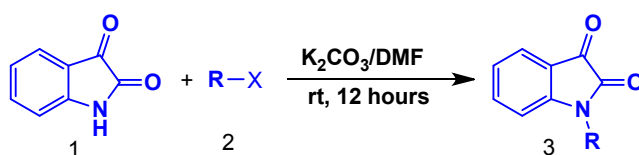


## Supporting Information file

### Ru(III) –catalyzed $\alpha$ -cross-coupling aldol type addition reaction of activated olefins with isatins

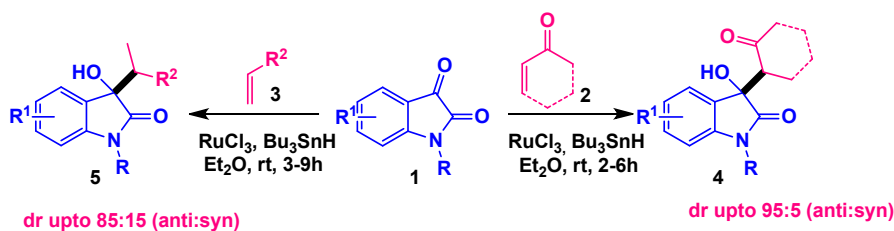
A. Sanjeeva Kumar<sup>a</sup>, Palakuri Ramesh<sup>a</sup>, G. Santosh Kumar<sup>a</sup>, A. Swetha<sup>a</sup>, Jagadeesh Babu Nanubolu<sup>b</sup> and H. M. Meshram<sup>a\*</sup>

**General procedure for preparation of N-alkyl Isatins:** A mixture of isatin **1** (1 mmol), alkyl bromide/iodide **2** (1.1 mmol) in 5 mL of DMF was added the K<sub>2</sub>CO<sub>3</sub> (1.5 mmol) and was stirred at rt for 12 hours under the argon atmosphere. After completion of the reaction, the reaction mixture was poured into ice-water and extracted by ethyl acetate (3×10 mL). Then, the combined organic layers were washed with brine, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduce pressure. The crude product was then purified by silica gel column chromatography (60–120 mesh) using ethyl acetate/hexane as eluent.



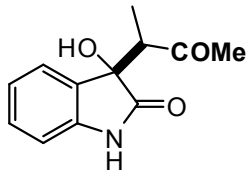
X = Br or I.  
R = Me, Et, Bu and Bn.

**General procedure for the synthesis of compounds 4 or 5:** A mixture of isatin **1** (1 mmol), activated olefin **2** or **3** (1.2 mmol) in 5 mL Et<sub>2</sub>O was added the TBTH (1.5 mmol), RuCl<sub>3</sub> (5 mol%) and was stirred at rt for stipulated time under argon atmosphere. The progress of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was quenched by adding aqueous NH<sub>4</sub>Cl solution. The aqueous layer was extracted by ethyl acetate (3×10 mL). Then, the combined organic layers were washed with brine, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduce pressure. The crude product was then purified by silica gel column chromatography (60–120 mesh) using ethyl acetate/hexane as eluent to yield the ene-carbonyl coupled products. All the obtained products **4** or **5** were characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, Mass and IR spectral data.



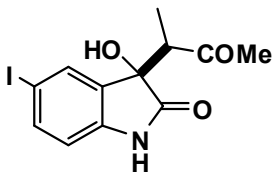
## Characterization Data of All Compounds

### 3-hydroxy-3-(3-oxobutan-2-yl)indolin-2-one (Table 2, 4a):



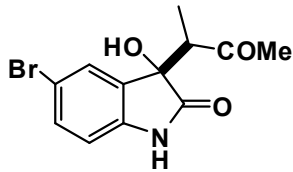
Pale yellow solid; Mp 110-112 °C; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>+DMSO-d<sub>6</sub>): δ 0.90 (d, *J* = 7.0 Hz, 3H), 2.36 (s, 3H), 3.29 (q, *J* = 7.0 Hz, 1H), 5.74 (s, 1H), 6.84 (d, *J* = 7.7 Hz, 1H), 6.96 (t, *J* = 7.7 Hz, 1H), 7.19 (t, *J* = 7.7 Hz, 1H), 7.26 (d, *J* = 7.4 Hz, 1H), 9.88 (s, 1H) (major); 1.28 (d, *J* = 7.7 Hz, 3H), 2.19 (s, 3H), 3.15 (q, *J* = 7.0 Hz, 1H), 5.74 (s, 1H), 6.99 (t, *J* = 7.0 Hz, 2H), 7.29 (d, *J* = 7.0 Hz, 2H), 9.82 (s, 1H) (minor); <sup>13</sup>C NMR (75 MHz, DMSO-d<sub>6</sub>): δ 10.6, 32.1, 50.4, 76.2, 111.3, 127.0, 127.8, 131.7, 131.8, 141.5, 177.3, 209.6 (major); 10.4, 29.6, 52.7, 75.5, 112.8, 127.0, 127.8, 131.4, 133.2, 141.6, 177.6, 208.0 (minor); IR (KBr) ν = 3326, 2929, 1715, 1621, 1485, 1191, 825 cm<sup>-1</sup>; MS-ESI: *m/z* = 242 [M+Na]<sup>+</sup>; HRMS (ESI) found: 242.0781, calcd. for C<sub>12</sub>H<sub>13</sub>NNaO<sub>3</sub>: 242.0793.

### 3-hydroxy-5-iodo-3-(3-oxobutan-2-yl)indolin-2-one (Table 2, 4b):



Pale brown solid; Mp 150-152 °C; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>+DMSO-d<sub>6</sub>): δ 0.76 (d, *J* = 6.9 Hz, 3H), 2.25 (s, 3H), 3.28 (q, *J* = 6.9 Hz, 1H), 6.32 (s, 1H), 6.75 (d, *J* = 8.1 Hz, 1H), 7.28 (d, *J* = 1.8 Hz, 1H), 7.3-7.41 (m, 1H), 10.46 (s, 1H) (major); 1.16 (d, *J* = 7.1 Hz, 3H), 2.10 (s, 3H), 3.15 (q, *J* = 7.1 Hz, 1H), 6.24 (s, 1H), 6.75 (d, *J* = 8.1 Hz, 1H), 7.35-7.38 (m, 2H), 10.39 (s, 1H) (minor); <sup>13</sup>C NMR (75 MHz, DMSO-d<sub>6</sub>): δ 10.6, 32.1, 50.4, 76.0, 84.0, 111.8, 132.1, 133.3, 137.5, 141.9, 177.0, 209.6 (major); 10.4, 29.6, 52.7, 75.3, 84.2, 111.7, 132.5, 133.6, 137.2, 141.8, 177.4, 208.0 (minor); IR (KBr) ν = 3318, 2990, 1699, 1625, 1175, 1051 cm<sup>-1</sup>; MS-ESI: *m/z* = 368 [M+Na]<sup>+</sup>; HRMS (ESI) found: 367.9758, calcd. for C<sub>12</sub>H<sub>12</sub>INNaO<sub>3</sub>: 367.9760.

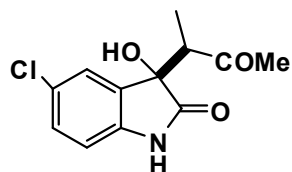
### 5-bromo-3-hydroxy-3-(3-oxobutan-2-yl)indolin-2-one (Table 2, 4c):



White solid; Mp 179-181 °C; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>+DMSO-d<sub>6</sub>): δ 0.89 (d, *J* = 6.9 Hz, 3H), 2.36 (s, 3H), 3.31 (q, *J* = 6.9 Hz, 1H), 5.98 (s, 1H), 6.75 (d, *J* = 8.3 Hz, 1H), 7.30-7.33 (m, 1H), 7.41 (d, *J* = 1.8 Hz, 1H), 10.12 (s, 1H) (major); 1.32 (d, *J* = 7.3 Hz, 3H), 2.19 (s, 3H), 3.19 (q, *J* = 7.3 Hz, 1H), 5.98 (s, 1H), 6.76 (d, *J* = 8.1 Hz, 1H), 7.31 (d, *J* = 8.3 Hz, 1H), 7.52-7.56 (m, 1H), 10.05 (s, 1H) (minor); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>+DMSO-d<sub>6</sub>): δ 10.5, 31.7, 50.2, 76.8, 110.9, 113.6, 128.1, 130.6, 131.4, 140.7, 177.5, 209.9 (major); 10.2, 29.1, 52.5, 75.8, 111.0, 113.4, 126.8, 131.1, 132.0, 140.8, 177.6, 208.7 (minor); IR (KBr) ν = 3316, 3216, 1699,

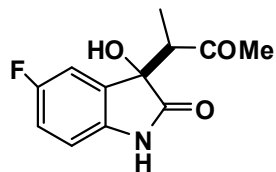
1620, 1176, 1051  $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 320$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 319.9890, calcd. for  $\text{C}_{12}\text{H}_{13}\text{BrNO}_3$ : 319.9898.

**5-chloro-3-hydroxy-3-(3-oxobutan-2-yl)indolin-2-one (Table 2, 4d):**



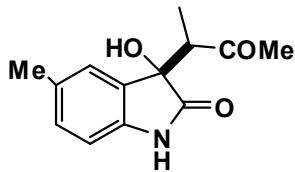
White solid; Mp 176-178  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  0.76 (d,  $J = 6.9$  Hz, 3H), 2.25 (s, 3H), 3.28 (q,  $J = 6.9$  Hz, 1H), 6.33 (s, 1H), 6.80 (d,  $J = 8.1$  Hz, 1H), 7.16 (d,  $J = 8.3$  Hz, 1H), 7.24 (d,  $J = 2.4$  Hz, 1H), 10.45 (s, 1H) (major); 1.17 (d,  $J = 7.3$  Hz, 3H), 2.10 (s, 3H), 3.16 (q,  $J = 7.3$  Hz, 1H), 6.24 (s, 1H), 6.80 (d,  $J = 8.1$  Hz, 1H), 7.16 (d,  $J = 8.3$  Hz, 1H), 7.27 (d,  $J = 2.0$  Hz, 1H), 10.38 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  10.3, 31.6, 50.1, 76.6, 110.2, 125.1, 125.9, 128.3, 130.1, 140.1, 177.5, 209.6 (major); 10.0, 28.9, 52.4, 75.6, 110.3, 123.9, 125.8, 128.1, 131.5, 140.2, 177.6, 208.3 (minor); IR (KBr)  $\nu = 3315$ , 2995, 1700, 1623, 1171, 1053  $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 276$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 276.0395, calcd. for  $\text{C}_{12}\text{H}_{12}\text{ClNNO}_3$ : 276.0403.

**5-fluoro-3-hydroxy-3-(3-oxobutan-2-yl)indolin-2-one (Table 2, 4e):**



Pale yellow solid; Mp 139-141  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  1.29 (d,  $J = 7.3$  Hz, 3H), 2.36 (s, 3H), 3.32 (q,  $J = 6.9$  Hz, 1H), 5.99 (s, 1H), 6.78-6.81 (m, 1H), 6.90 (d,  $J = 8.8$  Hz, 1H), 7.05 (d,  $J = 2.8$  Hz, 1H), 9.98 (s, 1H) (major); 0.85 (d,  $J = 7.3$  Hz, 3H), 2.19 (s, 3H), 3.18 (q,  $J = 7.3$  Hz, 1H), 5.99 (s, 1H), 6.76-6.78 (m, 1H), 6.87 (d,  $J = 8.8$  Hz, 1H), 7.02 (d,  $J = 2.8$  Hz, 1H), 10.05 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  10.5, 29.2, 50.1, 77.3, 111.8, 112.8, 114.7, 131.4, 137.6, 159.3, 178.0, 209.9 (major); 10.2, 31.9, 52.5, 76.1, 111.5, 113.1, 115.0, 131.5, 137.6, 159.4, 178.0, 208.6 (minor); IR (KBr)  $\nu = 3324$ , 2922, 1717, 1631, 1487, 1190, 828  $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 260$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 260.0691, calcd. for  $\text{C}_{12}\text{H}_{12}\text{FNNO}_3$ : 260.0699.

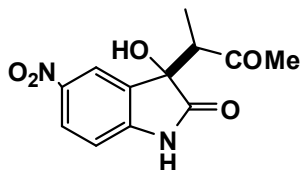
**3-hydroxy-5-methyl-3-(3-oxobutan-2-yl)indolin-2-one (Table 2, 4f):**



Pale brown solid; Mp 161-163  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  0.90 (d,  $J = 6.9$  Hz, 3H), 2.29 (s, 3H), 2.37 (s, 3H), 3.27 (q,  $J = 6.9$  Hz, 1H), 5.70 (s, 1H), 6.73 (d,  $J = 7.7$  Hz, 1H), 7.00 (d,  $J = 7.7$  Hz, 1H), 7.06 (s, 1H), 9.78 (s, 1H) (major); 1.26 (d,  $J = 7.3$  Hz, 3H), 2.20 (s, 3H), 2.31 (s, 3H), 3.13 (q,  $J = 7.3$  Hz, 1H), 5.70 (s, 1H), 6.73 (d,  $J = 7.7$  Hz, 1H), 7.00 (d,  $J = 7.7$  Hz, 1H), 7.10 (m, 1H), 9.78 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  10.1, 20.1, 31.5, 50.1, 77.1, 108.6, 125.1, 128.1, 128.6, 129.9, 138.7, 177.6, 209.6 (major); 9.9, 20.1, 28.9, 52.2, 75.8, 108.8, 124.1, 128.16, 128.5, 129.6, 138.7, 177.6, 209.6 (minor); IR (KBr)

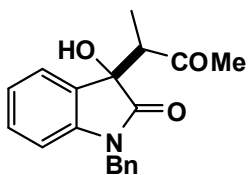
$\nu = 3323, 3209, 2921, 1698, 1629, 1494, 1154, 821 \text{ cm}^{-1}$ ; MS-ESI:  $m/z = 256 [M+Na]^+$ ; HRMS (ESI) found: 256.0941, calcd. for  $C_{13}H_{15}NNaO_3$ : 256.0950.

**3-hydroxy-5-nitro-3-(3-oxobutan-2-yl)indolin-2-one (Table 2, 4g):**



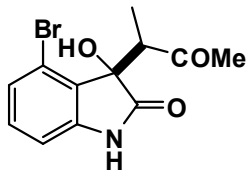
Pale brown solid; Mp 224-226 °C;  $^1H$  NMR (300 MHz,  $CDCl_3$ +DMSO- $d_6$ ):  $\delta$  0.97-1.03 (m, 3H), 2.36 (s, 3H), 3.38 (q,  $J = 7.1$  Hz, 1H), 6.05 (s, 1H), 7.43 (s, 1H), 8.15-8.20 (m, 2H), 10.63 (s, 1H) (major); 1.47 (d,  $J = 7.1$  Hz, 3H), 2.19 (s, 3H), 3.32 (q,  $J = 7.3$  Hz, 1H), 6.02 (s, 1H), 6.93-6.99 (m, 2H), 8.23 (s, 1H), 10.58 (s, 1H) (minor);  $^{13}C$  NMR (75 MHz,  $CDCl_3$ +DMSO- $d_6$ ):  $\delta$  10.1, 31.2, 50.3, 75.7, 108.8, 120.6, 125.3, 129.4, 141.7, 147.9, 177.9, 209.1 (major); 9.9, 28.5, 52.7, 74.5, 108.8, 119.3, 125.2, 130.6, 141.5, 148.3, 178.3, 207.9 (minor); IR (KBr)  $\nu = 3516, 3204, 1724, 1621, 1522, 1334, 1281, 1104 \text{ cm}^{-1}$ ; MS-ESI:  $m/z = 287 [M+Na]^+$ ; HRMS (ESI) found: 287.0638, calcd. for  $C_{12}H_{12}N_2NaO_5$ : 287.0644.

**1-benzyl-3-hydroxy-3-(3-oxobutan-2-yl)indolin-2-one (Table 2, 4h):**



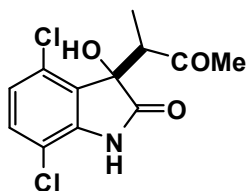
White solid; Mp 133-135 °C;  $^1H$  NMR (300 MHz,  $CDCl_3$ +DMSO- $d_6$ ):  $\delta$  0.93 (d,  $J = 6.9$  Hz, 3H), 2.35 (s, 3H), 3.40 (q,  $J = 6.9$  Hz, 1H), 4.88 (d,  $J = 15.6$  Hz, 2H), 6.00 (s, 1H), 6.69 (d,  $J = 7.7$  Hz, 1H), 7.00 (t,  $J = 8.3$  Hz, 1H), 7.18 (t,  $J = 7.7$  Hz, 1H), 7.33-7.38 (m, 6H) (major); 1.33 (d,  $J = 7.3$  Hz, 3H), 2.19 (s, 3H), 3.27 (q,  $J = 7.3$  Hz, 1H), 4.88 (d,  $J = 15.6$  Hz, 2H), 6.03 (s, 1H), 6.68 (d,  $J = 7.5$  Hz, 1H), 7.00 (t,  $J = 8.3$  Hz, 1H), 7.18 (t,  $J = 7.7$  Hz, 1H), 7.25-7.30 (m, 4H) 7.51-7.55 (m, 2H) (minor);  $^{13}C$  NMR (75 MHz,  $CDCl_3$ +DMSO- $d_6$ ): 10.3, 31.4, 42.7, 50.7, 75.8, 108.1, 121.6, 124.2, 126.5, 126.7, 127.7, 127.8, 128.5, 134.9, 142.1, 176.0, 209.4 (major); 10.2, 28.9, 42.7, 52.6, 75.2, 108.3, 121.6, 123.4, 126.5, 126.6, 127.7, 128.0, 129.2, 134.9, 142.2, 176.2, 208.4 (minor); IR (KBr)  $\nu = 3407, 3058, 1698, 1614, 1464, 1177, 1052 \text{ cm}^{-1}$ ; MS-ESI:  $m/z = 332 [M+Na]^+$ ; HRMS (ESI) found: 332.1253, calcd. for  $C_{19}H_{19}NNaO_3$ : 332.1263.

**4-bromo-3-hydroxy-3-(3-oxobutan-2-yl)indolin-2-one (Table 2, 4i):**



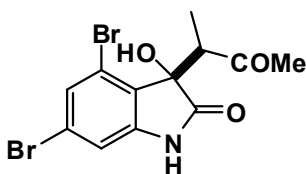
Pale yellow solid; Mp 165-168 °C;  $^1H$  NMR (300 MHz,  $CDCl_3$ +DMSO- $d_6$ ):  $\delta$  0.87 (d,  $J = 7.1$  Hz, 3H), 2.45 (s, 3H), 3.63 (q,  $J = 7.1$  Hz, 1H), 5.96 (s, 1H), 6.79-6.82 (m, 1H), 7.06 (d,  $J = 6.2$  Hz, 1H), 7.07-7.11 (m, 1H), 10.06 (s, 1H) (major); 1.48 (d,  $J = 7.3$  Hz, 3H), 2.35 (s, 3H), 4.09 (q,  $J = 7.1$  Hz, 1H), 5.47 (s, 1H), 6.74-6.77 (m, 1H), 7.00-7.05 (m, 1H), 7.13-7.18 (m, 1H), 9.83 (s, 1H) (minor);  $^{13}C$  NMR (75 MHz,  $CDCl_3$ +DMSO- $d_6$ ):  $\delta$  9.1, 30.3, 49.8, 77.8, 110.9, 122.2, 123.7, 124.1, 129.1, 142.6, 174.7, 206.5 (major); 8.8, 28.1, 51.4, 77.1, 111.0, 120.4, 124.3, 125.1, 129.0, 142.2, 175.1, 207.1 (minor); IR (KBr)  $\nu = 3314, 3211, 1701, 1625, 1177, 1051, 868 \text{ cm}^{-1}$ ; MS-ESI:  $m/z = 320 [M+Na]^+$ ; HRMS (ESI) found: 319.9891, calcd. for  $C_{12}H_{12}BrNNaO_3$ : 319.9898.

**4,7-dichloro-3-hydroxy-3-(3-oxobutan-2-yl)indolin-2-one (Table 2, 4j):**



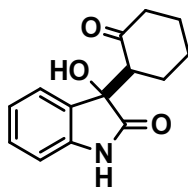
White solid; Mp 217-219 °C; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>+DMSO-d<sub>6</sub>): δ 0.89 (d, *J* = 7.1 Hz, 3H), 2.46 (s, 3H), 3.56 (q, *J* = 7.1 Hz, 1H), 6.23 (s, 1H), 6.92 (d, *J* = 8.6 Hz, 1H), 7.18 (d, *J* = 8.6 Hz, 1H), 10.25 (s, 1H) (major); 1.48 (d, *J* = 7.3 Hz, 3H), 2.09 (s, 3H), 3.98 (q, *J* = 7.3 Hz, 1H), 5.98 (s, 1H), 6.84 (d, *J* = 8.6 Hz, 1H), 7.12 (d, *J* = 8.6 Hz, 1H), 9.91 (s, 1H) (minor); <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): 10.6, 32.2, 50.4, 76.3, 110.8, 124.4, 125.1, 128.9, 131.4, 141.1, 177.4, 209.6 (major); 10.4, 29.6, 52.7, 75.5, 110.8, 124.4, 125.1, 128.6, 132.8, 141.2, 177.8, 208.0 (minor); IR (KBr) ν = 3420, 3155, 1729, 1686, 1615, 1472, 1314, 814 cm<sup>-1</sup>; MS-ESI: *m/z* = 310 [M+Na]<sup>+</sup>; HRMS (ESI) found: 310.0004, calcd. for C<sub>12</sub>H<sub>11</sub>Cl<sub>2</sub>NNaO<sub>3</sub>: 310.0014.

**4,6-dibromo-3-hydroxy-3-(3-oxobutan-2-yl)indolin-2-one (Table 2, 4k):**



Pale yellow solid; Mp 155-157 °C; <sup>1</sup>H NMR (300 MHz, DMSO-d<sub>6</sub>): δ 1.34 (d, *J* = 7.1 Hz, 3H), 2.37 (s, 3H), 3.92 (q, *J* = 7.1 Hz, 1H), 6.28 (s, 1H), 6.89 (d, *J* = 1.5 Hz, 1H), 7.27 (d, *J* = 1.5 Hz, 1H), 10.51 (s, 1H) (major); 0.55 (d, *J* = 7.0 Hz, 3H), 2.15 (s, 3H), 3.51 (q, *J* = 7.1 Hz, 1H), 6.53 (s, 1H), 6.97 (d, *J* = 1.5 Hz, 1H), 7.38 (d, *J* = 1.5 Hz, 1H), 10.66 (s, 1H) (minor); <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): 9.8, 29.5, 51.4, 74.9, 111.5, 118.8, 122.4, 126.8, 128.7, 145.8, 176.5, 209.1 (major); 10.4, 32.0, 48.5, 76.5, 112.0, 119.3, 122.5, 127.4, 128.4, 145.3, 176.1, 207.2 (minor); IR (KBr) ν = 3315, 3214, 1700, 1615, 1170, 1053 cm<sup>-1</sup>; MS-ESI: *m/z* = 375 [M+H]<sup>+</sup>; HRMS (ESI) found: 375.9173, calcd. for C<sub>12</sub>H<sub>12</sub>Br<sub>2</sub>NNaO<sub>3</sub>: 375.9184.

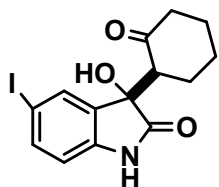
**3-hydroxy-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4l):**



White solid; Mp 189-191 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>+DMSO-d<sub>6</sub>): δ 1.52-1.68 (m, 3H), 1.93-2.10 (m, 4H), 2.28-2.34 (m, 1H), 3.16 (dd, *J* = 5.4, 13.2 Hz, 1H), 5.62 (s, 1H), 6.88 (d, *J* = 7.7 Hz, 1H), 6.92-6.95 (m, 1H), 7.20 (t, *J* = 7.7 Hz, 1H), 7.29 (d, *J* = 7.3 Hz, 1H), 9.88 (s, 1H) (major); 1.12-1.28 (m, 3H), 1.71-1.83 (m, 4H), 2.36-2.43 (m, 1H), 3.09 (dd, *J* = 5.2, 12.6 Hz, 1H), 5.12 (s, 1H), 6.85 (d, *J* = 7.5 Hz, 1H), 6.96-6.99 (m, 1H), 7.20 (t, *J* = 7.7 Hz, 1H), 7.39 (d, *J* = 7.5 Hz, 1H), 9.69 (s, 1H) (minor); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>+DMSO-d<sub>6</sub>): δ 24.2, 26.5, 27.6, 41.4, 56.6, 74.6, 109.4, 120.8, 124.1, 128.5, 129.9, 142.6, 178.7, 209.5 (major); 24.1, 26.1, 26.8, 42.2, 56.1, 75.8, 109.4, 121.4, 124.4, 128.4, 129.8, 142.0, 177.0, 209.4 (minor); IR (KBr) ν = 3338, 3166, 2943,

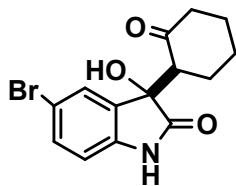
1721, 1618, 1469, 756  $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 268 [M+Na]^+$ ; HRMS (ESI) found: 268.0941, calcd. for  $\text{C}_{14}\text{H}_{15}\text{NNaO}_3$ : 268.0950.

**3-hydroxy-5-iodo-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4m):**



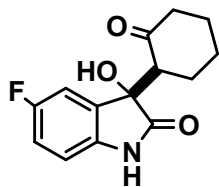
White solid; Mp 223-225  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3+\text{DMSO}-d_6$ ):  $\delta$  1.60-1.69 (m, 3H), 1.97-2.11 (m, 4H), 2.46-2.50 (m, 1H), 3.13-3.19 (m, 1H), 5.77 (s, 1H), 7.47 (s, 1H), 7.53-7.55 (m, 1H), 7.68-7.71 (m, 1H), 9.93 (s, 1H) (major); 1.76-1.87 (m, 3H), 2.27-2.33 (m, 2H), 2.36-2.44 (m, 2H), 2.51-2.54 (m, 1H), 3.08-3.12 (m, 1H), 5.25 (s, 1H), 6.64-6.71 (m, 2H), 7.48-7.52 (m, 1H), 10.08 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}-d_6$ ):  $\delta$  24.3, 26.5, 27.4, 41.3, 57.3, 73.6, 83.4, 111.5, 132.7, 135.3, 137.0, 143.1, 177.9, 209.1 (major); 24.4, 26.6, 27.6, 42.0, 56.9, 73.3, 83.7, 111.8, 132.0, 133.5, 136.8, 142.4, 177.2, 209.8 (minor); IR (KBr)  $\nu = 3293, 2934, 1726, 1613, 1197 \text{ cm}^{-1}$ ; MS-ESI:  $m/z = 394 [M+Na]^+$ ; HRMS (ESI) found: 393.9906, calcd. for  $\text{C}_{14}\text{H}_{14}\text{INaO}_3$ : 393.9916.

**5-bromo-3-hydroxy-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4n):**



White solid; Mp 225-227  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3+\text{DMSO}-d_6$ ):  $\delta$  1.55-1.69 (m, 3H), 1.99-2.13 (m, 4H), 2.24-2.31 (m, 1H), 3.16 (dd,  $J = 4.9, 13.2 \text{ Hz}$ , 1H), 5.87 (s, 1H), 6.78 (d,  $J = 8.8 \text{ Hz}$ , 1H), 7.29 (d,  $J = 8.3 \text{ Hz}$ , 1H), 7.36 (d,  $J = 1.7 \text{ Hz}$ , 1H), 10.17 (s, 1H) (major); 1.23-1.48 (m, 3H), 1.70-1.88 (m, 4H), 2.35-2.41 (m, 1H), 3.16 (dd,  $J = 4.9, 13.2 \text{ Hz}$ , 1H), 5.43 (s, 1H), 6.75 (d,  $J = 8.4 \text{ Hz}$ , 1H), 7.32 (d,  $J = 8.3 \text{ Hz}$ , 1H), 7.53 (d,  $J = 2.0 \text{ Hz}$ , 1H), 10.08 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}-d_6$ ):  $\delta$  24.3, 26.5, 27.4, 41.3, 57.3, 73.8, 111.2, 112.6, 127.3, 130.1, 133.2, 142.6, 178.1, 209.1 (major); 24.4, 26.6, 27.6, 42.0, 56.9, 73.5, 110.9, 112.3, 126.6, 131.0, 134.9, 142.0, 177.4, 209.8 (minor); IR (KBr)  $\nu = 3290, 2938, 1718, 1615, 1192, 825 \text{ cm}^{-1}$ ; MS-ESI:  $m/z = 346 [M+Na]^+$ ; HRMS (ESI) found: 346.0041, calcd. for  $\text{C}_{14}\text{H}_{14}\text{BrNaO}_3$ : 346.0055.

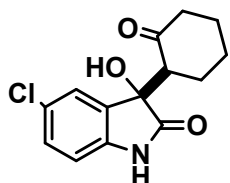
**5-fluoro-3-hydroxy-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4o):**



Pale yellow solid; Mp 188-190  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3+\text{DMSO}-d_6$ ):  $\delta$  1.54-1.74 (m, 3H), 1.92-2.02 (m, 4H), 2.28-2.35 (m, 1H), 3.12-3.20 (m, 1H), 5.73 (s, 1H), 6.78-6.85 (m, 1H), 7.01-7.06 (m, 1H), 7.44 (s, 1H), 9.74 (s, 1H) (major); 1.11-1.27 (m, 3H), 1.75-1.86 (m, 4H), 2.37-2.49 (m, 1H), 3.07-3.11 (m, 1H), 5.17 (s, 1H), 6.86-6.96 (m, 2H), 7.17-7.23 (m, 1H), 9.95 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3+\text{DMSO}-d_6$ ):  $\delta$  24.3, 26.1, 26.6, 41.6, 56.2, 77.2, 110.4, 112.3, 115.1, 131.1, 138.4, 159.6, 178.6, 210.3 (major); 24.0, 26.1, 27.7, 42.3,

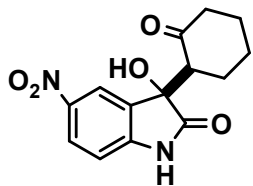
55.6, 75.7, 110.1, 111.9, 114.8, 131.2, 137.8, 156.5, 176.6, 212.7 (minor); IR (KBr)  $\nu$  = 3319, 2945, 1717, 1486, 1194, 827  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 286  $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 286.0846, calcd. for  $\text{C}_{14}\text{H}_{14}\text{FNNaO}_3$ : 286.0855.

**5-chloro-3-hydroxy-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4p):**



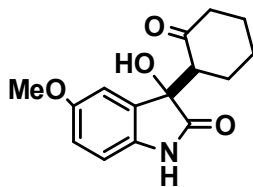
White solid; Mp 229-231  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  1.57-1.73 (m, 3H), 2.00-2.17 (m, 4H), 2.23-2.32 (m, 1H), 3.17-3.22 (m, 1H), 5.89 (s, 1H), 6.82 (d,  $J$  = 8.6 Hz, 1H), 7.13-7.19 (m, 1H), 7.64 (s, 1H), 10.11 (s, 1H) (major); 1.25-1.50 (m, 3H), 1.76-1.89 (m, 4H), 2.34-2.42 (m, 1H), 3.12-3.16 (m, 1H), 5.51 (s, 1H), 6.80 (d,  $J$  = 8.6 Hz, 1H), 7.21-7.26 (m, 1H), 7.36 (s, 1H), 10.19 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  23.8, 26.3, 27.3, 41.2, 56.5, 74.4, 110.2, 124.2, 125.5, 128.0, 131.4, 141.1, 178.1, 209.2 (major); 24.0, 26.0, 26.6, 41.9, 55.8, 75.7, 110.3, 124.7, 126.1, 128.1, 131.8, 140.4, 176.5, 211.1 (minor); IR (KBr)  $\nu$  = 3315, 2943, 1709, 1470, 1185, 823  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 302  $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 302.0552, calcd. for  $\text{C}_{14}\text{H}_{14}\text{ClNNaO}_3$ : 302.0560.

**3-hydroxy-5-nitro-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4q):**



Pale brown solid; Mp 236-238  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  1.54-1.73 (m, 3H), 2.23-2.29 (m, 4H), 2.71-2.74 (m, 1H), 3.28-3.32 (m, 1H), 6.11 (s, 1H), 7.00 (d,  $J$  = 8.4 Hz, 1H), 8.11-8.14 (m, 1H), 8.26 (d,  $J$  = 2.0 Hz, 1H), 10.71 (s, 1H) (major); 1.76-1.95 (m, 3H), 2.03-2.13 (m, 4H), 2.75-2.79 (m, 1H), 3.23-3.27 (m, 1H), 5.83 (s, 1H), 6.97 (d,  $J$  = 8.6 Hz, 1H), 8.15-8.18 (m, 1H), 8.19 (d,  $J$  = 2.0 Hz, 1H), 10.72 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  24.1, 26.4, 27.3, 41.1, 57.1, 73.7, 109.1, 119.8, 125.5, 130.5, 141.6, 149.2, 179.0, 209.3 (major); 24.1, 26.2, 26.9, 41.9, 56.6, 74.4, 109.1, 119.8, 125.5, 131.6, 142.0, 148.4, 177.6, 210.5 (minor); IR (KBr)  $\nu$  = 3337, 3211, 2946, 2864, 1712, 1625, 1339, 1180  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 313  $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 313.0795, calcd. for  $\text{C}_{14}\text{H}_{14}\text{N}_2\text{NaO}_5$ : 313.0800.

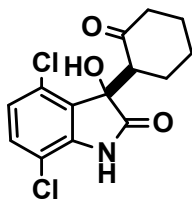
**3-hydroxy-5-methoxy-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4r):**



White solid; Mp 201-203  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  1.43-1.53 (m, 1H), 1.60-1.70 (m, 1H), 1.76-1.85 (m, 1H), 1.90-1.98 (m, 2H), 2.00-2.05 (m, 1H), 2.26-2.33 (m, 1H), 2.53-2.58 (m, 1H), 3.05 (dd,  $J$  = 5.0, 13.2 Hz, 1H), 3.67 (s, 3H), 5.85 (s, 1H), 6.71 (s, 1H), 6.74 (d,  $J$  = 2.4 Hz, 1H), 6.78 (d,  $J$  = 2.4 Hz, 1H), 10.03 (s, 1H) (major); 1.43-1.53 (m, 1H), 1.60-1.70 (m, 1H), 1.76-1.85 (m, 1H), 1.90-1.98 (m, 2H), 2.00-2.05 (m, 1H), 2.26-2.33 (m, 1H), 2.53-2.58 (m, 1H), 3.05 (dd,  $J$  = 5.0, 13.2 Hz, 1H), 3.66 (s, 3H), 5.74 (s, 1H), 6.70 (s, 1H), 6.75 (d,  $J$  = 2.4 Hz, 1H), 6.78 (d,  $J$  = 2.4 Hz, 1H), 9.97 (s, 1H) (major);  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  24.4, 26.6,

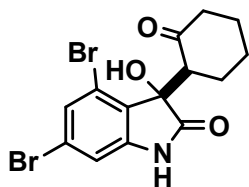
26.6, 41.5, 55.4, 57.3, 74.3, 109.6, 112.2, 112.7, 132.0, 136.6, 154.2, 178.6, 209.2 (major); 24.4, 26.6, 26.6, 41.5, 55.4, 57.3, 74.3, 109.6, 112.2, 112.7, 132.0, 136.6, 154.2, 178.6, 209.2 (minor); IR (KBr)  $\nu$  = 3342, 3221, 2954, 2871, 1724, 1618, 1325, 1162  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 298  $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 242.1052, calcd. for  $\text{C}_{15}\text{H}_{17}\text{NNaO}_4$ : 298.1055.

**4,7-dichloro-3-hydroxy-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4s):**



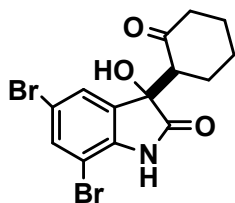
White solid; Mp 169-171  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  1.80-1.94 (m, 3H), 1.96-2.08 (m, 4H), 2.16-2.23 (m, 1H), 3.80 (dd,  $J$  = 5.2, 13.0 Hz, 1H), 6.26 (s, 1H), 6.87 (d,  $J$  = 8.8 Hz, 1H), 7.25 (d,  $J$  = 8.6 Hz, 1H), 10.81 (s, 1H) (major); 1.43-1.70 (m, 4H), 2.25-2.39 (m, 4H), 3.20-3.27 (m, 1H), 6.26 (s, 1H), 6.94 (d,  $J$  = 8.8 Hz, 1H), 7.31 (d,  $J$  = 8.6 Hz, 1H), 10.98 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  24.8, 26.9, 27.8, 41.9, 55.7, 74.6, 123.3, 124.0, 127.6, 130.2, 130.49, 142.5, 177.1, 210.4 (major); 24.4, 26.2, 29.0, 41.6, 56.9, 77.7, 123.3, 124.0, 127.6, 130.2, 130.49, 142.5, 178.1, 210.3 (minor); IR (KBr)  $\nu$  = 3386, 3309, 2952, 1729, 1615, 1467, 1157  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 336  $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 336.0162, calcd. for  $\text{C}_{14}\text{H}_{13}\text{Cl}_2\text{NNaO}_3$ : 336.0170.

**4,6-dibromo-3-hydroxy-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4t):**



White solid; Mp 179-181  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  1.53-1.72 (m, 3H), 2.17-2.42 (m, 4H), 2.61-2.66 (m, 1H), 3.96 (dd,  $J$  = 5.0, 12.8 Hz, 1H), 5.79 (s, 1H), 6.96 (d,  $J$  = 1.5 Hz, 1H), 7.14 (d,  $J$  = 1.5 Hz, 1H), 10.20 (s, 1H) (major); 1.25-1.42 (m, 4H), 1.76-1.89 (m, 2H), 1.96-2.13 (m, 1H), 2.67-2.72 (m, 1H), 3.48 (dd,  $J$  = 5.2, 12.0 Hz, 1H), 6.44 (s, 1H), 6.97 (d,  $J$  = 1.7 Hz, 1H), 7.27 (d,  $J$  = 1.7 Hz, 1H), 10.49 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  24.7, 26.4, 27.2, 41.7, 55.3, 74.0, 111.4, 117.5, 121.9, 126.7, 127.7, 145.5, 177.0, 20.9.7 (major); 22.9, 23.8, 25.8, 41.1, 48.8, 79.5, 112.0, 118.8, 123.0, 124.8, 128.7, 145.0, 176.8, 213.1 (minor); IR (KBr)  $\nu$  = 3285, 2932, 2865, 1725, 1615, 1455, 1166  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 426  $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found 425.9135, calcd. for  $\text{C}_{14}\text{H}_{13}\text{Br}_2\text{NNaO}_3$ : 425.9139.

**5,7-dibromo-3-hydroxy-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4u):**

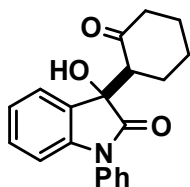


White solid; Mp 137-139  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  1.57-1.75 (m, 3H), 1.99-2.16 (m, 4H), 2.36-2.41 (m, 1H), 3.17 (dd,  $J$  = 5.2, 13.0 Hz, 1H), 5.50 (s, 1H), 7.34 (d,  $J$  = 1.5 Hz, 1H), 7.49 (s, 1H), 9.62 (s, 1H) (major); 1.79-1.90 (m, 3H), 2.27-2.33 (m, 4H), 2.53-2.56 (m, 1H), 3.17 (dd,  $J$  = 5.2, 13.0 Hz, 1H), 6.00 (s, 1H), 7.43 (s, 1H), 7.51 (s, 1H), 9.86 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  24.9, 26.5,



27.3, 41.8, 55.4, 74.3, 111.7, 117.7, 122.1, 127.0, 127.9, 145.5, 177.1, 213.3 (major); 23.1, 24.0, 26.0, 41.3, 48.9, 79.7, 112.2, 119.0, 123.3, 126.9, 128.8, 145.1, 176.9, 209.9 (minor); IR (KBr)  $\nu$  = 3283, 2935, 2861, 1730, 1613, 1457, 1164  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 426  $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found 425.9133, calcd. for  $\text{C}_{14}\text{H}_{13}\text{Br}_2\text{NNaO}_3$ : 425.9139.

**3-hydroxy-1-phenyl-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4v):**



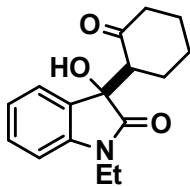
White solid; Mp 127-129 °C;  $^1\text{H}$ NMR (300 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  1.15-1.24 (m, 2H), 1.84-2.11 (m, 4H), 2.29-2.44 (m, 2H) 3.25 (dd,  $J$  = 4.7, 12.8 Hz, 1H), 6.20 (s, 1H), 6.69 (d,  $J$  = 7.7 Hz, 1H), 7.01 (t,  $J$  = 7.5 Hz, 1H), 7.22 (t,  $J$  = 7.5 Hz, 1H), 7.36-7.48 (m, 6H) (major); 1.45-1.55 (m, 2H), 1.63-1.78 (m, 4H), 2.64-2.74 (m, 2H) 3.46 (dd,  $J$  = 4.9, 13.0 Hz, 1H), 6.13 (s, 1H), 6.65 (d,  $J$  = 7.7 Hz, 1H), 7.01 (t,  $J$  = 7.5 Hz, 1H), 7.19 (t,  $J$  = 7.5 Hz, 1H), 7.55-7.62 (m, 6H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  24.2, 26.4, 27.8, 41.2, 58.2, 73.7, 108.6, 122.0, 125.0, 126.5, 127.7, 128.7, 129.4, 129.4, 134.7, 144.6, 175.6, 209.3 (major); 24.5, 26.5, 27.6, 42.0, 58.2, 72.8, 108.2, 122.2, 123.4, 126.5, 127.6, 128.6, 129.4, 129.7, 132.0, 143.9, 175.7, 210.1 (minor); IR (KBr)  $\nu$  = 3355, 2956, 1709, 1615, 1371, 1260, 1061  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 344  $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 344.1265, calcd. for  $\text{C}_{20}\text{H}_{19}\text{NNaO}_3$ : 344.1263.

**3-hydroxy-1-methyl-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4w):**



White solid; Mp 145-147 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  1.77-1.86 (m, 3H), 1.88-2.06 (m, 4H), 2.26-2.35 (m, 1H), 3.08 (s, 3H), 3.17 (dd,  $J$  = 5.0, 12.6 Hz, 1H), 5.95 (s, 1H), 6.92-6.95 (m, 2H), 7.20-7.27 (m, 2H) (major); 1.14-1.24 (m, 2H), 1.38-1.52 (m, 3H), 1.60-1.70 (m, 2H), 2.21-2.24 (m, 1H), 3.09 (s, 3H), 3.13 (dd,  $J$  = 4.9, 13.0 Hz, 1H), 5.86 (s, 1H), 6.87-6.91 (m, 1H), 6.96-6.98 (m, 1H), 7.28-7.32 (m, 2H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  22.6, 23.9, 24.9, 25.9, 39.6, 55.9, 71.7, 106.2, 119.7, 122.5, 126.9, 126.9, 142.9, 175.3, 207.2 (major); 22.7, 23.8, 24.7, 25.9, 40.3, 55.6, 71.5, 106.0, 119.9, 121.3, 128.1, 129.9, 142.2, 174.3, 208.0 (minor); IR (KBr)  $\nu$  = 3349, 2951, 1710, 1615, 1375, 1268, 1064  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 260  $[\text{M}+\text{H}]^+$ ; HRMS (ESI) found: 260.1283, calcd. for  $\text{C}_{15}\text{H}_{18}\text{NO}_3$ : 260.1287.

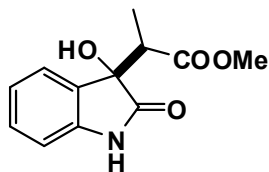
**1-ethyl-3-hydroxy-3-(2-oxocyclohexyl)indolin-2-one (Table 3, 4x):**



White solid; Mp 143-145 °C;  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  1.16 (t,  $J$  = 7.1 Hz, 3H), 1.34-1.52 (m, 2H), 1.89-2.04 (m, 4H), 2.24-2.40 (m, 2H), 3.13 (dd,  $J$  = 5.0, 13.2 Hz, 1H), 3.63-3.78 (m, 2H), 5.89 (s, 1H), 6.89-7.01 (m, 2H), 7.20-7.32 (m, 2H) (major); 1.16 (t,  $J$  = 7.1 Hz, 3H), 1.58-1.73 (m, 2H), 1.76-1.87 (m, 4H), 2.55-

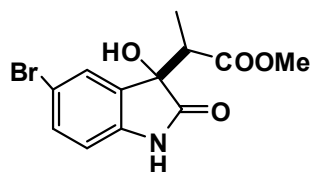
2.65 (m, 2H), 3.30 (dd,  $J = 4.7, 12.8$  Hz, 1H), 3.49-3.62 (m, 2H), 5.81 (s, 1H), 6.78-6.87 (m, 2H), 7.08-7.19 (m, 2H) (minor);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  11.9, 24.3, 26.4, 27.6, 33.6, 41.3, 57.6, 73.4, 108.1, 121.2, 124.5, 128.6, 130.1, 143.7, 176.5, 208.8 (major); 11.7, 24.5, 26.6, 27.7, 33.5, 42.0, 57.4, 73.1, 107.8, 121.4, 123.3, 128.6, 132.0, 143.1, 175.6, 209.5 (minor); IR (KBr)  $\nu = 3375, 2928, 1705, 1614, 1475, 1381, 1265, 1045$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 274$   $[\text{M}+\text{H}]^+$ ; HRMS (ESI) found: 274.1439, calcd. for  $\text{C}_{16}\text{H}_{20}\text{NO}_3$ : 274.1443.

**methyl 2-(3-hydroxy-2-oxoindolin-3-yl)propanoate (Table 4, 5a):**



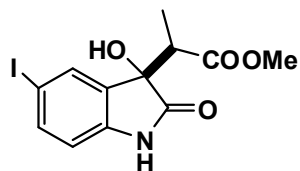
White solid; Mp 119-121  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  1.35 (d,  $J = 7.3$  Hz, 3H), 3.08 (q,  $J = 7.3$  Hz, 1H), 3.34 (s, 3H), 6.12 (s, 1H), 6.79 (d,  $J = 7.6$  Hz, 1H), 6.91 (t,  $J = 7.4$  Hz, 1H), 7.20 (t,  $J = 7.7$  Hz, 1H), 7.27 (d,  $J = 7.4$  Hz, 1H), 10.25 (s, 1H) (major); 0.92 (d,  $J = 7.0$  Hz, 3H), 3.03 (q,  $J = 7.1$  Hz, 1H), 3.54 (s, 3H), 6.14 (s, 1H), 6.80 (d,  $J = 7.4$  Hz, 1H), 6.95 (t,  $J = 7.4$  Hz, 1H), 7.21 (t,  $J = 7.7$  Hz, 1H), 7.39 (d,  $J = 7.3$  Hz, 1H), 10.34 (s, 1H) (minor);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  10.4, 45.5, 51.1, 74.9, 109.39, 121.10, 124.6, 129.0, 129.4, 142.1, 171.8, 177.4 (major); 11.5, 45.7, 51.2, 75.7, 109.3, 121.2, 125.3, 129.1, 129.7, 142.4, 173.0, 178.3 (minor); IR (KBr)  $\nu = 3283, 2979, 1725, 1625, 1472, 1190, 1048, 751$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 258$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 258.0736, calcd. for  $\text{C}_{12}\text{H}_{13}\text{NNaO}_4$ : 258.0742.

**methyl 2-(5-bromo-3-hydroxy-2-oxoindolin-3-yl)propanoate (Table 4, 5b):**



White solid; Mp 204-206  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ):  $\delta$  0.90 (d,  $J = 7.1$  Hz, 3H), 3.04 (q,  $J = 7.1$  Hz, 1H), 3.57 (s, 3H), 6.34 (s, 1H), 6.78 (d,  $J = 8.2$  Hz, 1H), 7.37 (d,  $J = 8.3$  Hz, 1H), 7.56 (d,  $J = 1.9$  Hz, 1H), 10.52 (s, 1H) (major); 1.34 (d,  $J = 7.3$  Hz, 3H), 3.07 (q,  $J = 7.1$  Hz, 1H), 3.38 (s, 3H), 6.32 (s, 1H), 6.77 (d,  $J = 8.2$  Hz, 1H), 7.38 (d,  $J = 8.3$  Hz, 1H), 7.41 (d,  $J = 1.9$  Hz, 1H), 10.43 (s, 1H) (minor);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  11.6, 45.5, 51.5, 75.8, 111.5, 113.1, 128.4, 131.8, 131.9, 141.6, 173.1, 177.1 (major); 10.5, 45.5, 51.3, 75.0, 111.5, 112.8, 127.4, 131.8, 132.2, 141.8, 171.9, 177.9 (minor); IR (KBr)  $\nu = 3251, 2947, 1731, 1699, 1618, 1474, 1206, 1179$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 336$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 335.9849, calcd. for  $\text{C}_{12}\text{H}_{12}\text{BrNNaO}_4$ : 335.9847.

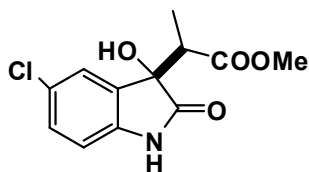
**methyl 2-(5-iodo-3-hydroxy-2-oxoindolin-3-yl)propanoate (Table 4, 5c):**



Pale yellow solid; Mp 209-211  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ):  $\delta$  1.34 (d,  $J = 7.3$  Hz, 3H), 3.03 (q,  $J = 7.1$  Hz, 1H), 3.57 (s, 3H), 6.29 (s, 1H), 6.66 (d,  $J = 8.2$  Hz, 1H), 7.51 (d,  $J = 1.6$  Hz, 1H), 7.56 (d,  $J = 8.2$  Hz, 1H), 10.49 (s, 1H) (major); 1.31 (d,  $J = 7.4$  Hz, 3H), 3.06 (q,  $J = 7.3$  Hz, 1H), 3.38 (s, 3H), 6.27 (s, 1H), 6.65 (d,  $J = 8.0$  Hz, 1H), 7.54 (d,  $J = 1.6$  Hz, 1H), 7.57 (d,  $J = 8.0$  Hz, 1H), 10.40 (s, 1H) (minor);  $^{13}\text{C}$  NMR

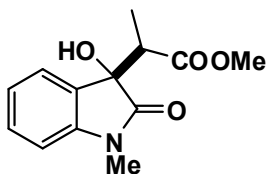
(100 MHz, DMSO- $d_6$ ):  $\delta$  11.5, 45.4, 51.4, 75.6, 84.1, 111.9, 132.0, 133.9, 137.6, 142.2, 173.0, 176.8 (major); 10.4, 45.4, 51.2, 74.7, 83.8, 111.9, 132.5, 132.8, 137.6, 142.0, 171.8, 177.6 (minor); IR (KBr)  $\nu$  = 3251, 2924, 1700, 1615, 1470, 1179  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 384  $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 383.9704, calcd. for  $\text{C}_{12}\text{H}_{12}\text{INNaO}_4$ : 383.9709.

**methyl 2-(5-chloro-3-hydroxy-2-oxoindolin-3-yl)propanoate (Table 4, 5d):**



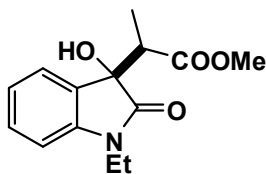
White solid; Mp 178-180  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (300 MHz, DMSO- $d_6$ ):  $\delta$  0.91 (d,  $J$  = 7.1 Hz, 3H), 3.05 (q,  $J$  = 7.1 Hz, 1H), 3.57 (s, 3H), 6.32 (s, 1H), 6.82 (d,  $J$  = 8.2 Hz, 1H), 7.27 (d,  $J$  = 7.3 Hz, 1H), 7.44 (d,  $J$  = 2.1 Hz, 1H), 10.51 (s, 1H) (major); 1.35 (d,  $J$  = 7.3 Hz, 3H), 3.08 (q,  $J$  = 7.3 Hz, 1H), 3.38 (s, 3H), 6.30 (s, 1H), 6.80 (d,  $J$  = 8.1 Hz, 1H), 7.26 (d,  $J$  = 7.1 Hz, 1H), 7.29 (d,  $J$  = 2.2 Hz, 1H), 10.42 (s, 1H) (minor);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  11.5, 45.4, 51.4, 75.8, 110.8, 124.6, 125.6, 129.0, 131.4, 141.1, 173.1, 177.1 (major); 10.4, 45.4, 51.2, 74.9, 110.8, 125.0, 125.2, 128.9, 131.7, 141.3, 171.8, 177.9 (minor); IR (KBr)  $\nu$  = 3438, 3234, 2992, 2953, 1732, 1700, 1621, 1208, 829  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 292  $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 270.0527, calcd. for  $\text{C}_{12}\text{H}_{13}\text{ClNO}_4$ : 270.0533.

**methyl 2-(3-hydroxy-1-methyl-2-oxoindolin-3-yl)propanoate (Table 4, 5e):**



Pale yellow solid; Mp 110-112  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ):  $\delta$  1.01 (d,  $J$  = 7.1 Hz, 3H), 3.18 (s, 3H), 3.16 (q,  $J$  = 7.1 Hz, 1H), 3.64 (s, 3H), 5.98 (s, 1H), 6.85 (d,  $J$  = 7.7 Hz, 1H), 7.06 (t,  $J$  = 7.3 Hz, 1H), 7.29-7.32 (m, 1H), 7.48 (d,  $J$  = 8.1 Hz, 1H) (major); 1.39 (d,  $J$  = 7.0 Hz, 3H), 3.18 (s, 3H), 3.21 (q,  $J$  = 7.3 Hz, 1H), 3.45 (s, 3H), 6.05 (s, 1H), 6.85 (d,  $J$  = 7.7 Hz, 1H), 7.06 (t,  $J$  = 7.3 Hz, 1H), 7.34-7.38 (m, 2H) (minor);  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ):  $\delta$  10.3, 26.1, 45.7, 51.2, 74.6, 108.2, 121.8, 124.2, 129.0, 129.2, 143.8, 171.7, 176.7 (major); 11.5, 25.7, 46.0, 51.3, 75.2, 108.1, 121.9, 124.7, 129.2, 129.3, 143.6, 172.9, 175.6 (minor); IR (KBr)  $\nu$  = 3372, 2926, 1725, 1615, 1473, 1273, 1050, 755  $\text{cm}^{-1}$ ; MS-ESI:  $m/z$  = 272  $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 272.0893, calcd. for  $\text{C}_{13}\text{H}_{15}\text{NNaO}_4$ : 272.0897.

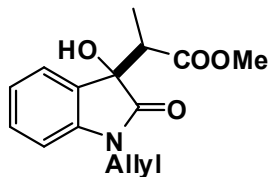
**methyl 2-(1-ethyl-3-hydroxy-2-oxoindolin-3-yl)propanoate (Table 4, 5f):**



Pale yellow solid; Mp 105-107  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ):  $\delta$  1.14 (t,  $J$  = 7.1 Hz, 3H), 1.37 (d,  $J$  = 7.3 Hz, 3H), 3.12 (q,  $J$  = 7.1 Hz, 1H), 3.29 (s, 3H), 3.55-3.65 (m, 2H), 6.19 (s, 1H), 7.01 (t,  $J$  = 7.1 Hz, 2H), 7.29-7.34 (m, 2H) (major); 0.94 (d,  $J$  = 7.1 Hz, 3H), 1.14 (t,  $J$  = 7.1 Hz, 3H), 3.08 (q,  $J$  = 7.1 Hz, 1H), 3.50 (s, 3H), 3.68-3.75 (m, 2H), 6.19 (s, 1H), 6.98 (t,  $J$  = 8.0 Hz, 2H), 7.28 (d,  $J$  = 7.7 Hz, 1H), 7.42 (d,  $J$  = 7.4 Hz, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ):  $\delta$  10.4, 12.1, 33.7, 45.6, 51.1, 74.5, 108.2, 121.6, 124.5, 129.1, 129.2,

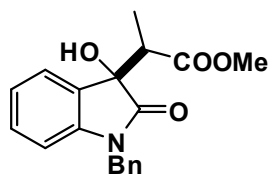
142.7, 171.6, 176.2 (major); 11.5, 12.1, 33.7, 46.1, 51.2, 75.0, 108.1, 121.7, 124.9, 129.1, 129.3, 142.5, 172.8, 175.2 (minor); IR (KBr)  $\nu = 3375, 2924, 1720, 1616, 1470, 1385, 1275, 1053 \text{ cm}^{-1}$ ; MS-ESI:  $m/z = 286 [M+Na]^+$ ; HRMS (ESI) found: 286.1049, calcd. for  $C_{14}H_{17}NNaO_4$ : 286.1056.

**methyl 2-(1-allyl-3-hydroxy-2-oxoindolin-3-yl)propanoate (Table 4, 5g):**



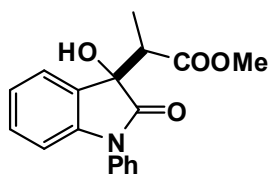
Pale yellow solid; Mp 99-101 °C;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3+\text{DMSO-}d_6$ ):  $\delta$  1.28 (d,  $J = 7.1 \text{ Hz}$ , 3H), 3.23 (q,  $J = 7.1 \text{ Hz}$ , 1H), 3.71 (s, 3H), 4.22-4.26 (m, 1H), 4.34-4.39 (m, 1H), 5.19-5.27 (m, 2H), 5.66 (s, 1H), 5.77-5.82 (m, 1H), 6.83 (d,  $J = 7.7 \text{ Hz}$ , 1H), 7.07 (t,  $J = 7.5 \text{ Hz}$ , 1H), 7.29 (t,  $J = 7.5 \text{ Hz}$ , 1H), 7.39 (d,  $J = 7.3 \text{ Hz}$ , 1H) (major); 1.08 (d,  $J = 7.1 \text{ Hz}$ , 3H), 3.18 (q,  $J = 7.1 \text{ Hz}$ , 1H), 3.59 (s, 3H), 4.17-4.20 (m, 1H), 4.41-4.45 (m, 1H), 5.29-5.32 (m, 2H), 5.39 (s, 1H), 5.84-5.90 (m, 1H), 6.83 (d,  $J = 7.7 \text{ Hz}$ , 1H), 7.07 (t,  $J = 7.5 \text{ Hz}$ , 1H), 7.29 (t,  $J = 7.5 \text{ Hz}$ , 1H), 7.48 (d,  $J = 7.3 \text{ Hz}$ , 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3+\text{DMSO-}d_6$ ):  $\delta$  11.5, 41.9, 45.2, 51.6, 76.1, 108.8, 117.4, 122.4, 123.9, 127.9, 129.3, 130.8, 142.8, 173.8, 176.2 (major); 10.4, 41.9, 45.4, 51.6, 75.8, 108.7, 117.4, 122.4, 124.9, 128.5, 129.3, 130.8, 142.6, 172.8, 175.7 (minor); IR (KBr)  $\nu = 3378, 2928, 1722, 1615, 1466, 1383, 1276, 1054 \text{ cm}^{-1}$ ; MS-ESI:  $m/z = 298 [M+Na]^+$ ; HRMS (ESI) found: 298.1048, calcd. for  $C_{15}H_{17}NNaO_4$ : 298.1055.

**methyl 2-(1-benzyl-3-hydroxy-2-oxoindolin-3-yl)propanoate (Table 4, 5h):**



Pale yellow solid; Mp 120-122 °C;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3+\text{DMSO-}d_6$ ):  $\delta$  1.33 (d,  $J = 7.1 \text{ Hz}$ , 3H), 3.27 (q,  $J = 7.3 \text{ Hz}$ , 1H), 3.51 (s, 3H), 4.79-4.86 (m, 2H), 5.85 (s, 1H), 6.72 (d,  $J = 7.7 \text{ Hz}$ , 1H), 7.02 (t,  $J = 7.5 \text{ Hz}$ , 1H), 7.30-7.38 (m, 7H) (major); 1.10 (d,  $J = 7.1 \text{ Hz}$ , 3H), 3.22 (q,  $J = 7.3 \text{ Hz}$ , 1H), 3.69 (s, 3H), 4.88-4.98 (m, 2H), 5.64 (s, 1H), 6.72 (d,  $J = 7.7 \text{ Hz}$ , 1H), 7.03 (t,  $J = 7.3 \text{ Hz}$ , 1H), 7.18-7.29 (m, 5H), 7.40-7.50 (m, 2H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3+\text{DMSO-}d_6$ ):  $\delta$  10.4, 43.3, 45.1, 51.4, 75.5, 108.7, 122.3, 123.9, 126.9, 127.0, 128.2, 128.5, 129.1, 135.2, 142.7, 172.6, 176.6 (major); 11.4, 43.3, 45.5, 51.4, 75.9, 108.7, 122.1, 124.9, 126.7, 127.1, 128.1, 128.5, 129.1, 135.1, 142.4, 173.6, 176.1 (minor); IR (KBr)  $\nu = 3388, 3030, 2955, 1723, 1614, 1495, 1358, 1180, 1056 \text{ cm}^{-1}$ ; MS-ESI:  $m/z = 348 [M+Na]^+$ ; HRMS (ESI) found: 326.1386, calcd. for  $C_{19}H_{20}NO_4$ : 326.1392.

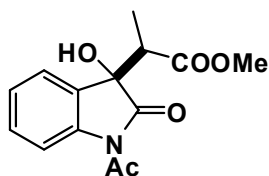
**methyl 2-(1-phenyl-3-hydroxy-2-oxoindolin-3-yl)propanoate (Table 4, 5i):**



White solid; Mp 133-135 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  1.47 (d,  $J = 7.1 \text{ Hz}$ , 3H), 3.26 (q,  $J = 7.0 \text{ Hz}$ , 1H), 3.37 (s, 3H), 6.48 (s, 1H), 6.72 (d,  $J = 7.9 \text{ Hz}$ , 1H), 7.10 (t,  $J = 7.4 \text{ Hz}$ , 1H), 7.26 (t,  $J = 7.6 \text{ Hz}$ , 1H), 7.40 (d,  $J = 7.6 \text{ Hz}$ , 2H), 7.44-7.48 (m, 2H) 7.59 (t,  $J = 7.7 \text{ Hz}$ , 2H) (major); 1.17 (d,  $J = 7.1 \text{ Hz}$ , 3H), 3.21

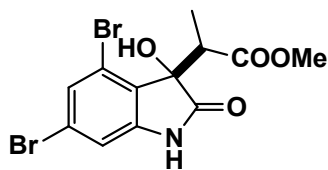
(q,  $J = 7.1$  Hz, 1H), 3.50 (s, 3H), 6.46 (s, 1H), 6.69 (d,  $J = 7.7$  Hz, 1H), 7.06 (t,  $J = 7.4$  Hz, 1H), 7.26 (t,  $J = 7.6$  Hz, 1H), 7.39 (d,  $J = 7.7$  Hz, 2H), 7.50-7.53 (m, 2H) 7.59 (t,  $J = 7.7$  Hz, 2H) (minor);  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ):  $\delta$  10.2, 46.0, 51.4, 74.5, 108.6, 122.4, 124.9, 126.2, 126.4, 127.8, 129.3, 129.5, 134.2, 143.5, 171.7, 176.3 (major); 11.4, 46.8, 51.4, 74.7, 108.5, 122.5, 124.9, 126.2, 126.4, 127.9, 128.8, 129.5, 134.1, 143.2, 172.9, 175.1 (minor); IR (KBr)  $\nu = 3351, 2952, 1736, 1718, 1613, 1376, 1204, 1065$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 334$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 312.1230, calcd. for  $\text{C}_{18}\text{H}_{18}\text{NO}_4$ : 312.1233.

**methyl 2-(1-acetyl-3-hydroxy-2-oxoindolin-3-yl)propanoate (Table 4, 5j):**



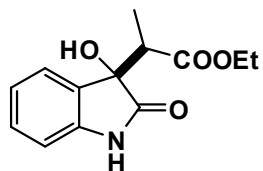
Pale yellow semi solid;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ):  $\delta$  1.42 (d,  $J = 7.3$  Hz, 3H), 2.58 (s, 3H), 3.27 (q,  $J = 7.1$  Hz, 1H), 3.39 (s, 3H), 6.66 (s, 1H), 7.20-7.26 (m, 2H), 7.46 (d,  $J = 7.3$  Hz, 1H), 8.10 (d,  $J = 8.2$  Hz, 1H) (major); 1.31 (d,  $J = 7.3$  Hz, 3H), 2.58 (s, 3H), 3.23 (q,  $J = 7.1$  Hz, 1H), 3.32 (s, 3H), 6.61 (s, 1H), 7.36-7.41 (m, 2H), 7.50 (d,  $J = 7.4$  Hz, 1H), 8.07 (d,  $J = 8.0$  Hz, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ):  $\delta$  9.8, 26.3, 46.6, 51.5, 74.6, 122.2, 124.7, 124.9, 129.5, 135.2, 139.8, 170.2, 172.9, 178.3 (major); 11.3, 27.5, 47.8, 51.5, 74.0, 120.2, 124.1, 125.0, 129.8, 132.9, 139.6, 168.9, 171.5, 176.8 (minor); IR (KBr)  $\nu = 3431, 2982, 1775, 1712, 1273, 1175, 1041, 762$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 300$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 300.0853, calcd. for  $\text{C}_{14}\text{H}_{15}\text{NNaO}_4$ : 300.0848.

**methyl 2-(4,6-dibromo-3-hydroxy-2-oxoindolin-3-yl)propanoate (Table 4, 5k):**



Pale yellow solid; Mp 133-135  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  1.41 (d,  $J = 7.1$  Hz, 3H), 3.33 (s, 3H), 3.71 (q,  $J = 7.1$  Hz, 1H), 6.40 (s, 1H), 6.91 (s, 1H), 7.29 (s, 1H), 10.55 (s, 1H) (major);  $\delta$  0.85 (d,  $J = 7.1$  Hz, 3H), 3.57 (s, 3H), 3.71 (q,  $J = 7.1$  Hz, 1H), 6.18 (s, 1H), 6.98 (s, 1H), 7.37 (s, 1H), 10.68 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ):  $\delta$  10.2, 44.5, 51.4, 75.0, 111.5, 119.2, 122.5, 126.9, 128.4, 145.6, 172.5, 176.1 (major); 11.6, 43.1, 51.5, 78.1, 112.0, 119.4, 122.7, 127.5, 127.8, 145.5, 171.7, 176.2 (minor); IR (KBr)  $\nu = 3314, 2925, 1720, 1705, 1615, 1475, 1180, 1116$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 391$   $[\text{M}+\text{H}]^+$ ; HRMS (ESI) found: 391.9129, calcd. for  $\text{C}_{12}\text{H}_{12}\text{Br}_2\text{NO}_4$ : 391.9133.

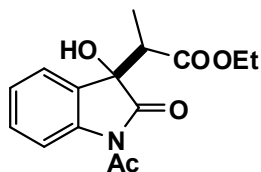
**ethyl 2-(3-hydroxy-2-oxoindolin-3-yl)propanoate (Table 4, 5l):**



White solid; Mp 105-107  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (300 MHz, DMSO- $d_6$ ):  $\delta$  0.87 (t,  $J = 7.0$  Hz, 3H), 1.36 (d,  $J = 7.1$  Hz, 3H), 3.05 (q,  $J = 7.3$  Hz, 1H), 3.76 (q,  $J = 7.0$  Hz, 2H), 6.13 (s, 1H), 6.77 (d,  $J = 7.7$  Hz, 1H), 6.90 (t,  $J = 7.4$  Hz, 1H), 7.17-7.19 (m, 1H), 7.27 (d,  $J = 7.3$  Hz, 1H), 10.26 (s, 1H) (major); 0.98 (d,  $J = 7.1$  Hz, 3H), 1.03 (t,  $J = 7.0$  Hz, 3H), 3.00 (q,  $J = 7.1$  Hz, 1H), 3.95 (q,  $J = 7.1$  Hz, 2H), 6.13 (s, 1H), 6.77 (d,  $J = 7.7$  Hz, 1H),

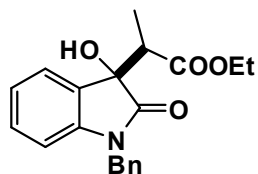
6.94 (t,  $J = 7.6$  Hz, 1H), 7.20-7.22 (m, 1H), 7.38 (d,  $J = 7.3$  Hz, 1H), 10.31 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ):  $\delta$  10.3, 13.4, 45.4, 59.7, 74.9, 109.4, 121.1, 124.7, 125.2, 129.7, 142.5, 171.3, 178.4 (major); 11.4, 13.7, 46.3, 59.8, 75.4, 109.3, 121.2, 124.8, 125.3, 129.8, 142.2, 172.5, 177.4 (minor); IR (KBr)  $\nu = 3284, 2984, 1724, 1621, 1470, 1193, 755$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 272$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 272.0895, calcd. for  $\text{C}_{13}\text{H}_{15}\text{NNaO}_4$ : 272.0899.

**ethyl 2-(1-acetyl-3-hydroxy-2-oxindolin-3-yl)propanoate (Table 4, 5n):**



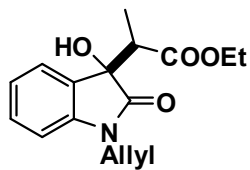
Pale yellow semi solid;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  0.81 (t,  $J = 7.0$  Hz, 3H), 1.42 (d,  $J = 7.3$  Hz, 3H), 2.60 (s, 3H), 3.25 (q,  $J = 7.1$  Hz, 1H), 3.76-3.82 (m, 2H), 6.67 (s, 1H), 7.22 (t,  $J = 6.7$  Hz, 1H), 7.36-7.41 (m, 2H), 8.12 (d,  $J = 8.0$  Hz, 1H) (major); 0.85 (t,  $J = 7.0$  Hz, 3H), 1.32 (d,  $J = 7.1$  Hz, 3H), 2.58 (s, 3H), 3.20 (q,  $J = 7.1$  Hz, 1H), 3.69-3.75 (m, 2H), 6.60 (s, 1H), 7.25 (t,  $J = 6.8$  Hz, 1H), 7.47-7.52 (m, 2H), 8.06 (d,  $J = 8.0$  Hz, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ):  $\delta$  9.7, 13.3, 26.1, 46.4, 60.2, 74.5, 115.6, 124.7, 124.9, 128.6, 129.6, 139.9, 170.3, 170.8, 178.3 (major); 11.2, 13.4, 26.1, 48.4, 60.1, 73.8, 115.4, 124.1, 125.0, 129.6, 130.1, 139.5, 170.2, 172.3, 176.7 (minor); IR (KBr)  $\nu = 3434, 2985, 1771, 1715, 1606, 1465, 1274, 1173$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 314$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 314.1001, calcd. for  $\text{C}_{15}\text{H}_{17}\text{NNaO}_5$ : 314.1004.

**ethyl 2-(1-benzyl-3-hydroxy-2-oxindolin-3-yl)propanoate (Table 4, 5m):**



Pale yellow solid; Mp 115-117  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ):  $\delta$  0.75 (t,  $J = 7.0$  Hz, 3H), 1.41 (d,  $J = 7.1$  Hz, 3H), 3.17 (q,  $J = 7.1$  Hz, 1H), 3.91 (q,  $J = 7.1$  Hz, 2H), 4.84-4.89 (m, 2H), 6.38 (s, 1H), 6.83 (t,  $J = 8.6$  Hz, 1H), 6.97 (t,  $J = 7.4$  Hz, 1H), 7.26 (t,  $J = 7.3$  Hz, 2H), 7.31-7.35 (m, 5H) (major); 0.95 (t,  $J = 7.1$  Hz, 3H), 1.06 (d,  $J = 7.1$  Hz, 3H), 3.13 (q,  $J = 7.1$  Hz, 1H), 3.65-3.76 (m, 2H), 4.77-4.81 (m, 2H), 6.36 (s, 1H), 6.83 (t,  $J = 8.6$  Hz, 1H), 7.01 (t,  $J = 7.4$  Hz, 1H), 7.21 (t,  $J = 7.7$  Hz, 2H), 7.36-7.40 (m, 4H), 7.45 (d,  $J = 7.0$  Hz, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ):  $\delta$  10.6, 13.5, 42.8, 45.7, 59.9, 74.7, 109.0, 122.1, 124.7, 125.0, 127.5, 128.5, 129.2, 129.5, 136.3, 143.1, 171.4, 177.1 (major); 11.5, 13.8, 42.8, 46.7, 60.0, 75.1, 109.0, 122.2, 124.6, 124.9, 127.5, 128.6, 129.3, 129.4, 136.3, 142.7, 172.5, 176.0 (minor); IR (KBr)  $\nu = 3397, 3323, 2985, 1720, 1694, 1613, 1376, 1180$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 362$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 362.1371, calcd. for  $\text{C}_{20}\text{H}_{21}\text{NNaO}_4$ : 362.1368.

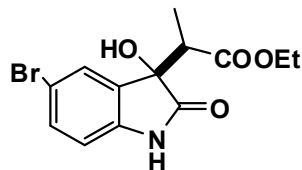
**ethyl 2-1-allyl-3-hydroxy-2-oxindolin-3-yl)propanoate (Table 4, 5o):**



Pale yellow solid; Mp 89-91  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  0.87 (t,  $J = 7.3$  Hz, 3H), 1.31 (d,  $J = 7.3$  Hz, 3H), 3.12 (q,  $J = 7.1$  Hz, 1H), 3.75 (q,  $J = 7.0$  Hz, 2H), 4.22-4.27 (m, 2H), 5.14-5.20 (m, 2H), 5.74-5.80 (m, 1H), 6.27 (s, 1H), 6.89 (d,  $J = 7.7$  Hz, 1H), 6.98 (t,  $J = 7.5$  Hz, 1H), 7.27 (t,  $J = 7.7$  Hz, 1H), 7.35

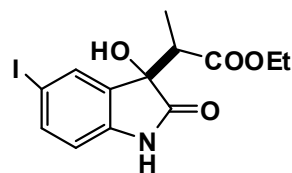
(d,  $J = 7.3$  Hz, 1H) (major); 0.85 (t,  $J = 7.1$  Hz, 3H), 1.39 (d,  $J = 7.1$  Hz, 3H), 3.09 (q,  $J = 7.1$  Hz, 1H), 3.93 (q,  $J = 6.9$  Hz, 2H), 4.28-4.34 (m, 2H), 5.22-5.32 (m, 2H), 5.81-5.88 (m, 1H), 6.26 (s, 1H), 6.89 (d,  $J = 7.7$  Hz, 1H), 7.02 (t,  $J = 7.5$  Hz, 1H), 7.27 (t,  $J = 7.7$  Hz, 1H), 7.44 (d,  $J = 7.3$  Hz, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ):  $\delta$  10.4, 13.5, 41.4, 45.6, 59.7, 74.4, 108.8, 117.0, 121.7, 124.4, 129.0, 129.1, 131.7, 143.0, 171.1, 176.4 (major); 11.3, 13.6, 41.3, 45.5, 59.7, 74.8, 108.7, 116.9, 121.8, 124.7, 129.0, 129.3, 131.7, 142.6, 172.3, 175.3 (minor); IR (KBr)  $\nu = 3434, 2985, 1771, 1715, 1606, 1465, 1274, 1173$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 312$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 312.1208, calcd. for  $\text{C}_{16}\text{H}_{19}\text{NNaO}_4$ : 312.1211.

**ethyl 2-(5-bromo-3-hydroxy-2-oxindolin-3-yl)propanoate (Table 4, 5p):**



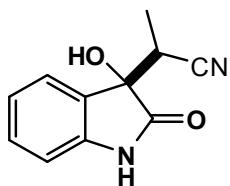
Pale yellow solid; Mp 228-230  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (300 MHz, DMSO- $d_6$ ):  $\delta$  0.95 (d,  $J = 7.1$  Hz, 3H), 1.07 (t,  $J = 7.1$  Hz, 3H), 3.00 (q,  $J = 7.1$  Hz, 1H), 3.98 (q,  $J = 7.1$  Hz, 2H), 6.28 (s, 1H), 6.65 (d,  $J = 8.2$  Hz, 1H), 7.54 (d,  $J = 4.5$  Hz, 1H), 7.71 (d,  $J = 1.6$  Hz, 1H), 10.47 (s, 1H) (major); 0.91 (t,  $J = 7.0$  Hz, 3H), 1.33 (d,  $J = 7.3$  Hz, 3H), 3.03 (q,  $J = 7.1$  Hz, 1H), 3.80 (q,  $J = 7.1$  Hz, 2H), 6.29 (s, 1H), 6.65 (d,  $J = 8.2$  Hz, 1H), 7.50 (d,  $J = 1.6$  Hz, 1H), 7.56 (d,  $J = 4.5$  Hz, 1H), 10.42 (s, 1H) (minor);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  11.3, 13.7, 46.0, 59.9, 75.5, 111.3, 112.9, 128.3, 131.8, 132.1, 141.5, 172.4, 176.9 (major); 10.3, 13.5, 45.3, 59.8, 74.9, 111.4, 112.7, 127.3, 131.8, 132.1, 141.8, 171.2, 177.9 (minor); IR (KBr)  $\nu = 3316, 2924, 1725, 1700, 1619, 1471, 1183, 1119$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 350$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 350.0021, calcd. for  $\text{C}_{13}\text{H}_{14}\text{BrNNaO}_3$ : 350.0004.

**ethyl 2-(3-hydroxy-5-iodo-2-oxindolin-3-yl)propanoate (Table 4, 5q):**



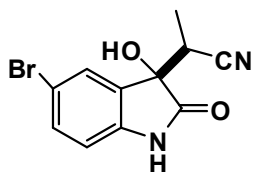
Pale brown solid; Mp 223-225  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  0.96 (d,  $J = 7.1$  Hz, 3H), 1.08 (t,  $J = 7.1$  Hz, 3H), 3.00 (q,  $J = 7.1$  Hz, 1H), 3.98 (q,  $J = 7.1$  Hz, 2H), 6.27 (s, 1H), 6.64 (d,  $J = 8.0$  Hz, 1H), 7.54 (d,  $J = 4.5$  Hz, 1H), 7.71 (d,  $J = 1.6$  Hz, 1H), 10.46 (s, 1H) (major); 0.92 (t,  $J = 7.0$  Hz, 3H), 1.34 (d,  $J = 7.3$  Hz, 3H), 3.03 (q,  $J = 7.3$  Hz, 1H), 3.80 (q,  $J = 7.0$  Hz, 2H), 6.28 (s, 1H), 6.64 (d,  $J = 8.0$  Hz, 1H), 7.51 (d,  $J = 1.6$  Hz, 1H), 7.56 (d,  $J = 4.7$  Hz, 1H), 10.41 (m, 1H) (minor);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  11.3, 13.7, 46.0, 59.9, 75.5, 84.0, 111.8, 132.3, 133.8, 137.6, 142.0, 172.4, 176.7 (major); 10.3, 13.4, 45.3, 59.8, 74.7, 83.7, 111.9, 132.4, 132.8, 137.6, 142.3, 171.2, 177.7 (minor); IR (KBr)  $\nu = 3325, 3244, 2921, 1700, 1615, 1469, 1181, 1053$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 398$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 376.0040, calcd. for  $\text{C}_{13}\text{H}_{15}\text{INNaO}_4$ : 376.0050.

**2-(3-hydroxy-2-oxoindolin-3-yl)propanenitrile (Table 5, 5r):**



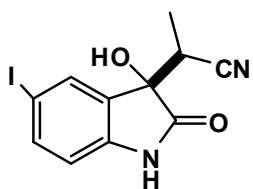
Yellow semi solid;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3+\text{DMSO}-d_6$ ):  $\delta$  0.97 (d,  $J = 7.1$  Hz, 3H), 3.29 (q,  $J = 7.1$  Hz, 1H), 6.62 (s, 1H), 6.91 (d,  $J = 7.7$  Hz, 1H), 7.06 (t,  $J = 7.5$  Hz, 1H), 7.28 (t,  $J = 6.7$  Hz, 1H), 7.62 (d,  $J = 7.3$  Hz, 1H), 10.29 (s, 1H) (major); 1.36 (d,  $J = 7.1$  Hz, 3H), 3.21 (q,  $J = 7.1$  Hz, 1H), 6.50 (s, 1H), 6.91 (d,  $J = 7.7$  Hz, 1H), 7.02 (t,  $J = 7.5$  Hz, 1H), 7.26 (t,  $J = 6.4$  Hz, 1H), 7.38 (d,  $J = 7.3$  Hz, 1H), 10.29 (s, 1H) (minor);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3+\text{DMSO}-d_6$ ):  $\delta$  12.0, 33.2, 75.0, 109.9, 120.0, 121.9, 124.0, 127.0, 129.7, 141.7, 176.5 (major); 11.3, 33.1, 74.8, 109.9, 119.1, 121.7, 124.0, 128.0, 129.5, 141.6, 176.5 (minor); IR (KBr)  $\nu = 3415, 2922, 2851, 2106, 1618, 1265, 1073$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 225$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 225.0635, calcd. for  $\text{C}_{11}\text{H}_{10}\text{NNaO}_2$ : 225.0640.

**2-(5-bromo-3-hydroxy-2-oxoindolin-3-yl)propanenitrile (Table 5, 5s):**



Yellow semi solid;  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ):  $\delta$  0.94 (d,  $J = 7.0$  Hz, 3H), 3.31 (q,  $J = 7.0$  Hz, 1H), 6.88 (s, 1H), 6.89-6.91 (m, 1H), 7.20 (d,  $J = 2.6$  Hz, 1H), 7.23 (d,  $J = 2.6$  Hz, 1H), 10.63 (s, 1H) (major); 1.16 (d,  $J = 7.0$  Hz, 3H), 3.40 (q,  $J = 7.0$  Hz, 1H), 6.75 (s, 1H), 6.84-6.87 (m, 1H), 7.11 (d,  $J = 2.6$  Hz, 1H), 7.29 (d,  $J = 2.6$  Hz, 1H), 10.58 (s, 1H) (minor);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ ):  $\delta$  11.9, 33.0, 75.0, 111.0, 111.6, 116.4, 120.4, 129.6, 138.2, 159.1, 176.1 (major); 11.5, 32.4, 74.7, 111.9, 113.5, 119.7, 127.3, 131.1, 132.6, 141.2, 175.8 (minor); IR (KBr)  $\nu = 3421, 2923, 2854, 2255, 1653, 1477, 1025$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 279$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 279.9838, calcd. for  $\text{C}_{11}\text{H}_9\text{BrNNaO}_2$ : 279.9847.

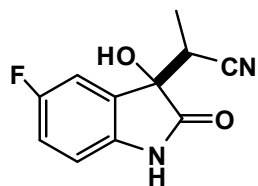
**2-(3-hydroxy-5-iodo-2-oxoindolin-3-yl)propanenitrile (Table 5, 5t):**



Yellow semi solid;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3+\text{DMSO}-d_6$ ):  $\delta$  1.01 (d,  $J = 7.1$  Hz, 3H), 3.30 (q,  $J = 6.9$  Hz, 1H), 6.72 (s, 1H), 7.51-7.56 (m, 2H), 7.89 (s, 1H), 10.37 (s, 1H) (major); 1.38 (d,  $J = 6.7$  Hz, 3H), 3.19 (q,  $J = 7.1$  Hz, 1H), 6.70 (s, 1H), 7.57-7.62 (m, 2H), 7.66 (s, 1H), 10.37 (s, 1H) (minor);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ ):  $\delta$  12.1, 33.1, 74.7, 84.9, 120.6, 124.2, 130.7, 132.4, 138.8, 141.9, 175.7 (major); 12.0, 33.2, 74.8, 84.8, 119.9, 124.2, 130.3, 132.8, 138.6, 142.1, 175.8 (minor); IR (KBr)  $\nu = 3423, 2918, 2850, 2251, 1720, 1475, 1022$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 350$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 350.9703, calcd. for  $\text{C}_{11}\text{H}_9\text{INNaO}_2$ : 350.9606.



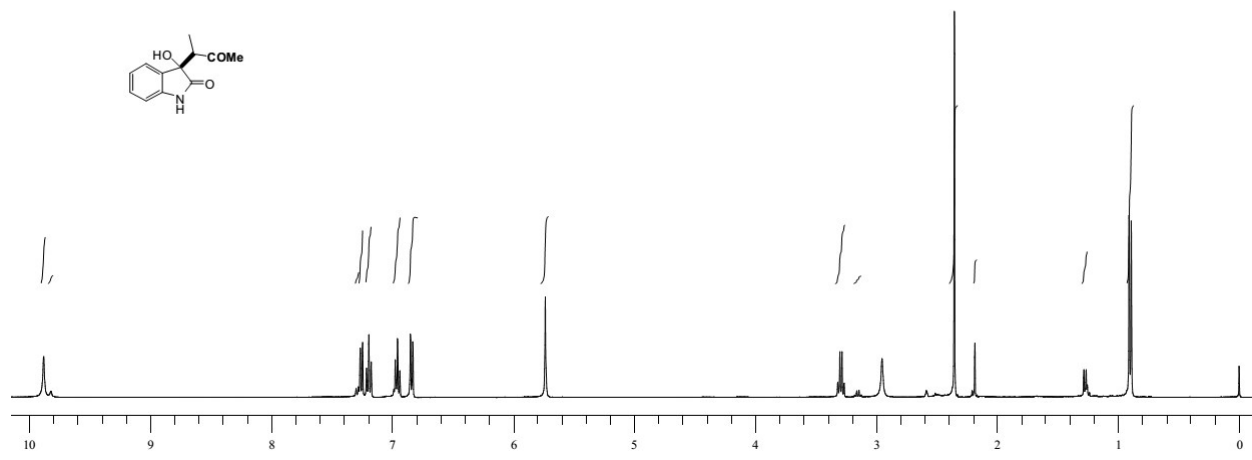
**2-(5-fluoro-3-hydroxy-2-oxindolin-3-yl)propanenitrile (Table 5, 5u):**



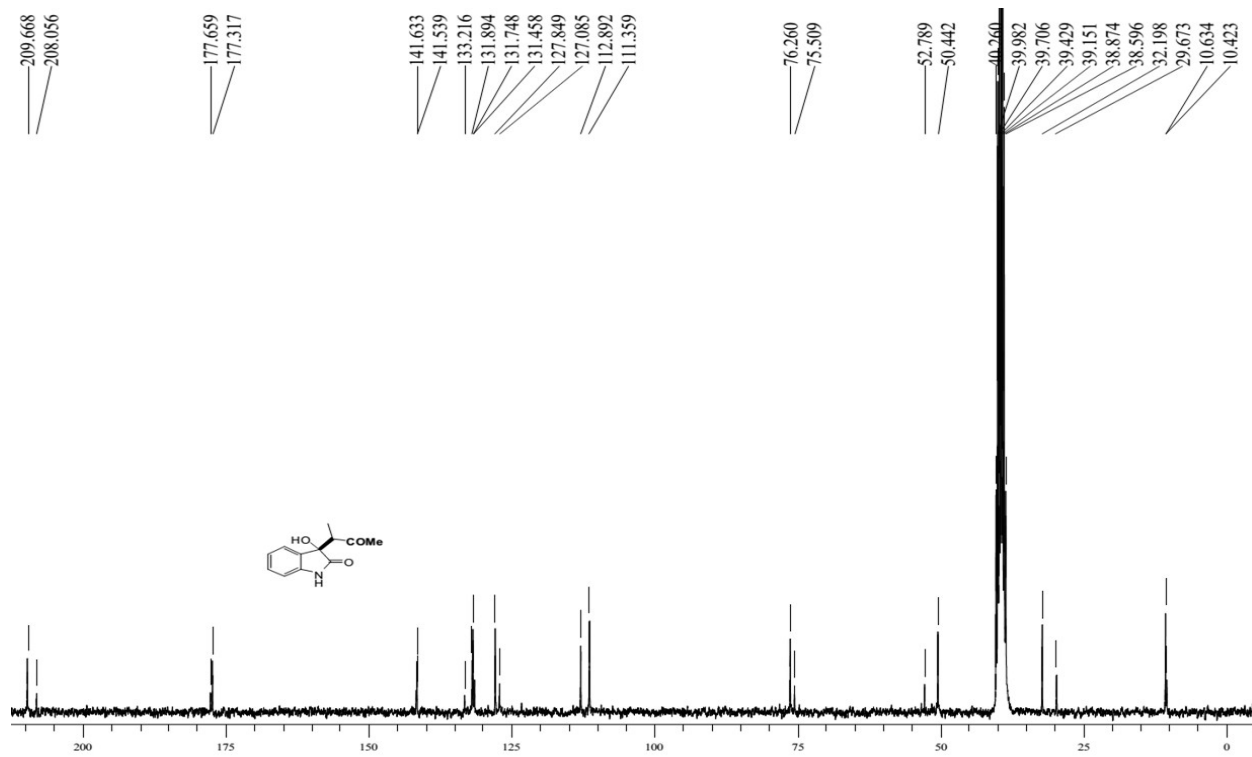
Yellow semi solid;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  0.94 (d,  $J = 7.0$  Hz, 3H), 3.32 (q,  $J = 7.0$  Hz, 1H), 6.86 (d,  $J = 8.1$  Hz, 1H), 6.89 (s, 1H), 7.50 (d,  $J = 2.0$  Hz, 1H), 7.52 (d,  $J = 2.0$  Hz, 1H), 10.75 (s, 1H) (major); 1.16 (d,  $J = 6.9$  Hz, 3H), 3.42 (q,  $J = 7.0$  Hz, 1H), 6.77 (d,  $J = 8.3$  Hz, 1H), 6.83 (s, 1H), 7.46 (d,  $J = 2.0$  Hz, 1H), 7.48 (d,  $J = 2.0$  Hz, 1H), 10.70 (s, 1H) (minor);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  11.8, 33.0, 74.8, 112.1, 113.6, 120.4, 126.7, 130.3, 132.8, 141.4, 175.7 (major); 11.8, 33.0, 74.8, 112.1, 113.6, 120.4, 126.7, 130.3, 132.8, 141.4, 175.7 (minor); IR (KBr)  $\nu = 3418, 2923, 2855, 2104, 1614, 1269, 1075$   $\text{cm}^{-1}$ ; MS-ESI:  $m/z = 243$   $[\text{M}+\text{Na}]^+$ ; HRMS (ESI) found: 243.0539, calcd. for  $\text{C}_{11}\text{H}_9\text{FNNaO}_2$ : 243.0545.

## Compound 4a

### <sup>1</sup>H NMR

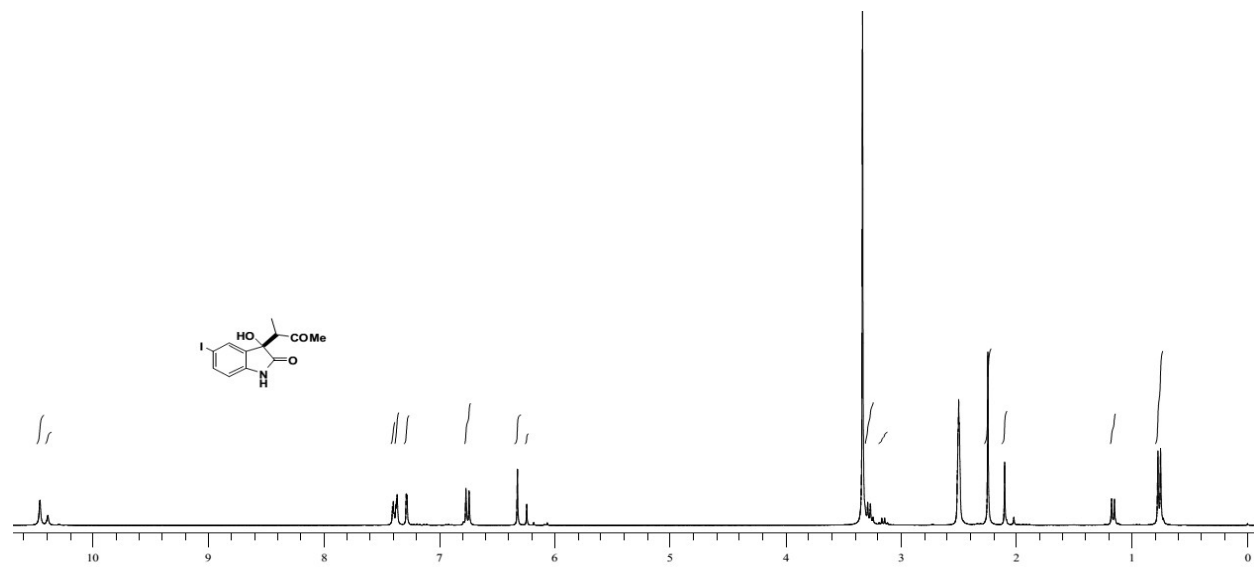


### <sup>13</sup>C NMR

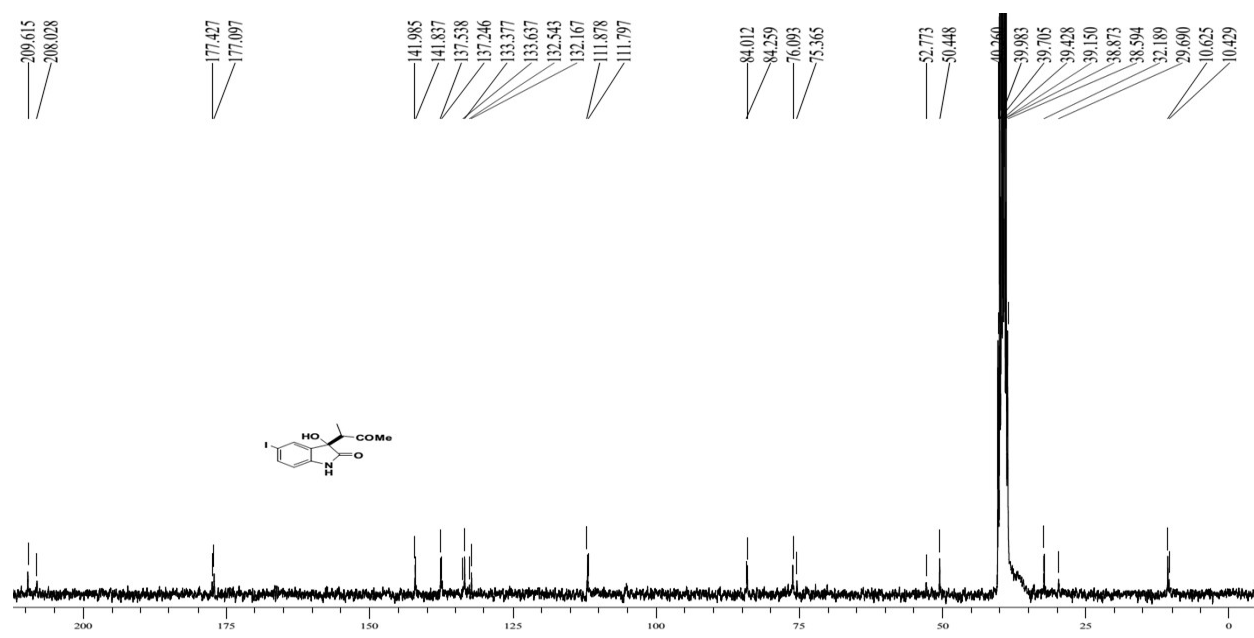


## Compound 4b

### <sup>1</sup>H NMR

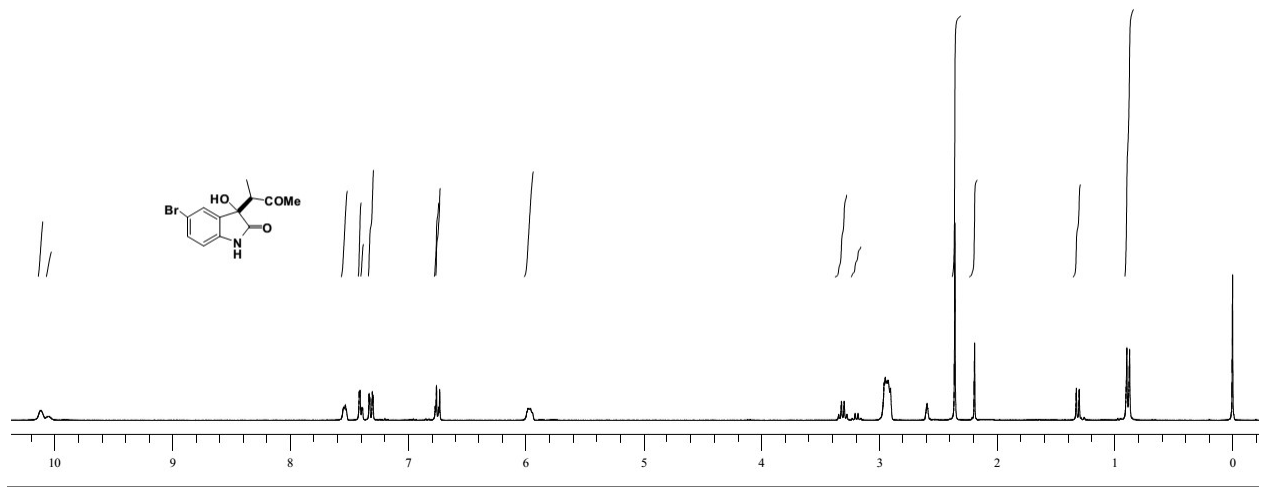


### <sup>13</sup>C NMR

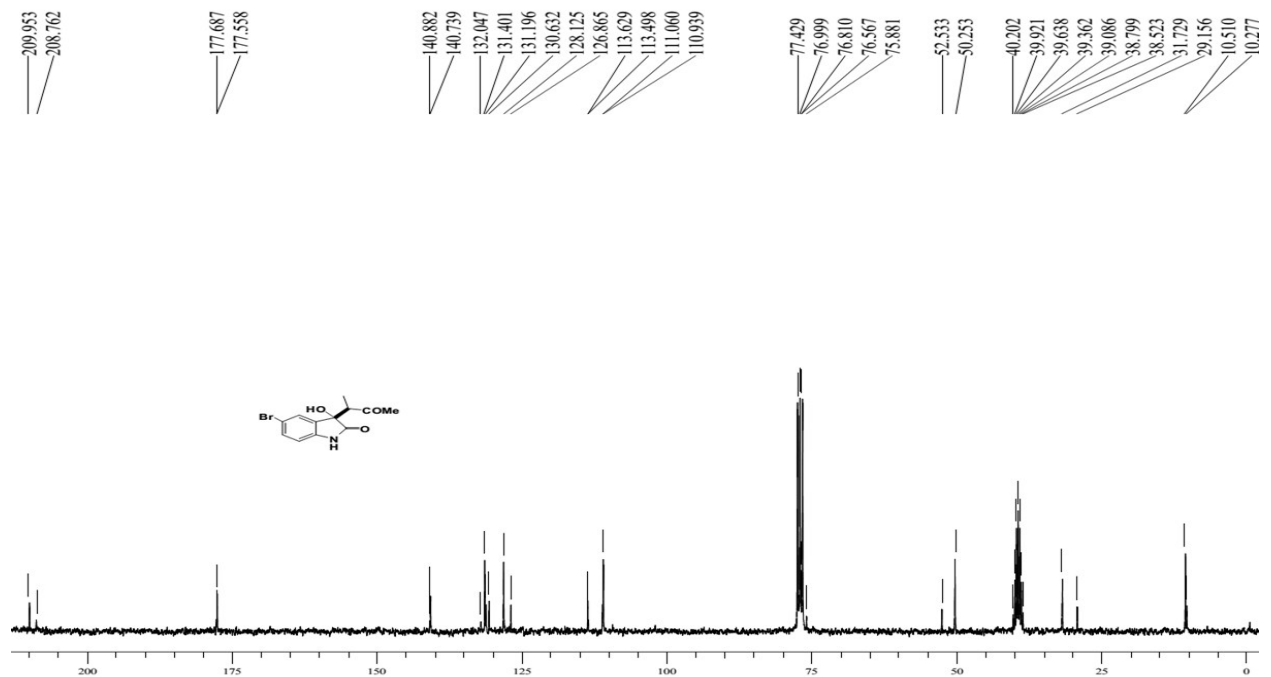


## Compound 4c

# <sup>1</sup>H NMR

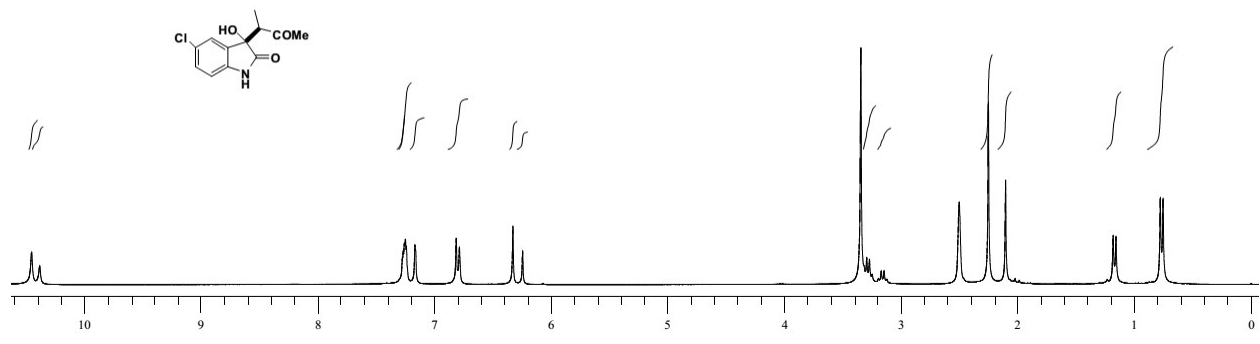


# <sup>13</sup>C NMR

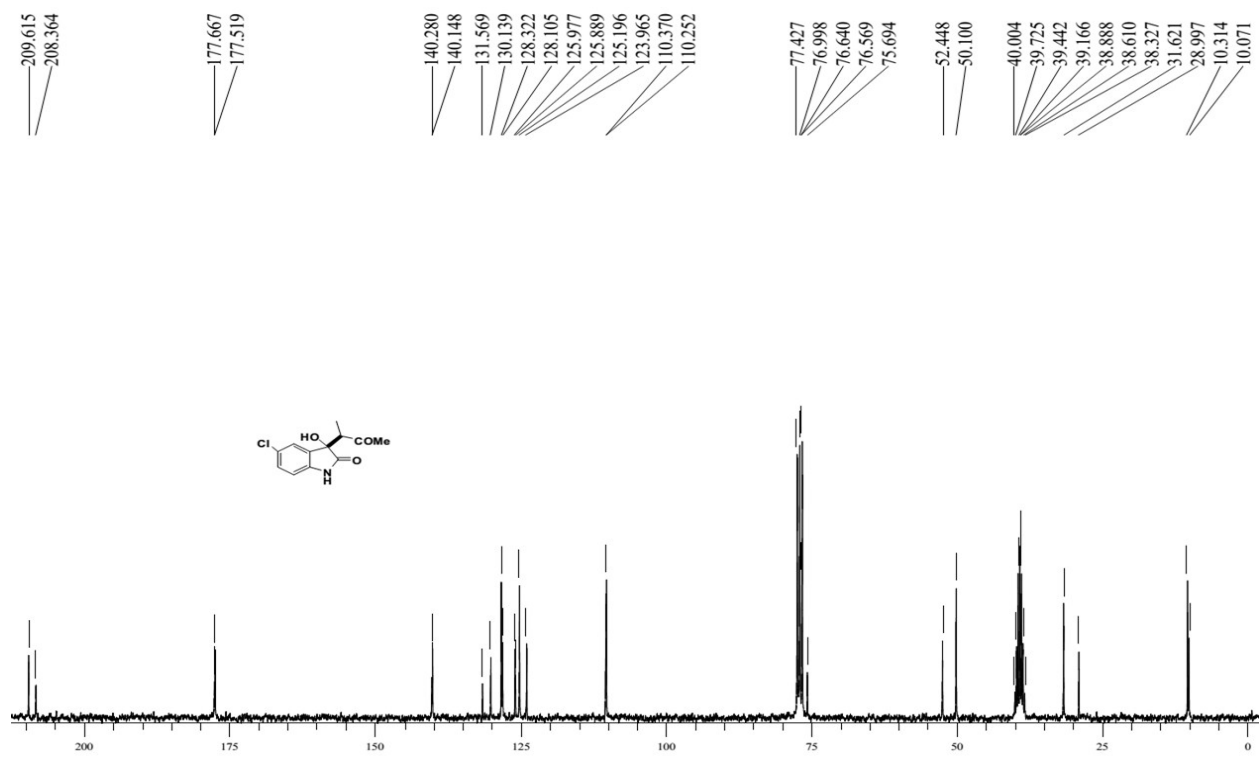


**Compound 4d**

## <sup>1</sup>H NMR

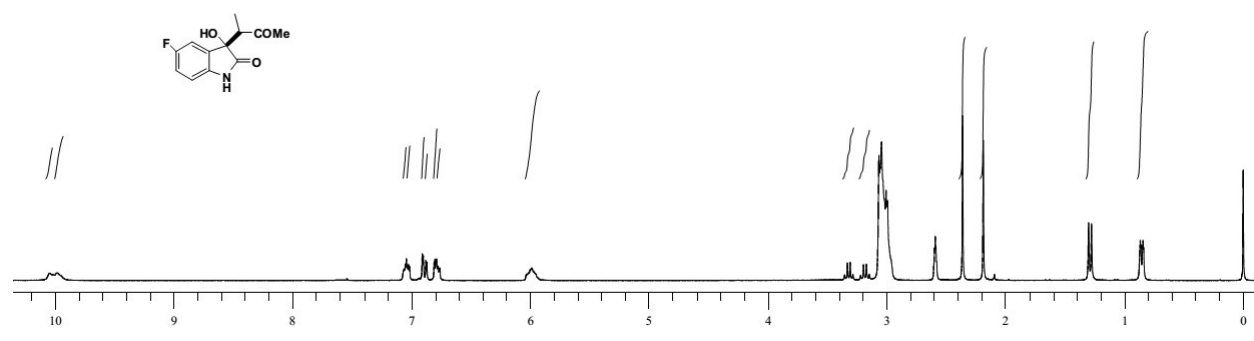


## <sup>13</sup>C NMR

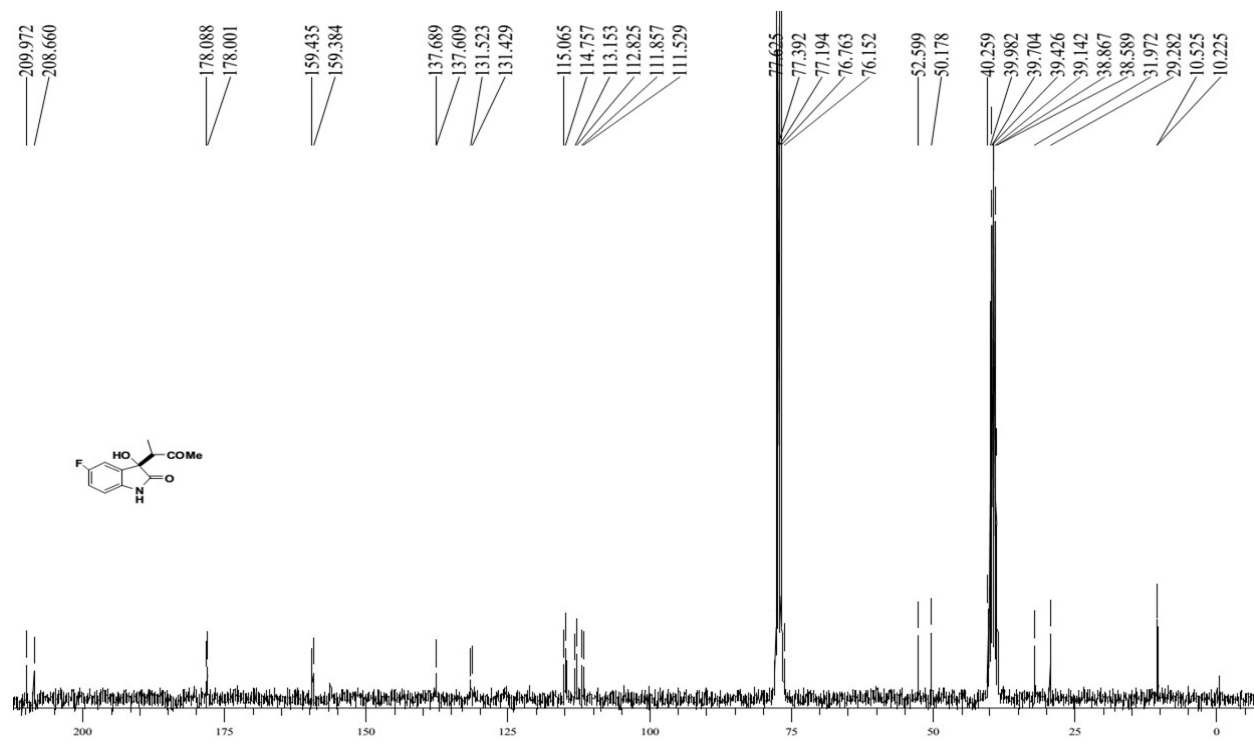


Compound 4e

## <sup>1</sup>H NMR

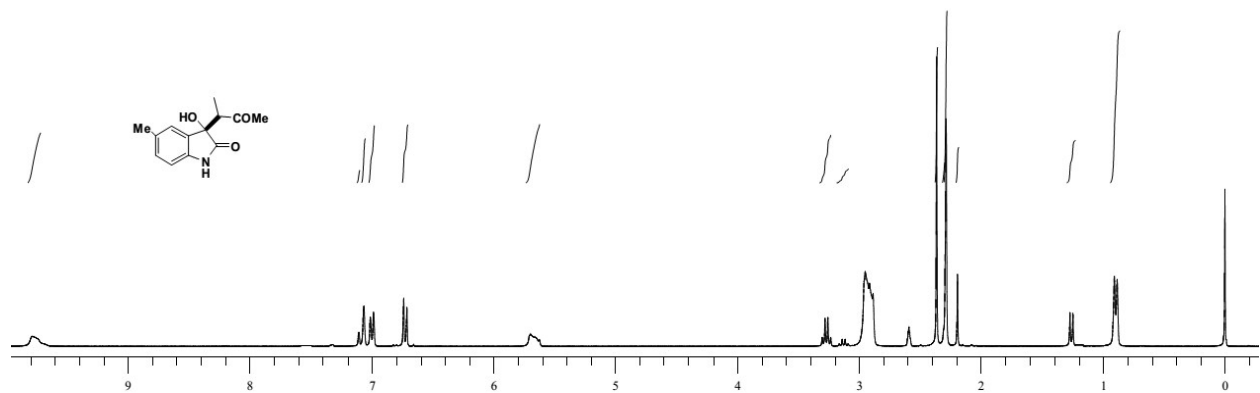


## <sup>13</sup>C NMR

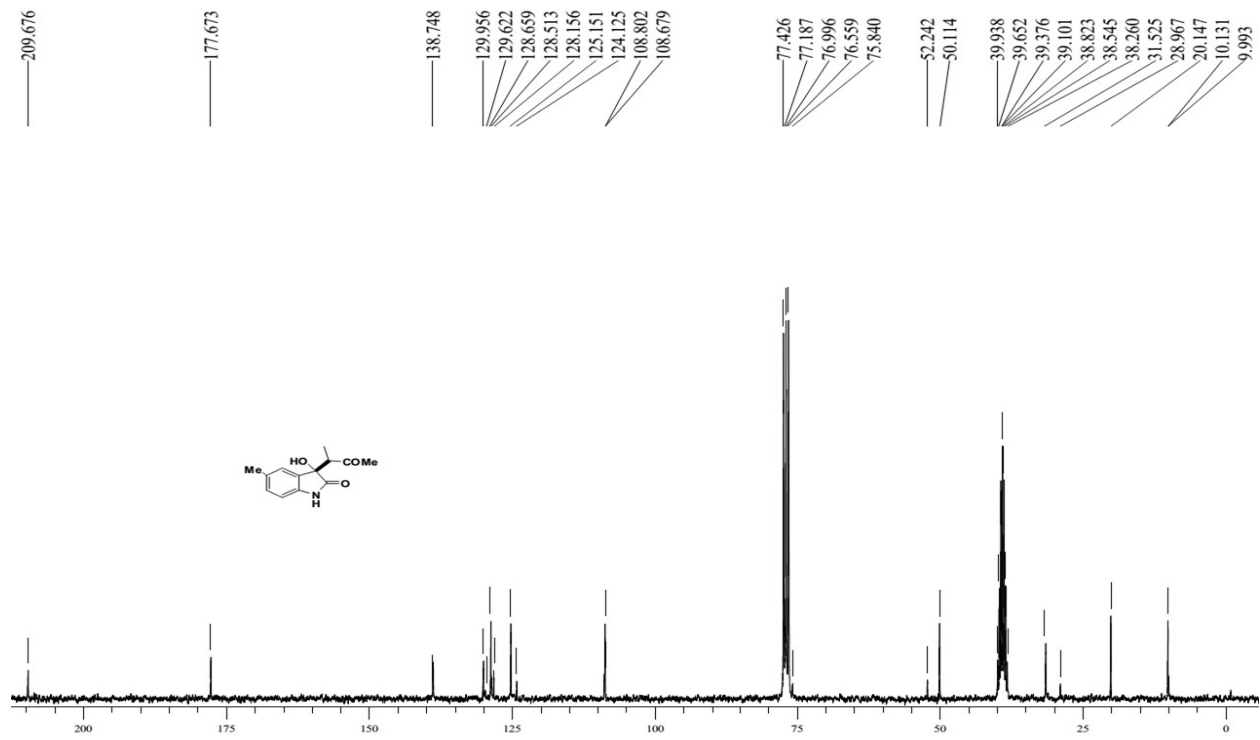


Compound 4f

# <sup>1</sup>H NMR

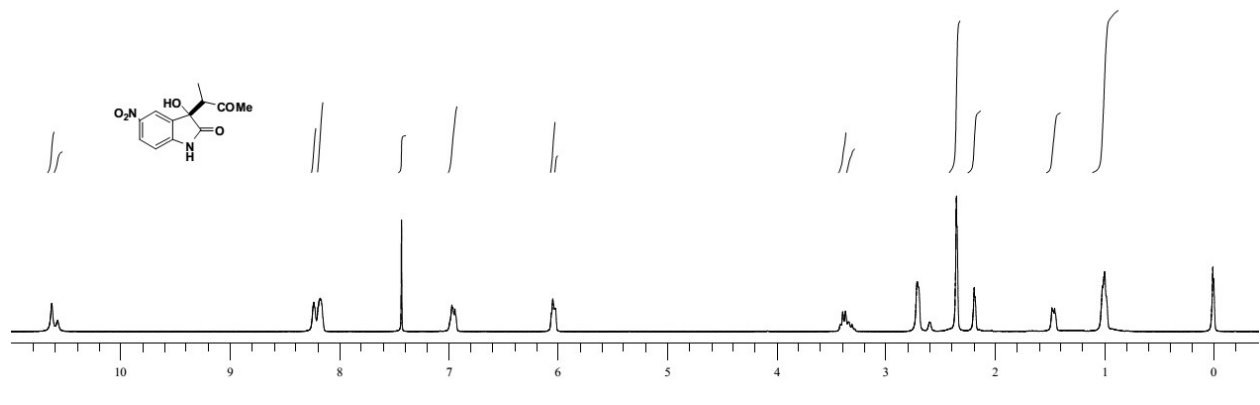


# <sup>13</sup>C NMR

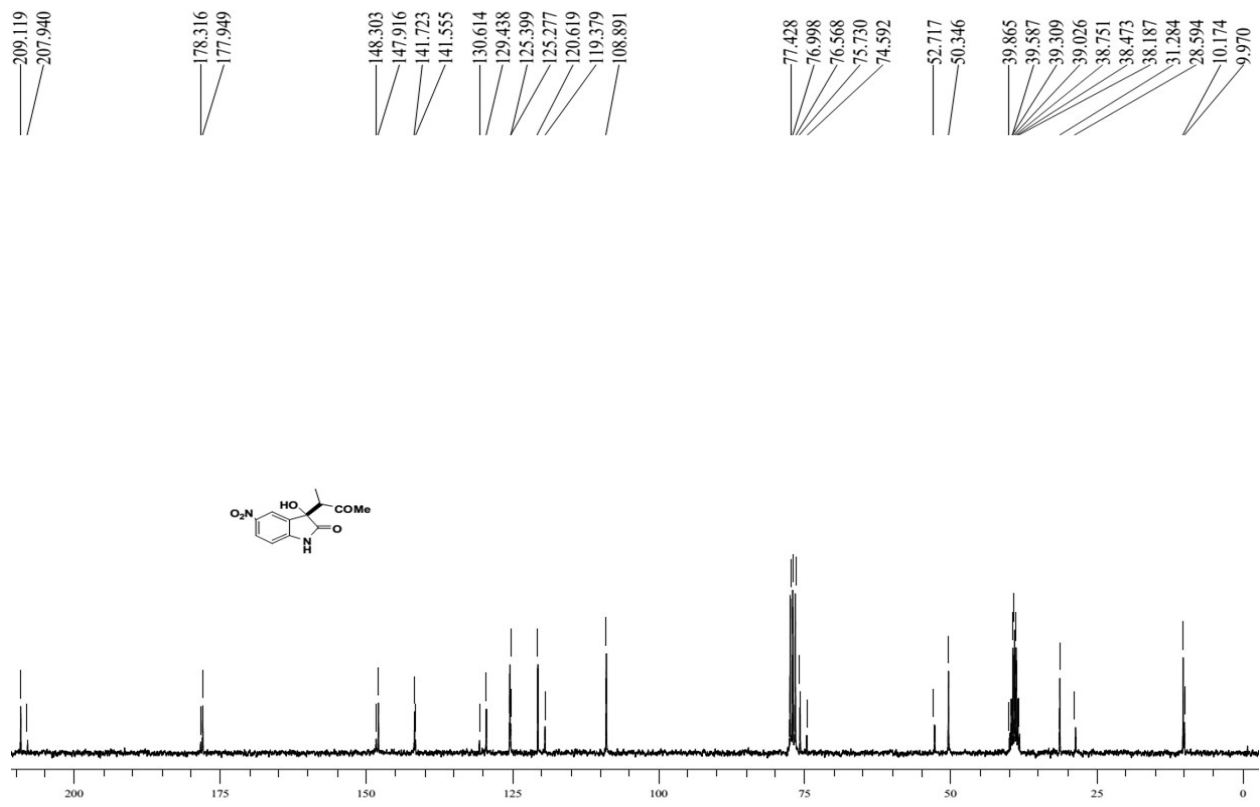


Compound 4g

## <sup>1</sup>H NMR



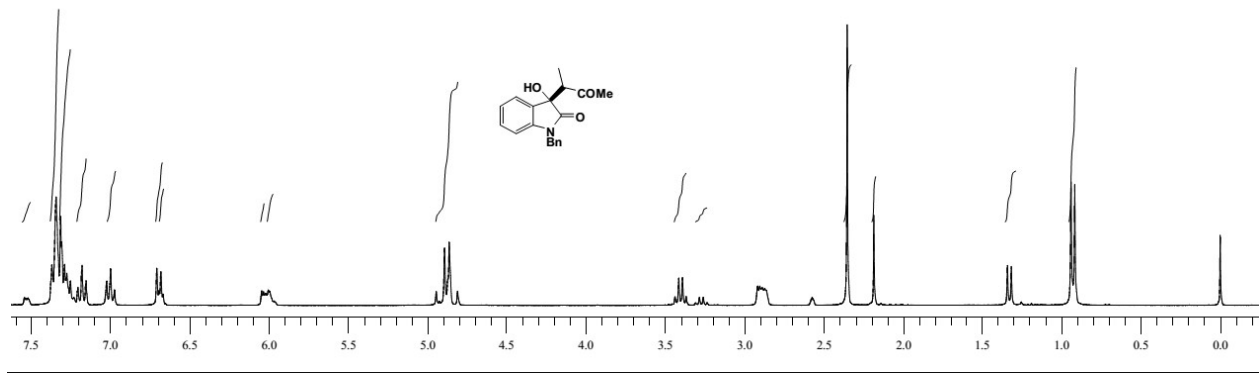
## <sup>13</sup>C NMR



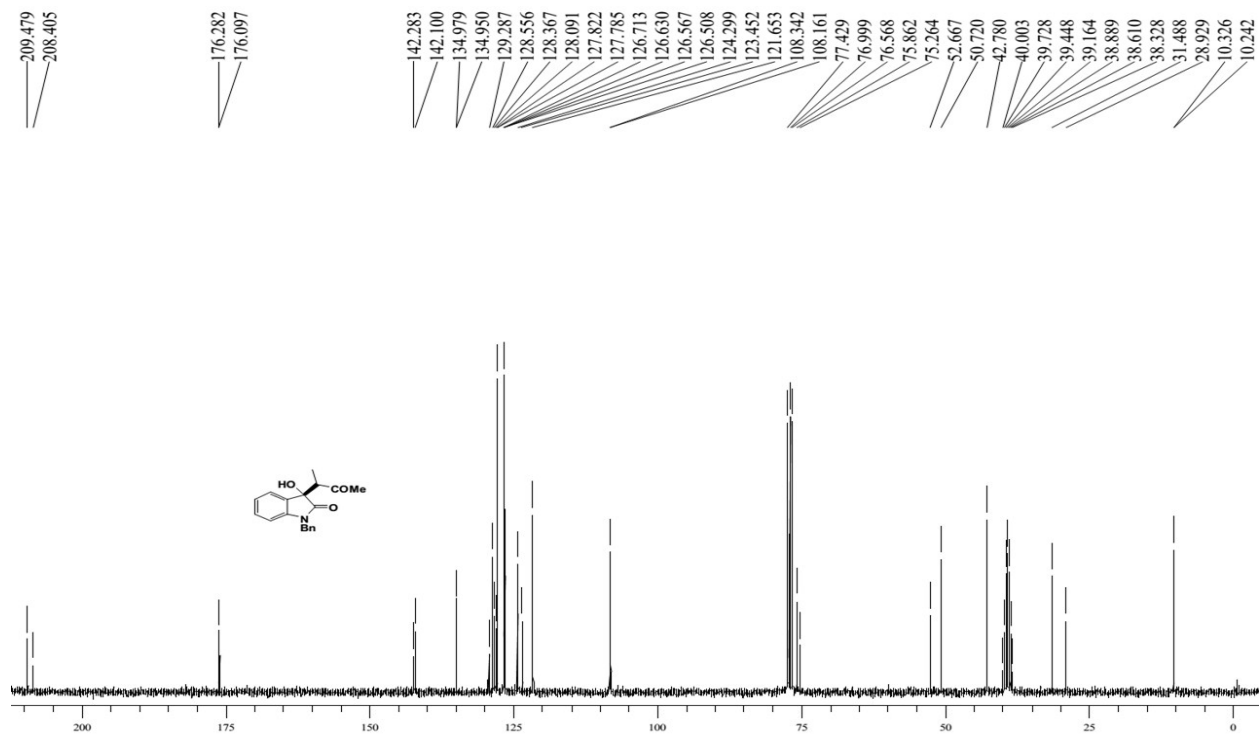
Compound 4h



## <sup>1</sup>H NMR

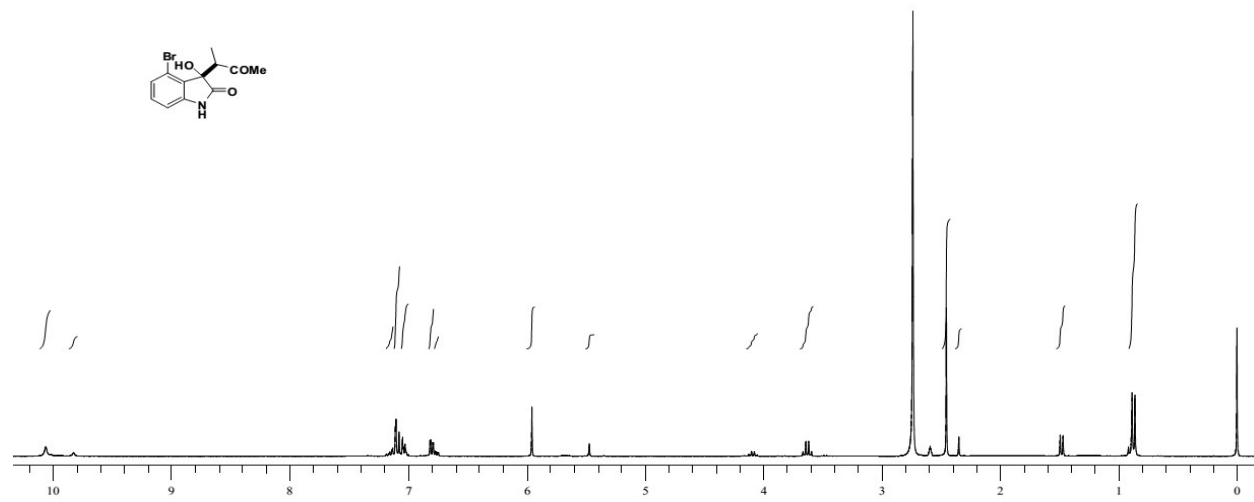


## <sup>13</sup>C NMR

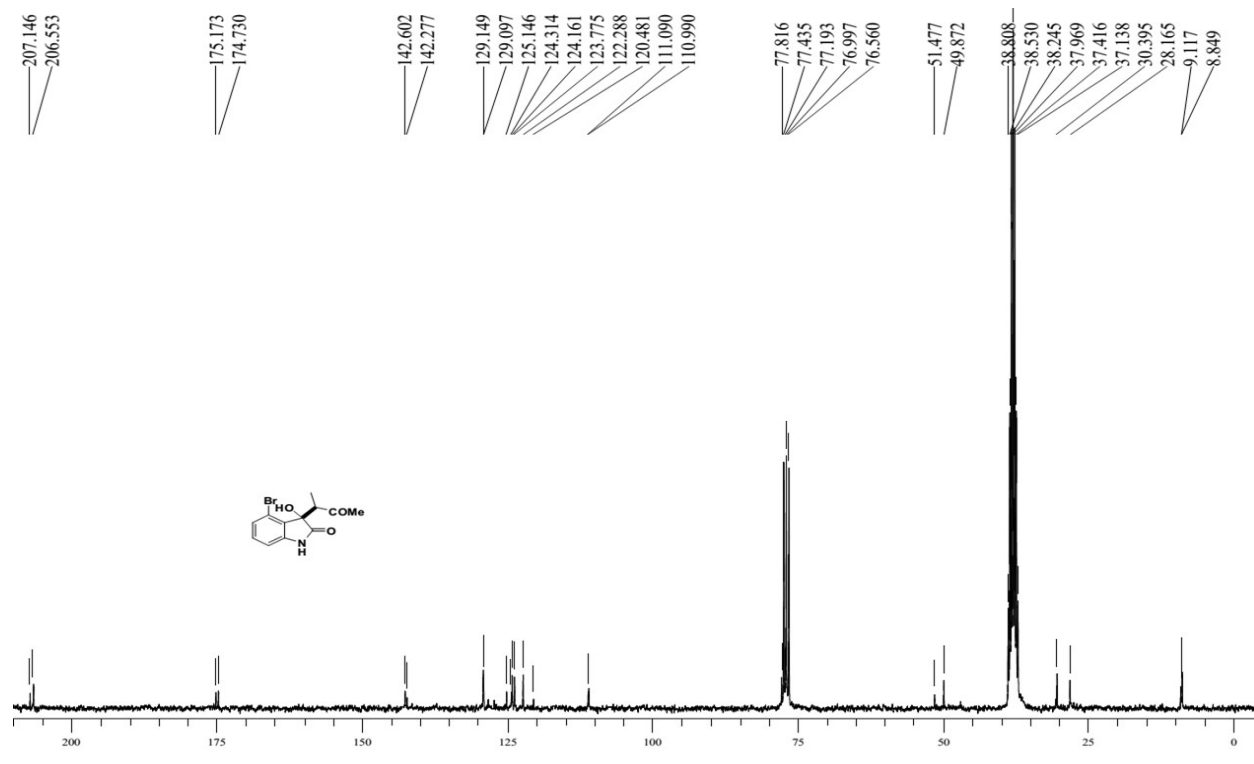


**Compound 4i**

# <sup>1</sup>H NMR

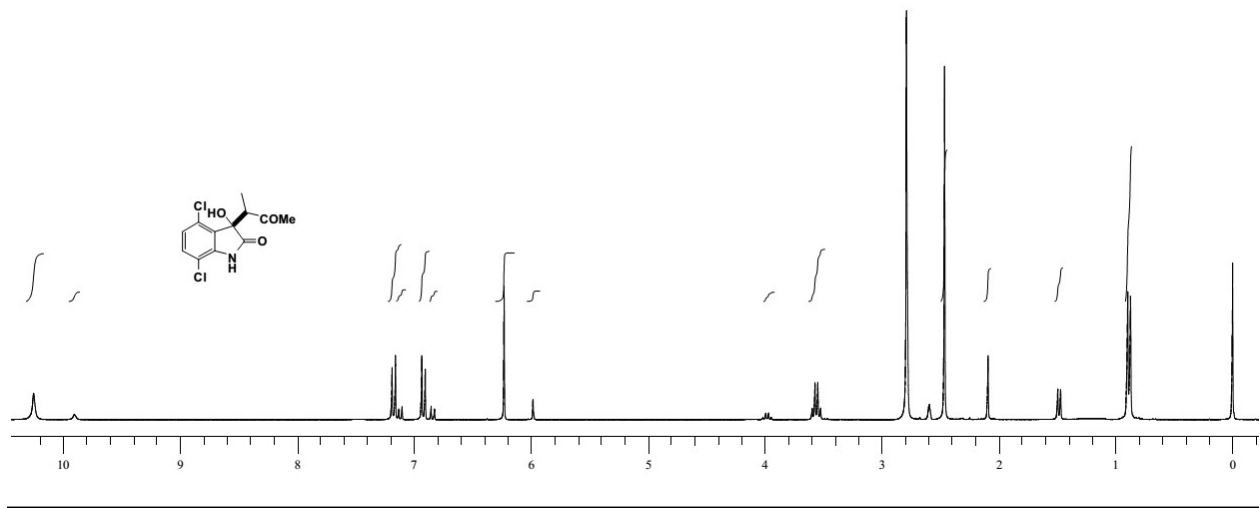


# <sup>13</sup>C NMR

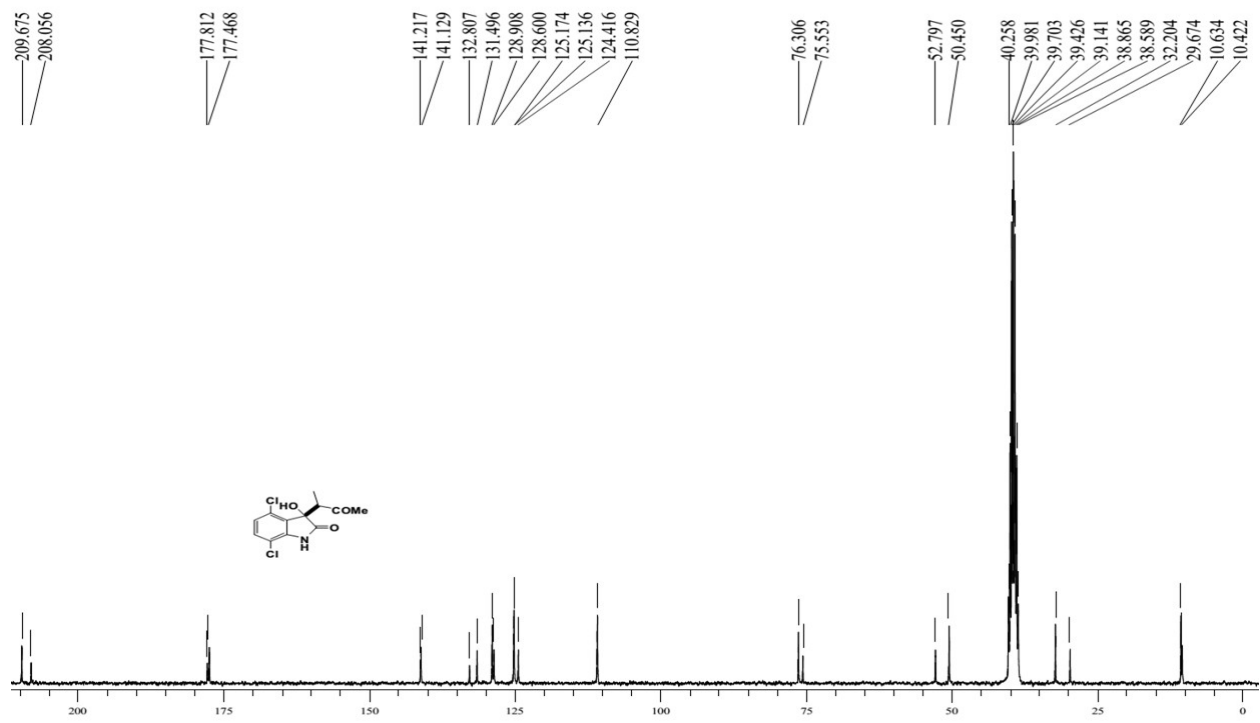


**Compound 4j**

### <sup>1</sup>H NMR

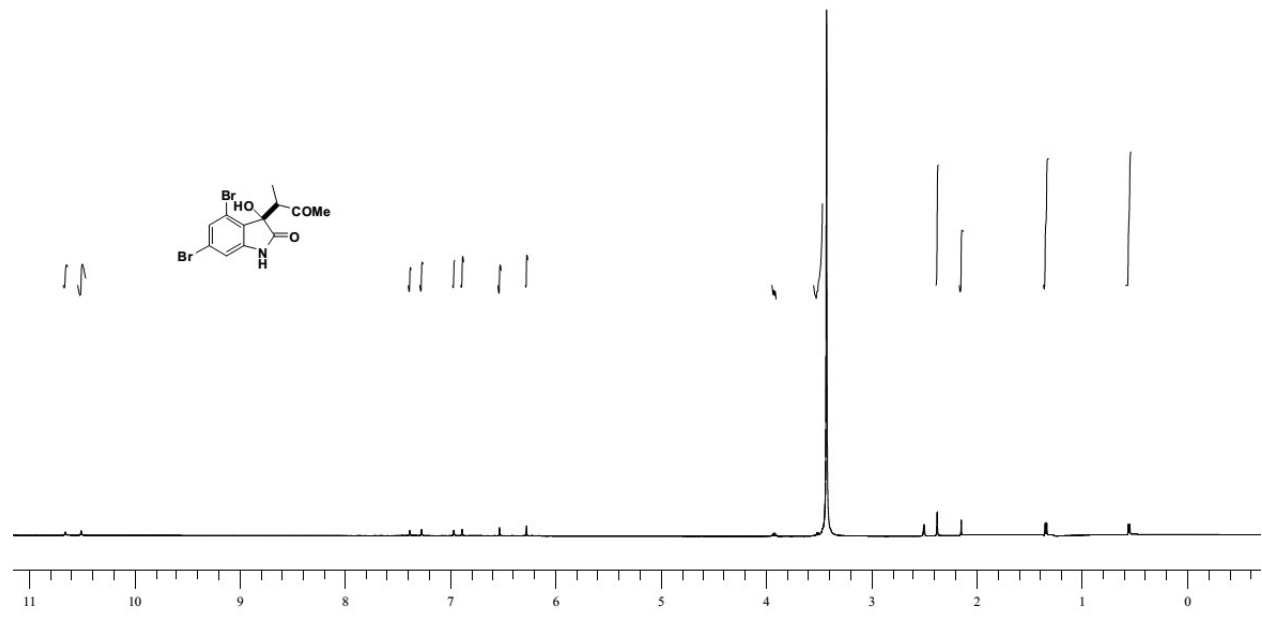


### <sup>13</sup>C NMR

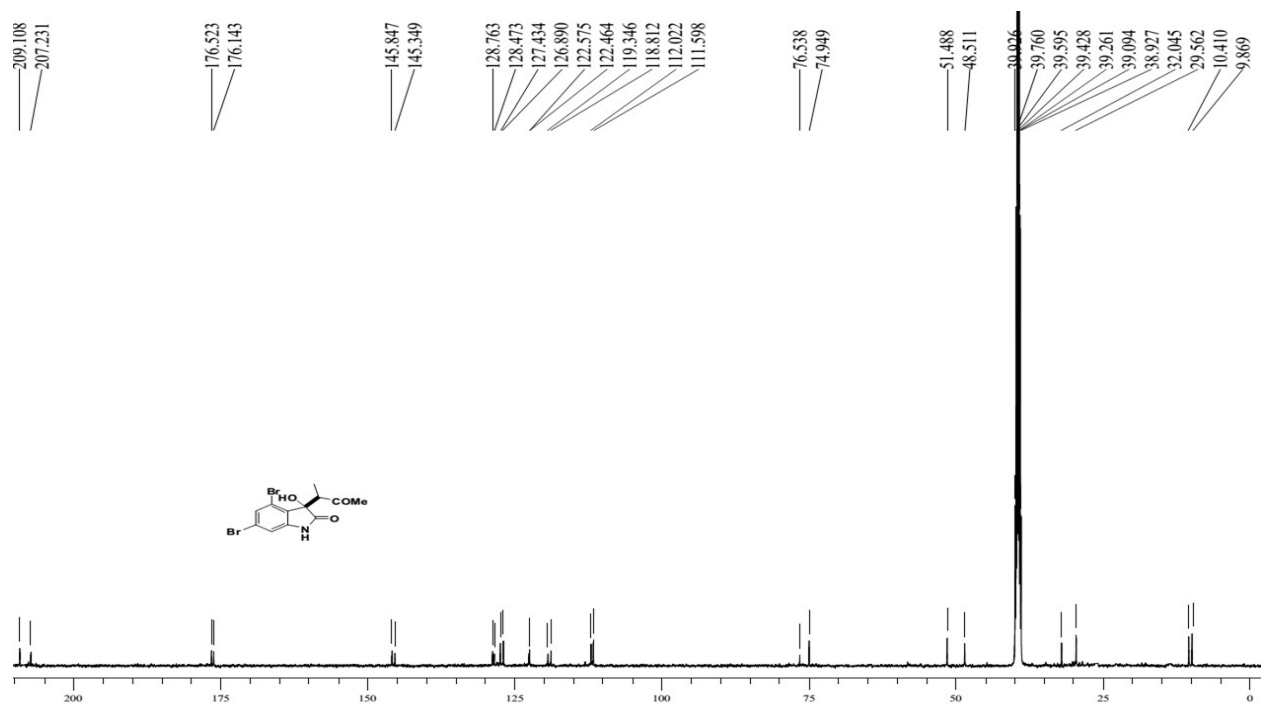


**Compound 4k**

### <sup>1</sup>H NMR

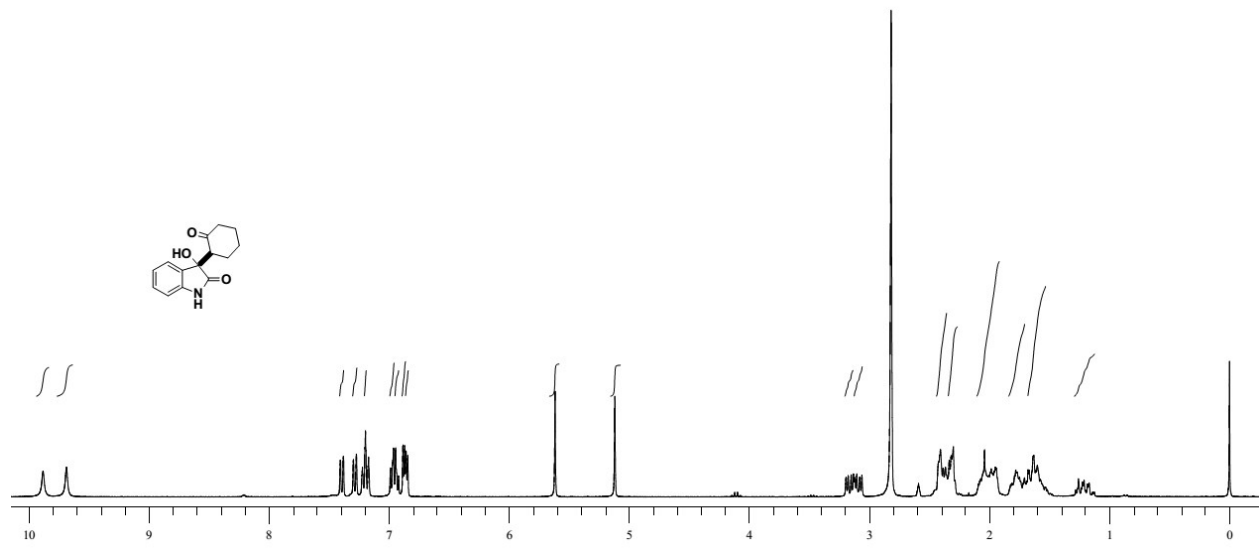


### <sup>13</sup>C NMR

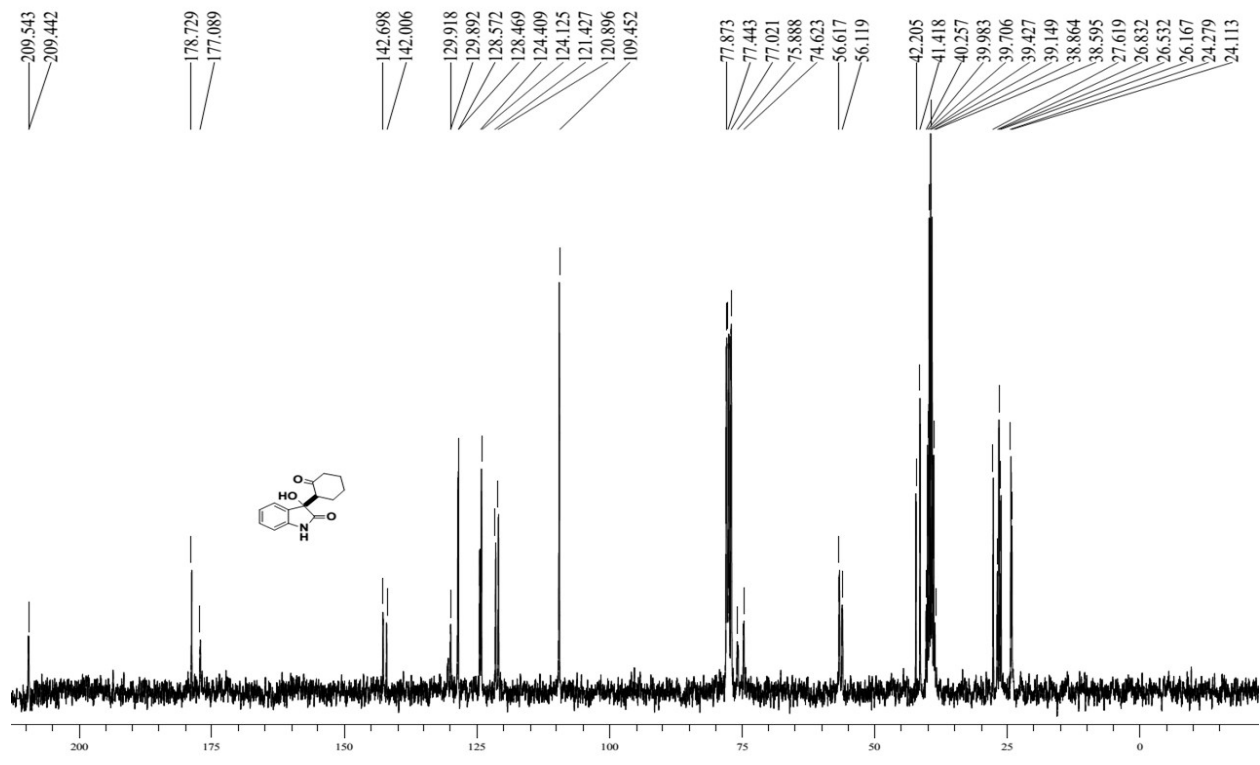


Compound 4l

### <sup>1</sup>H NMR

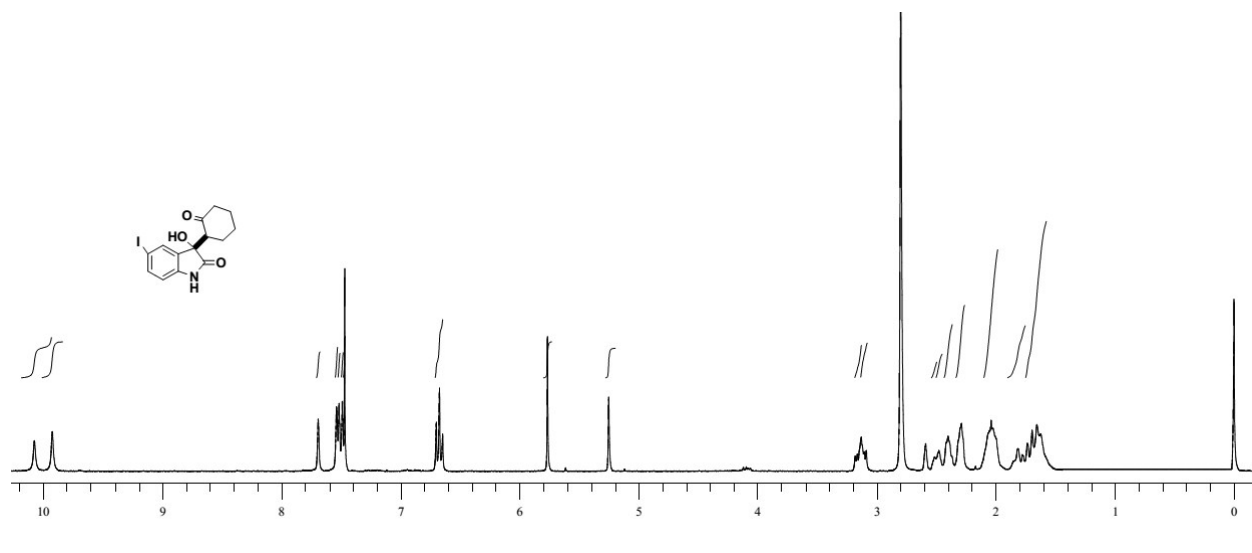


### <sup>13</sup>C NMR

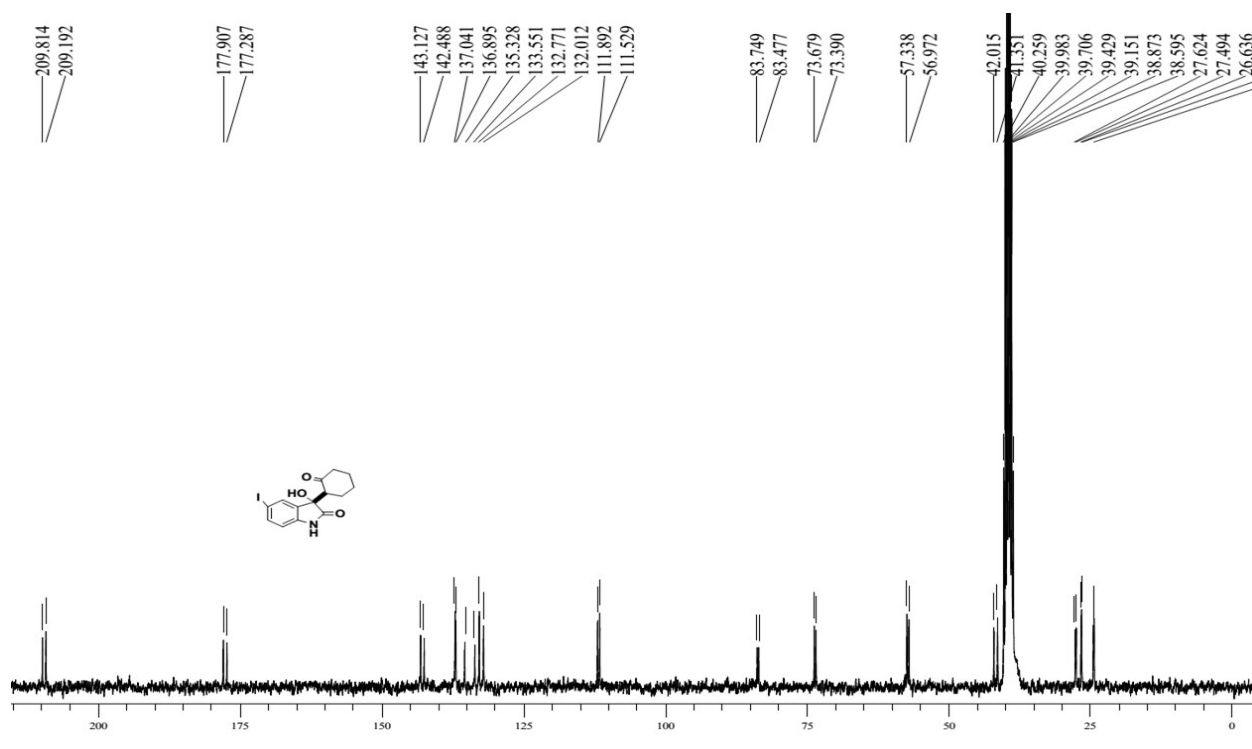


**Compound 4m**

### <sup>1</sup>H NMR

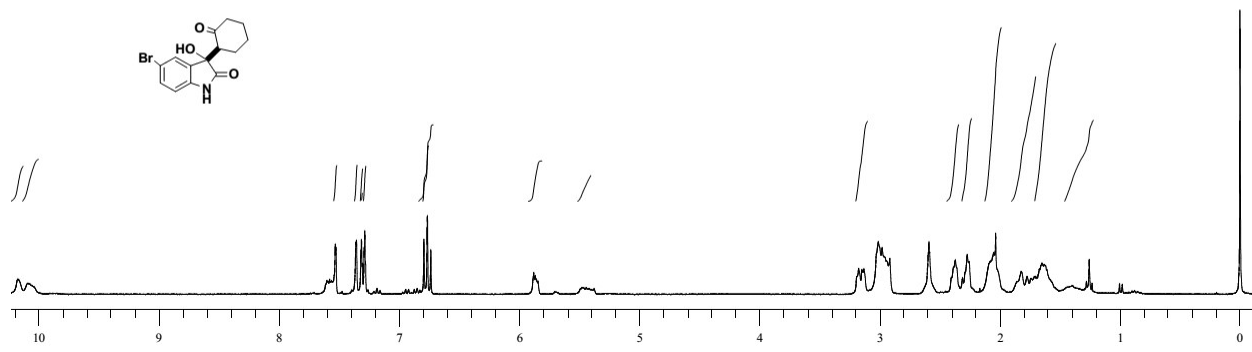


### <sup>13</sup>C NMR

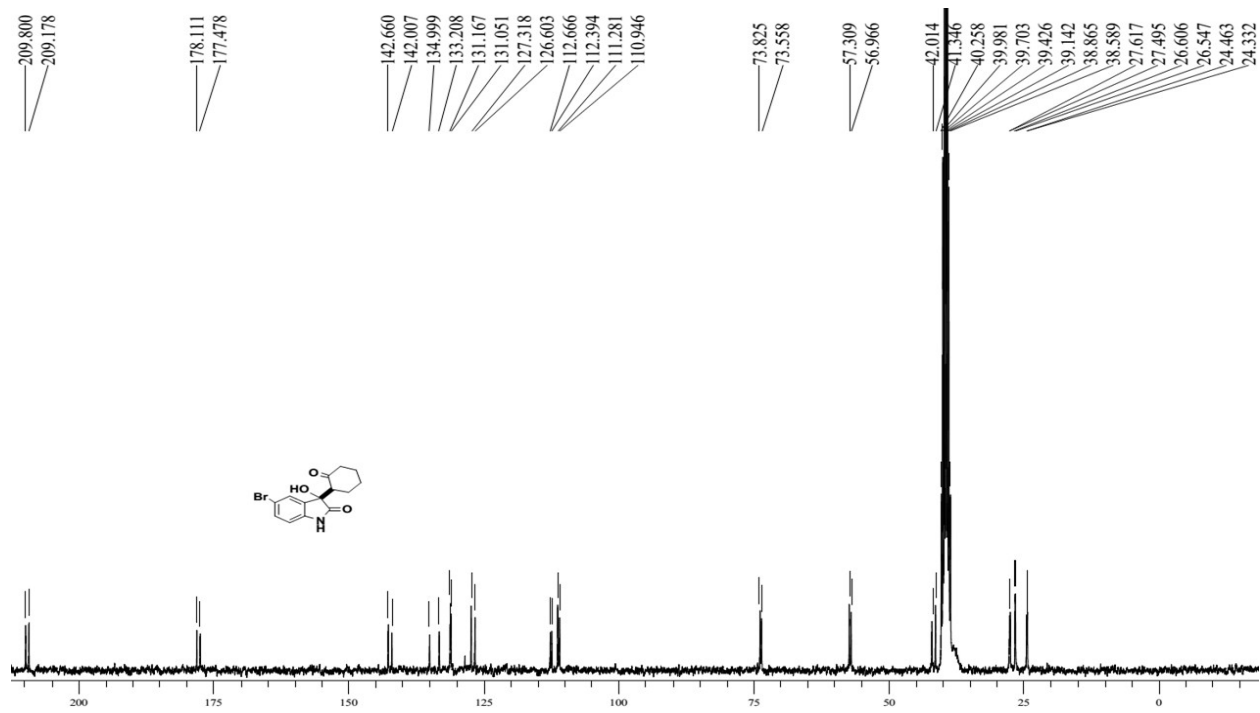


### Compound 4n

### <sup>1</sup>H NMR

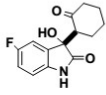
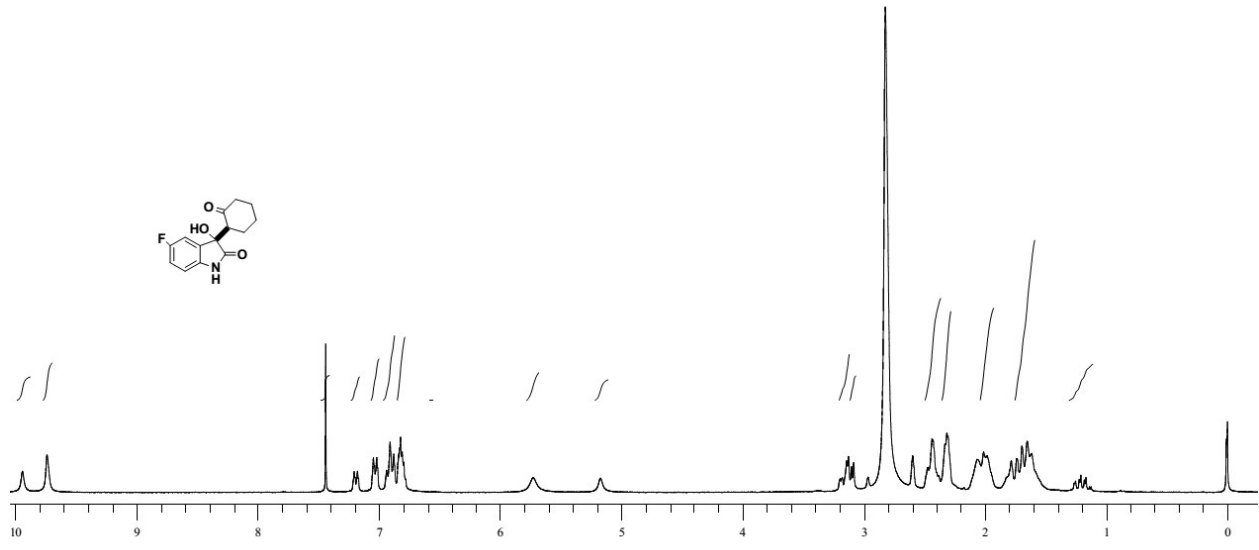


**<sup>13</sup>C NMR**

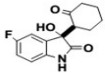
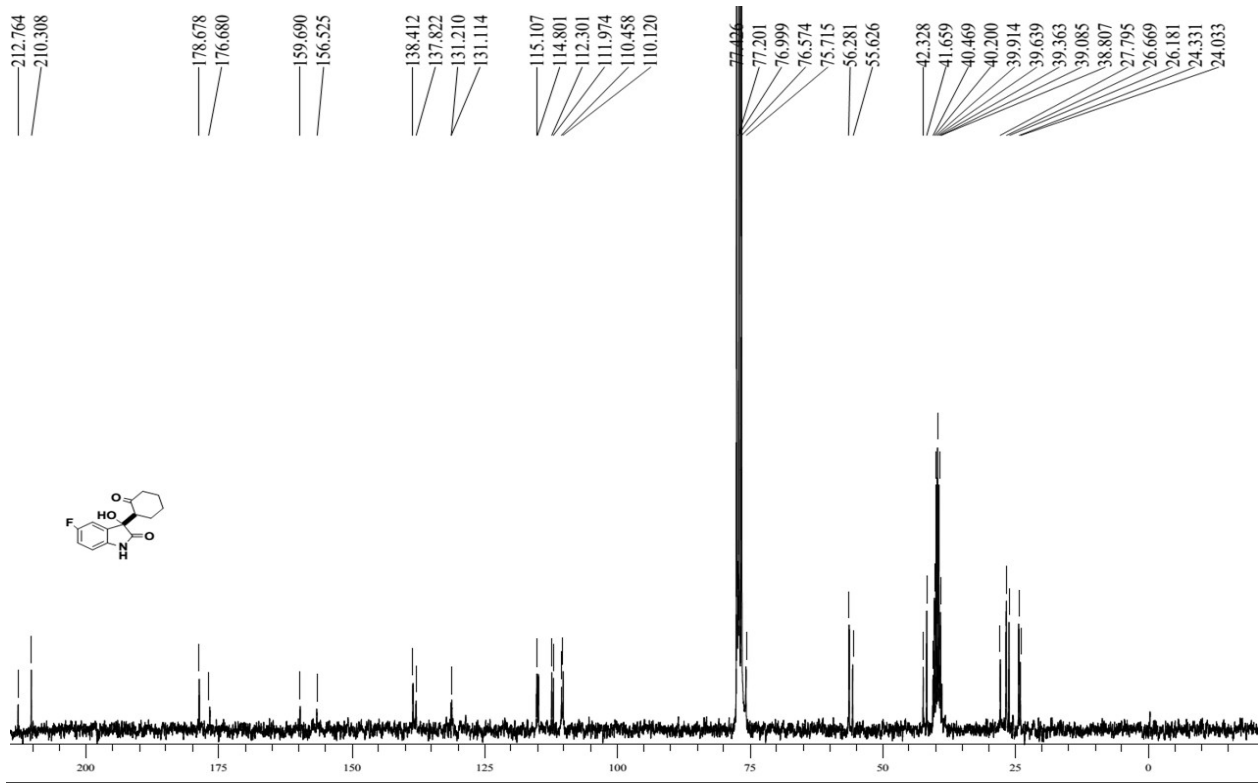


**Compound 40**

**<sup>1</sup>H NMR**



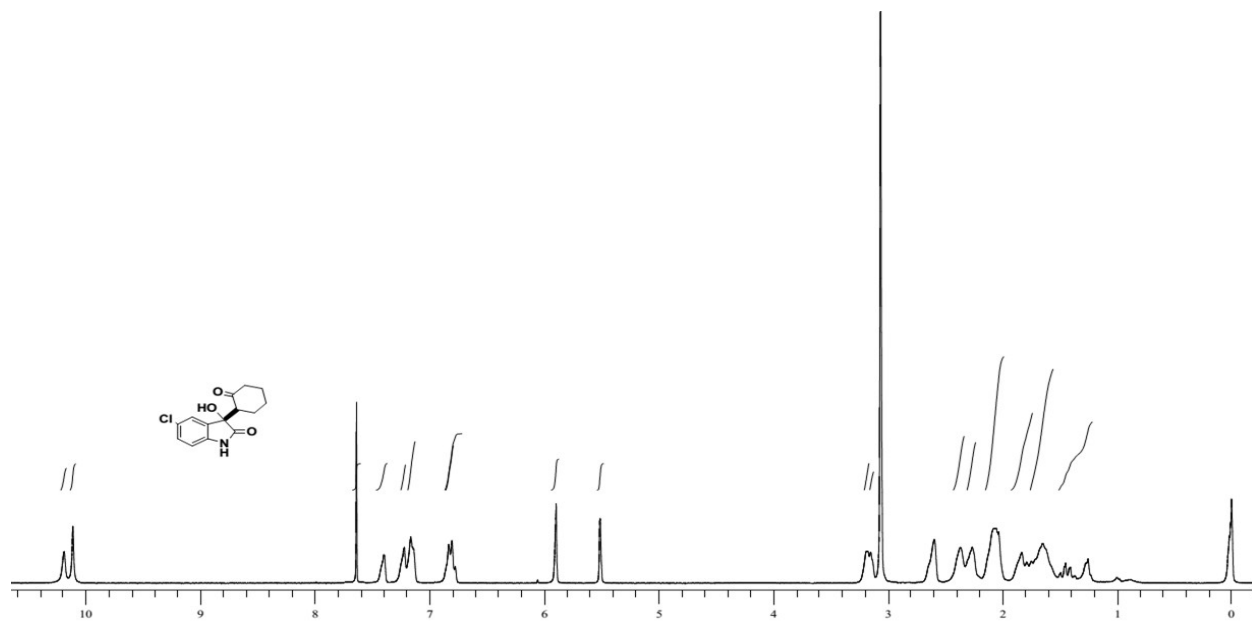
**<sup>13</sup>C NMR**



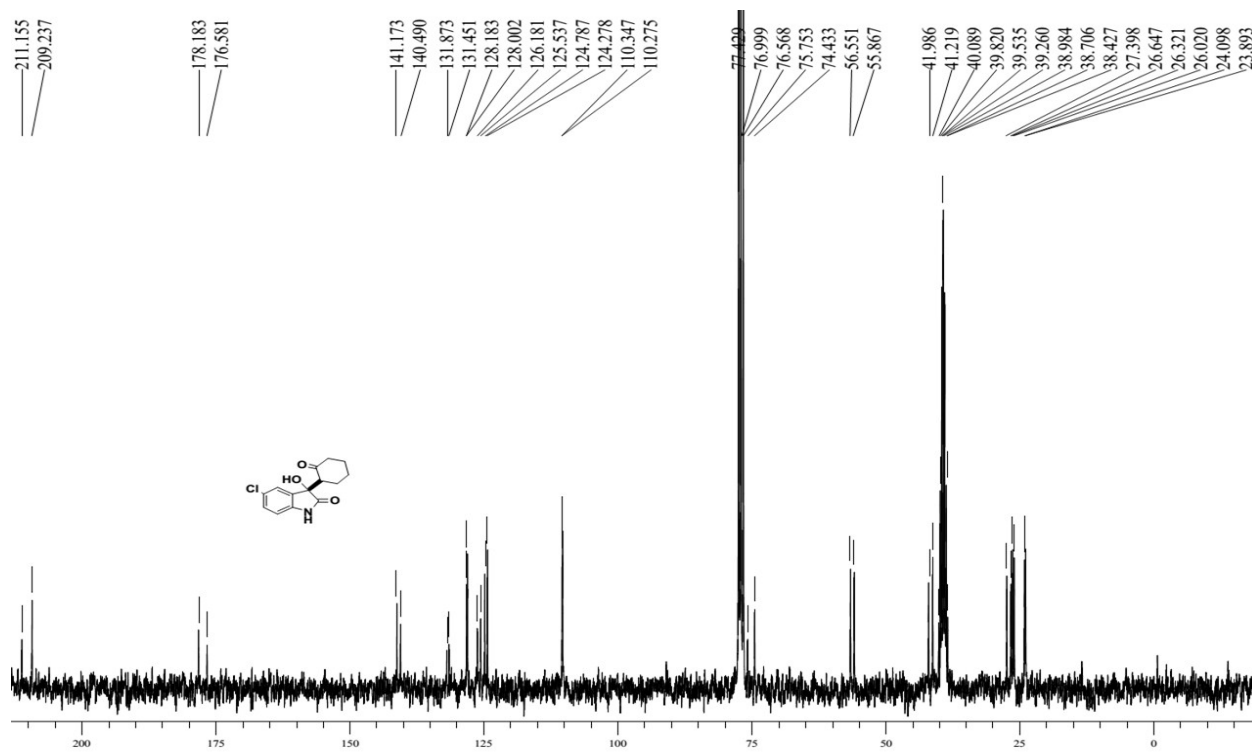
**Compound 4p**

**<sup>1</sup>H NMR**



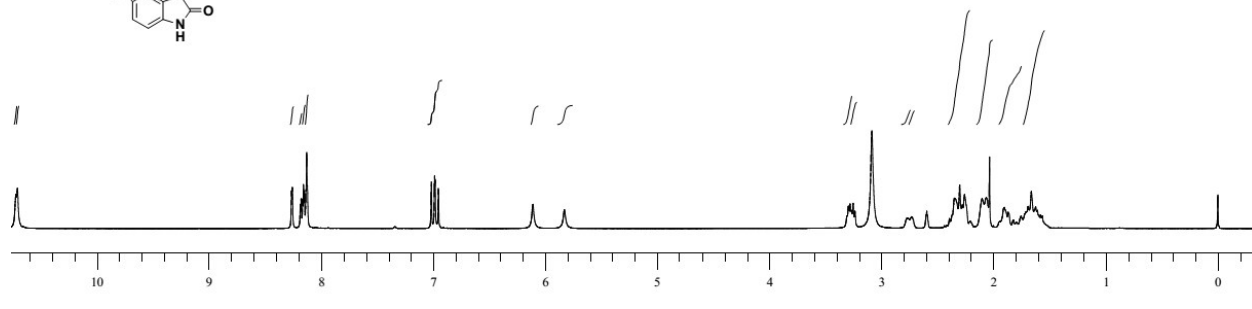
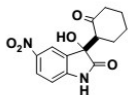


**<sup>13</sup>C NMR**

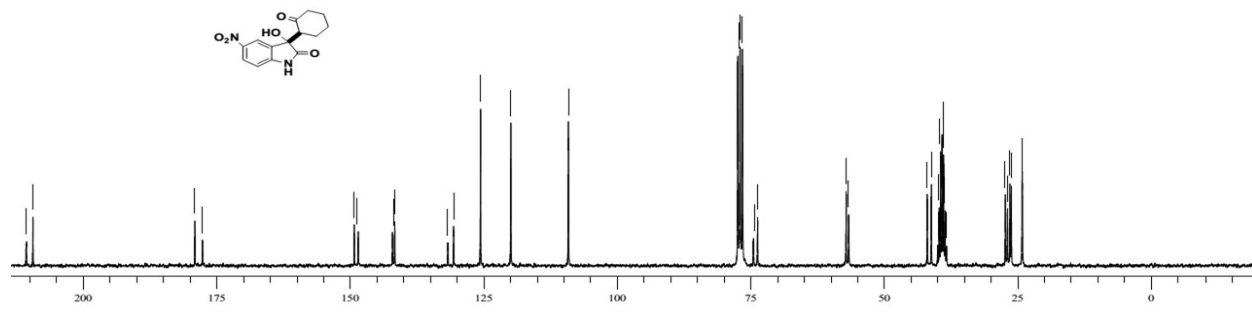


**Compound 4q**

**<sup>1</sup>H NMR**

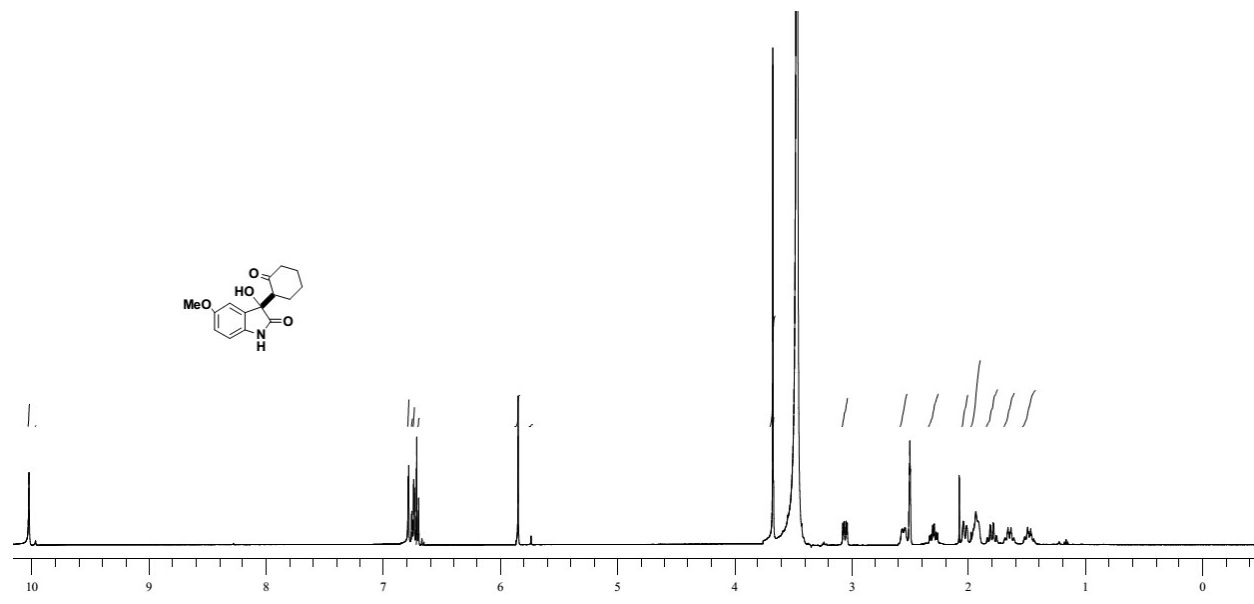


**<sup>13</sup>C NMR**

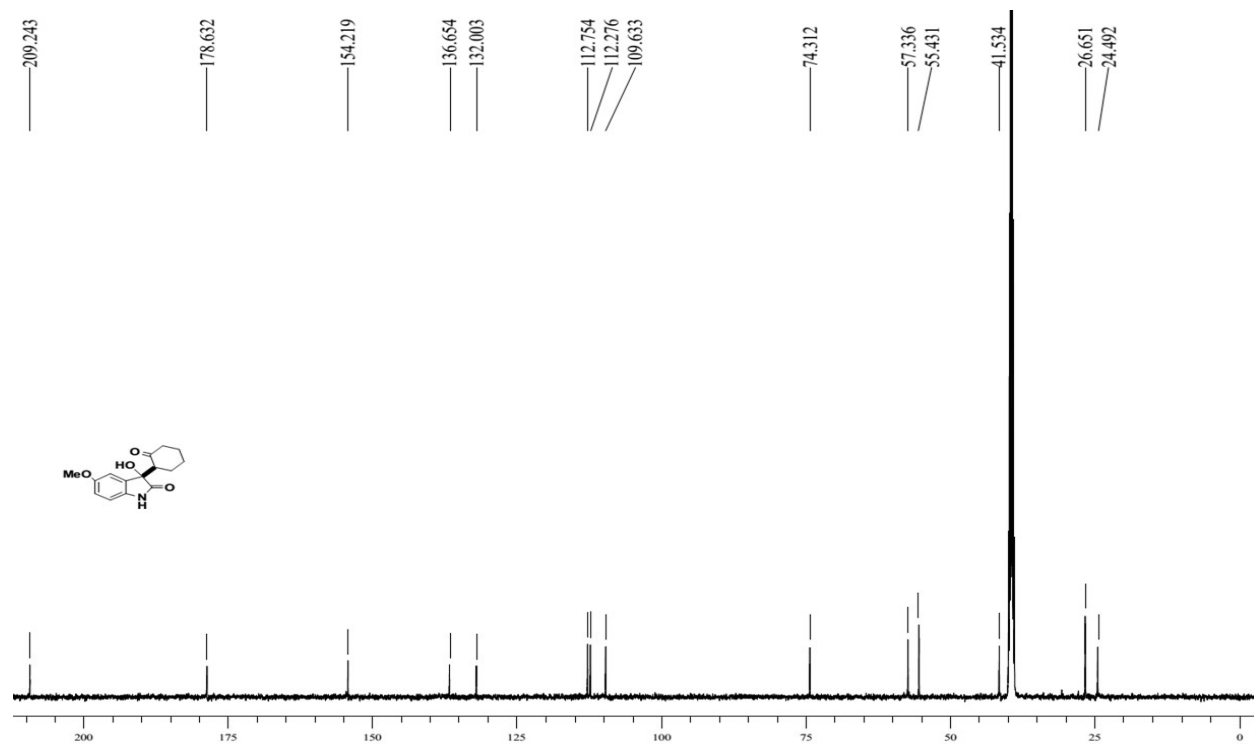


**Compound 4r**

# <sup>1</sup>H NMR

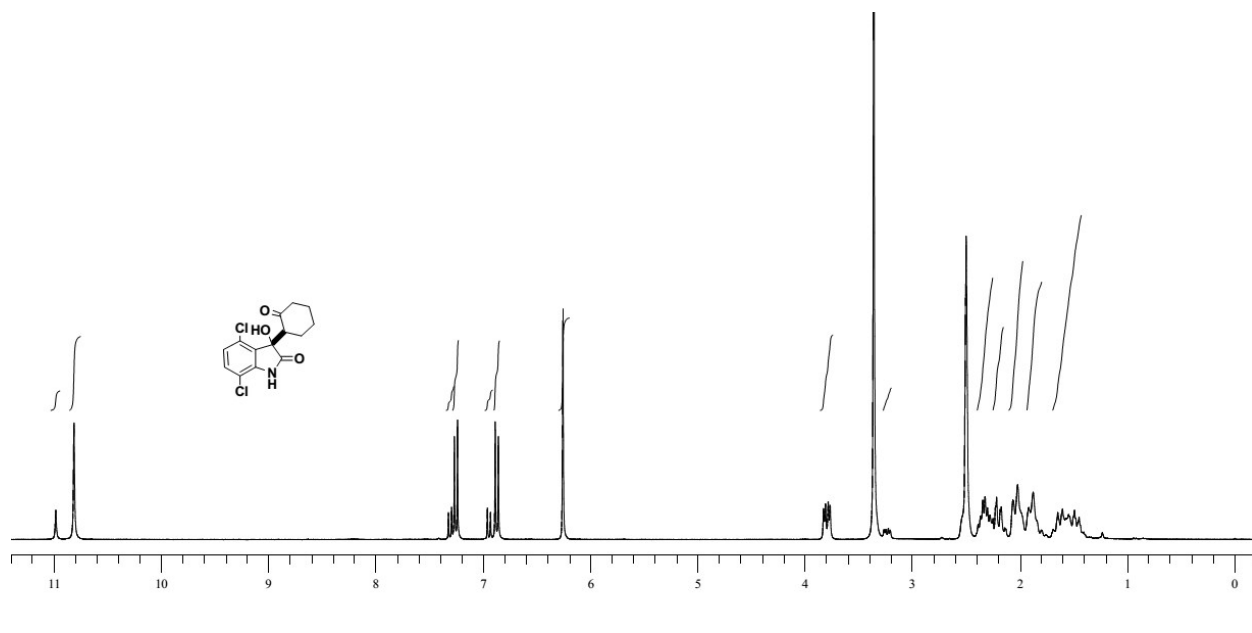


# <sup>13</sup>C NMR

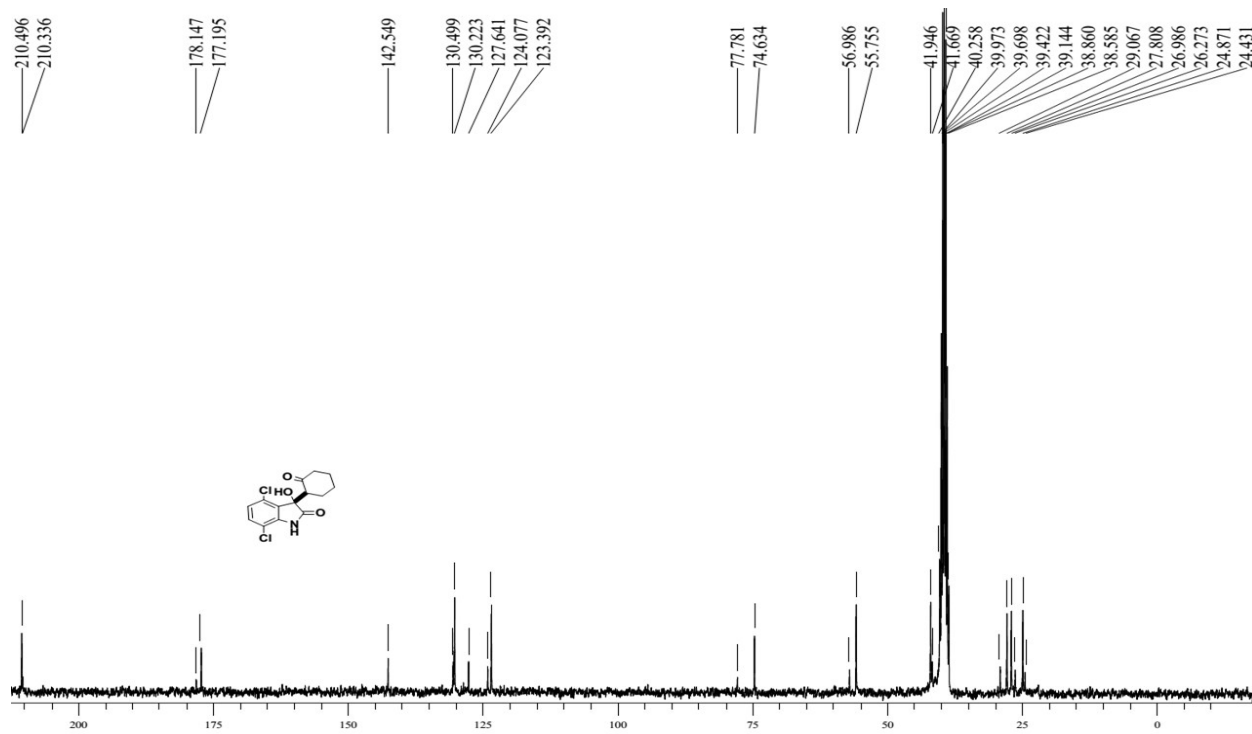


**Compound 4s**

# <sup>1</sup>H NMR

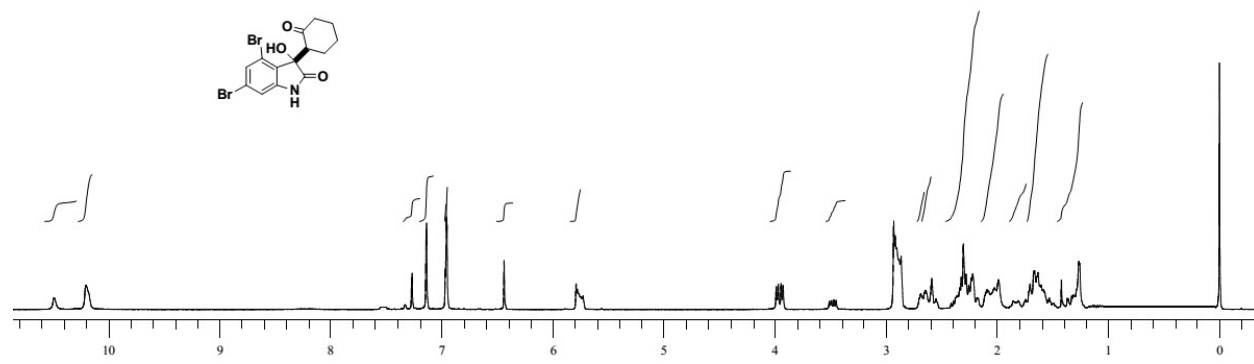


# <sup>13</sup>C NMR

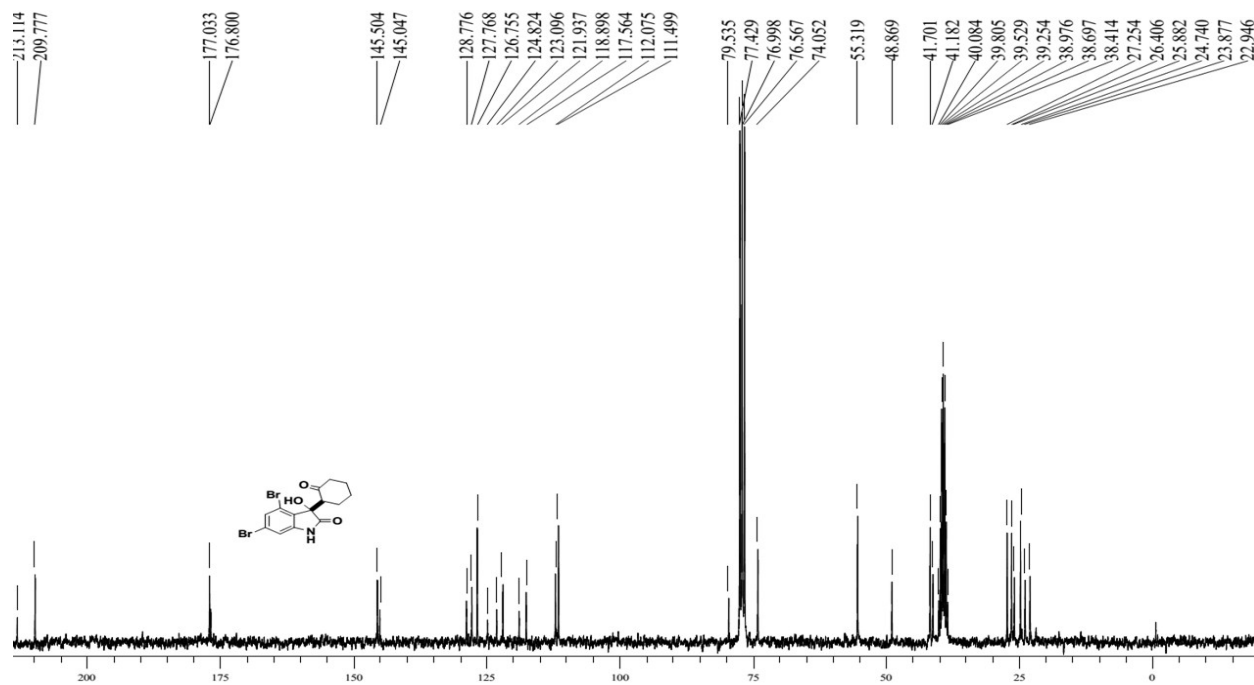


**Compound 4t**

# <sup>1</sup>H NMR

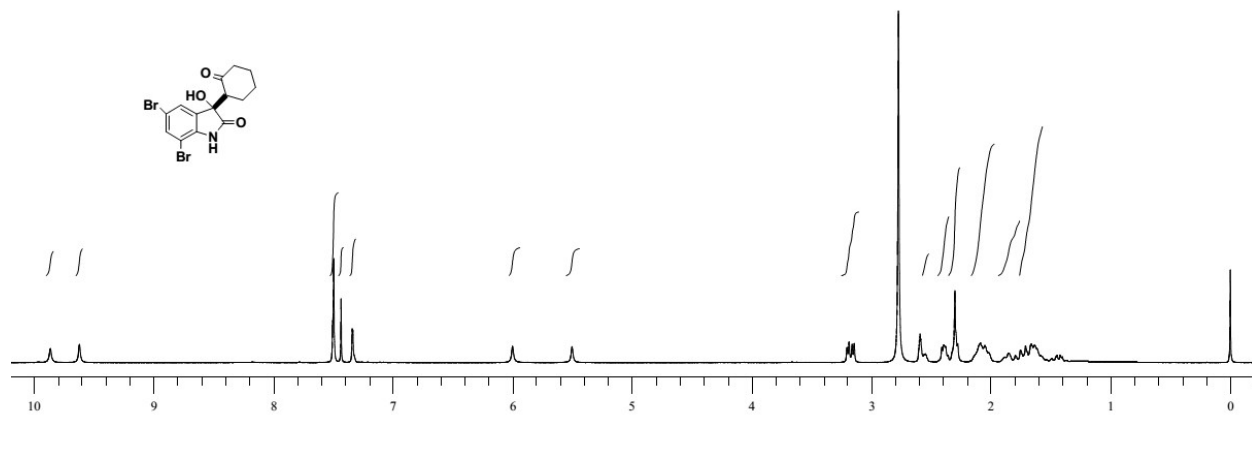


# <sup>13</sup>C NMR

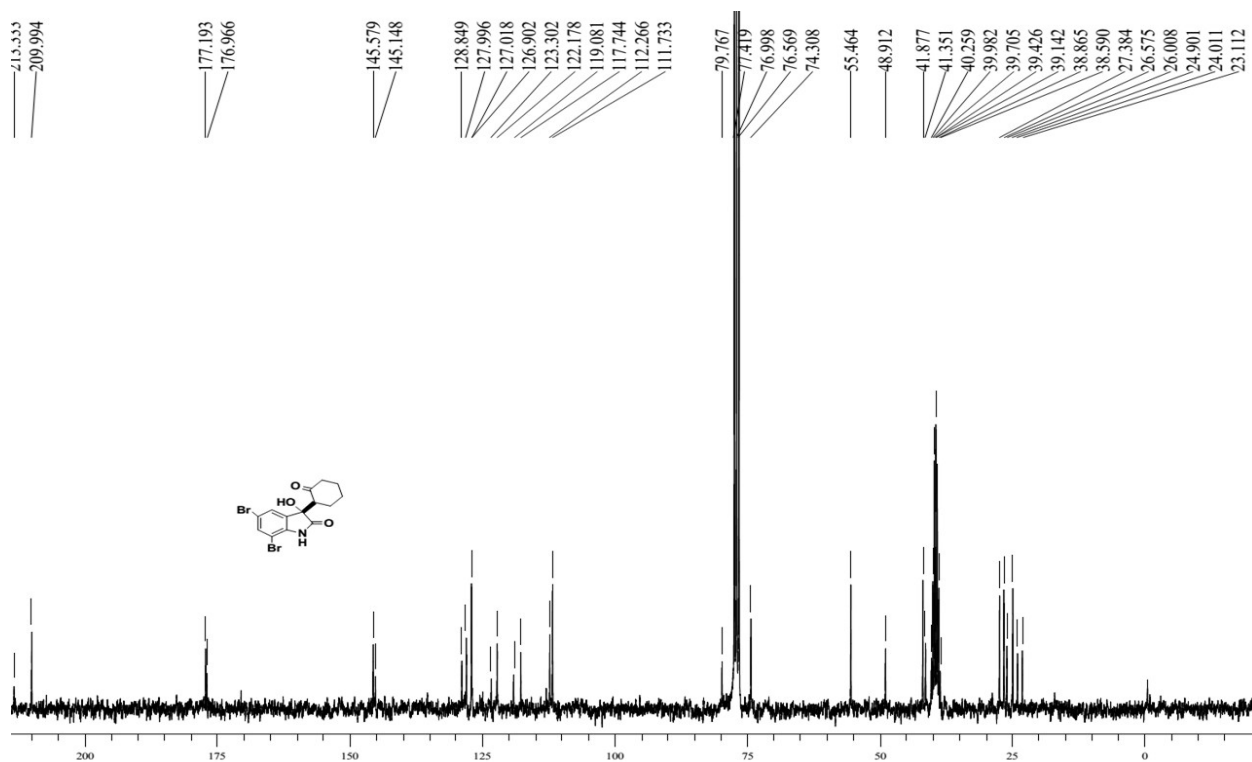


Compound 4u

### <sup>1</sup>H NMR

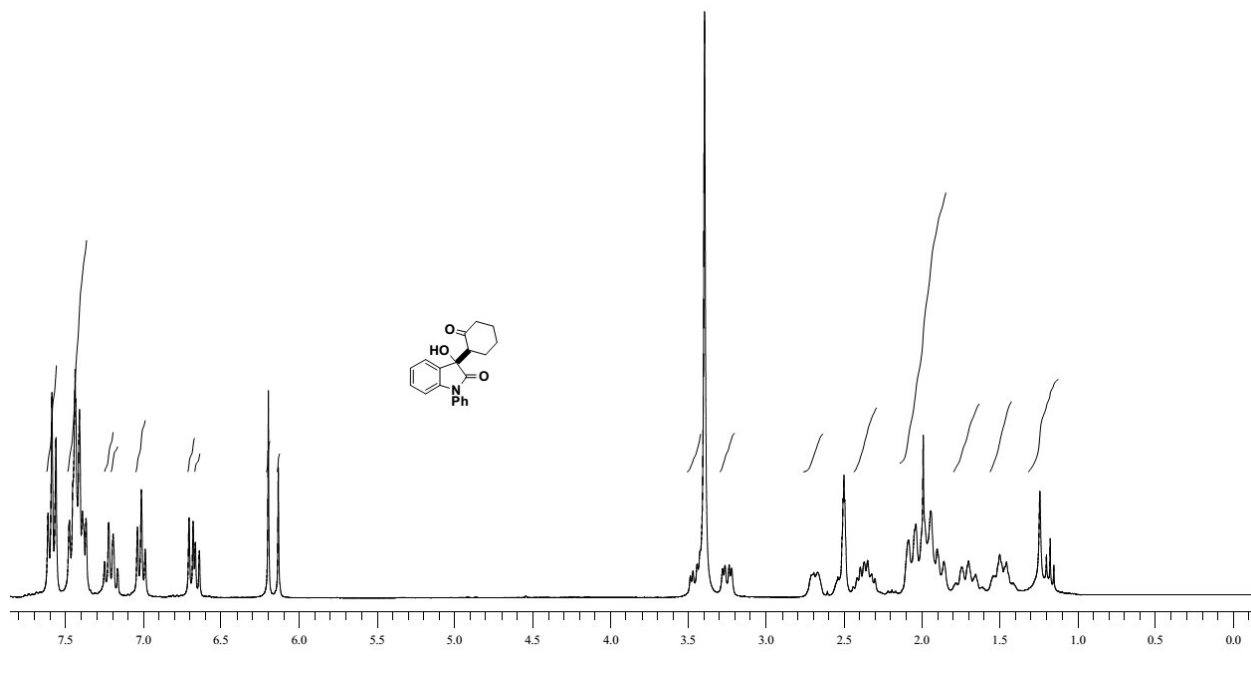


### <sup>13</sup>C NMR

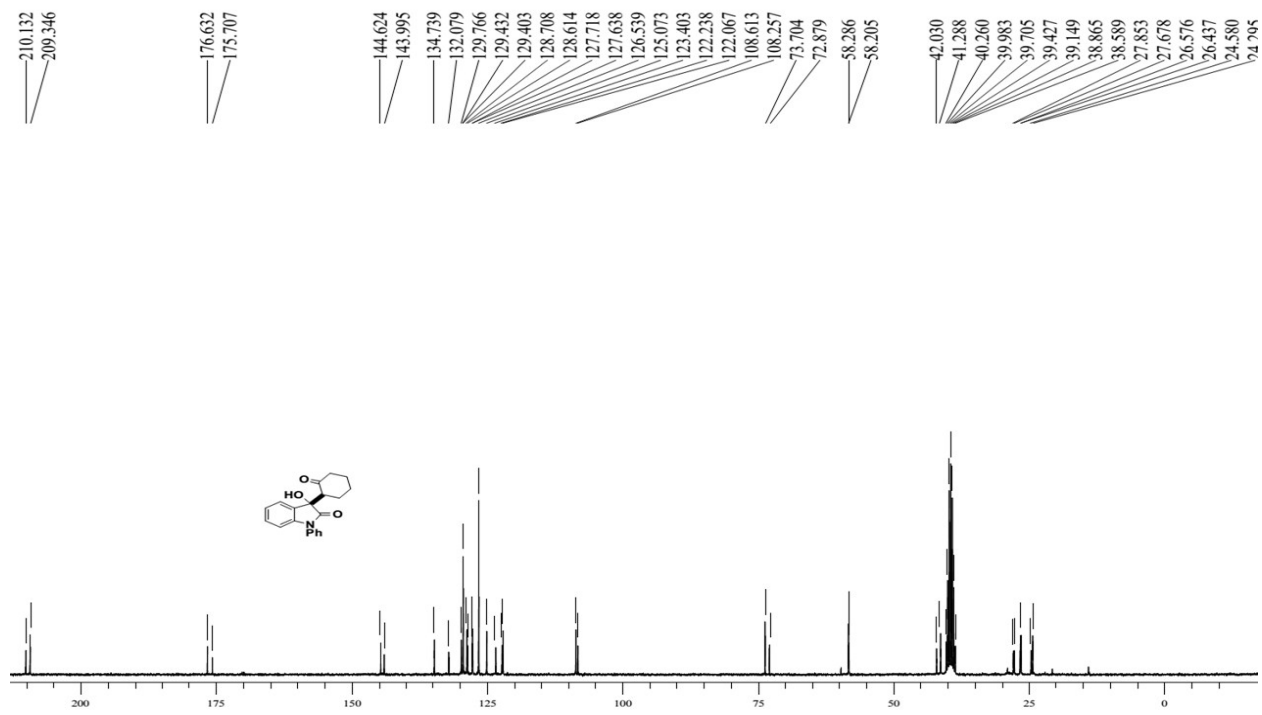


**Compound 4v**

# <sup>1</sup>H NMR

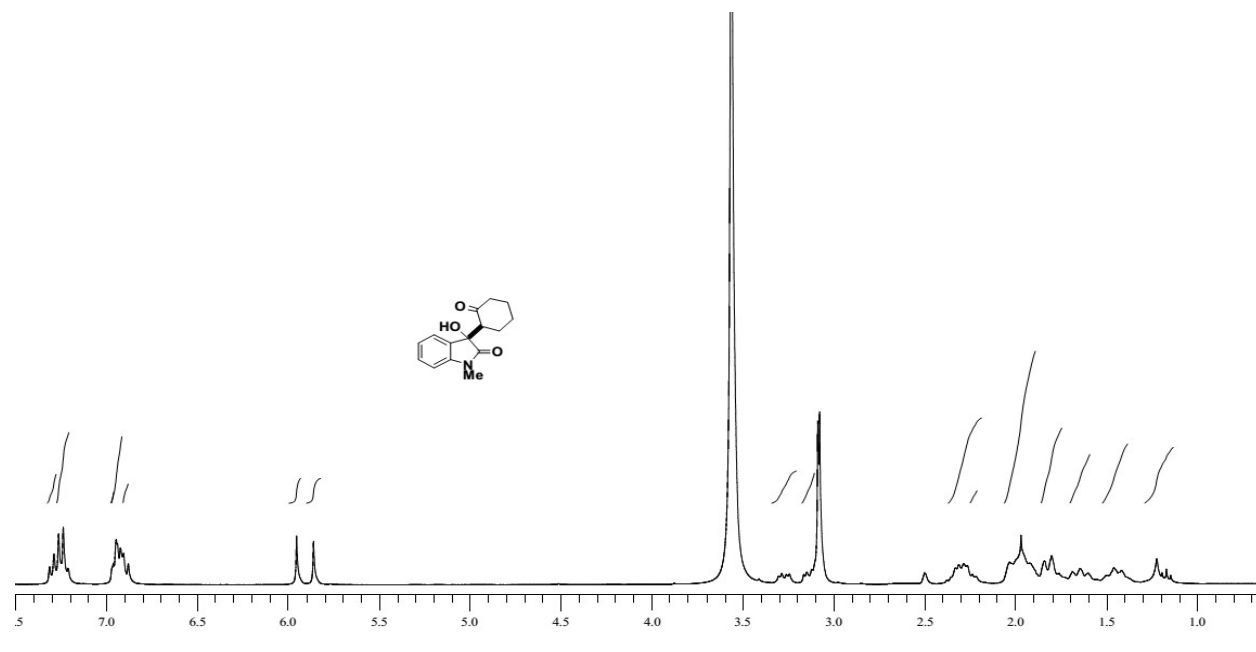


# <sup>13</sup>C NMR

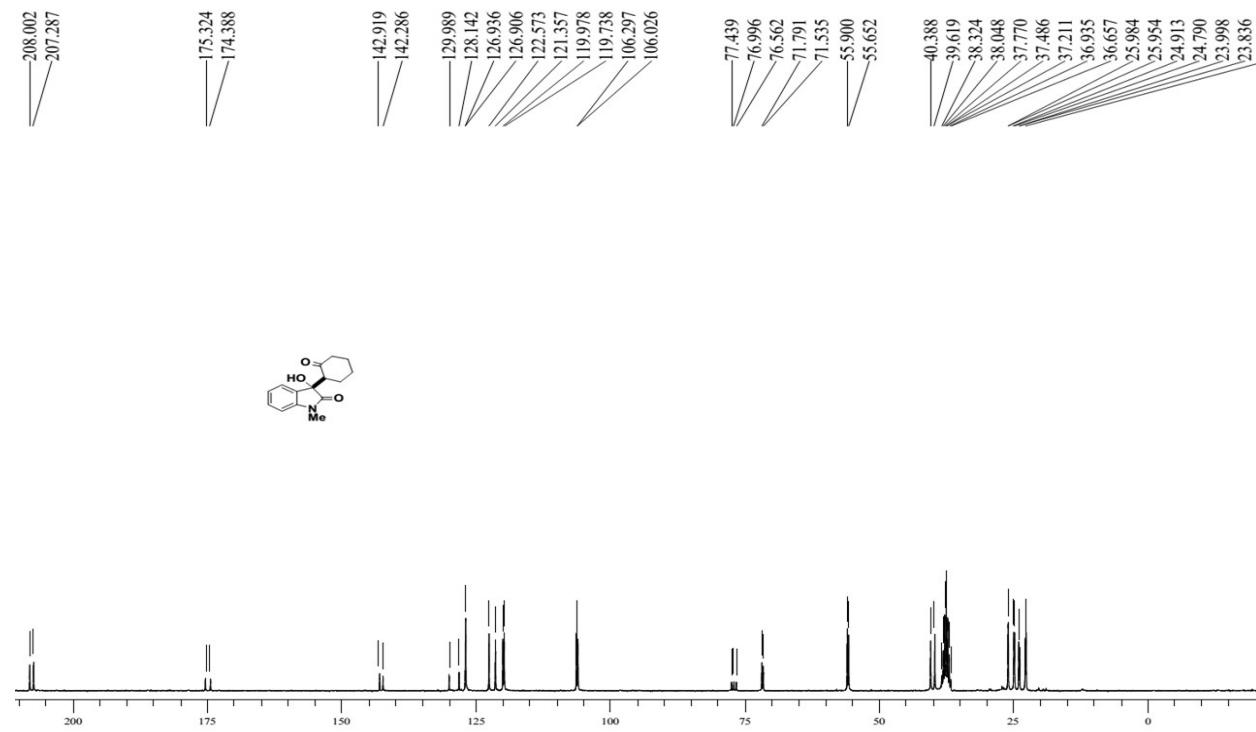


Compound 4w

# <sup>1</sup>H NMR



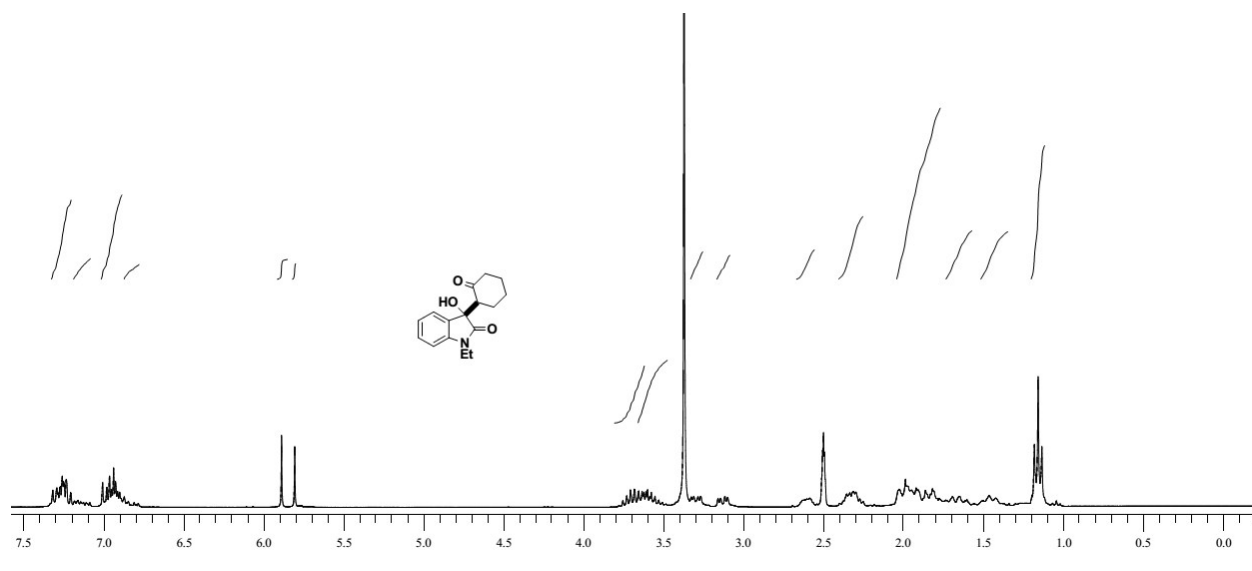
# <sup>13</sup>C NMR



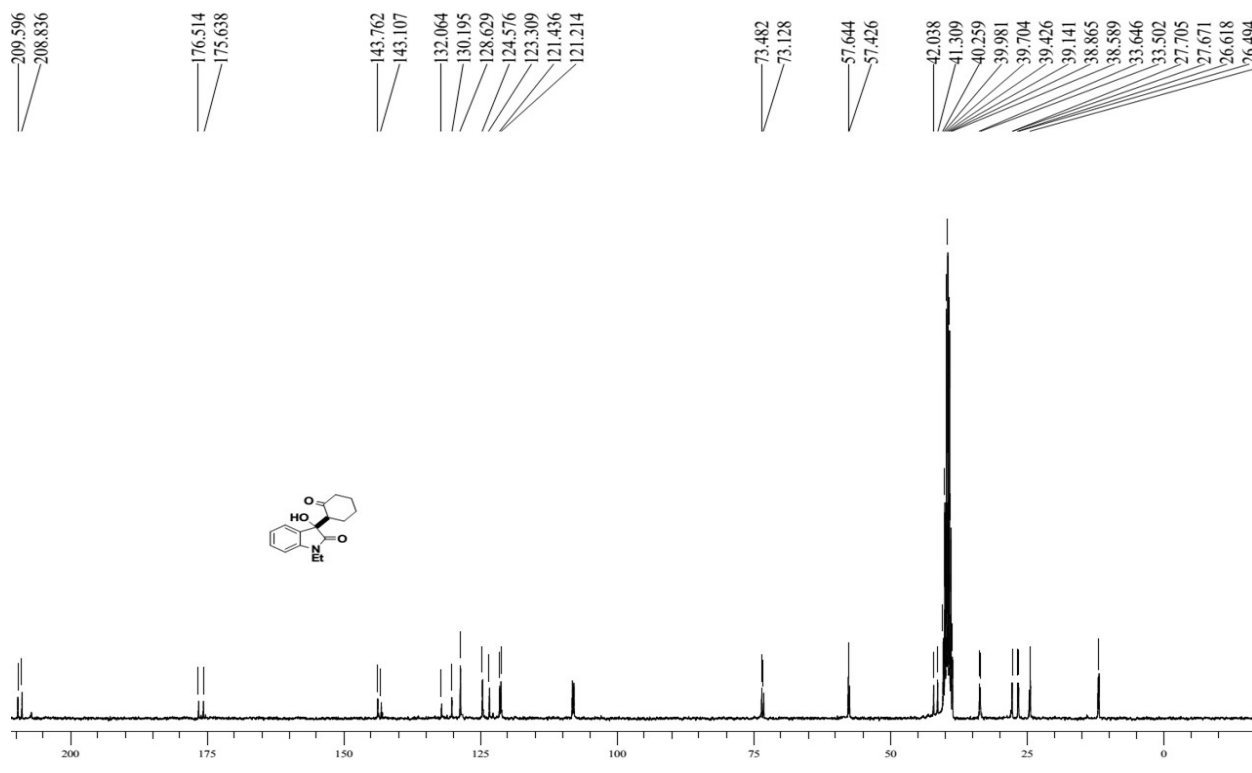
**Compound 4x**



### <sup>1</sup>H NMR

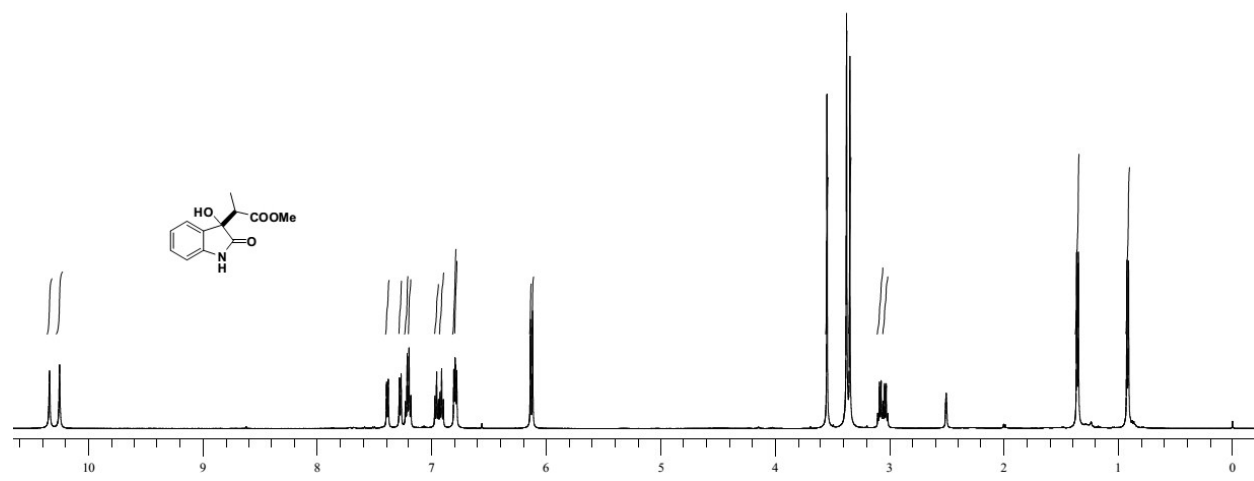


### <sup>13</sup>C NMR

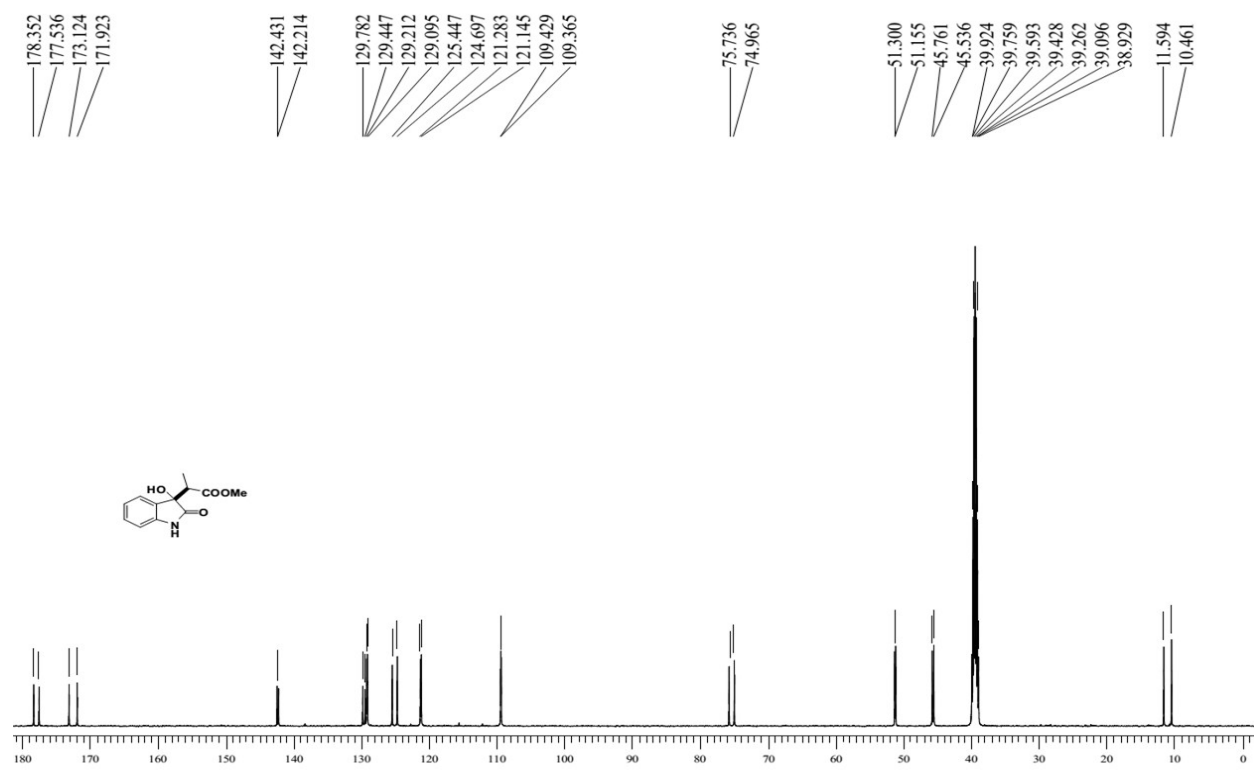


**Compound 5a**

### <sup>1</sup>H NMR

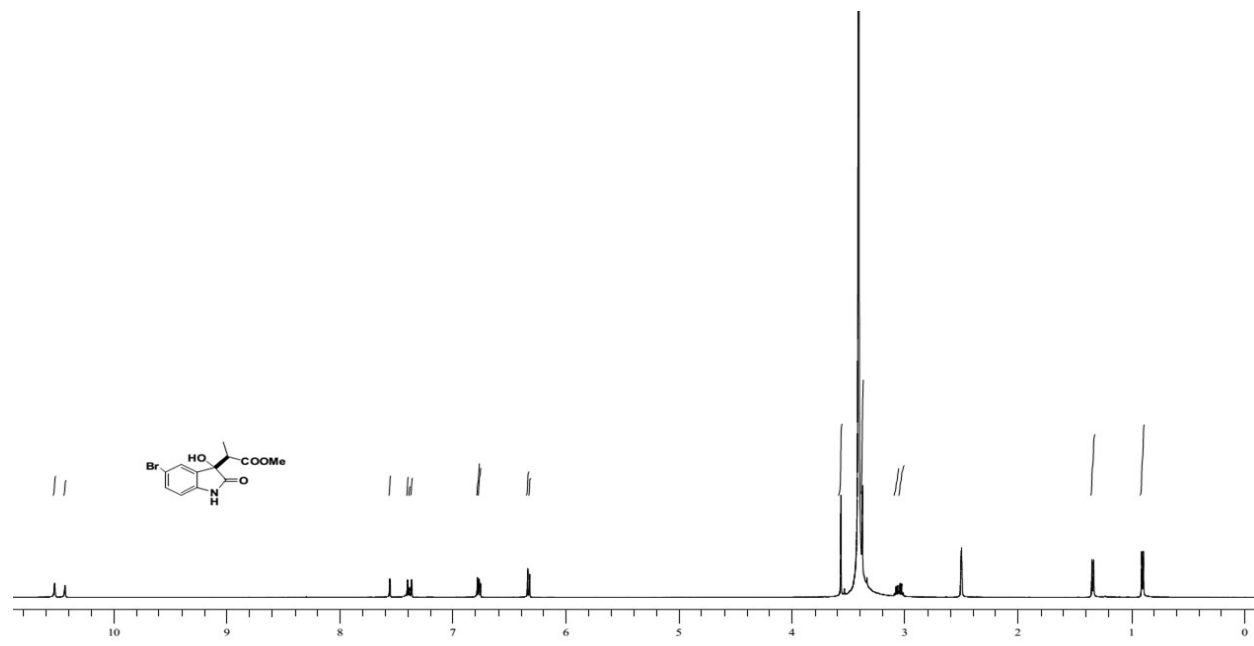


### <sup>13</sup>C NMR

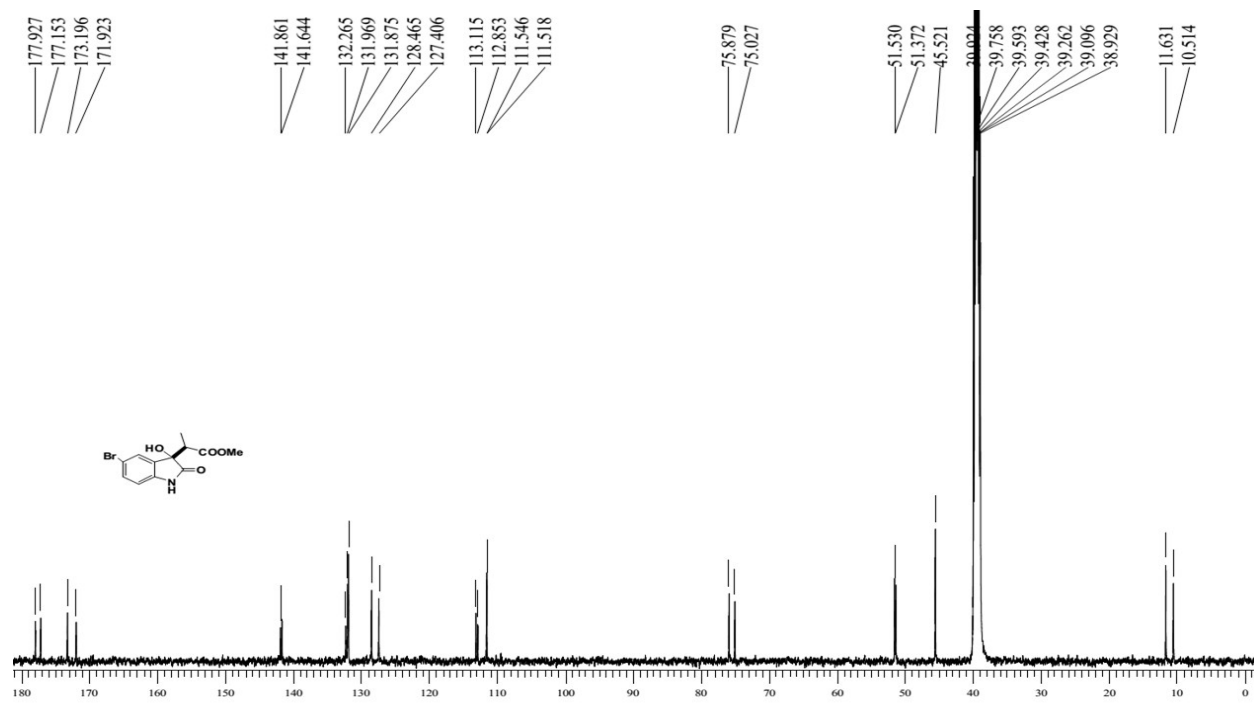


**Compound 5b**

# <sup>1</sup>H NMR

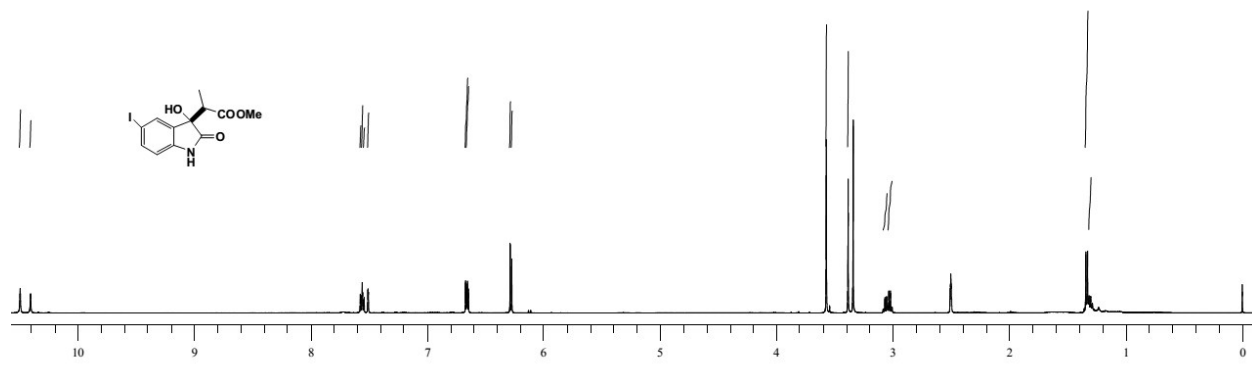


# <sup>13</sup>C NMR

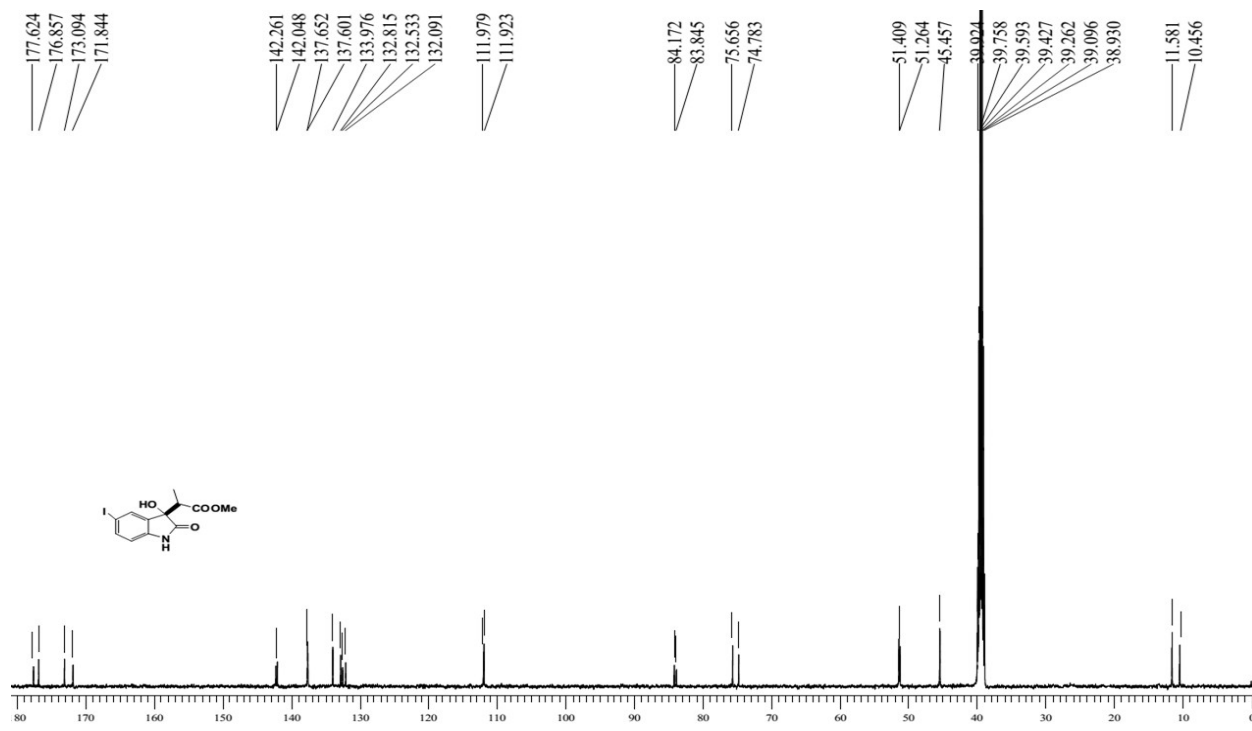


**Compound 5c**

## <sup>1</sup>H NMR

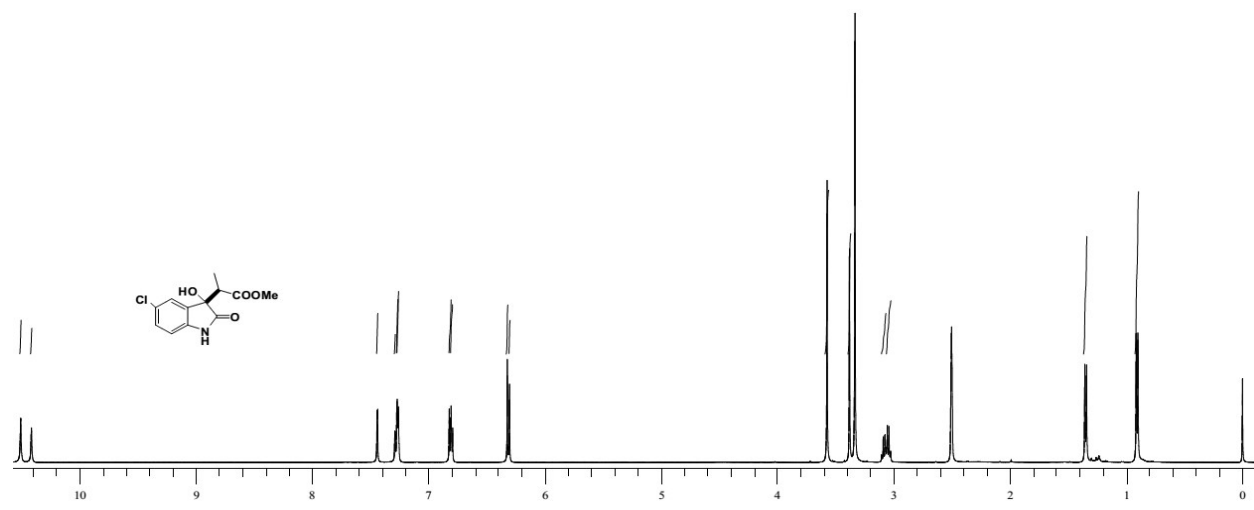


## <sup>13</sup>C NMR

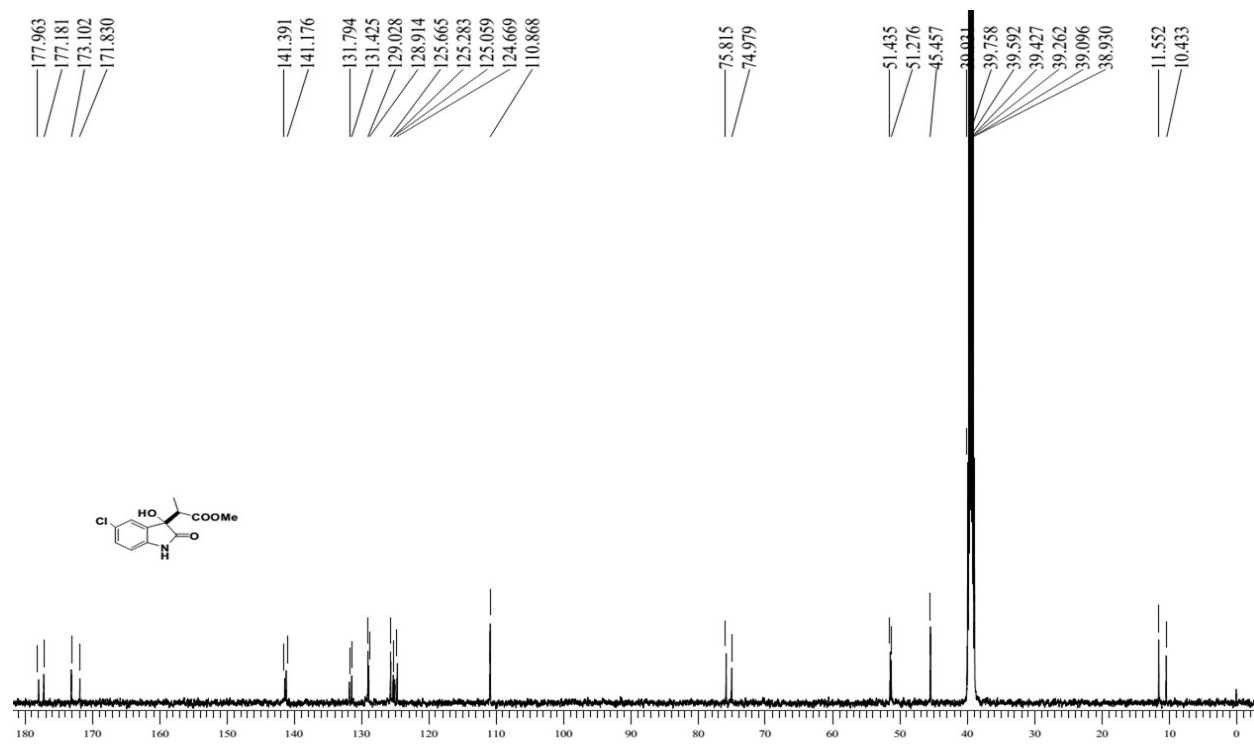


**Compound 5d**

### <sup>1</sup>H NMR

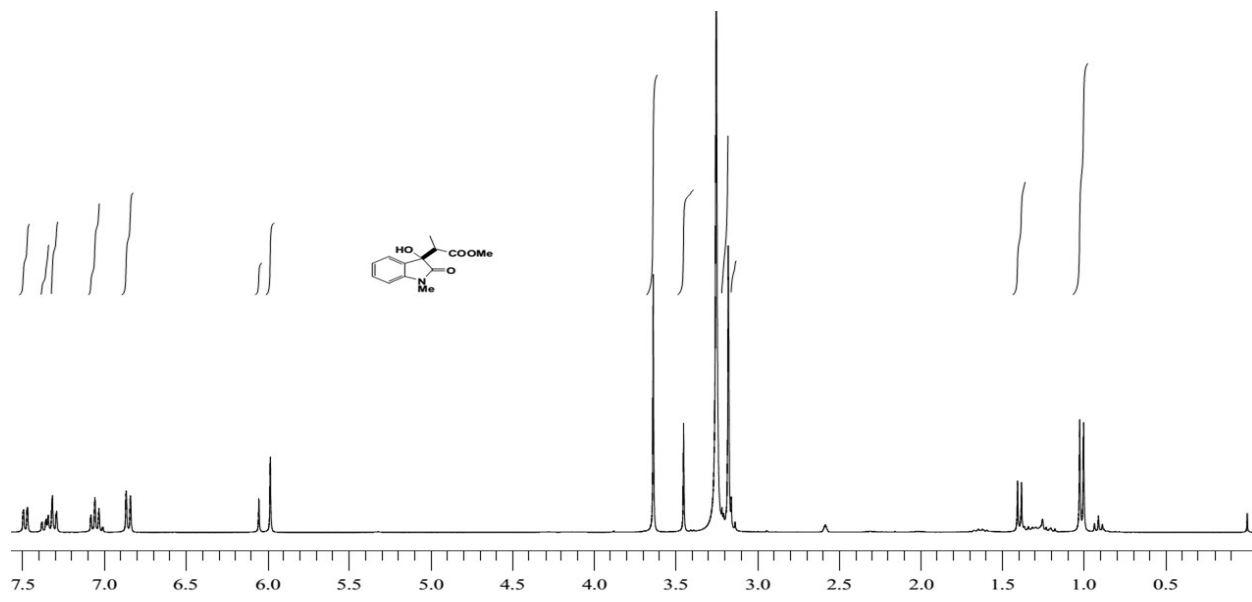


### <sup>13</sup>C NMR

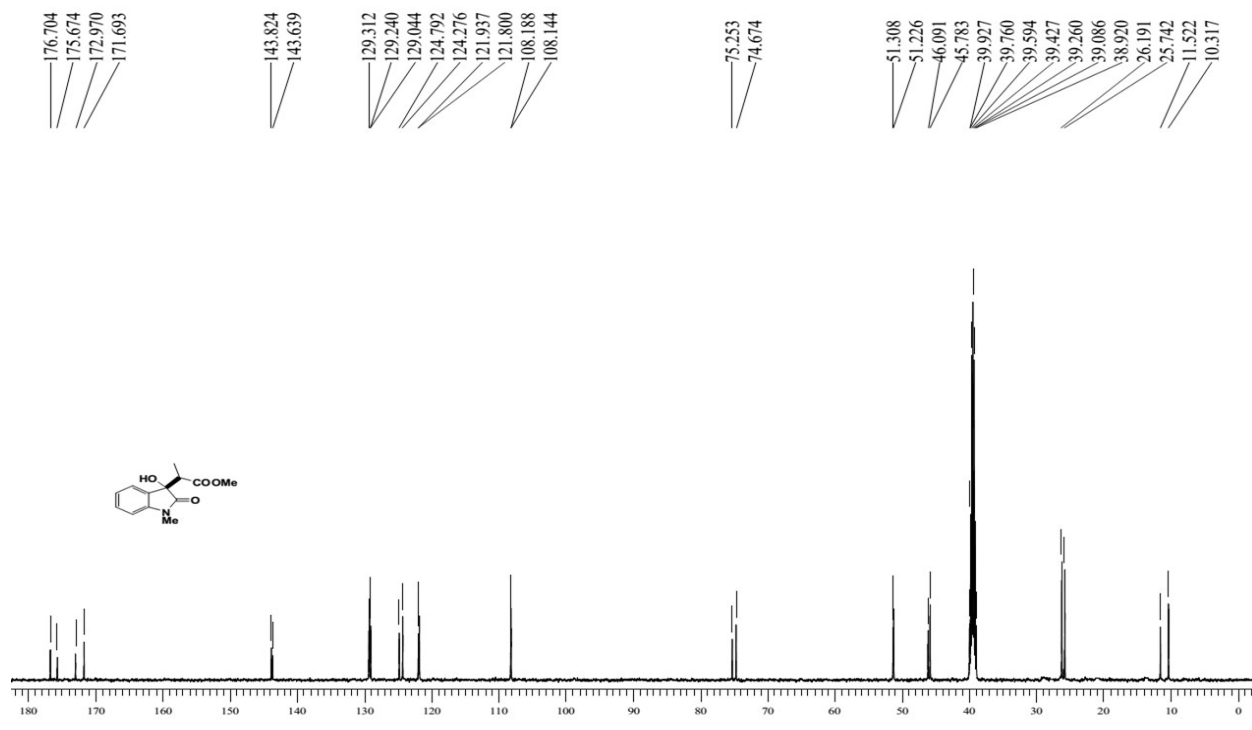


### Compound 5c

### <sup>1</sup>H NMR

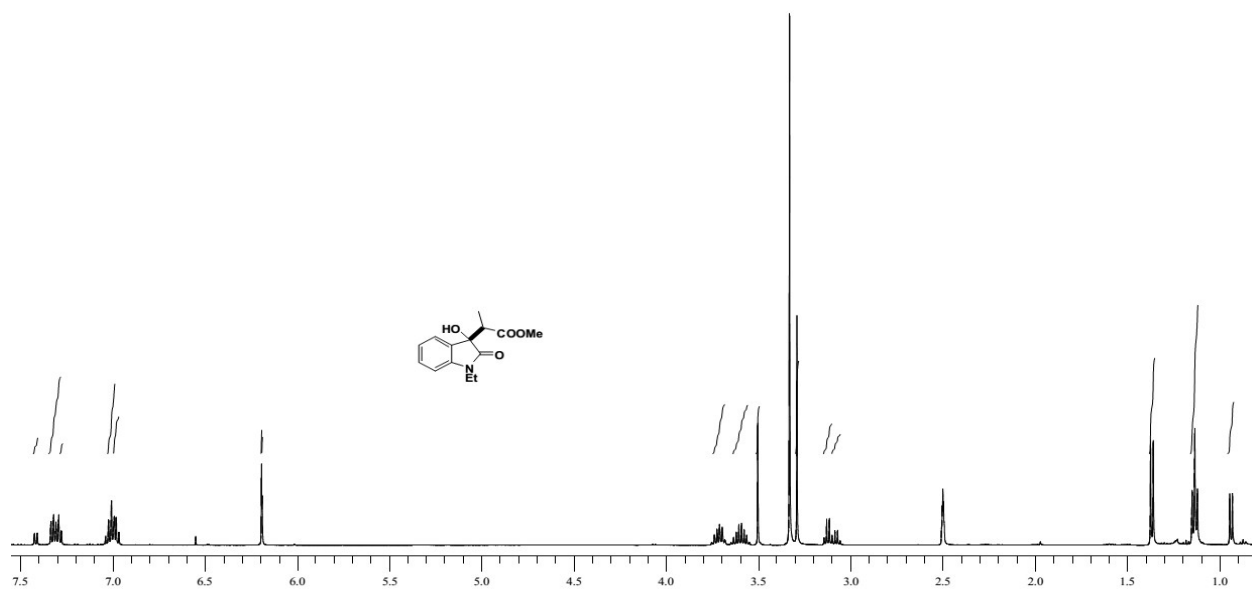


**<sup>13</sup>C NMR**

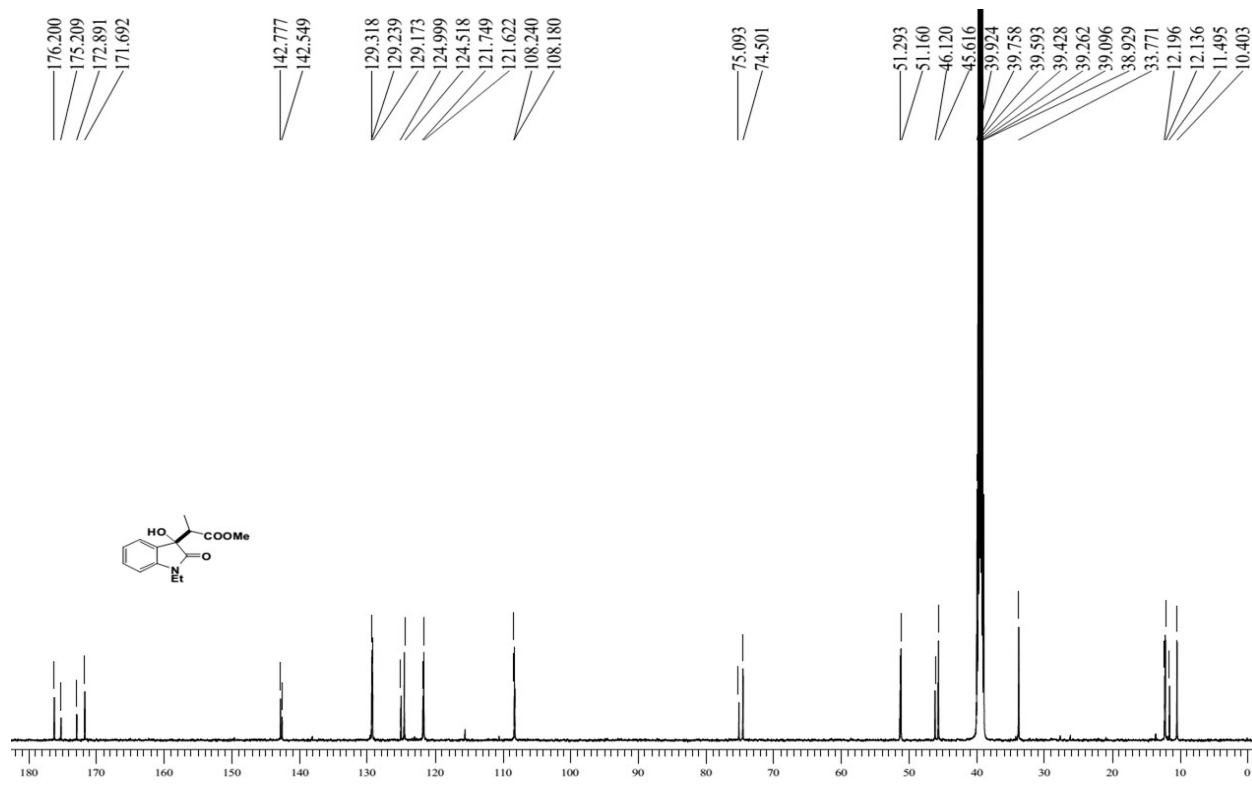


**Compound 5f**

**<sup>1</sup>H NMR**

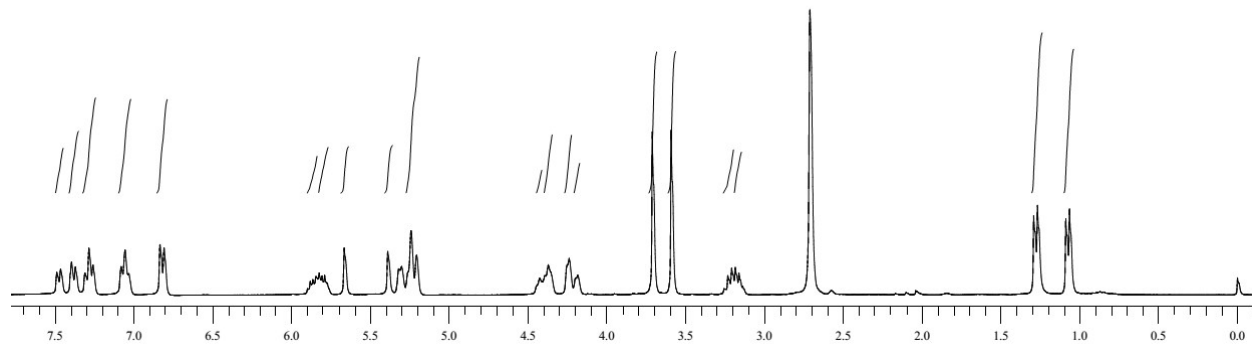
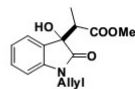


**<sup>13</sup>C NMR**

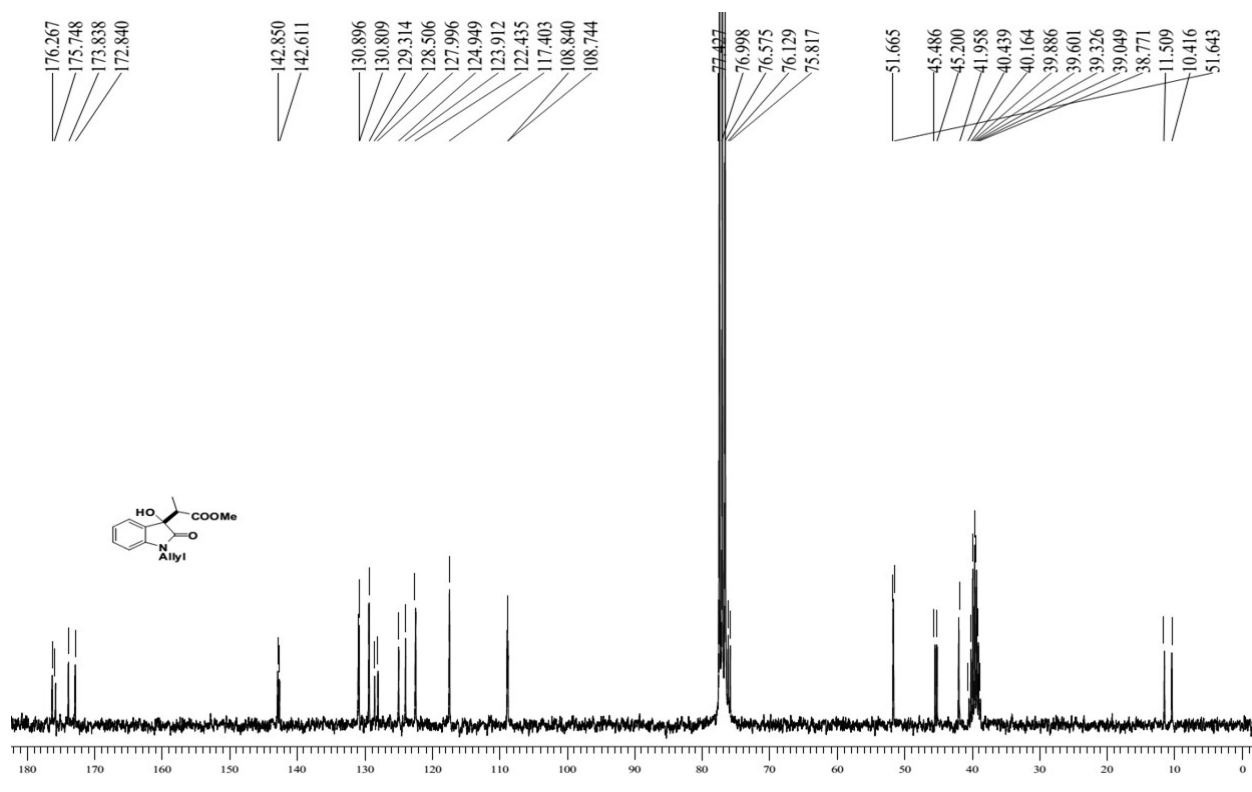


**Compound 5g**

**<sup>1</sup>H NMR**



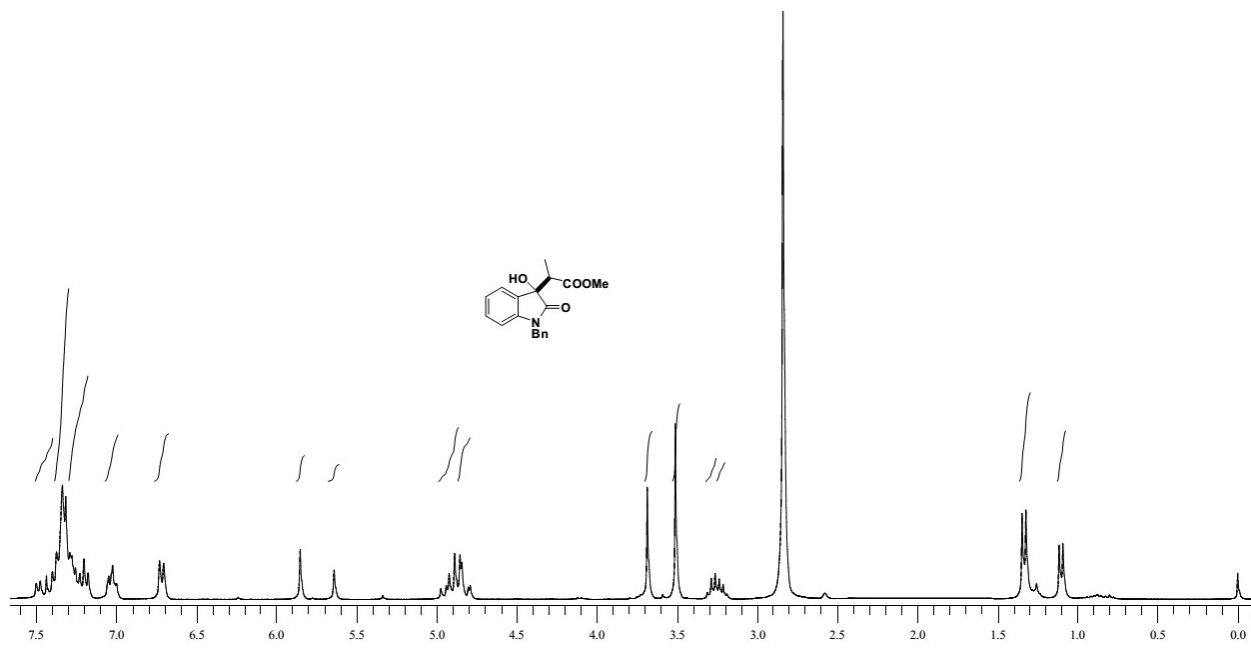
**<sup>13</sup>C NMR**



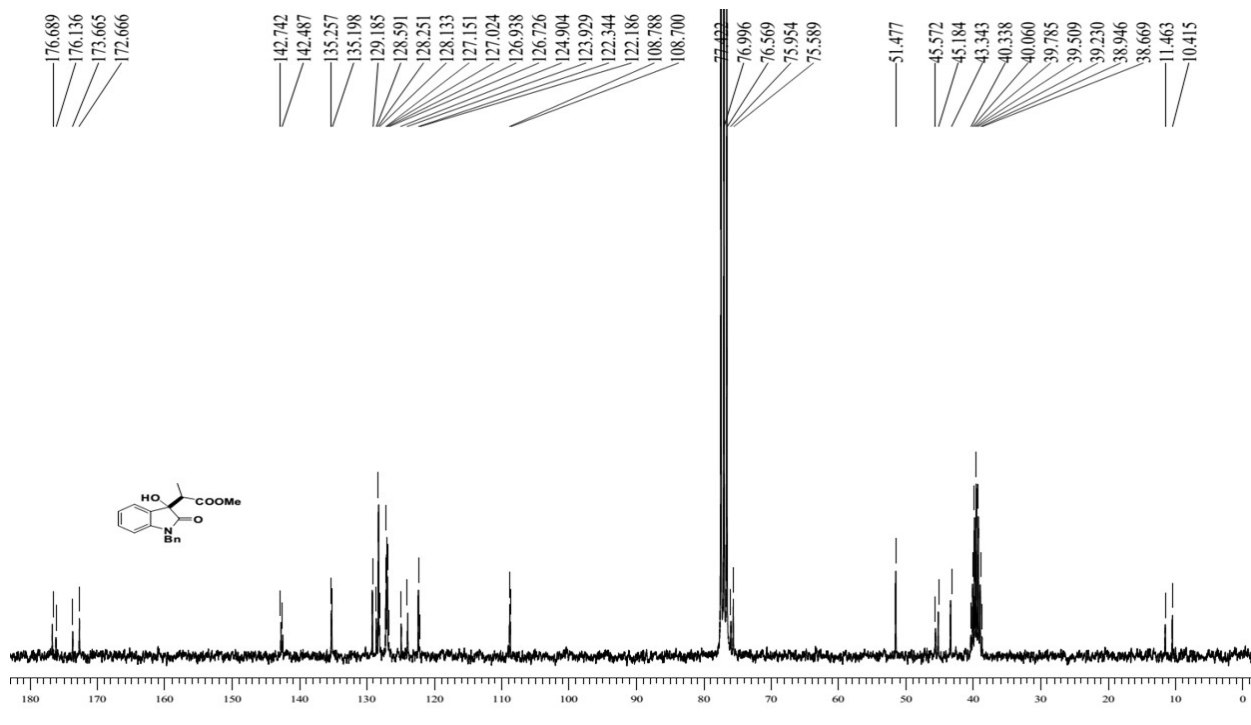
**Compound 5h**

**<sup>1</sup>H NMR**



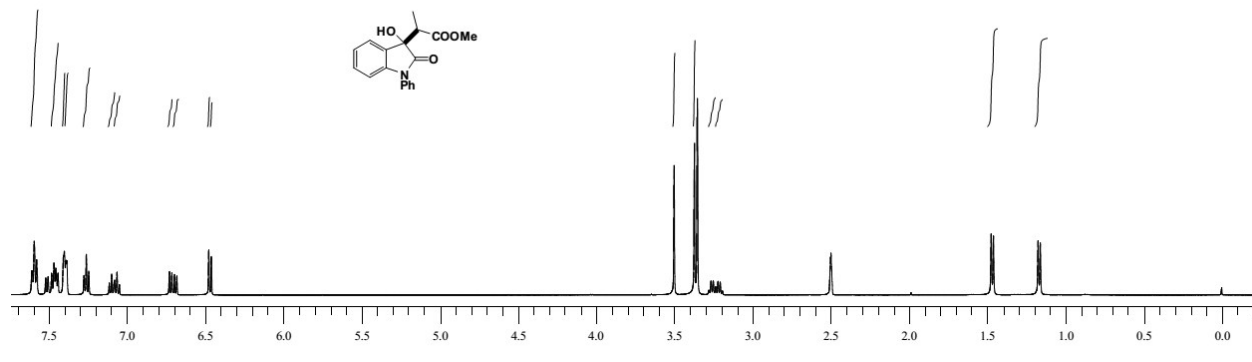


### <sup>13</sup>C NMR

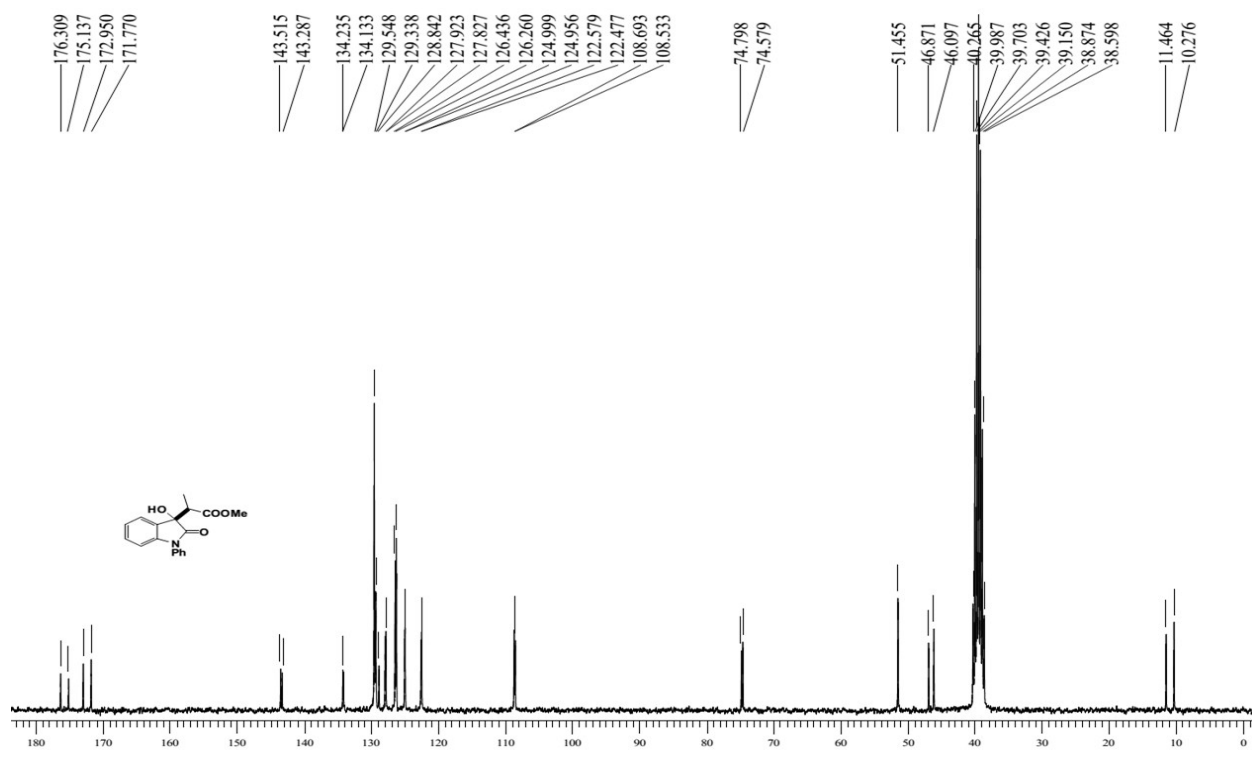


**Compound 5i**

### <sup>1</sup>H NMR

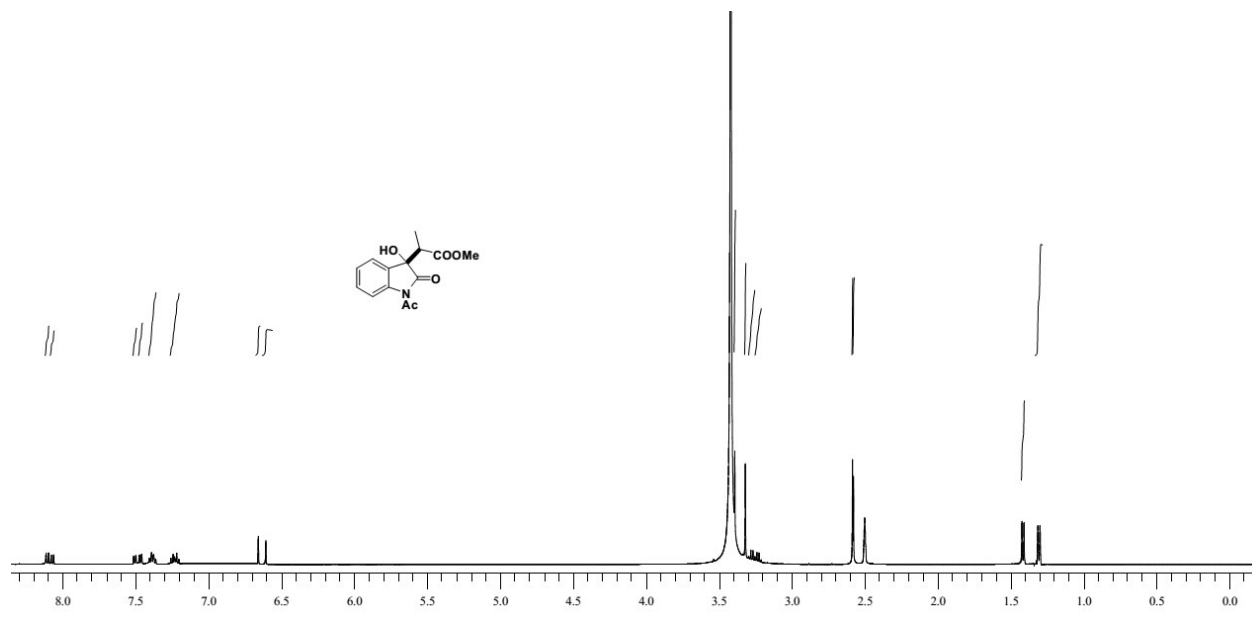


### <sup>13</sup>C NMR

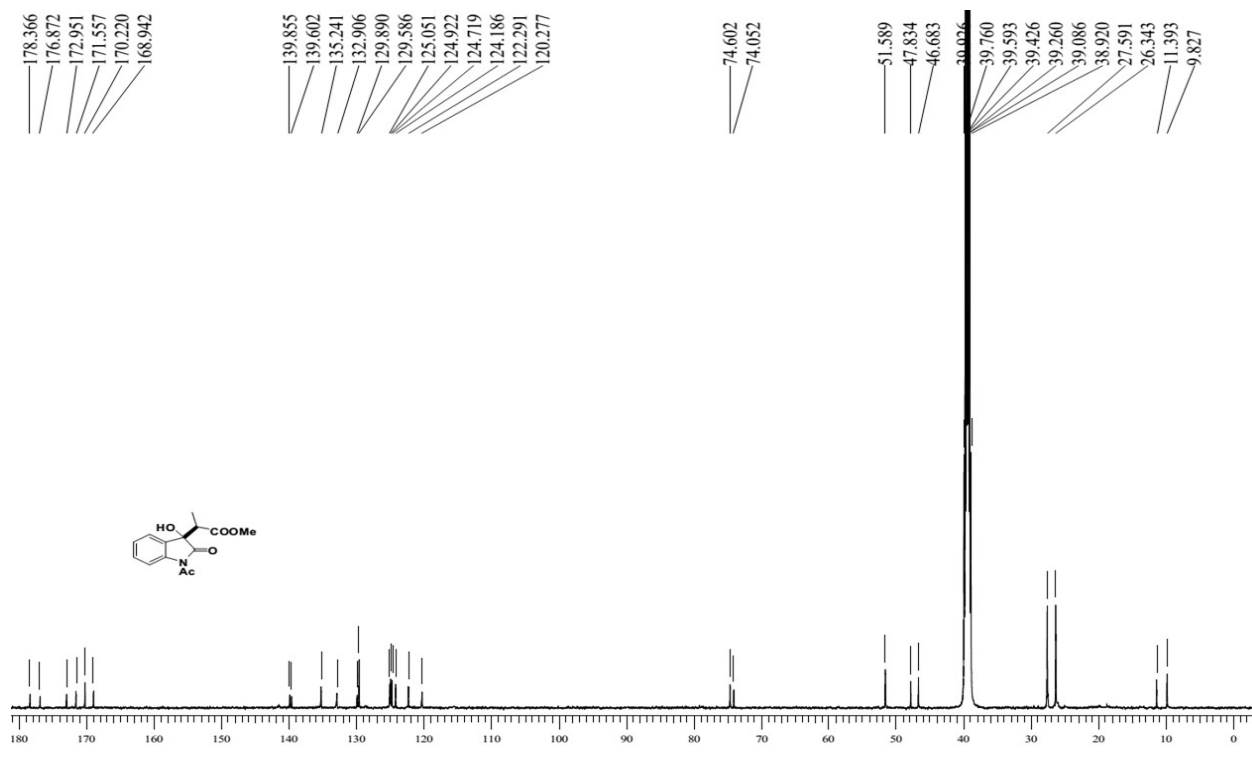


### Compound 5j

### <sup>1</sup>H NMR

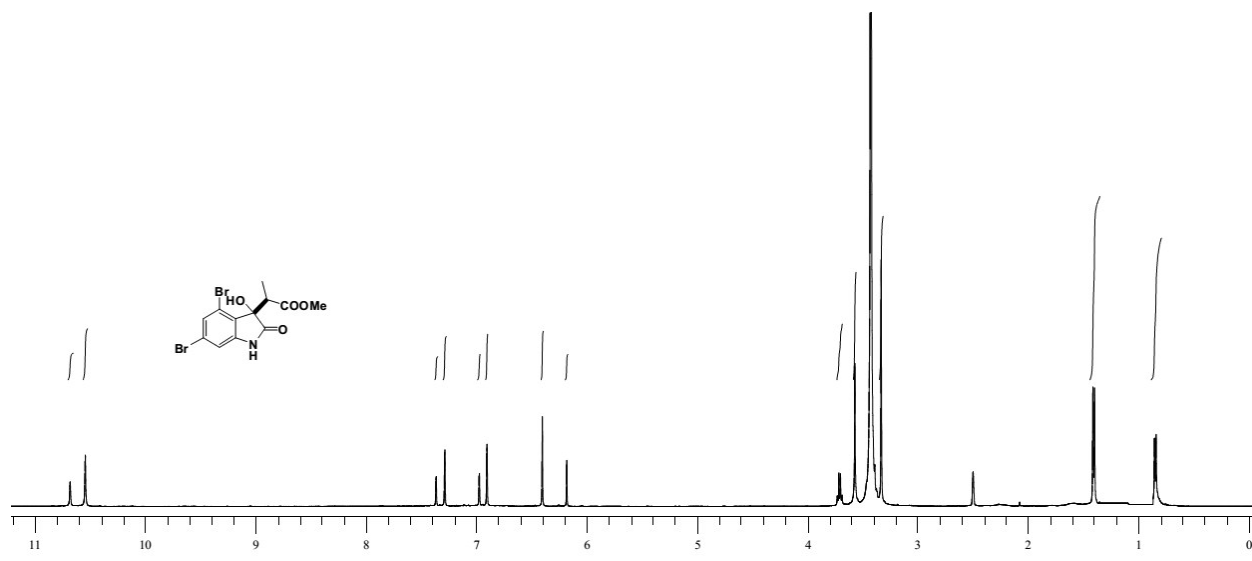


**<sup>13</sup>C NMR**

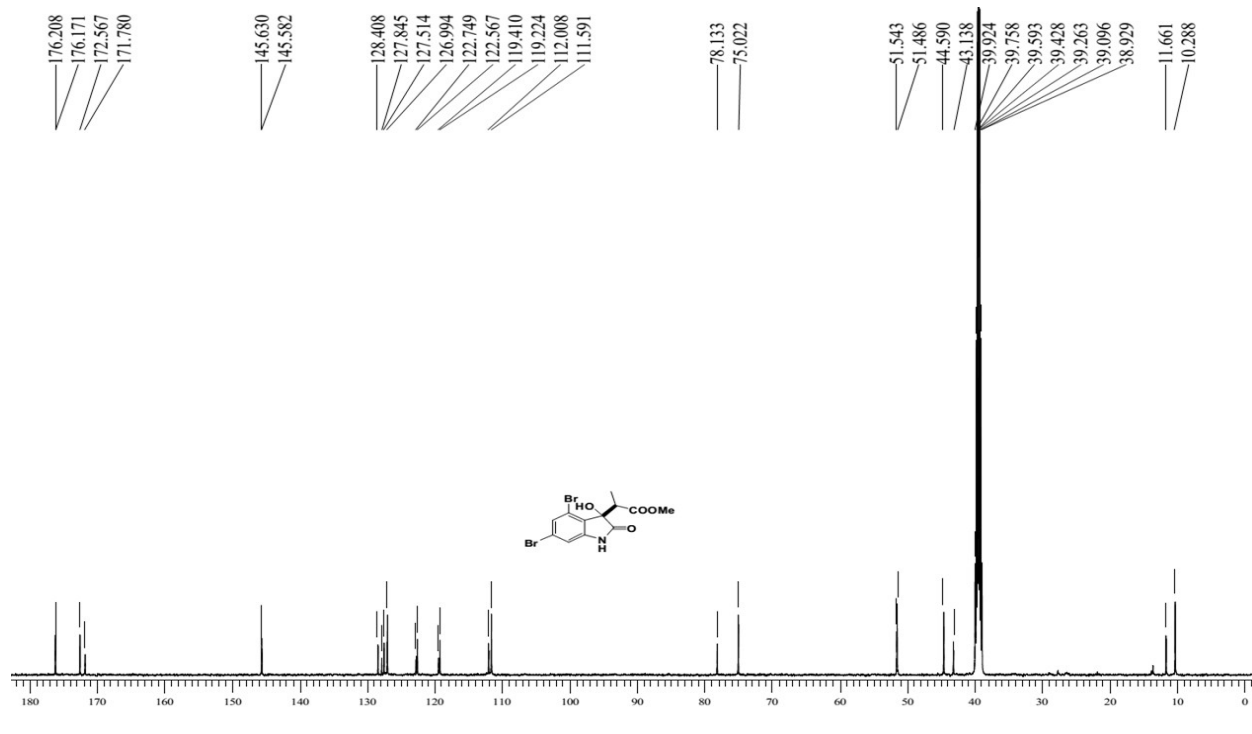


**Compound 5k**

**<sup>1</sup>H NMR**

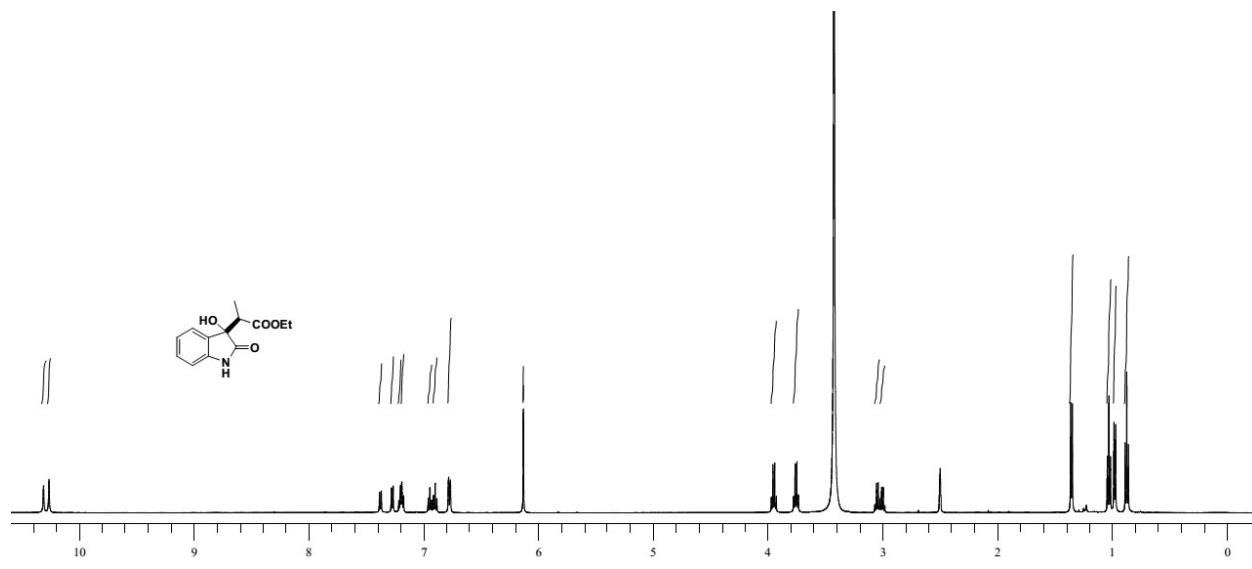


**<sup>13</sup>C NMR**

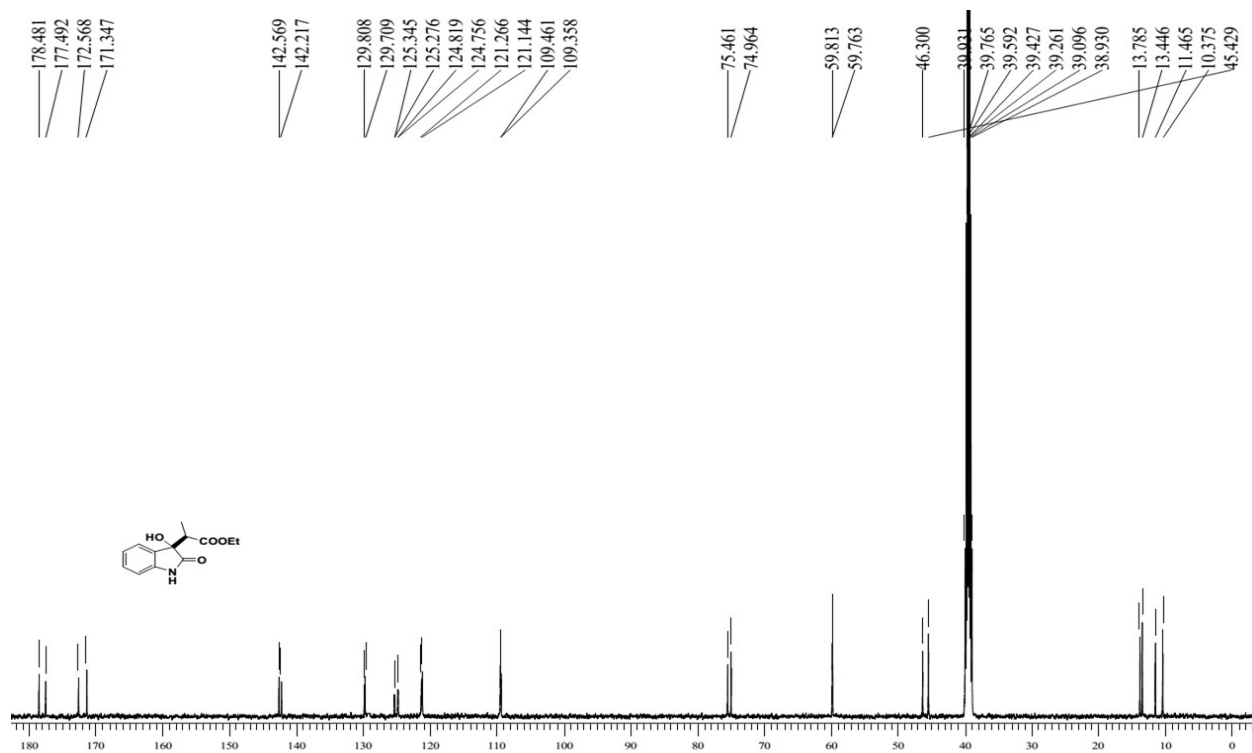


**Compound 51**

**<sup>1</sup>H NMR**

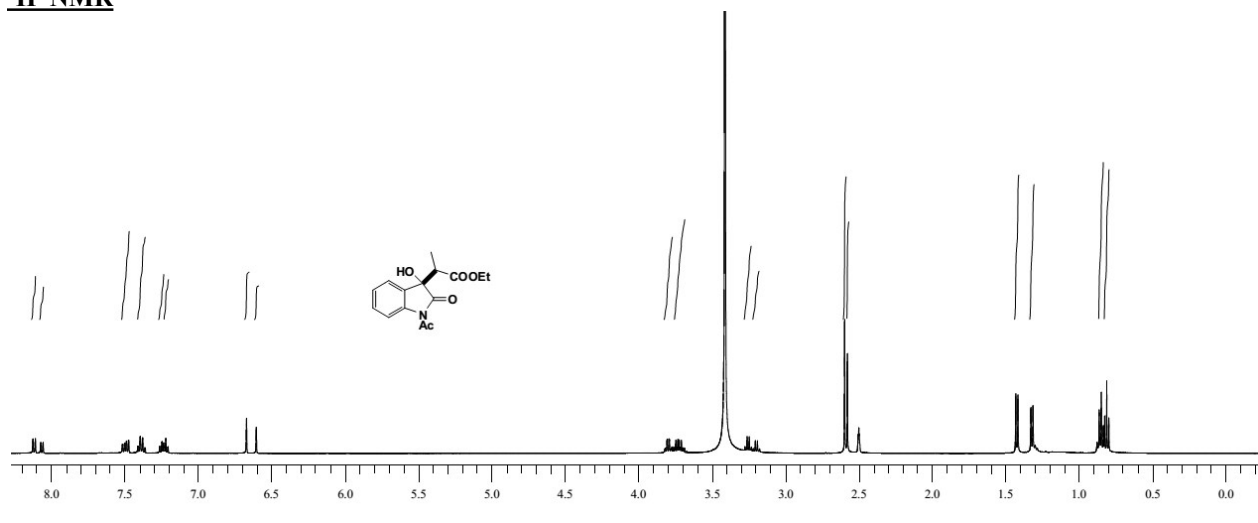


**<sup>13</sup>C NMR**

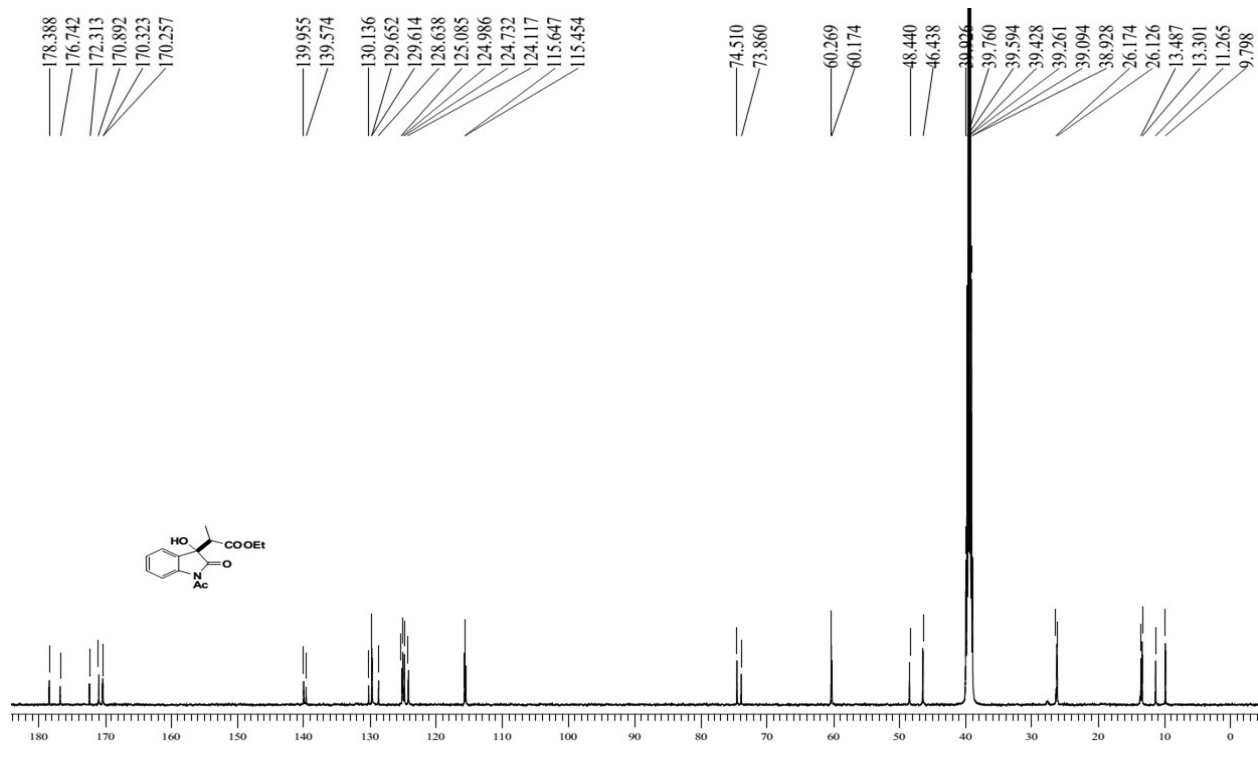


**Compound 5m**

### <sup>1</sup>H NMR

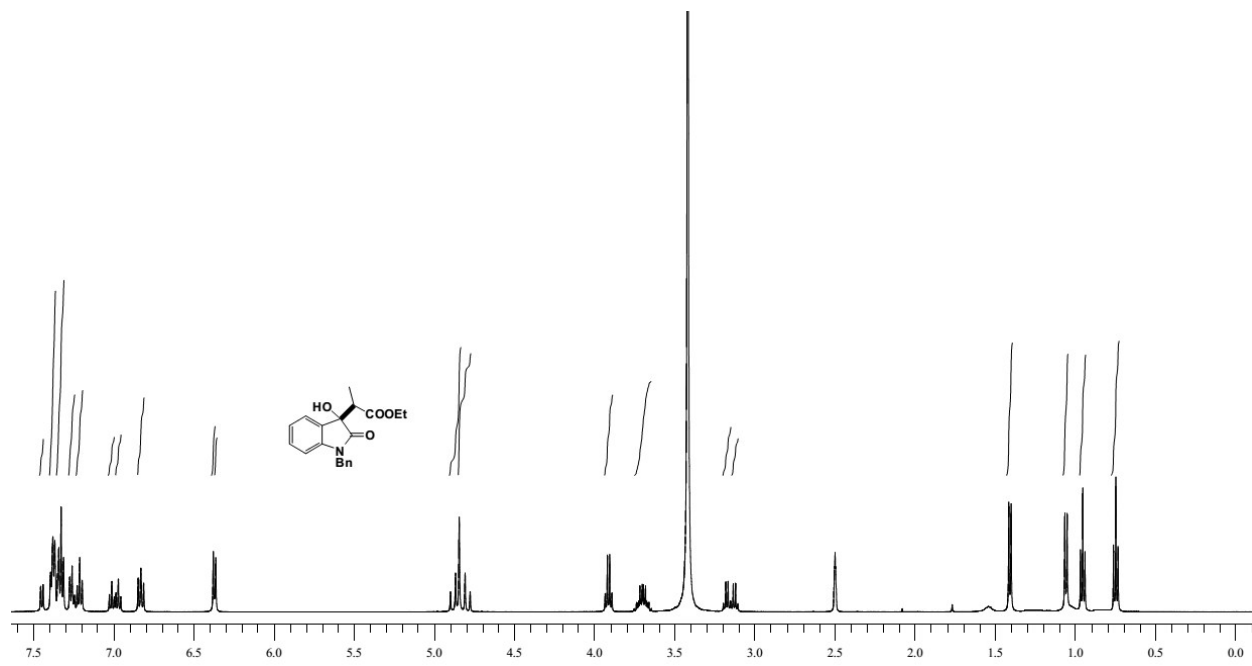


### <sup>13</sup>C NMR

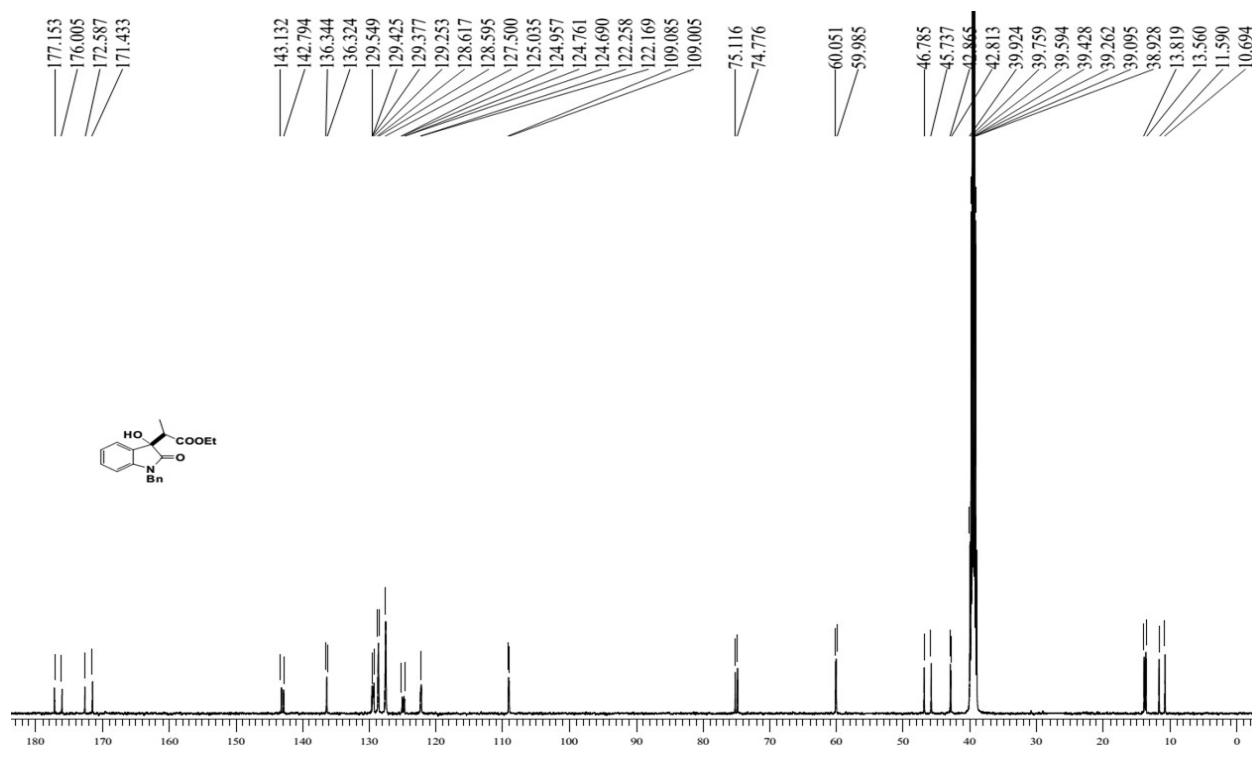


### Compound 5n

### <sup>1</sup>H NMR

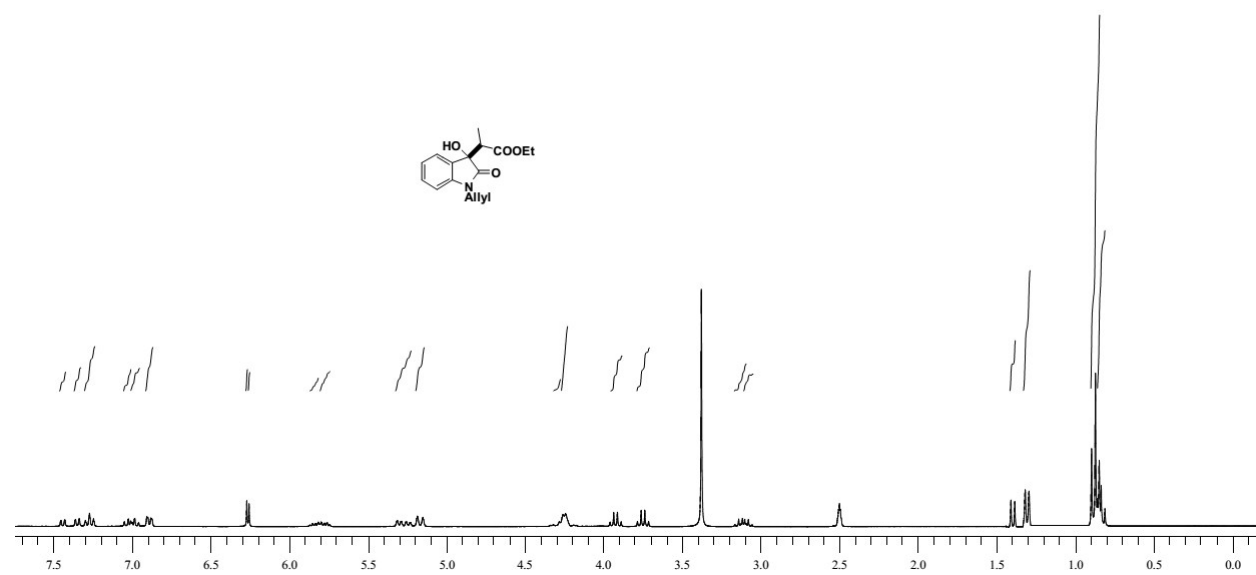


**<sup>13</sup>C NMR**

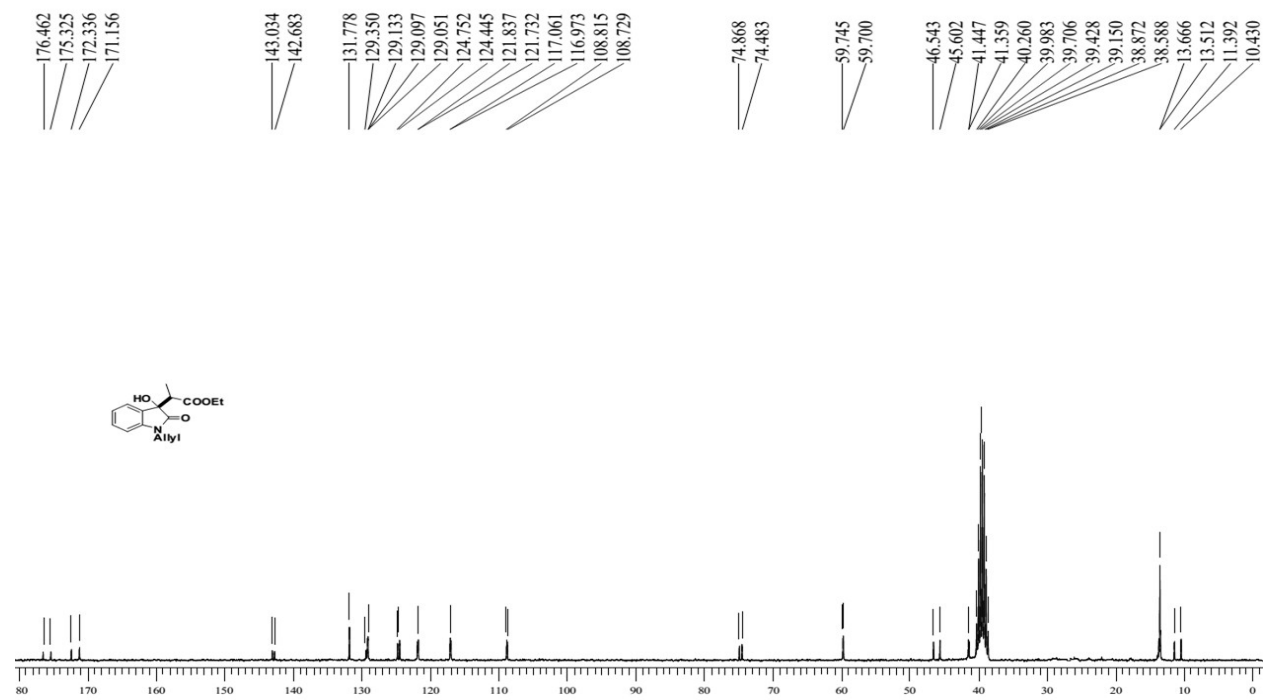


**Compound 50**

**<sup>1</sup>H NMR**



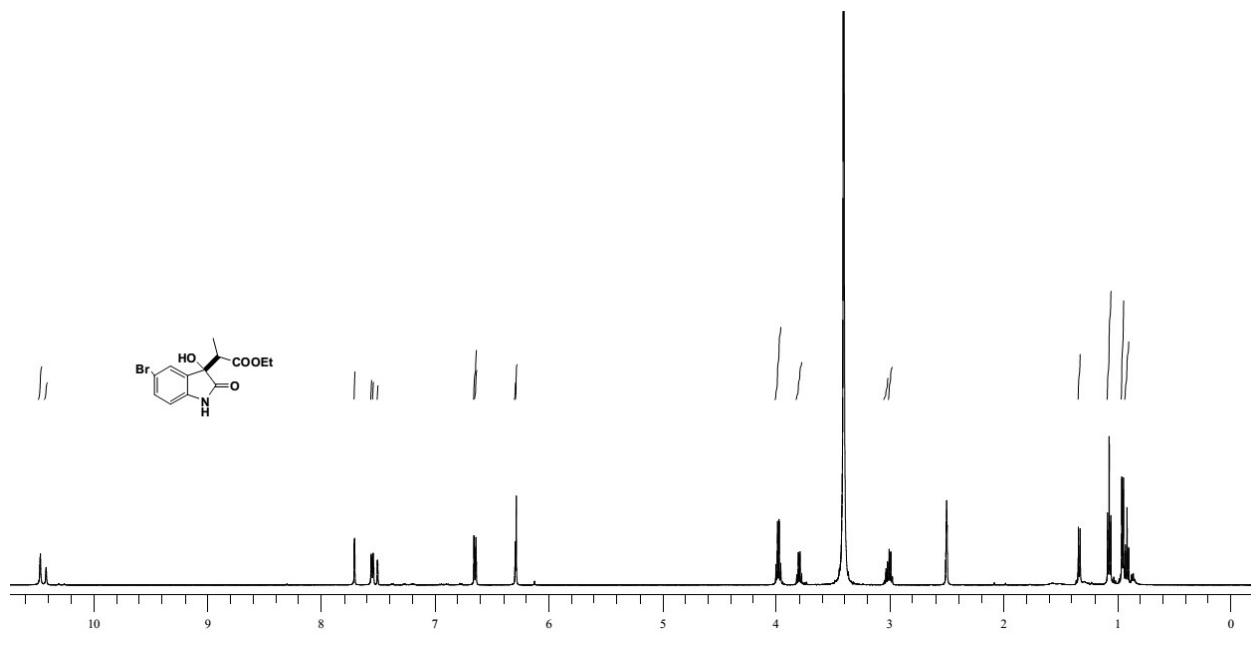
### <sup>13</sup>C NMR



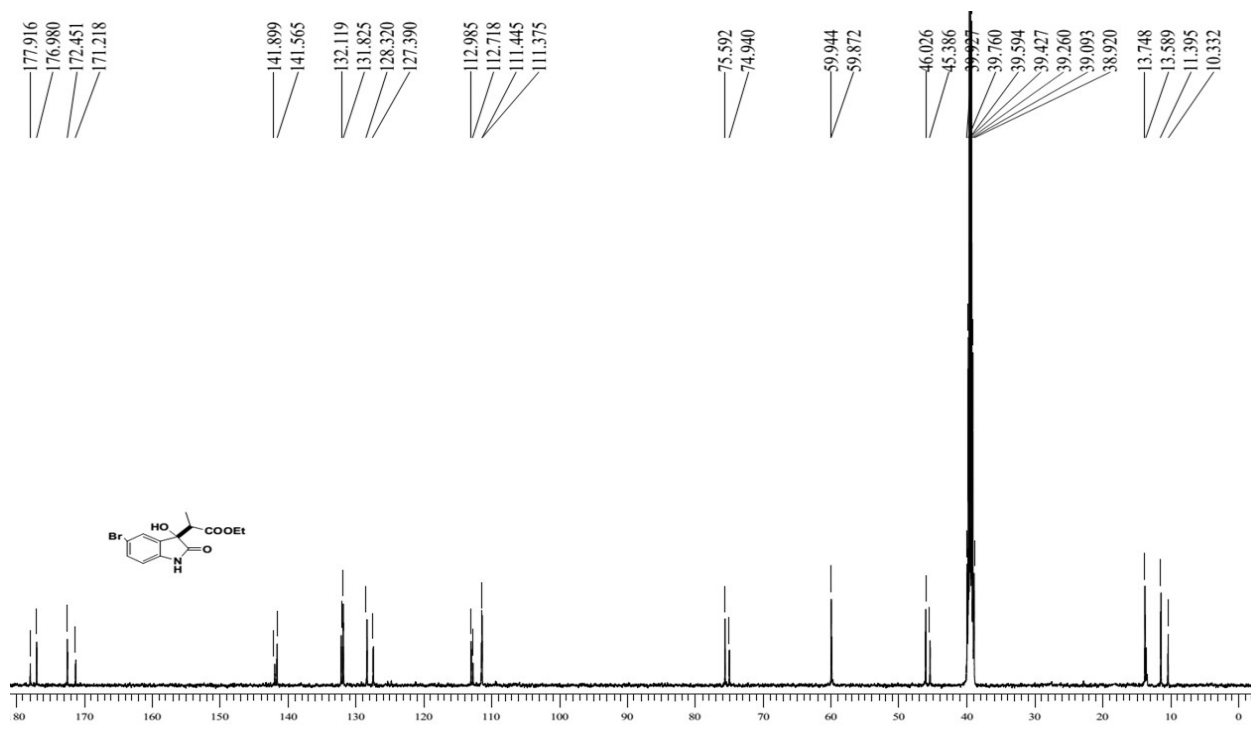
### Compound 5p

### <sup>1</sup>H NMR



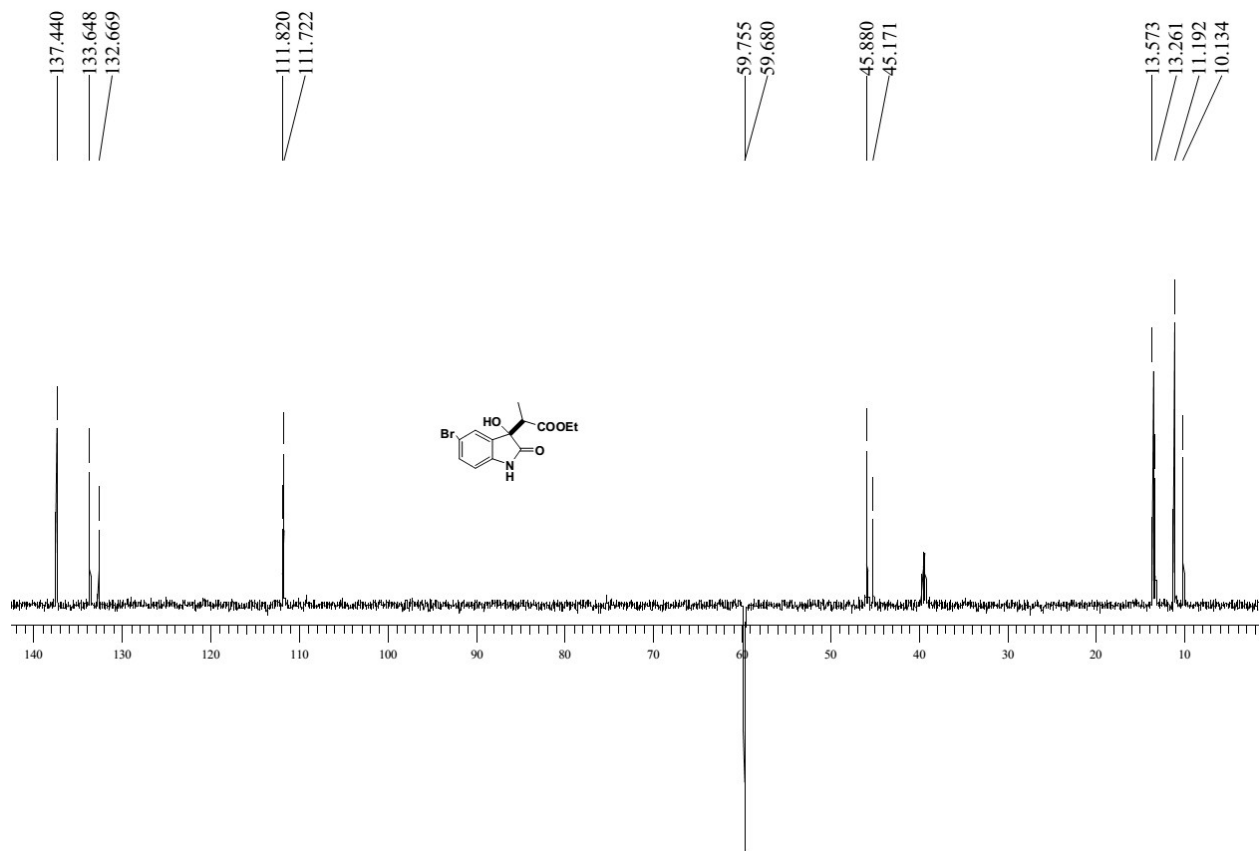


### <sup>13</sup>C NMR



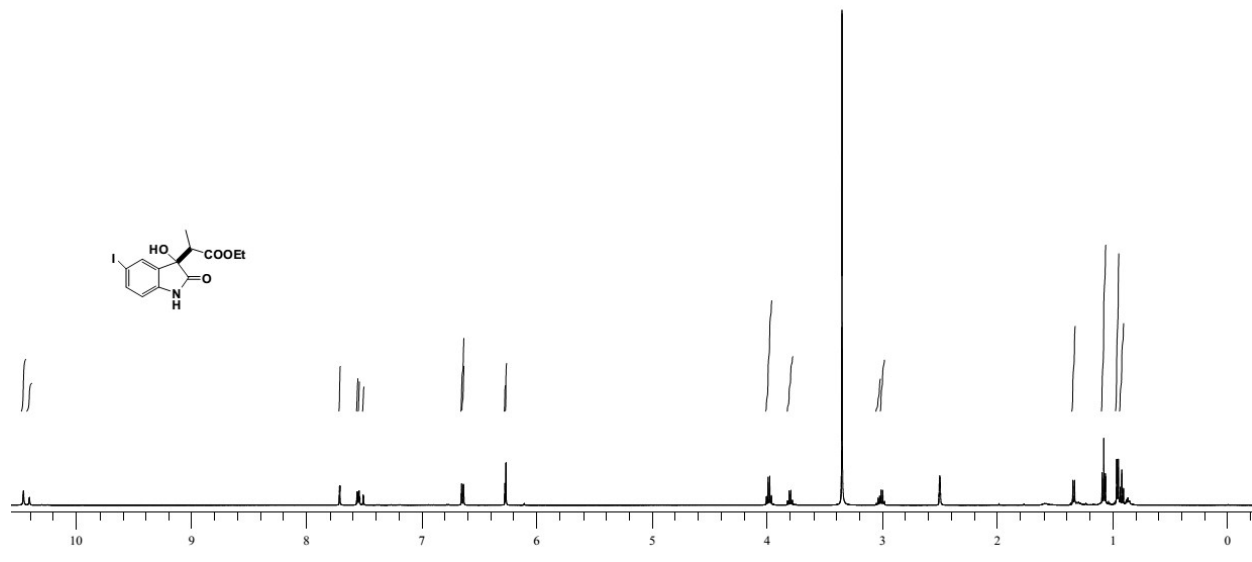
**Compound 5p**

### DEPT-<sup>13</sup>CMR

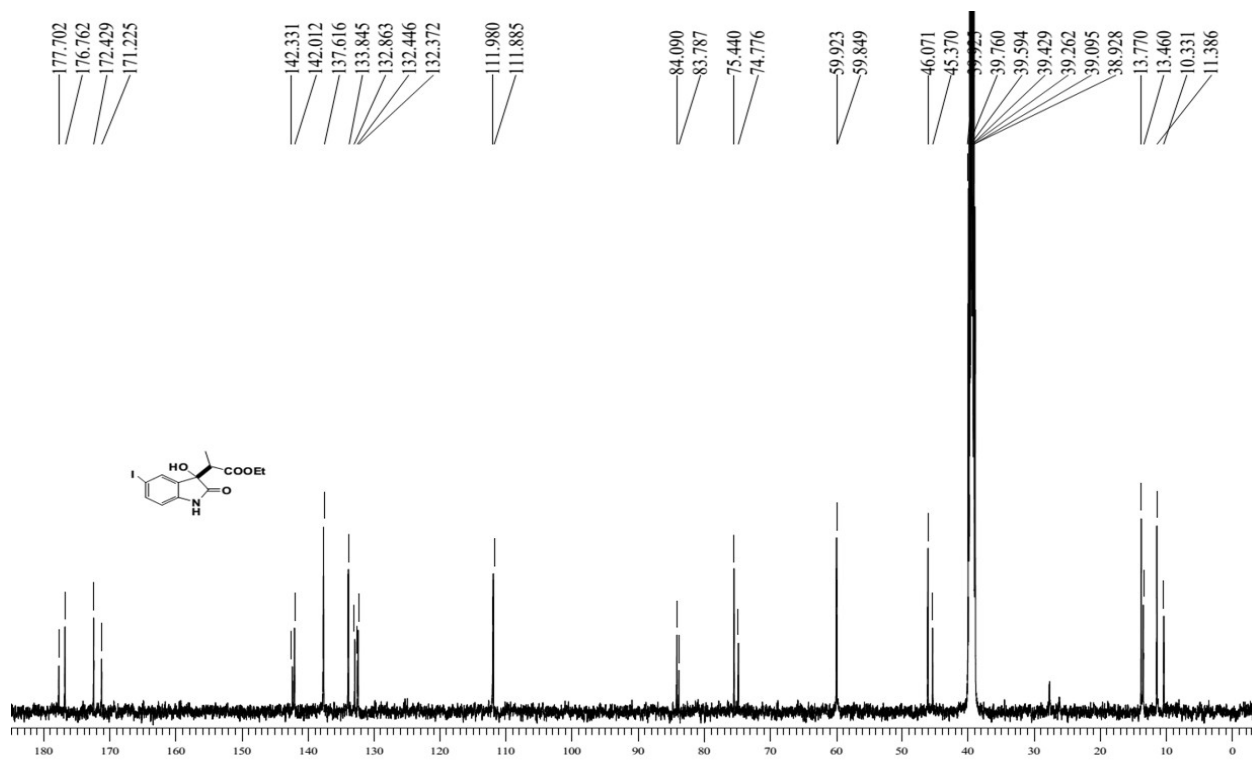


**Compound 5q**

**1H NMR**

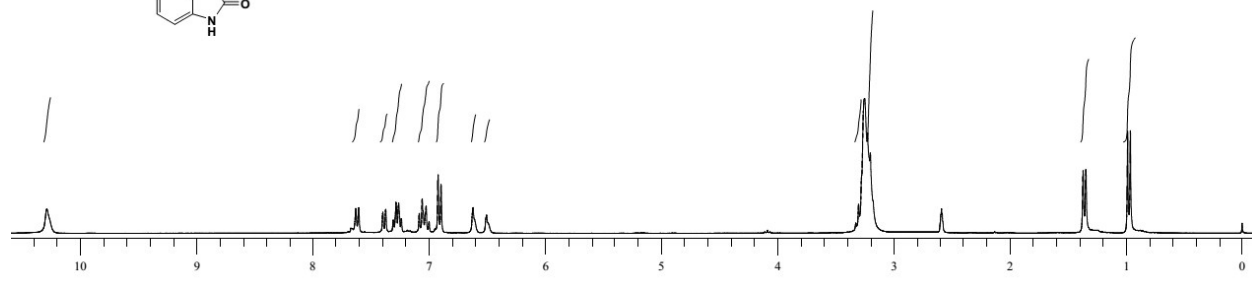
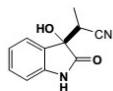


**<sup>13</sup>C NMR**



**Compound 5r**

**<sup>1</sup>H NMR**



### <sup>13</sup>C NMR

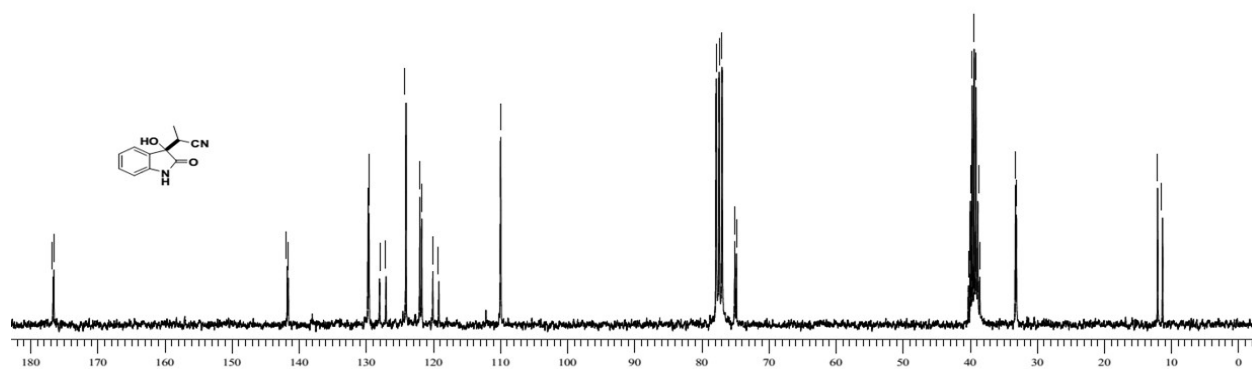
176.632  
176.513

141.751  
141.611

129.710  
129.570  
128.003  
127.032  
124.066  
121.998  
121.720  
120.062  
119.168  
109.954

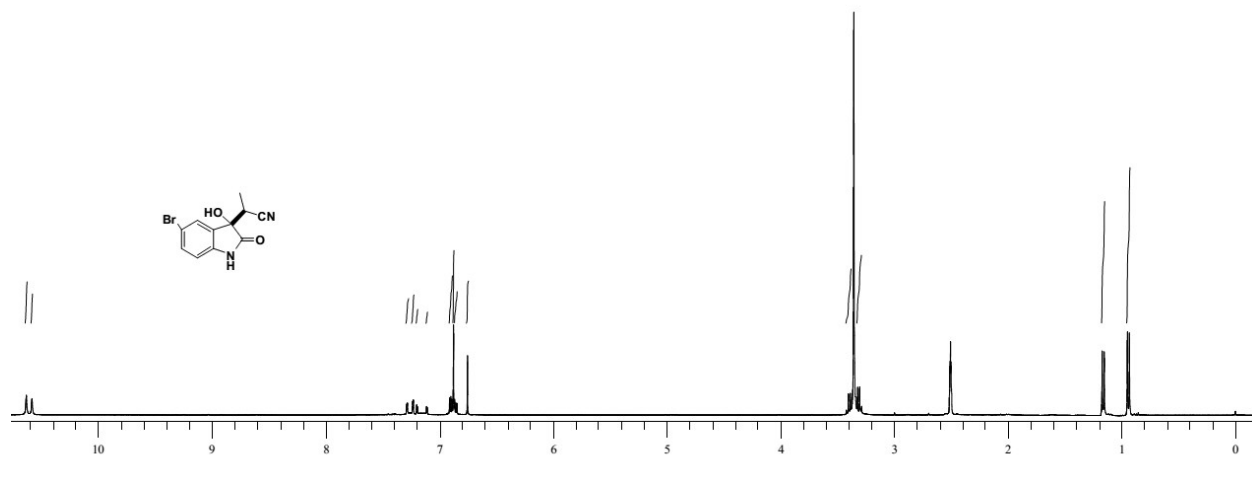
77.844  
77.413  
76.983  
75.074  
74.839

40.257  
39.981  
39.705  
39.429  
39.151  
38.873  
38.589  
33.275  
33.122  
12.091  
11.357

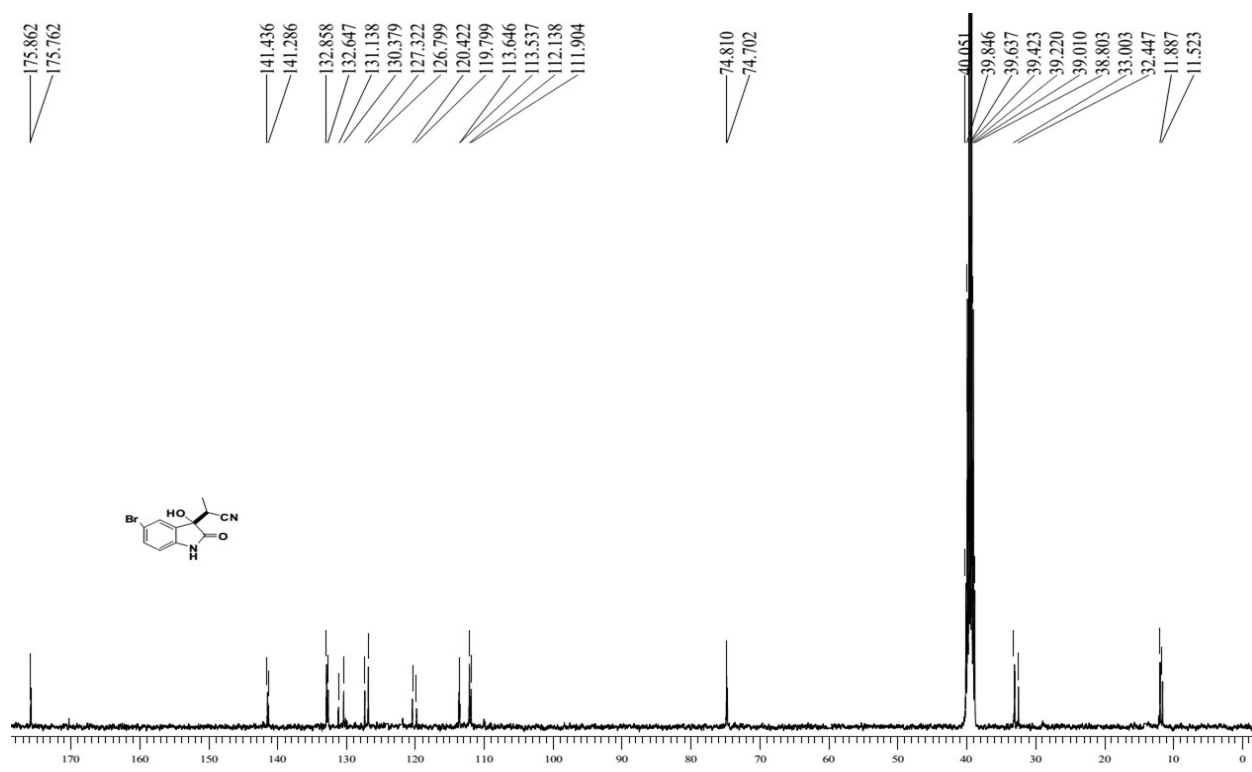


Compound 5s

### <sup>1</sup>H NMR

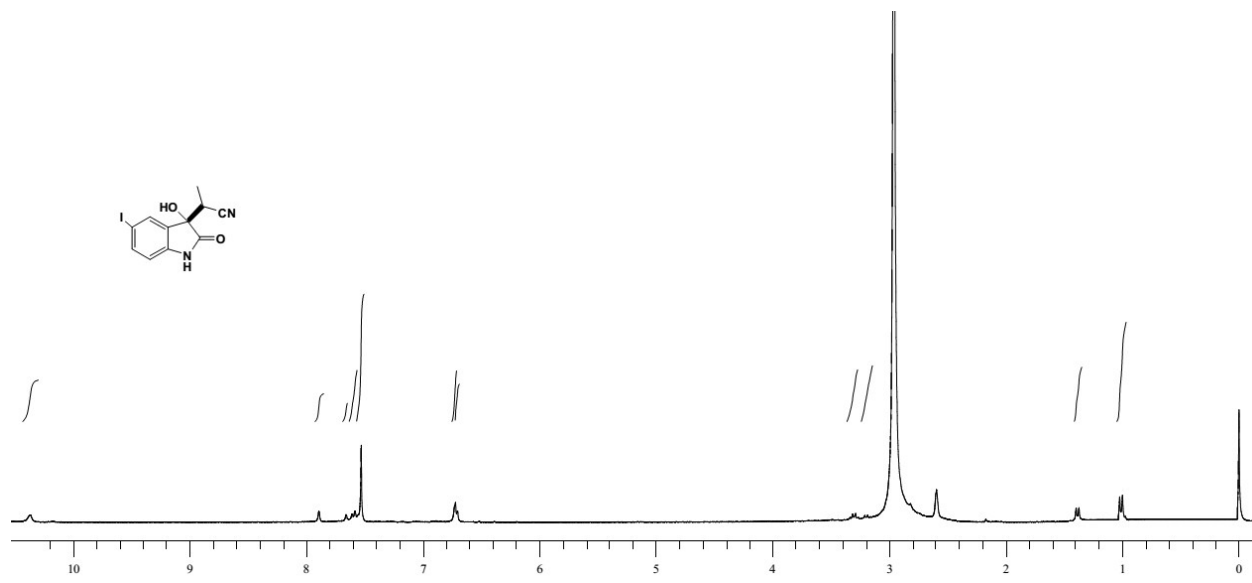


### <sup>13</sup>C NMR

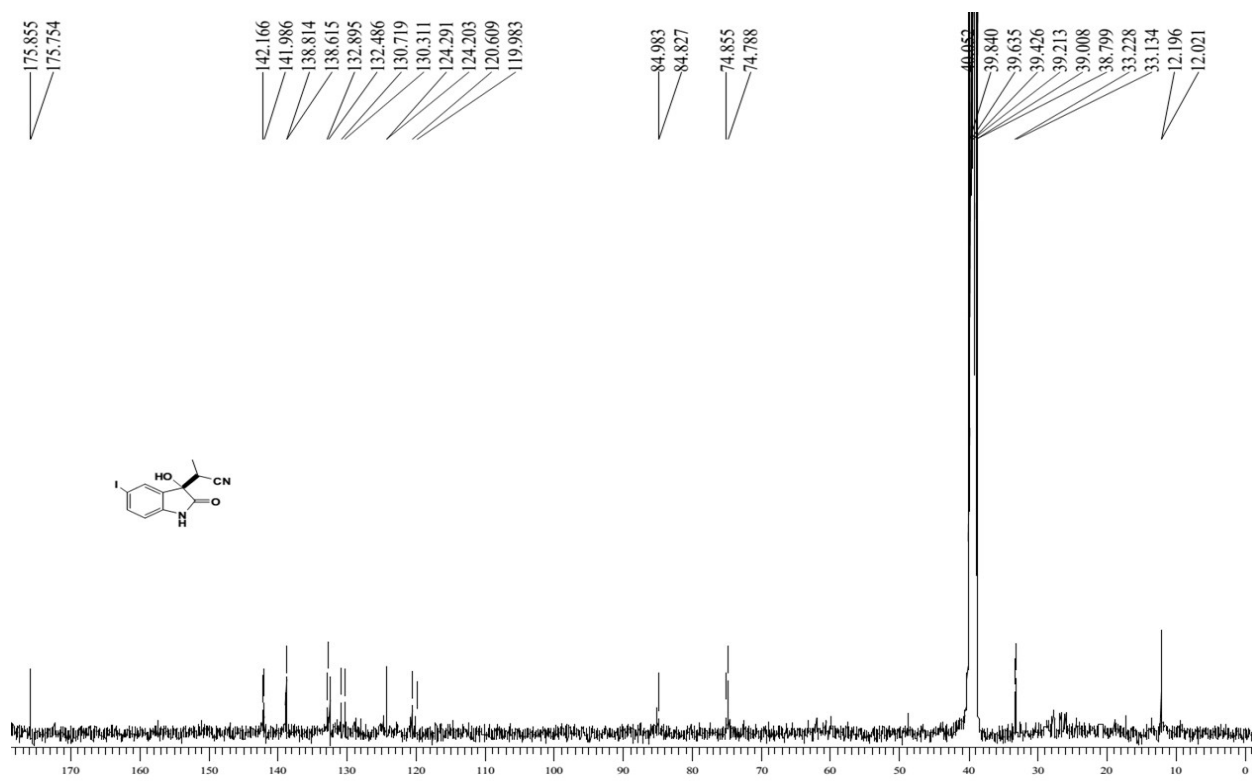


**Compound 5t**

### <sup>1</sup>H NMR

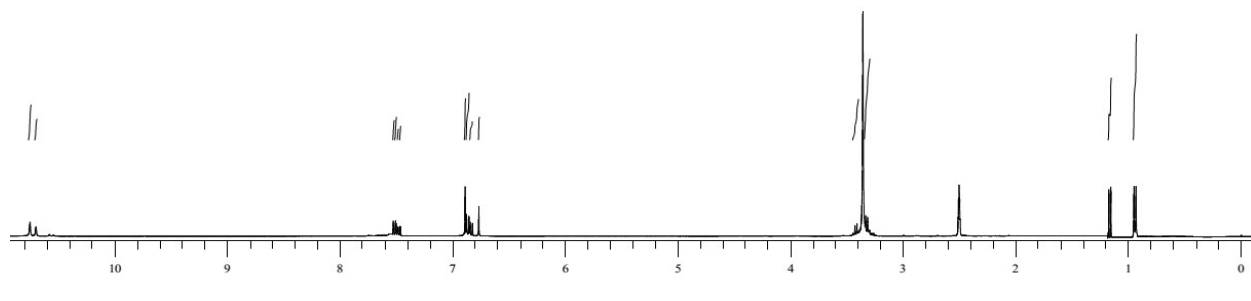
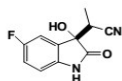


### <sup>13</sup>C NMR

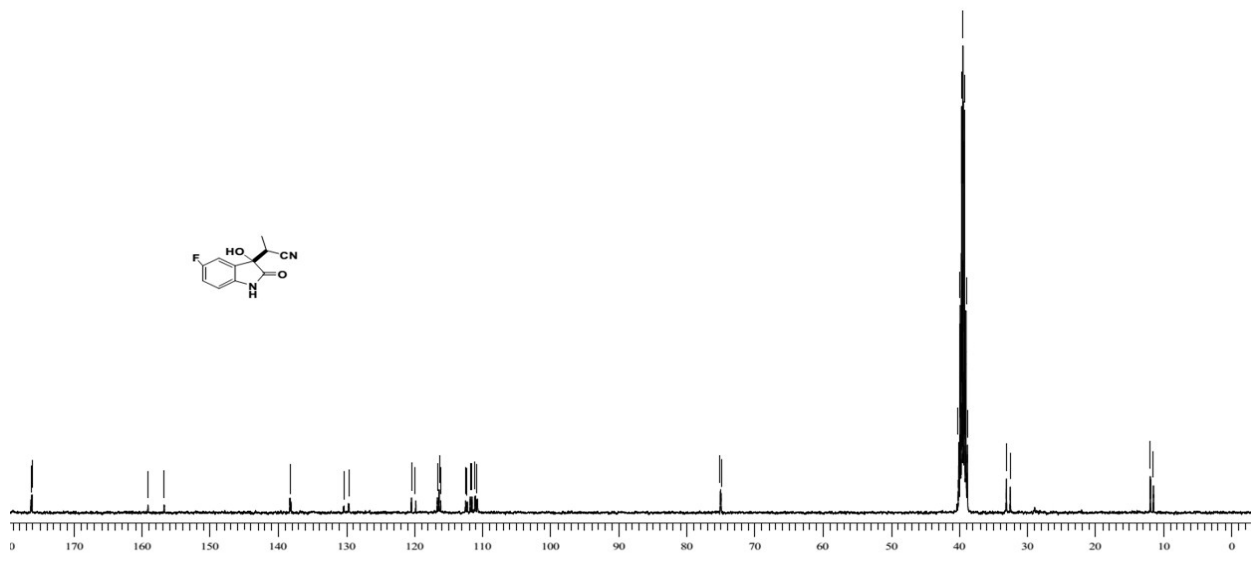
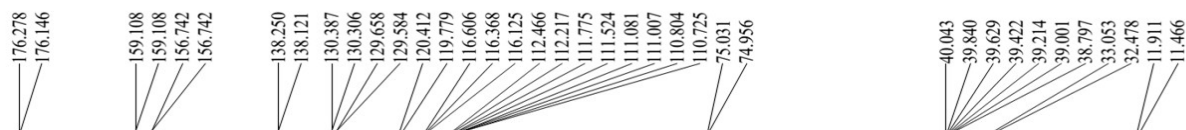


**Compound 5u**

### <sup>1</sup>H NMR



**<sup>13</sup>C NMR**



Crystallographic data for 4r

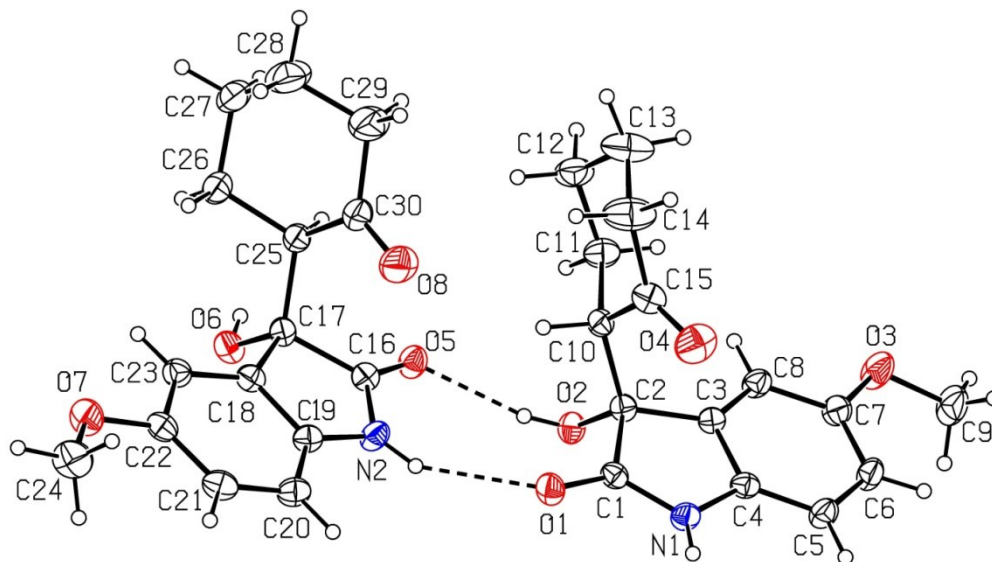
X-ray data for the compound (**4r**) were collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated MoK $\alpha$  radiation ( $\lambda=0.71073\text{\AA}$ ) with  $\omega$ -scan method.<sup>1</sup> Preliminary lattice parameters and orientation matrices were obtained from four sets of frames. Unit cell dimensions were determined using 7182 reflections for BB74 data. Integration and scaling of intensity data were accomplished using SAINT program.<sup>1</sup> The structures were solved by Direct Methods using SHELXS97<sup>2</sup> and refinement was carried out by full-matrix least-squares technique using SHELXL-2014/7.<sup>2</sup> Anisotropic displacement parameters were included for all non-hydrogen atoms. All H atoms were positioned geometrically and treated as riding on their parent C atoms with C-H distances of 0.93--0.97  $\text{\AA}$ , and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}$  for methyl atoms. Amide N and hydroxyl O bound H atoms were located from the difference Fourier map.

**Crystallographic data for 4r:** C<sub>15</sub>H<sub>17</sub>NO<sub>4</sub>,  $M = 275.30$ , colourless plate, 0.37 x 0.25 x 0.13 mm<sup>3</sup>, monoclinic, space group  $P2_1/n$  (No. 14),  $a = 7.5260(7)$ ,  $b = 15.1059(14)$ ,  $c = 24.110(2)$   $\text{\AA}$ ,  $\alpha = 90$ ,  $\beta = 96.277(2)$ ,  $\gamma = 90^\circ$ ,  $V = 2724.6(4)\text{\AA}^3$ ,  $Z = 8$ ,  $D_c = 1.342$  g/cm<sup>3</sup>,  $F_{000} = 1168$ , CCD area detector, MoK $\alpha$  radiation,  $\lambda = 0.71073$   $\text{\AA}$ ,  $T = 293(2)\text{K}$ ,  $2\theta_{\text{max}} = 50.0^\circ$ , 25936 reflections collected, 4796 unique ( $R_{\text{int}} = 0.033$ ), Final  $Goof = 1.23$ ,  $R_I = 0.0704$ ,  $wR_2 = 0.1629$ ,  $R$  indices based on 4356 reflections with  $I > 2\sigma(I)$  (refinement on  $F^2$ ), 379 parameters,  $\mu = 0.098$  mm<sup>-1</sup>, Minimum and Maximum Residual Densities = -0.18 and 0.38 e/  $\text{\AA}^3$ .

CCDC 1435101 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at <https://summary.ccdc.cam.ac.uk/structure-summary-form> or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk)

1. SMART & SAINT. Software Reference manuals. Versions 6.28a & 5.625, Bruker Analytical X-ray Systems Inc., Madison, Wisconsin, U.S.A., 2001.
2. Sheldrick, G. M. SHELXS97 and SHELXL Version 2014/7, <http://shelx.uni-ac.gwdg.de/SHELX/index.php>





**Figure 1.** The molecular structure of **4r** with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius. Racemic molecules in the asymmetric unit are connected by N-H $\cdots$ O and O-H $\cdots$ O hydrogen bonds (shown as dotted lines).