

## Supporting Information

### **Pd-catalyzed cross-coupling synthesis of 4-aryl-3-formylcoumarins**

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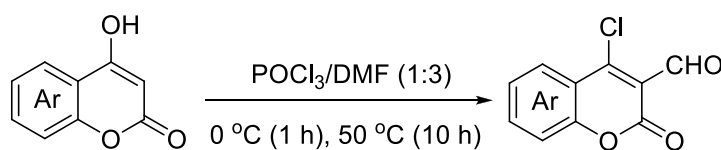
## General Information:

The coupling reactions were done in dry Schlenk tubes under N<sub>2</sub> atmosphere conditions. All solvents used in coupling reactions were dried following the standard procedures. These solvents after distillation were stored over oven-dried molecular sieves (4Å) in Schlenk bottles under N<sub>2</sub> atmosphere. Column chromatography was done with 100-200 mesh (Souvenir Chemicals) or 230-400 mesh silica gel (Merck) using EtOAc/hexane as eluent. The instruments of JEOL ECS 400 (400 MHz) and JEOL ECX 500 (500 MHz) were used to measure <sup>1</sup>H and <sup>13</sup>C NMR spectra. Agilent 6230 LC/TOF analyzer for atmospheric-pressure chemical ionization (APCI) and Agilent 6546 LC/Q-TOF analyzer for Electrospray Ionization (ESI) were used to measure high-resolution mass spectra (HRMS). The Perkin Elmer FT-IR machine was used for recording IR spectra. Chemical shifts in parts per million (ppm) were reported with reference to residual CHCl<sub>3</sub> ( $\delta$  = 7.26 ppm) for <sup>1</sup>H NMR and  $\delta$  = 77.16 ppm for CDCl<sub>3</sub> in <sup>13</sup>C NMR spectrum. Coupling constant (*J*) values were reported in Hertz (Hz). The JSGW melting point apparatus was used to measure the melting points of the products and are reported uncorrected.

## Experimental procedures:

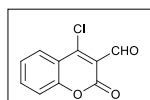
The synthesis of 4-hydroxy coumarins was carried out from corresponding 2-hydroxy acetophenone derivatives using the known procedure.<sup>1</sup> These compounds were further transformed into 4-chloro-3-formyl coumarin using POCl<sub>3</sub> and DMF conditions.<sup>2</sup>

### General procedure for preparation of 4-chloro -3-formylcoumarin derivatives (1a-1d):



In an oven-dried round-bottomed flask, DMF (10 mL) was taken and cooled to 0 °C. To this, the POCl<sub>3</sub> (5 mL) was added dropwise with stirring. To this mixture, 4-hydroxycoumarin (3 g, 1 equiv.) in DMF (5 mL) added dropwise. After the complete addition, the mixture was stirred at 50 °C for 10 h. Then, the mixture was cooled to rt and poured into ice-cold water. The resulted solid product was filtered off and dried under reduced pressure. The crudewas further purified by silica gel column chromatography using 100-200 silic and ethyl acetate/hexane as an eluent to obtain 4-chloro-3-formylcoumarin.

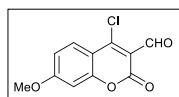
**4-chloro-2-oxo-2H-chromene-3-carbaldehyde (1a):** Yellow solid (2.9 g, 75%); m.p. 122-124 °C, <sup>1</sup>H



NMR (396 MHz, Chloroform-*d*)  $\delta$  = 10.36 (s, 1H), 8.12 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.76 – 7.71 (m, 1H), 7.47 – 7.42 (m, 1H), 7.40 – 7.37 (m, 1H). <sup>13</sup>C NMR (100 MHz, Chloroform-*d*)  $\delta$  = 186.94, 158.53, 153.70, 153.35, 135.85, 127.75, 125.71, 118.46, 118.26, 117.30. IR (neat, cm<sup>-1</sup>): 2875, 1702, 1602, 1540, 1300, 966, 751. APCI (m/z) calcd. for C<sub>10</sub>H<sub>6</sub>ClO<sub>3</sub> [M+H]<sup>+</sup> 209.0005; found

209.0019.

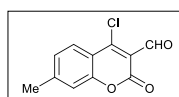
**4-chloro-7-methoxy-2-oxo-2H-chromene-3-carbaldehyde (1b):** Yellow solid (2.6 g, 70%); m.p. 176-



178 °C, <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  = 10.33 (s, 1H), 8.00 (d, *J* = 9.0 Hz, 1H), 6.97 (dd, *J* = 9.1, 2.4 Hz, 1H), 6.81 (d, *J* = 2.4 Hz, 1H), 3.94 (s, 3H). <sup>13</sup>C NMR (126 MHz, Chloroform-*d*)  $\delta$  = 186.94, 166.29, 159.00, 155.78, 154.16, 129.22, 115.12, 114.61, 112.05, 100.63, 56.43. IR (neat, cm<sup>-1</sup>): 1722, 1691, 1608, 1527, 1292, 1129, 844, 753. APCI (m/z) calcd. for C<sub>11</sub>H<sub>8</sub>ClO<sub>4</sub> [M+H]<sup>+</sup>

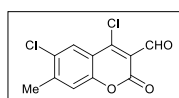
239.0106; found 239.0107.

**4-chloro-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (1c):** Yellow solid (2.8 g, 74%); m.p. 142-144



°C, <sup>1</sup>H NMR (500 MHz, Chloroform-*d*)  $\delta$  10.32 (s, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.23 (d, *J* = 8.8 Hz, 1H), 7.16 (s, 1H), 2.50 (s, 3H). <sup>13</sup>C NMR (126 MHz, Chloroform-*d*)  $\delta$  = 186.93, 158.75, 153.80, 153.45, 148.25, 127.46, 127.05, 117.30, 117.24, 116.16, 22.13. IR (neat, cm<sup>-1</sup>): 2868, 1755, 1610, 1534, 1324, 1157, 844, 723. APCI (m/z) calcd. for C<sub>11</sub>H<sub>8</sub>ClO<sub>3</sub> [M+H]<sup>+</sup> 223.0162; found 223.0166.

**4,6-dichloro-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (1d):** Yellow solid (2.5 g, 68%); m.p. 130-



132 °C, <sup>1</sup>H NMR (500 MHz, Chloroform-*d*)  $\delta$  = 10.32 (s, 1H), 8.04 (s, 1H), 7.25 (s, 1H), 2.51 (s, 3H). <sup>13</sup>C NMR (126 MHz, Chloroform-*d*)  $\delta$  = 186.63, 158.29, 152.18, 151.53, 145.77, 132.02, 127.13, 119.16, 118.01, 117.54, 21.09. IR (neat, cm<sup>-1</sup>): 2924, 1730, 1701, 1534, 1300, 1034, 889, 797. APCI (m/z) calcd. for C<sub>11</sub>H<sub>7</sub>Cl<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 256.9767; found 256.9767.

#### General procedure for synthesis of 4-aryl-3-formylcoumarins (2.1 - 2.11, 3.1 - 3.14, Table 2 and Table 3):

The cross-coupling reaction was carried out in an oven-dried Schlenk tube under a nitrogen atmosphere with 4-chloro-3-formylcoumarin derivative (0.825 mmol, 3.3 equiv.), BiAr<sub>3</sub> (0.25 mmol, 1 equiv.), K<sub>3</sub>PO<sub>4</sub> (1 mmol, 4 equiv.), Pd<sub>2</sub>(dba)<sub>3</sub> (0.0125 mmol, 0.05 equiv.), PPh<sub>3</sub> (0.025 mmol, 0.1 equiv.) in THF (3 mL). The mixture was heated in an oil bath at 60 °C for 4 h. It was then brought to rt and extracted with ethyl acetate (30 mL). The organic extract was washed with water, brine, dried over anhydrous MgSO<sub>4</sub>, and concentrated. The crude was purified by silica gel column chromatography using ethyl acetate/hexane as an eluent. The cross-coupled product yield was calculated considering 0.75 mmol as 100% yield.

## Procedure for one-pot synthesis of Wittig modified 3, 4-disubstituted couamrins (4.1 – 4.6,

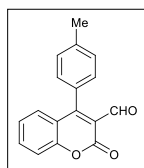
Table 4):

**Step 1:** The cross-coupling reaction was carried out in an oven-dried Schlenk tube under a nitrogen atmosphere with 4-chloro-3-formylcoumarin (0.825 mmol, 3.3 equiv.), BiAr<sub>3</sub> (0.25 mmol, 1 equiv.), K<sub>3</sub>PO<sub>4</sub> (1 mmol, 4 equiv.), Pd<sub>2</sub>(dba)<sub>3</sub> (0.0125 mmol, 0.05 equiv.), PPh<sub>3</sub> (0.025 mmol, 0.1 equiv.) in THF (3 mL). The mixture was heated in an oil bath at 60 °C for 4 h.

**Step 2:** The product mixture obtained in Schlenk tube from step 1 was cooled to rt. To this, Wittig salt (0.75 mmol, 3 equiv.), NaOMe (0.75 mmol, 3 equiv.) and THF (1 mL) were added under the nitrogen atmosphere. The mixture was heated at 60 °C for 6 h. It was then brought to rt, extracted with ethyl acetate (30 mL). The organic extract was washed with water, brine, dried over anhydrous MgSO<sub>4</sub>, and concentrated. The crude was subjected to silica gel column chromatography using ethyl acetate/hexane as an eluent to obtain Wittig modified 3, 4-disubstituted couamrin product. The overall yield was calculated considering 0. 75 mmol product as 100% yield.

### Spectral data of products:

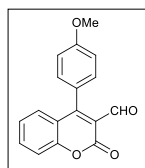
**2-oxo-4-*p*-tolyl-2*H*-chromene-3-carbaldehyde (2.1):** Yellow solid (166 mg, 84%); m.p. 134-136 °C, <sup>1</sup>H



NMR (400 MHz, Chloroform-*d*)  $\delta$  = 9.92 (s, 1H), 7.68 – 7.62 (m, 1H), 7.40 (d, *J* = 8.3 Hz, 1H), 7.36 (d, *J* = 7.9 Hz, 2H), 7.28 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.24 (d, *J* = 7.1 Hz, 1H), 7.20 (d, *J* = 7.8 Hz, 2H), 2.48 (s, 3H). <sup>13</sup>C NMR (101 MHz, Chloroform-*d*)  $\delta$  = 188.53, 161.89, 158.27, 154.65, 140.34, 134.80, 129.57, 129.49, 128.76, 128.50, 124.86, 119.97, 119.14, 117.29,

21.60. IR (neat, cm<sup>-1</sup>): 2862, 1753, 1722, 1605, 1548, 1365, 1041, 815, 759. APCI (m/z) calcd. for C<sub>17</sub>H<sub>13</sub>O<sub>3</sub> [M+H]<sup>+</sup> 265.0859; found 265.0858.

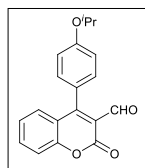
**4-(4-methoxyphenyl)-2-oxo-2*H*-chromene-3-carbaldehyde (2.2):** Yellow solid (176 mg, 84%); m.p.



156-158 °C, <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  = 9.94 (s, 1H), 7.68 (t, *J* = 7.1 Hz, 1H), 7.43 (d, *J* = 8.2 Hz, 1H), 7.37 (d, *J* = 7.9 Hz, 1H), 7.32 – 7.29 (m, 3H), 7.10 (d, *J* = 8.7 Hz, 2H), 3.94 (s, 3H). <sup>13</sup>C NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.55, 161.41, 161.16, 158.29, 154.70, 134.70, 130.67, 129.45, 124.84, 123.36, 120.06, 119.29, 117.34, 114.38, 55.59. IR (neat, cm<sup>-1</sup>):

2924, 1753, 1719, 1606, 1543, 1256, 1017, 835, 761. APCI (m/z) calcd. for C<sub>17</sub>H<sub>13</sub>O<sub>4</sub> [M+H]<sup>+</sup> 281.0808; found 281.0825.

**4-(4-isopropoxyphenyl)-2-oxo-2*H*-chromene-3-carbaldehyde (2.3):** Yellow solid (179 mg, 77%); m.p.

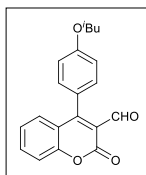


128-130 °C, <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  = 9.87 (s, 1H), 7.64 (td, *J* = 8.0, 7.4, 1.5 Hz, 1H), 7.40 – 7.34 (m, 2H), 7.26 – 7.21 (m, 3H), 7.05 – 6.99 (m, 2H), 4.64 (hept, *J* = 6.0 Hz, 1H), 1.39 (d, *J* = 6.0 Hz, 6H). <sup>13</sup>C NMR (100 MHz, Chloroform-*d*)  $\delta$  = 188.58, 161.78, 159.68, 158.07, 154.70, 134.70, 130.84, 129.42, 124.80, 122.74, 119.98, 119.26, 117.33, 115.79, 70.32,



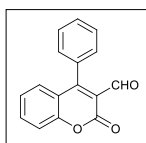
22.11. IR (neat,  $\text{cm}^{-1}$ ): 2978, 1754, 1722, 1605, 1546, 1249, 1106, 953, 758. APCI (m/z) calcd. for  $\text{C}_{19}\text{H}_{17}\text{O}_4$   $[\text{M}+\text{H}]^+$  309.1121; found 309.1129.

**4-(4-isobutoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.4):** Yellow solid (195 mg, 80%); m.p.



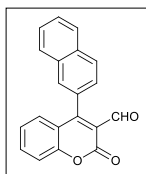
108–110 °C,  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  = 9.89 (s, 1H), 7.67 – 7.62 (m, 1H), 7.39 (d,  $J$  = 8.2 Hz, 1H), 7.36 (dd,  $J$  = 8.0, 1.3 Hz, 1H), 7.26 – 7.22 (m, 3H), 7.06 (d,  $J$  = 8.7 Hz, 2H), 3.81 (d,  $J$  = 6.4 Hz, 2H), 2.19 – 2.09 (m, 1H), 1.06 (d,  $J$  = 6.7 Hz, 6H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.56, 161.63, 160.90, 158.20, 154.70, 134.67, 130.70, 129.45, 124.80, 123.00, 120.05, 119.26, 117.32, 114.85, 74.72, 28.38, 19.36. IR (neat,  $\text{cm}^{-1}$ ): 2960, 1754, 1721, 1605, 1547, 1366, 1027, 758. APCI (m/z) calcd. for  $\text{C}_{20}\text{H}_{19}\text{O}_4$   $[\text{M}+\text{H}]^+$  323.1278; found 323.1275.

**2-oxo-4-phenyl-2H-chromene-3-carbaldehyde (2.5):** Yellow solid (121 mg, 64%); m.p. 140–142 °C,  $^1\text{H}$



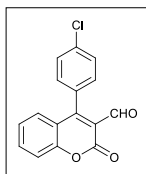
NMR (400 MHz, Chloroform-*d*)  $\delta$  = 9.95 (s, 1H), 7.68 – 7.64 (m, 1H), 7.57 – 7.53 (m, 3H), 7.41 (d,  $J$  = 8.2 Hz, 1H), 7.31 (dd,  $J$  = 6.5, 3.1 Hz, 2H), 7.24 – 7.21 (m, 2H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.38, 161.31, 158.41, 154.68, 134.86, 131.74, 129.97, 129.51, 128.88, 128.58, 124.95, 119.95, 119.13, 117.31. IR (neat,  $\text{cm}^{-1}$ ): 2767, 1748, 1676, 1604, 1548, 1372, 893, 762. APCI (m/z) calcd. for  $\text{C}_{16}\text{H}_{11}\text{O}_3$   $[\text{M}+\text{H}]^+$  251.0703; found 251.0713.

**4-(naphthalen-2-yl)-2-oxo-2H-chromene-3-carbaldehyde (2.6):** Yellow solid (204 mg, 90%); m.p.



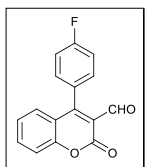
122–124 °C,  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  = 9.98 (s, 1H), 8.03 (d,  $J$  = 8.3 Hz, 1H), 7.93 (dd,  $J$  = 28.7, 7.4 Hz, 2H), 7.80 (s, 1H), 7.68 – 7.61 (m, 3H), 7.42 (dd,  $J$  = 15.0, 8.3 Hz, 2H), 7.24 (dd,  $J$  = 13.6, 6.2 Hz, 2H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.34, 161.27, 158.46, 154.70, 134.85, 133.63, 132.76, 129.65, 129.16, 128.75, 128.46, 128.44, 128.15, 127.70, 127.43, 125.70, 124.97, 120.06, 119.36, 117.35. IR (neat,  $\text{cm}^{-1}$ ): 2924, 1752, 1721, 1602, 1547, 1324, 821, 754. APCI (m/z) calcd. for  $\text{C}_{20}\text{H}_{13}\text{O}_3$   $[\text{M}+\text{H}]^+$  301.0859; found 301.0850.

**4-(4-chlorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.7):** Yellow solid (157 mg, 74%); m.p. 174–



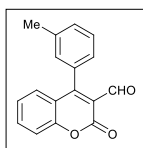
176 °C,  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  = 10.06 (s, 1H), 7.69 – 7.65 (m, 1H), 7.54 (d,  $J$  = 8.3 Hz, 2H), 7.42 (d,  $J$  = 8.4 Hz, 1H), 7.27 – 7.22 (m, 3H), 7.19 (dd,  $J$  = 8.0, 1.5 Hz, 1H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.32, 159.12, 159.02, 154.67, 136.13, 134.98, 130.46, 129.79, 129.41, 129.22, 125.13, 119.83, 119.07, 117.44. IR (neat,  $\text{cm}^{-1}$ ): 2924, 1749, 1705, 1596, 1541, 1362, 1089, 762. APCI (m/z) calcd. for  $\text{C}_{16}\text{H}_{10}\text{ClO}_3$   $[\text{M}+\text{H}]^+$  285.0313; found 285.0313.

**4-(4-fluorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.8):** Yellow solid (117 mg, 58%); m.p. 144–



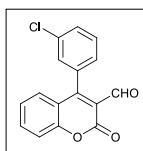
146 °C,  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  = 10.03 (s, 1H), 7.69 – 7.65 (m, 1H), 7.42 (d,  $J$  = 8.4 Hz, 1H), 7.31 – 7.19 (m, 6H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.36, 163.57 (d,  $J_{\text{C-F}}$  = 249.25 Hz), 159.55, 158.89, 154.66, 134.92, 130.55 (d,  $J_{\text{C-F}}$  = 8.33 Hz), 129.41, 127.81, 125.08, 120.00, 119.28, 117.42, 116.20 (d,  $J_{\text{C-F}}$  = 21.81 Hz). IR (neat,  $\text{cm}^{-1}$ ): 2867, 1752, 1725, 1604, 1548, 1223, 836, 760. APCI (m/z) calcd. for  $\text{C}_{16}\text{H}_{10}\text{FO}_3$   $[\text{M}+\text{H}]^+$  269.0608; found 269.0608.

**2-oxo-4-*m*-tolyl-2*H*-chromene-3-carbaldehyde (2.9):** Yellow solid (160 mg, 81%); m.p. 114-116 °C, <sup>1</sup>H



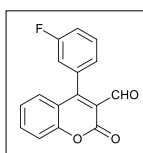
NMR (400 MHz, Chloroform-*d*)  $\delta$  = 9.91 (s, 1H), 7.68 – 7.64 (m, 1H), 7.41 (dq,  $J$  = 13.8, 7.7 Hz, 3H), 7.26 – 7.24 (m, 2H), 7.12 (s, 2H), 2.44 (s, 3H). <sup>13</sup>C NMR (101 MHz, Chloroform-*d*)  $\delta$  = 188.49, 162.05, 158.14, 154.65, 138.85, 134.88, 131.49, 130.82, 129.52, 129.15, 128.80, 125.80, 124.91, 119.92, 119.07, 117.29, 21.62. IR (neat, cm<sup>-1</sup>): 2861, 1755, 1721, 1604, 1548, 1364, 998, 758. APCI (m/z) calcd. for C<sub>17</sub>H<sub>13</sub>O<sub>3</sub> [M+H]<sup>+</sup> 265.0859; found 265.0857.

**4-(3-chlorophenyl)-2-oxo-2*H*-chromene-3-carbaldehyde (2.10):** Yellow solid (147 mg, 70%); m.p.



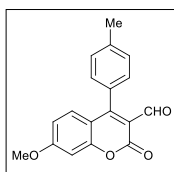
118-120 °C, <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  = 10.06 (d,  $J$  = 0.9 Hz, 1H), 7.70 – 7.66 (m, 1H), 7.55 – 7.48 (m, 2H), 7.42 (d,  $J$  = 8.4 Hz, 1H), 7.28 – 7.22 (m, 2H), 7.19 – 7.16 (m, 2H). <sup>13</sup>C NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.16, 158.93, 158.57, 154.65, 135.08, 135.04, 133.89, 130.23, 129.94, 129.42, 128.18, 126.52, 125.19, 119.71, 119.02, 117.40. IR (neat, cm<sup>-1</sup>): 2864, 1755, 1724, 1602, 1550, 1347, 1192, 758. APCI (m/z) calcd. for C<sub>16</sub>H<sub>10</sub>ClO<sub>3</sub> [M+H]<sup>+</sup> 285.0313; found 285.0313.

**4-(3-fluorophenyl)-2-oxo-2*H*-chromene-3-carbaldehyde (2.11):** Yellow solid (143 mg, 71%); m.p.



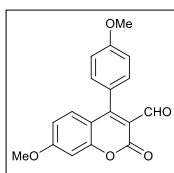
136-138 °C, <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  = 10.05 (s, 1H), 7.70 – 7.66 (m, 1H), 7.54 (td,  $J$  = 8.0, 5.8 Hz, 1H), 7.43 (d,  $J$  = 8.3 Hz, 1H), 7.29 – 7.24 (m, 2H), 7.19 (dd,  $J$  = 8.0, 1.5 Hz, 1H), 7.07 (d,  $J$  = 7.7 Hz, 1H), 7.02 (dt,  $J$  = 8.5, 1.8 Hz, 1H). <sup>13</sup>C NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.15, 162.77 (d,  $J_{C-F}$  = 247.68 Hz), 158.88, 158.76, 154.67, 135.02, 134.13 (d,  $J_{C-F}$  = 7.86 Hz), 130.81 (d,  $J_{C-F}$  = 8.31 Hz), 129.39, 125.16, 124.14, 124.12, 119.70, 119.04, 117.41, 116.86 (d,  $J_{C-F}$  = 20.68 Hz), 115.68 (d,  $J_{C-F}$  = 23.11 Hz). IR (neat, cm<sup>-1</sup>): 2888, 1728, 1703, 1606, 1586, 1347, 1149, 760. APCI (m/z) calcd. for C<sub>16</sub>H<sub>10</sub>FO<sub>3</sub> [M+H]<sup>+</sup> 269.0608; found 269.0608.

**7-methoxy-2-oxo-4-*p*-tolyl-2*H*-chromene-3-carbaldehyde (3.1):** Yellow solid (148 mg, 67%); m.p.



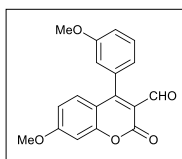
146-148 °C, <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  = 9.87 (d,  $J$  = 1.4 Hz, 1H), 7.34 (d,  $J$  = 7.8 Hz, 2H), 7.19 – 7.15 (m, 3H), 6.85 (s, 1H), 6.78 (dd,  $J$  = 9.0, 2.4 Hz, 1H), 3.91 (s, 3H), 2.46 (s, 3H). <sup>13</sup>C NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.47, 165.48, 162.43, 158.65, 157.01, 140.09, 130.84, 129.48, 129.00, 128.64, 116.10, 113.65, 113.51, 100.71, 56.22, 21.56. IR (neat, cm<sup>-1</sup>): 2924, 1755, 1725, 1614, 1584, 1370, 1287, 771. APCI (m/z) calcd. for C<sub>18</sub>H<sub>15</sub>O<sub>4</sub> [M+H]<sup>+</sup> 295.0965; found 295.0965.

**7-methoxy-4-(4-methoxyphenyl)-2-oxo-2*H*-chromene-3-carbaldehyde (3.2):** Yellow solid (196 mg,



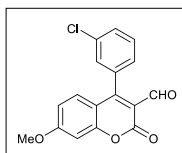
84%); m.p. 144-146 °C, <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  = 9.86 (d,  $J$  = 4.1 Hz, 1H), 7.26 – 7.20 (m, 3H), 7.07 – 7.05 (m, 2H), 6.85 (t,  $J$  = 2.8 Hz, 1H), 6.81 – 6.78 (m, 1H), 3.91 – 3.90 (m, 6H). <sup>13</sup>C NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.52, 165.42, 162.13, 160.97, 158.59, 156.99, 130.78, 130.52, 123.75, 116.15, 114.25, 113.59, 113.51, 100.74, 56.20, 55.55. IR (neat, cm<sup>-1</sup>): 2845, 1752, 1719, 1611, 1507, 1287, 1116, 836. APCI (m/z) calcd. for C<sub>18</sub>H<sub>15</sub>O<sub>5</sub> [M+H]<sup>+</sup> 311.0914; found 311.0913.

**7-methoxy-4-(3-methoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (3.3):** Yellow solid (150 mg,



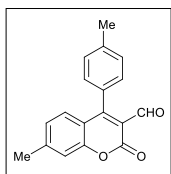
65%); m.p. 154-156 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 9.87 (s, 1H), 7.44 (t,  $J$  = 7.9 Hz, 1H), 7.14 (d,  $J$  = 9.0 Hz, 1H), 7.06 (dd,  $J$  = 8.4, 2.4 Hz, 1H), 6.87 – 6.84 (m, 2H), 6.81 – 6.80 (m, 1H), 6.78 (dd,  $J$  = 9.1, 2.4 Hz, 1H), 3.90 (s, 3H), 3.84 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.25, 165.59, 161.96, 159.78, 158.46, 157.01, 133.34, 130.79, 130.07, 120.80, 115.96, 115.15, 114.28, 113.73, 113.29, 100.71, 56.22, 55.53. IR (neat,  $\text{cm}^{-1}$ ): 2845, 1755, 1721, 1614, 1535, 1288, 1164, 770. APCI (m/z) calcd. for  $\text{C}_{18}\text{H}_{15}\text{O}_5$   $[\text{M}+\text{H}]^+$  311.0914; found 311.0919.

**4-(3-chlorophenyl)-7-methoxy-2-oxo-2H-chromene-3-carbaldehyde (3.4):** Yellow solid (145 mg,



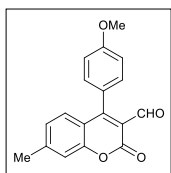
62%); m.p. 108-110 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 10.00 (s, 1H), 7.52 – 7.46 (m, 3H), 7.15 (d,  $J$  = 7.4 Hz, 1H), 7.05 (d,  $J$  = 8.9 Hz, 1H), 6.87 (d,  $J$  = 2.6 Hz, 1H), 6.80 (dd,  $J$  = 9.0, 2.4 Hz, 1H), 3.91 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.11, 165.69, 159.34, 159.20, 157.06, 134.98, 134.36, 130.74, 130.15, 129.77, 129.14, 128.11, 126.44, 115.79, 113.98, 113.20, 100.90, 56.29. IR (neat,  $\text{cm}^{-1}$ ): 2962, 1756, 1724, 1614, 1536, 1298, 1141, 741. APCI (m/z) calcd. for  $\text{C}_{17}\text{H}_{12}\text{ClO}_4$   $[\text{M}+\text{H}]^+$  315.0424; found 315.0423.

**7-methyl-2-oxo-4-*p*-tolyl-2H-chromene-3-carbaldehyde (3.5):** Yellow solid (156 mg, 75%); m.p. 136-



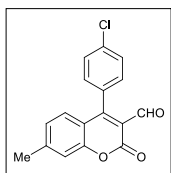
138 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 9.89 (s, 1H), 7.34 (d,  $J$  = 7.9 Hz, 2H), 7.18 (d,  $J$  = 7.9 Hz, 3H), 7.14 (d,  $J$  = 8.2 Hz, 1H), 7.03 (d,  $J$  = 7.2 Hz, 1H), 2.46 (s, 6H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.53, 162.05, 158.50, 154.77, 146.91, 140.15, 129.47, 129.21, 128.69, 126.19, 118.09, 117.57, 117.33, 22.06, 21.55. IR (neat,  $\text{cm}^{-1}$ ): 2861, 1755, 1722, 1619, 1538, 1369, 1262, 1137, 773. APCI (m/z) calcd. for  $\text{C}_{18}\text{H}_{15}\text{O}_3$   $[\text{M}+\text{H}]^+$  279.1016; found 279.1017.

**4-(4-methoxyphenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.6):** Yellow solid (171 mg,



77%); m.p. 140-142 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 9.88 (s, 1H), 7.24 (d,  $J$  = 8.6 Hz, 2H), 7.20 (d,  $J$  = 8.5 Hz, 2H), 7.06 – 7.04 (m, 3H), 3.89 (s, 3H), 2.47 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.62, 161.73, 161.03, 158.50, 154.79, 146.84, 130.61, 129.17, 126.18, 123.52, 118.18, 117.62, 117.39, 114.27, 55.56, 22.05. IR (neat,  $\text{cm}^{-1}$ ): 2841, 1753, 1719, 1608, 1509, 1370, 1252, 1178, 631. APCI (m/z) calcd. for  $\text{C}_{18}\text{H}_{15}\text{O}_4$   $[\text{M}+\text{H}]^+$  295.0965; found 295.0965.

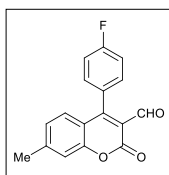
**4-(4-chlorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.7):** Yellow solid (147 mg,



66%); m.p. 158-160 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 10.03 (s, 1H), 7.53 – 7.50 (m, 2H), 7.23 – 7.20 (m, 3H), 7.05 (s, 2H), 2.48 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.37, 159.39, 159.25, 154.77, 147.23, 135.94, 130.65, 129.74, 129.11, 126.46, 117.93, 117.49, 117.41, 22.11. IR (neat,  $\text{cm}^{-1}$ ): 2862, 1755, 1724, 1620, 1537, 1369, 1261, 1091, 736.

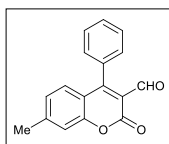
APCI (m/z) calcd. for  $\text{C}_{17}\text{H}_{12}\text{ClO}_3$   $[\text{M}+\text{H}]^+$  299.0469; found 299.0469.

**4-(4-fluorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.8):** Yellow solid (145 mg,



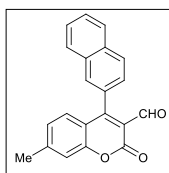
69%); m.p. 124-126 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 10.00 (s, 1H), 7.28 – 7.21 (m, 5H), 7.08 – 7.04 (m, 2H), 2.47 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.42, 163.46 (d,  $J_{\text{C-F}}$  = 248.75 Hz), 159.86, 159.11, 154.76, 147.17, 130.49 (d,  $J_{\text{C-F}}$  = 8.31 Hz), 129.13, 127.98 (d,  $J_{\text{C-F}}$  = 3.03 Hz), 126.42, 118.14, 117.57, 117.46, 116.09 (d,  $J_{\text{C-F}}$  = 21.76 Hz), 22.09. IR (neat,  $\text{cm}^{-1}$ ): 2856, 1753, 1720, 1619, 1537, 1369, 1230, 1015, 673. APCI (m/z) calcd. for  $\text{C}_{17}\text{H}_{12}\text{FO}_3$   $[\text{M}+\text{H}]^+$  283.0765; found 283.0765.

**7-methyl-2-oxo-4-phenyl-2H-chromene-3-carbaldehyde (3.9):** Yellow solid (136 mg, 69%); m.p. 146-



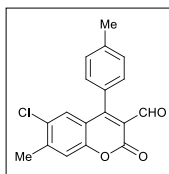
148 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 9.93 (s, 1H), 7.56 – 7.53 (m, 3H), 7.29 (dd,  $J$  = 6.6, 2.8 Hz, 2H), 7.21 (s, 1H), 7.09 (d,  $J$  = 8.2 Hz, 1H), 7.04 (d,  $J$  = 8.4 Hz, 1H), 2.48 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.45, 161.52, 158.69, 154.85, 147.03, 132.00, 129.85, 129.25, 128.82, 128.55, 126.30, 118.11, 117.59, 117.42, 22.11. IR (neat,  $\text{cm}^{-1}$ ): 2859, 1754, 1722, 1618, 1537, 1370, 1261, 1076, 755. APCI (m/z) calcd. for  $\text{C}_{17}\text{H}_{13}\text{O}_3$   $[\text{M}+\text{H}]^+$  265.0859; found 265.0858.

**7-methyl-4-(naphthalen-2-yl)-2-oxo-2H-chromene-3-carbaldehyde (3.10):** Yellow solid (168 mg,



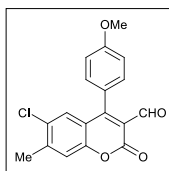
71%); m.p. 148-150 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 9.97 (s, 1H), 8.01 (d,  $J$  = 8.4 Hz, 1H), 7.96 (d,  $J$  = 7.4 Hz, 1H), 7.89 – 7.87 (m, 1H), 7.78 (s, 1H), 7.63 – 7.58 (m, 2H), 7.38 (dd,  $J$  = 8.4, 1.6 Hz, 1H), 7.24 (s, 1H), 7.12 (d,  $J$  = 8.2 Hz, 1H), 7.02 (d,  $J$  = 8.3 Hz, 1H), 2.48 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.40, 161.47, 158.73, 154.84, 147.03, 133.58, 132.74, 129.39, 128.65, 128.41, 128.36, 128.13, 127.60, 127.35, 126.32, 125.75, 118.31, 117.68, 117.43, 22.10. IR (neat,  $\text{cm}^{-1}$ ): 2861, 1753, 1721, 1620, 1537, 1384, 1263, 1045, 749. APCI (m/z) calcd. for  $\text{C}_{21}\text{H}_{15}\text{O}_3$   $[\text{M}+\text{H}]^+$  315.1016; found 315.1016.

**6-chloro-7-methyl-2-oxo-4-*p*-tolyl-2H-chromene-3-carbaldehyde (3.11):** Yellow solid (176 mg,



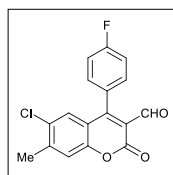
75%); m.p. 180-182 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 9.89 (s, 1H), 7.37 (d,  $J$  = 7.9 Hz, 2H), 7.28 (s, 1H), 7.21 (s, 1H), 7.18 (d,  $J$  = 8.0 Hz, 2H), 2.48 (s, 6H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.21, 160.61, 158.02, 152.93, 144.35, 140.61, 131.05, 129.75, 128.72, 128.65, 128.11, 119.19, 119.12, 118.97, 21.62, 21.01. IR (neat,  $\text{cm}^{-1}$ ): 2854, 1760, 1726, 1612, 1537, 1366, 1160, 919, 730. APCI (m/z) calcd. for  $\text{C}_{18}\text{H}_{14}\text{ClO}_3$   $[\text{M}+\text{H}]^+$  313.0626; found 313.0626.

**6-chloro-4-(4-methoxyphenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.12):** Yellow solid



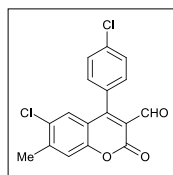
(175 mg, 71%); m.p. 178-180 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 9.89 (s, 1H), 7.28 (s, 1H), 7.26 – 7.23 (m, 3H), 7.10 – 7.07 (m, 2H), 3.91 (s, 3H), 2.48 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.29, 161.32, 160.28, 158.02, 152.95, 144.29, 131.03, 130.59, 128.69, 122.89, 119.24, 119.17, 119.04, 114.56, 55.61, 20.99. IR (neat,  $\text{cm}^{-1}$ ): 2841, 1758, 1723, 1607, 1533, 1366, 1253, 1021, 890. APCI (m/z) calcd. for  $\text{C}_{18}\text{H}_{14}\text{ClO}_4$   $[\text{M}+\text{H}]^+$  329.0575; found 329.0575.

**6-chloro-4-(4-fluorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.13):** Yellow solid



(155 mg, 65%); m.p. 184-186 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 10.00 (s, 1H), 7.30 (s, 1H), 7.27 (s, 2H), 7.26 (s, 2H), 7.12 (s, 1H), 2.49 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.08, 163.66 (d,  $J_{\text{C-F}}$  = 249.45 Hz), 158.61, 158.43, 152.89, 144.62, 131.27, 130.48 (d,  $J_{\text{C-F}}$  = 8.34 Hz), 128.62, 127.33 (d,  $J_{\text{C-F}}$  = 3.36 Hz), 119.30, 119.07, 119.04, 116.40 (d,  $J_{\text{C-F}}$  = 22.11 Hz), 21.04. IR (neat,  $\text{cm}^{-1}$ ): 2859, 1758, 1726, 1605, 1536, 1365, 1160, 1021, 889. APCI (m/z) calcd. for  $\text{C}_{17}\text{H}_{11}\text{ClFO}_3$   $[\text{M}+\text{H}]^+$  317.0375; found 317.0378.

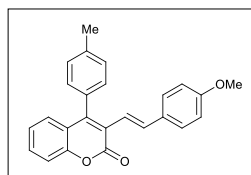
**6-chloro-4-(4-chlorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.14):** Yellow



solid (151 mg, 60%); m.p. 138-140 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 10.03 (s, 1H), 7.56 – 7.53 (m, 2H), 7.30 (s, 1H), 7.22 – 7.20 (m, 2H), 7.10 (s, 1H), 2.49 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 188.03, 158.71, 158.00, 152.88, 144.69, 136.36, 131.32, 129.96, 129.69, 129.38, 128.58, 119.30, 118.89, 118.83, 21.04. IR (neat,  $\text{cm}^{-1}$ ):

2863, 1759, 1727, 1613, 1534, 1366, 1160, 1015, 889. APCI (m/z) calcd. for  $\text{C}_{17}\text{H}_{11}\text{Cl}_2\text{O}_3$   $[\text{M}+\text{H}]^+$  333.0080; found 333.0084.

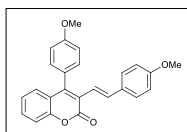
**(E)-3-(4-methoxystyryl)-4-*p*-tolyl-2H-chromen-2-one (4.1):** Yellow solid (154 mg, 56%); m.p. 146-148



°C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 7.92 (d,  $J$  = 16.2 Hz, 1H), 7.45 (td,  $J$  = 7.8, 7.2, 1.5 Hz, 1H), 7.37 (dd,  $J$  = 8.0, 2.4 Hz, 3H), 7.21 (dd,  $J$  = 12.0, 8.3 Hz, 4H), 7.15 – 7.11 (m, 1H), 7.08 (dd,  $J$  = 8.0, 1.5 Hz, 1H), 6.80 (d,  $J$  = 8.7 Hz, 2H), 6.61 (d,  $J$  = 16.2 Hz, 1H), 3.78 (s, 3H), 2.50 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  =

160.20, 159.77, 152.20, 149.77, 138.81, 135.19, 131.83, 130.82, 130.71, 129.67, 129.18, 128.30, 127.53, 124.12, 121.78, 121.27, 119.99, 116.46, 114.14, 55.40, 21.59. IR (neat,  $\text{cm}^{-1}$ ): 2834, 1723, 1605, 1511, 1249, 1074, 755. APCI (m/z) calcd. for  $\text{C}_{25}\text{H}_{21}\text{O}_3$   $[\text{M}+\text{H}]^+$  369.1485; found 369.1481.

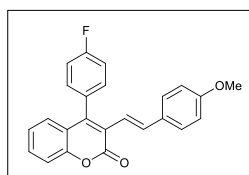
**(E)-4-(4-methoxyphenyl)-3-(4-methoxystyryl)-2H-chromen-2-one (4.2):** Yellow solid (150 mg,



52%); m.p. 122-124 °C,  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  = 7.93 (d,  $J$  = 16.2 Hz, 1H), 7.49 – 7.43 (m, 1H), 7.37 (d,  $J$  = 8.3 Hz, 1H), 7.24 (dd,  $J$  = 8.7, 2.4 Hz, 4H), 7.17 – 7.06 (m, 4H), 6.81 (d,  $J$  = 8.7 Hz, 2H), 6.63 (d,  $J$  = 16.2 Hz, 1H), 3.93 (s, 3H), 3.79 (s, 3H).  $^{13}\text{C}$

NMR (101 MHz, Chloroform-*d*)  $\delta$  = 160.21, 159.99, 159.78, 152.21, 149.47, 135.17, 130.83, 130.73, 128.30, 127.50, 126.89, 124.14, 121.96, 121.38, 120.01, 116.50, 114.40, 114.17, 55.54, 55.41. IR (neat,  $\text{cm}^{-1}$ ): 2926, 1722, 1605, 1511, 1249, 1174, 1074, 755. APCI (m/z) calcd. for  $\text{C}_{25}\text{H}_{21}\text{O}_4$   $[\text{M}+\text{H}]^+$  385.1434; found 385.1433.

**(E)-4-(4-fluorophenyl)-3-(4-methoxystyryl)-2H-chromen-2-one (4.3):** Yellow solid (106 mg, 38%);

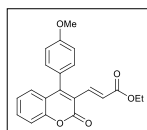


m.p. 118-120 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  = 7.92 (d,  $J$  = 16.2 Hz, 1H), 7.47 (td,  $J$  = 8.0, 7.5, 1.5 Hz, 1H), 7.38 – 7.36 (m, 1H), 7.30 (dd,  $J$  = 6.9, 4.7 Hz, 4H), 7.21 (d,  $J$  = 8.7 Hz, 2H), 7.17 – 7.14 (m, 1H), 7.02 (dd,  $J$  = 8.0, 1.1 Hz, 1H), 6.81 (d,  $J$  = 8.8 Hz, 2H), 6.53 (d,  $J$  = 16.2 Hz, 1H), 3.79 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, Chloroform-*d*)  $\delta$  = 162.96 (d,  $J_{\text{C-F}}$  = 247.68 Hz), 159.95, 152.15, 148.26,

135.79, 131.21 (d,  $J_{\text{C-F}}$  = 8.10 Hz), 131.02, 130.81, 130.42, 128.32, 127.14, 124.29, 122.24, 121.04, 119.43,

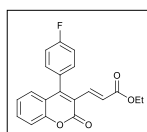
116.59, 116.30 (d,  $J_{\text{C-F}} = 21.53$  Hz), 114.22, 55.41. IR (neat,  $\text{cm}^{-1}$ ): 2836, 1724, 1604, 1511, 1249, 1075, 755. APCI (m/z) calcd. for  $\text{C}_{24}\text{H}_{18}\text{FO}_3$   $[\text{M}+\text{H}]^+$  373.1234; found 373.1234.

**(E)-ethyl 3-(4-(4-methoxyphenyl)-2-oxo-2H-chromen-3-yl)acrylate (4.4):** White solid (121 mg,



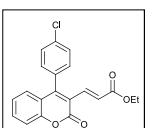
46%); m.p. 146-148 °C,  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta = 7.57$  (ddd,  $J = 8.5, 5.8, 2.9$  Hz, 1H), 7.42 – 7.36 (m, 1H), 7.34 – 7.28 (m, 2H), 7.25 – 7.17 (m, 4H), 7.12 – 7.07 (m, 2H), 4.19 (q,  $J = 7.1$  Hz, 2H), 3.93 (s, 3H), 1.28 (t,  $J = 7.2$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta = 167.65, 160.59, 159.38, 155.97, 153.05, 136.86, 132.69, 130.62, 128.57, 125.42, 124.45, 120.62, 119.49, 116.82, 114.52, 60.57, 55.52, 14.34$ . IR (neat,  $\text{cm}^{-1}$ ): 2923, 1726, 1634, 1510, 1277, 1170, 750. APCI (m/z) calcd. for  $\text{C}_{21}\text{H}_{19}\text{O}_5$   $[\text{M}+\text{H}]^+$  351.1227; found 351.1229.

**(E)-ethyl 3-(4-(4-fluorophenyl)-2-oxo-2H-chromen-3-yl)acrylate (4.5):** White solid (102 mg, 40%);



m.p. 140-142 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta = 7.60$  (ddd,  $J = 8.5, 7.3, 1.5$  Hz, 1H), 7.42 (d,  $J = 8.9$  Hz, 1H), 7.33 – 7.27 (m, 6H), 7.24 – 7.20 (m, 1H), 7.11 (dd,  $J = 8.1, 1.4$  Hz, 1H), 4.19 (q,  $J = 7.1$  Hz, 2H), 1.29 (t,  $J = 7.1$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta = 167.44, 163.39$  (d,  $J_{\text{C-F}} = 248.72$  Hz), 159.10, 154.80, 153.02, 136.16, 132.95, 131.04 (d,  $J_{\text{C-F}} = 8.15$  Hz), 129.40 (d,  $J_{\text{C-F}} = 3.26$  Hz), 128.23, 125.31, 124.65, 120.34, 119.88, 116.95, 116.48 (d,  $J_{\text{C-F}} = 21.78$  Hz), 60.70, 14.33. IR (neat,  $\text{cm}^{-1}$ ): 2985, 1729, 1706, 1604, 1508, 1278, 1187, 762. APCI (m/z) calcd. for  $\text{C}_{20}\text{H}_{16}\text{FO}_4$   $[\text{M}+\text{H}]^+$  339.1027; found 339.1022.

**(E)-ethyl 3-(4-(4-chlorophenyl)-2-oxo-2H-chromen-3-yl)acrylate (4.6):** White solid (120 mg, 45%);

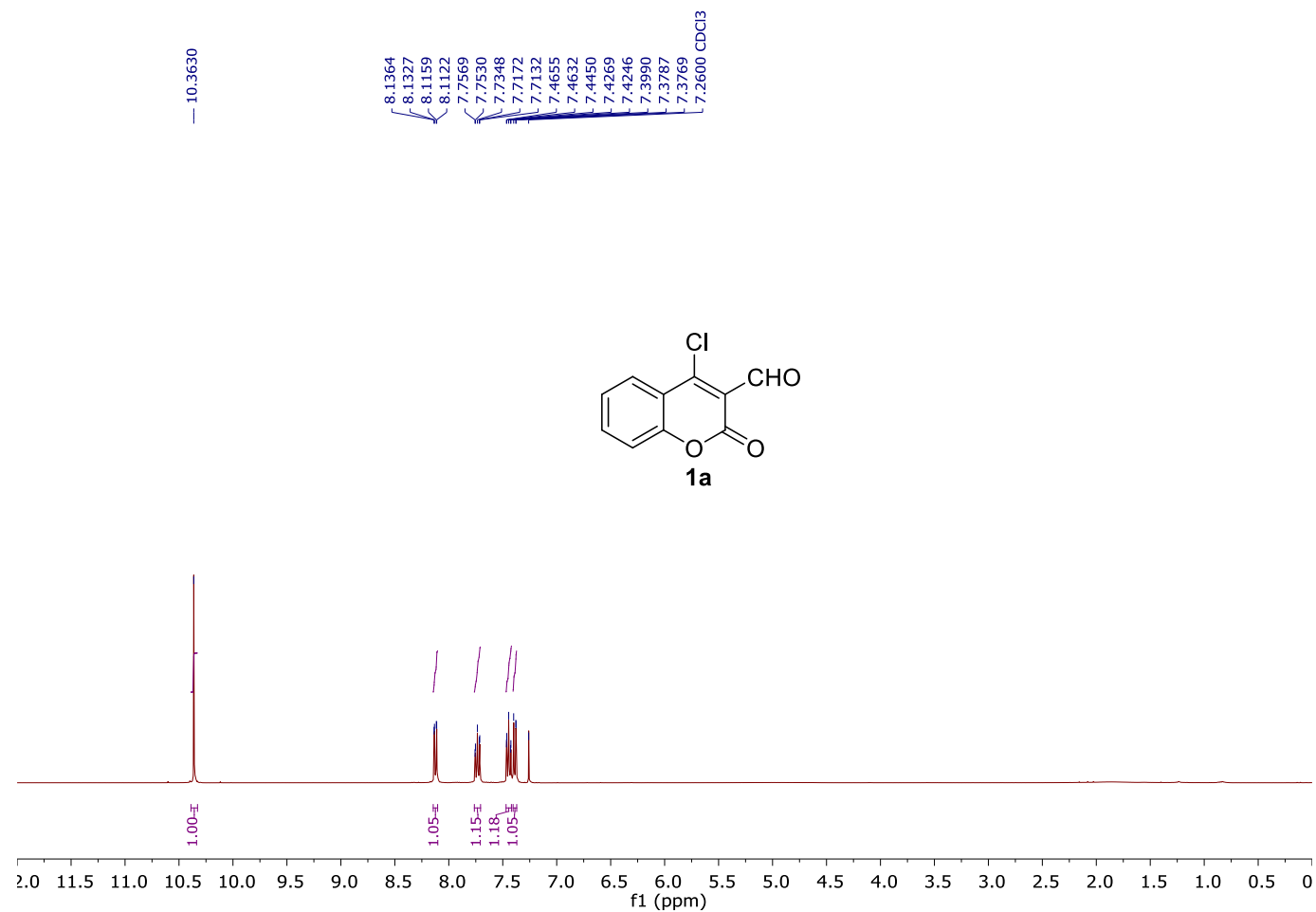


m.p. 138-140 °C,  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta = 7.59 - 7.54$  (m, 3H), 7.41 – 7.38 (m, 1H), 7.31 – 7.26 (m, 2H), 7.24 – 7.17 (m, 3H), 7.08 (dd,  $J = 8.1, 1.4$  Hz, 1H), 4.17 (q,  $J = 7.1$  Hz, 2H), 1.27 (t,  $J = 7.1$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz, Chloroform-*d*)  $\delta = 167.44, 159.01, 154.54, 153.03, 136.03, 133.02, 131.87, 130.44, 129.57, 128.17, 125.46, 124.69, 120.13, 119.75, 116.99, 60.74, 14.35$ . IR (neat,  $\text{cm}^{-1}$ ): 2980, 1724, 1643, 1496, 1276, 1189, 758. APCI (m/z) calcd. for  $\text{C}_{20}\text{H}_{16}\text{ClO}_4$   $[\text{M}+\text{H}]^+$  355.0737; found 355.0743.

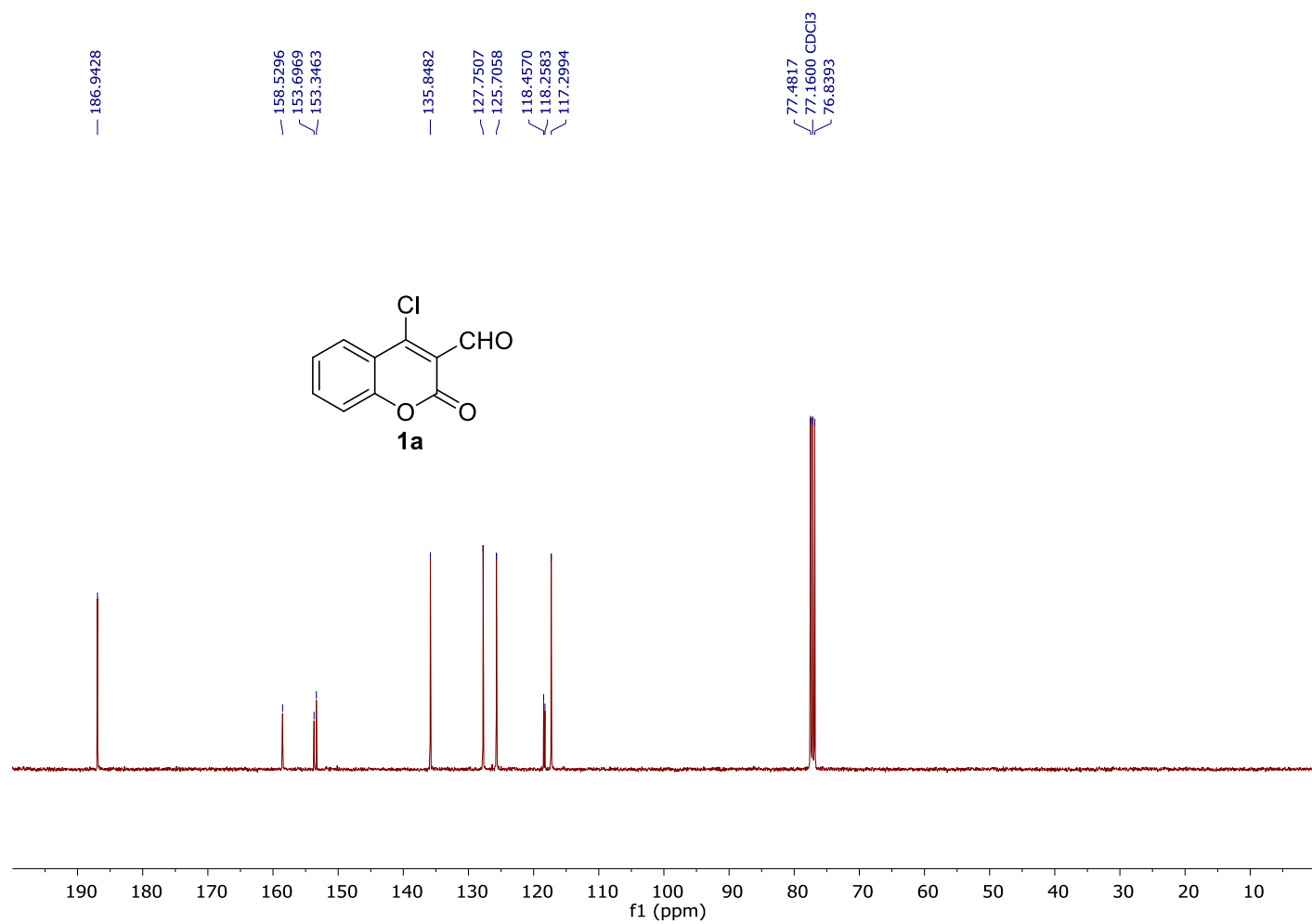
## References:

- (1) J. Liu, Y.Q. Sun, Y. Huo, H. Zhang, L. Wang, P. Zhang, D. Song, Y. Shi and W. Guo, *J. Am. Chem. Soc.*, 2014, **136**, 574-577.
- (2) U. R. Saeed, H. C. Zahid, G. Farzana and T. S. Claudius, *J. Enzyme Inhib. Med. Chem.* 2005, **20**, 333.

**$^1\text{H}$ ,  $^{13}\text{C}$  NMR, HRMS spectra:**

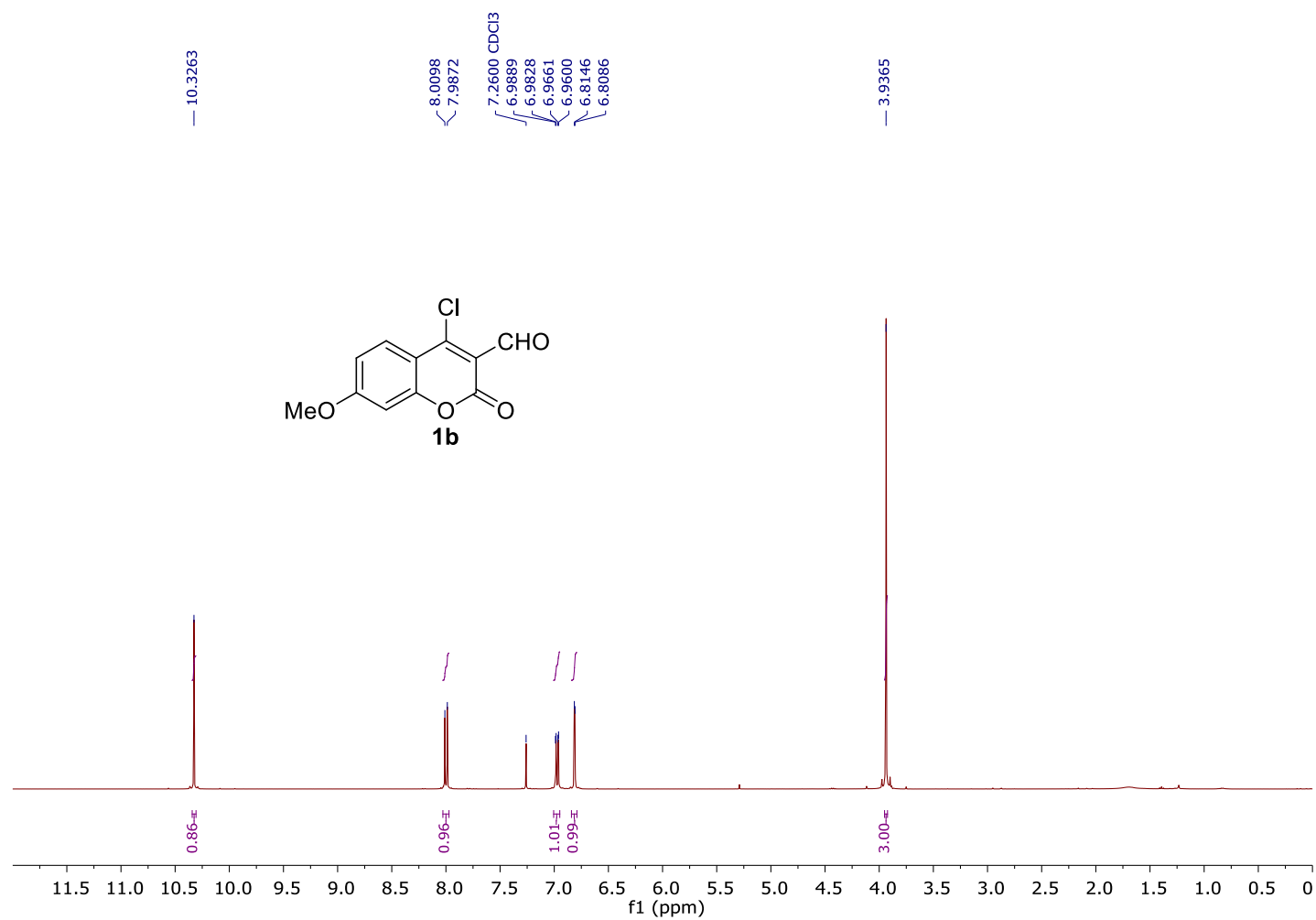


**$^1\text{H}$  Spectrum of 4-chloro-2-oxo-2H-chromene-3-carbaldehyde (1a)**

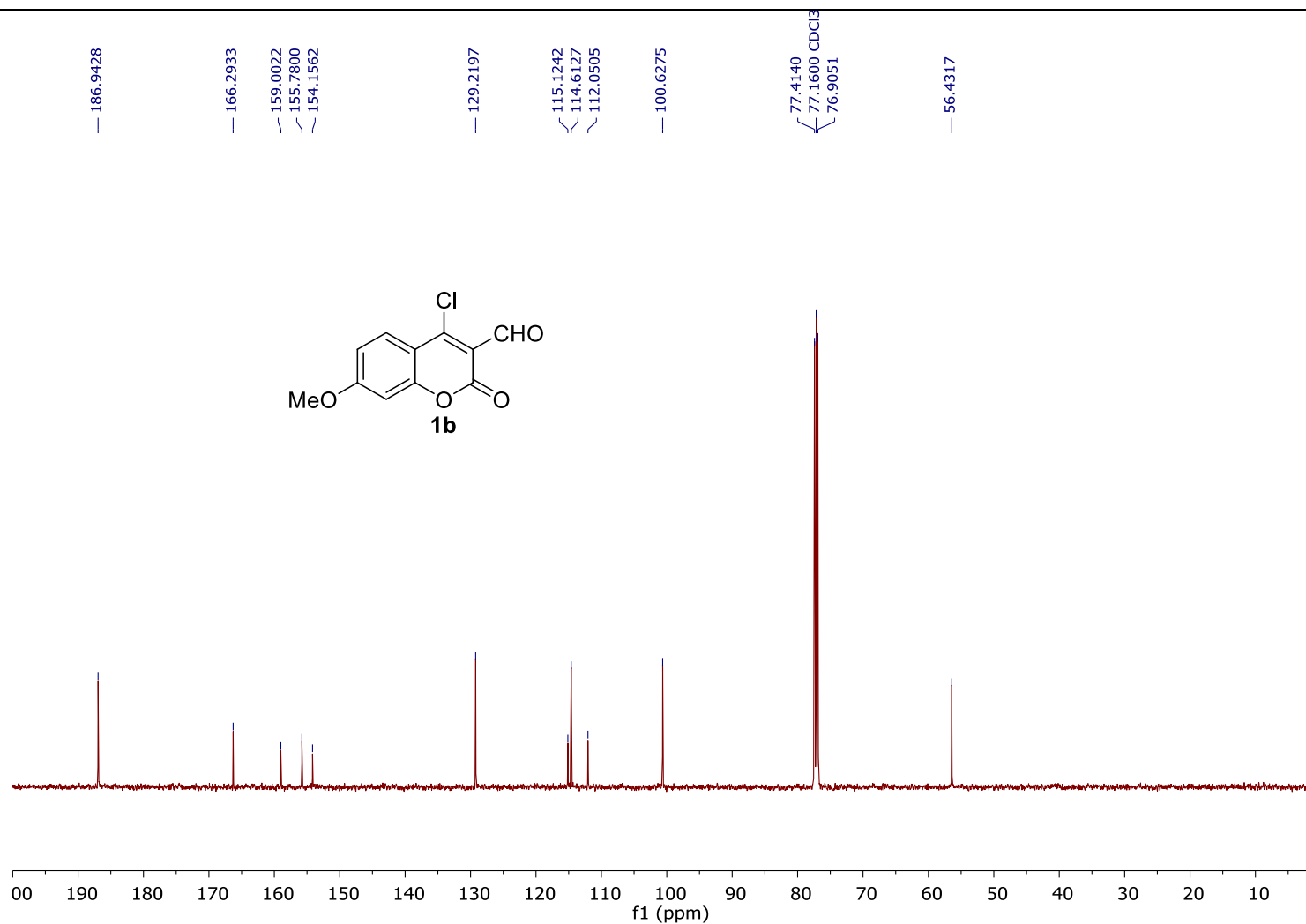


<sup>13</sup>C Spectrum of 4-chloro-2-oxo-2H-chromene-3-carbaldehyde (1a)

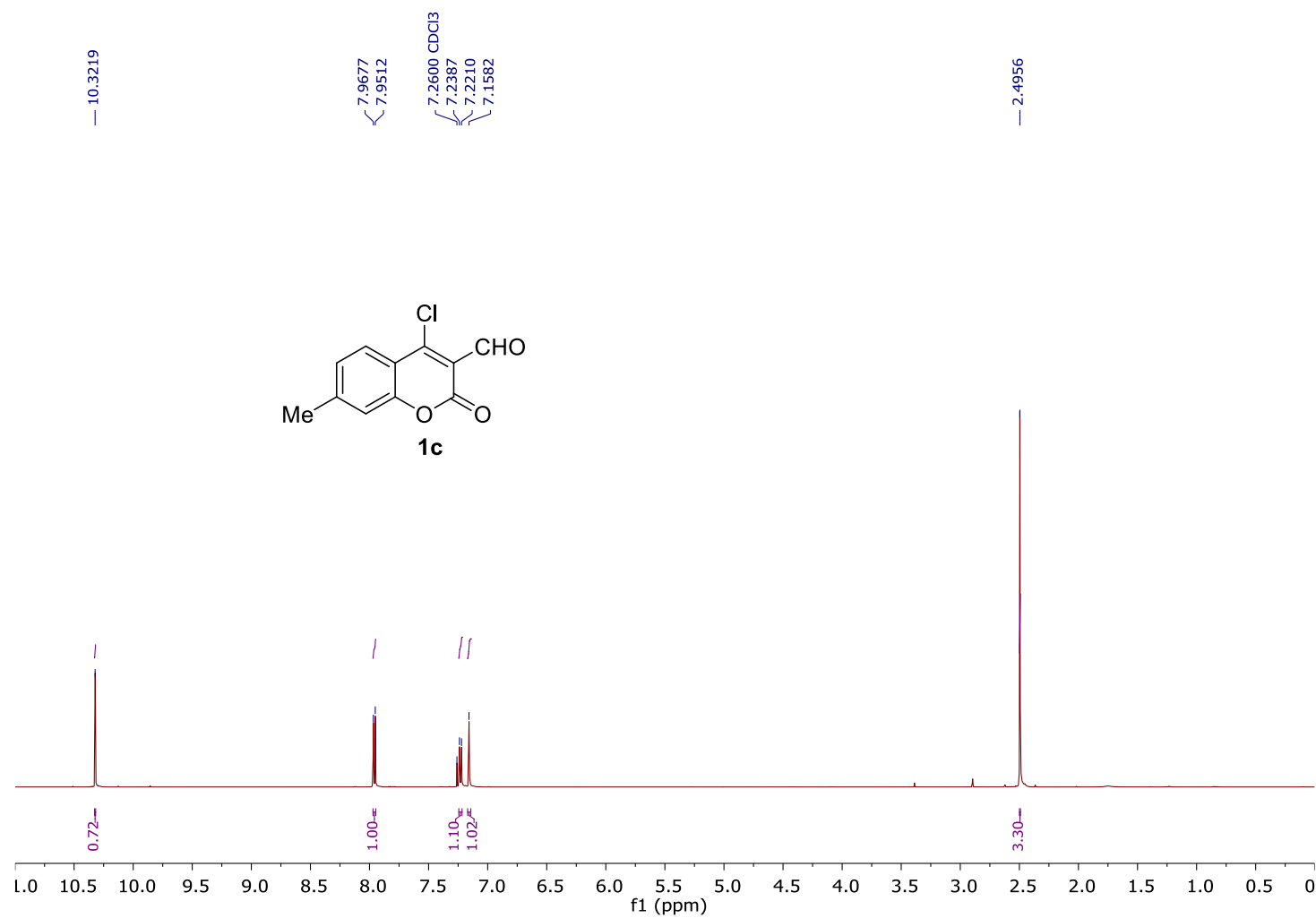




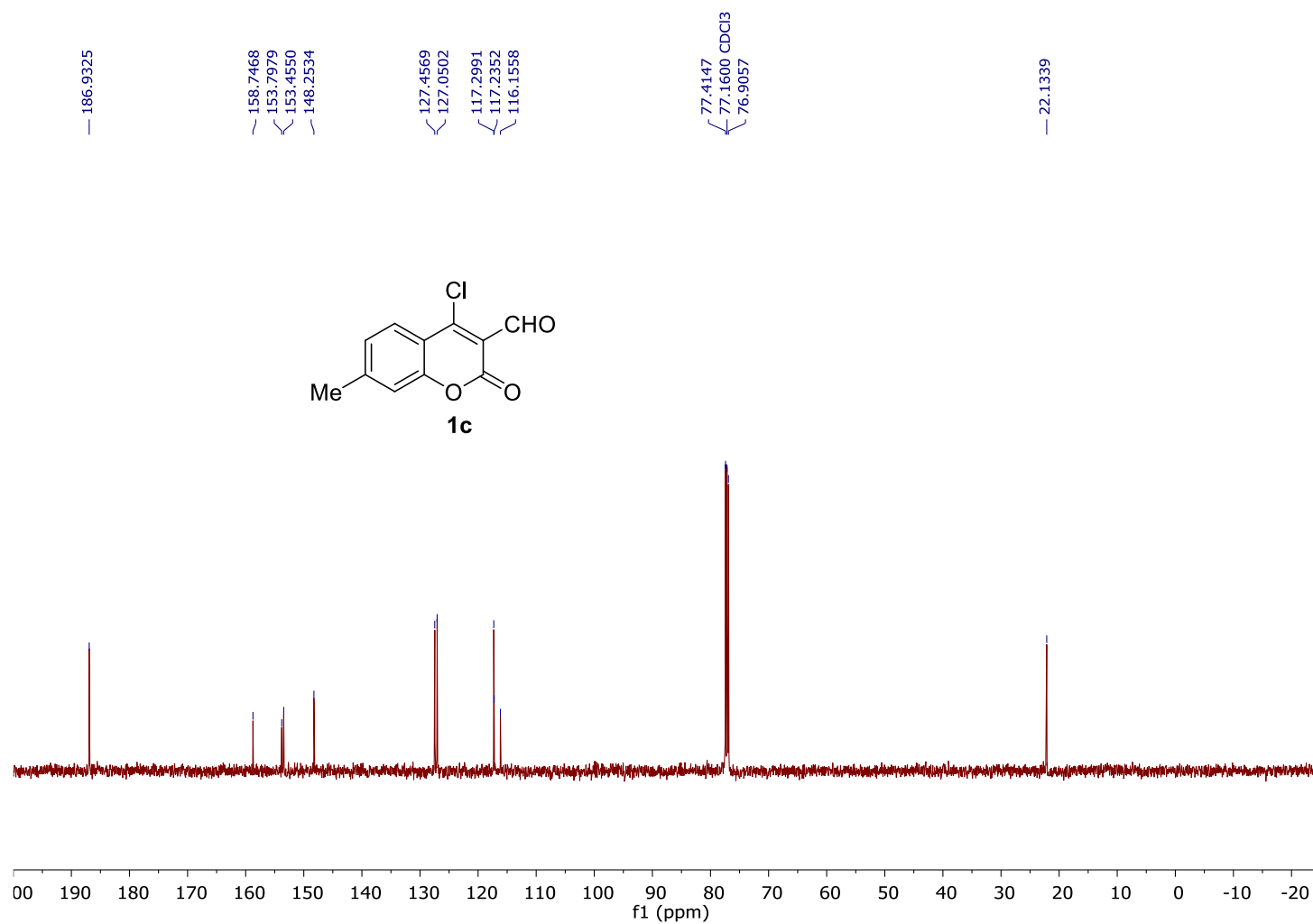
**<sup>1</sup>H Spectrum of 4-chloro-7-methoxy-2-oxo-2H-chromene-3-carbaldehyde (1b)**

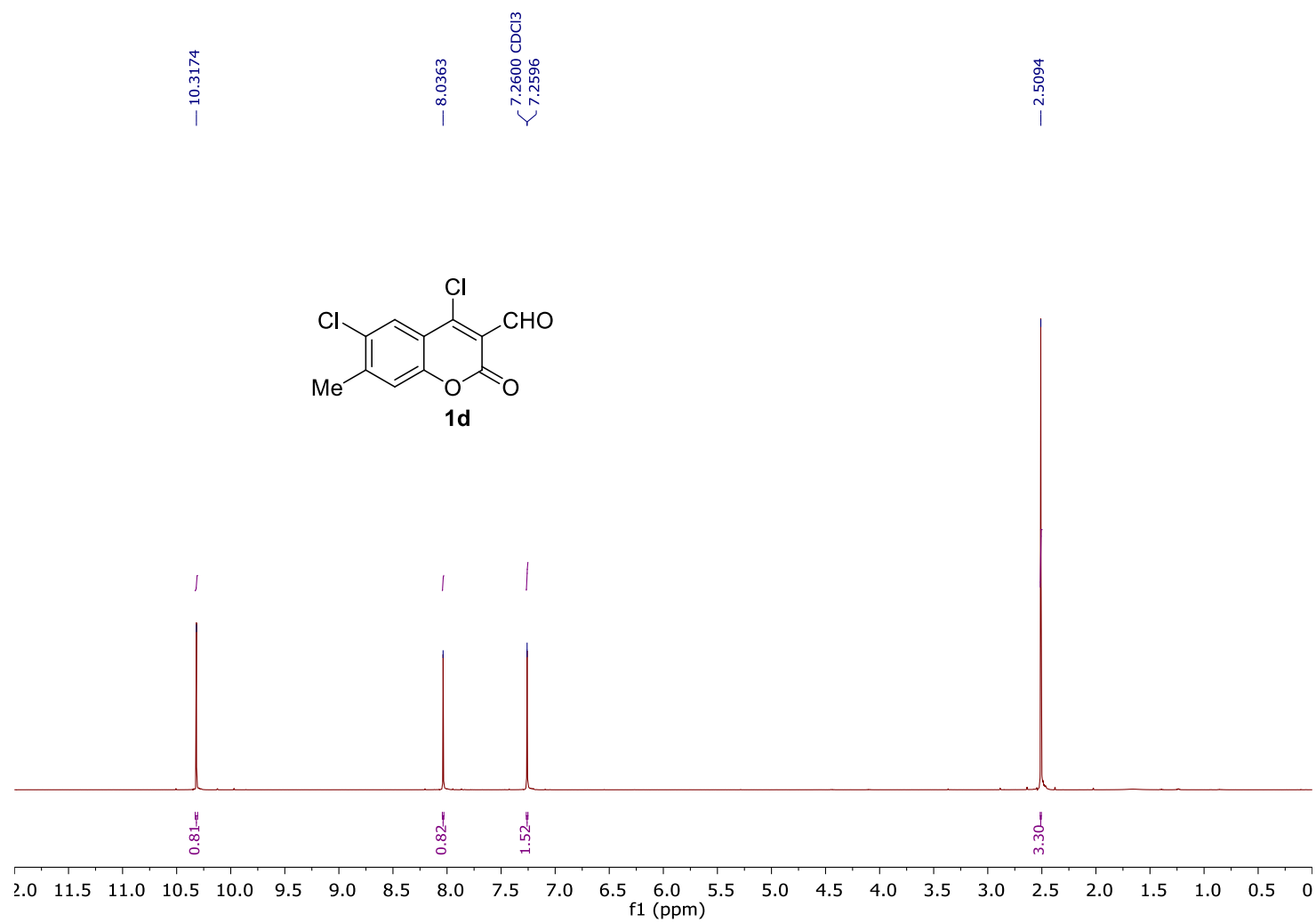


<sup>13</sup>C Spectrum of 4-chloro-7-methoxy-2-oxo-2H-chromene-3-carbaldehyde (**1b**)

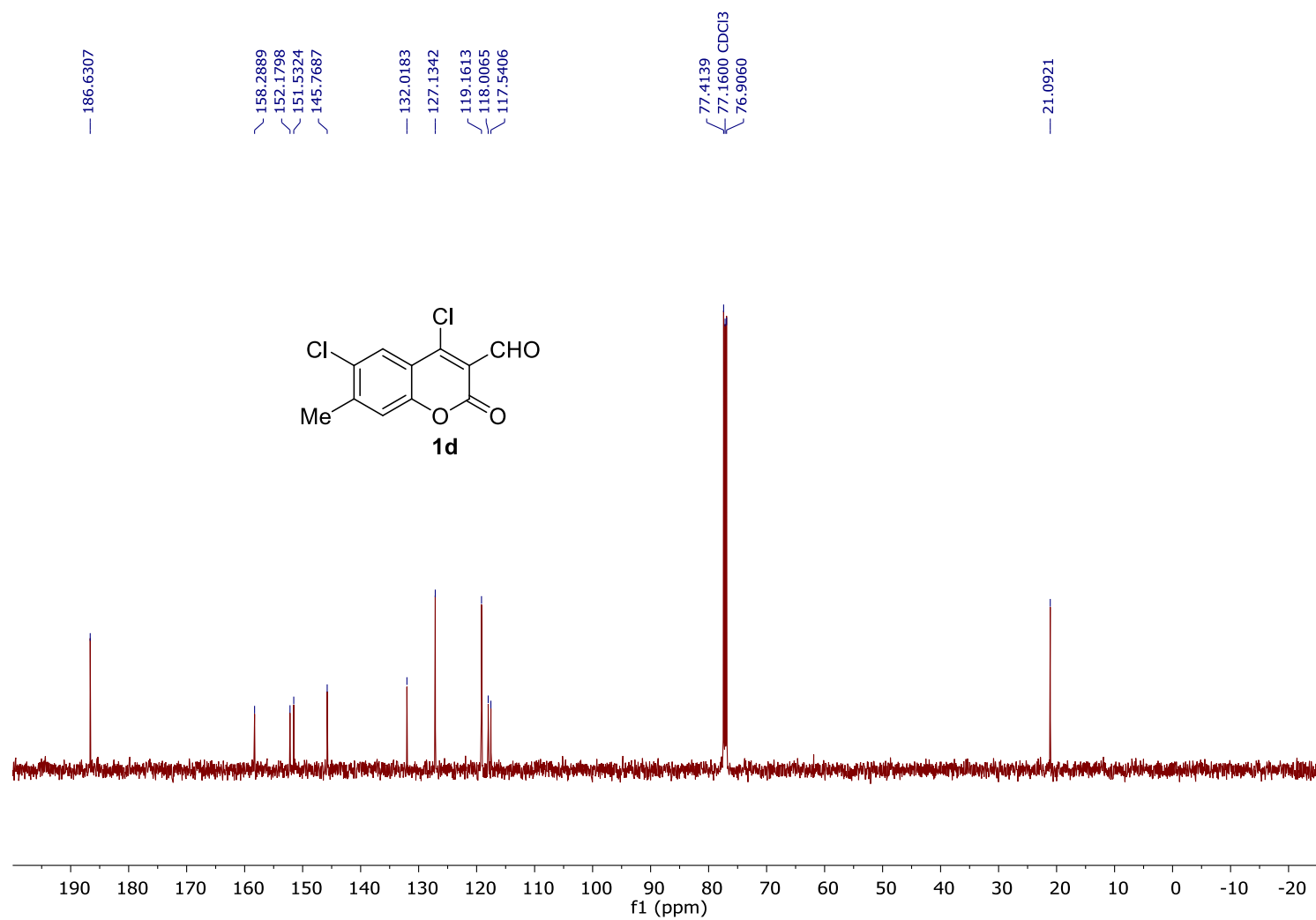


**<sup>1</sup>H Spectrum of 4-chloro-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (1c)**

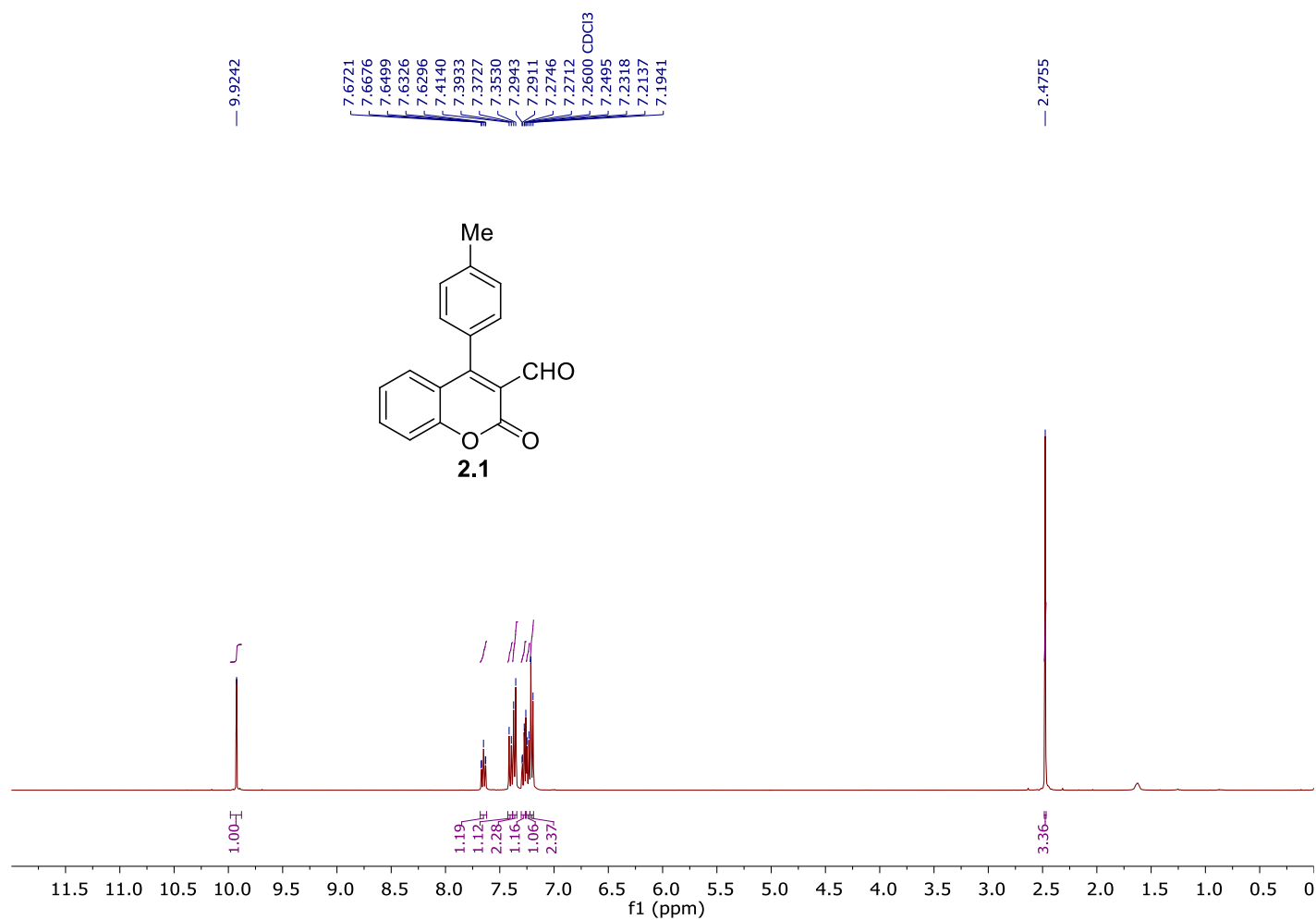




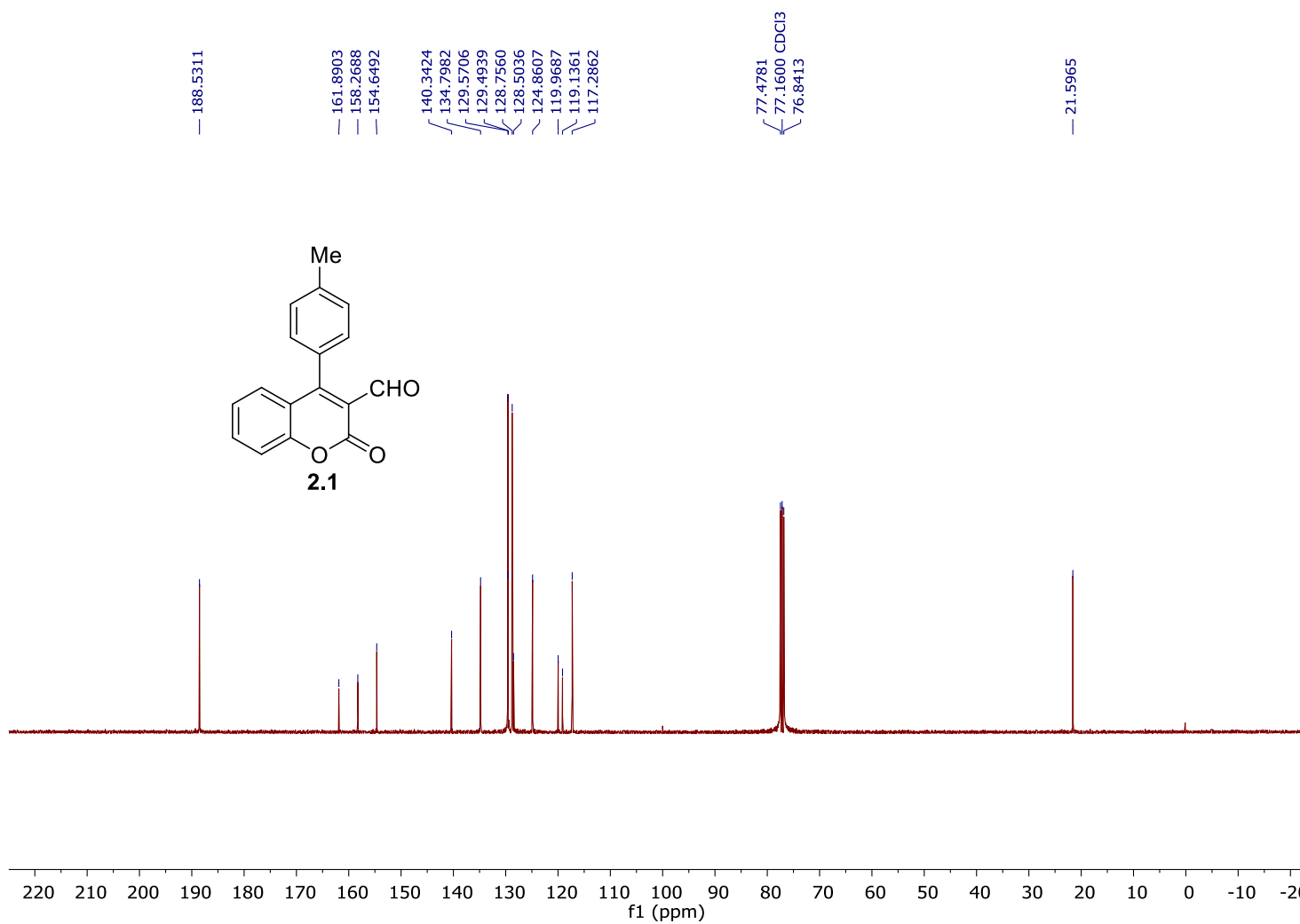
**<sup>1</sup>H Spectrum of 4,6-dichloro-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (1d)**



<sup>13</sup>C Spectrum of 4,6-dichloro-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (**1d**)

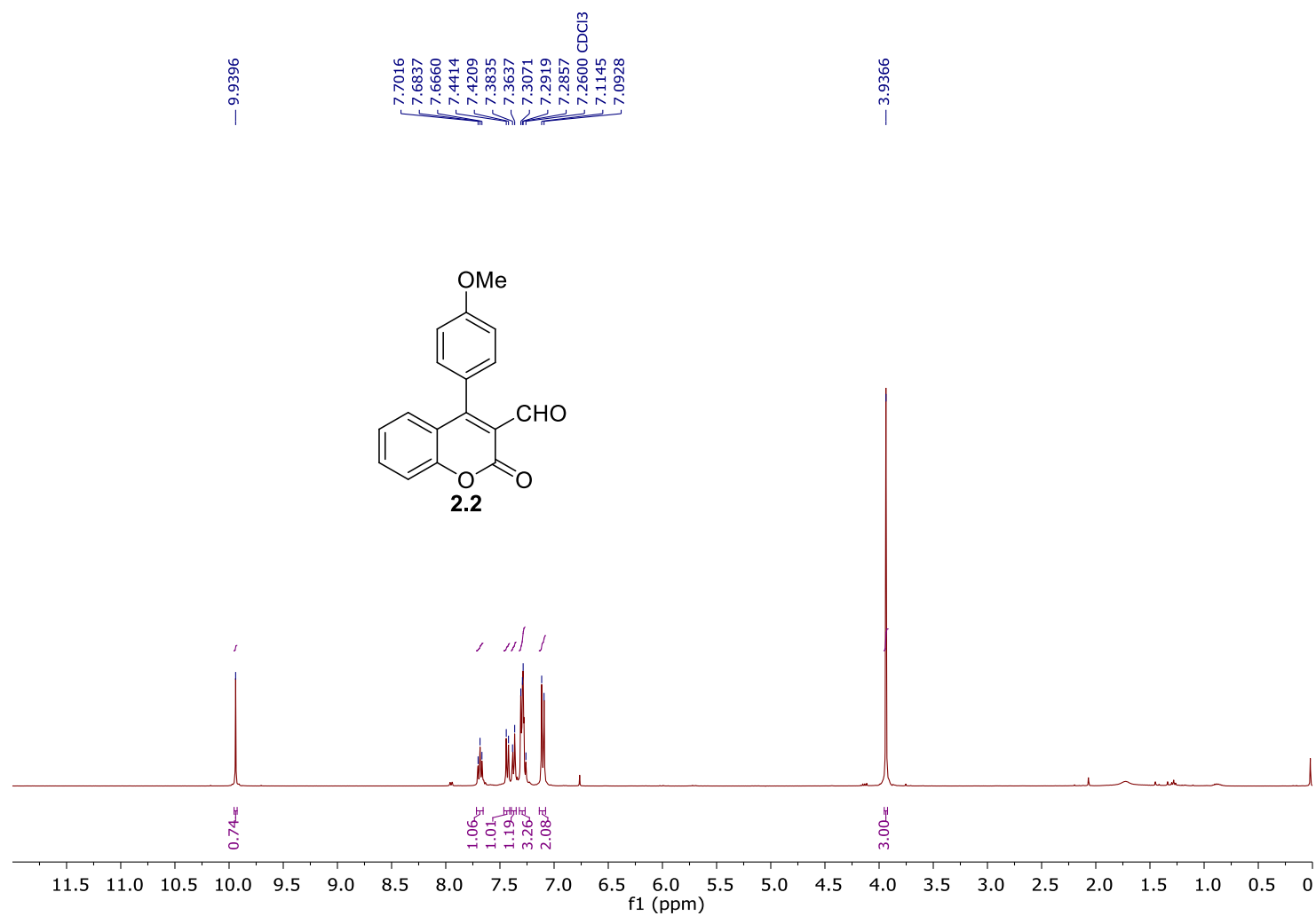


<sup>1</sup>H Spectrum of 2-oxo-4-*p*-tolyl-2*H*-chromene-3-carbaldehyde (2.1)

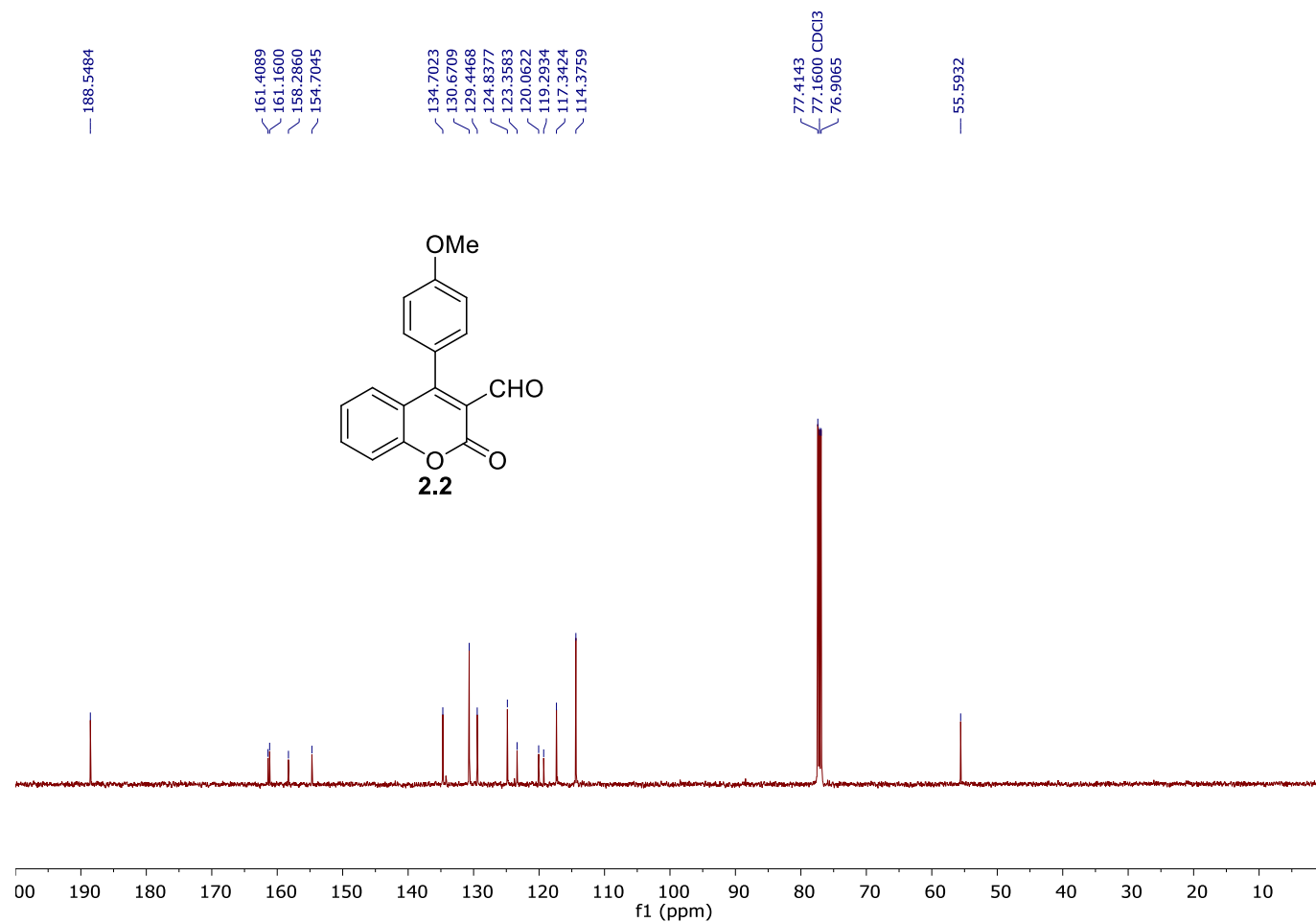


**<sup>13</sup>C Spectrum 2-oxo-4-*p*-tolyl-2*H*-chromene-3-carbaldehyde (2.1)**

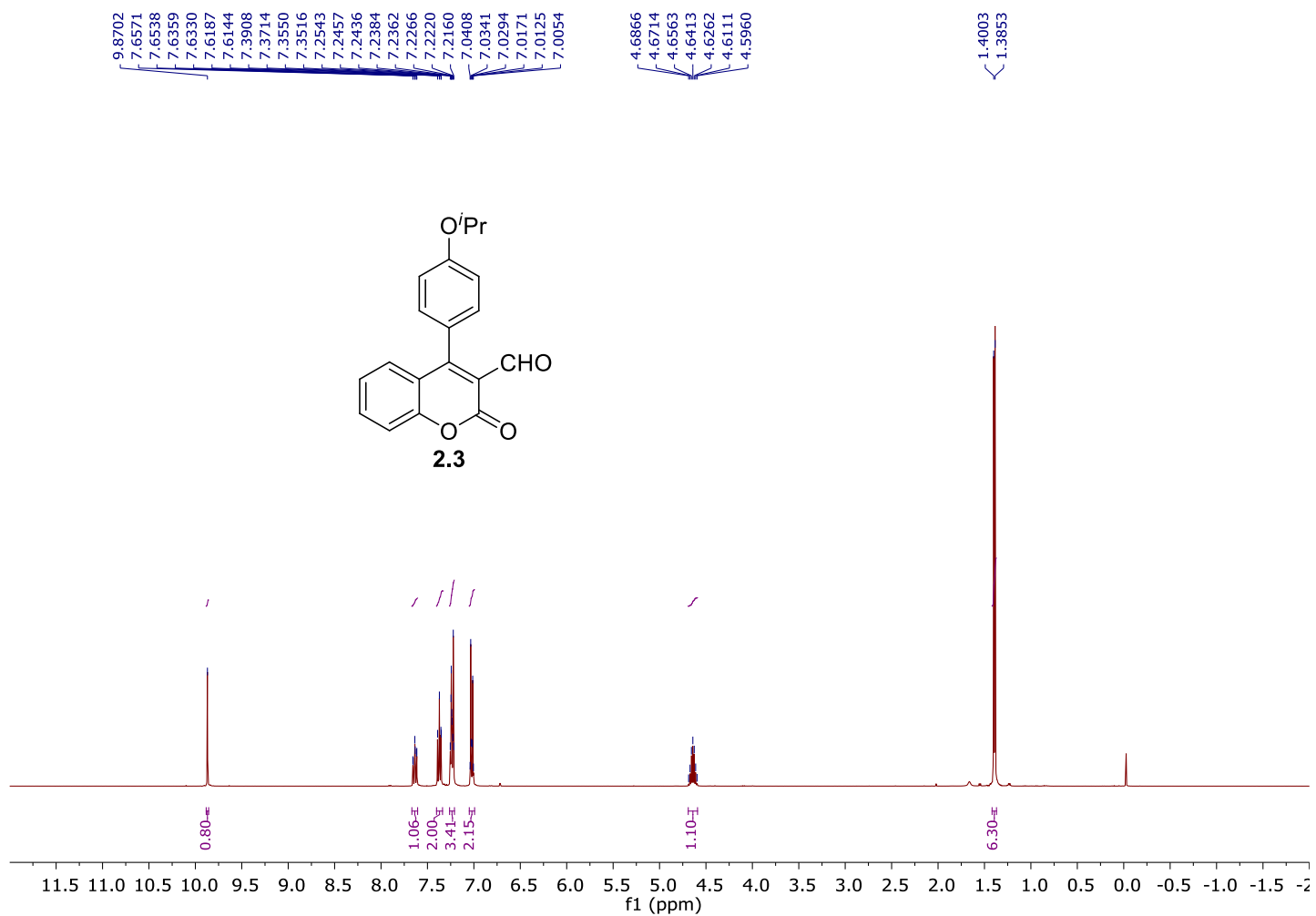




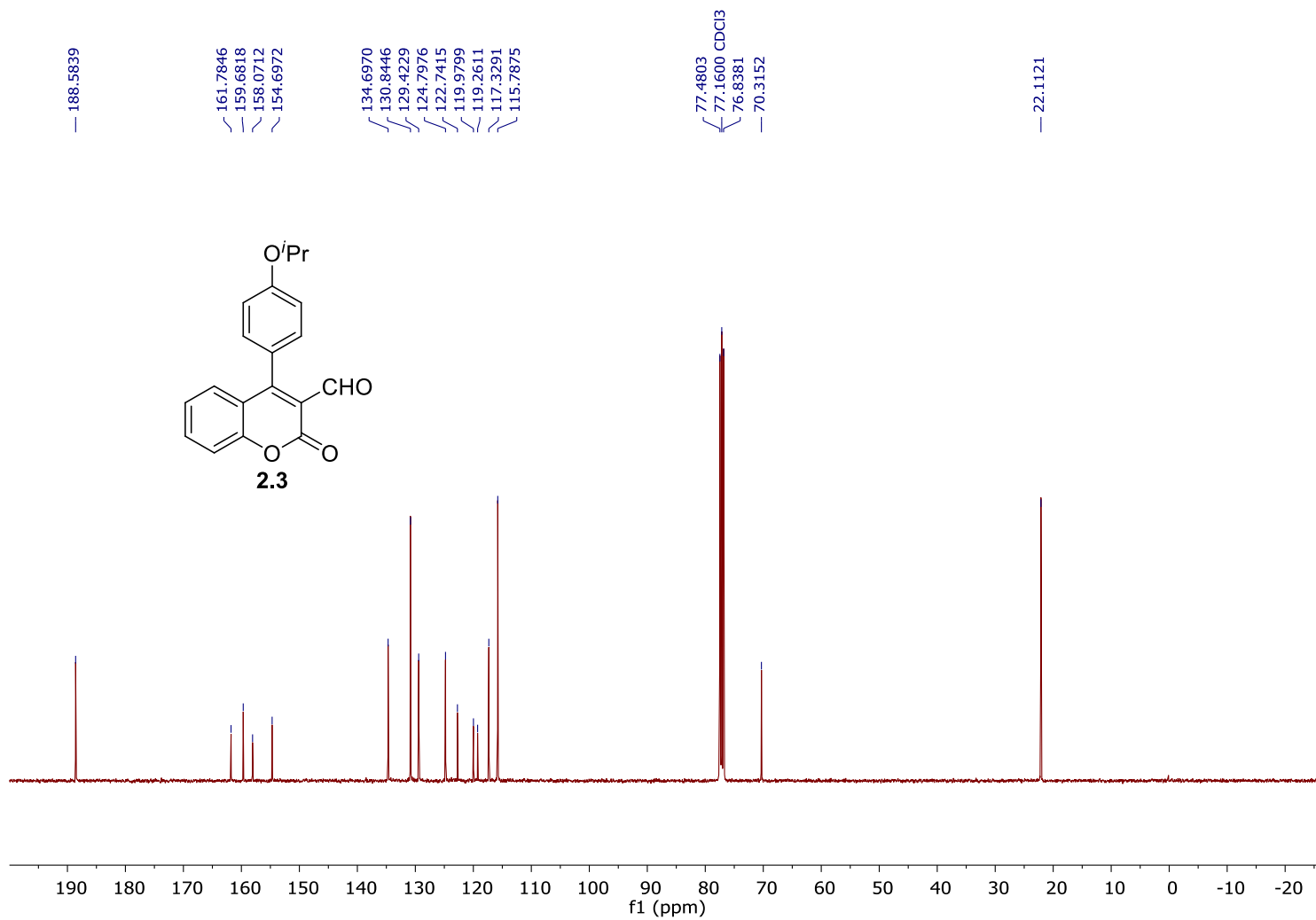
<sup>1</sup>H Spectrum of 4-(4-methoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.2)



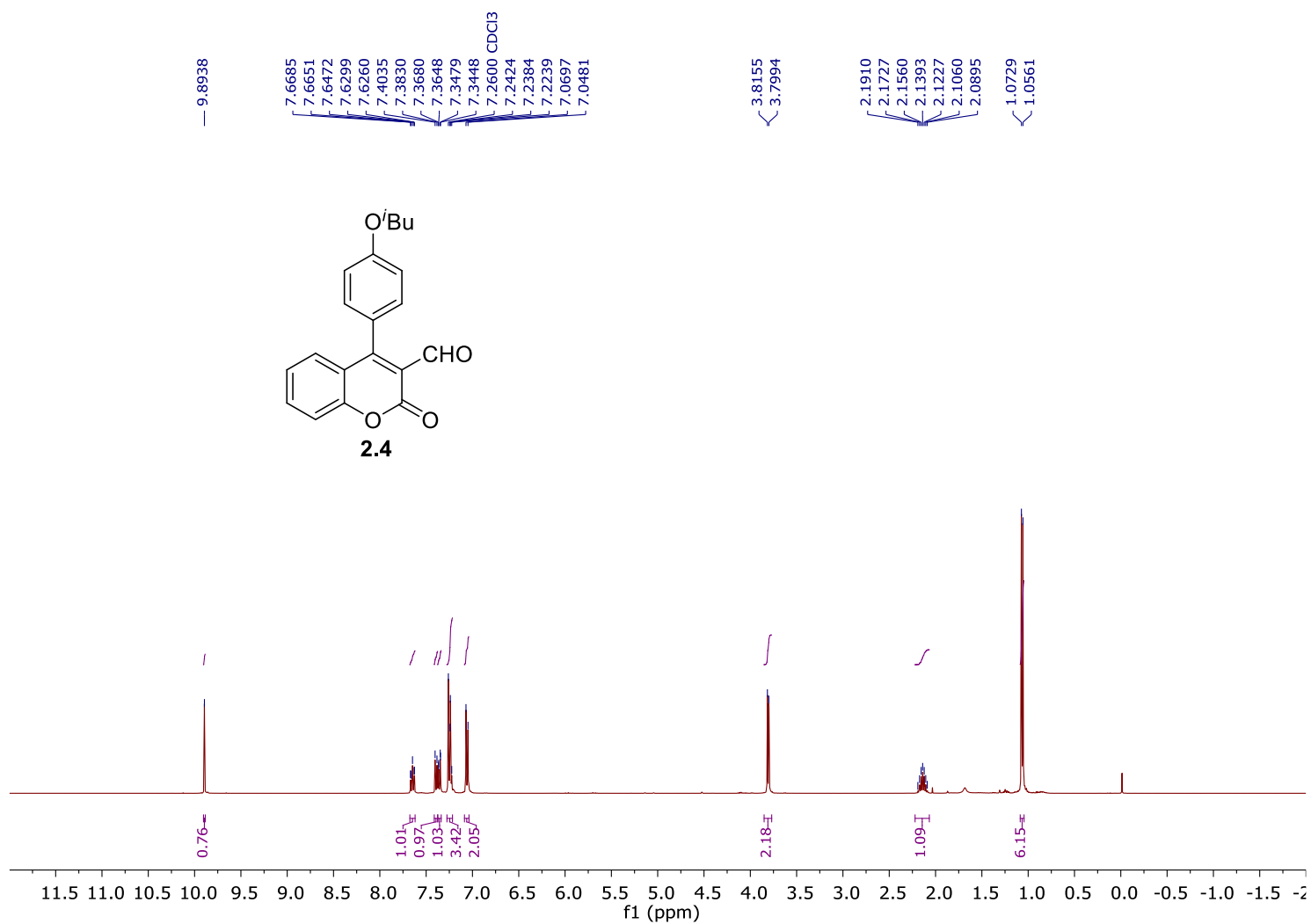
<sup>13</sup>C Spectrum of 4-(4-methoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.2)



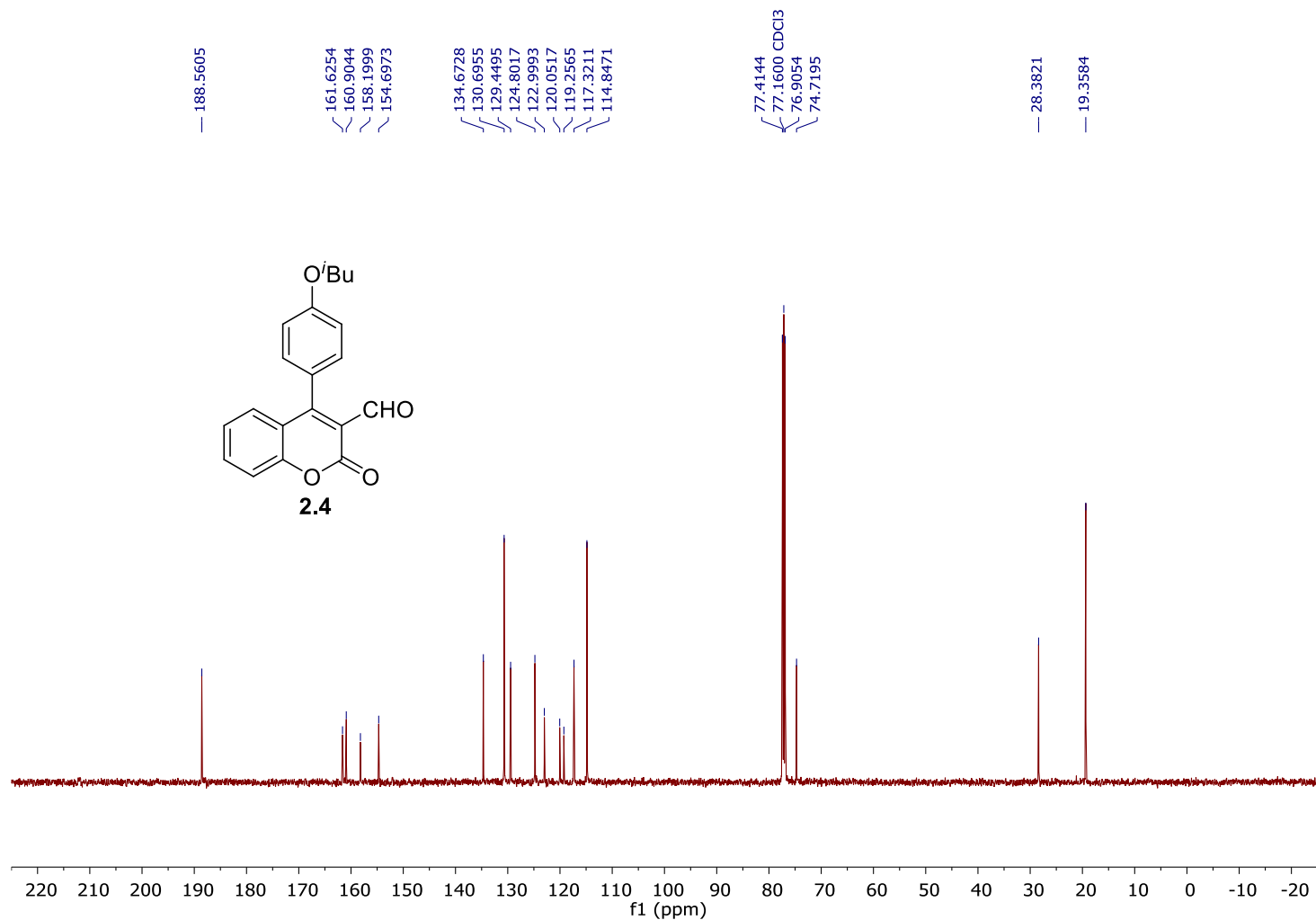
**<sup>1</sup>H Spectrum of 4-(4-isopropoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.3)**



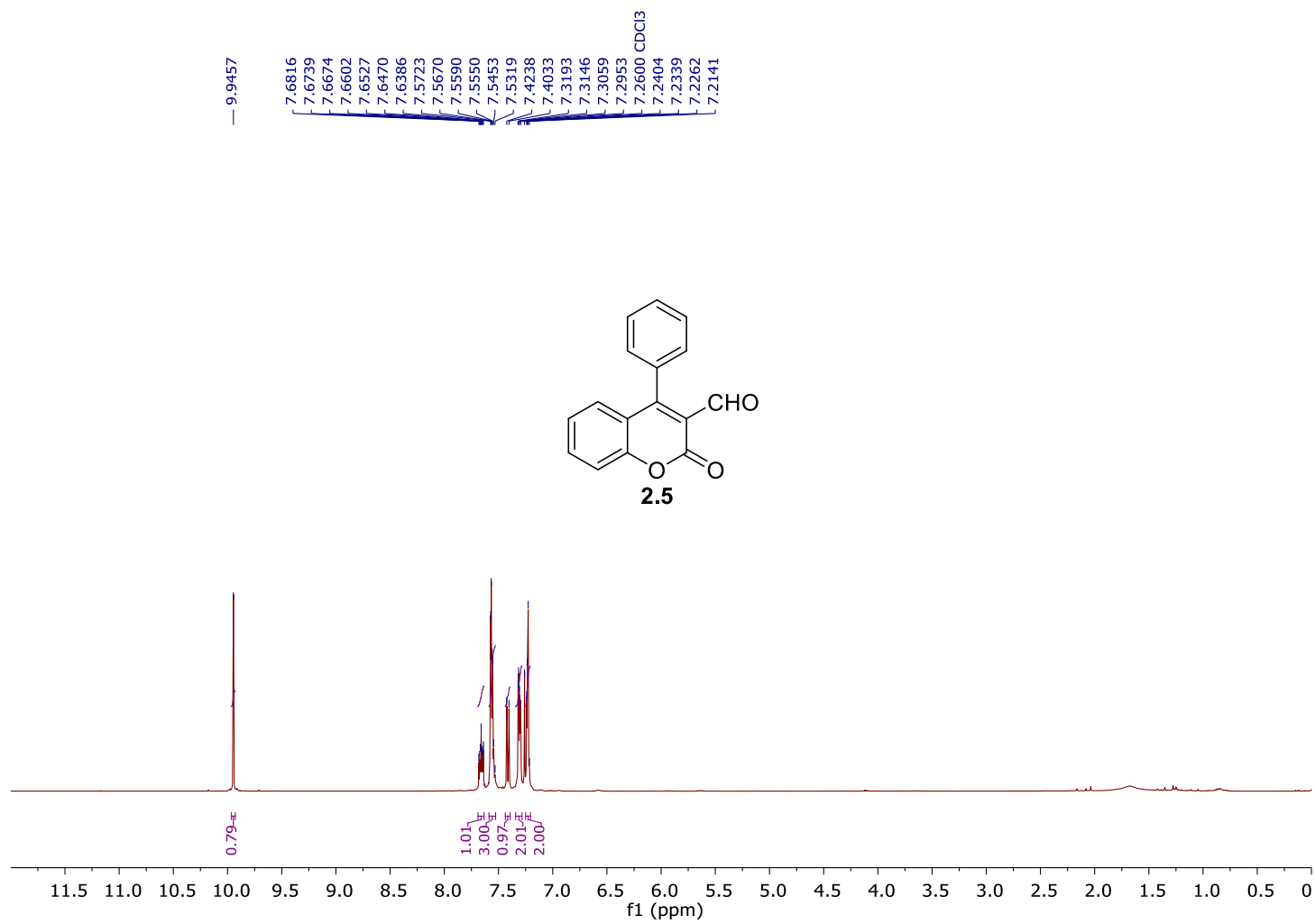
<sup>13</sup>C Spectrum of 4-(4-isopropoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.3)



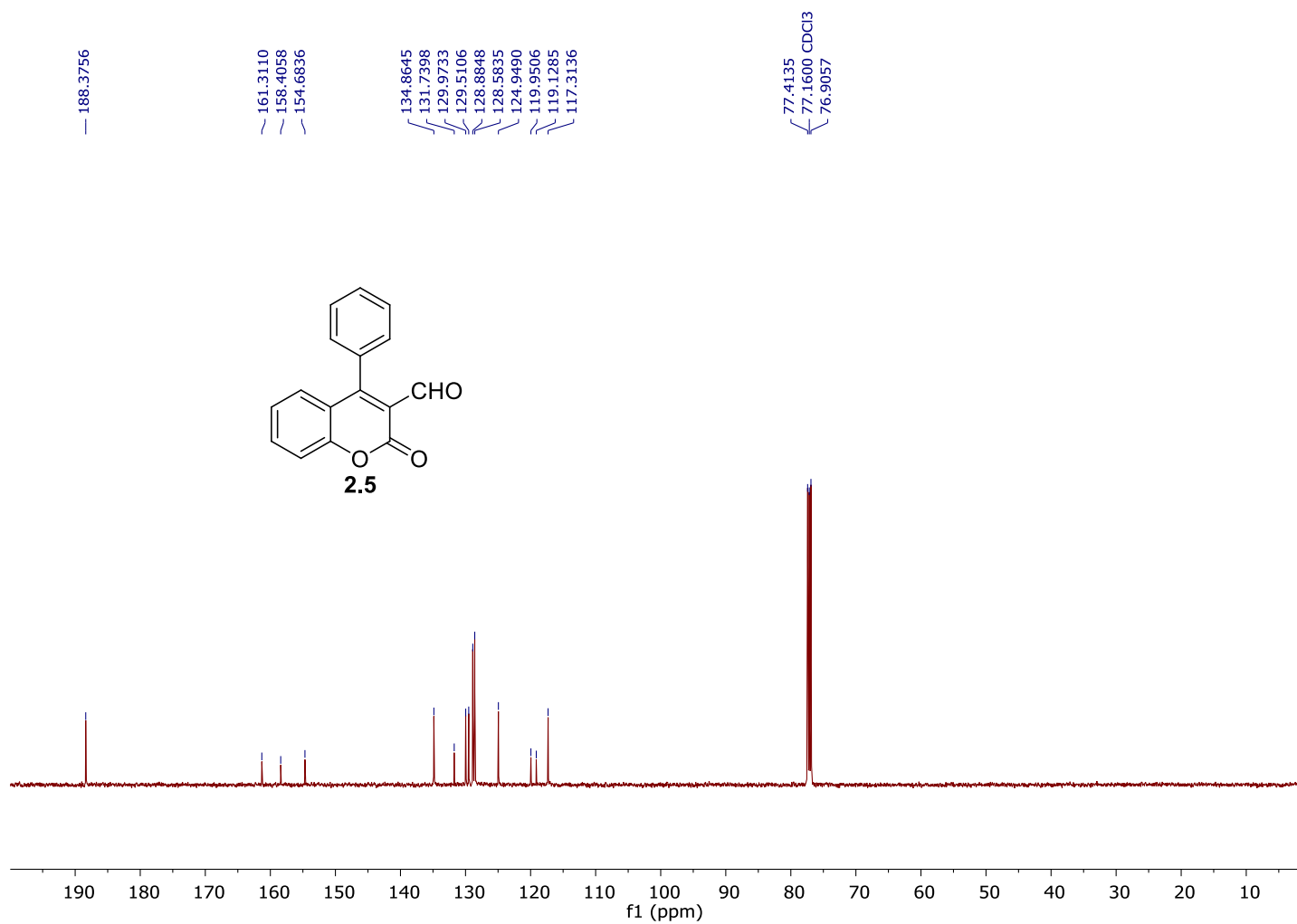
**<sup>1</sup>H Spectrum of 4-(4-isobutoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.4)**



<sup>13</sup>C Spectrum of 4-(4-isobutoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.4)

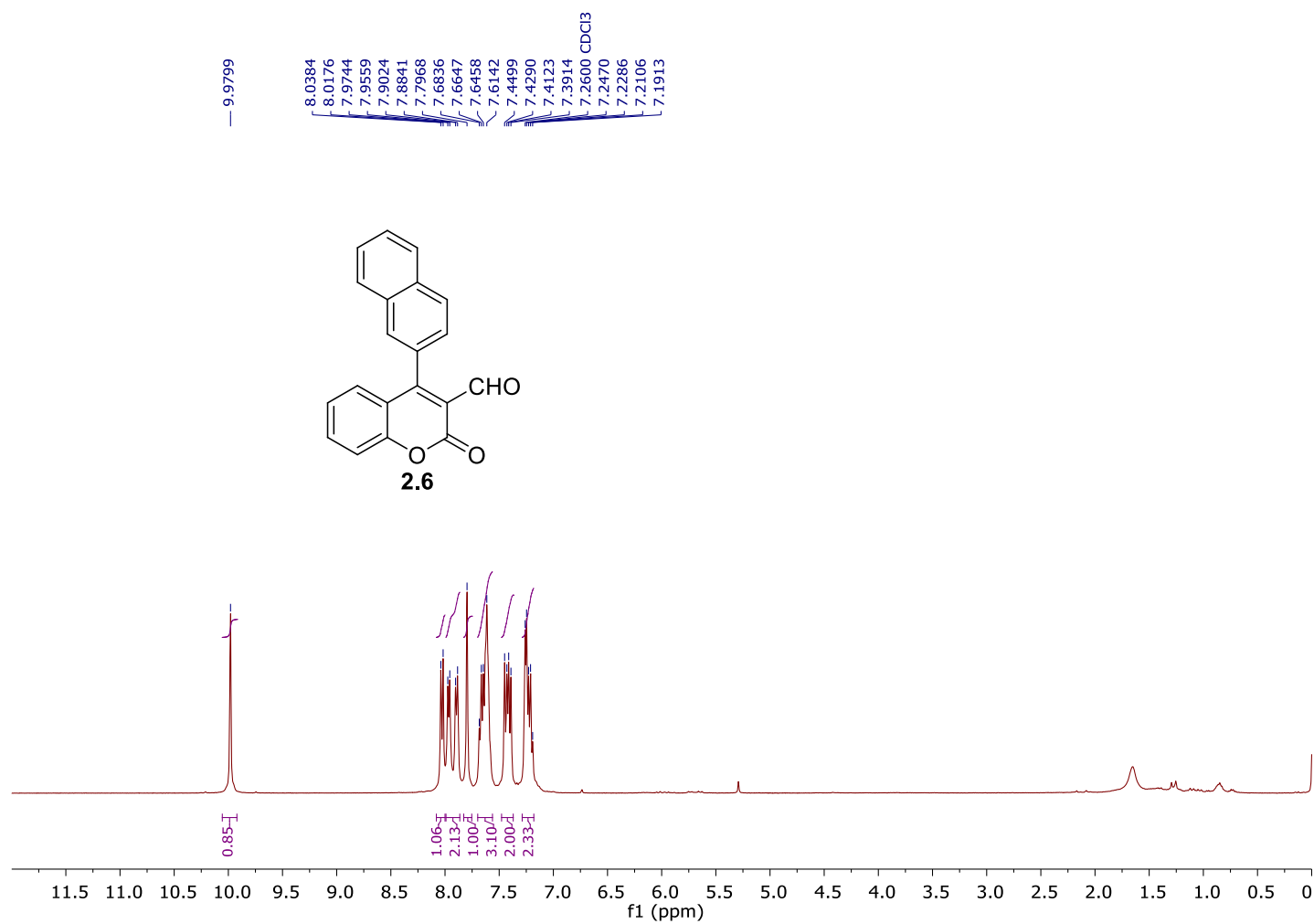


**<sup>1</sup>H Spectrum of 2-oxo-4-phenyl-2H-chromene-3-carbaldehyde (2.5)**

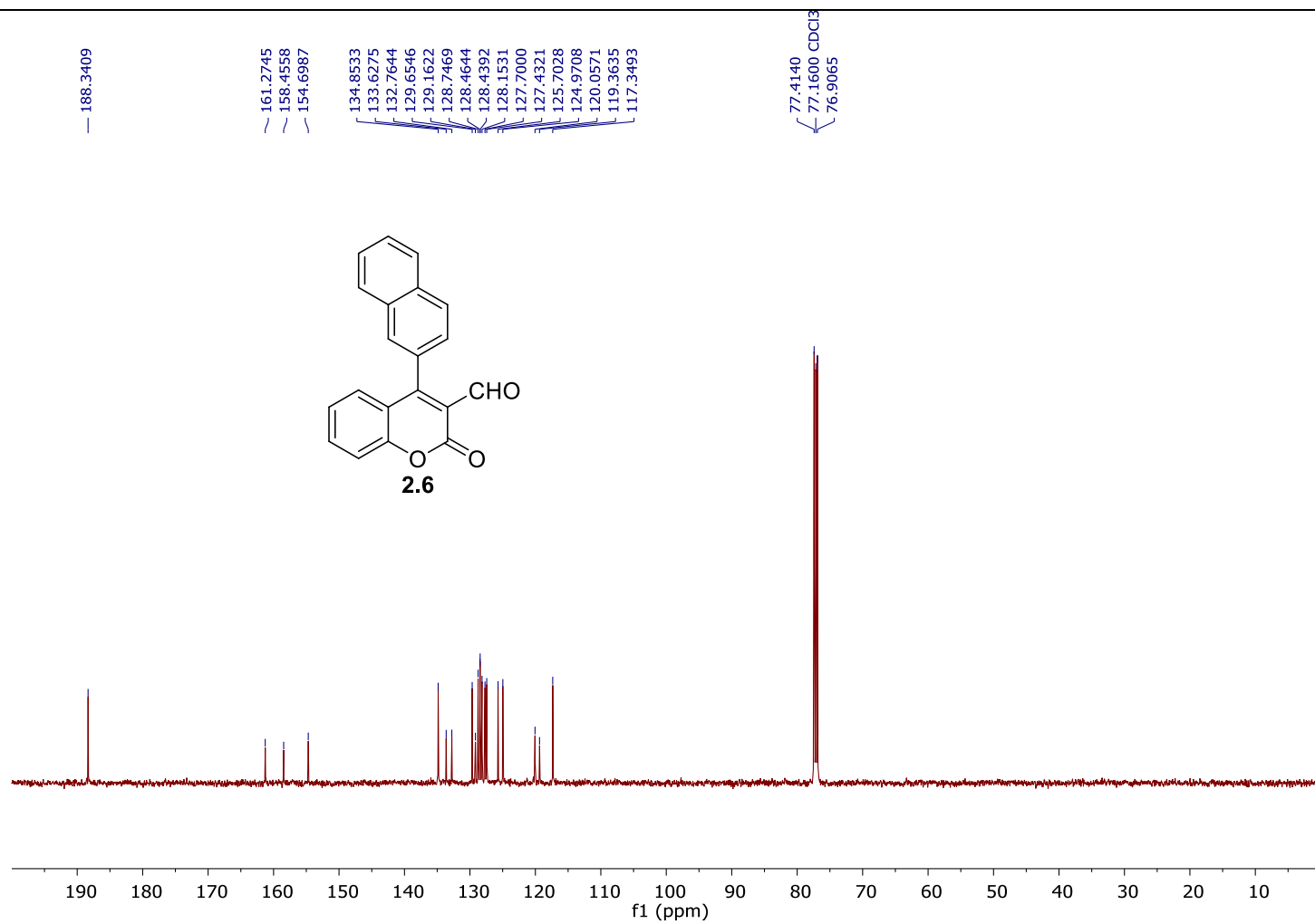


**<sup>13</sup>C Spectrum of 2-oxo-4-phenyl-2H-chromene-3-carbaldehyde (2.5)**

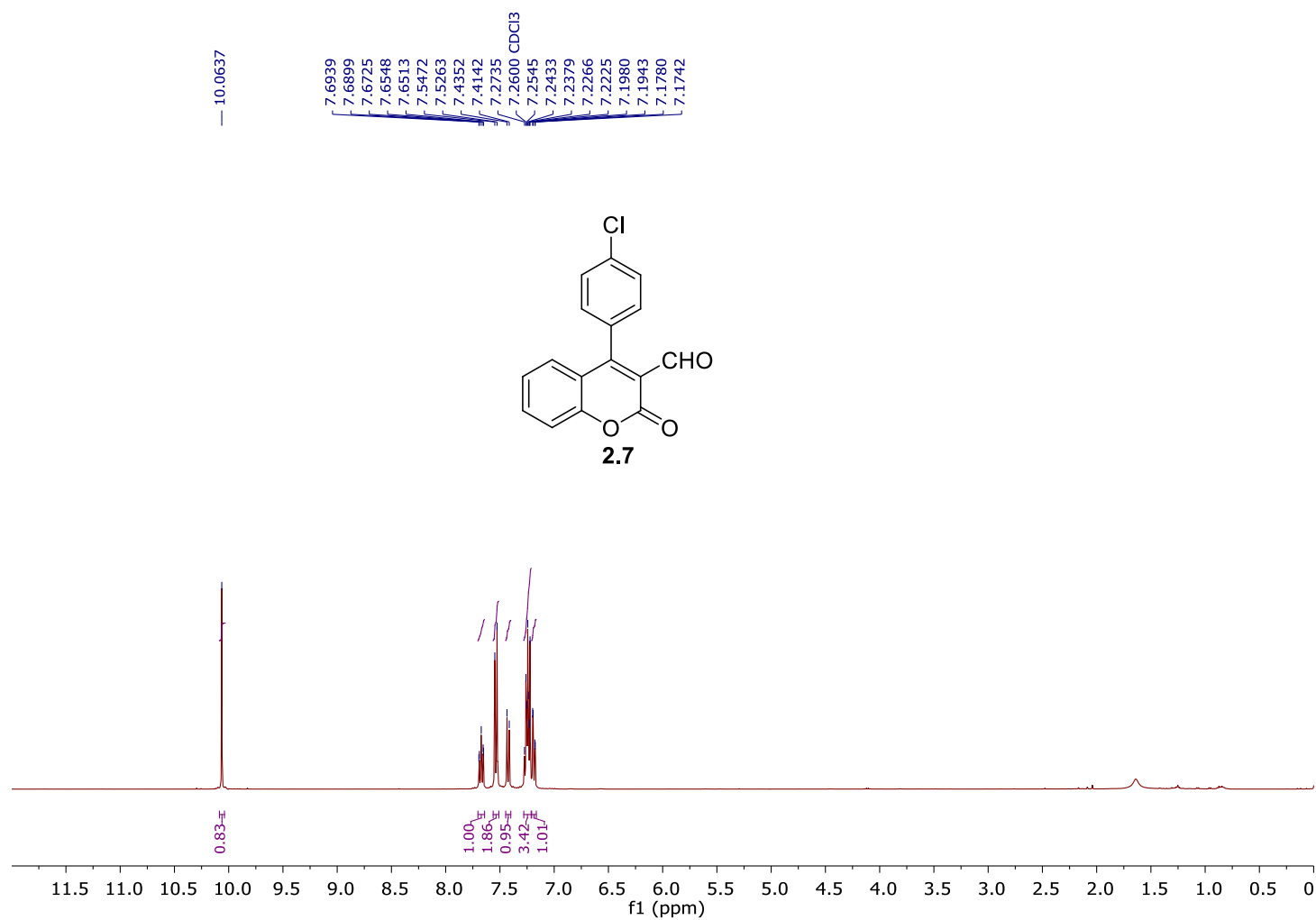




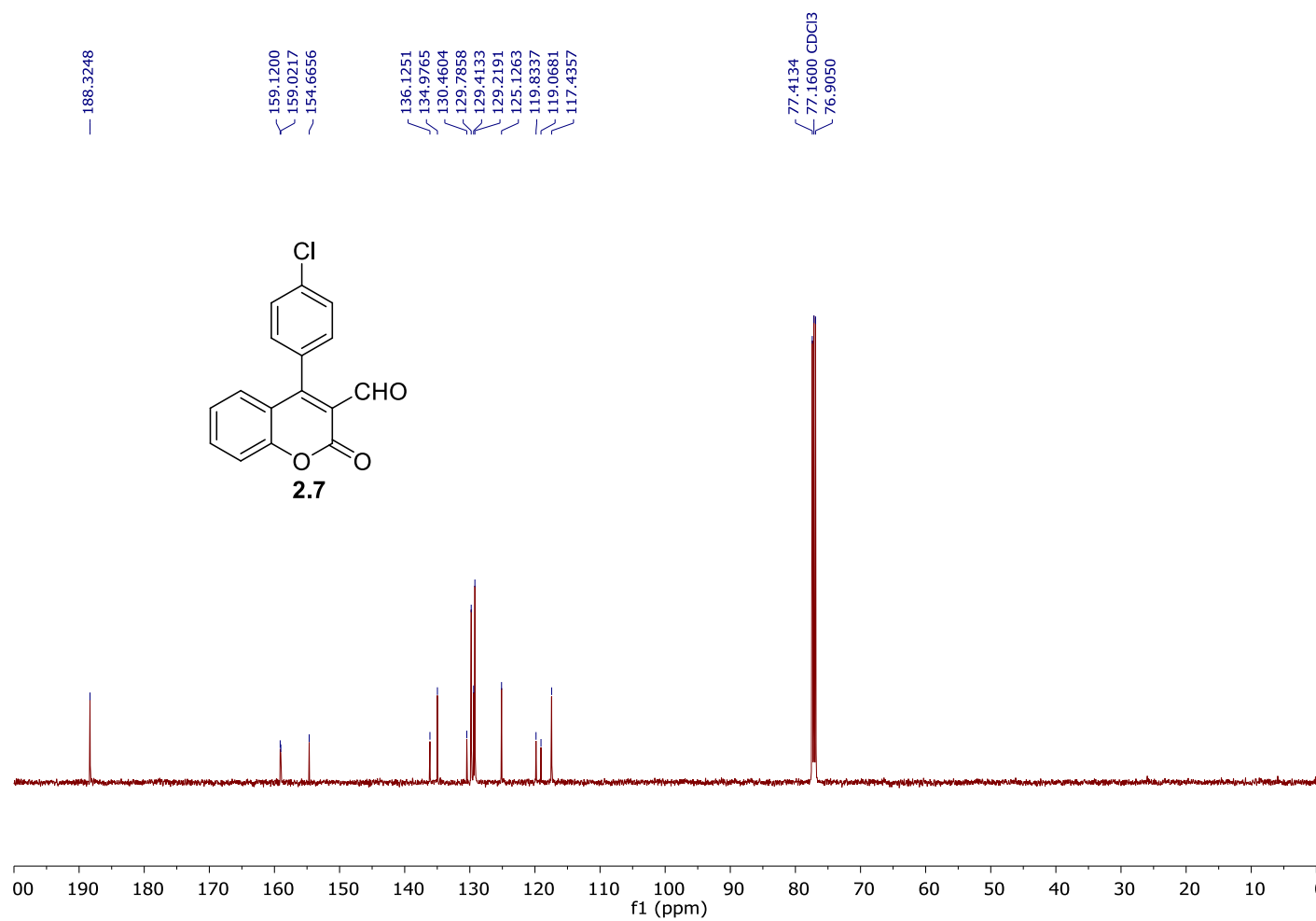
**<sup>1</sup>H Spectrum of 4-(naphthalen-2-yl)-2-oxo-2H-chromene-3-carbaldehyde (2.6)**



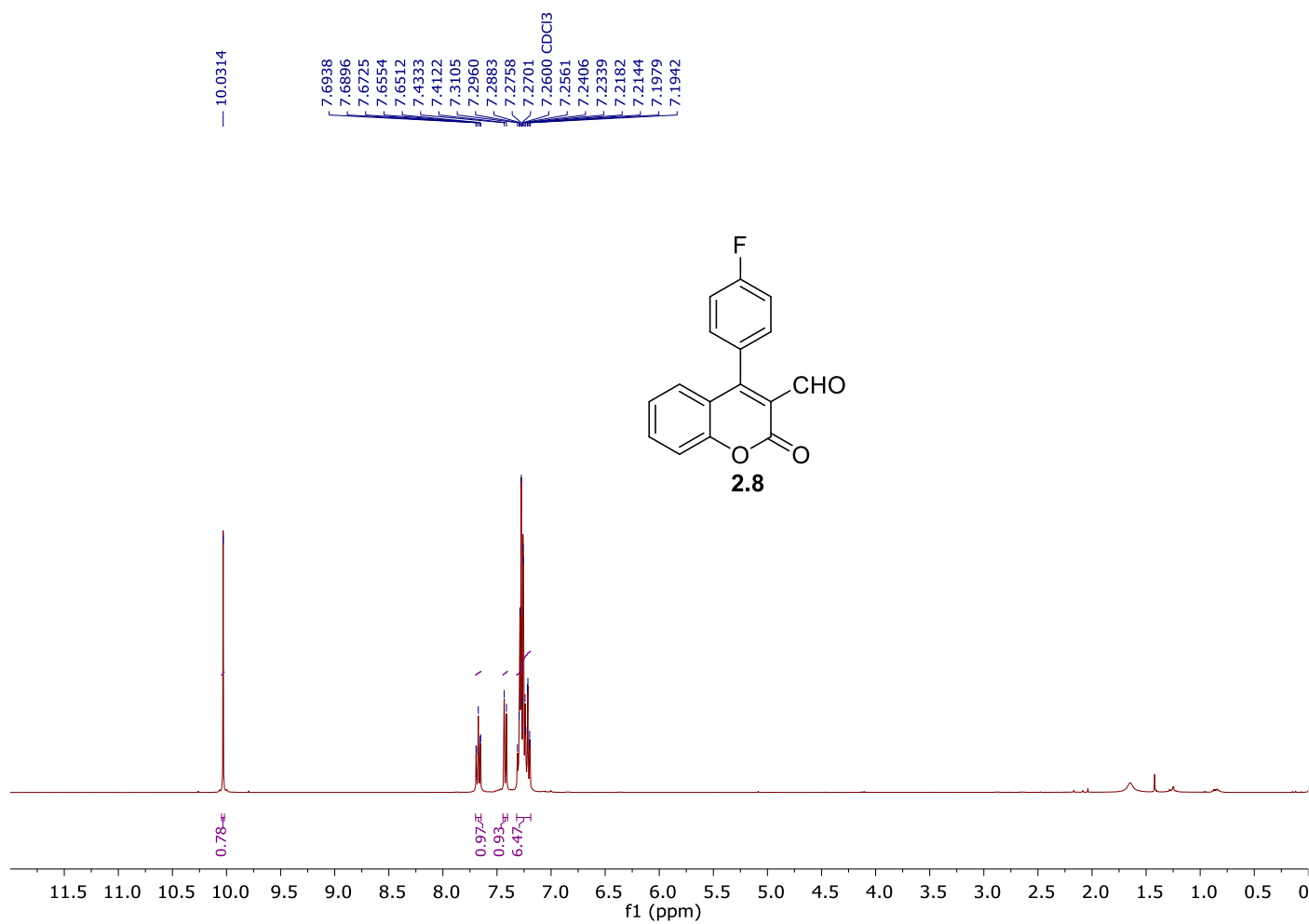
<sup>13</sup>C Spectrum of 4-(naphthalen-2-yl)-2-oxo-2H-chromene-3-carbaldehyde (2.6)



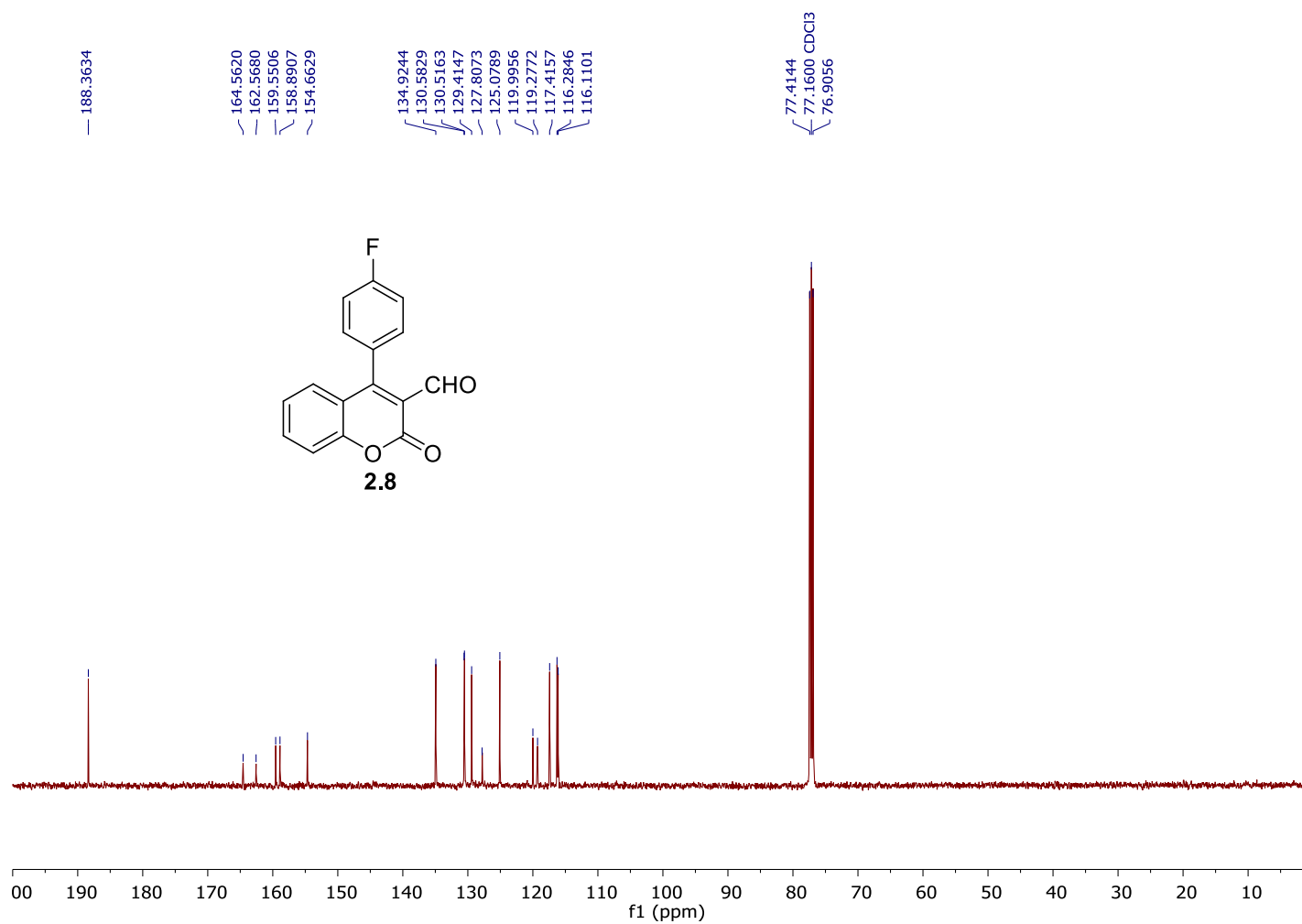
<sup>1</sup>H Spectrum of 4-(4-chlorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.7)



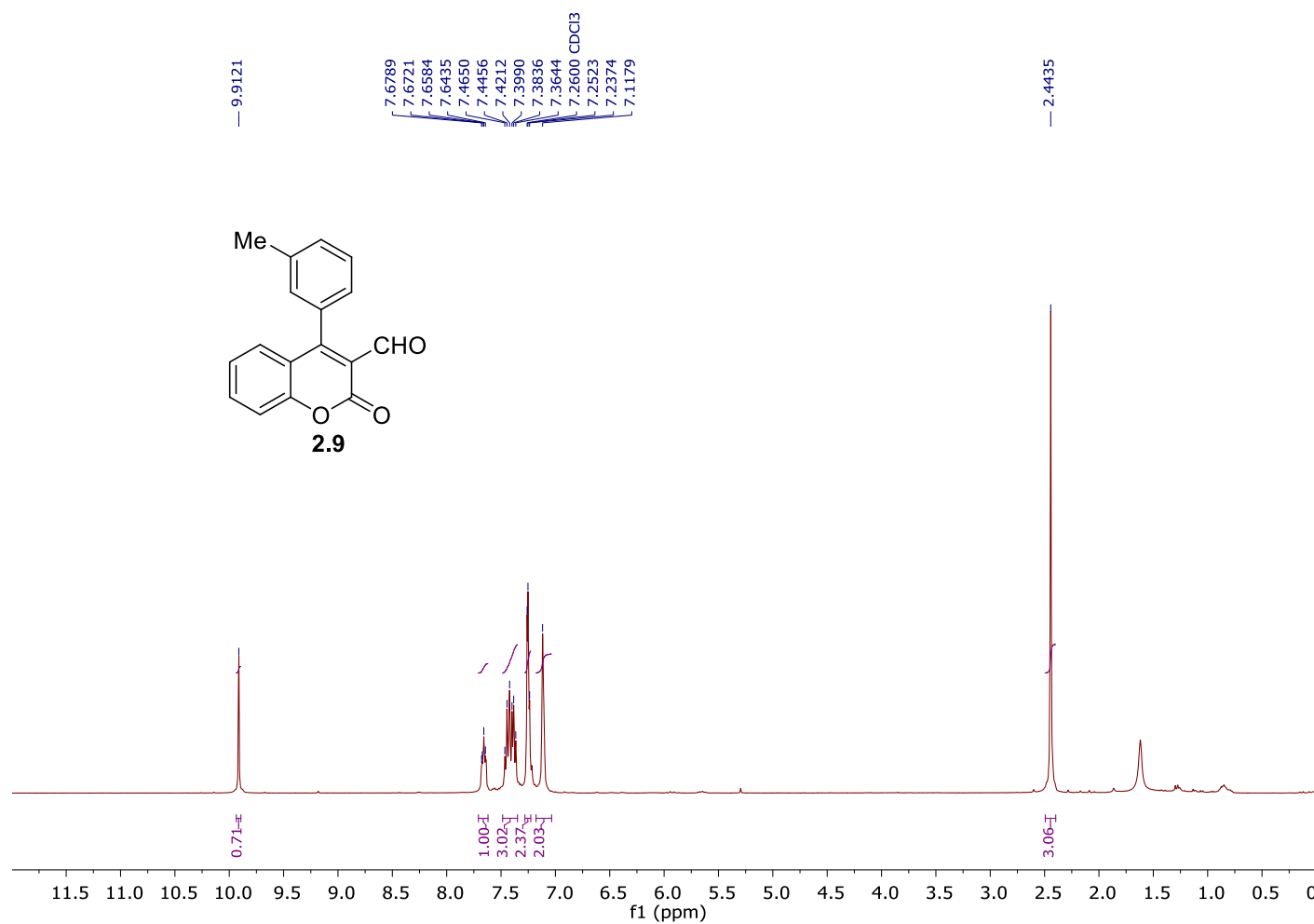
<sup>13</sup>C Spectrum of 4-(4-chlorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.7)



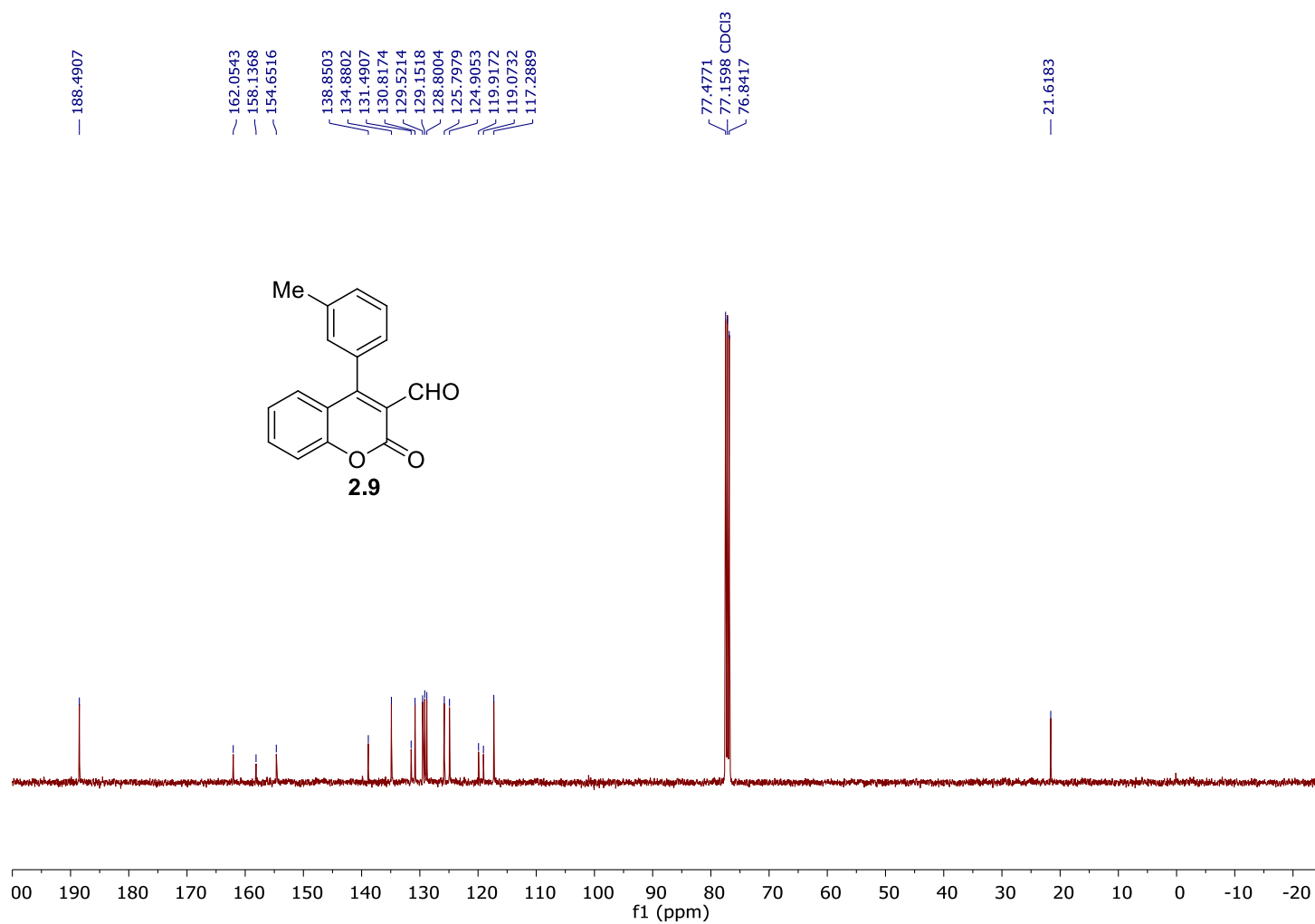
**<sup>1</sup>H Spectrum of 4-(4-fluorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.8)**



**<sup>13</sup>C Spectrum of 4-(4-fluorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.8)**

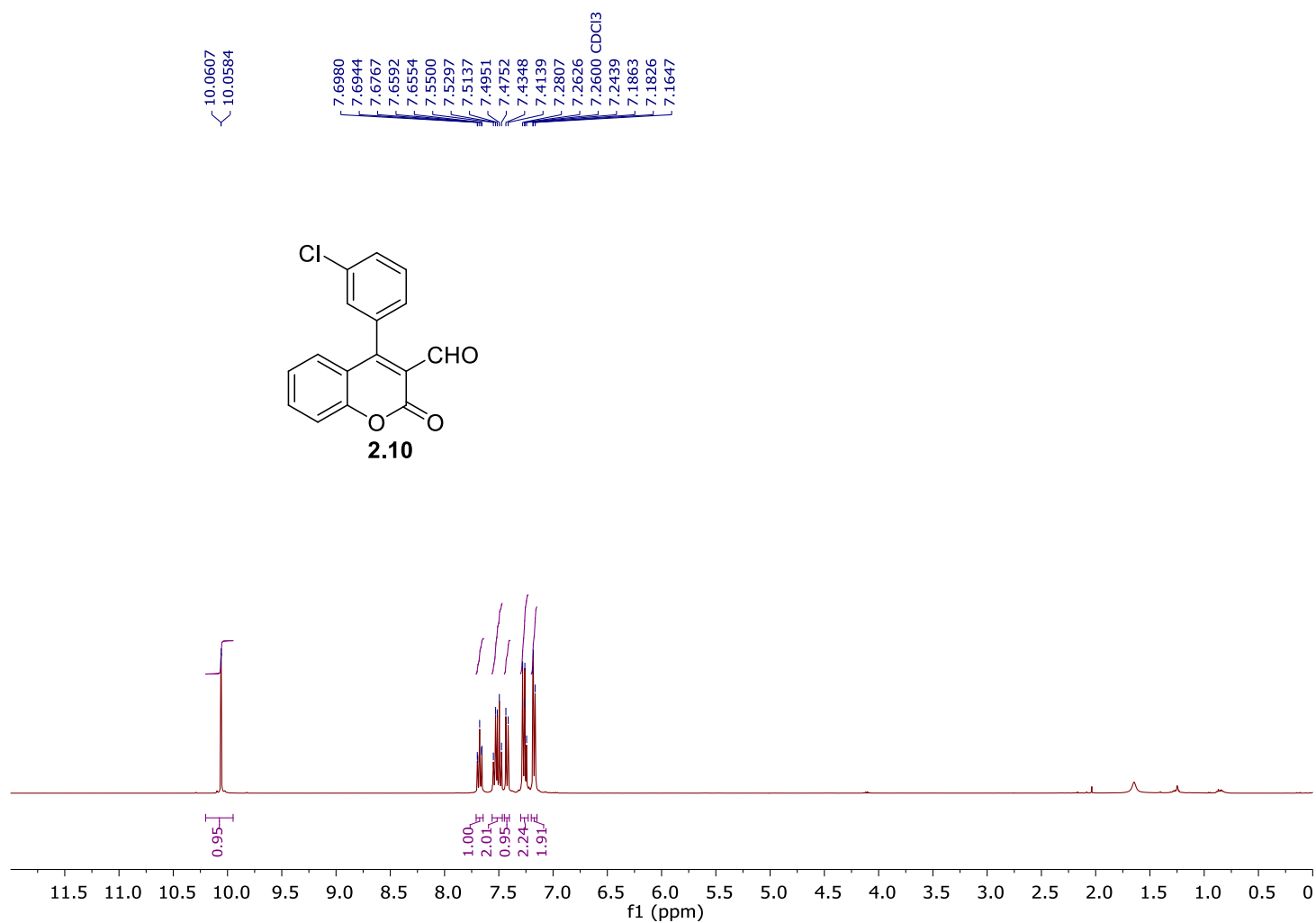


**<sup>1</sup>H Spectrum of 2-oxo-4-m-tolyl-2H-chromene-3-carbaldehyde (2.9)**

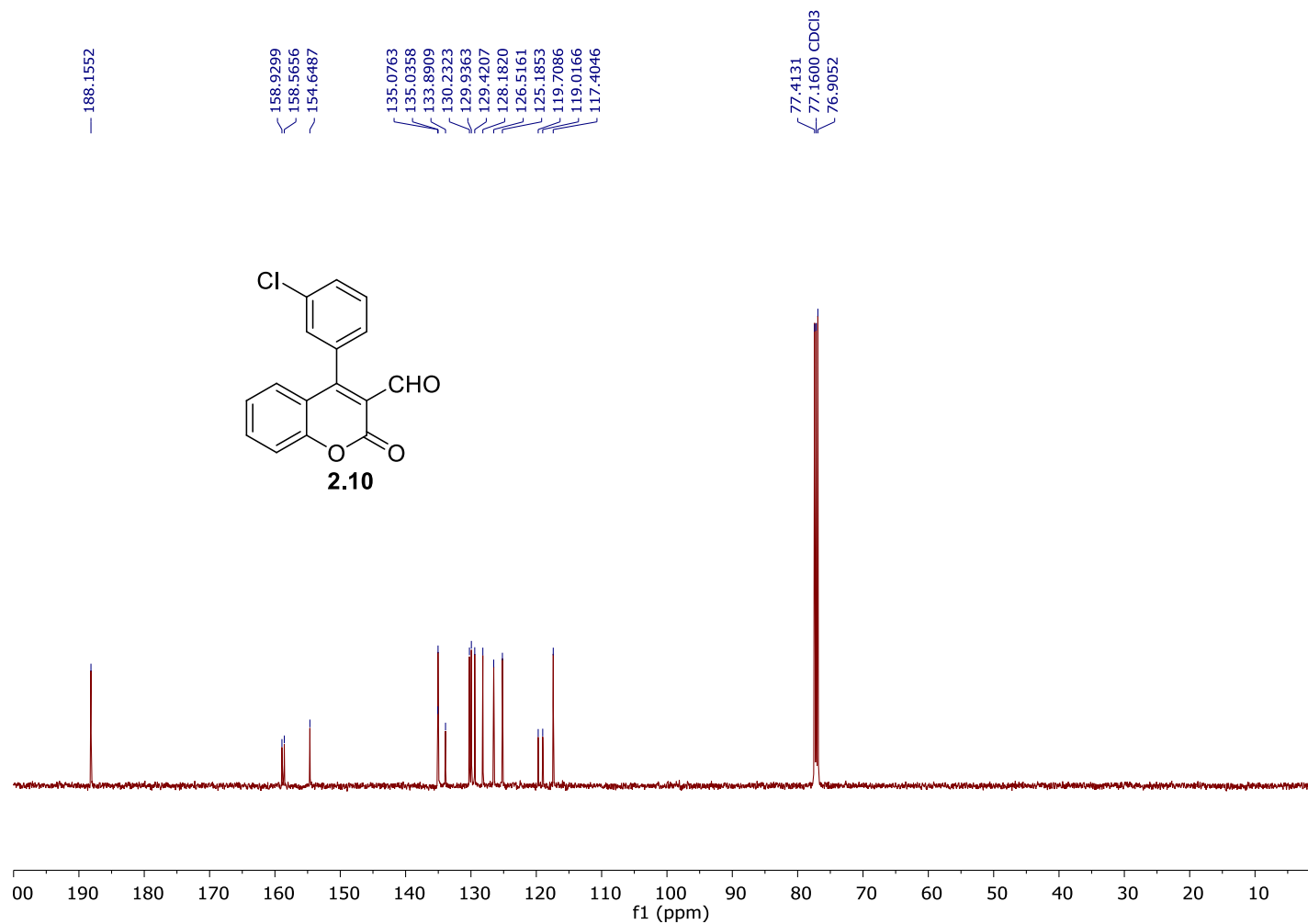


<sup>13</sup>C Spectrum of 2-oxo-4-*m*-tolyl-2*H*-chromene-3-carbaldehyde (2.9)

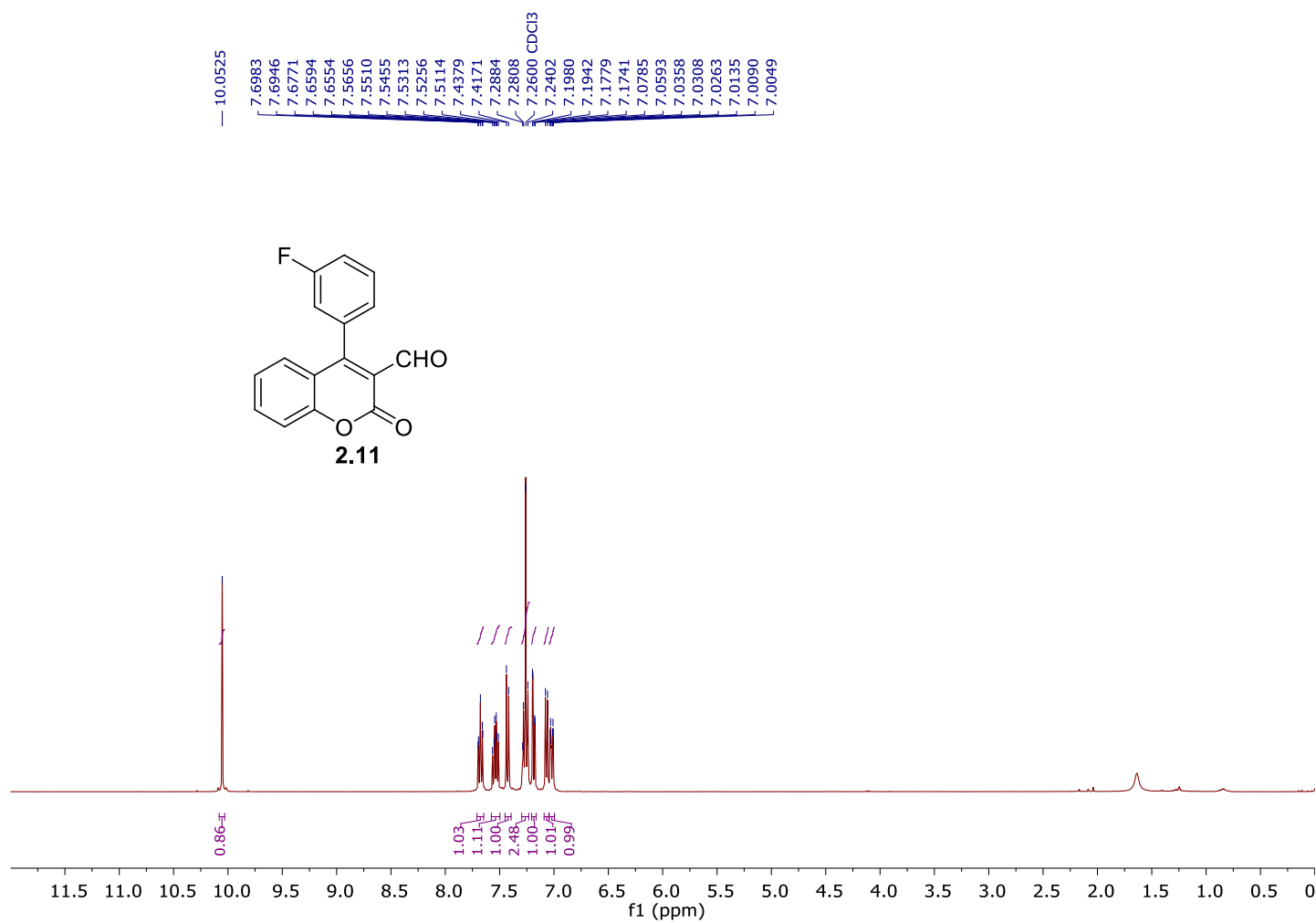




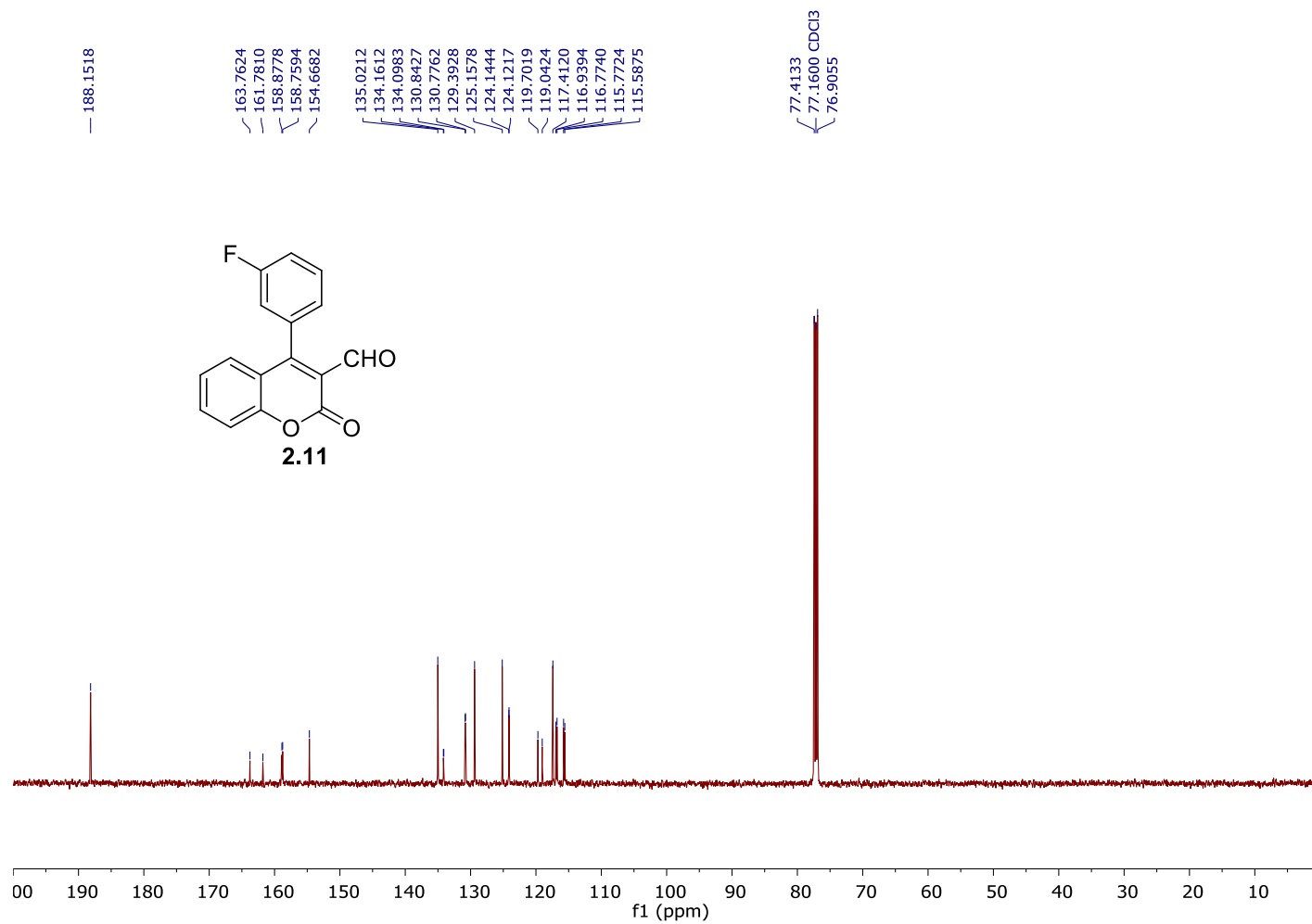
**<sup>1</sup>H Spectrum of 4-(3-chlorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.10)**



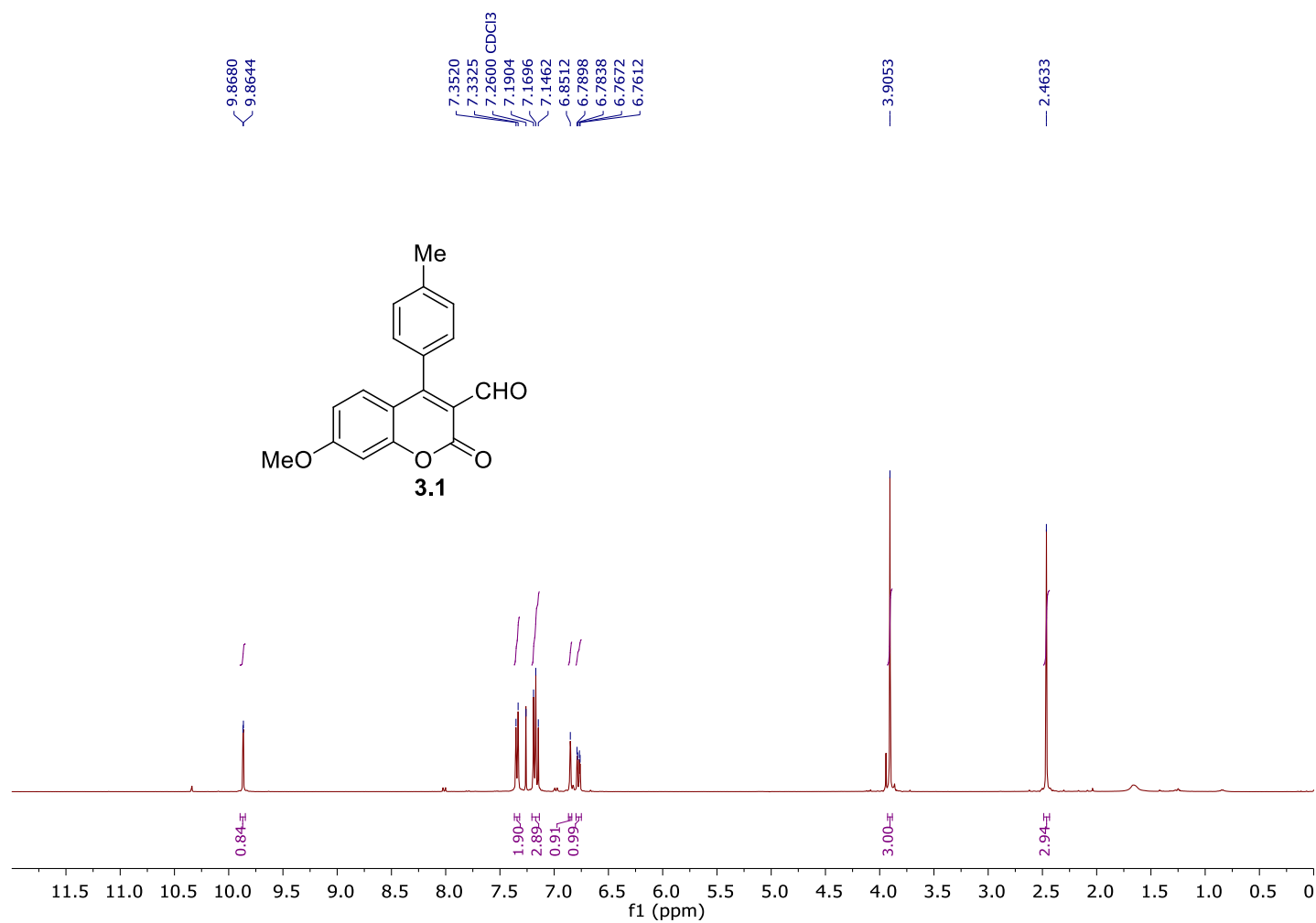
<sup>13</sup>C Spectrum of 4-(3-chlorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.10)



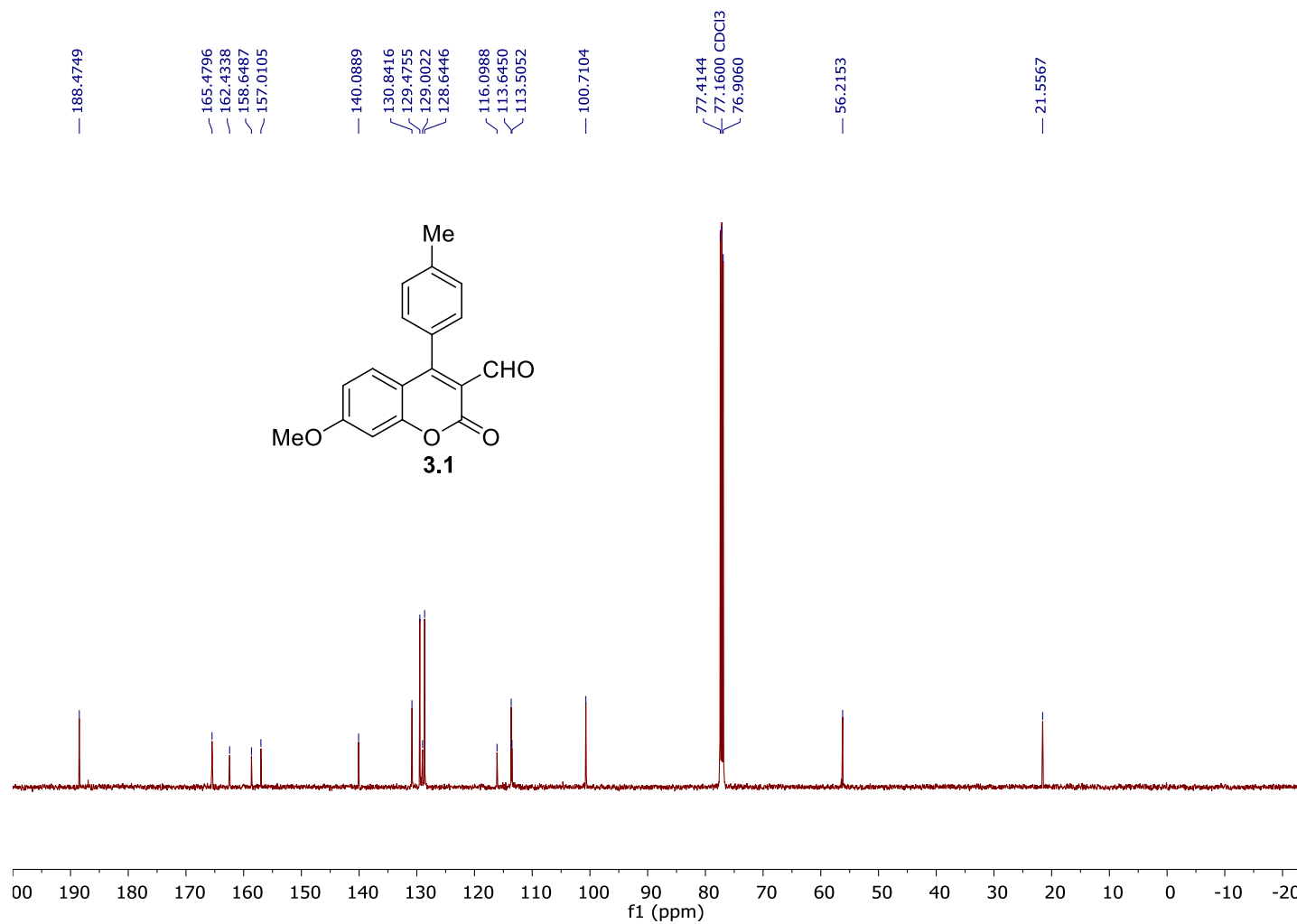
<sup>1</sup>H Spectrum of 4-(3-fluorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.11)



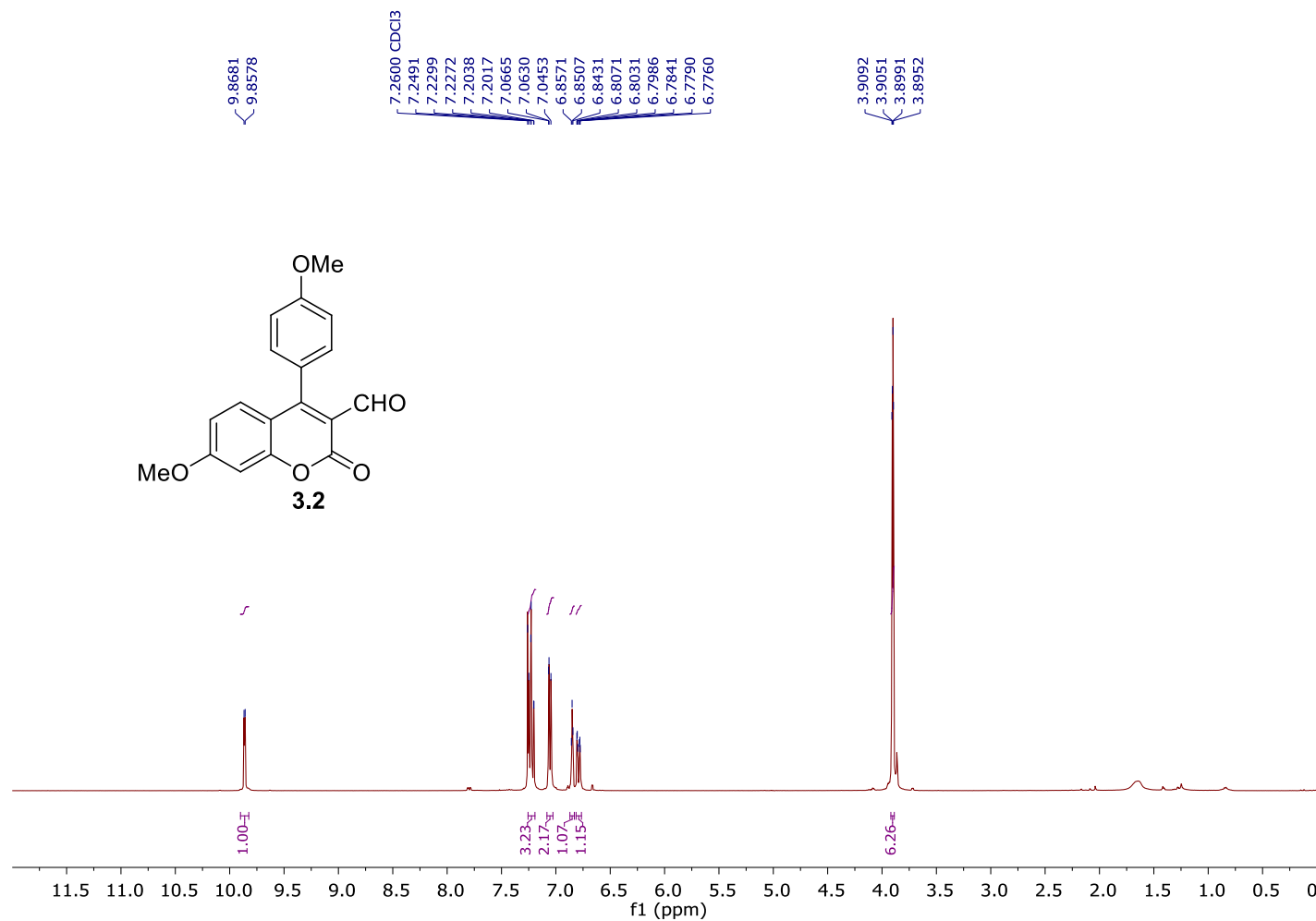
<sup>13</sup>C Spectrum of 4-(3-fluorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.11)



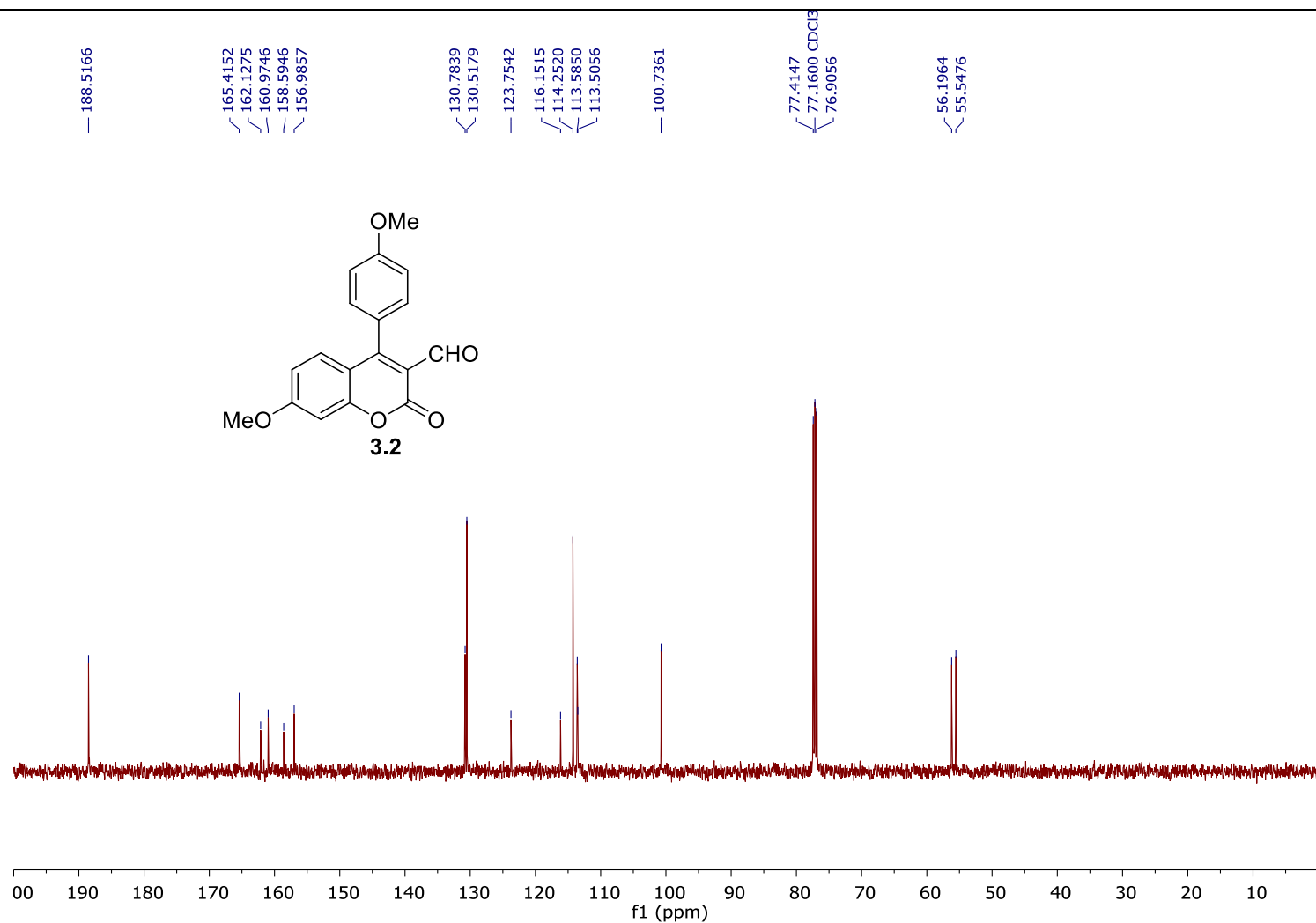
**<sup>1</sup>H Spectrum of 7-methoxy-2-oxo-4-p-tolyl-2H-chromene-3-carbaldehyde (3.1)**



<sup>13</sup>C Spectrum of 7-methoxy-2-oxo-4-*p*-tolyl-2*H*-chromene-3-carbaldehyde (3.1)

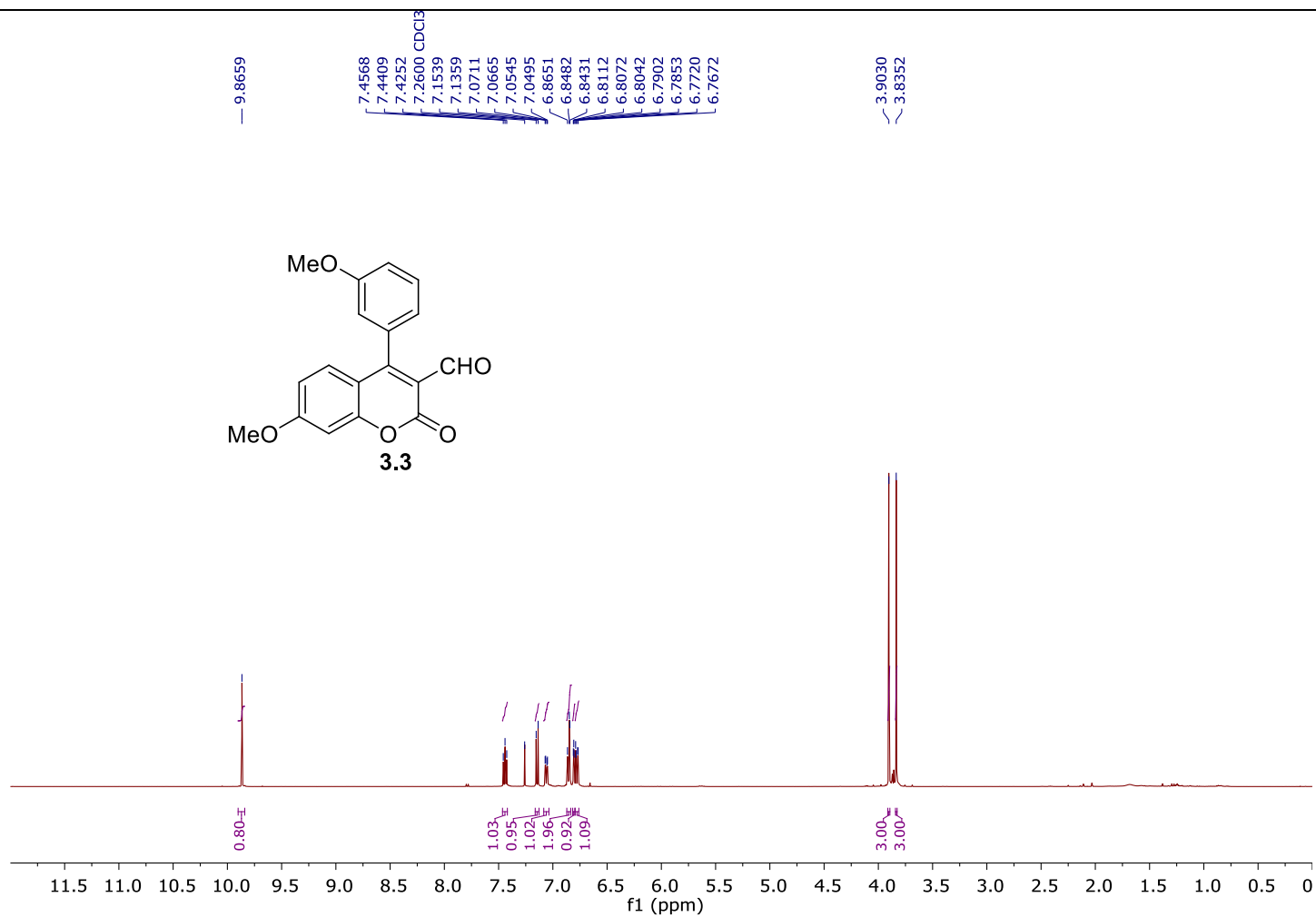


**<sup>1</sup>H Spectrum of 7-methoxy-4-(4-methoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (3.2)**

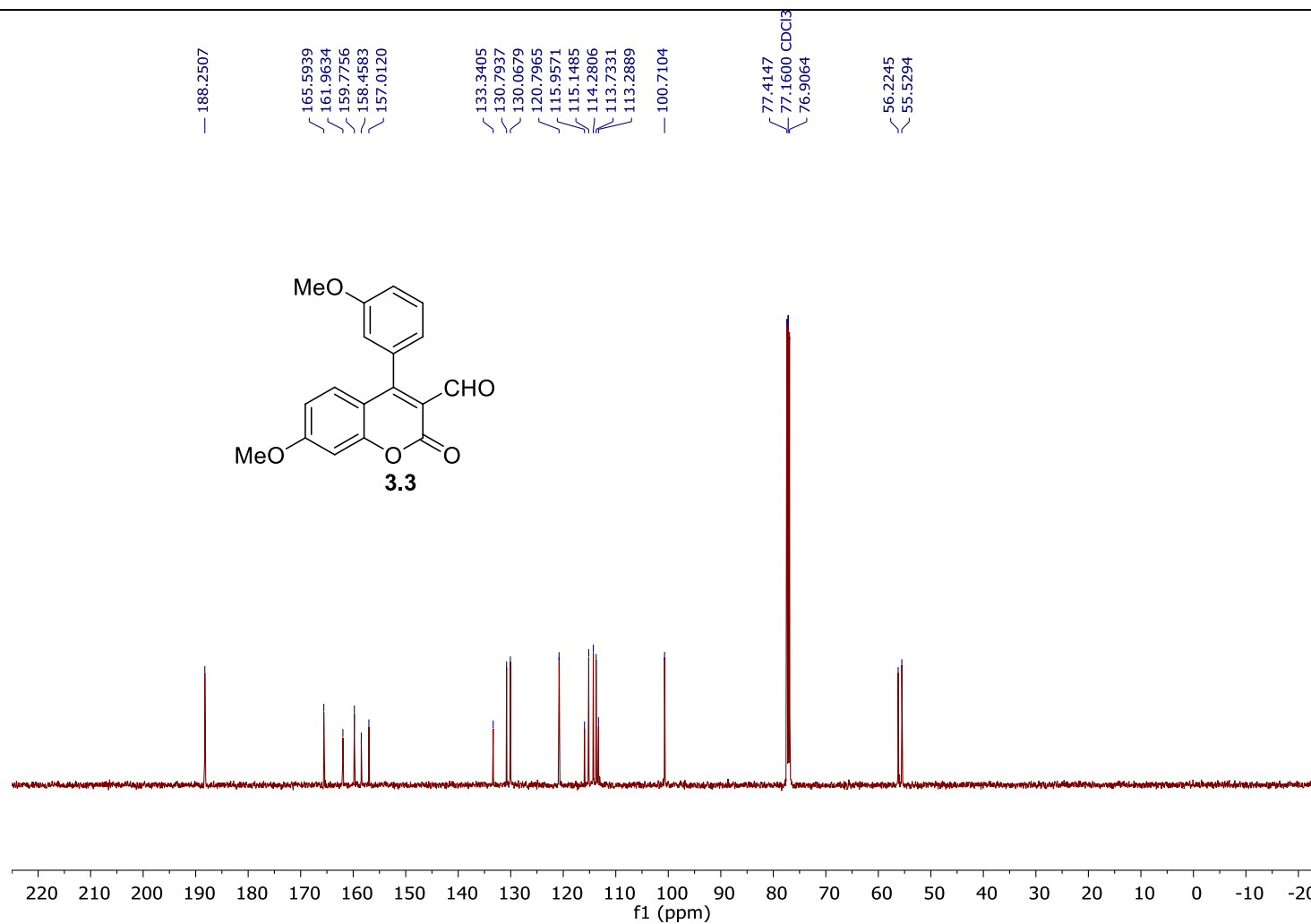


**<sup>13</sup>C Spectrum of 7-methoxy-4-(4-methoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (3.2)**

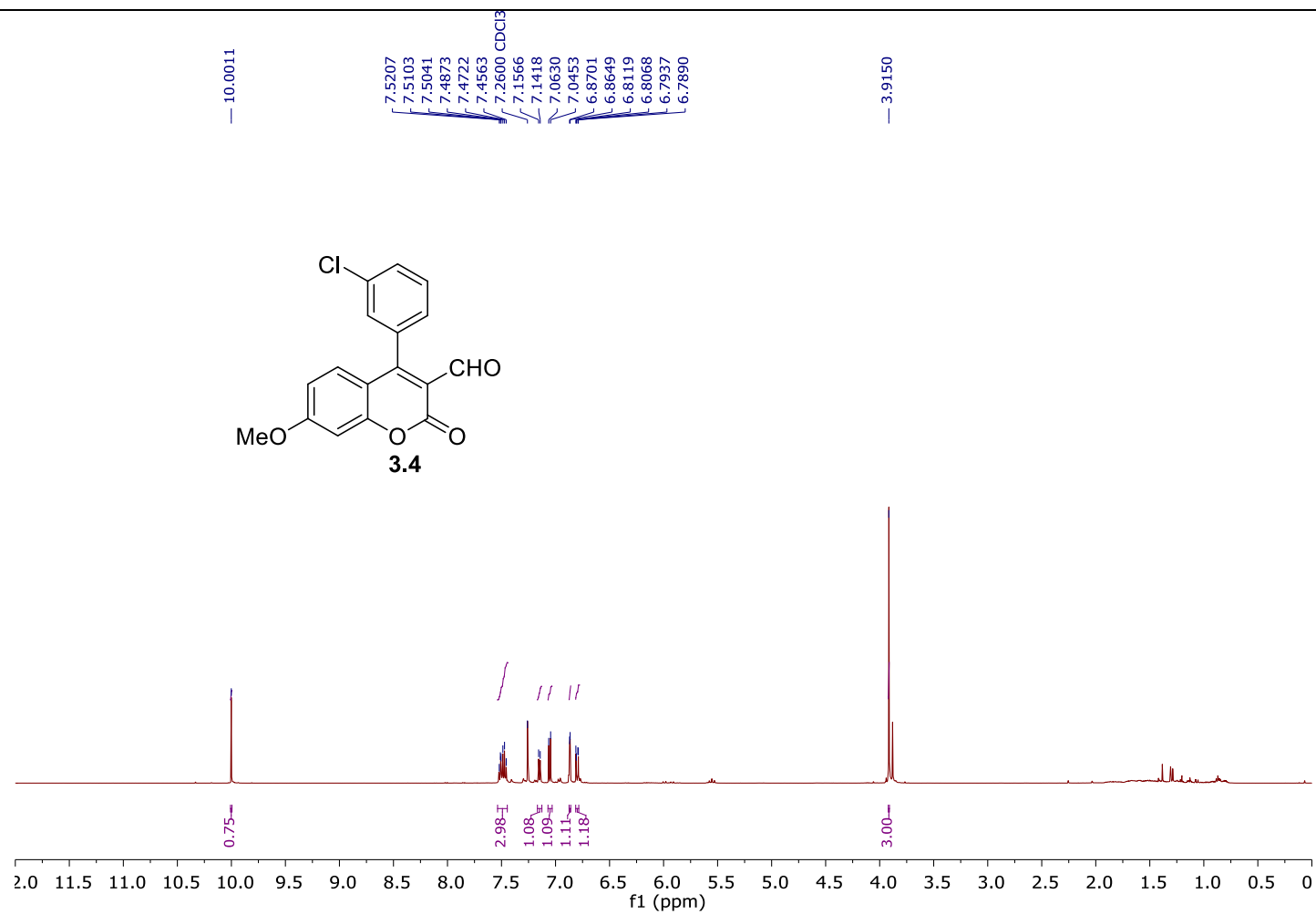




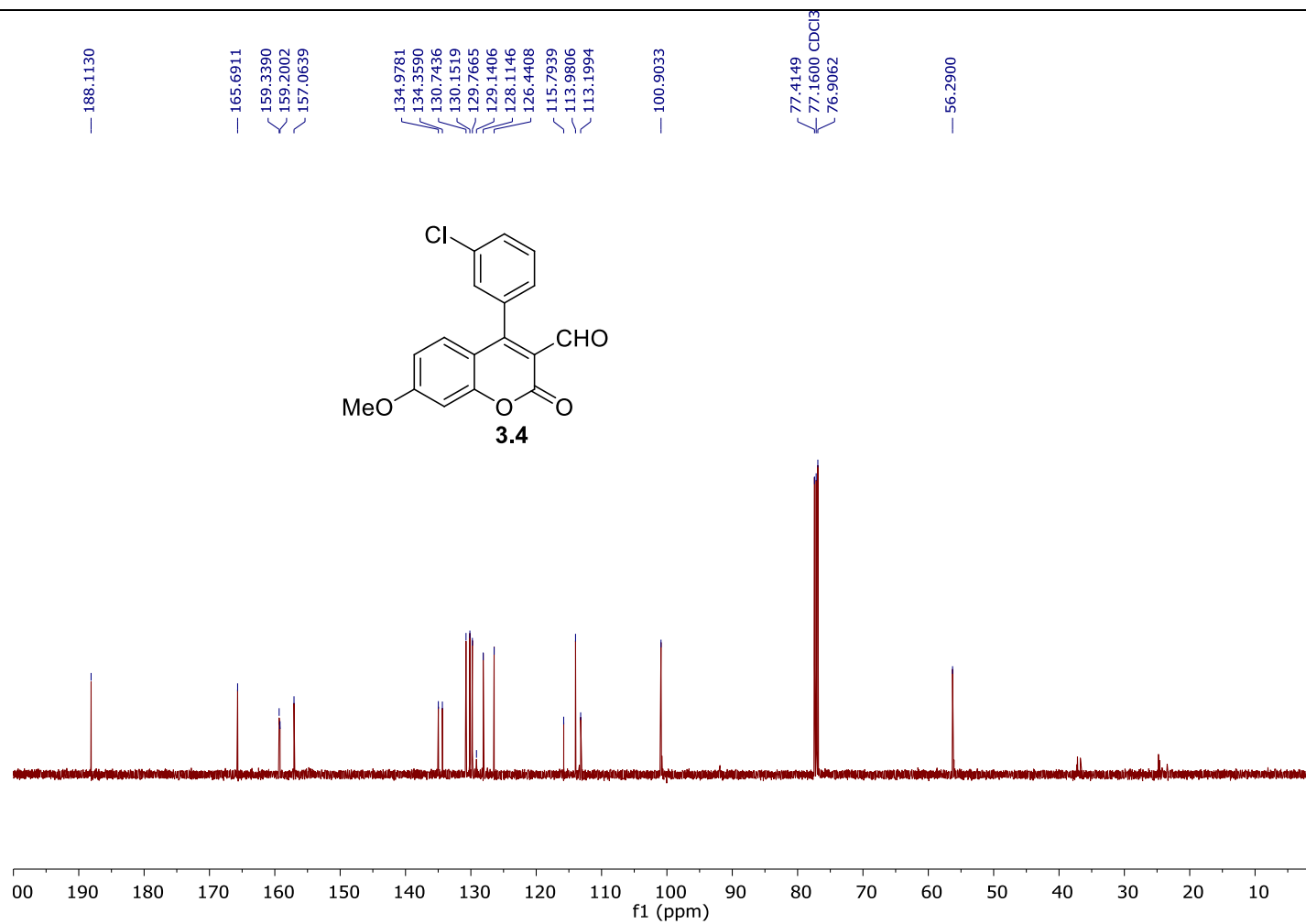
**<sup>1</sup>H Spectrum of 7-methoxy-4-(3-methoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (3.3)**



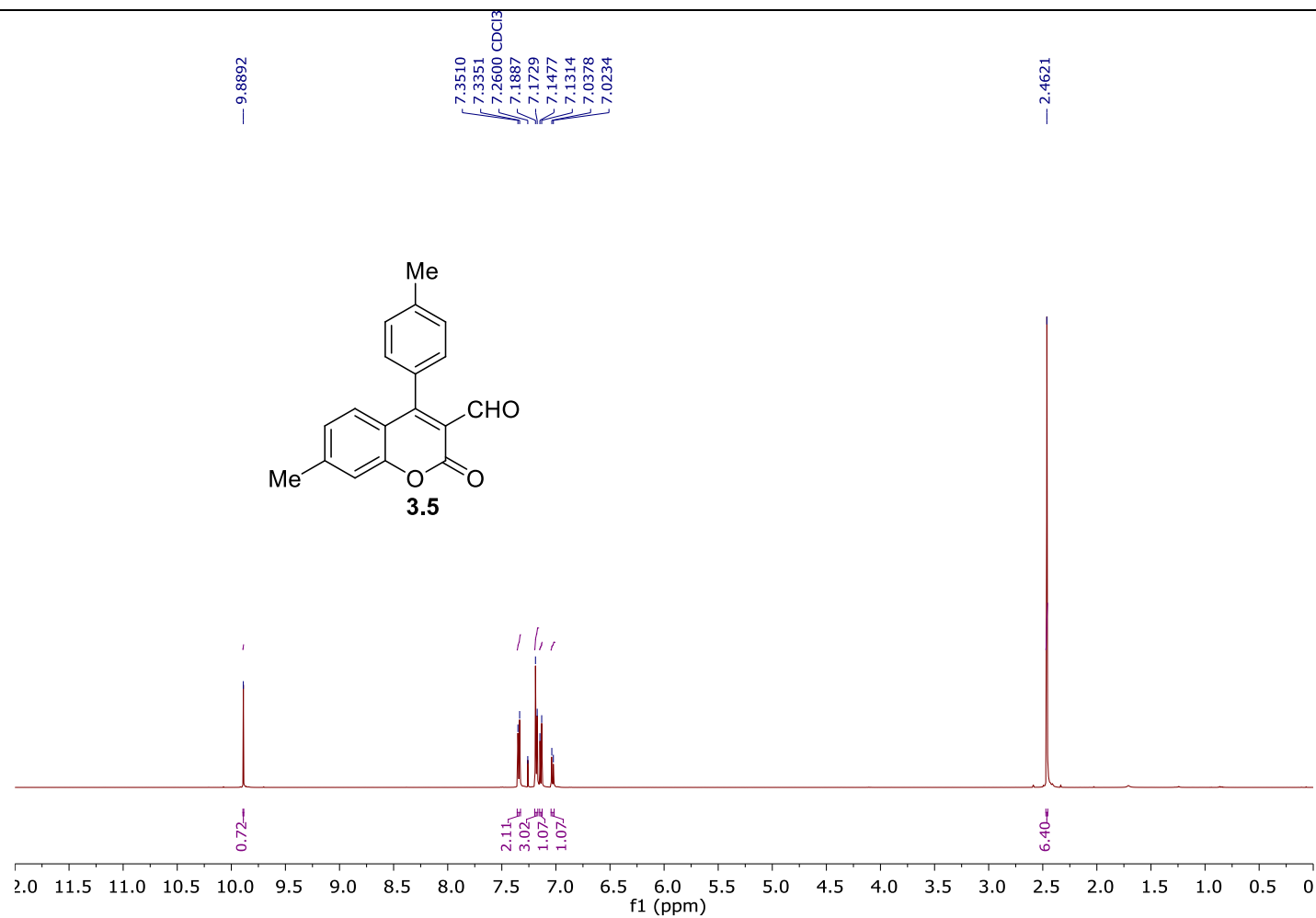
<sup>13</sup>C Spectrum of 7-methoxy-4-(3-methoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (3.3)



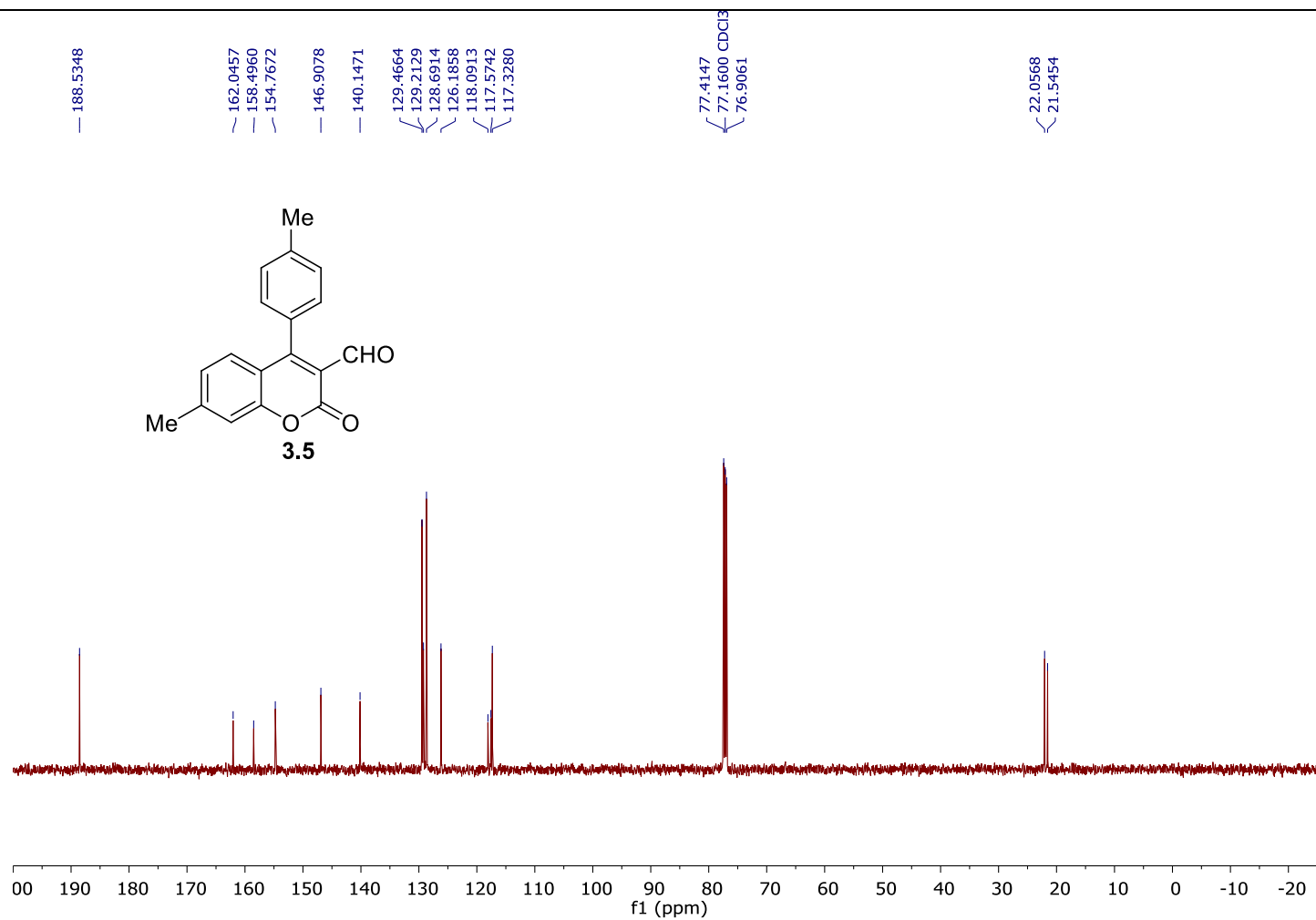
$^1\text{H}$  Spectrum of 4-(3-chlorophenyl)-7-methoxy-2-oxo-2H-chromene-3-carbaldehyde (3.4)



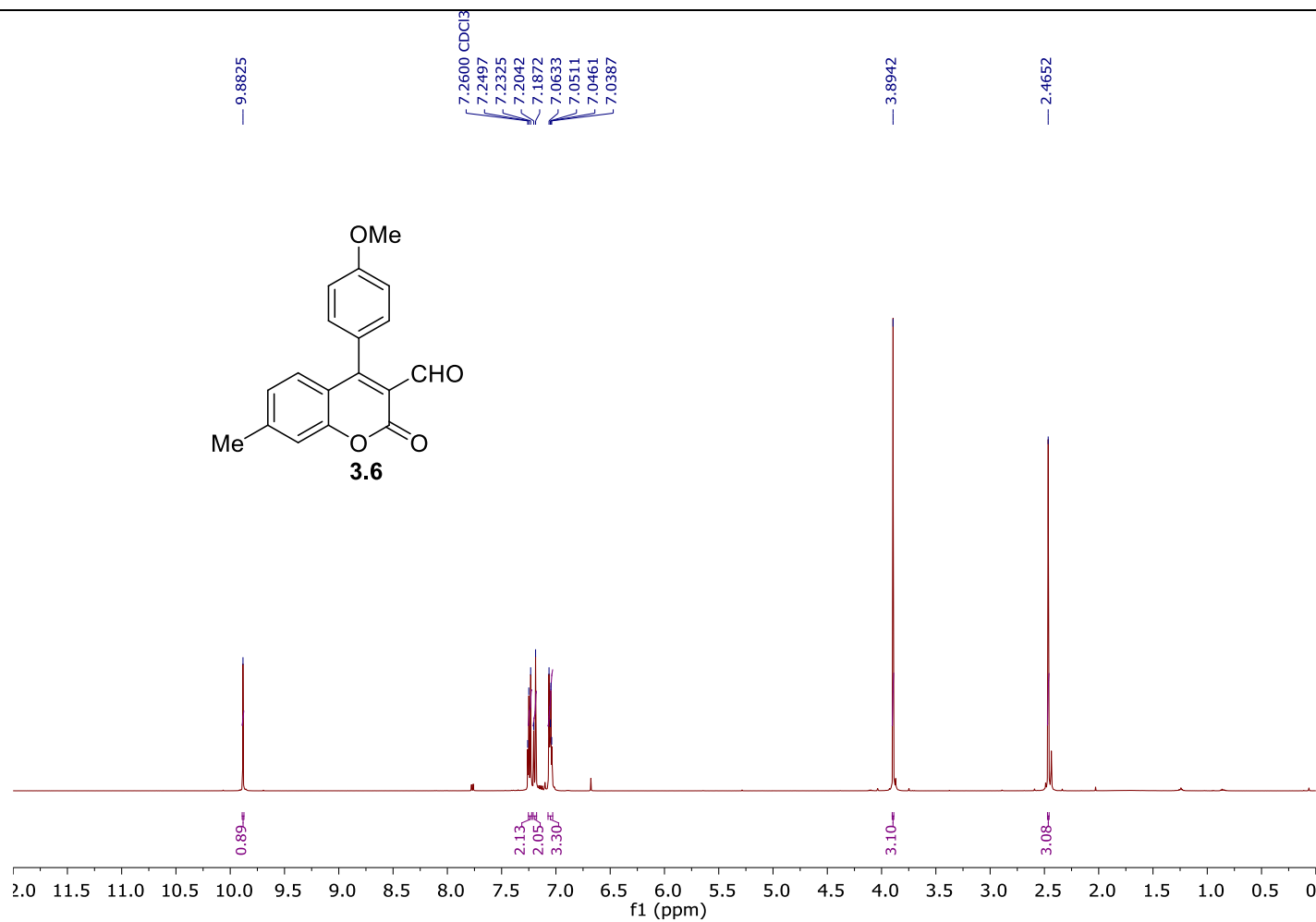
**<sup>13</sup>C Spectrum of 4-(3-chlorophenyl)-7-methoxy-2-oxo-2H-chromene-3-carbaldehyde (3.4)**



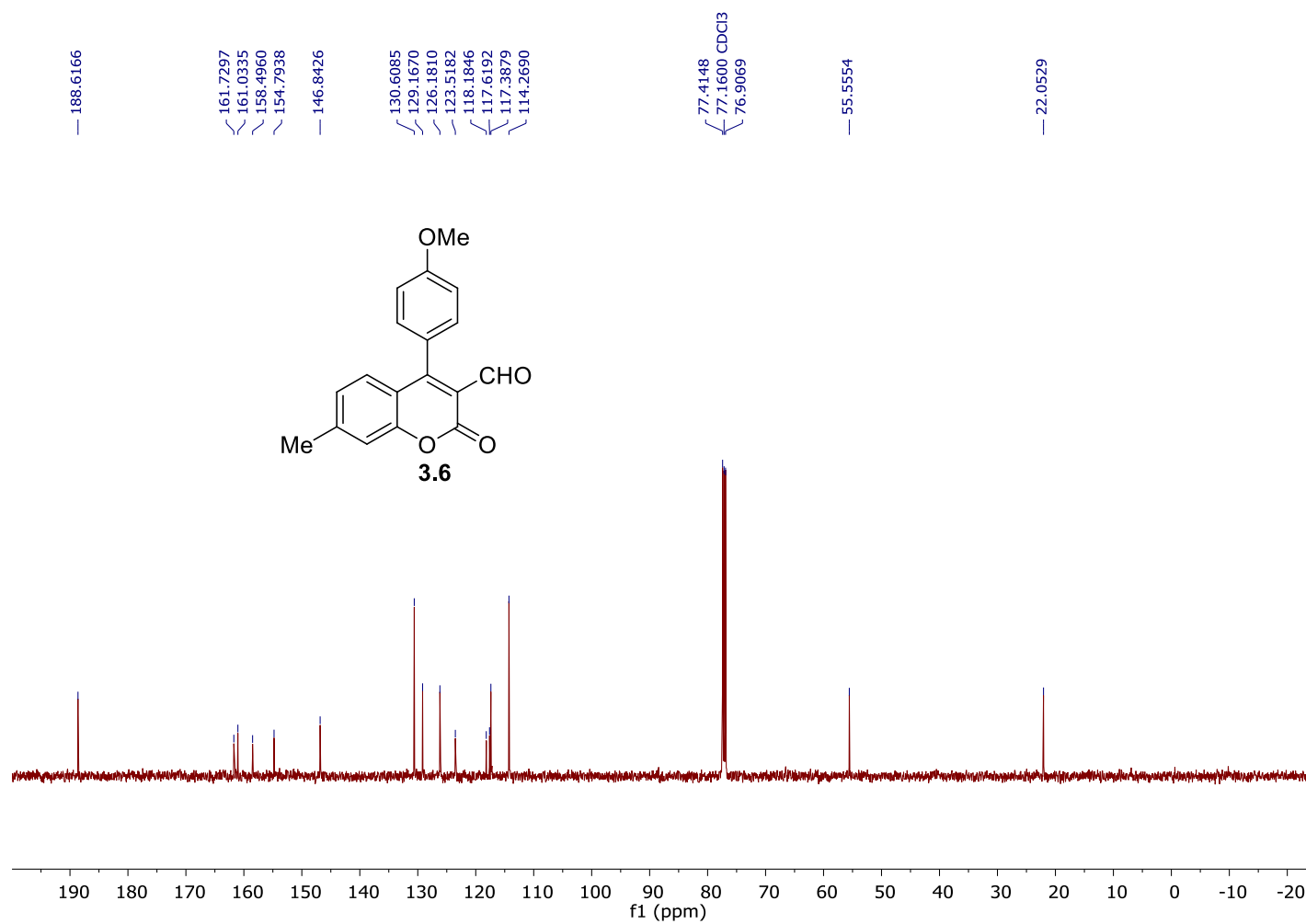
**<sup>1</sup>H Spectrum of 7-methyl-2-oxo-4-p-tolyl-2H-chromene-3-carbaldehyde (3.5)**



<sup>13</sup>C Spectrum of 7-methyl-2-oxo-4-p-tolyl-2H-chromene-3-carbaldehyde (3.5)

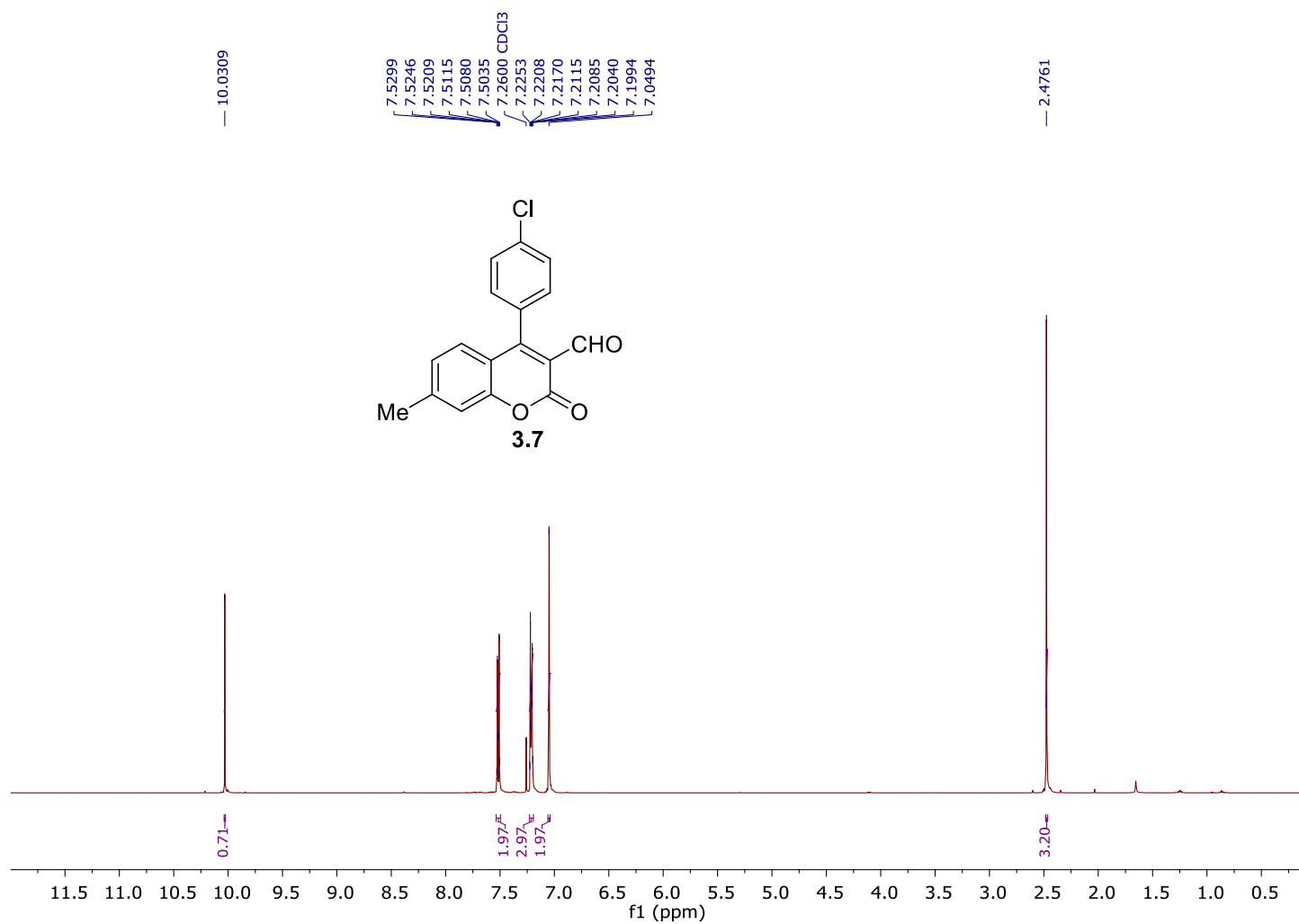


<sup>1</sup>H Spectrum of 4-(4-methoxyphenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.6)

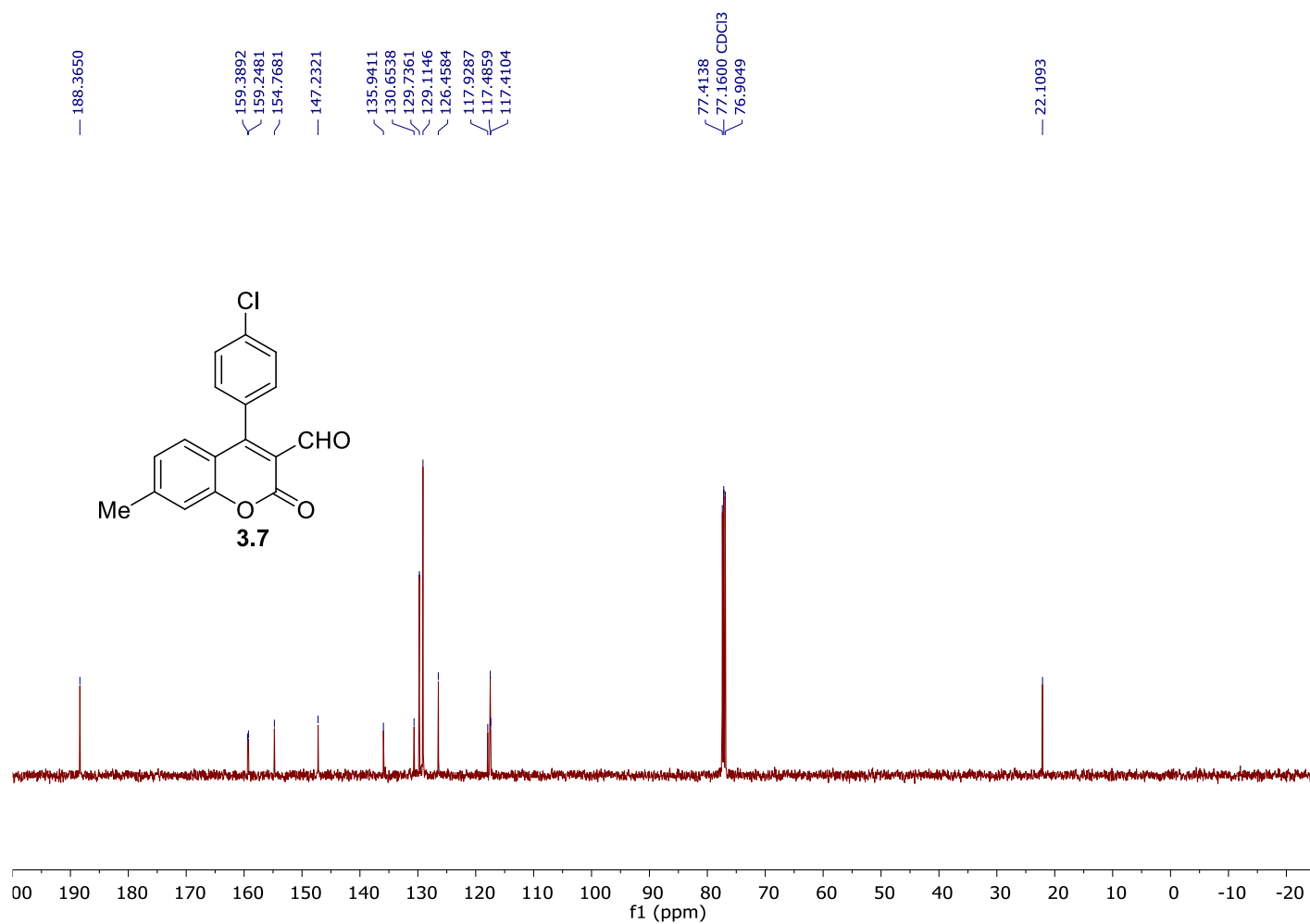


<sup>13</sup>C Spectrum of 4-(4-methoxyphenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.6)

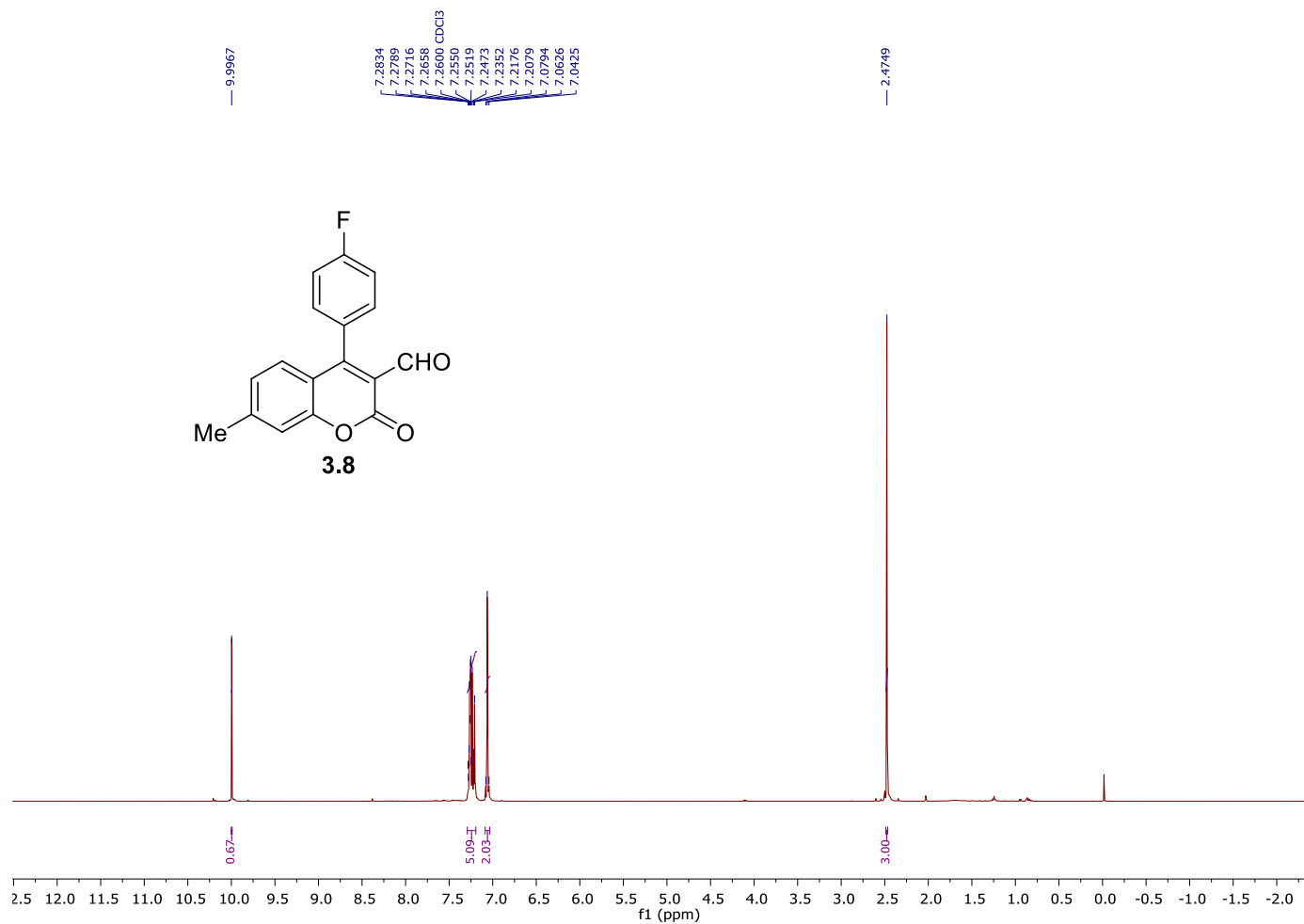




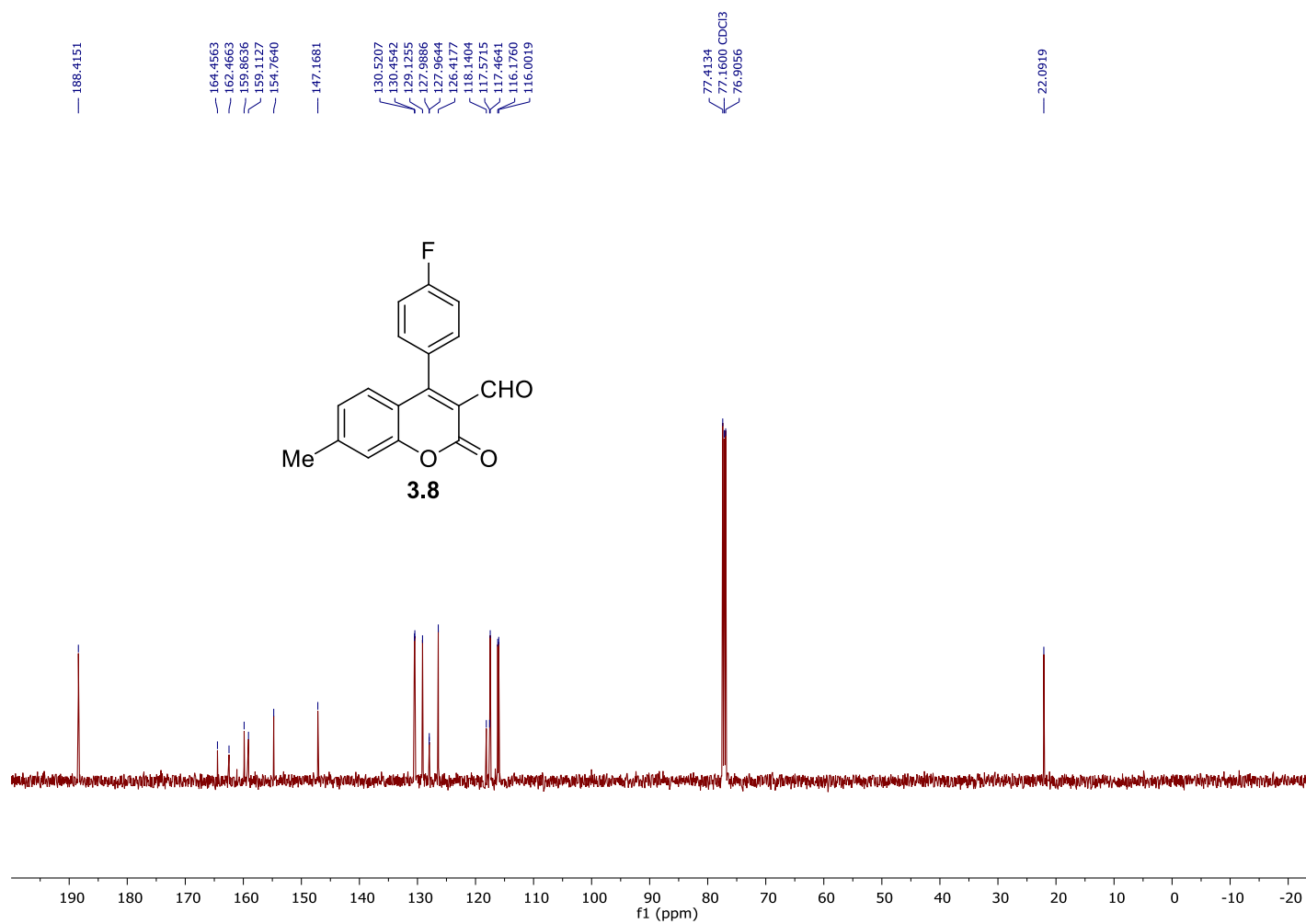
<sup>1</sup>H Spectrum of 4-(4-chlorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.7)



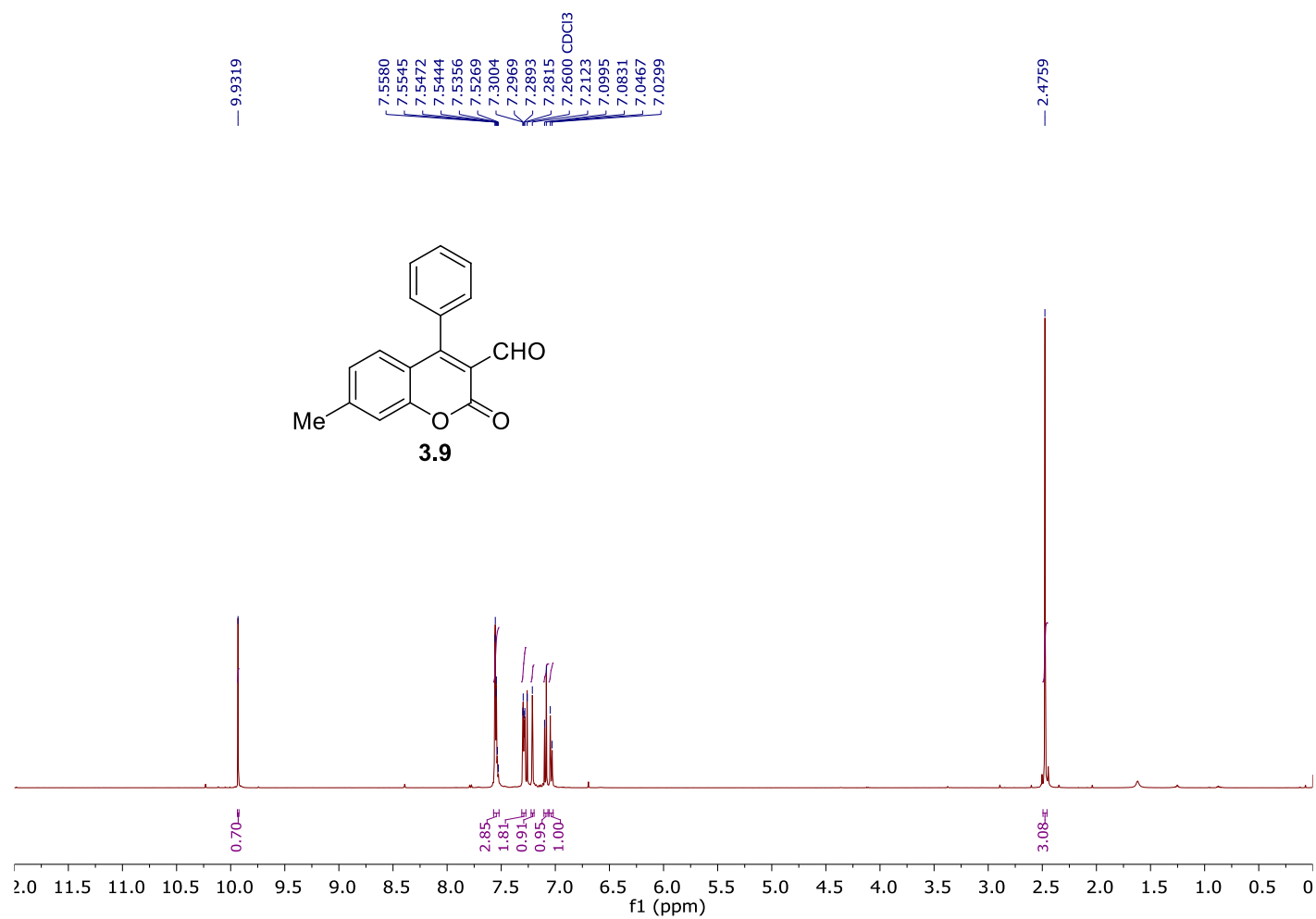
<sup>13</sup>C Spectrum of 4-(4-chlorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.7)



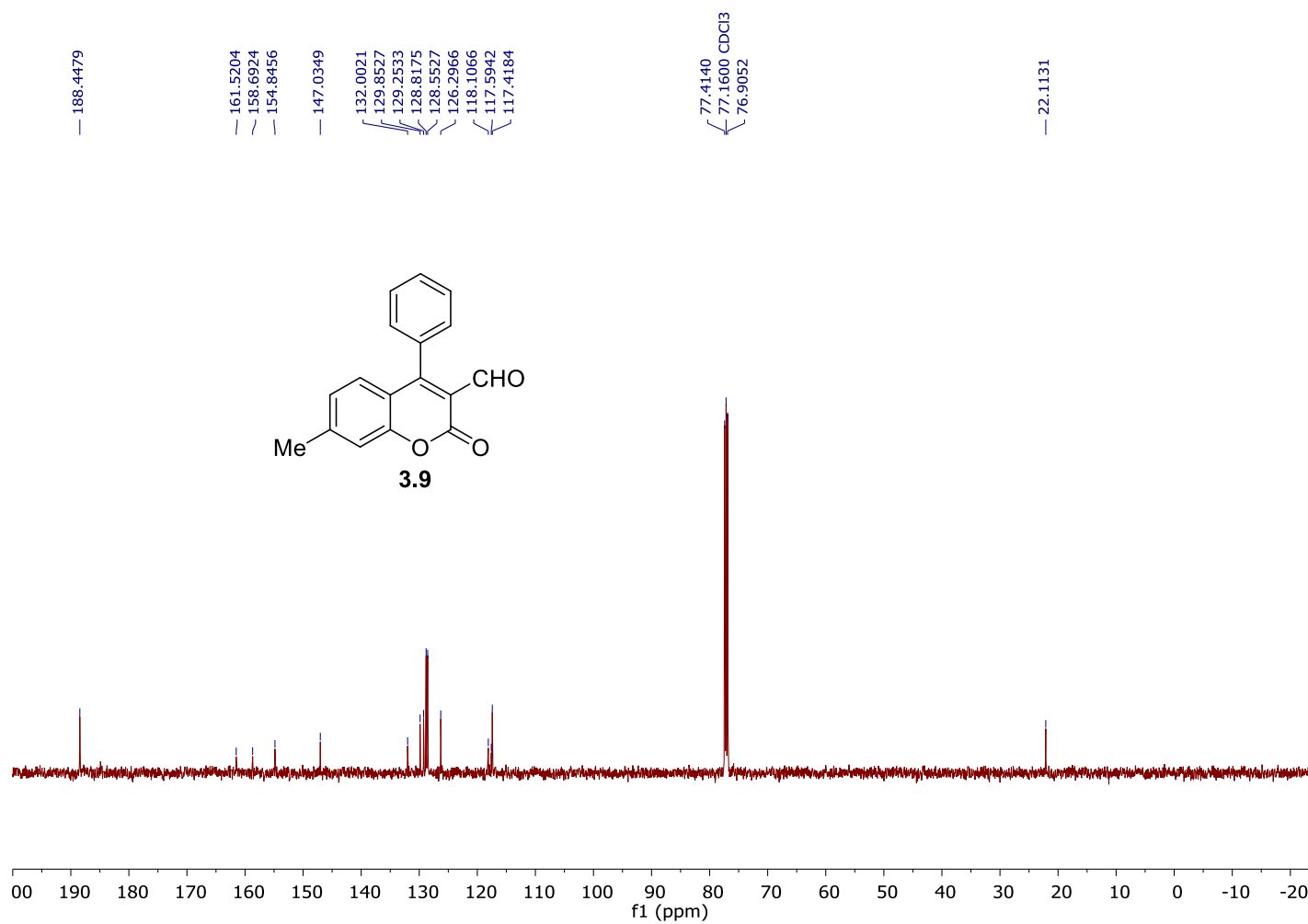
**<sup>1</sup>H Spectrum of 4-(4-fluorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.8)**



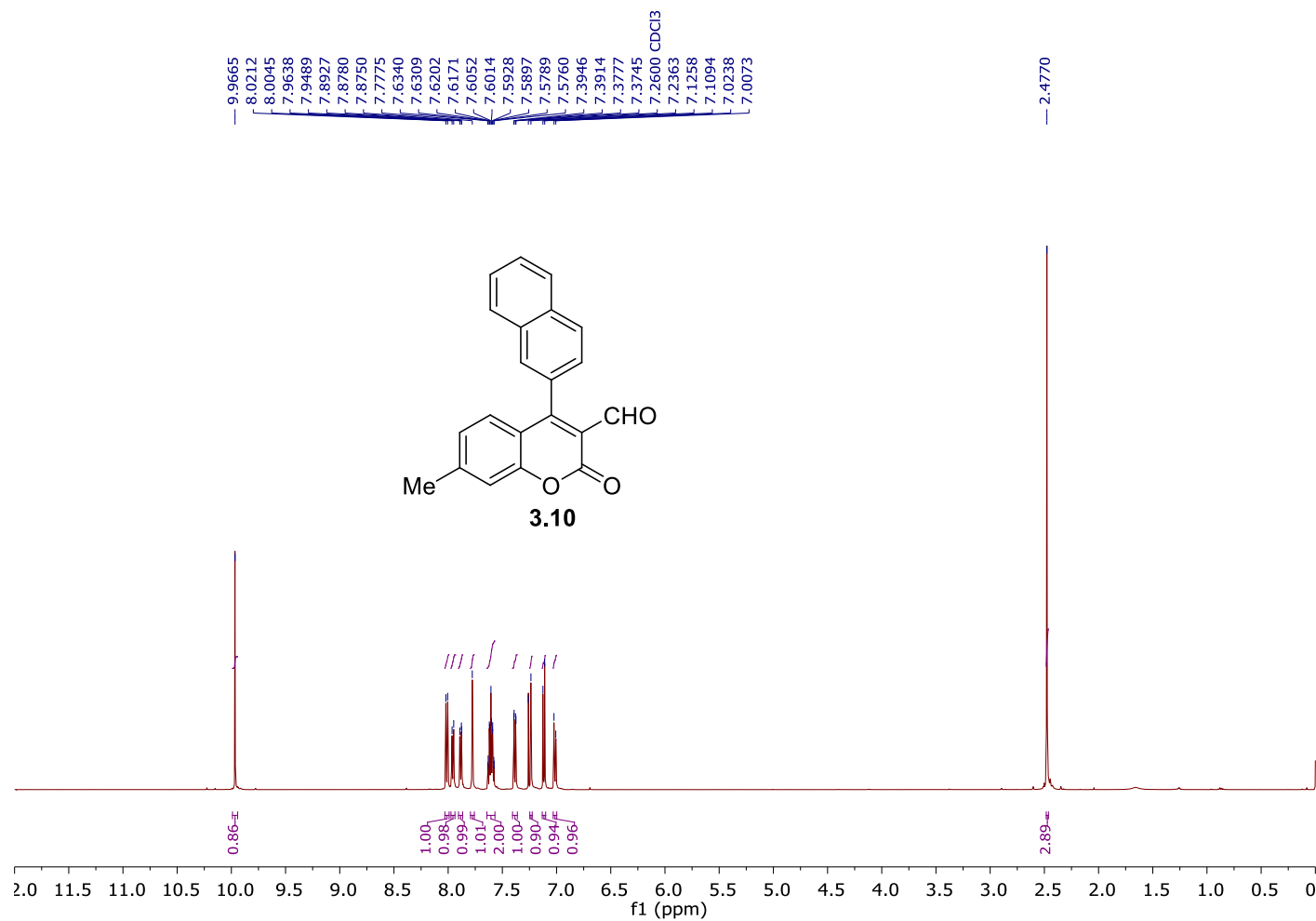
**<sup>13</sup>C Spectrum of 4-(4-fluorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.8)**



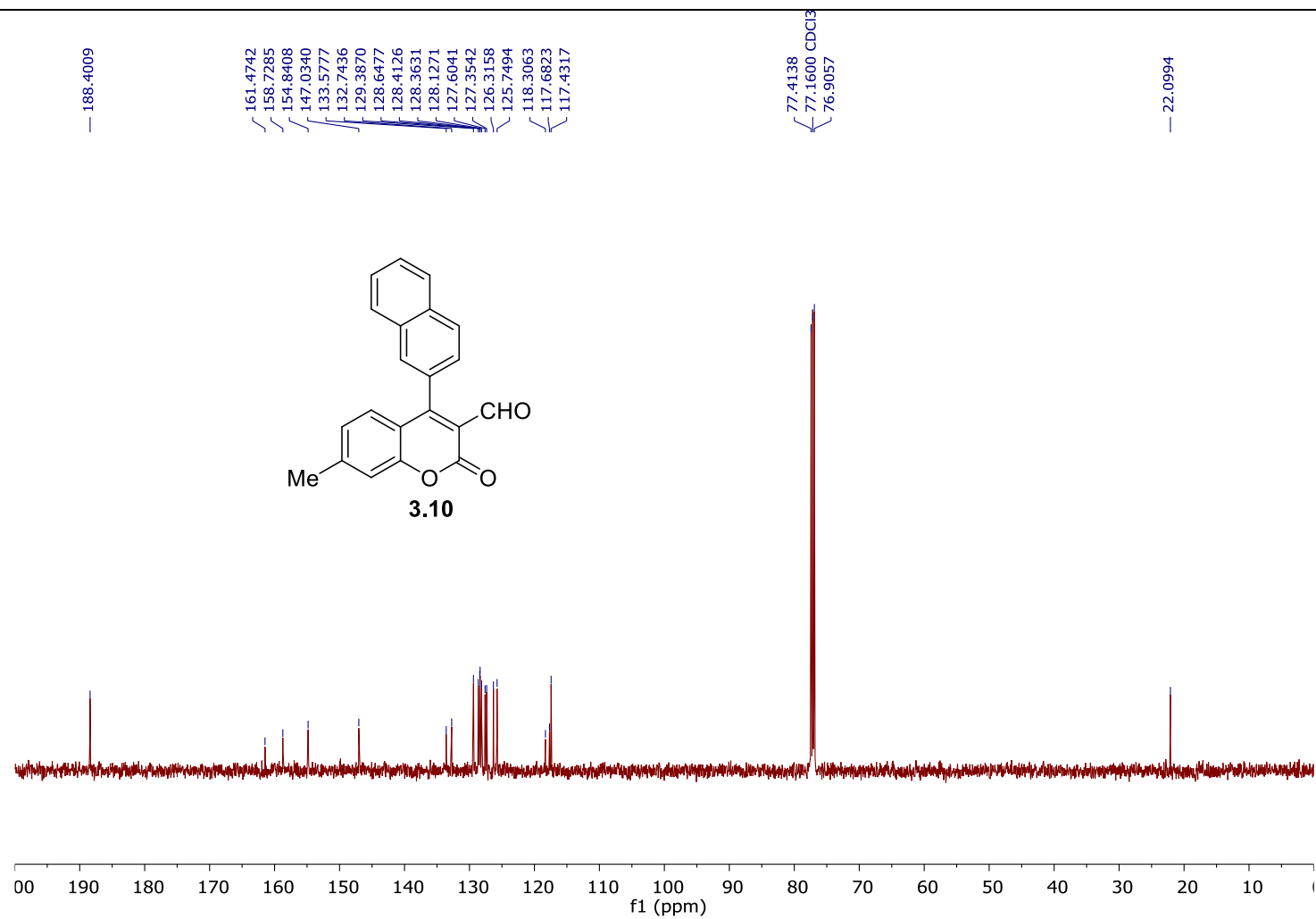
<sup>1</sup>H Spectrum of 7-methyl-2-oxo-4-phenyl-2H-chromene-3-carbaldehyde (3.9)



<sup>13</sup>C Spectrum of 7-methyl-2-oxo-4-phenyl-2H-chromene-3-carbaldehyde (3.9)

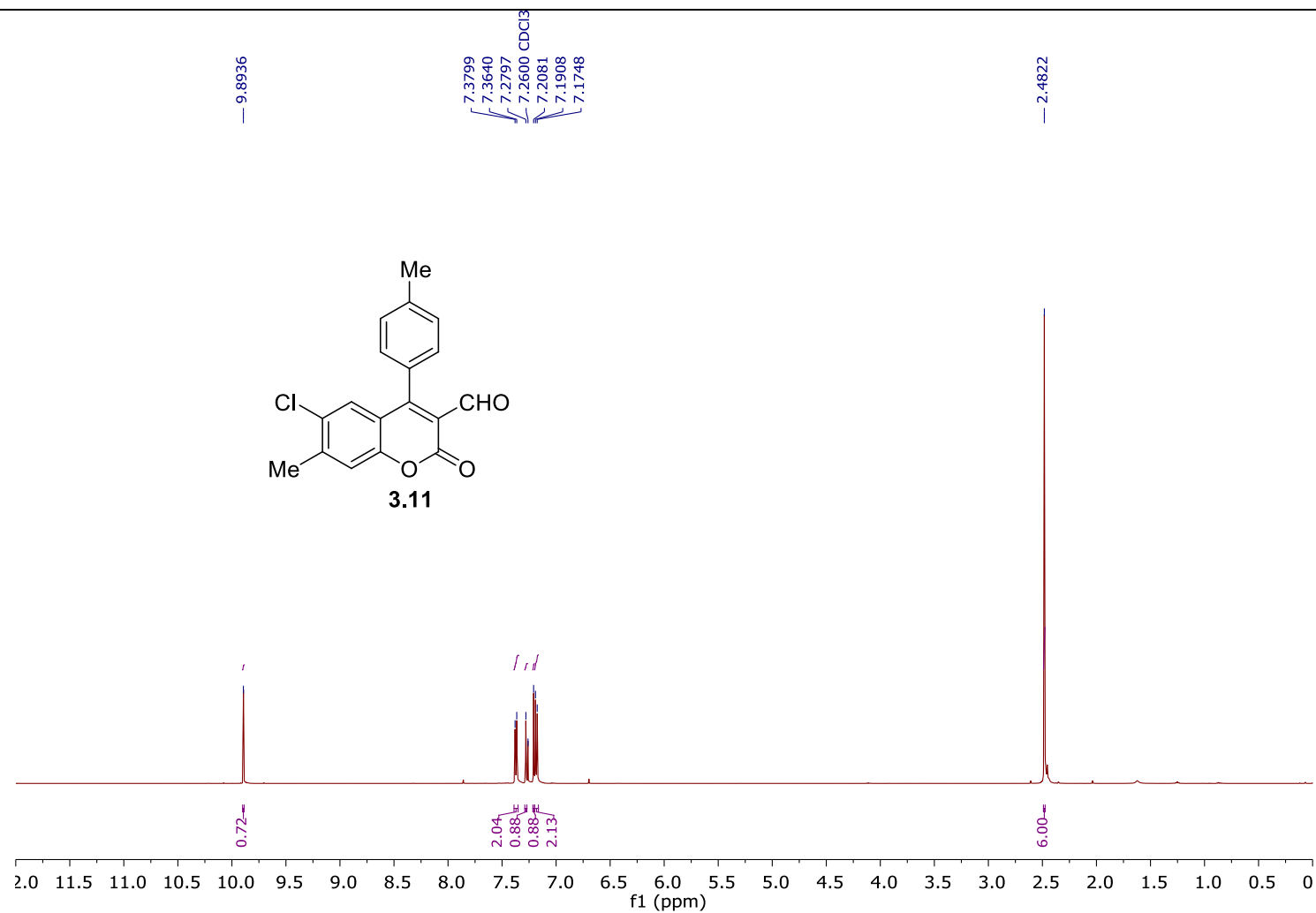


<sup>1</sup>H Spectrum of 7-methyl-4-(naphthalen-2-yl)-2-oxo-2H-chromene-3-carbaldehyde (3.10)

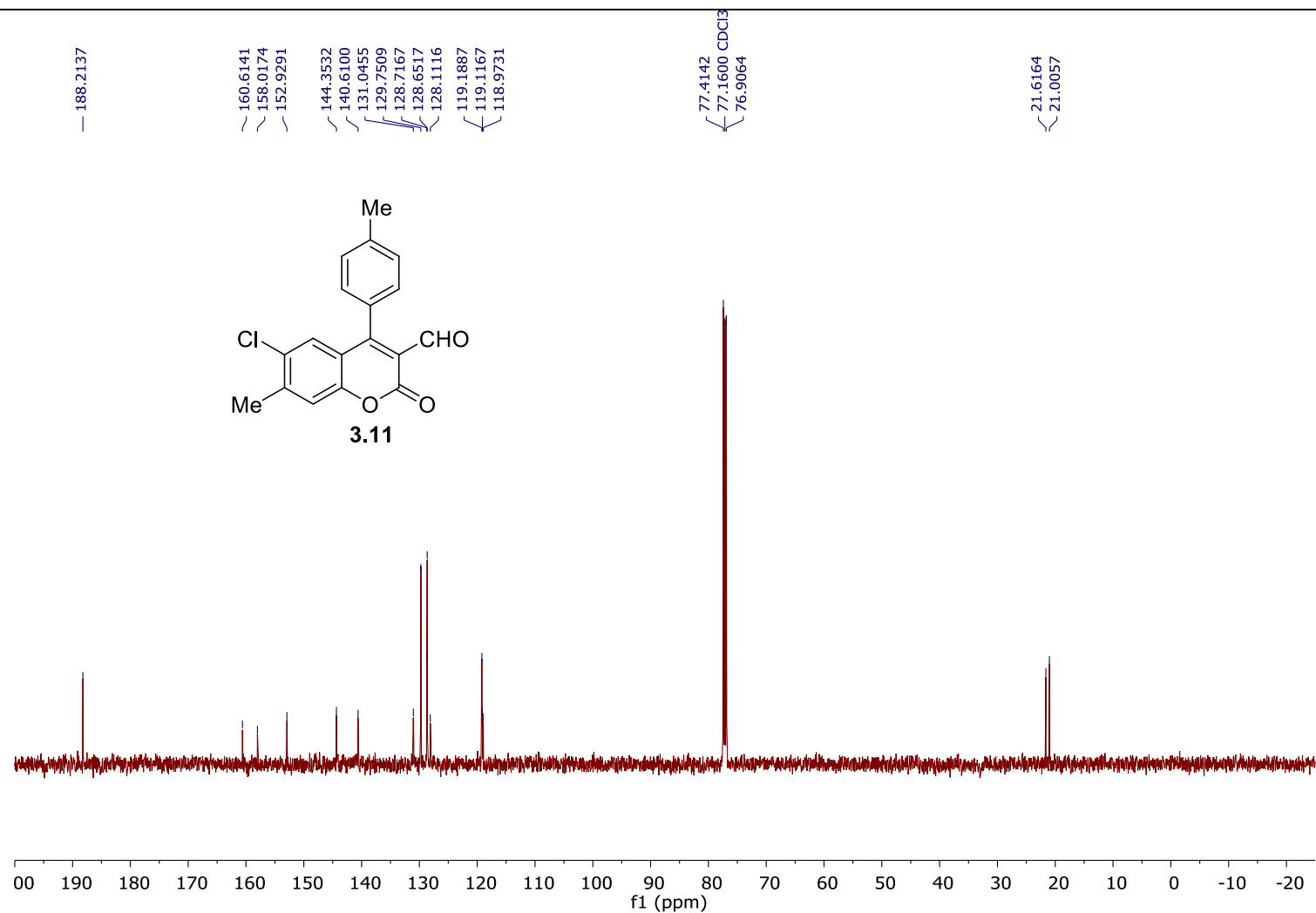


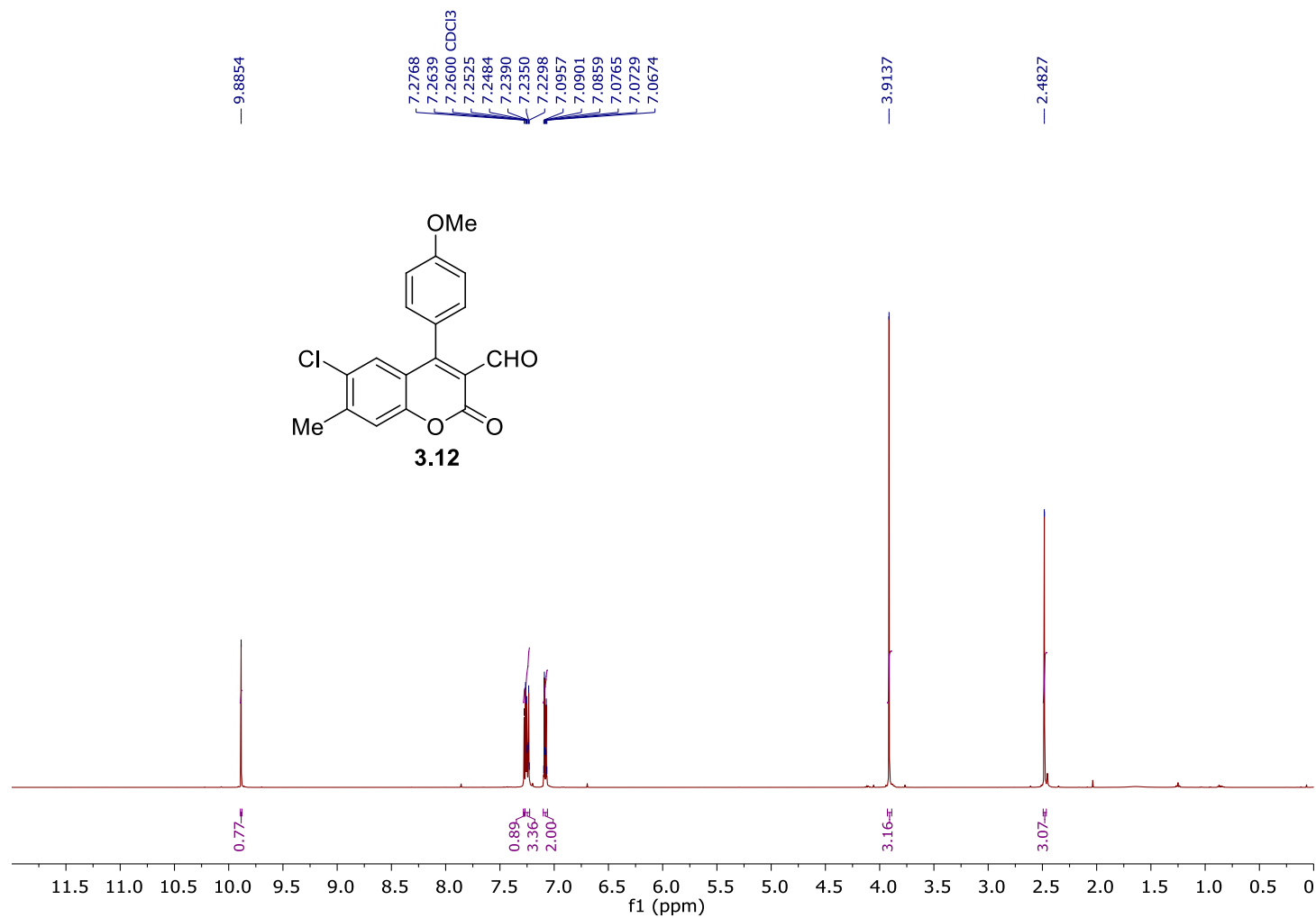
<sup>13</sup>C Spectrum of 7-methyl-4-(naphthalen-2-yl)-2-oxo-2H-chromene-3-carbaldehyde (3.10)



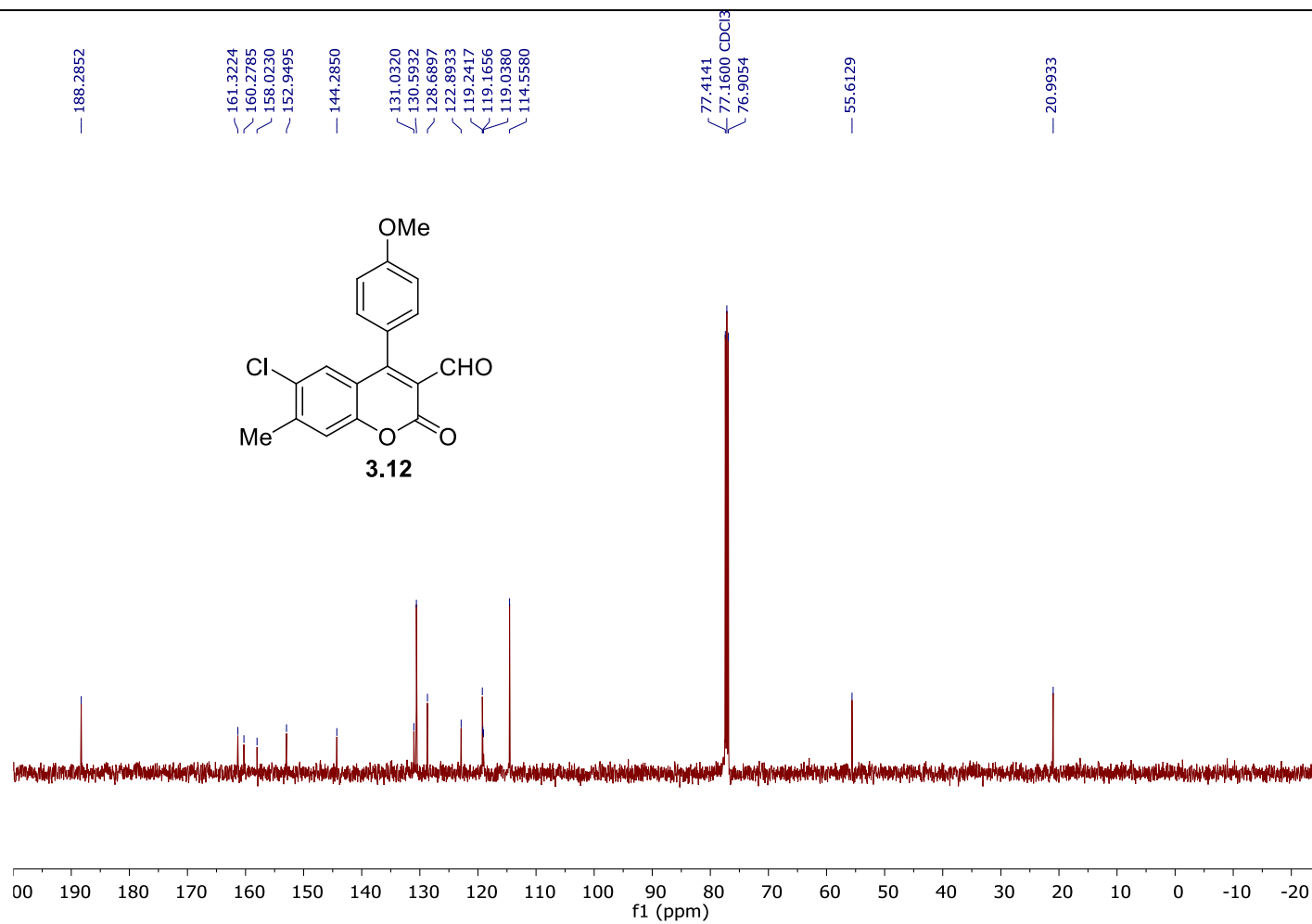


<sup>1</sup>H Spectrum of 6-chloro-7-methyl-2-oxo-4-*p*-tolyl-2*H*-chromene-3-carbaldehyde (3.11)

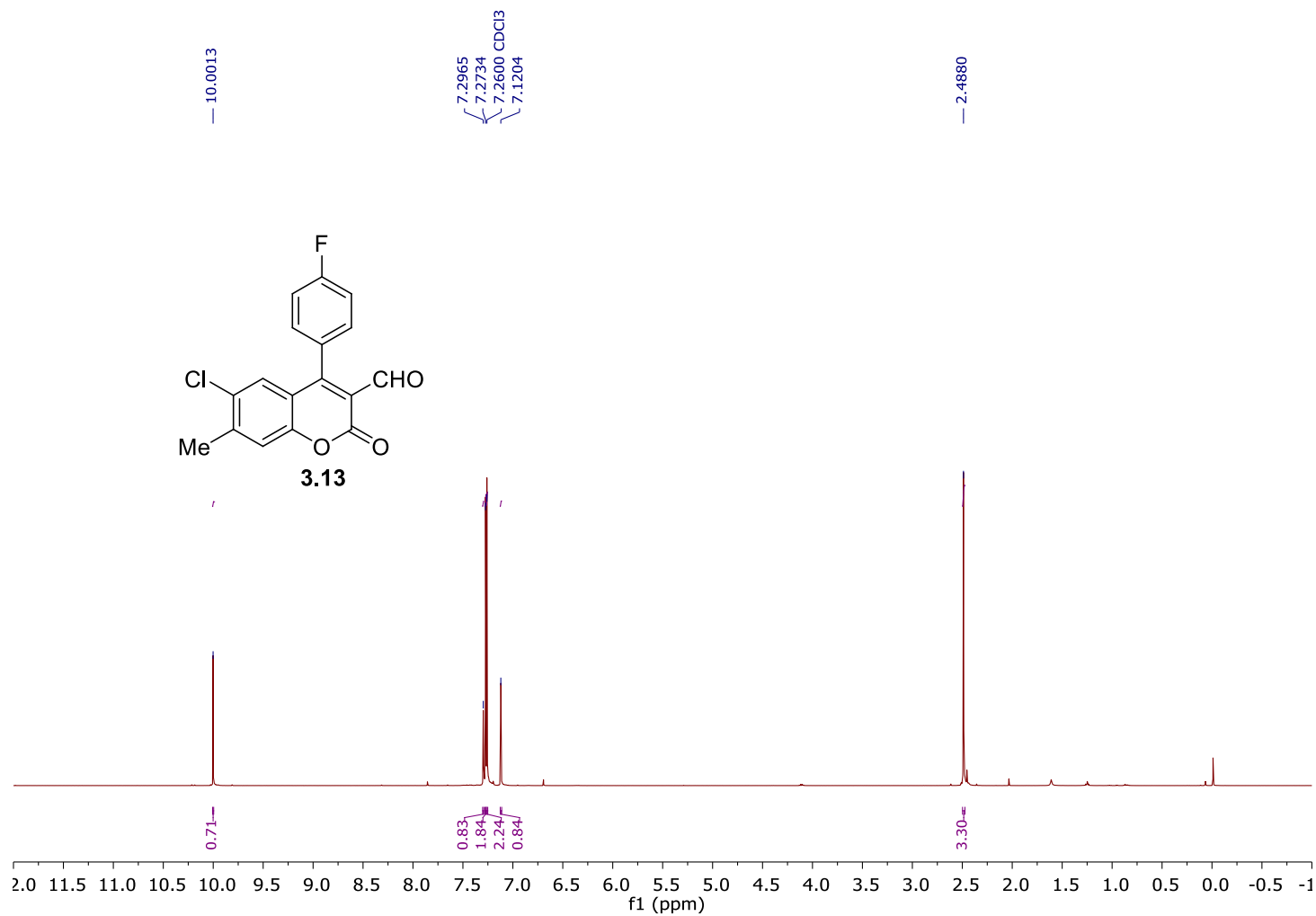




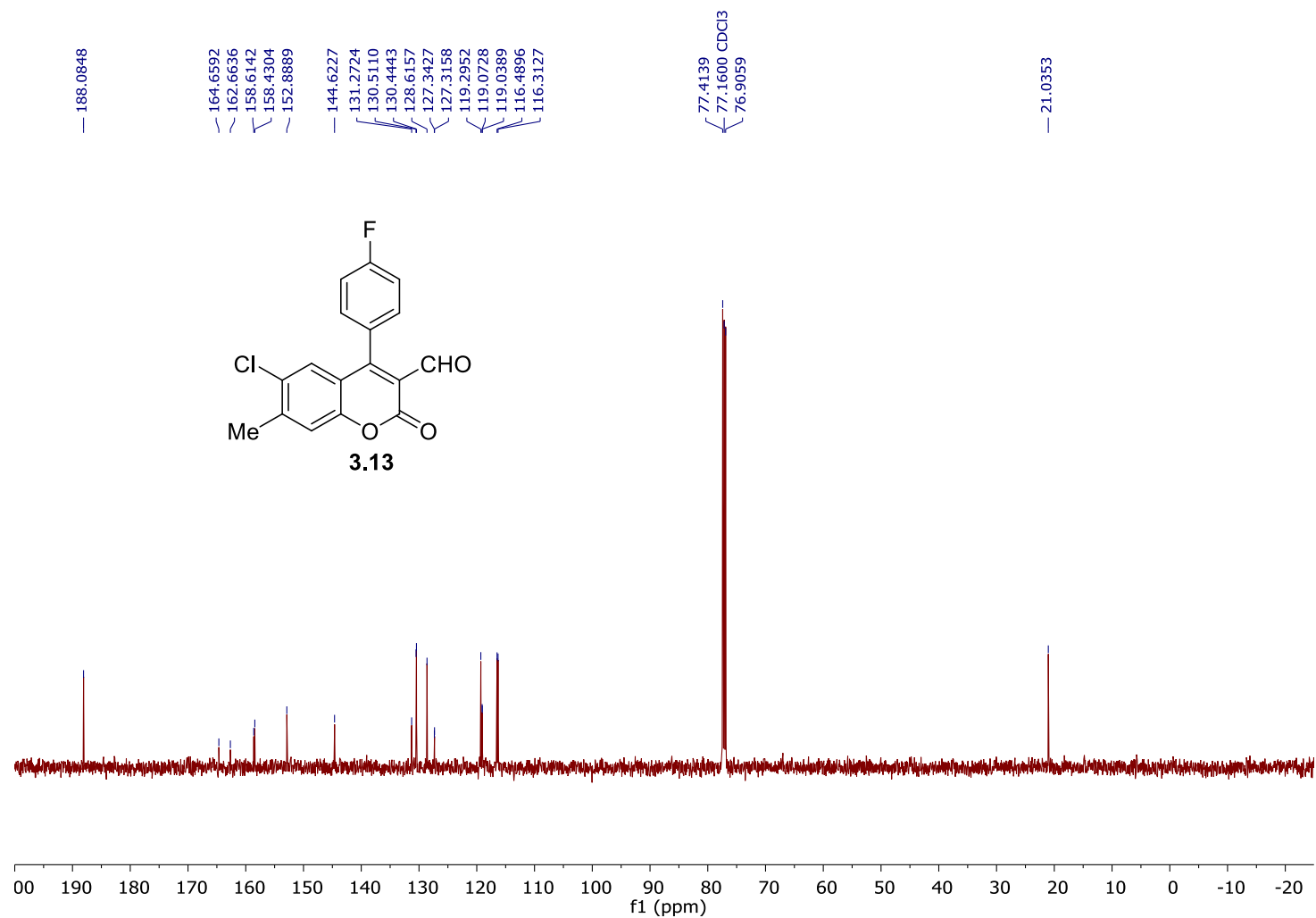
<sup>1</sup>H Spectrum of 6-chloro-4-(4-methoxyphenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.12)



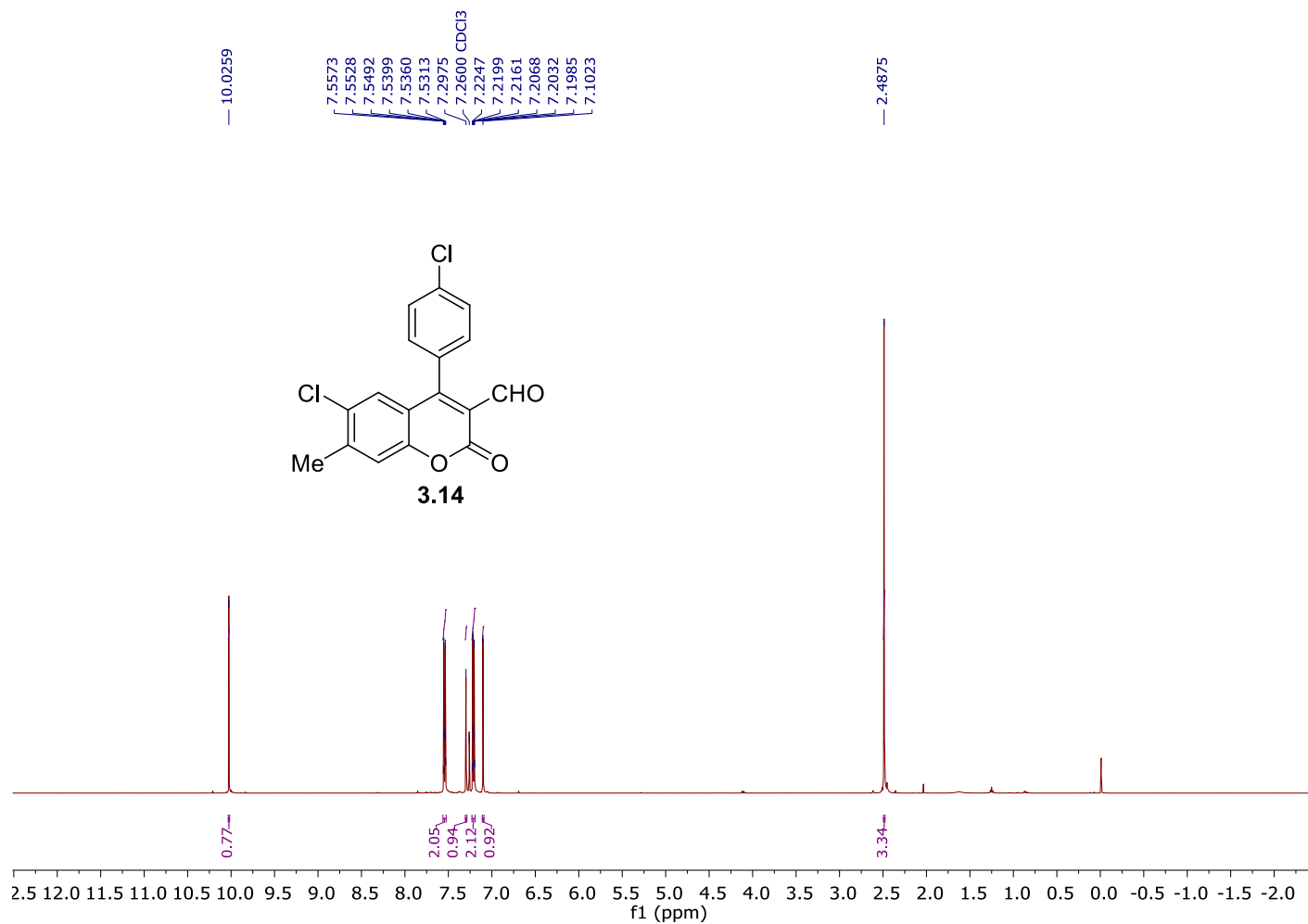
<sup>13</sup>C Spectrum of 6-chloro-4-(4-methoxyphenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.12)



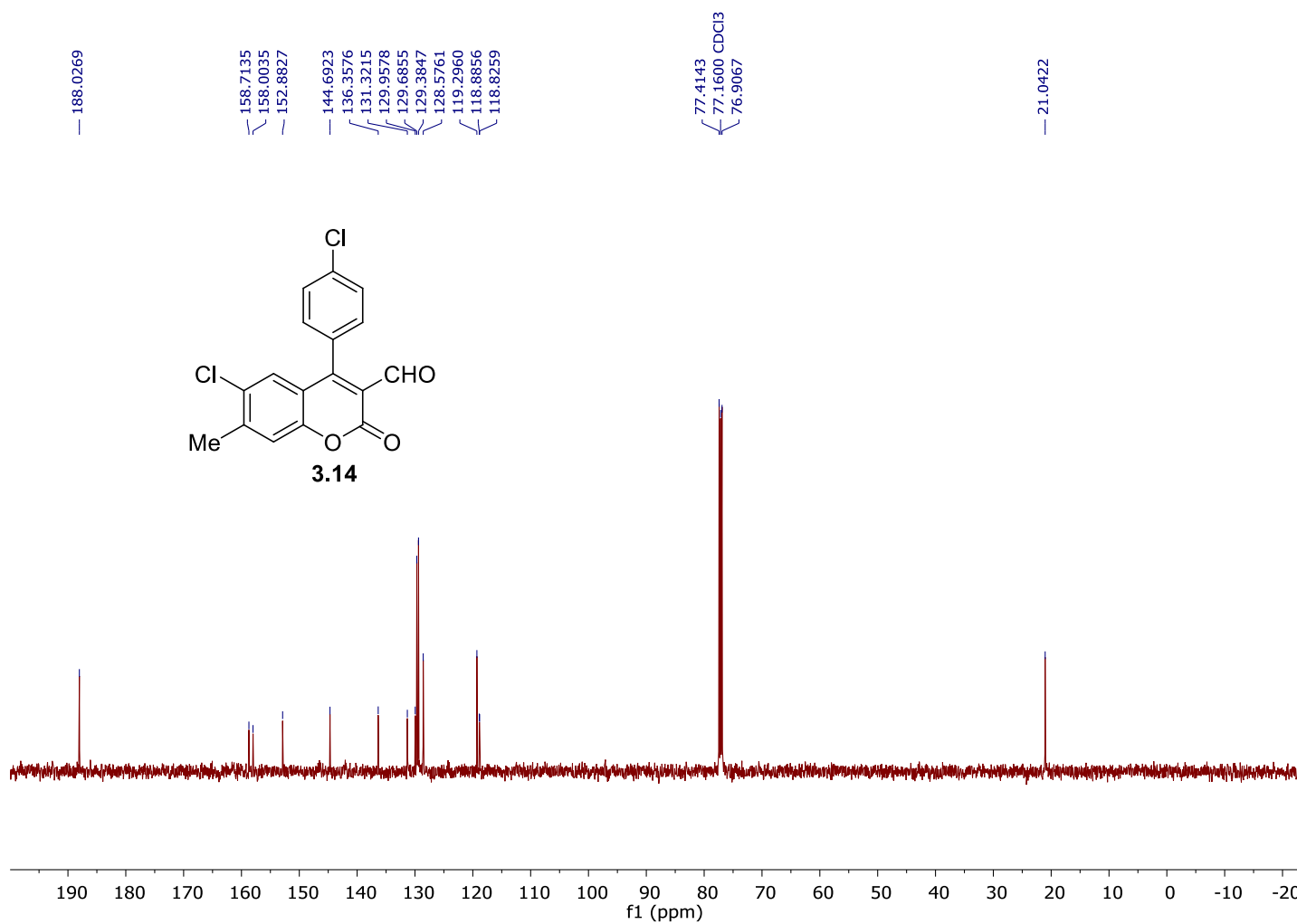
**<sup>1</sup>H Spectrum of 6-chloro-4-(4-fluorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.13)**



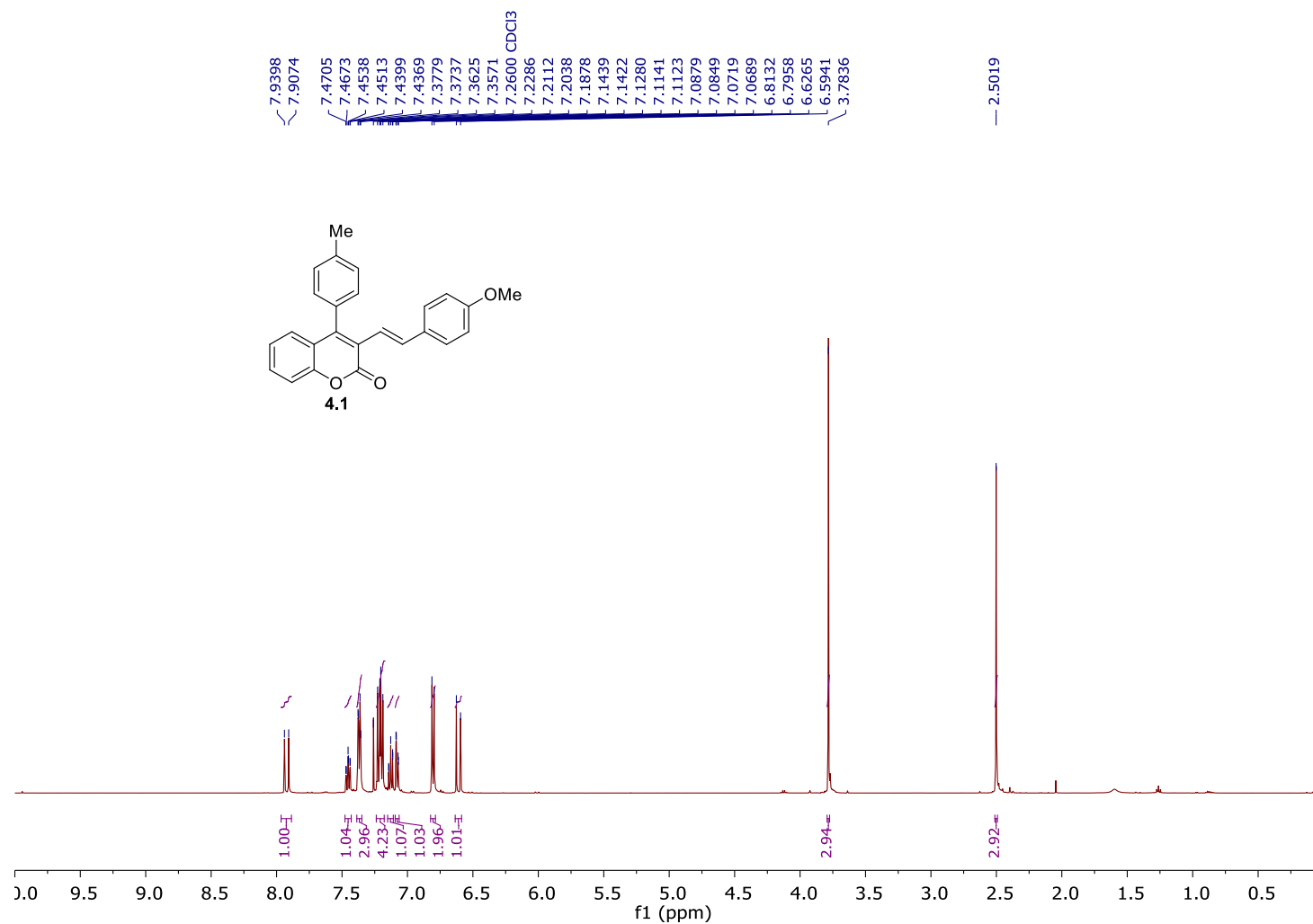
<sup>13</sup>C Spectrum of 6-chloro-4-(4-fluorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.13)



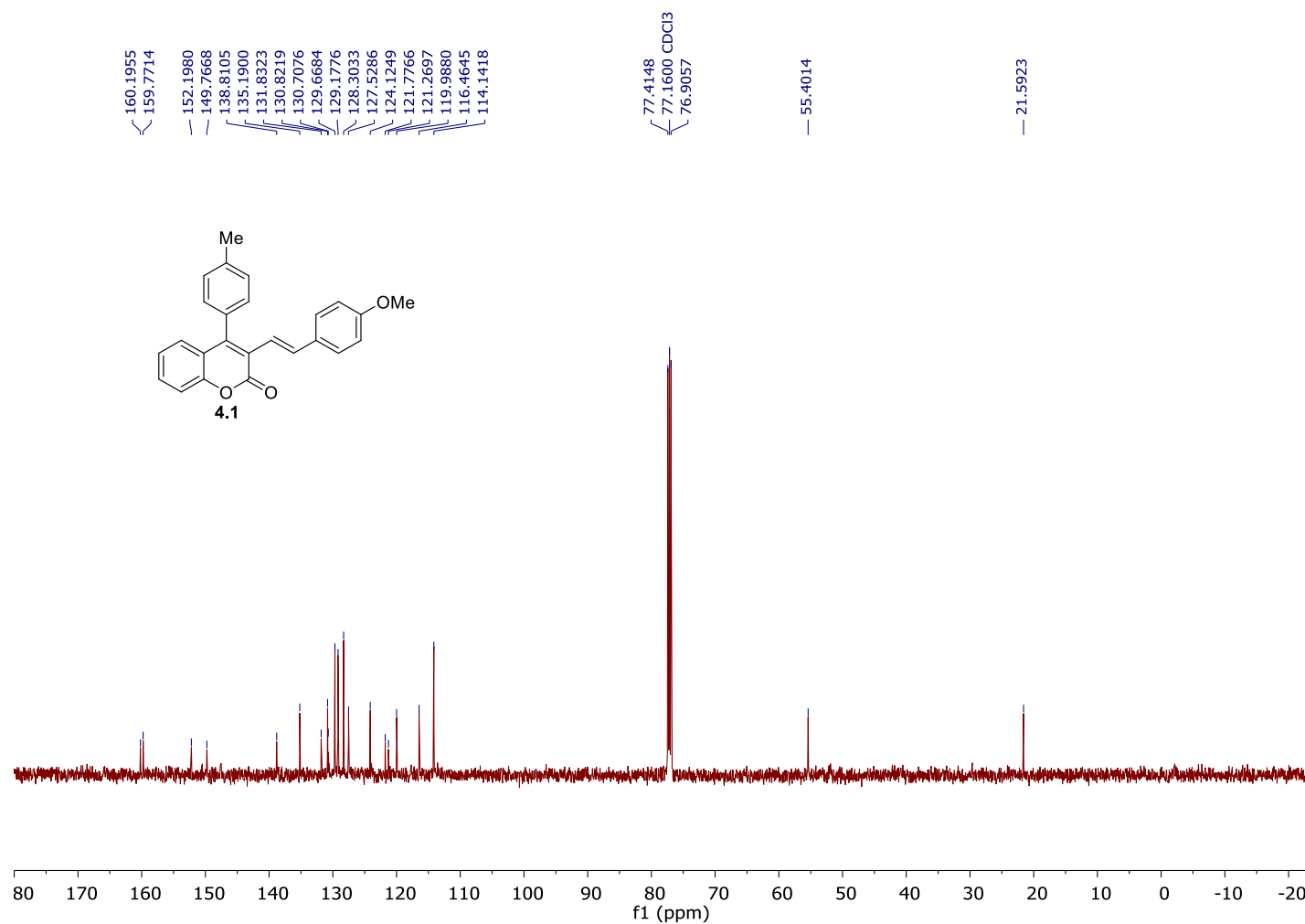
<sup>1</sup>H Spectrum of 6-chloro-4-(4-chlorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.14)



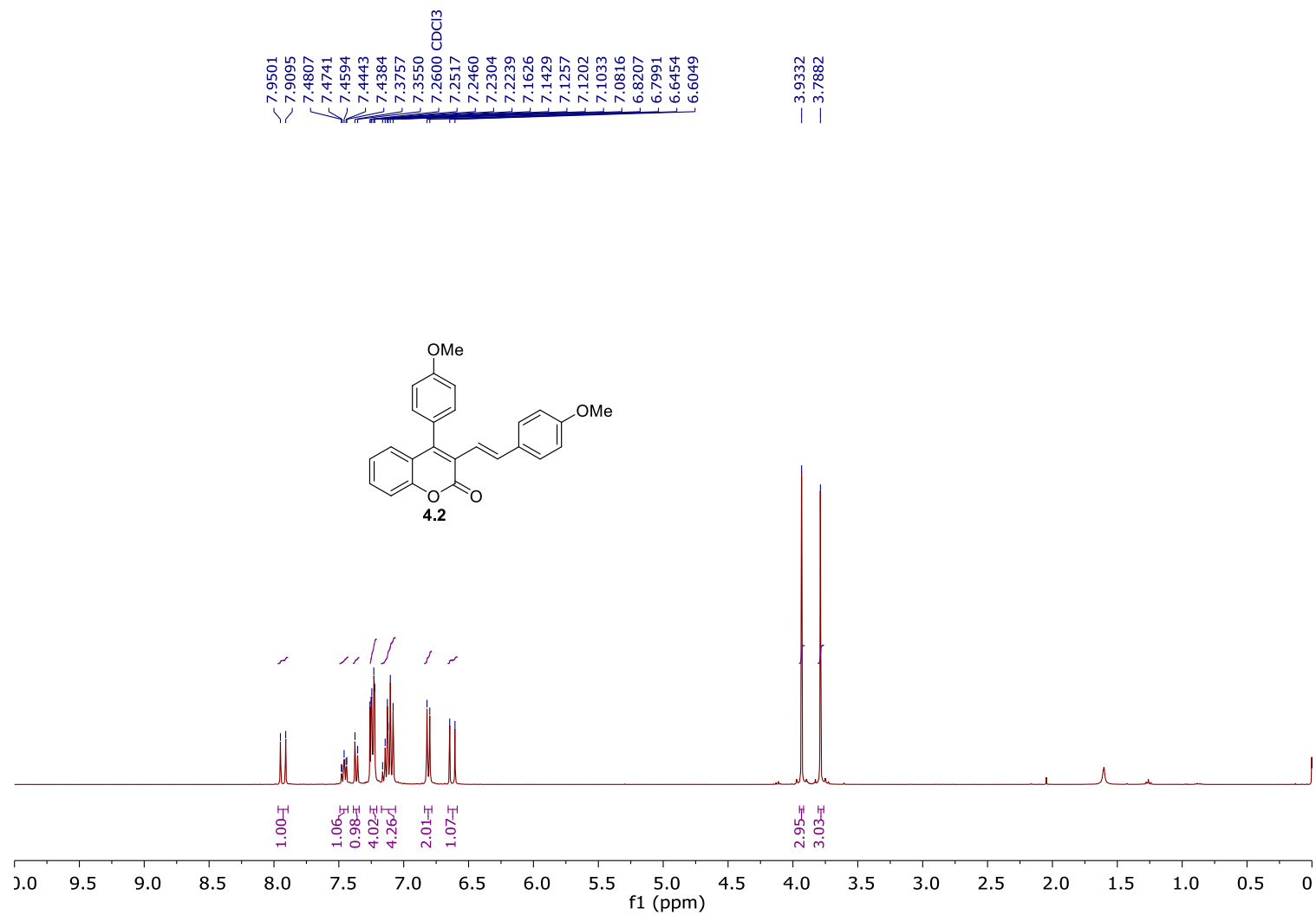




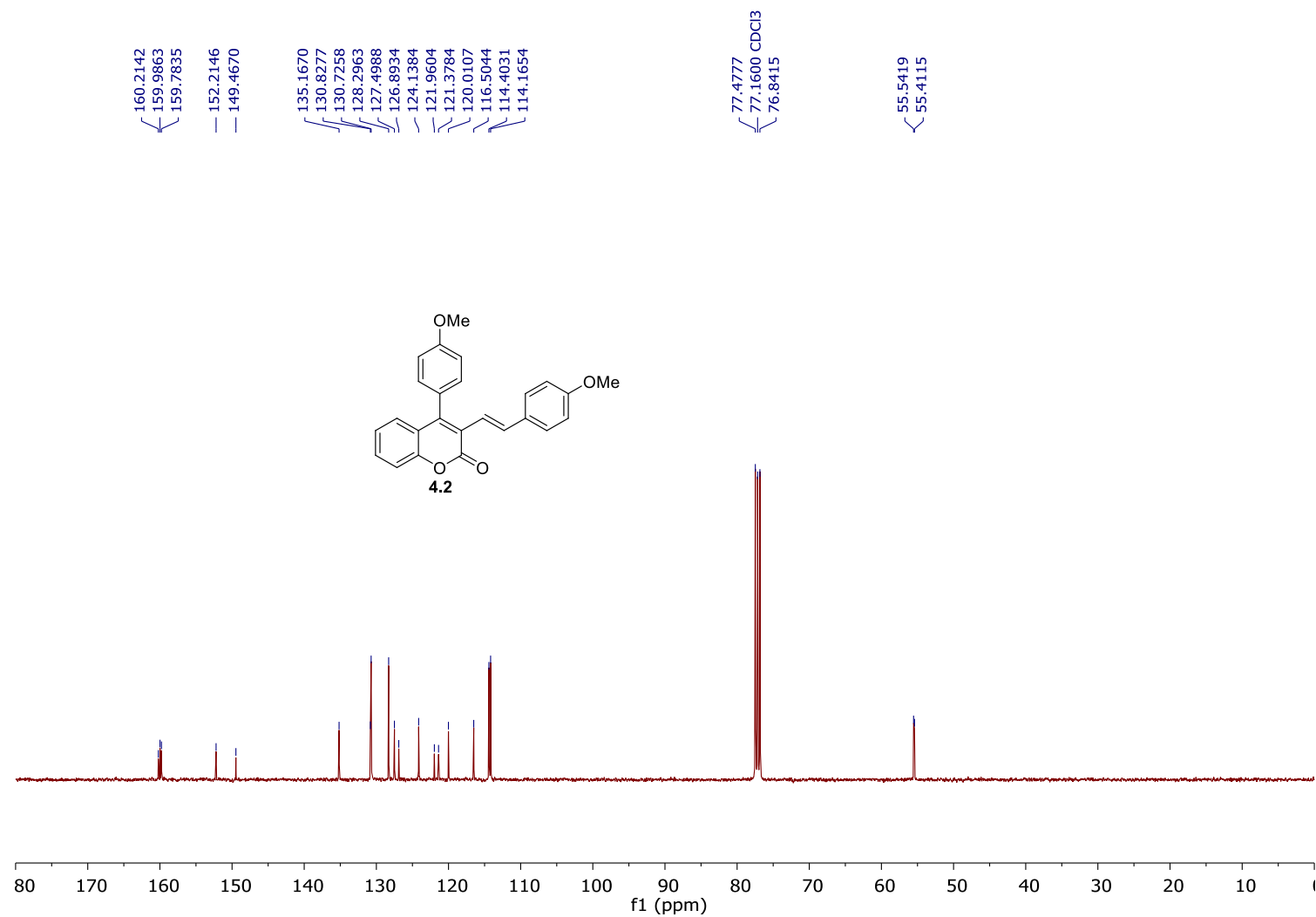
**<sup>1</sup>H Spectrum of (*E*)-3-(4-methoxystyryl)-4-*p*-tolyl-2H-chromen-2-one (4.1)**



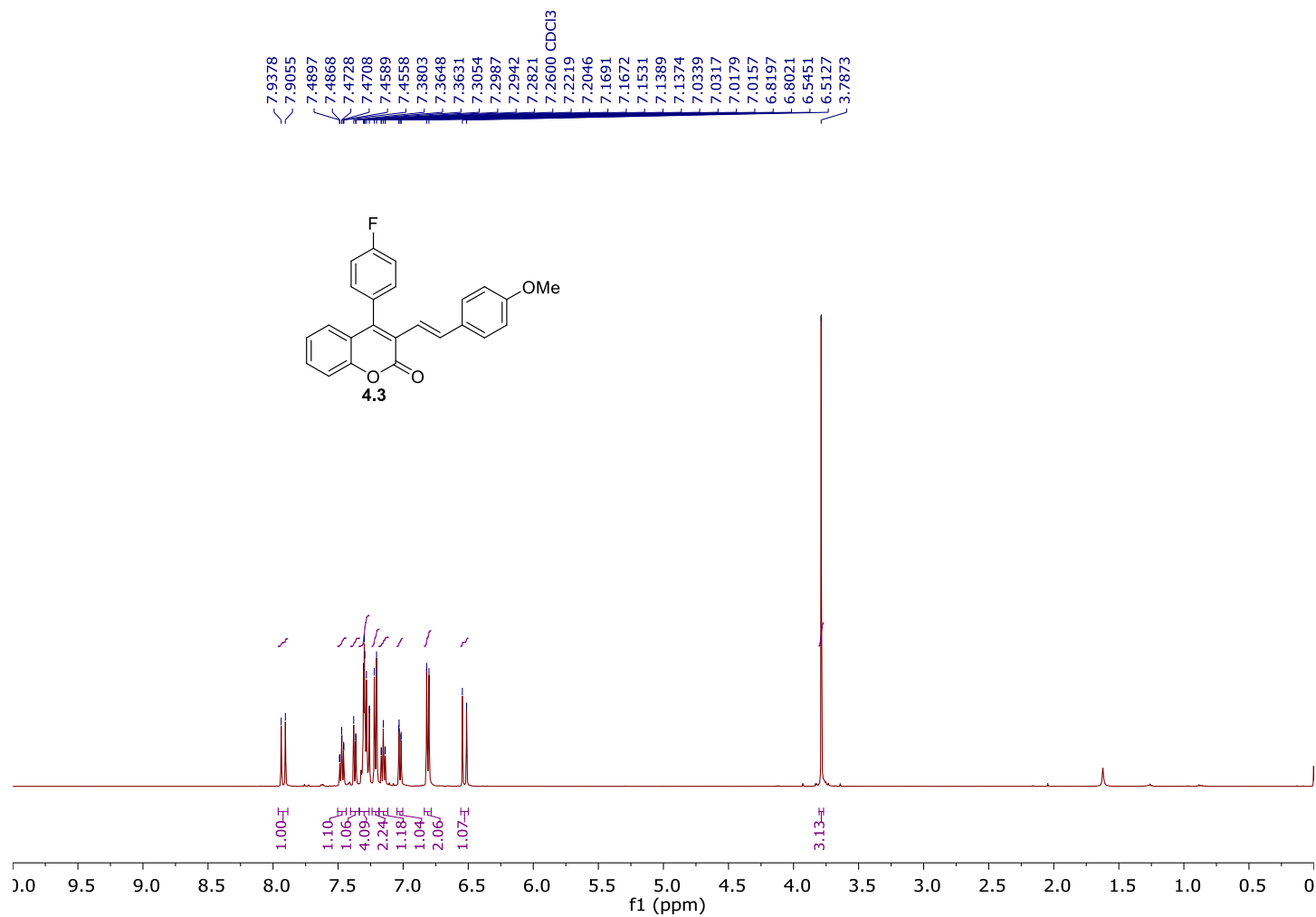
<sup>13</sup>C Spectrum of (*E*)-3-(4-methoxystyryl)-4-*p*-tolyl-2*H*-chromen-2-one (**4.1**)



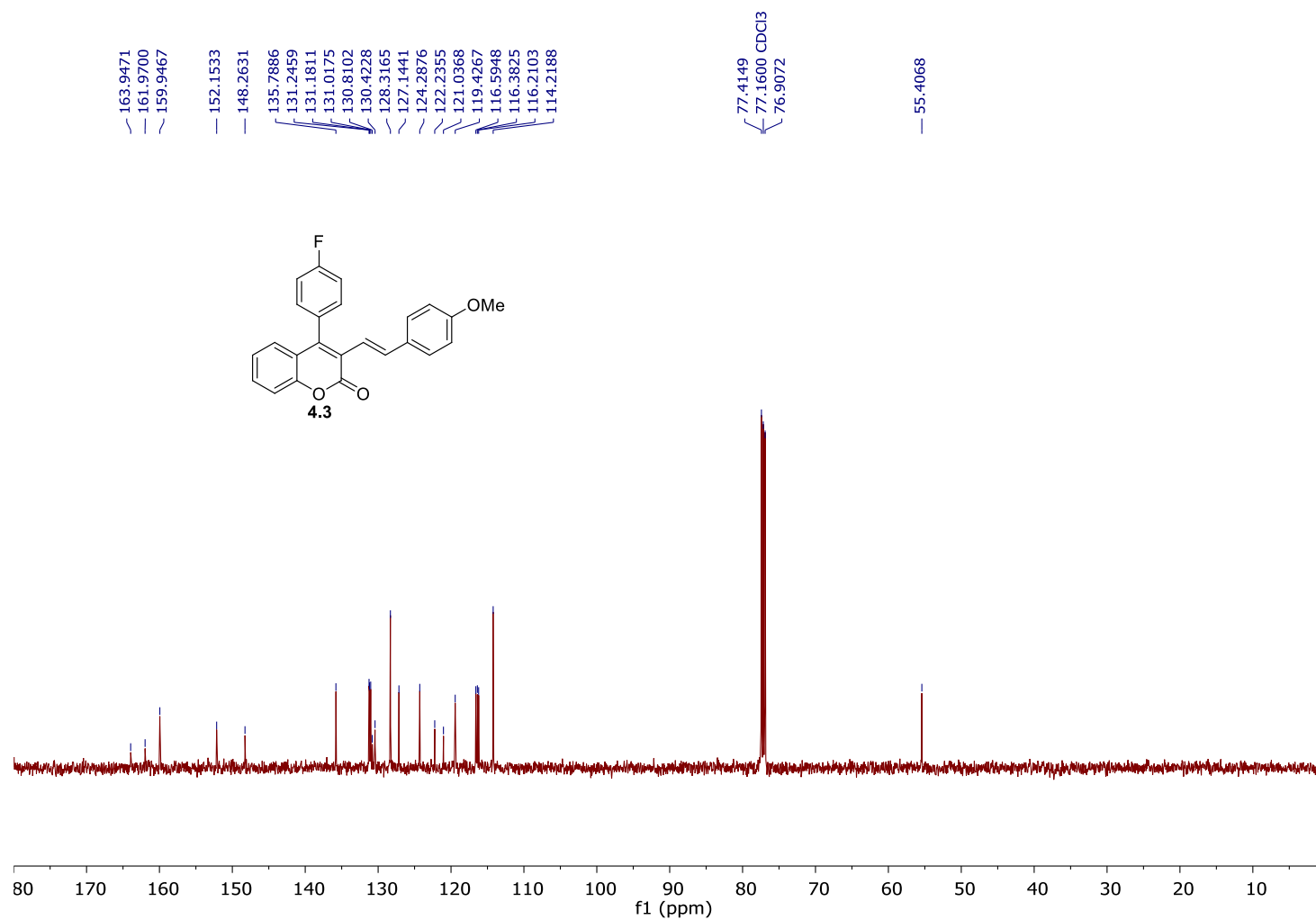
**<sup>1</sup>H Spectrum of (E)-4-(4-methoxyphenyl)-3-(4-methoxystyryl)-2H-chromen-2-one (4.2)**



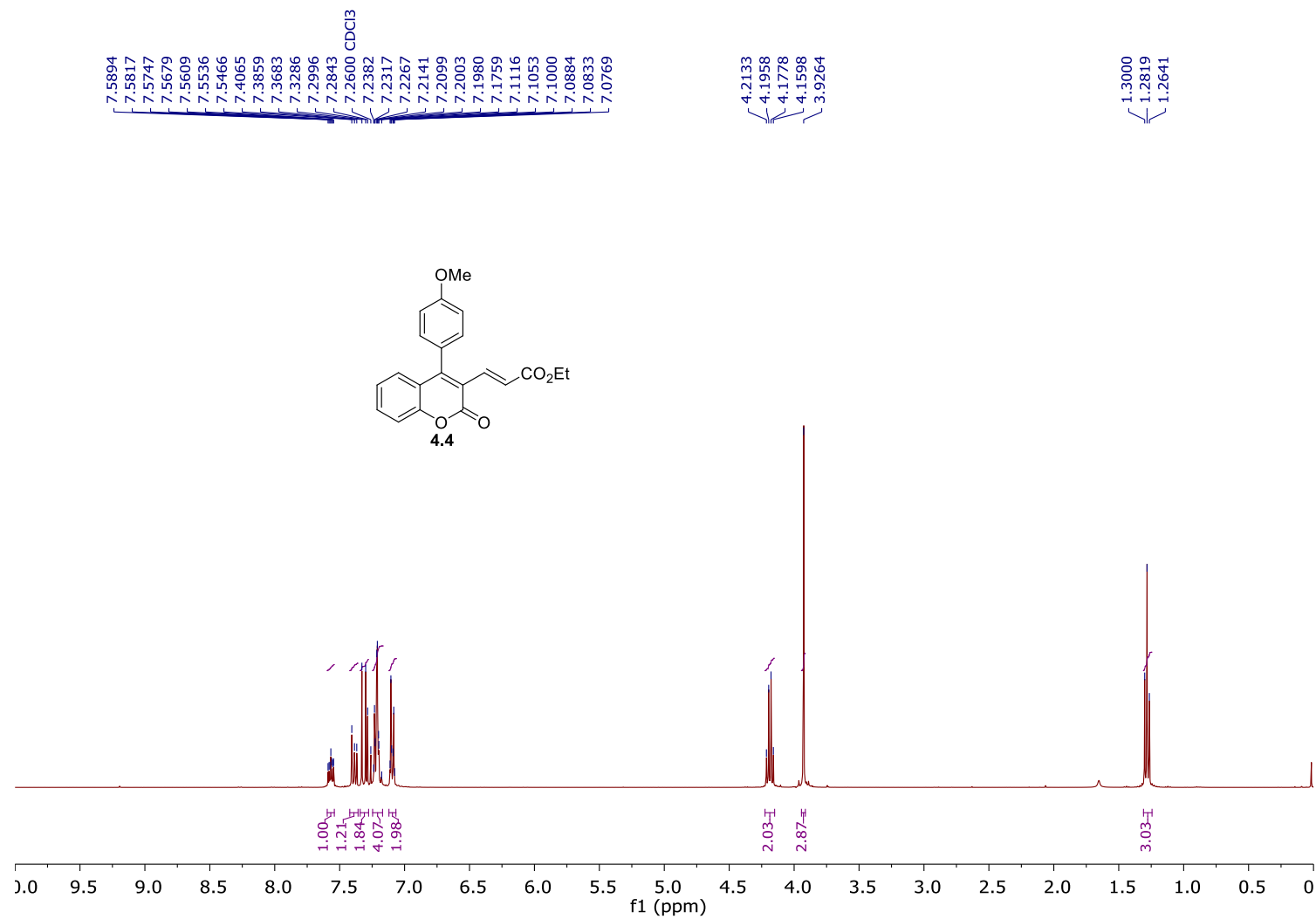
<sup>13</sup>C Spectrum of *(E)*-4-(4-methoxyphenyl)-3-(4-methoxystyryl)-2*H*-chromen-2-one (**4.2**)



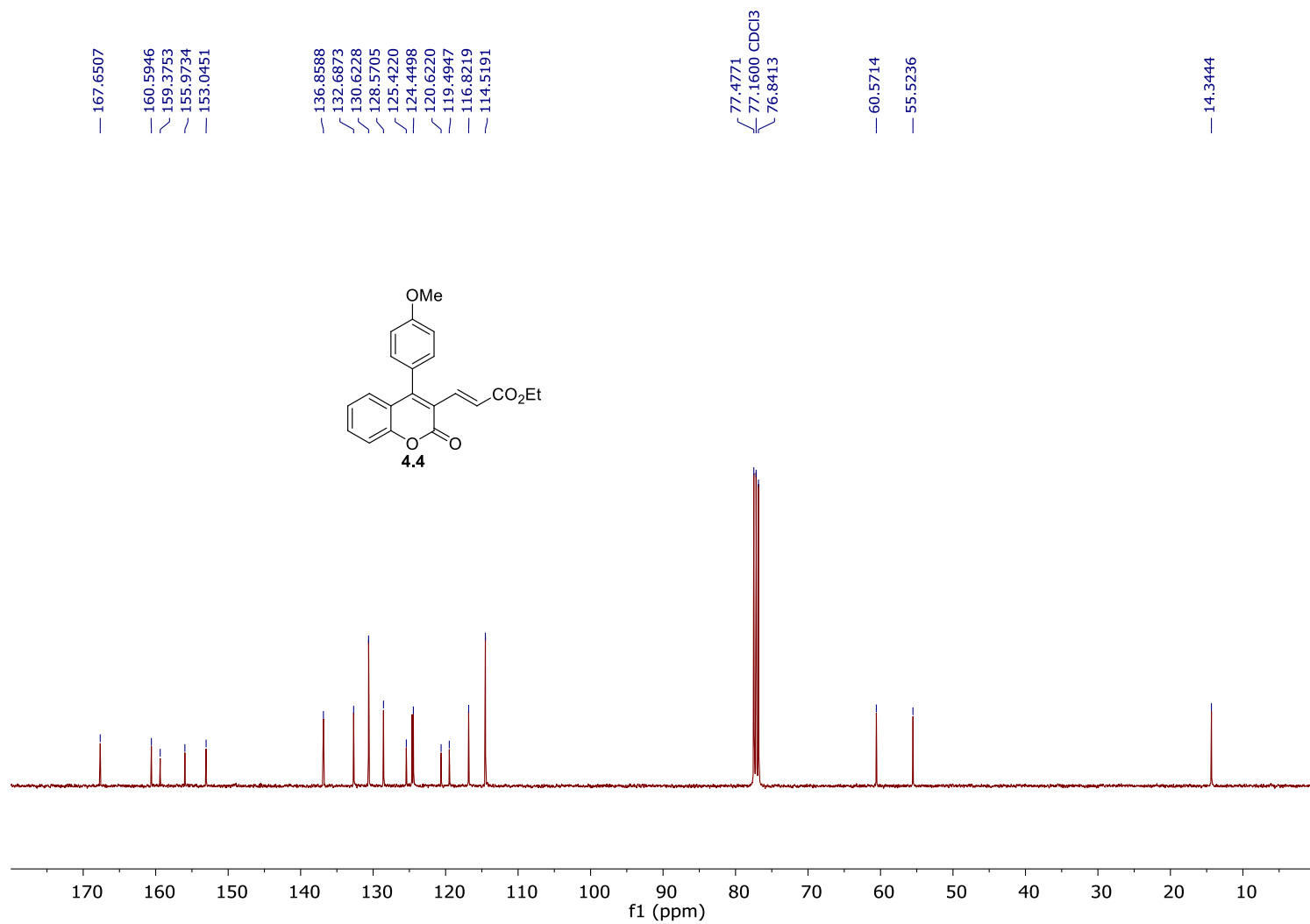
**<sup>1</sup>H Spectrum of (E)-4-(4-fluorophenyl)-3-(4-methoxystyryl)-2H-chromen-2-one (4.3)**



<sup>13</sup>C Spectrum of (E)-4-(4-fluorophenyl)-3-(4-methoxystyryl)-2H-chromen-2-one (4.3)

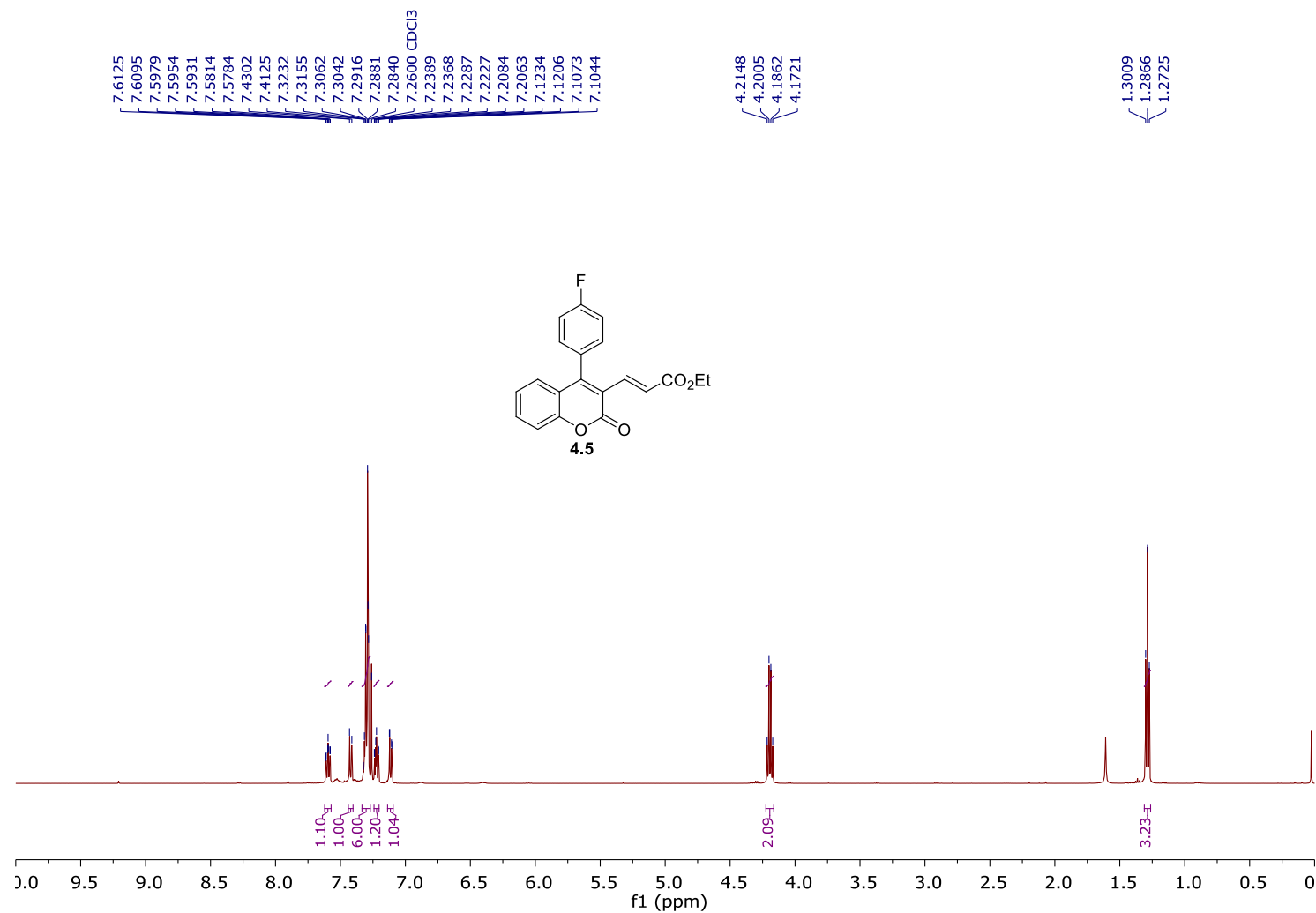


**<sup>1</sup>H Spectrum of (E)-ethyl 3-(4-(4-methoxyphenyl)-2-oxo-2H-chromen-3-yl)acrylate (4.4)**

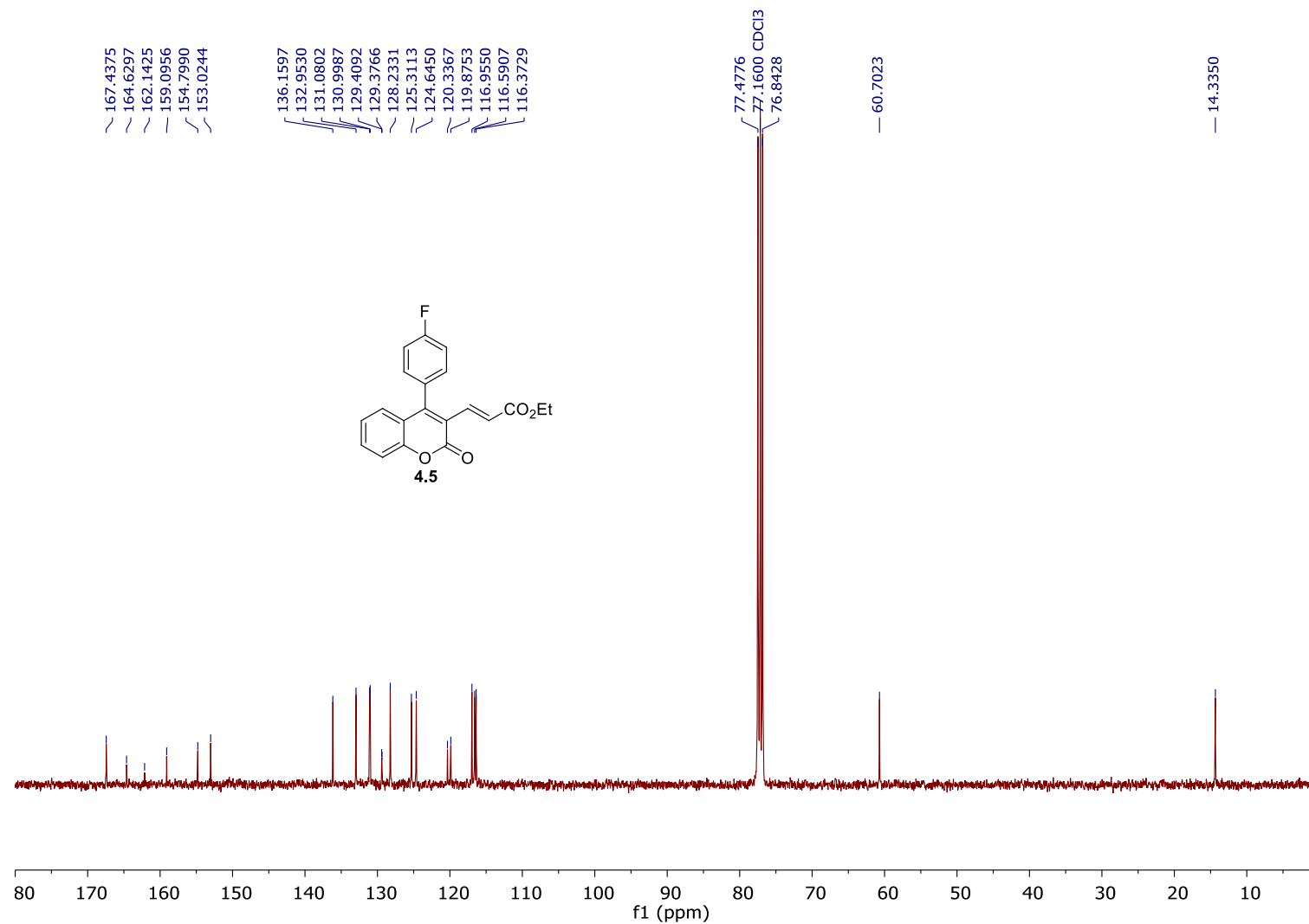


<sup>13</sup>C Spectrum of *(E)*-ethyl 3-(4-(4-methoxyphenyl)-2-oxo-2H-chromen-3-yl)acrylate (**4.4**)

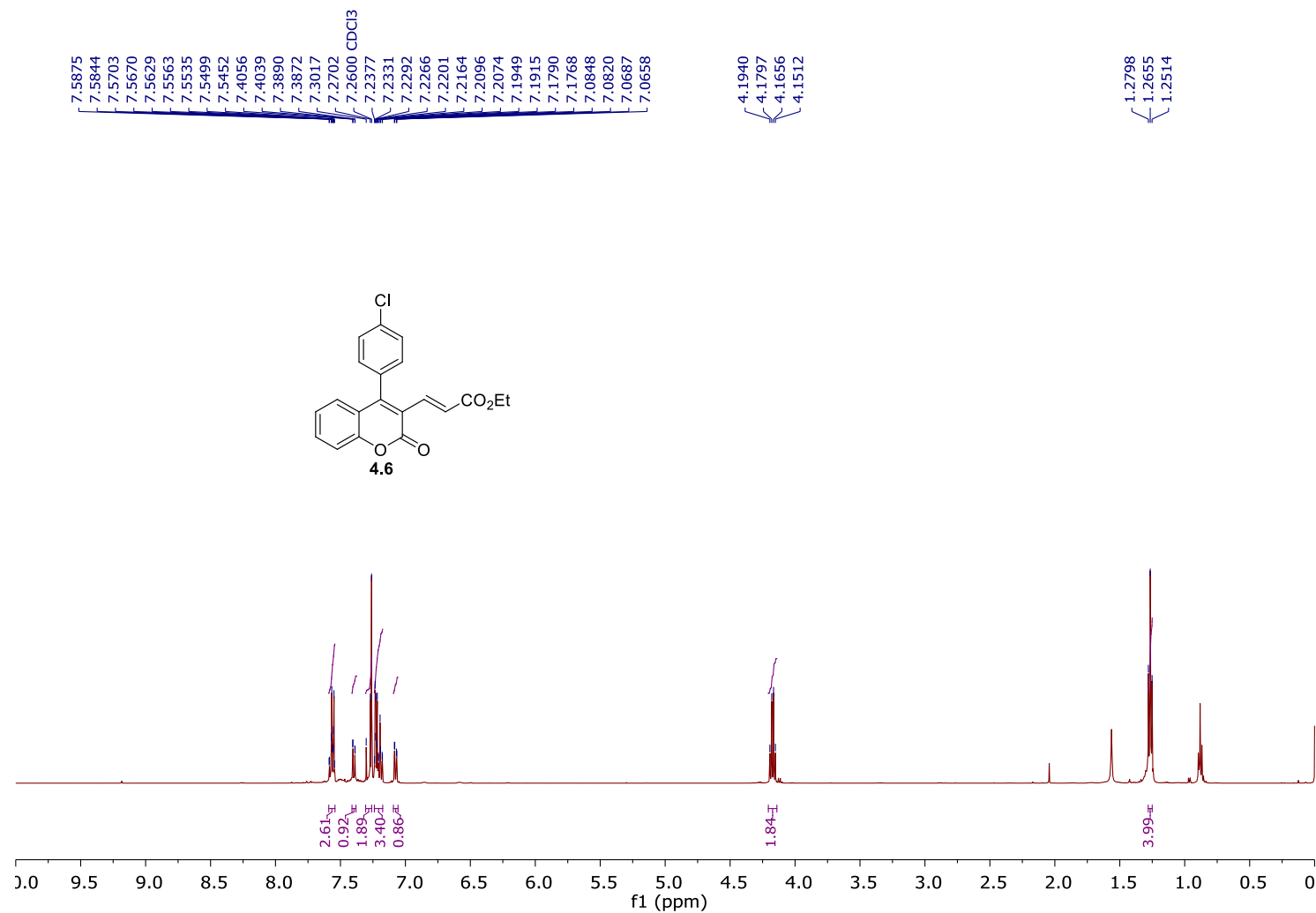




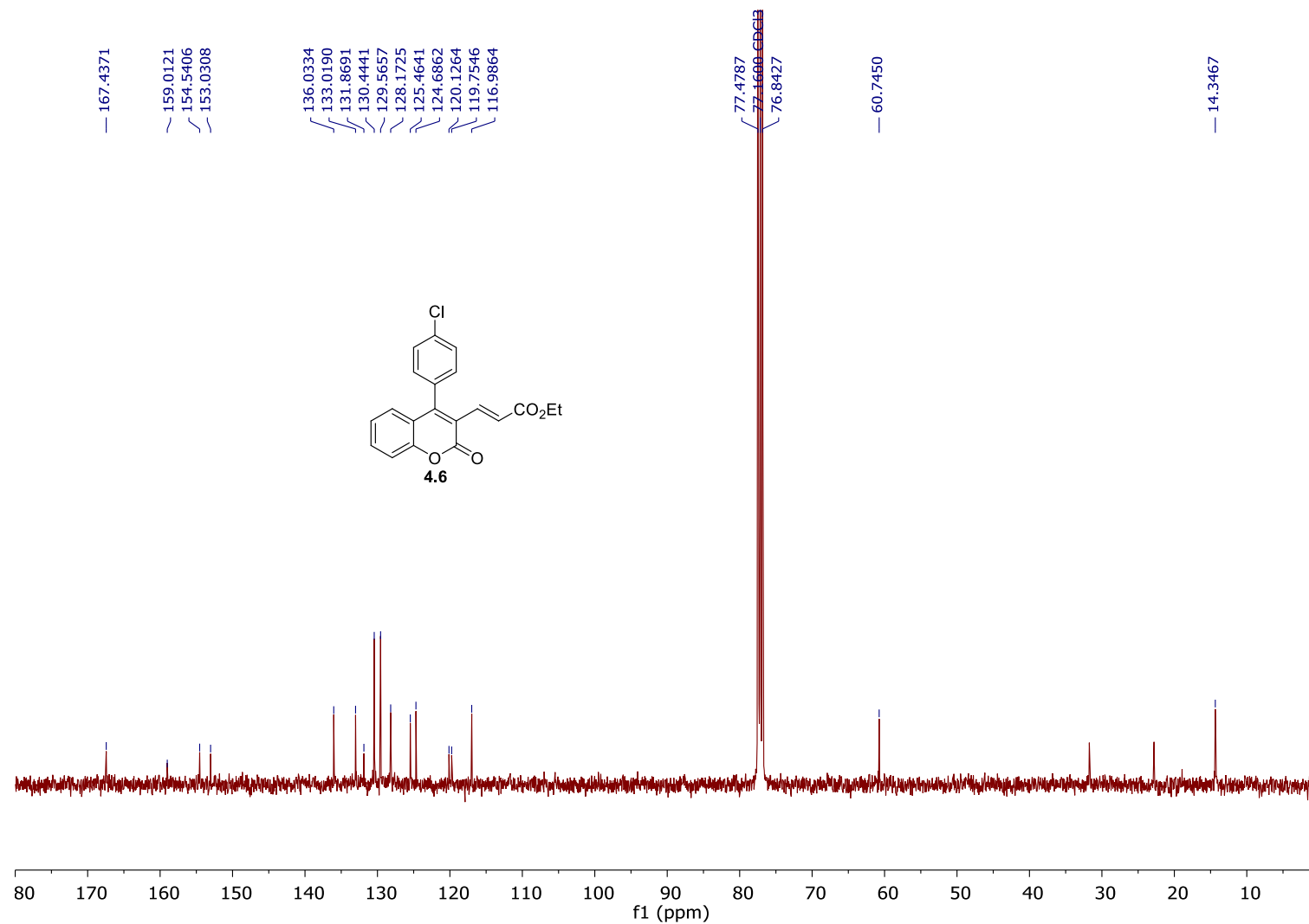
**<sup>1</sup>H Spectrum of (E)-ethyl 3-(4-(4-fluorophenyl)-2-oxo-2H-chromen-3-yl)acrylate (4.5)**



<sup>13</sup>C Spectrum of (E)-ethyl 3-(4-(4-fluorophenyl)-2-oxo-2H-chromen-3-yl)acrylate (4.5)



**<sup>1</sup>H Spectrum of (E)-ethyl 3-(4-(4-chlorophenyl)-2-oxo-2H-chromen-3-yl)acrylate (4.6)**

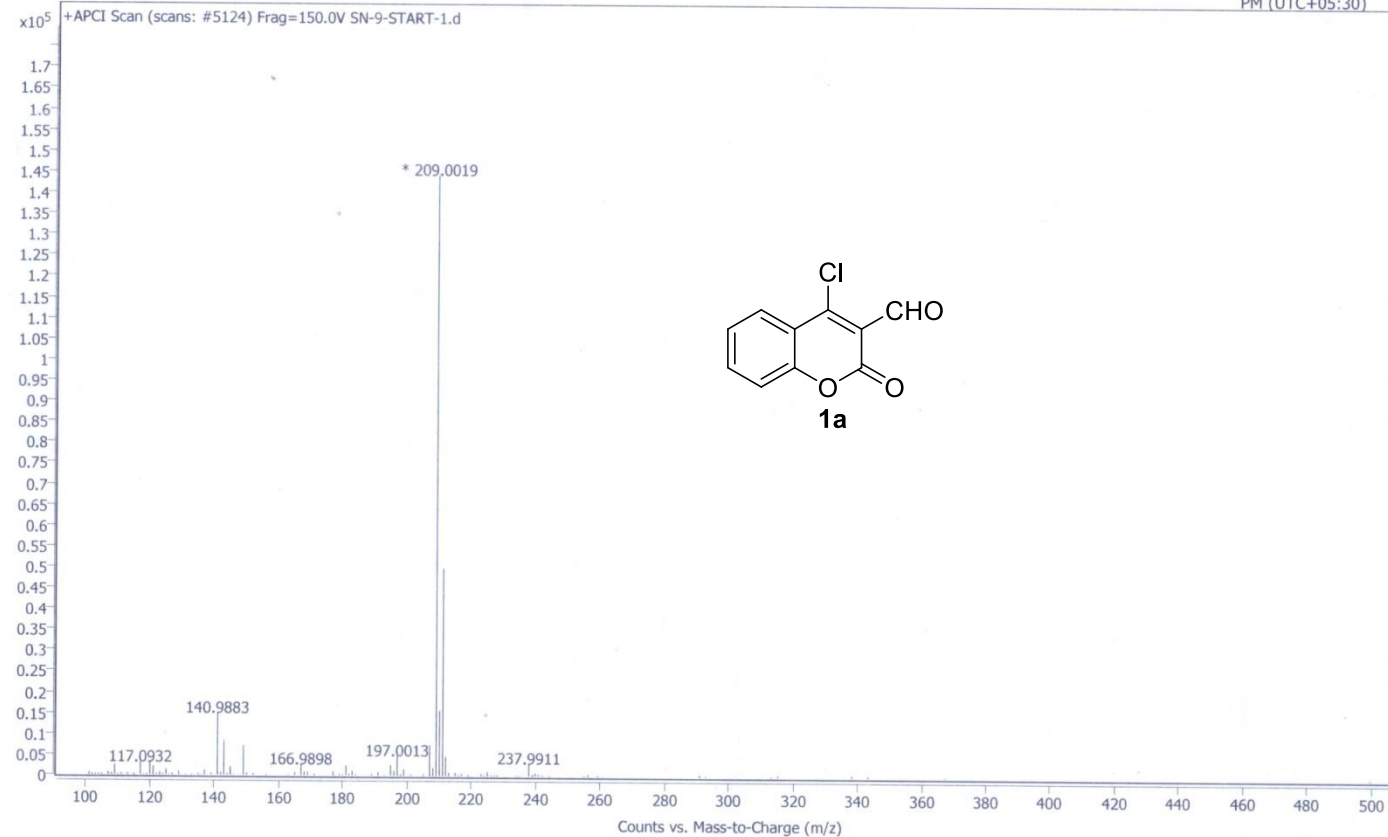


<sup>13</sup>C Spectrum of (E)-ethyl 3-(4-(4-chlorophenyl)-2-oxo-2H-chromen-3-yl)acrylate (4.6)

# User Spectrum Plot Report



| Name           | Rack Pos.    | Instrument | Success | Operator | Acq. Time (Local)   |
|----------------|--------------|------------|---------|----------|---------------------|
| Inj. Vol. (ul) | Plate Pos.   | IRM Status |         |          | 13-04-2021 12:49:38 |
| Data File      | Method (Acq) | Comment    |         |          | PM (UTC+05:30)      |

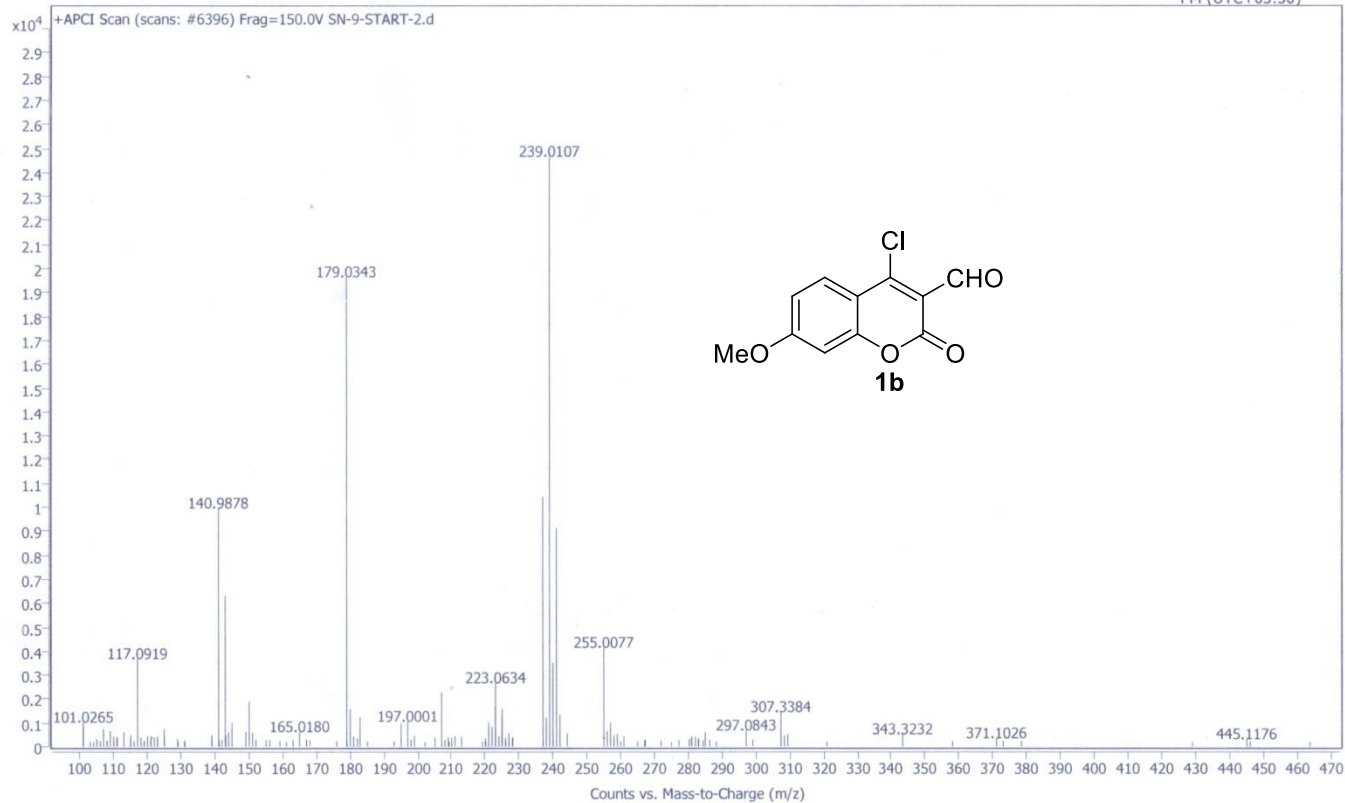


**Mass Spectrum of 4-chloro-2-oxo-2H-chromene-3-carbaldehyde (1a)**

## User Spectrum Plot Report



| Name           | Rack Pos.    | Instrument | Operator                           |
|----------------|--------------|------------|------------------------------------|
| Inj. Vol. (ul) | Plate Pos.   | IRM Status |                                    |
| Data File      | Method (Acq) | Comment    | Success                            |
| SN-9-START-2.d |              |            | Acq. Time (Local)                  |
|                |              |            | 13-04-2021 12:06:27 PM (UTC+05:30) |

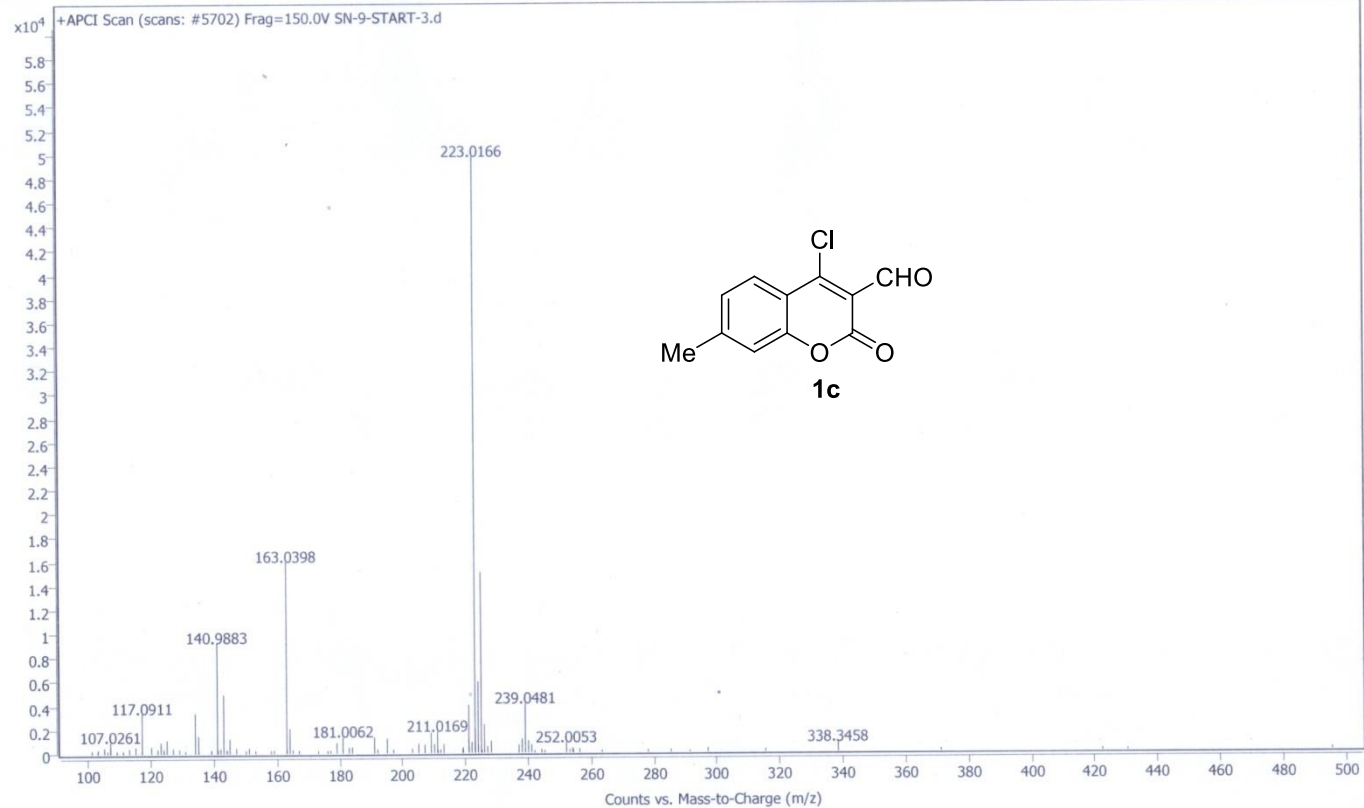


**Mass Spectrum of 4-chloro-7-methoxy-2-oxo-2H-chromene-3-carbaldehyde (1b)**

# User Spectrum Plot Report



| Name           | Rack Pos.    | Instrument | Success | Operator                           |
|----------------|--------------|------------|---------|------------------------------------|
| Inj. Vol. (ul) | Plate Pos.   | IRM Status |         |                                    |
| Data File      | Method (Acq) | Comment    |         |                                    |
| SN-9-START-3.d |              |            |         |                                    |
|                |              |            |         | Acq. Time (Local)                  |
|                |              |            |         | 13-04-2021 12:24:32 PM (UTC+05:30) |

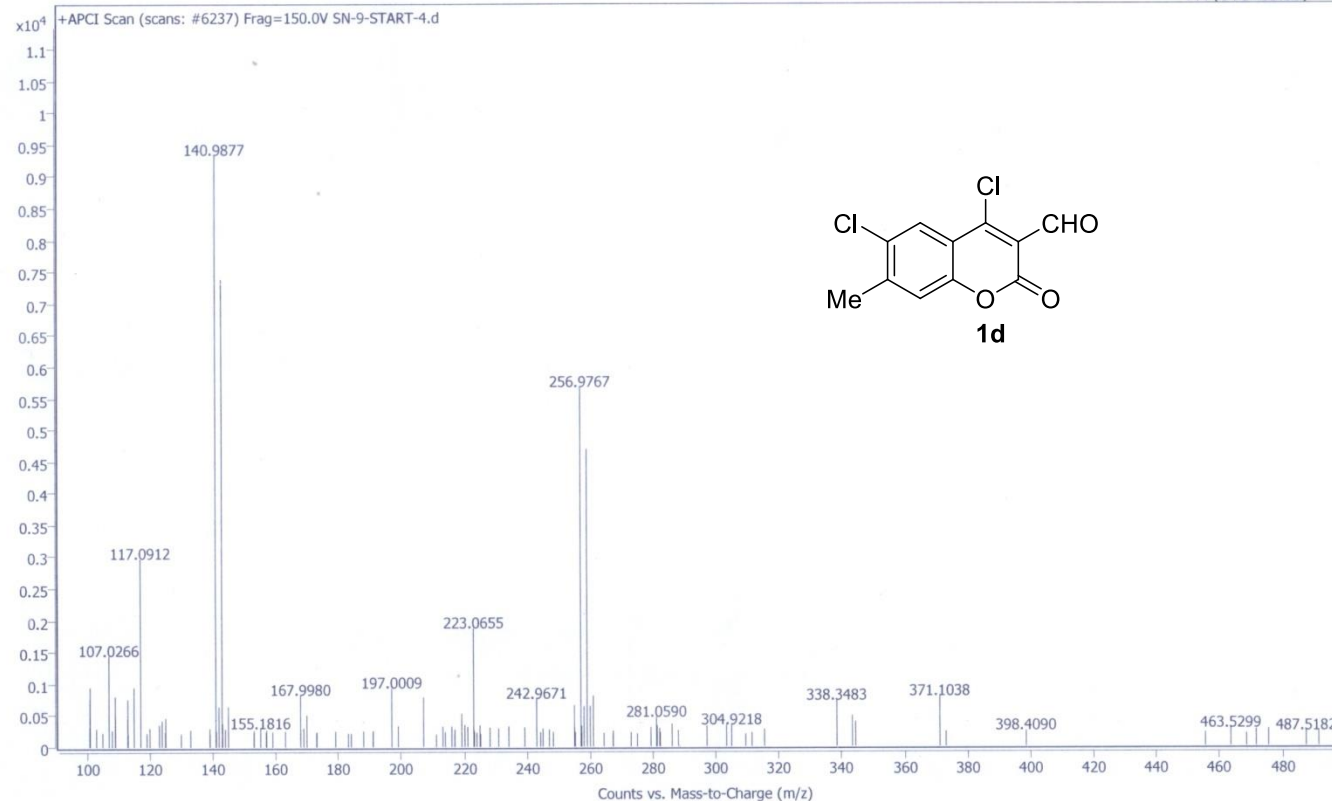


**Mass Spectrum of 4-chloro-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (1c)**

## User Spectrum Plot Report



|                |                             |              |             |           |                   |                                    |
|----------------|-----------------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-START-4                | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection Program | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-START-4.d              | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 13-04-2021 01:09:26 PM (UTC+05:30) |



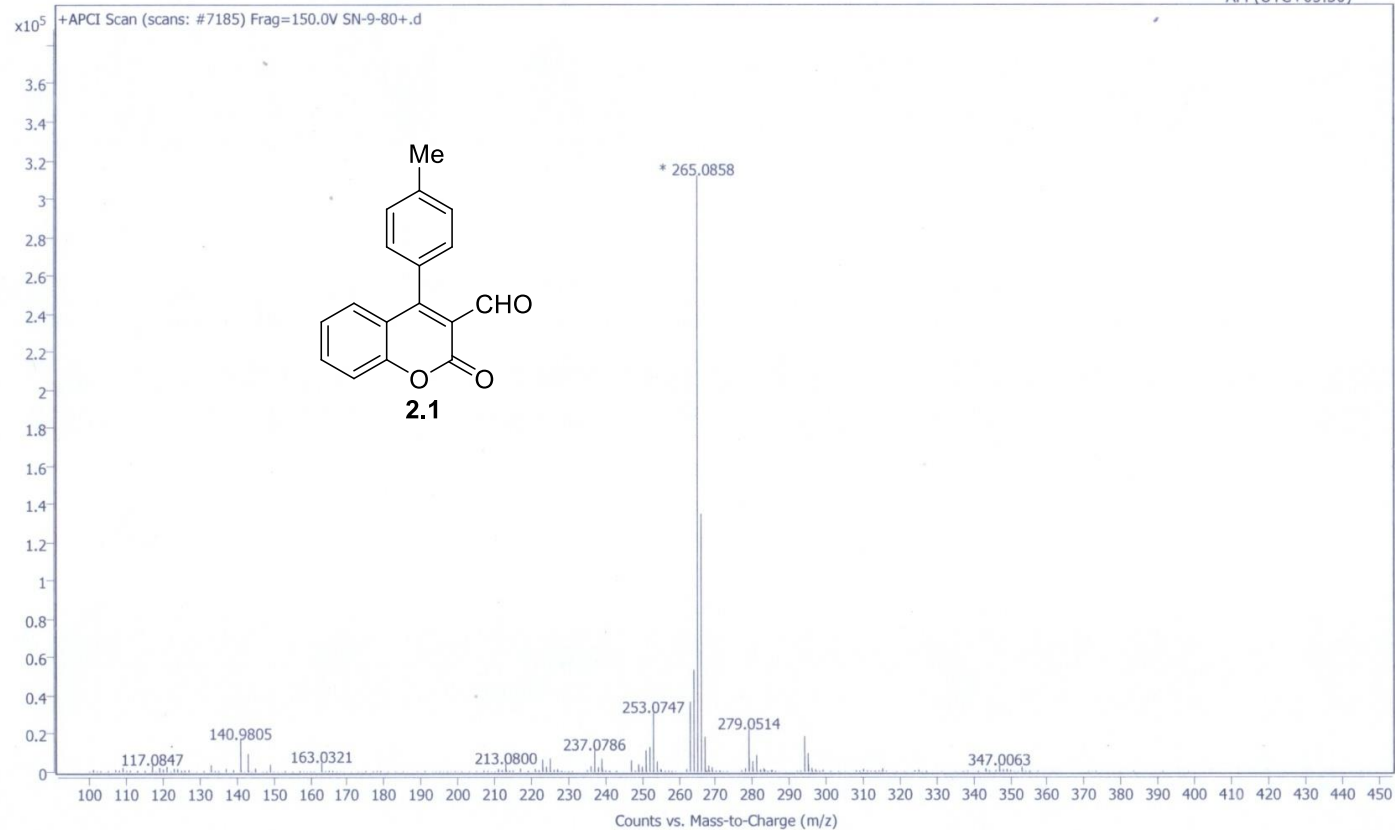
**Mass Spectrum of 4,6-dichloro-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (1d)**



# User Spectrum Plot Report



|                |                     |              |             |            |           |                   |                                    |
|----------------|---------------------|--------------|-------------|------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-80             | Rack Pos.    |             | Instrument | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   |             | IRM Status | Success   |                   |                                    |
| Data File      | SN-9-80+.d          | Method (Acq) | GCAPCIITK.m | Comment    |           | Acq. Time (Local) | 20-04-2021 11:12:22 AM (UTC+05:30) |

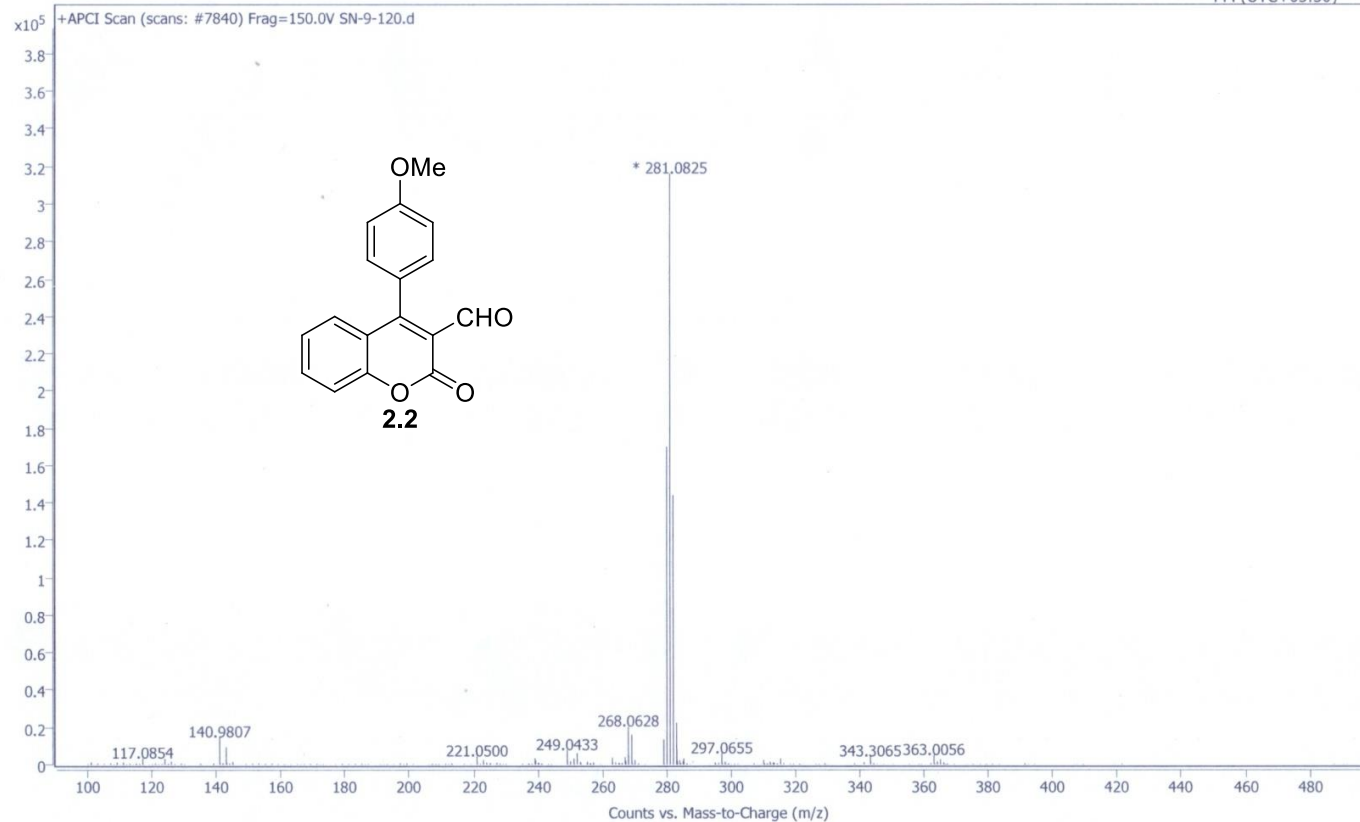


**Mass Spectrum of 2-oxo-4-p-tolyl-2H-chromene-3-carbaldehyde (2.1)**

## User Spectrum Plot Report



|                |                             |              |             |           |                   |                                    |
|----------------|-----------------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-120                    | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection Program | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-120.d                  | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 19-04-2021 02:38:12 PM (UTC+05:30) |

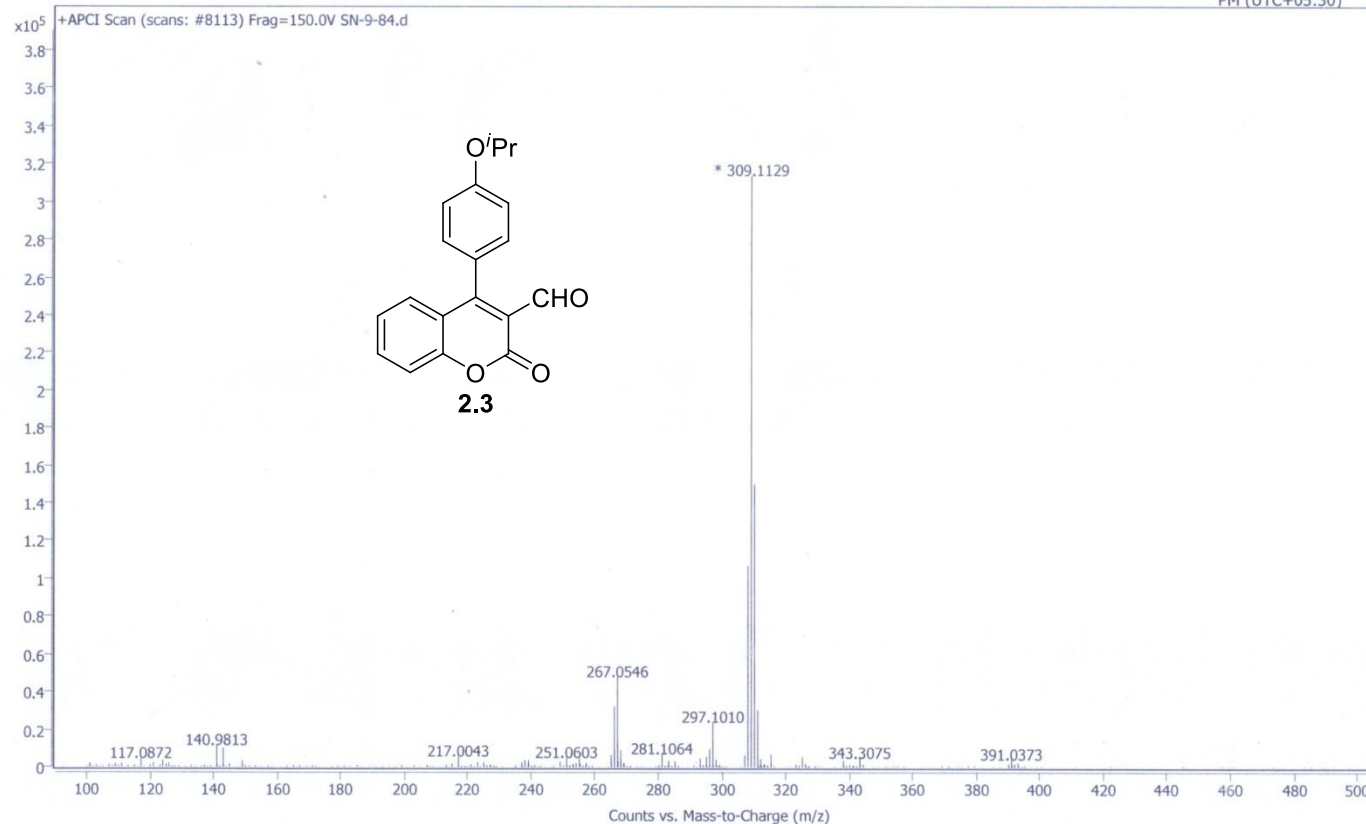


**Mass Spectrum of 4-(4-methoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.2)**

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-84             | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-84.d           | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 19-04-2021 01:53:19 PM (UTC+05:30) |

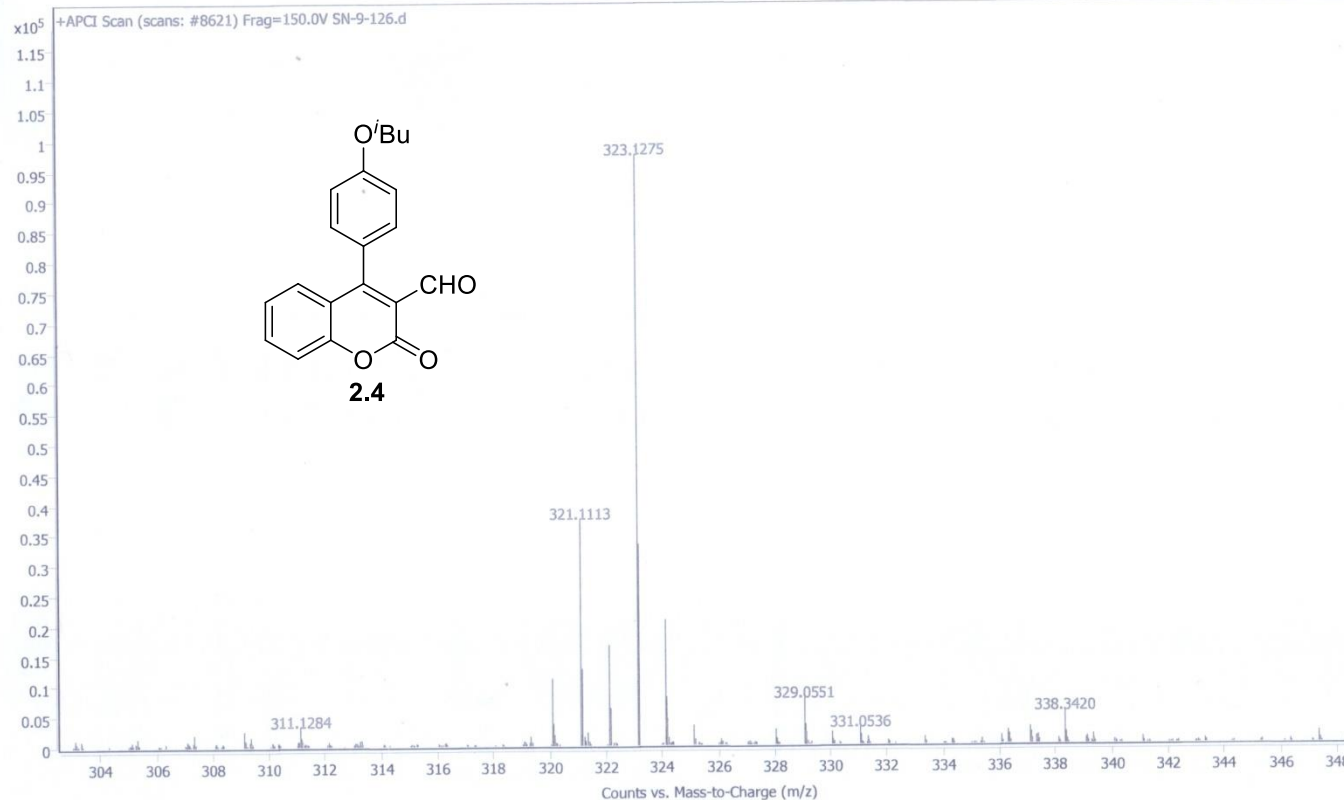


**Mass Spectrum of 4-(4-isopropoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.3)**

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-126            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-126.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 22-07-2021 02:29:24 PM (UTC+05:30) |

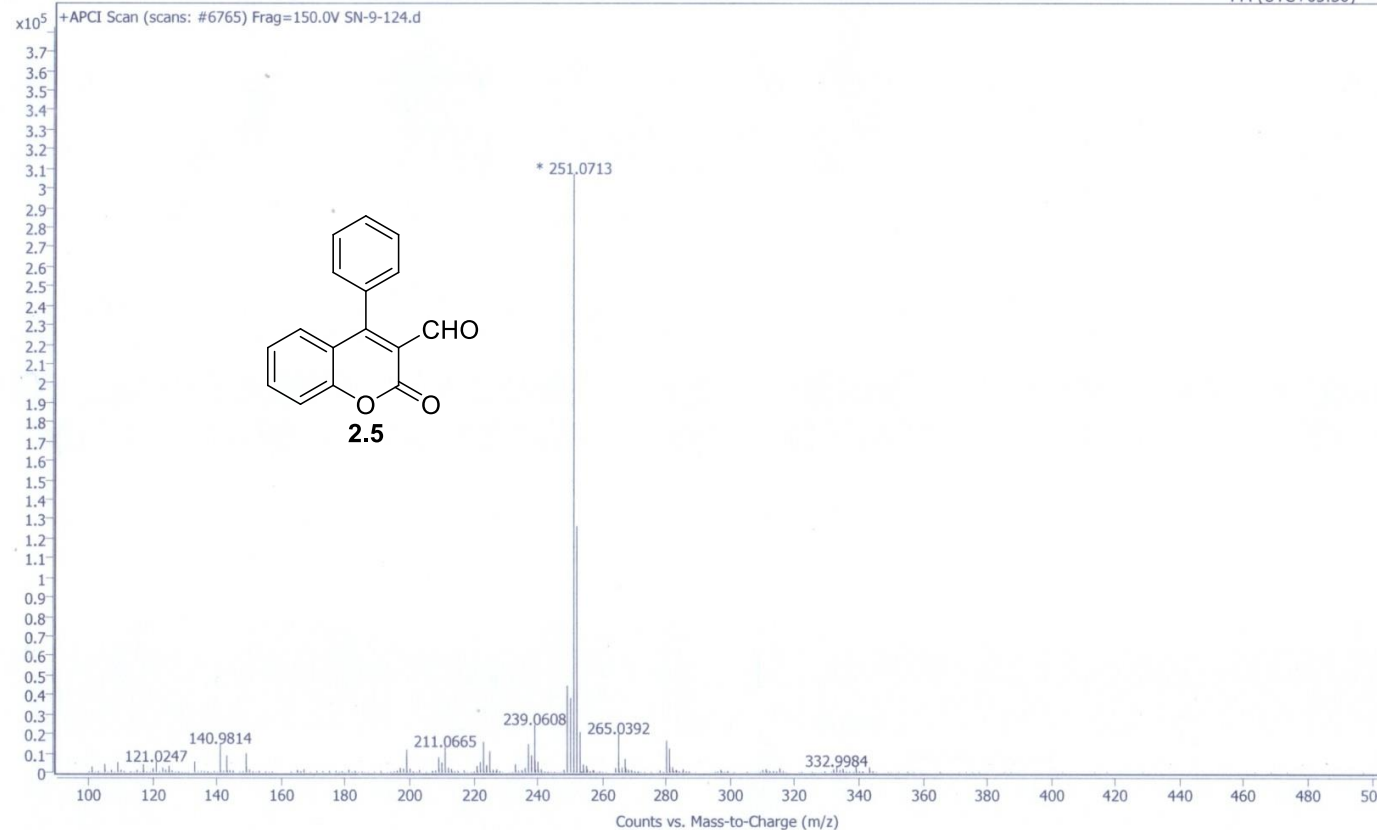


Mass Spectrum of 4-(4-isobutoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.4)

# User Spectrum Plot Report



| Name           | Rack Pos.    | Instrument        | Operator            |
|----------------|--------------|-------------------|---------------------|
| Inj. Vol. (ul) | Plate Pos.   | IRM Status        |                     |
| Data File      | Method (Acq) | Comment           |                     |
| SN-9-124.d     |              |                   |                     |
|                |              | Success           |                     |
|                |              | Acq. Time (Local) | 19-04-2021 03:38:22 |
|                |              |                   | PM (UTC+05:30)      |

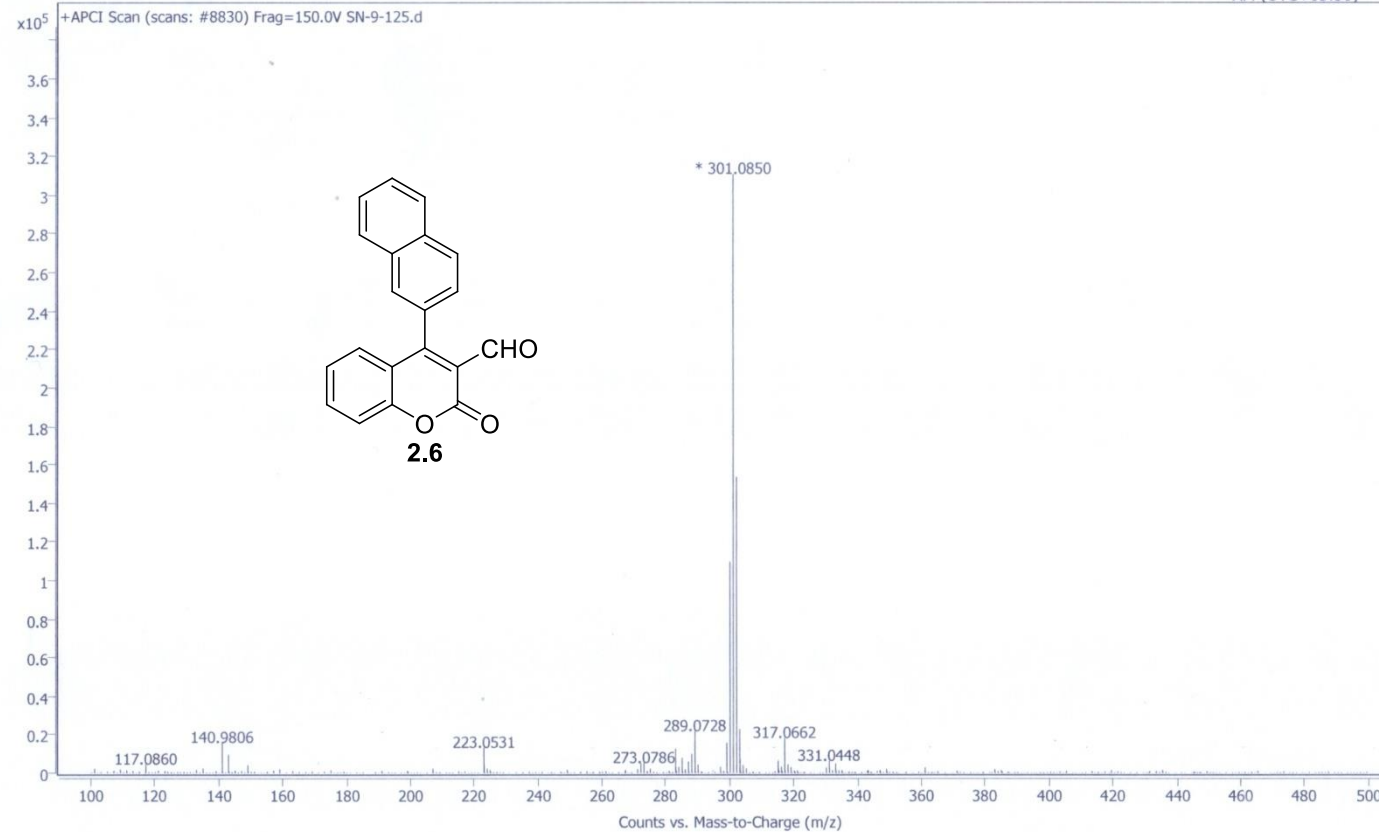


Mass Spectrum of 2-oxo-4-phenyl-2H-chromene-3-carbaldehyde (2.5)

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-125            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-125.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 20-04-2021 11:52:56 AM (UTC+05:30) |

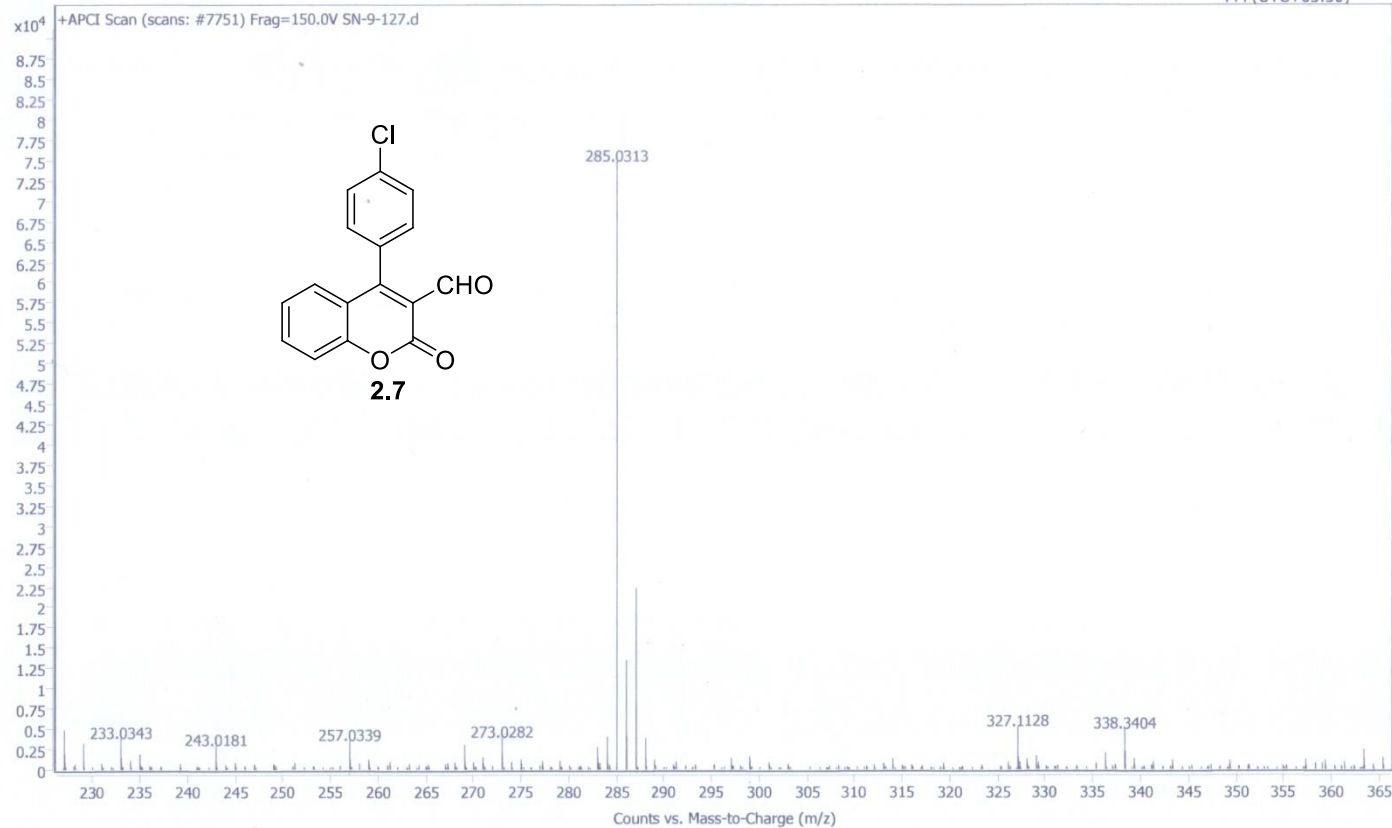


**Mass Spectrum of 4-(naphthalen-2-yl)-2-oxo-2H-chromene-3-carbaldehyde (2.6)**

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-127            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-127.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 22-07-2021 12:45:43 PM (UTC+05:30) |

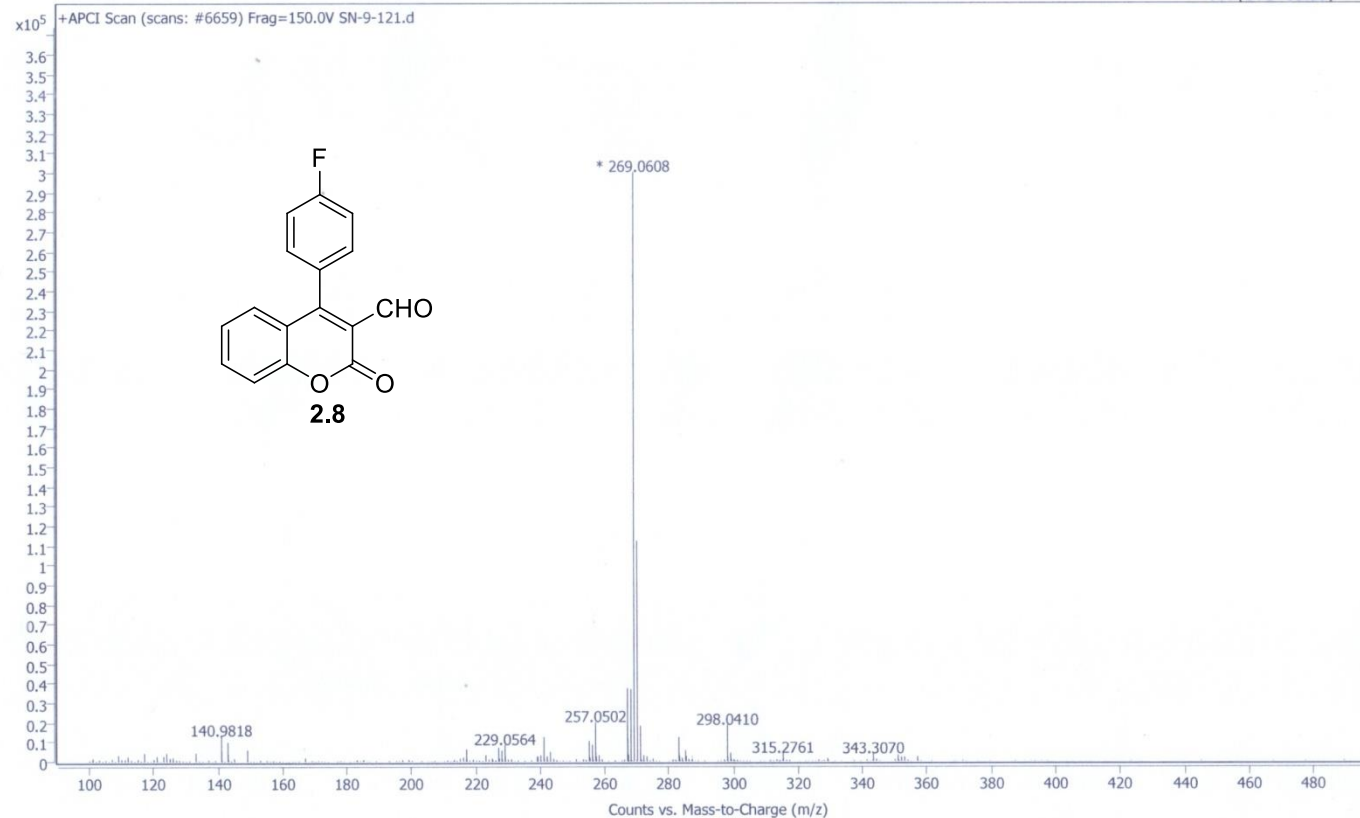


**Mass Spectrum of 4-(4-chlorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.7)**

# User Spectrum Plot Report



|                |                             |              |             |           |                   |                                    |
|----------------|-----------------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-121                    | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection Program | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-121.d                  | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 19-04-2021 02:15:43 PM (UTC+05:30) |



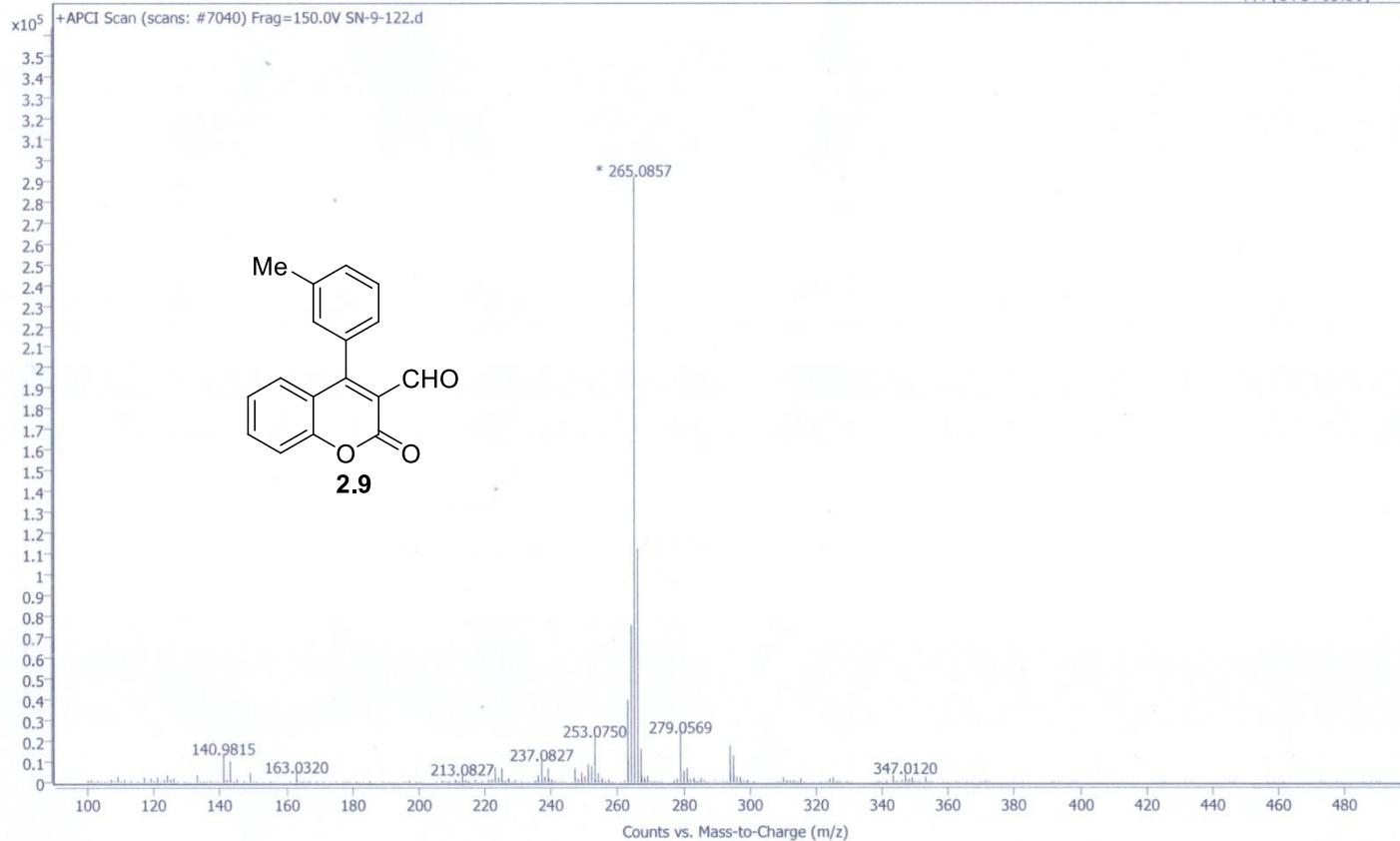
**Mass Spectrum of 4-(4-fluorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.8)**



# User Spectrum Plot Report



|                |                     |              |             |            |           |                   |                                    |
|----------------|---------------------|--------------|-------------|------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-122            | Rack Pos.    |             | Instrument | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   |             | IRM Status | Success   |                   |                                    |
| Data File      | SN-9-122.d          | Method (Acq) | GCAPCIITK.m | Comment    |           | Acq. Time (Local) | 19-04-2021 03:20:43 PM (UTC+05:30) |

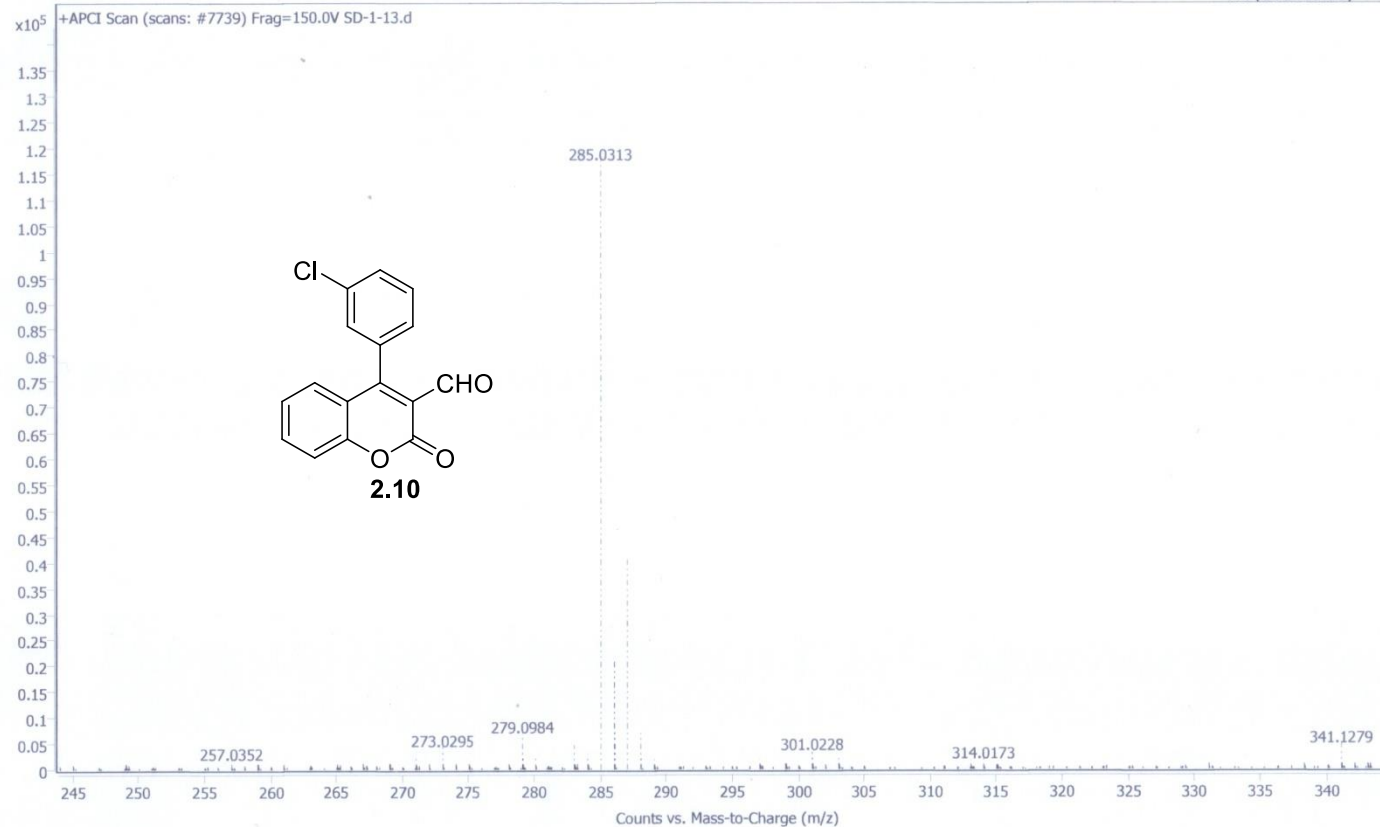


**Mass Spectrum of 2-oxo-4-*m*-tolyl-2*H*-chromene-3-carbaldehyde (2.9)**

# User Spectrum Plot Report



|                |                     |              |             |            |           |                   |                                    |
|----------------|---------------------|--------------|-------------|------------|-----------|-------------------|------------------------------------|
| Name           | SD-1-13             | Rack Pos.    |             | Instrument | APCI-GCMS | Operator          | ABHISHEK16ITK                      |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   |             | IRM Status | Success   |                   |                                    |
| Data File      | SD-1-13.d           | Method (Acq) | GCAPCIITK.m | Comment    |           | Acq. Time (Local) | 22-07-2021 12:23:10 PM (UTC+05:30) |

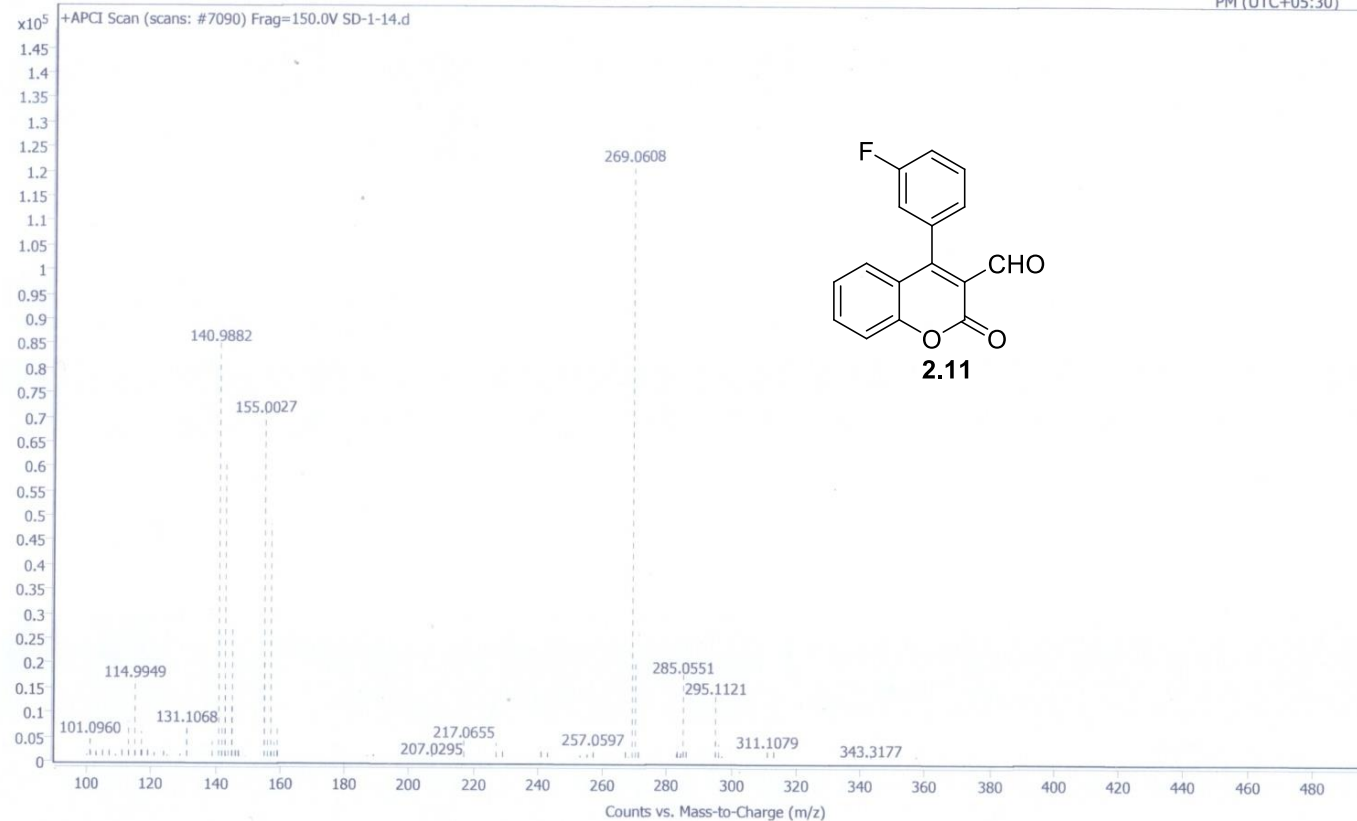


Mass Spectrum of 4-(3-chlorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.10)

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SD-1-14             | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SD-1-14.d           | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 13-07-2021 03:03:30 PM (UTC+05:30) |

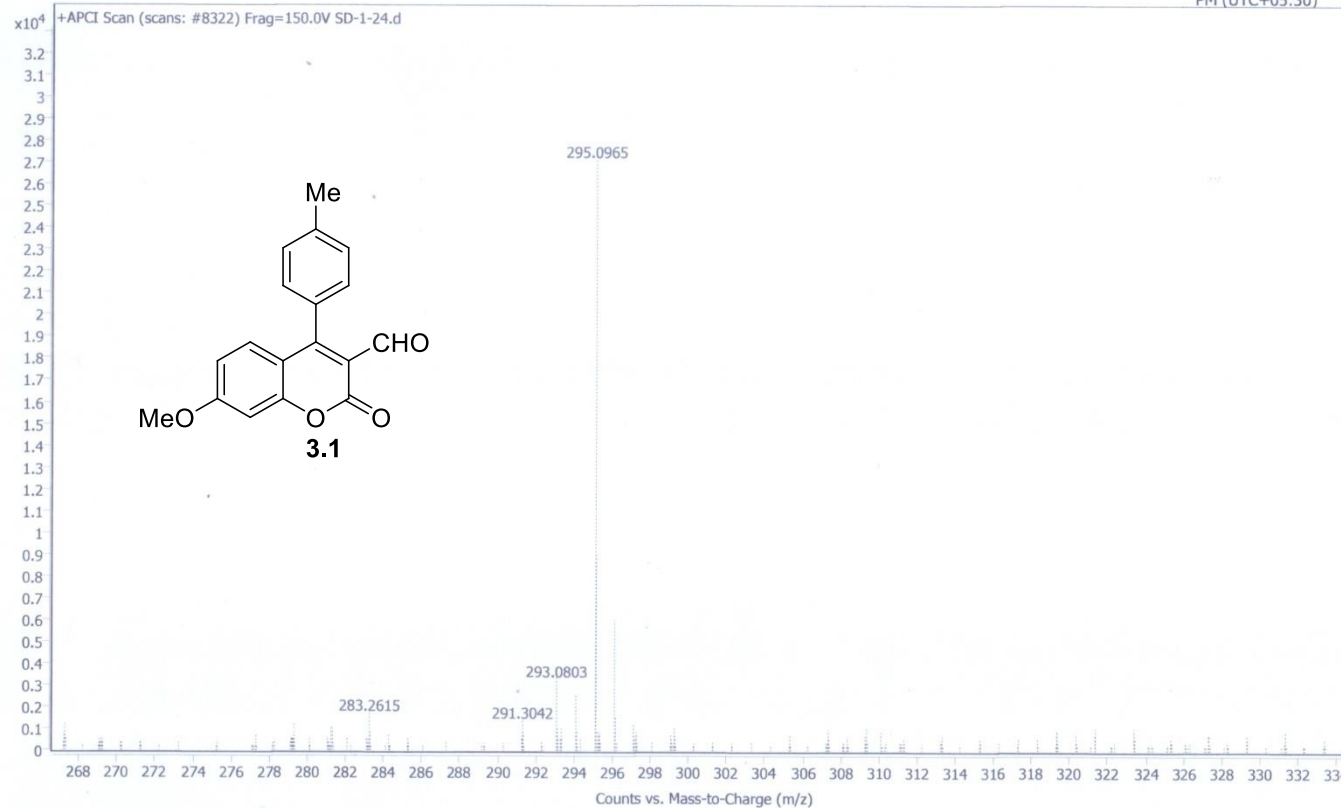


Mass Spectrum of 4-(3-fluorophenyl)-2-oxo-2H-chromene-3-carbaldehyde (2.11)

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SD-1-24             | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SD-1-24.d           | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 13-07-2021 03:26:03 PM (UTC+05:30) |

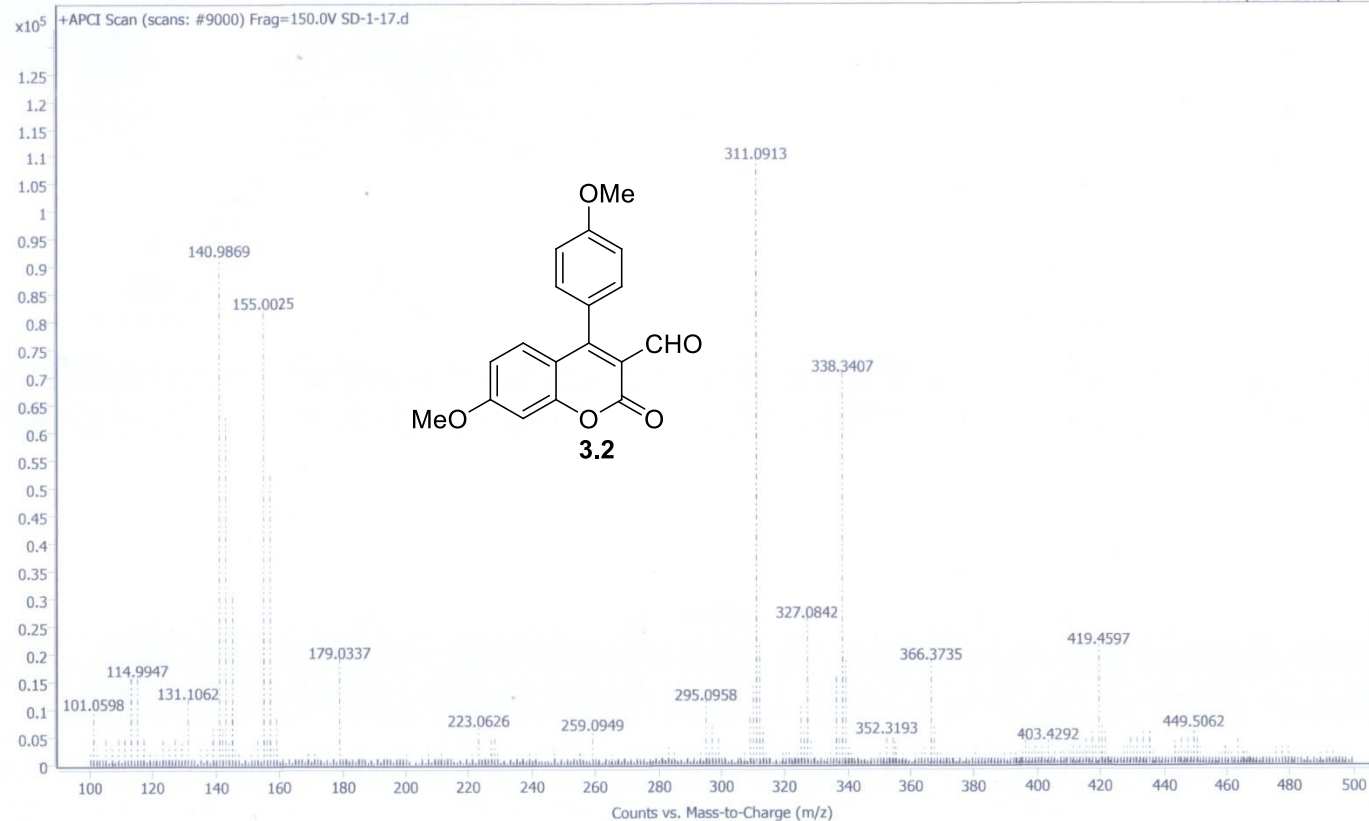


**Mass Spectrum of 7-methoxy-2-oxo-4-*p*-tolyl-2*H*-chromene-3-carbaldehyde (3.1)**

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SD-1-17             | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SD-1-17.d           | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 13-07-2021 02:20:48 PM (UTC+05:30) |

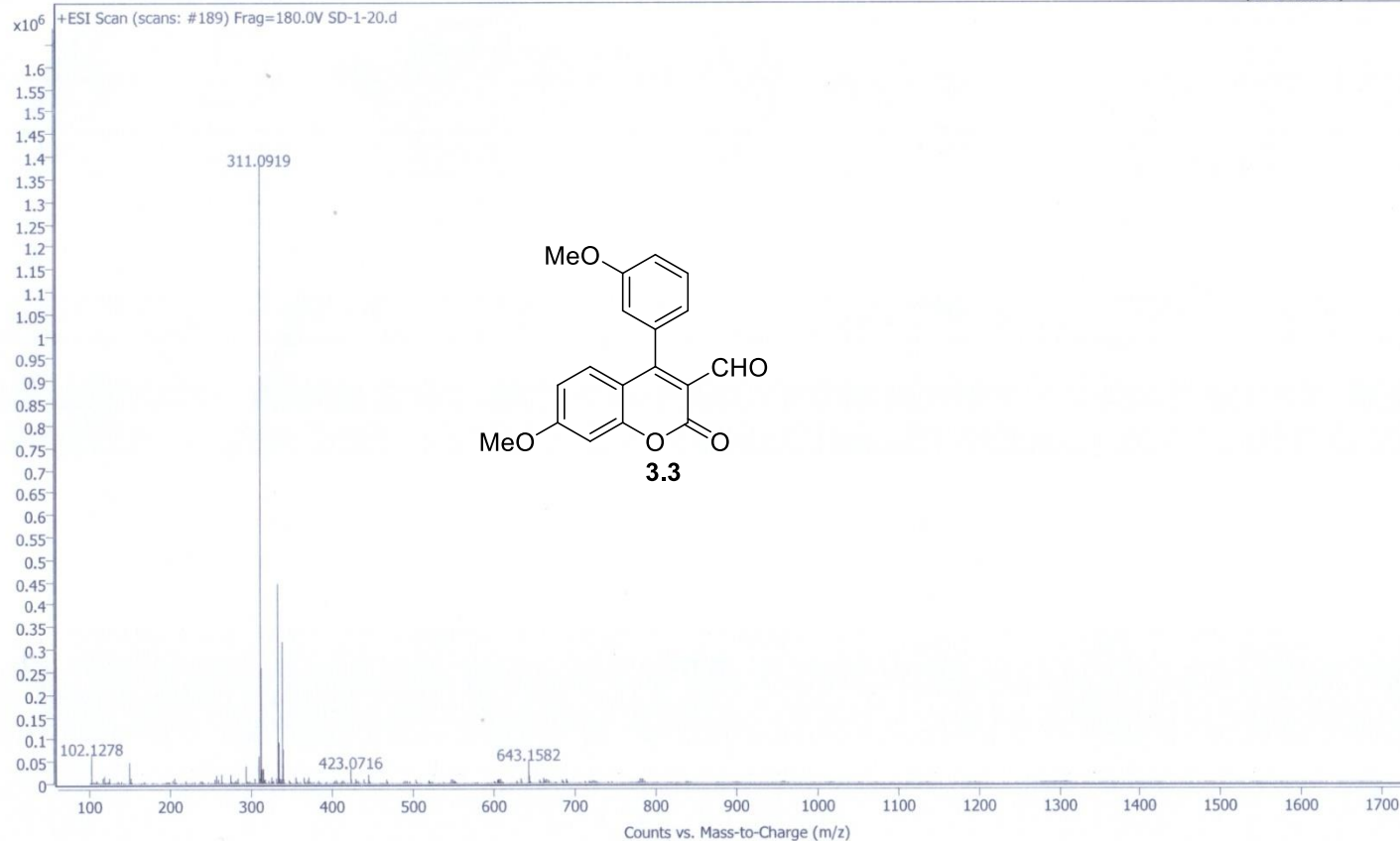


**Mass Spectrum of 7-methoxy-4-(4-methoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (3.2)**

# User Spectrum Plot Report



| Name           | Rack Pos.    | Instrument | Operator                        |
|----------------|--------------|------------|---------------------------------|
| Inj. Vol. (ul) | Plate Pos.   | IRM Status |                                 |
| Data File      | Method (Acq) | Comment    | Success                         |
| SD-1-20.d      |              |            | Acq. Time (Local)               |
|                |              |            | 22-06-2021 15:20:36 (UTC+05:30) |

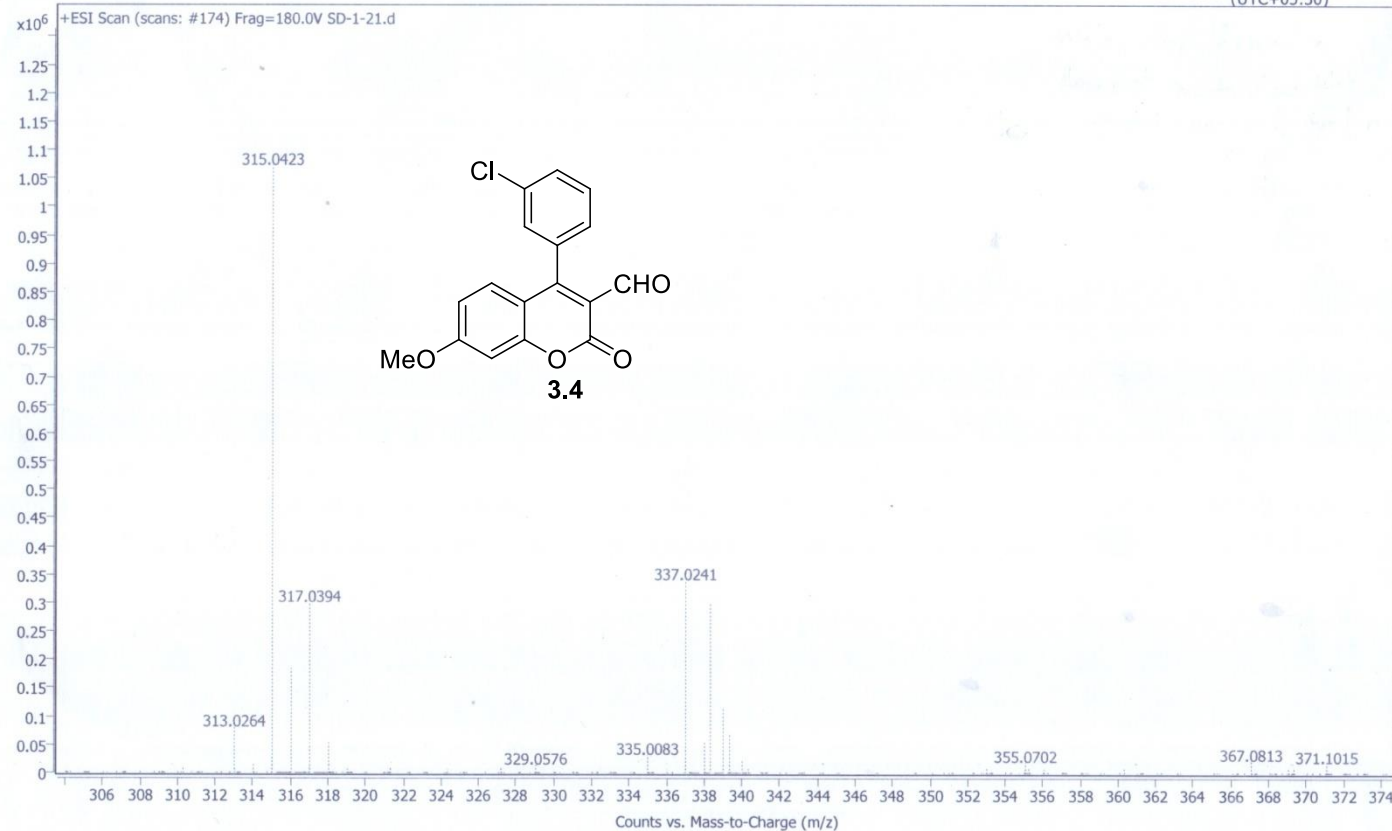


**Mass Spectrum of 7-methoxy-4-(3-methoxyphenyl)-2-oxo-2H-chromene-3-carbaldehyde (3.3)**

# User Spectrum Plot Report



|                |           |              |                   |         |                                 |
|----------------|-----------|--------------|-------------------|---------|---------------------------------|
| Name           | SD-1-21   | Rack Pos.    | Instrument        | ESI-MS  | Operator                        |
| Inj. Vol. (ul) | 1         | Plate Pos.   | IRM Status        | Success |                                 |
| Data File      | SD-1-21.d | Method (Acq) | ORGANIC METHODE.m | Comment | Acq. Time (Local)               |
|                |           |              |                   |         | 22-06-2021 15:07:33 (UTC+05:30) |

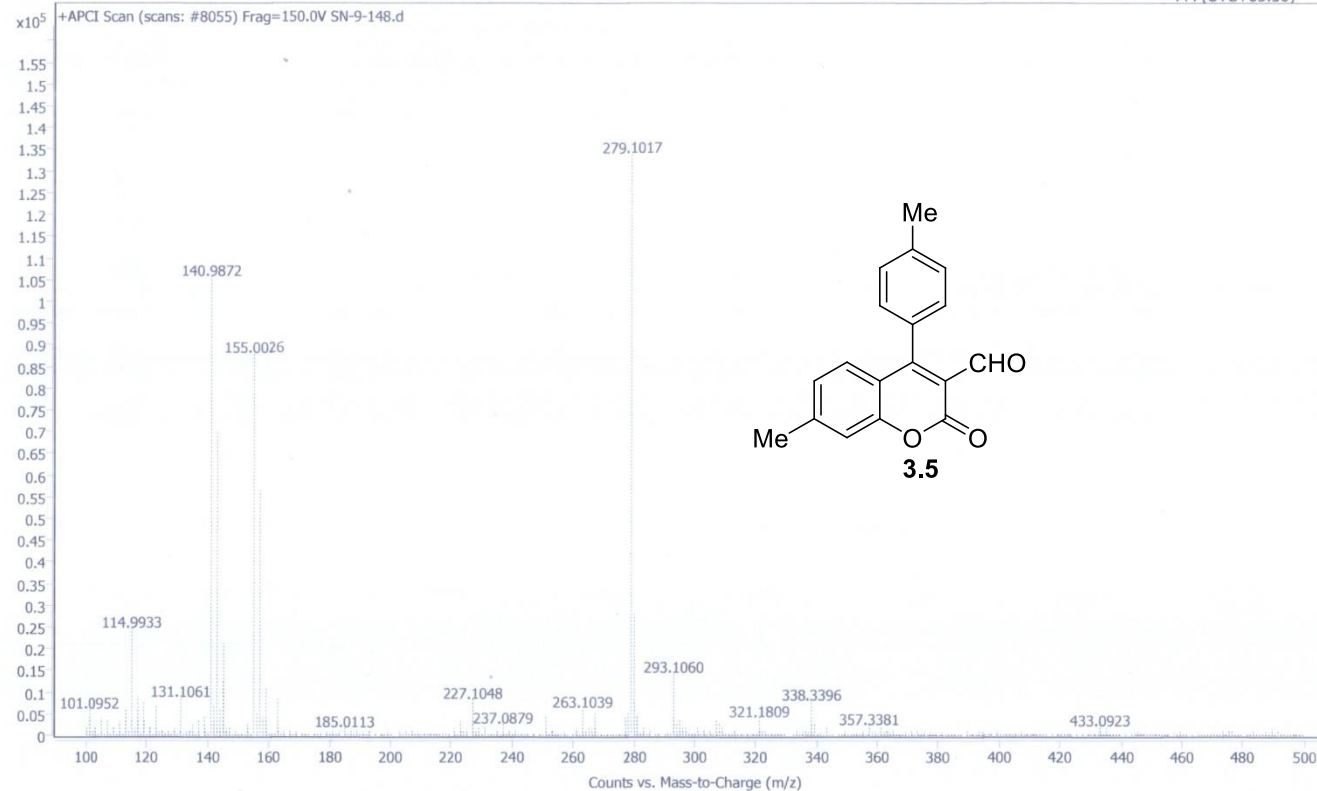


**Mass Spectrum of 4-(3-chlorophenyl)-7-methoxy-2-oxo-2H-chromene-3-carbaldehyde (3.4)**

## User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-148            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-148.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 15-07-2021 01:49:34 PM (UTC+05:30) |



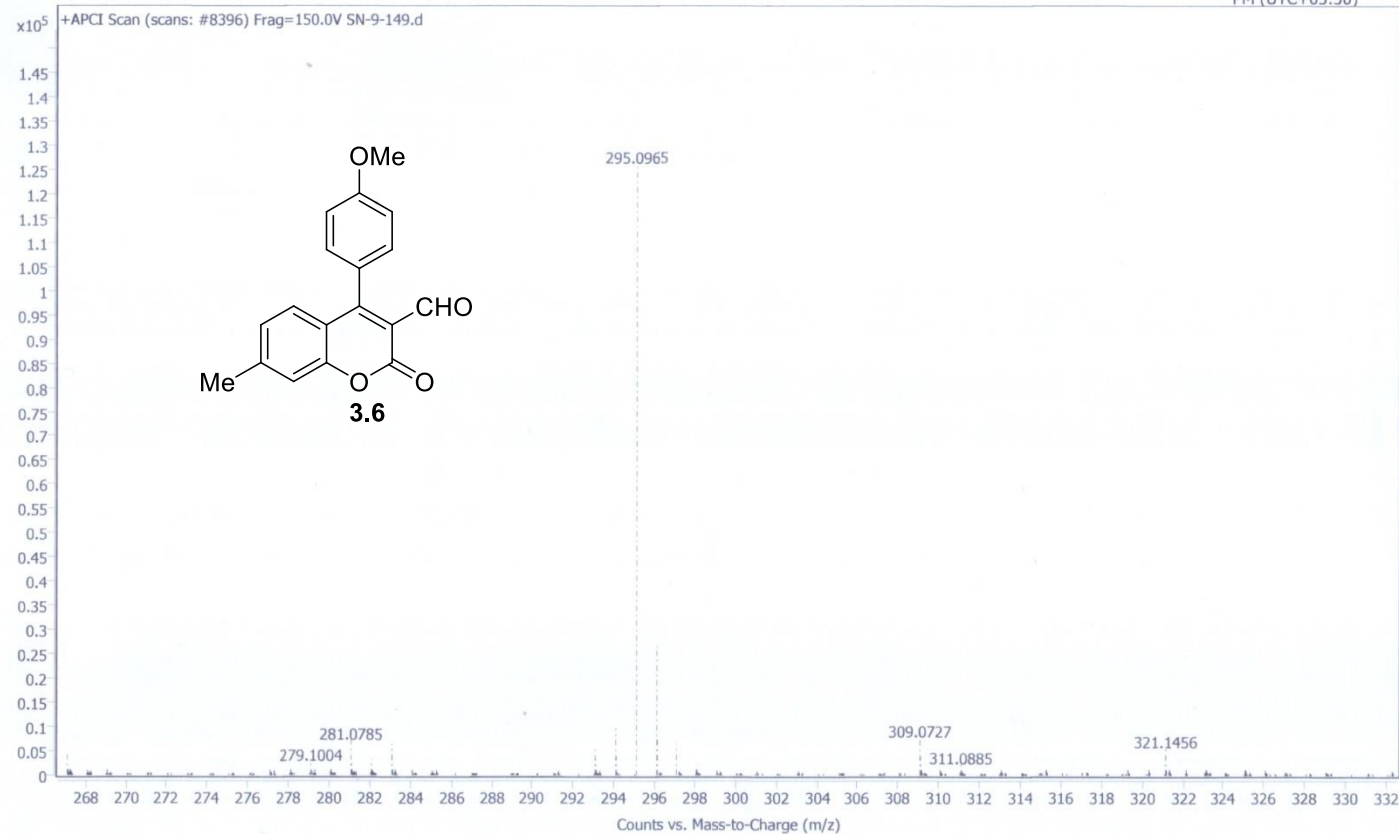
**Mass Spectrum of 7-methyl-2-oxo-4-p-tolyl-2H-chromene-3-carbaldehyde (3.5)**



# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-149            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-149.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 15-07-2021 02:12:07 PM (UTC+05:30) |

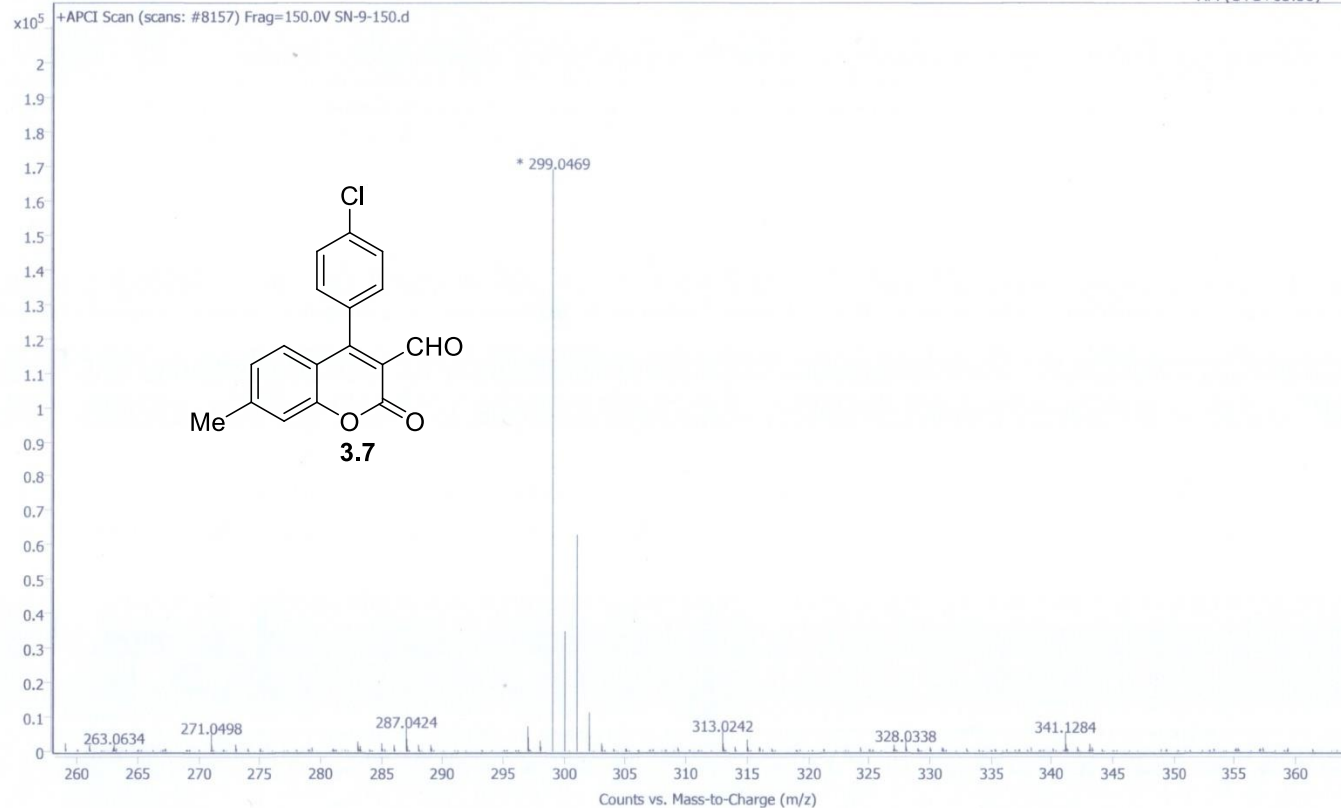


**Mass Spectrum of 4-(4-methoxyphenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.6)**

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-150            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-150.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 22-07-2021 10:53:23 AM (UTC+05:30) |

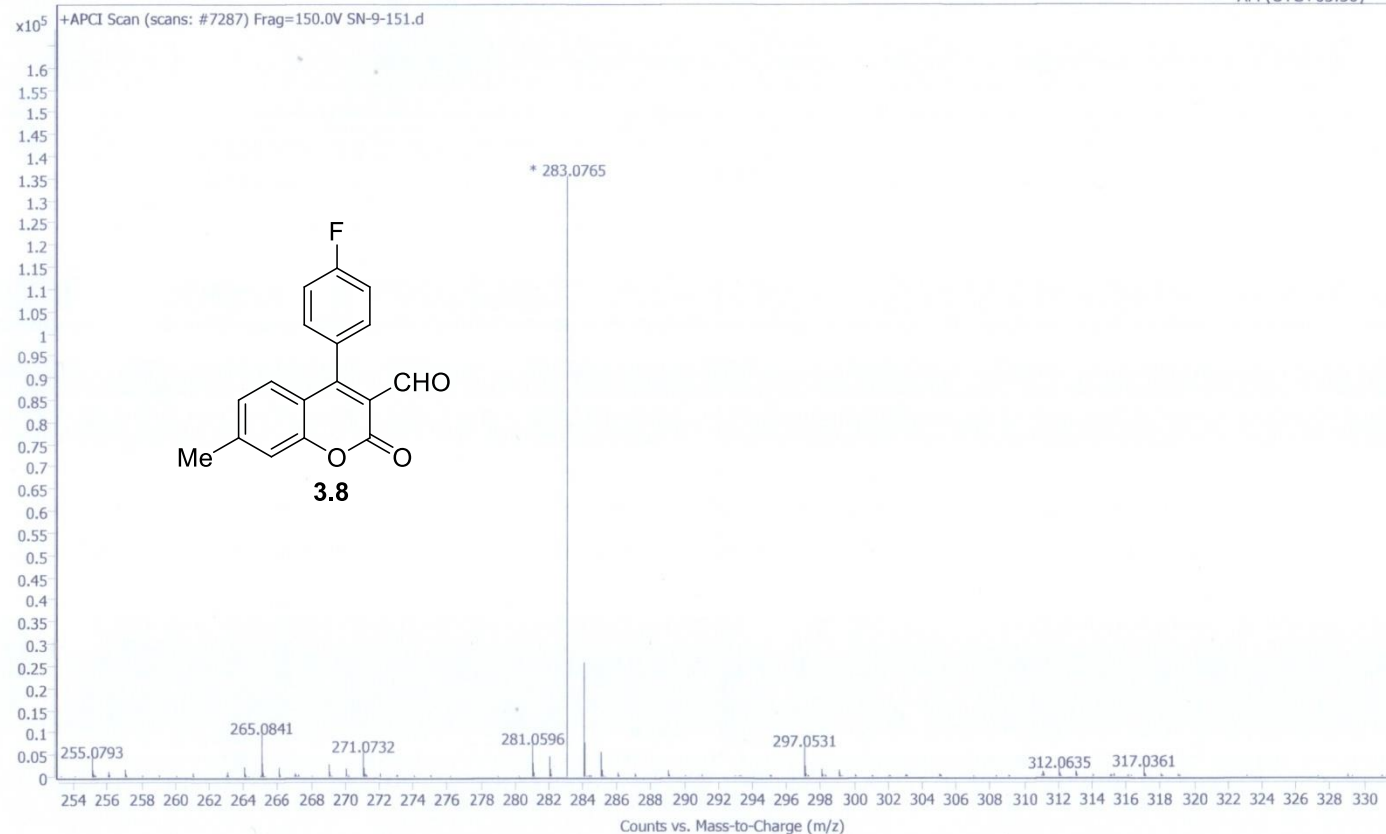


**Mass Spectrum of 4-(4-chlorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.7)**

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-151            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-151.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 22-07-2021 10:34:44 AM (UTC+05:30) |

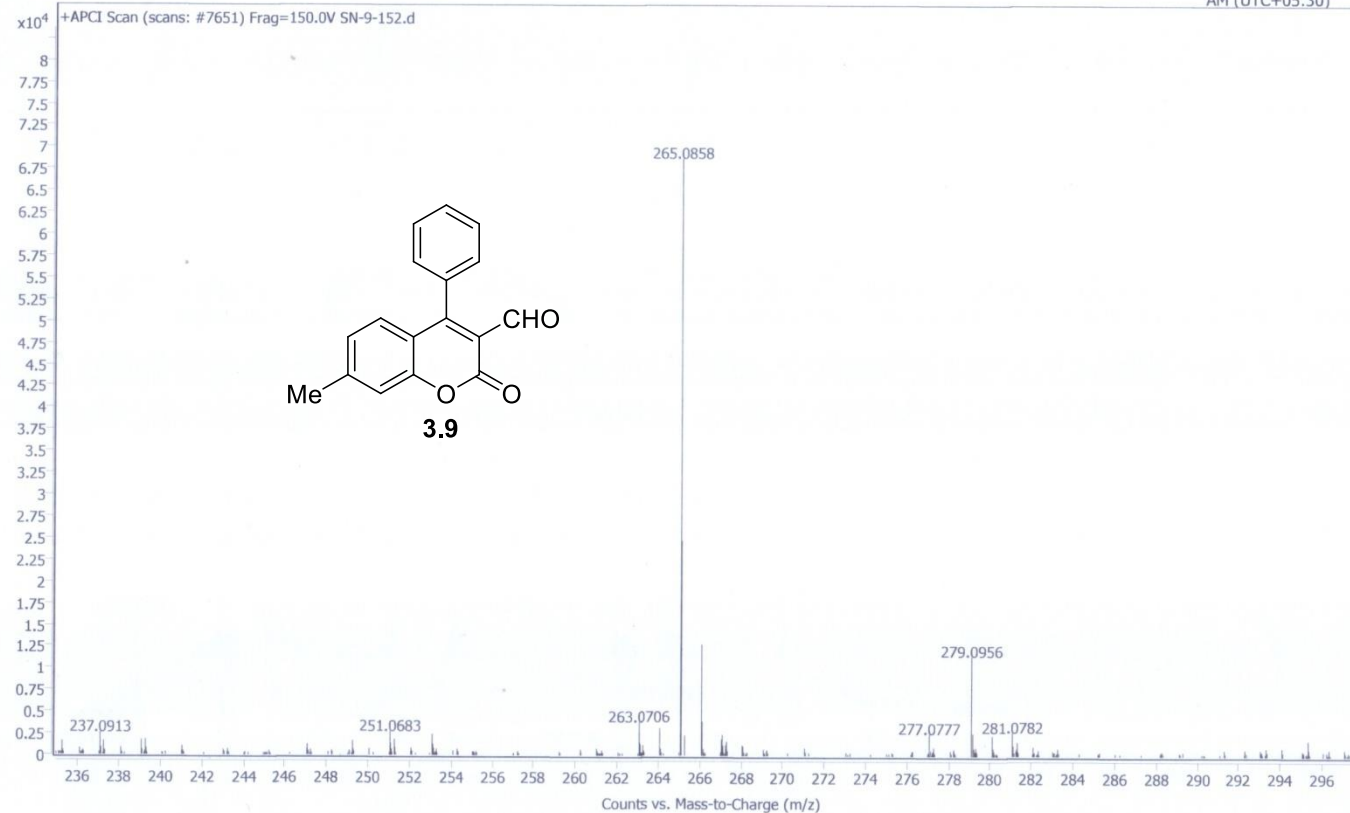


**Mass Spectrum of 4-(4-fluorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.8)**

# User Spectrum Plot Report



|                |                             |              |             |           |                   |                                    |
|----------------|-----------------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-152                    | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection Program | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-152.d                  | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 23-07-2021 11:00:30 AM (UTC+05:30) |

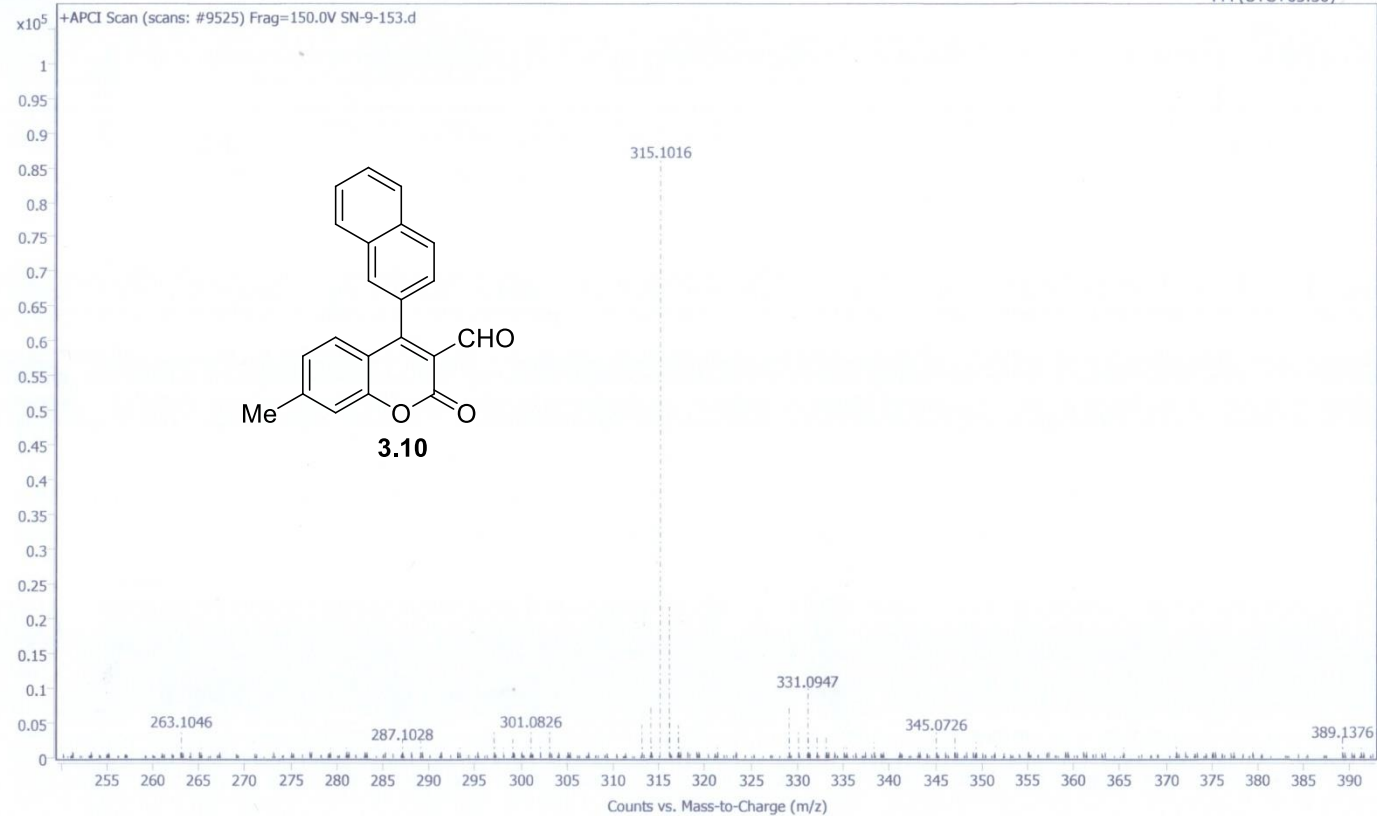


**Mass Spectrum of 7-methyl-2-oxo-4-phenyl-2H-chromene-3-carbaldehyde (3.9)**

# User Spectrum Plot Report



|                |                             |              |             |           |                   |                                    |
|----------------|-----------------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-153                    | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection Program | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-153.d                  | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 22-07-2021 12:00:47 PM (UTC+05:30) |

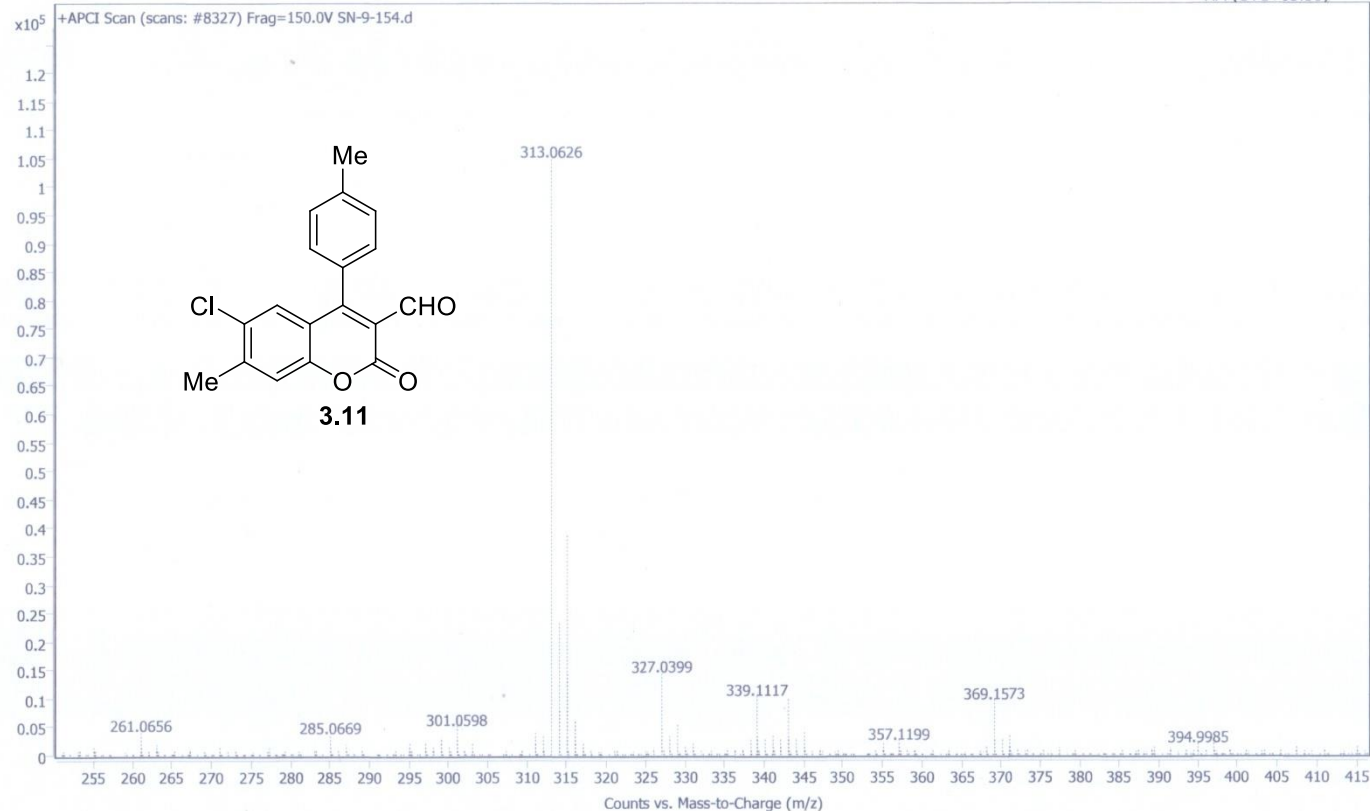


**Mass Spectrum of 7-methyl-4-(naphthalen-2-yl)-2-oxo-2H-chromene-3-carbaldehyde (3.10)**

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-154            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-154.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 22-07-2021 11:38:14 AM (UTC+05:30) |

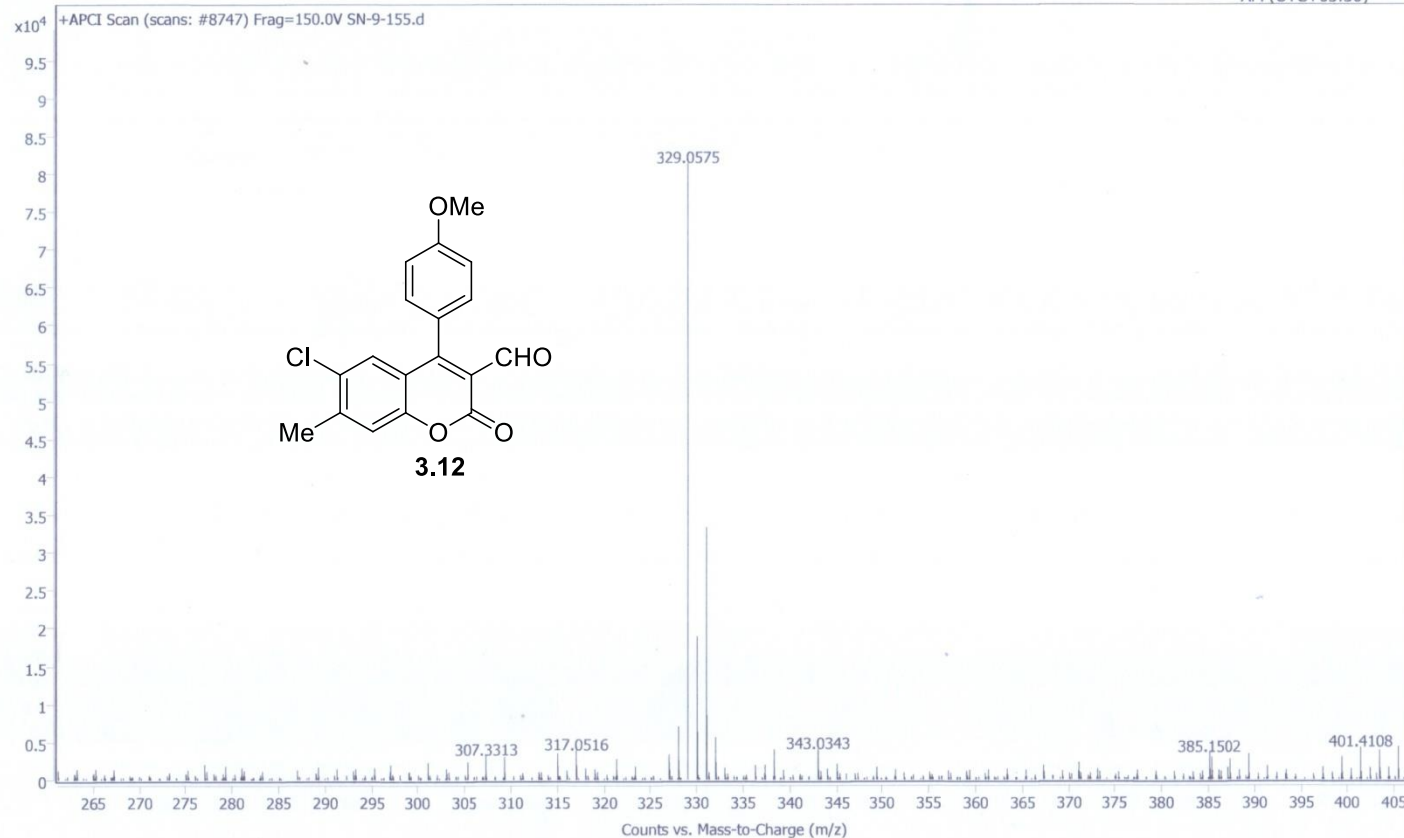


**Mass Spectrum of 6-chloro-7-methyl-2-oxo-4-p-tolyl-2H-chromene-3-carbaldehyde (3.11)**

# User Spectrum Plot Report



|                |                     |              |             |            |           |                   |                                    |
|----------------|---------------------|--------------|-------------|------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-155            | Rack Pos.    |             | Instrument | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   |             | IRM Status | Success   |                   |                                    |
| Data File      | SN-9-155.d          | Method (Acq) | GCAPCIITK.m | Comment    |           | Acq. Time (Local) | 22-07-2021 11:15:47 AM (UTC+05:30) |

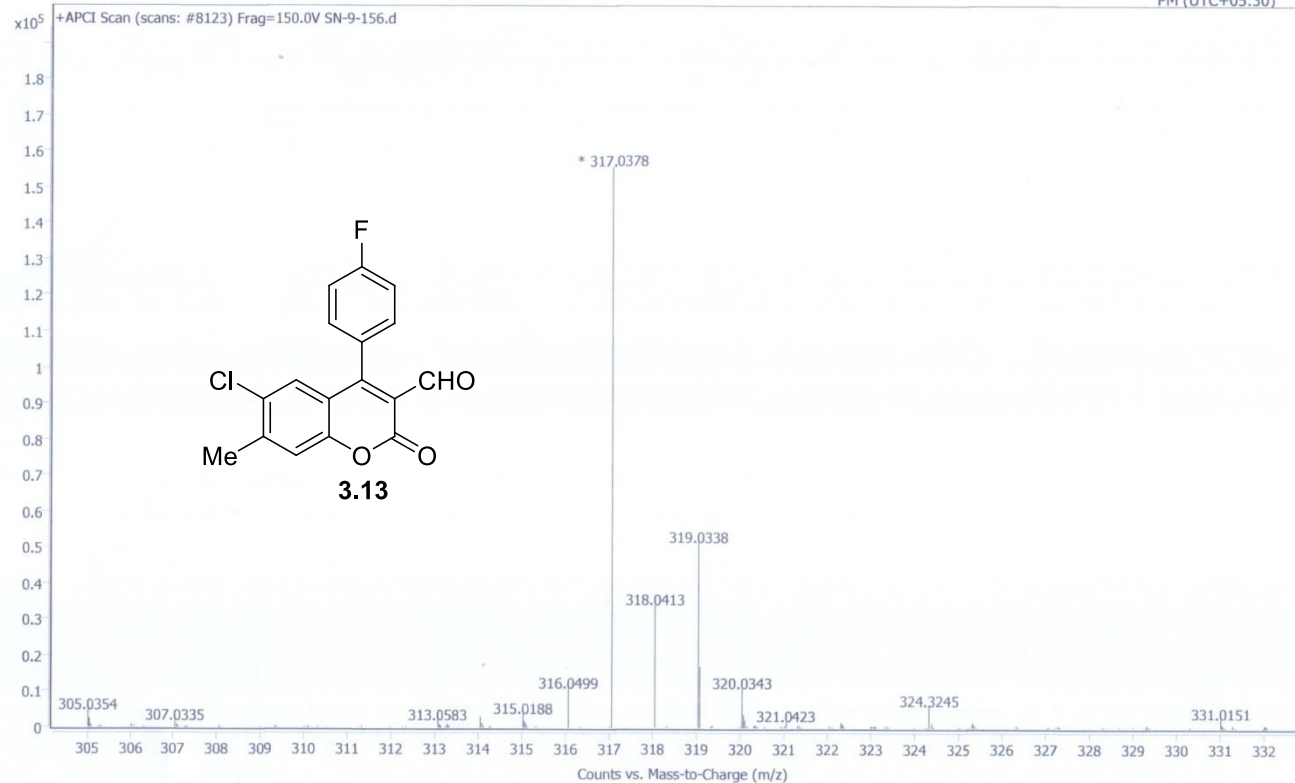


Mass Spectrum of 6-chloro-4-(4-methoxyphenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.12)

## User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-156            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-156.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 15-07-2021 12:46:29 PM (UTC+05:30) |



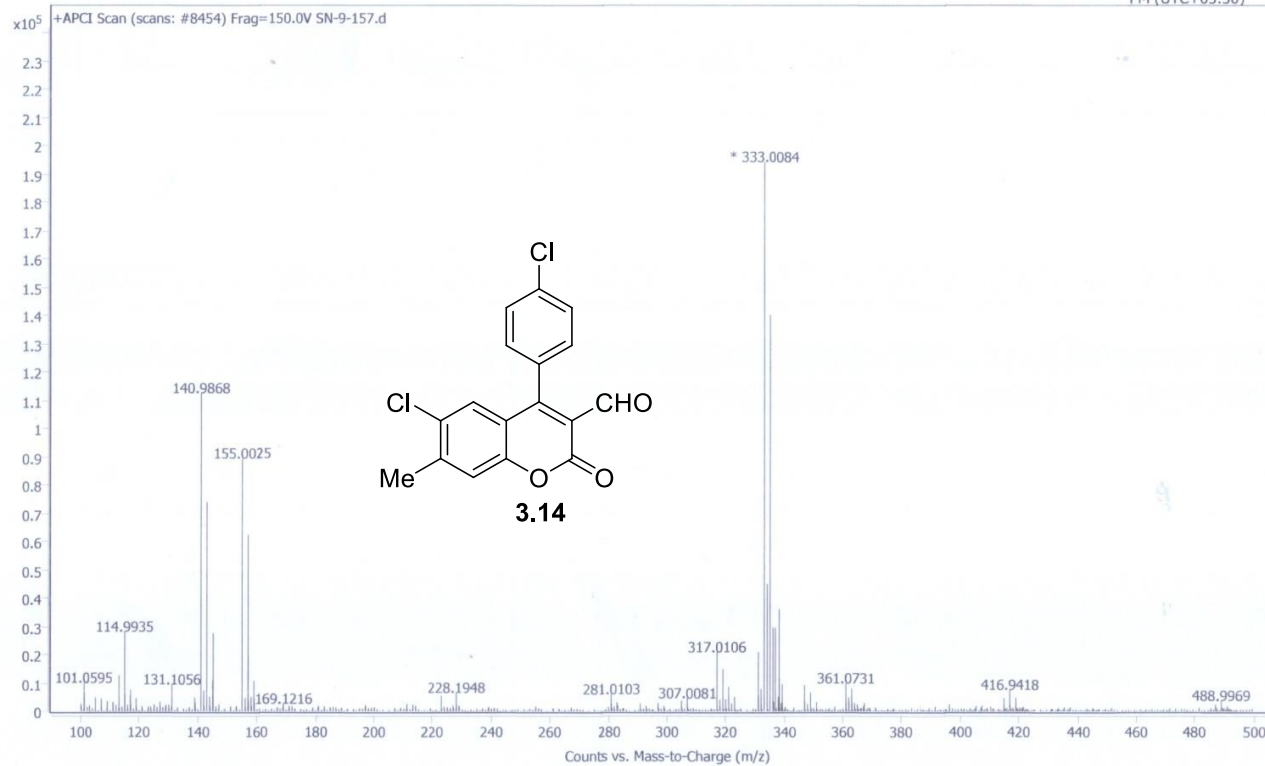
**Mass Spectrum of 6-chloro-4-(4-fluorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.13)**



## User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-157            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-157.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 15-07-2021 01:04:53 PM (UTC+05:30) |

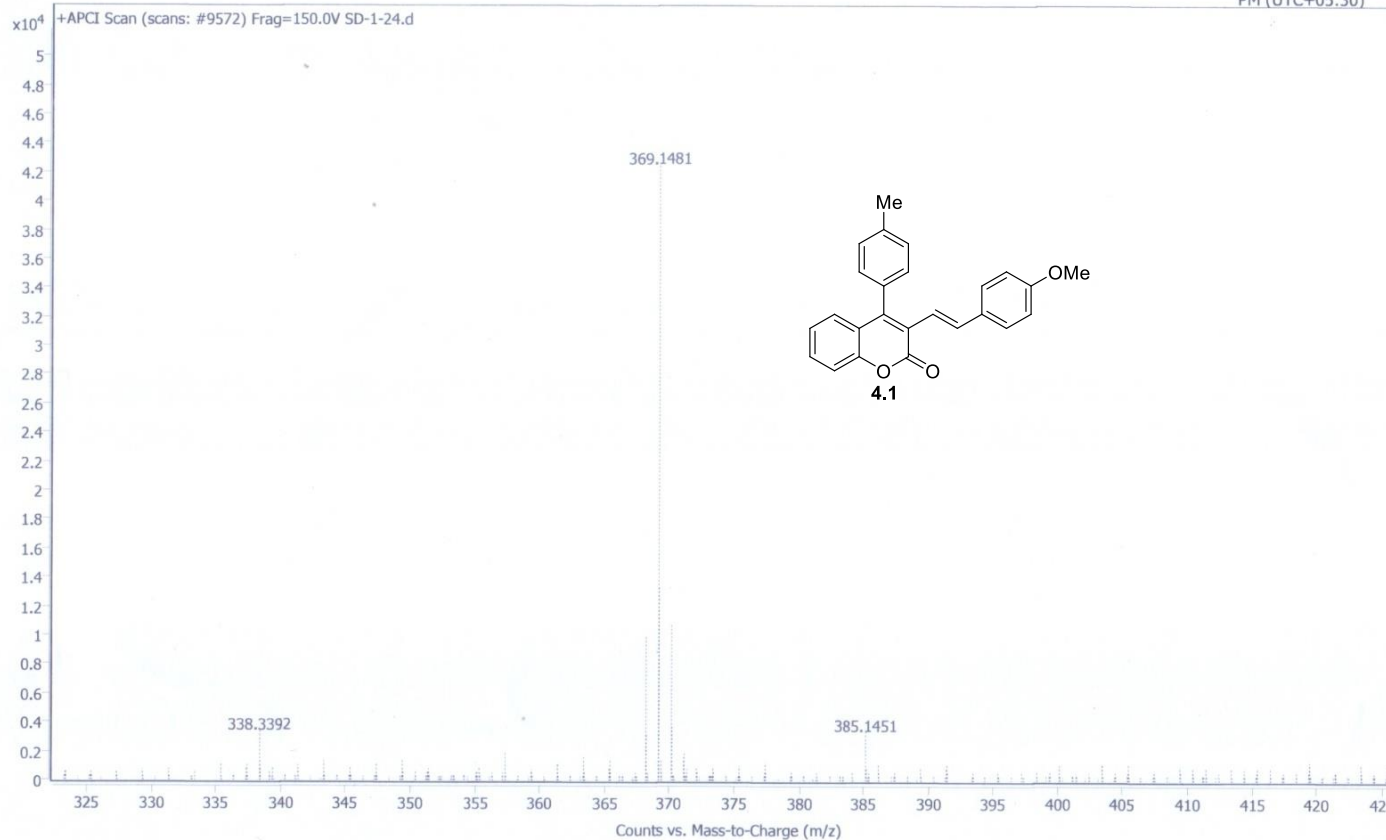


**Mass Spectrum of 6-chloro-4-(4-chlorophenyl)-7-methyl-2-oxo-2H-chromene-3-carbaldehyde (3.14)**

# User Spectrum Plot Report



|                |                     |              |             |            |           |                   |                                    |
|----------------|---------------------|--------------|-------------|------------|-----------|-------------------|------------------------------------|
| Name           | SD-1-24             | Rack Pos.    |             | Instrument | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   |             | IRM Status | Success   |                   |                                    |
| Data File      | SD-1-24.d           | Method (Acq) | GCAPCIITK.m | Comment    |           | Acq. Time (Local) | 13-07-2021 03:26:03 PM (UTC+05:30) |

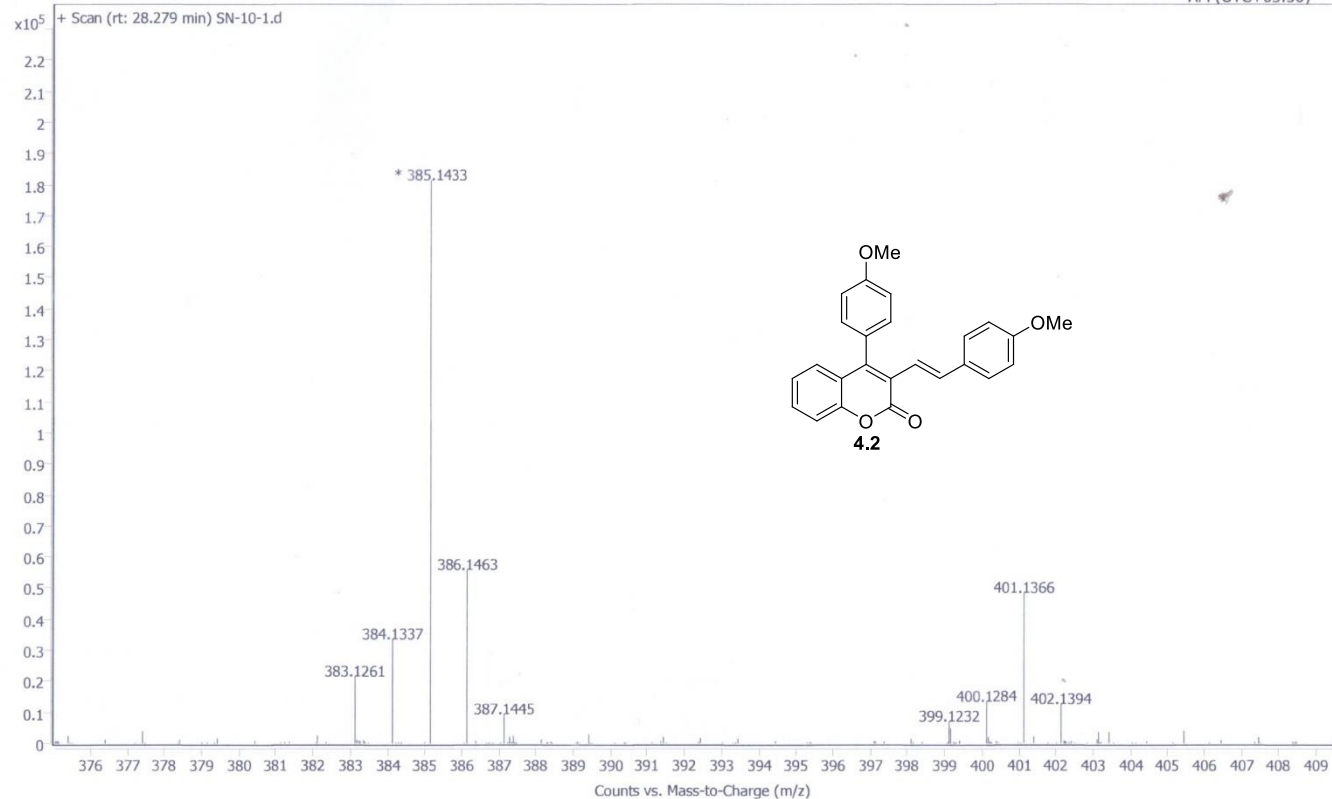


Mass Spectrum of (*E*)-3-(4-methoxystyryl)-4-*p*-tolyl-2*H*-chromen-2-one (4.1)

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-10-1             | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-10-1.d           | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 16-12-2021 10:38:14 AM (UTC+05:30) |

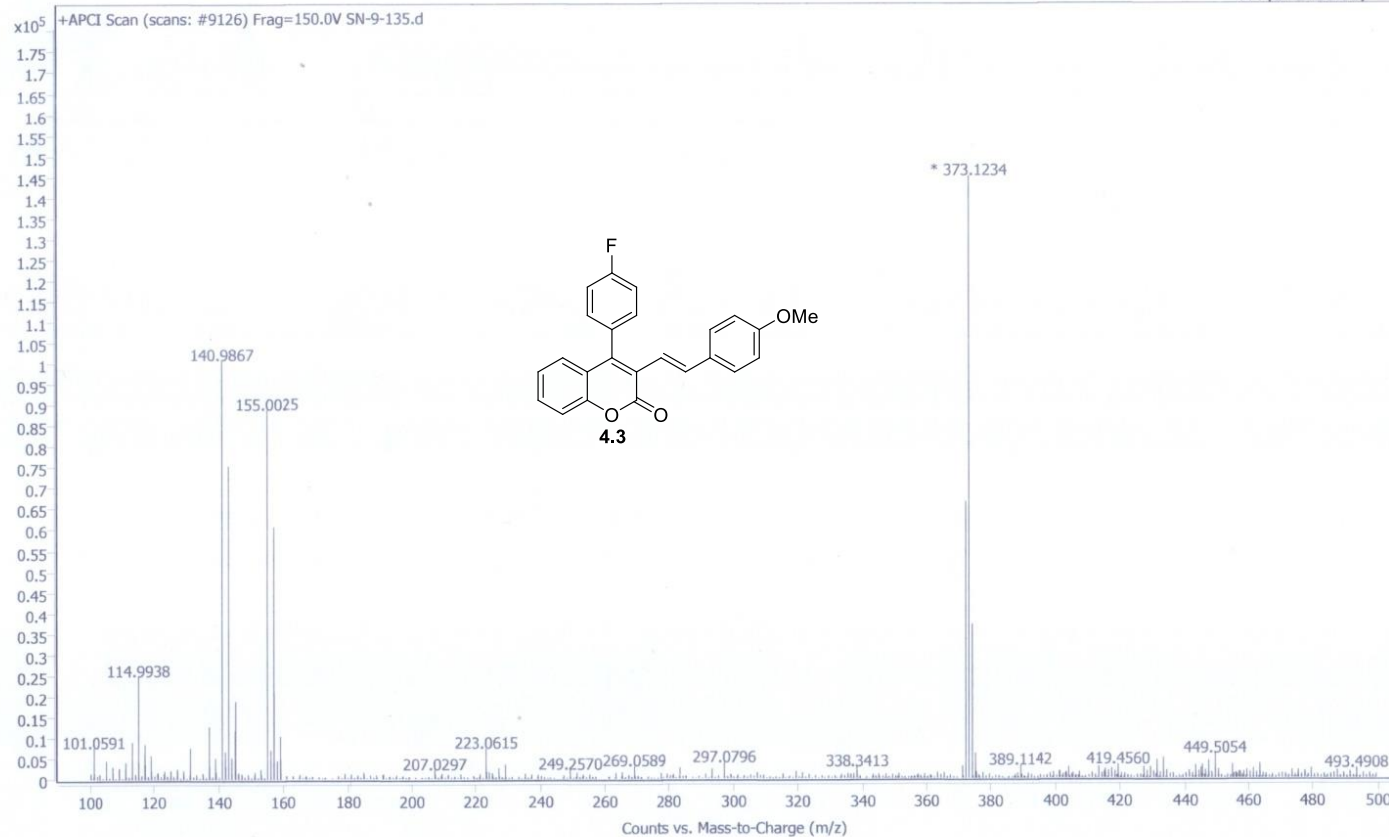


**Mass Spectrum of (E)-4-(4-methoxyphenyl)-3-(4-methoxystyryl)-2H-chromen-2-one (4.2)**

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-135            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-135.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 15-07-2021 01:27:12 PM (UTC+05:30) |

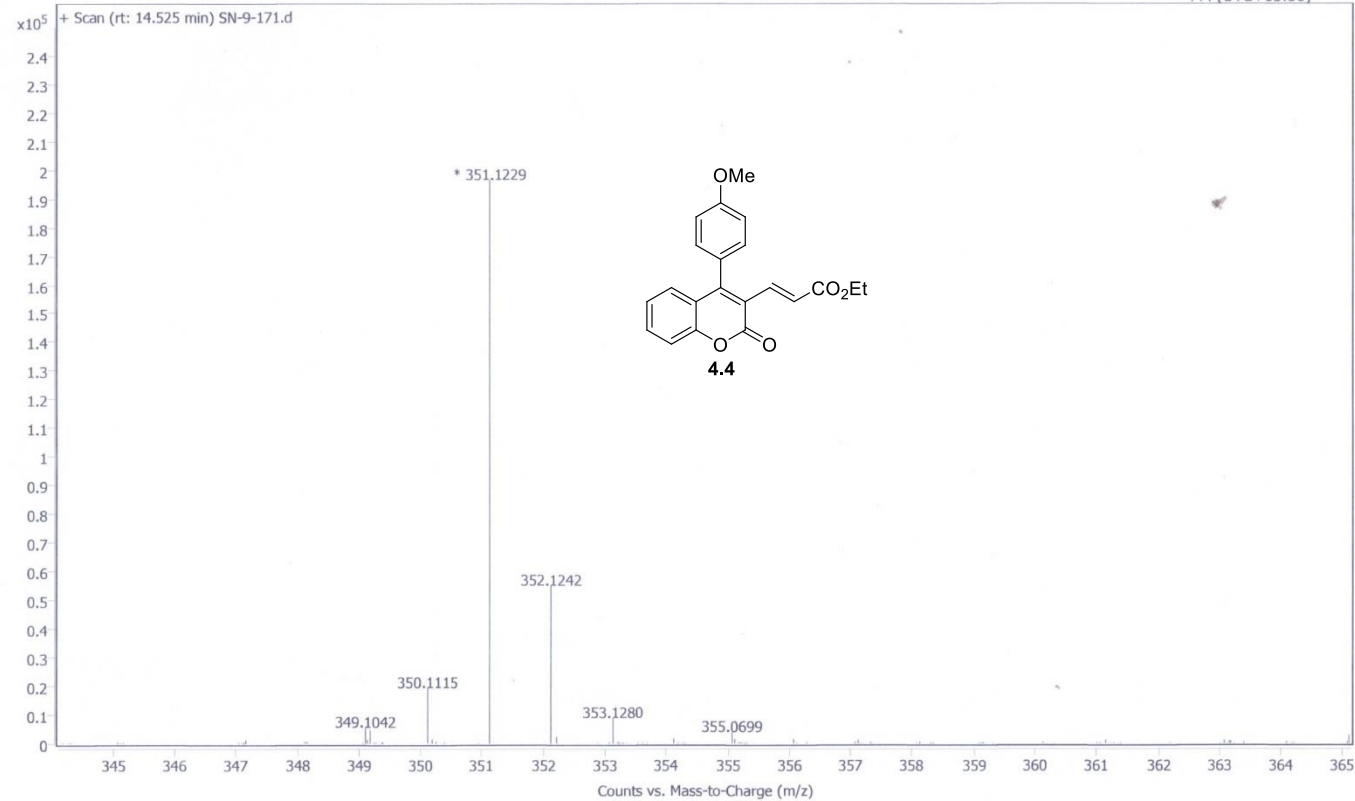


**Mass Spectrum of (E)-4-(4-fluorophenyl)-3-(4-methoxystyryl)-2H-chromen-2-one (4.3)**

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-171            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-171.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 08-12-2021 02:38:11 PM (UTC+05:30) |

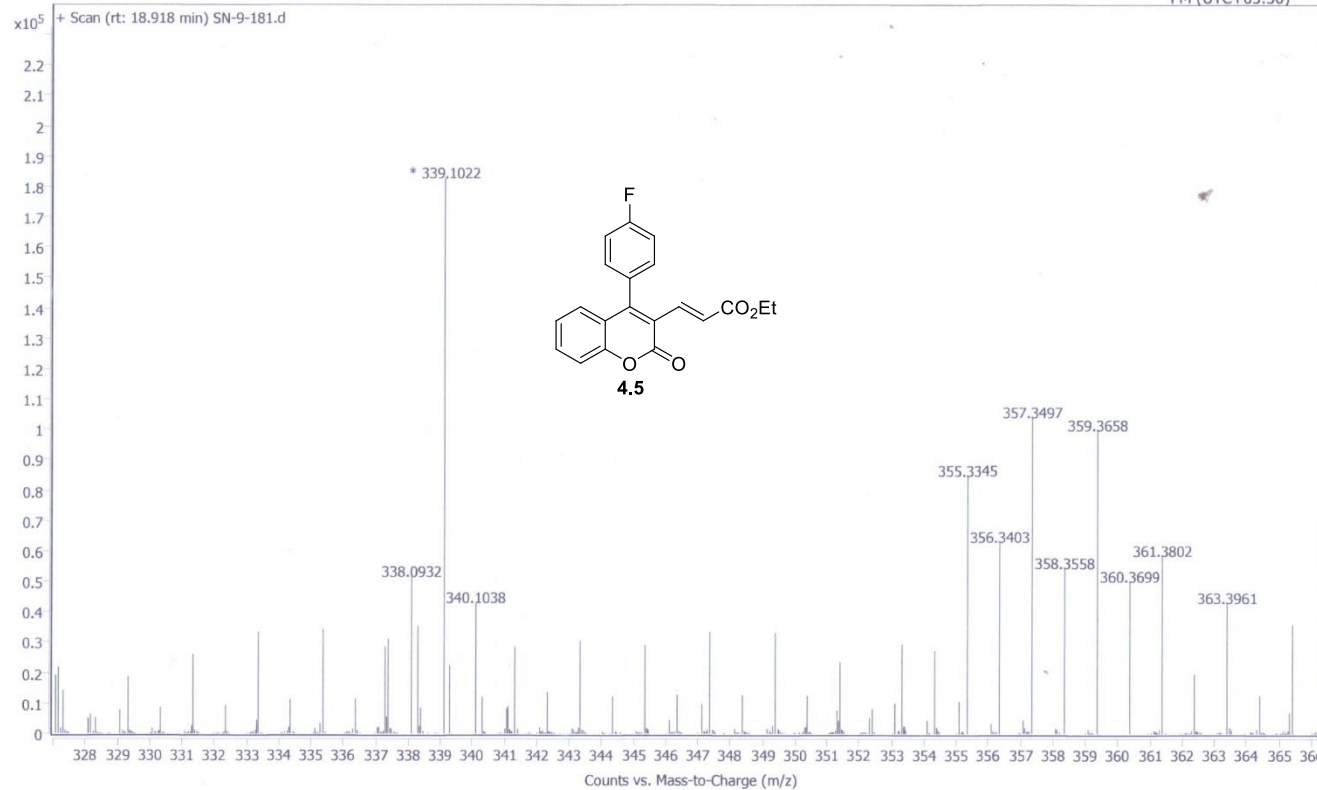


**Mass Spectrum of (E)-ethyl 3-(4-(4-methoxyphenyl)-2-oxo-2H-chromen-3-yl)acrylate (4.4)**

# User Spectrum Plot Report



|                |                             |              |             |            |           |                   |                                    |
|----------------|-----------------------------|--------------|-------------|------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-181                    | Rack Pos.    |             | Instrument | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection Program | Plate Pos.   |             | IRM Status | Success   |                   |                                    |
| Data File      | SN-9-181.d                  | Method (Acq) | GCAPCIITK.m | Comment    |           | Acq. Time (Local) | 15-12-2021 12:20:51 PM (UTC+05:30) |

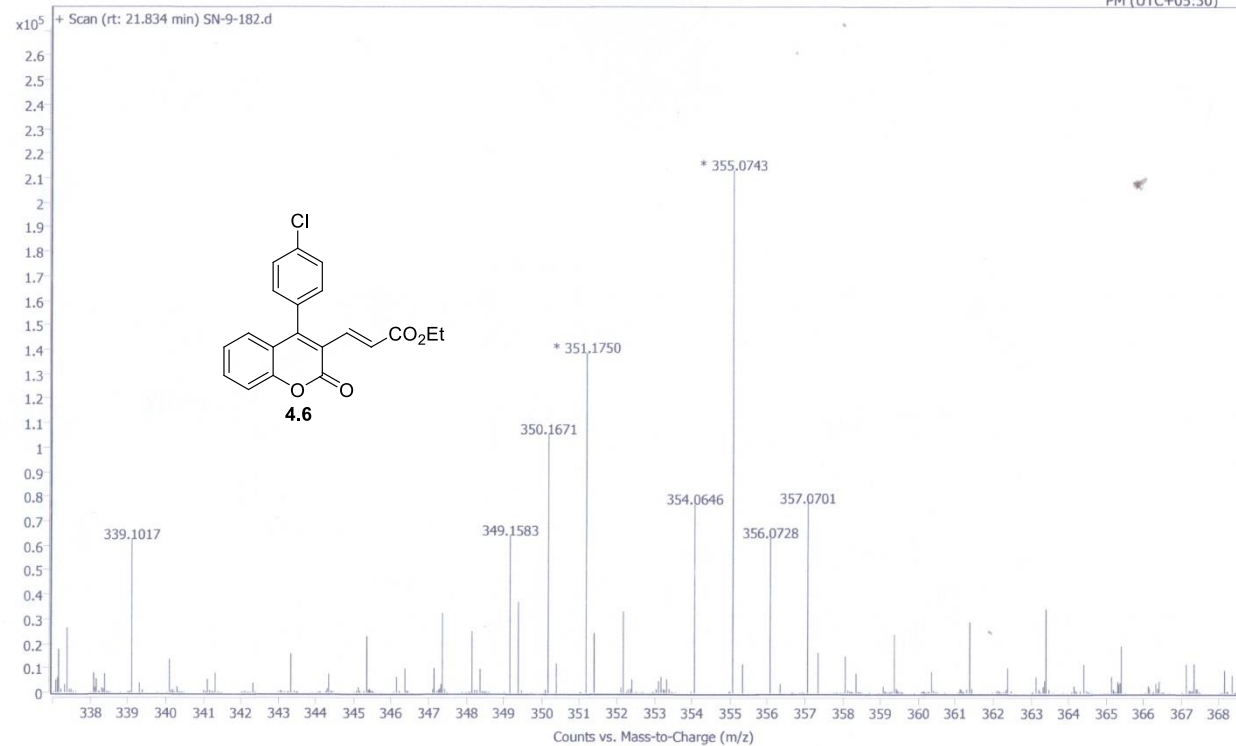


**Mass Spectrum of (E)-ethyl 3-(4-(4-fluorophenyl)-2-oxo-2H-chromen-3-yl)acrylate (4.5)**

# User Spectrum Plot Report



|                |                     |              |             |           |                   |                                    |
|----------------|---------------------|--------------|-------------|-----------|-------------------|------------------------------------|
| Name           | SN-9-182            | Rack Pos.    | Instrument  | APCI-GCMS | Operator          | ABHISHEK16IITK                     |
| Inj. Vol. (ul) | Unknown / Injection | Plate Pos.   | IRM Status  | Success   |                   |                                    |
| Data File      | SN-9-182.d          | Method (Acq) | GCAPCIITK.m | Comment   | Acq. Time (Local) | 15-12-2021 01:33:24 PM (UTC+05:30) |



**Mass Spectrum of (*E*)-ethyl 3-(4-(4-chlorophenyl)-2-oxo-2*H*-chromen-3-yl)acrylate (4.6)**