

## *Supporting Information*

### **Gold-Catalyzed Oxidative Cycloalkenations of Alkynes with Quinoline *N*-Oxides**

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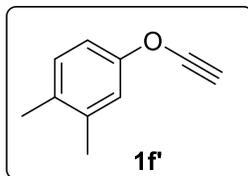
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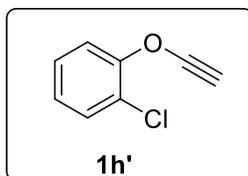
## (1) Spectral Data of Key Compounds:

### Spectral data of compound 4-(ethynyloxy)-1,2-dimethylbenzene (1f’):



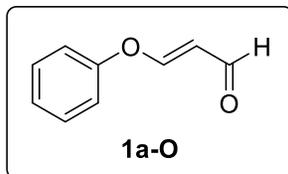
Black oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.08 (d,  $J = 8.4$  Hz, 1H), 7.04 (s, 1H), 7.99 (d,  $J = 8.0$  Hz, 1H), 2.25 (s, 3 H), 2.21 (s, 3H), 2.03 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  153.6, 138.3, 132.8, 130.5, 115.9, 112.0, 85.0, 32.8, 20.0, 19.0; EI-MS calcd. for  $\text{C}_{10}\text{H}_{10}\text{NaO}$  (M+Na): 169.0629; Found: 169.0634.

### Spectral data of compound 4-(ethynyloxy)-1,2-dimethylbenzene (1h’):



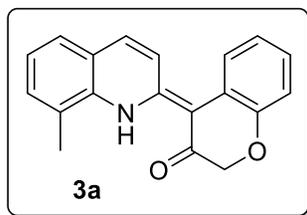
Black oil;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.58 (d,  $J = 8.3$  Hz, 1H), 7.37 (d,  $J = 8.0$  Hz, 1H), 7.29 (t,  $J = 7.7$  Hz, 1H), 7.08 (t,  $J = 7.7$  Hz, 1H), 2.17 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  151.1, 130.5, 127.8, 125.3, 121.6, 115.2, 83.4, 34.6; EI-MS calcd. for  $\text{C}_8\text{H}_6\text{ClO}$ (M+H): 153.0107; Found: 153.0125.

### Spectral data of compound (*E*)-3-phenoxyacrylaldehyde (1a-O):



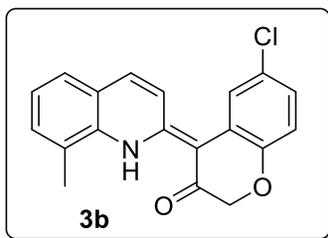
Pale yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  9.47 (d,  $J = 8.1$  Hz, 1H), 7.58 (d,  $J = 12.4$  Hz, 1H), 7.42-7.37 (m, 2H), 7.25-7.21 (m, 1H), 7.10-7.07 (m, 2H), 5.84 (dd,  $J = 8.0, 12.3$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  190.8, 167.2, 155.5, 130.1, 125.7, 118.3, 114.3; EI-MS calcd. for  $\text{C}_9\text{H}_8\text{O}_2$ : 148.0524; Found: 148.0510.

**Spectral data for (Z)-4-(8-methylquinolin-2(1H)-ylidene)chroman-3-one (3a):**



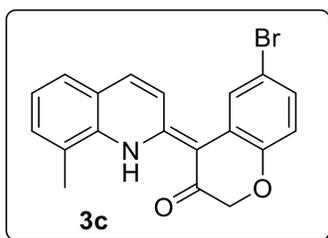
Orange solid; m.p 182-183 °C;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  16.22 (s, 1H), 7.83 (d,  $J = 9.4$  Hz, 1H), 7.70 (d,  $J = 9.4$  Hz, 1H), 7.47 (t,  $J = 8.5$  Hz, 3H), 7.26-7.25 (m, 1H), 7.06-7.01 (m, 3H), 4.55 (s, 2H), 2.67 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.6, 152.7, 149.4, 138.1, 136.4, 132.2, 126.0, 125.3, 125.0, 124.5, 124.0, 123.6, 123.3, 122.0, 118.7, 117.2, 97.2, 72.0, 17.0; EI-MS calcd. for  $\text{C}_{19}\text{H}_{15}\text{NO}_2$ : 289.1103; Found: 289.1106.

**Spectral data for (Z)-6-chloro-4-(8-methylquinolin-2(1H)-ylidene)chroman-3-one (3b):**



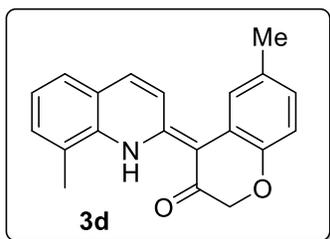
Orange solid; m.p 243-244 °C;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  16.26 (s, 1H), 7.90 (d,  $J = 9.4$  Hz, 1H), 7.66 (d,  $J = 9.4$  Hz, 1H), 7.49-7.47 (m, 2H), 7.41 (d,  $J = 2.2$  Hz, 1H), 7.26 (t,  $J = 7.6$  Hz, 1H), 6.97-6.93 (m, 2H), 4.50 (s, 2H), 2.66 (s, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.3, 151.2, 149.5, 138.8, 136.3, 132.5, 127.0, 126.4, 126.1, 125.5, 124.4, 124.3, 123.4, 123.0, 118.3, 118.1, 96.4, 72.0, 17.0; EI-MS calcd. for  $\text{C}_{19}\text{H}_{14}\text{ClNO}_2$ : 323.0713; Found: 323.0722.

**Spectral data for (Z)-6-bromo-4-(8-methylquinolin-2(1H)-ylidene)chroman-3-one (3c):**



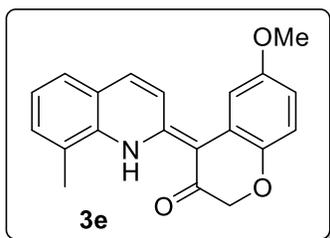
Orange solid; m.p 261-261 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  16.26 (s, 1H), 7.90 (d,  $J = 9.5$  Hz, 1H), 7.66 (d,  $J = 9.4$  Hz, 1H), 7.55 (s, 1H), 7.47 (d,  $J = 2.2$  Hz, 2H), 7.26 (t,  $J = 8.0$  Hz, 1H), 7.11 (d,  $J = 8.0$  Hz, 1H), 6.88 (d,  $J = 8.0$  Hz, 1H), 4.50 (s, 2H), 2.66 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.3, 151.7, 149.5, 138.9, 136.3, 132.5, 127.3, 126.9, 126.1, 125.8, 125.5, 124.3, 123.5, 118.8, 118.1, 114.5, 96.3, 72.0, 17.0; EI-MS calcd. for  $\text{C}_{19}\text{H}_{14}\text{BrNO}_2$ : 367.0208; Found: 367.0089.

**Spectral data for (Z)-6-methyl-4-(8-methylquinolin-2(1H)-ylidene)chroman-3-one (3d):**



Orange solid; m.p 174-175 °C;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  16.18 (s, 1H), 7.81 (d,  $J = 9.4$  Hz, 1H), 7.69 (d,  $J = 9.4$  Hz, 1H), 7.44 (d,  $J = 7.6$  Hz, 2H), 7.27 (d,  $J = 1.6$  Hz, 1H), 7.23 (t,  $J = 7.5$  Hz, 1H), 6.92 (d,  $J = 8.1$  Hz, 1H), 6.84 (dd,  $J = 8.1, 1.6$  Hz, 1H), 4.50 (s, 2H), 2.65 (s, 3H), 2.33 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.9, 150.6, 149.4, 138.1, 136.5, 132.2, 131.2, 126.0, 125.5, 125.3, 124.3, 124.1, 123.9, 123.3, 118.8, 116.9, 97.3, 72.2, 21.1, 17.0; EI-MS calcd. for  $\text{C}_{20}\text{H}_{17}\text{NO}_2$ : 303.1259; Found: 303.1256.

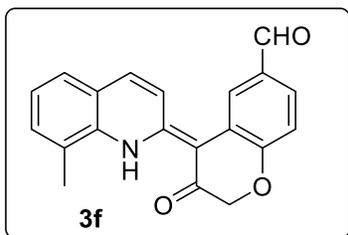
**Spectral data for (Z)-6-methoxy-4-(8-methylquinolin-2(1H)-ylidene)chroman-3-one (3e):**



Orange solid; m.p 197-198 °C;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  16.23 (s, 1H), 7.82 (d,  $J = 9.4$  Hz, 1H), 7.74 (dd,  $J = 9.4, 0.8$  Hz, 1H), 7.45 (d,  $J = 7.6$  Hz, 2H), 7.25-7.22 (m, 1H), 7.03 (d,  $J = 2.3$  Hz, 1H), 6.96 (d,  $J = 8.6$  Hz, 1H), 6.58 (dd,  $J = 8.1, 2.9$  Hz, 1H), 4.48 (s, 2H), 3.79 (s, 3H), 2.65 (s, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  189.1, 154.6, 149.5, 146.9, 138.2, 136.4, 132.3, 126.0,

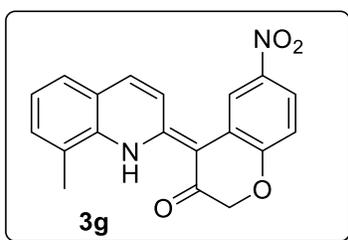
125.6, 125.4, 124.0, 123.3, 118.6, 117.4, 110.2, 108.8, 97.3, 72.3, 55.7, 17.0; EI-MS calcd. for  $C_{20}H_{17}NO_3$ : 319.1208; Found: 319.1205.

**Spectral data for (Z)-6-chloro-7-methyl-4-(8-methylquinolin-2(1H)-ylidene)chroman-3-one (3f):**



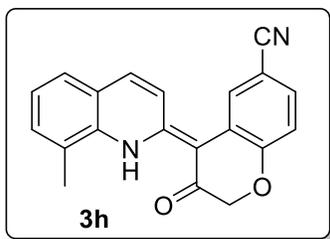
Orange solid; m.p 195-196 °C;  $^1H$  NMR (600 MHz,  $CDCl_3$ ):  $\delta$  16.21 (s, 1H), 7.88 (d,  $J = 9.4$  Hz, 1H), 7.65 (d,  $J = 9.4$  Hz, 1H), 7.48-7.46 (m, 2H), 7.47 (s, 1H), 7.27-7.23 (m, 1H), 6.88 (s, 1H), 4.49 (s, 2H), 2.65 (s, 3H), 2.32 (s, 3H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ ):  $\delta$  188.2, 151.2, 149.3, 138.6, 136.4, 132.4, 132.2, 127.0, 126.1, 125.5, 124.2, 123.8, 123.3, 119.4, 118.3, 96.3, 72.1, 19.7, 17.0, one carbon merged with others; EI-MS calcd. for  $C_{20}H_{16}ClNO_2$ : 337.0870; Found: 337.0872.

**Spectral data for (Z)-7-bromo-4-(8-methylquinolin-2(1H)-ylidene) chroman-3-one (3g):**



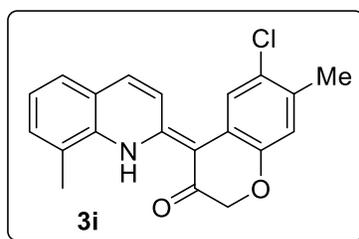
Orange solid; m.p 231-232 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  16.20 (s, 1H), 7.84 (d,  $J = 9.3$  Hz, 1H), 7.59 (d,  $J = 9.3$  Hz, 1H), 7.46 (d,  $J = 7.4$  Hz, 2H), 7.31-7.25 (m, 2H), 7.16-7.10 (m, 2H), 4.51 (s, 2H), 2.64 (s, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  187.9, 153.5, 149.4, 138.5, 136.3, 132.4, 126.1, 125.4, 124.9, 124.4, 124.2, 123.7, 123.4, 120.5, 118.3, 116.8, 96.5, 72.1, 17.0; EI-MS calcd. for  $C_{19}H_{14}BrNO_2$ : 367.0208; Found: 367.0203.

**Spectral data for (Z)-8-bromo-4-(8-methylquinolin-2(1H)-ylidene) chroman-3-one (3h):**



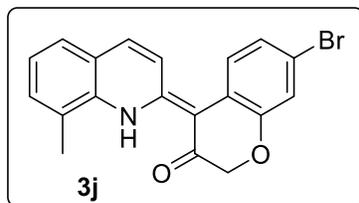
Orange solid; m.p 224-225 °C;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  16.23 (s, 1H), 7.84 (d,  $J = 9.4$  Hz, 1H), 7.62 (d,  $J = 9.4$  Hz, 1H), 7.47 (d,  $J = 7.6$  Hz, 2H), 7.37 (d,  $J = 7.7$  Hz, 1H), 7.27-7.24 (m, 2H), 6.86 (t,  $J = 7.8$  Hz, 1H), 4.61 (s, 2H), 2.65 (s, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  187.9, 149.6, 149.3, 138.5, 136.3, 132.4, 128.5, 126.2, 126.1, 125.4, 124.3, 123.4, 122.8, 122.5, 118.3, 111.6, 96.6, 72.2, 17.0; EI-MS calcd. for  $\text{C}_{19}\text{H}_{14}\text{BrNO}_2$ : 367.0208; Found: 367.0209.

**Spectral data for (Z)-6-chloro-7-methyl-4-(8-methylquinolin-2(1H)-ylidene)chroman-3-one (3i):**



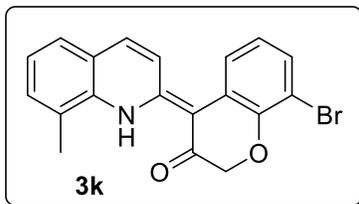
Orange solid; m.p 195-196 °C;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  16.21 (s, 1H), 7.88 (d,  $J = 9.4$  Hz, 1H), 7.65 (d,  $J = 9.4$  Hz, 1H), 7.48-7.46 (m, 2H), 7.47 (s, 1H), 7.27-7.23 (m, 1H), 6.88 (s, 1H), 4.49 (s, 2H), 2.65 (s, 3H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.2, 151.2, 149.3, 138.6, 136.4, 132.4, 132.2, 127.0, 126.1, 125.5, 124.2, 123.8, 123.3, 119.4, 118.3, 96.3, 72.1, 19.7, 17.0, one carbon merged with others; EI-MS calcd. for  $\text{C}_{20}\text{H}_{16}\text{ClNO}_2$ : 337.0870; Found: 337.0872.

**Spectral data for (Z)-7-bromo-4-(8-methylquinolin-2(1H)-ylidene)chroman-3-one (3j):**



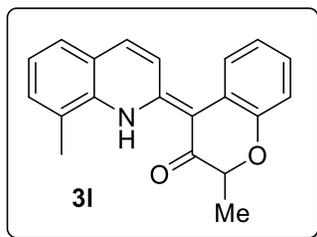
Orange solid; m.p 231-232 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 16.20 (s, 1H), 7.84 (d, *J* = 9.3 Hz, 1H), 7.59 (d, *J* = 9.3 Hz, 1H), 7.46 (d, *J* = 7.4 Hz, 2H), 7.31-7.25 (m, 2H), 7.16-7.10 (m, 2H), 4.51 (s, 2H), 2.64 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 187.9, 153.5, 149.4, 138.5, 136.3, 132.4, 126.1, 125.4, 124.9, 124.4, 124.2, 123.7, 123.4, 120.5, 118.3, 116.8, 96.5, 72.1, 17.0; EI-MS calcd. for C<sub>19</sub>H<sub>14</sub>BrNO<sub>2</sub>: 367.0208; Found: 367.0203.

**Spectral data for (*Z*)-8-bromo-4-(8-methylquinolin-2(1*H*)-ylidene)chroman-3-one (3k):**



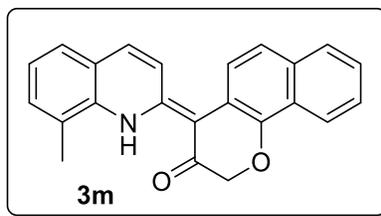
Orange solid; m.p 224-225 °C; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 16.23 (s, 1H), 7.84 (d, *J* = 9.4 Hz, 1H), 7.62 (d, *J* = 9.4 Hz, 1H), 7.47 (d, *J* = 7.6 Hz, 2H), 7.37 (d, *J* = 7.7 Hz, 1H), 7.27-7.24 (m, 2H), 6.86 (t, *J* = 7.8 Hz, 1H), 4.61 (s, 2H), 2.65 (s, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): δ 187.9, 149.6, 149.3, 138.5, 136.3, 132.4, 128.5, 126.2, 126.1, 125.4, 124.3, 123.4, 122.8, 122.5, 118.3, 111.6, 96.6, 72.2, 17.0; EI-MS calcd. for C<sub>19</sub>H<sub>14</sub>BrNO<sub>2</sub>: 367.0208; Found: 367.0209.

**Spectral data for (*Z*)-2-methyl-4-(8-methylquinolin-2(1*H*)-ylidene)chroman-3-one (3l):**



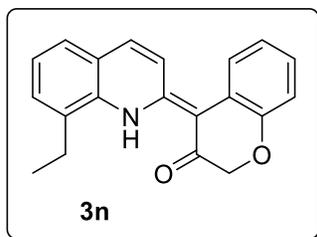
Orange solid; m.p 133-134 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 16.27 (s, 1H), 7.80 (d, *J* = 9.5 Hz, 1H), 7.70 (d, *J* = 9.4 Hz, 1H), 7.45 (t, *J* = 7.3 Hz, 3H), 7.22-7.20 (m, 1H), 7.07-6.98 (m, 3H), 4.57 (q, *J* = 6.8 Hz, 1H), 2.67 (s, 3H), 1.51 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): δ 190.8, 151.5, 149.7, 137.9, 136.5, 132.1, 126.0, 125.3, 125.0, 124.5, 123.9, 123.5, 123.3, 121.8, 119.0, 117.8, 96.4, 77.0, 17.2, 16.3; EI-MS calcd. for C<sub>20</sub>H<sub>17</sub>NO<sub>2</sub>: 303.1259; Found: 303.1258.

**Spectral data for (*Z*)-4-(8-methylquinolin-2(1*H*)-ylidene)-2*H*-benzo[*h*]chromen-3(4*H*)-one (3m):**



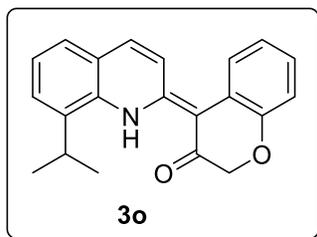
Orange solid; m.p 261-262 °C;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  16.06 (s, 1H), 8.19 (d,  $J = 9.3$  Hz, 1H), 7.81 (d,  $J = 9.4$  Hz, 1H), 7.77 (d,  $J = 9.4$  Hz, 1H), 7.65 (d,  $J = 9.3$  Hz, 1H), 7.62 (d,  $J = 8.5$  Hz, 1H), 7.50 (d,  $J = 9.4$  Hz, 1H), 7.46-7.43 (m, 3H), 7.39-7.38 (m, 1H), 7.23 (t,  $J = 7.4$  Hz, 1H), 4.70 (s, 2H), 2.67 (s, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  189.3, 148.9, 147.1, 138.1, 136.5, 132.3, 131.9, 127.4, 125.9, 125.7, 125.6, 125.4, 125.1, 123.9, 123.3, 122.9, 121.4, 121.2, 119.1, 118.8, 97.8, 72.4, 17.0; ESI-MS ( $\text{M}+\text{H}$ ) calcd. for  $\text{C}_{23}\text{H}_{18}\text{NO}_2$ : 340.1338; Found: 340.1328.

**Spectral data for (Z)-4-(8-ethylquinolin-2(1H)-ylidene)chroman-3-one (3n):**



Orange solid; m.p 184-185 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  16.29 (s, 1H), 7.82 (d,  $J = 9.4$  Hz, 1H), 7.68 (d,  $J = 9.4$  Hz, 1H), 7.47-7.44 (m, 3H), 7.27 (t,  $J = 7.3$  Hz, 1H), 7.03-6.99 (m, 3H), 4.53 (s, 2H), 3.04 (q,  $J = 7.4$  Hz, 2H), 1.44 (t,  $J = 7.4$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.6, 152.7, 149.4, 138.2, 135.7, 131.7, 130.2, 125.3, 124.9, 124.5, 124.1, 123.6, 123.4, 121.9, 118.6, 117.2, 97.1, 72.0, 23.7, 12.9; EI-MS calcd. for  $\text{C}_{20}\text{H}_{17}\text{NO}_2$ : 303.1259; Found: 303.1255.

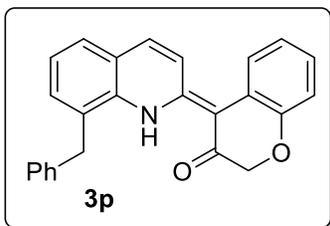
**Spectral data for (Z)-4-(8-isopropylquinolin-2(1H)-ylidene)chroman-3-one (3o):**



Orange solid; m.p 173-174 °C;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  16.41 (s, 1H), 7.84 (d,  $J = 9.4$  Hz, 1H), 7.70 (dd,  $J = 9.4, 1.0$  Hz, 1H), 7.54 (d,  $J = 9.3$  Hz, 1H), 7.47-7.44 (m, 2H), 7.31 (t,  $J = 7.6$

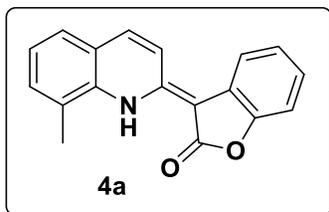
Hz, 1H), 7.04-6.99 (m, 3H), 4.53 (s, 2H), 3.66-3.59 (m, 1H), 1.44 (d,  $J = 6.8$  Hz, 6H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.6, 152.8, 149.6, 138.5, 136.5, 135.2, 127.7, 125.4, 125.0, 124.6, 124.3, 123.6, 122.0, 118.6, 117.3, 97.1, 72.1, 29.6 (grease peak), 27.7, 22.4, one carbon merged with others; EI-MS calcd. for  $\text{C}_{21}\text{H}_{19}\text{NO}_2$ : 317.1416; Found: 317.1414.

**Spectral data for (Z)-4-(8-benzylquinolin-2(1H)-ylidene)chroman-3-one (3p):**



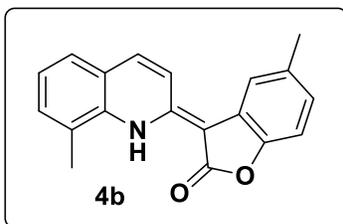
Orange solid; m.p 194-195 °C;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  16.29 (s, 1H), 7.81 (d,  $J = 9.4$  Hz, 1H), 7.68 (d,  $J = 9.4$  Hz, 1H), 7.48-7.43 (m, 2H), 7.34-7.31 (m, 5H), 7.25-7.23 (m, 2H), 7.04-7.00 (m, 3H), 4.36 (s, 2H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.5, 152.8, 149.5, 138.1, 137.8, 136.0, 132.1, 129.3, 128.6, 126.6, 125.9, 125.1, 124.5, 124.0, 123.7, 122.0, 119.0, 117.2, 97.4, 72.0, 36.4, other carbons merged with others; EI-MS calcd. for  $\text{C}_{25}\text{H}_{19}\text{NO}_2$ : 365.1416; Found: 365.1414.

**Spectral Data of (Z)-3-(8-methylquinolin-2(1H)-ylidene)benzofuran-2(3H)-one (4a):**



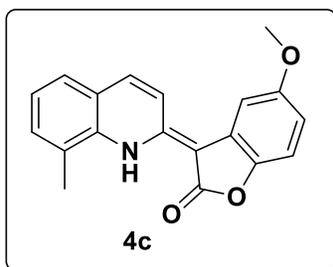
Orange solid, m.p 219-220 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.23 (bs, 1H), 7.86 (d,  $J = 9.2$  Hz, 1H), 7.51 (d,  $J = 9.6$  Hz, 1H), 7.46-7.43 (m, 3H), 7.21 (t,  $J = 8.0$  Hz, 1H), 7.17-7.11 (m, 2H), 7.08-7.04 (m, 1H), 2.61 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 171.7, 149.1, 148.3, 138.8, 136.1, 132.9, 125.9, 125.8, 125.0, 123.8, 122.9, 122.6, 122.0, 117.8, 117.3, 110.1, 85.2, 16.6 ; ESI-MS calcd for  $\text{C}_{18}\text{H}_{14}\text{NO}_2$  [ $\text{M}+\text{H}$ ]: 276.1025 found: 276.1016.

**Spectral Data of (Z)-5-methyl-3-(8-methylquinolin-2(1H)-ylidene)benzofuran-2(3H)-one (4b):**



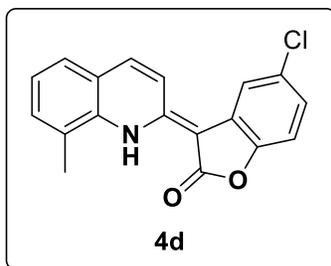
Orange solid, m.p 228-229 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.22 (bs, 1H), 7.85 (dd,  $J = 9.2$ , 2.0 Hz, 1H), 7.50 (d,  $J = 9.2$  Hz, 1H), 7.43 (t,  $J = 8.0$  Hz, 2H), 7.24-7.19 (m, 2H), 7.03 (dd,  $J = 8.0$  Hz, 1H), 6.86 (d,  $J = 8.0$  Hz, 1H), 2.60 (s, 3H), 2.39 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 172.1, 148.2, 147.3, 138.6, 136.1, 132.8, 132.3, 125.9, 125.8, 125.0, 123.7, 123.2, 122.0, 118.0, 109.7, 85.4, 21.6, 16.6, one carbon merged with others; ESI-MS calcd for  $\text{C}_{19}\text{H}_{16}\text{NO}_2$  [M+H]: 290.1181 found: 290.1178.

**Spectral Data of (Z)-5-methoxy-3-(8-methylquinolin-2(1H)-ylidene)benzofuran-2(3H)-one (4c):**



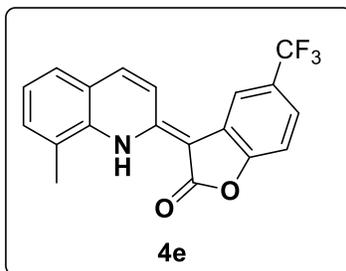
Orange solid, m.p 222-223 °C;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.30 (bs, 1H), 7.87 (d,  $J = 9.3$  Hz, 1H), 7.48-7.44 (m, 3H), 7.21 (t,  $J = 7.6$  Hz, 1H), 7.05 (d,  $J = 8.6$  Hz, 1H), 6.99 (d,  $J = 2.4$  Hz, 1H), 6.60 (dd,  $J = 8.6$ , 2.5 Hz, 1H), 3.84 (s, 3H), 2.61 (s, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): 172.3, 155.9, 148.3, 143.7, 138.8, 136.1, 132.9, 126.6, 125.9, 125.1, 123.8, 122.1, 117.7, 110.0, 107.0, 104.3, 85.7, 56.0, 16.6; ESI-MS calcd for  $\text{C}_{19}\text{H}_{16}\text{NO}_3$  [M+H]: 306.1130 found: 306.1141.

**Spectral Data of (Z)-5-chloro-3-(8-methylquinolin-2(1H)-ylidene)benzofuran-2(3H)-one (4d):**



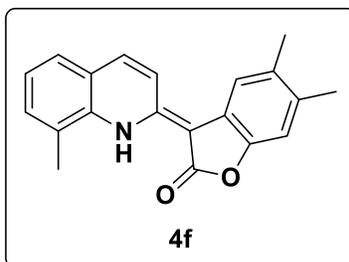
Orange solid, m.p 288-289 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 13.36 (bs, 1H), 7.96 (d, *J* = 9.2 Hz, 1H), 7.51-7.48 (m, 3H), 7.40 (s, 1H), 7.27 (d, *J* = 7.2 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 2.64 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 171.7, 148.5, 147.3, 139.5, 136.0, 133.2, 128.3, 127.4, 126.1, 125.3, 124.3, 122.3, 122.1, 117.6, 117.1, 110.9, 84.7, 16.6; ESI-MS calcd for C<sub>18</sub>H<sub>13</sub>ClNO<sub>2</sub> [M+H]: 310.0635 found: 310.0639.

**Spectral Data of (Z)-3-(8-methylquinolin-2(1H)-ylidene)-5-(trifluoromethyl)benzofuran-2(3H)-one (4e):**



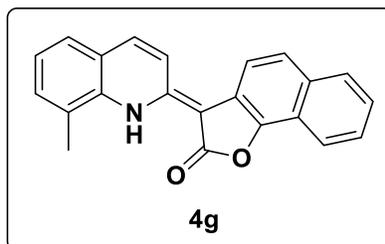
Orange solid, m.p 271-271 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 13.40 (bs, 1H), 8.01 (d, *J* = 9.2 Hz, 1H), 7.66 (s, 1H), 7.57-7.50 (m, 3H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.28 (d, *J* = 7.6 Hz, 1H), 7.26-7.21 (m, 1H), 2.66 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 171.5, 150.8, 148.7, 139.8, 136.0, 133.3, 126.5, 127.0, 125.4 (*J*<sub>C-F</sub> = 29.0 Hz), 124.4, 123.4, 122.4, 119.8, 117.5, 113.9, 109.9, 84.2, 16.6, other carbon peaks are merged; ESI-MS calcd for C<sub>19</sub>H<sub>13</sub>F<sub>3</sub>NO<sub>2</sub> [M+H]: 344.0898 found: 344.0882.

**Spectral Data of (Z)-5,6-dimethyl-3-(8-methylquinolin-2(1H)-ylidene)benzofuran-2(3H)-one (4f):**



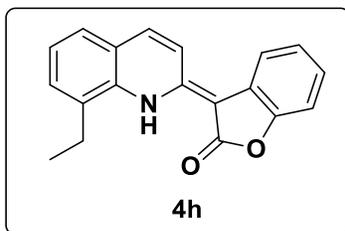
Orange solid, m.p 249-250 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.07 (bs, 1H), 7.80 (dd,  $J = 9.2$ , 1.6 Hz, 1H), 7.46 (d,  $J = 9.6$  Hz, 1H), 7.41 (t,  $J = 6.8$  Hz, 2H), 7.19-7.15 (m, 2H), 6.93 (s, 1H), 2.58 (s, 3H), 2.29 (s, 3H), 2.26 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 172.0, 147.7, 138.2, 136.2, 132.7, 131.1, 130.7, 128.8, 124.8, 123.4, 123.2, 121.9, 118.5, 118.1, 111.1, 85.5, 20.0, 19.9, 16.5, one carbon merged with others; ESI-MS calcd for  $\text{C}_{20}\text{H}_{18}\text{NO}_2$   $[\text{M}+\text{H}]$ : 304.1338 found: 304.1346.

**Spectral Data of (Z)-3-(8-methylquinolin-2(1H)-ylidene)naphtho[1,2-b]furan-2(3H)-one (4g):**



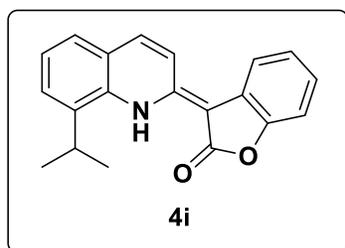
Orange solid, m.p 123-124 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.30 (bs, 1H), 8.12 (d,  $J = 8.4$  Hz, 1H), 7.86 (d,  $J = 9.6$  Hz, 1H), 7.80 (d,  $J = 8.0$  Hz, 1H), 7.68 (d,  $J = 8.8$  Hz, 1H), 7.64-7.61 (m, 2H), 7.48 (d,  $J = 7.2$  Hz, 1H), 7.44 (d,  $J = 7.6$  Hz, 2H), 7.37-7.33 (m, 1H), 7.21 (t,  $J = 7.2$  Hz, 1H), 2.64 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 171.8, 148.2, 143.1, 138.6, 136.2, 132.9, 130.4, 128.0, 126.3, 125.8, 125.1, 124.2, 123.8, 122.9, 122.2, 120.5, 120.3, 120.1, 118.0, 117.1, 86.7, 16.6; ESI-MS calcd for  $\text{C}_{22}\text{H}_{16}\text{NO}_2$   $[\text{M}+\text{H}]$ : 326.1181 found: 326.1170.

**Spectral Data of (Z)-3-(8-ethylquinolin-2(1H)-ylidene)benzofuran-2(3H)-one (4h):**



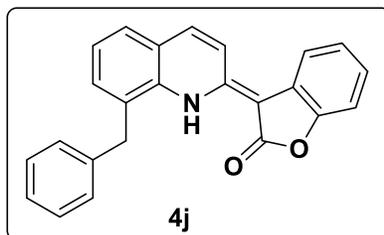
Orange solid, m.p 182-183 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.38 (bs, 1H), 7.88 (d,  $J = 9.6$  Hz, 1H), 7.54-7.44 (m, 4H), 7.26 (d,  $J = 7.6$  Hz, 1H), 7.18-7.06 (m, 3H), 2.99 (q,  $J = 7.2$  Hz, 2H), 1.44 (t,  $J = 7.6$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 171.8, 149.1, 148.3, 138.9, 135.4, 130.9, 130.8, 125.9, 124.0, 122.9, 122.6, 122.2, 117.8, 117.2, 110.1, 85.1, 23.3, 13.0, one carbon merged with others; ESI-MS calcd for  $\text{C}_{19}\text{H}_{16}\text{NO}_2$   $[\text{M}+\text{H}]$ : 290.1181 found: 290.1178.

**Spectral Data of (Z)-3-(8-isopropylquinolin-2(1H)-ylidene)benzofuran-2(3H)-one (4i):**



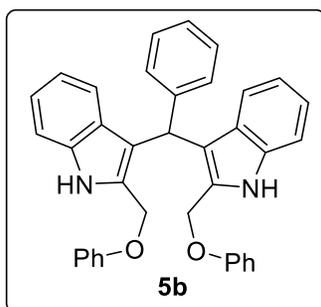
Orange solid, m.p 185-186 °C =  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.54 (bs, 1H), 7.89 (d,  $J = 9.2$  Hz, 1H), 7.55 (d,  $J = 8.4$  Hz, 2H), 7.46 (d,  $J = 7.6$  Hz, 2H), 7.29 (t,  $J = 7.6$  Hz, 1H), 7.19-7.11 (m, 2H), 7.09-7.05 (m, 1H), 3.58-3.51 (m, 1H), 1.45 (s, 3H), 1.43 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 171.8, 149.1, 148.4, 139.1, 135.5, 134.8, 128.3, 125.9, 124.1, 122.9, 122.5, 122.3, 117.7, 117.2, 110.1, 85.1, 27.4, 22.3, other carbon peaks are merged; ESI-MS calcd for  $\text{C}_{20}\text{H}_{18}\text{NO}_2$   $[\text{M}+\text{H}]$ : 304.1338 found: 304.1337.

**Spectral Data of (Z)-3-(8-benzylquinolin-2(1H)-ylidene)benzofuran-2(3H)-one (4j):**



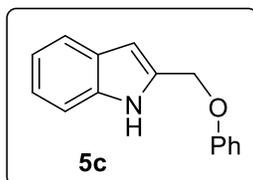
Orange red solid, m.p 239-240 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.38 (bs, 1H), 7.86 (dd,  $J = 9.6, 2.8$  Hz, 1H), 7.54-7.48 (m, 2H), 7.43 (d,  $J = 7.2$  Hz, 1H), 7.38-7.36 (m, 3H), 7.33-7.29 (m, 2H), 7.27-7.22 (m, 2H), 7.17-7.07 (m, 3H), 4.32 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 171.6, 149.1, 148.3, 138.8, 137.3, 135.6, 132.9, 129.3, 128.7, 128.3, 126.9, 126.5, 125.8, 123.8, 123.0, 122.7, 122.5, 118.1, 117.3, 110.2, 85.5, 36.2; ESI-MS calcd for  $\text{C}_{24}\text{H}_{18}\text{NO}_2$   $[\text{M}+\text{H}]$ : 352.1338 found: 352.1331.

**Spectral Data of 3,3'-(phenylmethylene)bis(2-(phoxymethyl)-1H-indole) (5b):**



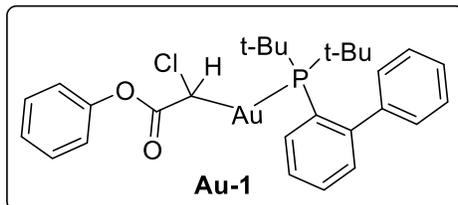
Yellow solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.29 (s, 2H), 7.35-7.33 (m, 4H), 7.29-7.25 (m, 3H), 7.20 (d,  $J = 8.0$  Hz, 2H), 7.17-7.13 (m, 6H), 6.97-6.95 (m, 2H), 6.91-6.89 (m, 2H), 6.60 (dd,  $J = 8.8, 1.0$  Hz, 4H), 4.60 (d,  $J = 12.9$  Hz, 2H), 4.48 (d,  $J = 12.9$  Hz, 2H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ): 158.0, 142.8, 135.3, 130.9, 129.3, 128.9, 128.4, 128.2, 126.6, 122.0, 121.1, 119.7, 119.6, 114.4, 114.0, 110.8, 62.1, 39.1; EI-MS calcd for  $\text{C}_{37}\text{H}_{30}\text{N}_2\text{O}_2$ : 534.2307 found: 534.2308

**Spectral Data of 2-(phoxymethyl)-1H-indole (5c):**



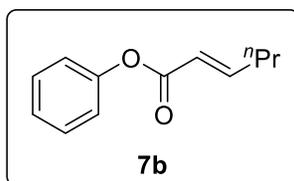
Pale yellow oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.35 (s, 1H), 7.59 (d,  $J = 7.8$  Hz, 1H), 7.35 (d,  $J = 8.1$  Hz, 1H), 7.28 (t,  $J = 8.5$  Hz, 2H), 7.17 (t,  $J = 7.2$  Hz, 1H), 7.09 (t,  $J = 7.3$  Hz, 1H), 6.99 (d,  $J = 8.4$  Hz, 2H), 6.96 (d,  $J = 7.3$  Hz, 1H), 6.52 (s, 1H), 5.21 (s, 2H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ): 158.1, 136.3, 133.7, 129.5, 127.9, 122.2, 121.3, 120.6, 119.9, 114.7, 110.9, 101.7, 63.6 ; ESI-MS calcd for  $\text{C}_{15}\text{H}_{14}\text{NO}$   $[\text{M}+\text{H}]$ : 224.1075, found: 224.1122

### Spectral Data of Compound Au-1:



Off White Solid; m.p 173-174 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.85 (t, *J* = 6.8 Hz, 1H), 7.50-7.39 (m, 5H), 7.30-7.25 (m, 3H), 7.18-7.09 (m, 3H), 7.00 (d, *J* = 8.0 Hz, 2H), 3.47 (d, *J* = 8.8 Hz, 1H), 1.38 (t, *J* = 14.8 Hz, 18 H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 174.7, 151.9, 150.1 (*J*<sub>C-P</sub> = 15.4 Hz), 142.8 (*J*<sub>C-P</sub> = 134.3 Hz), 134.3, 132.9 (*J*<sub>C-P</sub> = 7.3 Hz), 130.4, 129.3, 129.1, 128.8 (*J*<sub>C-P</sub> = 10.4 Hz), 127.5, 127.4, 127.1, 126.7 (*J*<sub>C-P</sub> = 5.5 Hz), 124.7, 121.7, 37.5 (*J*<sub>C-P</sub> = 10.2 Hz), 37.2 (*J*<sub>C-P</sub> = 10.2 Hz), 31.1 (*J*<sub>C-P</sub> = 6.8 Hz), 30.9 (*J*<sub>C-P</sub> = 6.6 Hz); ESI-MS calcd for C<sub>28</sub>H<sub>33</sub>AuClNaO<sub>2</sub>P [M+Na]: 687.1470, found: 687.1463.

### Spectral Data of (*E*)-hex-2-enoate (7b):



Sticky Solid; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.40-7.35 (m, 2H), 7.23-7.17 (m, 2H), 7.13-7.10 (m, 2H), 6.01 (d, *J* = 15.6 Hz, 1H), 2.28-2.22 (m, 2H), 1.58-1.49 (m, 2H), 0.97(t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 165.1, 151.7, 150.8, 129.4, 125.7, 121.7, 120.7, 34.4, 21.2, 13.7; ESI-MS calcd for C<sub>12</sub>H<sub>14</sub>NaO<sub>2</sub> [M+Na]: 213.0891, found: 213.0882.

## (2) X-Ray crystallographic Data:

### (a) X-Ray Data of Compound 3a:

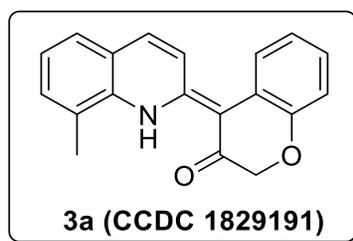
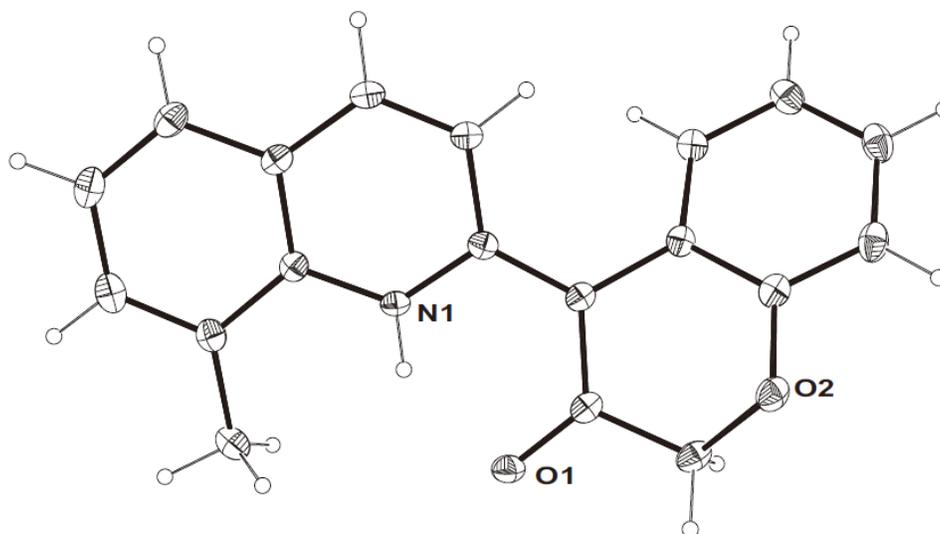


Table S1. Crystal data and structure refinement for d19251.

Identification code	d19251	
Empirical formula	C <sub>19</sub> H <sub>15</sub> N O <sub>2</sub>	
Formula weight	289.32	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P c	
Unit cell dimensions	a = 21.0827(15) Å	α = 90°.
	b = 8.2829(6) Å	β = 95.222(2)°.
	c = 8.2169(4) Å	γ = 90°.
Volume	1428.93(16) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.345 Mg/m <sup>3</sup>	
Absorption coefficient	0.087 mm <sup>-1</sup>	

F(000)	608
Crystal size	0.79 x 0.28 x 0.04 mm <sup>3</sup>
Theta range for data collection	2.46 to 25.06°.
Index ranges	-25<=h<=25, -9<=k<=9, -9<=l<=9
Reflections collected	16223
Independent reflections	4764 [R(int) = 0.0851]
Completeness to theta = 25.06°	99.6 %
Absorption correction	multi-scan
Max. and min. transmission	0.9965 and 0.9341
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	4764 / 2 / 398
Goodness-of-fit on F <sup>2</sup>	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.1034
R indices (all data)	R1 = 0.0603, wR2 = 0.1156
Absolute structure parameter	0.3(12)
Extinction coefficient	0.052(5)
Largest diff. peak and hole	0.168 and -0.149 e.Å <sup>-3</sup>

Table S2. Atomic coordinates ( x 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup>x 10<sup>3</sup>) for d19251. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	x	y	z	U(eq)
C(1)	2648(1)	1027(3)	5570(3)	34(1)
C(2)	3024(2)	-120(4)	6685(3)	40(1)
C(3)	3750(1)	1901(4)	7562(3)	37(1)
C(4)	4332(2)	2124(4)	8454(4)	46(1)
C(5)	4736(2)	3337(4)	8001(4)	48(1)
C(6)	4558(1)	4295(4)	6665(4)	46(1)
C(7)	3970(1)	4055(4)	5785(3)	39(1)
C(8)	3536(1)	2893(3)	6247(3)	33(1)
C(9)	2896(1)	2602(3)	5418(3)	32(1)
C(10)	2518(1)	3831(3)	4625(3)	31(1)
C(11)	2626(1)	5528(3)	4779(3)	36(1)
C(12)	2210(1)	6600(4)	4042(3)	37(1)
C(13)	1656(1)	6091(4)	3069(3)	34(1)

C(14)	1545(1)	4432(3)	2908(3)	32(1)
C(15)	1009(1)	3801(4)	1956(3)	38(1)
C(16)	920(1)	2025(4)	1743(4)	48(1)
C(17)	592(2)	4928(4)	1198(4)	49(1)
C(18)	687(2)	6589(4)	1361(4)	49(1)
C(19)	1212(2)	7176(4)	2271(3)	43(1)
C(20)	7351(1)	6044(3)	6664(3)	34(1)
C(21)	6969(2)	4888(4)	7611(3)	40(1)
C(22)	6245(1)	6915(3)	8146(3)	36(1)
C(23)	5660(1)	7130(4)	8767(4)	45(1)
C(24)	5258(1)	8338(4)	8122(4)	49(1)
C(25)	5438(1)	9287(4)	6872(4)	45(1)
C(26)	6026(1)	9062(4)	6262(3)	39(1)
C(27)	6456(1)	7902(3)	6938(3)	33(1)
C(28)	7101(1)	7612(3)	6410(3)	31(1)
C(29)	7481(1)	8841(3)	5788(3)	30(1)
C(30)	7370(1)	10543(3)	5894(3)	35(1)
C(31)	7784(1)	11617(4)	5352(3)	37(1)
C(32)	8344(1)	11102(4)	4637(3)	33(1)
C(33)	8453(1)	9447(3)	4538(3)	32(1)
C(34)	8993(1)	8820(4)	3844(3)	36(1)
C(35)	9084(1)	7041(4)	3694(4)	46(1)
C(36)	9411(1)	9941(4)	3288(4)	45(1)
C(37)	9317(2)	11592(4)	3398(4)	48(1)
C(38)	8785(1)	12183(4)	4053(4)	43(1)
N(1)	1978(1)	3388(3)	3705(3)	31(1)
N(2)	8021(1)	8397(3)	5127(2)	32(1)
O(1)	2130(1)	512(2)	4827(2)	40(1)
O(2)	3369(1)	673(2)	8045(2)	43(1)
O(3)	7867(1)	5522(2)	6177(2)	39(1)
O(4)	6630(1)	5680(2)	8809(2)	42(1)

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Table S3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for d19251.

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C(1)-O(1)	1.274(3)
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C(1)-C(9)	1.415(4)
C(1)-C(2)	1.496(4)
C(2)-O(2)	1.436(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-O(2)	1.377(4)
C(3)-C(4)	1.383(4)
C(3)-C(8)	1.399(4)
C(4)-C(5)	1.390(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.378(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.392(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.405(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.475(4)
C(9)-C(10)	1.414(4)
C(10)-N(1)	1.358(3)
C(10)-C(11)	1.428(4)
C(11)-C(12)	1.350(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.419(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.398(4)
C(13)-C(19)	1.415(4)
C(14)-N(1)	1.378(3)
C(14)-C(15)	1.415(4)
C(15)-C(17)	1.389(4)
C(15)-C(16)	1.491(4)
C(16)-H(16A)	0.9984
C(16)-H(16B)	0.9343
C(16)-H(16C)	0.9491
C(17)-C(18)	1.395(5)
C(17)-H(17)	0.9500
C(18)-C(19)	1.366(4)

C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-O(3)	1.269(3)
C(20)-C(28)	1.411(4)
C(20)-C(21)	1.511(4)
C(21)-O(4)	1.428(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-O(4)	1.386(3)
C(22)-C(23)	1.388(4)
C(22)-C(27)	1.390(4)
C(23)-C(24)	1.385(5)
C(23)-H(23)	0.9500
C(24)-C(25)	1.374(5)
C(24)-H(24)	0.9500
C(25)-C(26)	1.393(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.400(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.485(4)
C(28)-C(29)	1.419(4)
C(29)-N(2)	1.357(3)
C(29)-C(30)	1.433(4)
C(30)-C(31)	1.350(4)
C(30)-H(30)	0.9500
C(31)-C(32)	1.430(4)
C(31)-H(31)	0.9500
C(32)-C(33)	1.394(4)
C(32)-C(38)	1.407(4)
C(33)-N(2)	1.378(3)
C(33)-C(34)	1.418(4)
C(34)-C(36)	1.384(4)
C(34)-C(35)	1.492(4)
C(35)-H(35A)	1.0528
C(35)-H(35B)	0.9714
C(35)-H(35C)	1.0150

C(36)-C(37)	1.386(5)
C(36)-H(36)	0.9500
C(37)-C(38)	1.378(5)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
N(1)-H(1)	0.8800
N(2)-H(2)	0.8800
O(1)-C(1)-C(9)	125.0(3)
O(1)-C(1)-C(2)	117.7(3)
C(9)-C(1)-C(2)	117.4(3)
O(2)-C(2)-C(1)	112.9(2)
O(2)-C(2)-H(2A)	109.0
C(1)-C(2)-H(2A)	109.0
O(2)-C(2)-H(2B)	109.0
C(1)-C(2)-H(2B)	109.0
H(2A)-C(2)-H(2B)	107.8
O(2)-C(3)-C(4)	117.3(3)
O(2)-C(3)-C(8)	120.1(3)
C(4)-C(3)-C(8)	122.7(3)
C(3)-C(4)-C(5)	119.4(3)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3
C(6)-C(5)-C(4)	120.0(3)
C(6)-C(5)-H(5)	120.0
C(4)-C(5)-H(5)	120.0
C(5)-C(6)-C(7)	119.8(3)
C(5)-C(6)-H(6)	120.1
C(7)-C(6)-H(6)	120.1
C(6)-C(7)-C(8)	122.0(3)
C(6)-C(7)-H(7)	119.0
C(8)-C(7)-H(7)	119.0
C(3)-C(8)-C(7)	116.0(3)
C(3)-C(8)-C(9)	118.6(2)
C(7)-C(8)-C(9)	125.4(3)
C(10)-C(9)-C(1)	120.5(2)
C(10)-C(9)-C(8)	123.2(3)

C(1)-C(9)-C(8)	116.1(2)
N(1)-C(10)-C(9)	118.1(2)
N(1)-C(10)-C(11)	115.7(2)
C(9)-C(10)-C(11)	126.1(3)
C(12)-C(11)-C(10)	121.0(3)
C(12)-C(11)-H(11)	119.5
C(10)-C(11)-H(11)	119.5
C(11)-C(12)-C(13)	121.7(3)
C(11)-C(12)-H(12)	119.2
C(13)-C(12)-H(12)	119.2
C(14)-C(13)-C(19)	118.9(3)
C(14)-C(13)-C(12)	117.8(3)
C(19)-C(13)-C(12)	123.3(3)
N(1)-C(14)-C(13)	118.3(2)
N(1)-C(14)-C(15)	119.5(2)
C(13)-C(14)-C(15)	122.2(3)
C(17)-C(15)-C(14)	116.1(3)
C(17)-C(15)-C(16)	122.9(3)
C(14)-C(15)-C(16)	121.0(3)
C(15)-C(16)-H(16A)	107.2
C(15)-C(16)-H(16B)	112.7
H(16A)-C(16)-H(16B)	104.3
C(15)-C(16)-H(16C)	113.4
H(16A)-C(16)-H(16C)	108.7
H(16B)-C(16)-H(16C)	110.1
C(15)-C(17)-C(18)	122.7(3)
C(15)-C(17)-H(17)	118.7
C(18)-C(17)-H(17)	118.7
C(19)-C(18)-C(17)	120.4(3)
C(19)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(18)-C(19)-C(13)	119.7(3)
C(18)-C(19)-H(19)	120.1
C(13)-C(19)-H(19)	120.1
O(3)-C(20)-C(28)	125.9(3)
O(3)-C(20)-C(21)	117.4(2)

C(28)-C(20)-C(21)	116.7(3)
O(4)-C(21)-C(20)	112.8(2)
O(4)-C(21)-H(21A)	109.0
C(20)-C(21)-H(21A)	109.0
O(4)-C(21)-H(21B)	109.0
C(20)-C(21)-H(21B)	109.0
H(21A)-C(21)-H(21B)	107.8
O(4)-C(22)-C(23)	117.3(3)
O(4)-C(22)-C(27)	120.1(2)
C(23)-C(22)-C(27)	122.6(3)
C(24)-C(23)-C(22)	119.1(3)
C(24)-C(23)-H(23)	120.5
C(22)-C(23)-H(23)	120.5
C(25)-C(24)-C(23)	119.8(3)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	120.6(3)
C(24)-C(25)-H(25)	119.7
C(26)-C(25)-H(25)	119.7
C(25)-C(26)-C(27)	120.9(3)
C(25)-C(26)-H(26)	119.6
C(27)-C(26)-H(26)	119.6
C(22)-C(27)-C(26)	116.8(3)
C(22)-C(27)-C(28)	118.3(2)
C(26)-C(27)-C(28)	124.8(3)
C(20)-C(28)-C(29)	119.9(2)
C(20)-C(28)-C(27)	116.5(2)
C(29)-C(28)-C(27)	123.5(2)
N(2)-C(29)-C(28)	118.2(2)
N(2)-C(29)-C(30)	115.9(2)
C(28)-C(29)-C(30)	125.8(2)
C(31)-C(30)-C(29)	121.0(3)
C(31)-C(30)-H(30)	119.5
C(29)-C(30)-H(30)	119.5
C(30)-C(31)-C(32)	121.4(3)
C(30)-C(31)-H(31)	119.3

C(32)-C(31)-H(31)	119.3
C(33)-C(32)-C(38)	119.2(3)
C(33)-C(32)-C(31)	117.7(2)
C(38)-C(32)-C(31)	123.1(3)
N(2)-C(33)-C(32)	118.8(2)
N(2)-C(33)-C(34)	119.4(2)
C(32)-C(33)-C(34)	121.8(3)
C(36)-C(34)-C(33)	116.4(3)
C(36)-C(34)-C(35)	123.0(3)
C(33)-C(34)-C(35)	120.5(3)
C(34)-C(35)-H(35A)	107.2
C(34)-C(35)-H(35B)	116.1
H(35A)-C(35)-H(35B)	106.5
C(34)-C(35)-H(35C)	107.5
H(35A)-C(35)-H(35C)	106.3
H(35B)-C(35)-H(35C)	112.7
C(34)-C(36)-C(37)	122.8(3)
C(34)-C(36)-H(36)	118.6
C(37)-C(36)-H(36)	118.6
C(38)-C(37)-C(36)	120.1(3)
C(38)-C(37)-H(37)	119.9
C(36)-C(37)-H(37)	119.9
C(37)-C(38)-C(32)	119.7(3)
C(37)-C(38)-H(38)	120.2
C(32)-C(38)-H(38)	120.2
C(10)-N(1)-C(14)	125.5(2)
C(10)-N(1)-H(1)	117.3
C(14)-N(1)-H(1)	117.3
C(29)-N(2)-C(33)	125.2(2)
C(29)-N(2)-H(2)	117.4
C(33)-N(2)-H(2)	117.4
C(3)-O(2)-C(2)	112.4(2)
C(22)-O(4)-C(21)	112.4(2)

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Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for d19251. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U11	U22	U33	U23	U13	U12
C(1)	45(2)	33(2)	27(1)	-1(1)	10(1)	5(1)
C(2)	60(2)	33(2)	29(2)	1(1)	10(1)	2(2)
C(3)	43(2)	38(2)	31(2)	-2(1)	8(1)	7(1)
C(4)	51(2)	52(2)	34(2)	-4(1)	-2(1)	16(2)
C(5)	37(2)	59(2)	48(2)	-13(2)	-3(1)	10(2)
C(6)	36(2)	52(2)	50(2)	-11(2)	6(1)	1(2)
C(7)	38(2)	42(2)	36(2)	-1(1)	6(1)	2(1)
C(8)	36(2)	37(2)	26(1)	-2(1)	5(1)	4(1)
C(9)	38(2)	31(2)	27(1)	0(1)	7(1)	2(1)
C(10)	33(2)	35(2)	26(1)	1(1)	9(1)	-3(1)
C(11)	39(2)	31(2)	37(2)	-1(1)	6(1)	-3(1)
C(12)	44(2)	28(2)	38(2)	-1(1)	10(1)	-3(1)
C(13)	37(2)	33(2)	34(2)	3(1)	13(1)	4(1)
C(14)	31(1)	35(2)	32(2)	0(1)	9(1)	3(1)
C(15)	34(2)	47(2)	34(2)	-1(1)	6(1)	0(1)
C(16)	39(2)	52(2)	52(2)	-8(2)	3(2)	-8(2)
C(17)	37(2)	67(3)	41(2)	-1(2)	2(1)	3(2)
C(18)	44(2)	58(2)	44(2)	10(2)	7(2)	15(2)
C(19)	48(2)	40(2)	41(2)	6(1)	14(1)	10(2)
C(20)	44(2)	31(2)	26(1)	-1(1)	-1(1)	0(1)
C(21)	55(2)	35(2)	31(2)	2(1)	5(1)	0(1)
C(22)	40(2)	37(2)	29(1)	-4(1)	-1(1)	-3(1)
C(23)	48(2)	51(2)	38(2)	-11(1)	11(1)	-14(2)
C(24)	37(2)	58(2)	52(2)	-14(2)	7(1)	-6(2)
C(25)	35(2)	52(2)	46(2)	-12(2)	-3(1)	4(1)
C(26)	39(2)	45(2)	34(2)	-1(1)	1(1)	1(1)
C(27)	34(1)	38(2)	27(1)	-3(1)	0(1)	-2(1)
C(28)	37(1)	30(2)	25(1)	-2(1)	0(1)	1(1)
C(29)	35(2)	32(2)	24(1)	-2(1)	-2(1)	6(1)
C(30)	38(2)	31(2)	36(2)	-1(1)	2(1)	5(1)
C(31)	43(2)	29(2)	37(2)	-1(1)	-3(1)	4(1)

C(32)	38(2)	30(2)	30(1)	2(1)	-6(1)	-1(1)
C(33)	32(1)	36(2)	28(1)	3(1)	-4(1)	-3(1)
C(34)	33(2)	44(2)	31(1)	1(1)	-4(1)	-1(1)
C(35)	40(2)	46(2)	53(2)	2(2)	8(1)	8(2)
C(36)	34(2)	59(2)	42(2)	4(2)	3(1)	-4(2)
C(37)	45(2)	51(2)	47(2)	8(2)	0(1)	-13(2)
C(38)	46(2)	40(2)	40(2)	4(1)	-6(1)	-9(1)
N(1)	36(1)	25(1)	33(1)	-2(1)	4(1)	-2(1)
N(2)	37(1)	25(1)	32(1)	-3(1)	3(1)	2(1)
O(1)	46(1)	31(1)	43(1)	-2(1)	4(1)	-5(1)
O(2)	56(1)	43(1)	28(1)	4(1)	4(1)	2(1)
O(3)	43(1)	32(1)	42(1)	0(1)	5(1)	5(1)
O(4)	55(1)	44(1)	27(1)	3(1)	6(1)	1(1)

Table S5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for d19251.

	x	y	z	U(eq)
H(2A)	2731	-923	7102	48
H(2B)	3329	-709	6055	48
H(4)	4454	1455	9368	55
H(5)	5135	3506	8613	58
H(6)	4836	5116	6347	55
H(7)	3859	4695	4843	46
H(11)	2995	5910	5411	43
H(12)	2292	7722	4179	44
H(17)	228	4552	542	58
H(18)	386	7316	837	58
H(19)	1278	8308	2367	51
H(21A)	6662	4307	6838	49
H(21B)	7260	4079	8161	49
H(23)	5538	6459	9622	54
H(24)	4858	8509	8542	58
H(25)	5159	10104	6421	54

H(26)	6138	9705	5374	47
H(30)	7000	10922	6352	42
H(31)	7702	12739	5447	44
H(36)	9777	9561	2811	54
H(37)	9620	12318	3020	57
H(38)	8717	13314	4111	51
H(1)	1898	2348	3610	38
H(2)	8102	7358	5070	38
H(16A)	507	1857	1072	50
H(16B)	869	1495	2726	50
H(16C)	1249	1524	1207	50
H(35A)	8687	6592	2965	50
H(35B)	9110	6433	4709	50
H(35C)	9467	6863	3051	50

**(b) X-Ray Data of Compound 4c:**

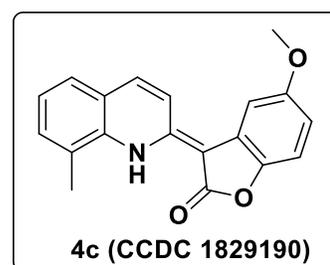
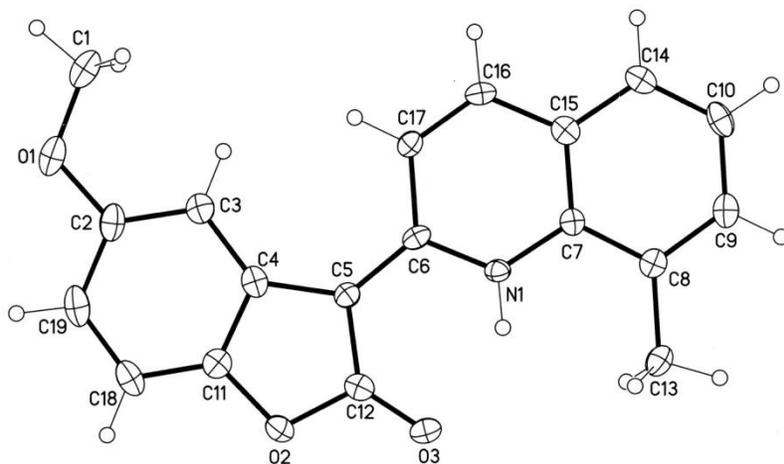


Table S6. Crystal data and structure refinement for 170929LT.

Identification code	170929LT
Empirical formula	C <sub>19</sub> H <sub>15</sub> N O <sub>3</sub>
Formula weight	305.32

Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P c a 21	
Unit cell dimensions	a = 14.3845(14) Å	$\alpha = 90^\circ$ .
	b = 4.3448(4) Å	$\beta = 90^\circ$ .
	c = 23.199(2) Å	$\gamma = 90^\circ$ .
Volume	1449.9(2) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.399 Mg/m <sup>3</sup>	
Absorption coefficient	0.095 mm <sup>-1</sup>	
F(000)	640	
Crystal size	0.15 x 0.14 x 0.06 mm <sup>3</sup>	
Theta range for data collection	1.756 to 26.337°.	
Index ranges	-17<=h<=17, -3<=k<=5, -28<=l<=28	
Reflections collected	10448	
Independent reflections	2941 [R(int) = 0.0542]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8324	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2941 / 1 / 211	
Goodness-of-fit on F <sup>2</sup>	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0375, wR2 = 0.0747	
R indices (all data)	R1 = 0.0510, wR2 = 0.0802	
Absolute structure parameter	-1.7(17)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.147 and -0.211 e.Å <sup>-3</sup>	

Table S7. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) for 170929LT.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
O(1)	8573(1)	12185(5)	6294(1)	28(1)
O(2)	11520(1)	12421(5)	4790(1)	22(1)

O(3)	11722(1)	10118(5)	3923(1)	21(1)
N(1)	10295(2)	6371(5)	3625(1)	15(1)
C(1)	7812(2)	10168(8)	6180(1)	30(1)
C(2)	9297(2)	12156(7)	5903(1)	22(1)
C(3)	9268(2)	10583(7)	5383(1)	19(1)
C(4)	10048(2)	10757(6)	5020(1)	17(1)
C(5)	10300(2)	9439(7)	4469(1)	15(1)
C(6)	9840(2)	7400(7)	4103(1)	15(1)
C(7)	9940(2)	4304(6)	3232(1)	15(1)
C(8)	10485(2)	3318(6)	2764(1)	16(1)
C(9)	10085(2)	1257(7)	2382(1)	20(1)
C(10)	9179(2)	142(7)	2456(1)	21(1)
C(11)	10804(2)	12496(7)	5197(1)	20(1)
C(12)	11215(2)	10544(6)	4342(1)	18(1)
C(13)	11464(2)	4482(7)	2688(1)	21(1)
C(14)	8657(2)	1107(7)	2917(1)	19(1)
C(15)	9030(2)	3193(6)	3315(1)	16(1)
C(16)	8530(2)	4288(7)	3808(1)	18(1)
C(17)	8909(2)	6273(7)	4183(1)	17(1)
C(18)	10844(2)	14051(7)	5712(1)	25(1)
C(19)	10073(2)	13878(7)	6066(1)	26(1)

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Table S8. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 170929LT.

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O(1)-C(2)	1.380(4)
O(1)-C(1)	1.427(4)
O(2)-C(12)	1.392(4)
O(2)-C(11)	1.398(3)
O(3)-C(12)	1.231(3)
N(1)-C(6)	1.363(3)
N(1)-C(7)	1.378(4)
N(1)-H(5)	0.8800
C(1)-H(3)	0.9800
C(1)-H(1)	0.9800
C(1)-H(15)	0.9800

C(2)-C(3)	1.387(4)
C(2)-C(19)	1.396(5)
C(3)-C(4)	1.406(4)
C(3)-H(4)	0.9500
C(4)-C(11)	1.386(4)
C(4)-C(5)	1.446(4)
C(5)-C(6)	1.393(4)
C(5)-C(12)	1.431(4)
C(6)-C(17)	1.438(4)
C(7)-C(8)	1.408(4)
C(7)-C(15)	1.408(4)
C(8)-C(9)	1.384(4)
C(8)-C(13)	1.507(4)
C(9)-C(10)	1.401(4)
C(9)-H(12)	0.9500
C(10)-C(14)	1.373(4)
C(10)-H(2)	0.9500
C(11)-C(18)	1.373(4)
C(13)-H(6)	0.9800
C(13)-H(7)	0.9800
C(13)-H(8)	0.9800
C(14)-C(15)	1.400(4)
C(14)-H(9)	0.9500
C(15)-C(16)	1.432(4)
C(16)-C(17)	1.341(4)
C(16)-H(10)	0.9500
C(17)-H(11)	0.9500
C(18)-C(19)	1.383(5)
C(18)-H(13)	0.9500
C(19)-H(14)	0.9500
C(2)-O(1)-C(1)	116.9(2)
C(12)-O(2)-C(11)	106.5(2)
C(6)-N(1)-C(7)	125.0(2)
C(6)-N(1)-H(5)	117.5
C(7)-N(1)-H(5)	117.5

O(1)-C(1)-H(3)	109.5
O(1)-C(1)-H(1)	109.5
H(3)-C(1)-H(1)	109.5
O(1)-C(1)-H(15)	109.5
H(3)-C(1)-H(15)	109.5
H(1)-C(1)-H(15)	109.5
O(1)-C(2)-C(3)	123.5(3)
O(1)-C(2)-C(19)	114.9(3)
C(3)-C(2)-C(19)	121.6(3)
C(2)-C(3)-C(4)	118.1(3)
C(2)-C(3)-H(4)	120.9
C(4)-C(3)-H(4)	120.9
C(11)-C(4)-C(3)	118.5(3)
C(11)-C(4)-C(5)	106.3(2)
C(3)-C(4)-C(5)	135.2(3)
C(6)-C(5)-C(12)	121.6(2)
C(6)-C(5)-C(4)	132.1(3)
C(12)-C(5)-C(4)	106.2(2)
N(1)-C(6)-C(5)	118.5(2)
N(1)-C(6)-C(17)	116.1(2)
C(5)-C(6)-C(17)	125.4(3)
N(1)-C(7)-C(8)	120.1(3)
N(1)-C(7)-C(15)	118.6(2)
C(8)-C(7)-C(15)	121.3(3)
C(9)-C(8)-C(7)	117.3(3)
C(9)-C(8)-C(13)	122.1(3)
C(7)-C(8)-C(13)	120.6(3)
C(8)-C(9)-C(10)	122.2(3)
C(8)-C(9)-H(12)	118.9
C(10)-C(9)-H(12)	118.9
C(14)-C(10)-C(9)	119.9(3)
C(14)-C(10)-H(2)	120.0
C(9)-C(10)-H(2)	120.0
C(18)-C(11)-C(4)	124.0(3)
C(18)-C(11)-O(2)	124.5(3)
C(4)-C(11)-O(2)	111.5(2)

O(3)-C(12)-O(2)	119.4(2)
O(3)-C(12)-C(5)	131.1(3)
O(2)-C(12)-C(5)	109.5(2)
C(8)-C(13)-H(6)	109.5
C(8)-C(13)-H(7)	109.5
H(6)-C(13)-H(7)	109.5
C(8)-C(13)-H(8)	109.5
H(6)-C(13)-H(8)	109.5
H(7)-C(13)-H(8)	109.5
C(10)-C(14)-C(15)	120.1(3)
C(10)-C(14)-H(9)	119.9
C(15)-C(14)-H(9)	119.9
C(14)-C(15)-C(7)	119.2(3)
C(14)-C(15)-C(16)	123.3(3)
C(7)-C(15)-C(16)	117.5(3)
C(17)-C(16)-C(15)	121.8(3)
C(17)-C(16)-H(10)	119.1
C(15)-C(16)-H(10)	119.1
C(16)-C(17)-C(6)	121.0(3)
C(16)-C(17)-H(11)	119.5
C(6)-C(17)-H(11)	119.5
C(11)-C(18)-C(19)	117.2(3)
C(11)-C(18)-H(13)	121.4
C(19)-C(18)-H(13)	121.4
C(18)-C(19)-C(2)	120.6(3)
C(18)-C(19)-H(14)	119.7
C(2)-C(19)-H(14)	119.7

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Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 170929LT. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^*2U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

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	U11	U22	U33	U23	U13	U12
O(1)	36(1)	30(1)	19(1)	-2(1)	7(1)	6(1)

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O(2)	18(1)	24(1)	22(1)	-4(1)	-3(1)	-3(1)
O(3)	15(1)	24(1)	24(1)	1(1)	2(1)	0(1)
N(1)	11(1)	15(1)	19(1)	0(1)	0(1)	0(1)
C(1)	32(2)	34(2)	23(2)	1(2)	10(2)	5(2)
C(2)	32(2)	18(2)	14(2)	2(1)	1(1)	7(1)
C(3)	20(1)	17(2)	21(2)	1(1)	-2(1)	4(1)
C(4)	22(2)	14(1)	16(2)	2(1)	-4(1)	4(1)
C(5)	14(1)	15(1)	16(2)	1(1)	0(1)	2(1)
C(6)	12(1)	14(1)	18(2)	5(1)	2(1)	3(1)
C(7)	16(1)	14(1)	13(2)	2(1)	-2(1)	2(1)
C(8)	20(1)	13(1)	16(2)	5(1)	0(1)	3(1)
C(9)	26(2)	18(2)	16(2)	0(1)	-2(1)	6(1)
C(10)	29(2)	16(2)	19(2)	-2(1)	-9(1)	3(1)
C(11)	20(2)	19(2)	19(2)	2(1)	-1(1)	2(1)
C(12)	17(1)	15(2)	22(2)	2(1)	-3(1)	1(1)
C(13)	20(1)	24(2)	19(2)	0(1)	3(1)	5(1)
C(14)	20(1)	16(2)	22(2)	3(1)	-6(1)	-2(1)
C(15)	18(1)	12(1)	19(2)	3(1)	-4(1)	4(1)
C(16)	13(1)	19(1)	21(2)	5(1)	1(1)	-2(1)
C(17)	16(1)	17(1)	17(2)	-1(1)	2(1)	2(1)
C(18)	33(2)	19(2)	22(2)	-3(1)	-7(2)	-2(1)
C(19)	42(2)	19(2)	16(2)	-2(1)	-4(2)	5(2)

Table S10. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 170929LT.

	x	y	z	U(eq)
H(5)	10859	7082	3562	18
H(3)	7530	10706	5809	45
H(1)	7347	10374	6486	45
H(15)	8036	8039	6167	45
H(4)	8736	9421	5276	23
H(12)	10437	575	2060	24

H(2)	8927	-1282	2188	26
H(6)	11743	3520	2346	31
H(7)	11833	3960	3029	31
H(8)	11454	6721	2637	31
H(9)	8041	359	2966	23
H(10)	7912	3590	3871	21
H(11)	8558	6943	4506	20
H(13)	11379	15197	5819	30
H(14)	10071	14941	6424	31

**(c) X-Ray Data of Compound Au-1:**

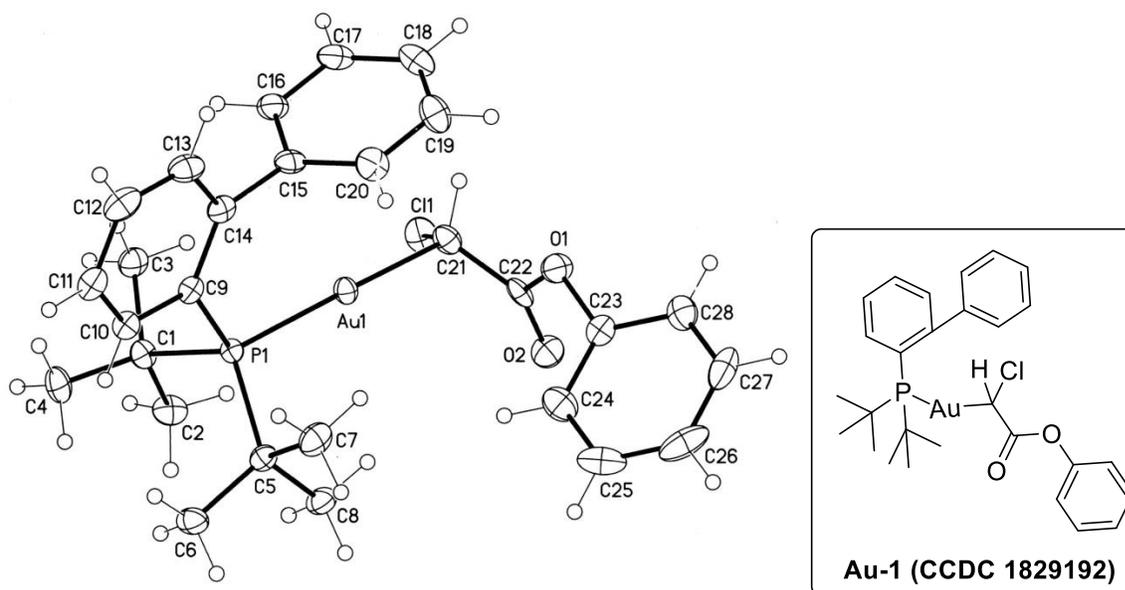


Table S11. Crystal data and structure refinement for 170934LT\_0M\_A.

Identification code	170934lt_0m_a	
Empirical formula	C <sub>28</sub> H <sub>33</sub> Au Cl O <sub>2</sub> P	
Formula weight	664.93	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.2179(4) Å	α = 100.062(2)°.
	b = 10.4777(5) Å	β = 92.031(2)°.

	$c = 14.2247(7) \text{ \AA}$	$\gamma = 103.287(2)^\circ$ .
Volume	1312.41(11) $\text{\AA}^3$	
Z	2	
Density (calculated)	1.683 Mg/m <sup>3</sup>	
Absorption coefficient	5.790 mm <sup>-1</sup>	
F(000)	656	
Crystal size	0.10 x 0.08 x 0.02 mm <sup>3</sup>	
Theta range for data collection	1.458 to 26.432°.	
Index ranges	-11<=h<=11, -13<=k<=13, -17<=l<=17	
Reflections collected	19696	
Independent reflections	5361 [R(int) = 0.0197]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.7527	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	5361 / 0 / 304	
Goodness-of-fit on F <sup>2</sup>	1.137	
Final R indices [I>2sigma(I)]	R1 = 0.0186, wR2 = 0.0442	
R indices (all data)	R1 = 0.0196, wR2 = 0.0480	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.390 and -0.666 e. $\text{\AA}^{-3}$	

Table S12. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 170934LT\_0M\_A. U(eq) is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Au(1)	3140(1)	5408(1)	6972(1)	17(1)
C(1)	2097(3)	2113(3)	6056(2)	18(1)
C(2)	2330(4)	2483(4)	5063(2)	24(1)
C(3)	575(3)	2337(3)	6360(2)	22(1)
C(4)	2074(4)	639(3)	6001(2)	25(1)
C(5)	5537(3)	3355(3)	6690(2)	18(1)
C(6)	5907(4)	2010(3)	6323(2)	24(1)
C(7)	6483(4)	4054(4)	7629(2)	27(1)
C(8)	5959(4)	4232(3)	5930(2)	23(1)

C(9)	3258(3)	2718(3)	8088(2)	17(1)
C(10)	3610(3)	1508(3)	8177(2)	19(1)
C(11)	3443(4)	990(3)	9009(2)	23(1)
C(12)	2904(4)	1681(4)	9784(2)	28(1)
C(13)	2555(4)	2875(4)	9714(2)	26(1)
C(14)	2717(3)	3418(3)	8882(2)	19(1)
C(15)	2301(3)	4726(3)	8930(2)	20(1)
C(16)	850(4)	4779(4)	8661(2)	24(1)
C(17)	438(4)	5986(4)	8794(2)	28(1)
C(18)	1456(4)	7153(4)	9208(3)	31(1)
C(19)	2898(4)	7116(4)	9481(3)	31(1)
C(20)	3315(4)	5909(4)	9347(2)	26(1)
C(21)	2721(4)	7275(3)	6875(2)	21(1)
C(22)	4155(4)	8173(3)	6815(2)	20(1)
C(23)	6431(4)	9040(3)	7805(2)	21(1)
C(24)	7236(4)	8114(4)	7464(2)	30(1)
C(25)	8771(4)	8457(5)	7630(3)	37(1)
C(26)	9491(4)	9721(5)	8135(3)	41(1)
C(27)	8653(4)	10631(4)	8468(3)	34(1)
C(28)	7136(4)	10298(3)	8296(2)	26(1)
Cl(1)	1428(1)	7116(1)	5867(1)	28(1)
O(1)	4864(3)	8669(2)	7727(2)	25(1)
O(2)	4749(3)	8478(2)	6111(2)	26(1)
P(1)	3533(1)	3323(1)	6952(1)	14(1)

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Table S13. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 170934LT\_0M\_A.

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Au(1)-C(21)	2.105(3)
Au(1)-P(1)	2.2911(8)
C(1)-C(4)	1.528(4)
C(1)-C(2)	1.538(4)
C(1)-C(3)	1.539(4)
C(1)-P(1)	1.879(3)
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800

C(2)-H(2C)	0.9800
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(6)	1.533(4)
C(5)-C(7)	1.537(4)
C(5)-C(8)	1.542(4)
C(5)-P(1)	1.891(3)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.403(4)
C(9)-C(14)	1.408(4)
C(9)-P(1)	1.841(3)
C(10)-C(11)	1.386(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.382(5)
C(11)-H(11)	0.9500
C(12)-C(13)	1.380(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.398(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.497(5)
C(15)-C(20)	1.390(5)
C(15)-C(16)	1.395(4)
C(16)-C(17)	1.387(5)
C(16)-H(16)	0.9500

C(17)-C(18)	1.380(5)
C(17)-H(17)	0.9500
C(18)-C(19)	1.383(5)
C(18)-H(18)	0.9500
C(19)-C(20)	1.388(5)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(22)	1.450(5)
C(21)-Cl(1)	1.791(3)
C(21)-H(21)	1.0000
C(22)-O(2)	1.214(4)
C(22)-O(1)	1.389(4)
C(23)-C(28)	1.378(5)
C(23)-C(24)	1.385(5)
C(23)-O(1)	1.402(4)
C(24)-C(25)	1.378(5)
C(24)-H(24)	0.9500
C(25)-C(26)	1.392(6)
C(25)-H(25)	0.9500
C(26)-C(27)	1.392(6)
C(26)-H(26)	0.9500
C(27)-C(28)	1.364(5)
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500
C(21)-Au(1)-P(1)	175.48(9)
C(4)-C(1)-C(2)	109.7(3)
C(4)-C(1)-C(3)	108.5(3)
C(2)-C(1)-C(3)	108.5(3)
C(4)-C(1)-P(1)	115.7(2)
C(2)-C(1)-P(1)	108.6(2)
C(3)-C(1)-P(1)	105.6(2)
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5

H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(1)-C(3)-H(3A)	109.5
C(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(1)-C(4)-H(4A)	109.5
C(1)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(1)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(6)-C(5)-C(7)	110.1(3)
C(6)-C(5)-C(8)	107.3(3)
C(7)-C(5)-C(8)	108.3(3)
C(6)-C(5)-P(1)	117.1(2)
C(7)-C(5)-P(1)	105.7(2)
C(8)-C(5)-P(1)	108.0(2)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5

H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-C(14)	117.9(3)
C(10)-C(9)-P(1)	119.0(2)
C(14)-C(9)-P(1)	123.1(2)
C(11)-C(10)-C(9)	122.5(3)
C(11)-C(10)-H(10)	118.7
C(9)-C(10)-H(10)	118.7
C(12)-C(11)-C(10)	119.2(3)
C(12)-C(11)-H(11)	120.4
C(10)-C(11)-H(11)	120.4
C(13)-C(12)-C(11)	119.3(3)
C(13)-C(12)-H(12)	120.4
C(11)-C(12)-H(12)	120.4
C(12)-C(13)-C(14)	122.5(3)
C(12)-C(13)-H(13)	118.8
C(14)-C(13)-H(13)	118.8
C(13)-C(14)-C(9)	118.6(3)
C(13)-C(14)-C(15)	115.6(3)
C(9)-C(14)-C(15)	125.8(3)
C(20)-C(15)-C(16)	118.4(3)
C(20)-C(15)-C(14)	120.2(3)
C(16)-C(15)-C(14)	121.1(3)
C(17)-C(16)-C(15)	120.7(3)
C(17)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(18)-C(17)-C(16)	120.3(3)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(17)-C(18)-C(19)	119.7(3)
C(17)-C(18)-H(18)	120.2
C(19)-C(18)-H(18)	120.2
C(18)-C(19)-C(20)	120.1(3)
C(18)-C(19)-H(19)	119.9
C(20)-C(19)-H(19)	119.9
C(19)-C(20)-C(15)	120.8(3)

C(19)-C(20)-H(20)	119.6
C(15)-C(20)-H(20)	119.6
C(22)-C(21)-Cl(1)	112.8(2)
C(22)-C(21)-Au(1)	106.9(2)
Cl(1)-C(21)-Au(1)	110.37(16)
C(22)-C(21)-H(21)	108.9
Cl(1)-C(21)-H(21)	108.9
Au(1)-C(21)-H(21)	108.9
O(2)-C(22)-O(1)	121.1(3)
O(2)-C(22)-C(21)	129.2(3)
O(1)-C(22)-C(21)	109.7(3)
C(28)-C(23)-C(24)	121.3(3)
C(28)-C(23)-O(1)	118.4(3)
C(24)-C(23)-O(1)	120.0(3)
C(25)-C(24)-C(23)	119.1(4)
C(25)-C(24)-H(24)	120.4
C(23)-C(24)-H(24)	120.4
C(24)-C(25)-C(26)	119.9(4)
C(24)-C(25)-H(25)	120.0
C(26)-C(25)-H(25)	120.0
C(27)-C(26)-C(25)	119.7(3)
C(27)-C(26)-H(26)	120.2
C(25)-C(26)-H(26)	120.2
C(28)-C(27)-C(26)	120.5(4)
C(28)-C(27)-H(27)	119.8
C(26)-C(27)-H(27)	119.8
C(27)-C(28)-C(23)	119.5(3)
C(27)-C(28)-H(28)	120.3
C(23)-C(28)-H(28)	120.3
C(22)-O(1)-C(23)	117.3(2)
C(9)-P(1)-C(1)	105.15(14)
C(9)-P(1)-C(5)	106.37(13)
C(1)-P(1)-C(5)	114.52(14)
C(9)-P(1)-Au(1)	114.75(10)
C(1)-P(1)-Au(1)	107.44(10)
C(5)-P(1)-Au(1)	108.78(10)

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Symmetry transformations used to generate equivalent atoms:

Table S14. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 170934LT\_0M\_A. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U11	U22	U33	U23	U13	U12
Au(1)	18(1)	14(1)	19(1)	4(1)	0(1)	5(1)
C(1)	18(2)	18(2)	15(1)	1(1)	-4(1)	3(1)
C(2)	24(2)	33(2)	14(2)	2(1)	-2(1)	8(1)
C(3)	18(2)	25(2)	22(2)	2(1)	-1(1)	3(1)
C(4)	27(2)	18(2)	27(2)	-2(1)	-8(1)	3(1)
C(5)	16(1)	21(2)	19(2)	6(1)	1(1)	4(1)
C(6)	26(2)	25(2)	28(2)	11(1)	9(1)	13(1)
C(7)	19(2)	33(2)	26(2)	5(2)	-2(1)	1(1)
C(8)	22(2)	24(2)	24(2)	9(1)	7(1)	6(1)
C(9)	15(1)	18(2)	15(1)	5(1)	-1(1)	1(1)
C(10)	19(2)	21(2)	18(2)	5(1)	0(1)	4(1)
C(11)	19(2)	26(2)	27(2)	11(1)	-1(1)	4(1)
C(12)	26(2)	41(2)	21(2)	17(2)	2(1)	5(2)
C(13)	25(2)	36(2)	17(2)	5(1)	4(1)	7(1)
C(14)	14(1)	24(2)	17(2)	2(1)	-2(1)	2(1)
C(15)	21(2)	27(2)	12(1)	1(1)	3(1)	7(1)
C(16)	18(2)	28(2)	24(2)	-2(1)	3(1)	5(1)
C(17)	23(2)	35(2)	26(2)	1(2)	6(1)	12(2)
C(18)	40(2)	29(2)	25(2)	-2(2)	4(2)	16(2)
C(19)	38(2)	26(2)	24(2)	-5(1)	-5(2)	5(2)
C(20)	23(2)	30(2)	24(2)	0(1)	-5(1)	6(1)
C(21)	22(2)	20(2)	22(2)	2(1)	-1(1)	9(1)
C(22)	23(2)	14(2)	22(2)	-2(1)	-3(1)	11(1)
C(23)	20(2)	24(2)	20(2)	7(1)	-1(1)	4(1)
C(24)	36(2)	31(2)	22(2)	1(2)	-1(1)	11(2)
C(25)	35(2)	60(3)	26(2)	9(2)	8(2)	28(2)
C(26)	15(2)	77(3)	33(2)	22(2)	2(2)	4(2)
C(27)	36(2)	34(2)	23(2)	9(2)	-1(2)	-12(2)

C(28)	32(2)	23(2)	24(2)	8(1)	1(1)	7(1)
Cl(1)	24(1)	26(1)	33(1)	4(1)	-7(1)	9(1)
O(1)	21(1)	29(1)	21(1)	0(1)	1(1)	3(1)
O(2)	27(1)	29(1)	24(1)	7(1)	2(1)	6(1)
P(1)	16(1)	14(1)	13(1)	4(1)	0(1)	4(1)

Table S15. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 170934LT\_0M\_A.

	x	y	z	U(eq)
H(2A)	3242	2254	4829	36
H(2B)	2426	3444	5112	36
H(2C)	1471	1988	4616	36
H(3A)	-224	1758	5900	34
H(3B)	560	3272	6376	34
H(3C)	419	2122	6998	34
H(4A)	1322	94	5496	38
H(4B)	1823	383	6617	38
H(4C)	3060	493	5854	38
H(6A)	6974	2156	6221	36
H(6B)	5316	1583	5717	36
H(6C)	5667	1432	6796	36
H(7A)	6284	3480	8108	41
H(7B)	6223	4902	7865	41
H(7C)	7546	4224	7513	41
H(8A)	7031	4368	5848	35
H(8B)	5722	5098	6138	35
H(8C)	5391	3787	5319	35
H(10)	3978	1027	7646	23
H(11)	3696	170	9047	28
H(12)	2776	1337	10359	34
H(13)	2190	3345	10251	31
H(16)	137	3980	8382	29

H(17)	-551	6010	8600	33
H(18)	1167	7977	9305	37
H(19)	3605	7918	9762	37
H(20)	4306	5892	9541	32
H(21)	2280	7617	7472	25
H(24)	6737	7254	7120	35
H(25)	9338	7832	7401	45
H(26)	10548	9961	8251	50
H(27)	9142	11491	8817	41
H(28)	6568	10927	8514	31

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### **(3) $^1\text{H}$ & $^{13}\text{C}$ Spectra OF Key Compounds:**

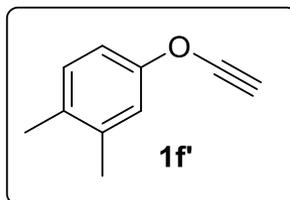


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7.0936  
7.0728  
7.0415  
7.0080  
6.9878

2.2501  
2.2119  
2.0335  
2.0307  
1.5682

Current Data Parameters  
NAME 08022018  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameter  
Date\_ 20180208  
Time 21.10  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 14  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 se  
RG 4  
DW 78.000 us  
DE 6.00 us  
TE 300.0 K  
D1 2.00000000 se  
TDO 1



----- CHANNEL f1 -----  
NUC1 1H  
P1 10.00 us  
PL1 -2.40 dB  
SFO1 400.1528010 MH

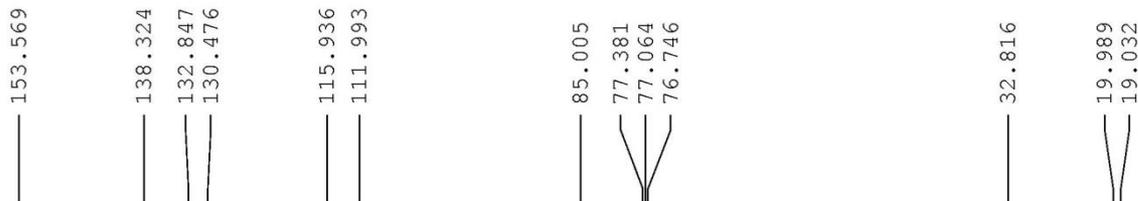
F2 - Processing parameters  
SI 16384  
SF 400.1500168 MH  
WDW EM  
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LB 0.00 Hz  
GB 0  
PC 1.00



10 9 8 7 6 5 4 3 2 1 ppm

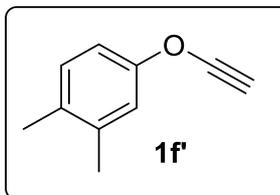
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1.10  
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3.19  
3.10  
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EXPNO 3  
PROCNO 1

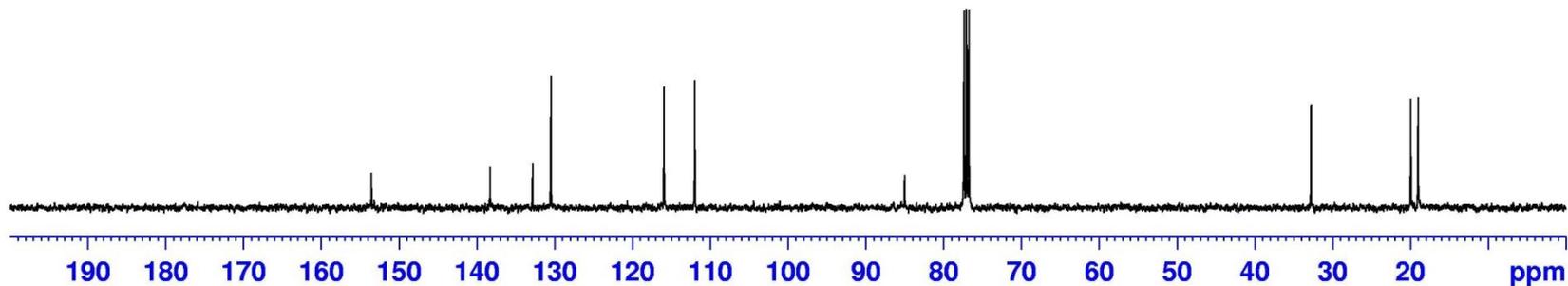
F2 - Acquisition Parameters  
Date\_ 20180324  
Time 17.54  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 102  
DS 0  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
RG 57  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1



=====  
CHANNEL f1  
NUC1 13C  
P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.40 dB  
PL12 15.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6177980 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



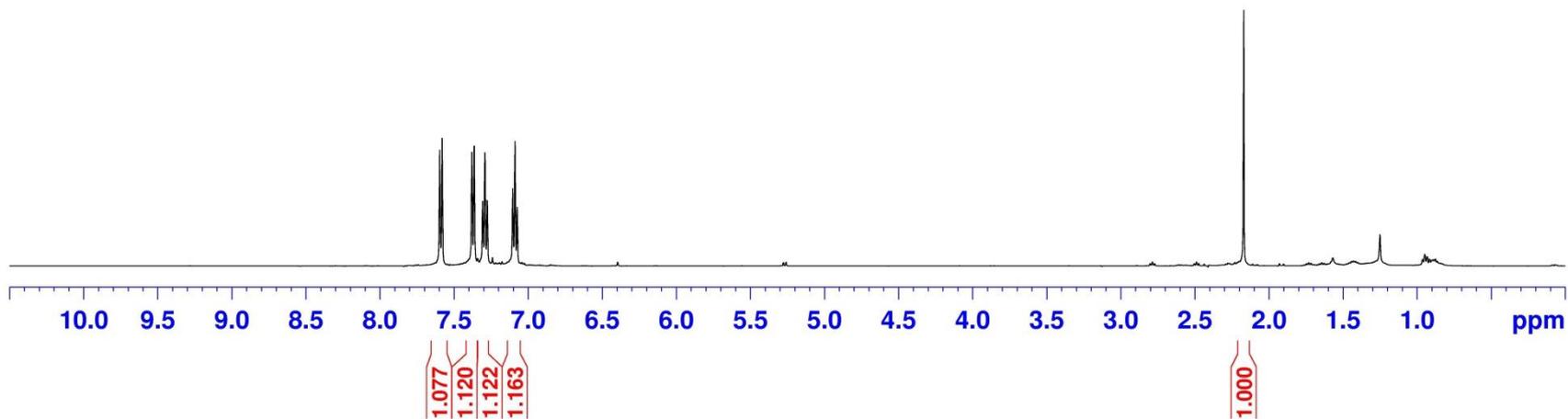
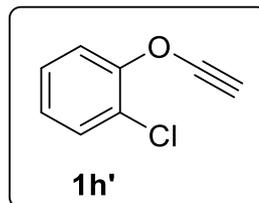
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7.5795  
7.3794  
7.3635  
7.3063  
7.2910  
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7.2400  
7.1034  
7.0880  
7.0726

2.1702

1.2506

Current Data Parameters  
NAME MDP-115-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 16384  
SF 499.7938787 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



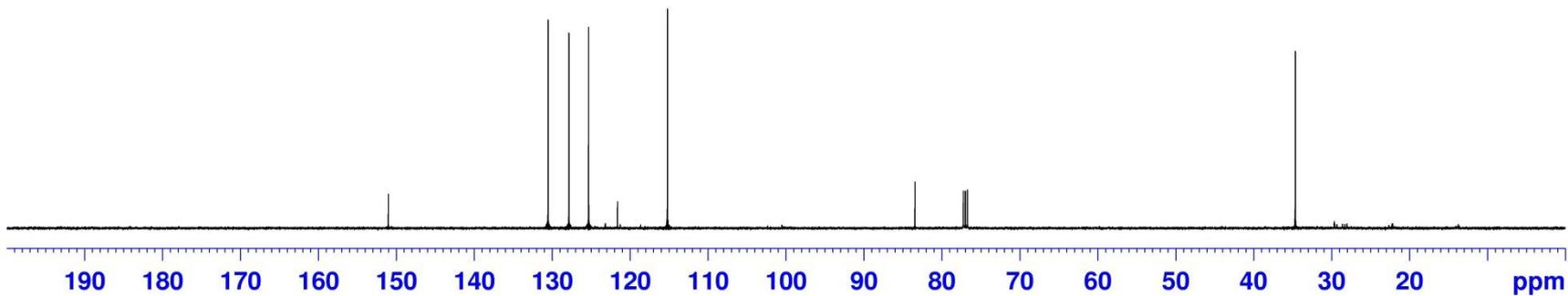
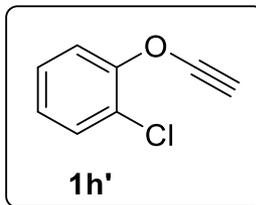


Current Data Parameters

NAME MDP-115--C  
 EXPNO 1  
 PROCNO 1

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 SF 125.6761648 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



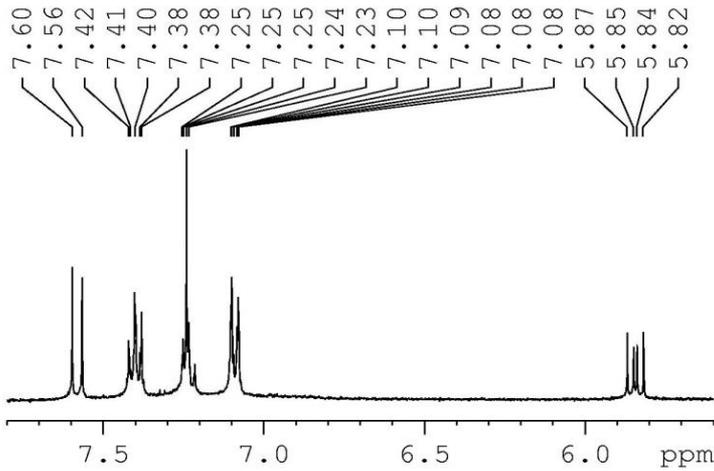
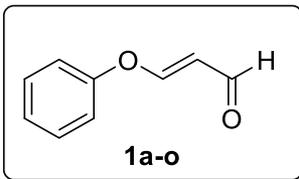


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9.4682  
7.5958  
7.5648  
7.4254  
7.4199  
7.4146  
7.4010  
7.3845  
7.3797  
7.3737  
7.2542  
7.2515  
7.2487  
7.2400  
7.2330  
7.2292  
7.2144  
7.2116  
7.1017  
7.0989  
7.0933  
7.0824  
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7.0777  
5.8691  
5.8492  
5.8385  
5.8182

1.5726  
1.2316

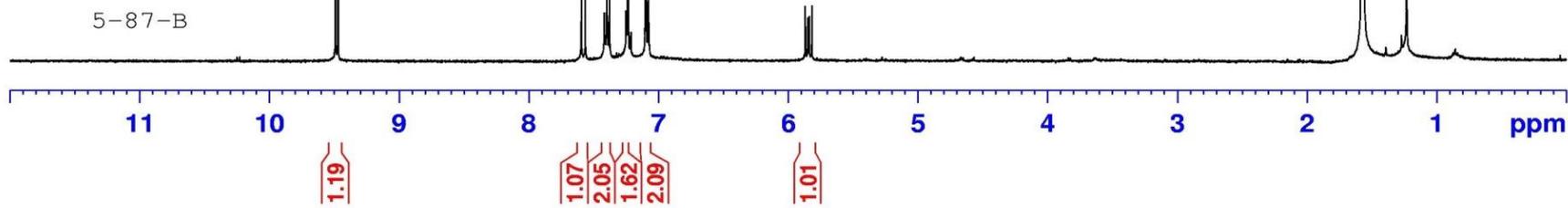
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EXPNO 2  
PROCNO 1

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INSTRUM spect  
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PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 12  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 se  
RG 645  
DW 78.000 us  
DE 6.00 us  
TE 300.0 K  
D1 2.00000000 se  
TDO 1



----- CHANNEL f1 -----  
NUC1 1H  
P1 10.00 us  
PL1 -2.40 dB  
SFO1 400.1528010 MH

F2 - Processing parameters  
SI 16384  
SF 400.1500167 MH  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00





190.84  
167.21  
155.52  
130.17  
125.76  
118.35  
114.38  
77.32  
77.00  
76.68

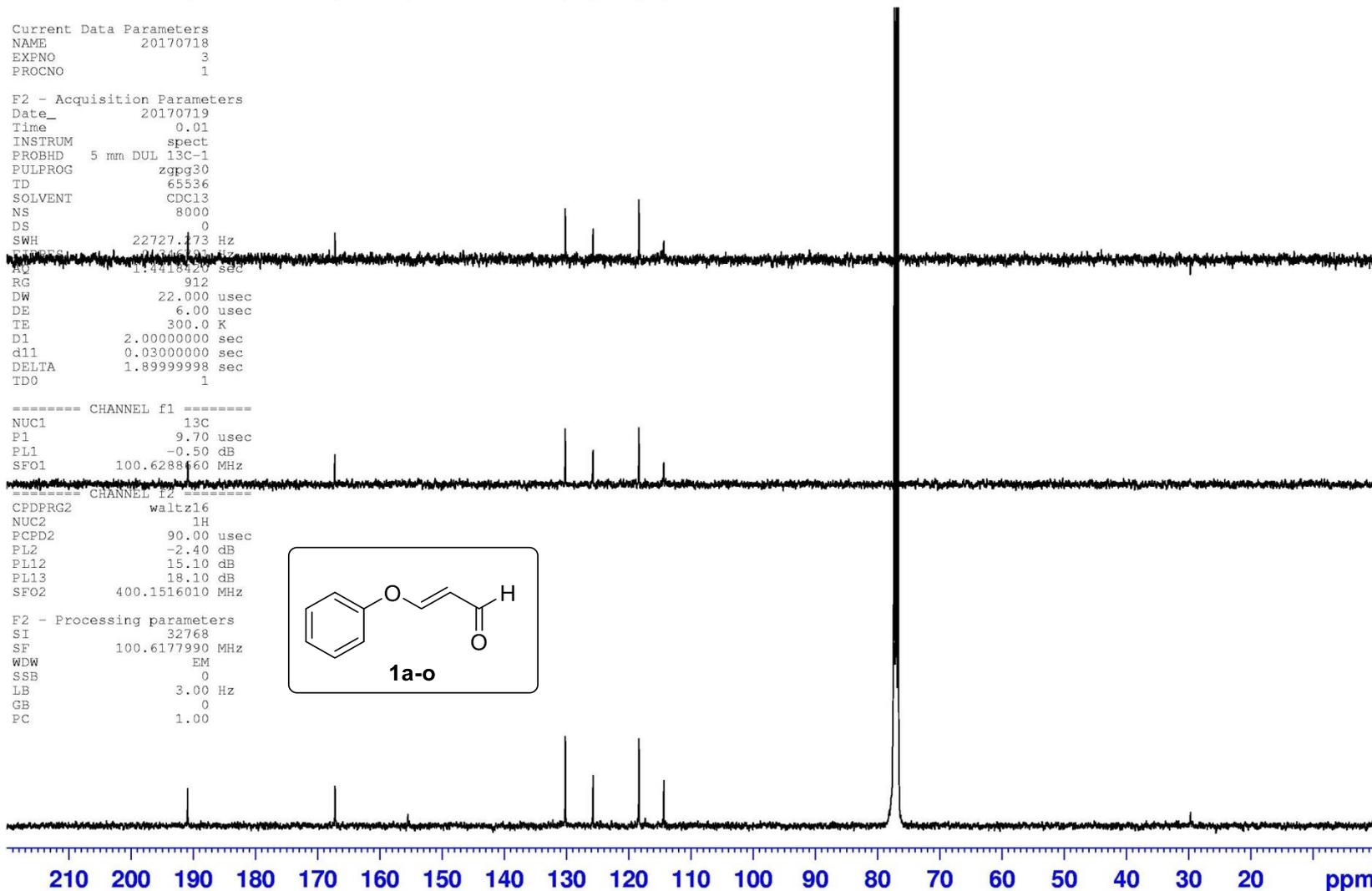
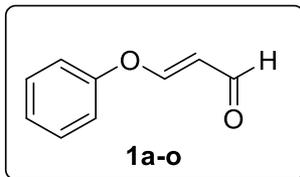
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EXPNO 3  
PROCNO 1

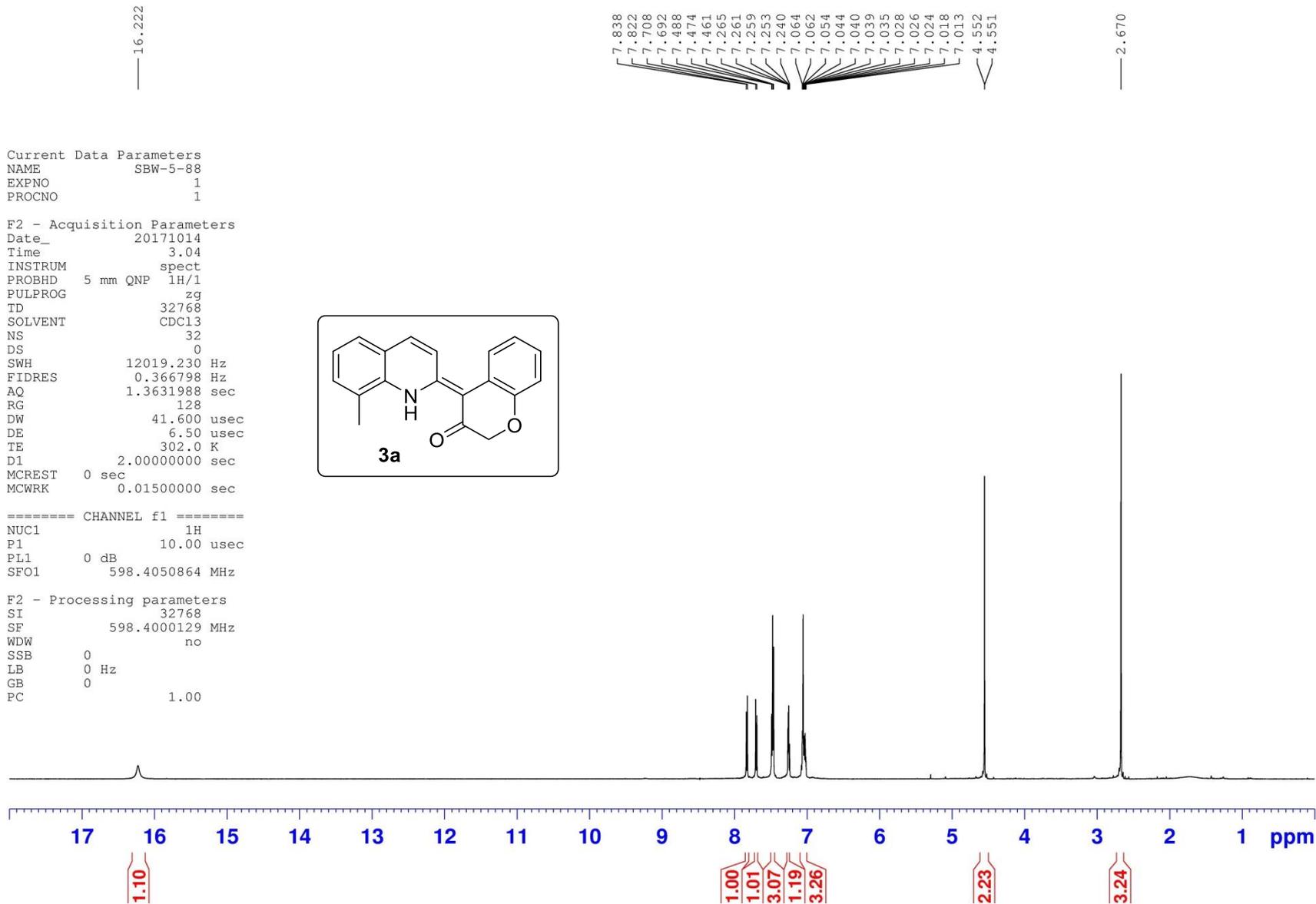
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Date\_ 20170719  
Time 0.01  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 8000  
DS 0  
SWH 22727.473 Hz  
RG 14418420 sec  
RG 912  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.628860 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.40 dB  
PL12 15.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6177990 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00







188.671

152.754  
149.469  
138.167  
136.444  
132.252  
126.015  
125.392  
125.042  
124.565  
124.031  
123.640  
123.354  
122.014  
118.707  
117.276

97.205

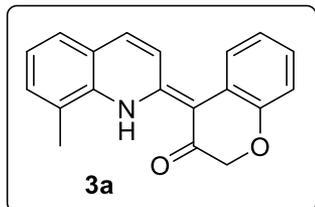
77.317  
77.000  
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72.098

17.047

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NAME 20171004  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171004  
Time 23.40  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 4000  
DS 0

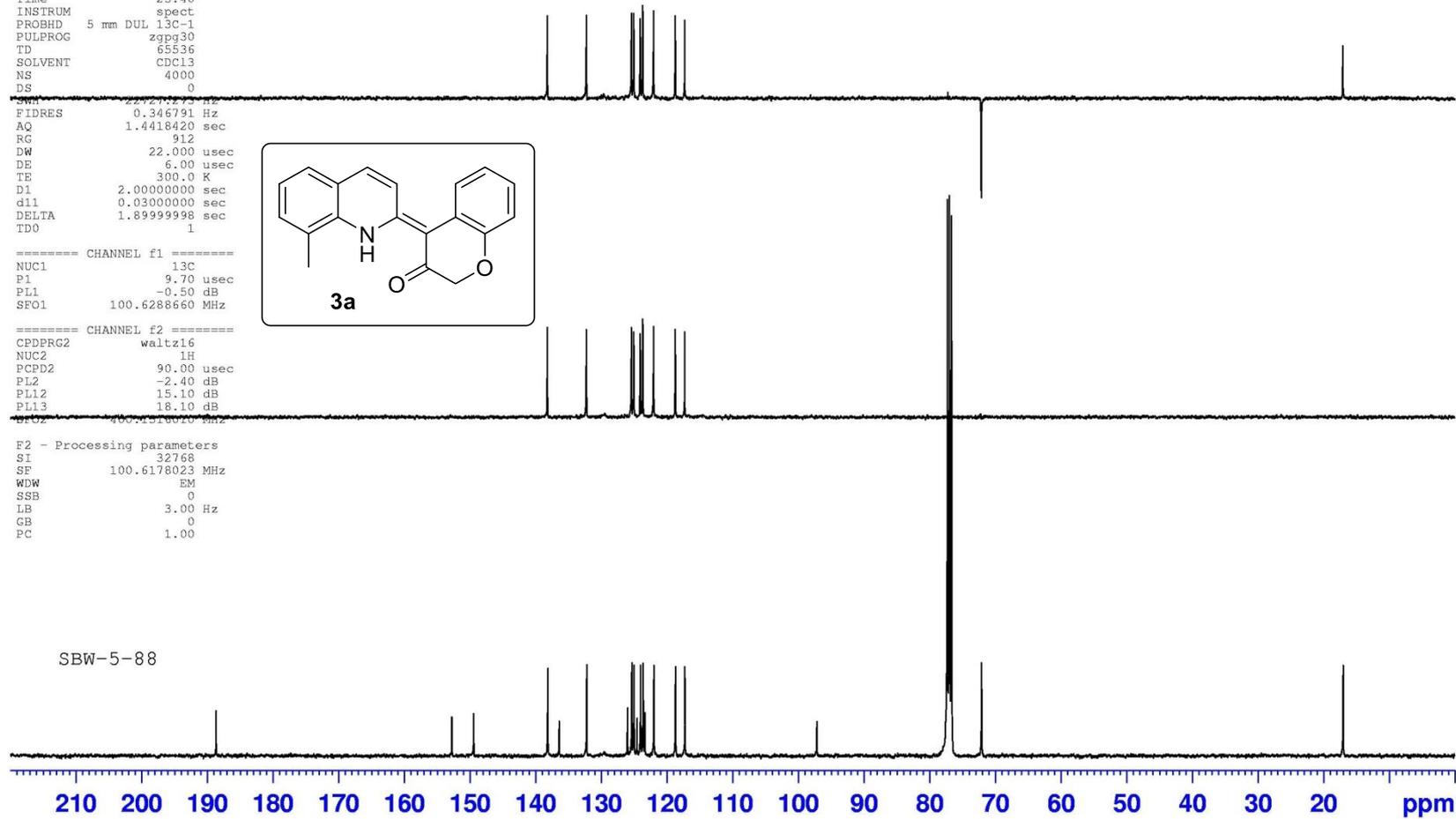
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P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

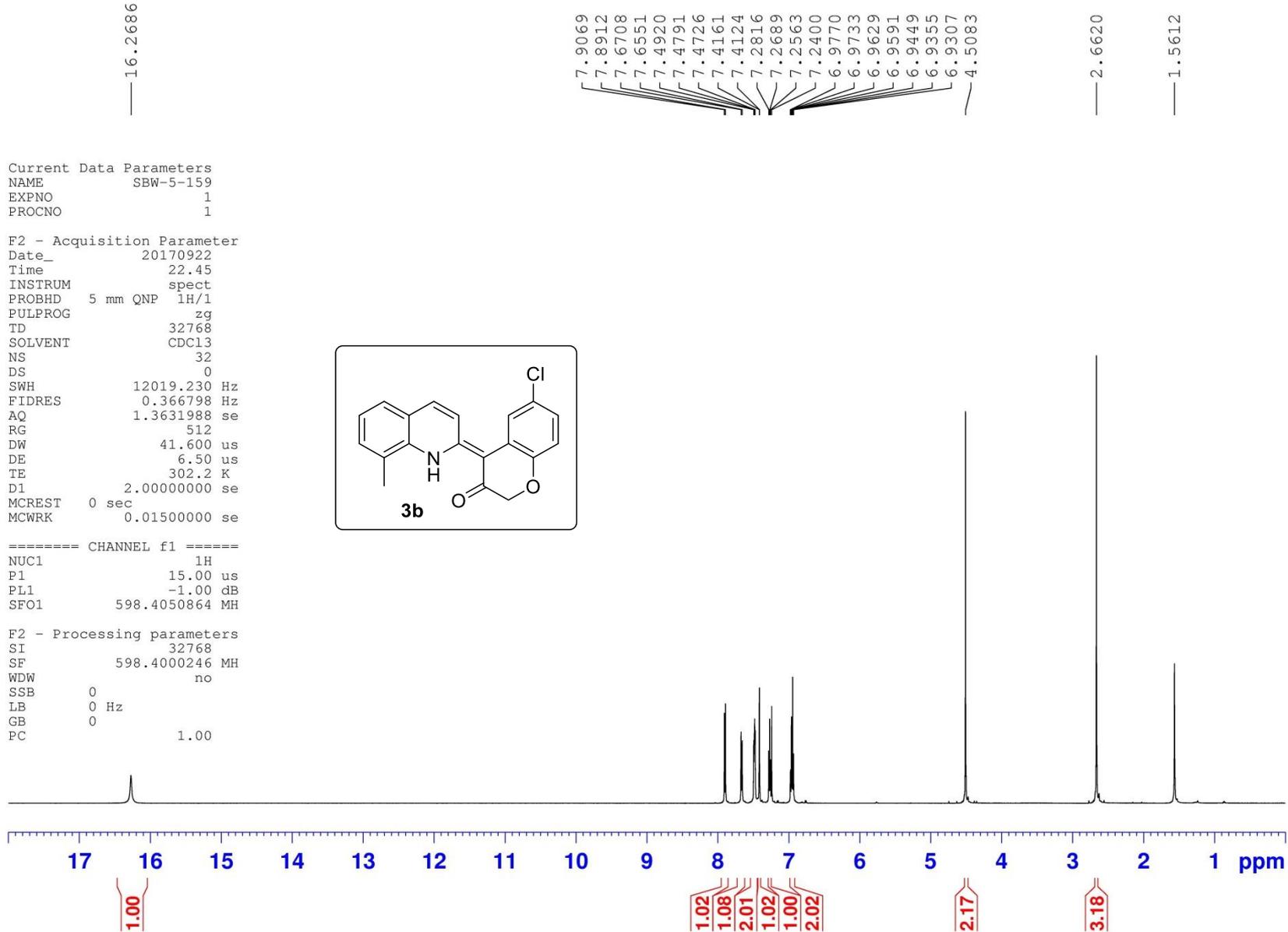


===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.40 dB  
PL12 15.10 dB  
PL13 18.10 dB

F2 - Processing parameters  
SI 32768  
SF 100.6178023 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

SBW-5-88





Current Data Parameters  
 NAME 554-5-159  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170922  
 Time 6.33  
 INSTRUM spect  
 PROBED 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 518  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DA 11.100 usec  
 DE 6.50 usec  
 TE 301.9 K  
 DL 3.5000000 sec  
 SFL 0.0300000 sec  
 DELTA 3.4000010 sec  
 ACQRES 0.0000000 sec  
 NSMRK 0.0150000 sec

===== CHANNEL f1 =====

NUC1 13C  
 P1 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.4828468 MHz

===== CHANNEL f2 =====

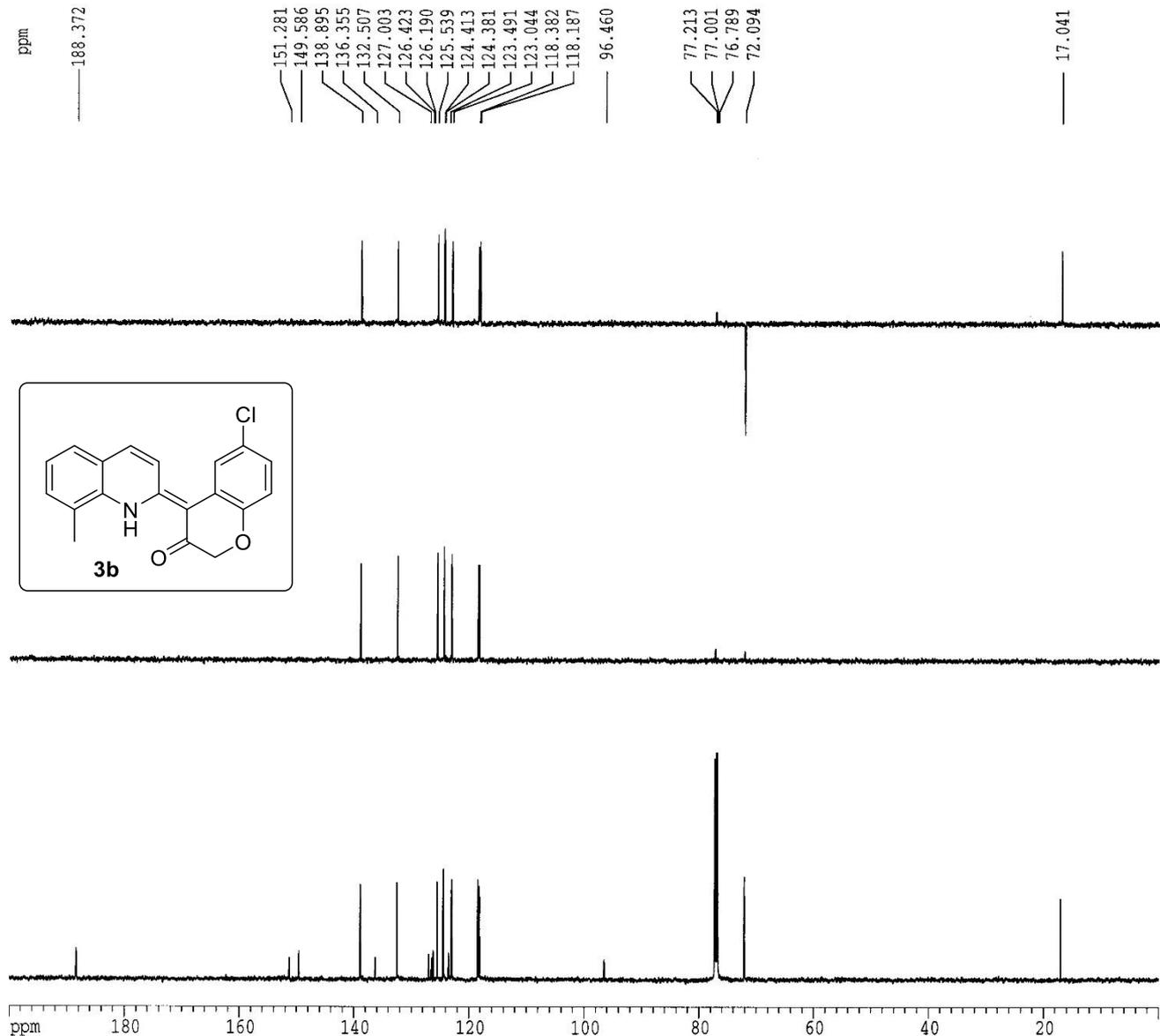
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 NUC2 1H  
 P2 92.00 usec  
 PL2 120.00 dB  
 PL12 5.50 dB  
 PL13 9.00 dB  
 SFO2 598.4029920 MHz

F2 - Processing parameters

SI 65536  
 SF 150.4678021 MHz  
 WDWT EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters

CK 20.00 cm  
 CY 4.00 cm  
 FLP 200.000 ppm  
 F1 30093.56 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 FREQM 10.00000 ppm/cm  
 NSCH 1504.67798 Hz/cm

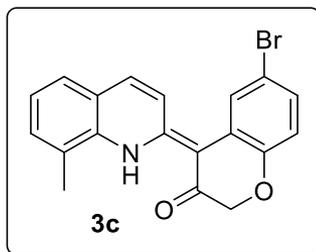


Current Data Parameters  
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 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170810  
 Time 16.58 h  
 INSTRUM spect  
 PROBHD Z119470\_0234 ( )  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 0  
 SWH 10997.067 Hz  
 FIDRES 0.335604 Hz  
 AQ 1.4898517 sec  
 RG 154.01  
 DW 45.467 usec  
 DE 6.88 usec  
 TE 299.9 K  
 D1 2.0000000 sec  
 TD0 1  
 SFO1 500.1645014 MHz  
 NUC1 1H  
 P1 10.00 usec  
 PLW1 23.39999962 W

F2 - Processing parameters  
 SI 16384  
 SF 500.1600211 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

— 16.261

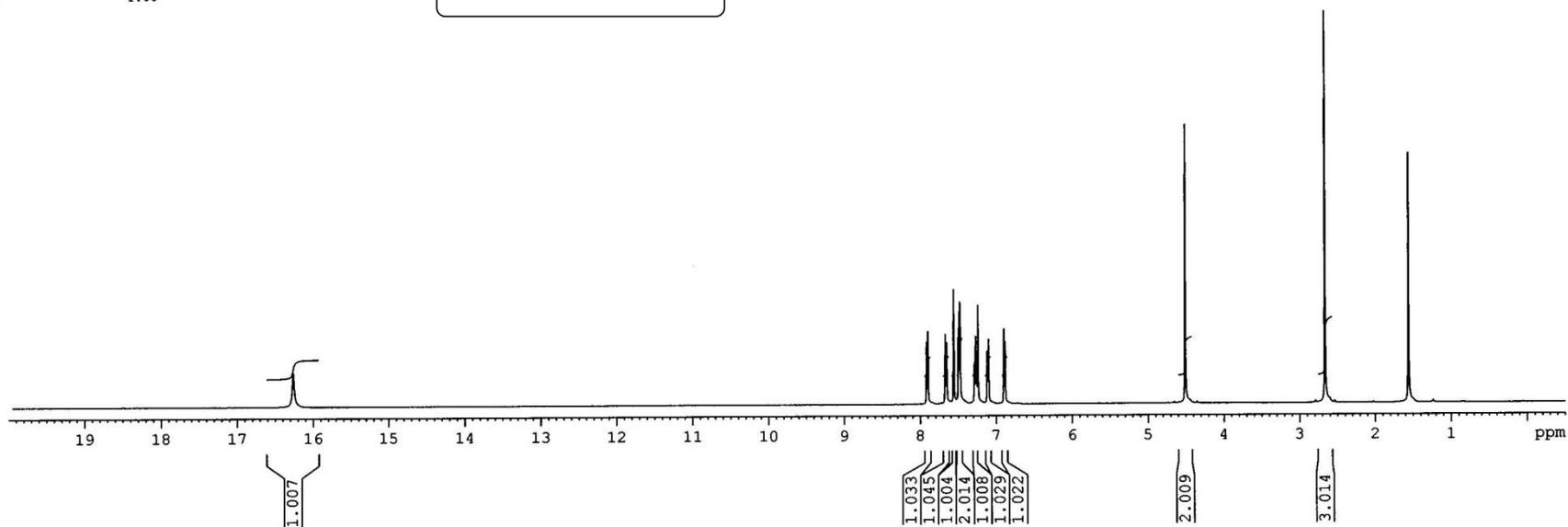


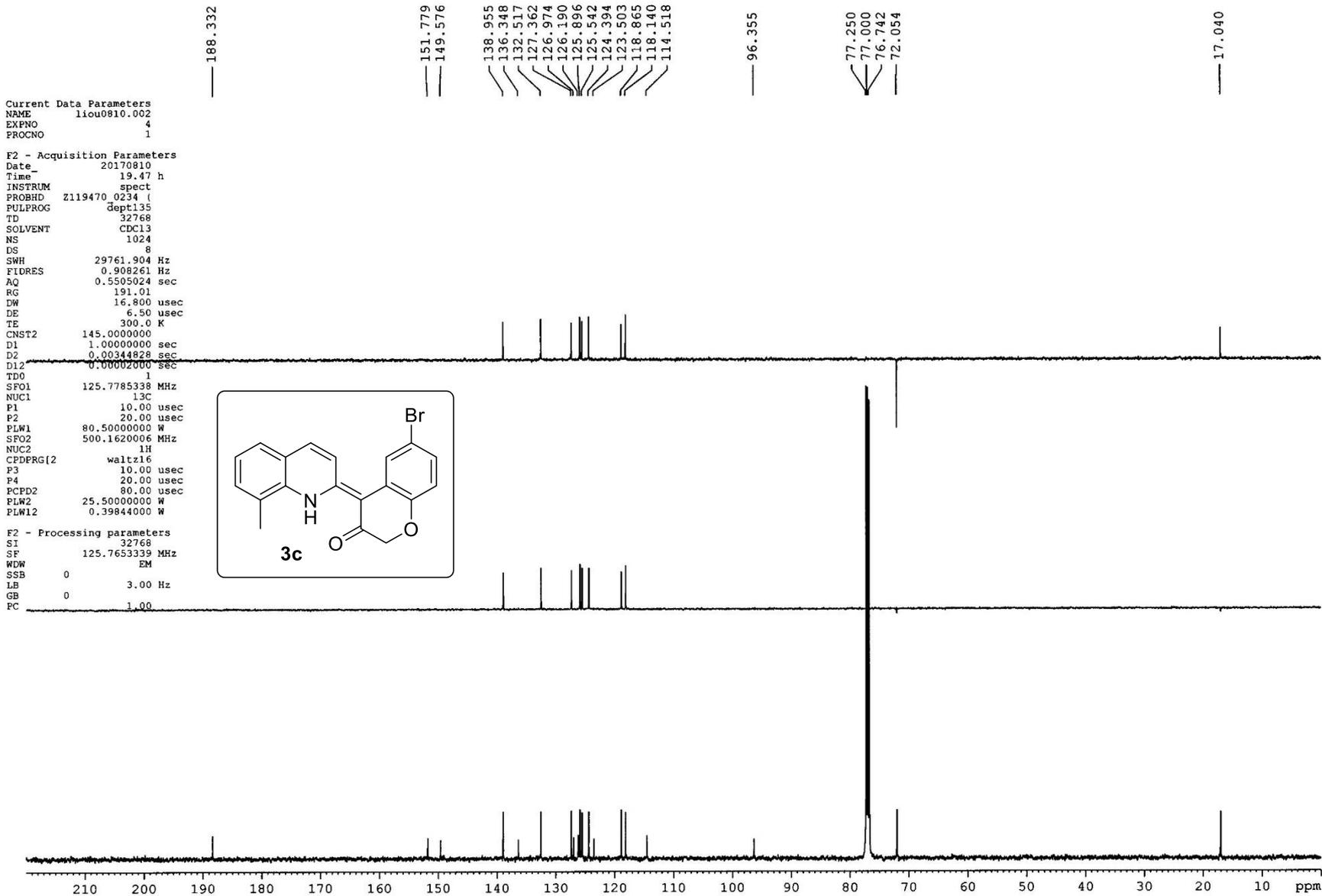
7.915  
 7.896  
 7.870  
 7.652  
 7.559  
 7.479  
 7.285  
 7.269  
 7.254  
 7.240  
 7.116  
 7.100  
 6.896  
 6.882  
 6.880

— 4.506

— 2.663

— 1.557





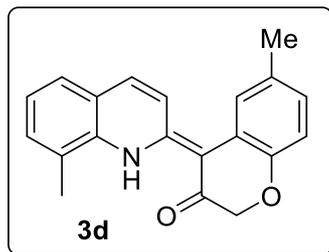
— 16.1864

7.8280  
7.8123  
7.7030  
7.6873  
7.4538  
7.4411  
7.2739  
7.2713  
7.2441  
7.2400  
7.2315  
7.2187  
6.9347  
6.9212  
6.8509  
6.8482  
6.8374  
6.8347  
— 4.5006

— 2.6516  
— 2.3308

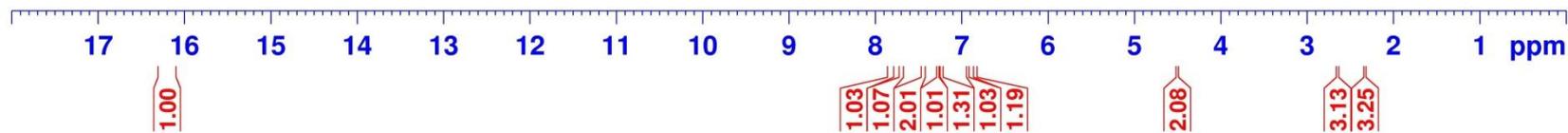
Current Data Parameters  
NAME SBW-5-105  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameter  
Date\_ 20170815  
Time 22.46  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDC13  
NS 64  
DS 0  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 se  
RG 512  
DW 41.600 us  
DE 6.50 us  
TE 300.4 K  
D1 2.00000000 se  
MCREST 0 sec  
MCWRK 0.01500000 se



==== CHANNEL f1 =====  
NUC1 1H  
P1 15.00 us  
PL1 -1.00 dB  
SFO1 598.4047872 MH

F2 - Processing parameters  
SI 32768  
SF 598.4000238 MH  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00





188.97

150.65  
149.44  
138.10  
136.50  
132.23  
131.23  
126.02  
125.57  
125.38  
124.37  
124.16  
123.99  
123.35  
118.86  
116.97

97.33

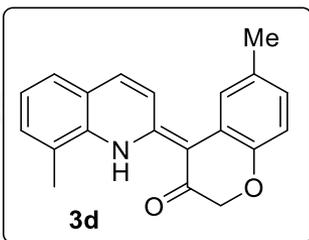
77.32  
77.00  
76.68  
72.22

21.11  
17.06

Current Data Parameters  
NAME 20170805  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170805  
Time 19.13  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536

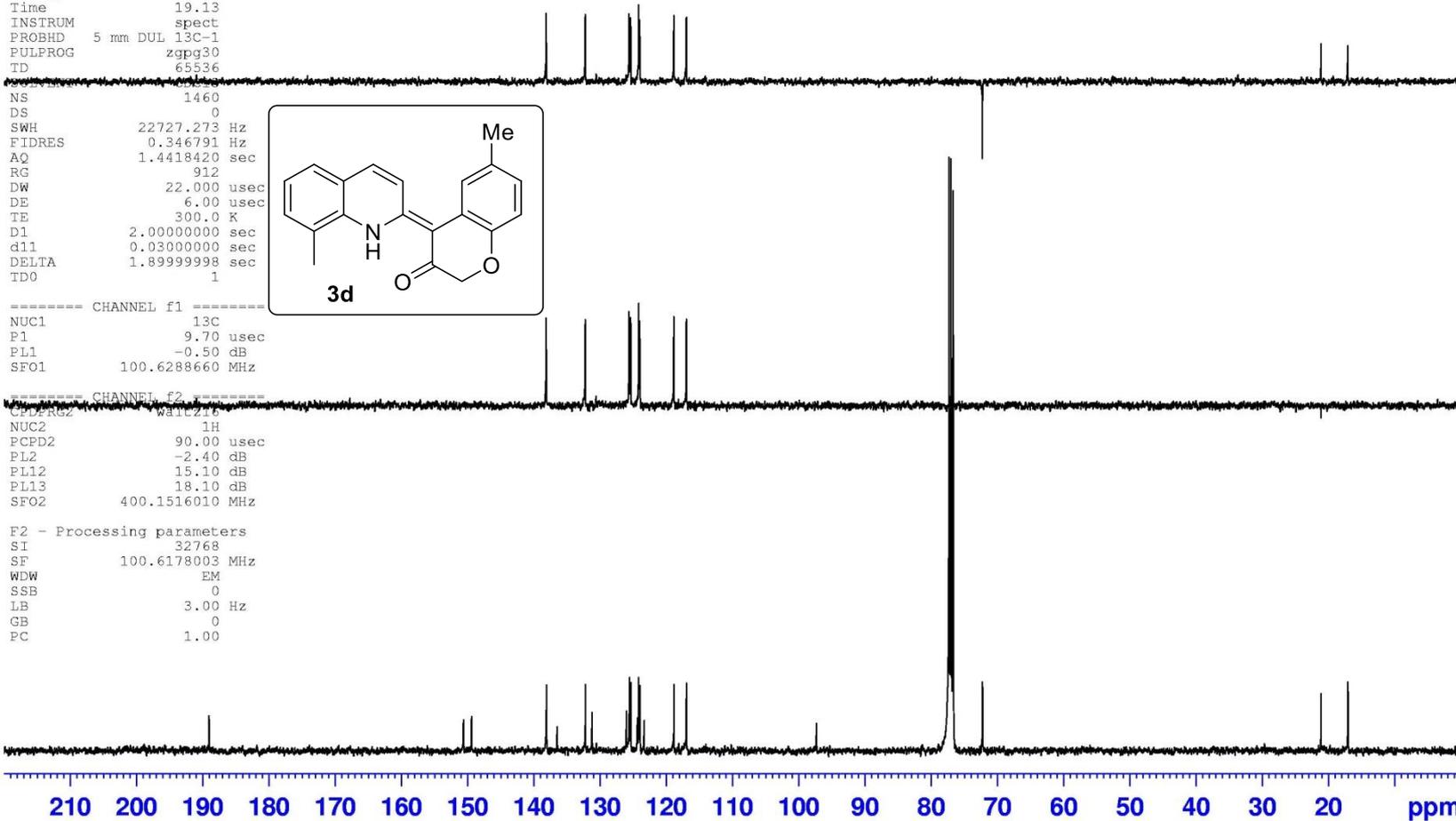
NS 1460  
DS 0  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
RG 912  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.40 dB  
PL12 15.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6178003 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



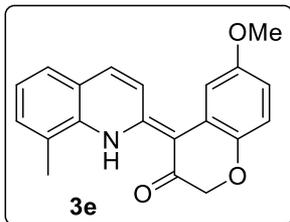
— 16.2343

Current Data Parameter  
NAME SBW-5-1  
EXPNO  
PROCNO

F2 - Acquisition Parameter  
Date\_ 201708  
Time 8.  
INSTRUM spe  
PROBHD 5 mm QNP 1H  
PULPROG  
TD 327  
SOLVENT CDC  
NS  
DS  
SWH 12019.2  
FIDRES 0.3667  
AQ 1.36319  
RG 5  
DW 41.6  
DE 6.  
TE 300  
D1 2.000000  
MCREST 0.000000  
MCWRK 0.015000

==== CHANNEL f1 =  
NUC1  
P1 15.  
PL1 -1.  
SFO1 598.40478

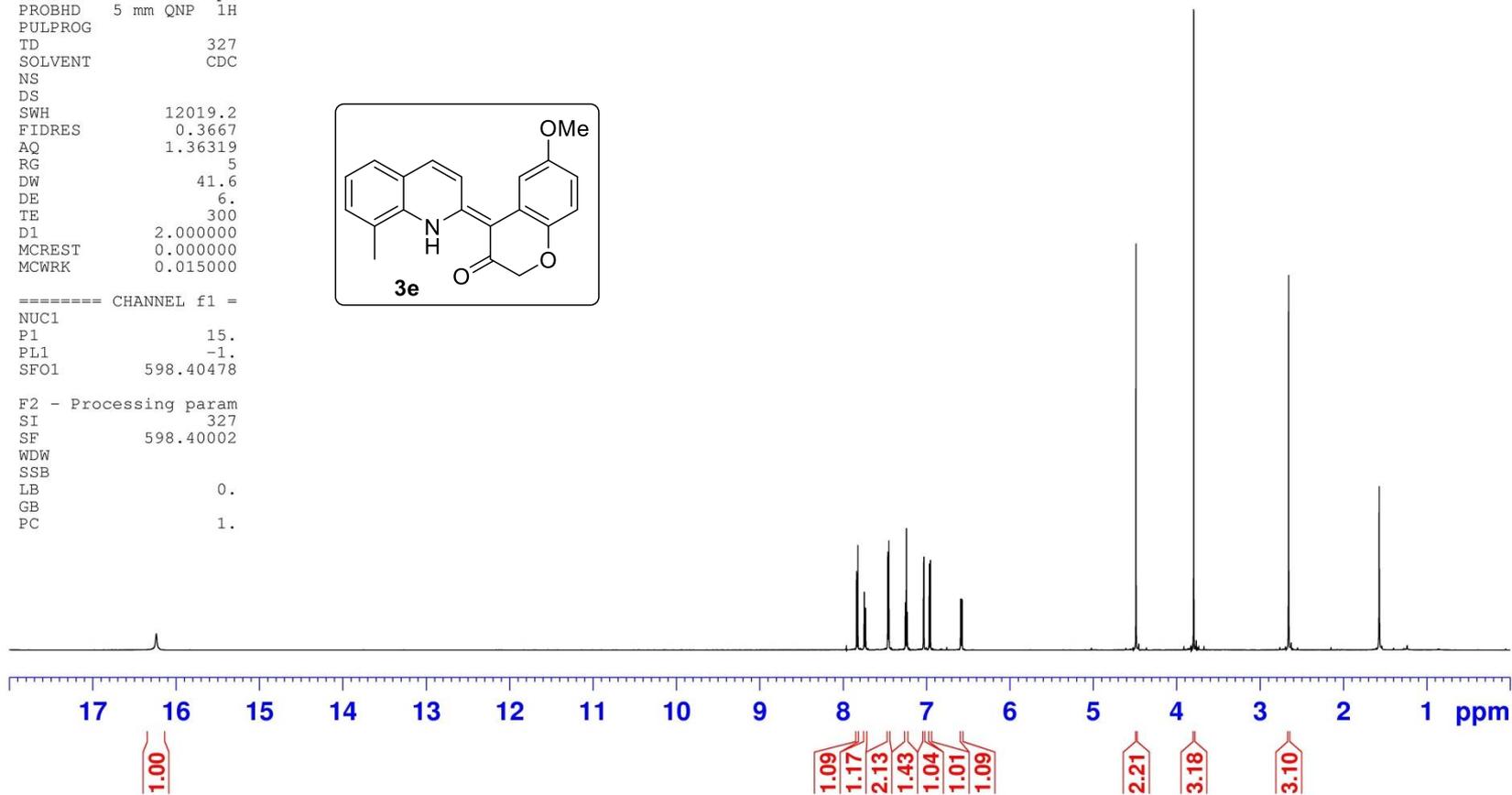
F2 - Processing parameter  
SI 327  
SF 598.40002  
WDW  
SSB  
LB 0.  
GB  
PC 1.



7.8391  
7.8234  
7.7474  
7.7460  
7.7316  
7.7301  
7.4644  
7.4517  
7.2549  
7.2423  
7.2400  
7.2384  
7.2371  
7.2360  
7.2296  
7.0357  
7.0309  
6.9675  
6.9531  
6.5914  
6.5865  
6.5768  
6.5720  
4.4874  
3.7950

— 2.6573

— 1.5697



Current Data Parameters  
 NAME SBM-5-115  
 EXPNO 2  
 PROCNO 1

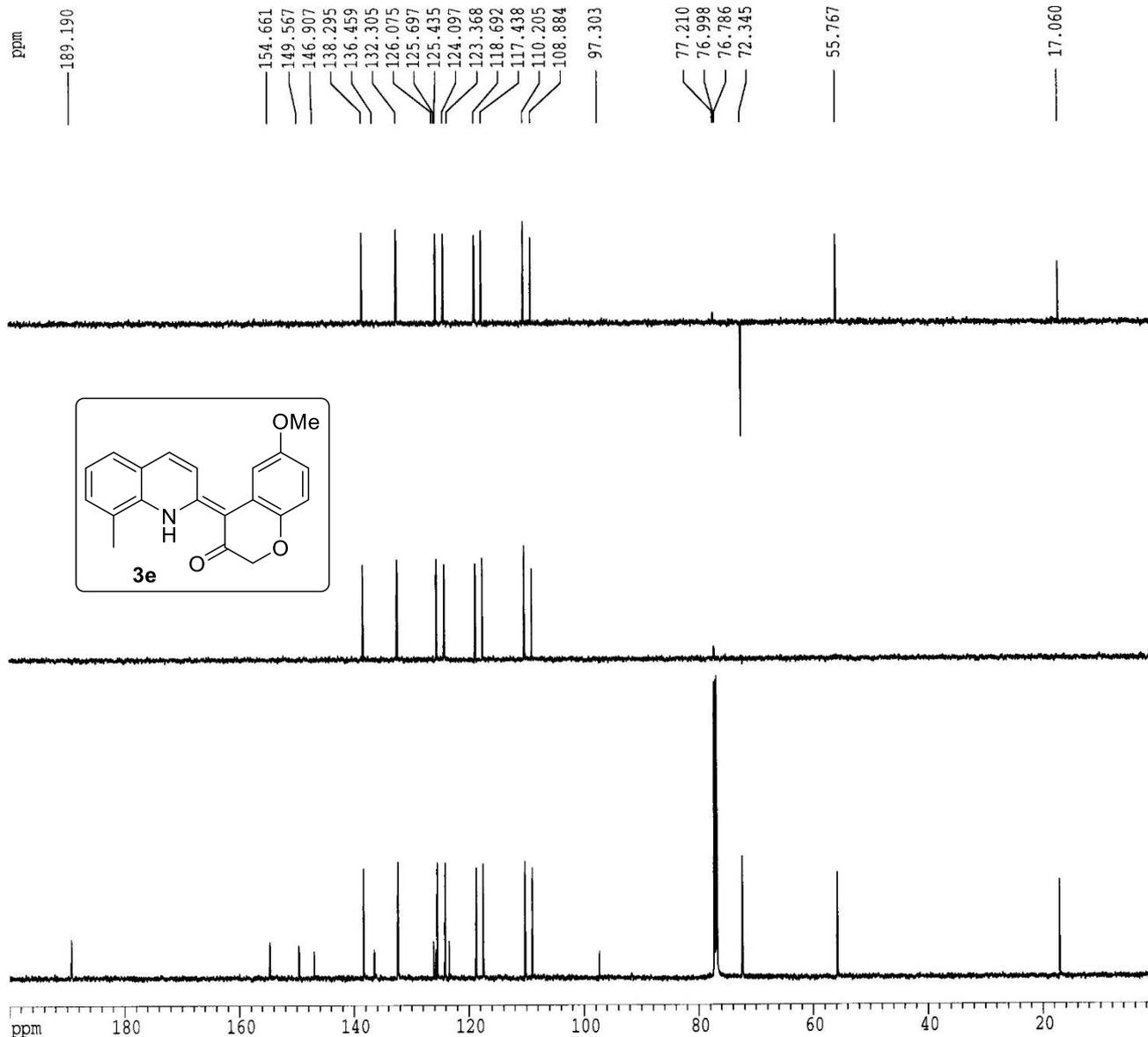
F2 - Acquisition Parameters  
 Date\_ 20170821  
 Time 8.57  
 INSTRUM spect  
 PROBED 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDC13  
 NS 811  
 DS 0  
 SFE 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 TM 11.100 usec  
 DE 6.50 usec  
 TE 300.5 K  
 HI 3.5000000 sec  
 H1 0.0300000 sec  
 DELTA 3.4000010 sec  
 DELTAREST 0.0000000 sec  
 MONRES 0.0150000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.4843515 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 P2 92.00 usec  
 PL2 120.00 dB  
 PL12 5.50 dB  
 PL13 9.00 dB  
 SFO2 598.4029920 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4678036 MHz  
 'WDW' EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 AC 1.00

1D NMR plot parameters  
 SX 20.00 cm  
 SY 5.30 cm  
 FIP 200.000 ppm  
 FI 30093.56 Hz  
 FIP 0.000 ppm  
 FZ 0.00 Hz  
 PPKCM 10.00000 ppm/cm  
 HZCM 1504.67798 Hz/cm



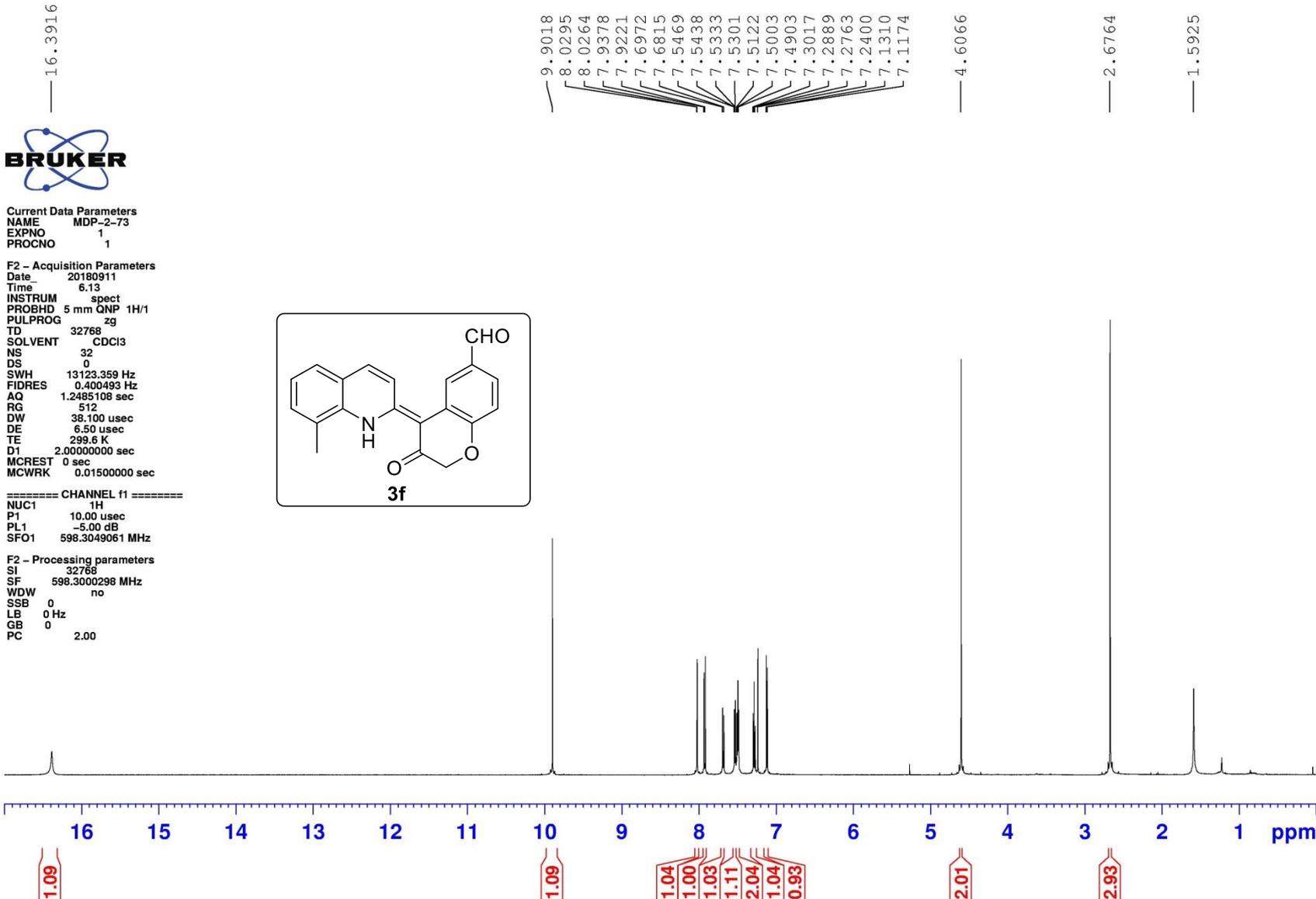
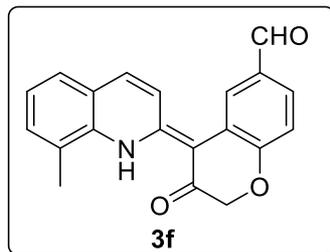


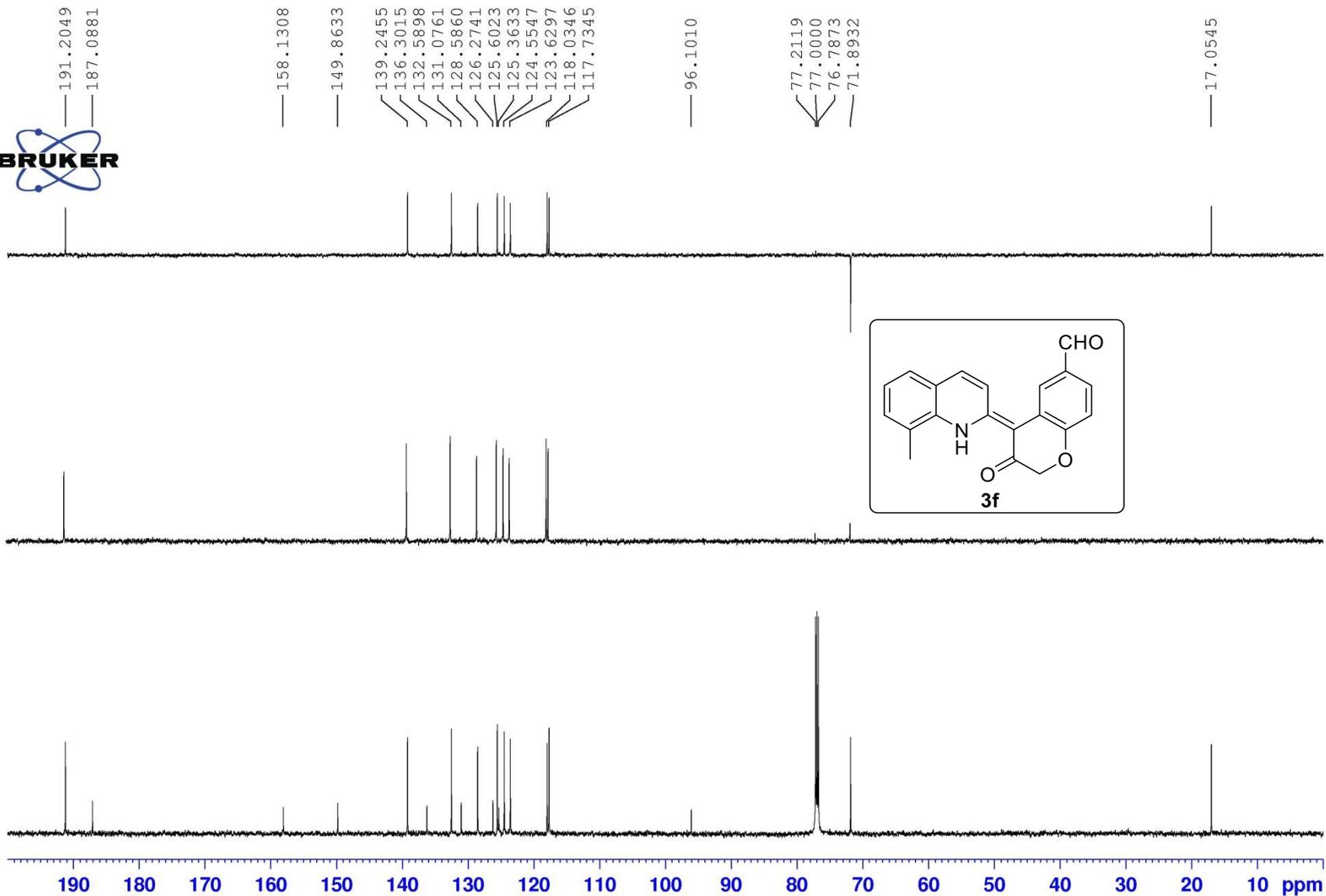
Current Data Parameters  
NAME MDP-2-73  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180911  
Time 6.13  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 13123.359 Hz  
FIDRES 0.400493 Hz  
AQ 1.2485108 sec  
RG 512  
DW 38.100 usec  
DE 6.50 usec  
TE 299.6 K  
D1 2.00000000 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -5.00 dB  
SFO1 598.3049061 MHz

F2 - Processing parameters  
SI 32768  
SF 598.3000298 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 2.00





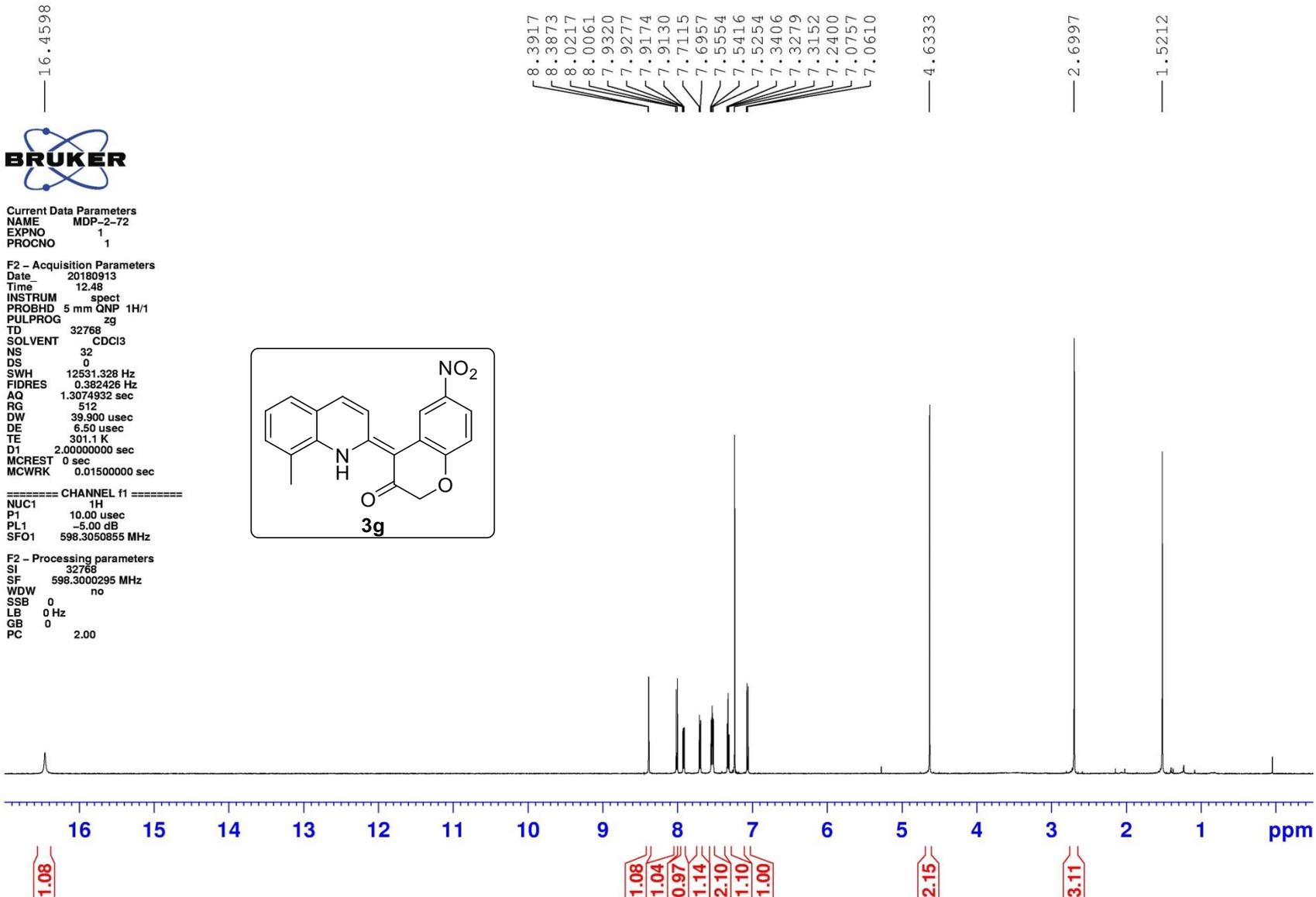
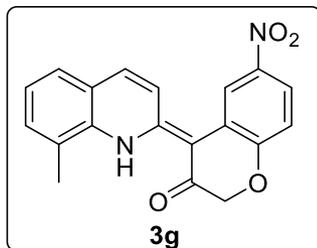


Current Data Parameters  
NAME MDP-2-72  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180913  
Time 12.48  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 12531.328 Hz  
FIDRES 0.382426 Hz  
AQ 1.3074932 sec  
RG 512  
DW 39.900 usec  
DE 6.50 usec  
TE 301.1 K  
D1 2.00000000 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -5.00 dB  
SFO1 598.3050855 MHz

F2 - Processing parameters  
SI 32768  
SF 598.3000295 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 2.00





Current Data Parameters  
NAME MDP-2-72  
EXPNO 2  
PROCNO 1

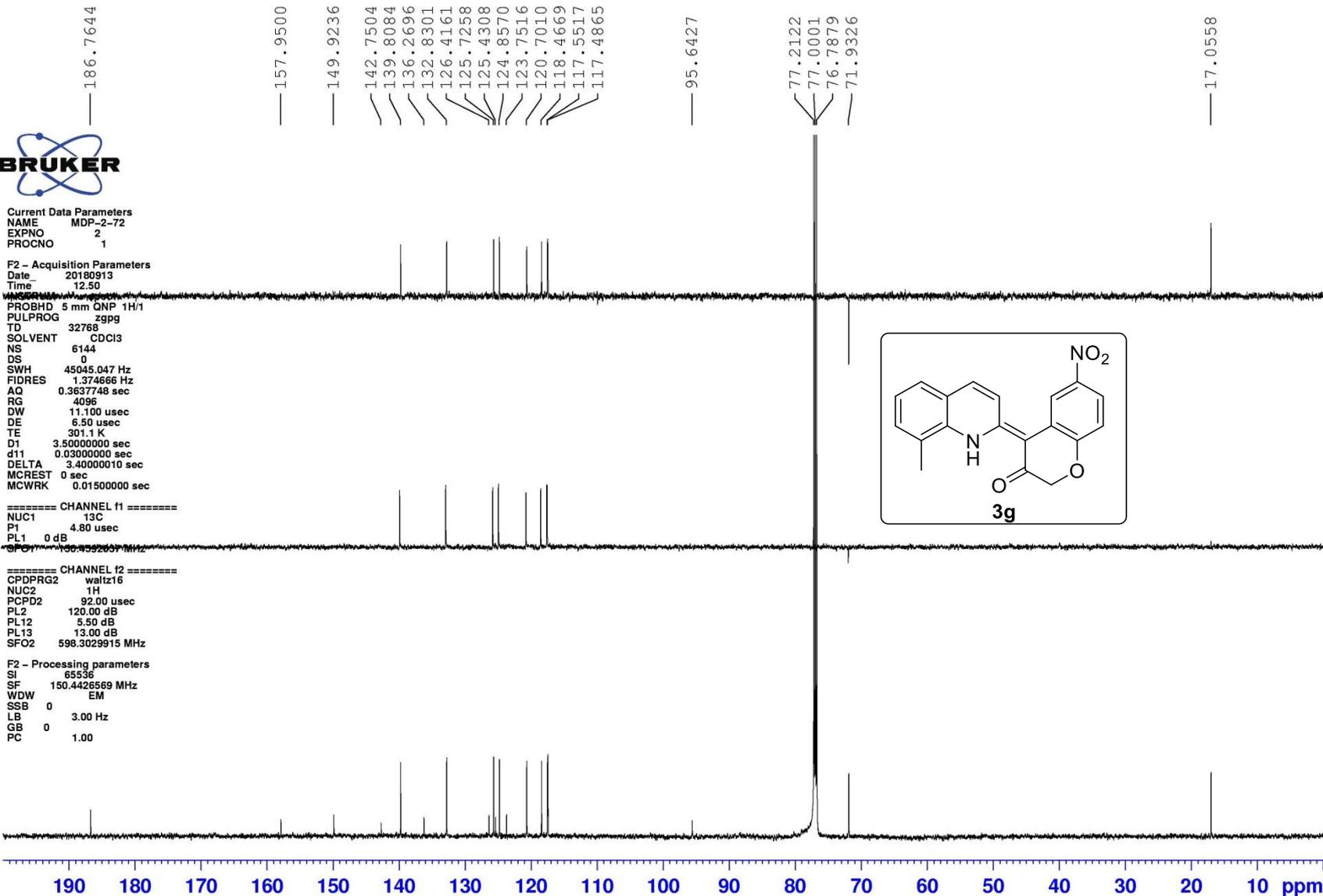
F2 - Acquisition Parameters  
Date\_ 20180913  
Time\_ 12.50

PROBHD 5 mm QNP 1H/1  
PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 6144  
DS 0  
SWH 45045.047 Hz  
FIDRES 1.374666 Hz  
AQ 0.3637748 sec  
RG 4096  
DW 11.100 usec  
DE 6.50 usec  
TE 301.1 K  
D1 3.50000000 sec  
d11 0.03000000 sec  
DELTA 3.40000010 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

==== CHANNEL f1 =====  
NUC1 13C  
P1 4.80 usec  
PL1 0 dB  
SFO1 100.625000 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 92.00 usec  
PL2 120.00 dB  
PL12 5.50 dB  
PL13 13.00 dB  
SFO2 598.3029915 MHz

F2 - Processing parameters  
SI 6556  
SF 150.4426569 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



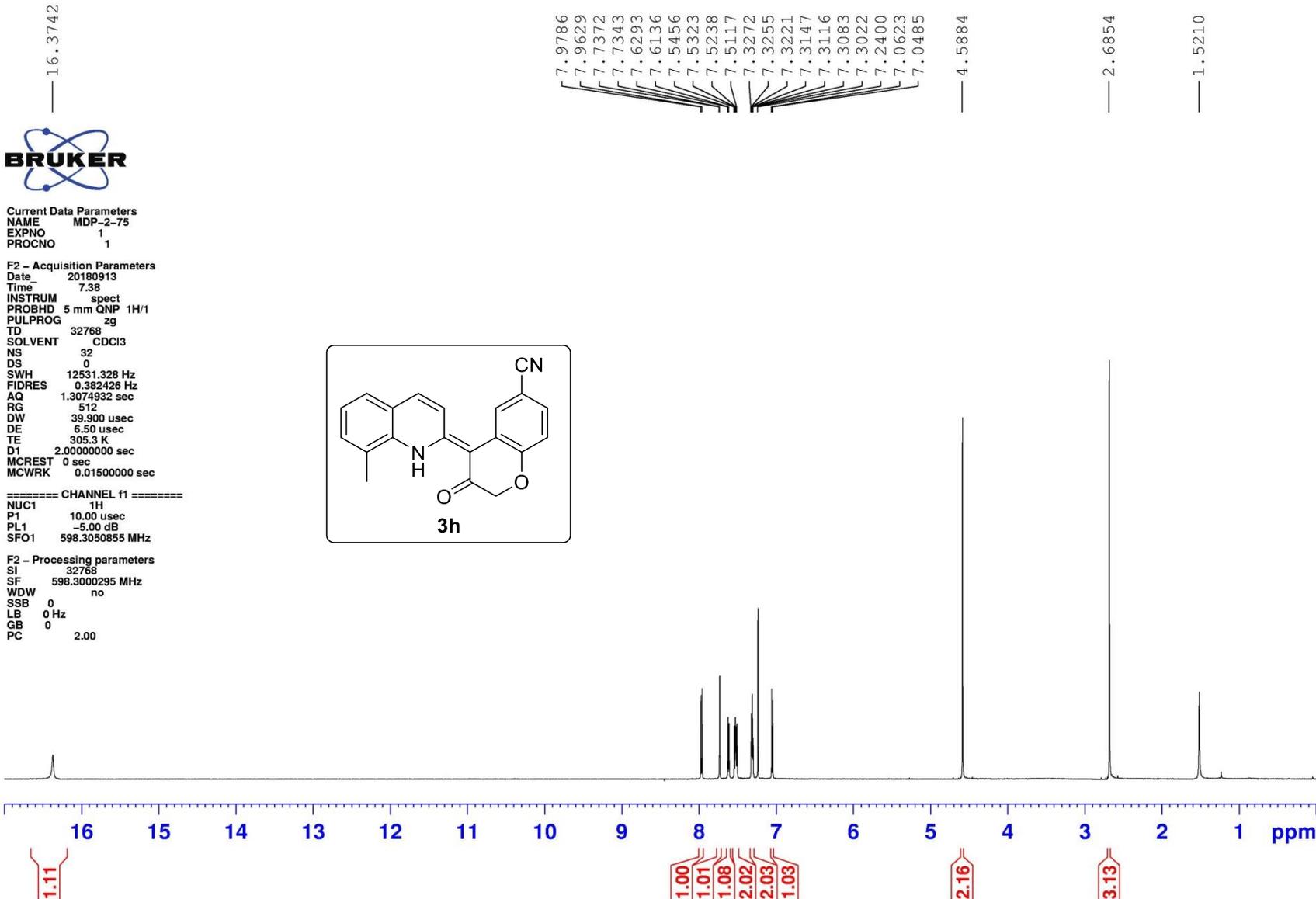
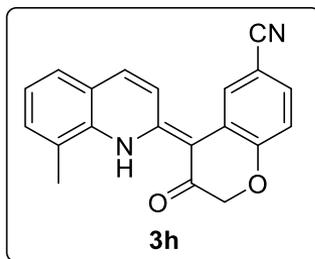


Current Data Parameters  
NAME MDP-2-75  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180913  
Time 7.38  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 12531.328 Hz  
FIDRES 0.382426 Hz  
AQ 1.3074932 sec  
RG 512  
DW 39.900 usec  
DE 6.50 usec  
TE 305.3 K  
D1 2.00000000 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -5.00 dB  
SFO1 598.3050855 MHz

F2 - Processing parameters  
SI 32768  
SF 598.3000295 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 2.00





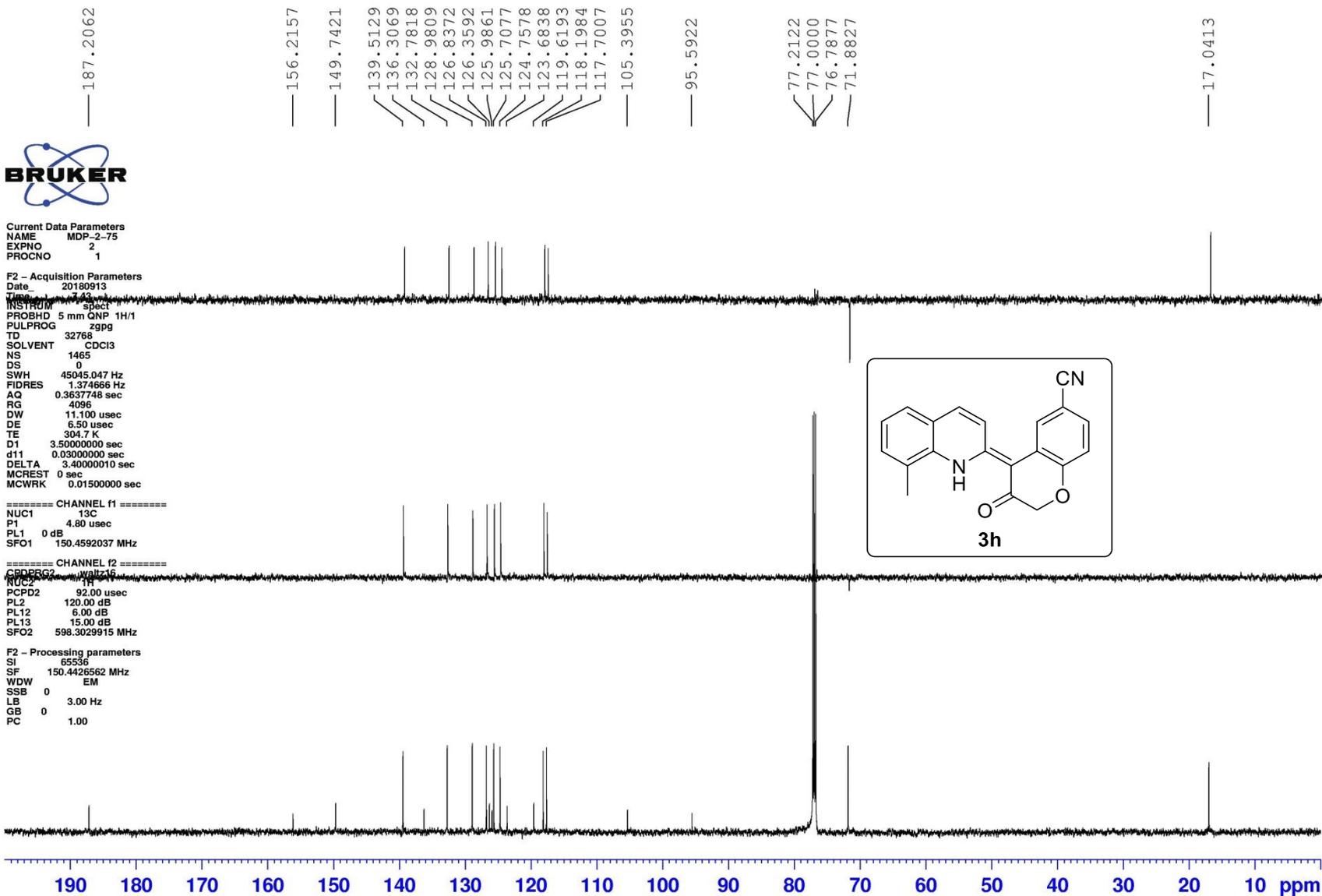
Current Data Parameters  
NAME MDP-2-75  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180913  
Time 14.43  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 1465  
DS 0  
SWH 45045.047 Hz  
FIDRES 1.374666 Hz  
AQ 0.3637748 sec  
RG 4096  
DW 11.100 usec  
DE 6.50 usec  
TE 304.7 K  
D1 3.50000000 sec  
d11 0.03000000 sec  
DELTA 3.40000010 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 4.80 usec  
PL1 0 dB  
SFO1 150.4592037 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 92.00 usec  
PL2 120.00 dB  
PL12 6.00 dB  
PL13 15.00 dB  
SFO2 598.3029915 MHz

F2 - Processing parameters  
SI 65536  
SF 150.4426562 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



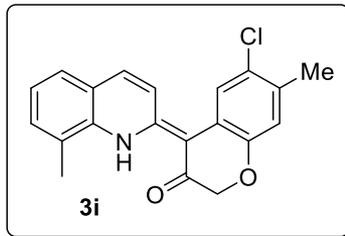
16.215

Current Data Parameters  
NAME SBW-5-113  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameter  
Date\_ 20170816  
Time\_ 0.04  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 64  
DS 0  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 se  
RG 512  
DW 41.600 us  
DE 6.50 us  
TE 300.7 K  
D1 2.00000000 se  
MCREST 0 sec  
MCWRK 0.01500000 se

----- CHANNEL f1 -----  
NUCL1 1H  
P1 15.00 us  
PL1 -1.00 dB  
SFO1 598.4047872 MHz

F2 - Processing parameters  
SI 32768  
SF 598.4000258 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

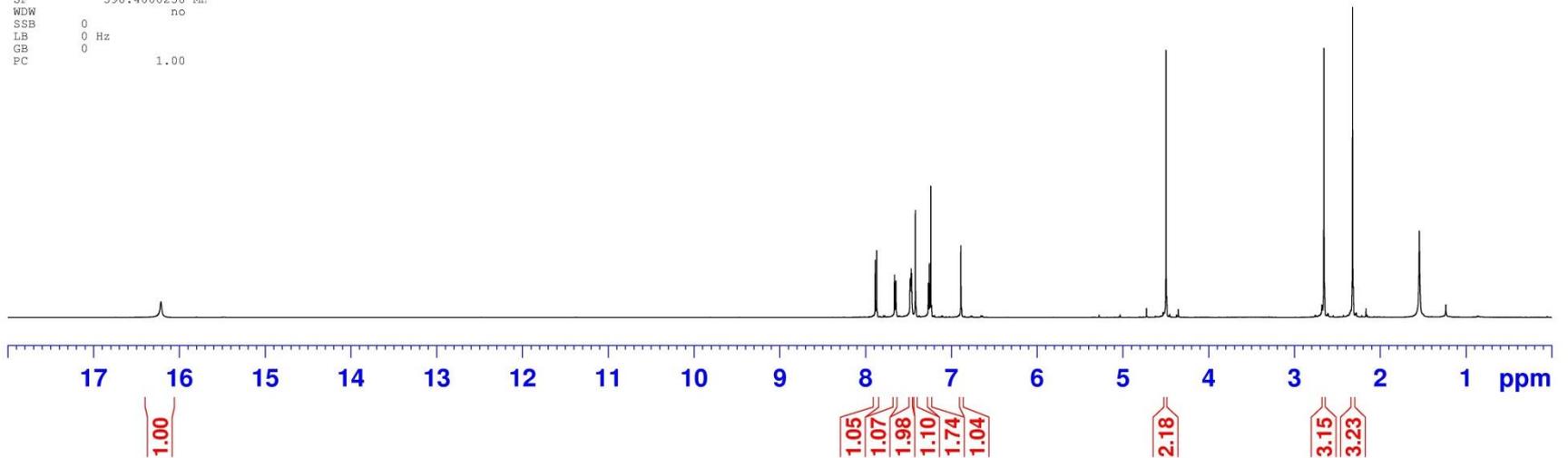


7.888  
7.872  
7.662  
7.647  
7.481  
7.475  
7.468  
7.463  
7.419  
7.274  
7.269  
7.256  
7.249  
7.244  
7.240  
7.230  
6.888

4.498

2.657  
2.323

1.544





188.24

151.27  
149.39  
138.68  
136.43  
132.42  
132.21  
127.06  
126.11  
125.50  
124.22  
123.83  
123.39  
119.40  
118.33

96.36

77.32  
77.00  
76.68  
72.17

19.72  
17.05

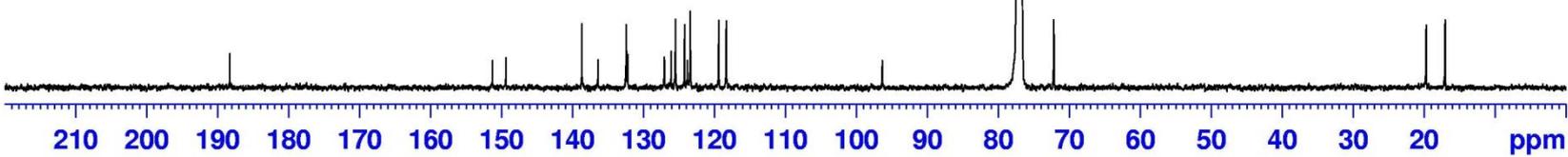
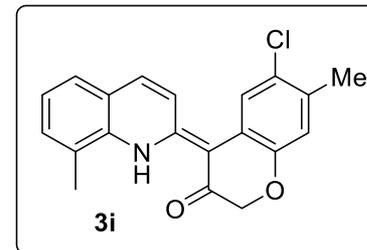
Current Data Parameters  
NAME 20170821  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170821  
Time 22.52  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 7000  
DS 0  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
RG 912  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.40 dB  
PL12 15.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6177990 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

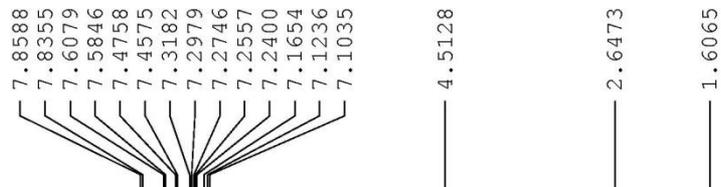
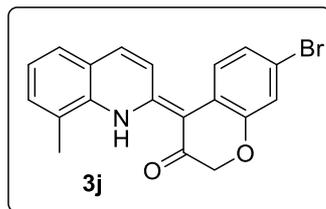




16.202

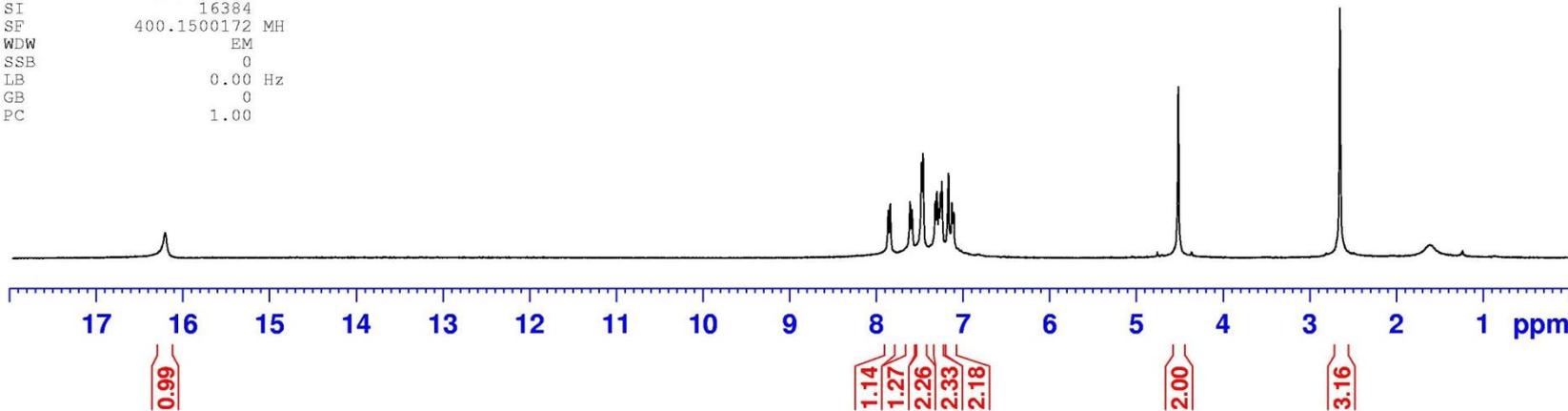
Current Data Parameters  
NAME 20170930  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameter  
Date\_ 20170930  
Time 9.17  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 30  
DS 0  
SWH 8802.817 Hz  
FIDRES 0.268641 Hz  
AQ 1.8612725 se  
RG 456  
DW 56.800 us  
DE 6.00 us  
TE 300.0 K  
D1 2.00000000 se  
TD0 1



----- CHANNEL f1 -----  
NUC1 1H  
P1 10.00 us  
PL1 -2.40 dB  
SFO1 400.1528010 MH

F2 - Processing parameters  
SI 16384  
SF 400.1500172 MH  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00





187.997

153.512  
149.409  
138.581  
136.383  
132.460  
126.120  
125.482  
124.999  
124.460  
124.287  
123.776  
123.415  
120.553  
118.304  
116.810

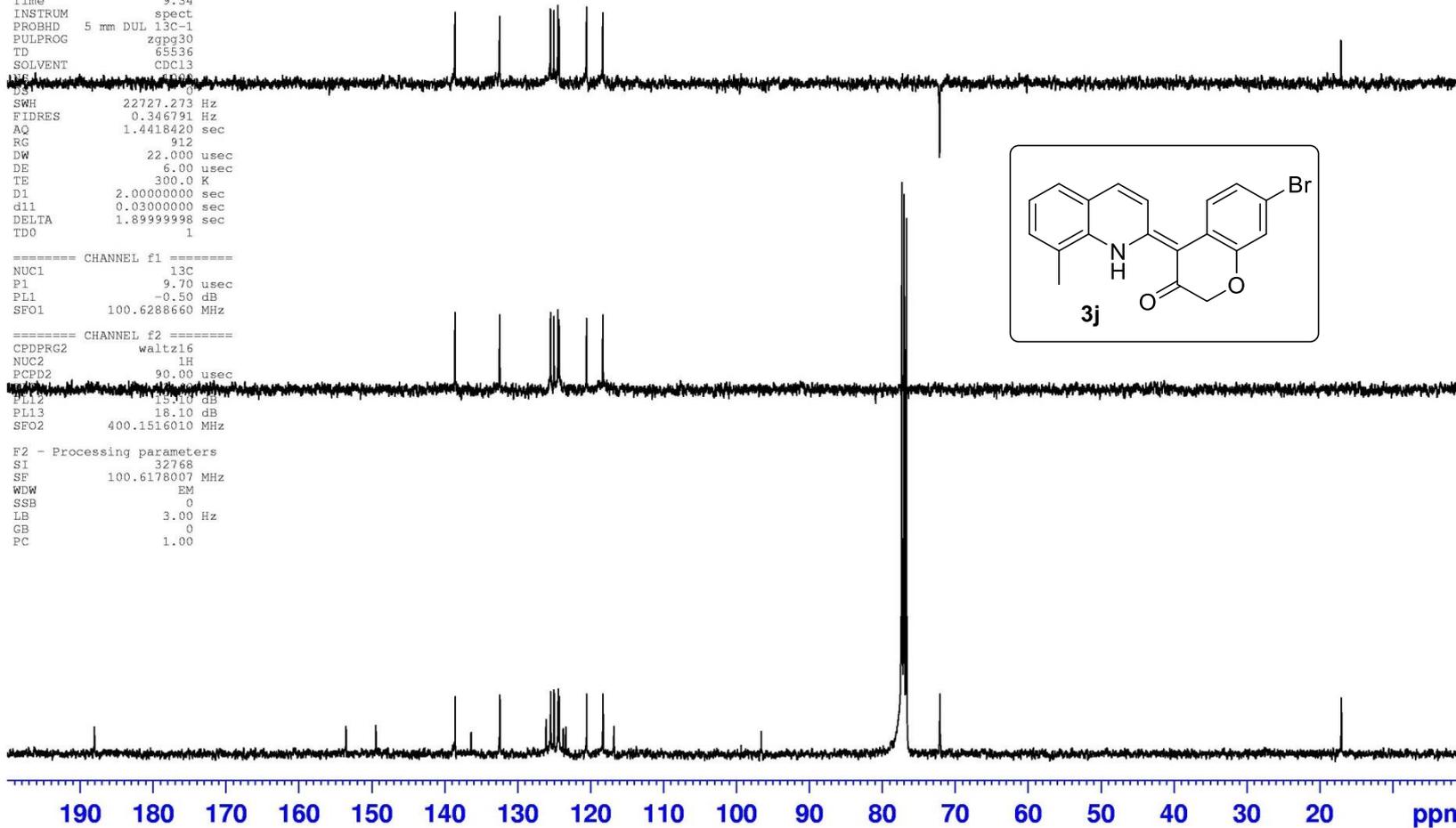
96.567

77.318  
77.000  
76.683  
72.100

17.029

Current Data Parameters  
NAME 20170930  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170930  
Time 9.34  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz  
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 19.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz  
F2 - Processing parameters  
SI 32768  
SF 100.6178007 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



```

Current Data Parameters
NAME      SBM 5-119
EXPNO    1
PROCNO   1

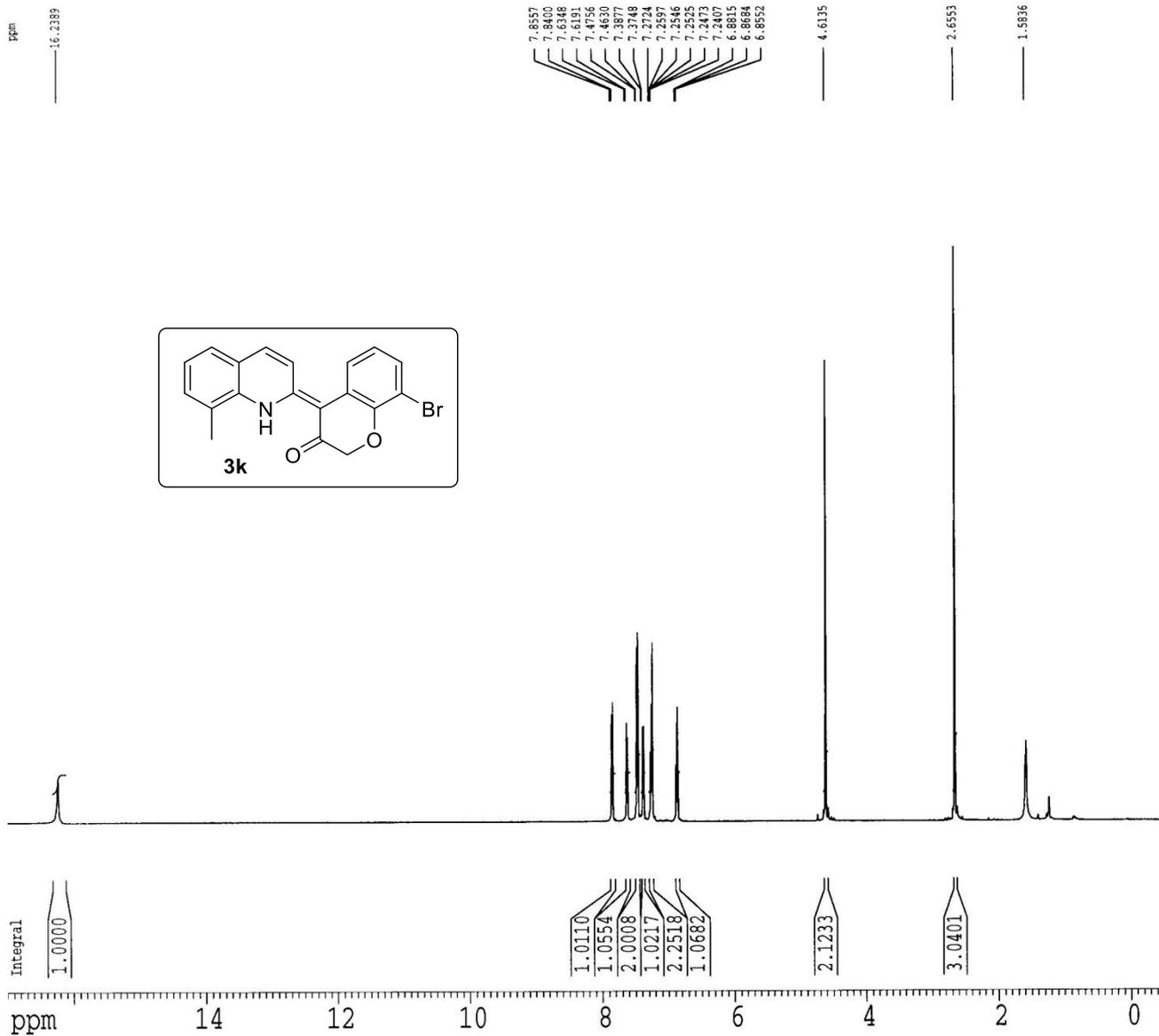
F2 Acquisition Parameters
Date_    20170817
Time     7.01
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD       32768
SOLVENT  CDCl3
NS       32
DS       0
SWH      12019.230 Hz
FIDRES   0.366798 Hz
AQ       1.3631888 sec
RG       512
TE       41.400 usec
LB       0.50 usec
GB       0
PC       300.2 K
PI       0.00000000 sec
MKREF   0.00000000 sec
NOREF   0.01500000 sec

** CHANNEL f1 *****
NAME     1H
P1       13.00 usec
PL       -1.00 dB
SFO1     598.4047872 MHz

F2 Processing parameters
SI       32768
SF       598.4000252 MHz
WDW      no
SSB      0
GB       0
LB       0.00 Hz
GB       0
PC       1.00

ID NMR plot parameters
CX       20.00 cm
CY       10.00 cm
FID      17.000 ppm
FO       10172.80 Hz
FQ1      -0.500 ppm
FL       299.20 Hz
PULPROG 0.47500 ppm/cm
RG1      523.60004 Hz/cm

```



Current Data Parameters  
 NAME SBM-5-119  
 EXPNO 2  
 PROCNO 1

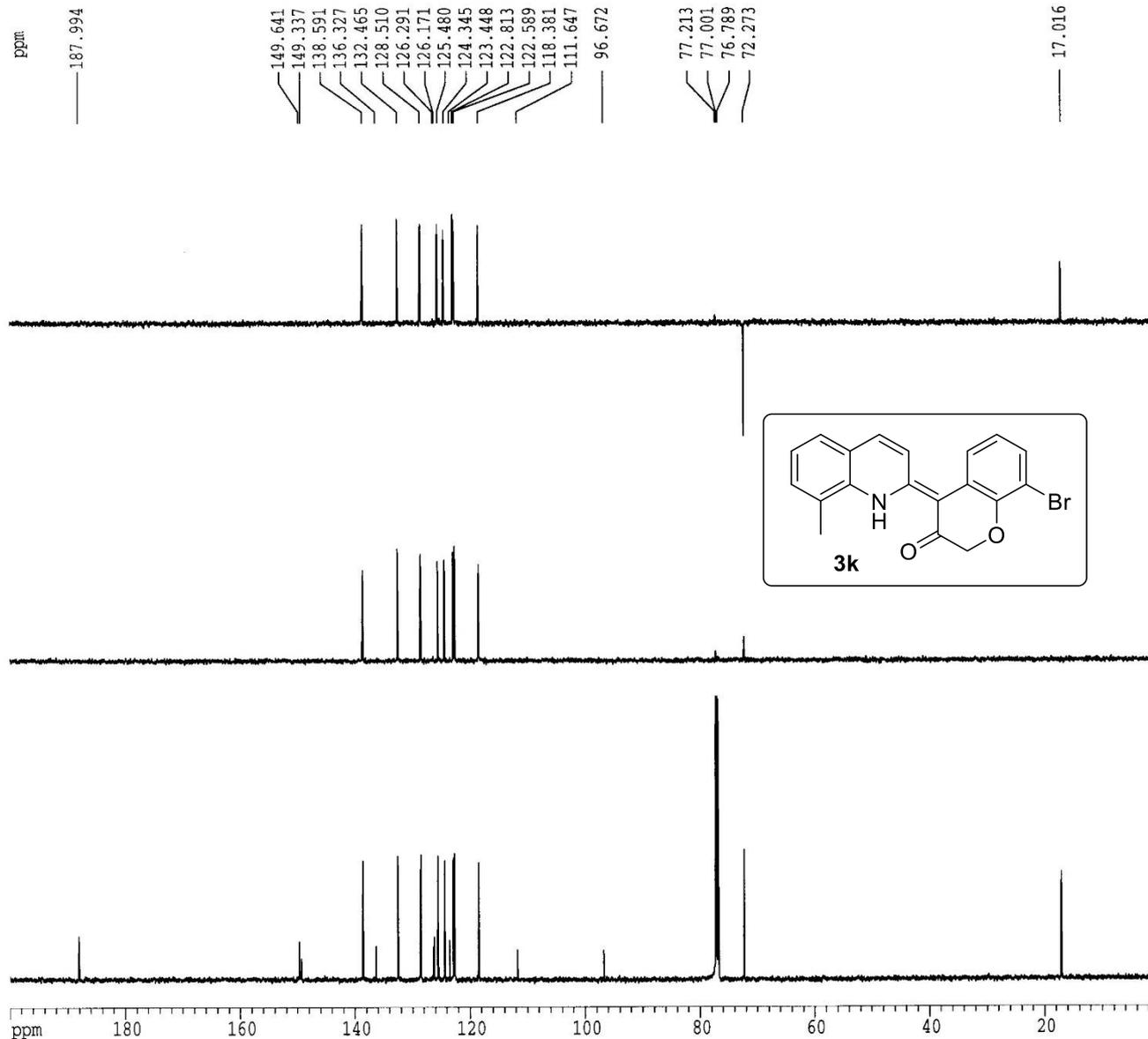
F2 - Acquisition Parameters  
 Date\_ 20170817  
 Time 7.05  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 589  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 EQ 4096  
 WT 11.100 usec  
 DE 6.50 usec  
 TE 300.3 K  
 DQ 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0.00000000 sec  
 MCHKE 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUCL 13C  
 PL 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.4843515 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NUC2 1H  
 PULPROG 92.00 usec  
 PL2 120.00 dB  
 PL11 5.50 dB  
 PL13 9.00 dB  
 SFO2 598.4029920 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4678043 MHz  
 EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 SI 20.00 cm  
 SF 5.00 cm  
 FID 200.000 ppm  
 FI 30093.56 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 10.00000 ppm/cm  
 HZCM 1504.67798 Hz/cm



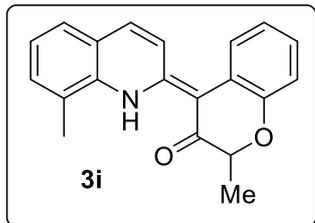


16.278

7.8133  
7.7894  
7.7195  
7.6959  
7.4698  
7.4550  
7.4363  
7.2478  
7.2400  
7.2291  
7.2202  
7.2099  
7.0710  
7.0520  
7.0480  
7.0397  
7.0372  
7.0336  
7.0226  
7.0158  
7.0076  
7.0042  
6.9970  
6.9903  
6.9823  
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4.5808  
4.5640  
4.5467  
2.6705  
1.5252  
1.5081  
0.0507

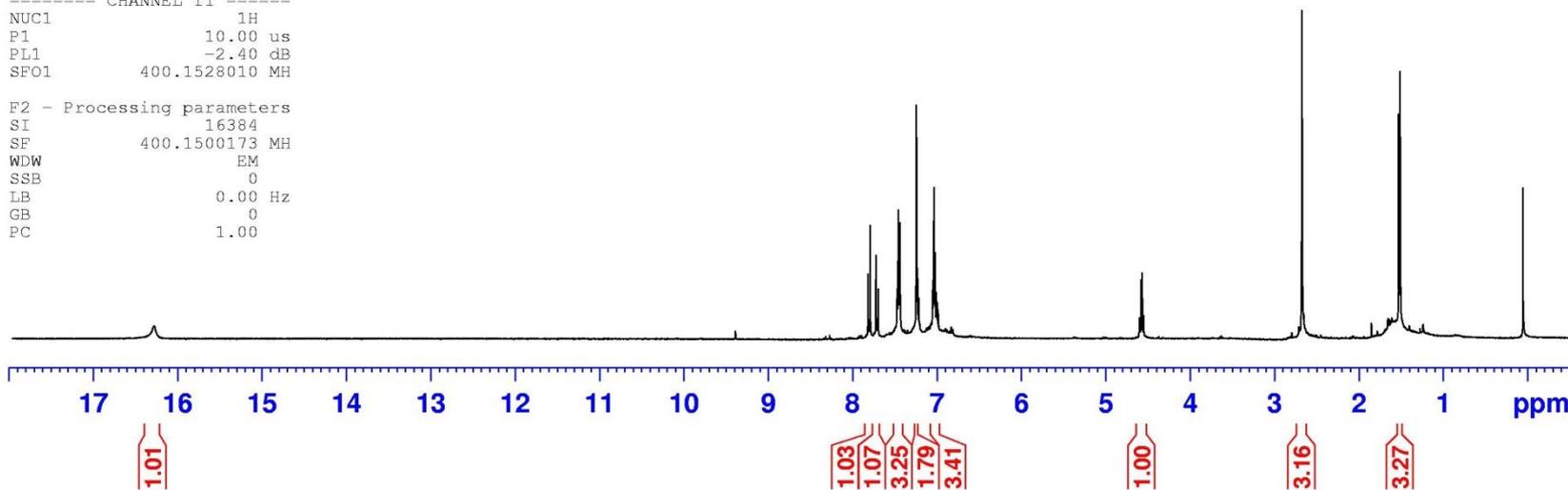
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NAME 20171115  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameter  
Date\_ 20171116  
Time 10.43  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 33  
DS 0  
SWH 8802.817 Hz  
FIDRES 0.268641 Hz  
AQ 1.8612725 se  
RG 512  
DW 56.800 us  
DE 6.00 us  
TE 300.0 K  
D1 2.00000000 se  
TD0 1



==== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 us  
PL1 -2.40 dB  
SFO1 400.1528010 MH

F2 - Processing parameters  
SI 16384  
SF 400.1500173 MH  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00



Current Data Parameters  
 NAME SMF-5-112A  
 EXPNO 2  
 PROCNO 1

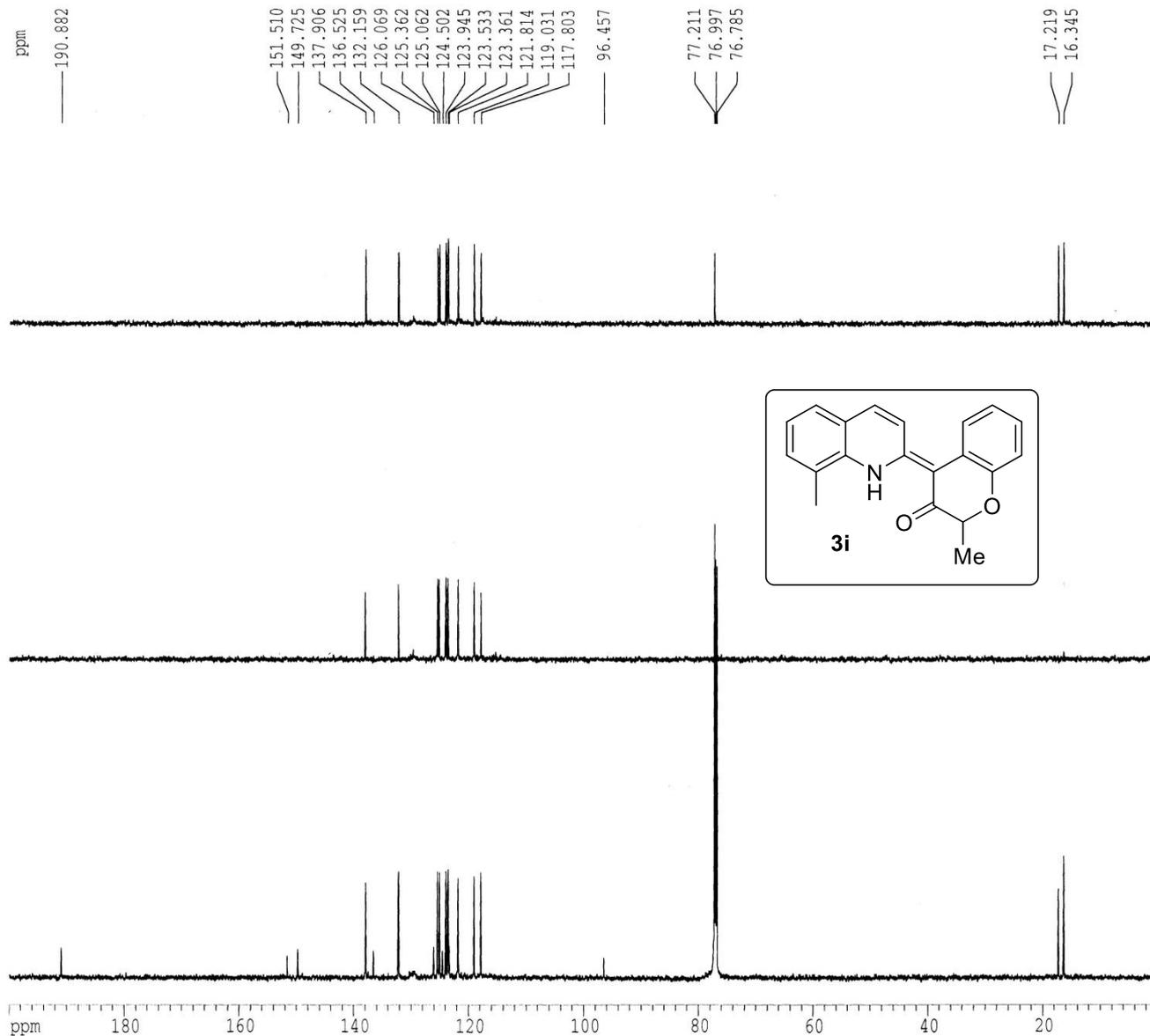
F2 - Acquisition Parameters  
 Date\_ 20171117  
 Time 6.32  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 2193  
 DS 0  
 SSB 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DM 11.100 usec  
 DE 6.50 usec  
 TE 300.8 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0.00000000 sec  
 MCHRX 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.4426598 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 5.50 dB  
 PL13 9.00 dB  
 SFO2 598.3029915 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4426598 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 8.00 cm  
 F1P 200.000 ppm  
 F1 30098.53 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 10.00000 ppm/cm  
 HZCM 1504.42651 Hz/cm



```

Current Data Parameters
NAME      SBM-5-150
EXPNO    1
PROCNO   1

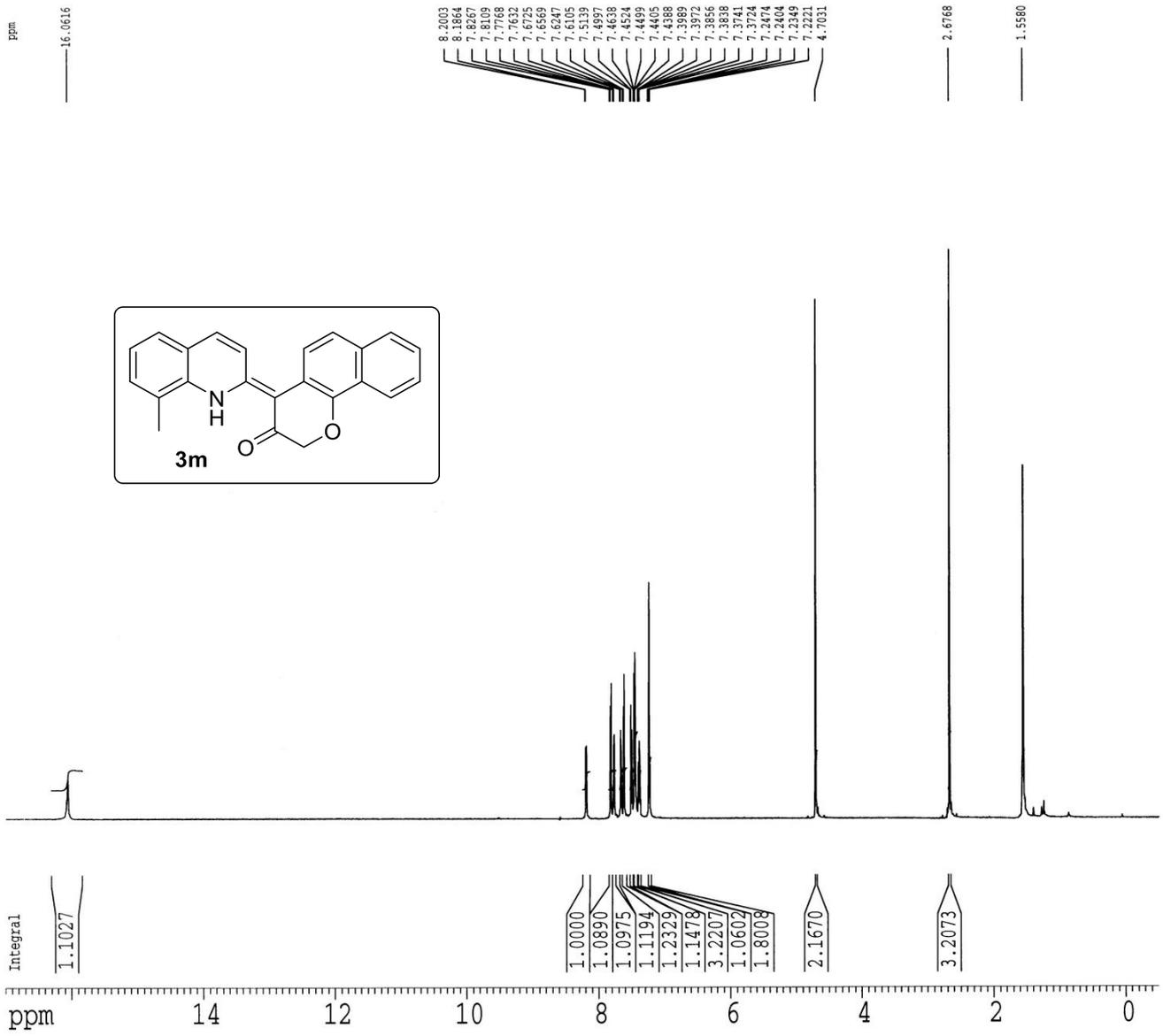
F2 - Acquisition Parameters
Date_    20170915
Time     7.33
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        32
DS        0
SWH       12019.210 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG         512
DW         41.600 usec
DE         6.50 usec
TE        300.9 K
D1         2.00000000 sec
MORREST   0.00000000 sec
MORMRK    0.01500000 sec

***** CHANNEL f1 *****
NUC1      1H
P1        15.00 usec
PL1       -1.00 dB
SFO1      598.4051663 MHz

F2 - Processing parameters
SI         32768
SF         598.4000247 MHz
WDW        no
SSB         0
LB          0.00 Hz
GB          0
PC          1.00

ID NMR plot parameters
CH         30.00 cm
CY         10.00 cm
F1F        17.000 ppm
F1         10172.80 Hz
F2F         0.500 ppm
F2         299.20 Hz
F2F2CM     0.87500 ppm/cm
H2H2C      523.60004 Hz/cm

```



Current Data Parameters  
 NAME SB0-5-150  
 EXPNO 2  
 PROCNO 1

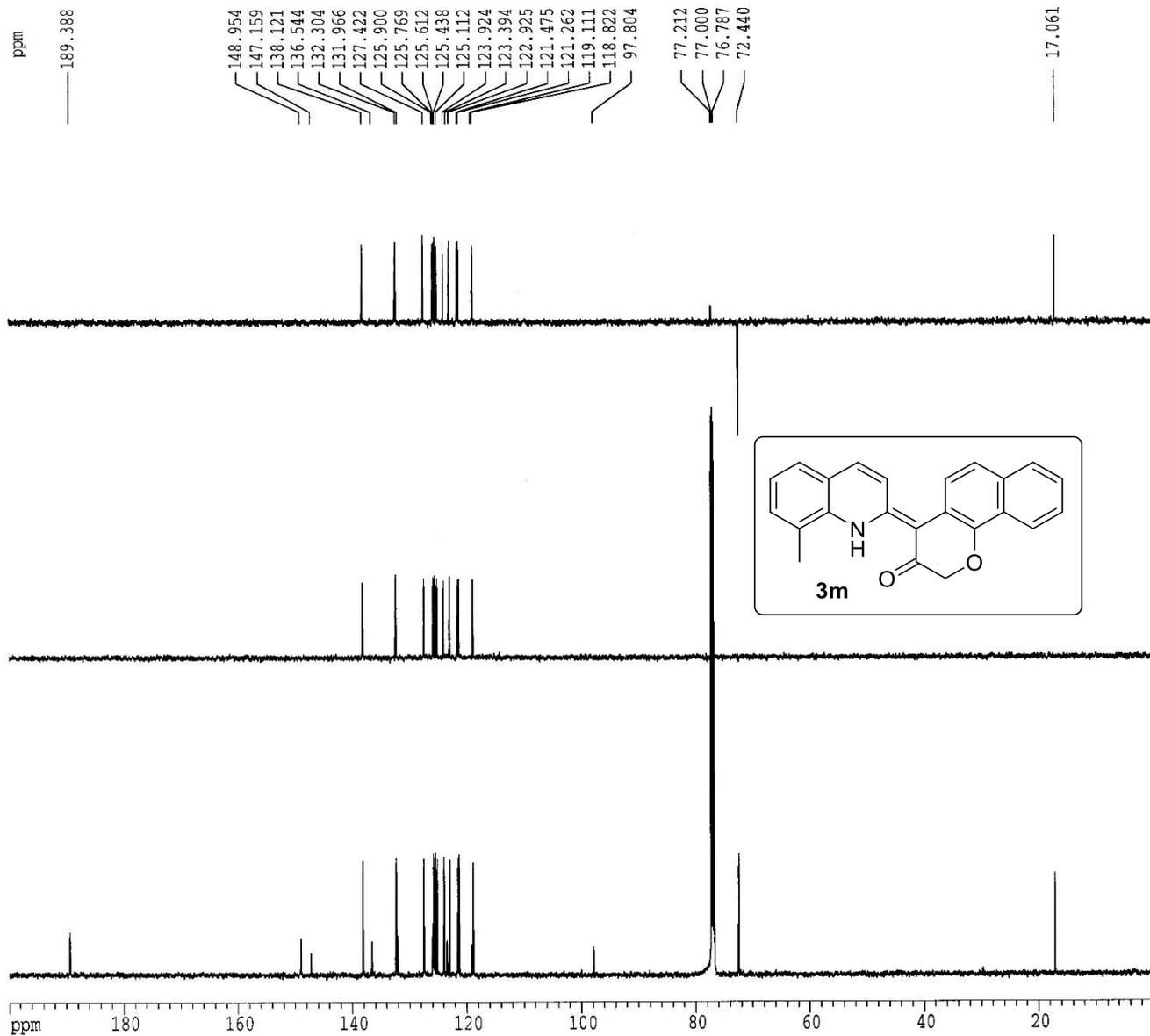
F2 - Acquisition Parameters  
 Date\_ 20170915  
 Time 8.04  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 2307  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 301.1 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 INCRST 0.00000000 sec  
 MCYCLE 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.4828468 MHz

===== CHANNEL f2 =====  
 CPDPRG2 walzr16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 5.50 dB  
 PL13 9.00 dB  
 SFO2 598.4029920 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4678028 MHz  
 WDM EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CA 20.00 cm  
 CB 10.00 cm  
 F1P 200.000 ppm  
 F1 30093.56 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 TEMPC 10.00000 ppm/cm  
 HSCN 1504.67798 Hz/cm



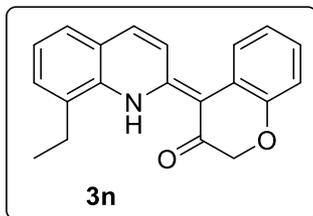


16.292.

7.8343  
7.8106  
7.6941  
7.6705  
7.4793  
7.4709  
7.4634  
7.4455  
7.2960  
7.2770  
7.2578  
7.2400  
7.0394  
7.0331  
7.0089  
7.0034  
6.9985  
4.5313  
3.0712  
3.0525  
3.0338  
3.0151  
1.6076  
1.4645  
1.4458  
1.4271

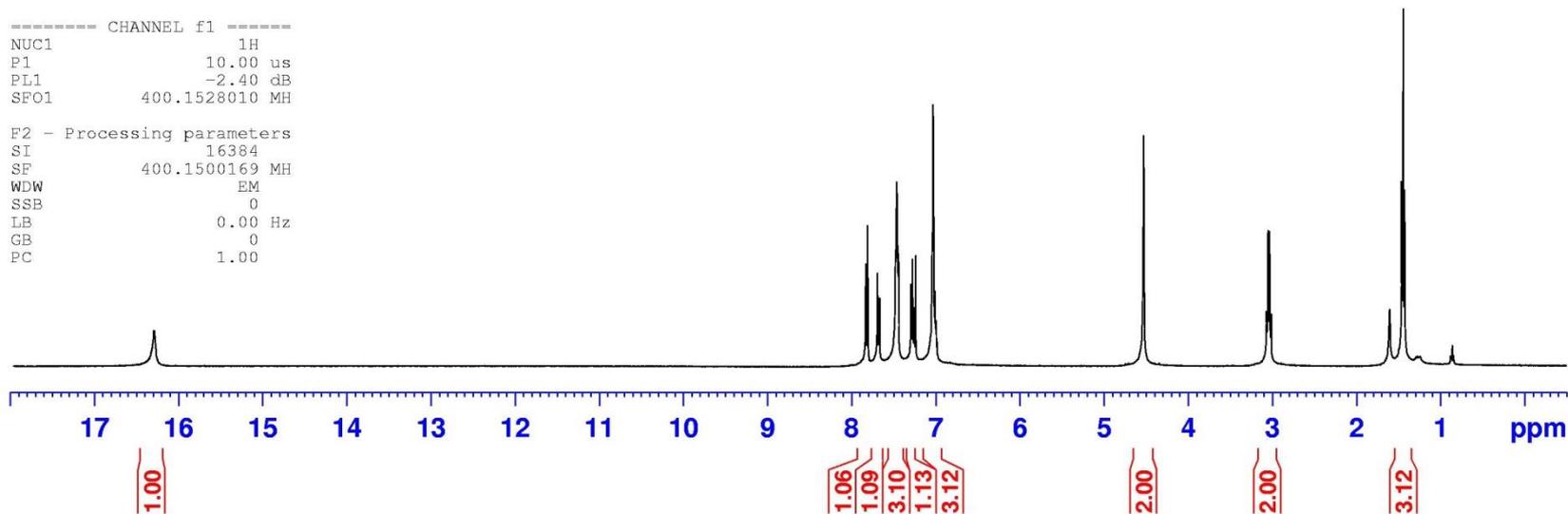
Current Data Parameters  
NAME 20171023  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameter  
Date\_ 20171023  
Time 13.43  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 26  
DS 0  
SWH 8802.817 Hz  
FIDRES 0.268641 Hz  
AQ 1.8612725 se  
RG 362  
DW 56.800 us  
DE 6.00 us  
TE 300.0 K  
D1 2.00000000 se  
TD0 1



----- CHANNEL f1 -----  
NUC1 1H  
P1 10.00 us  
PL1 -2.40 dB  
SFO1 400.1528010 MH

F2 - Processing parameters  
SI 16384  
SF 400.1500169 MH  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00





188.658

152.746  
149.415  
138.265  
135.738  
131.740  
130.249  
125.385  
124.984  
124.566  
124.182  
123.628  
123.448  
121.982  
118.617  
117.236

97.133

77.310  
76.992  
76.675  
72.096

23.717

12.983

Current Data Parameters  
NAME 20171023  
EXPNO 2  
PROCNO 1

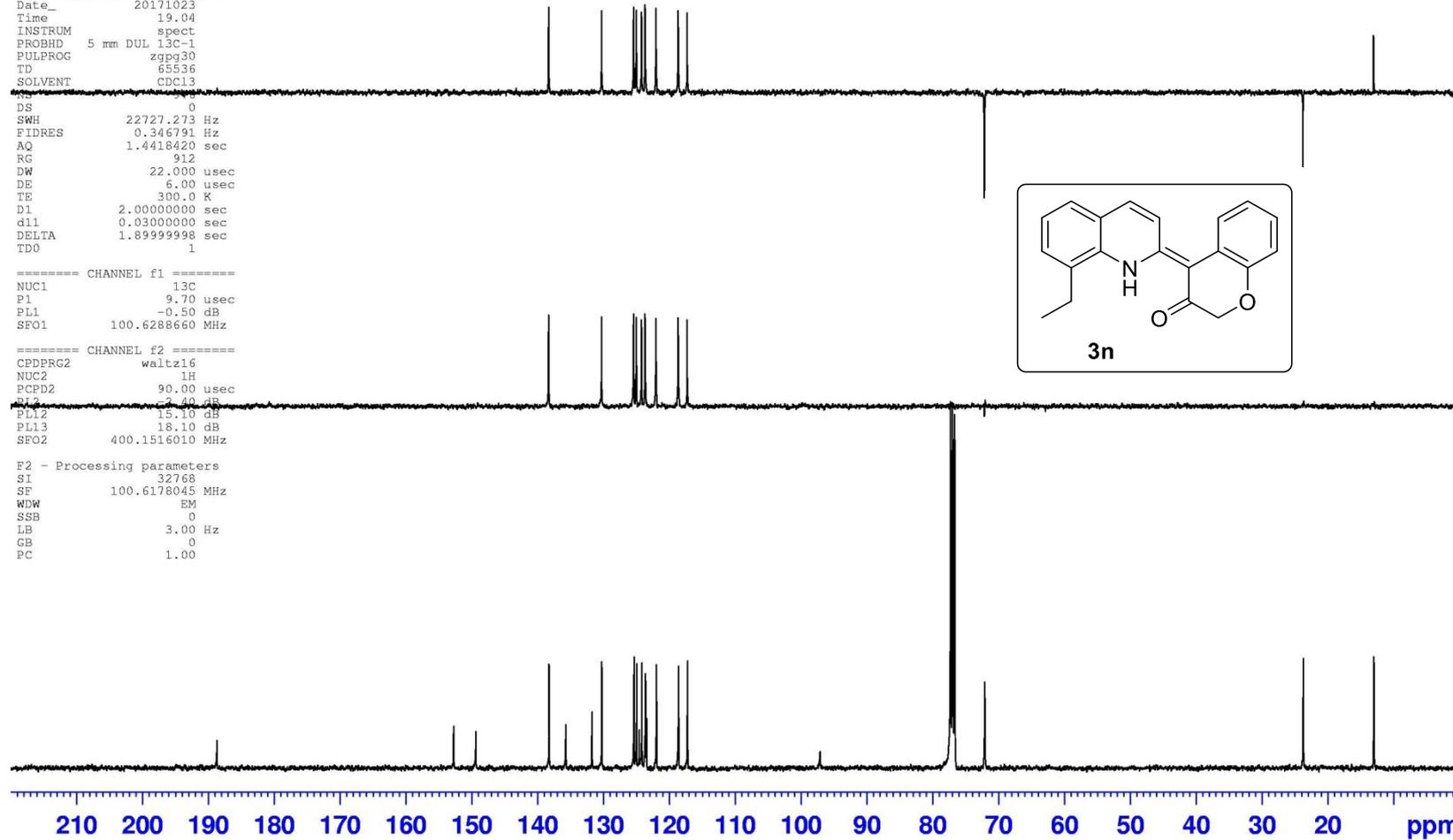
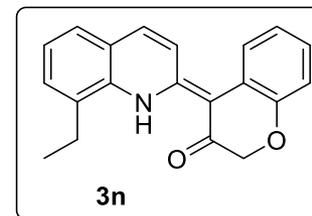
F2 - Acquisition Parameters  
Date\_ 20171023  
Time 19.04  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3

DS 0  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
RG 912  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

==== CHANNEL f2 =====  
CDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.40 dB  
PL12 18.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6178045 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



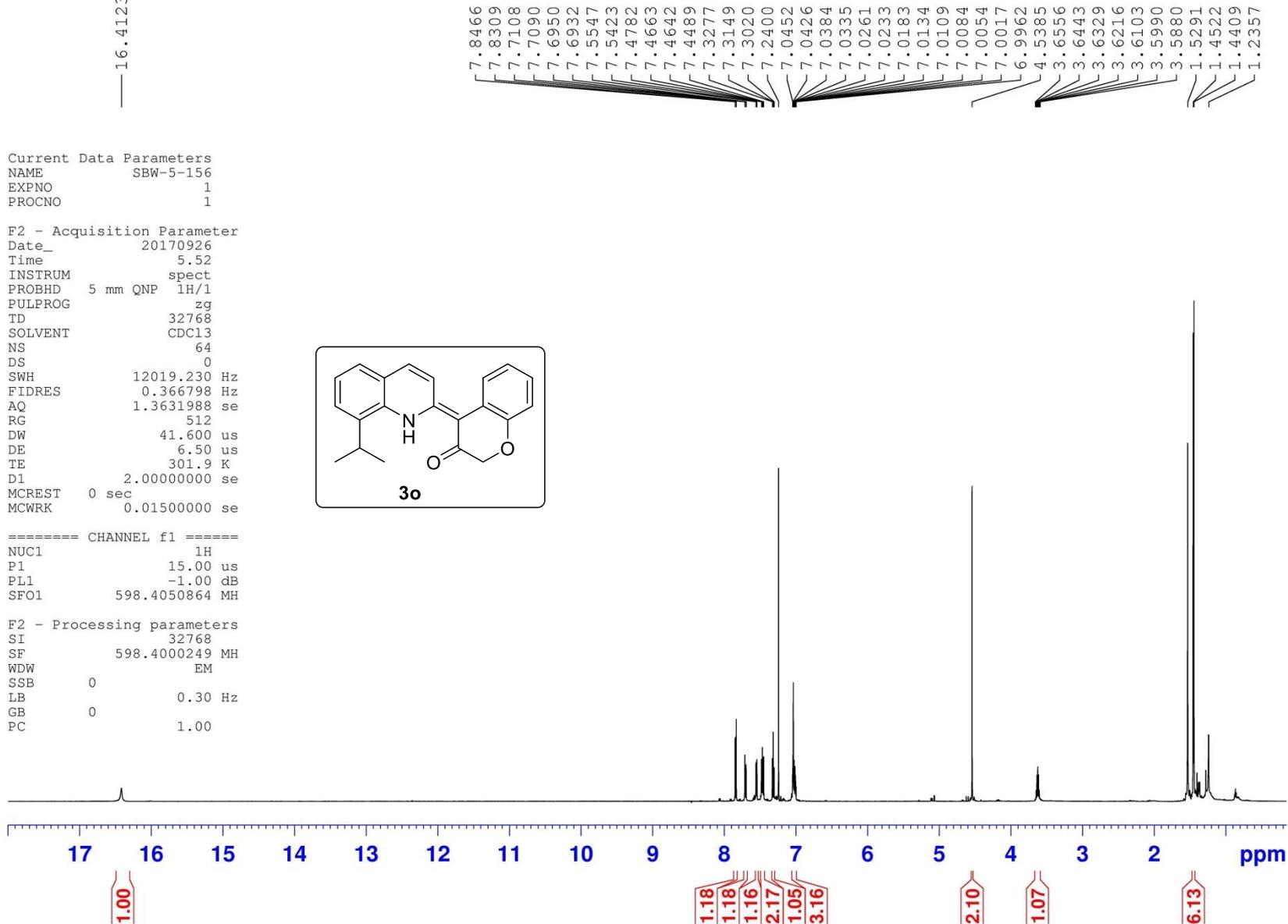
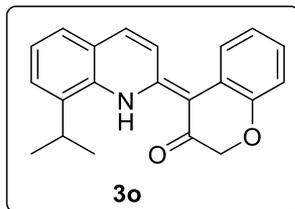
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Current Data Parameters  
NAME SBW-5-156  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameter  
Date\_ 20170926  
Time 5.52  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 64  
DS 0  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 se  
RG 512  
DW 41.600 us  
DE 6.50 us  
TE 301.9 K  
D1 2.00000000 se  
MCREST 0 sec  
MCWRK 0.01500000 se

==== CHANNEL f1 =====  
NUC1 1H  
P1 15.00 us  
PL1 -1.00 dB  
SFO1 598.4050864 MH

F2 - Processing parameters  
SI 32768  
SF 598.4000249 MH  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
 NAME SBN-5-156  
 EXPNO 2  
 PROCNO 1

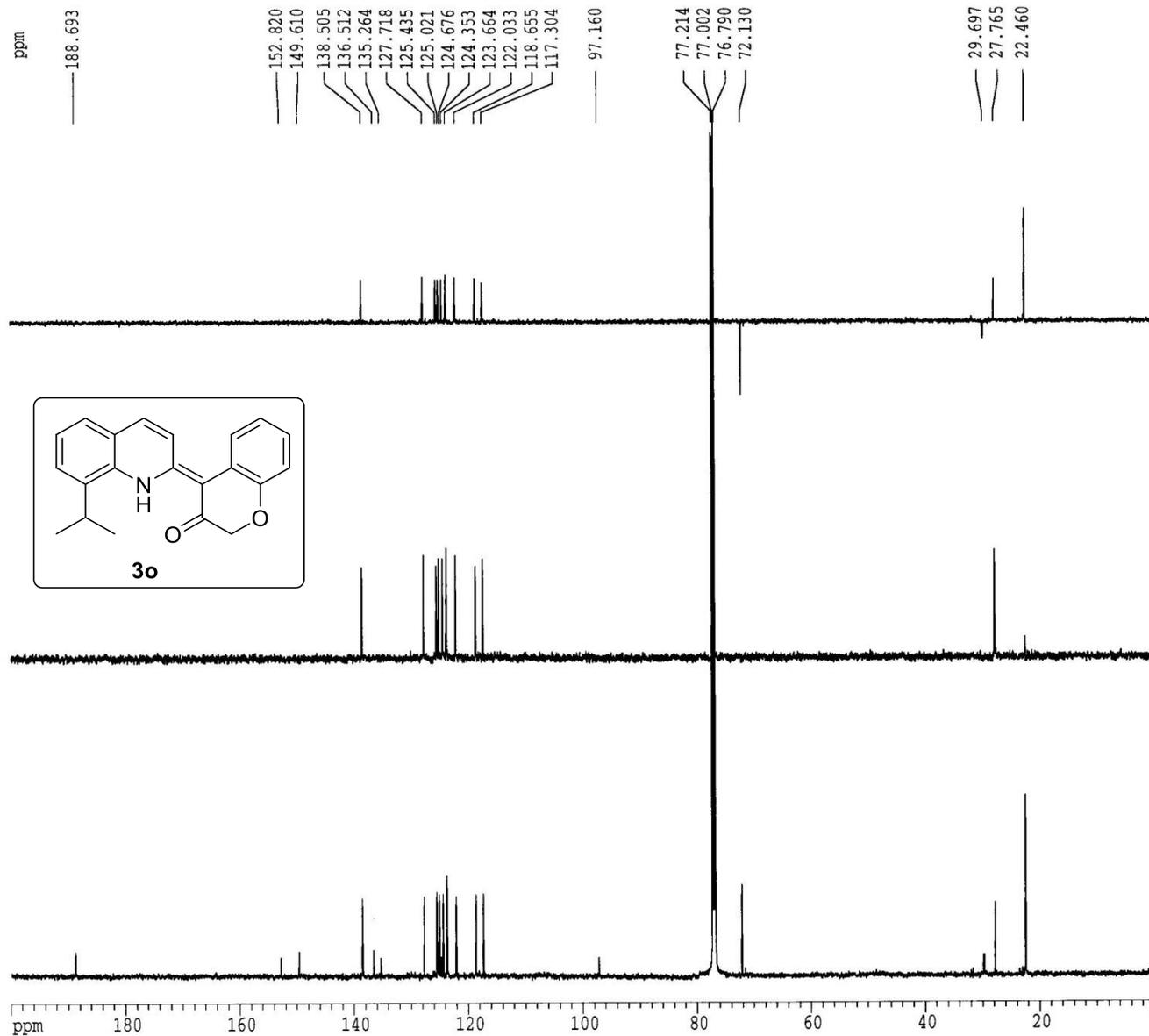
F2 - Acquisition Parameters  
 Date\_ 20170925  
 Time 14.57  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDC13  
 NS 6144  
 DS 0  
 FWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 A\_ 0.3637748 sec  
 RG 4096  
 IFT 11.100 usec  
 DE 6.50 usec  
 TE 301.9 K  
 OL 3.5000000 sec  
 H11 0.0300000 sec  
 DELTA 3.4000010 sec  
 MCREST 0.0000000 sec  
 MARRA 0.0150000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.4828468 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 5.50 dB  
 PL13 9.00 dB  
 SFO2 598.4029920 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4678007 MHz  
 EQN EM  
 SNR 0  
 LP 3.00 Hz  
 GB 0  
 DC 1.00

ED NMR plot parameters  
 CA 20.00 cm  
 CY 15.00 cm  
 F1P 200.000 ppm  
 F1 30093.56 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 FPMCM 10.00000 ppm/cm  
 HECM 1504.67798 Hz/cm



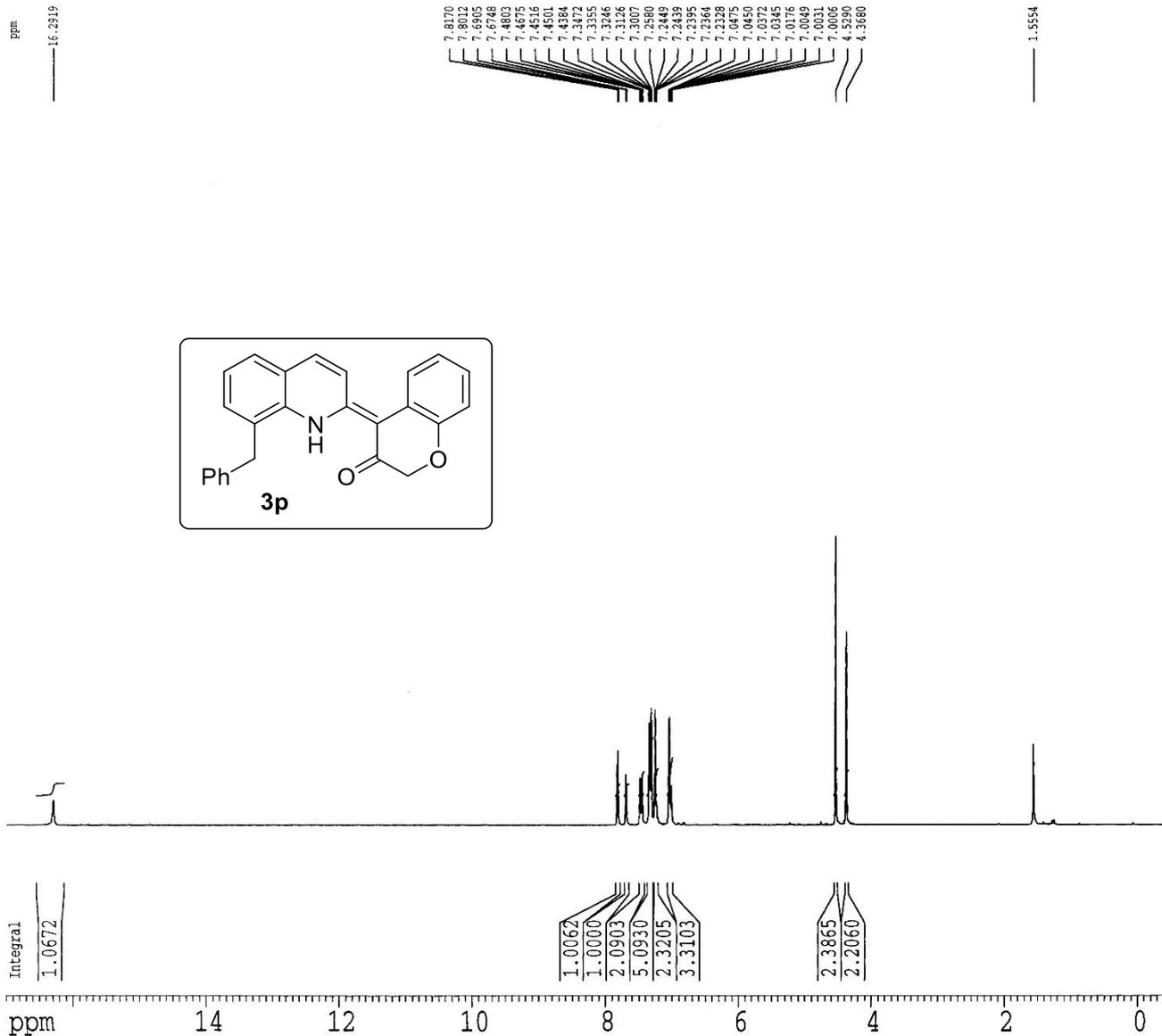
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 NAME JEU-5-105  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170926  
 Time 13.29  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zg  
 PC 32768  
 SOLVENT C6D6  
 NS 32  
 DS 6  
 SWH 12019.330 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631986 sec  
 RG 512  
 DN 41.630 usec  
 DE 6.50 usec  
 TE 302.6 K  
 D1 2.0600000 sec  
 DELT 0.0000000 sec  
 DELT2 0.0150000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 15.00 usec  
 PL1 -1.00 dB  
 SFO1 500.1364262 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1364262 MHz  
 MW no  
 SUB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 X 50.00 cm  
 Y 5.00 cm  
 F1P 17.000 ppm  
 F1 10173.30 Hz  
 F1P 0.500 ppm  
 SF 500.1364262 MHz  
 SFMCX 0.87500 ppm/cm  
 FZCM 523.60004 Hz/cm



Current Data Parameters  
 NAME SSW-5-165  
 EXPNO 2  
 PROCNO 1

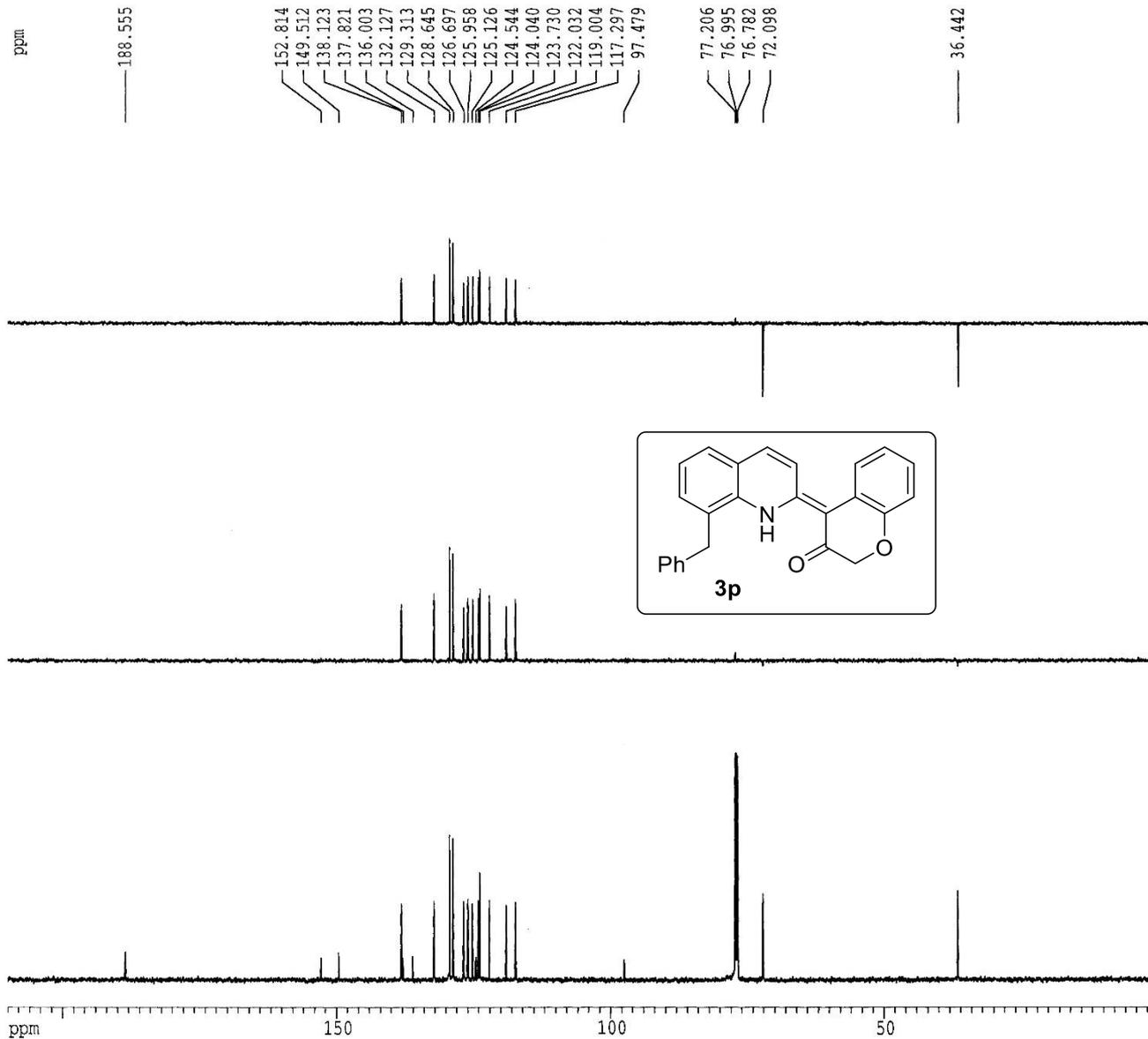
F2 - Acquisition Parameters  
 Date\_ 20170926  
 Time 11.25  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 799  
 DS 0  
 SFO 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 302.4 K  
 D1 3.5000000 sec  
 a11 0.0300000 sec  
 DELTA 3.4000010 sec  
 MCREST 0.0000000 sec  
 MCVRK 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.4828468 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 5.50 dB  
 PL13 9.00 dB  
 SFO2 598.4029920 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4678090 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 FC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 4.00 cm  
 FLP 210.000 ppm  
 F1 31598.24 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 10.50000 ppm/cm  
 HZCM 1579.91199 Hz/cm





Current Data Parameters  
NAME 24082017  
EXPNO 1  
PROCNO 1

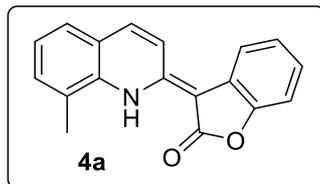
F2 - Acquisition Parameters  
Date\_ 20170824  
Time 23.05  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
PD 32768  
SOLVENT CDCl3  
NS 26  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 4  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
D0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500164 MHz  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

PS-D-033-A-2

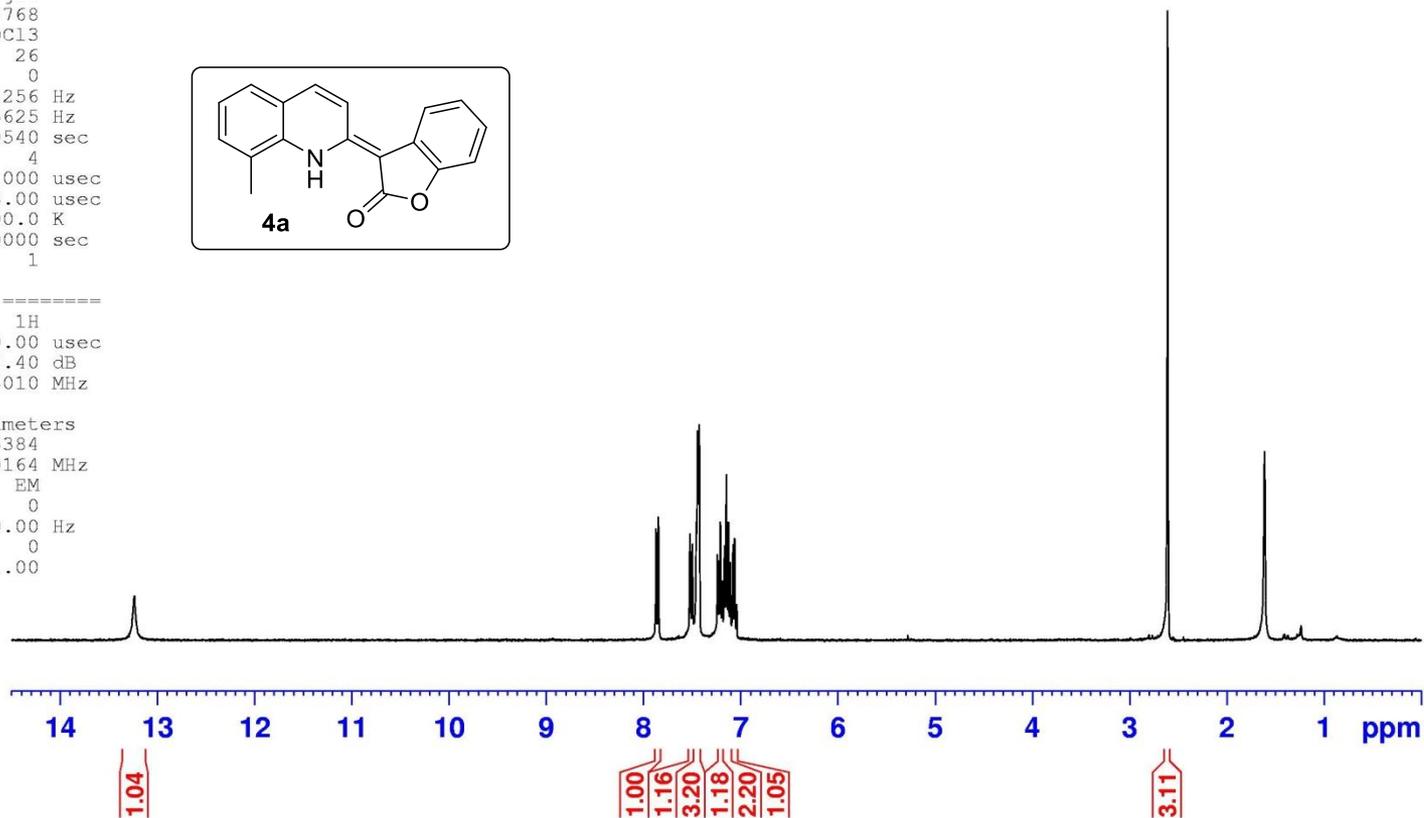
13.233

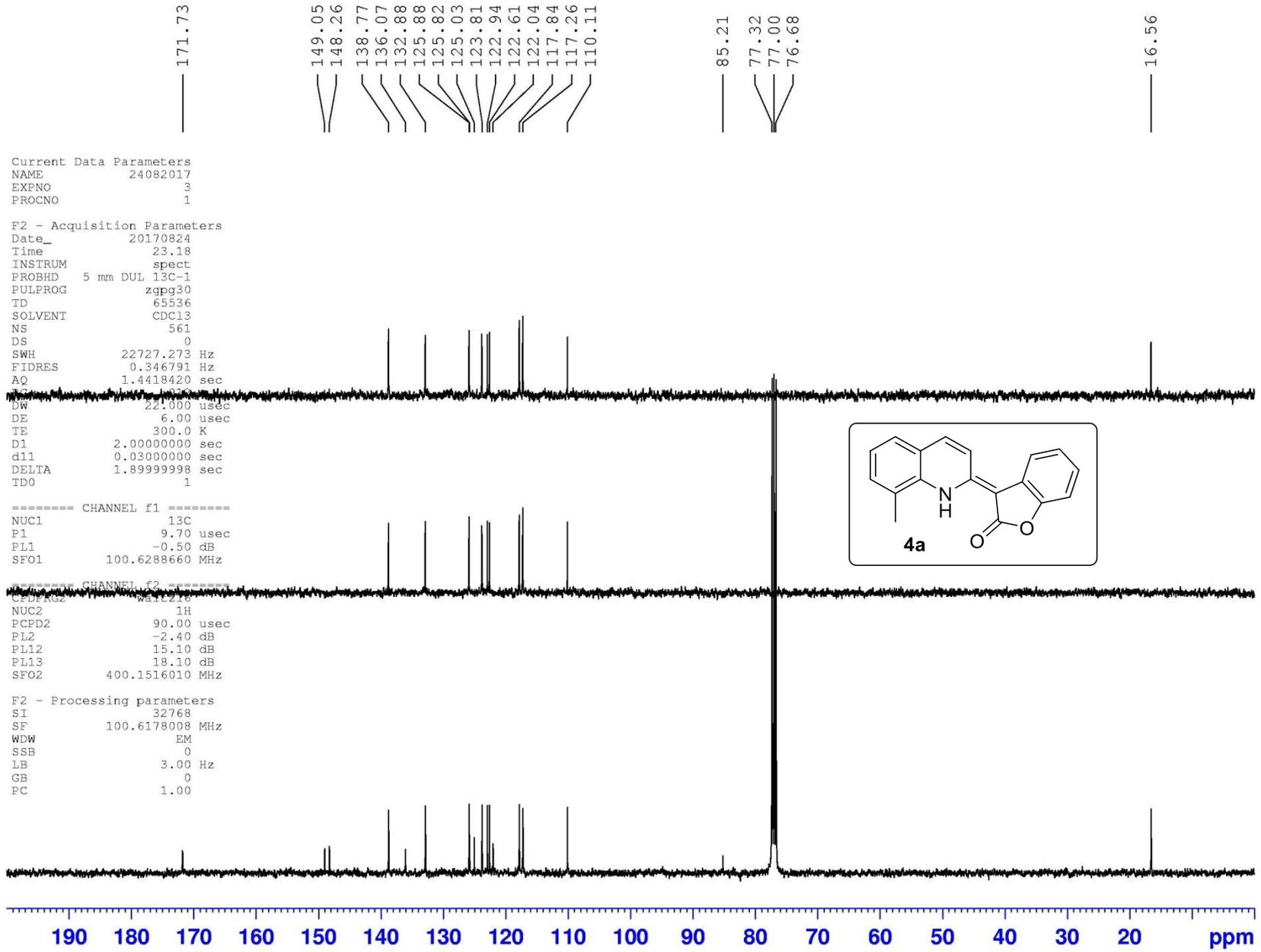


7.870  
7.847  
7.522  
7.498  
7.456  
7.445  
7.427  
7.243  
7.241  
7.228  
7.208  
7.189  
7.166  
7.146  
7.126  
7.107  
7.079  
7.060  
7.041

2.607

1.611





Current Data Parameters  
 NAME 24082017  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170824  
 Time 23.18  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 561  
 DS 0  
 SWH 22727.273 Hz  
 FIDRES 0.346791 Hz  
 AQ 1.4418420 sec  
 EQ 3.0000000 sec  
 DW 221.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.70 usec  
 PL1 -0.50 dB  
 SFO1 100.6288660 MHz

===== CHANNEL f2 =====  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -2.40 dB  
 PL12 15.10 dB  
 PL13 18.10 dB  
 SFO2 400.1516010 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6178008 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
NAME 09092017  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170909  
Time 22.59  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
ID 32768  
SOLVENT CDCl3  
NS 31  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 4  
OW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
D0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

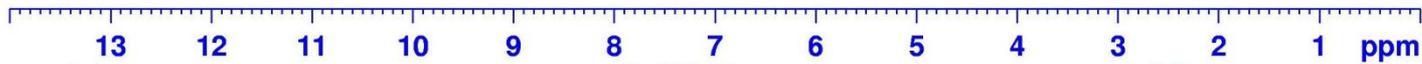
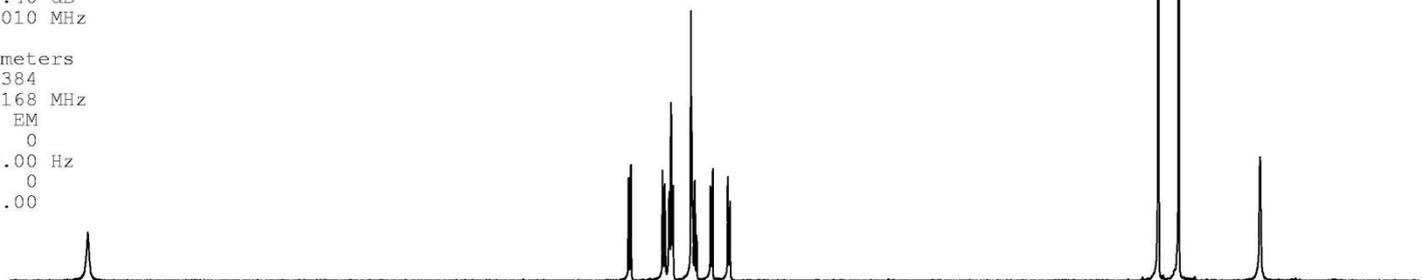
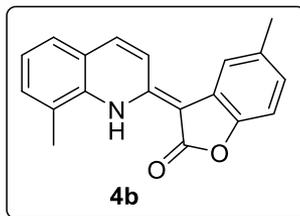
F2 - Processing parameters  
SI 16384  
SF 400.1500168 MHz  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

13.223

7.860  
7.855  
7.837  
7.832  
7.520  
7.497  
7.456  
7.436  
7.418  
7.244  
7.239  
7.234  
7.224  
7.218  
7.200  
7.186  
7.048  
7.043  
7.028  
7.023  
6.873  
6.853

2.597  
2.394

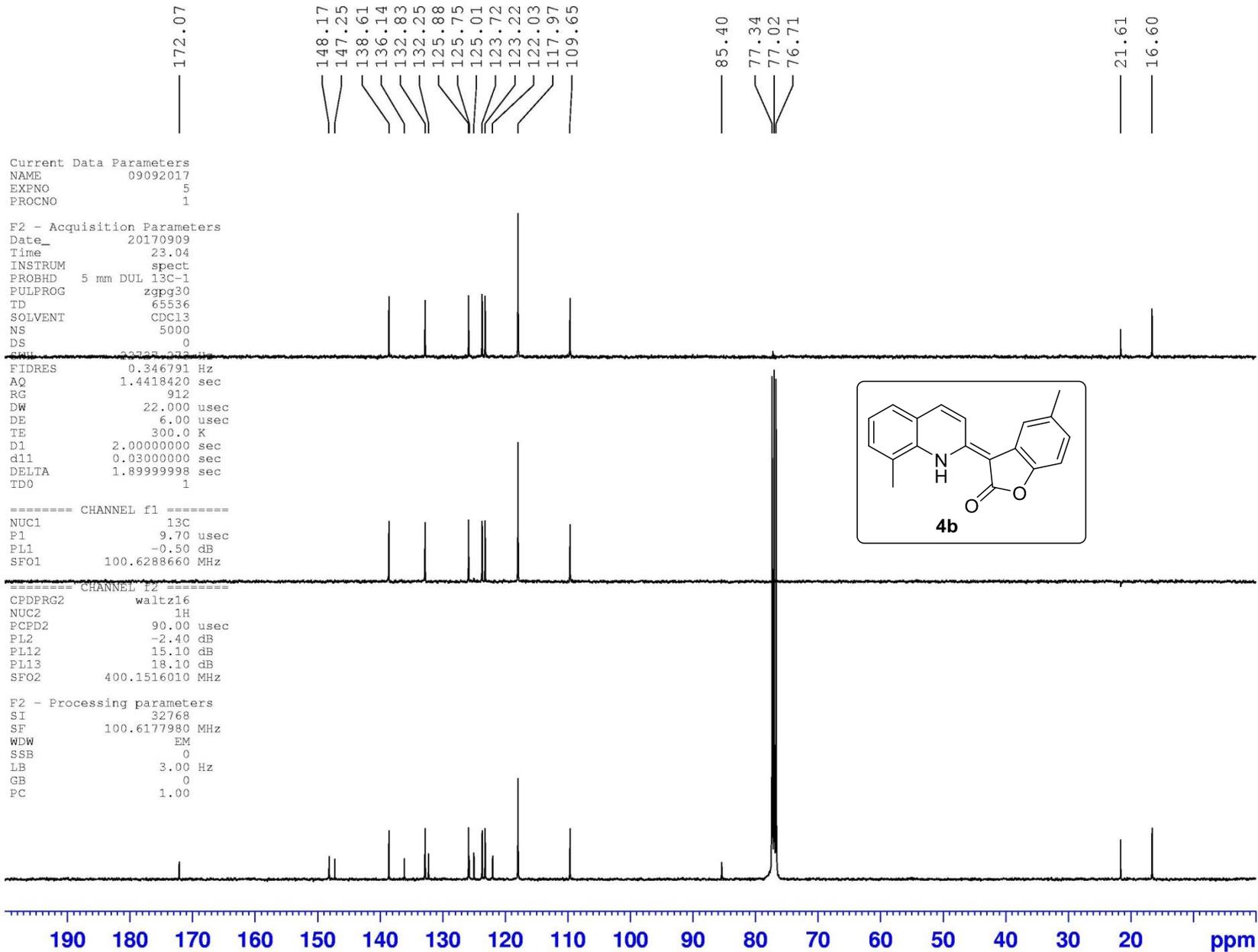
1.587



1.07

1.00  
1.11  
2.09  
2.29  
1.04  
1.06

3.14  
3.13



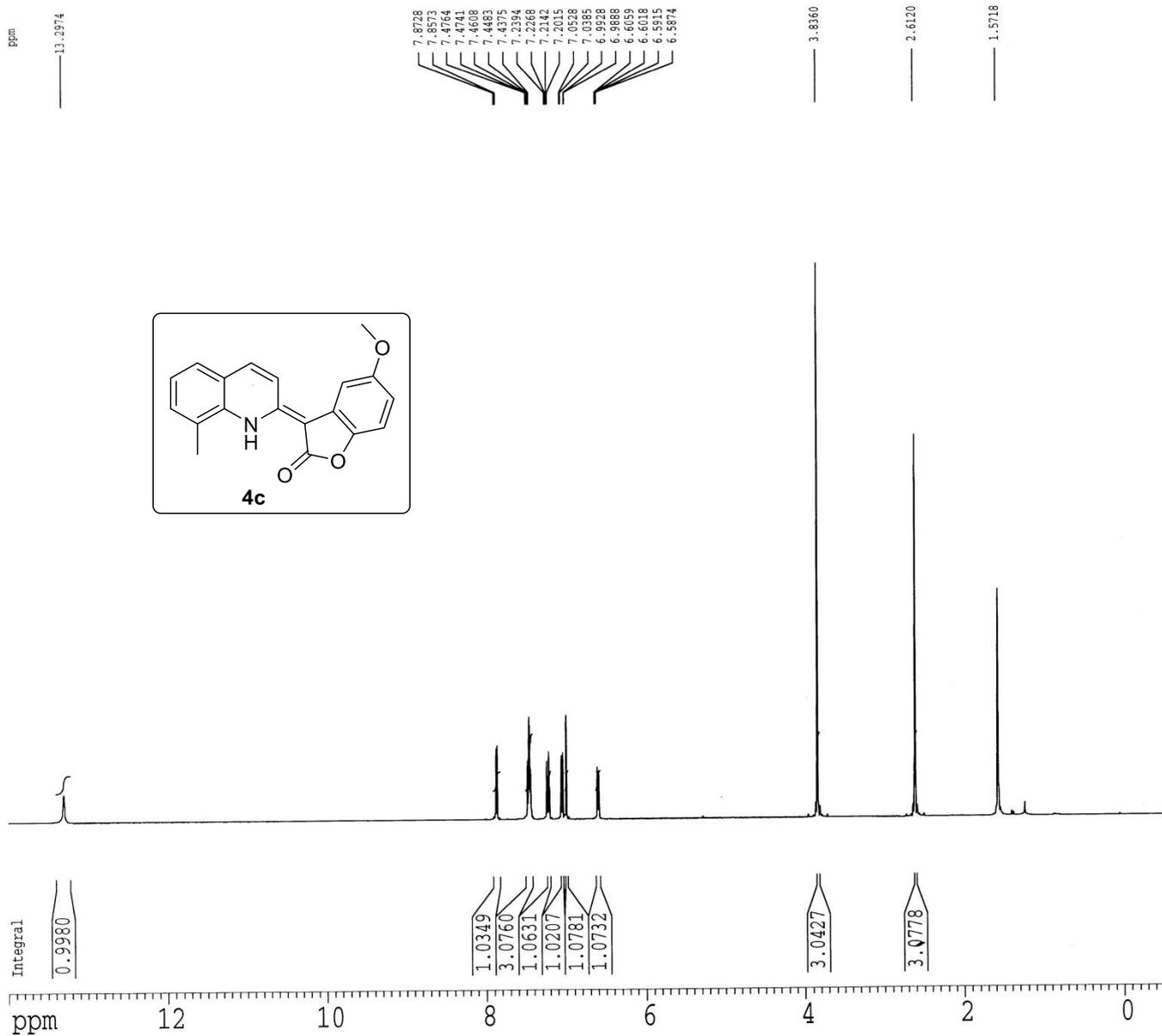
Current Data Parameters  
 NAME PS-D-045  
 EXFNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 DATE\_ 20170914  
 TIME 11.02  
 INSTRUM spect  
 PROBRHD 5 mm QNP 1H/1  
 PULPROG zg  
 DS 12768  
 SOLVENT CDCl3  
 NS 32  
 DS 0  
 SFR 10775.862 Hz  
 FIDRES 0.138853 Hz  
 AQ 1.5204852 sec  
 RG 512  
 DU 46.400 usec  
 DE 8.50 usec  
 TE 300.9 K  
 TI 2.00000000 sec  
 MPREST 0.00000000 sec  
 MWPK 0.01500000 sec

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 15.00 usec  
 PL1 -1.00 dB  
 SFO1 500.14035904 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.14000247 MHz  
 DS 0  
 SFR 0 Hz  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

F2 NMR plot parameters  
 SI 30.00 cm  
 SF 10.00 cm  
 FID 14.000 ppm  
 FI 8377.60 Hz  
 F2 0.500 ppm  
 F3 -0.942 Hz  
 F4 0.7500 ppm/cm  
 SFO1 433.94003 Hz/cm



Current Data Parameters  
 NAME PS-D-045  
 EXPNO 2  
 PROCNO 1

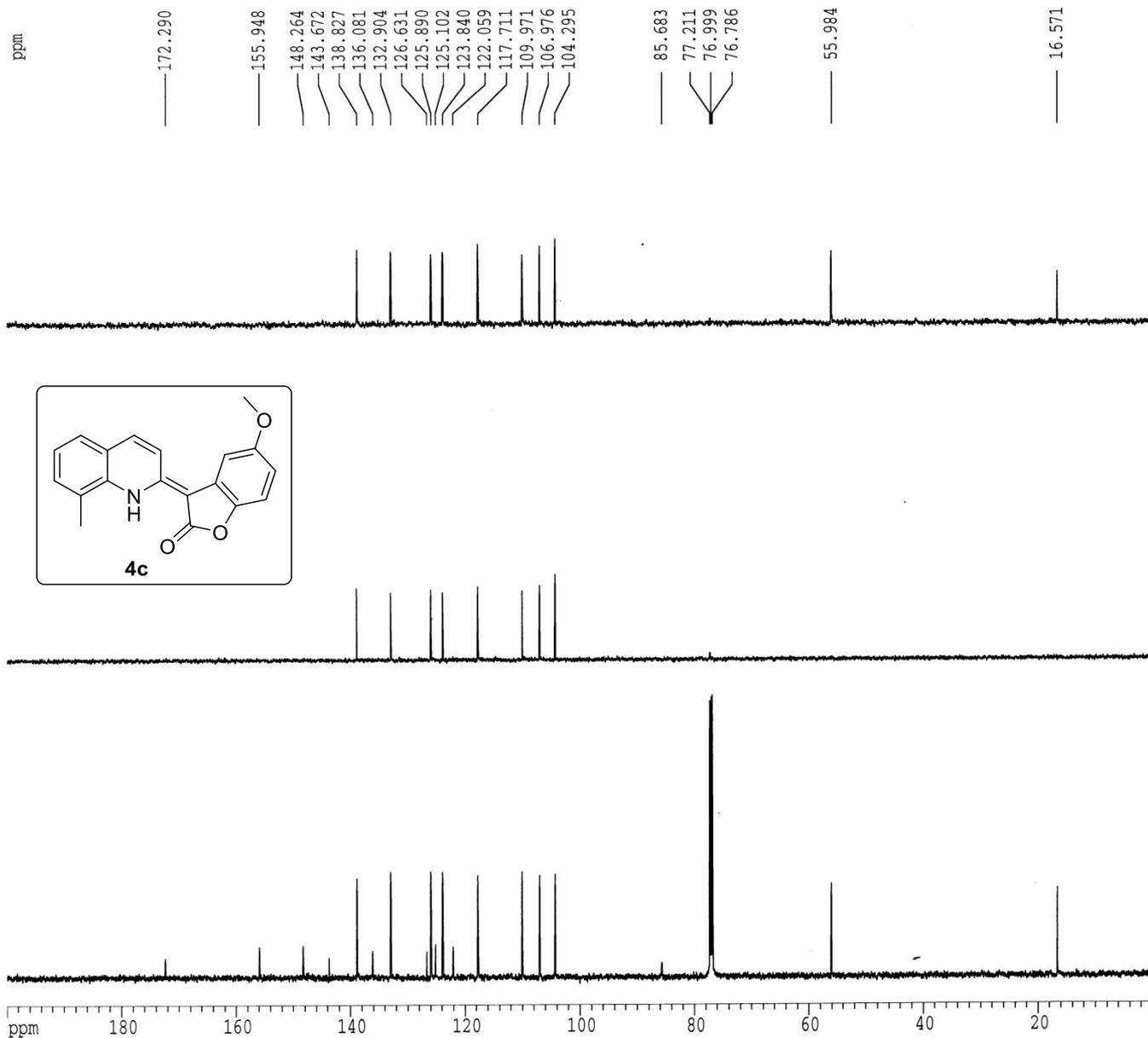
F2 - Acquisition Parameters  
 Date\_ 20170914  
 Time 11.22  
 INSTRUM spect  
 FREQID 5 mm QNP 1H/1  
 PULPROG zgpg  
 ID 32768  
 SOLVENT CDCl3  
 NS 500  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DQ 11.100 usec  
 DE 6.50 usec  
 TE 301.1 K  
 D1 3.5000000 sec  
 d11 0.0300000 sec  
 DELTA 3.4000010 sec  
 NOEPRG 0.0000000 sec  
 NOETX 0.0150000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 PC 4.80 usec  
 PL1 0.00 dB  
 PPR1 150.4828468 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PULPR2 92.00 usec  
 PL2 120.00 dB  
 PL12 5.50 dB  
 PL13 9.00 dB  
 PPR2 500.4029920 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4678028 MHz  
 TD 1  
 GB 0  
 LB 3.00 Hz  
 GB 0  
 FQ 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 5.00 cm  
 FIP 200.000 ppm  
 FL 30093.56 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 10.00000 ppm/cm  
 HZCM 1504.67798 Hz/cm





Current Data Parameters  
NAME 05092017  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170906  
Time 0.03  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
ID 32768  
SOLVENT CDC13  
NS 76  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 4  
OW 78.000 usec  
DE 6.00 usec  
FE 300.0 K  
D1 2.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

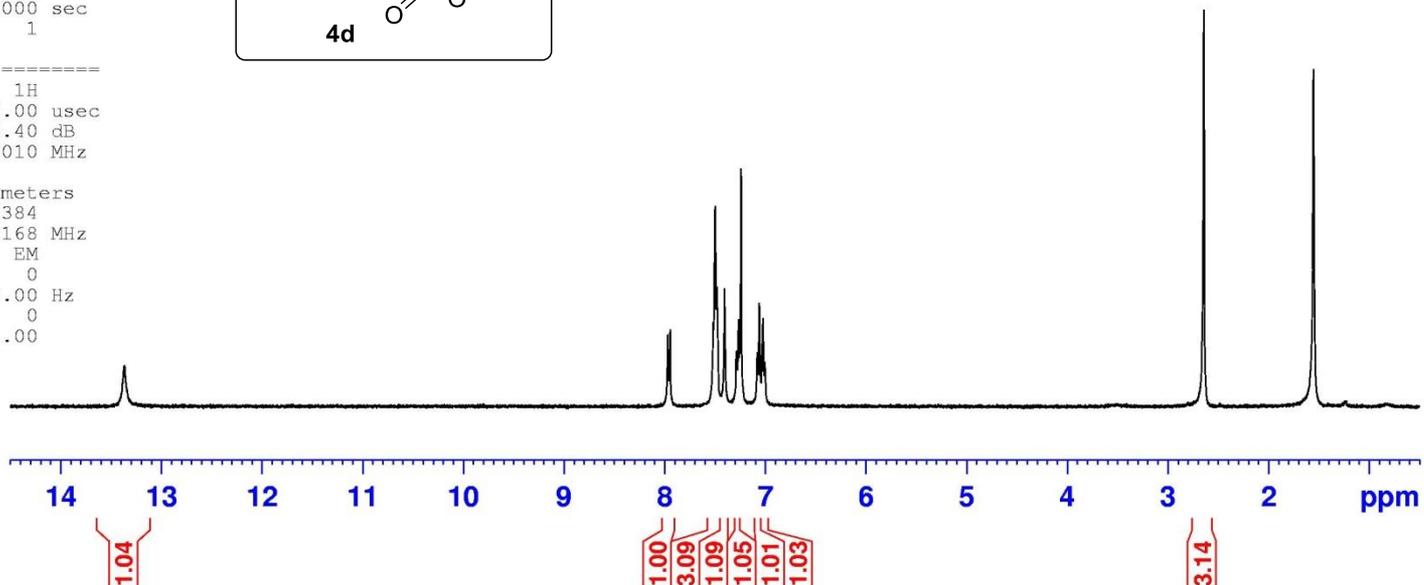
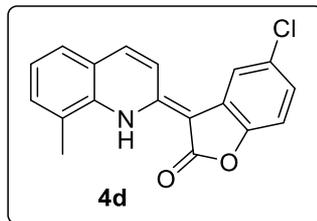
F2 - Processing parameters  
SI 16384  
SF 400.1500168 MHz  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

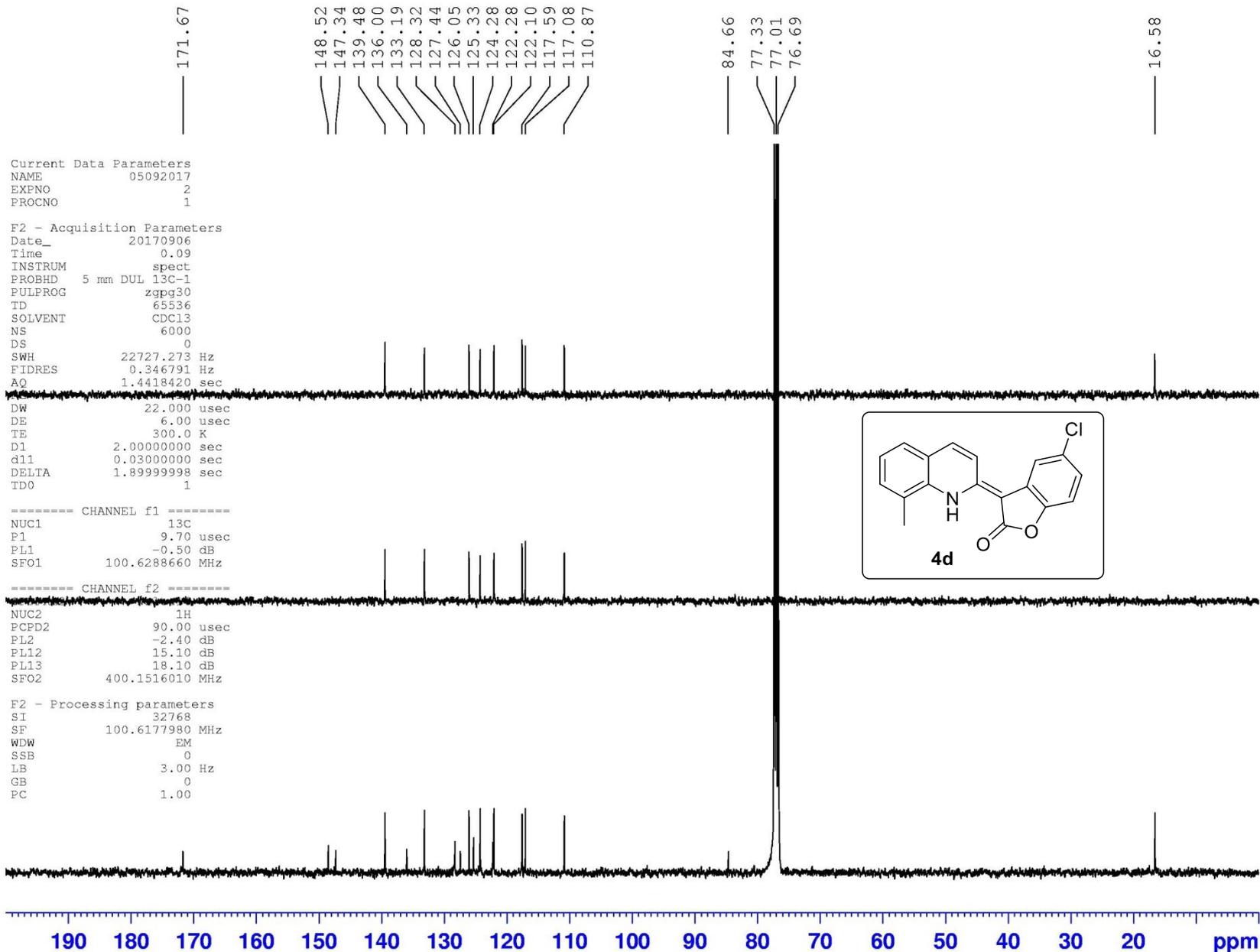
13.364

7.969  
7.946  
7.517  
7.500  
7.483  
7.403  
7.286  
7.268  
7.242  
7.079  
7.058  
7.023  
7.002

2.643

1.553







Current Data Parameters  
NAME 19092017  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170919  
Time 10.33  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 38  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 4  
OW 78.000 usec  
OE 6.00 usec  
FE 300.0 K  
OI 2.00000000 sec  
FO 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

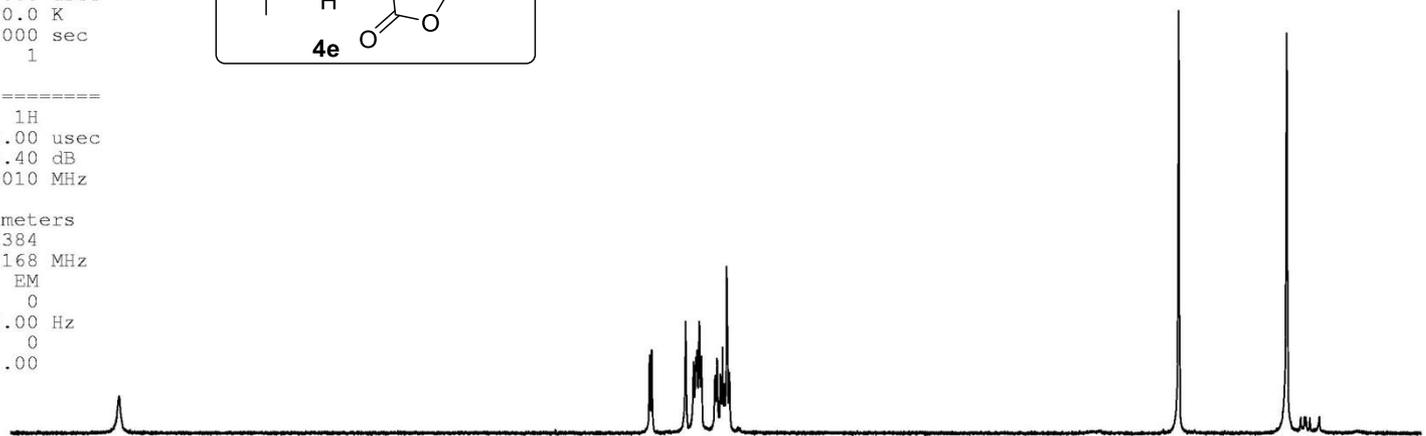
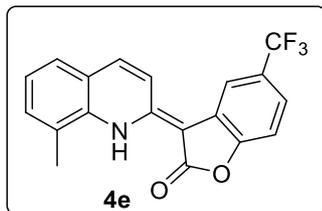
F2 - Processing parameters  
SI 16384  
SF 400.1500168 MHz  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

13.400

8.022  
7.999  
7.657  
7.577  
7.554  
7.541  
7.519  
7.498  
7.358  
7.338  
7.303  
7.284  
7.265  
7.241  
7.234  
7.213

2.657

1.562



1.07

1.00  
1.05  
3.14  
1.09  
1.07  
0.91

3.08

PS-D-048-A



171.499

150.770  
148.702  
139.761  
135.952  
133.293  
126.490  
126.096  
125.519  
125.395  
125.202  
124.435  
123.385  
122.352  
119.752  
117.516  
113.866  
109.924

84.212  
77.314  
76.997  
76.680

16.551

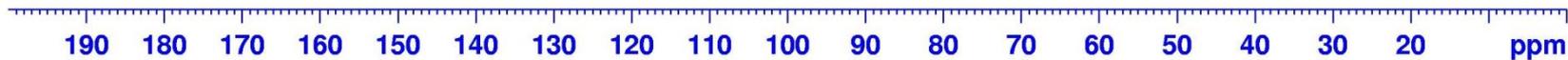
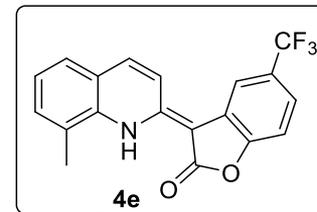
Current Data Parameters  
NAME 21092017  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170921  
Time 0.14  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
NS 6000  
DS 0  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
RG 57  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

----- CHANNEL f1 -----  
NUC1 13C  
P1 9.70 usec  
SFO1 100.6288660 MHz

----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.40 dB  
PL12 15.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6177997 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME 11092017  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170911  
Time 23.10  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
PD 32768  
SOLVENT CDCl3  
NS 20  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 4  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
ED0 1

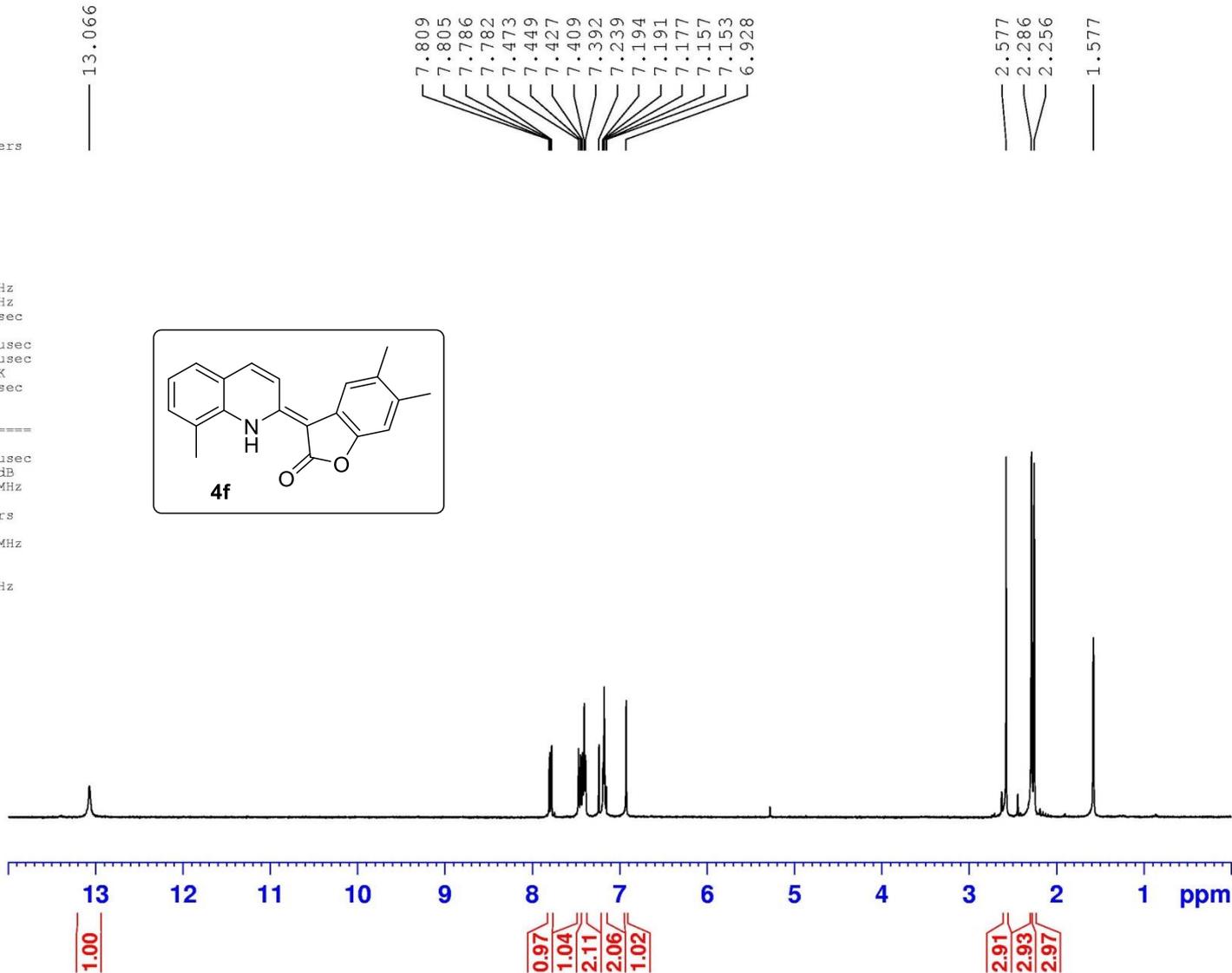
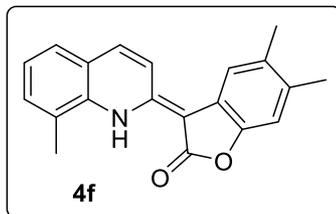
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500168 MHz  
WDW EM  
SSB 0  
LB 0.00 Hz  
SB 0  
GC 1.00

13.066

7.809  
7.805  
7.786  
7.782  
7.473  
7.449  
7.427  
7.409  
7.392  
7.239  
7.194  
7.191  
7.177  
7.157  
7.153  
6.928

2.577  
2.286  
2.256  
1.577





Current Data Parameters  
NAME 11092017  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170911  
Time 23.12

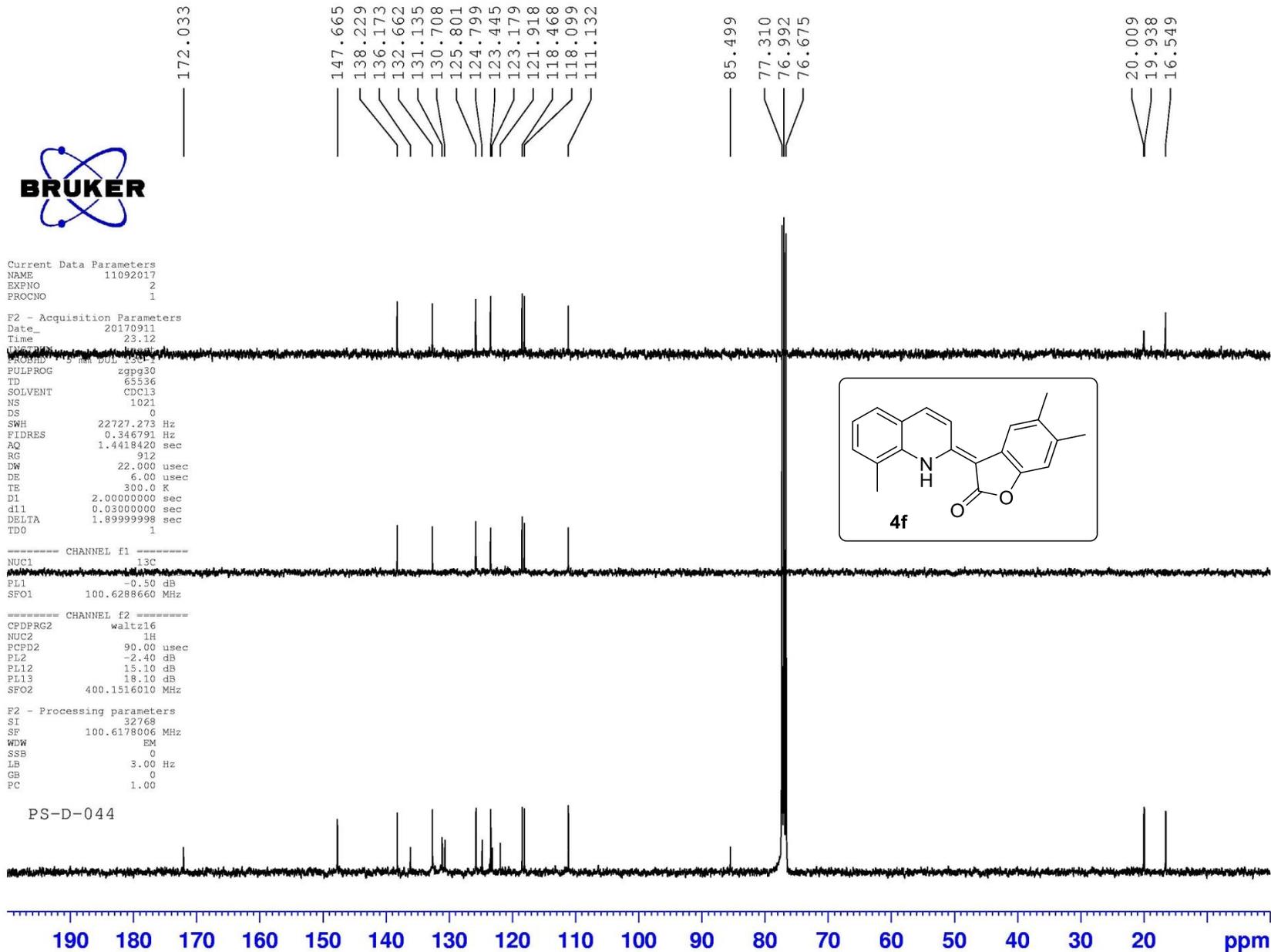
PROBHD 5 mm DUL 1301-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1021  
DS 0  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
RG 912  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999999 sec  
TDC 1

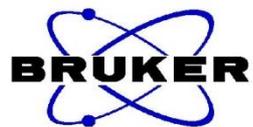
===== CHANNEL f1 =====  
NUC1 13C  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.40 dB  
PL12 15.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6178006 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

PS-D-044





Current Data Parameters  
NAME 19092017  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170919  
Time 0.04  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
ID 32768  
SOLVENT CDCl3  
NS 53  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 4  
OW 78.000 usec  
OE 6.00 usec  
FE 300.0 K  
SI 2.00000000 sec  
EO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

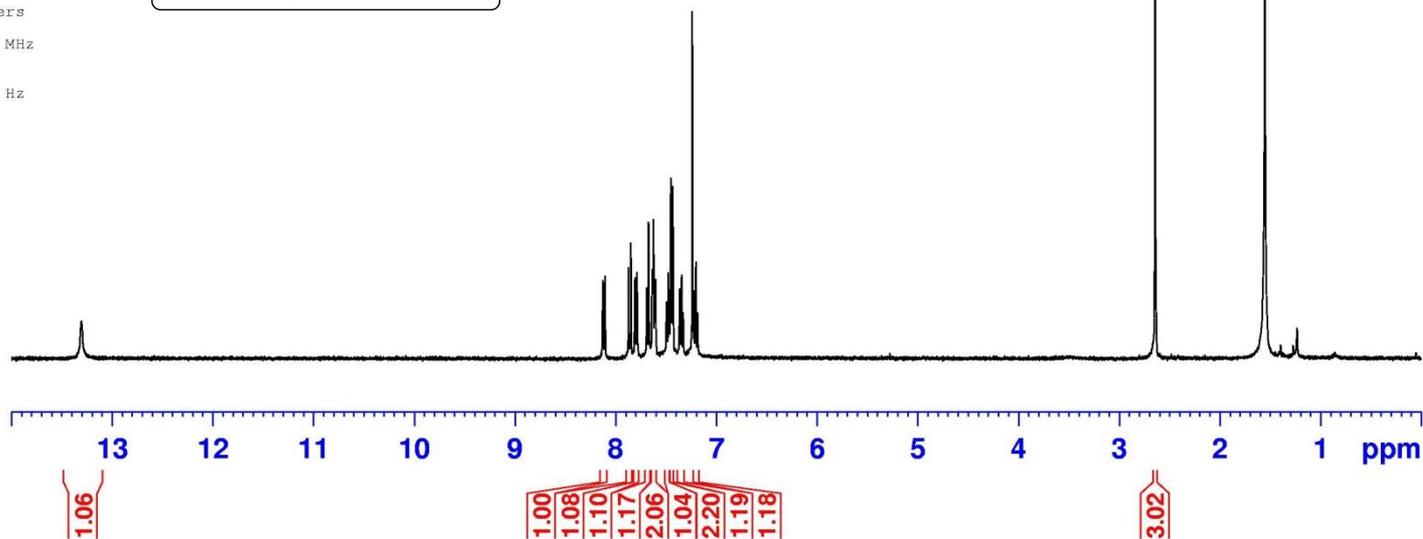
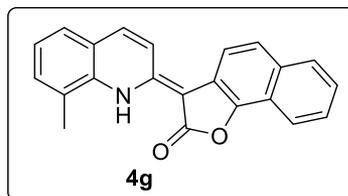
F2 - Processing parameters  
SI 16384  
SF 400.1500168 MHz  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

13.304

8.132  
8.111  
7.878  
7.854  
7.810  
7.790  
7.695  
7.673  
7.636  
7.628  
7.613  
7.607  
7.497  
7.479  
7.455  
7.436  
7.371  
7.369  
7.351  
7.348  
7.331  
7.242  
7.227  
7.207  
7.189

2.644

1.554



PS-D-048



Current Data Parameters  
NAME 19092017  
EXPNO 2  
PROCNO 1

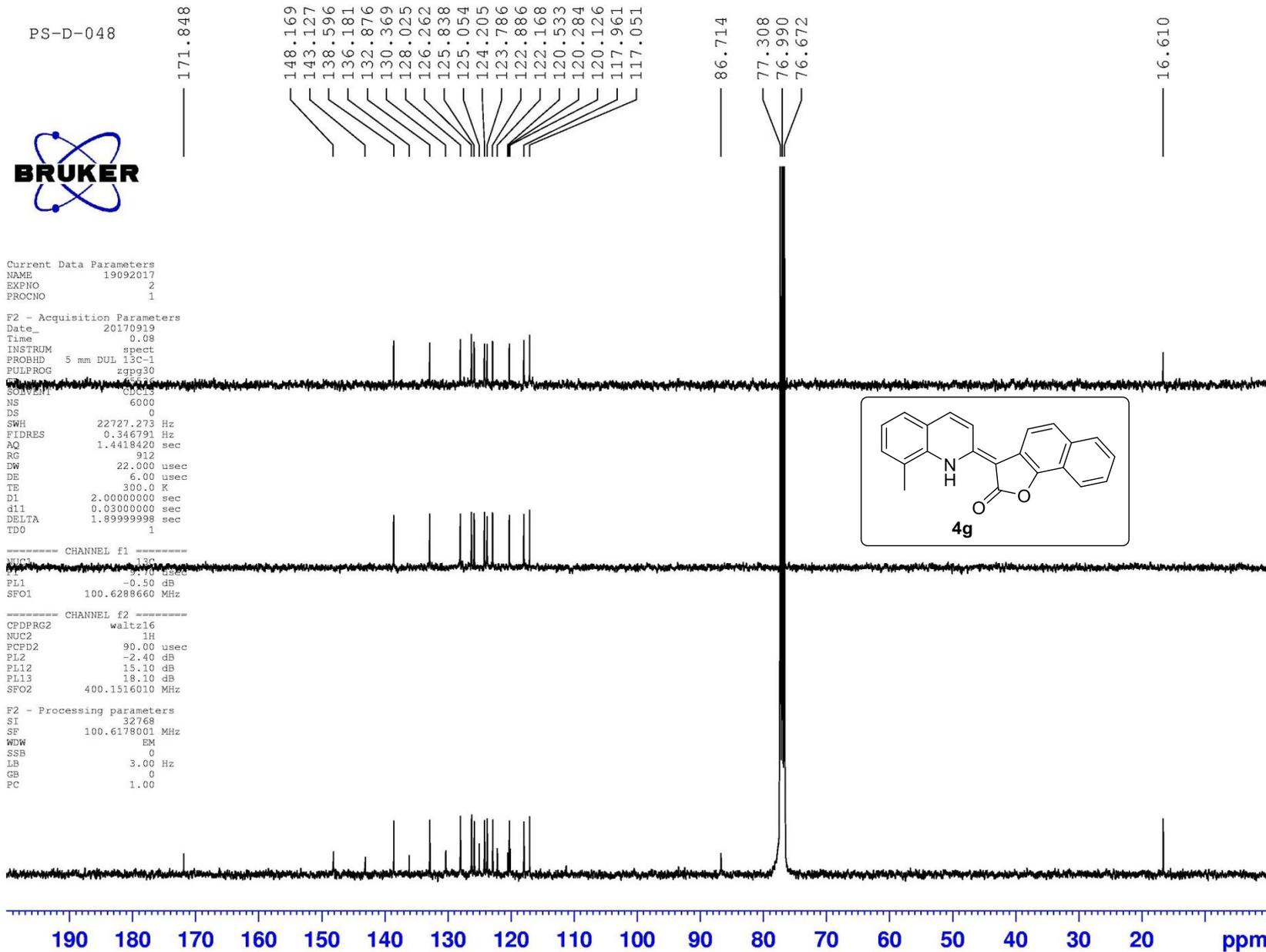
F2 - Acquisition Parameters  
Date\_ 20170919  
Time 0.08  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30

SOLVENT CDCl3  
NS 6000  
DS 0  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
RG 912  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999999 sec  
TD0 1

----- CHANNEL f1 -----  
NUC1 13C  
P1 9.170 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.40 dB  
PL12 15.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6178001 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME 07112017  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171107  
Time 23.16  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
ID 32768  
SOLVENT CDCl3  
NS 30  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 4  
WDW 78.000 usec  
DE 6.00 usec  
FE 300.0 K  
SI 2.00000000 sec  
DO 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

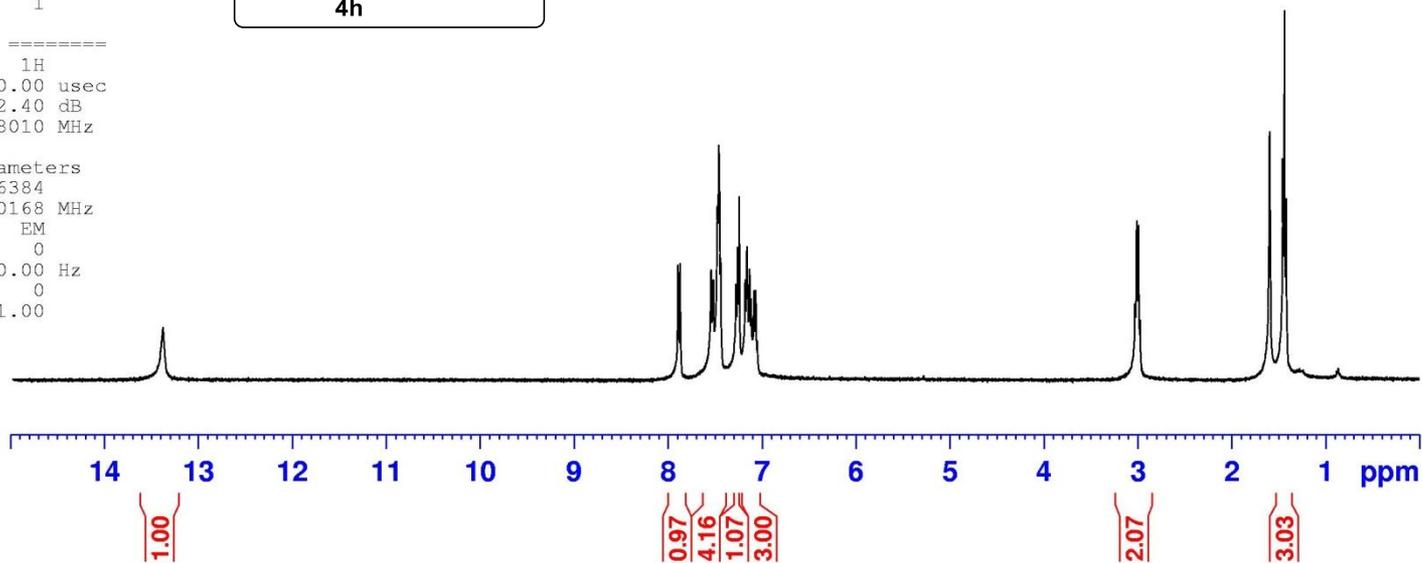
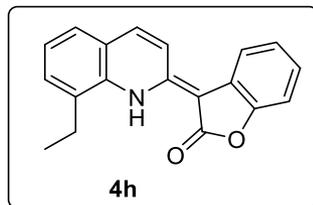
F2 - Processing parameters  
SI 16384  
SF 400.1500168 MHz  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

13.376

7.891  
7.867  
7.540  
7.519  
7.470  
7.457  
7.438  
7.276  
7.257  
7.240  
7.176  
7.157  
7.129  
7.112  
7.083  
7.064

3.026  
3.008  
2.989  
2.971

1.592  
1.454  
1.435  
1.417





171.764

149.066  
148.269  
138.924  
135.438  
130.868  
130.813  
125.866  
123.970  
122.928  
122.564  
122.163  
117.802  
117.217  
110.106

85.136  
77.309  
76.992  
76.674

23.260  
12.899

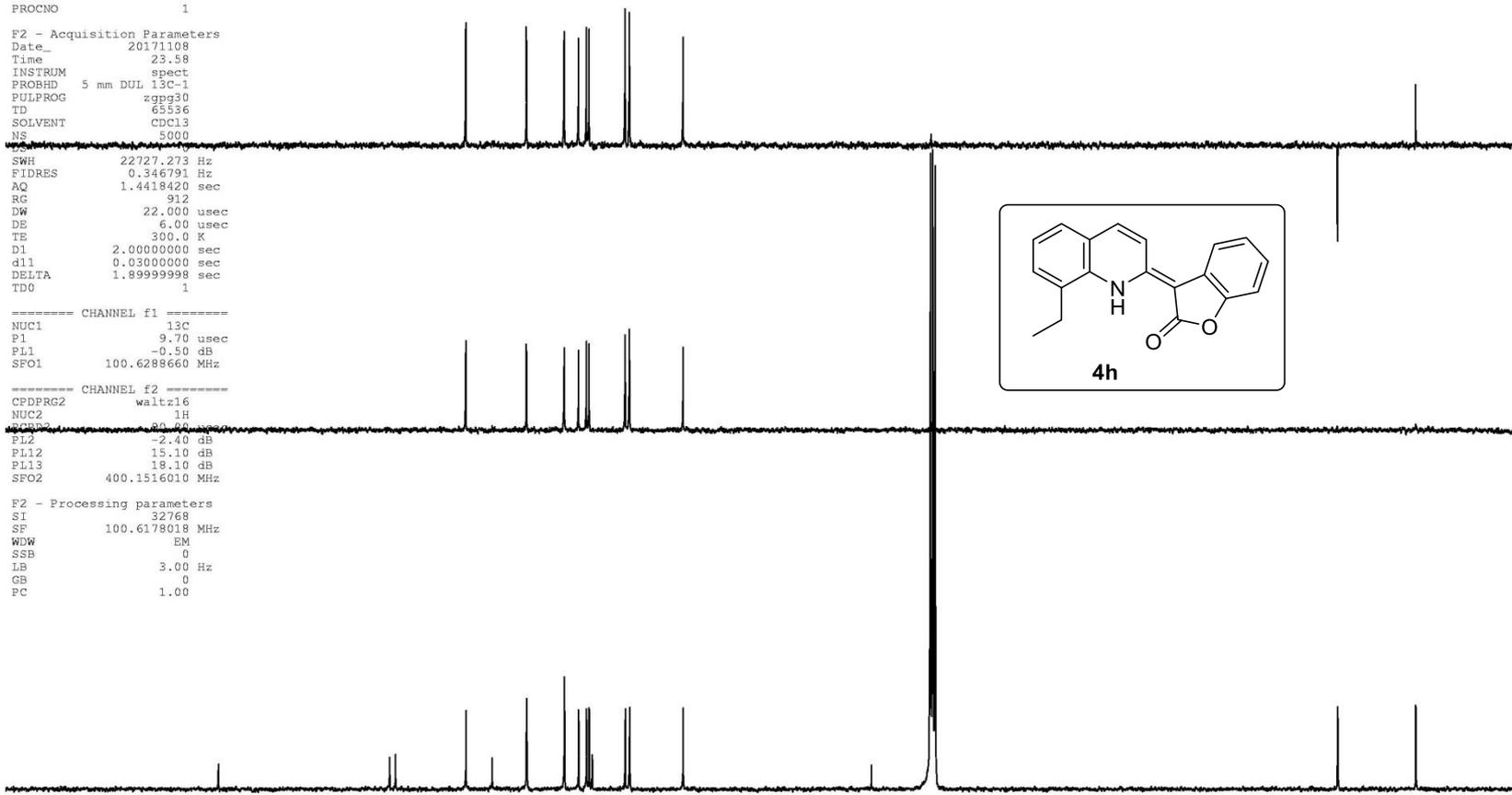
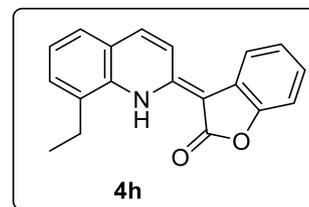
Current Data Parameters  
NAME 09112017  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171108  
Time 23.58  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 5000  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
RG 912  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

----- CHANNEL f1 -----  
NUC1 13C  
P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
P2 12.00 usec  
PL2 -2.40 dB  
PL12 15.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6178018 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm



Current Data Parameters  
NAME 20112017  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171120  
Time 23.37  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
PD 32768  
SOLVENT CDCl3  
NS 10  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 4  
OW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
SI 2.00000000 sec  
FDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

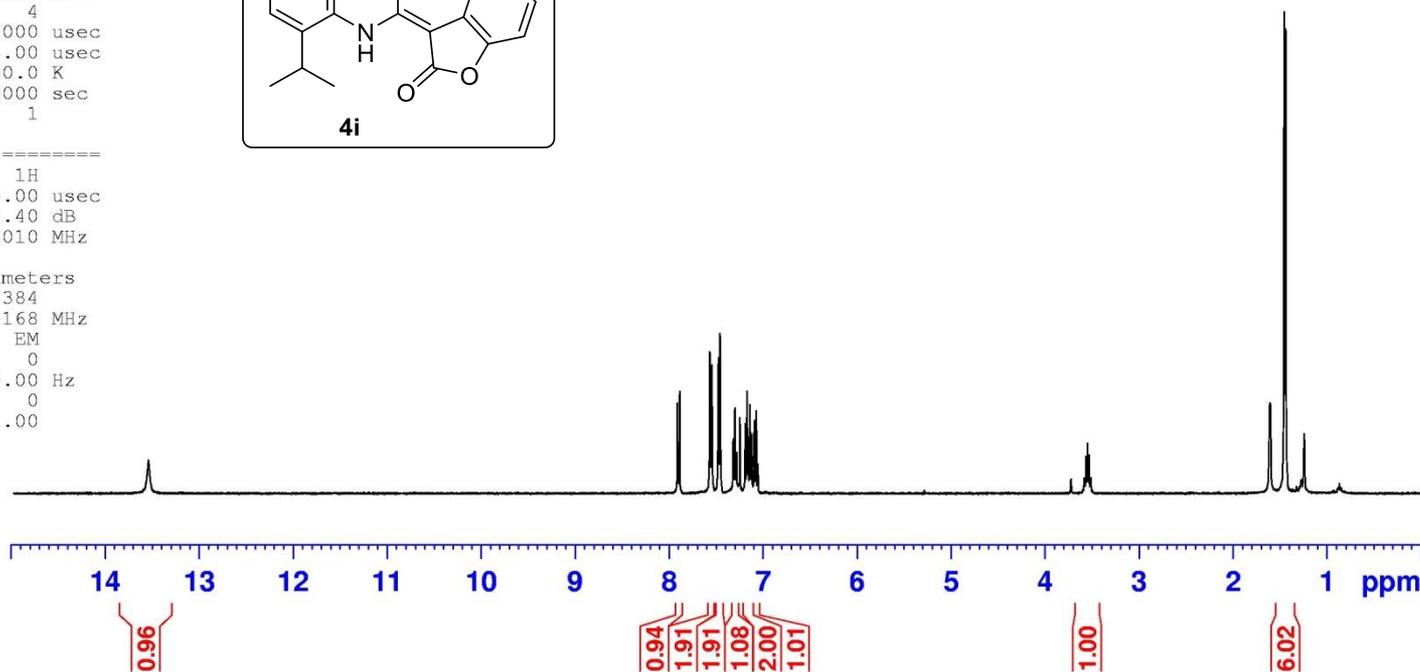
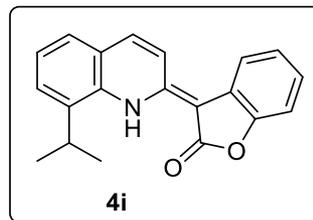
F2 - Processing parameters  
SI 16384  
SF 400.1500168 MHz  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

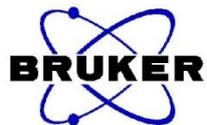
13.537

7.907  
7.884  
7.562  
7.541  
7.471  
7.452  
7.314  
7.295  
7.275  
7.186  
7.167  
7.155  
7.136  
7.117  
7.088  
7.069  
7.050

3.575  
3.558  
3.542  
3.525  
3.508

1.451  
1.434





171.817

149.069  
148.350  
139.125  
135.486  
134.837  
128.306  
125.852  
124.077  
122.925  
122.531  
122.308  
117.724  
117.192  
110.114

85.072  
77.309  
76.991  
76.674

27.397  
22.337

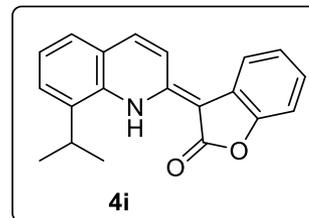
Current Data Parameters  
NAME 20112017  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171120  
Time 23.38  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65336  
SOLVENT CDCl3  
NS 614  
DS 0  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
SFO1 100.6288660 MHz  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.8999999 sec  
TD0 1

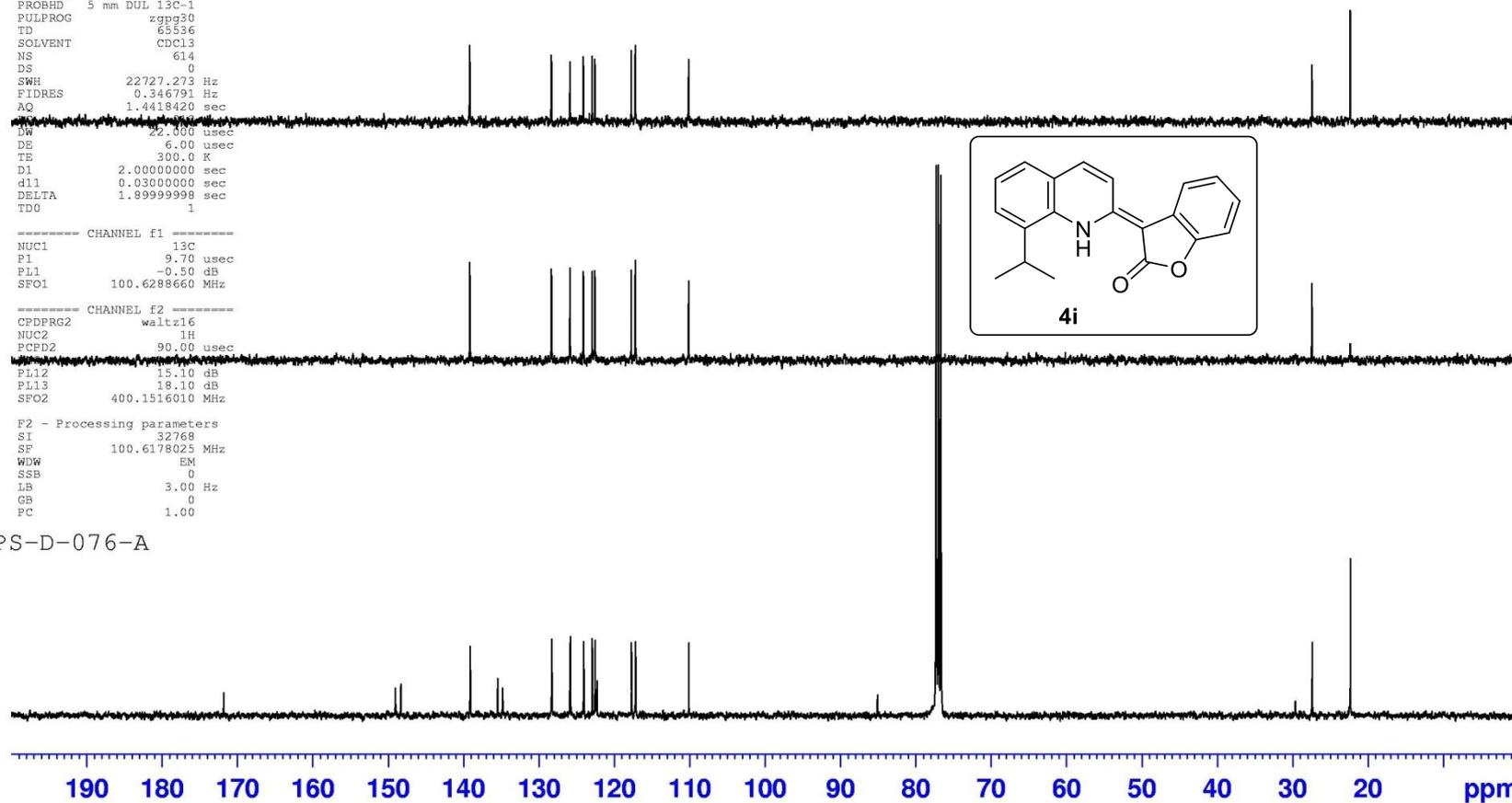
----- CHANNEL f1 -----  
NUC1 13C  
P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 15.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6178025 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



PS-D-076-A





Current Data Parameters  
NAME 22032018  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180322  
Time 14.58  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 54  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 4  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
TDO 1

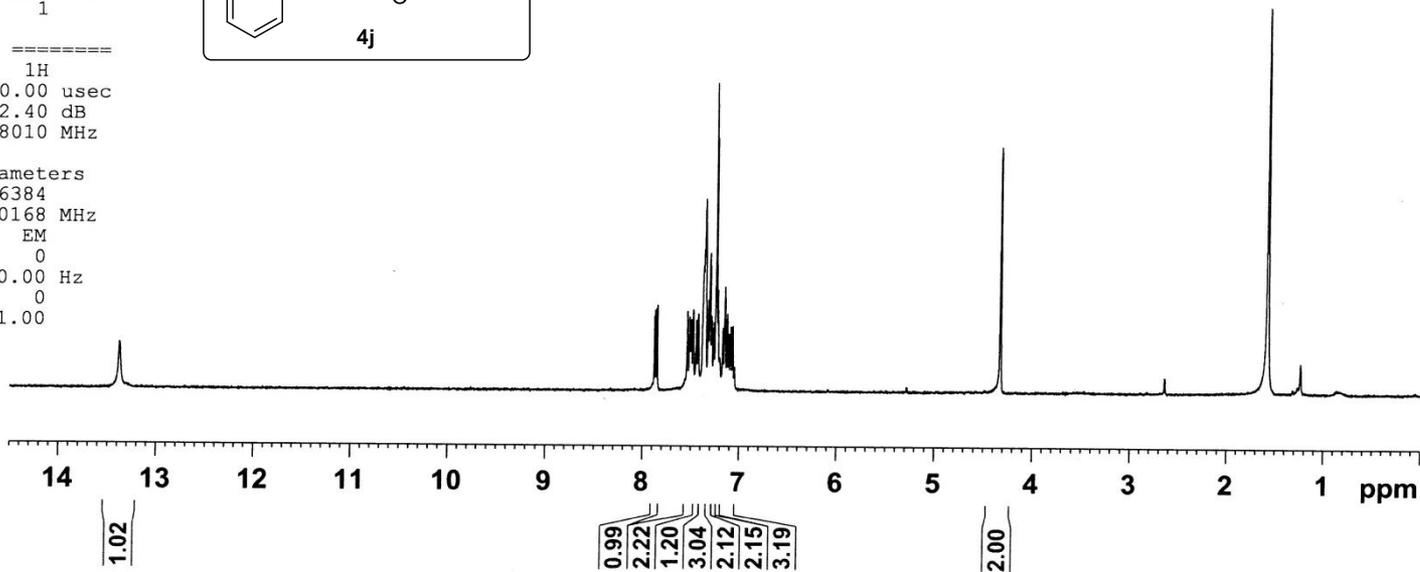
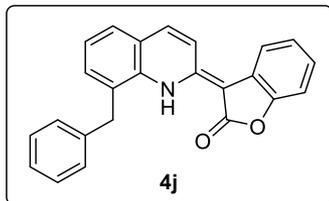
==== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500168 MHz  
WDM EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

13.378

7.881  
7.874  
7.857  
7.851  
7.841  
7.816  
7.501  
7.481  
7.445  
7.427  
7.377  
7.369  
7.359  
7.330  
7.325  
7.312  
7.306  
7.292  
7.272  
7.265  
7.252  
7.235  
7.227  
7.222  
7.172  
7.152  
7.150  
7.130  
7.127  
7.115  
7.111  
7.108  
7.092  
7.089  
7.073  
7.070  
7.051  
4.329  
4.325

1.577





171.608

149.143  
148.298  
138.767  
137.284  
135.557  
132.921  
129.280  
128.691  
128.294  
126.854  
126.514  
125.772  
123.830  
122.974  
122.745  
122.458  
118.124  
117.312  
110.151

85.516

77.323  
77.005  
76.688

36.214

Current Data Parameters  
NAME 21112017  
EXPNO 1  
PROCNO 1

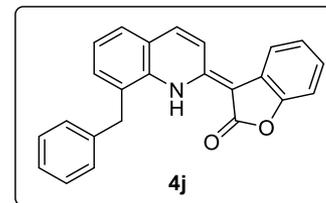
F2 - Acquisition Parameters  
Date\_ 20171121  
Time 0.33  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 4500

SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
RG 912  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TDO 1

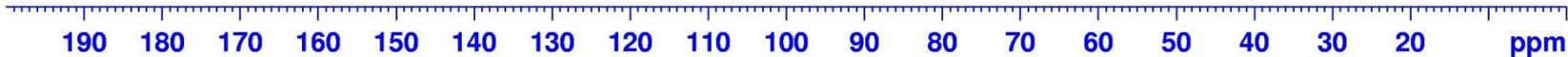
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

===== CHANNEL f2 =====  
CFDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.40 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6177995 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



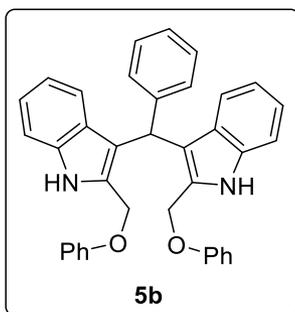
PS-D-076



8.2924  
7.3563  
7.3532  
7.3436  
7.3425  
7.3411  
7.3330  
7.3195  
7.2916  
7.2889  
7.2867  
7.2836  
7.2821  
7.2774  
7.2743  
7.2711  
7.2678  
7.2646  
7.2619  
7.2552  
7.2534  
7.2400  
7.2102  
7.1969  
7.1765  
7.1747  
7.1645  
7.1629  
7.1611  
7.1584  
7.1549  
7.1510  
7.1492  
7.1461  
7.1439  
7.1349  
7.1315  
6.9778  
6.9763  
6.9658  
6.9644  
6.9630  
6.9525  
6.9510  
6.9160  
6.9147  
6.9132  
6.9025  
6.8902  
6.6152  
6.6136  
6.6005  
6.5990  
6.2713  
4.6112  
4.5897  
4.4901  
4.4686

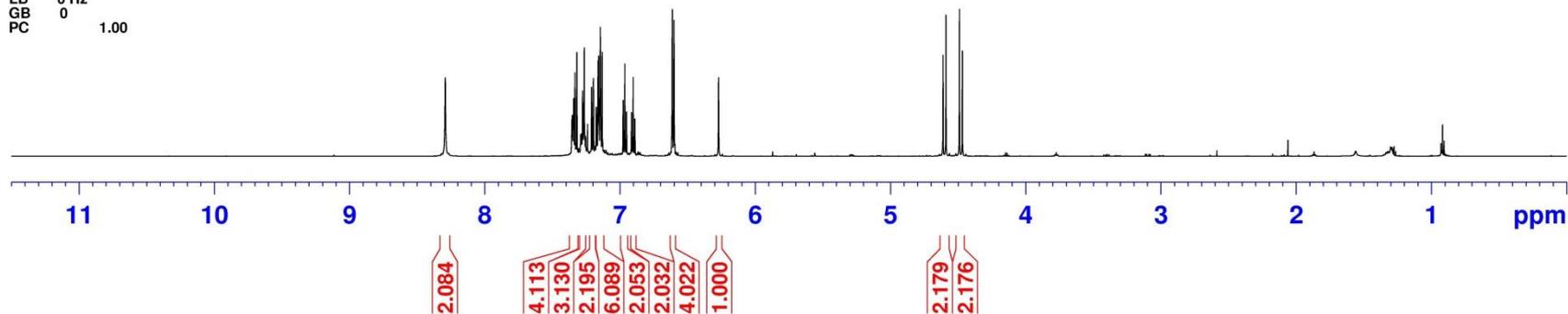
Current Data Parameters  
NAME SBW-5-203  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170801  
Time 23.13  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpr  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 1.6384000 sec  
RG 128  
DW 50.000 usec  
DE 6.50 usec  
TE 299.1 K  
D1 2.00000000 sec  
d12 0.00002000 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec



===== CHANNEL f1 =====  
NUC1 1H  
P1 20.00 usec  
PL1 -1.00 dB  
PL9 35.00 dB  
SFO1 598.4035904 MHz

F2 - Processing parameters  
SI 32768  
SF 598.4000248 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



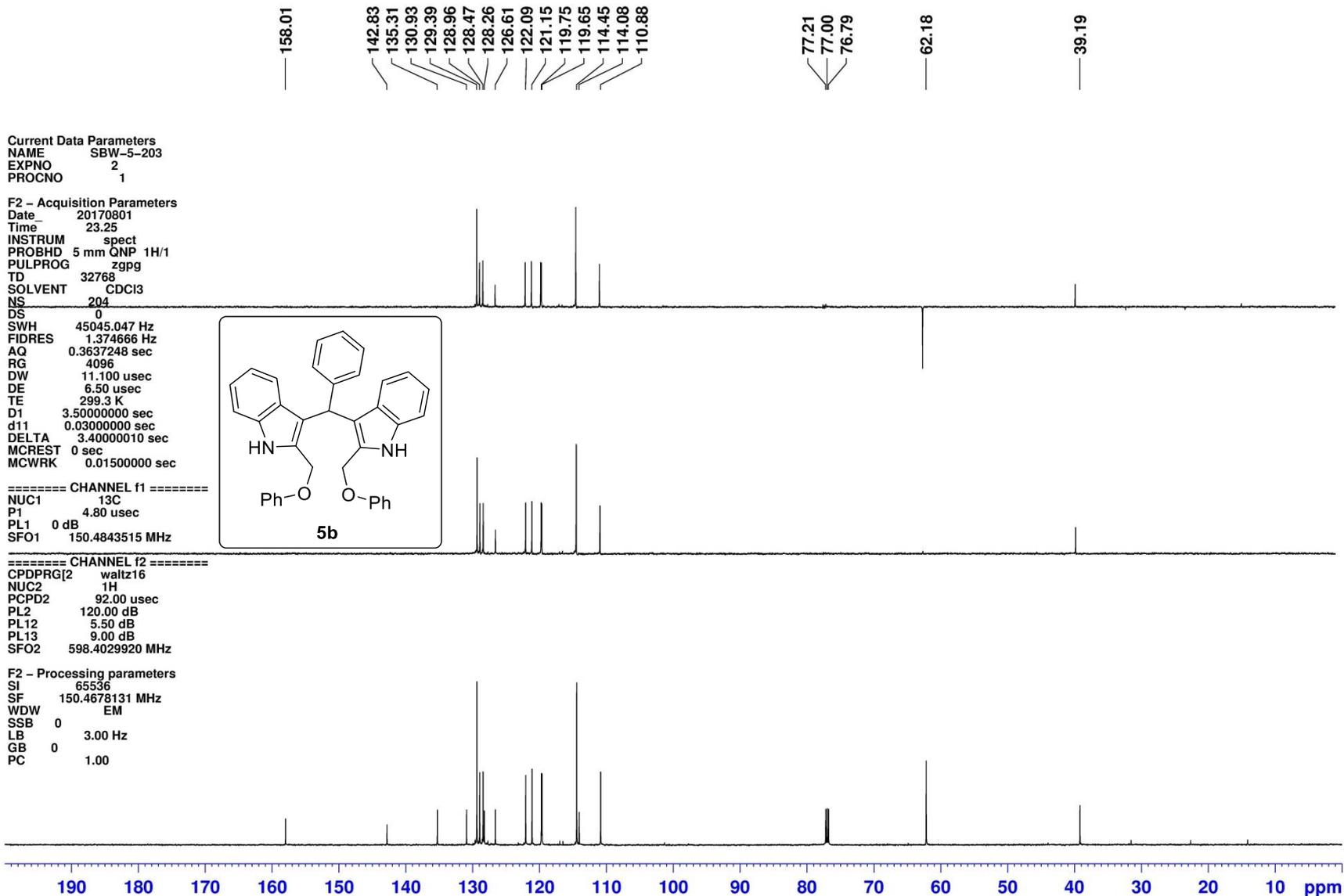
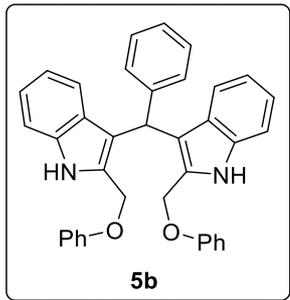
Current Data Parameters  
NAME SBW-5-203  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170801  
Time\_ 23.25  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 204  
DS 0  
SWH 45045.047 Hz  
FIDRES 1.374666 Hz  
AQ 0.3637248 sec  
RG 4096  
DW 11.100 usec  
DE 6.50 usec  
TE 299.3 K  
D1 3.5000000 sec  
d11 0.0300000 sec  
DELTA 3.40000010 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 4.80 usec  
PL1 0 dB  
SFO1 150.4843515 MHz

===== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 92.00 usec  
PL2 120.00 dB  
PL12 5.50 dB  
PL13 9.00 dB  
SFO2 598.4029920 MHz

F2 - Processing parameters  
SI 65536  
SF 150.4678131 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



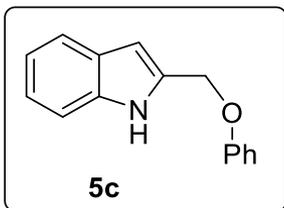
8.3551  
7.5957  
7.5826  
7.3597  
7.3461  
7.3031  
7.2889  
7.2764  
7.2400  
7.1891  
7.1771  
7.1638  
7.1089  
7.0966  
7.0841  
7.0008  
6.9867  
6.9734  
6.9611  
6.5245

5.2143

1.5675

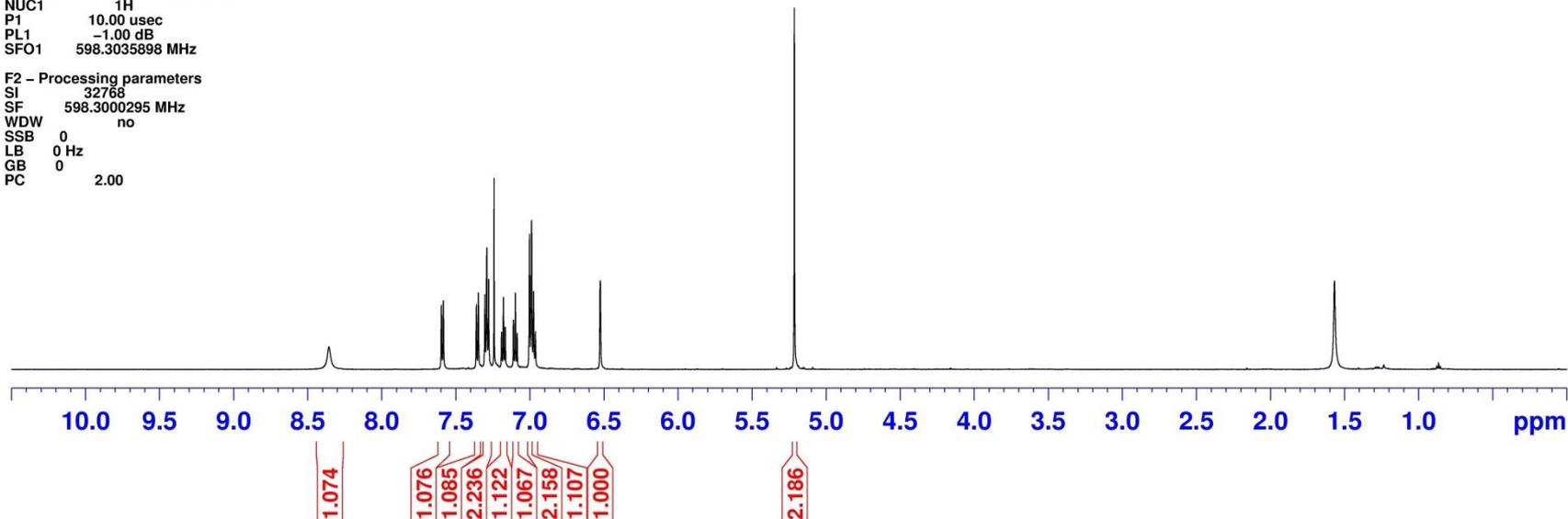
Current Data Parameters  
NAME SBW-5-203-C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180205  
Time\_ 10.52  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 9541.984 Hz  
FIDRES 0.291198 Hz  
AQ 1.7170432 sec  
RG 512  
DW 52.400 usec  
DE 6.50 usec  
TE 287.5 K  
D1 2.0000000 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec



===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -1.00 dB  
SFO1 598.3035898 MHz

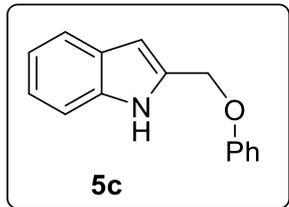
F2 - Processing parameters  
SI 32768  
SF 598.3000295 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 2.00



158.19  
 136.34  
 133.76  
 129.59  
 127.97  
 122.27  
 121.37  
 120.65  
 119.96  
 114.70  
 110.95  
 101.71  
 77.21  
 77.00  
 76.79  
 63.61

Current Data Parameters  
 NAME SBW-5-203-C  
 EXPNO 2  
 PROCNO 1

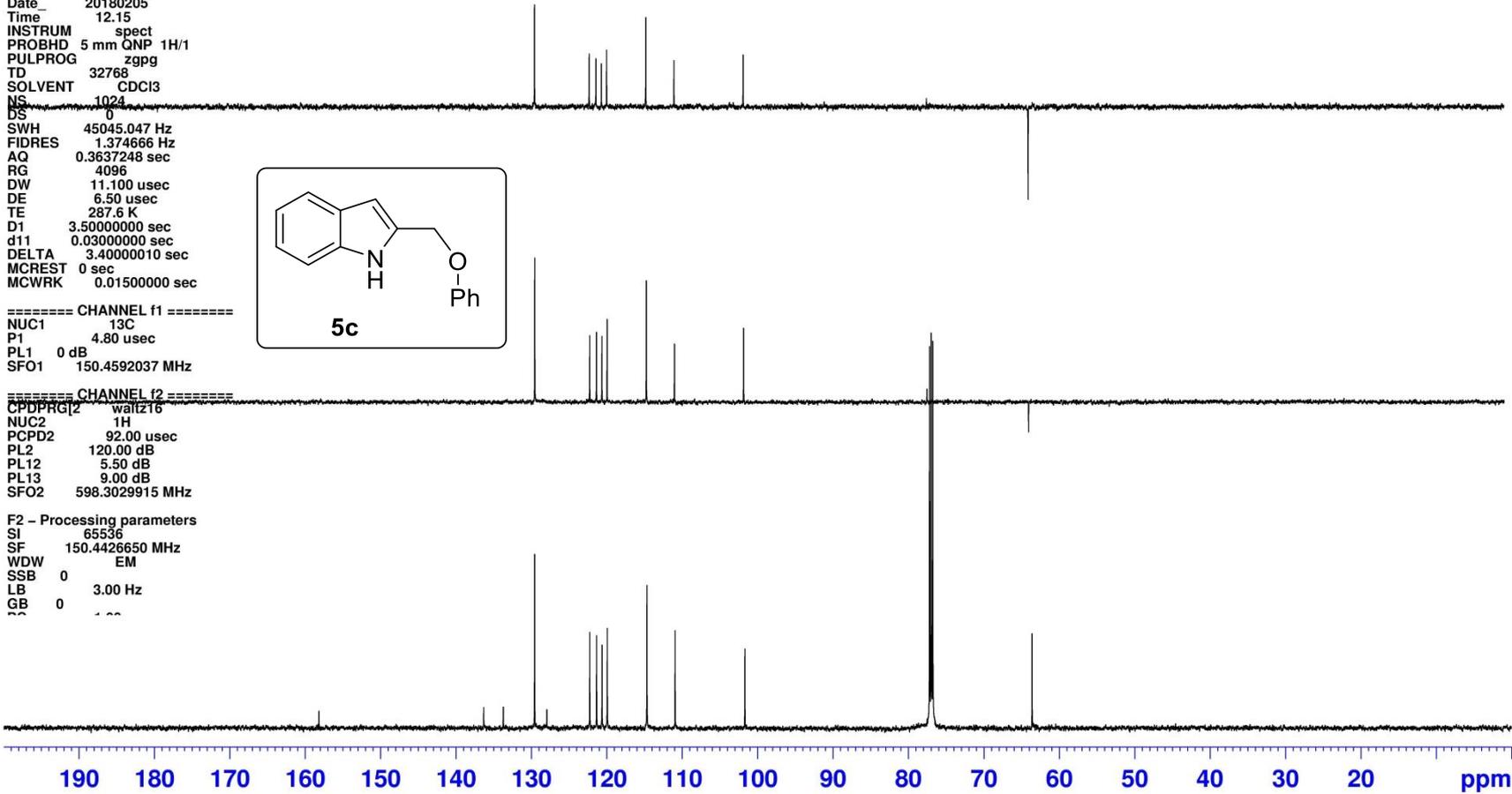
F2 - Acquisition Parameters  
 Date\_ 20180205  
 Time 12.15  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 1024  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637248 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 287.6 K  
 D1 3.5000000 sec  
 d11 0.0300000 sec  
 DELTA 3.4000010 sec  
 MCREST 0 sec  
 MCWRK 0.01500000 sec



===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0 dB  
 SFO1 150.4592037 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 5.50 dB  
 PL13 9.00 dB  
 SFO2 598.3029915 MHz

F2 - Processing parameters  
 SI 6536  
 SF 150.4426650 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0





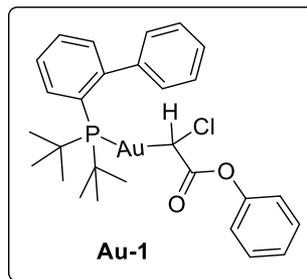
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7.8271  
7.5043  
7.4960  
7.4673  
7.4463  
7.4304  
7.3941  
7.3043  
7.2854  
7.2662  
7.2445  
7.1848  
7.1390  
7.1249  
7.1114  
7.0929  
7.0123  
6.9922

3.4876  
3.4657

1.5960  
1.4198  
1.3829  
1.3460

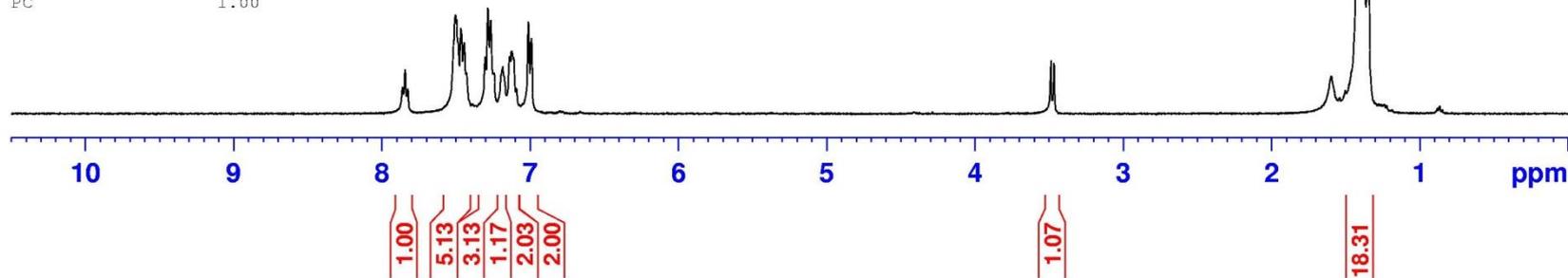
Current Data Parameters  
NAME 30092017  
EXPNO 1  
PROCNO 1

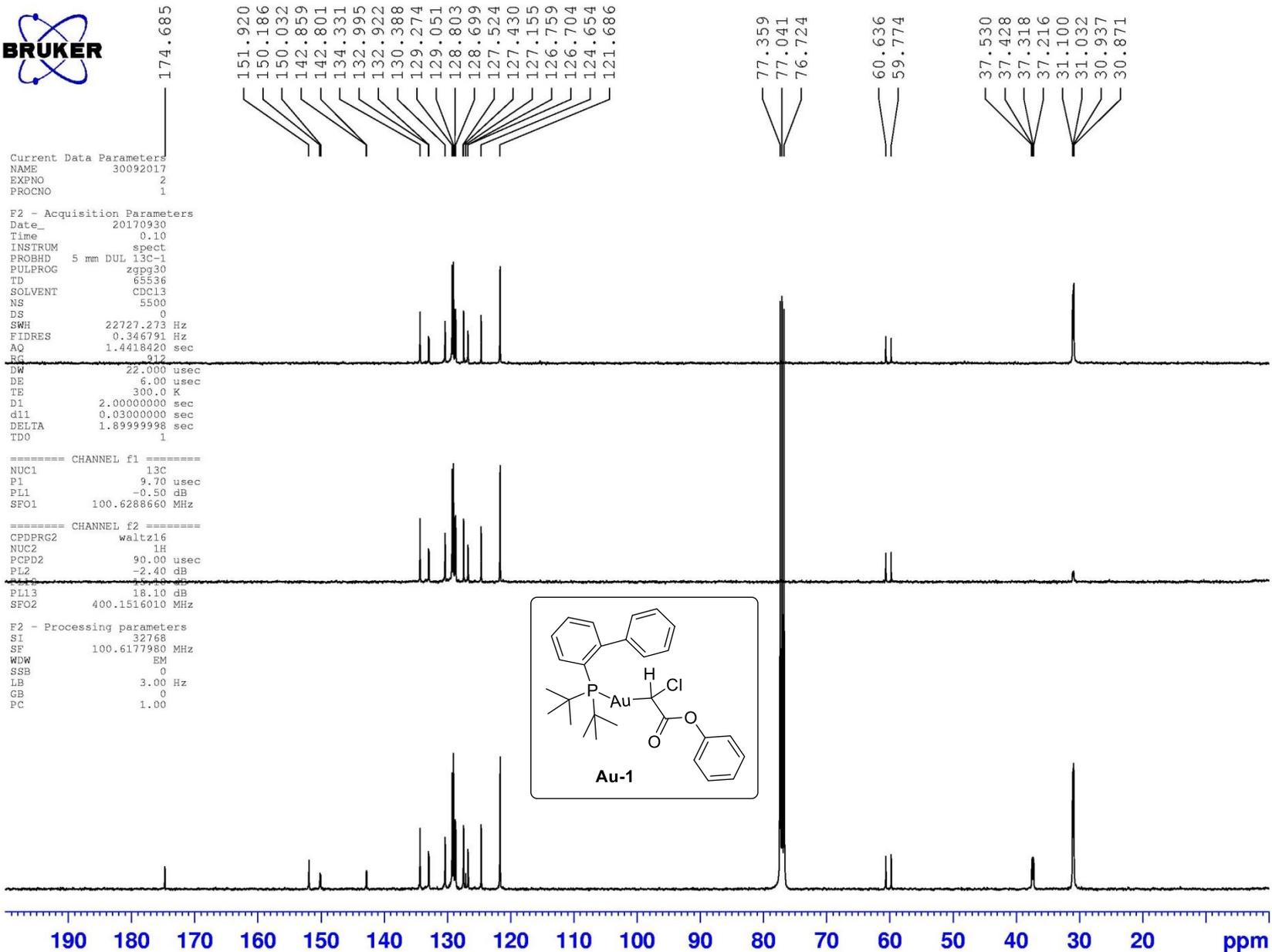
F2 - Acquisition Parameter  
Date\_ 20170930  
Time 0.08  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 9  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 se  
RG 4  
DW 78.000 us  
DE 6.00 us  
TE 300.0 K  
D1 2.00000000 se  
TD0 1

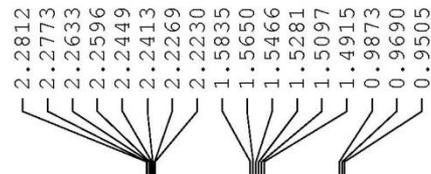
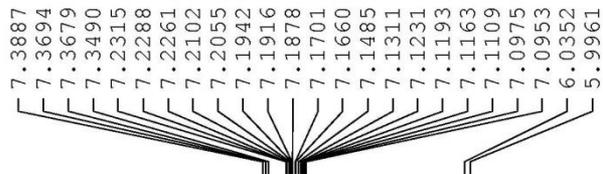


==== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 us  
PL1 -2.40 dB  
SFO1 400.1528010 MH

F2 - Processing parameters  
SI 16384  
SF 400.1500168 MH  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

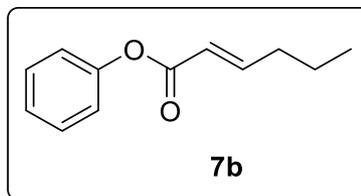






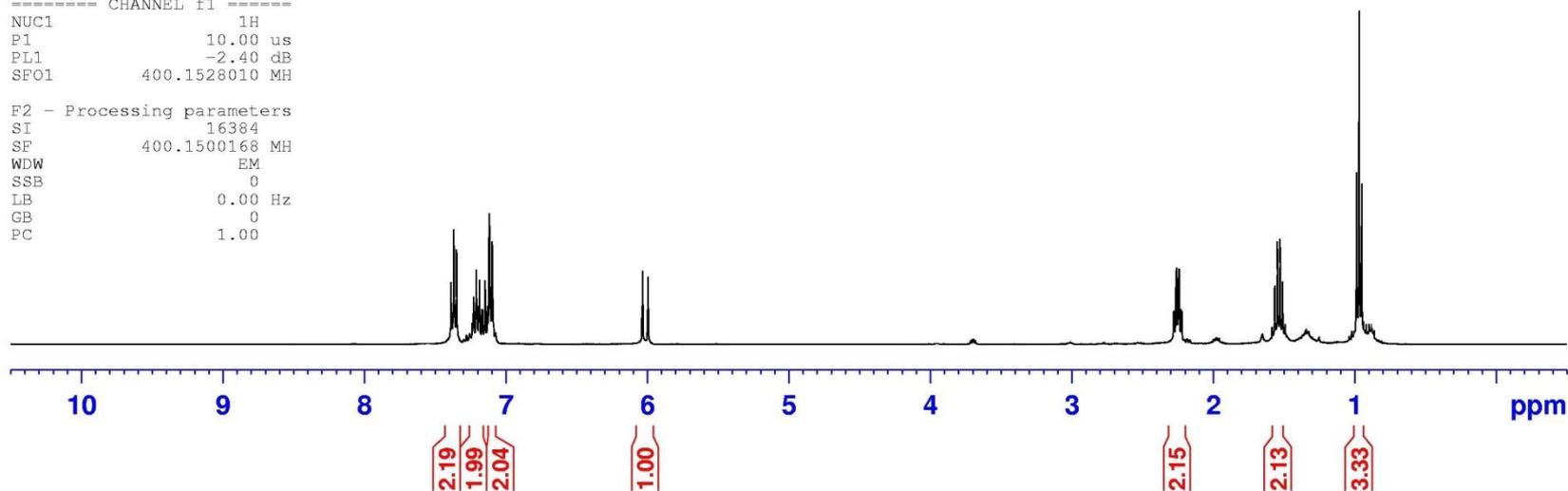
Current Data Parameters  
NAME 24032018  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameter  
Date\_ 20180324  
Time 19.01  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 7  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 se  
RG 4  
DW 78.000 us  
DE 6.00 us  
TE 300.0 K  
D1 2.00000000 se  
TD0 1



----- CHANNEL f1 -----  
NUC1 1H  
P1 10.00 us  
PL1 -2.40 dB  
SFO1 400.1528010 MH

F2 - Processing parameters  
SI 16384  
SF 400.1500168 MH  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00





165.073  
151.689  
150.796  
129.394  
125.684  
121.676  
120.675  
77.424  
77.106  
76.788  
34.436  
21.241  
13.739

Current Data Parameters  
NAME 24032018  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180324  
Time 19.05  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 54  
DS 0  
SWH 22727.273 Hz  
F2 101.626101 MHz  
AQ 1.4418420 sec  
RG 912  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 15.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6177980 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

