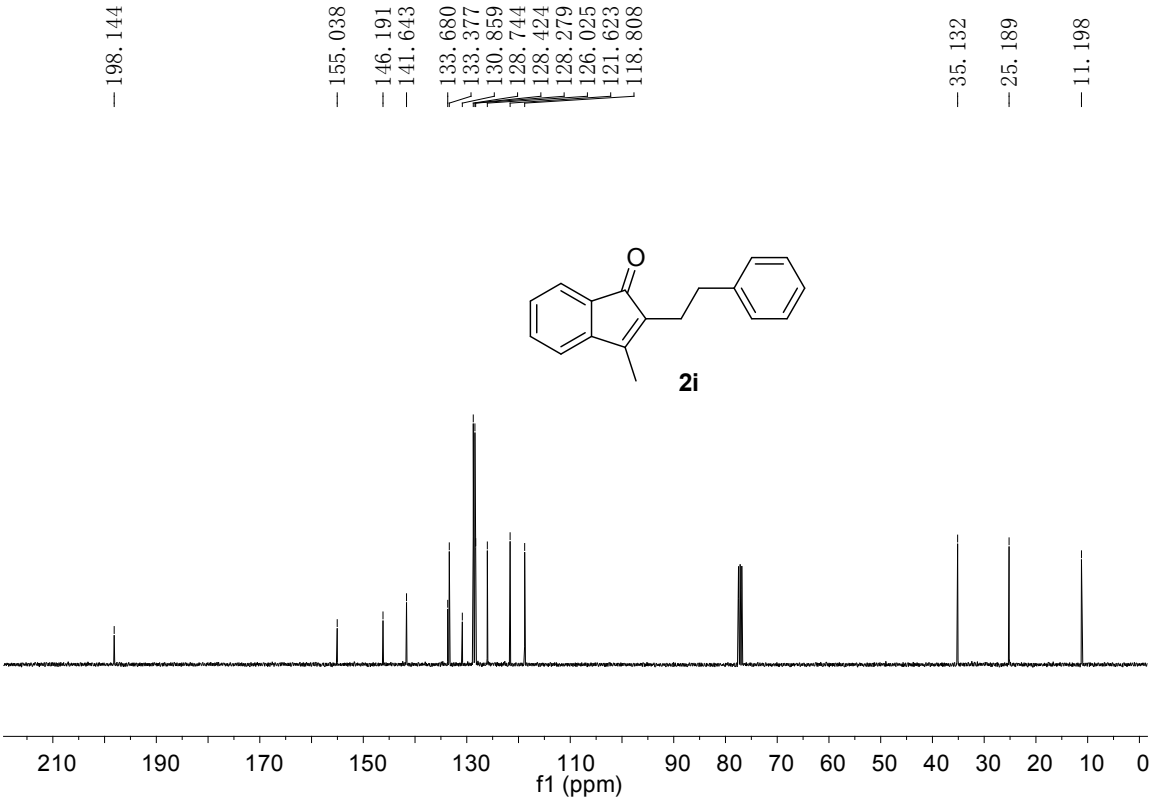
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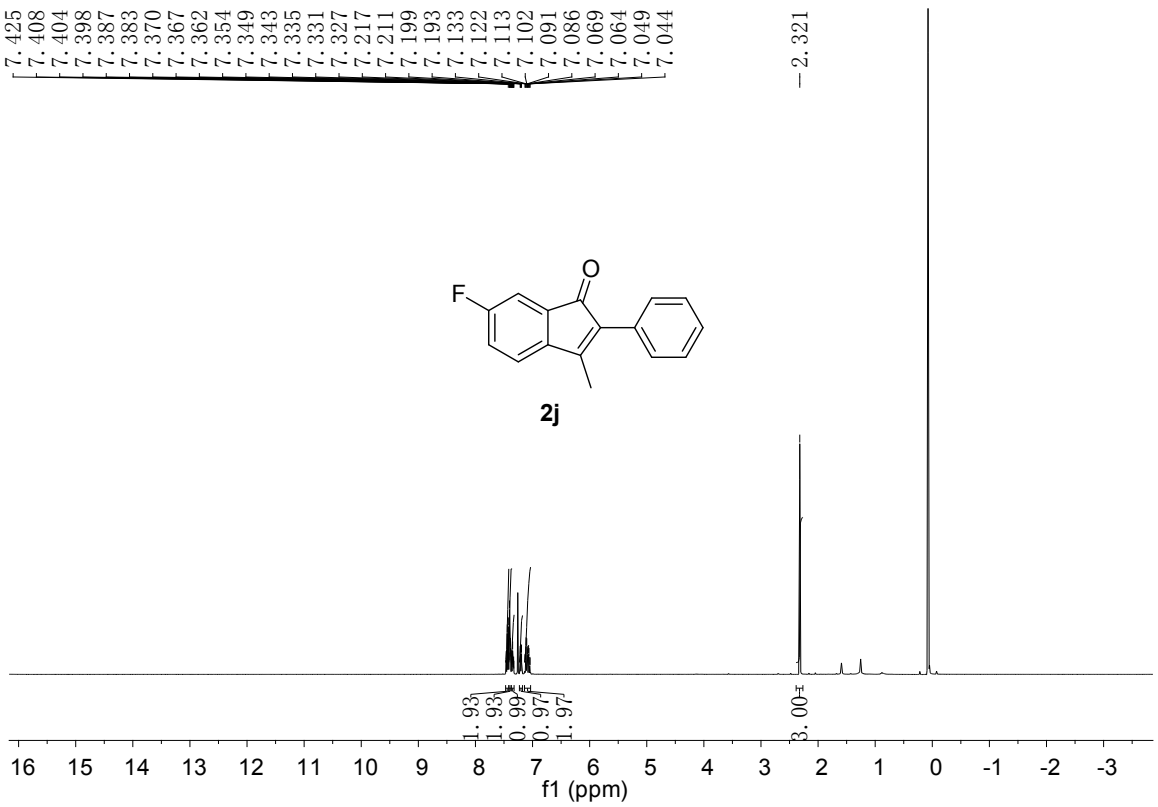
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2.321
F
O
2j
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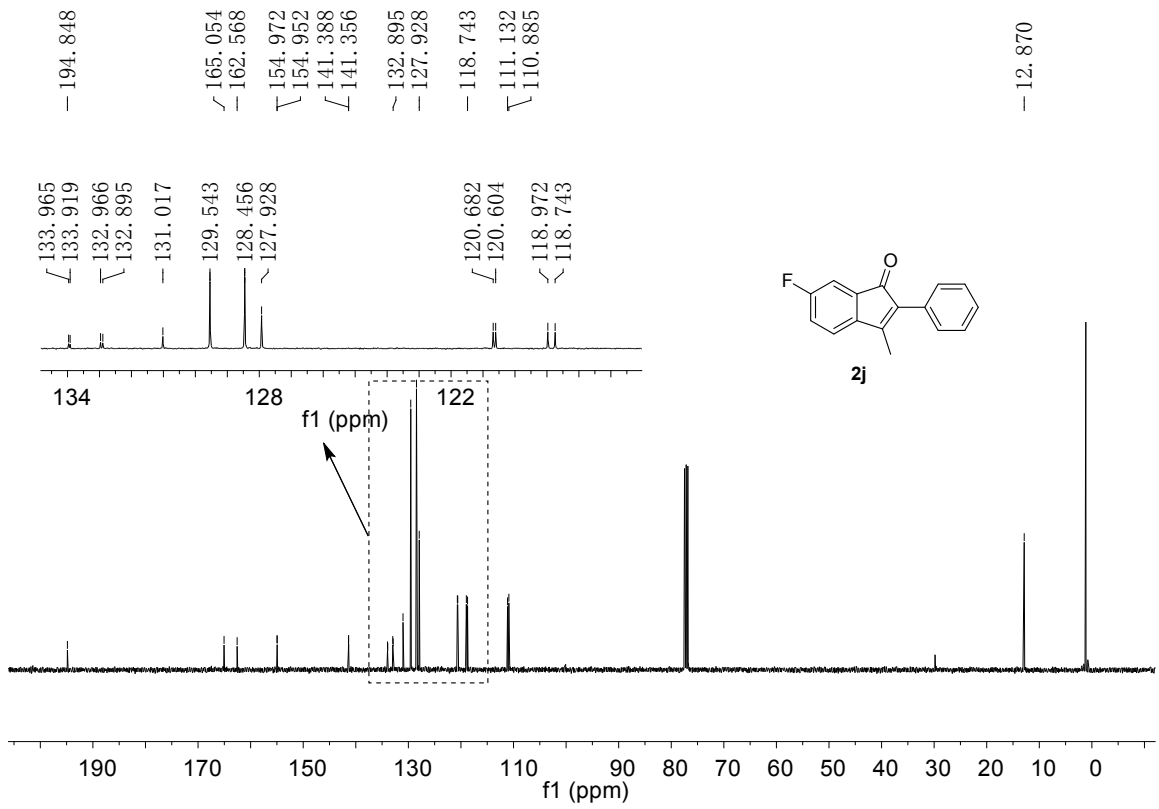
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120.604
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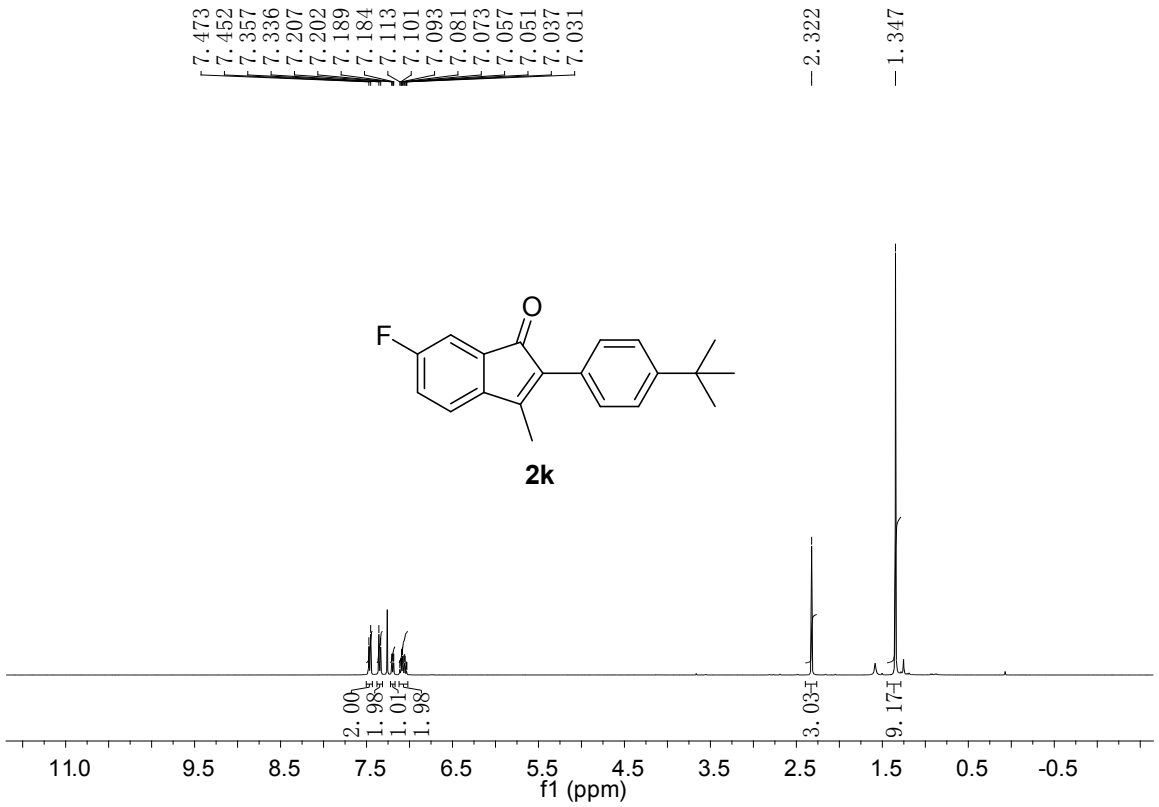
f1 (ppm)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7.057
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7.037
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O
F
2k
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1.01
1.98
3.03
9.17
11.0
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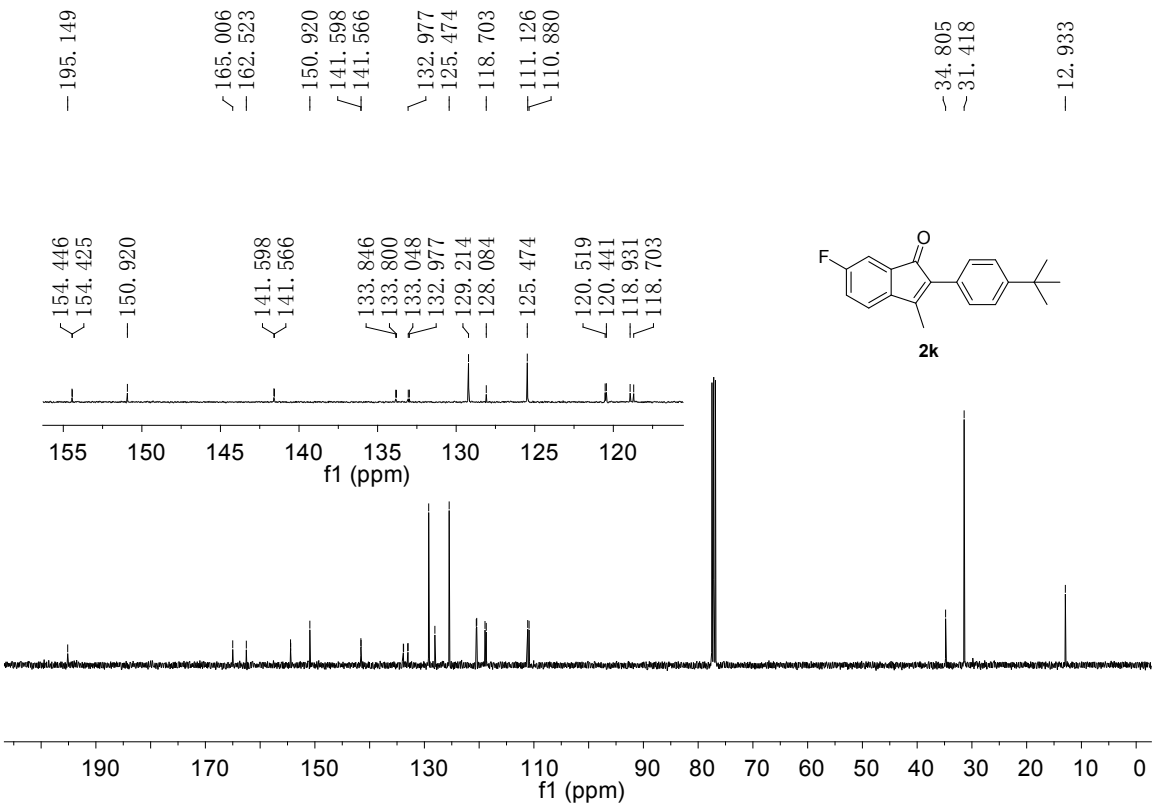
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141.598
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133.800
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129.214
128.084
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O
F
2k
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130
125
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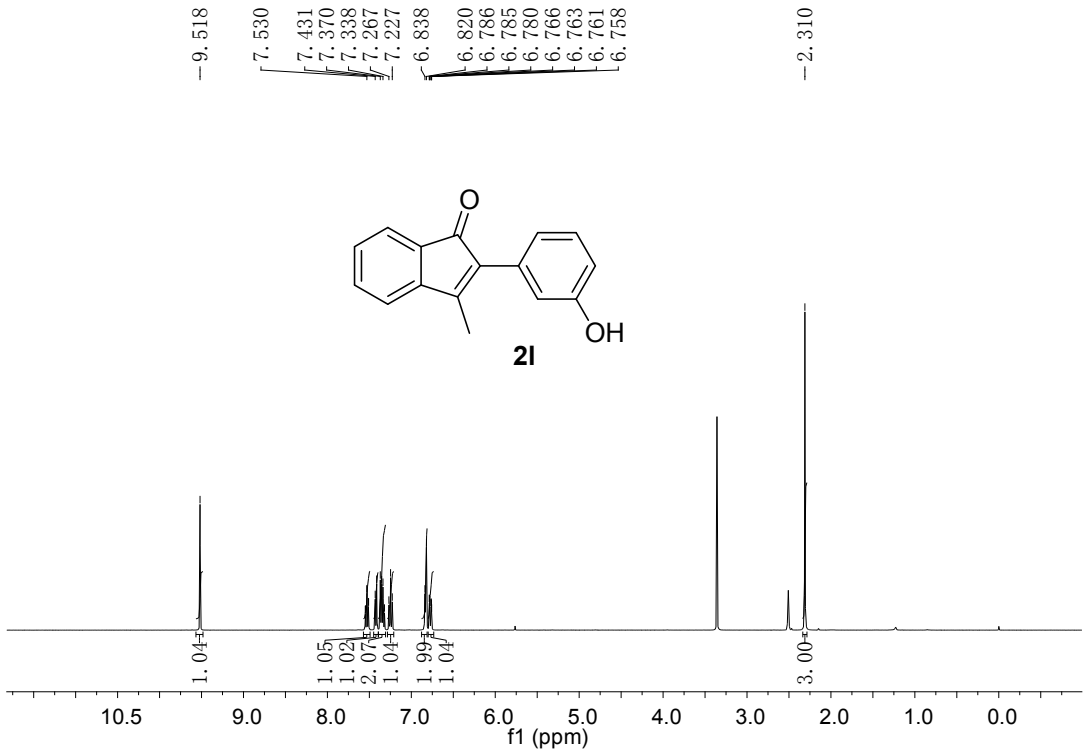
f1 (ppm)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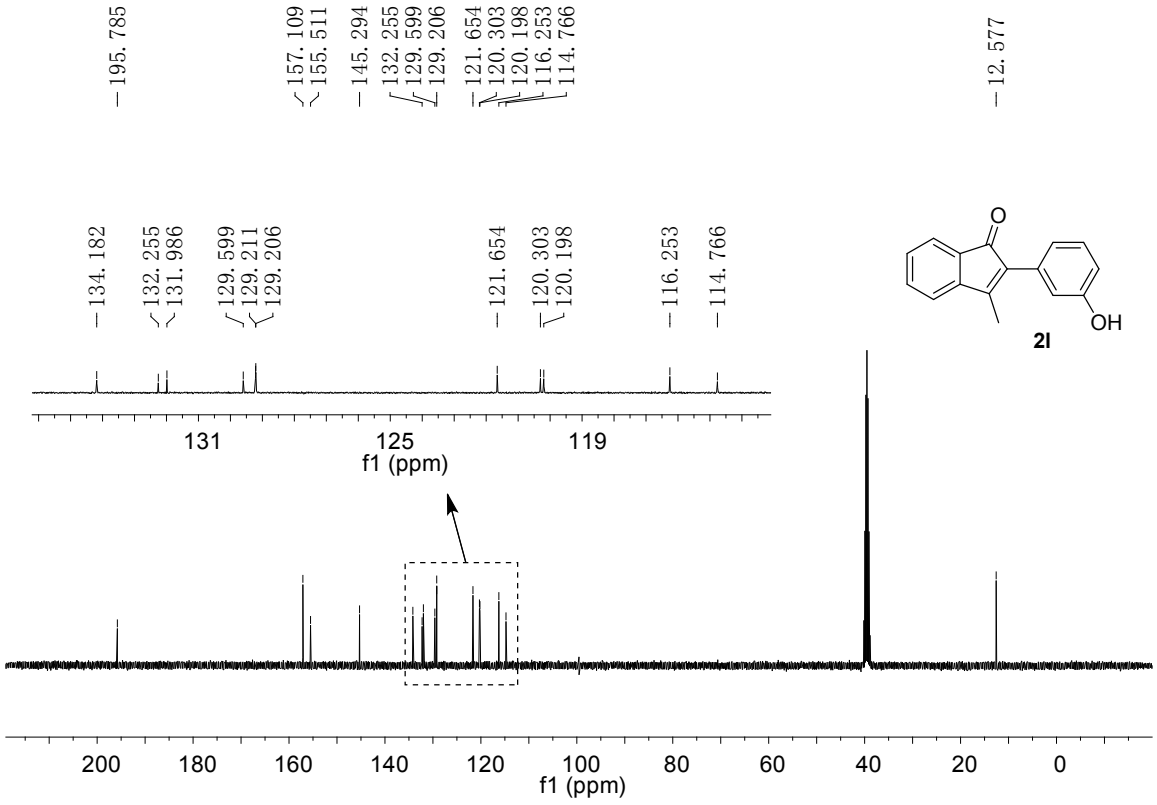
f1 (ppm)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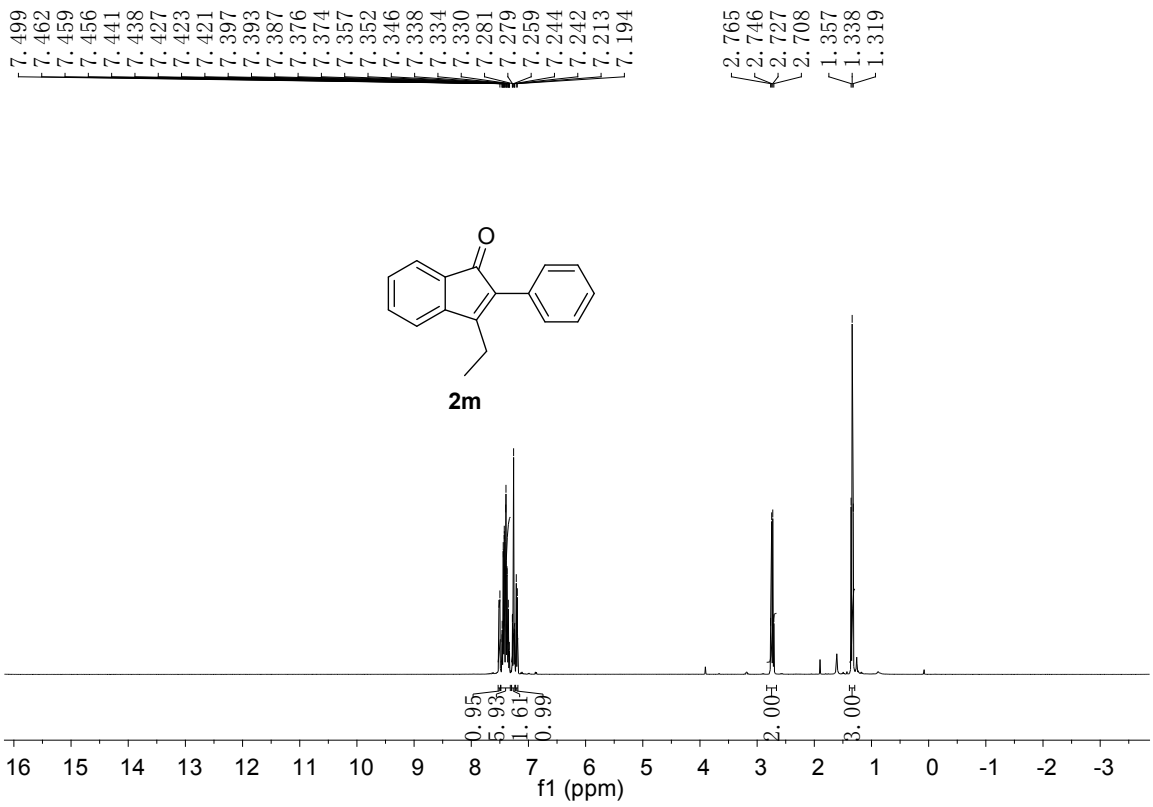
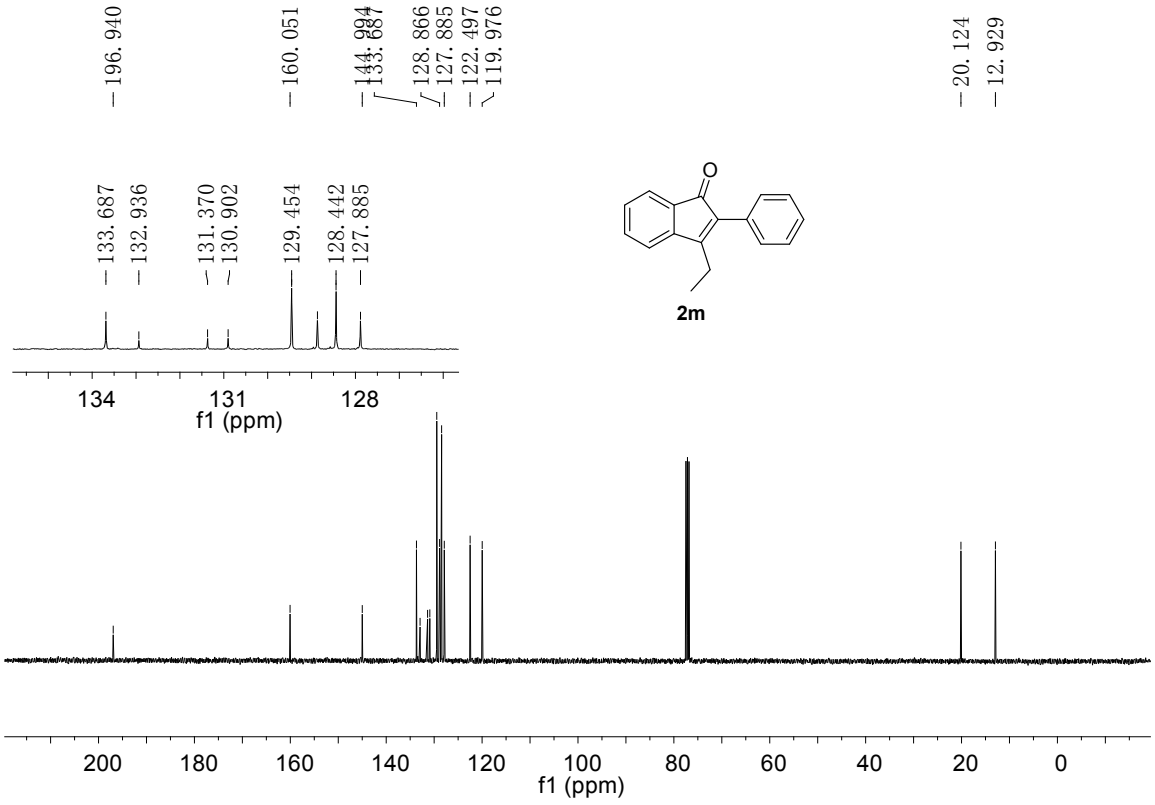
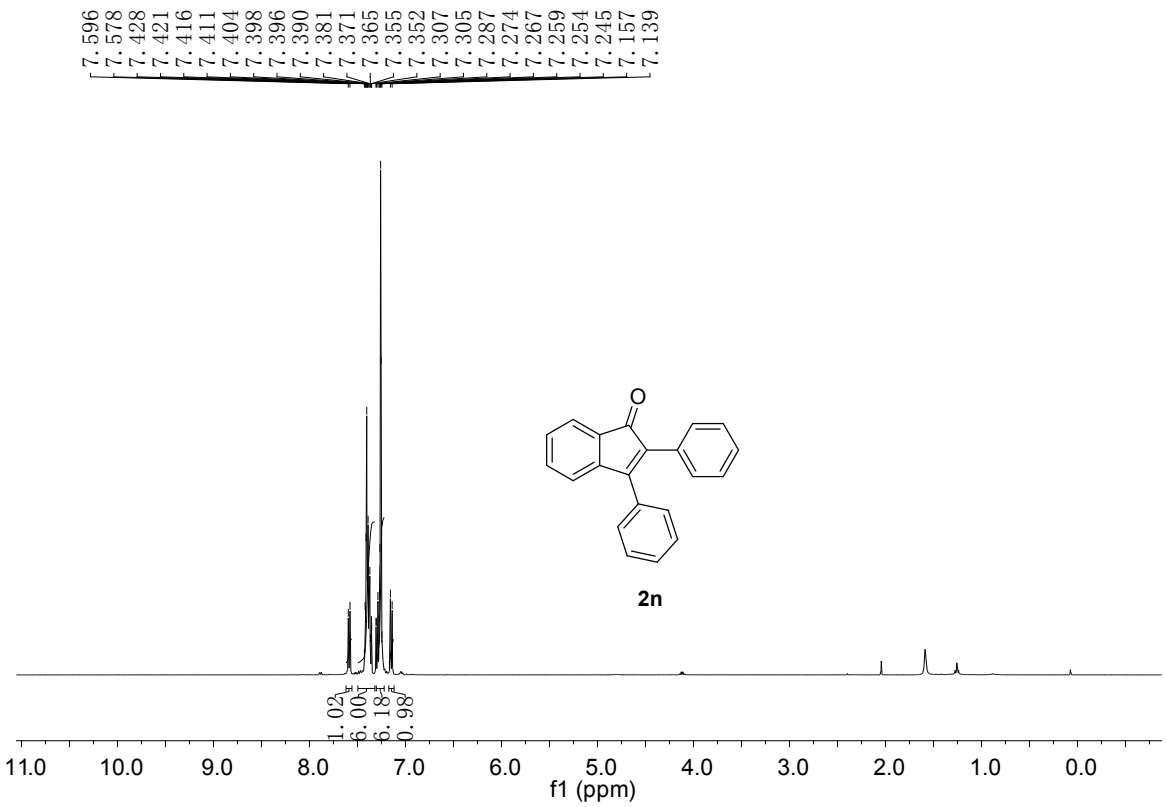
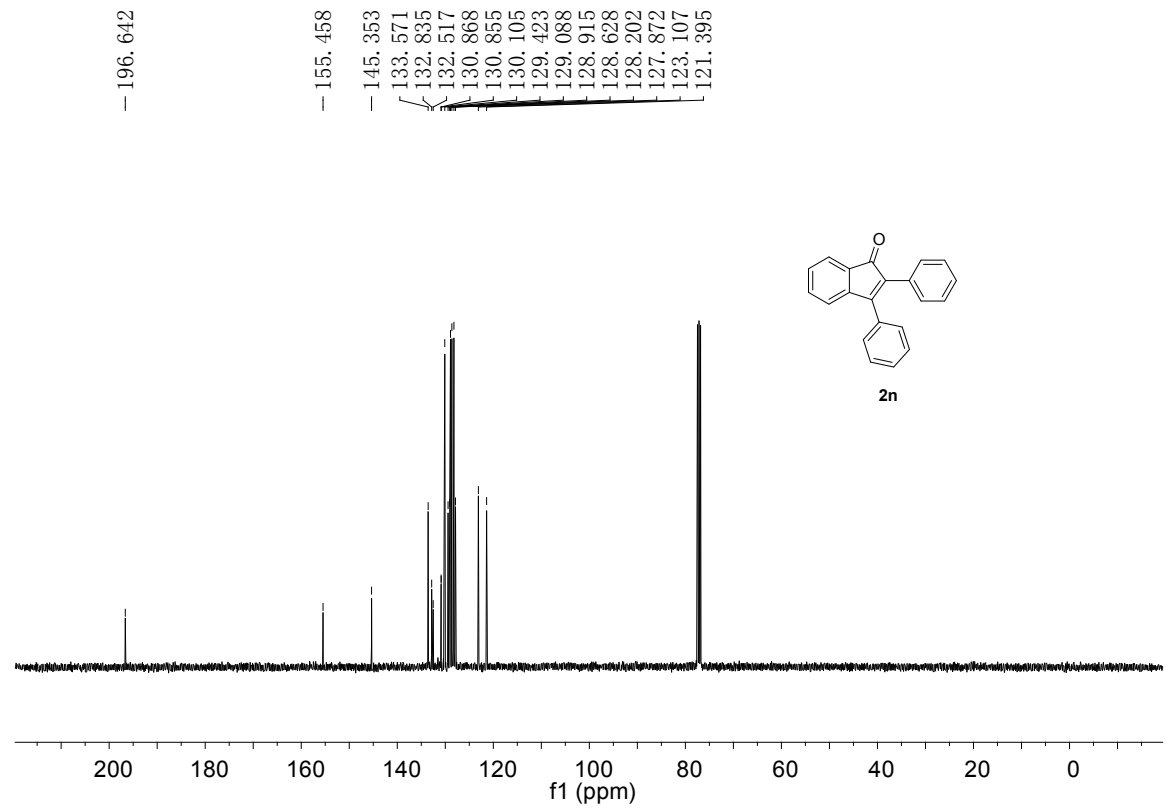
120.198
116.253
114.766
12.577
134.182
132.255
131.986
129.599
129.211
129.206
121.654
120.303
120.198
116.253
114.766
O
OH
2l
131
125
119
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


7.499
7.462
7.459
7.456
7.441
7.438
7.427
7.423
7.421
7.397
7.393
7.387
7.376
7.374
7.357
7.352
7.346
7.338
7.334
7.330
7.281
7.279
7.259
7.244
7.242
7.213
7.194
2.765
2.746
2.727
2.708
1.357
1.338
1.319
O
2m
0.95
5.93
1.61
0.99
2.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


196.940
160.051
144.994
133.687
128.866
127.885
122.497
119.976
20.124
12.929
133.687
132.936
131.370
130.902
129.454
128.442
127.885
O
2m
134
131
128
f1 (ppm)
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)


7.596
7.578
7.428
7.421
7.416
7.411
7.404
7.398
7.396
7.390
7.381
7.371
7.365
7.355
7.352
7.307
7.305
7.287
7.274
7.267
7.259
7.254
7.245
7.157
7.139
O
2n
1.02
6.00
6.18
0.98
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


196.642
155.458
145.353
133.571
132.835
132.517
130.868
130.855
130.105
129.423
129.088
128.915
128.628
128.202
127.872
123.107
121.395
O
2n
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

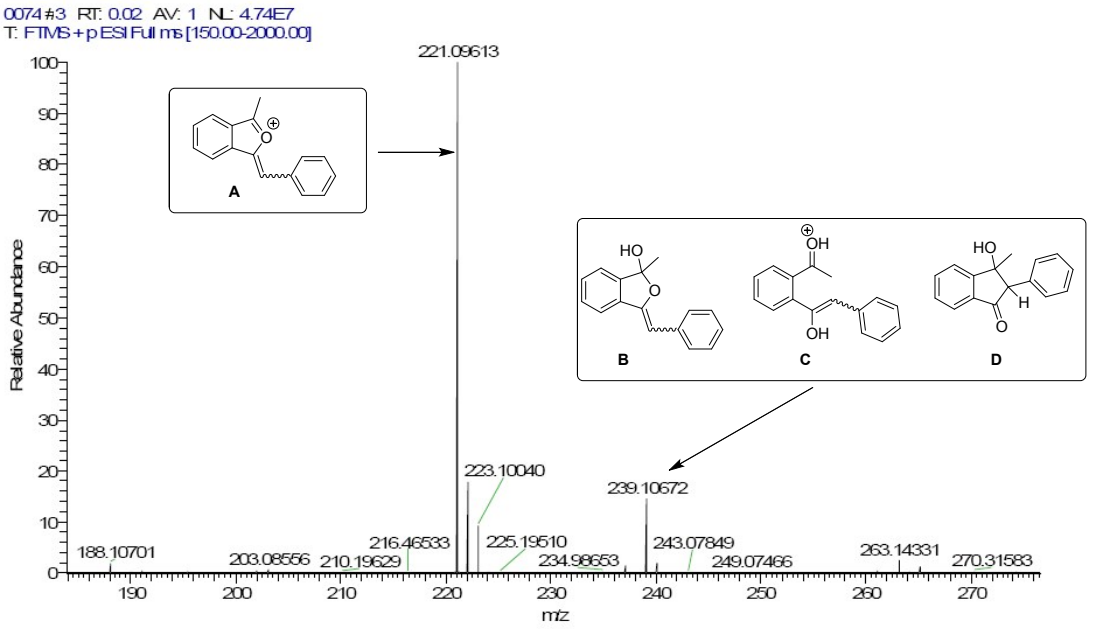


Figure S1. ESI-HRMS detection of the reaction mixture using **1a** as substrate with 1h under the standard conditions.