

## Supporting Information

### Visible Light-induced Deoxygenation/Coupling Cyclization of Salicylic Acid Derivatives and Aryl Acetylene for Synthesis of Flavonoids

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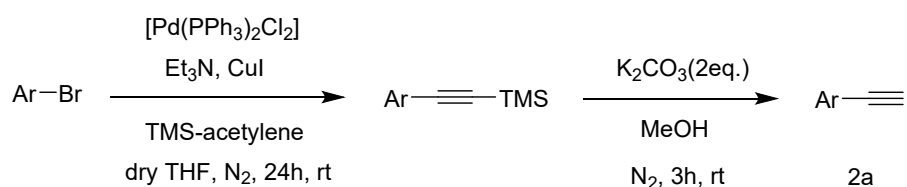
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## General Information

All starting materials and the reagents were purchased from TCI and J&K Chemical Company, and the reagents were used without further purification unless specified. The reactions were monitored by thin layer chromatography (TLC), and the products were purified by column chromatography on silica gel (300 ~ 400 mesh).  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on a Bruker Ultrashield™ 400 spectrometer operating at 400 MHz and 100 MHz in  $\text{CDCl}_3$  or DMSO. Chemical shifts were reported in ppm with tetramethylsilane (TMS) as internal standard. The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, t = triplet, m = multiple. Coupling constants (J) were reported in Hertz (Hz). Melting points were recorded on a WRR melting point apparatus. Infrared spectra were recorded with the Perkin-Elmer Spectrum100 Fourier transform infrared spectroscopy. Elemental analyses of C, H and N were performed on a Elementar Vario MICRO cube. High resolution mass spectrum (HRMS) was accomplished on Agilent1100 (VL) mass spectrometer.

## Experimental Section

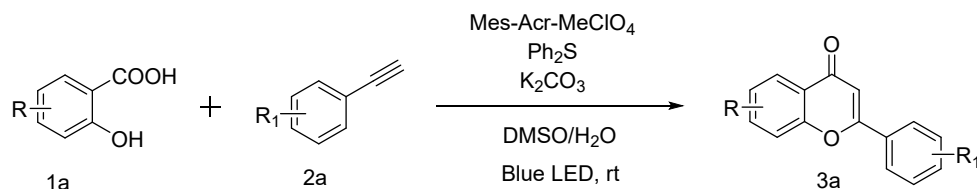
### 1. General procedure for the synthesis of 2a



The an oven-dried screw cap reaction tube was charged with a magnetic stir-bar  $[\text{Pd}(\text{PPh}_3)_2\text{Cl}_2]$  (0.02 mmol; 14 mg), CuI (0.04 mmol; 7.6 mg) and bromo-substrate (1 mmol). To that, dry THF (1 mL) followed by triethylamine (1.55 mmol; 216  $\mu\text{L}$ ) was added under nitrogen atmosphere with stirring at room temperature. Under nitrogen atmosphere, trimethylsilylacetylene (1.25 mmol; 176  $\mu\text{L}$ ) was added to the reaction mixture slowly. Gradually the reaction turned dark. The reaction was stirred continuously for 24 h at room temperature. The progress of the reaction was monitored by TLC. Once the reaction was done, the mixture was diluted with 5 mL

EtOAc and filtered through the celite. The filtrate was evaporated under reduced pressure and the compound was isolated through silica column (100-200 mesh).<sup>1</sup>

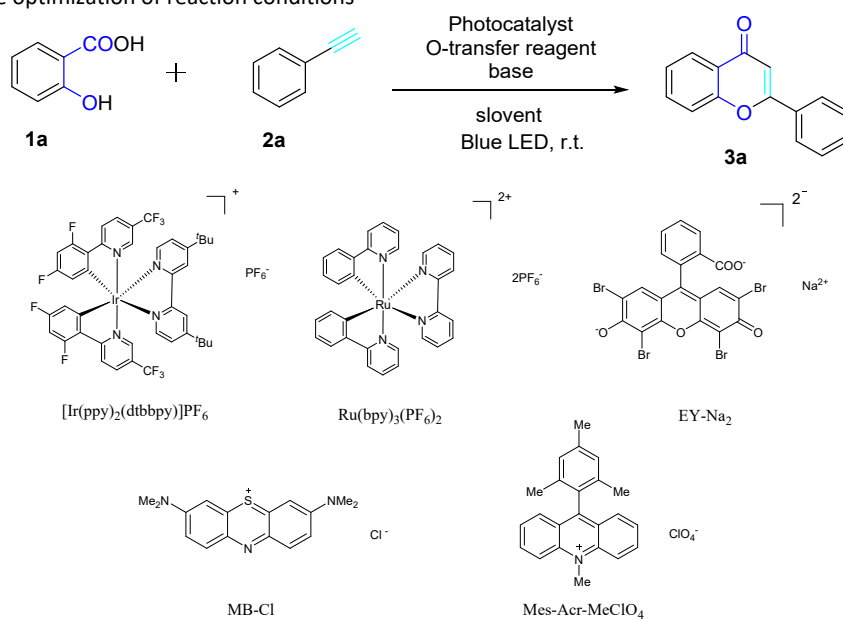
## 2. General procedure for the synthesis of 3a



The corresponding salicylic acid (1a, 0.2 mmol), Phenylacetylene (2a, 0.24 mmol), Mes-Acr-MeClO<sub>4</sub> (5 mol%), Ph<sub>2</sub>S(0.3 mmol), and K<sub>2</sub>CO<sub>3</sub>(0.04 mmol) were dissolved in 2 mL DMSO/H<sub>2</sub>O (4:1) in a sealed quartz tube. Next, the reaction mixture was placed under a blue LED and irradiated at room temperature. After the reaction was completed (monitored by TLC), an appropriate amount of water was added to the mixture, and the mixed solution was extracted with ethyl acetate (15 mL×3). The combined organic phases were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, concentrated in vacuo and the crude product was obtained. The pure product was obtained by silica gel chromatography using petroleum ether/ ethyl acetate (10:1) as eluent.

## 3. Optimisation Studies

**Table S1.** The optimization of reaction conditions <sup>[a]</sup>

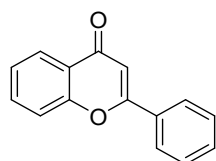


entry	catalyst	O-transfer reagent <sup>l</sup>	base	solvent	Yield(%) <sup>b</sup>
1	[Ir(ppy) <sub>2</sub> (dtbbpy)]PF <sub>6</sub>	Ph <sub>2</sub> S	Na <sub>2</sub> CO <sub>3</sub>	DCM	25
2	Ru(bpy) <sub>3</sub> (PF <sub>6</sub> ) <sub>2</sub>	Ph <sub>2</sub> S	Na <sub>2</sub> CO <sub>3</sub>	DCM	0
3	EY-Na <sub>2</sub>	Ph <sub>2</sub> S	Na <sub>2</sub> CO <sub>3</sub>	DCM	0
4	MB-Cl	Ph <sub>2</sub> S	Na <sub>2</sub> CO <sub>3</sub>	DCM	12
5	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	Na <sub>2</sub> CO <sub>3</sub>	DCM	42
6	Mes-Acr-MeClO <sub>4</sub>	Thianthrene	Na <sub>2</sub> CO <sub>3</sub>	DCM	11
7	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>3</sub> P	Na <sub>2</sub> CO <sub>3</sub>	DCM	trace
8	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	Cs <sub>2</sub> CO <sub>3</sub>	DCM	21
9	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	K <sub>2</sub> HPO <sub>4</sub>	DCM	35
10	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	K <sub>2</sub> CO <sub>3</sub>	DCM	50
11	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	Et <sub>3</sub> N	DCM	10
12	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	2,4,6-collidine	DCM	40
13	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	K <sub>2</sub> CO <sub>3</sub>	CH <sub>3</sub> CN	22
14	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	K <sub>2</sub> CO <sub>3</sub>	DMF	56
15	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	K <sub>2</sub> CO <sub>3</sub>	DMSO	60
16	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	K <sub>2</sub> CO <sub>3</sub>	(DCM)/H <sub>2</sub> O (4:1)	60
17	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	K <sub>2</sub> CO <sub>3</sub>	(DMF)/H <sub>2</sub> O (4:1)	68
18	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	K <sub>2</sub> CO <sub>3</sub>	(DMSO)/H <sub>2</sub> O (4:1)	75,0 <sup>c</sup>
19	-	Ph <sub>2</sub> S	K <sub>2</sub> CO <sub>3</sub>	(DMSO)/H <sub>2</sub> O (4:1)	0
20	Mes-Acr-MeClO <sub>4</sub>	-	K <sub>2</sub> CO <sub>3</sub>	(DMSO)/H <sub>2</sub> O (4:1)	0
21	Mes-Acr-MeClO <sub>4</sub>	Ph <sub>2</sub> S	-	(DMSO)/H <sub>2</sub> O (4:1)	trace

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.24 mmol), Mes-Acr-MeClO<sub>4</sub> (5.0 mol%), Ph<sub>2</sub>S (1.5 eq.) and K<sub>2</sub>CO<sub>3</sub> (0.2 eq.) in (DMSO)/H<sub>2</sub>O 2 ml, irradiation with blue light LEDs at 25 °C, the reaction completed (monitored by TLC). [b] isolated yield. [c] Control experiment without blue LEDs.

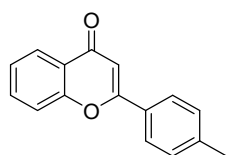
## Characterization of the data

### 2-Phenyl-4H-chromen-4-one<sup>2</sup> (3a):



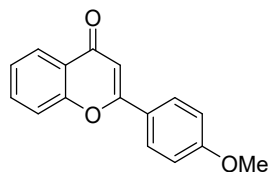
White solid, m.p.: 95-96 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.24 (d, *J* = 8.9 Hz, 1H), 7.93 (dd, *J* = 7.3, 2.2 Hz, 2H), 7.70 (t, *J* = 8.4 Hz, 1H), 7.55 (dd, *J* = 16.8, 7.7 Hz, 4H), 7.42 (t, *J* = 7.5 Hz, 1H), 6.83 (s, 1H) (**Figure S1**). <sup>13</sup>C NMR (101 MHz, Chloroform-*d*) δ 178.39, 163.31, 156.20, 133.76, 131.69, 131.60, 129.02, 126.24, 125.64, 125.20, 123.94, 118.09, 107.53 (**Figure S2**). Anal.calcd for: C<sub>15</sub>H<sub>10</sub>O<sub>2</sub>: C 81.07, H 4.54; Found: C 81.12, H 4.56. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1645, 1607, 1570, 1133, 770.

### 2-(*p*-Tolyl)-4H-chromen-4-one<sup>2</sup> (3b):



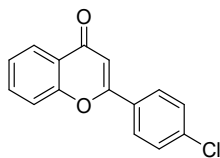
Yellow solid, m.p.: 109-110 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.22 (d, *J* = 7.7 Hz, 1H), 7.81 (d, *J* = 7.9 Hz, 2H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.41 (t, *J* = 7.4 Hz, 1H), 7.31 (d, *J* = 7.9 Hz, 2H), 6.79 (s, 1H), 2.43 (s, 3H) (**Figure S3**). <sup>13</sup>C NMR (101 MHz, Chloroform-*d*) δ 178.88, 163.88, 156.27, 142.38, 133.81, 129.79, 129.18, 126.30, 125.73, 125.23, 123.82, 118.07, 106.83, 21.76 (**Figure S4**). Anal.calcd for: C<sub>16</sub>H<sub>12</sub>O<sub>2</sub>: C 81.34, H 5.12; Found: C 81.35, H 5.14. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1639, 1465, 1370, 1225, 815, 750, 632.

### 2-(4-Methoxyphenyl)-4H-chromen-4-one<sup>3</sup> (3c):



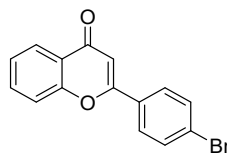
White solid, m.p.: 133-135 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.14 (d, *J* = 8.6 Hz, 1H), 7.94-7.90 (m, 2H), 7.55-7.51 (m, 3H), 6.99 (d, *J* = 10.0 Hz, 2H), 6.78 (s, 1H), 3.94 (s, 3H) (**Figure S5**). <sup>13</sup>C NMR (101 MHz, Chloroform-*d*) δ 178.54, 163.64, 162.53, 156.28, 133.73, 128.18, 125.72, 125.27, 124.05, 123.95, 118.11, 114.60, 106.20, 55.82 (**Figure S6**). Anal.calcd for: C<sub>16</sub>H<sub>12</sub>O<sub>3</sub>: C 76.18, H 4.79; Found: C 76.22, H 4.82. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 3425, 2920, 1650, 1610, 1465, 1380, 1131, 826, 769.

### 2-(4-Chlorophenyl)-4H-chromen-4-one<sup>2</sup> (3d):



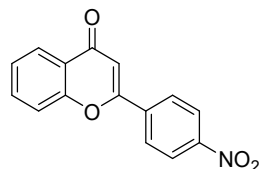
White solid, m.p.: 177-178 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.23 (d,  $J$  = 9.3 Hz, 1H), 7.87 (d,  $J$  = 8.7 Hz, 2H), 7.71 (t,  $J$  = 8.6 Hz, 1H), 7.58-7.40 (m, 4H), 6.79 (s, 1H) (**Figure S7**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  178.18, 162.13, 156.10, 137.86, 133.90, 130.17, 129.35, 127.50, 125.70, 125.36, 123.87, 118.03, 107.63 (**Figure S8**). Anal.calcd for:  $\text{C}_{15}\text{H}_9\text{ClO}_2$ : C 70.19, H 3.53, Cl 13.81; Found: C 70.21, H 3.54; Cl 13.78. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1666, 1376, 1095, 824, 753.

**2-(4-Bromophenyl)-4H-chromen-4-one<sup>4</sup> (3e):**



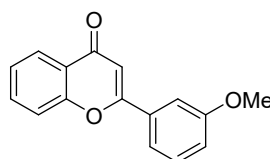
Yellow solid, m.p.: 148-151 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.22 (d,  $J$  = 7.7 Hz, 1H), 7.78 (d,  $J$  = 8.5 Hz, 2H), 7.68 (dt,  $J$  = 14.3, 7.7 Hz, 3H), 7.55 (d,  $J$  = 8.0 Hz, 1H), 7.42 (t,  $J$  = 7.0 Hz, 1H), 6.79 (s, 1H) (**Figure S9**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  178.21, 162.23, 156.12, 133.93, 132.34, 130.66, 127.67, 126.31, 125.73, 125.38, 123.89, 118.05, 107.67 (**Figure S10**). Anal.calcd for:  $\text{C}_{15}\text{H}_9\text{BrO}_2$ : C 59.83, H 3.01, Br 26.53; Found: C 59.86, H 3.02; Br 26.51. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1644, 1609, 1471, 1363.

**2-(4-Nitrophenyl)-4H-chromen-4-one<sup>5</sup> (3f):**



Yellow solid, m.p.: 232-235 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.39 (d,  $J$  = 8.7 Hz, 2H), 8.25 (d,  $J$  = 7.9 Hz, 1H), 8.12 (d,  $J$  = 8.7 Hz, 2H), 7.76 (t,  $J$  = 7.3 Hz, 1H), 7.61 (d,  $J$  = 8.4 Hz, 1H), 7.48 (t,  $J$  = 7.5 Hz, 1H), 6.92 (s, 1H) (**Figure S11**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  177.97, 160.58, 156.18, 149.45, 137.66, 134.34, 127.23, 125.89, 125.77, 124.25, 123.93, 118.14, 109.64 (**Figure S12**). Anal.calcd for:  $\text{C}_{15}\text{H}_9\text{NO}_4$ : C 67.42, H 3.39, N 5.24; Found: C 67.44, H 3.43, N 5.22. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1660, 1523, 1347, 857.

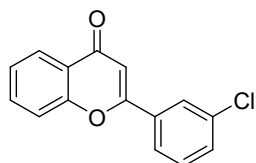
**2-(3-methoxyphenyl)-4H-chromen-4-one<sup>2</sup> (3g):**



White solid, m.p.: 126-128 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.24 (d,  $J$  = 7.9 Hz, 1H), 7.70 (d,  $J$  = 8.6 Hz, 1H), 7.58 (d,  $J$  = 8.4 Hz, 1H), 7.52 (d,  $J$  = 7.9 Hz, 1H), 7.47-7.41 (m, 3H), 7.09 (d,  $J$  = 10.0 Hz, 1H), 6.83 (s, 1H), 3.90 (s, 3H). (**Figure S13**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  179.08, 163.36, 160.14,

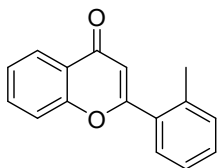
156.43, 133.94, 133.27, 130.29, 125.84, 125.39, 118.87, 118.27, 117.31, 111.90, 108.04, 55.54 (**Figure S14**). Anal.calcd for: C<sub>16</sub>H<sub>12</sub>O<sub>3</sub>: C 76.18, H 4.79; Found: C 76.21, H 4.82. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 3078, 3000, 2922, 2842, 1653, 1606, 1572, 1491, 1469, 1446, 1434, 1369, 1346, 1330, 1295, 1275, 1249, 1228, 1213, 1192, 1130.

**2-(3-chlorophenyl)-4H-chromen-4-one<sup>2</sup> (3h):**



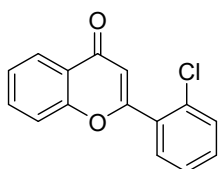
White solid, m.p.: 117-119 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  8.22 (d,  $J = 9.3$  Hz, 1H), 7.91 (s, 1H), 7.80 - 7.69 (m, 2H), 7.60 -7.41 (m, 4H), 6.79 (s, 1H) (**Figure S15**). <sup>13</sup>C NMR (101 MHz, Chloroform-*d*)  $\delta$  177.85, 161.37, 155.89, 135.08, 133.87, 133.27, 131.36, 130.22, 126.08, 125.52, 125.30, 124.19, 123.72, 117.99, 107.88 (**Figure S16**). Anal.calcd for: C<sub>15</sub>H<sub>9</sub>ClO<sub>2</sub>: C 70.19, H 3.53, Cl 13.81; Found: C 70.21, H 3.54; Cl 13.80. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 3085, 1645, 1565, 1466, 1422, 1372, 1335, 1304, 1261, 1226, 1131.

**2-(o-tolyl)-4H-chromen-4-one<sup>2</sup> (3i):**



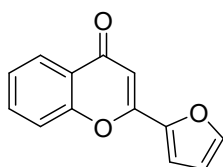
Yellow solid, m.p.: 104-106 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  8.25 (s, 1H), 7.72-7.63 (m, 1H), 7.54-7.45 (m, 2H), 7.40 (s, 2H), 7.30 (s, 1H), 6.56-6.41 (m, 1H), 2.48 (s, 3H) (**Figure S17**). <sup>13</sup>C NMR (101 MHz, Chloroform-*d*)  $\delta$  178.11, 165.98, 156.40, 136.74, 133.77, 132.54, 131.28, 130.73, 129.17, 126.21, 125.66, 125.21, 123.78, 118.06, 111.89, 20.59 (**Figure S18**). Anal.calcd for: C<sub>16</sub>H<sub>12</sub>O<sub>2</sub>: C 81.34, H 5.12; Found: C 81.35, H 5.14. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 2926, 1652, 1571, 1465, 1370, 1220, 1130.

**2-(2-chlorophenyl)-4H-chromen-4-one<sup>2</sup> (3j):**



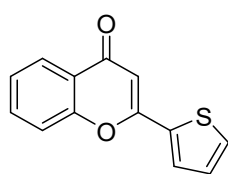
White solid, m.p.: 118-120 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  8.26 (dd,  $J = 7.9, 1.4$  Hz, 1H), 7.74-7.67 (m, 1H), 7.64 (dd,  $J = 7.4, 1.8$  Hz, 1H), 7.57-7.49 (m, 2H), 7.49-7.38 (m, 3H), 6.66 (s, 1H) (**Figure S19**). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.04, 162.56, 156.54, 133.93, 132.83, 131.81, 130.79, 130.63, 127.12, 125.68, 125.33, 123.79, 118.20, 112.97 (**Figure S20**). Anal.calcd for: C<sub>15</sub>H<sub>9</sub>ClO<sub>2</sub>: C 70.19, H 3.53, Cl 13.81; Found: C 70.21, H 3.54; Cl 13.78. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 2926, 1652, 1571, 1465, 1370, 1220, 1130.

**2-(Furan-2-yl)-4H-chromen-4-one<sup>6</sup> (3k):**



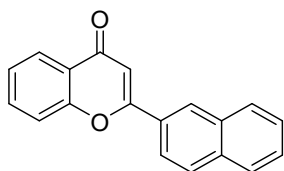
White solid, m.p.: 126-128 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.21 (d,  $J = 7.7$  Hz, 1H), 7.71-7.61 (m, 2H), 7.50 (d,  $J = 8.4$  Hz, 1H), 7.40 (t,  $J = 7.5$  Hz, 1H), 7.14 (d,  $J = 3.4$  Hz, 1H), 6.74 (s, 1H), 6.61 (s, 1H) (**Figure S21**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  177.76, 155.79, 155.14, 146.39, 145.77, 133.70, 125.74, 125.16, 124.22, 117.87, 113.02, 112.51, 105.50 (**Figure S22**). Anal.calcd for:  $\text{C}_{13}\text{H}_8\text{O}_3$ : C 73.58, H 3.80; Found: C 73.61, H 3.82. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1649, 1605, 1577, 1130, 775.

#### 2-(Thiophen-2-yl)-4H-chromen-4-one<sup>2</sup> (3l):



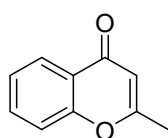
White solid, m.p.: 93-94 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.20 (d,  $J = 7.8$  Hz, 1H), 7.74 – 7.64 (m, 2H), 7.57 (d,  $J = 4.8$  Hz, 1H), 7.52 (d,  $J = 8.4$  Hz, 1H), 7.40 (t,  $J = 7.5$  Hz, 1H), 7.18 (t,  $J = 4.0$  Hz, 1H), 6.69 (s, 1H) (**Figure S23**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  177.86, 159.00, 155.89, 135.12, 133.74, 130.26, 128.49, 128.44, 125.65, 125.25, 123.97, 117.93, 106.17 (**Figure S24**). Anal.calcd for:  $\text{C}_{13}\text{H}_8\text{O}_2\text{S}$ : C 68.40, H 3.53, S 14.05; Found: C 68.41, H 3.55, S 14.03. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3070, 1634, 1462, 1260, 1127.

#### 2-(naphthalen-2-yl)-4H-chromen-4-one<sup>2</sup> (3m):



Yellow solid, m.p.: 159-161 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.41 (s, 1H), 8.23 (dd,  $J = 7.9, 1.5$  Hz, 1H), 7.97-7.82 (m, 4H), 7.69 (dd,  $J = 8.6, 7.1, 1.6$  Hz, 1H), 7.62 - 7.50 (m, 3H), 7.45-7.36 (m, 1H), 6.91 (s, 1H) (**Figure S25**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  178.35, 163.22, 156.29, 134.63, 133.75, 132.87, 129.03, 128.89, 127.99, 127.80, 127.05, 126.86, 125.70, 125.21, 122.45, 118.09, 107.84 (**Figure S26**). Anal.calcd for:  $\text{C}_{19}\text{H}_{12}\text{O}_2$ : C 83.81, H 4.44; Found: C 83.82, H 4.46. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3070, 1637, 1567, 1503, 1463, 1437, 1380, 1347, 1330, 1283, 1225, 1202, 1131.

#### 2-Methyl-4H-chromen-4-one (3n):

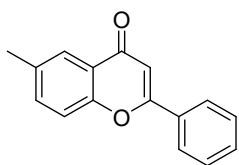


Yellow solid, m.p.: 71-73 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.18 (d,  $J = 9.4$  Hz, 1H), 7.63 (ddd,  $J = 8.6, 7.3, 1.6$  Hz, 1H), 7.41 (d,  $J = 8.3$  Hz, 1H), 7.37 (t,  $J = 7.6$  Hz, 1H), 6.17 (s, 1H), 2.39 (s, 3H)



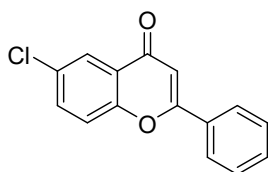
(**Figure S27**).  $^{13}\text{C}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  178.20, 166.14, 156.47, 133.41, 125.64, 124.89, 123.57, 117.77, 110.57 (**Figure S28**). HRMS:  $\text{C}_{10}\text{H}_8\text{O}_2$  for  $[\text{M}+\text{H}]^+$ : 161.0525; Found: 161.0530. Anal.calcd for:  $\text{C}_{10}\text{H}_8\text{O}_2$ : C 74.99, H 5.03; Found: C 75.01, H 5.05. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1652.

**6-methyl-2-phenyl-4H-chromen-4-one<sup>2</sup> (3o):**



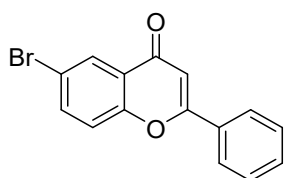
White solid, m.p.: 111-113 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.01 (s, 1H), 7.97-7.87 (m, 2H), 7.49 (dt,  $J = 16.4, 5.7$  Hz, 5H), 6.81 (s, 1H), 2.46 (s, 3H) (**Figure S29**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  178.43, 163.09, 154.43, 135.11, 134.92, 131.76, 131.45, 128.96, 126.17, 124.95, 123.54, 117.81, 107.30, 20.91 (**Figure S30**). Anal.calcd for:  $\text{C}_{16}\text{H}_{12}\text{O}_2$ : C, 81.34; H, 5.12; Found: C, 81.35; H, 5.14. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3064, 2920, 1645, 1615, 1569, 1494, 1483, 1450, 1431, 1361, 1302, 1255, 1223, 1139.

**6-chloro-2-phenyl-4H-chromen-4-one<sup>2</sup> (3p):**



White solid, m.p.: 182-184 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.21 (d,  $J = 2.5$  Hz, 1H), 7.94-7.90 (m, 2H), 7.65 (dd,  $J = 8.9, 2.5$  Hz, 1H), 7.55 (d,  $J = 6.9$  Hz, 4H), 6.83 (s, 1H) (**Figure S31**).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  177.10, 163.61, 154.50, 133.92, 131.87, 131.31, 131.16, 129.10, 126.28, 125.11, 124.88, 119.81, 107.40 (**Figure S32**). Anal.calcd for:  $\text{C}_{15}\text{H}_9\text{ClO}_2$ : C, 70.19; H, 3.53; Cl, 13.81; Found: C, 70.21; H, 3.54; Cl, 13.78. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3085, 1648, 1615, 1601, 1566, 1494, 1456, 1436, 1353, 1306, 1291, 1272, 1253, 1132.

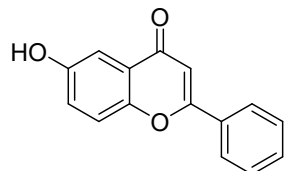
**6-bromo-2-phenyl-4H-chromen-4-one<sup>2</sup> (3q):**



White solid, m.p.: 188-190 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.36 (d,  $J = 2.4$  Hz, 1H), 7.93-7.90 (m, 2H), 7.79 (dd,  $J = 8.9, 2.4$  Hz, 1H), 7.54 (d,  $J = 7.4$  Hz, 3H), 7.48 (d,  $J = 8.9$  Hz, 1H), 6.84 (s, 1H) (**Figure S33**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  177.05, 163.72, 154.96, 136.74, 131.92, 131.28, 129.12, 128.33, 126.32, 125.21, 120.05, 118.70, 107.48 (**Figure S34**). Anal.calcd for:  $\text{C}_{15}\text{H}_9\text{BrO}_2$ : C, 59.83; H, 3.01; Br, 26.53; Found: C, 59.86; H, 3.02; Br, 26.52. IR

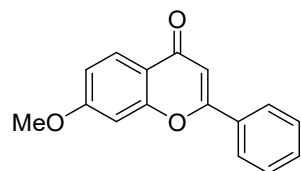
(KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 3083, 2920, 1648, 1614, 1597, 1563, 1494, 1456, 1434, 1350, 1304, 1271, 1253, 1210, 1133.

**6-hydroxy-2-phenyl-4H-chromen-4-one<sup>8</sup> (3r):**



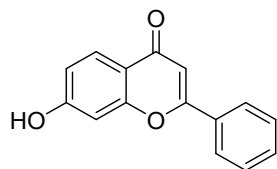
Yellow solid, m. p.: 231-233 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  9.87 (s, 1H), 7.82 (d, *J* = 5.6 Hz, 2H), 7.44-7.30 (m, 4H), 7.14 (d, *J* = 2.9 Hz, 1H), 7.05 (dd, *J* = 8.9, 2.6 Hz, 1H), 6.71 (s, 1H) (**Figure S35**). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  177.51, 162.63, 155.34, 149.82, 132.02, 131.75, 129.49, 126.62, 124.65, 123.55, 120.26, 107.95, 106.32 (**Figure S36**). Anal.calcd for: C<sub>15</sub>H<sub>10</sub>O<sub>3</sub>: C, 75.62; H, 4.23; Found: C, 75.66; H, 4.25. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 3068, 2949, 2864, 1624, 1593, 1577, 1568, 1494, 1473, 1454, 1400, 1375, 1363, 1328, 1255, 1197, 1184, 1132.

**7-methoxy-2-phenyl-4H-chromen-4-one<sup>2</sup> (3s):**



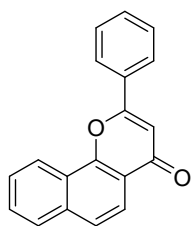
Yellow solid, m.p.: 96-98 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  8.09 (d, *J* = 8.7 Hz, 1H), 7.86 (dd, *J* = 7.5, 2.0 Hz, 2H), 7.56-7.42 (m, 3H), 7.00-6.86 (m, 2H), 6.72 (s, 1H), 3.90 (s, 3H) (**Figure S37**). <sup>13</sup>C NMR (101 MHz, Chloroform-*d*)  $\delta$  177.78, 164.20, 163.02, 157.99, 131.42, 128.99, 127.01, 126.14, 117.78, 114.43, 107.46, 100.41, 55.85 (**Figure S38**). Anal.calcd for: C<sub>16</sub>H<sub>12</sub>O<sub>3</sub>: C, 76.18; H, 4.79; Found: C, 76.22; H, 4.82. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 3026, 3002, 2924, 2845, 1653, 1626, 1606, 1494, 1450, 1439, 1348, 1357, 1284, 1247, 1190, 1165, 1131.

**7-Hydroxy-2-phenyl-4H-chromen-4-one<sup>9</sup> (3t):**



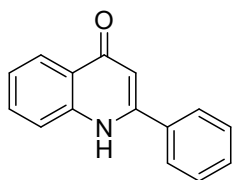
White solid, m.p.: 265-268 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  10.06 (s, 1H), 8.09 (d, *J* = 6.8 Hz, 2H), 7.67 (d, *J* = 9.0 Hz, 1H), 7.59 (d, *J* = 6.6 Hz, 3H), 7.36 (d, *J* = 3.0 Hz, 1H), 7.28 (dd, *J* = 9.0, 3.0 Hz, 1H), 6.97 (s, 1H) (**Figure S39**). <sup>13</sup>C NMR (101 MHz, DMSO)  $\delta$  176.33, 162.72, 161.89, 157.48, 131.52, 131.23, 129.03, 126.53, 126.15, 116.13, 115.05, 106.61, 102.53 (**Figure S40**). Anal.calcd for: C<sub>16</sub>H<sub>12</sub>O<sub>3</sub>: C, 75.62; H, 4.23; Found: C, 75.65; H, 4.25. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 3000, 1620, 1580, 1550, 1510, 1490, 1450, 1380, 1250.

**2-Phenyl-4H-benzo[*h*]chromen-4-one<sup>9</sup> (3u):**



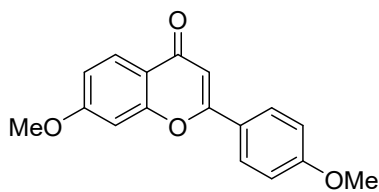
Yellow solid, m.p.: 166-168 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.61-8.49 (m, 1H), 8.15 (d,  $J = 8.7$  Hz, 1H), 8.04-7.96 (m, 2H), 7.91 (dd,  $J = 6.7, 2.6$  Hz, 1H), 7.75 (d,  $J = 8.7$  Hz, 1H), 7.71 -7.64 (m, 2H), 7.61 -7.51 (m, 3H), 6.94 (s, 1H) (**Figure S41**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  178.23, 162.60, 153.50, 135.99, 131.93, 131.56, 129.25, 129.20, 128.23, 127.16, 126.22, 125.34, 124.11, 122.33, 120.74, 120.26, 108.79 (**Figure S42**). Anal.calcd for:  $\text{C}_{19}\text{H}_{12}\text{O}_2$ : C, 83.81; H, 4.44; Found: C, 83.84; H, 4.47. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1630, 1560.

**2-phenylquinolin-4(1H)-one<sup>10</sup> (3v):**



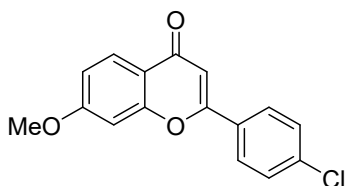
White solid, m.p.: 255-257 °C.  $^1\text{H}$  NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  8.12 (d,  $J = 7.5$  Hz, 1H), 7.93-7.86 (m, 2H), 7.81 (d,  $J = 7.7$  Hz, 1H), 7.64-7.58 (m, 1H), 7.52 (s, 3H), 7.29 (t,  $J = 6.2$  Hz, 1H), 6.45 (s, 1H) (**Figure S43**).  $^{13}\text{C}$  NMR (101 MHz, DMSO)  $\delta$  176.95, 150.04, 140.52, 134.20, 131.83, 130.52, 129.04, 127.44, 124.92, 124.75, 123.29, 118.76, 107.34 (**Figure S44**). Anal.calcd for:  $\text{C}_{15}\text{H}_{11}\text{NO}$ : C, 81.43; H, 5.01; N, 6.33; Found: C, 81.47; H, 5.03; N, 6.35. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3545, 2922, 1692, 1627, 1589, 1502, 756.

**7-Methoxy-2-(4-methoxyphenyl)-4H-chromen-4-one<sup>11</sup> (3w):**



White solid, m.p.: 149-150 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.13 (d,  $J = 8.7$  Hz, 1H), 7.86 (d,  $J = 8.9$  Hz, 2H), 7.08-6.91 (m, 4H), 6.68 (s, 1H), 3.91 (d,  $J = 16.3$  Hz, 6H) (**Figure S45**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  177.82, 164.03, 163.04, 162.24, 157.89, 127.82, 127.00, 124.11, 117.77, 114.40, 114.14, 106.09, 100.40, 55.80, 55.47 (**Figure S46**). Anal.calcd for:  $\text{C}_{17}\text{H}_{14}\text{O}_4$ : C, 72.33; H, 5.00; Found: C, 72.36; H, 5.05. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3361, 2925, 1626, 1607, 1258, 1180, 1165.

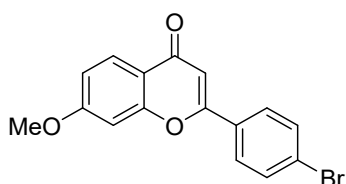
**2-(4-Chlorophenyl)-7-methoxy-4H-chromen-4-one<sup>6</sup> (3x):**



White solid, m.p.: 128-130 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.11 (d,  $J = 8.8$  Hz, 1H), 7.83 (d,  $J = 8.7$  Hz, 2H), 7.48 (d,  $J = 8.7$  Hz, 2H), 7.00-6.94 (m, 2H),

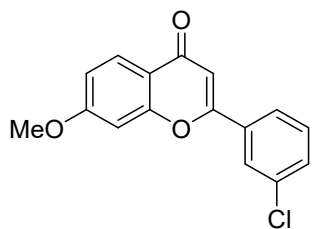
6.72 (s, 1H), 3.93 (s, 3H) (**Figure S47**).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  177.54, 164.23, 161.69, 157.82, 137.61, 130.21, 129.28, 127.33, 126.99, 117.69, 114.51, 107.54, 100.35, 55.87 (**FigureS48**). Anal.calcd for:  $\text{C}_{16}\text{H}_{11}\text{ClO}_3$ : C, 67.03; H, 3.87; Cl, 12.36; Found: C, 67.07; H, 3.89; Cl, 12.34. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3425, 1660, 1372, 1092, 832, 750.

**2-(4-Bromophenyl)-7-methoxy-4H-chromen-4-one<sup>12</sup> (3y):**



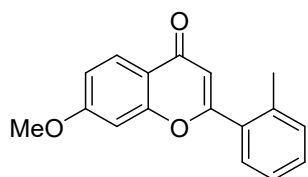
White solid, m.p.: 181-183 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.12 (d,  $J = 7.6$  Hz, 1H), 7.77 (d,  $J = 6.5$  Hz, 2H), 7.65 (d,  $J = 7.0$  Hz, 2H), 7.05 – 6.90 (m, 2H), 6.73 (s, 1H), 3.94 (s, 3H) (**Figure S49**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  177.64, 164.30, 161.88, 132.30, 127.57, 127.09, 126.07, 117.77, 114.57, 107.66, 100.40, 55.88 (**Figure S50**). Anal.calcd for:  $\text{C}_{16}\text{H}_{11}\text{BrO}_3$ : C, 58.03; H, 3.35; Br, 24.13; Found: C, 58.05 H, 3.38; Br, 24.10. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3059, 1604, 1489, 1440, 1348, 1274, 1246, 1201, 1166, 1139.

**2-(3-chloro-phenyl)-7-methoxy-chromen-4-one (3z):**



Yellow solid, m.p.: 124-126 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.14 (d,  $J = 8.6$  Hz, 1H), 7.92 (s, 1H), 7.77 (d,  $J = 6.6$  Hz, 1H), 7.48 (dt,  $J = 15.4, 7.6$  Hz, 2H), 7.00 (d,  $J = 11.1$  Hz, 2H), 6.76 (s, 1H), 3.95 (s, 3H) (**Figure S51**).  $^{13}\text{C}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  177.61, 164.39, 161.43, 157.96, 131.33, 130.29, 127.13, 126.25, 124.26, 117.80, 114.72, 108.16, 100.39, 55.90 (**Figure S52**). HRMS:  $\text{C}_{16}\text{H}_{11}\text{ClO}_3$  for  $[\text{M}+\text{H}]^+$ : 287.0512; Found: 287.0519. Anal.calcd for:  $\text{C}_{16}\text{H}_{11}\text{ClO}_3$ : C, 67.03; H, 3.87; Cl, 12.36; Found: C, 67.04; H, 3.90; Cl, 12.32. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3074, 2978, 2839, 1635, 1604, 1570, 1539, 1504, 1477, 1438, 1373, 1354, 1273, 1249, 1234, 1195, 1165, 1126, 1087, 1045, 1014.

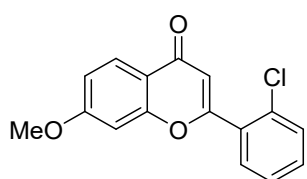
**2-(2-methylphenyl)-7-methoxy-chromen-4-one (3aa):**



Yellow solid, m.p.: 119-121 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.15 (d,  $J = 8.9$  Hz, 1H), 7.50 (d,  $J = 7.2$  Hz, 1H), 7.40 (t,  $J = 7.4$  Hz, 1H), 7.31 (d,  $J = 7.4$  Hz, 2H), 6.98 (dd,  $J = 8.9, 2.3$  Hz, 1H), 6.88 (d,  $J = 2.2$  Hz, 1H),

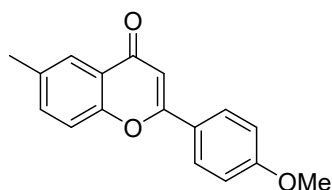
6.42 (s, 1H), 3.90 (s, 3H), 2.48 (s, 3H) (**Figure S53**).  $^{13}\text{C}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  177.67, 165.56, 164.19, 158.23, 136.70, 132.65, 131.22, 130.61, 129.15, 127.07, 126.18, 117.62, 114.46, 111.86, 100.33, 55.82, 20.55. (**Figure S54**). HRMS:  $\text{C}_{17}\text{H}_{14}\text{O}_3$  for  $[\text{M}+\text{H}]^+$ : 267.1054; Found: 267.1061. Anal.calcd for:  $\text{C}_{17}\text{H}_{14}\text{O}_3$ : C, 76.68; H, 5.30; Found: C, 76.70; H, 5.33. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3070, 2954, 2839, 1631, 1604, 1589, 1504, 1438, 1373, 1350, 1276, 1249, 1238, 1199, 1161, 1083, 1022.

**2-(2-chloro-phenyl)-7-methoxy-chromen-4-one (3ab):**



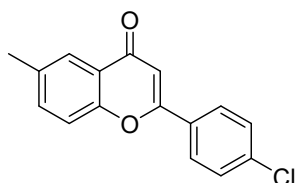
Yellow solid, m.p.: 142-144 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.15 (d,  $J = 8.9$  Hz, 1H), 7.62 (dd,  $J = 7.4$ , 1.8 Hz, 1H), 7.56 -7.50 (m, 1H), 7.38-7.47 (dtd,  $J = 18.2$ , 7.4, 1.4 Hz, 2H), 7.00 (dd,  $J = 8.9$ , 2.3 Hz, 1H), 6.91 (d,  $J = 2.3$  Hz, 1H), 6.59 (s, 1H), 3.91 (s, 3H) (**Figure S55**).  $^{13}\text{C}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  177.48, 164.31, 131.67, 130.76, 130.63, 127.11, 127.07, 114.70, 112.93, 100.36, 55.85 (**Figure S56**). HRMS:  $\text{C}_{16}\text{H}_{11}\text{ClO}_3$  for  $[\text{M}+\text{H}]^+$ : 287.0512; Found: 287.0518. Anal.calcd for:  $\text{C}_{16}\text{H}_{11}\text{ClO}_3$ : C, 67.03; H, 3.87; Cl, 12.36; Found: C, 67.04; H, 3.91; Cl, 12.22. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3070, 2974, 2843, 1643, 1608, 1573, 1504, 1477, 1442, 1373, 1354, 1273, 1249, 1203, 1168, 1126, 1083, 1033, 1026.

**2-(4-methoxyphenyl)-6-methyl-4H-chromen-4-one (3ac):**



Yellow solid, m.p.: 167-169 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.00 (s, 1H), 7.87 (d,  $J = 8.8$  Hz, 2H), 7.50-7.47 (m, 1H), 7.44 (d,  $J = 8.5$  Hz, 1H), 7.01 (d,  $J = 8.8$  Hz, 2H), 6.73 (s, 1H), 3.88 (s, 3H), 2.45 (s, 3H) (**Figure S57**).  $^{13}\text{C}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  178.5, 163.6, 162.5, 154.5, 135.2, 134.9, 128.1, 125.0, 124.1, 123.4, 117.7, 114.5, 105.9, 55.5, 20.9. (**Figure S58**). HRMS:  $\text{C}_{17}\text{H}_{14}\text{O}_3$  for  $[\text{M}+\text{H}]^+$ : 267.1021; Found: 267.1016. Anal.calcd for:  $\text{C}_{17}\text{H}_{14}\text{O}_3$ : C, 76.68; H, 5.30; Found: C, 76.70; H, 5.33. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3430, 1638, 1467, 1367, 1228, 822, 630.

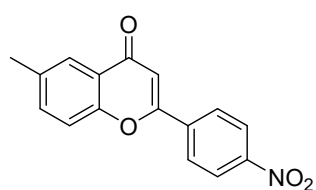
**2-(4-chlorophenyl)-6-methyl-4H-chromen-4-one<sup>2</sup> (3ad):**



White solid, m.p.: 193-195 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.00 (s, 1H), 7.86 (s, 1H), 7.84 (s, 1H),

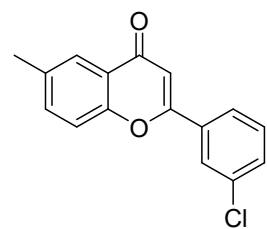
7.47 (dd,  $J = 15.6, 8.6$  Hz, 4H), 6.77 (s, 1H), 2.47 (s, 3H) (**Figure S59**).  $^{13}\text{C}$  NMR (100 MHz, Chloroform- $d$ )  $\delta$  178.3, 162.0, 154.4, 137.8, 135.4, 135.1, 130.3, 129.3, 127.5, 125.1, 123.5, 117.8, 107.5, 21.0 (**Figure S60**). HRMS:  $\text{C}_{16}\text{H}_{11}\text{ClO}_2$  for  $[\text{M}+\text{H}]^+$ : 271.0526; Found: 271.0522 Anal.calcd for:  $\text{C}_{16}\text{H}_{11}\text{ClO}_2$ : C, 70.99; H, 4.10; Cl, 13.10; Found: C, 71.02; H, 4.14; Cl, 13.06. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3427, 3063, 3028, 2922, 2856, 1642, 1622, 1594, 1577, 1490, 1453, 1407, 1378, 1364, 1285, 1228.

**6-methyl-2-(4-nitrophenyl)-4H-chromen-4-one<sup>13</sup> (3ae):**



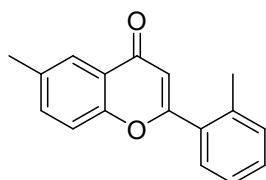
Yellow solid, m.p.: 276-278 °C.  $^1\text{H}$  NMR (400MHz, Chloroform- $d$ ):  $\delta$  8.38 (d,  $J = 8.7$  Hz, 2H), 8.11 (d,  $J = 9.0$  Hz, 2H), 8.03 (s, 1H), 7.54 (m, 2H), 6.89 (s, 1H), 2.49 (s, 3H) (**Figure S61**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform- $d$ )  $\delta$  178.13, 160.42, 154.47, 149.36, 137.78, 135.89, 135.59, 127.19, 125.20, 124.23, 123.57, 117.90, 109.46, 21.00 (**Figure S62**). Anal.calcd for:  $\text{C}_{16}\text{H}_{11}\text{NO}_4$ : C, 68.33; H, 3.94; N 4.98; Found: C, 68.36; H, 3.95; N 4.96. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1640, 1617, 1523, 1484, 1343.

**6-chloro-2-phenylquinazolin-4(3H)-one<sup>14</sup> (3af):**



Yellow solid, m.p.: 131-133 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform- $d$ )  $\delta$  8.00 (s, 1H), 7.94-7.87 (m, 1H), 7.77 (d,  $J = 7.6$  Hz, 1H), 7.54-7.42 (m, 4H), 6.78 (s, 1H), 2.47 (s, 3H) (**Figure S63**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform- $d$ )  $\delta$  178.32, 161.63, 154.46, 135.47, 135.25, 135.21, 133.73, 131.40, 130.29, 126.34, 125.10, 124.34, 123.58, 117.85, 108.01, 20.95 (**Figure S64**). Anal.calcd for:  $\text{C}_{16}\text{H}_{11}\text{ClO}_2$ : C, 70.99; H, 4.10; Cl, 13.10; Found: C, 71.02; H, 4.14; Cl, 13.06. IR (CCl $_4$ ):  $\nu = 3080$  (w), 3040 (w), 2930 (w), 1660 (s), 1620 (m), 1585 (m), 1570 (m), 1490 (m), 1440 (m), 1360 (s), 1290 (m), 1255 (w), 1230 (m), 1140 (m), 1105 (w), 1085 (m), 1045 (m), 930 (w), 855 (m), 700 (m)  $\text{cm}^{-1}$ .

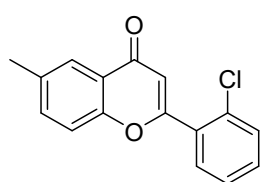
**6-methyl-2-(2-methylphenyl)-4H-chromen-4-one (3ag):**



Yellow solid, m.p.: 132-134 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform- $d$ )  $\delta$  8.05 (s, 1H), 7.54-7.48 (m, 2H), 7.40 (t,  $J = 6.9$  Hz, 2H), 7.33 (d,  $J = 7.4$  Hz, 2H), 6.47 (s, 1H), 2.48 (s, 6H)

(**Figure S65**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  178.42, 165.97, 136.81, 135.24, 134.99, 132.78, 131.25, 130.65, 129.21, 126.20, 125.10, 123.48, 117.82, 111.82, 20.96, 20.55 (**Figure S66**). HRMS:  $\text{C}_{17}\text{H}_{14}\text{O}_2$  for  $[\text{M}+\text{H}]^+$ : 251.1134. Found: 251.1142. Anal.calcd for:  $\text{C}_{17}\text{H}_{14}\text{O}_2$ : C, 81.58; H, 5.64; Found: C, 81.62; H, 5.68. IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3020, 2924, 2858, 1639, 1612, 1573, 1558, 1485, 1446, 1365, 1296, 1253, 1219, 1138, 1122, 1033.

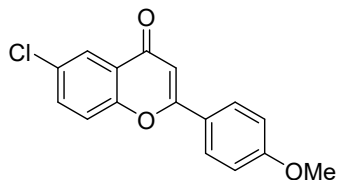
**2-(2-chlorophenyl)-6-methyl-4H-chromen-4-one<sup>15</sup> (3ah):**



Yellow solid. m.p.: 124-126 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.04 (s, 1H), 7.63 (dd,  $J = 7.5, 1.8$  Hz, 1H), 7.56-7.48 (m, 2H), 7.48-7.37 (m, 3H), 6.64 (s, 1H), 2.48 (s, 3H)

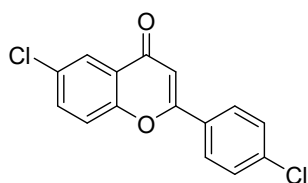
(**Figure S67**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  178.23, 162.50, 154.89, 135.35, 135.14, 132.94, 132.07, 131.69, 130.79, 130.64, 127.06, 125.08, 117.95, 112.83, 20.96 (**Figure S68**). Anal.calcd for:  $\text{C}_{16}\text{H}_{11}\text{ClO}_2$ : C, 70.99; H, 4.10; Cl, 13.10; Found: C, 71.02; H, 4.14; Cl, 13.06. IR (KBr)( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3444, 3070, 1658, 1620, 1485, 1440, 1340, 1224, 1072, 1025, 813, 761.

**6-chloro-2-(4-methoxyphenyl)-4H-chromen-4-one (3ai):**



Cream yellow solid, m.p.: 186-188 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.19 (d,  $J = 2.75$  Hz, 1H), 7.87 (d,  $J = 8.94$  Hz, 2H), 7.62 (dd,  $J = 2.75$  and  $8.94$  Hz, 1H), 7.51 (d,  $J = 8.94$  Hz, 1H), 7.03 (d,  $J = 8.94$  Hz, 2H), 6.75 (s, 1H), 3.90 (s, 3H) (**Figure S69**).  $^{13}\text{C}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  177.1, 163.7, 162.7, 154.5, 133.7, 131.1, 128.1, 125.2, 124.9, 123.6, 119.7, 114.6, 106.0, 55.6 (**Figure S70**). HRMS:  $\text{C}_{16}\text{H}_{11}\text{ClO}_3$  for  $[\text{M}+\text{H}]^+$ : 287.0512. Found: 287.0517. Anal.calcd for:  $\text{C}_{16}\text{H}_{11}\text{ClO}_3$ : C, 67.03; H, 3.87; Cl, 12.36; Found: C, 67.07; H, 3.91; Cl, 12.31. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3082, 2993, 2843, 1658, 1604, 1566, 1512, 1465, 1438, 1357, 1315, 1269, 1253, 1188, 1122, 1022.

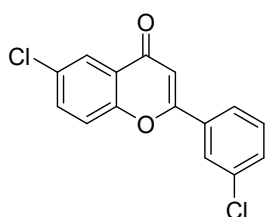
**6-chloro-2-(4-chlorophenyl)-4H-chromen-4-one<sup>16</sup> (3aj):**



Yellow solid, m.p.: 253-255 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.19 (s, 1H), 7.85 (d,  $J = 7.9$  Hz, 2H), 7.65 (d,  $J = 7.3$  Hz, 1H), 7.51 (d,  $J = 7.0$  Hz, 3H), 6.79 (s,

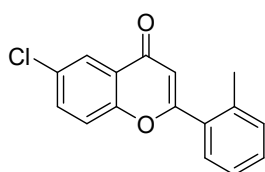
1H) (**Figure S71**). <sup>13</sup>C NMR (101 MHz, Chloroform-*d*) δ 177.01, 162.52, 154.47, 138.21, 134.11, 131.40, 129.87, 129.48, 127.58, 125.24, 124.87, 119.78, 107.60 (**Figure S72**). Anal.calcd for: C<sub>15</sub>H<sub>8</sub>Cl<sub>2</sub>O<sub>2</sub>: C, 61.89; H, 2.77; Cl, 24.35; Found: C, 61.93; H, 2.80; Cl, 24.32. IR (KBr) (ν<sub>max</sub>/cm<sup>-1</sup>): 1132, 1253, 1353, 1456, 1566, 1601, 1647, 2361, 2922, 3086.

**6-chloro-2-(3-chlorophenyl)-4H-chromen-4-one (3ak):**



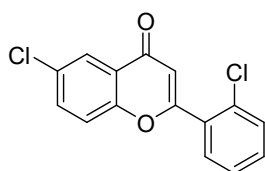
Yellow solid, m.p.: 209-211 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.19 (d, J = 2.4 Hz, 1H), 7.91 (s, 1H), 7.78 (d, J = 7.7 Hz, 1H), 7.66 (dd, J = 8.9, 2.5 Hz, 1H), 7.58-7.44 (m, 3H), 6.81 (s, 1H) (**Figure S73**). <sup>13</sup>C NMR (100 MHz, Chloroform-*d*) δ 162.07, 154.48, 135.38, 134.20, 133.23, 131.77, 130.41, 126.40, 125.24, 124.88, 124.42, 119.83, 108.08 (**Figure S74**). HRMS: C<sub>15</sub>H<sub>8</sub>Cl<sub>2</sub>O<sub>2</sub> for [M+H]<sup>+</sup>: 291.0054; Found: 291.0060. Anal.calcd for: C<sub>15</sub>H<sub>8</sub>Cl<sub>2</sub>O<sub>2</sub>: C, 61.89; H, 2.77; Cl, 24.35; Found: C, 61.93; H, 2.81; Cl, 24.31. IR (KBr) (ν<sub>max</sub>/cm<sup>-1</sup>): 3059, 1654, 1600, 1562, 1469, 1446, 1346, 1276, 1230, 1111.

**6-chloro-2-(2-methylphenyl)-4H-chromen-4-one (3al):**



Yellow solid, m.p.: 133-135 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.22 (d, J = 2.3 Hz, 1H), 7.63 (dd, J = 8.9, 2.4 Hz, 1H), 7.52 (d, J = 7.4 Hz, 1H), 7.44 (dd, J = 11.5, 8.2 Hz, 2H), 7.36-7.30 (m, 2H), 6.49 (s, 1H), 2.48 (s, 3H) (**Figure S75**). <sup>13</sup>C NMR (100 MHz, Chloroform-*d*) δ 177.06, 154.79, 136.82, 133.99, 132.27, 131.37, 131.23, 130.96, 129.23, 126.31, 125.22, 124.77, 119.82, 111.90, 20.61 (**Figure S76**). HRMS: C<sub>16</sub>H<sub>11</sub>ClO<sub>2</sub> for [M+H]<sup>+</sup>: 271.0526; Found: 271.0534. Anal.calcd for: C<sub>16</sub>H<sub>11</sub>ClO<sub>2</sub>: C, 70.99; H, 4.10; Cl, 13.10; Found: C, 71.02; H, 4.14; Cl, 13.06. IR (KBr) (ν<sub>max</sub>/cm<sup>-1</sup>): 3066, 2931, 1639, 1612, 1465, 1438, 1357, 1288, 1269, 1249, 1211, 1168, 1141, 1122, 1107.

**6-chloro-2-(2-chlorophenyl)-4H-chromen-4-one (3am):**



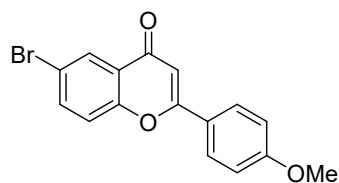
Yellow solid, m.p.: 153-155 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.22 (d, J = 2.4 Hz, 1H), 7.67-7.61 (m, 2H), 7.55 (d, J = 7.8 Hz, 1H), 7.50-7.40 (m, 3H), 6.67 (s, 1H)



(Figure S77).  $^{13}\text{C}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  176.91, 162.92, 154.90, 134.14, 132.95, 132.00, 131.59, 131.36, 130.88, 130.63, 127.16, 125.22, 119.95, 112.93

(Figure S78). HRMS:  $\text{C}_{15}\text{H}_8\text{Cl}_2\text{O}_2$  for  $[\text{M}+\text{H}]^+$ : 291.0054; Found: 291.0049. Anal.calcd for:  $\text{C}_{15}\text{H}_8\text{Cl}_2\text{O}_2$ : C, 61.89; H, 2.77; Cl, 24.35; Found: C, 61.92; H, 2.81; Cl, 24.31. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3028, 1647, 1606, 1566, 1469, 1438, 1350, 1296, 1276, 1141, 1107, 1068, 1026.

**6-Bromo-2-(4-methoxyphenyl)-4H-chromen-4-one<sup>17</sup> (3an):**

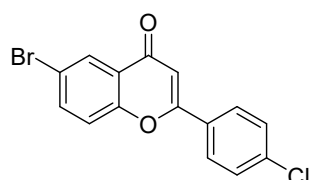


Cream yellow solid, m.p.: 185-187 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.32 (d,  $J = 2.2$  Hz, 1H), 7.84 (d,  $J = 8.8$  Hz, 2H), 7.75 (d,  $J = 2.2$  Hz, 1H), 7.43 (d,  $J = 8.8$  Hz, 1H), 7.01 (d,  $J = 8.8$  Hz, 2H), 6.72 (s, 1H), 3.89 (s,

3H) (Figure S79).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  176.83, 163.59, 162.60, 154.84, 136.43, 128.25, 128.00, 125.21, 119.89, 118.46, 114.51, 105.99, 55.52

(Figure S80). Anal.calcd for:  $\text{C}_{16}\text{H}_{11}\text{BrO}_3$ : C, 58.03; H, 3.35; Br, 24.13; Found: C, 58.06; H, 3.38; Br, 24.10. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3074, 2993, 2843, 1651, 1604, 1562, 1512, 1462, 1438, 1357, 1315, 1269, 1253, 1188, 1138, 1122, 1018.

**6-bromo-2-(4-chlorophenyl)-4H-chromen-4-one<sup>18</sup> (3ao):**

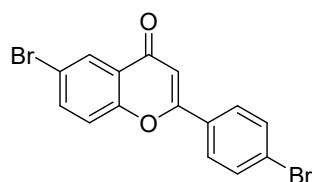


Yellow solid, m.p.: 191-193 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.34 (d,  $J = 2.3$  Hz, 1H), 7.84 (d,  $J = 8.6$  Hz, 2H), 7.79 (dd,  $J = 8.9, 2.3$  Hz, 1H), 7.51 (d,  $J = 8.6$  Hz, 2H), 7.46 (d,  $J = 8.9$  Hz, 1H), 6.79 (s, 1H) (Figure S81).

$^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta$  176.81, 162.49, 138.21, 154.90, 138.21, 136.86, 129.83, 129.47, 128.42, 127.56, 125.22, 119.99, 118.85, 107.66 (Figure S82).

Anal.calcd for:  $\text{C}_{15}\text{H}_8\text{BrClO}_2$ : C, 53.69; H, 2.40; Br, 23.81; Cl, 10.56; Found: C, 53.73; H, 2.41; Br, 23.79; Cl, 10.54. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1092, 1282, 1357, 1436, 1560, 1601, 1638, 2361, 2919, 3073.

**6-Bromo-2-(4-bromophenyl)-4H-chromen-4-one<sup>4</sup> (3ap):**

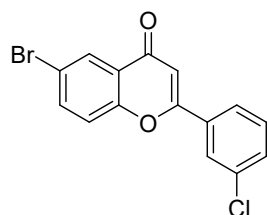


Yellow solid, m.p.: 245-247 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.35 (s, 1H), 7.88-7.59 (m, 5H), 7.46 (d,  $J = 8.8$  Hz, 1H), 6.80 (s, 1H) (Figure S83).  $^{13}\text{C}$  NMR (101

MHz, Chloroform-*d*)  $\delta$  176.83, 162.58, 154.91, 136.89, 132.45, 130.32, 128.44, 127.72, 126.66, 125.24, 120.01, 118.87, 107.69 (**Figure S84**).

Anal.calcd for: C<sub>15</sub>H<sub>8</sub>Br<sub>2</sub>O<sub>2</sub>: C, 47.41; H, 2.12; Br, 42.05; Found: C, 47.43; H, 2.16; Br, 42.01. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 3072, 1635, 1560, 1460, 1436, 1355, 1280, 1259, 1136, 1074, 1074, 1033, 1006.

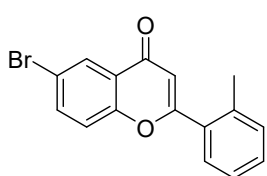
**6-bromo-2-(3-chlorophenyl)-4H-chromen-4-one (3aq):**



Yellow solid, m.p.: 204-206 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  8.35 (d, *J* = 2.3 Hz, 1H), 7.91 (s, 1H), 7.82-7.75 (m, 2H), 7.51 (dd, *J* = 19.0, 8.4 Hz, 3H), 6.81 (s, 1H) (**Figure S85**). <sup>13</sup>C NMR (100 MHz, Chloroform-*d*)  $\delta$  176.79, 162.07, 154.92, 136.96, 135.38, 133.21, 131.78, 130.41,

128.44, 126.39, 125.24, 124.42, 120.05, 118.93, 108.16 (**Figure S86**). HRMS: C<sub>15</sub>H<sub>8</sub>BrClO<sub>2</sub> for [M+H]<sup>+</sup>: 334.9569; Found: 334.9573. Anal.calcd for: C<sub>15</sub>H<sub>8</sub>BrClO<sub>2</sub>: C, 53.69; H, 2.40; Br, 23.81; Cl, 10.56; Found: C, 53.73; H, 2.41; Br, 23.79; Cl, 10.54. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 3062, 1651, 1616, 1600, 1562, 1473, 1465, 1438, 1346, 1276, 1257, 1141, 1107.

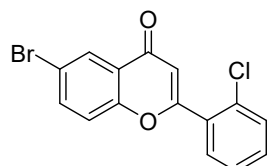
**6-Bromo-2-(2-methylphenyl)-4H-chromen-4-one (3ar):**



Yellow solid, m.p.: 114-116 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  8.38 (d, *J* = 2.3 Hz, 1H), 7.77 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.52 (d, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.39 (d, *J* = 8.9 Hz, 1H), 7.33 (d, *J* = 7.4 Hz, 2H), 6.49 (s, 1H), 2.48

(s, 3H) (**Figure S87**). <sup>13</sup>C NMR (101 MHz, Chloroform-*d*)  $\delta$  176.87, 166.34, 155.23, 136.81, 136.73, 132.27, 131.36, 130.96, 129.22, 128.43, 126.30, 125.16, 120.03, 118.70, 111.98, 20.58 (**Figure S88**). HRMS: C<sub>16</sub>H<sub>11</sub>BrO<sub>2</sub> for [M+H]<sup>+</sup>: 315.0048. Found: 315.0045. Anal.calcd for: C<sub>16</sub>H<sub>11</sub>BrO<sub>2</sub>: C, 60.98; H, 3.52; Br, 25.35; Found: C, 61.01; H, 3.54; Br, 25.37. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 3062, 2931, 1639, 1608, 1597, 1554, 1462, 1435, 1354, 1288, 1246, 1207, 1168, 1141, 1029.

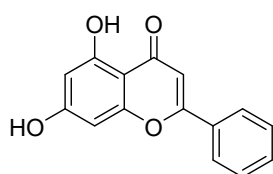
**6-Bromo-2-(2-chlorophenyl)-4H-chromen-4-one (3as):**



Yellow solid, m.p.: 196-198 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  8.38 (d, *J* = 2.2 Hz, 1H), 7.78 (dd, *J* = 8.9, 2.2

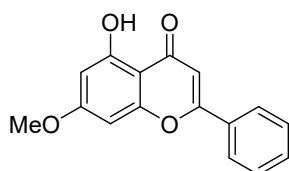
Hz, 1H), 7.66-7.60 (m, 1H), 7.55 (d,  $J = 7.9$  Hz, 1H), 7.51-7.39 (m, 3H), 6.67 (s, 1H) (**Figure S89**).  $^{13}\text{C}$  NMR (101 MHz, Chloroform- $d$ )  $\delta$  176.73, 155.33, 136.89, 132.94, 132.01, 130.88, 130.62, 128.41, 127.16, 125.16, 120.17, 118.82, 113.01 (**Figure S90**). HRMS:  $\text{C}_{15}\text{H}_8\text{BrClO}_2$  for  $[\text{M}+\text{H}]^+$ : 334.9569. Found: 334.9575. Anal.calcd for:  $\text{C}_{15}\text{H}_8\text{BrClO}_2$ : C, 53.69; H, 2.40; Br, 23.81; Cl, 10.56; Found: C, 53.73; H, 2.41; Br, 23.79; Cl, 10.54. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3028, 2920, 2854, 1651, 1600, 1562, 1465, 1435, 1350, 1292, 1276, 1141.

#### Chrysin<sup>19</sup>:



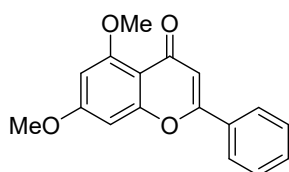
Yellow solid, m.p.: 283-284 °C.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  12.58 (s, 1H), 10.62 (s, 1H), 7.77 (d,  $J = 6.6$  Hz, 2H), 7.31 (q,  $J = 7.7, 6.2$  Hz, 3H), 6.70-6.56 (m, 1H), 6.25 (s, 1H), 6.05-5.92 (m, 1H) (**Figure S91**).  $^{13}\text{C}$  NMR (101 MHz, DMSO- $d_6$ )  $\delta$  182.21, 164.82, 163.49, 161.88, 157.82, 132.31, 131.10, 129.46, 126.71, 105.51, 104.39, 99.43, 94.51 (**Figure S92**). Anal.calcd for:  $\text{C}_{15}\text{H}_{10}\text{O}_4$ : C, 70.86; H, 3.96; Found: C, 70.88; H, 3.97. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3527, 3083, 1656, 1609, 1580, 1556, 1445.

#### Tectochrysin<sup>20</sup>:



Yellow solid, m.p.: 162-164 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform- $d$ )  $\delta$  12.70 (s, 1H), 7.89-7.81 (m, 2H), 7.51 (q,  $J = 6.8, 6.2$  Hz, 3H), 6.63 (s, 1H), 6.47 (d,  $J = 2.1$  Hz, 1H), 6.35 (d,  $J = 2.1$  Hz, 1H), 3.86 (s, 3H) (**Figure S93**).  $^{13}\text{C}$  NMR (100 MHz, Chloroform- $d$ )  $\delta$  182.42, 165.59, 163.91, 162.16, 157.75, 131.81, 131.28, 129.05, 126.25, 105.81, 105.68, 98.19, 92.63, 55.79. (**Figure S94**). HRMS:  $\text{C}_{16}\text{H}_{12}\text{O}_4$  for  $[\text{M}+\text{H}]^+$ : 269.0812. Found: 269.0808. Anal.calcd for:  $\text{C}_{16}\text{H}_{12}\text{O}_4$ : C, 71.64; H, 4.51; Found: C, 71.65; H, 4.53. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3450, 2925, 1654, 1621, 1016.

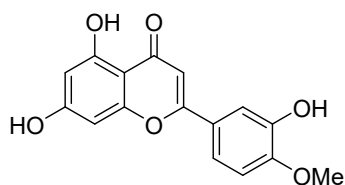
#### 5,7-Dimethoxyflavone<sup>21</sup>:



Yellow solid, m.p.: 147-149 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform- $d$ )  $\delta$  7.84 (dd,  $J = 7.1, 2.1$  Hz, 2H), 7.50-7.45 (m, 3H), 6.65 (s, 1H), 6.54 (d,  $J = 2.1$  Hz, 1H), 6.34 (d,  $J = 2.0$  Hz, 1H), 3.93 (s, 3H), 3.89 (s, 3H) (**Figure S95**).  $^{13}\text{C}$  NMR

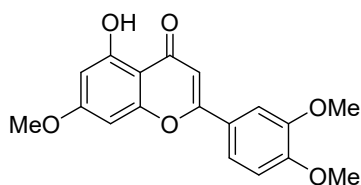
(100 MHz, Chloroform-*d*)  $\delta$  177.58, 164.02, 160.79, 160.55, 159.82, 131.41, 131.16, 128.89, 125.86, 109.18, 108.92, 96.15, 92.79, 56.38, 55.77 (**Figure S96**). HRMS:  $C_{17}H_{14}O_4$  for  $[M+H]^+$ : 283.1025. Found: 283.1029. Anal.calcd for:  $C_{17}H_{14}O_4$ : C, 72.33; H, 5.00; Found: C, 72.37; H, 5.04. IR (KBr) ( $\nu_{max}/cm^{-1}$ ): 3140, 1645, 1600, 1505.

#### Diosmetin<sup>22</sup>:



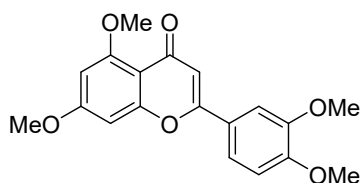
Yellow solid, m.p.: 287-289 °C.  $^1H$  NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  12.93 (s, 1H), 10.83 (s, 1H), 9.45 (s, 1H), 7.51 (dd,  $J = 8.5, 2.2$  Hz, 1H), 7.41 (d,  $J = 2.2$  Hz, 1H), 7.05 (d,  $J = 8.6$  Hz, 1H), 6.72 (s, 1H), 6.45 (d,  $J = 2.0$  Hz, 1H), 6.19 (d,  $J = 2.0$  Hz, 1H), 3.85 (s, 3H) (**Figure S97**).  $^{13}C$  NMR (100 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  182.12, 164.62, 163.93, 161.92, 157.75, 151.54, 147.22, 123.45, 119.12, 113.38, 112.51, 104.21, 103.95, 99.32, 94.34, 56.17 (**Figure S98**). HRMS:  $C_{16}H_{12}O_6$  for  $[M+H]^+$ : 301.0728. Found: 301.0731. Anal.calcd for:  $C_{16}H_{12}O_6$ : C, 64.00; H, 4.03; Found: C, 64.03; H, 4.05. IR (KBr) ( $\nu_{max}/cm^{-1}$ ): 3387, 3089, 2940, 2844, 1652, 1610, 1507, 1166.

#### 7,3',4'-Tri-O-methylfluteolin<sup>23</sup>:



Yellow solid, m.p.: 159-161 °C.  $^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  12.80 (s, 1H), 7.52 (dd,  $J = 8.5, 2.0$  Hz, 1H), 7.33 (d,  $J = 1.9$  Hz, 1H), 6.98 (d,  $J = 8.5$  Hz, 1H), 6.58 (s, 1H), 6.49 (d,  $J = 2.1$  Hz, 1H), 6.37 (d,  $J = 2.1$  Hz, 1H), 3.98 (d,  $J = 6.3$  Hz, 6H), 3.89 (s, 3H) (**Figure S99**).  $^{13}C$  NMR (100 MHz, Chloroform-*d*)  $\delta$  182.37, 165.45, 163.96, 162.17, 152.25, 149.29, 123.77, 120.10, 111.13, 108.75, 104.66, 98.07, 92.66, 56.11, 55.82 (**Figure S100**). HRMS:  $C_{18}H_{16}O_6$  for  $[M+H]^+$ : 329.1065. Found: 329.1070. Anal.calcd for:  $C_{18}H_{16}O_6$ : C, 65.85; H, 4.91; Found: C, 65.88; H, 4.93. IR (KBr) ( $\nu_{max}/cm^{-1}$ ): 3045~2900, 2835, 1660, 1625, 1505, 1446, 810.

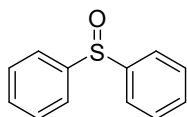
#### 5,7,3',4'-Tetramethoxyflavone<sup>20</sup>:



Yellow solid, m.p.: 192-194 °C.  $^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  7.49 (d,  $J = 8.5$  Hz, 1H), 7.30 (d,  $J =$

2.0 Hz, 1H), 6.95 (d,  $J = 8.5$  Hz, 1H), 6.61 (s, 1H), 6.55 (d,  $J = 2.2$  Hz, 1H), 6.36 (d,  $J = 2.2$  Hz, 1H), 3.98 -3.91 (m, 12H) (**Figure S101**).  $^{13}\text{C}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  182.37, 165.45, 163.96, 162.17, 152.25, 149.29, 123.77, 120.10, 111.13, 108.75, 104.66, 98.07, 92.66, 56.11, 55.82 (**Figure S102**). HRMS:  $\text{C}_{19}\text{H}_{18}\text{O}_6$  for  $[\text{M}+\text{H}]^+$ : 343.1231. Found: 343.1225. Anal.calcd for:  $\text{C}_{19}\text{H}_{18}\text{O}_6$ : C, 66.66; H, 5.30; Found: C, 66.67; H, 5.31. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3215, 3108, 3085, 3004, 2942, 2840, 1645, 1604, 1516, 1486, 1461, 1421, 1387, 1356, 1269, 1254, 1120, 1201, 1159, 1139, 1118, 1099, 870, 834, 806.

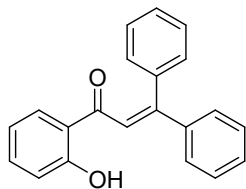
**Diphenyl sulfoxide<sup>24</sup>(5):**



White solid, m.p.: 68-70 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  7.70-7.61 (m, 4H), 7.48-7.40 (m, 6H) (**Figure S103**).  $^{13}\text{C}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  145.52, 131.07, 129.33, 124.19 (**Figure S104**).

HRMS:  $\text{C}_{12}\text{H}_{10}\text{OS}$  for  $[\text{M}+\text{H}]^+$ : 203.0553; Found: 203.0559. Anal.calcd for:  $\text{C}_{12}\text{H}_{10}\text{OS}$ : C, 71.26; H, 4.98; Found: C, 71.28; H, 5.02. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3020, 1440, 1080, 1030, 685.

**1,3,3-triphenylprop-2-en-1-one<sup>25</sup> (6):**



Yellow solid, m.p.: 77-79 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  12.28 (s, 1H), 7.93-7.84 (m, 1H), 7.49-7.41 (m, 6H), 7.39-7.34 (m, 3H), 7.26 (dd,  $J = 7.7, 1.8$  Hz, 2H), 7.21 (s, 1H), 7.00 (d,  $J = 8.4$  Hz, 1H), 6.88 (t,  $J = 7.6$  Hz, 1H) (**Figure S105**).  $^{13}\text{C}$

NMR (100 MHz, Chloroform-*d*)  $\delta$  197.19, 162.98, 155.69, 141.27, 138.94, 136.23, 130.81, 129.65, 128.71, 128.63, 128.55, 128.26, 122.61, 120.67, 118.79, 118.39 (**Figure S106**). HRMS:  $\text{C}_{21}\text{H}_{16}\text{O}_2$  for  $[\text{M}+\text{H}]^+$ : 301.1214; Found: 301.1220. Anal.calcd for:  $\text{C}_{21}\text{H}_{16}\text{O}_2$ : C, 83.98; H, 5.37; Found: C, 83.99; H, 5.39. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3057, 2925, 1735, 1628, 1568, 1485, 1444, 1349, 1297, 1030, 756, 697, 604.

**NMR spectra**

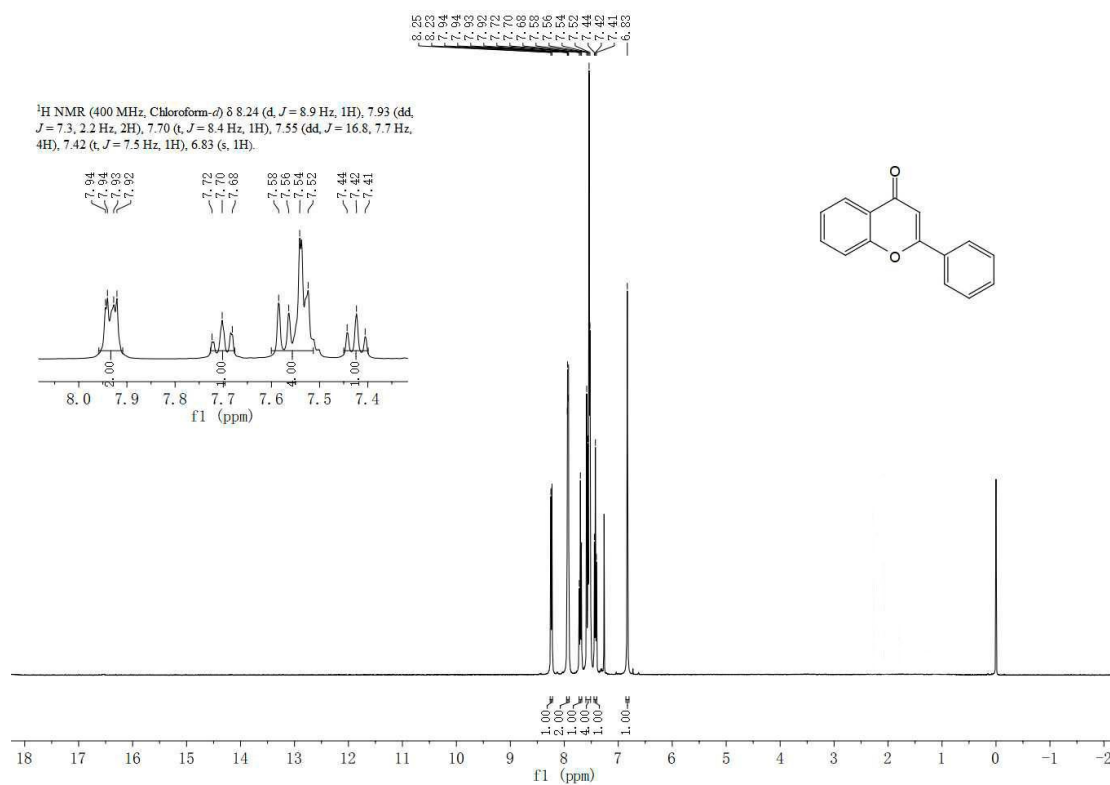


Figure S1 <sup>1</sup>H NMR spectrum of 2-Phenyl-4H-chromen-4-one (3a)

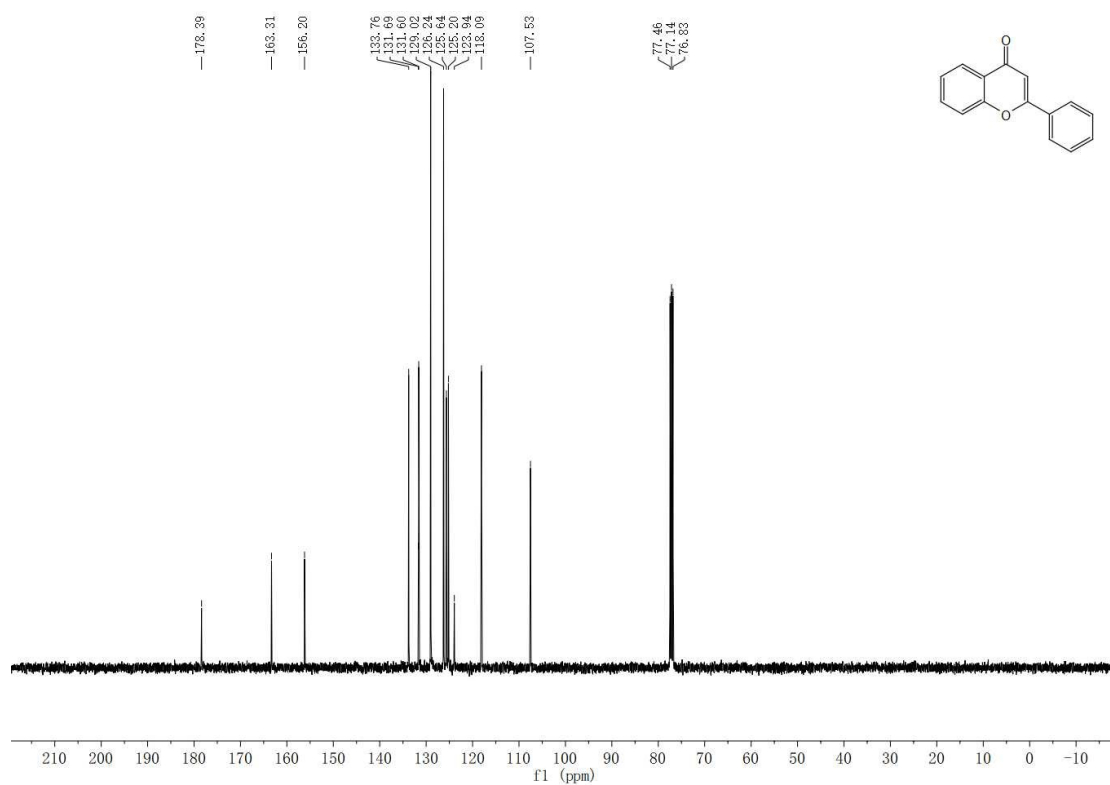


Figure S2 <sup>13</sup>C NMR spectrum of 2-Phenyl-4H-chromen-4-one (3a)

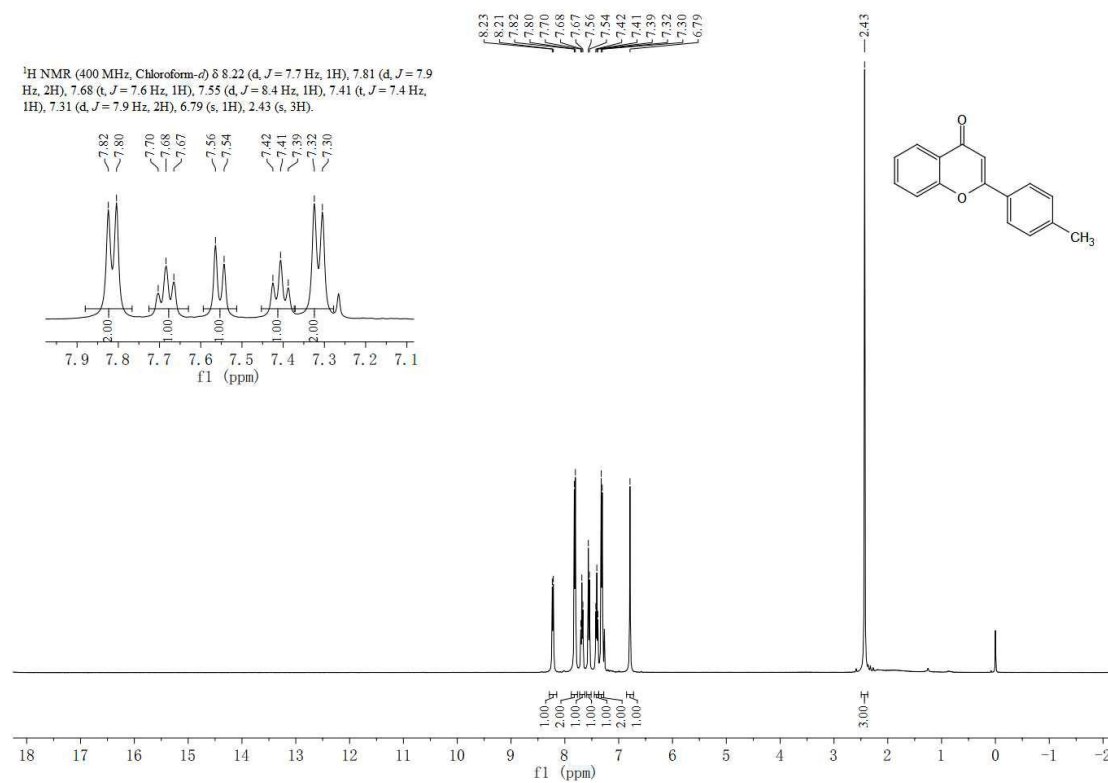


Figure S3 <sup>1</sup>H NMR spectrum of 2-(*p*-Tolyl)-4*H*-chromen-4-one (3b)

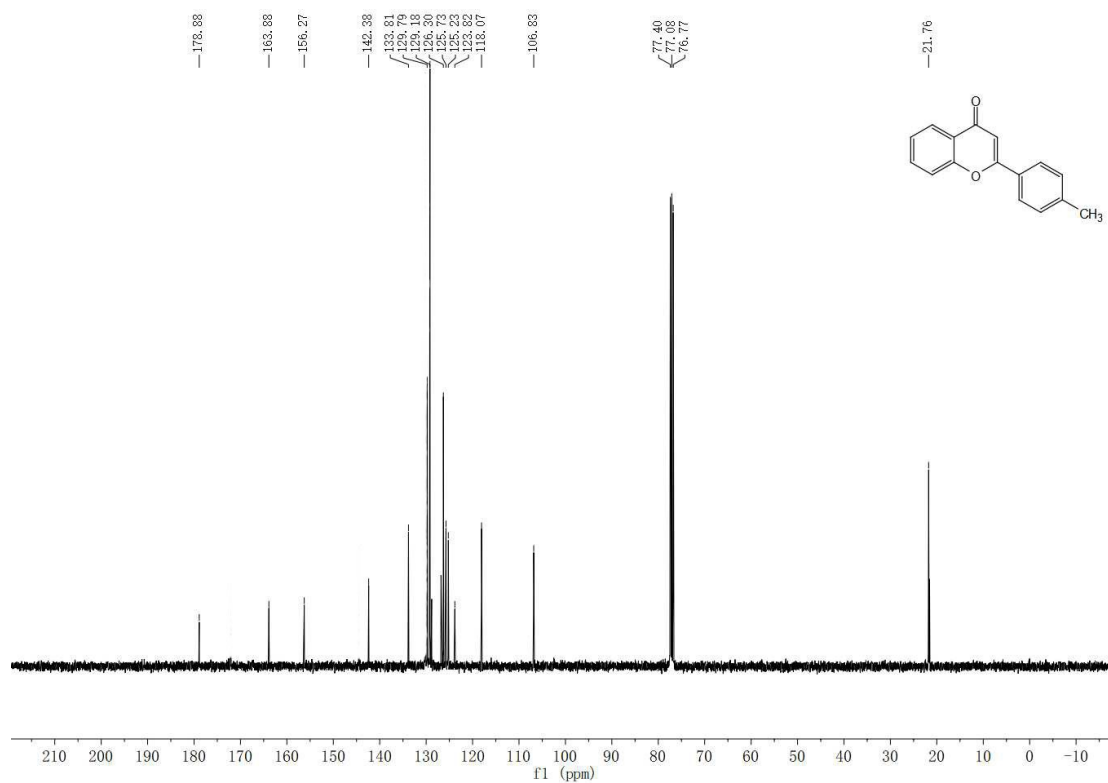


Figure S4 <sup>13</sup>C NMR spectrum of 2-(*p*-Tolyl)-4*H*-chromen-4-one (3b)



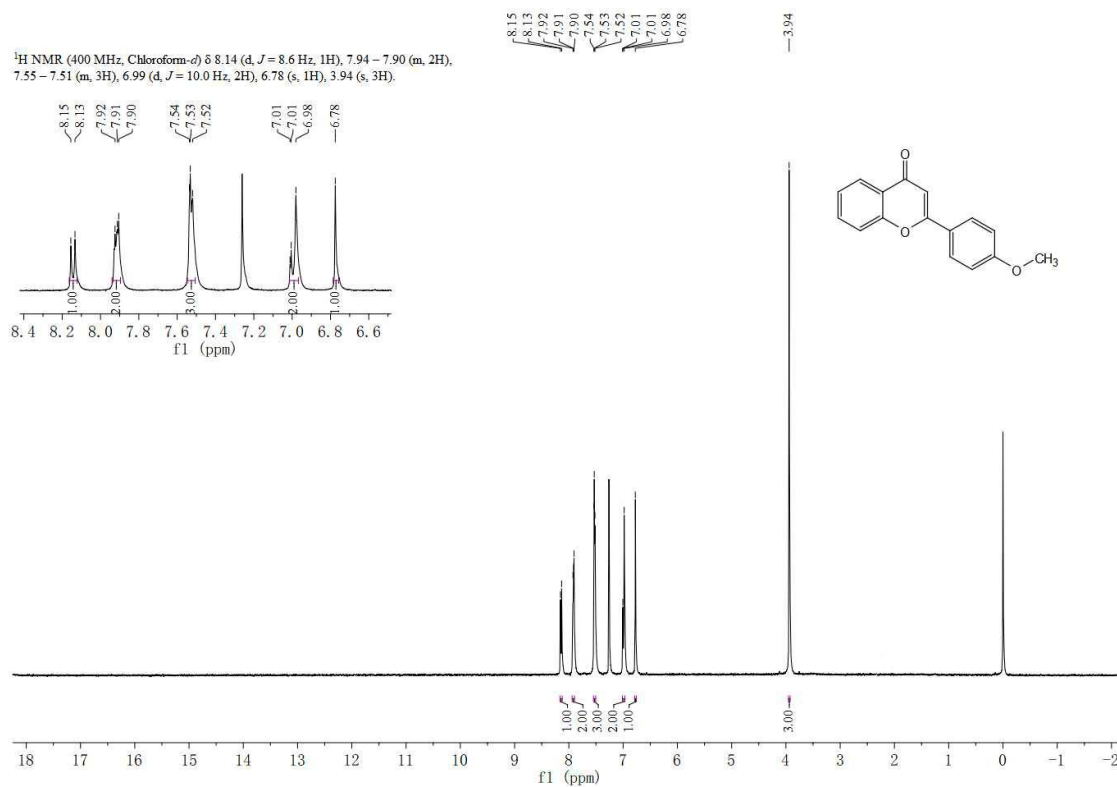


Figure S5 <sup>1</sup>H NMR spectrum of 2-(4-Methoxyphenyl)-4H-chromen-4-one (3c)

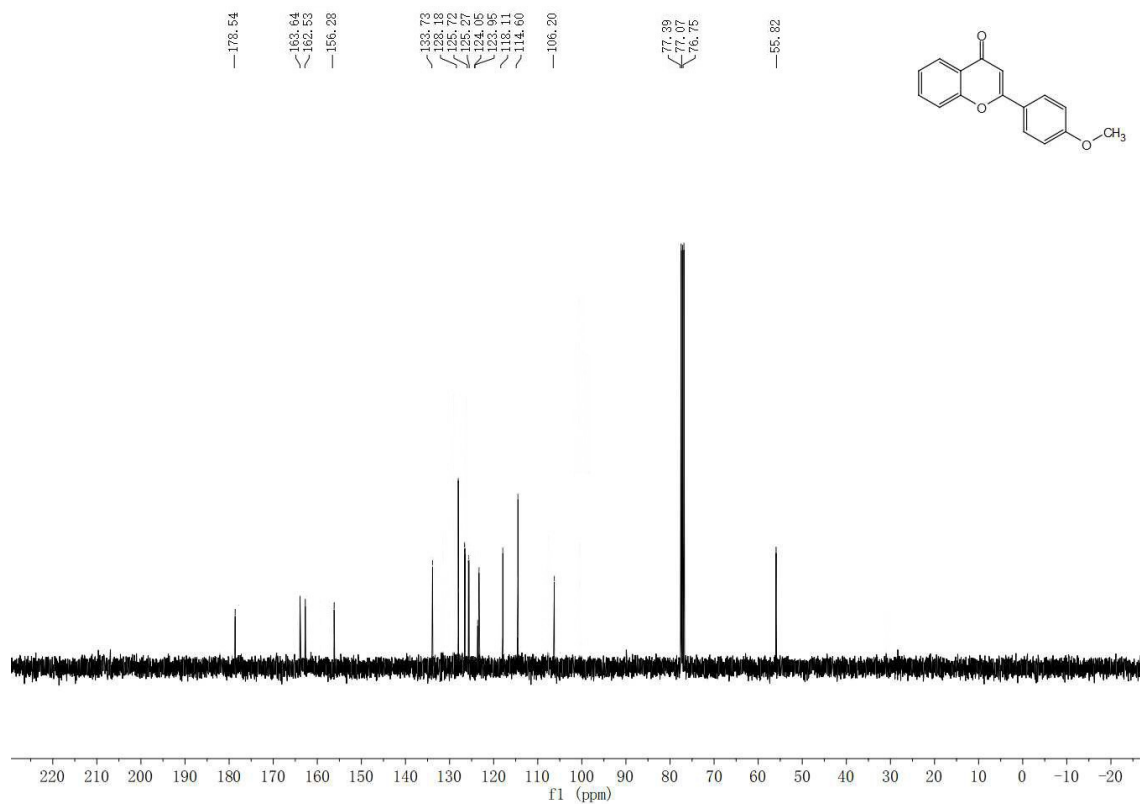


Figure S6 <sup>13</sup>C NMR spectrum of 2-(4-Methoxyphenyl)-4H-chromen-4-one (3c)

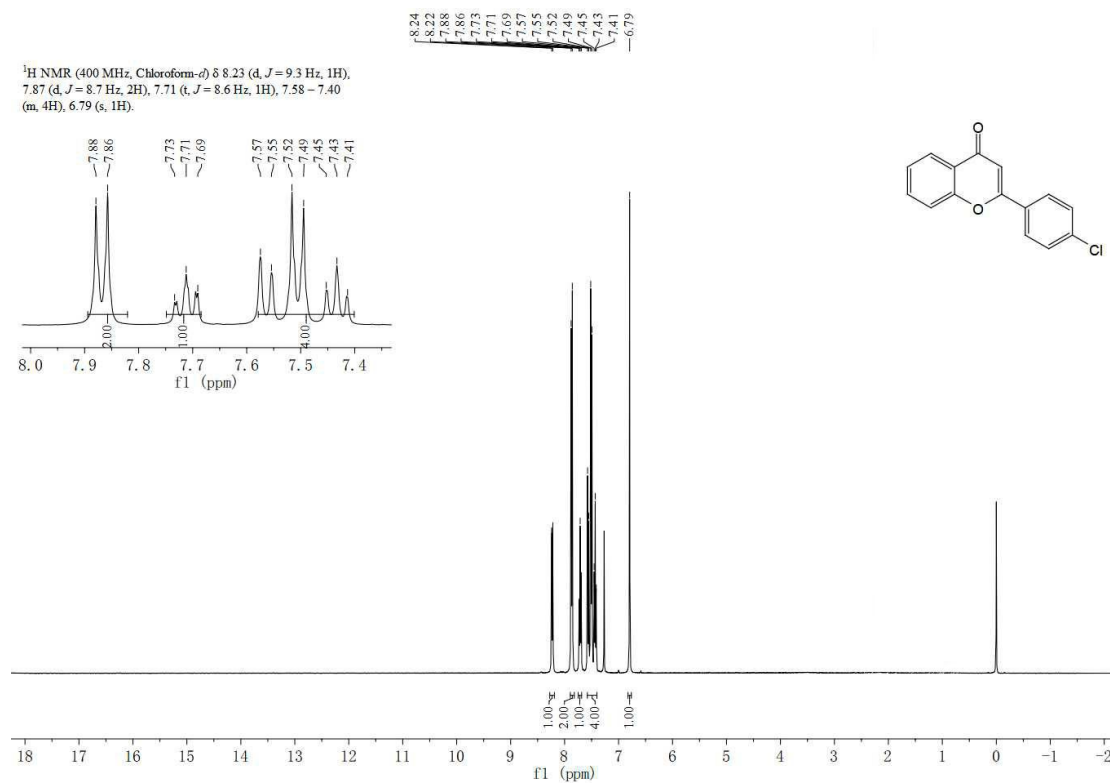


Figure S7 <sup>1</sup>H NMR spectrum of 2-(4-Chlorophenyl)-4H-chromen-4-one (3d)

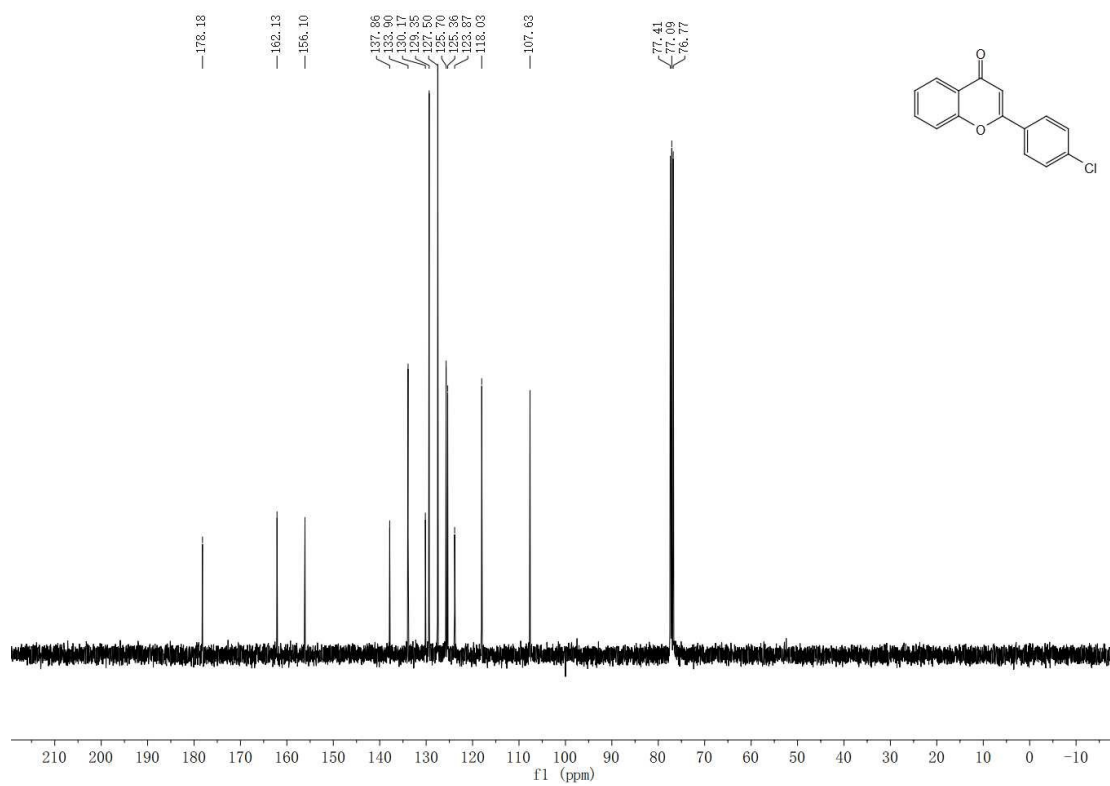


Figure S8 <sup>13</sup>C NMR spectrum of 2-(4-Chlorophenyl)-4H-chromen-4-one (3d)

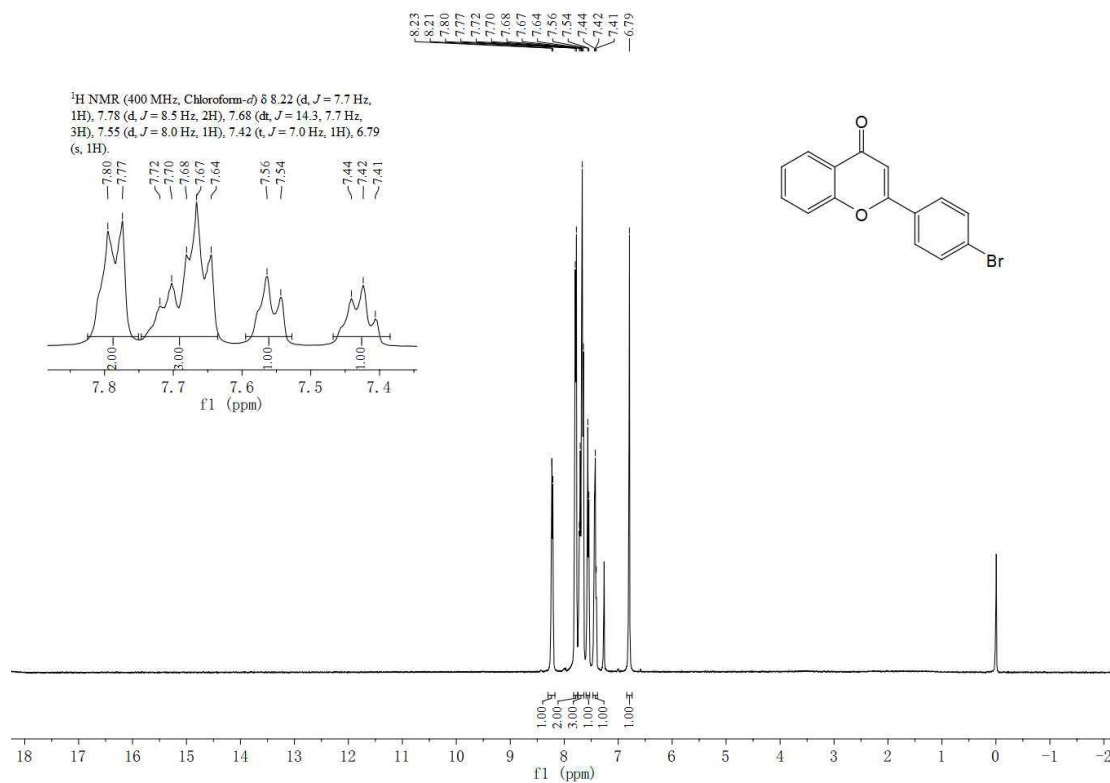


Figure S9 <sup>1</sup>H NMR spectrum of 2-(4-Bromophenyl)-4H-chromen-4-one (3e)

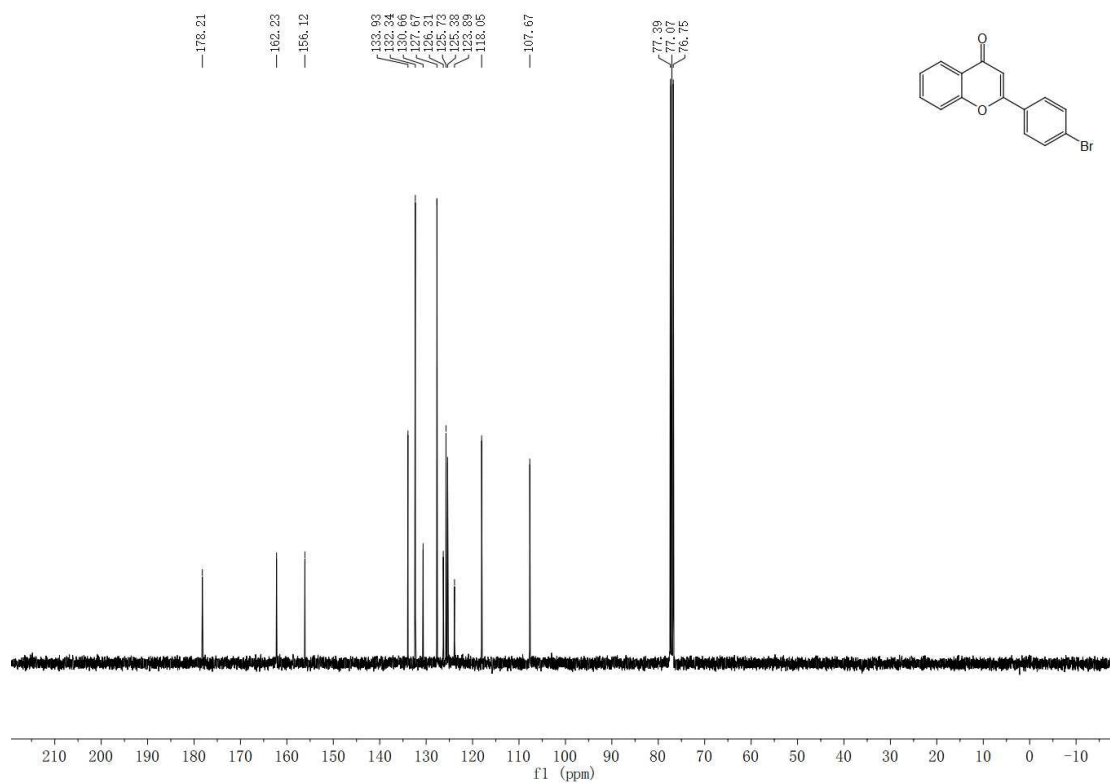


Figure S10 <sup>13</sup>C NMR spectrum of 2-(4-Bromophenyl)-4H-chromen-4-one (3e)

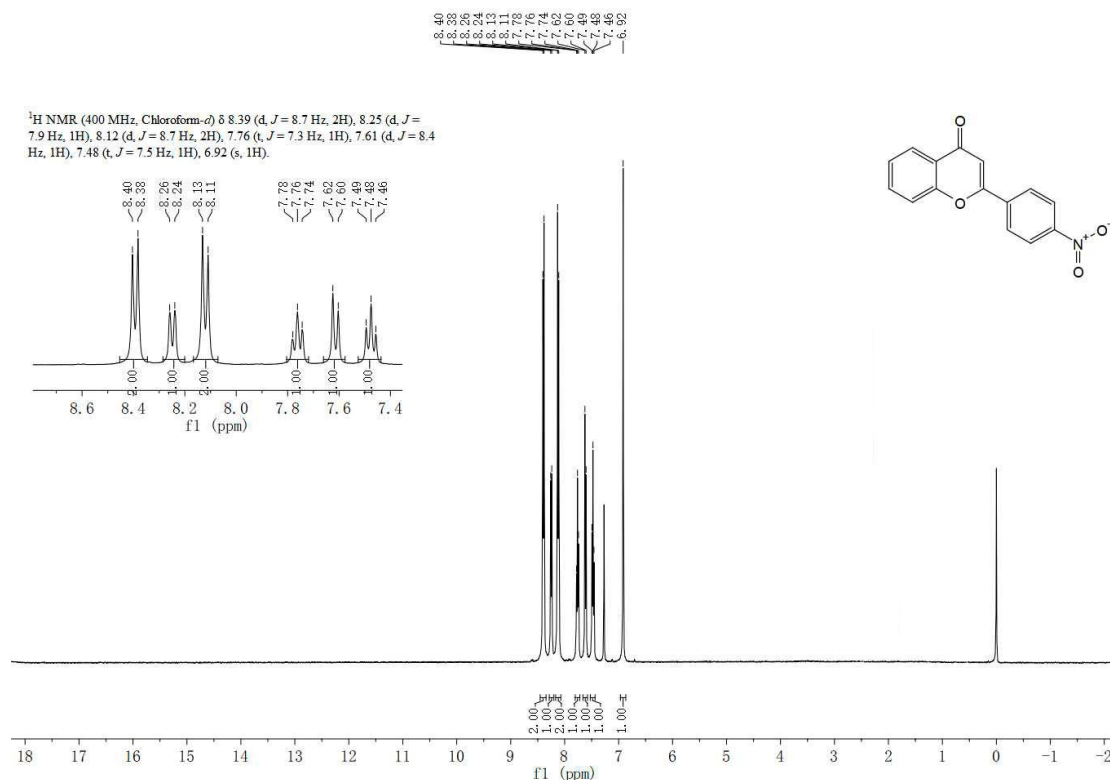


Figure S11 <sup>1</sup>H NMR spectrum of 2-(4-Nitrophenyl)-4H-chromen-4-one (3f)

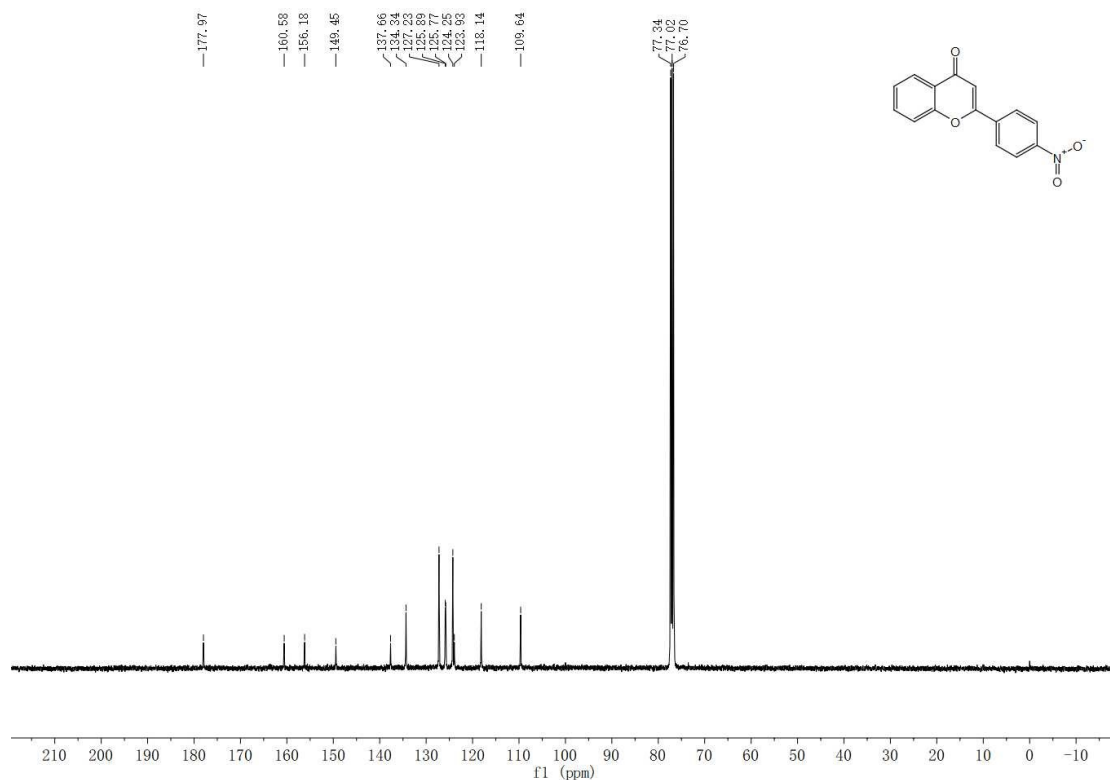


Figure S12 <sup>13</sup>C NMR spectrum of 2-(4-Nitrophenyl)-4H-chromen-4-one (3f)

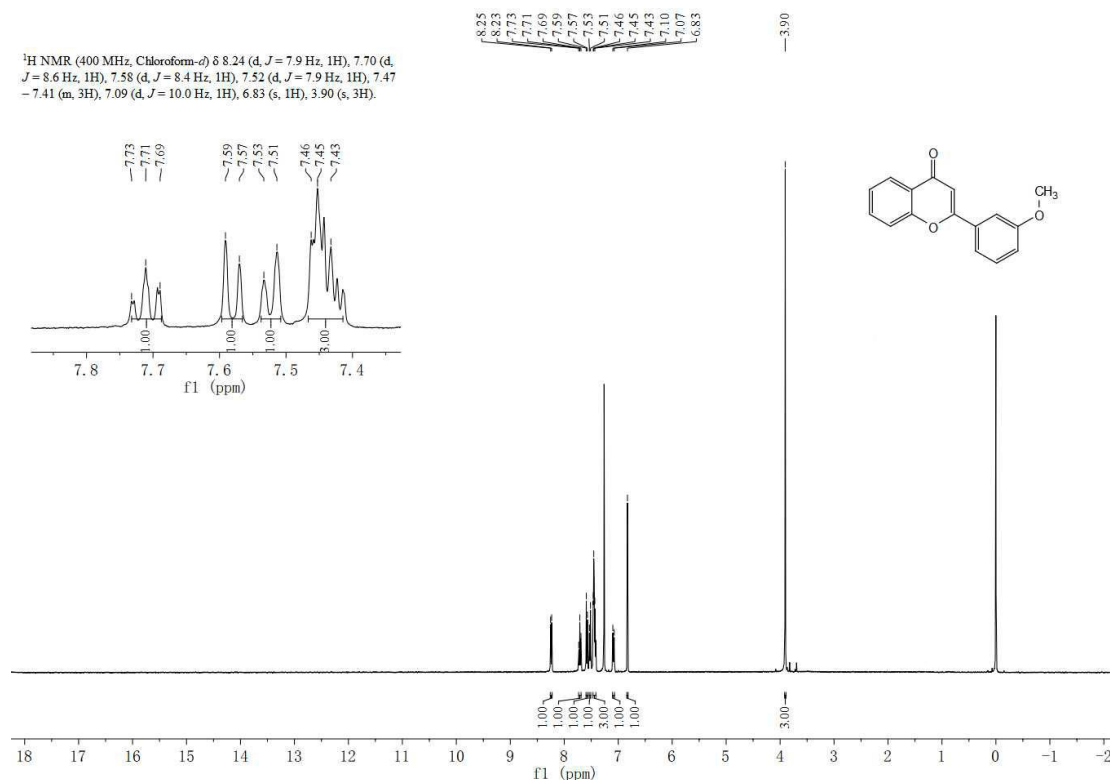


Figure S13 <sup>1</sup>H NMR spectrum of 2-(3-methoxyphenyl)-4H-chromen-4-one (3g)

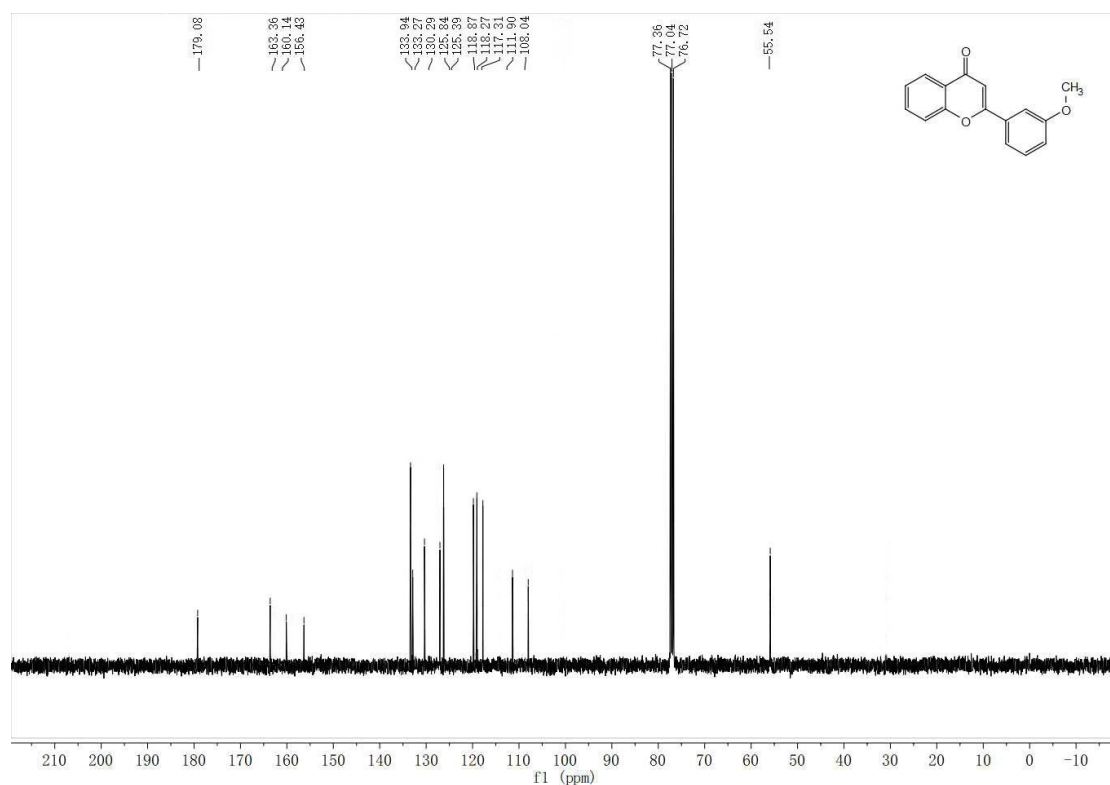


Figure S14 <sup>13</sup>C NMR spectrum of 2-(3-methoxyphenyl)-4H-chromen-4-one (3g)

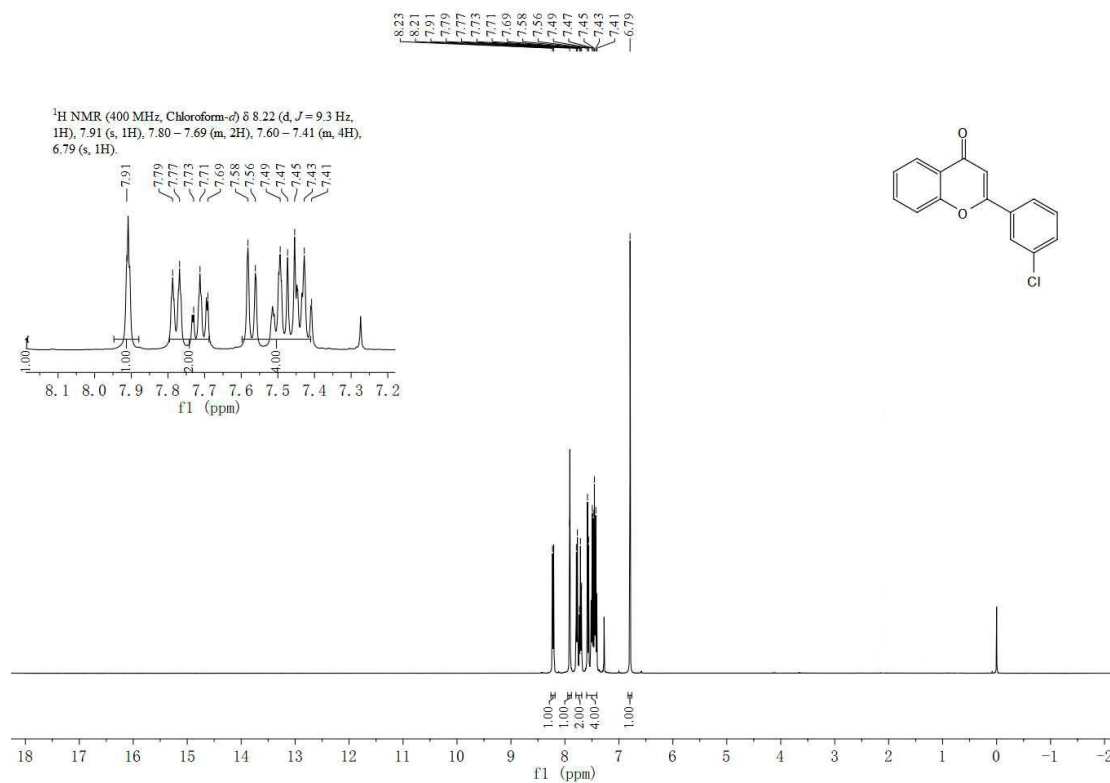


Figure S15 <sup>1</sup>H NMR spectrum of 2-(3-chlorophenyl)-4H-chromen-4-one (3h)

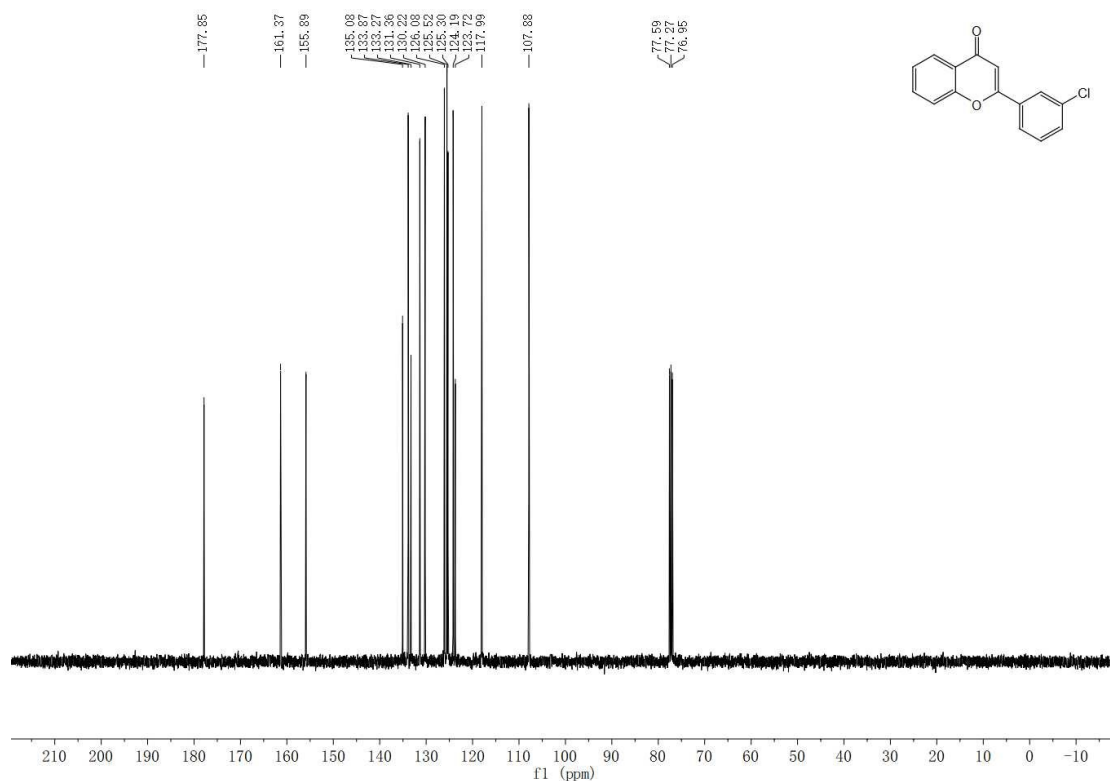


Figure S16 <sup>13</sup>C NMR spectrum of 2-(3-chlorophenyl)-4H-chromen-4-one (3h)

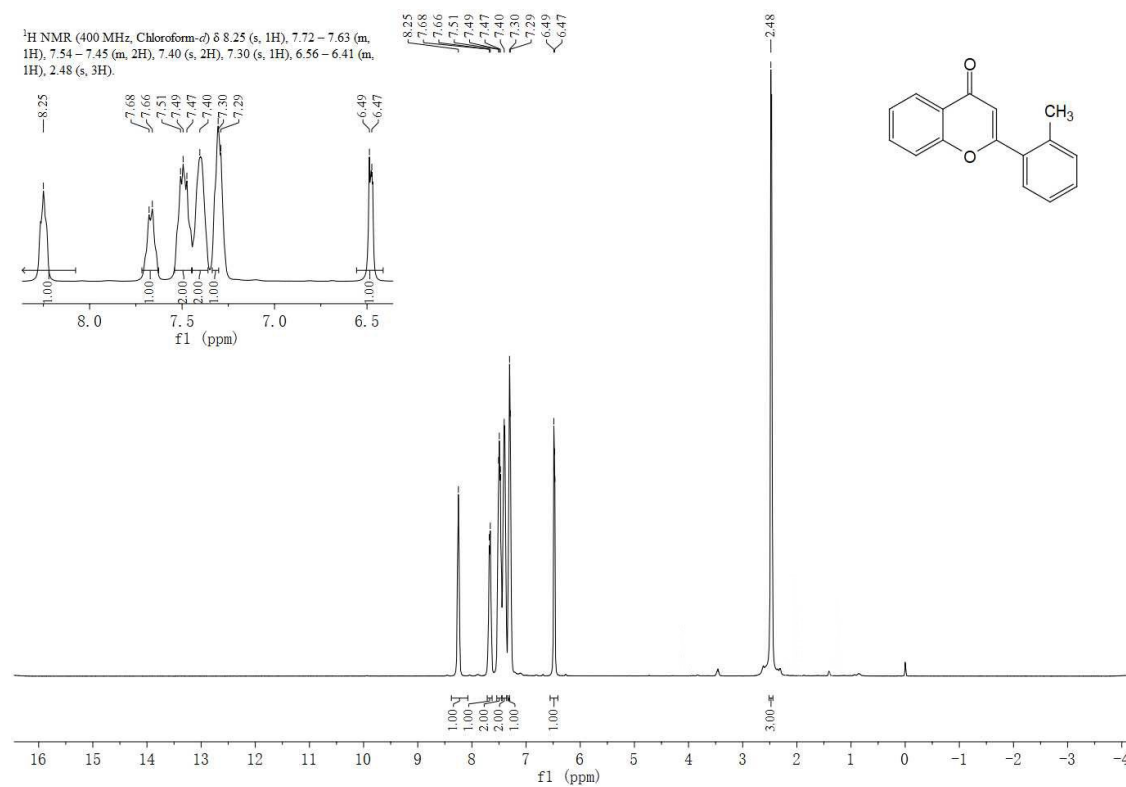


Figure S17 <sup>1</sup>H NMR spectrum of 2-(o-tolyl)-4H-chromen-4-one (3i)

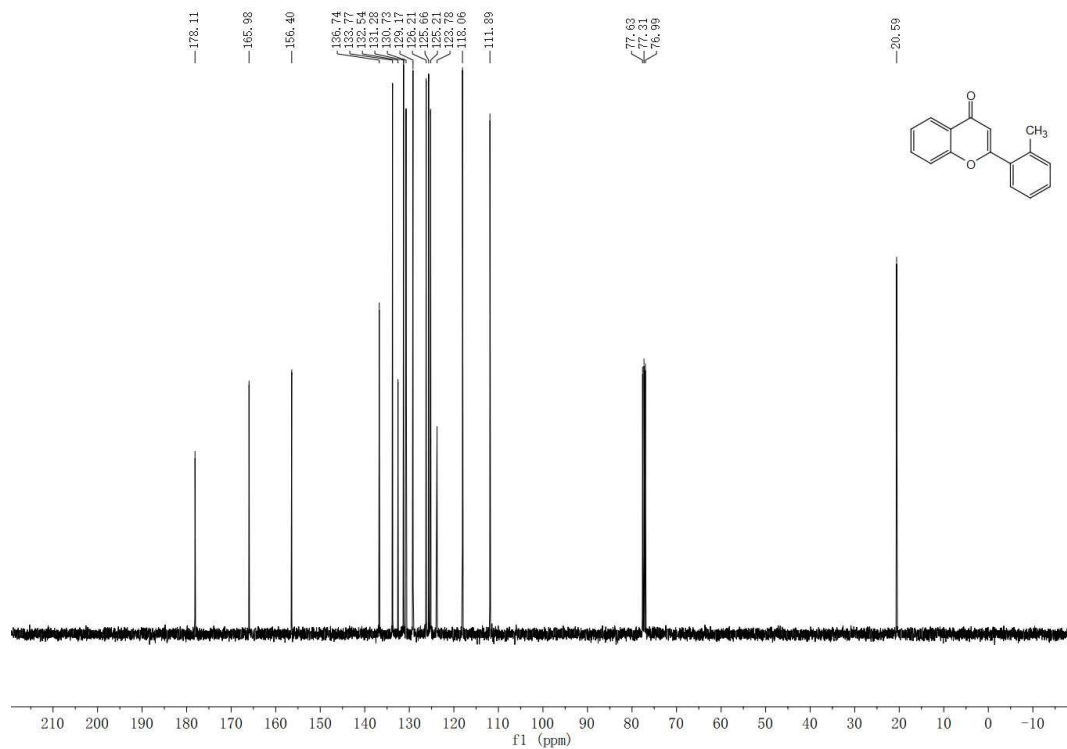
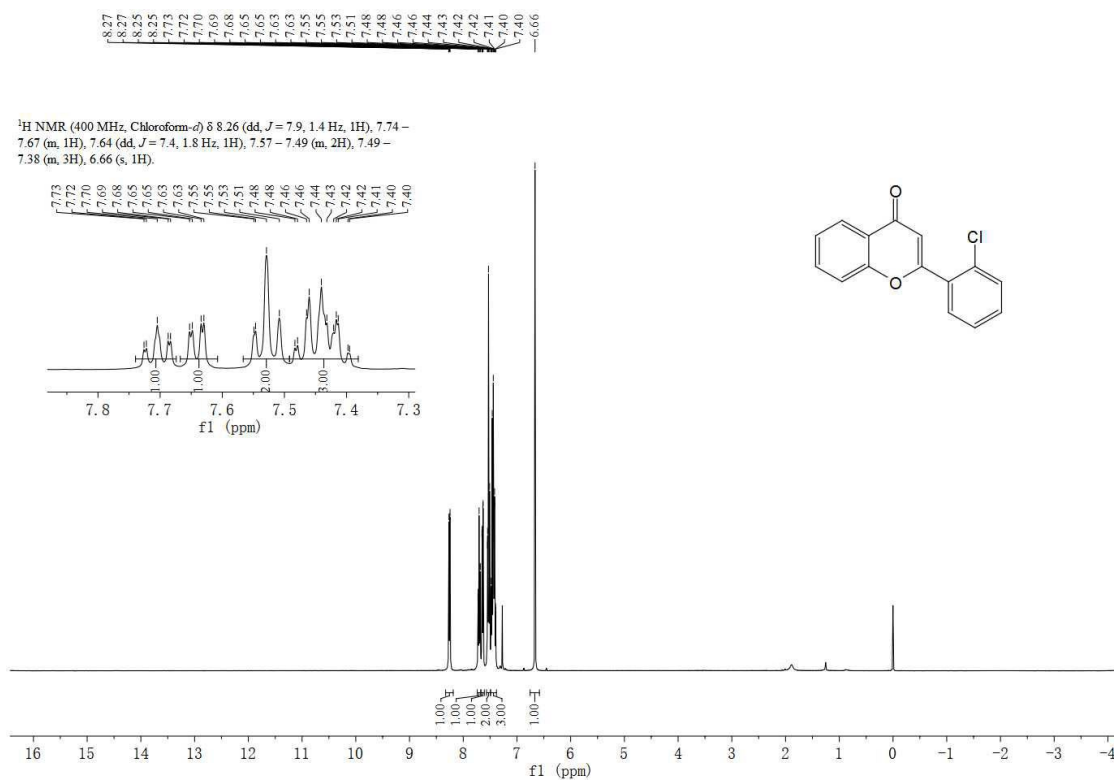
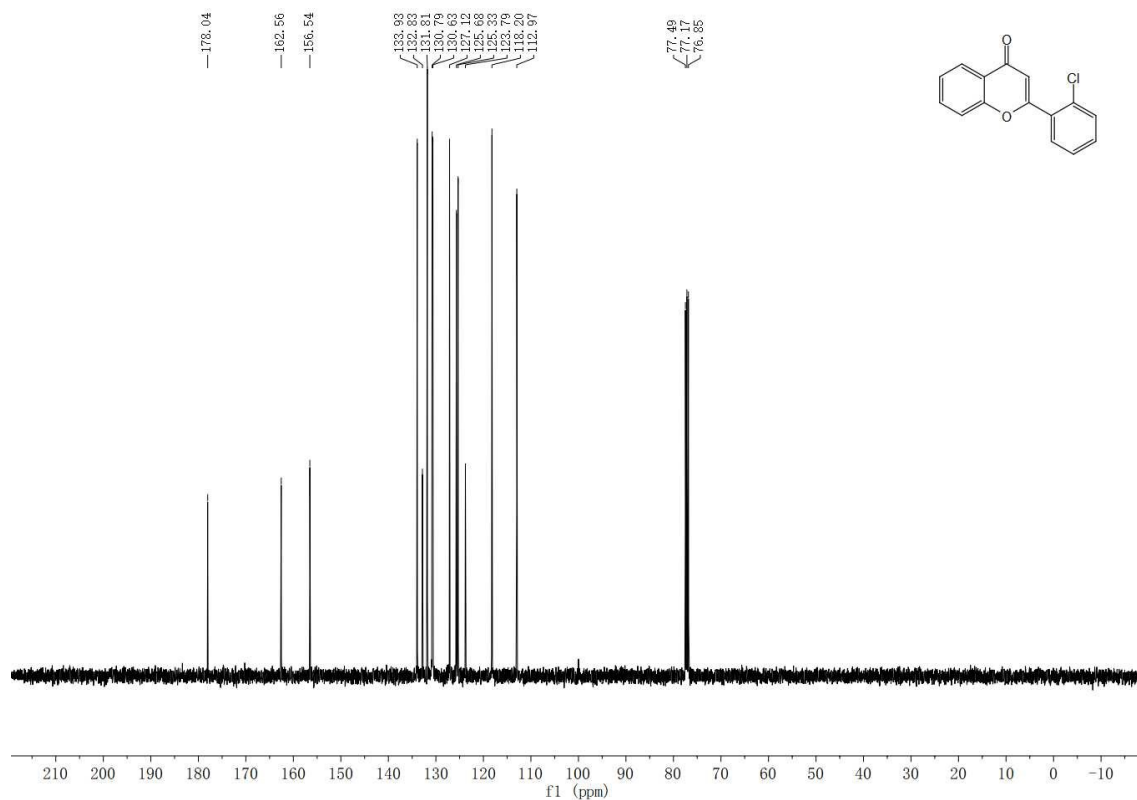


Figure S18 <sup>13</sup>C NMR spectrum of 2-(o-tolyl)-4H-chromen-4-one (3i)



**Figure S19** <sup>1</sup>H NMR spectrum of 2-(3-chlorophenyl)-4H-chromen-4-one (3j)



**Figure S20** <sup>13</sup>C NMR spectrum of 2-(3-chlorophenyl)-4H-chromen-4-one (3j)





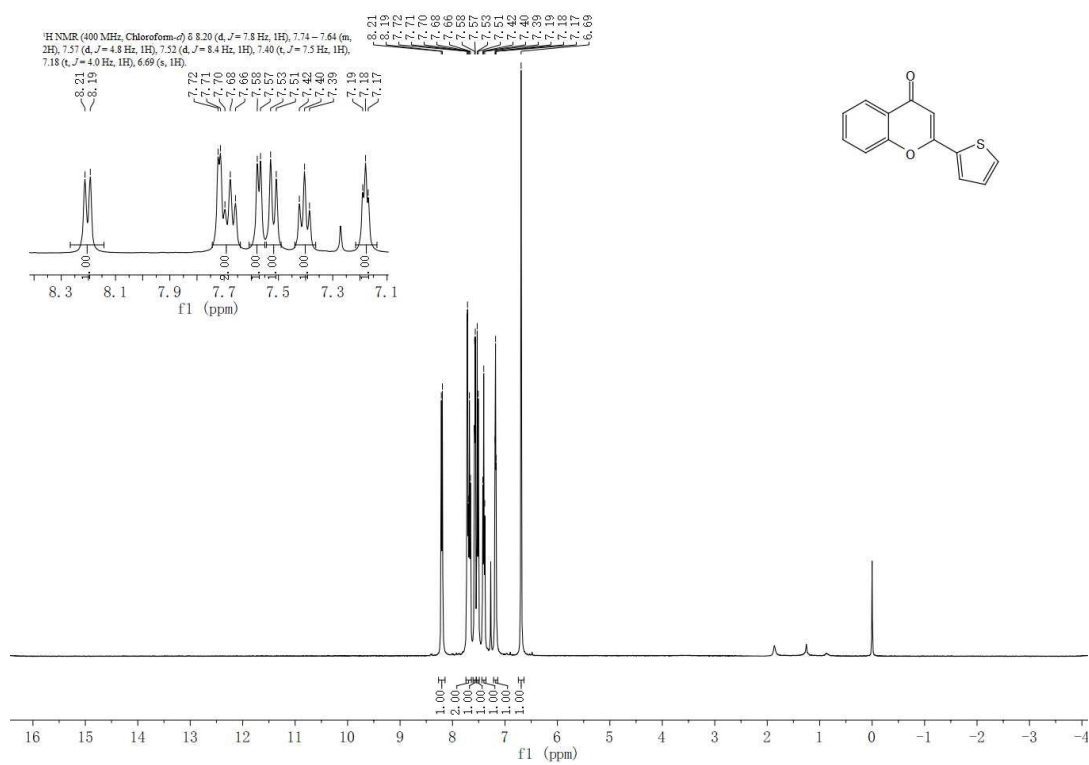


Figure S23 <sup>1</sup>H NMR spectrum of 2-(Thiophen-2-yl)-4H-chromen-4-one (3I)

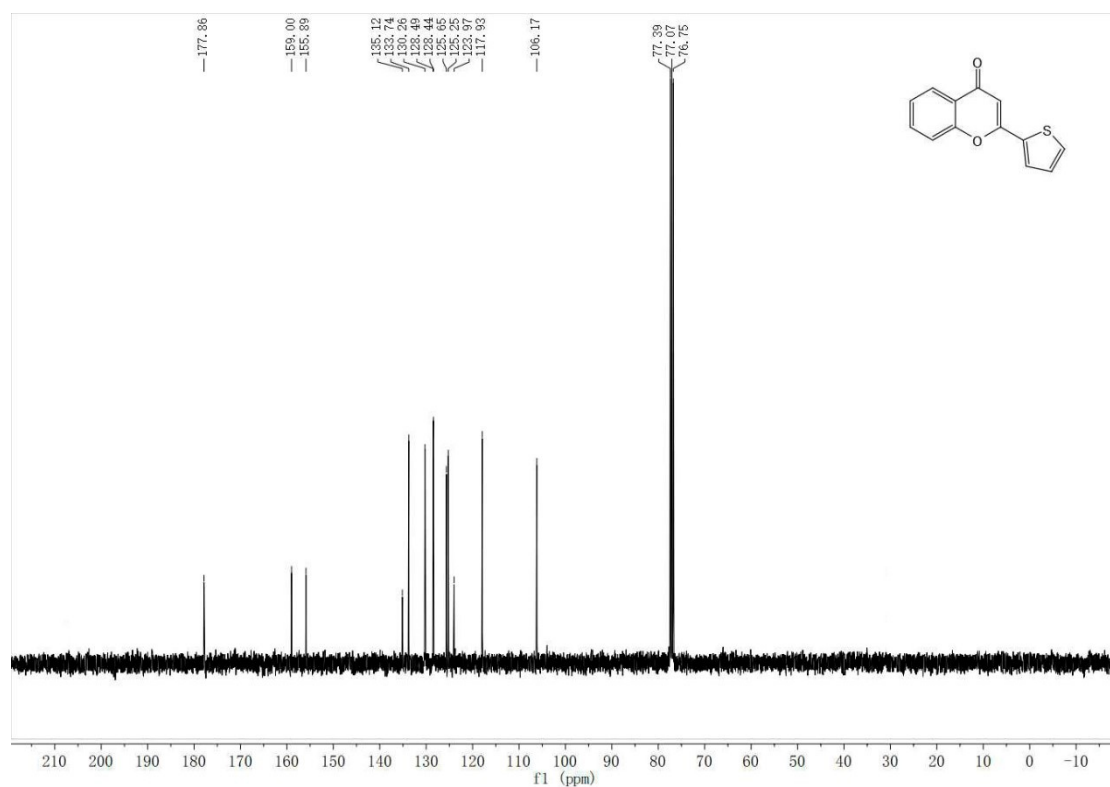
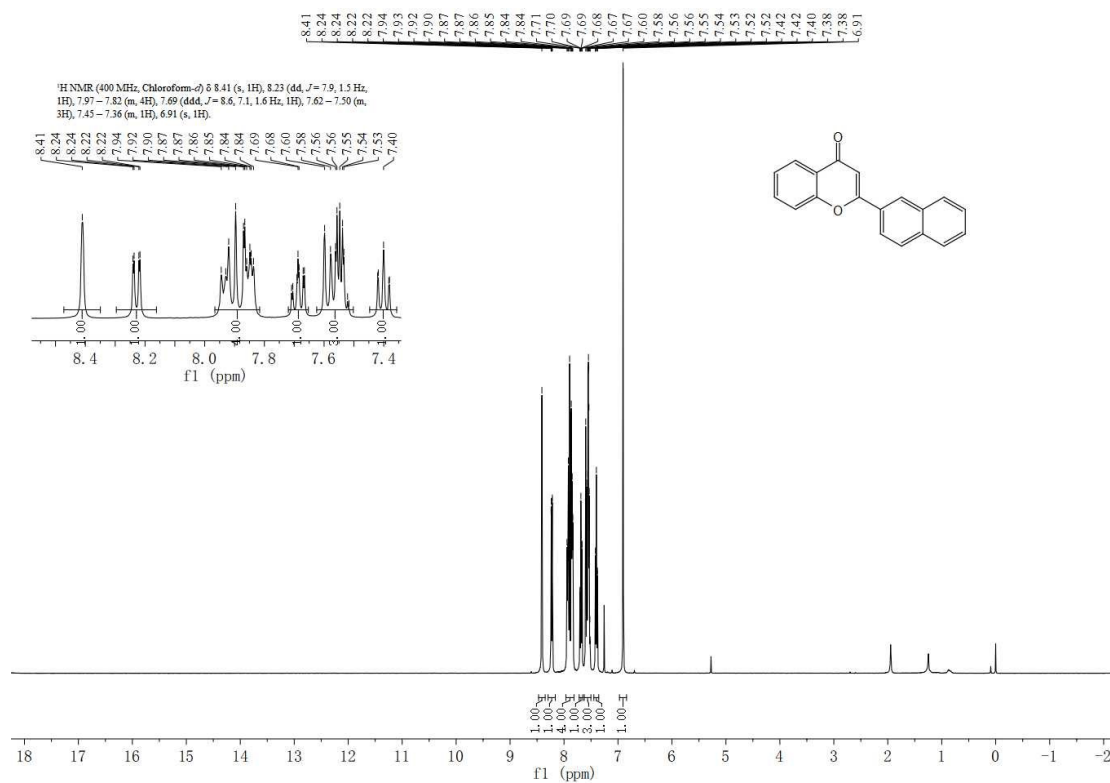
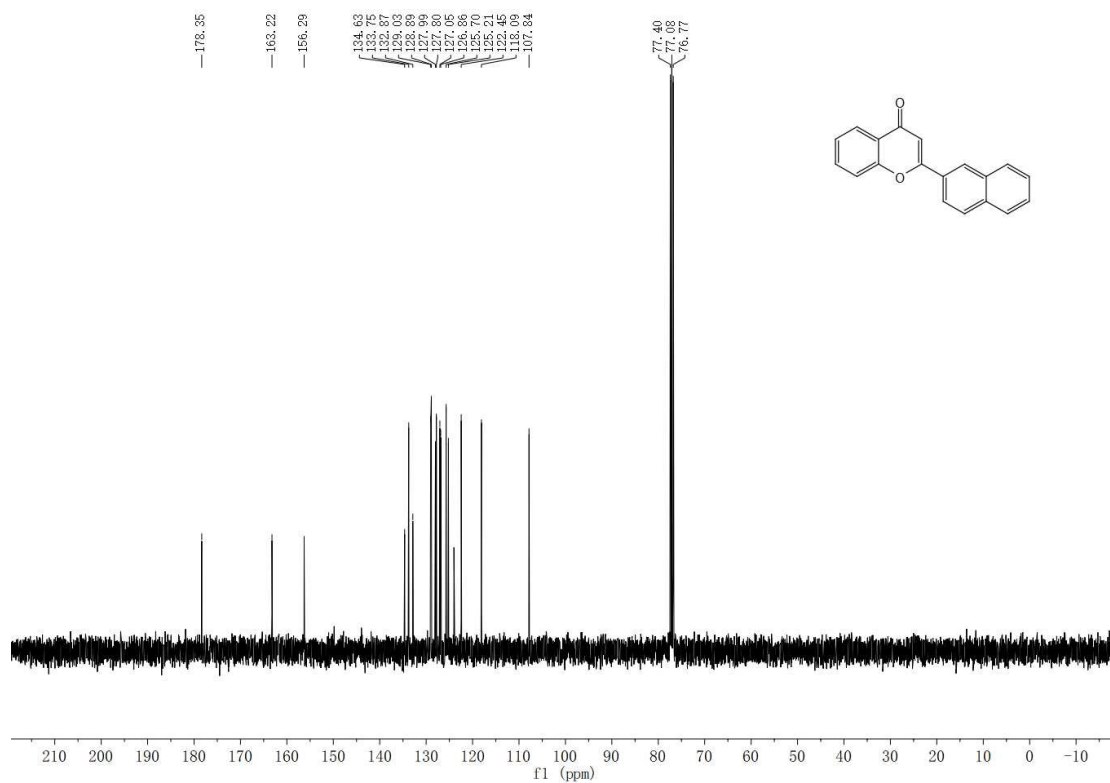


Figure S24 <sup>13</sup>C NMR spectrum of 2-(Thiophen-2-yl)-4H-chromen-4-one (3I)



**Figure S25**  $^1\text{H NMR}$  spectrum of 2-(naphthalen-2-yl)-4H-chromen-4-one (3m)



**Figure S26**  $^{13}\text{C NMR}$  spectrum of 2-(naphthalen-2-yl)-4H-chromen-4-one (3m)

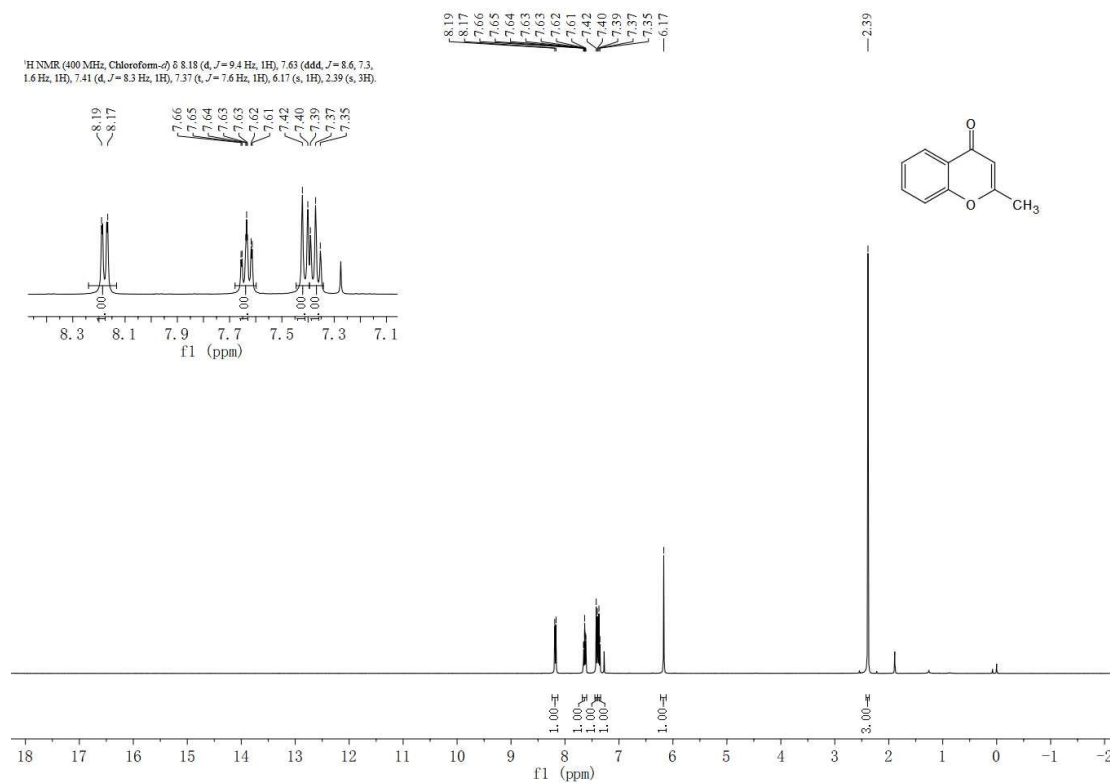


Figure S27 <sup>1</sup>H NMR spectrum of 2-Methyl-4H-chromen-4-one (3n)

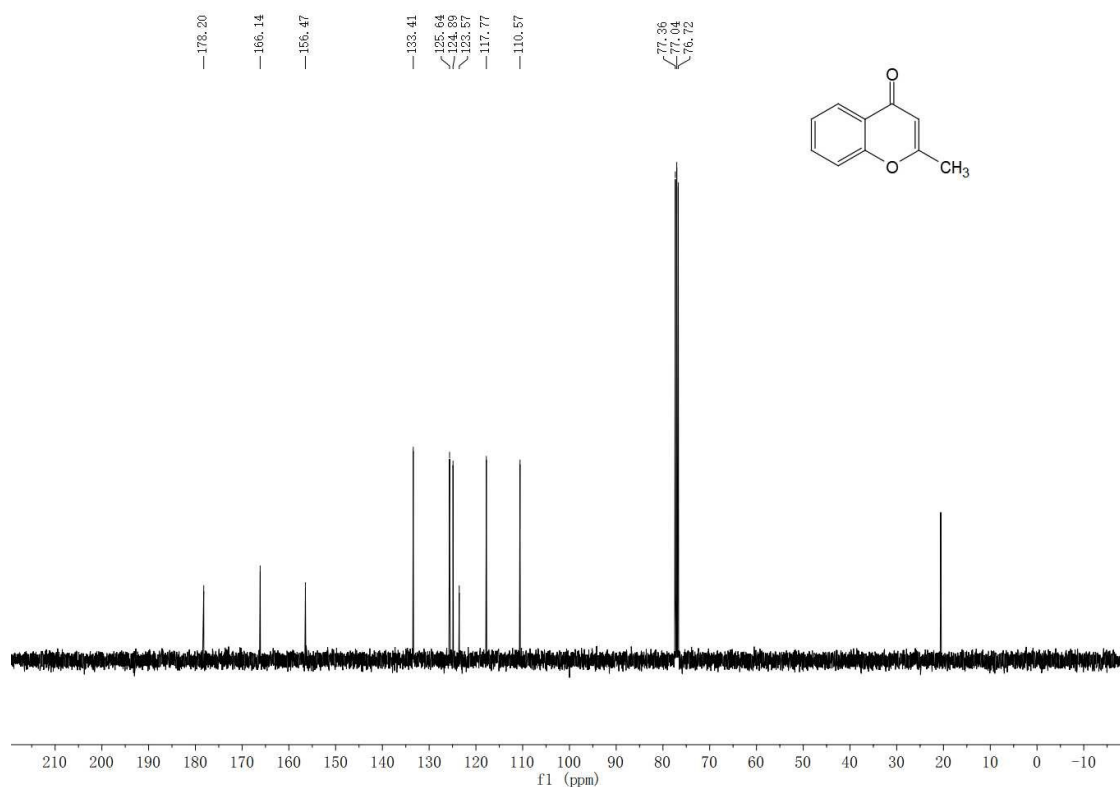


Figure S28 <sup>13</sup>C NMR spectrum of 2-Methyl-4H-chromen-4-one (3n)

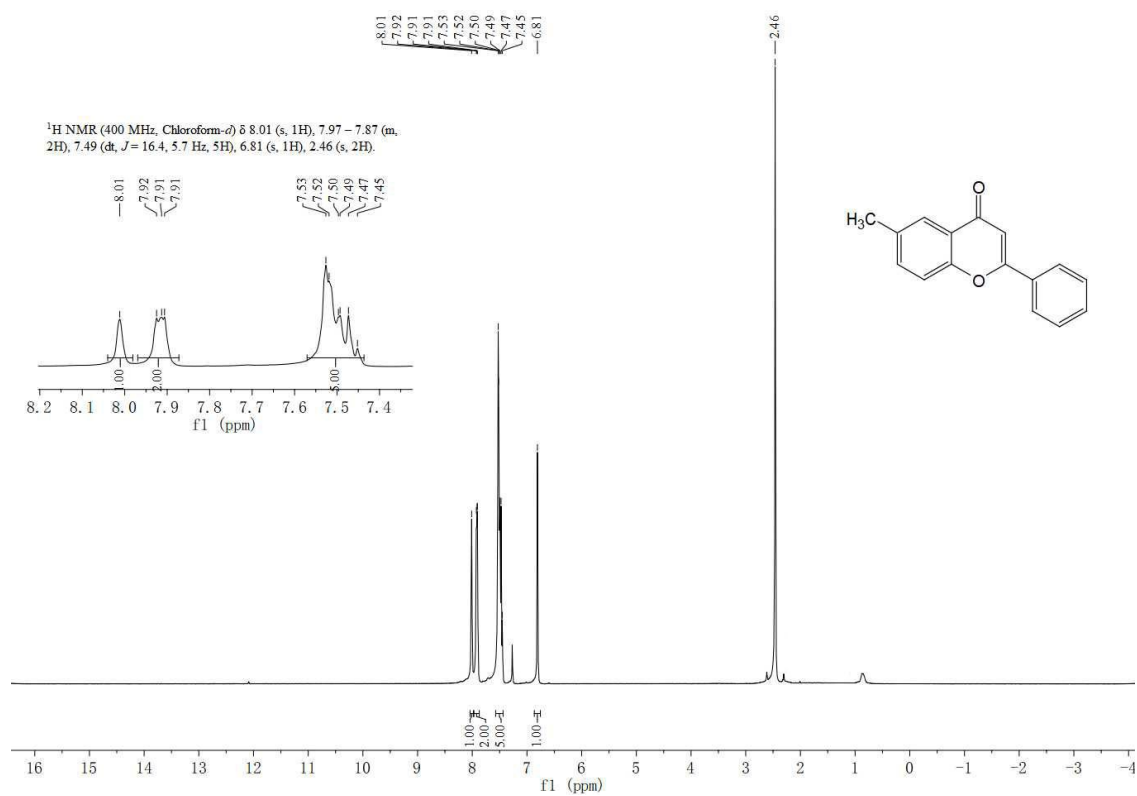


Figure S29 <sup>1</sup>H NMR spectrum of 6-methyl-2-phenyl-4H-chromen-4-one (3o)

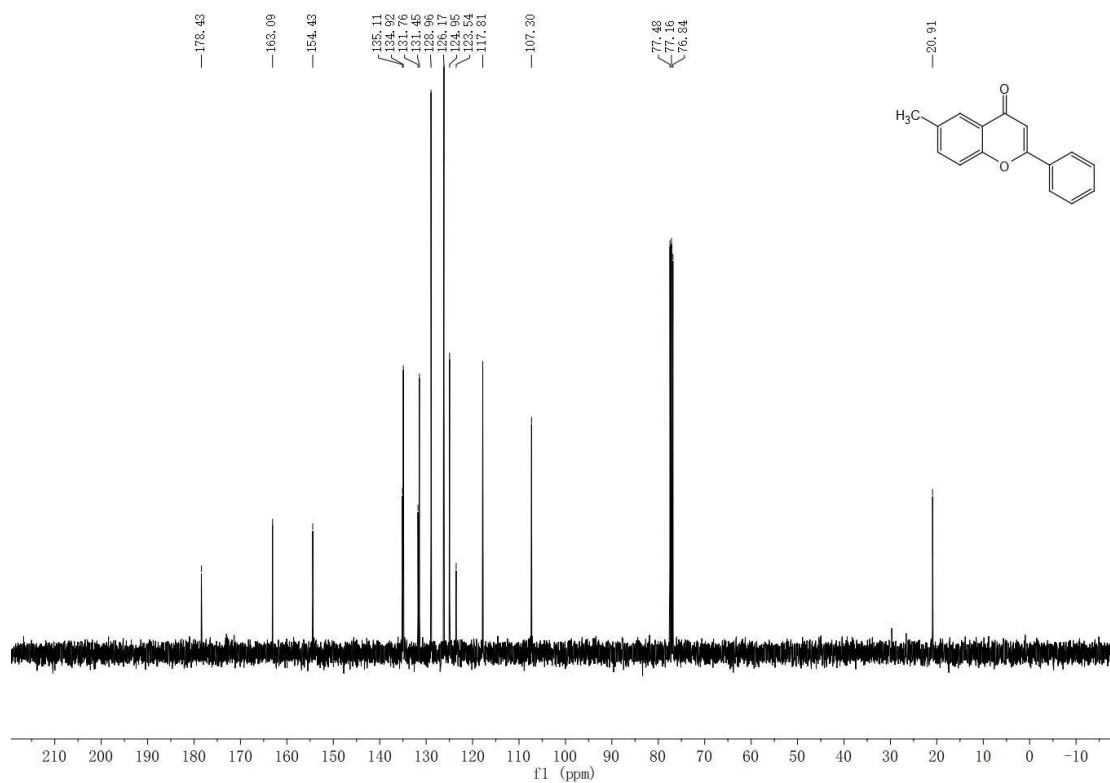


Figure S30 <sup>13</sup>C NMR spectrum of 6-methyl-2-phenyl-4H-chromen-4-one (3o)



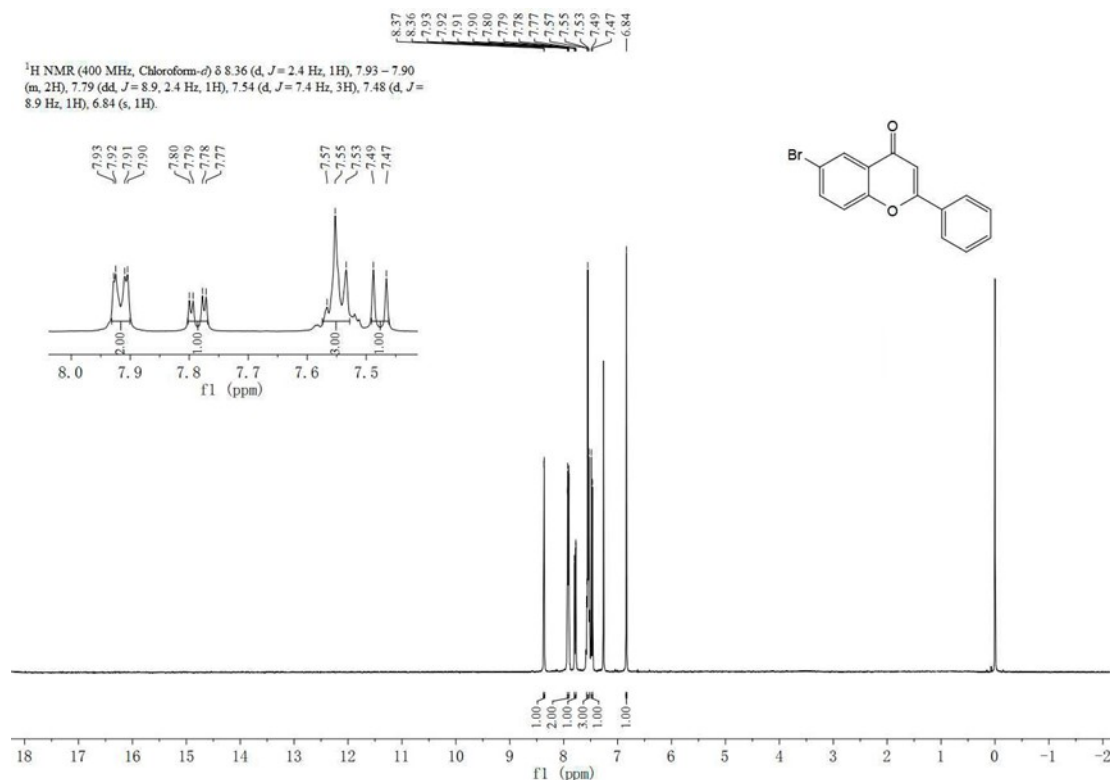


Figure S33 <sup>1</sup>H NMR spectrum of 6-bromo-2-phenyl-4H-chromen-4-one (3q)

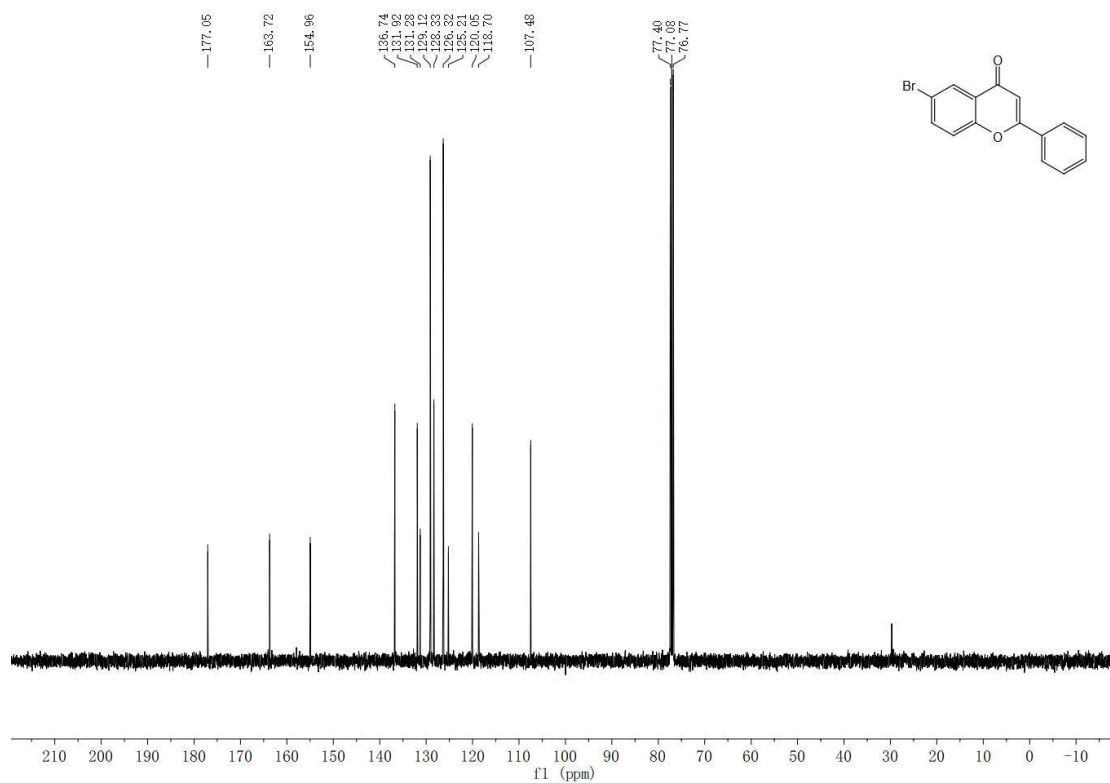


Figure S34 <sup>13</sup>C NMR spectrum of 6-bromo-2-phenyl-4H-chromen-4-one (3q)

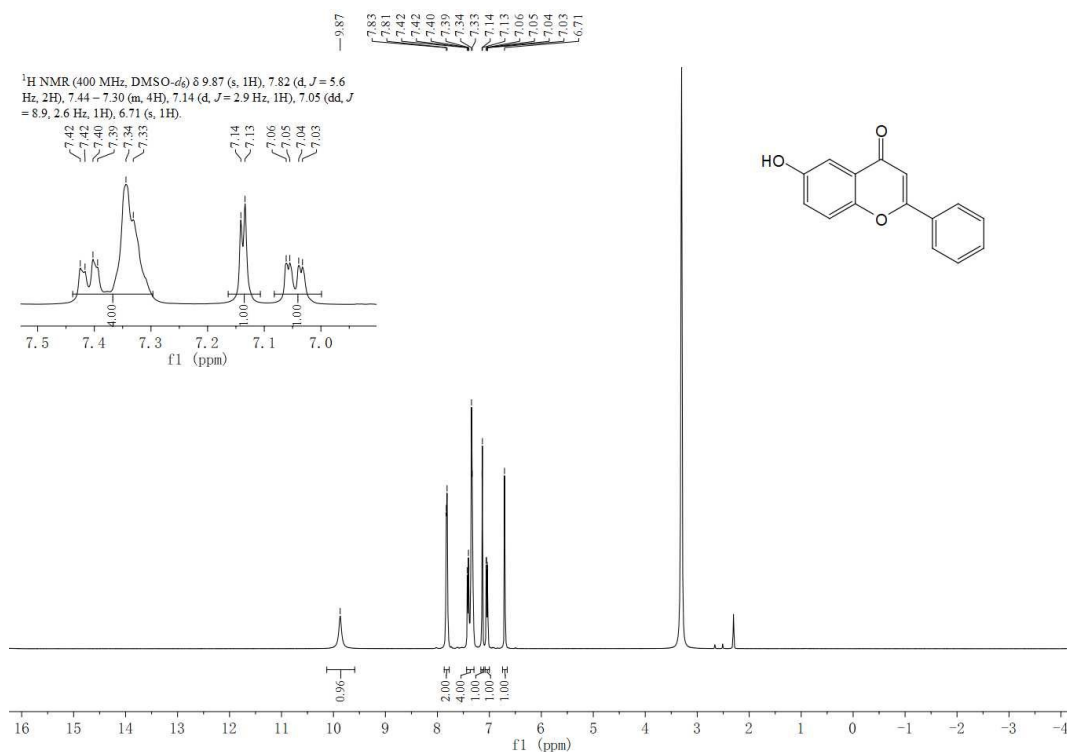


Figure S35 <sup>1</sup>H NMR spectrum of 6-Hydroxy-2-phenyl-4H-chromen-4-one (3r)

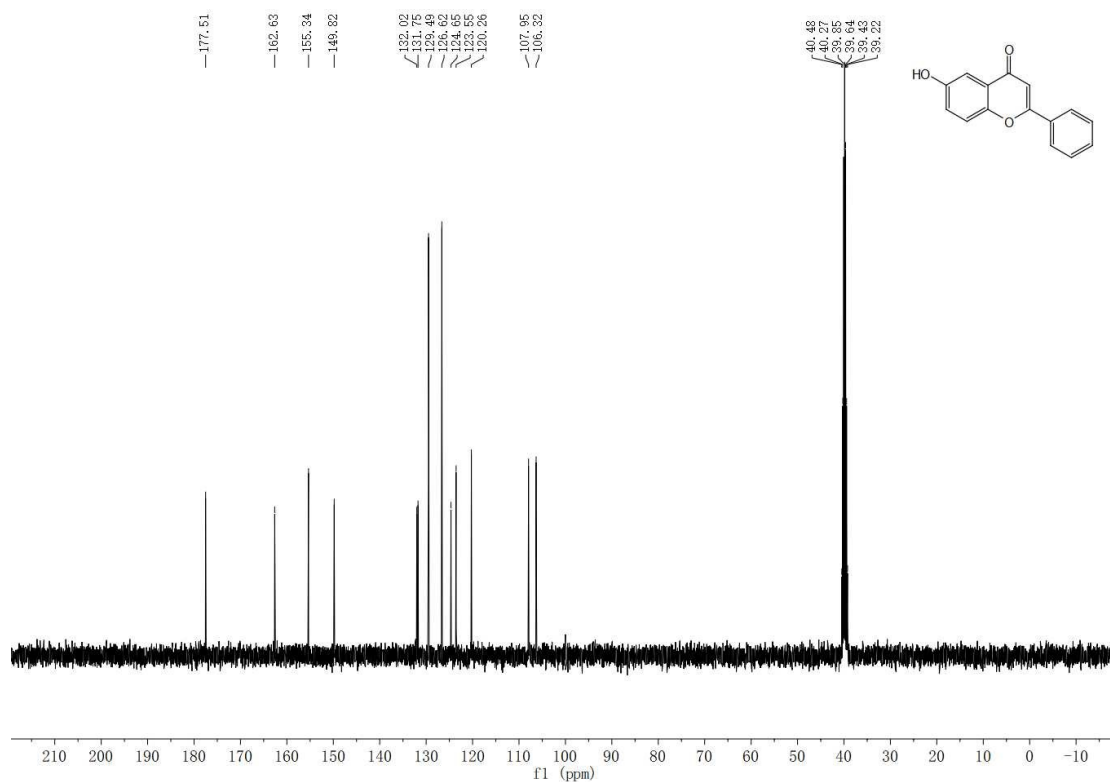


Figure S36 <sup>13</sup>C NMR spectrum of 6-Hydroxy-2-phenyl-4H-chromen-4-one (3r)



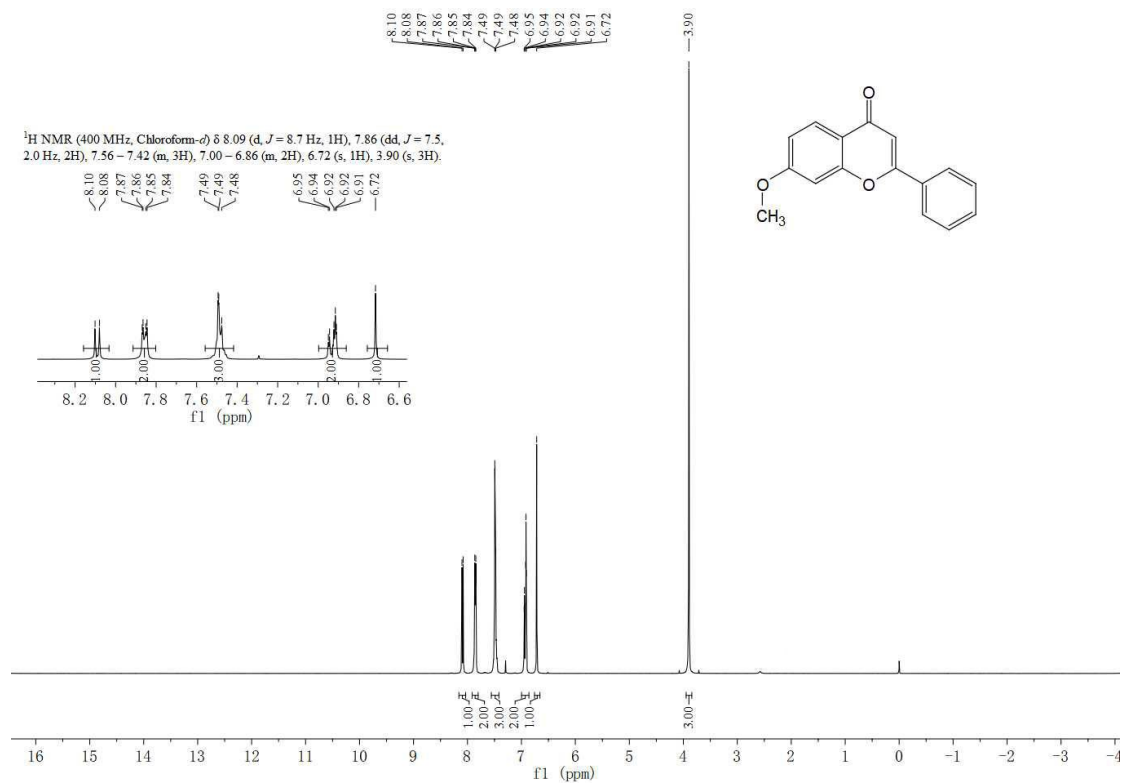


Figure S37 <sup>1</sup>H NMR spectrum of 7-methoxy-2-phenyl-4H-chromen-4-one (3s)

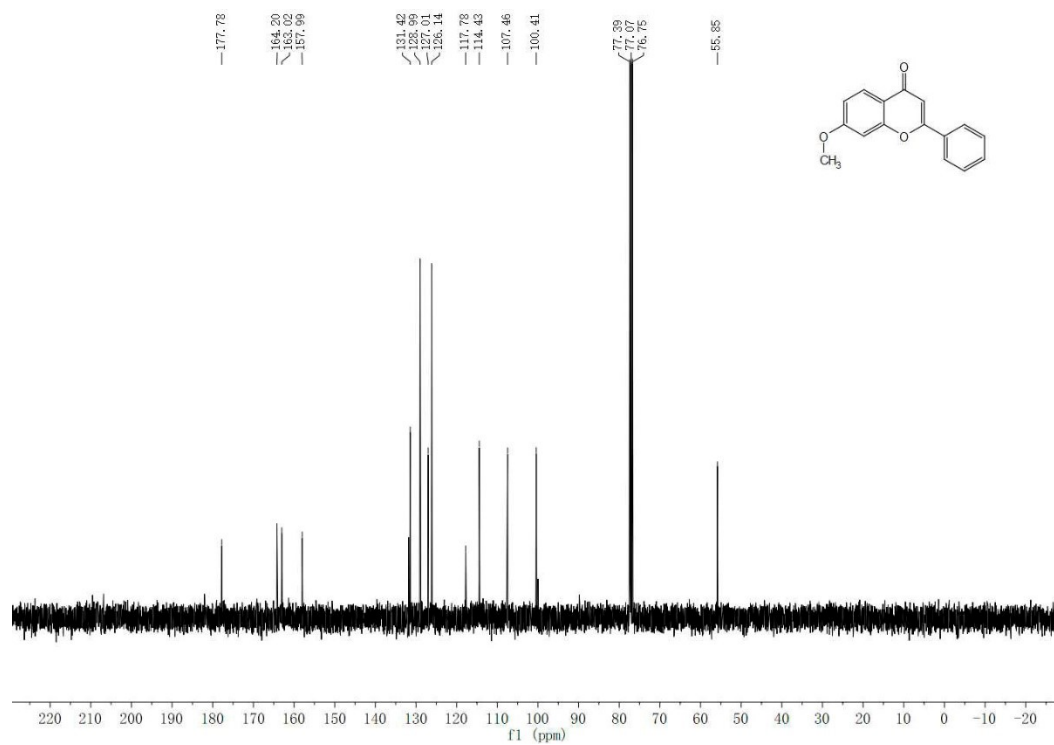


Figure S38 <sup>13</sup>C NMR spectrum of 7-methoxy-2-phenyl-4H-chromen-4-one (3s)

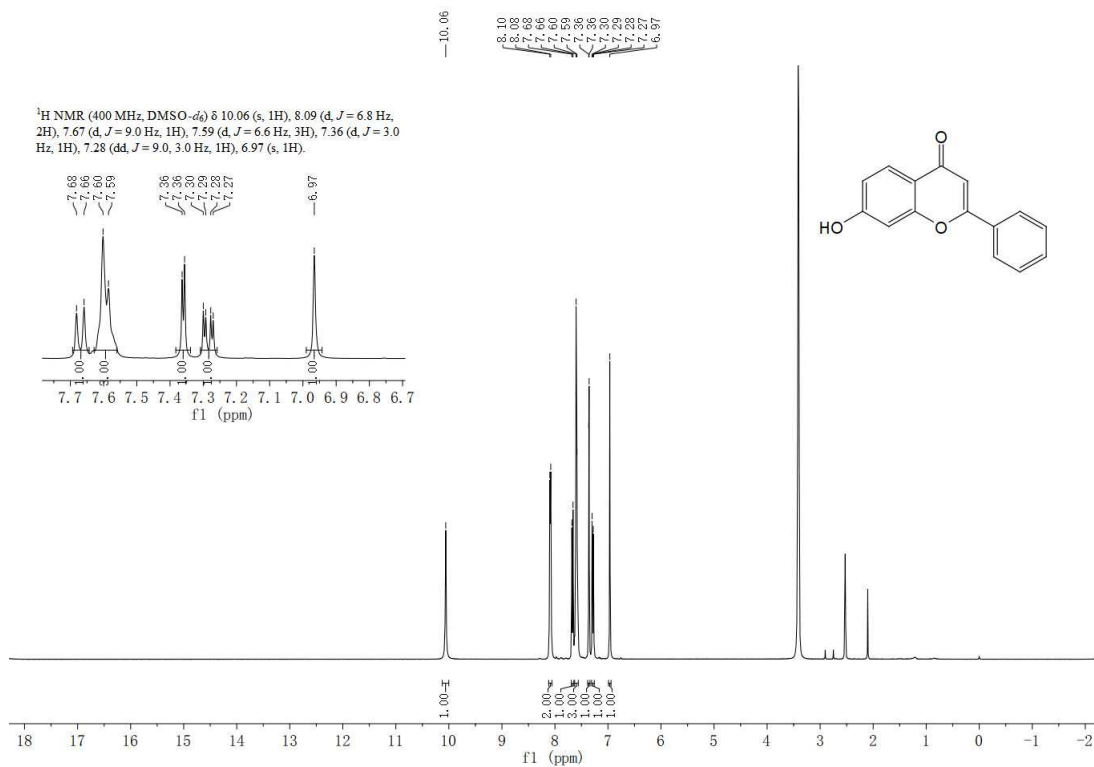


Figure S39 <sup>1</sup>H NMR spectrum of 7-Hydroxy-2-phenyl-4H-chromen-4-one (3t)

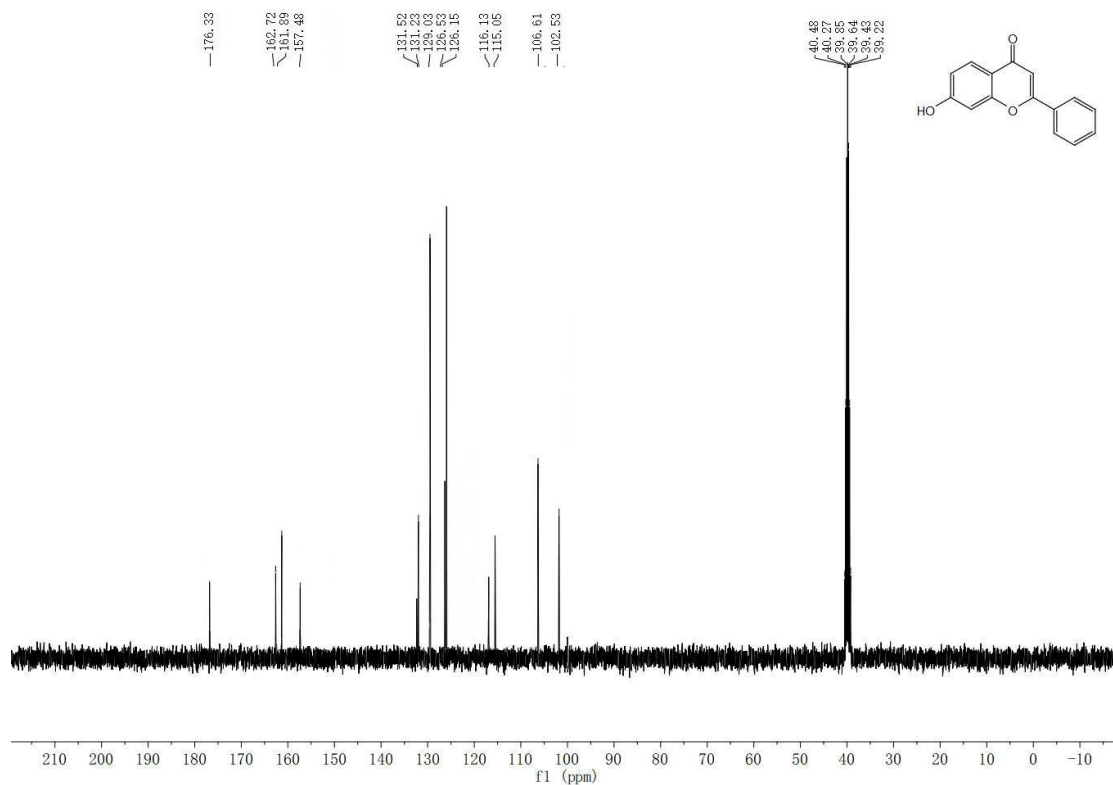


Figure S40 <sup>13</sup>C NMR spectrum of 7-Hydroxy-2-phenyl-4H-chromen-4-one (3t)

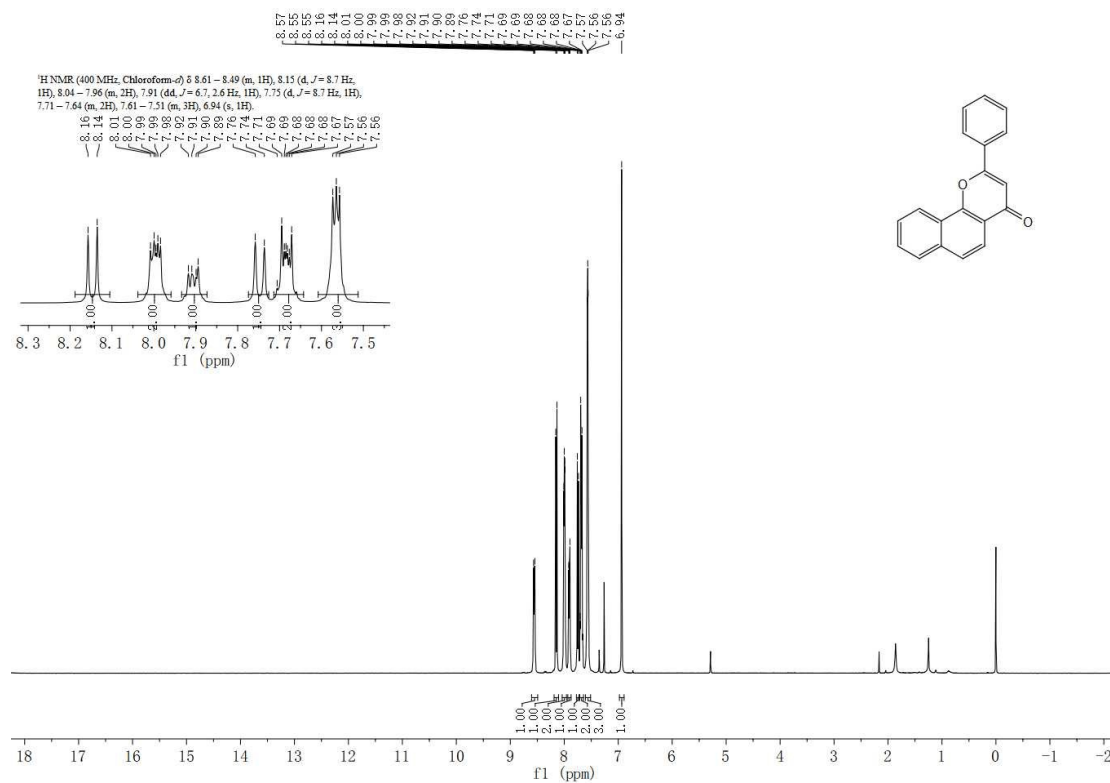


Figure S41 <sup>1</sup>H NMR spectrum of 2-Phenyl-4*H*-benzo[*h*]chromen-4-one (3u)

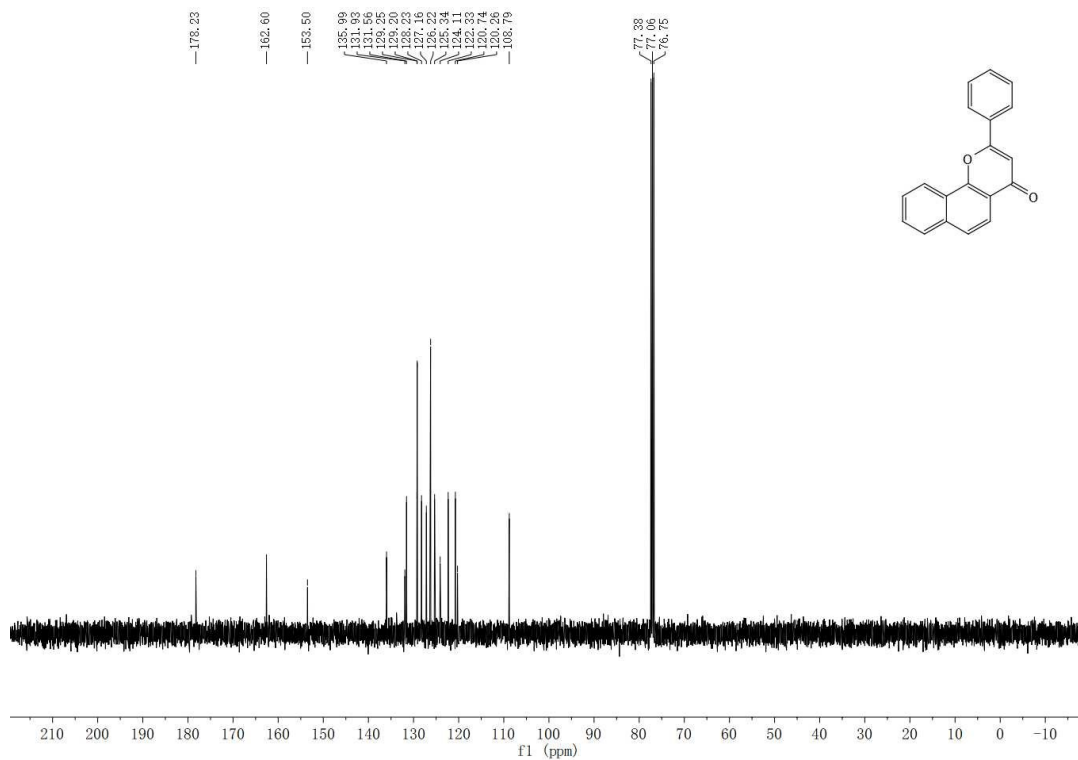


Figure S42 <sup>13</sup>C NMR spectrum of 2-Phenyl-4*H*-benzo[*h*]chromen-4-one (3u)

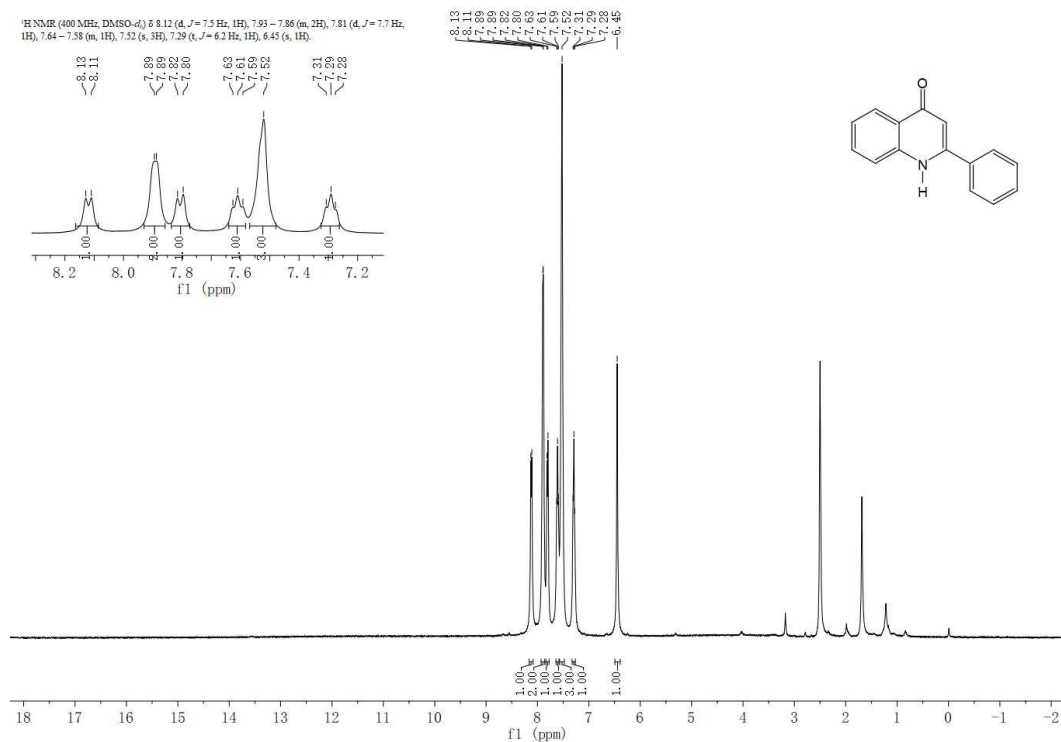


Figure S43 <sup>1</sup>H NMR spectrum of 2-phenylquinolin-4(1H)-one (3v)

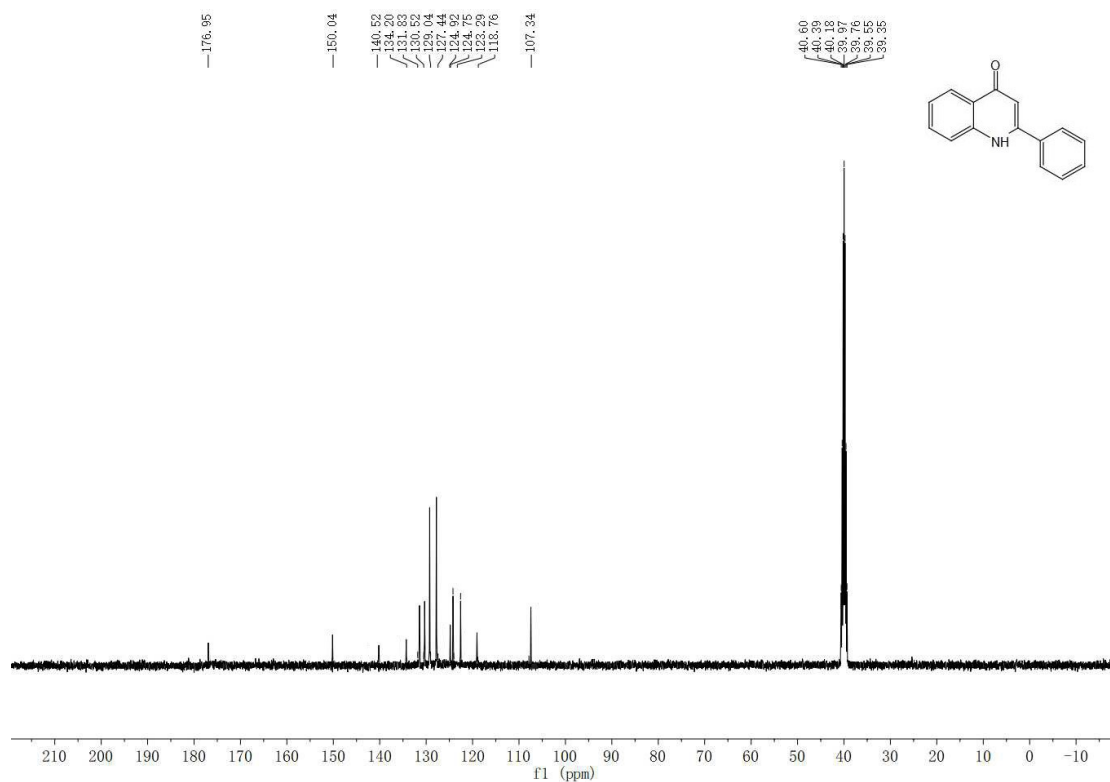


Figure S44 <sup>13</sup>C NMR spectrum of 2-phenylquinolin-4(1H)-one (3v)

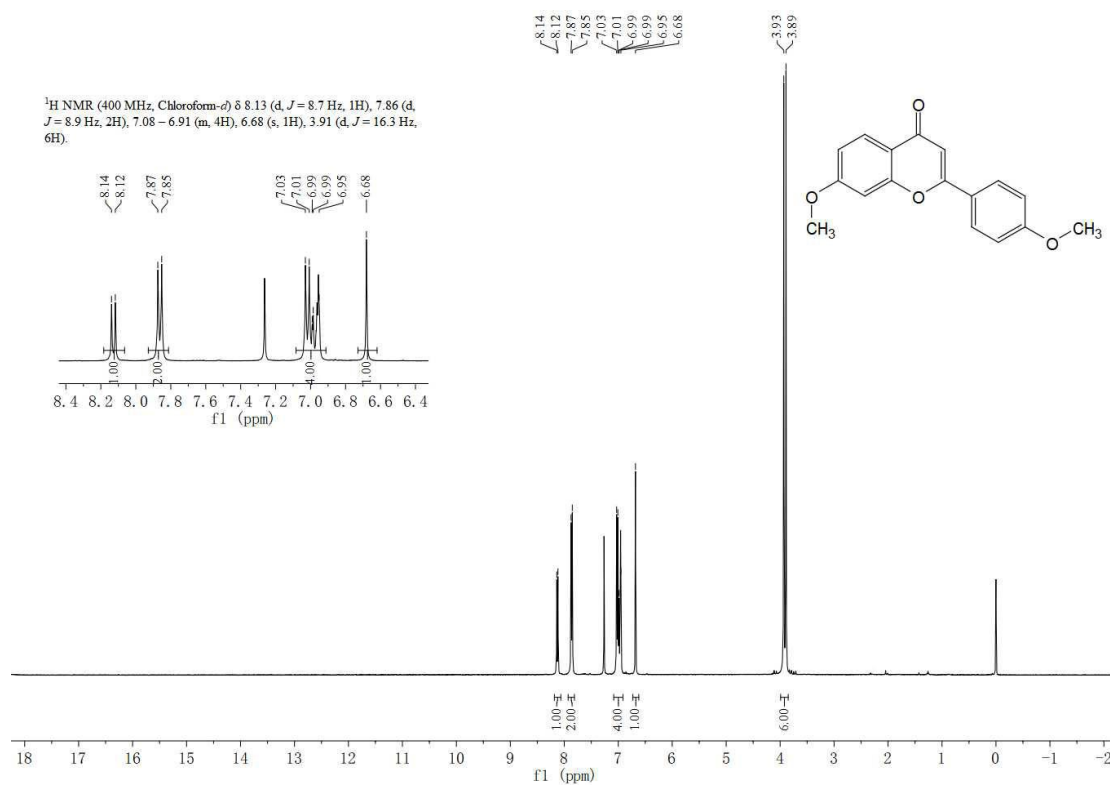


Figure S45 <sup>1</sup>H NMR spectrum of 7-Methoxy-2-(4-methoxyphenyl)-4H-chromen-4-one (3w)

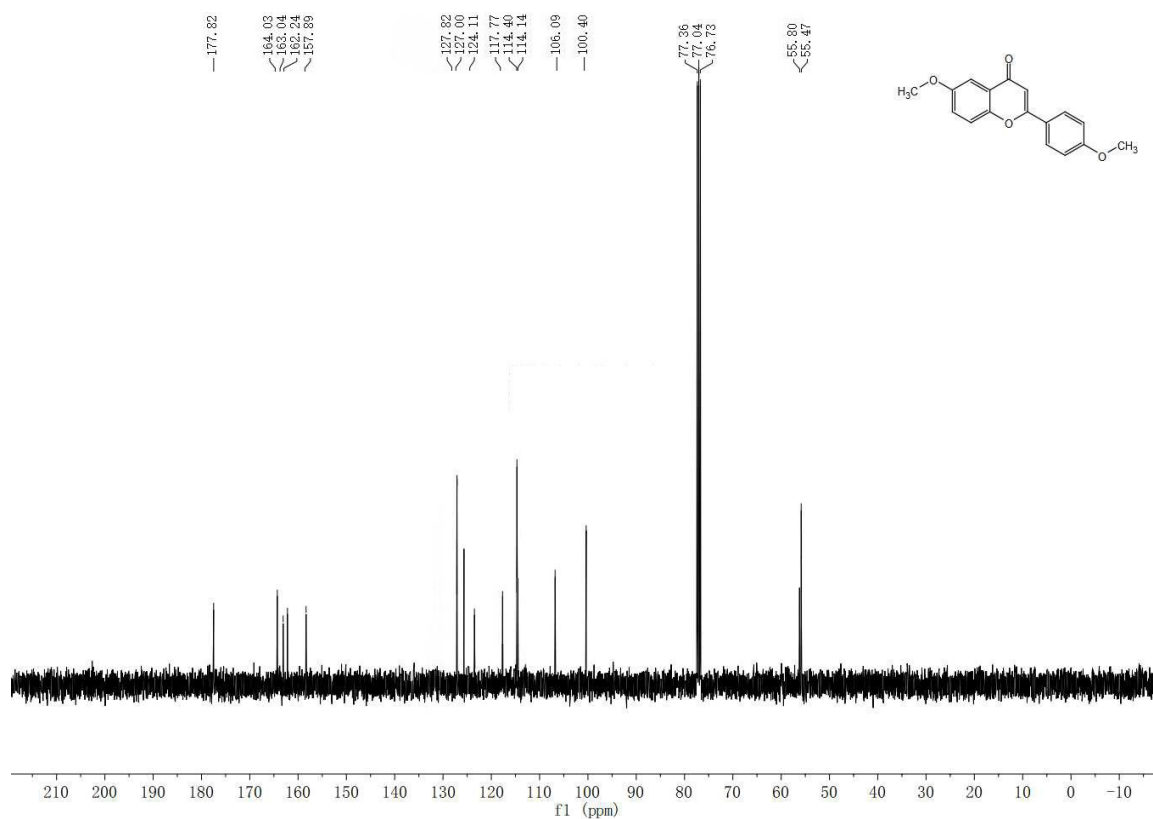


Figure S46 <sup>13</sup>C NMR spectrum of 7-Methoxy-2-(4-methoxyphenyl)-4H-chromen-4-one (3w)

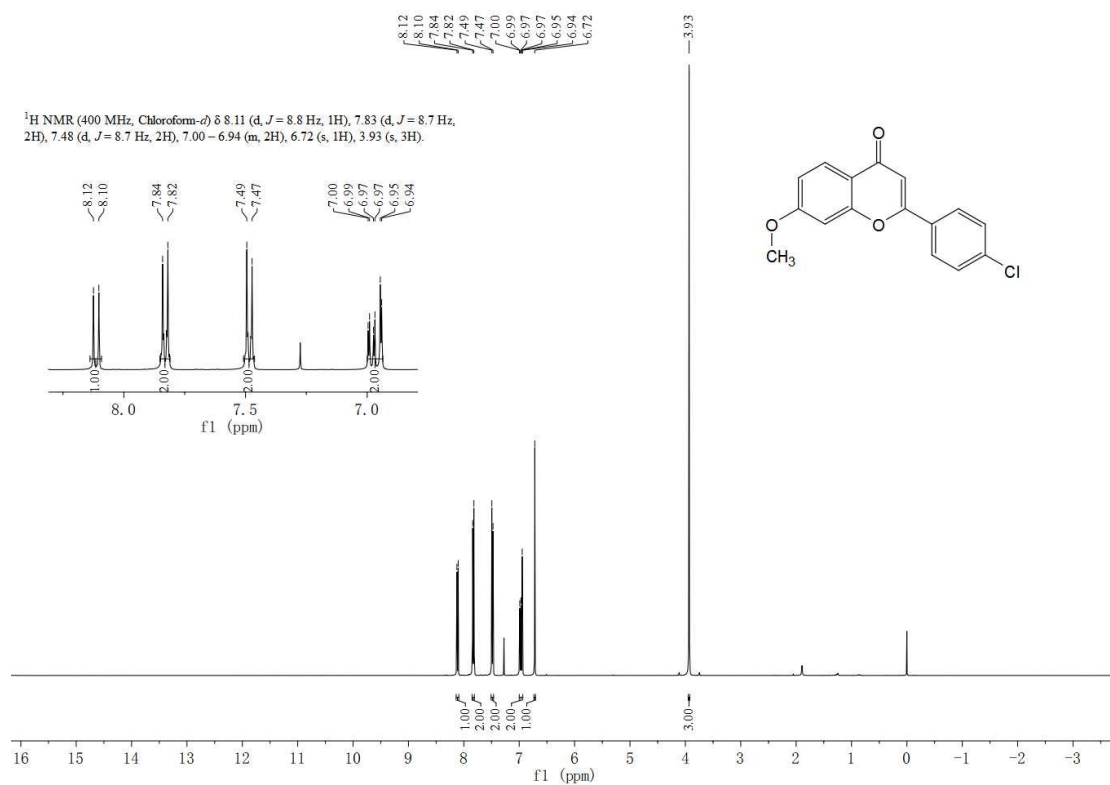


Figure S47 <sup>1</sup>H NMR spectrum of 2-(4-Chlorophenyl)-7-methoxy-4*H*-chromen-4-one (3x)

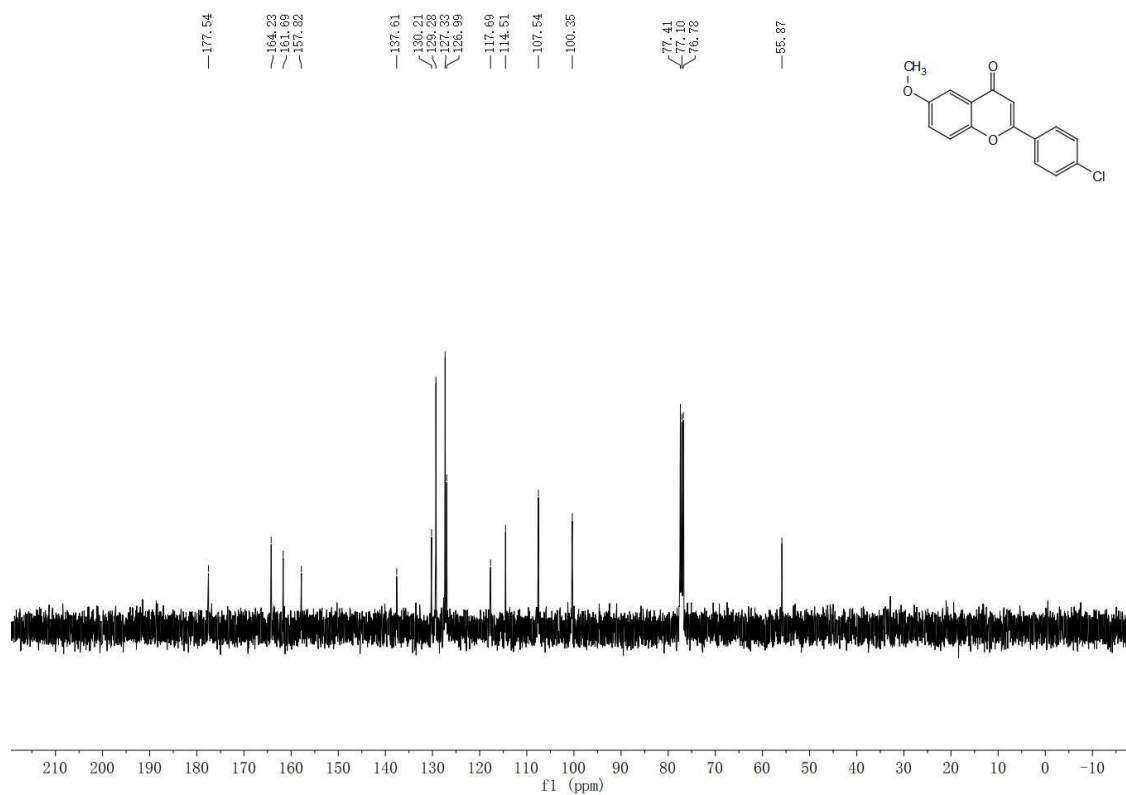
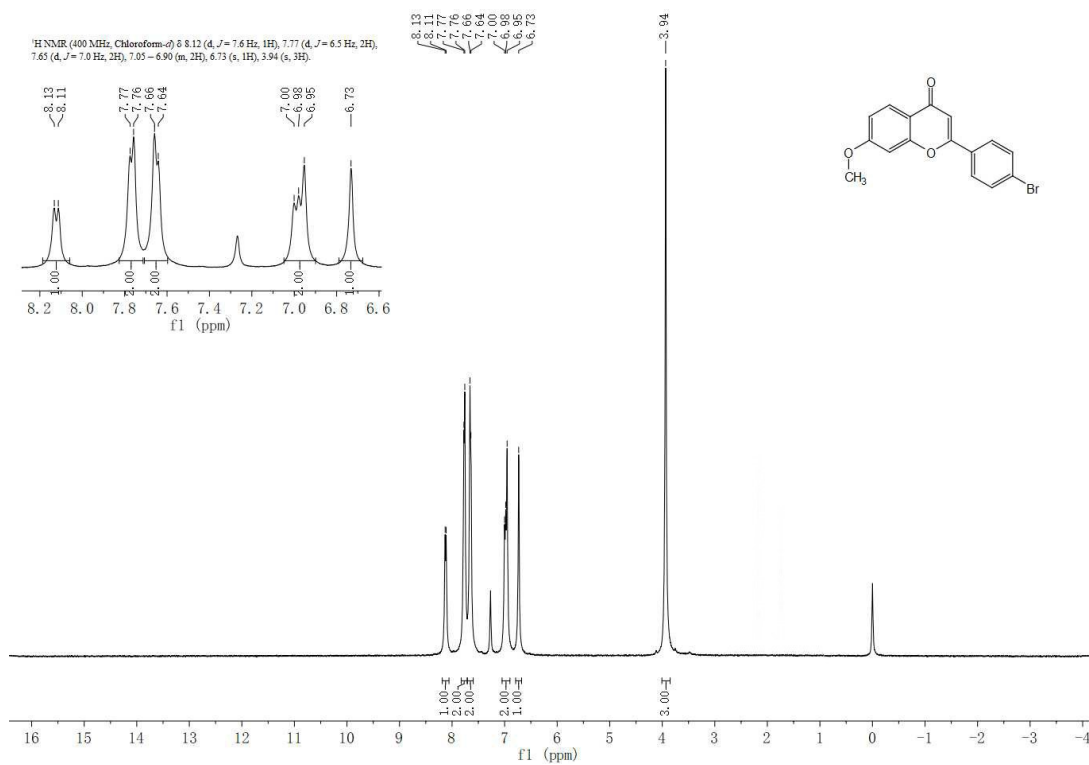
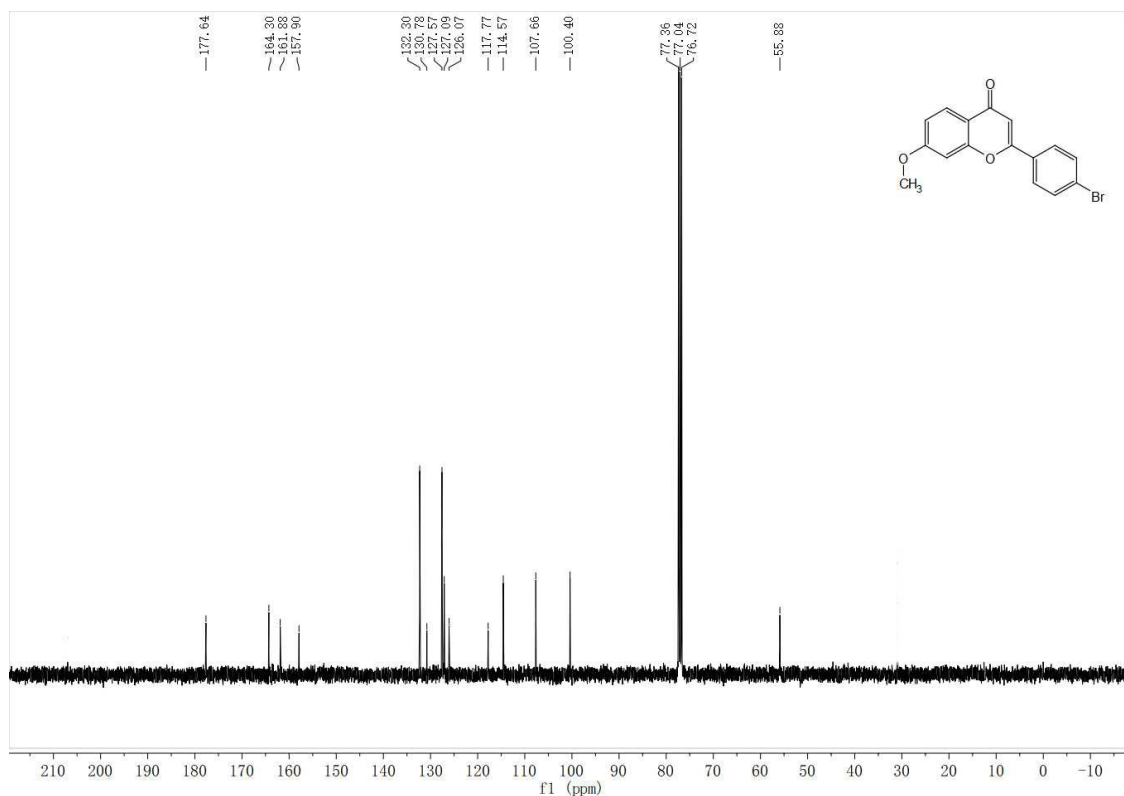


Figure S48 <sup>13</sup>C NMR spectrum of 2-(4-Chlorophenyl)-7-methoxy-4*H*-chromen-4-one (3x)



**Figure S49** <sup>1</sup>H NMR spectrum of 2-(4-Bromophenyl)-7-methoxy-4H-chromen-4-one (3y)



**Figure S50** <sup>13</sup>C NMR spectrum of 2-(4-Bromophenyl)-7-methoxy-4H-chromen-4-one (3y)

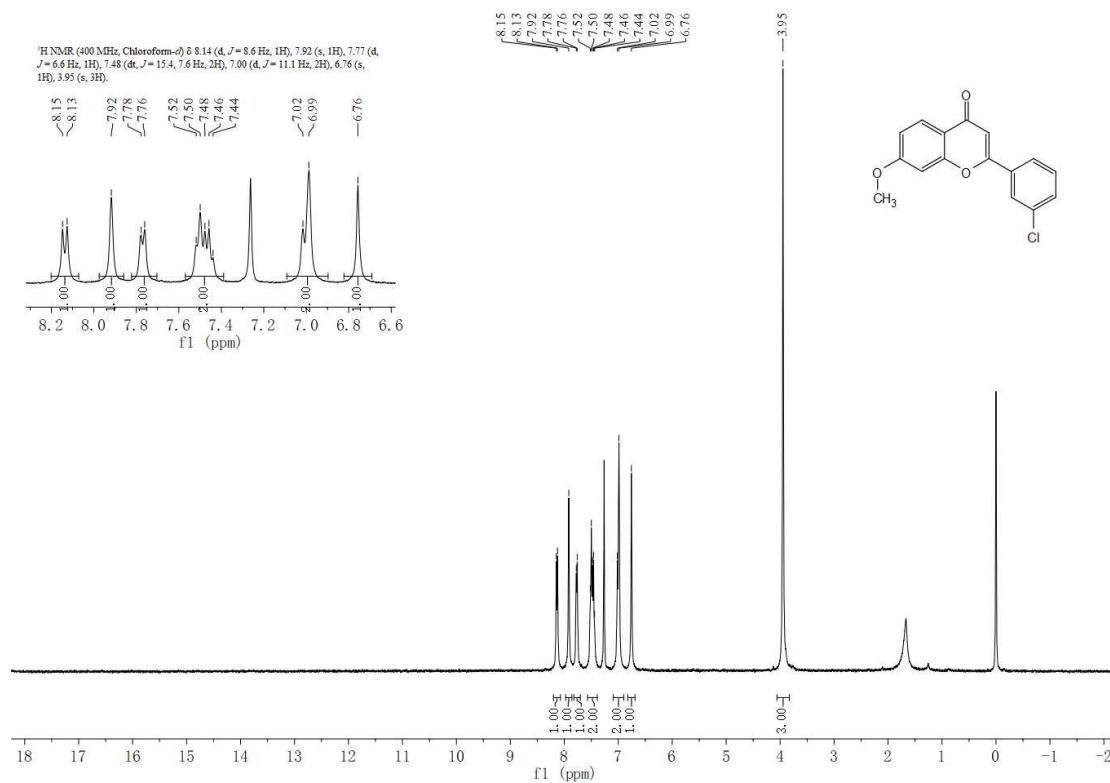


Figure S51 <sup>1</sup>H NMR spectrum of 2-(3-chloro-phenyl)-7-methoxy-chromen-4-one (3z)

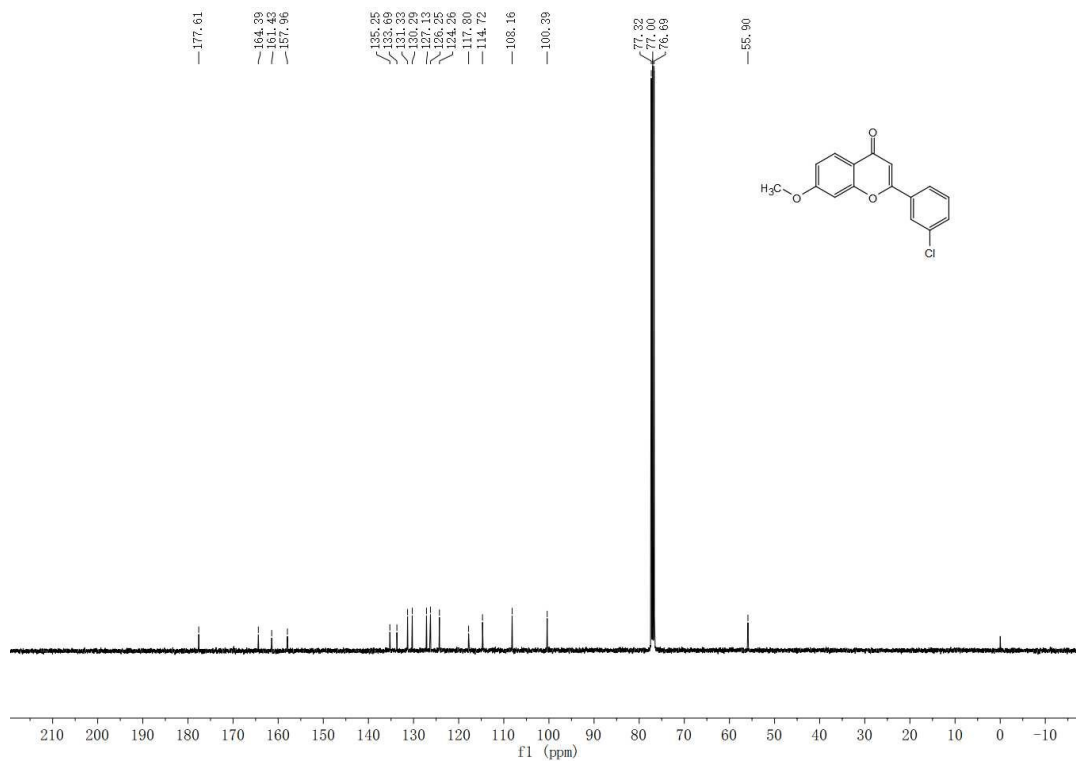


Figure S52 <sup>13</sup>C NMR spectrum of 2-(3-chloro-phenyl)-7-methoxy-chromen-4-one (3z)



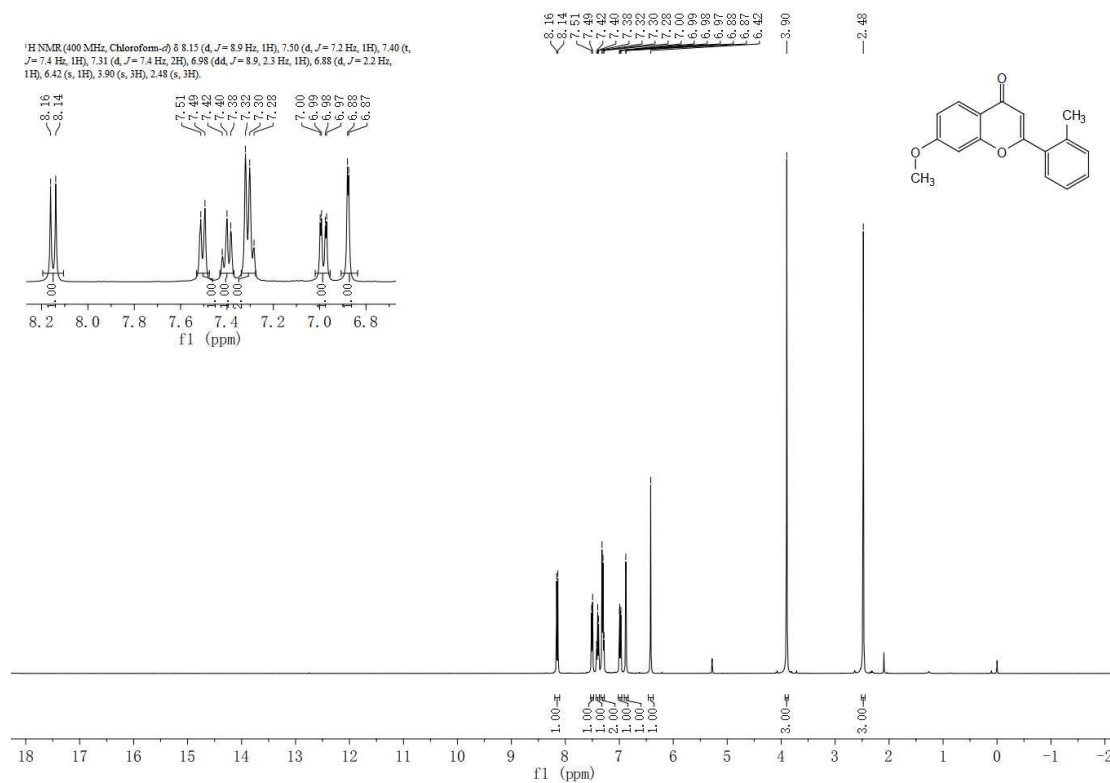


Figure S53 <sup>1</sup>H NMR spectrum of 2-(2-methylphenyl)-7-methoxy-chromen-4-one (3aa)

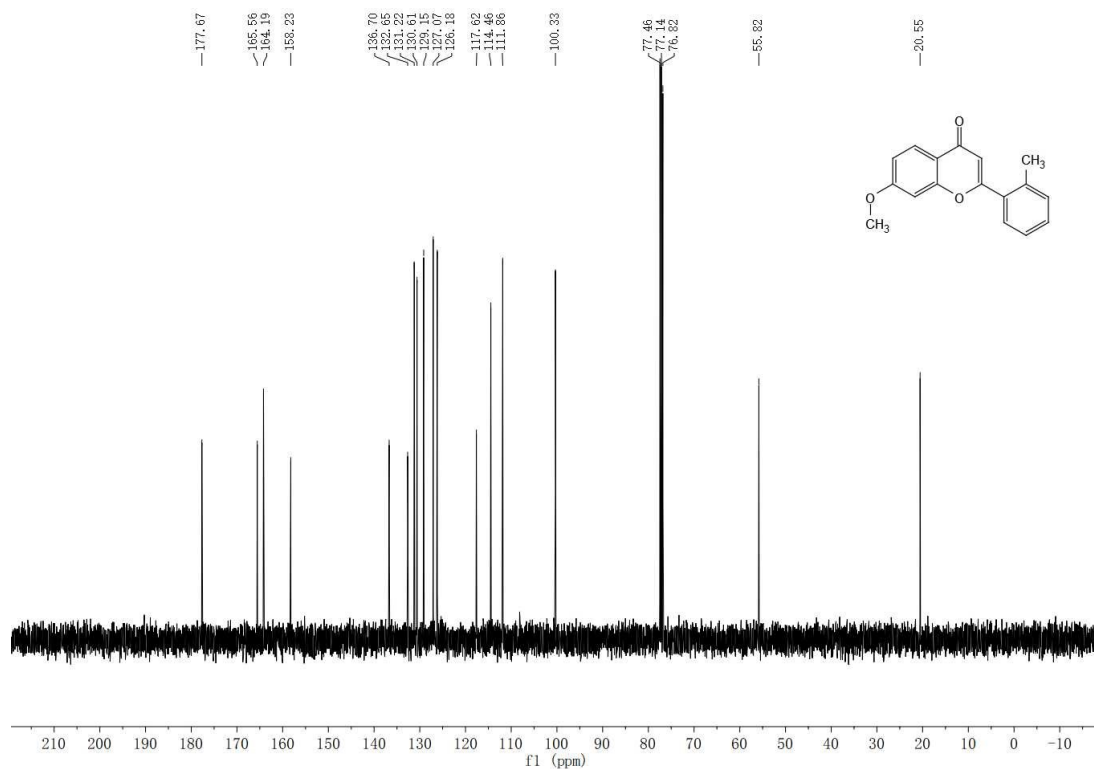


Figure S54 <sup>13</sup>C NMR spectrum of 2-(2-methylphenyl)-7-methoxy-chromen-4-one (3aa)

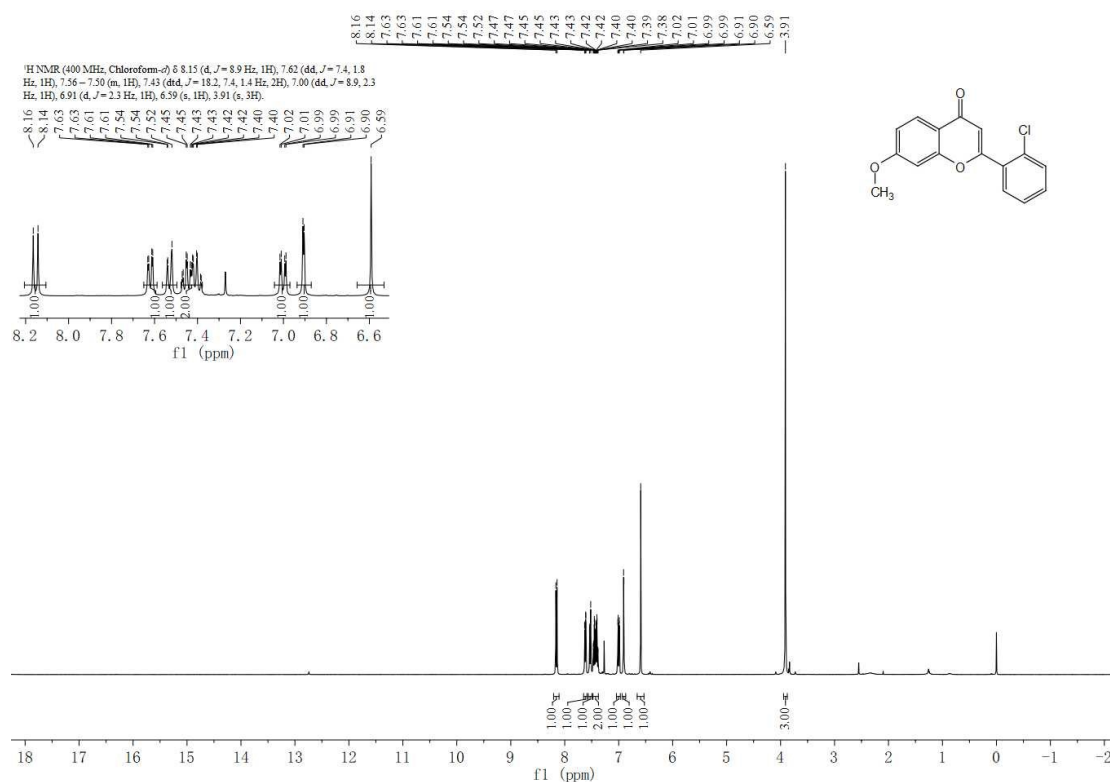


Figure S55 <sup>1</sup>H NMR spectrum of 2-(2-chloro-phenyl)-7-methoxy-chromen-4-one (3ab)

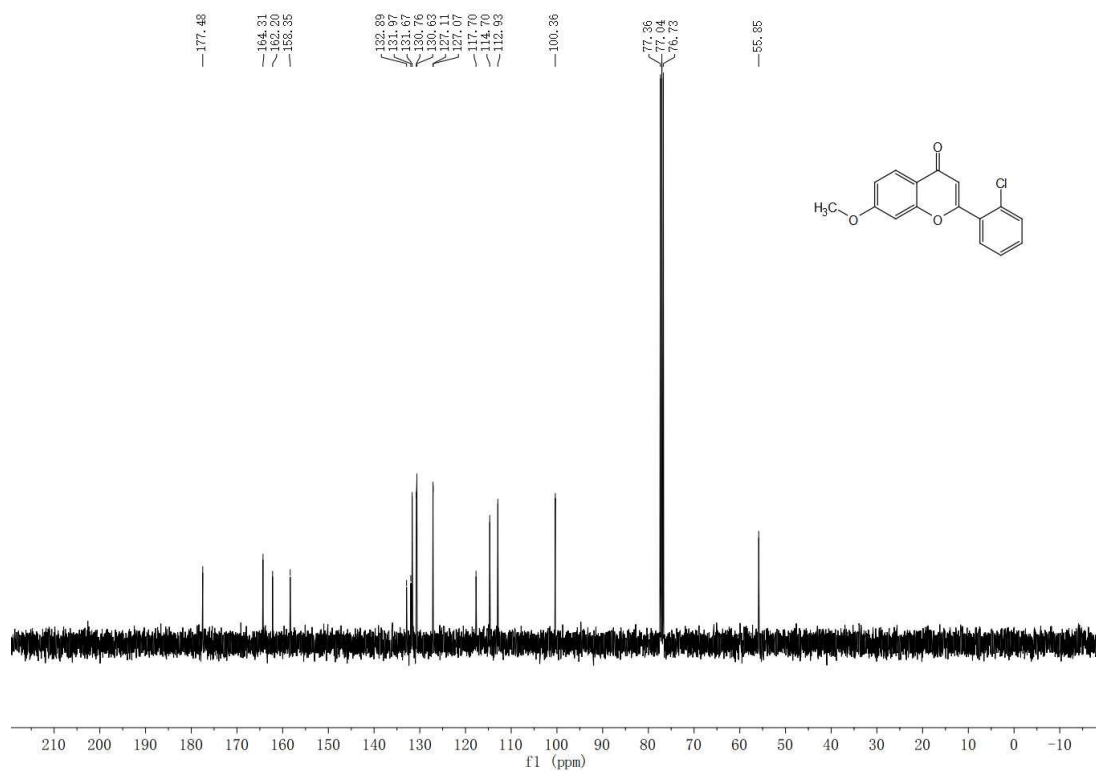
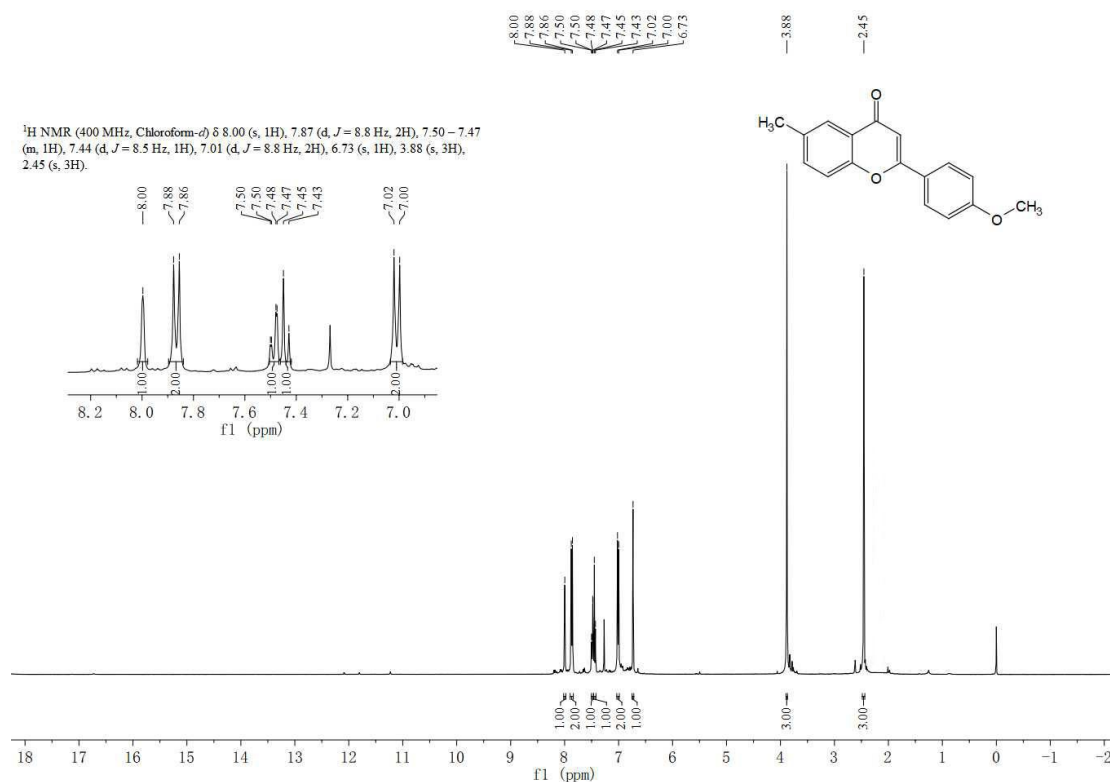
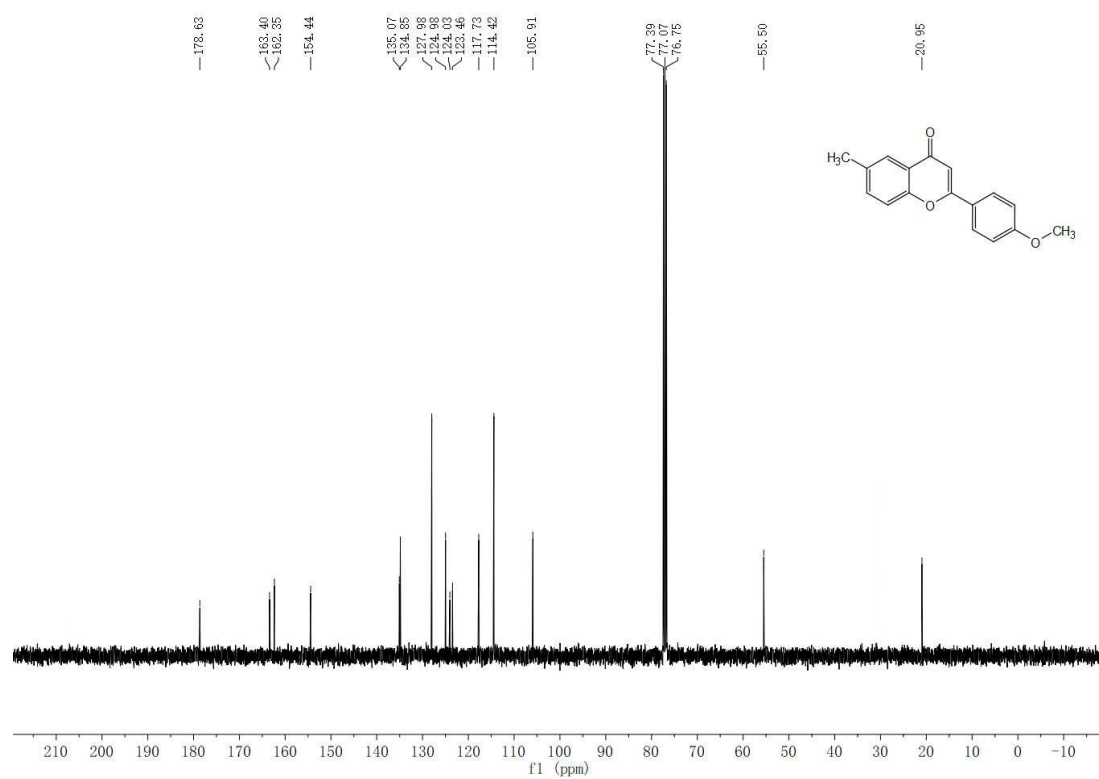


Figure S56 <sup>13</sup>C NMR spectrum of 2-(2-chloro-phenyl)-7-methoxy-chromen-4-one (3ab)



**Figure S57** <sup>1</sup>H NMR spectrum of 2-(4-Methoxyphenyl)-6-methyl-4*H*-chromen-4-one (3ac)



**Figure S58** <sup>13</sup>C NMR spectrum of 2-(4-Methoxyphenyl)-6-methyl-4*H*-chromen-4-one (3ac)

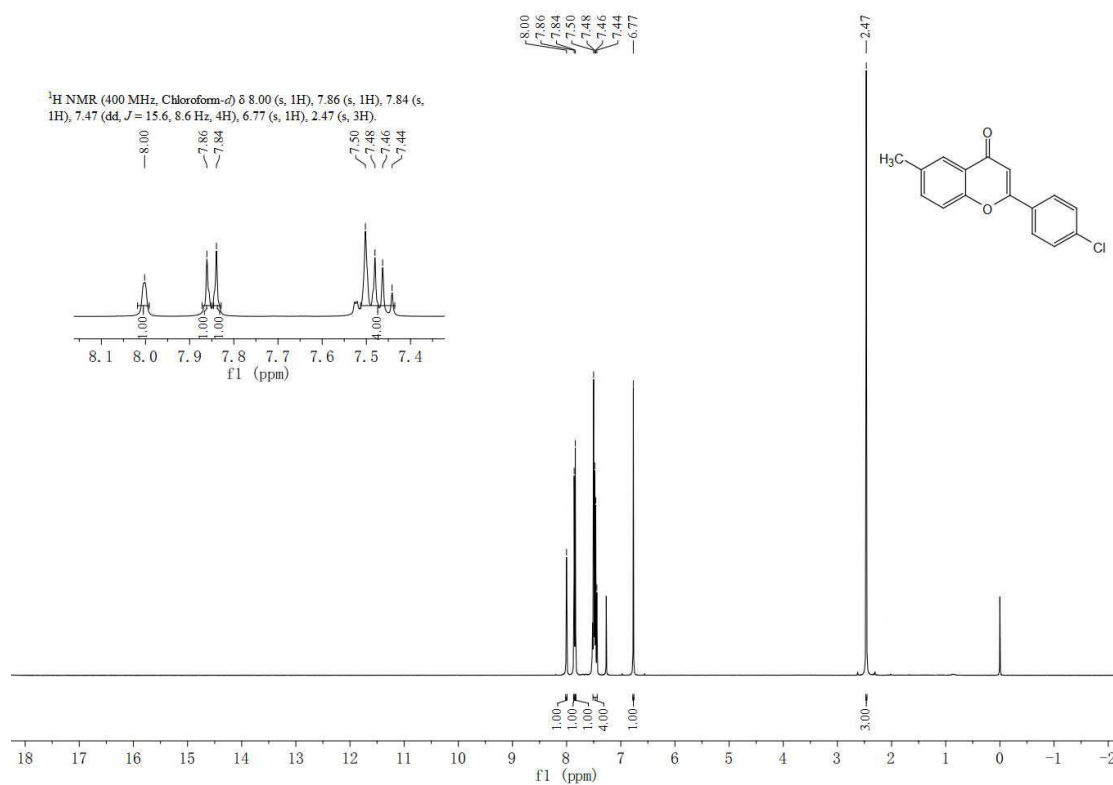


Figure S59 <sup>1</sup>H NMR spectrum of 2-(4-chlorophenyl)-6-methyl-4H-chromen-4-one (3ad)

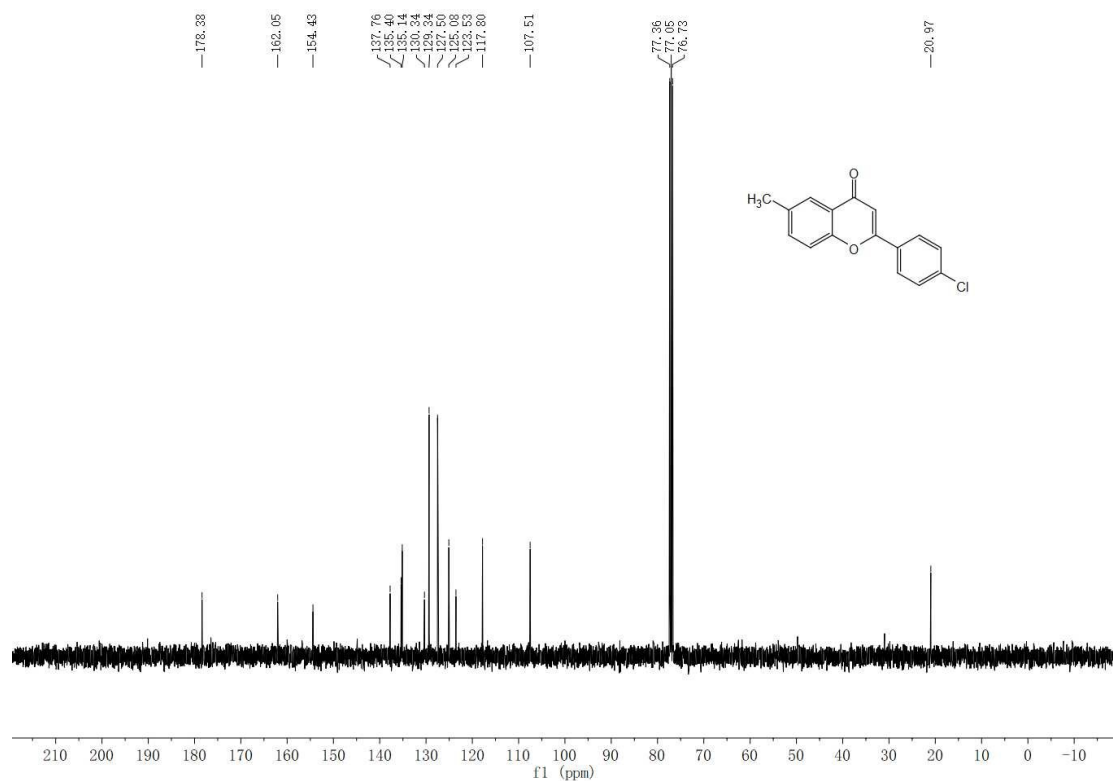


Figure S60 <sup>13</sup>C NMR spectrum of 2-(4-chlorophenyl)-6-methyl-4H-chromen-4-one (3ad)

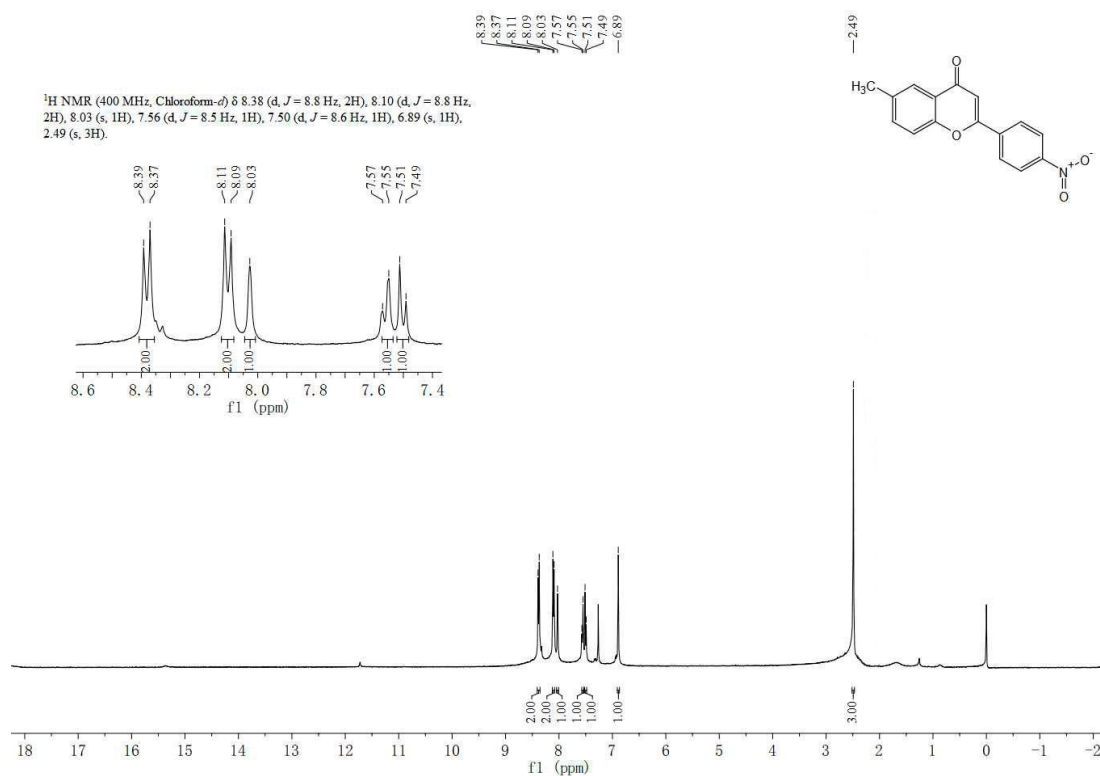


Figure S61 <sup>1</sup>H NMR spectrum of 6-methyl-2-(4-nitrophenyl)-4H-chromen-4-one (3ae)

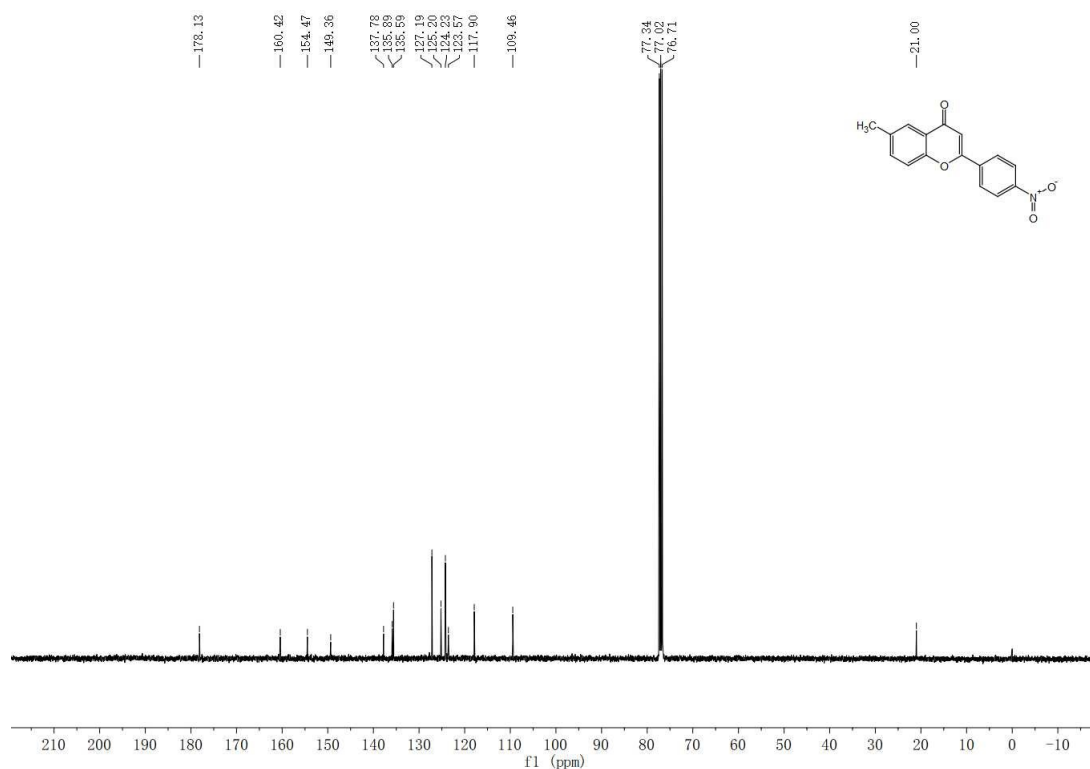


Figure S62 <sup>13</sup>C NMR spectrum of 6-methyl-2-(4-nitrophenyl)-4H-chromen-4-one (3ae)

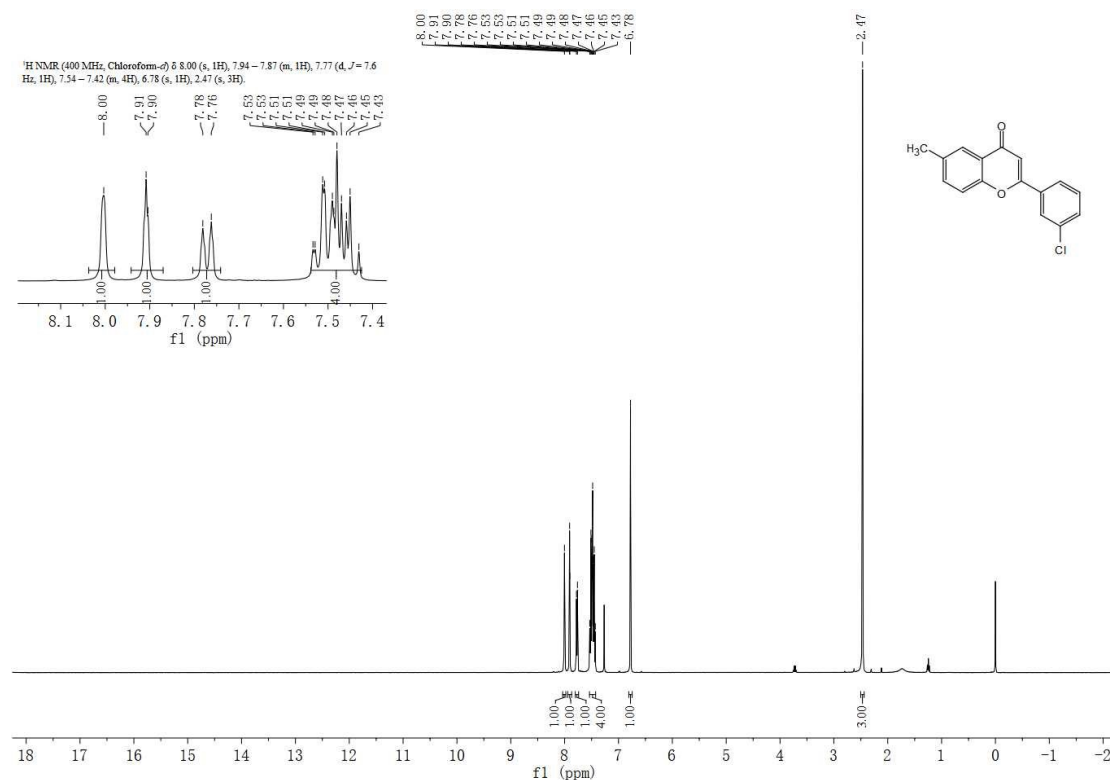


Figure S63 <sup>1</sup>H NMR spectrum of 2-(4-chlorophenyl)-6-methyl-4H-chromen-4-one (3af)

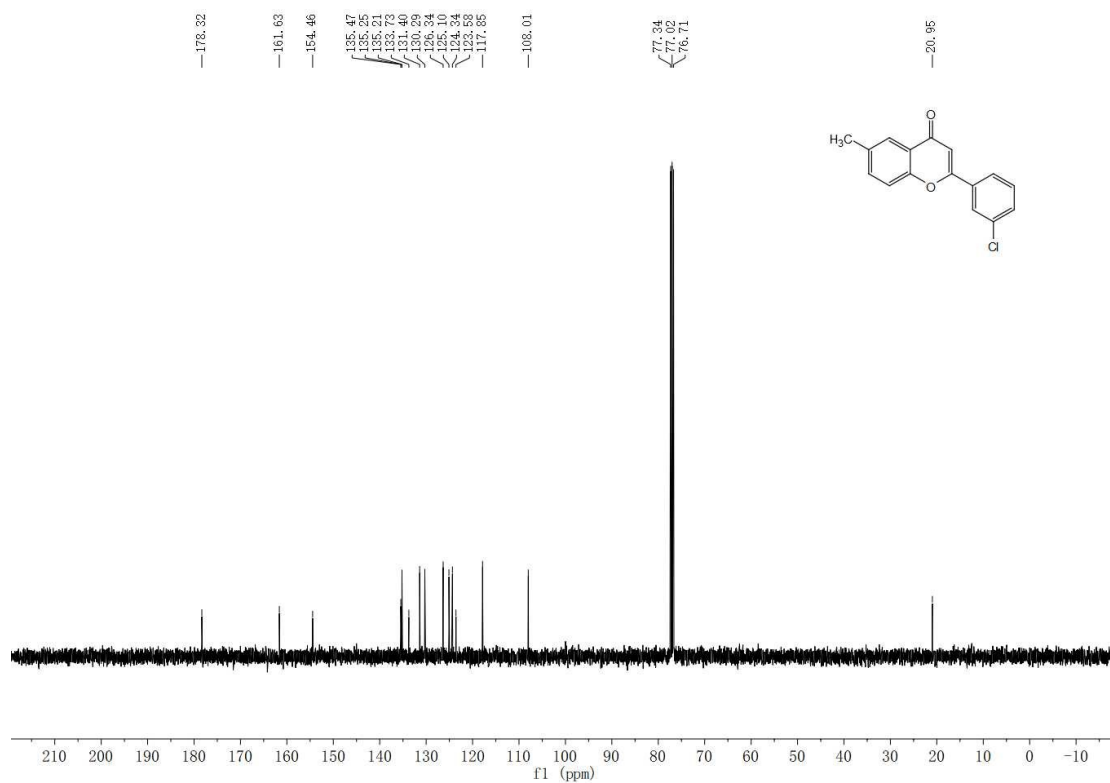


Figure S64 <sup>13</sup>C NMR spectrum of 2-(4-chlorophenyl)-6-methyl-4H-chromen-4-one (3af)

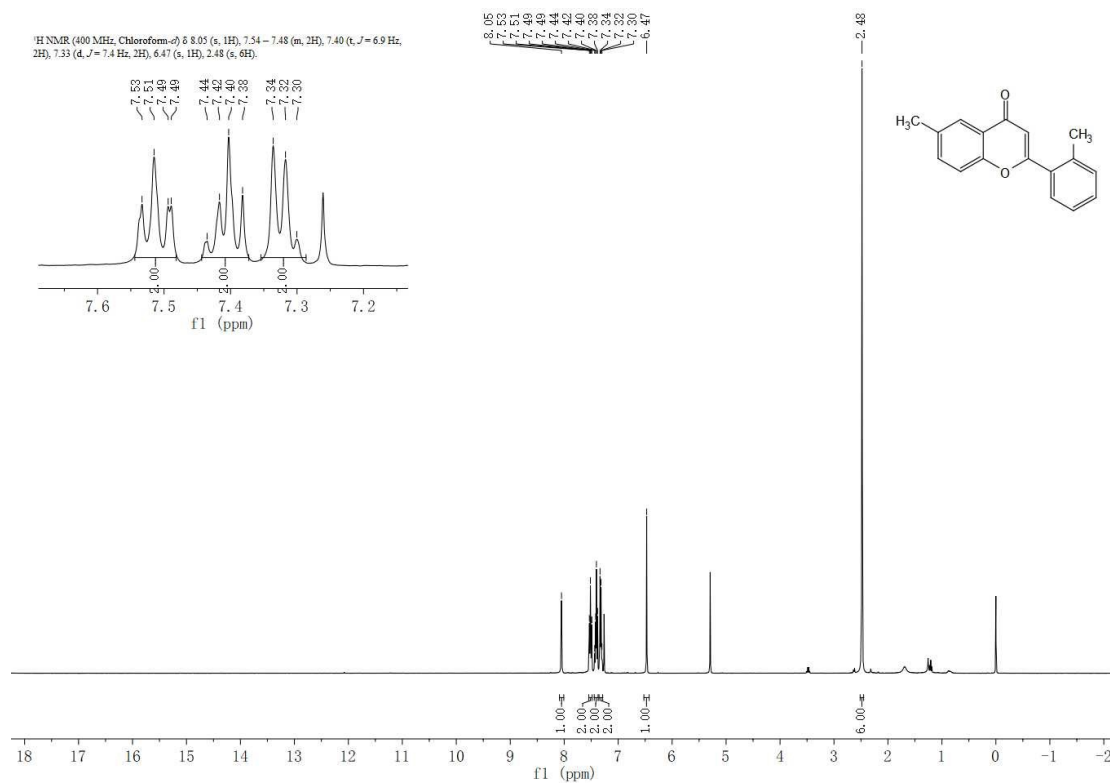


Figure S65 <sup>1</sup>H NMR spectrum of 6-methyl-2-(2-methylphenyl)-4H-chromen-4-one (3ag)

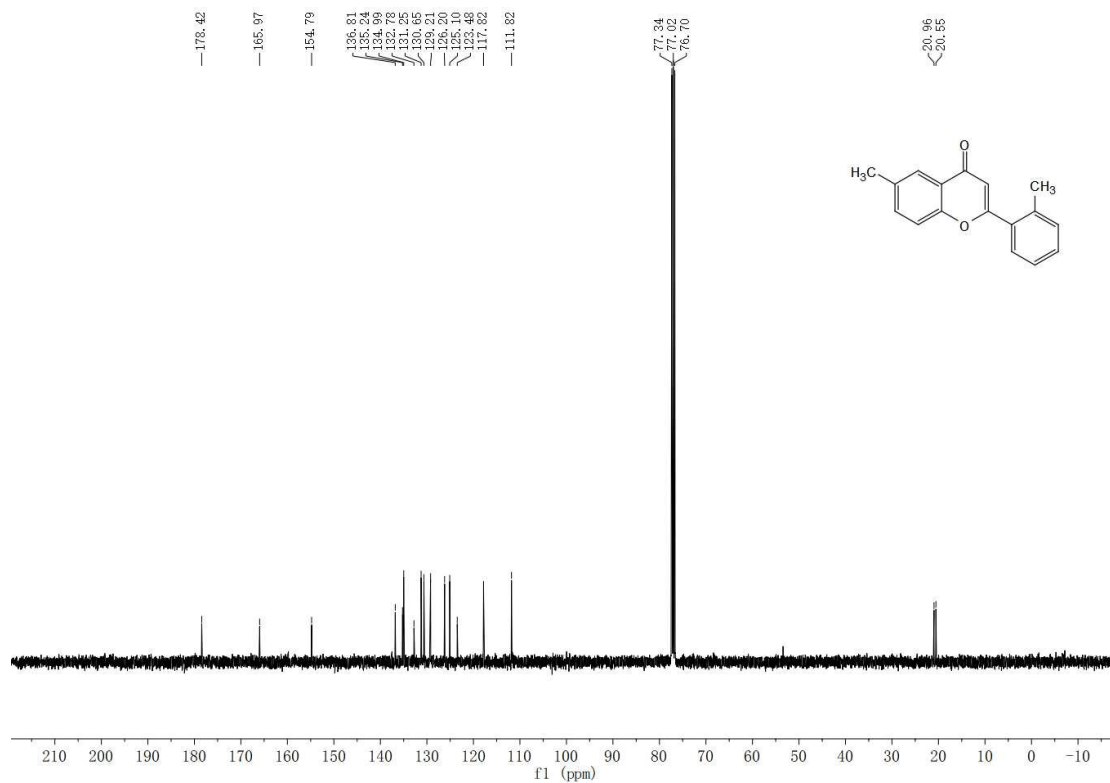


Figure S66 <sup>13</sup>C NMR spectrum of 6-methyl-2-(2-methylphenyl)-4H-chromen-4-one (3ag)

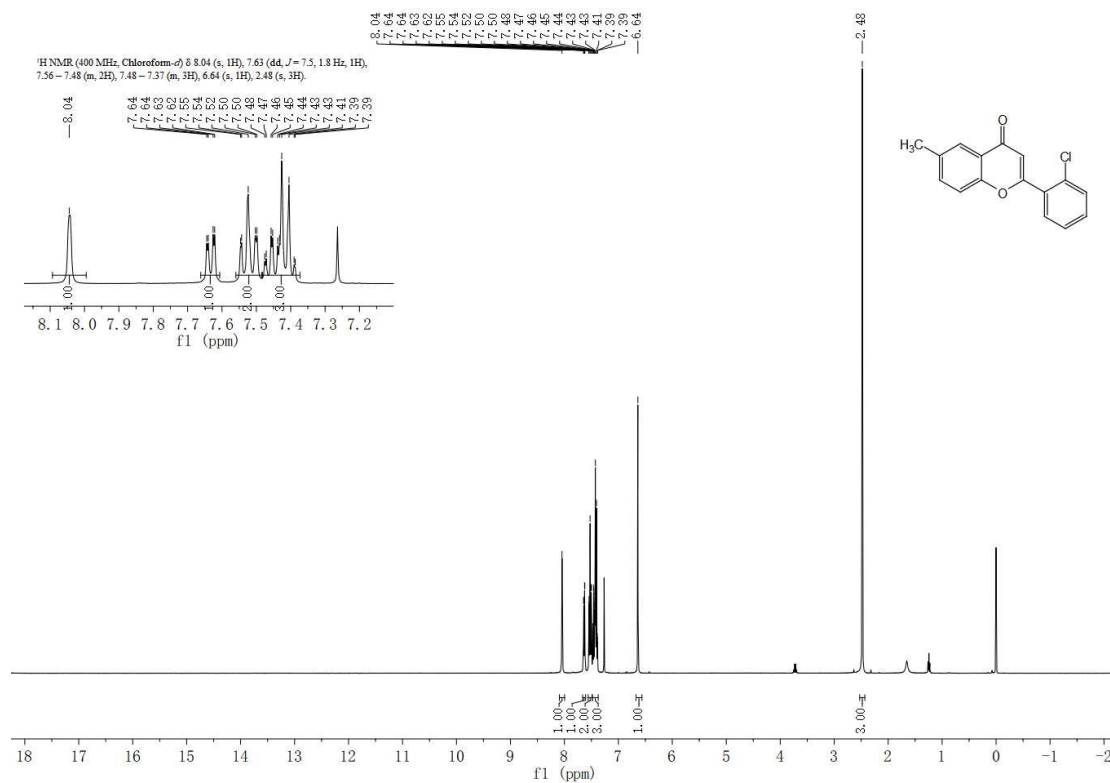


Figure S67 <sup>1</sup>H NMR spectrum of 2-(2-chlorophenyl)-6-methyl-4H-chromen-4-one (3ah)

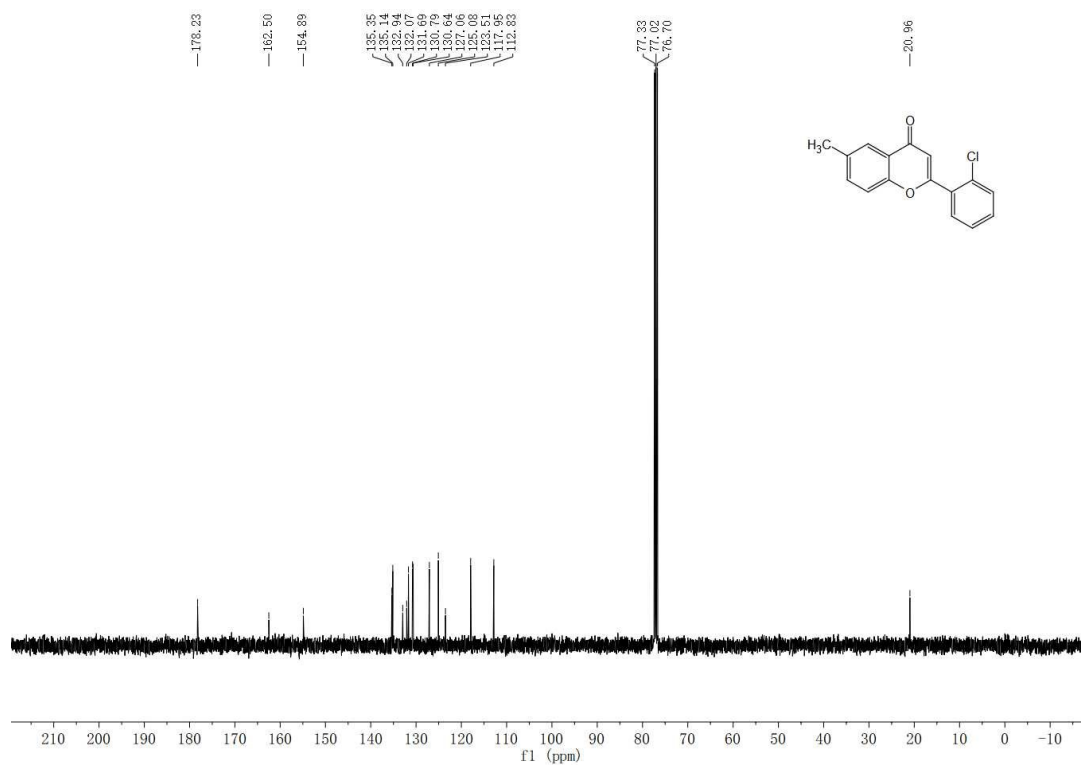


Figure S68 <sup>13</sup>C NMR spectrum of 2-(2-chlorophenyl)-6-methyl-4H-chromen-4-one (3ah)



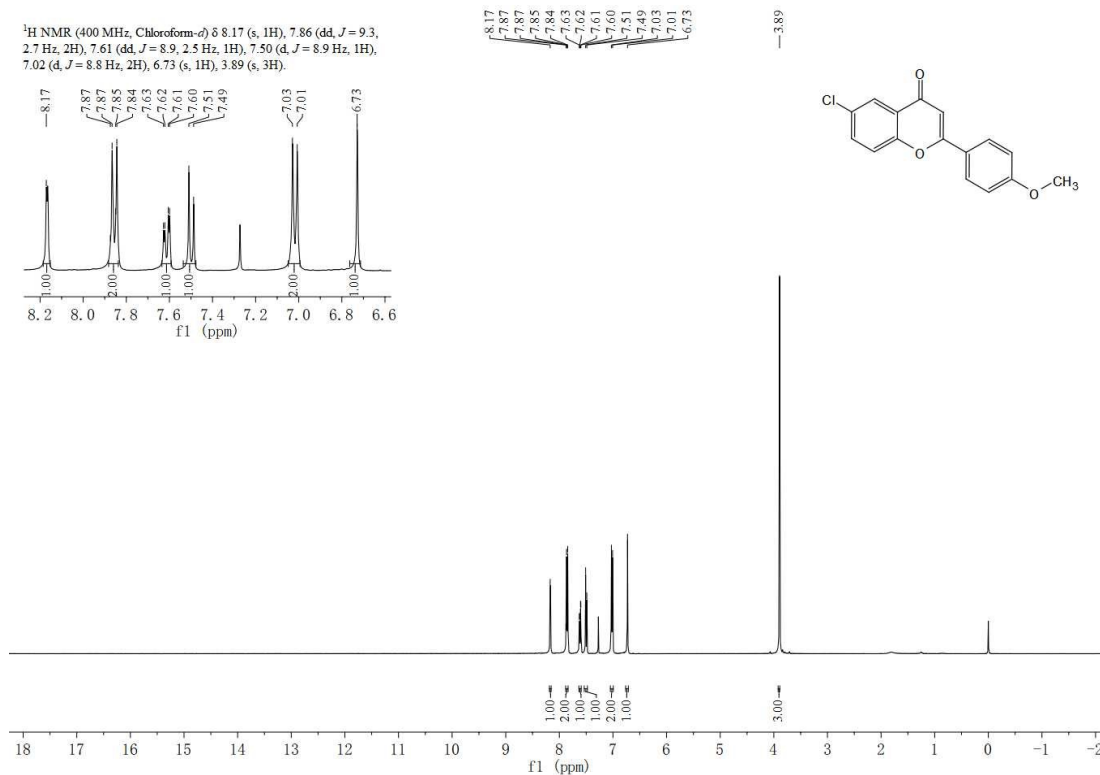


Figure S69 <sup>1</sup>H NMR spectrum of 6-chloro-2-(4-methoxyphenyl)-4H-chromen-4-one (3ai)

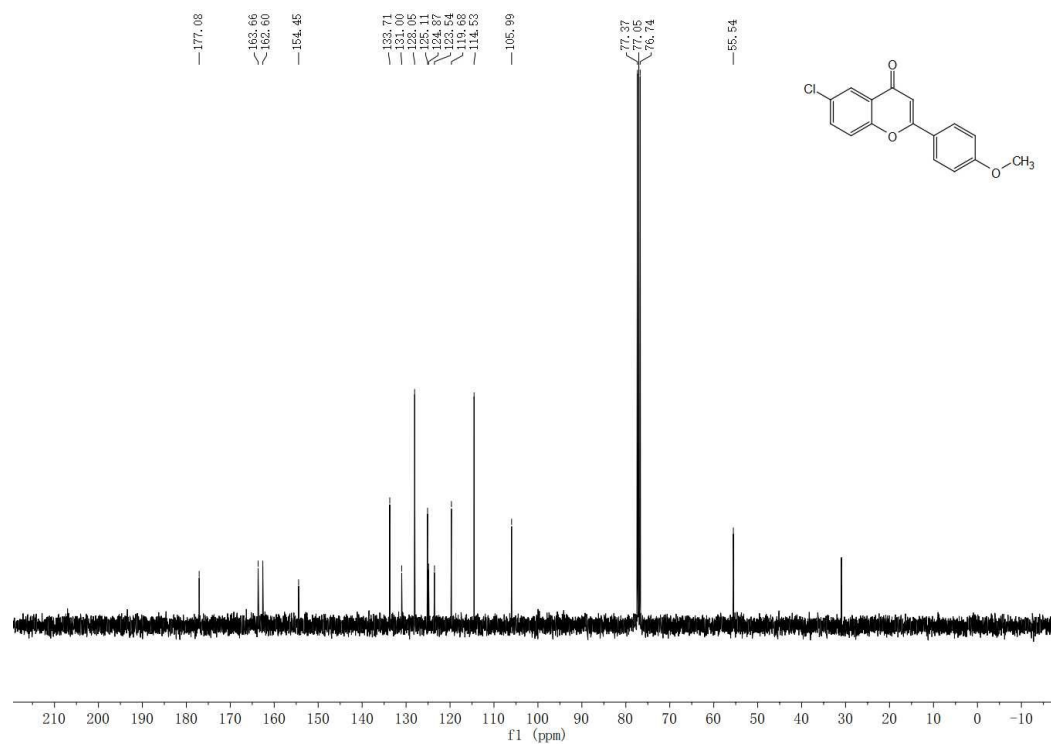


Figure S70 <sup>13</sup>C NMR spectrum of 6-chloro-2-(4-methoxyphenyl)-4H-chromen-4-one (3ai)

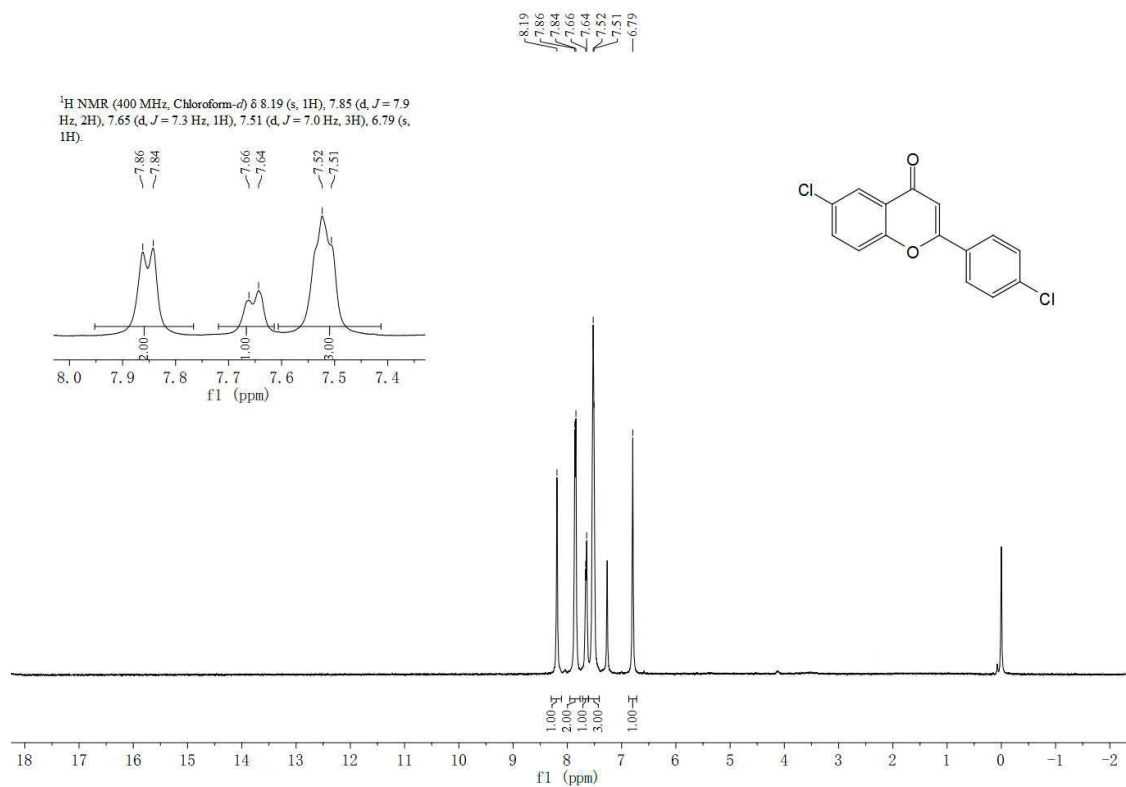


Figure S71 <sup>1</sup>H NMR spectrum of 6-chloro-2-(4-chlorophenyl)-4H-chromen-4-one (3aj)

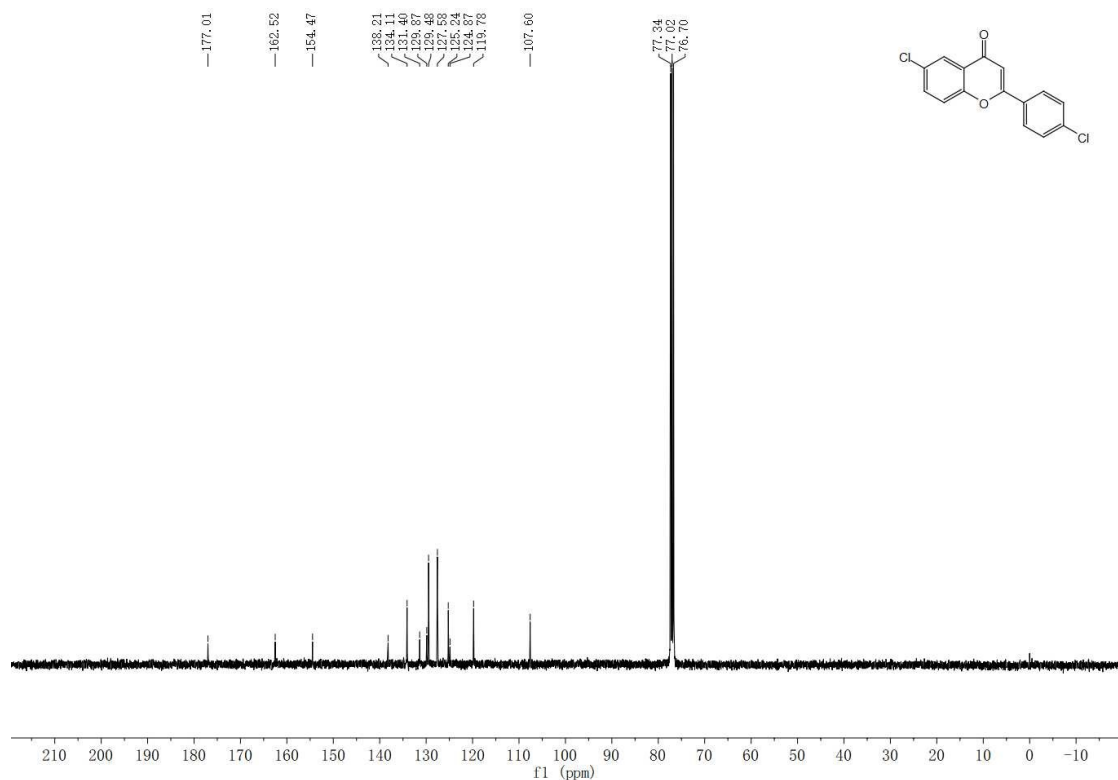
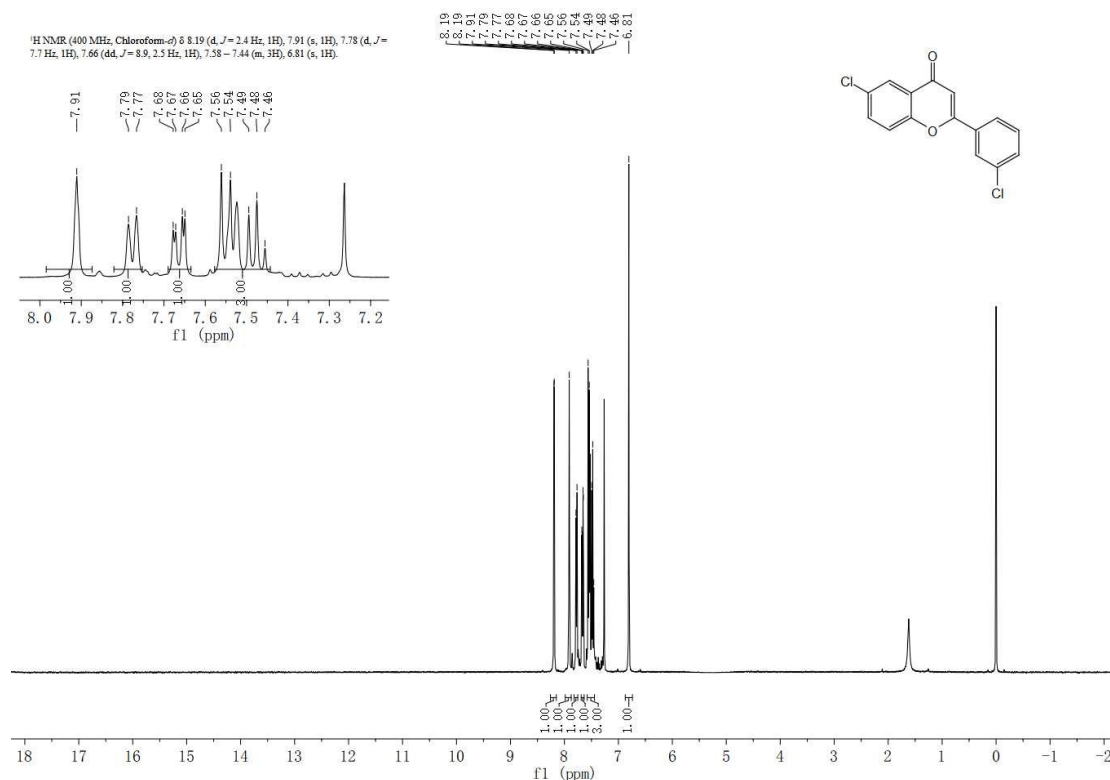
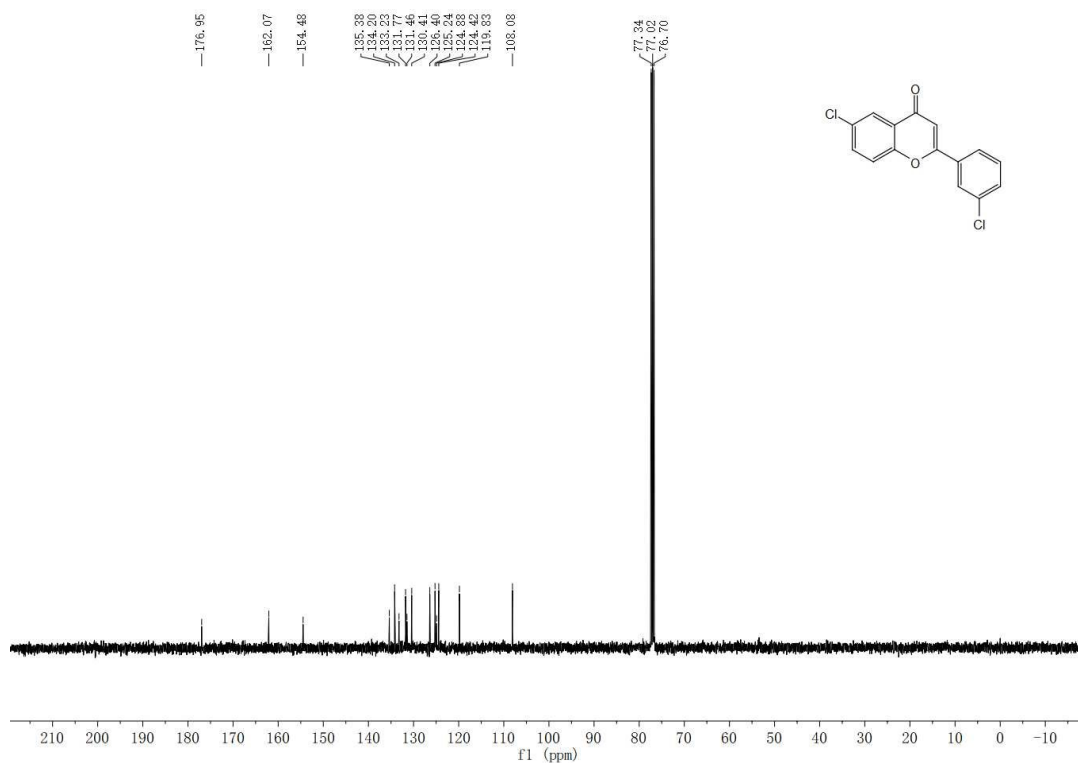


Figure S72 <sup>13</sup>C NMR spectrum of 6-chloro-2-(4-chlorophenyl)-4H-chromen-4-one (3aj)



**Figure S73** <sup>1</sup>H NMR spectrum of 6-chloro-2-(3-chlorophenyl)-4H-chromen-4-one (3ak)



**Figure S74** <sup>13</sup>C NMR spectrum of 6-chloro-2-(3-chlorophenyl)-4H-chromen-4-one (3ak)

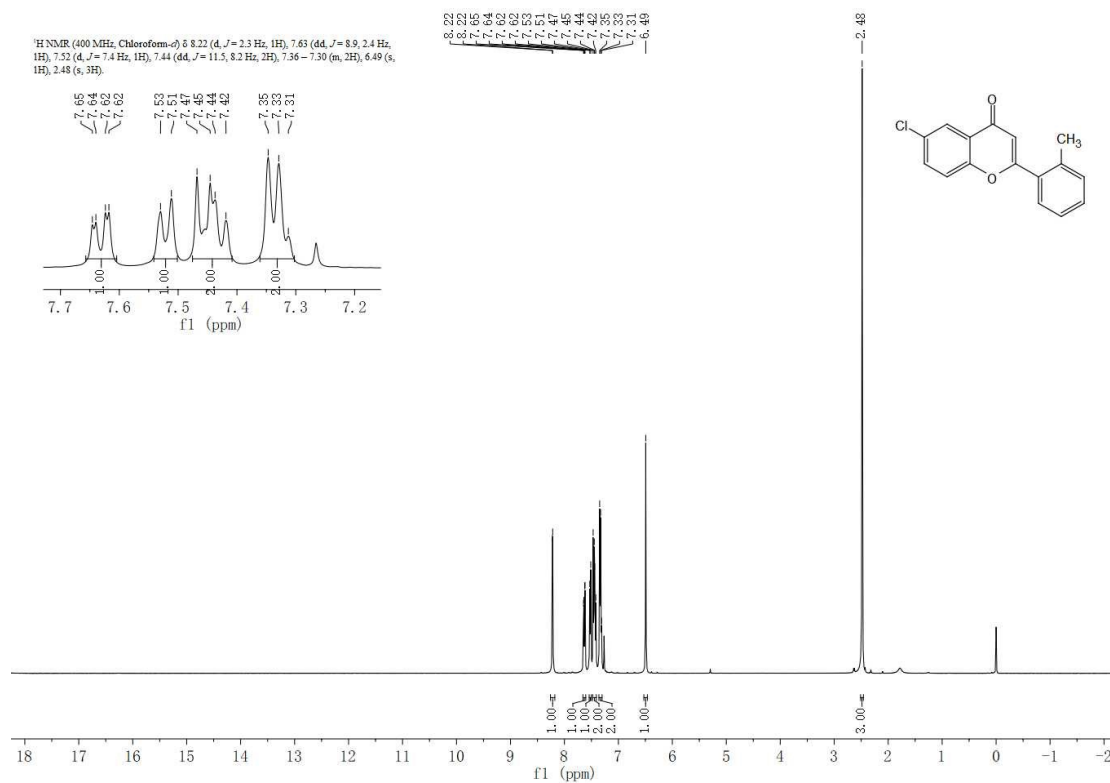


Figure S75 <sup>1</sup>H NMR spectrum of 6-chloro-2-(2-methylphenyl)-4H-chromen-4-one (3aI)

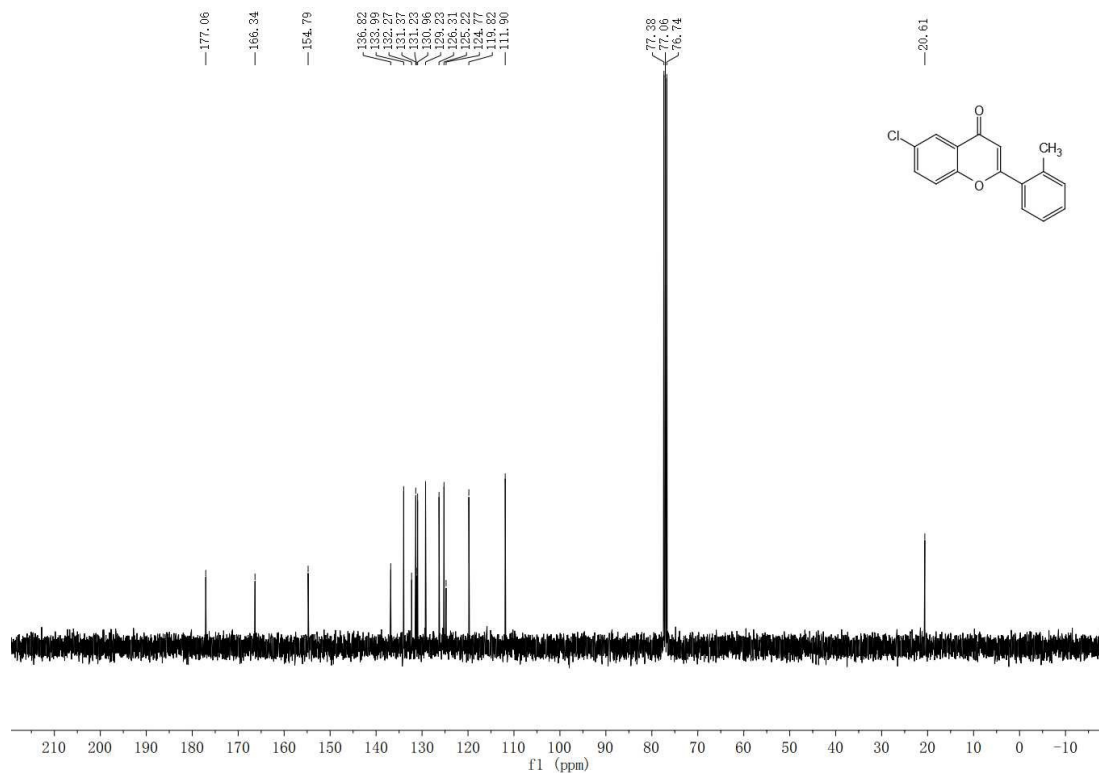


Figure S76 <sup>13</sup>C NMR spectrum of 6-chloro-2-(2-methylphenyl)-4H-chromen-4-one (3aI)

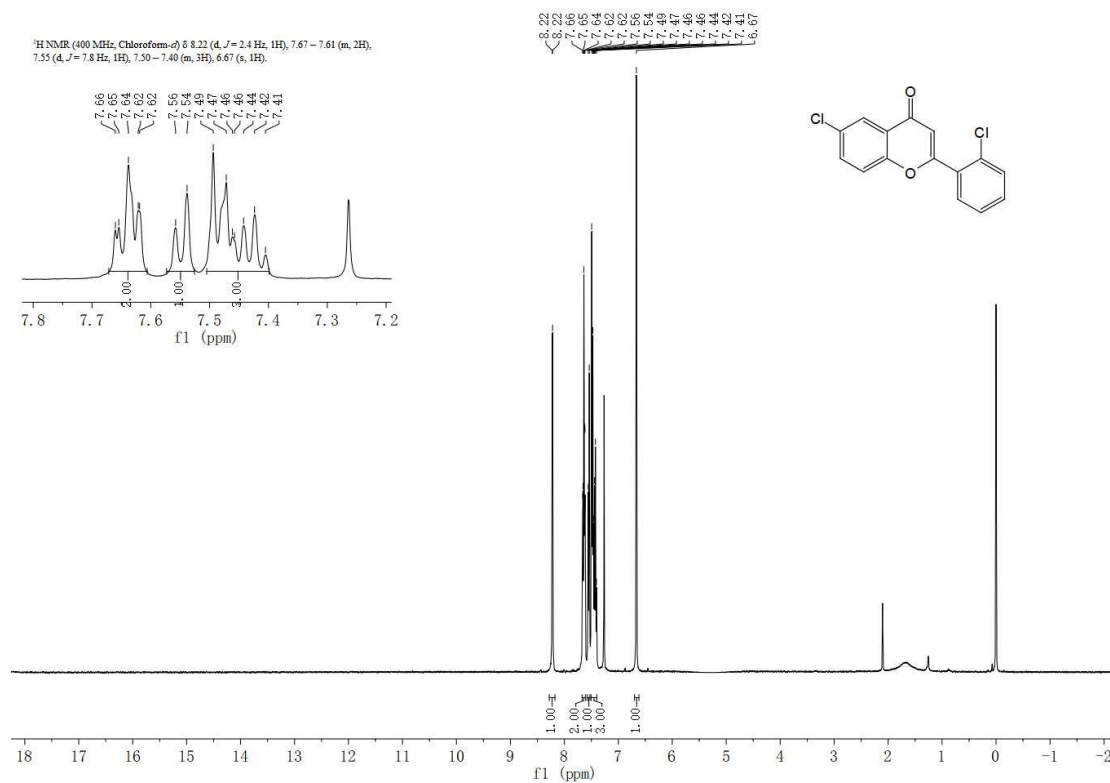


Figure S77 <sup>1</sup>H NMR spectrum of 6-chloro-2-(2-chlorophenyl)-4H-chromen-4-one (3am)

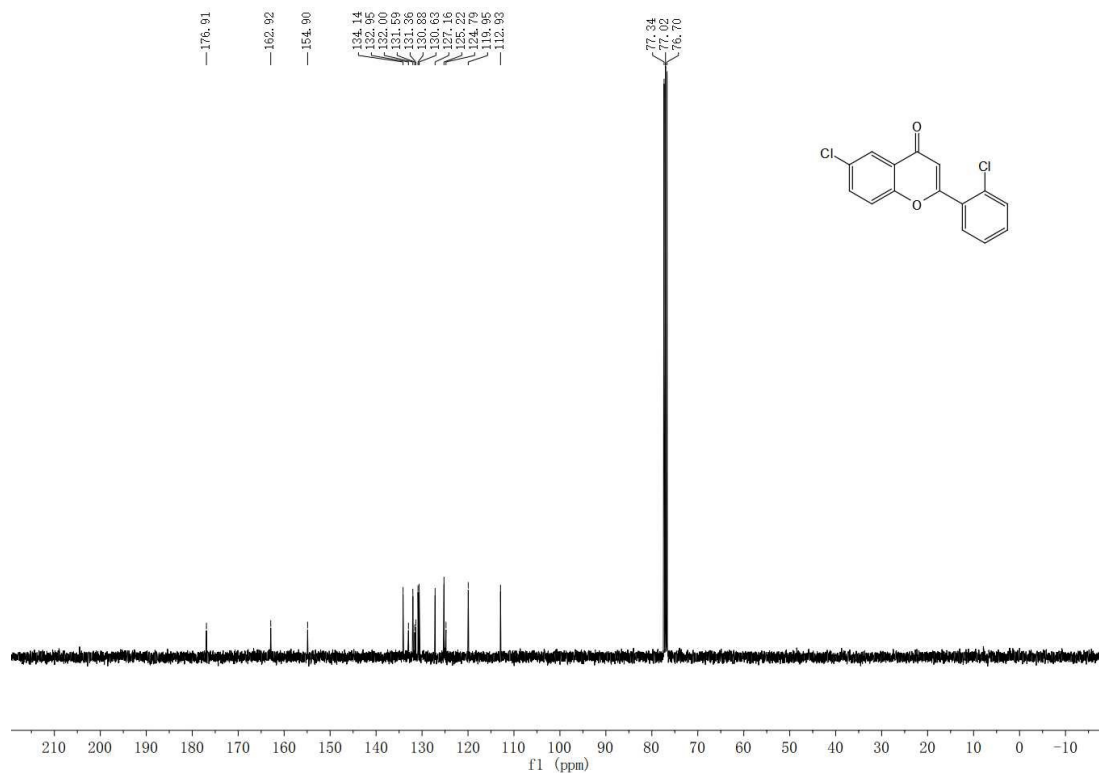


Figure S78 <sup>13</sup>C NMR spectrum of 6-chloro-2-(2-chlorophenyl)-4H-chromen-4-one (3am)

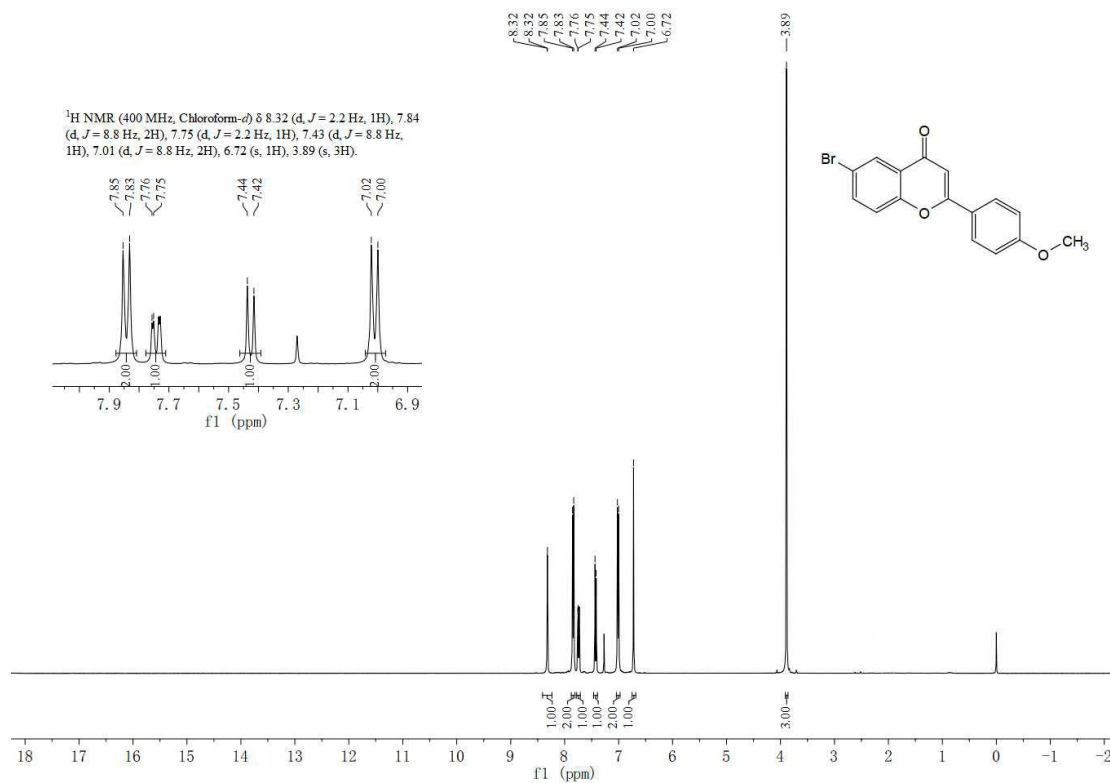


Figure S79 <sup>1</sup>H NMR spectrum of 6-bromo-2-(4-methoxyphenyl)-4H-chromen-4-one (3an)

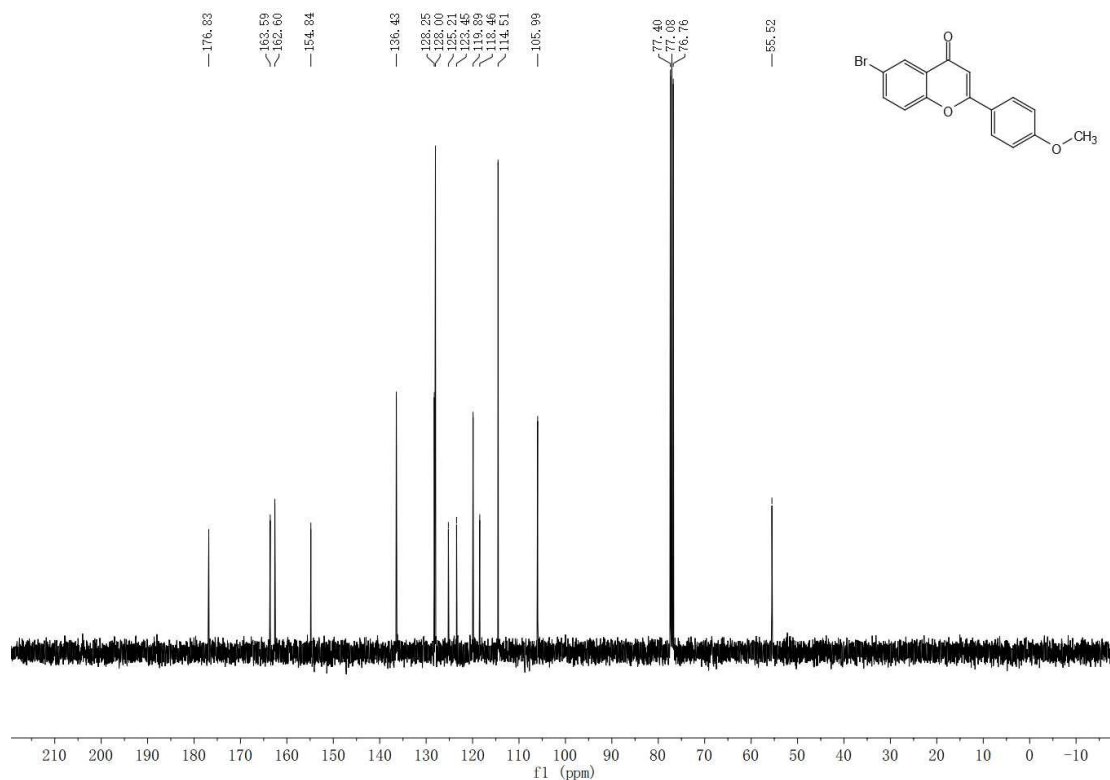


Figure S80 <sup>13</sup>C NMR spectrum of 6-bromo-2-(4-methoxyphenyl)-4H-chromen-4-one (3an)

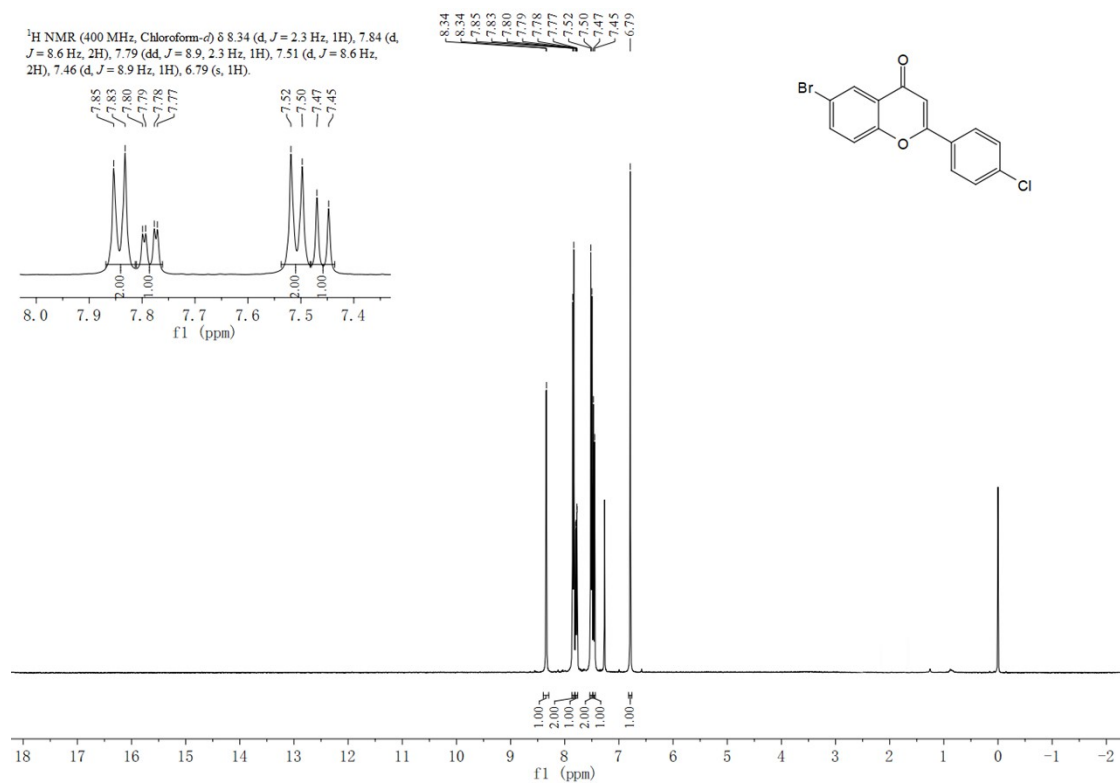


Figure S81 <sup>1</sup>H NMR spectrum of 6-bromo-2-(4-chlorophenyl)-4H-chromen-4-one (3ao)

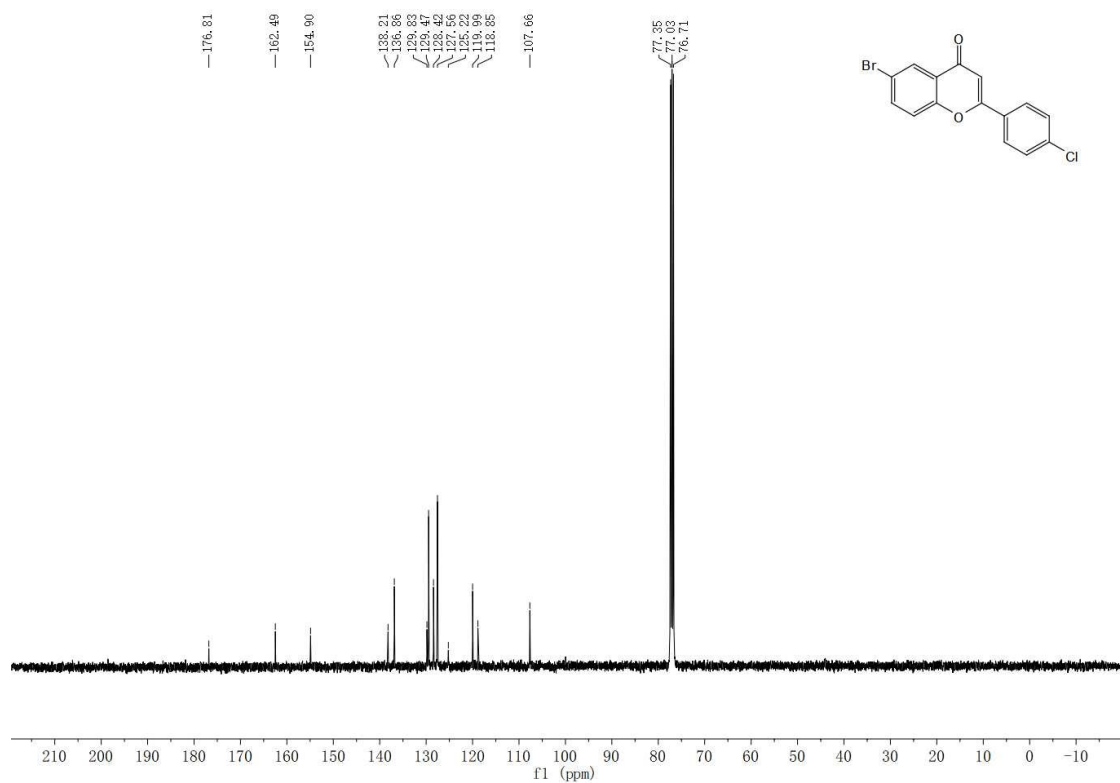
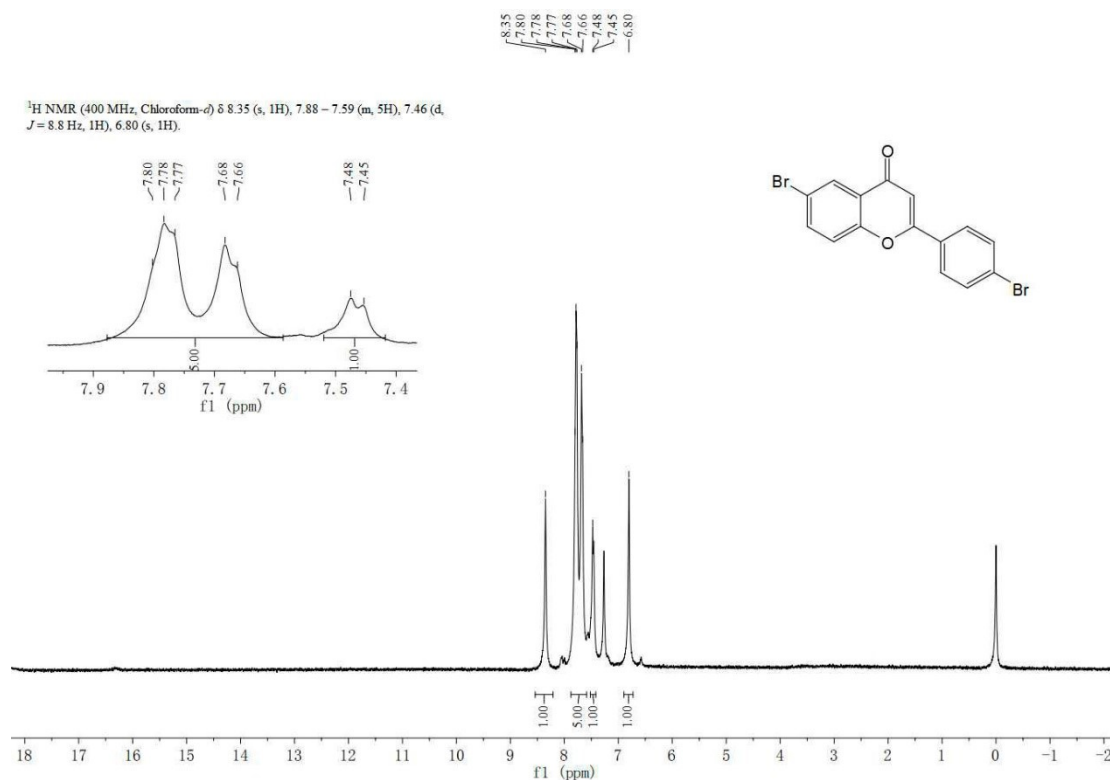
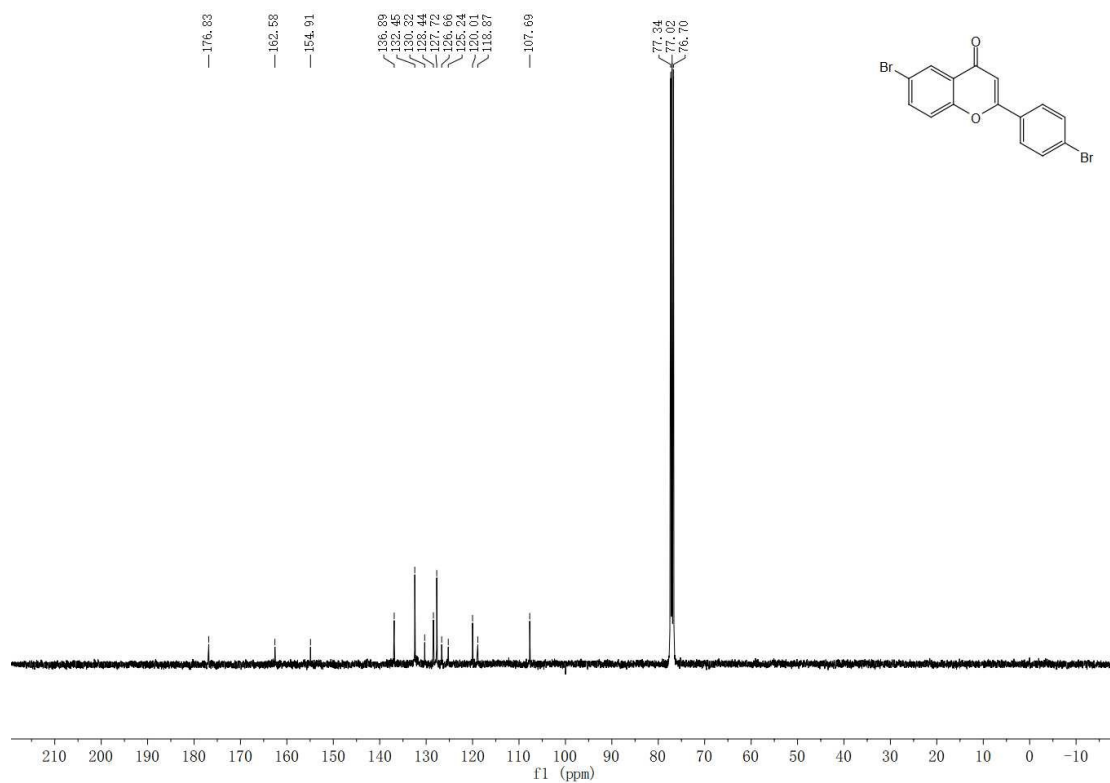


Figure S82 <sup>13</sup>C NMR spectrum of 6-bromo-2-(4-chlorophenyl)-4H-chromen-4-one (3ao)

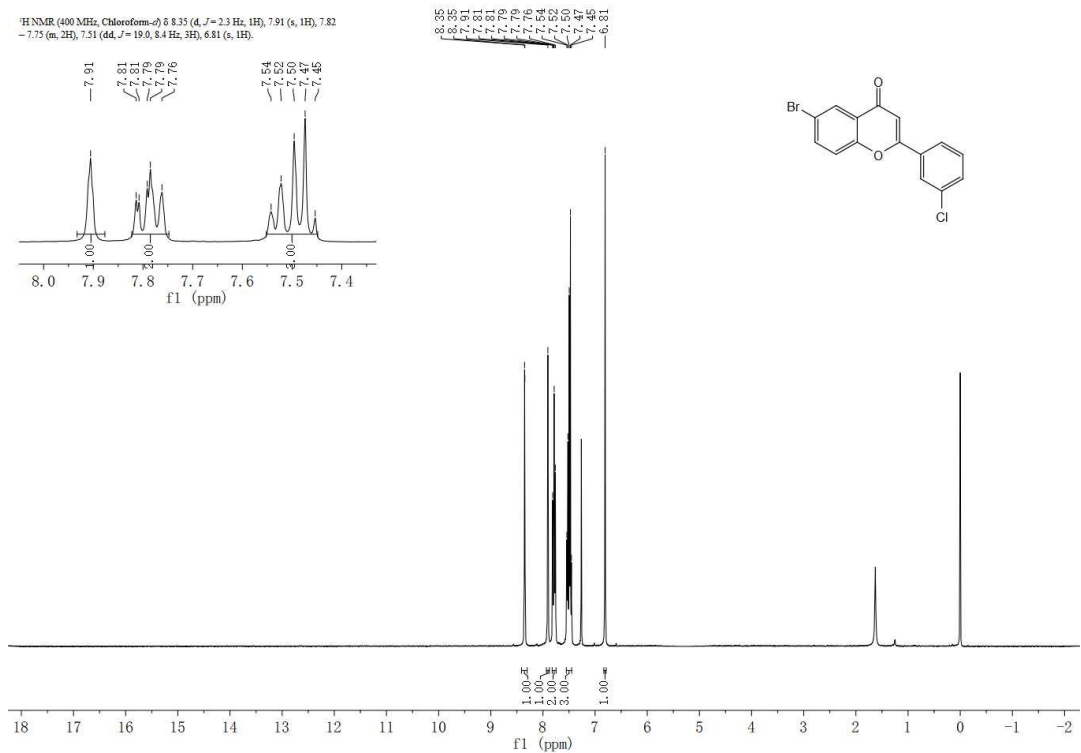


**Figure S83** <sup>1</sup>H NMR spectrum of 6-Bromo-2-(4-bromophenyl)-4H-chromen-4-one (3ap)

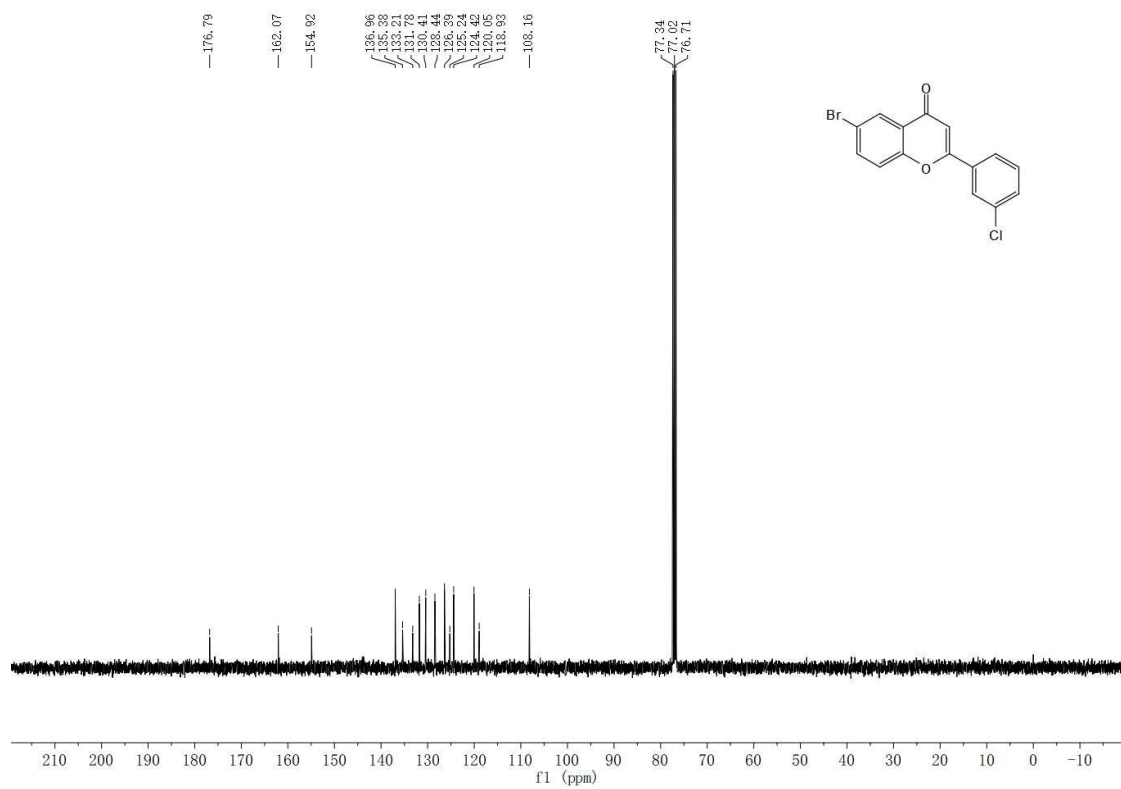


**Figure S84** <sup>13</sup>C NMR spectrum of 6-Bromo-2-(4-bromophenyl)-4H-chromen-4-one (3ap)





**Figure S85** <sup>1</sup>H NMR spectrum of 6-bromo-2-(3-chlorophenyl)-4H-chromen-4-one (3aq)



**Figure S86** <sup>13</sup>C NMR spectrum of 6-bromo-2-(3-chlorophenyl)-4H-chromen-4-one (3aq)

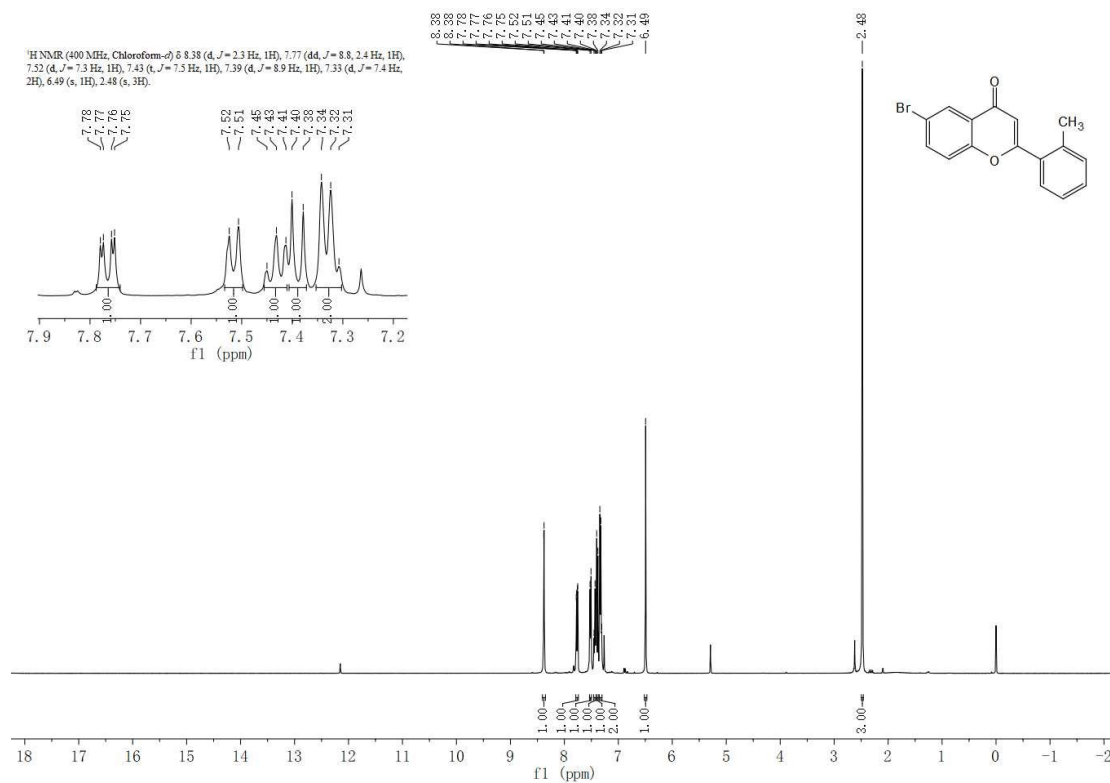


Figure S87 <sup>1</sup>H NMR spectrum of 6-Bromo-2-(2-methylphenyl)-4H-chromen-4-one (3ar)

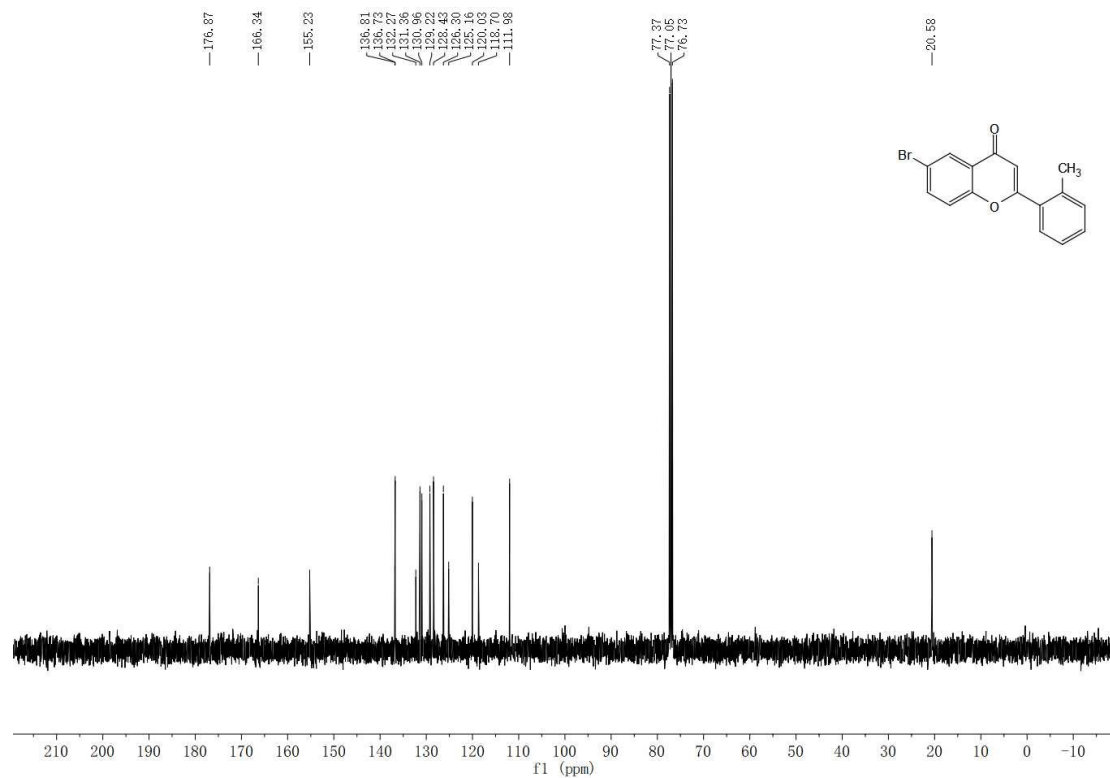


Figure S88 <sup>13</sup>C NMR spectrum of 6-Bromo-2-(2-methylphenyl)-4H-chromen-4-one (3ar)



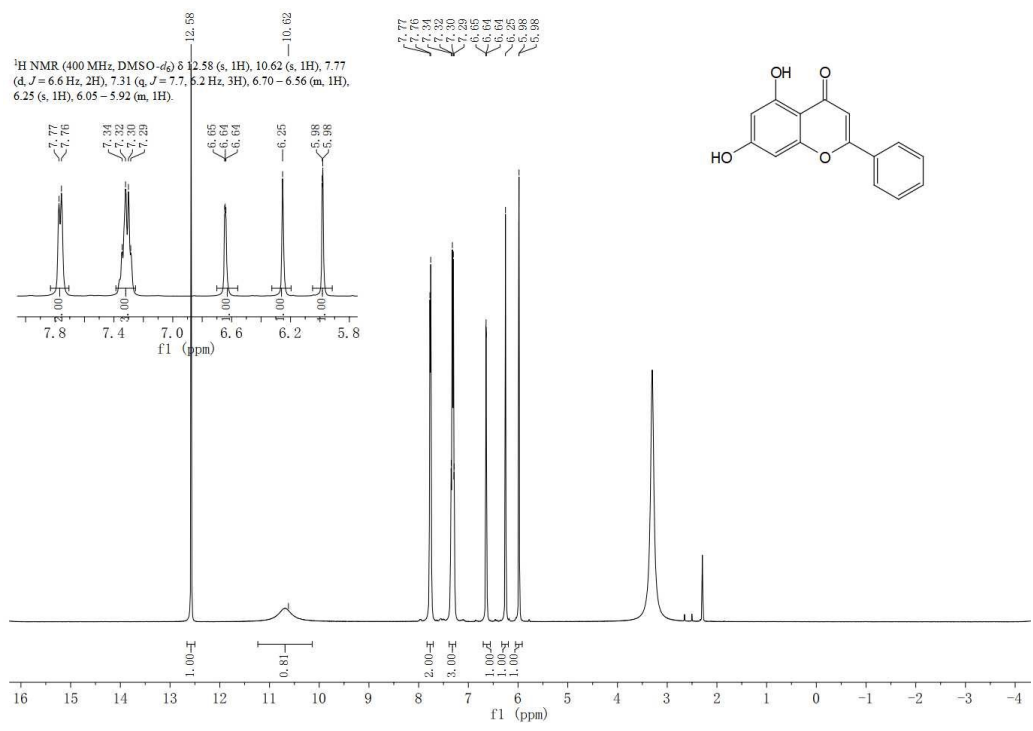


Figure S91 <sup>1</sup>H NMR spectrum of Chrysin

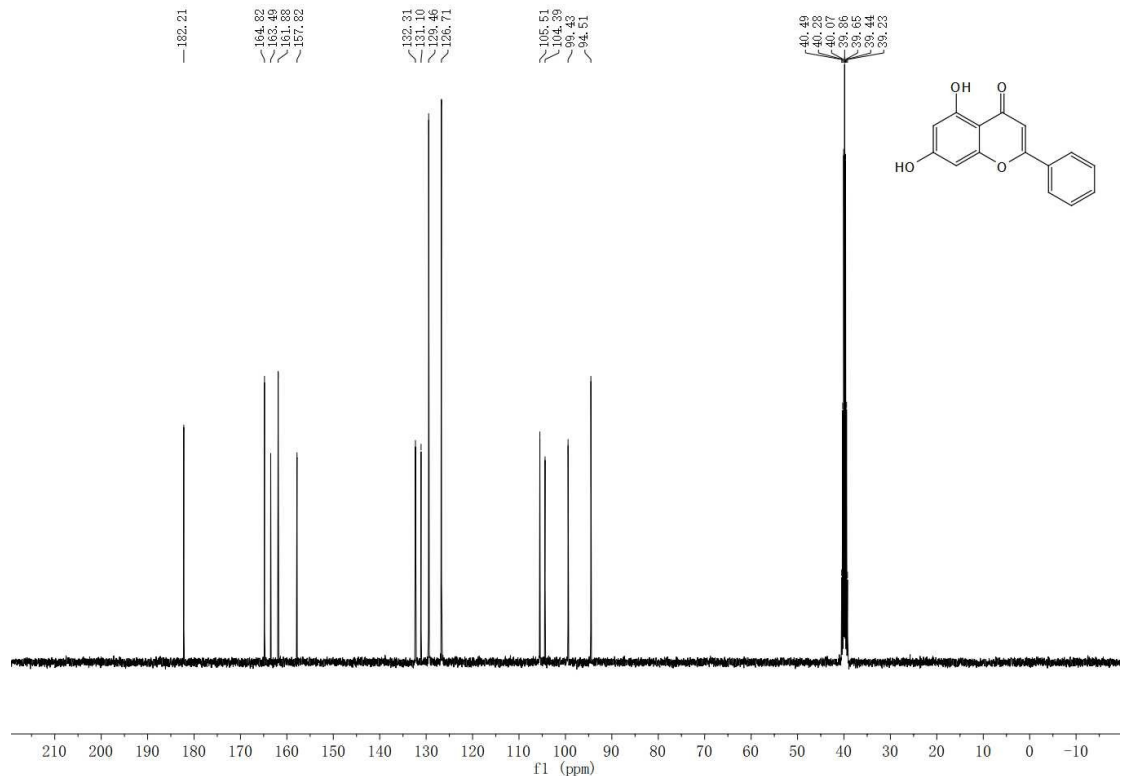


Figure S92 <sup>13</sup>C NMR spectrum of Chrysin

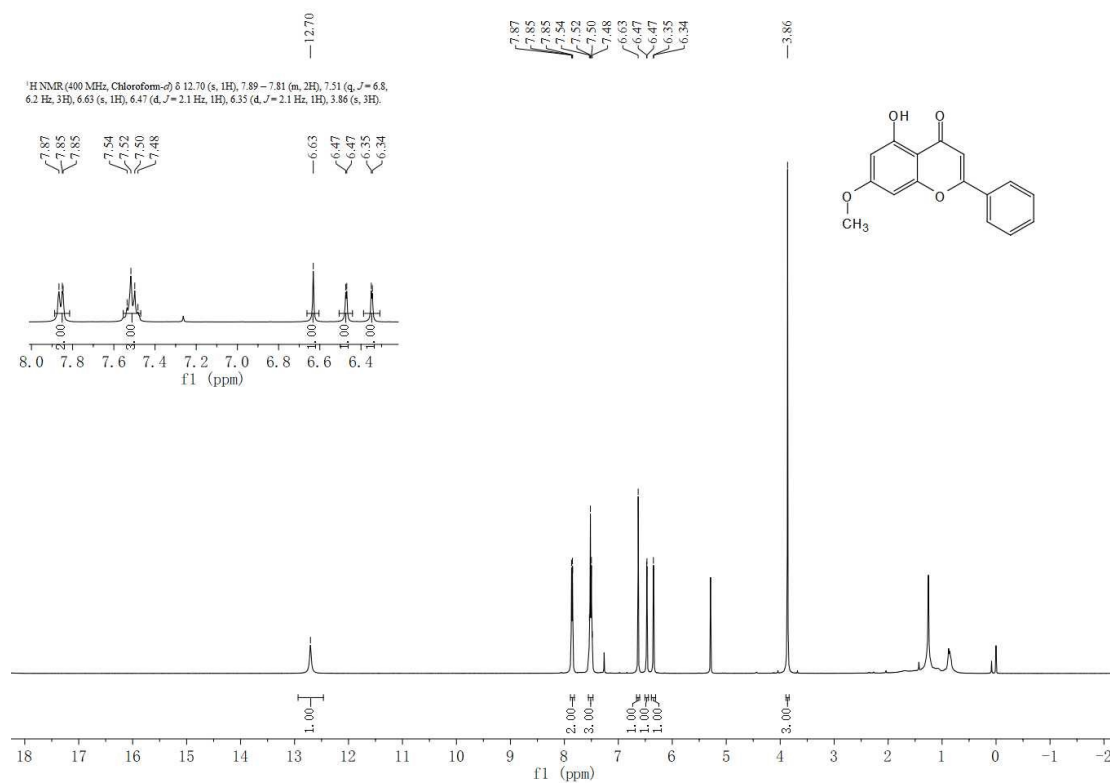


Figure S93 <sup>1</sup>H NMR spectrum of Tectochrysin

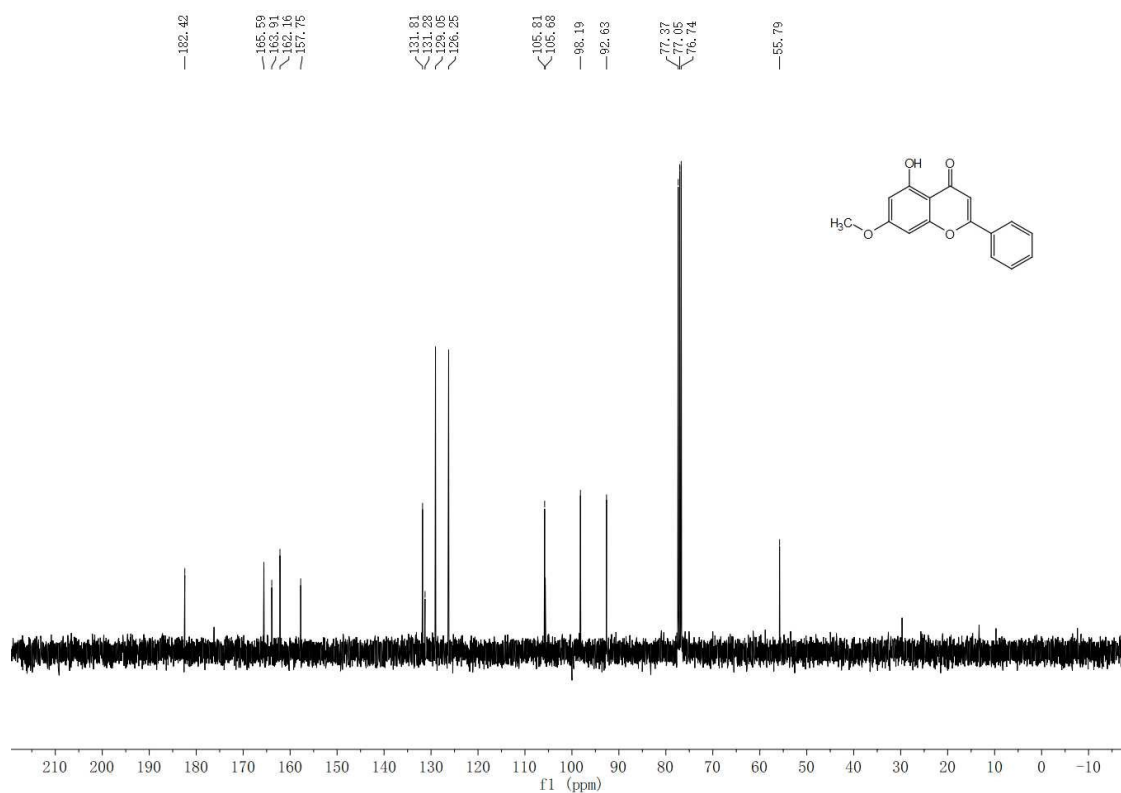


Figure S94 <sup>13</sup>C NMR spectrum of Tectochrysin

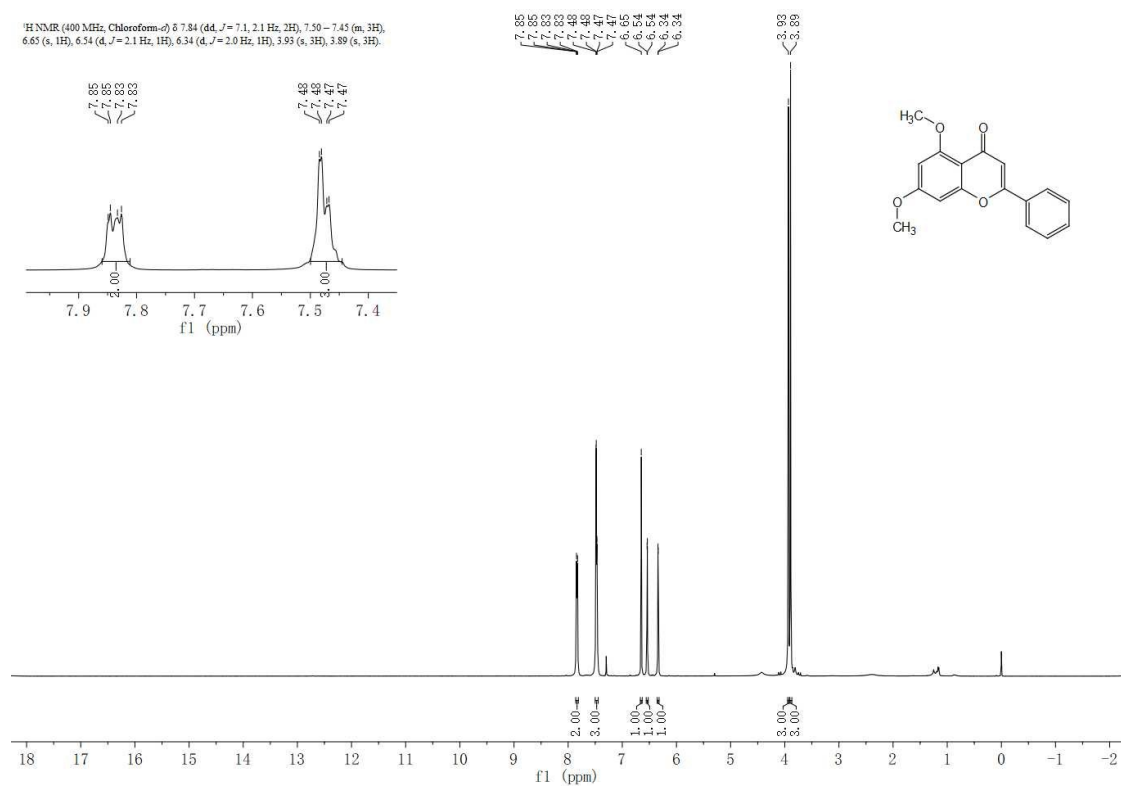


Figure S95 <sup>1</sup>H NMR spectrum of 5,7-Dimethoxyflavone

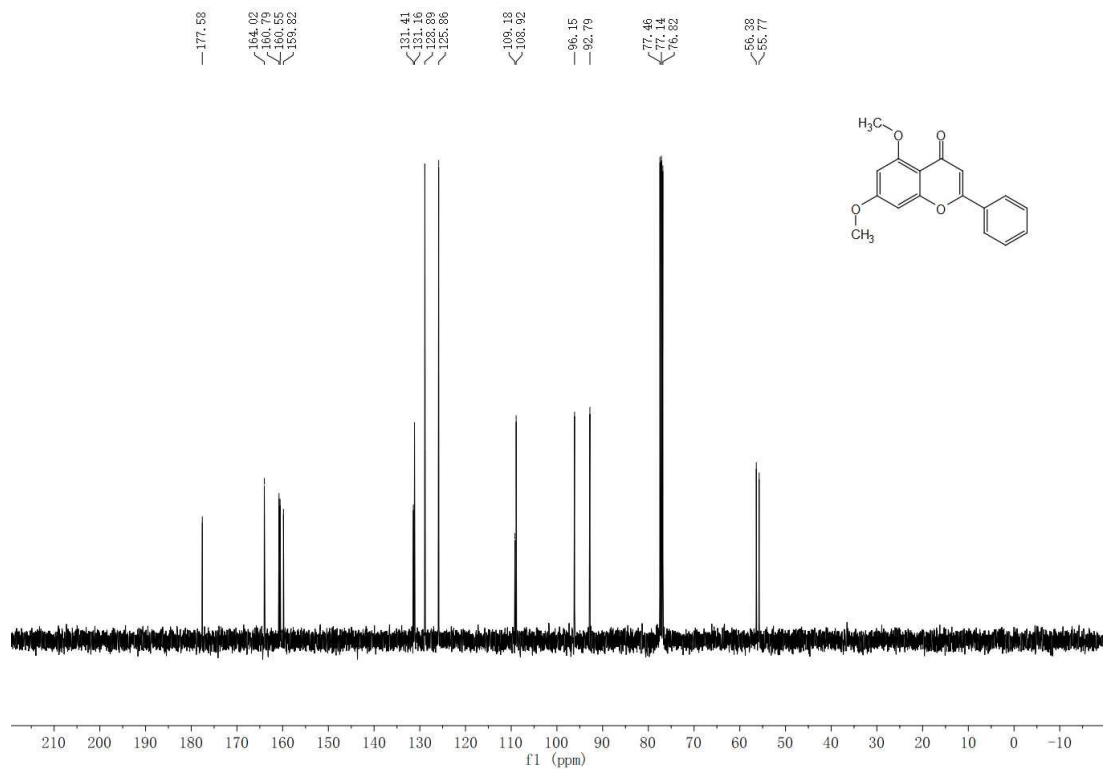


Figure S96 <sup>13</sup>C NMR spectrum of 5,7-Dimethoxyflavone

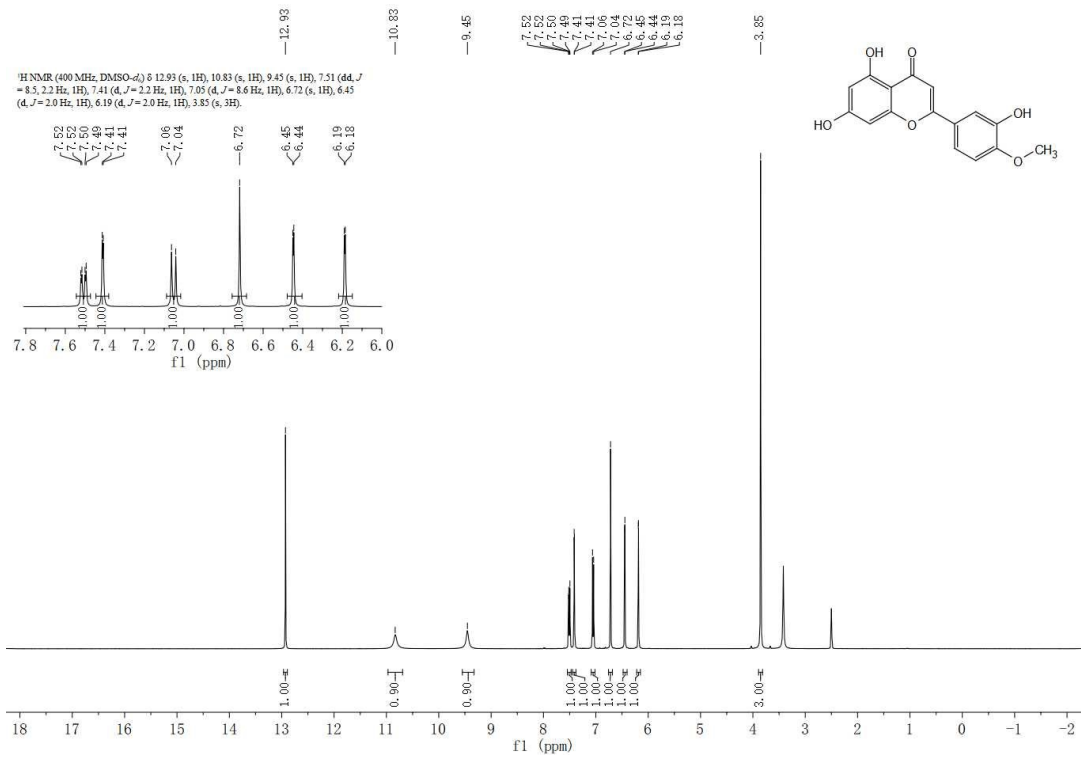


Figure S97 <sup>1</sup>H NMR spectrum of Diosmetin

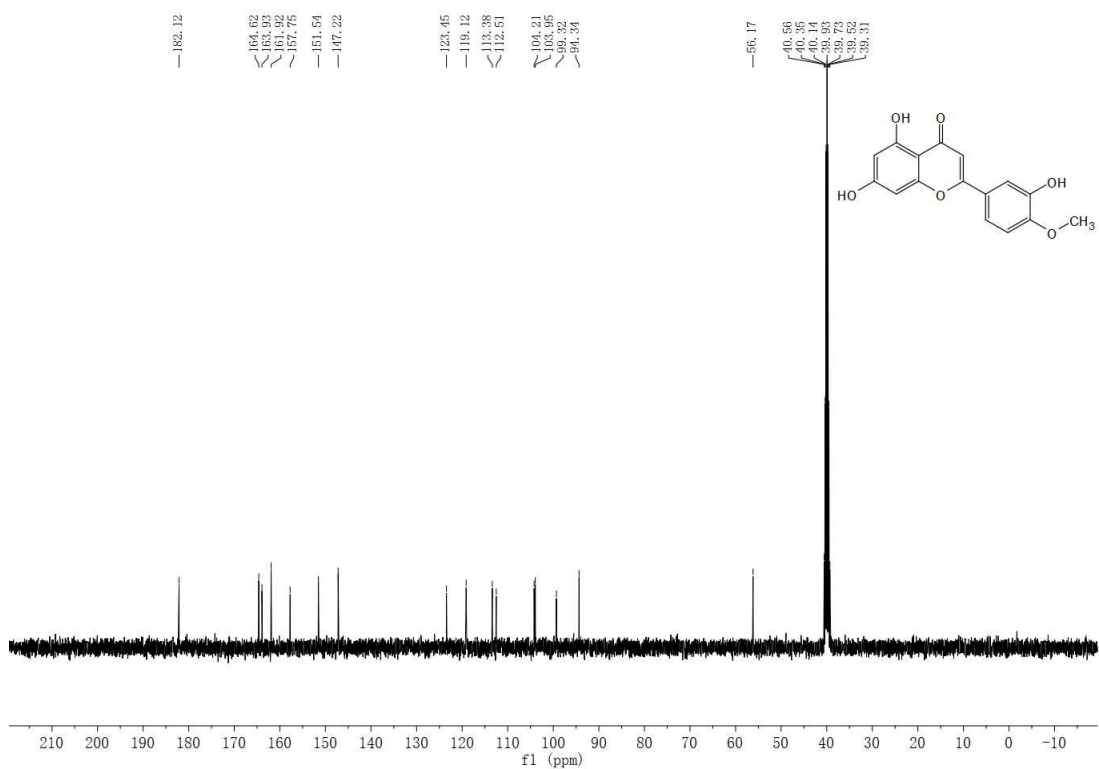


Figure S98 <sup>13</sup>C NMR spectrum of Diosmetin

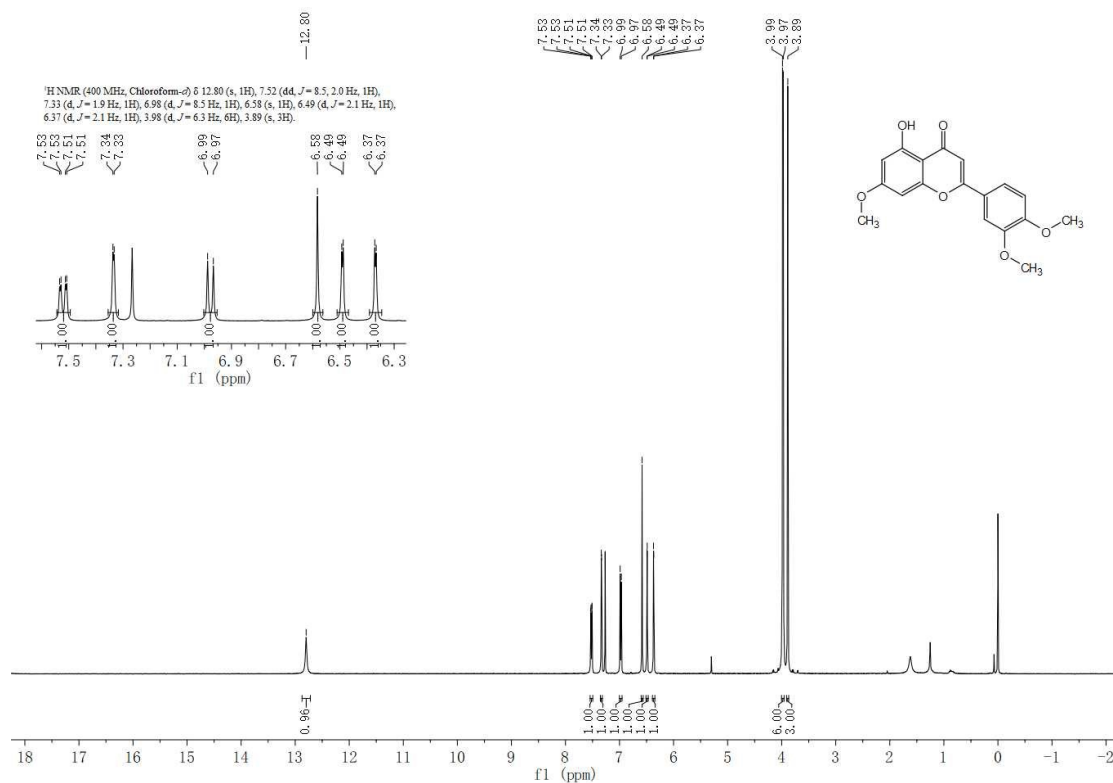


Figure S99 <sup>1</sup>H NMR spectrum of 7,3',4' -Tri-methyluteolin

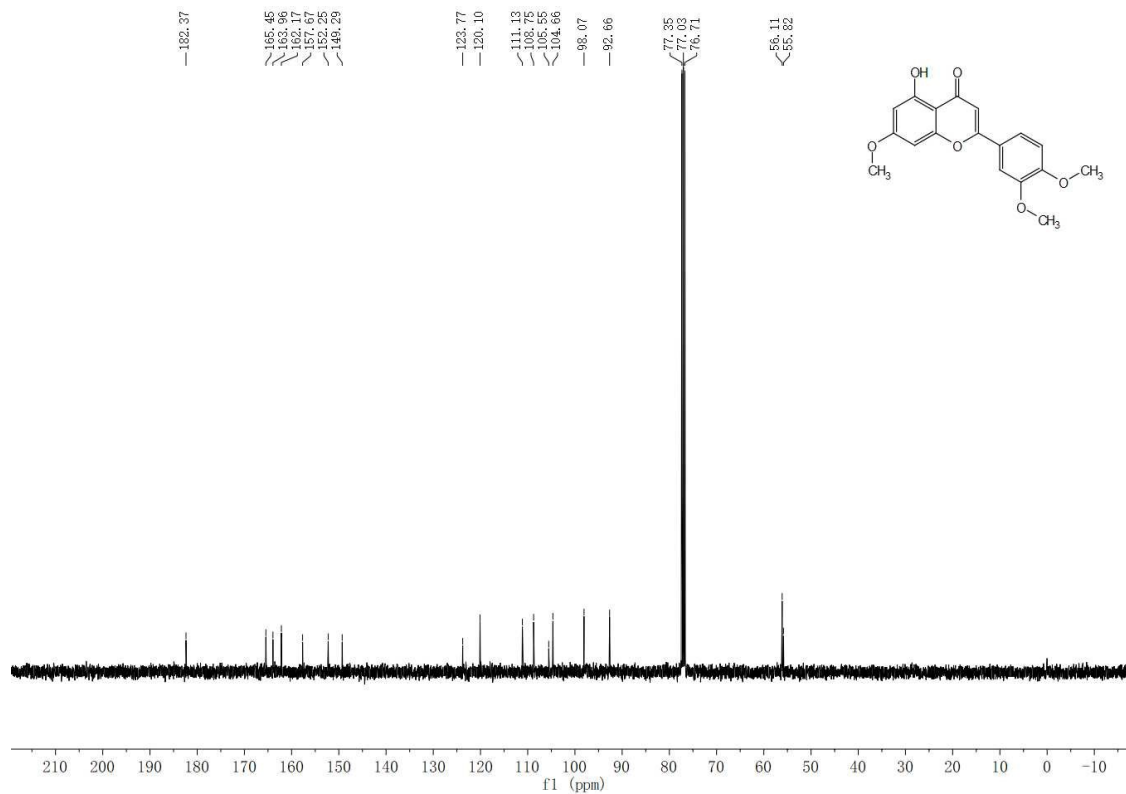


Figure S100 <sup>13</sup>C NMR spectrum of 7,3',4' -Tri-methyluteolin



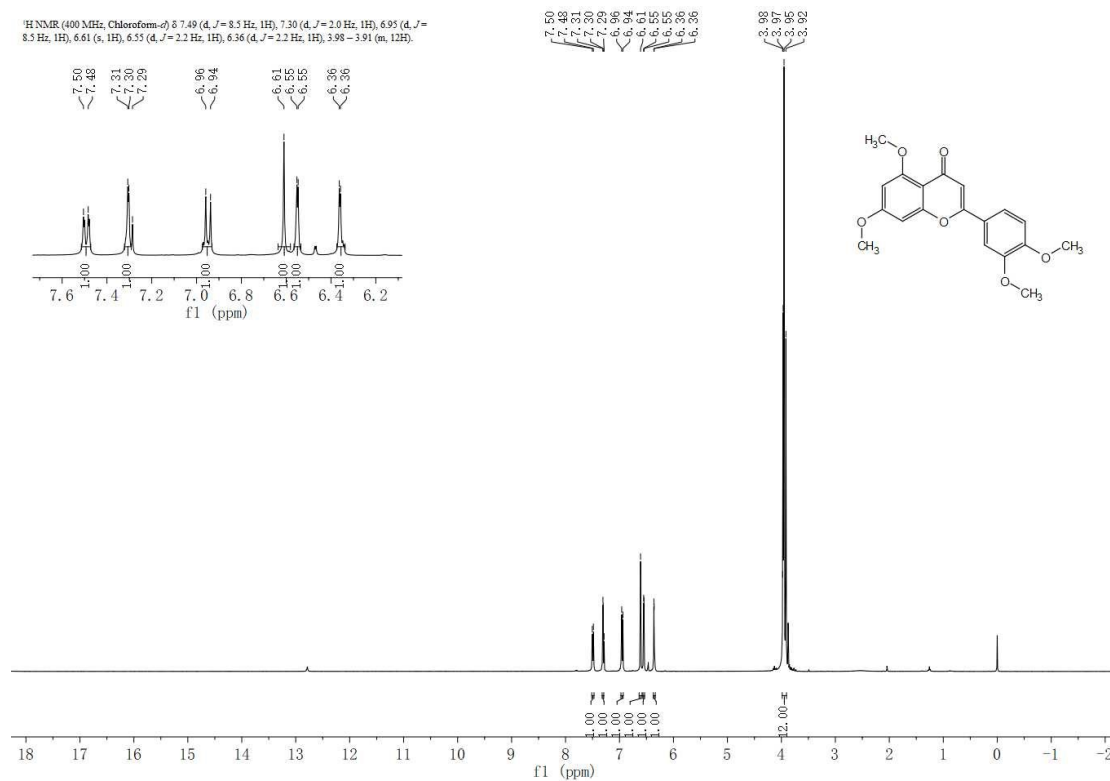


Figure S101 <sup>1</sup>H NMR spectrum of 5,7,3',4'-Tetramethoxyflavone

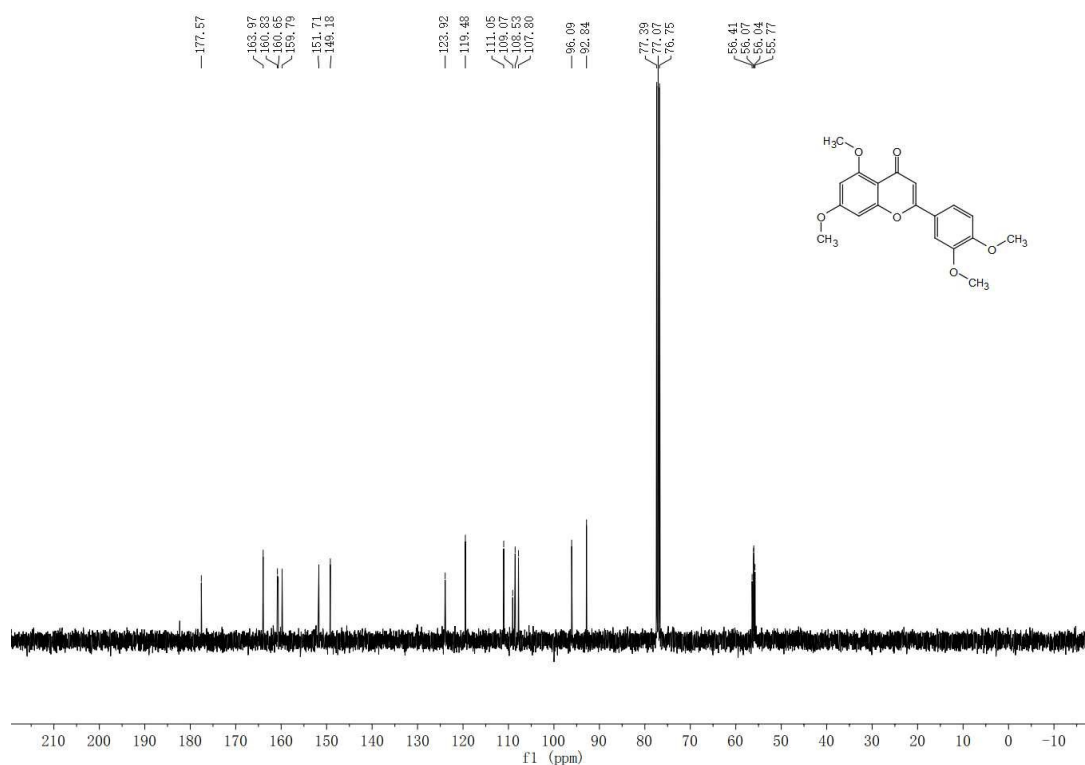


Figure S102 <sup>13</sup>C NMR spectrum of 5,7,3',4'-Tetramethoxyflavone

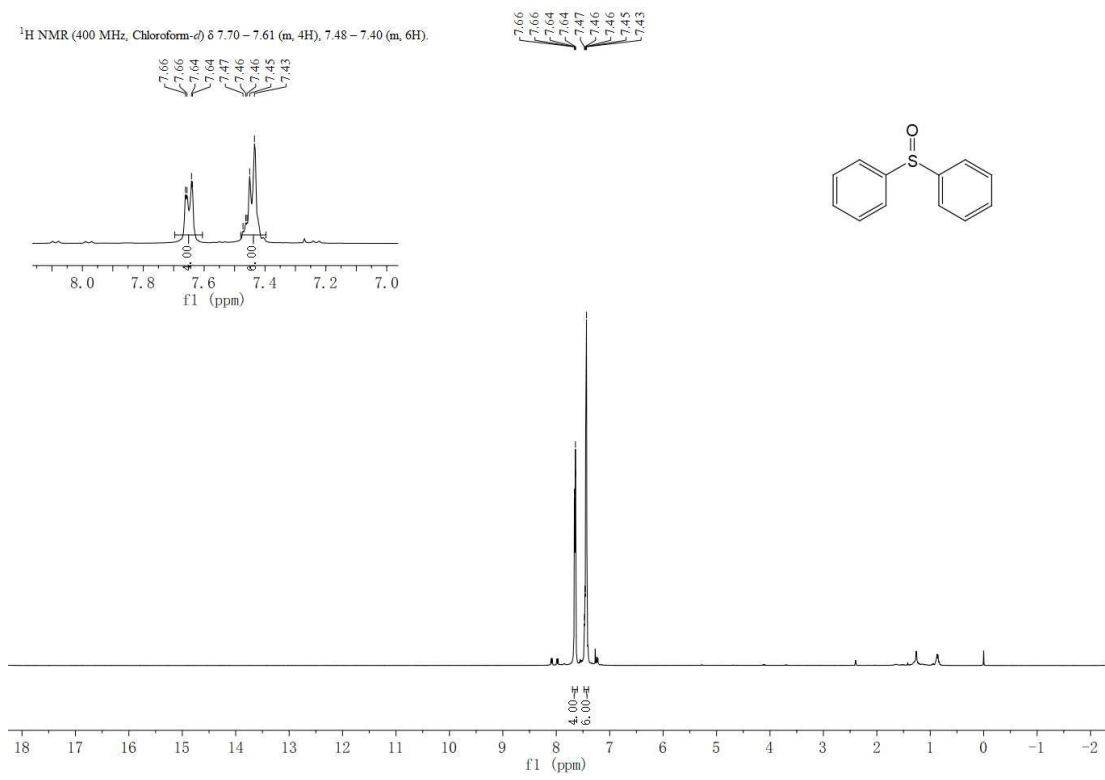


Figure 103 <sup>1</sup>H NMR spectrum of 1,1'-sulfinylbisbenzene

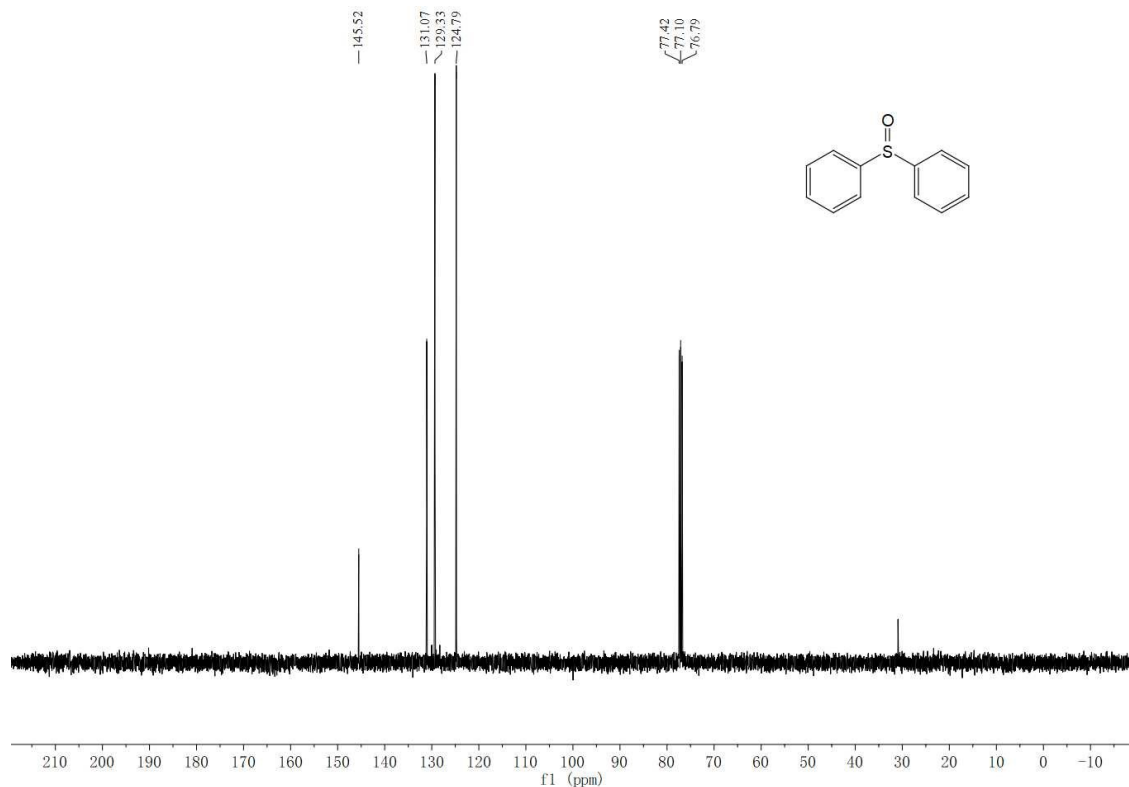


Figure S104 <sup>13</sup>C NMR spectrum of 1,1'-sulfinylbisbenzene

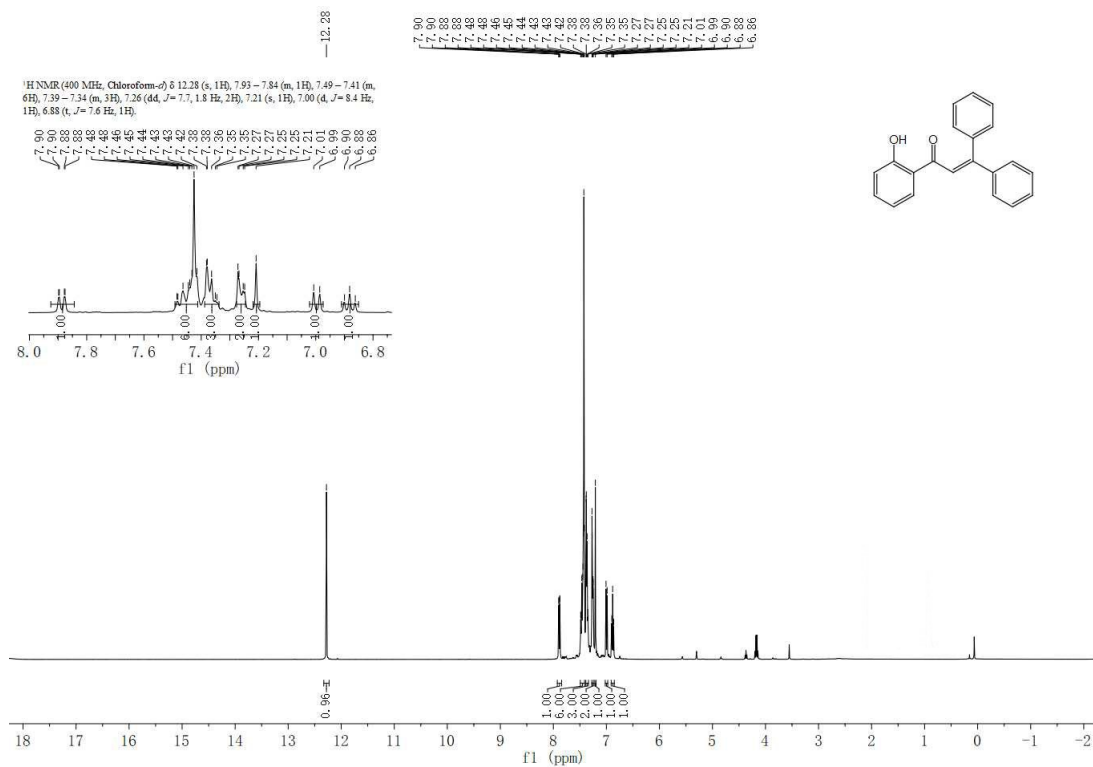


Figure S105 <sup>1</sup>H NMR spectrum of 1,3,3-triphenylprop-2-en-1-one

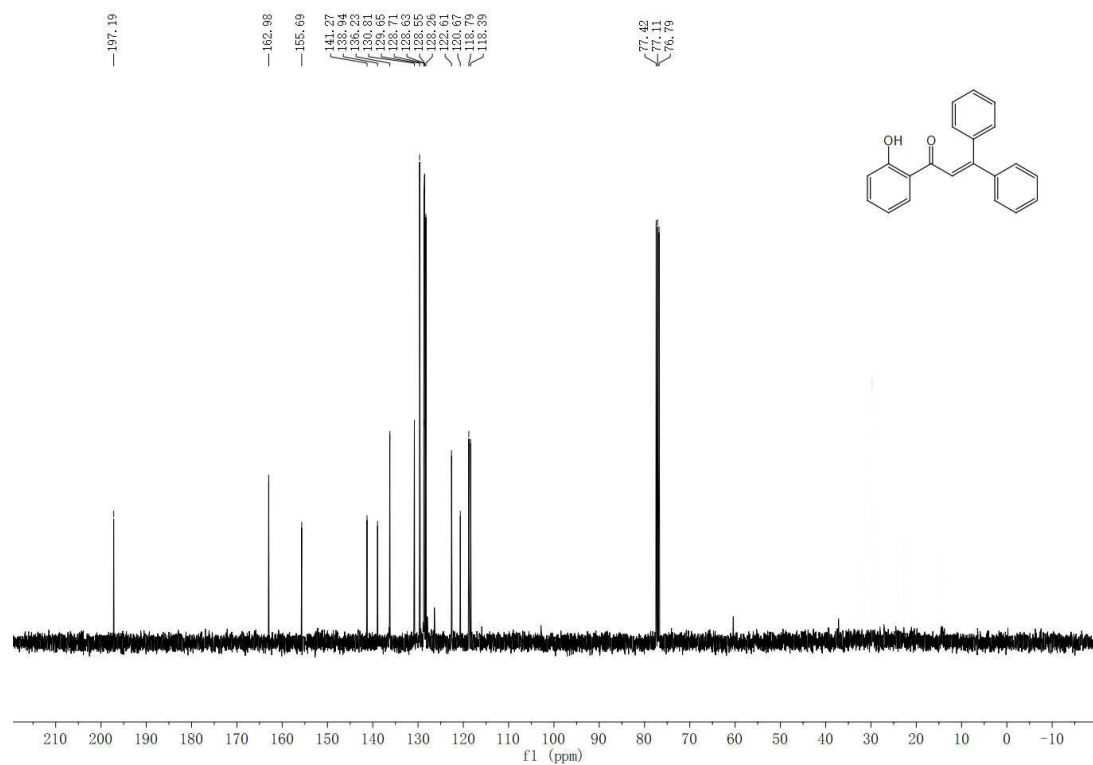


Figure S106 <sup>13</sup>C NMR spectrum of 1,3,3-triphenylprop-2-en-1-one

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