Atom-Economical Chemoselective Synthesis of Furocoumarins *via* Cascade Palladium Catalyzed Oxidative Alkoxylation of 4-Oxohydrocoumarins and Alkenes

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General Procedures.

Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Column chromatography was performed on silica gel (300−400 mesh). NMR spectra were obtained using a Bruker Avance 500 spectrometer (^{1}H at 500 MHz, and ^{13}C at 125 MHz). Chemical shifts for ^{1}H NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 7.26 ppm). Chemical shifts for ^{13}C NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent as the internal standard ($CDCl_3$: δ 77.0 ppm).

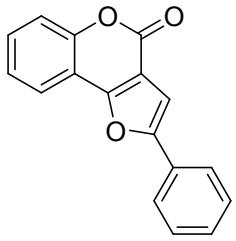
Materials. Unless stated otherwise, commercial reagents were used without further purification. All reagents were weighed and handled in air at room temperature.

Experimental Section

The mixture of 4-hydroxycoumarin **1** (0.5 mmol), alkenes **2** (0.5 mmol) and $Pd(CF_3COO)_2$ (0.1 mmol) in PhCl (2 mL) was stirred at 90 ^{o}C for 4 h. The progress of the reaction was monitored by thin-layer chromatography. Upon completion, the mixture was then cooled and evaporated under reduced pressure. The target product **3** was purified by flash chromatography on silica gel using a mixture of ethyl acetate and petroleum ether.

Characterization Data

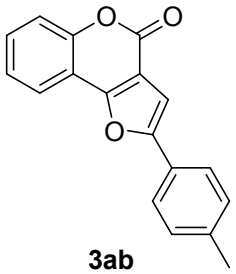
2-Phenyl-furo[3,2-c]coumarin (3aa)



3aa

White solid, m.p. 176-178 °C. **FTIR** (KBr) w: 3066, 2923, 2855, 1707, 1639, 1566, 1499, 898, 753. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.97-7-95 (m, 1H), 7.82-7.80 (m, 2H), 7.54-7.51 (m, 1H), 7.49-7.45 (m, 3H), 7.41-7.36 (m, 2H), 7.18 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 158.2, 156.9, 156.6, 152.6, 130.6, 129.1, 129.0, 128.9, 124.6, 124.5, 120.8, 117.4, 112.7, 112.5, 102.7. **HRMS** (m/z) (ESI): calcd for $C_{17}H_{11}O_3$ 263.0708 [M+H$^+$]; found 263.0704.

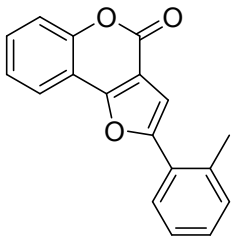
2-(*p*-Tolyl)-furo[3,2-c]coumarin (3ab)



3ab

White solid, m.p. 212-214 °C. **FTIR** (KBr) w: 3066, 3027, 2917, 1741, 1630, 1568, 1494, 961, 747. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.94-7.92 (m, 1H), 7.68 (d, *J* = 8.1 Hz, 2H), 7.52-7.49(m, 1H), 7.44 (d, *J* = 8.2 Hz, 1H), 7.38-7.35 (m, 1H), 7.26 (d, *J* = 7.6 Hz, 2H), 7.09 (s, 1H), 2.40 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 158.3, 156.8, 156.5, 152.5, 139.3, 130.4, 129.6, 126.2, 124.5, 124.4, 120.7, 117.3, 112.7, 112.5, 101.8, 21.4. **HRMS** (m/z) (ESI): calcd for $C_{18}H_{13}O_3$ 277.0865 [M+H$^+$]; found 277.0857.

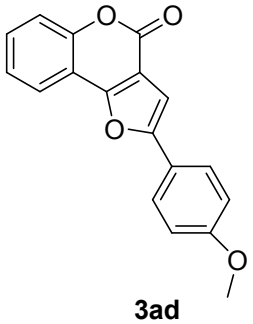
2-(*o*-Tolyl)-furo[3,2-c]coumarin (3ac)



3ac

White solid, m.p. 132-138 °C. **FTIR** (KBr) w: 3060, 3019, 1740, 1631, 1566, 1490, 959, 751. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.95-9.93 (m, 1H), 7.84-7.82 (m, 1H), 7.55-7.51 (m, 1H), 7.47-7.46 (m, 1H), 7.38-7.32 (m, 4H), 7.08 (s, 1H), 2.58 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 158.4, 156.5, 156.2, 152.6, 135.5, 131.5, 130.6, 129.1, 128.3, 127.6, 126.3, 124.6, 120.8, 117.4, 112.7, 112.3, 106.2, 21.9. **HRMS** (m/z) (ESI): calcd for $C_{18}H_{13}O_3$ 277.0865 [M+H$^+$]; found 277.0858.

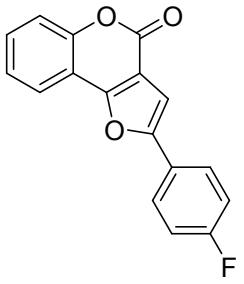
2-(4-Methoxyphenyl)-furo[3,2-c]coumarin (3ad)



3ad

White solid, m.p. 189-191 °C. **FTIR** (KBr) w: 3081, 2955, 2845, 1747, 1609, 1568, 1498, 971, 748. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.94-7.92 (m, 1H), 7.74-7.72 (m, 2H), 7.52-7.49 (m, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.38-7.35 (m, 1H), 7.02 (s, 1H), 6.99 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.3, 158.4, 156.8, 156.4, 152.4, 130.3, 126.1, 124.5, 121.8, 120.6, 117.3, 114.4, 112.8, 112.6, 100.9, 55.4. **HRMS** (m/z) (ESI): calcd for $C_{18}H_{13}O_4$ 293.0814 [M+H$^+$]; found 293.0808.

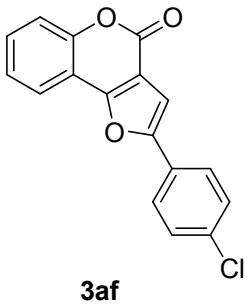
2-(4-Fluorophenyl)-furo[3,2-c]coumarin (3ae)



3ae

White solid, m.p. 231 °C. **FTIR** (KBr) w: 3085, 2966, 2926, 1752, 1632, 1571, 1495, 965, 753. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.8 Hz, 1H), 7.83-7.81 (m, 2H), 7.56 (t, *J* = 7.9 Hz, 1H), 7.49 (d, *J* = 8.3 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.29 (s, 2H), 7.20 (t, *J* = 8.4 Hz, 2H), 7.14 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 163.1 ($^1J_{CF}$ = 250 Hz), 158.1, 156.9, 155.7, 152.6, 130.7, 126.5 ($^2J_{CF}$ = 8.8 Hz), 125.3, 124.6, 120.7, 117.4, 116.3, 116.1, 112.6 ($^2J_{CF}$ = 12.5 Hz), 102.4. **HRMS** (m/z) (ESI): calcd for $C_{17}H_{10}FO_3$ 281.0614 [M+H$^+$]; found 281.0611.

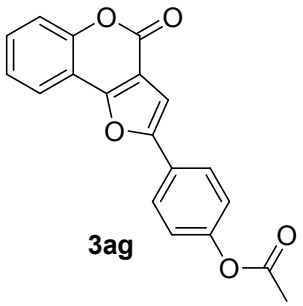
2-(4-Chlorophenyl)-furo[3,2-c]coumarin (3af)



3af

White solid, m.p. 276 °C. **FTIR** (KBr) w: 3095, 2963, 2866, 1743, 1635, 1574, 1493, 967, 758. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 8.5 Hz, 2H), 7.54 (dd, *J* = 14.0, 6.6 Hz, 1H), 7.47 (dd, *J* = 15.5, 9.6 Hz, 3H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.18 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 158.1, 157.1, 155.5, 152.7, 135.1, 130.8, 129.3, 127.5, 125.8, 124.7, 120.8, 117.5, 112.6, 112.5, 103.2. **HRMS** (m/z) (ESI): calcd for $C_{17}H_{10}ClO_3$ 297.0319 [M+H$^+$]; found 297.0314.

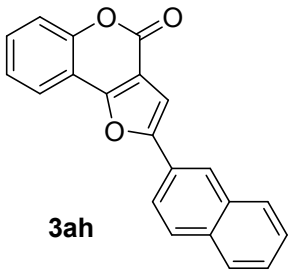
4-(4-Oxo-furo[3,2-c]coumarin)phenyl acetate (3ag)



3ag

White solid, m.p. 180-182 °C. **FTIR** (KBr) w: 3132, 2923, 2851, 1764, 1681, 1635, 1557, 1495, 964, 746. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92-7.90 (m, 1H), 7.80-7.78 (m, 2H), 7.52-7.49 (m, 1H), 7.42 (d, *J* = 8.4 Hz, 1H), 7.37-7.34 (m, 1H), 7.21-7.19 (m, 23H), 7.11 (d, *J* = 1.7 Hz, 1H), 2.33 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 169.2, 158.1, 156.9, 155.8, 152.6, 151.2, 130.7, 126.6, 125.7, 124.6, 122.3, 120.8, 117.4, 112.7, 112.5, 102.7, 21.1. **HRMS** (m/z) (ESI): calcd for $C_{19}H_{13}O_5$ 321.0763 [M+H$^+$]; found 321.0757.

2-Naphthalen-furo[3,2-c]coumarin (3ah)

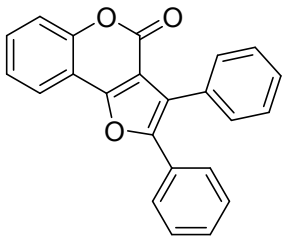


3ah

White solid, m.p. 230-234 °C. **FTIR** (KBr) w: 3052, 2922, 2852, 1749, 1629, 1559, 1503, 967, 751. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.32 (s, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.95-7.92 (m, 2H), 7.88-7.84 (m, 2H), 7.56-7.53 (m, 3H), 7.49-7.47 (m, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.30 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 158.2, 157.1, 156.7, 152.7, 133.4, 133.3, 130.7, 128.9, 128.4, 127.9, 127.0, 126.9, 126.2, 124.6, 123.7, 122.1, 120.9, 117.4, 112.8, 112.7, 103.2. **HRMS** (m/z) (ESI): calcd for $C_{21}H_{13}O_3$

313.0865 [M+H$^+$]; found 313.0861.

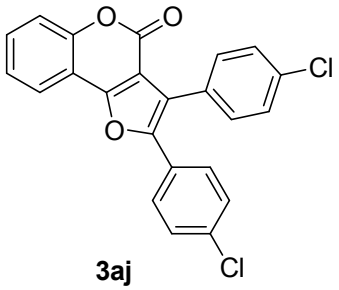
2,3-Diphenyl-furo[3,2-c]coumarin (3ai)



3ai

White solid, m.p. 181 ^{o}C. FTIR (KBr) w: 3053, 2942, 2853, 1743, 1628, 1553, 1501, 963, 769. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.8 Hz, 1H), 7.56-7.52 (m, 5H), 7.48-7.43 (m, 4H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.33-7.31 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.4, 156.4, 152.6, 151.3, 130.7, 130.2, 130.1, 129.2, 128.8, 128.54, 128.52, 128.4, 126.6, 124.4, 120.83, 120.79, 117.2, 112.7, 111.2. **HRMS** (m/z) (ESI): calcd for $C_{23}H_{15}O_3$ 339.1021 [M+H$^+$]; found 339.1017.

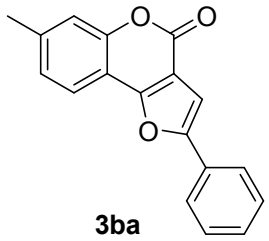
2,3-Bis(4-chlorophenyl)-furo[3,2-c]coumarin (3aj)



3aj

White solid, m.p. 191-193 ^{o}C. **FTI**R (KBr) w: 3055, 2923, 2853, 1743, 1628, 1553, 1507, 963, 768. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98-7.96 (m, 1H), 7.57-7.54 (m, 1H), 7.47-7.44 (m, 3H), 7.43- 7.37 (m, 5H), 7.34-7.31 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.3, 156.7, 152.7, 150.4, 135.1, 134.7, 131.5, 131.1, 129.04, 129.01, 128.3, 127.9, 127.4, 124.6, 120.9, 120.1, 117.3, 112.5, 111.0. HRMS (m/z) (ESI): calcd for $C_{23}H_{13}Cl_2O_3$ 407.0242 [M+H$^+$]; found 407.0242.

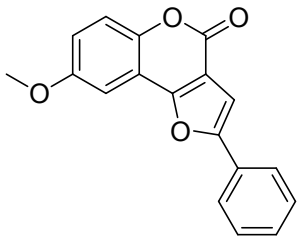
7-Methyl-2-phenyl-furo[3,2-c]coumarin (3ba)



3ba

White solid, m.p. 144 °C. **FTIR** (KBr) w: 3063, 2928, 2857, 1743, 1602, 1552, 1498, 976, 759. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.82-7.80 (m, 2H), 7.73 (s, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.39 (t, *J* = 7.1 Hz, 1H), 7.33-7.30 (m, 2H), 7.16 (d, *J* = 2.0 Hz, 1H), 2.48 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 158.4, 156.9, 156.4, 150.8, 134.4, 131.7, 129.1, 120.0, 124.5, 120.5, 117.1, 112.4, 102.7, 21.0. **HRMS** (m/z) (ESI): calcd for $C_{18}H_{13}O_3$ 277.0865 [M+H$^+$]; found 277.0860.

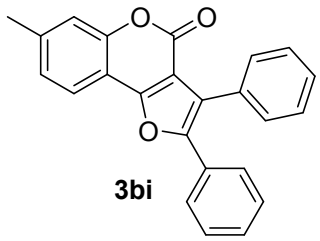
8-Methoxy-2-phenyl-furo[3,2-c]coumarin (3ca)



3cb

White solid, m.p. 178 °C. **FTIR** (KBr) w: 3063, 2925, 2852, 1742, 1639 , 1566, 1489, 932, 754. **^{1}H NMR** (500 MHz, $CDCl_3$) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.9 Hz, 1H), 7.79- 7.77 (m, 2H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.39-7.36 (m, 1H), 7.13 (s, 1H), 6.98-6.95 (m, 2H), 3.89 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.0, 158.5, 157.6, 155.7, 154.4, 129.1, 129.0, 128.8, 124.4, 121.7, 112.9, 110.0, 106.2, 102.5, 101.5, 55.8. **HRMS** (m/z) (ESI): calcd for $C_{18}H_{13}O_4$ 293.0814 [M+H$^+$]; found 293.0808.

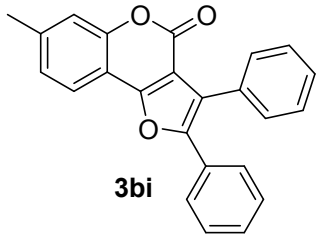
7-Methyl-2,3-diphenyl-furo[3,2-c]coumarin (3bi)



3bi

White solid, m.p. 175 °C. **FTIR** (KBr) w: 3064, 2934, 2855, 1738, 1636, 1572, 1503, 986, 778. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 0.7 Hz, 1H), 7.57-7.54 (m, 2H), 7.52-7.50 (m, 2H), 7.48-7.42 (m, 3H), 7.33-7.31 (m, 5H), 7.26 (s, 1H), 2.49 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.6, 156.5, 151.2, 150.9, 134.2, 131.8, 130.21, 130.20, 129.3, 128.7, 128.54, 128.51, 128.3, 126.6, 120.8, 120.5, 116.9, 112.4, 111.2, 21.0. **HRMS** (m/z) (ESI): calcd for $C_{24}H_{17}O_3$ 353.1178 [M+H$^+$]; found 353.1176.

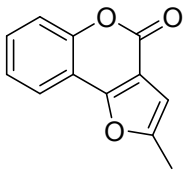
8-Methoxy-2,3-diphenyl-furo[3,2-c]coumarin (3ci)



3bi

White solid, m.p. 247-248 °C. **FTIR** (KBr) w: 3053, 2944, 2852, 1745, 1638, 1556, 1501, 953, 759. **^{1}H NMR** (500 MHz, CDCl3) δ 7.88 (d, *J* = 9.3 Hz, 1H), 7.54-7.49 (m, 4H), 7.45-7.41 (m, 3H), 7.33-7.30 (m, 3H), 6.97-6.96 (m, 2H), 3.89 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.1, 157.8, 157.1, 154.5, 150.4, 130.3, 130.2, 129.5, 128.53, 128.51, 128.3, 126.5, 121.9, 120.6, 112.8, 108.9, 106.1, 101.2, 55.8. **HRMS** (m/z) (ESI): calcd for $C_{24}H_{17}O_4$ 369.1127 [M+H$^+$]; found 369.1123.

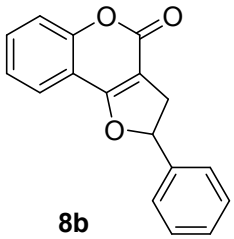
2-Methyl-furo[3,2-c]coumarin (3al)



3al

White solid, m.p. 211-213 °C. **FTIR** (KBr) w: 3085, 3045, 2943, 1743, 1638, 1567, 1493, 956, 764. **^{1}H NMR** (500 MHz, CDCl3) δ 8.04-8.03 (m, 1H), 7.78 (d, *J* = 1.3 Hz, 1H), 7.66-7.62 (m, 1H), 7.41-7.36 (m, 2H), 7.26 (s, 1H), 2.23 (d, *J* = 1.3 Hz, 3H). **^{13}C NMR** (125 MHz, CDCl3) δ 159.9, 159.8, 159.0, 153.1, 136.3, 133.8, 125.9, 125.1, 123.1, 117.3, 113.2, 103.6, 17.1. **HRMS** (m/z) (ESI): calcd for $C_{12}H_9O_3$ 201.0552 [M+H$^+$]; found 201.0548.

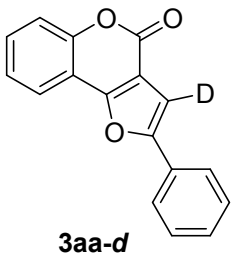
2-Phenyl-2H-furo[3,2-c]coumarin (8b)



8b

White solid, m.p. 105 °C. **FTIR** (KBr) w: 3045, 2924, 2844, 1754, 1631, 1565, 1489, 960, 750. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.8 Hz, 1H), 7.58 (t, *J* = 7.9 Hz, 1H), 7.48-7.38 (m, 6H), 7.30 (t, *J* = 7.6 Hz, 1H), 6.07 (t, *J* = 9.2 Hz, 1H), 3.65 (dd, *J* = 15.3, 10.5 Hz, 1H), 3.23 (dd, *J* = 15.3, 8.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 166.5, 160.5, 155.1, 139.9, 132.5, 129.0, 126.0, 124.0, 122.8, 117.0, 112.5, 101.9, 87.9.0, 35.0, 29.7. **HRMS** (m/z) (ESI): calcd for $C_{17}H_{13}O_3$ 265.0865 [M+H$^+$]; found 265.00858.

3aa-*d*



3aa-*d*

FTIR (KBr) w: 3065, 2922, 2854, 1708, 1637, 1567, 1495, 904, 752. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.94-7.92 (m, 1H), 7.79-7.77 (m, 2H), 7.53-7.49 (m, 1H), 7.47-7.42 (m, 3H), 7.39-7.35 (m, 2H), 7.14 (s, 0.04H).


7.9663
7.9635
7.9507
7.9479
7.8187
7.8160
7.8123
7.8017
7.5440
7.5408
7.5294
7.5268
7.5241
7.5127
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7.4916
7.4882
7.4768
7.4614
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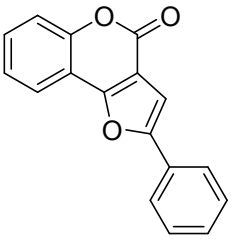
7.1750



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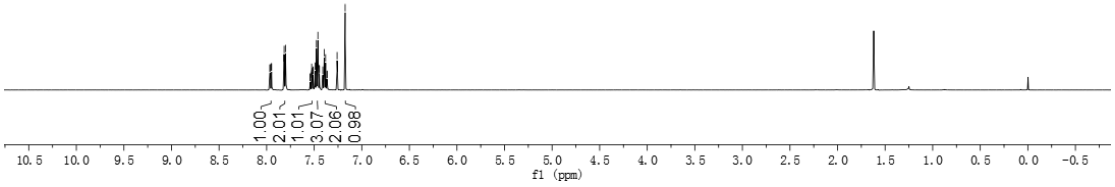
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1.01
3.07
2.06
0.98
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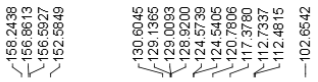
f1 (ppm)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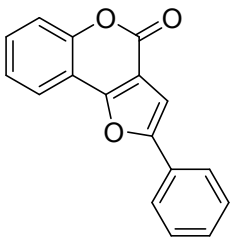
76.7456



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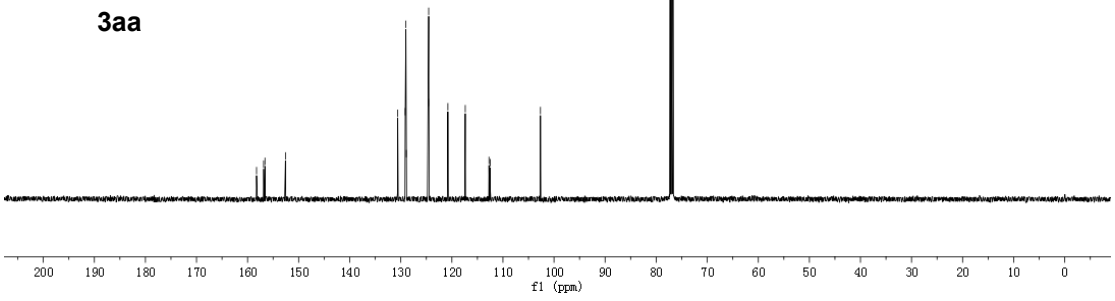
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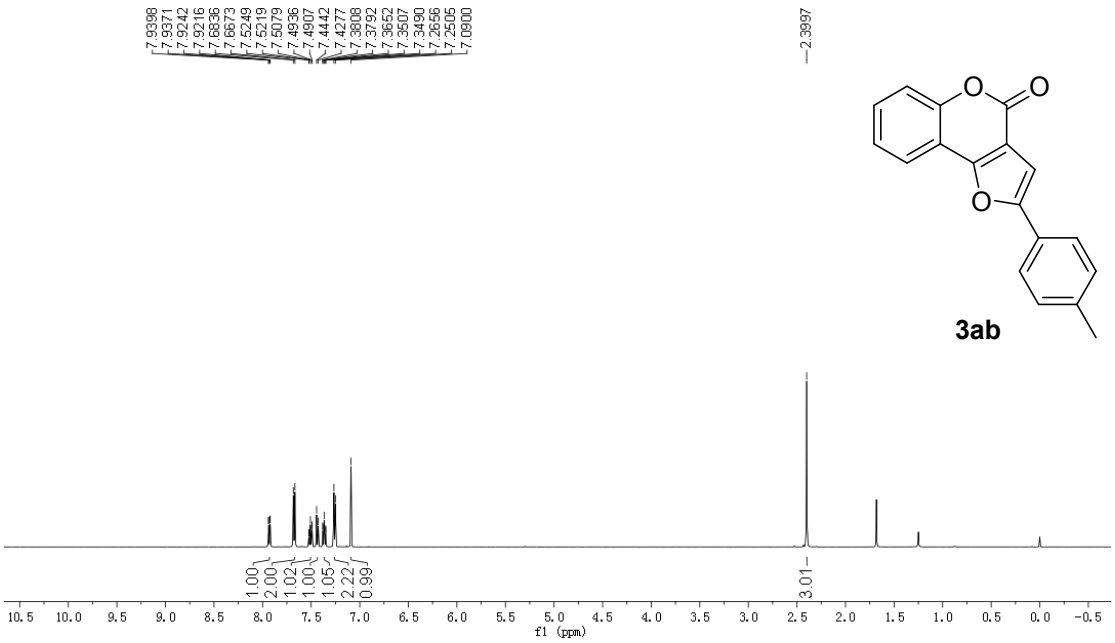
f1 (ppm)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7.4442
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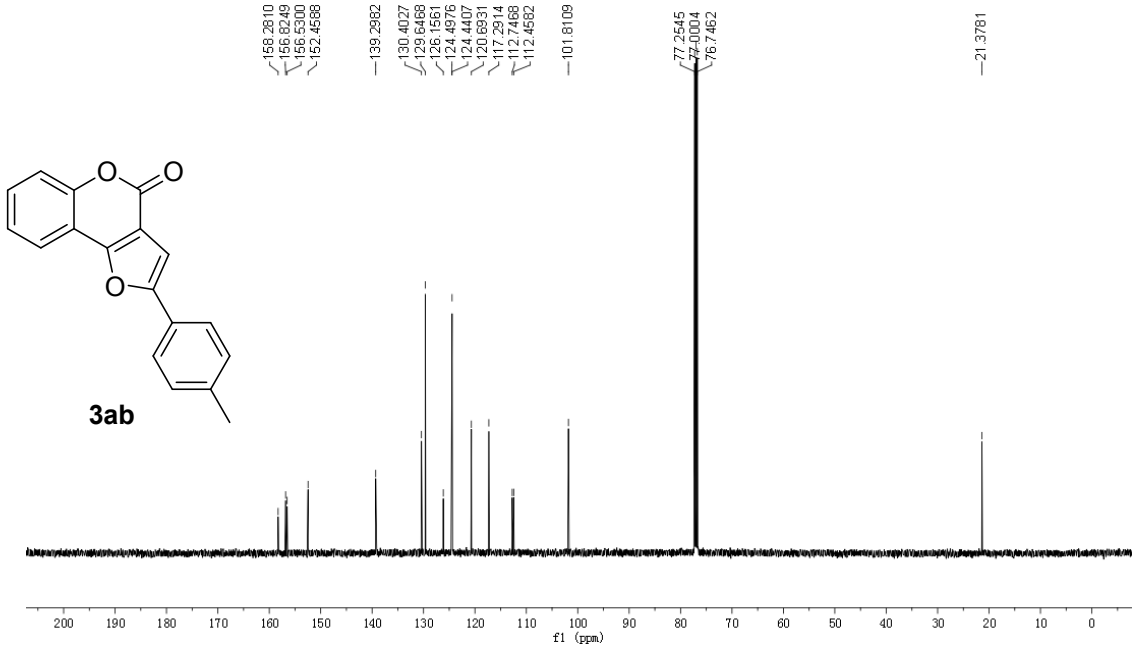
7.3808
7.3792
7.3652
7.3507
7.3490
7.2666
7.2505
7.0900
2.3997
3ab
1.00
2.00
1.02
1.00
1.05
2.22
0.99
3.01
f1 (ppm)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120.6931
117.2914
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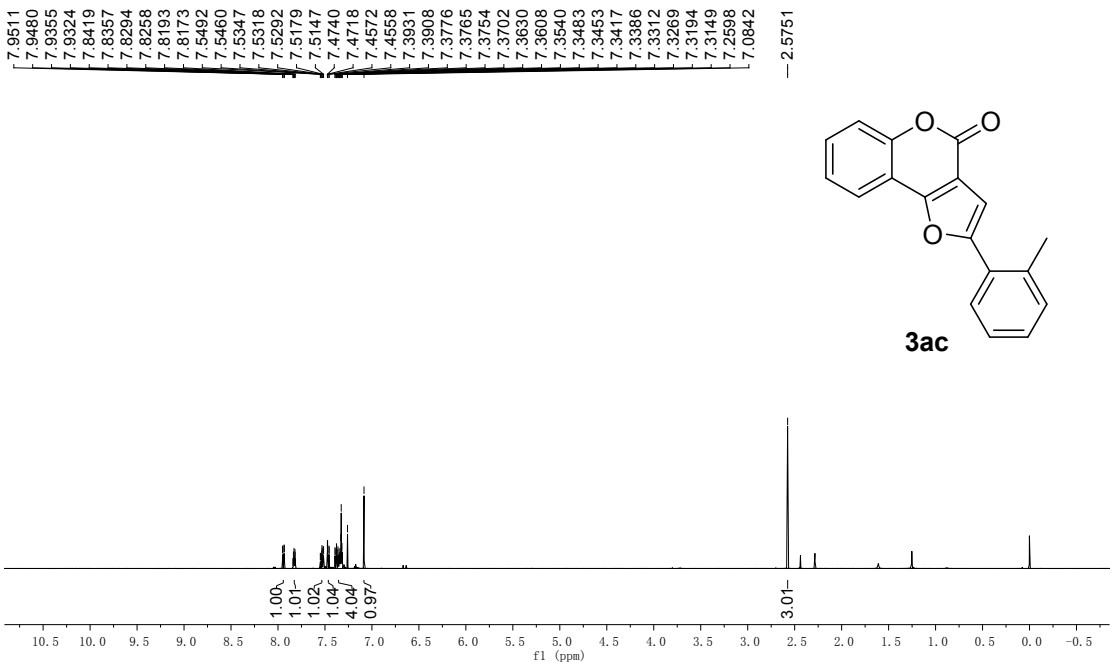
112.4562
101.8109
77.2545
77.0004
76.7462
21.3781
3ab
f1 (ppm)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7.5460
7.5347
7.5318
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7.5179
7.5147
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7.4718
7.4572
7.4558
7.3931
7.3908
7.3776
7.3765
7.3754
7.3702
7.3630
7.3608
7.3540
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7.3453
7.3417
7.3386
7.3312
7.3269
7.3194
7.3149
7.2598
7.0842
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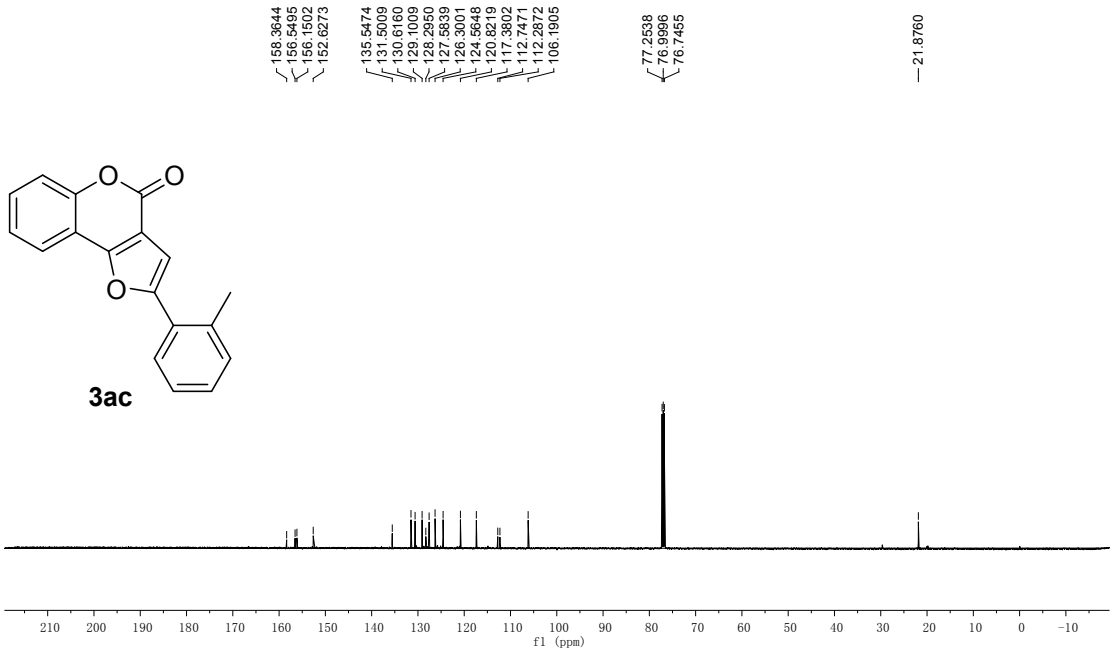
1.01
1.02
1.04
4.04
0.97
3.01
f1 (ppm)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130.6160
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126.3001
124.5648
120.8219
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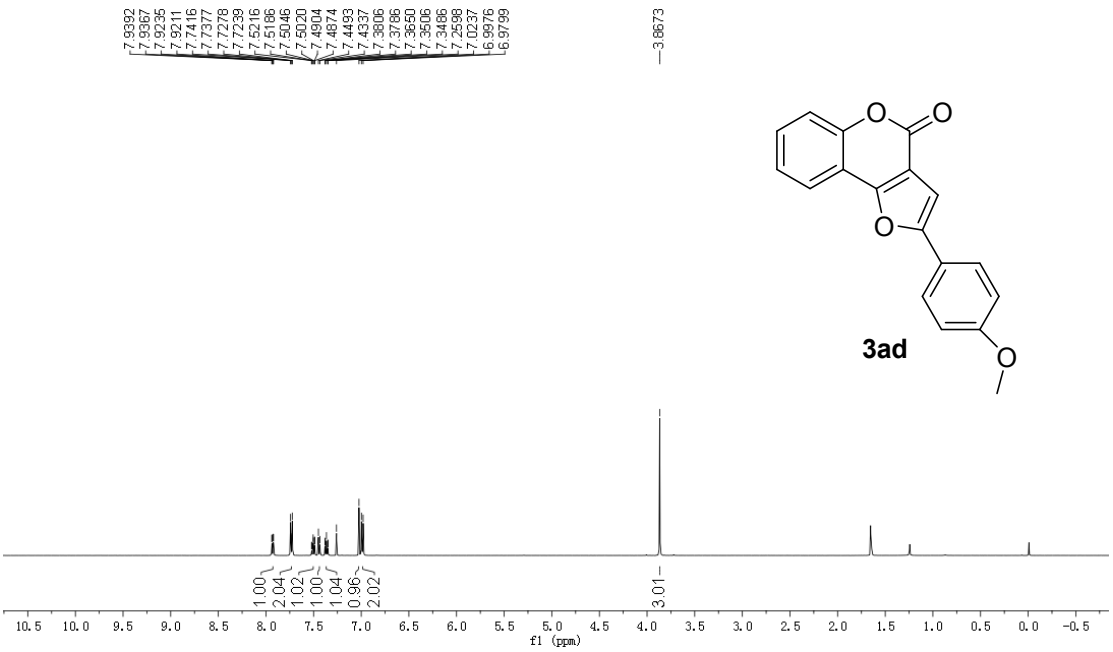
76.9996
76.7455
21.8760
3ac
f1 (ppm)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7.5216
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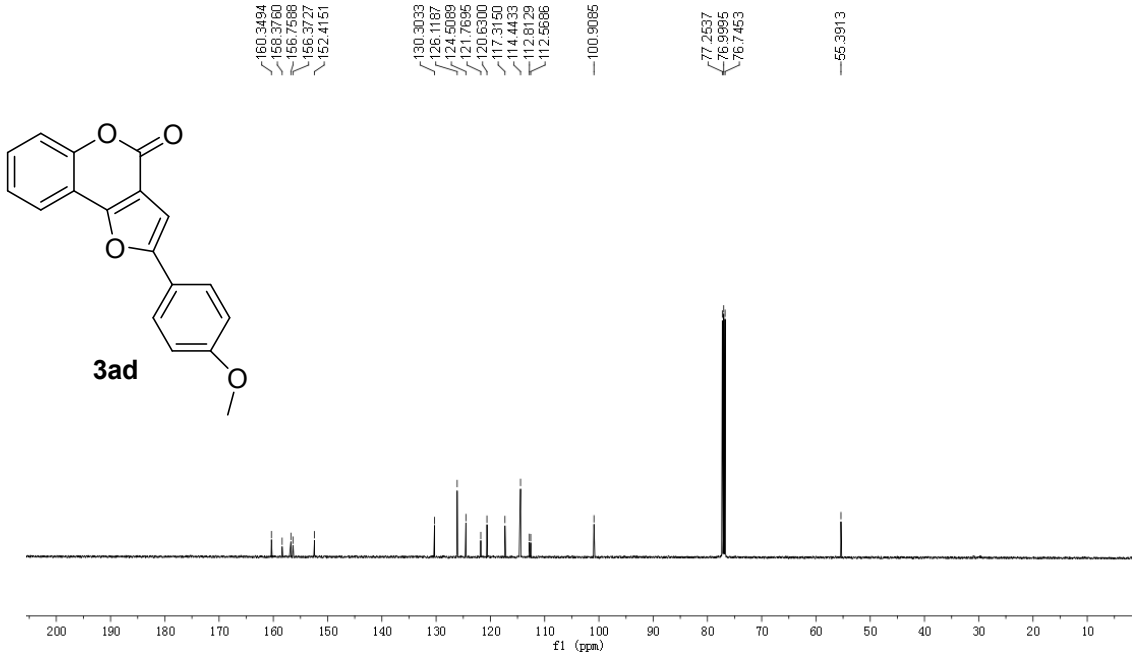
7.5046
7.5020
7.4904
7.4874
7.4493
7.4337
7.3806
7.3786
7.3650
7.3506
7.3486
7.2598
7.0237
6.9976
6.9799
3.8673
3ad
1.00
2.04
1.02
1.00
1.04
0.96
2.02
3.01
f1 (ppm)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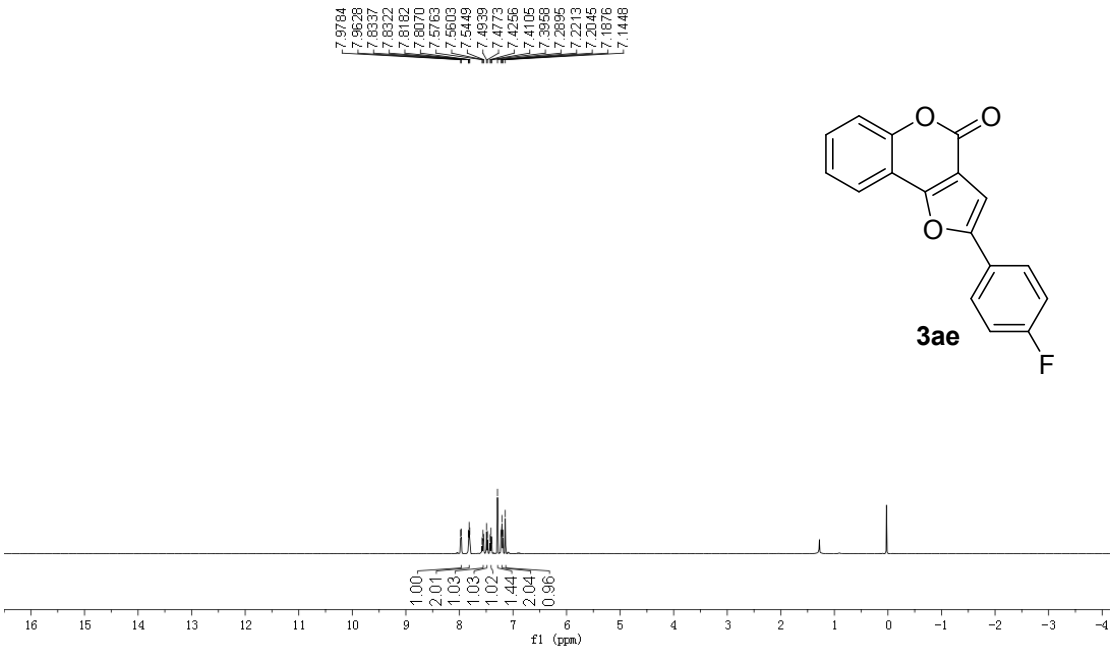
76.7453
55.3913
3ad
f1 (ppm)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7.8070
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7.5603
7.5449
7.4939
7.4773
7.4256
7.4105
7.3958
7.2895
7.2213
7.2045
7.1876
7.1448
3ae
F
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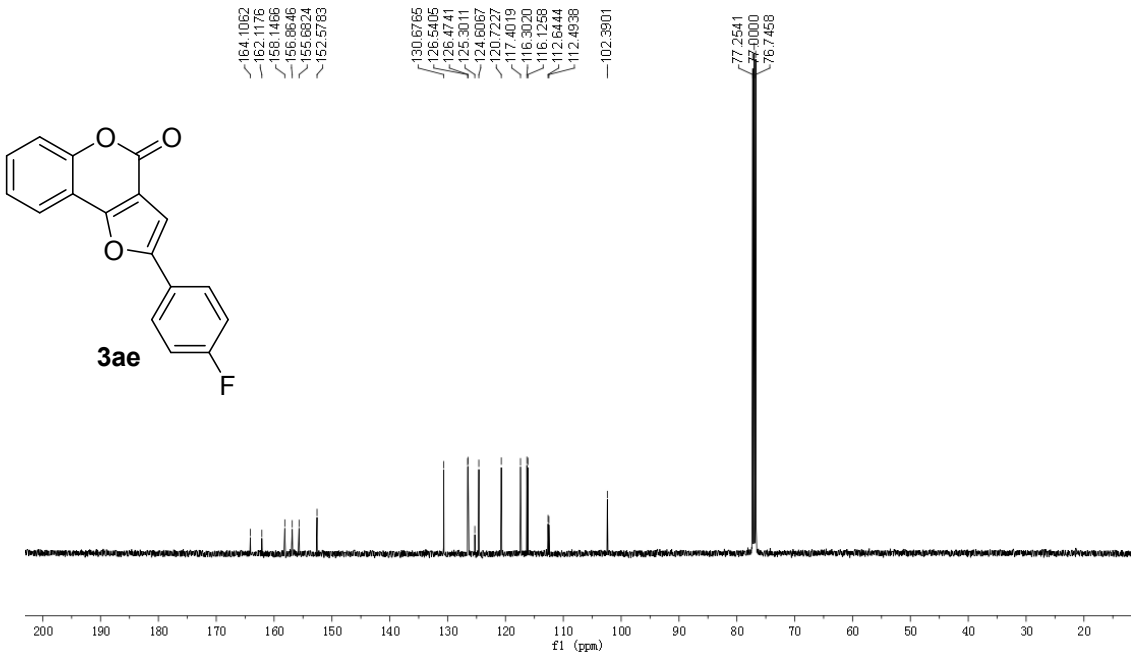
2.01
1.03
1.03
1.02
1.44
2.04
0.96
f1 (ppm)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126.5405
126.4741
125.3011
124.6067
120.7227
117.4019
116.3020
116.1258
112.6444
112.4938
102.3901
77.2541
77.0000
76.7458
3ae
F
f1 (ppm)


7.9680
7.9524
7.7590
7.7421
7.5632
7.5466
7.5318
7.5220
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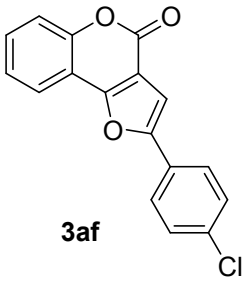
7.4774
7.4655
7.4487
7.4073
7.3922
7.3771
7.2605
7.1613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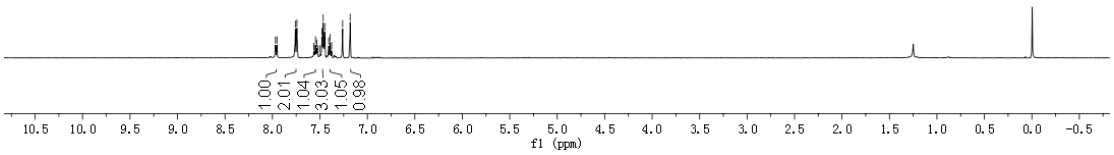
O
O
Cl

3af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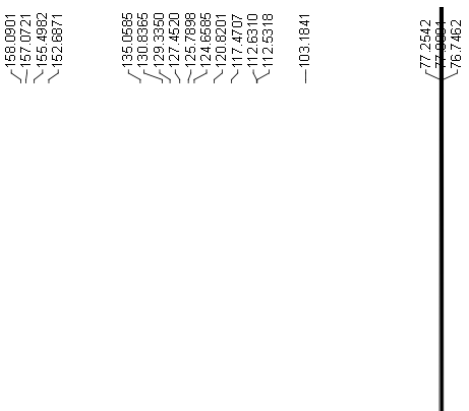
2.01
1.04
3.03
1.05
0.98
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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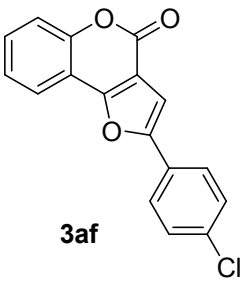
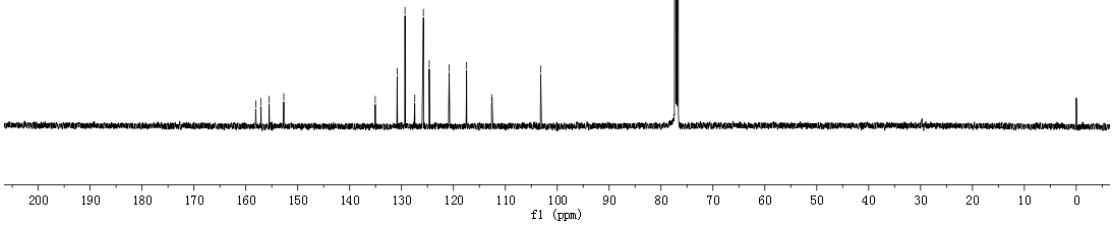
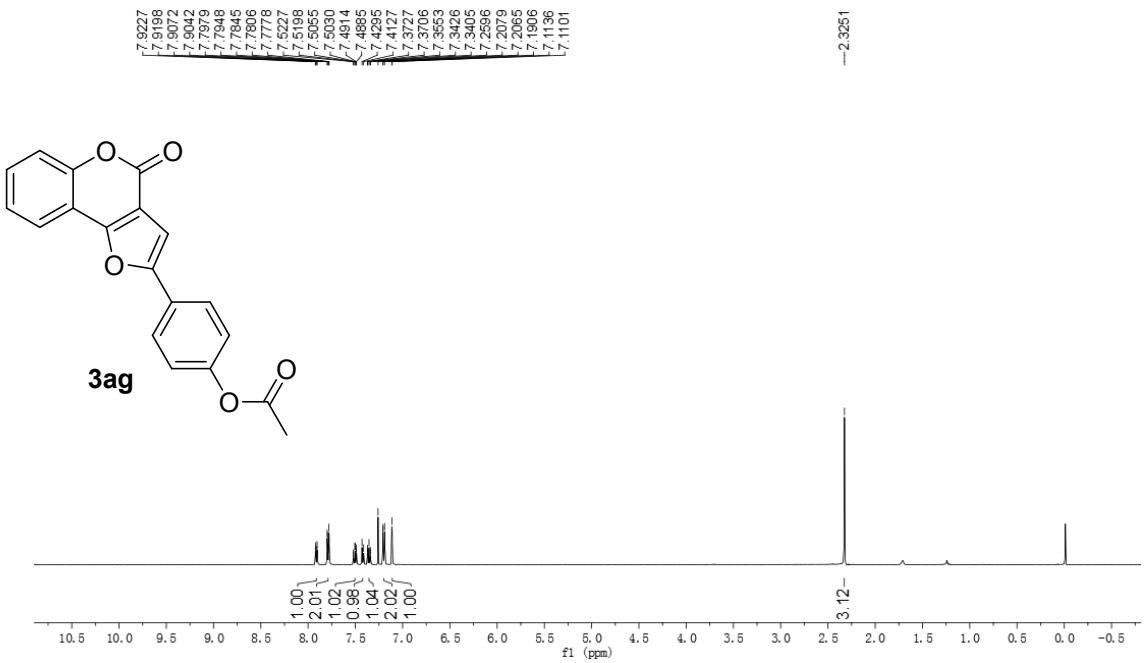
76.7462


O
O
O
Cl

3af


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.7948
7.7845
7.7806
7.7778
7.5227
7.5198
7.5055
7.5030
7.4914
7.4885
7.4295
7.4127
7.3727
7.3706
7.3553
7.3426
7.3405
7.2596
7.2079
7.2065
7.1906
7.1136
7.1101
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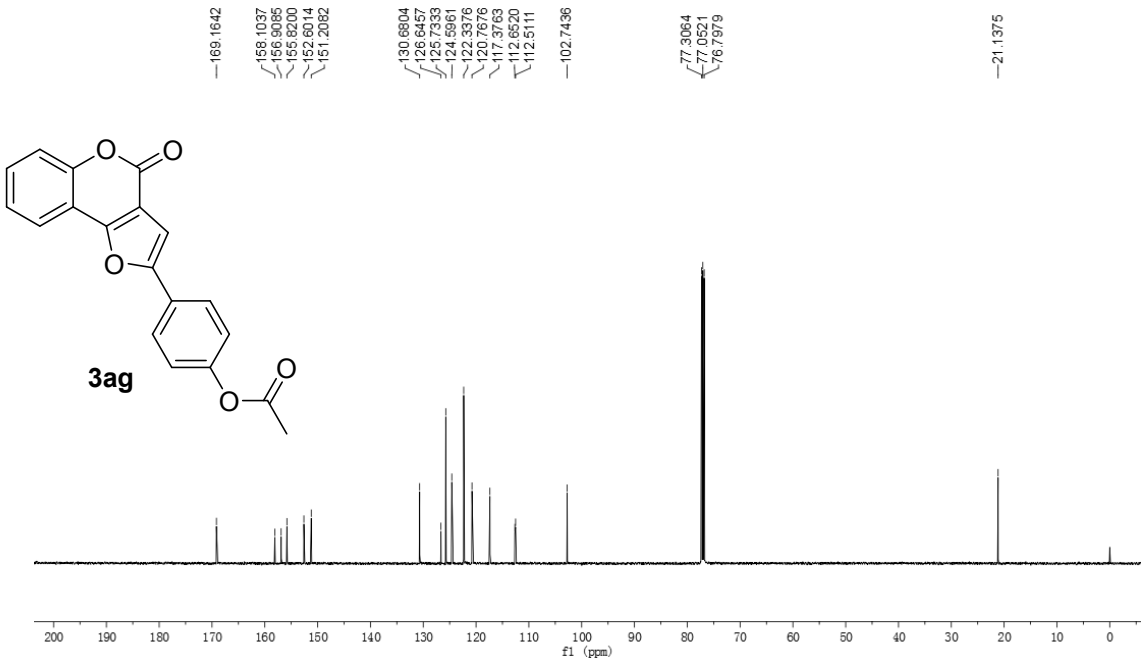
3ag
1.00
2.01
1.02
0.98
1.04
2.02
1.00
3.12
f1 (ppm)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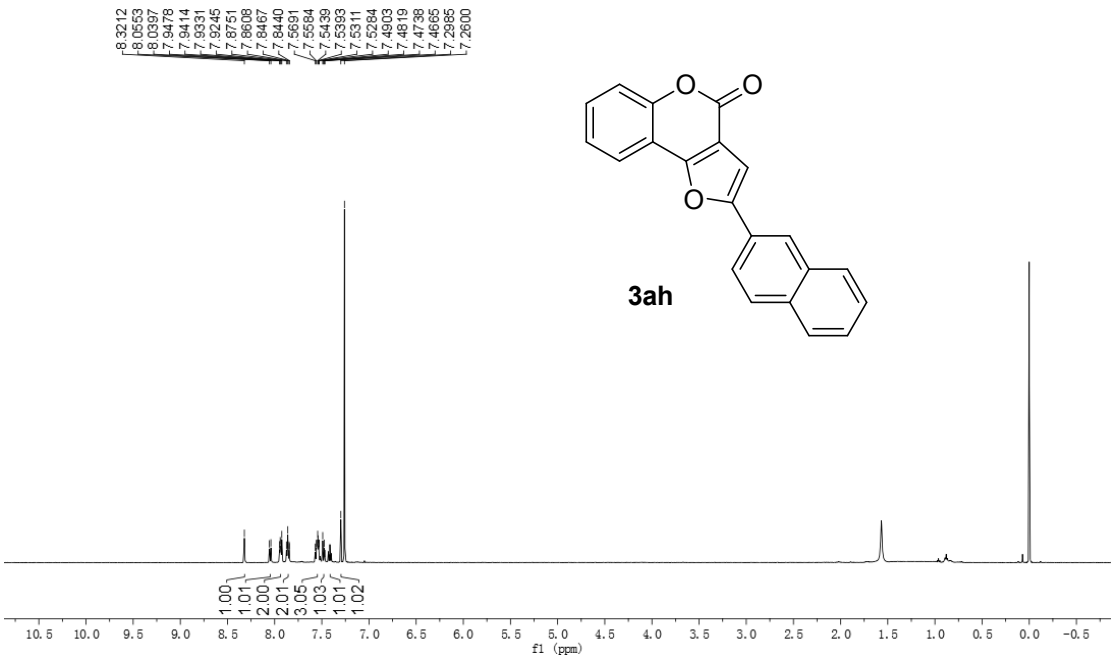
f1 (ppm)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7.5393
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7.5284
7.4903
7.4819
7.4738
7.4665
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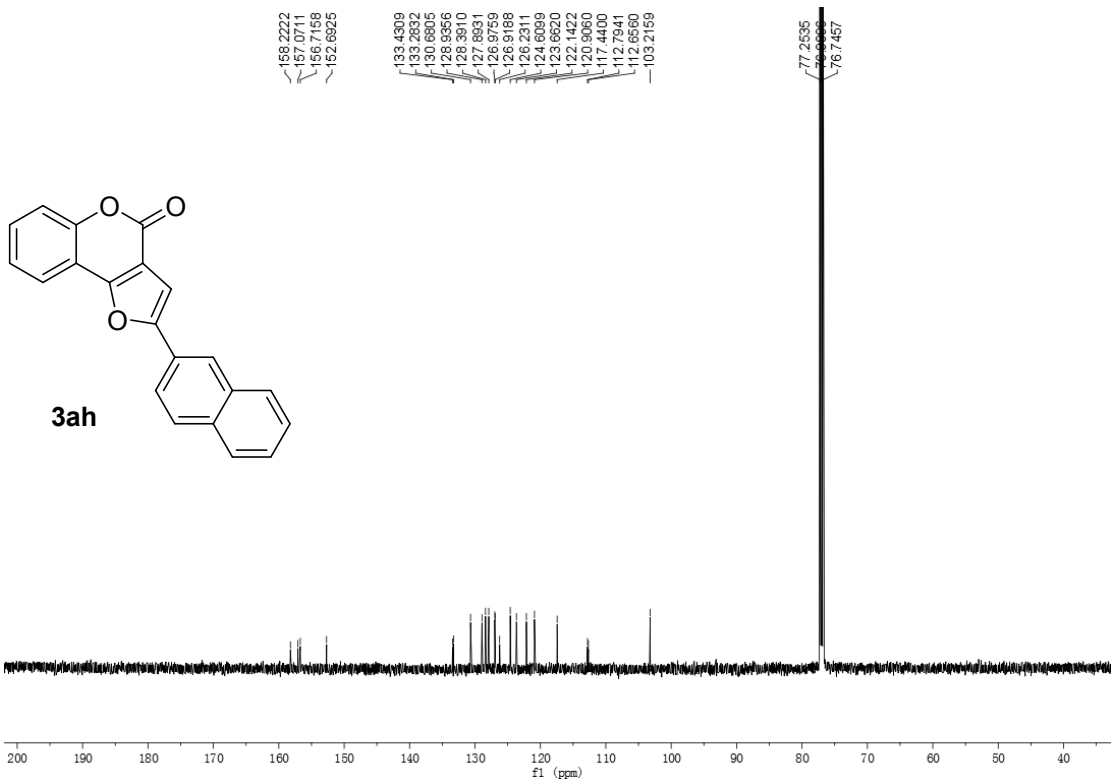
2.00
2.01
3.05
1.03
1.01
1.02
f1 (ppm)

3ah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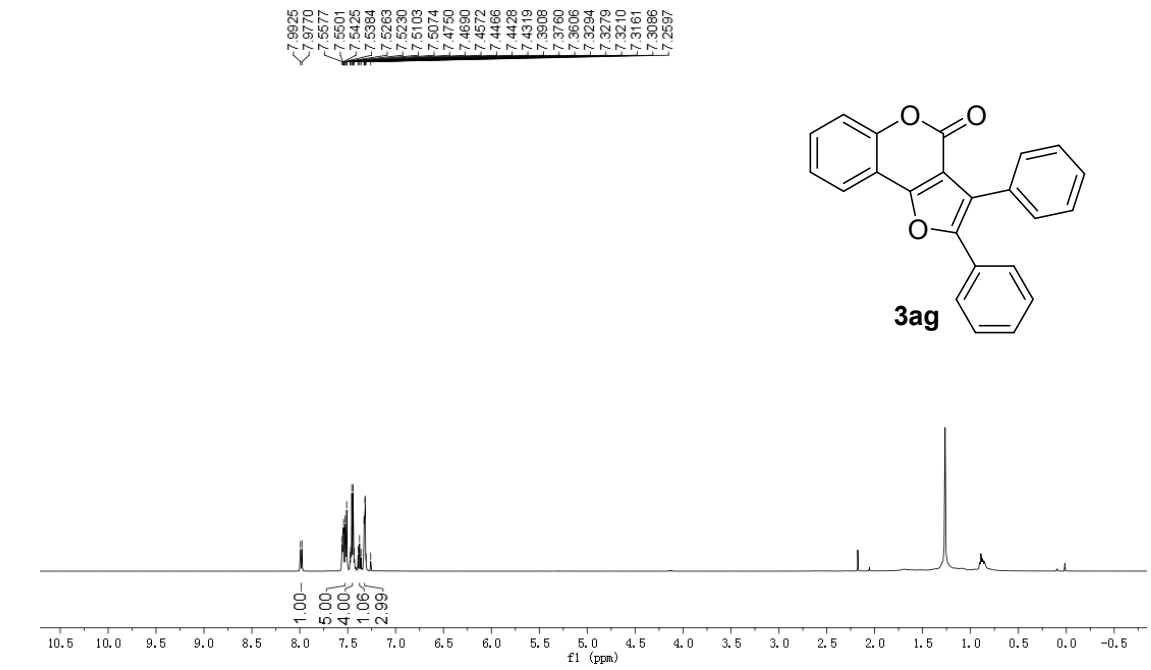
f1 (ppm)

3ah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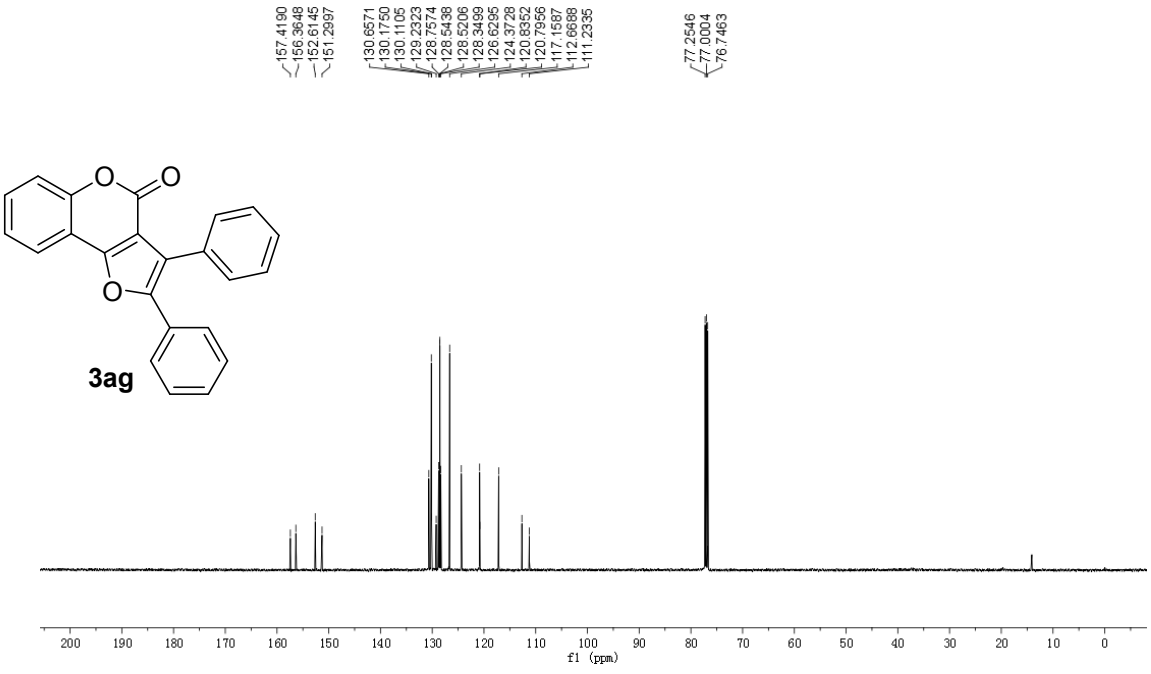
7.4690
7.4572
7.4486
7.4428
7.4319
7.3908
7.3760
7.3606
7.3294
7.3279
7.3210
7.3161
7.3086
7.2597
O
O
O
3ag
1.00
5.00
4.00
1.06
2.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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120.7956
117.1587
112.6688
111.2335
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76.7463
O
O
O
3ag
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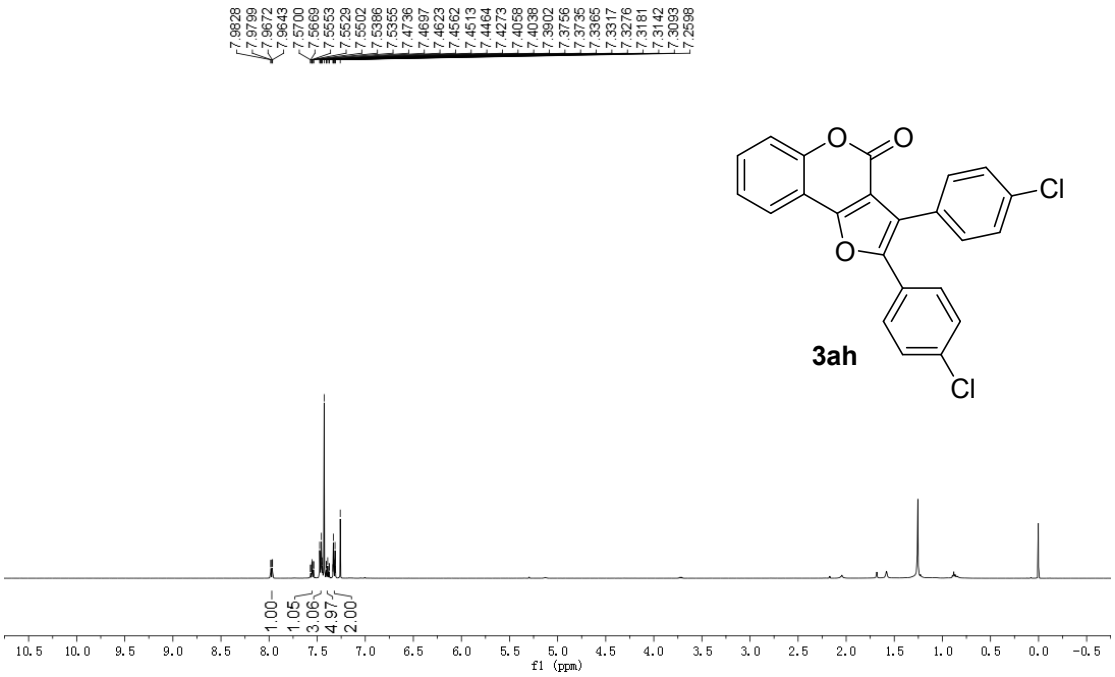
f1 (ppm)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7.4513
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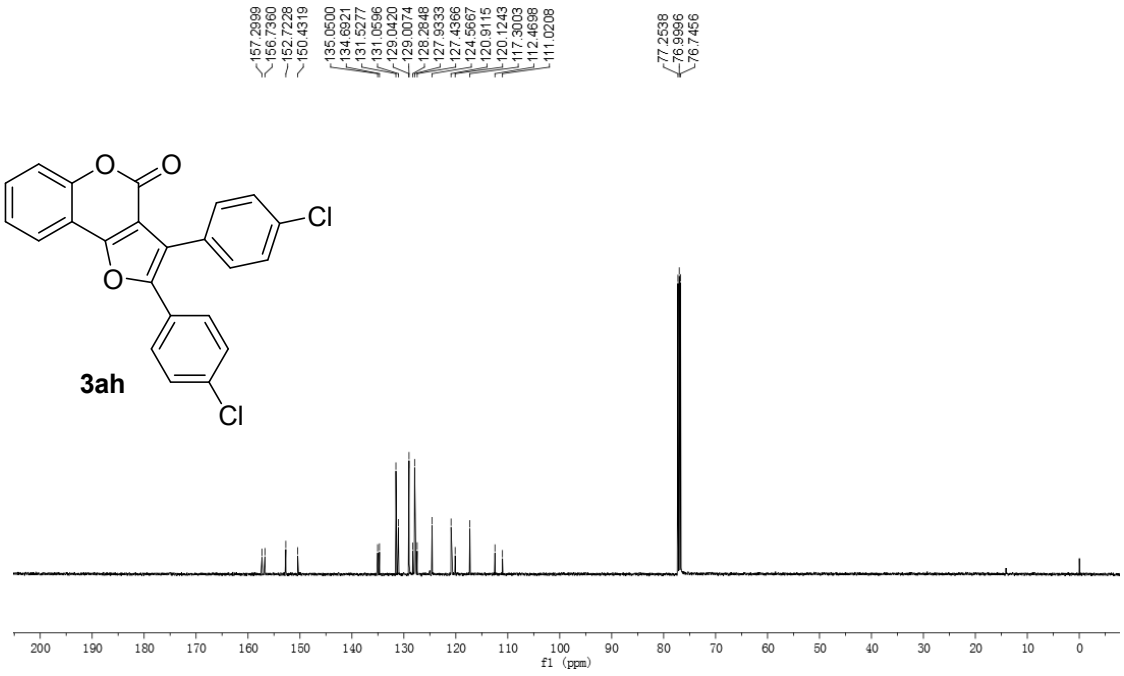
7.3902
7.3756
7.3735
7.3365
7.3317
7.3276
7.3181
7.3142
7.3093
7.2598
O
O
Cl
O
Cl
3ah
1.00
1.05
3.06
4.97
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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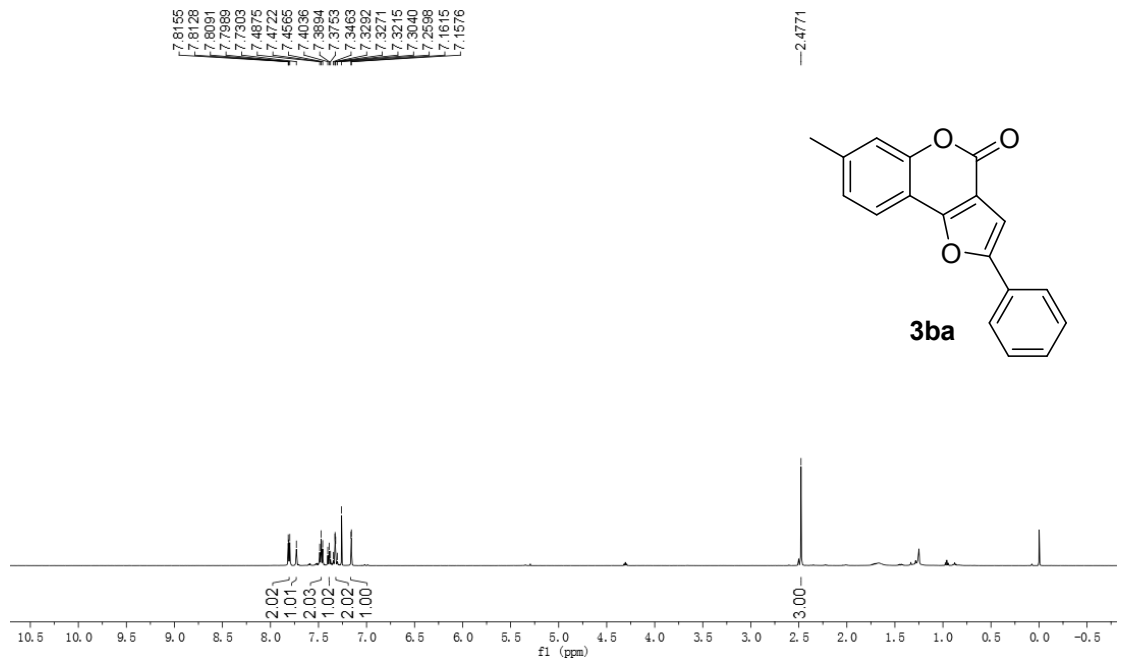
128.2848
127.9333
127.4366
124.5667
120.9115
120.1243
117.3003
112.4698
111.0208
77.2538
76.9996
76.7456
O
O
Cl
O
Cl
3ah
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.3271
7.3215
7.3040
7.2598
7.1615
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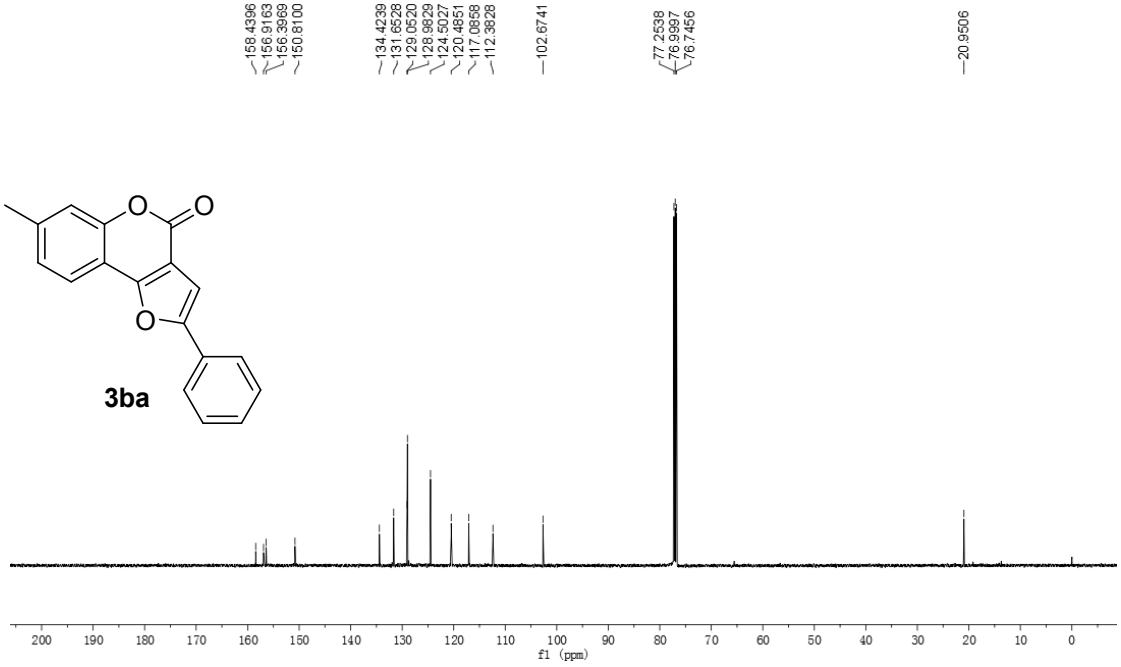
2.02
1.01
2.03
1.02
2.02
1.00
3.00
f1 (ppm)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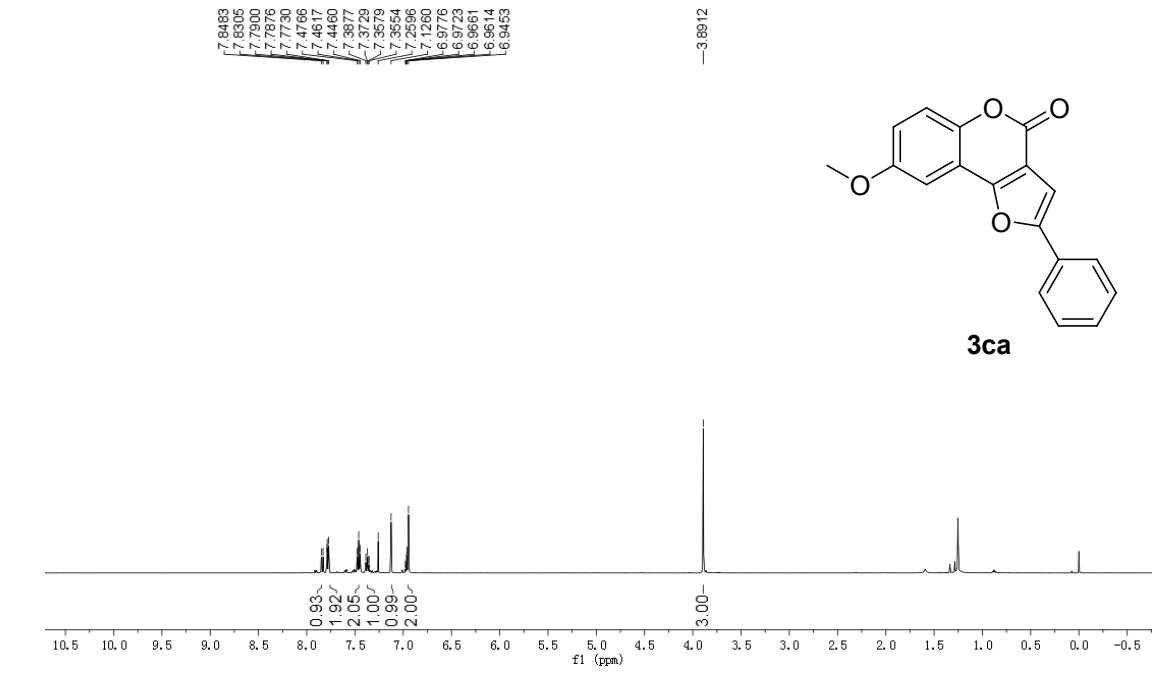
3ba
f1 (ppm)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7.2596
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6.9614
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3ca
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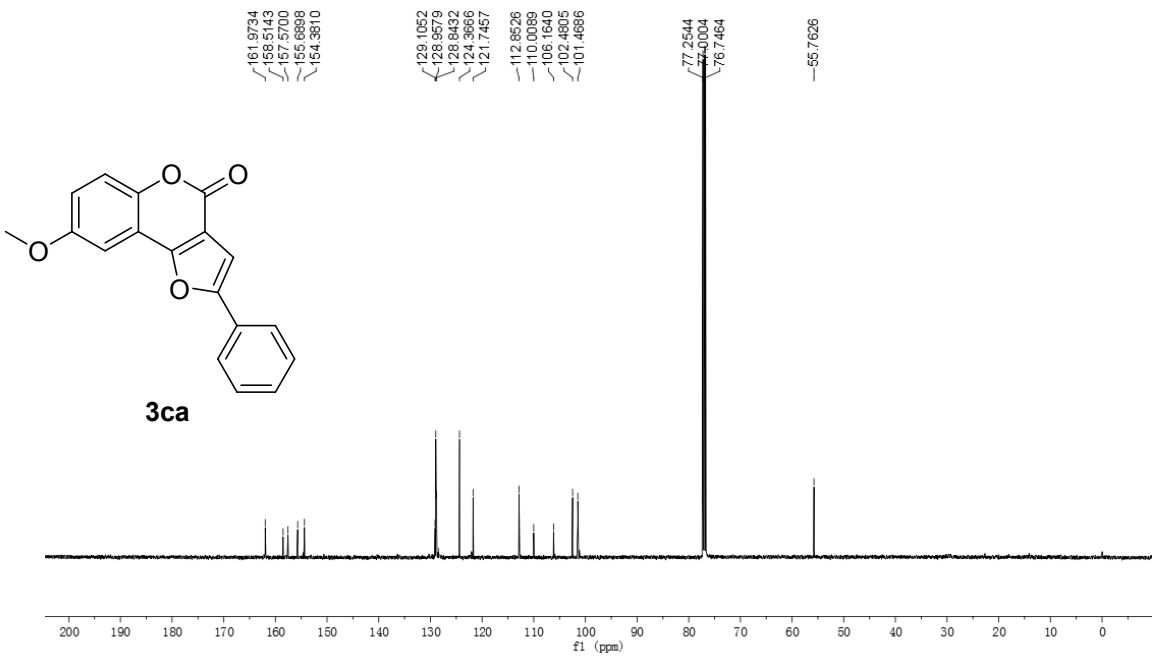
1.92
2.05
1.00
0.99
2.00
3.00
f1 (ppm)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110.0089
106.1640
102.4805
101.4686
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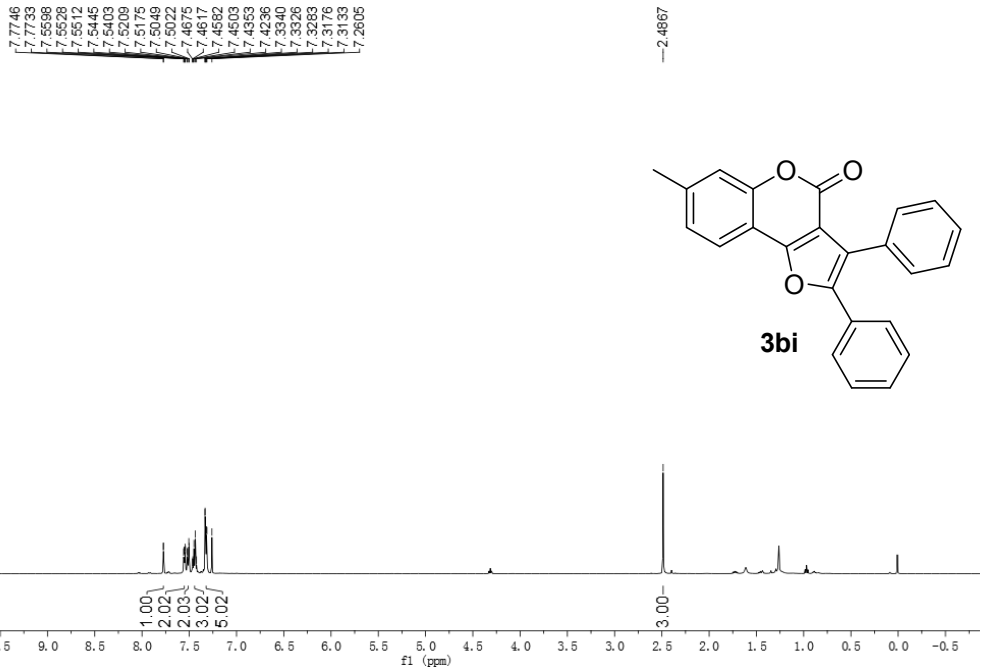
76.7464
55.7626
3ca
f1 (ppm)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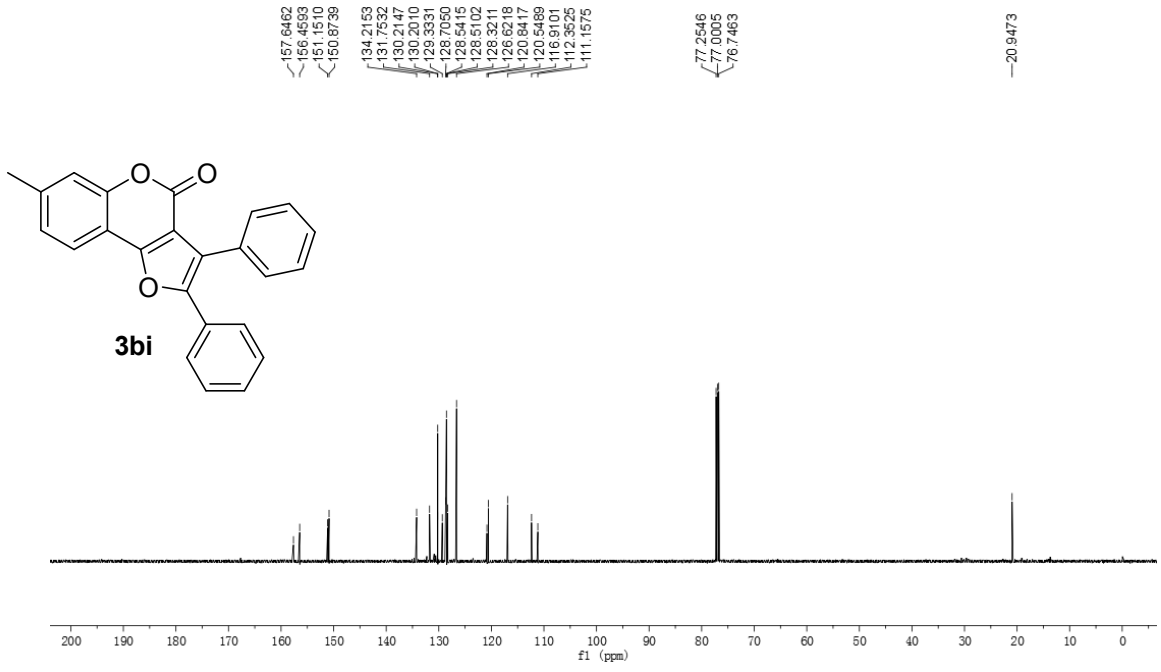
7.7733
7.5598
7.5528
7.5512
7.5445
7.5403
7.5209
7.5175
7.5049
7.5022
7.4675
7.4617
7.4582
7.4503
7.4353
7.4236
7.3340
7.3326
7.3283
7.3176
7.3133
7.2605
2.4867
3bi
1.00
2.02
2.03
3.02
5.02
3.00
f1 (ppm)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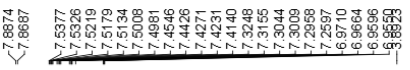
156.4593
151.1510
150.8739
134.2153
131.7532
130.2147
130.2010
129.3331
128.7050
128.5415
128.5102
128.3211
126.6218
120.8417
120.5489
116.9101
112.3625
111.1575
77.2546
77.0005
76.7463
20.9473
3bi
f1 (ppm)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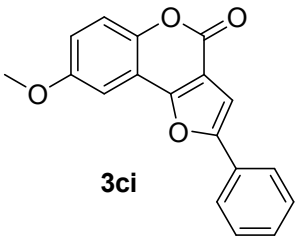
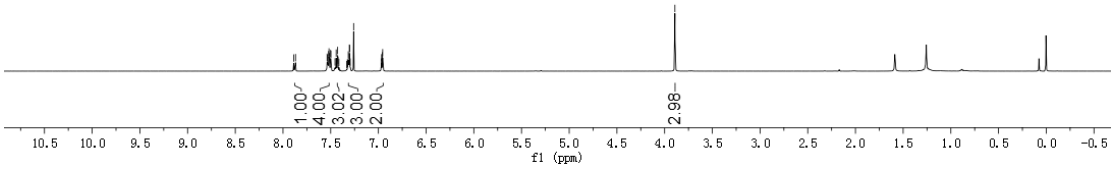
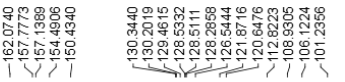
7.8687
7.5377
7.5326
7.5219
7.5179
7.5134
7.5008
7.4981
7.4546
7.4426
7.4271
7.4231
7.4140
7.3248
7.3155
7.3044
7.3009
7.2958
7.2597
6.9710
6.9664
6.9596
3.8923


O
O
O
O

3ci


1.00
4.00
3.02
3.00
2.00
2.98
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 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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157.7773
157.1389
154.4906
150.4340
130.3440
130.2019
129.4615
128.5332
128.5111
128.2858
126.5444
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112.8223
108.9305
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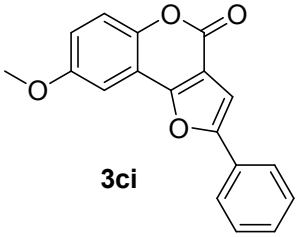
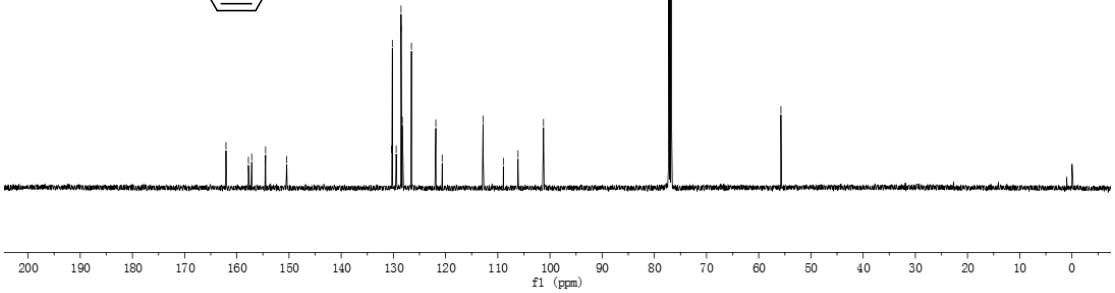
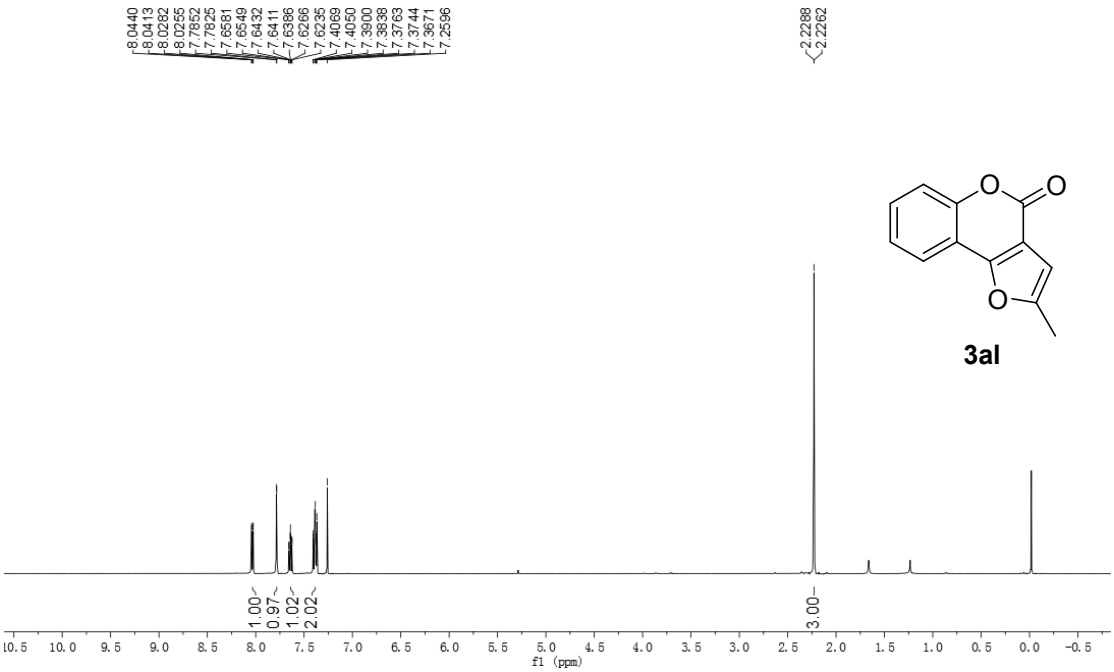
101.2356
77.2538
76.9999
76.7458
55.7504

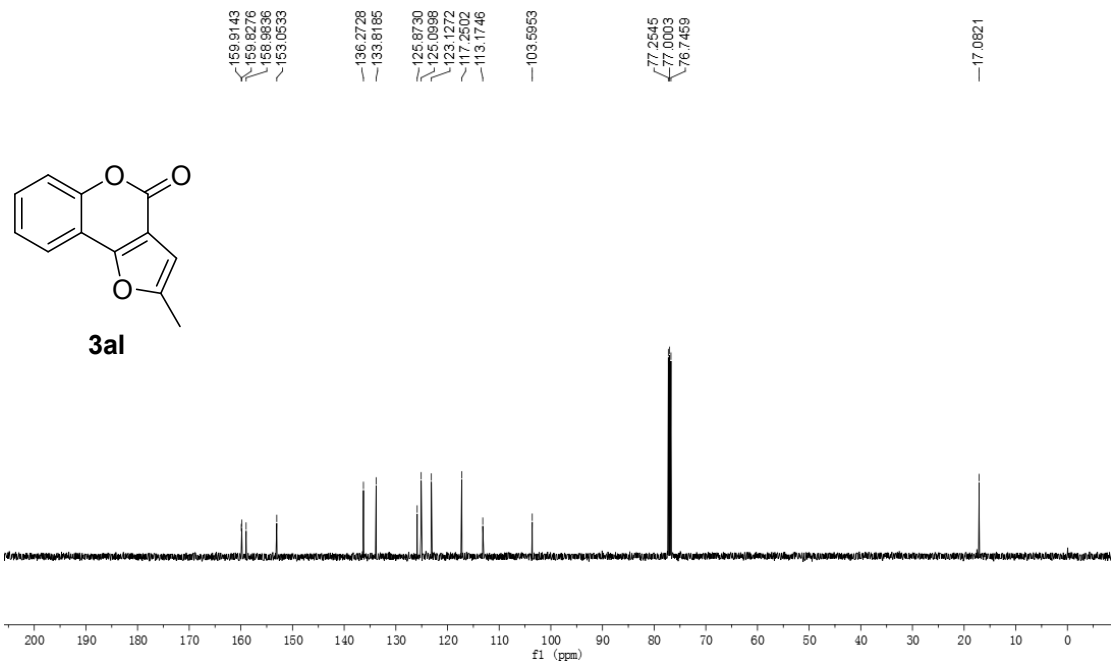

O
O
O
O

3ci

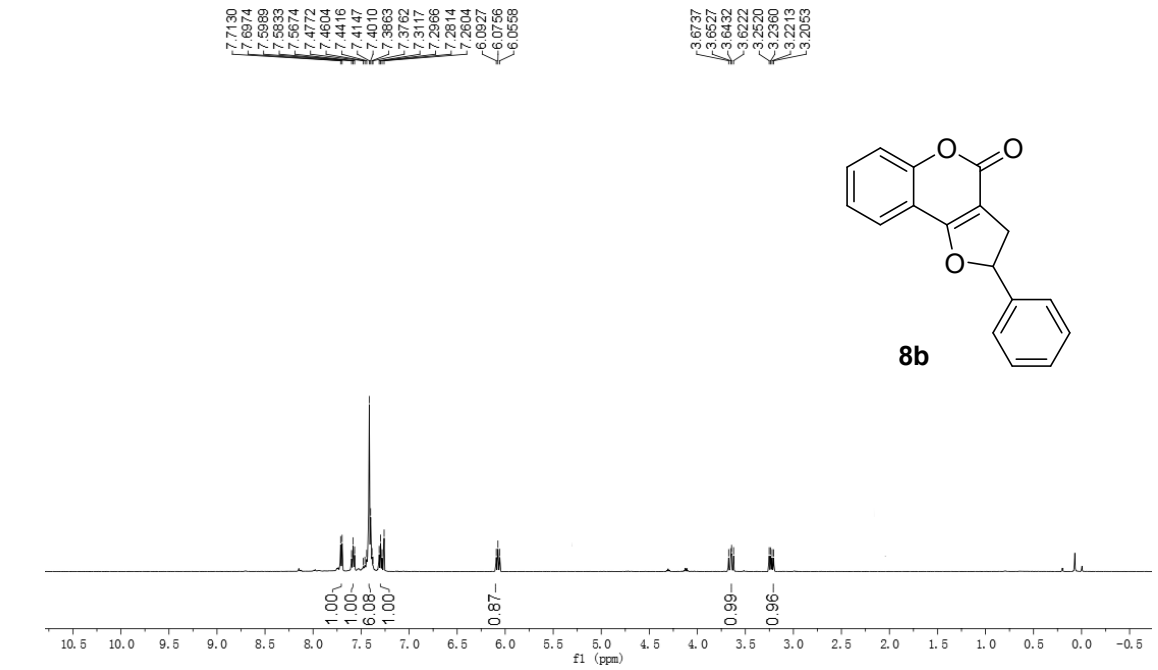

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

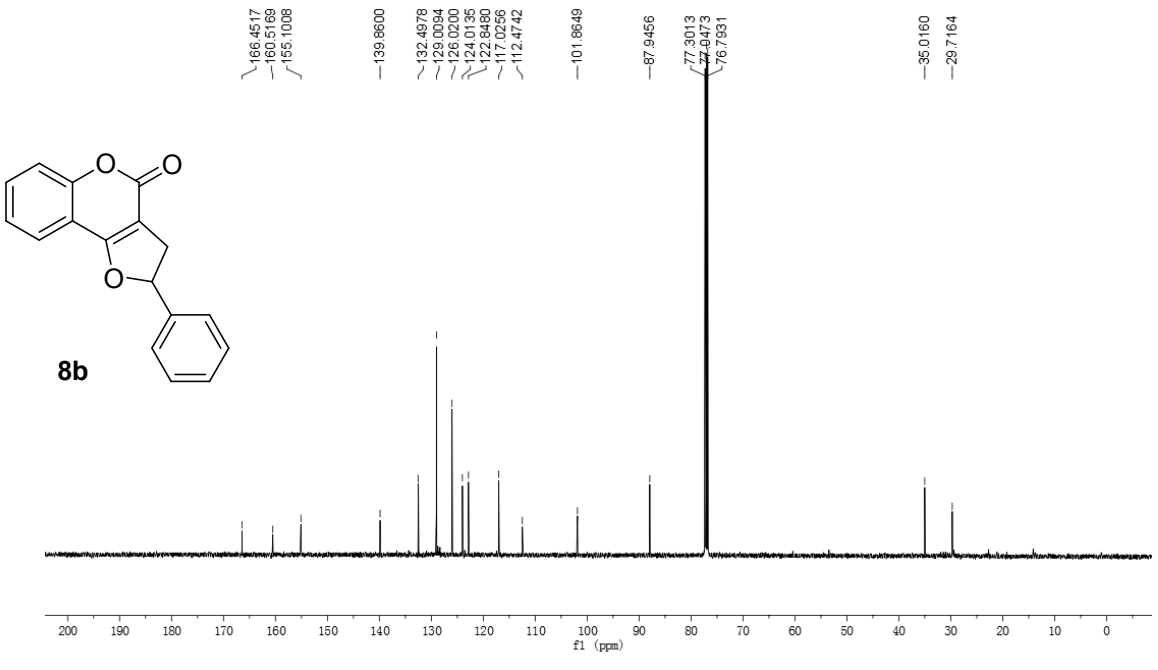

8.0440
8.0413
8.0282
8.0255
7.7852
7.7825
7.6581
7.6549
7.6432
7.6411
7.6386
7.6266
7.6235
7.4069
7.4050
7.3900
7.3838
7.3763
7.3744
7.3671
7.2596
2.2288
2.2262
1.00
0.97
1.02
2.02
3.00
f1 (ppm)

3al

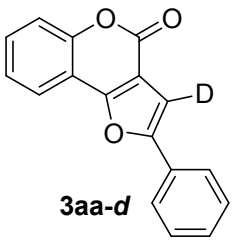

159.9143
159.8276
158.9836
153.0533
136.2728
133.8185
125.8730
125.0998
123.1272
117.2502
113.1746
103.5953
77.2545
77.0003
76.7459
17.0821
f1 (ppm)

3al

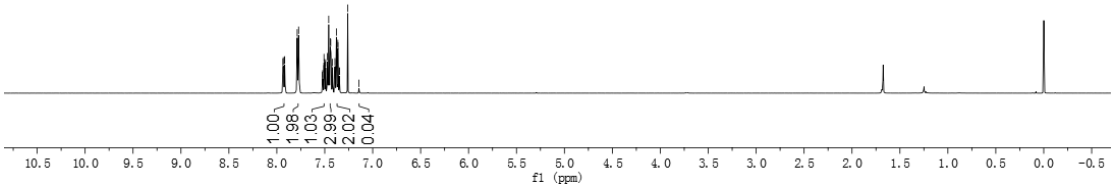

7.7130
7.6974
7.5989
7.5833
7.5674
7.4772
7.4604
7.4416
7.4147
7.4010
7.3863
7.3762
7.3117
7.2966
7.2814
7.2604
6.0927
6.0756
6.0558
3.6737
3.6527
3.6432
3.6222
3.2520
3.2360
3.2213
3.2053
8b
1.00
1.00
6.08
1.00
0.87
0.99
0.96
f1 (ppm)

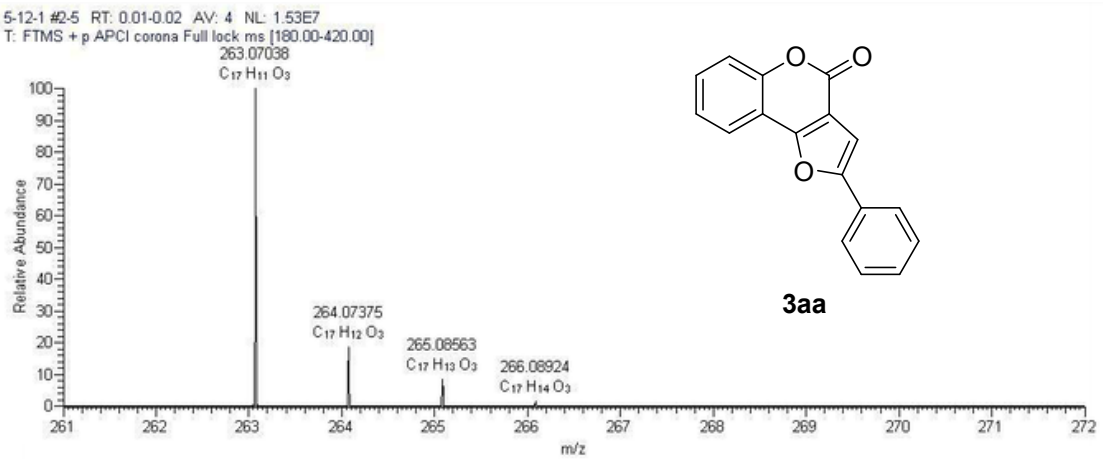

166.4517
160.5169
155.1008
139.8600
132.4978
129.0094
126.0200
124.0135
122.8480
117.0256
112.4742
101.8649
87.9456
77.3013
77.0473
76.7931
35.0160
29.7164
8b
f1 (ppm)


7.9362
7.9334
7.9207
7.9178
7.7902
7.7876
7.7730
7.5251
7.5220
7.5104
7.5079
7.5053
7.4939
7.4907
7.4734
7.4701
7.4587
7.4429
7.4378
7.4207
7.3937
7.3914
7.3789
7.3637
7.3622
7.3488
7.3467
7.2604
7.1437


O
O
D
O

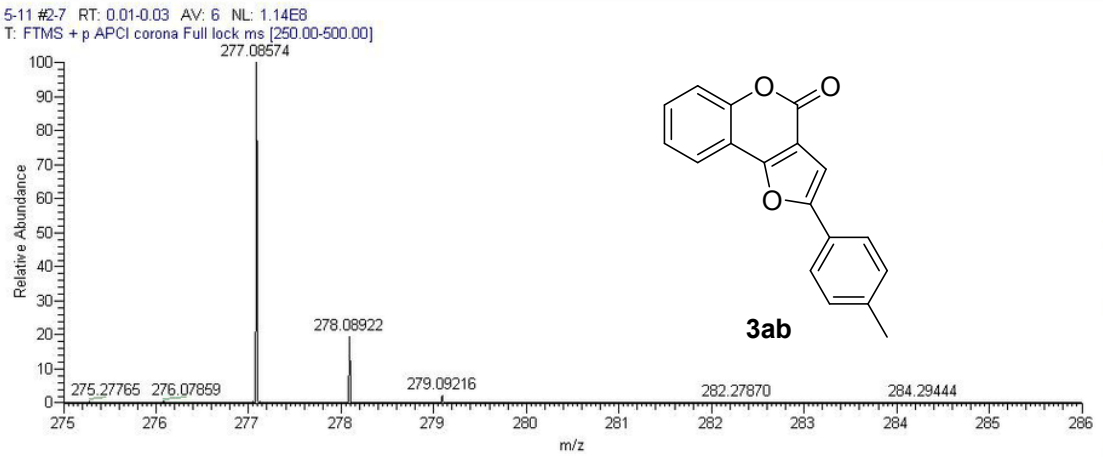
3aa-*d*


1.00
1.98
1.03
2.99
2.02
0.04
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 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


5-12-1 #2-5 RT: 0.01-0.02 AV: 4 NL: 1.53E7
T: FTMS + p APCI corona Full lock ms [180.00-420.00]
263.07038
C17 H11 O3
264.07375
C17 H12 O3
265.08563
C17 H13 O3
266.08924
C17 H14 O3
Relative Abundance
m/z

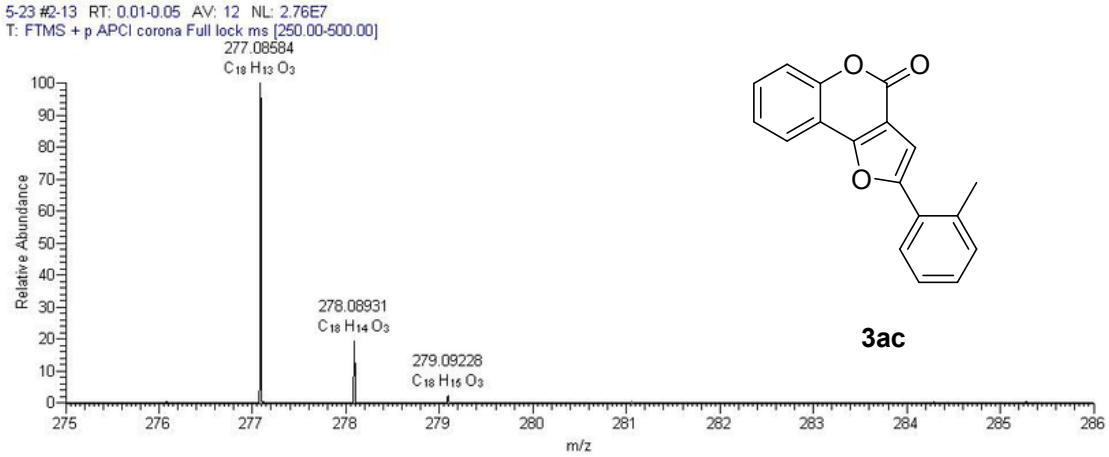
O
O
O

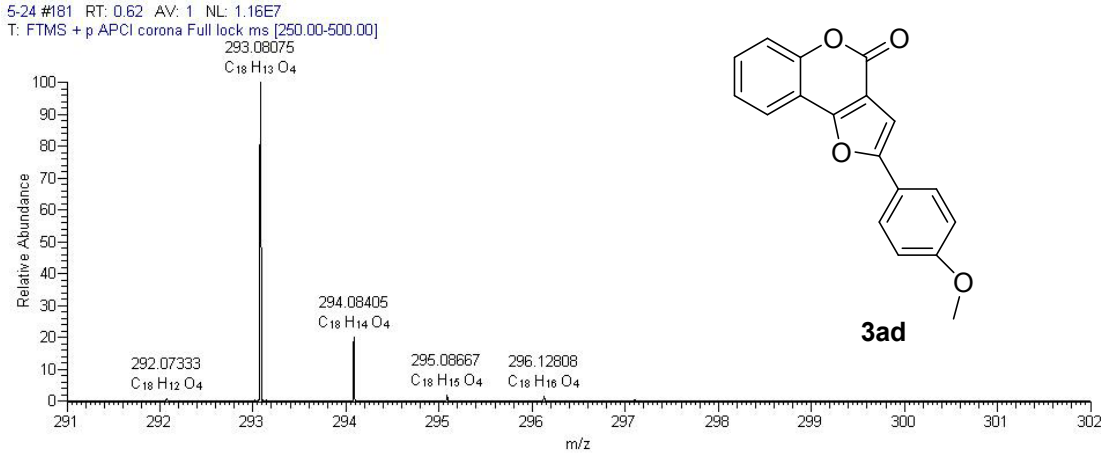
3aa

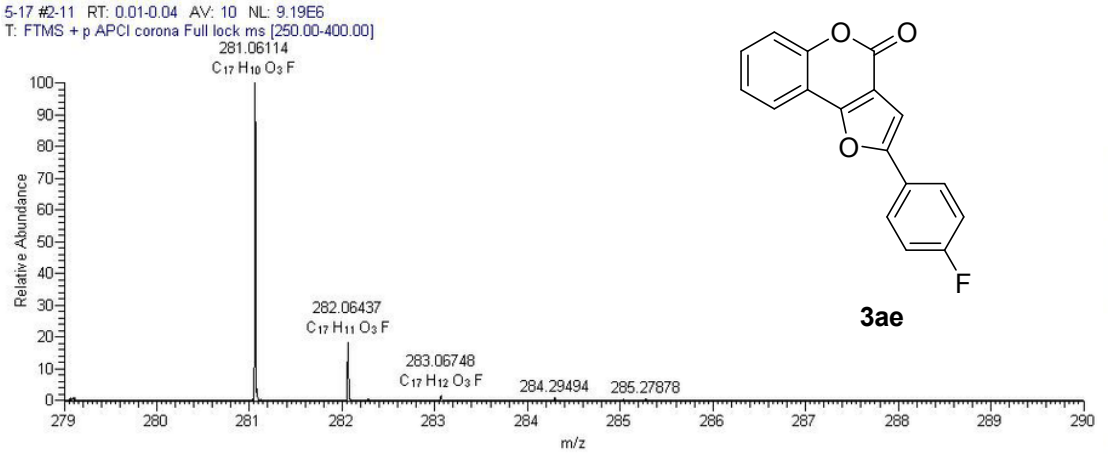

5-11 #2-7 RT: 0.01-0.03 AV: 6 NL: 1.14E8
T: FTMS + p APCI corona Full lock ms [250.00-500.00]
277.08574
278.08922
275.27765
276.07859
279.09216
282.27870
284.29444
Relative Abundance
m/z

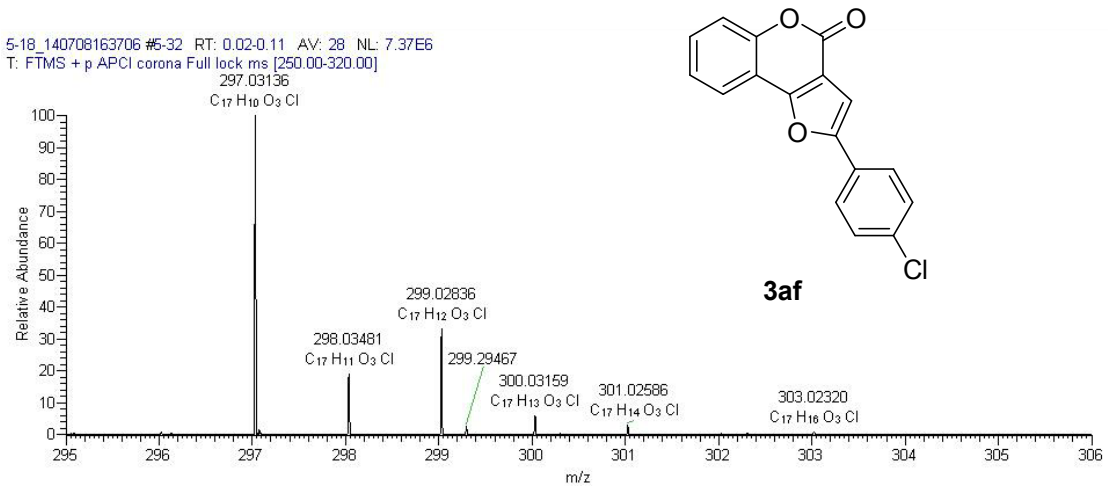
O
O
O

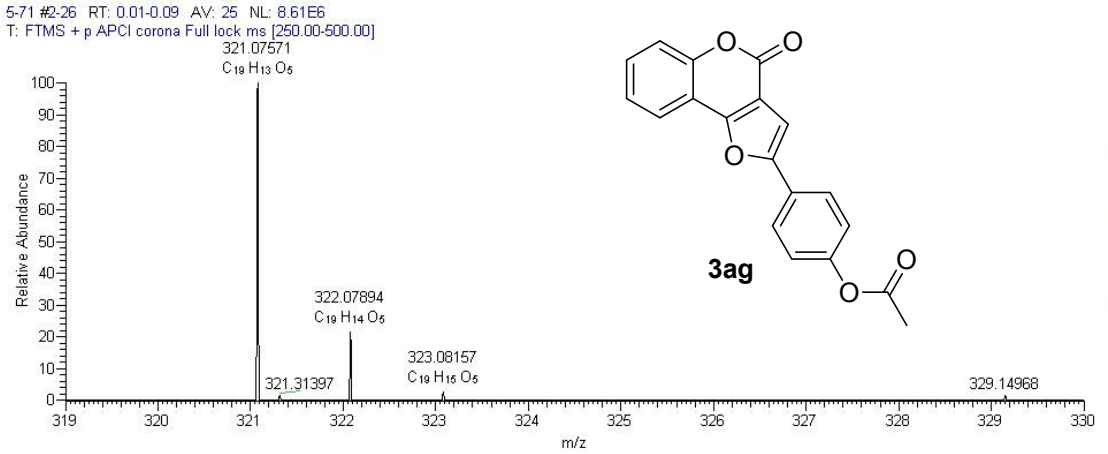
3ab

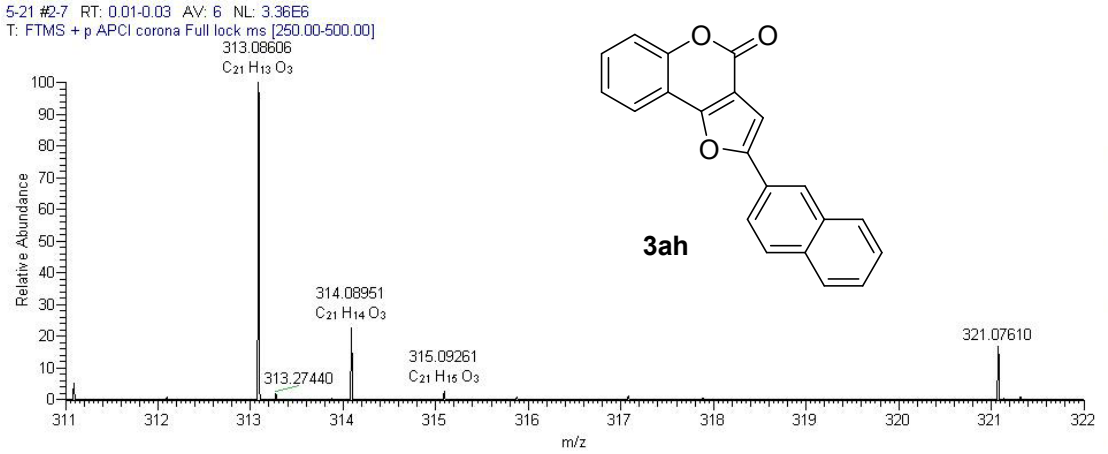

5-23 #2-13 RT: 0.01-0.05 AV: 12 NL: 2.76E7
T: FTMS + p APCI corona Full lock ms [250.00-500.00]
277.08584
C18 H13 O3
278.08931
C18 H14 O3
279.09228
C18 H15 O3
Relative Abundance
m/z
3ac

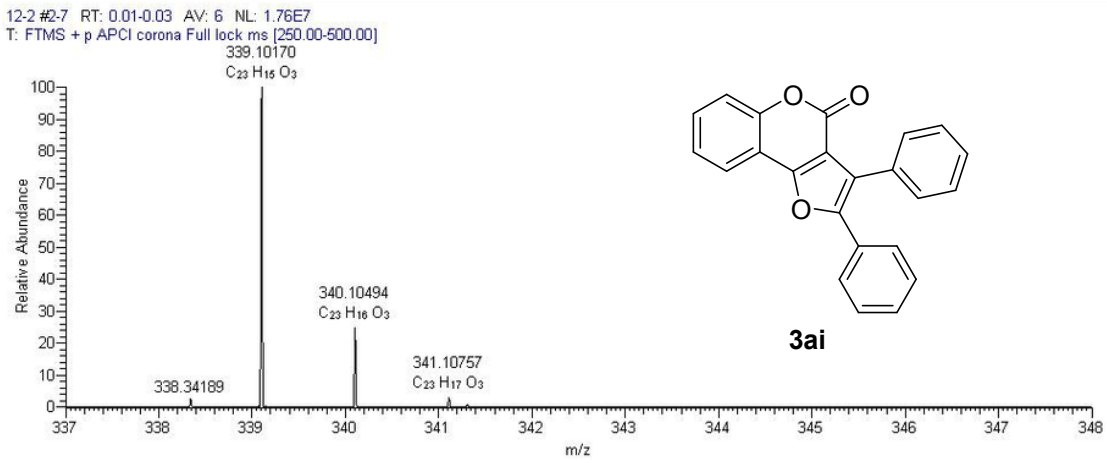

5-24 #181 RT: 0.62 AV: 1 NL: 1.16E7
T: FTMS + p APCI corona Full lock ms [250.00-500.00]
293.08075
C18 H13 O4
294.08405
C18 H14 O4
292.07333
C18 H12 O4
295.08667
C18 H15 O4
296.12808
C18 H16 O4
Relative Abundance
m/z
3ad

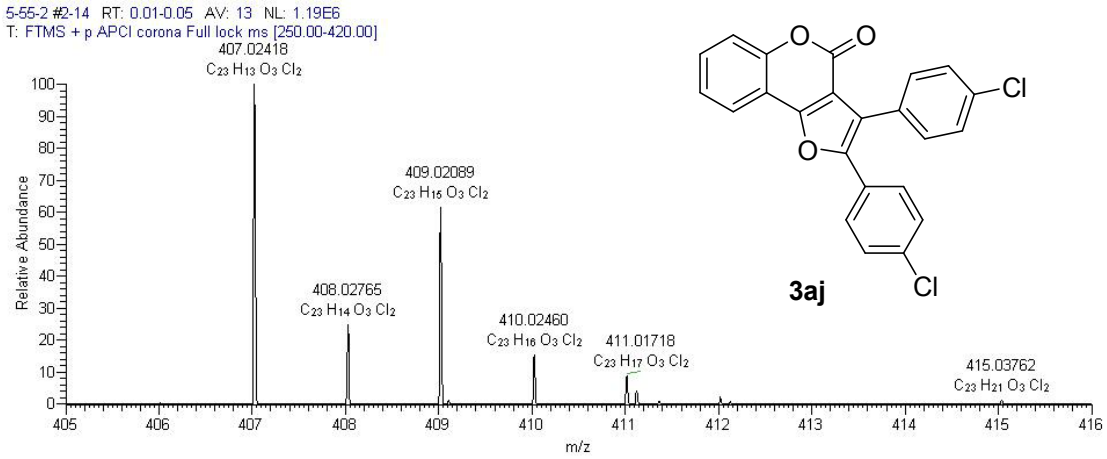

5-17 #2-11 RT: 0.01-0.04 AV: 10 NL: 9.19E6
T: FTMS + p APCI corona Full lock ms [250.00-400.00]
281.06114
C17 H10 O3 F
282.06437
C17 H11 O3 F
283.06748
C17 H12 O3 F
284.29494
285.27878
Relative Abundance
m/z
3ae

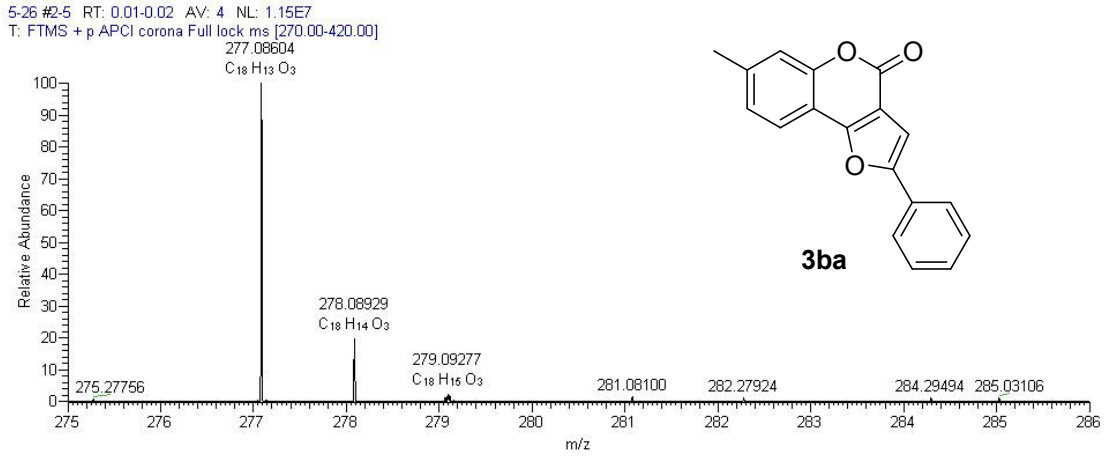

5-18_140708163706 #5-32 RT: 0.02-0.11 AV: 28 NL: 7.37E6
T: FTMS + p APCI corona Full lock ms [250.00-320.00]
297.03136
C17 H10 O3 Cl
299.02836
C17 H12 O3 Cl
298.03481
C17 H11 O3 Cl
299.29467
300.03159
C17 H13 O3 Cl
301.02586
C17 H14 O3 Cl
303.02320
C17 H16 O3 Cl
Relative Abundance
m/z
3af

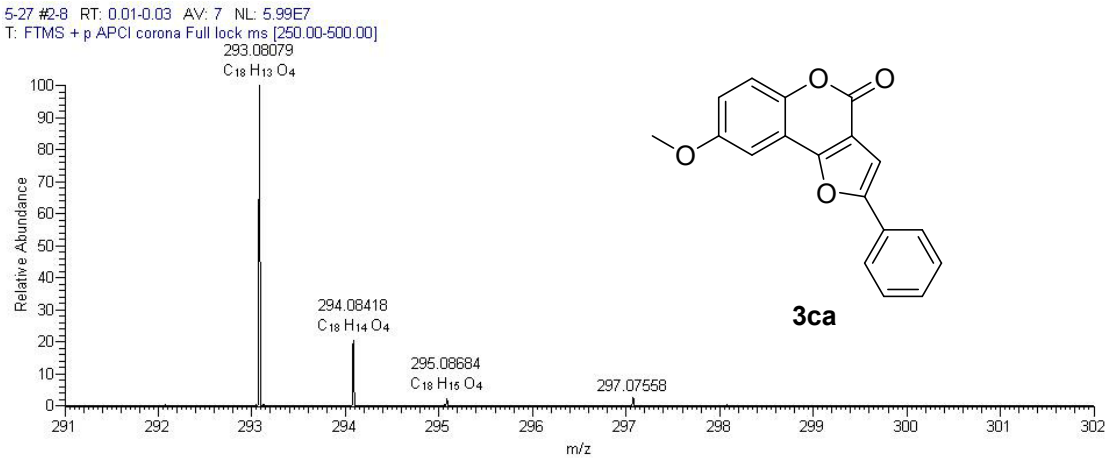

5-71 #2-26 RT: 0.01-0.09 AV: 25 NL: 8.61E6
T: FTMS + p APCI corona Full lock ms [250.00-500.00]
321.07571
C19 H13 O5
322.07894
C19 H14 O5
323.08157
C19 H15 O5
321.31397
329.14968
Relative Abundance
m/z
3ag

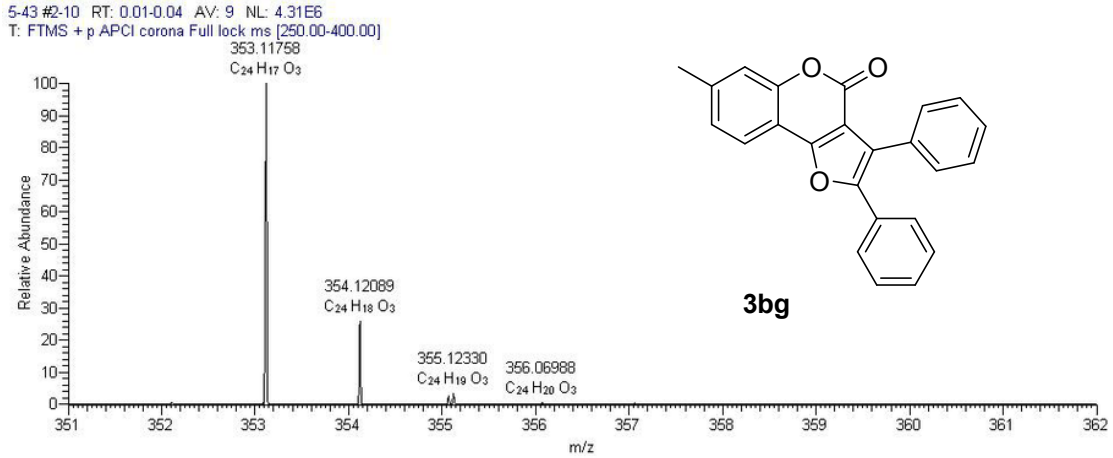

5-21 #2-7 RT: 0.01-0.03 AV: 6 NL: 3.36E6
T: FTMS + p APCI corona Full lock ms [250.00-500.00]
313.08606
C21 H13 O3
314.08951
C21 H14 O3
315.09261
C21 H15 O3
313.27440
321.07610
Relative Abundance
m/z
3ah

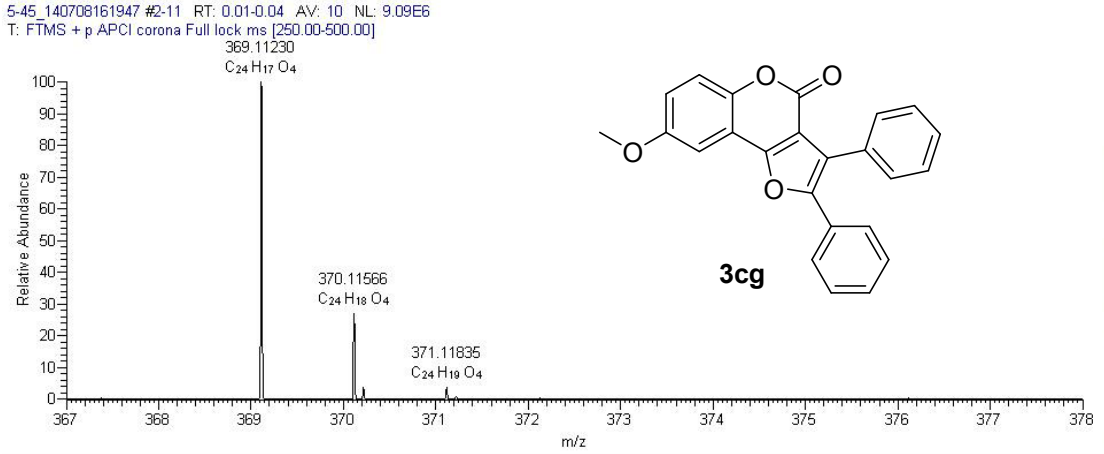

12-2 #2-7 RT: 0.01-0.03 AV: 6 NL: 1.76E7
T: FTMS + p APCI corona Full lock ms [250.00-500.00]
339.10170
C23 H15 O3
340.10494
C23 H16 O3
341.10757
C23 H17 O3
338.34189
Relative Abundance
m/z
3ai

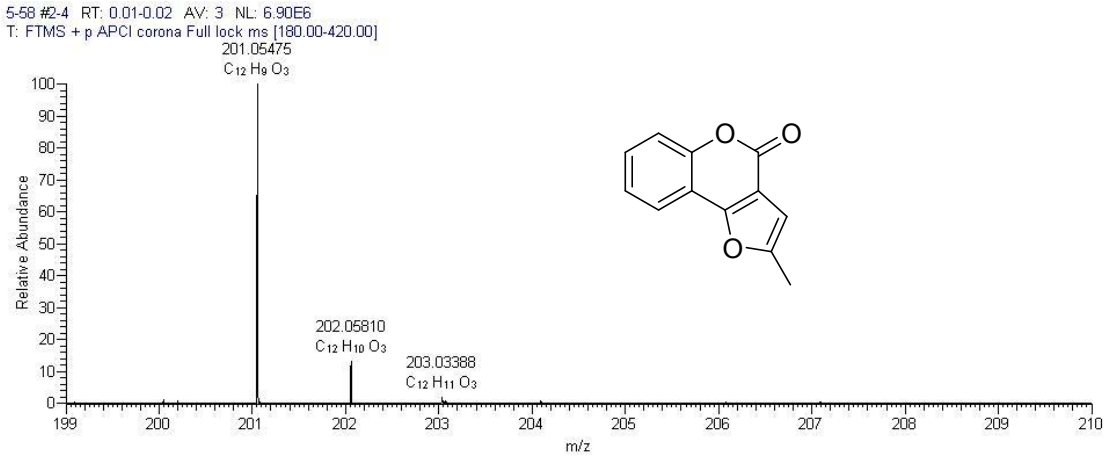

5-55-2 #2-14 RT: 0.01-0.05 AV: 13 NL: 1.19E6
T: FTMS + p APCI corona Full lock ms [250.00-420.00]
407.02418
C23 H13 O3 Cl2
409.02089
C23 H15 O3 Cl2
408.02765
C23 H14 O3 Cl2
410.02460
C23 H16 O3 Cl2
411.01718
C23 H17 O3 Cl2
415.03762
C23 H21 O3 Cl2
Relative Abundance
m/z
Cl
Cl
3aj

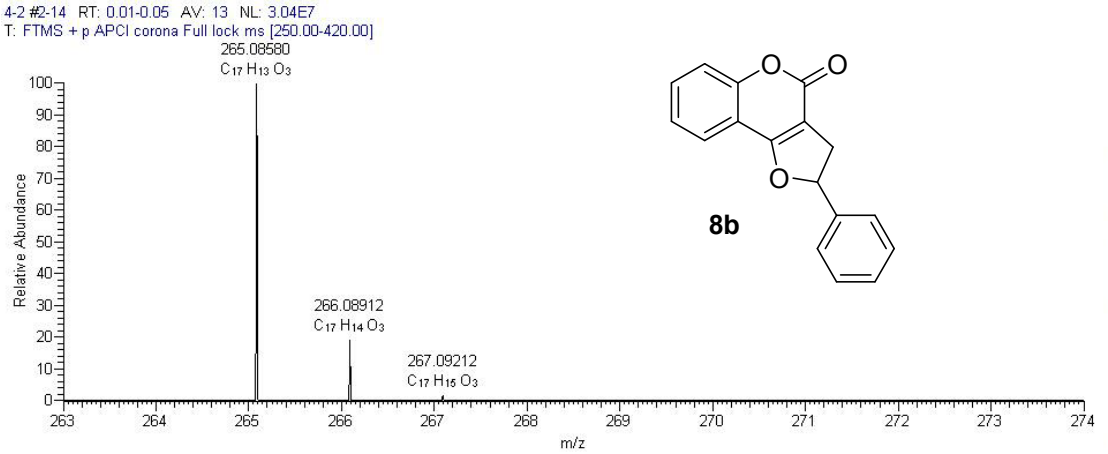

5-26 #2-5 RT: 0.01-0.02 AV: 4 NL: 1.15E7
T: FTMS + p APCI corona Full lock ms [270.00-420.00]
277.08604
C18 H13 O3
278.08929
C18 H14 O3
279.09277
C18 H15 O3
275.27756
281.08100
282.27924
284.29494
285.03106
Relative Abundance
m/z
3ba


5-27 #2-8 RT: 0.01-0.03 AV: 7 NL: 5.99E7
T: FTMS + p APCI corona Full lock ms [250.00-500.00]
293.08079
C18 H13 O4
294.08418
C18 H14 O4
295.08684
C18 H15 O4
297.07558
Relative Abundance
m/z
3ca


5-43 #2-10 RT: 0.01-0.04 AV: 9 NL: 4.31E6
T: FTMS + p APCI corona Full lock ms [250.00-400.00]
353.11758
C24 H17 O3
354.12089
C24 H18 O3
355.12330
C24 H19 O3
356.06988
C24 H20 O3
Relative Abundance
m/z
3bg


5-45_140708161947 #2-11 RT: 0.01-0.04 AV: 10 NL: 9.09E6
T: FTMS + p APCI corona Full lock ms [250.00-500.00]
369.11230
C24 H17 O4
370.11566
C24 H18 O4
371.11835
C24 H19 O4
Relative Abundance
m/z
3cg


5-58 #2-4 RT: 0.01-0.02 AV: 3 NL: 6.90E6
T: FTMS + p APCI corona Full lock ms [180.00-420.00]
201.05475
C12 H9 O3
202.05810
C12 H10 O3
203.03388
C12 H11 O3
Relative Abundance
m/z


4-2 #2-14 RT: 0.01-0.05 AV: 13 NL: 3.04E7
T: FTMS + p APCI corona Full lock ms [250.00-420.00]
265.08580
C17 H13 O3
266.08912
C17 H14 O3
267.09212
C17 H15 O3
Relative Abundance
m/z

8b