

## A novel domino strategy for forming poly-substituted quaternary imidazoles through Cs<sub>2</sub>CO<sub>3</sub>-promoted aryl migration process

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### General

Microwave irradiation was carried out with initiator from Biotage Company, Sweden. Melting points were determined in open capillaries and were uncorrected. IR spectra were taken on a FT-IR-Tensor 27 spectrometer in KBr pellets and reported in cm<sup>-1</sup>. <sup>1</sup>H NMR spectra were measured on a Bruker DPX 400 MHz spectrometer in DMSO-d<sub>6</sub> with chemical shift (δ) given in ppm relative to TMS as internal standard. HRMS (ESI) was determined by using microTOF-Q II

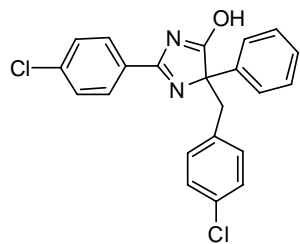
HRMS/MS instrument (Bruker). X-Ray crystallographic analysis was performed with a Siemens SMART CCD and a Siemens P4 diffractometer.

### Example for the synthesis of **3a**:

#### **4-(4-chlorobenzyl)-2-(4-chlorophenyl)-4-phenyl-4H-imidazol-5-ol (3a)**

Typically, (3-(4-chlorophenyl)oxiran-2-yl)(phenyl)methanone (**2a**, 1 mmol, 0.258 g, 1.0 equiv.) was introduced in a 10-mL Initiator<sup>TM</sup> reaction vial, 4-chlorobenzimidamide (**1a**, 1.0 mmol, 0.154 g, 1.0 equiv.) and Cs<sub>2</sub>CO<sub>3</sub> (1.0 mmol, 0.326 g, 1.0 equiv.) as well as ethylene glycol (1.5 mL) were then successively added. Subsequently, the reaction vial was closed and then pre-stirred for 20 second. The mixture was irradiated (Time: 15 min, Temperature: 120 °C; Absorption Level: High; Fixed Hold Time) until TLC (petroleum ether : acetone 3:1) revealed that conversion of the starting material **2a** was complete. The reaction mixture was then cooled to room temperature and then diluted with cold water (20 ml). The solid product was collected by Büchner filtration and was purified by recrystallization from 60% ethanol to afford the desired pure imidazoles **3a** as a white solid (mp: 253-254 °C).

#### 4-(4-Chlorobenzyl)-2-(4-chlorophenyl)-4-phenyl-4H-imidazol-5-ol (3a)



White solid, mp: 253-254 °C;

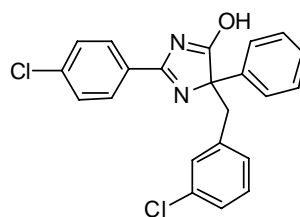
IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3164, 3058, 2846, 1682, 1495, 1299, 1165, 1018, 830, 730, 694 $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 8.76 (s, 1H, OH), 7.74 (t,  $J = 7.2$  Hz, 4H, ArH), 7.48 (d,  $J = 8.4$  Hz, 2H, ArH), 7.37 (t,  $J = 7.2$  Hz, 2H, ArH), 7.31 (t,  $J = 7.2$  Hz, 1H, ArH), 7.14-7.08 (m, 4H, ArH), 3.43 (s, 2H,  $\text{CH}_2$ );

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 184.6, 158.7, 139.6, 137.2, 134.9, 132.5, 131.8, 129.5, 129.2, 128.8, 128.1, 127.9, 127.6, 126.5, 76.7, 44.9.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{22}\text{H}_{16}\text{Cl}_2\text{N}_2\text{NaO}$ : 417.0537  $[\text{M}+\text{Na}]^+$ , found:417.0544.

#### 4-(3-Chlorobenzyl)-2-(4-chlorophenyl)-4-phenyl-4H-imidazol-5-ol (3b)



White solid, mp: 216-217 °C;

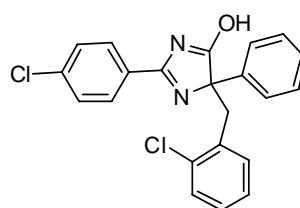
IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3166, 3090, 1722, 1626, 1434, 1260, 1092, 838, 740, 687 $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 8.91 (s, 1H, OH), 7.76 (d,  $J = 7.2$  Hz, 4H, ArH), 7.49 (d,  $J = 8.4$  Hz, 2H, ArH), 7.38 (t,  $J = 7.2$  Hz, 2H, ArH), 7.32 (t,  $J = 6.8$  Hz, 1H, ArH), 7.22 (s, 1H, ArH), 7.07 (d,  $J = 7.6$  Hz, 2H, ArH), 7.02 (t,  $J = 8.8$  Hz, 1H, ArH), 3.44 (s, 2H,  $\text{CH}_2$ );

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 184.8, 158.8, 139.6, 138.4, 137.2, 132.5, 130.5, 129.7, 129.5, 129.1, 128.8, 128.1, 127.6, 127.1, 126.5, 76.7, 45.0.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{22}\text{H}_{16}\text{Cl}_2\text{N}_2\text{NaO}$ : 417.0537  $[\text{M}+\text{Na}]^+$ , found:417.0546.

#### 4-(2-Chlorobenzyl)-2-(4-chlorophenyl)-4-phenyl-4H-imidazol-5-ol (3c)



Pale White solid, mp: 209-210 °C;

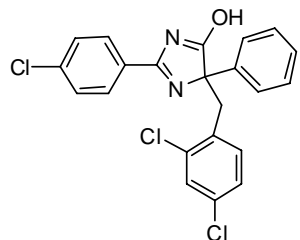
IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3174, 3088, 1718, 1598, 1475, 1324, 1259, 1091, 825, 729, 697  $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 9.83 (s, 1H, OH), 7.84 (d,  $J = 8.0$  Hz, 2H, ArH), 7.76 (d,  $J = 4.8$  Hz, 2H, ArH), 7.48 (d,  $J = 8.4$  Hz, 2H, ArH), 7.37 (t,  $J = 7.2$  Hz, 2H, ArH), 7.31 (t,  $J = 7.2$  Hz, 1H, ArH), 7.22 (d,  $J = 7.6$  Hz, 1H, ArH), 7.17 (d,  $J = 6.4$  Hz, 1H, ArH), 7.03 (t,  $J = 7.2$  Hz, 1H, ArH), 6.97 (d,  $J = 6.4$  Hz, 1H, ArH), 3.74-3.62 (m, 2H,  $\text{CH}_2$ );

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 185.1, 158.5, 139.5, 137.2, 134.9, 133.8, 132.2, 129.5, 129.4, 129.1, 128.9, 128.8, 128.1, 127.7, 126.8, 126.5, 76.7, 42.0.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{22}\text{H}_{16}\text{Cl}_2\text{N}_2\text{NaO}$ : 417.0537  $[\text{M}+\text{Na}]^+$ , found:417.0544.

#### 2-(4-Chlorophenyl)-4-(2,4-dichlorobenzyl)-4-phenyl-4H-imidazol-5-ol (3d)



White solid, mp: 219-220 °C;

IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3149, 3058, 1684, 1602, 1542, 1469, 1344, 1811, 844, 732, 696  $\text{cm}^{-1}$ ;

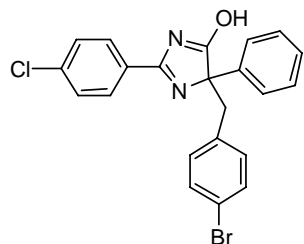
$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 9.49 (s, 1H, OH), 7.83 (d,  $J = 8.4$  Hz, 2H, ArH), 7.73 (d,  $J = 6.8$  Hz, 2H, ArH), 7.50 (d,  $J = 8.4$  Hz, 2H, ArH), 7.38-7.29 (m, 3H, ArH), 7.27 (s, 1H, ArH), 7.10 (d,  $J = 8.0$  Hz, 1H, ArH), 6.99 (d,  $J = 8.4$  Hz, 1H,

ArH), 3.69-3.55 (m, 2H,  $\text{CH}_2$ );

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 185.0, 158.7, 139.2, 137.3, 135.9, 133.5, 133.1, 132.5, 129.5, 129.2, 128.9, 128.8, 128.2, 127.6, 127.0, 126.5, 76.5, 41.3.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{22}\text{H}_{15}\text{Cl}_3\text{N}_2\text{NaO}$ : 451.0148 $[\text{M}+\text{Na}]^+$ , found:451.0428.

#### 4-(4-Bromobenzyl)-2-(4-chlorophenyl)-4-phenyl-4H-imidazol-5-ol (3e)



Pale White solid, mp: 276-277 °C;

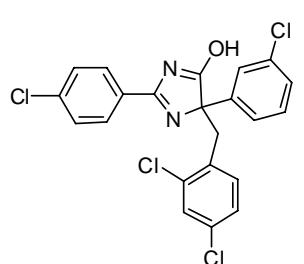
IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3166, 3058, 1680, 1501, 1411, 1298, 1165, 1015, 843, 734, 699 $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 8.90 (s, 1H, OH), 7.75 (d,  $J = 6.8$  Hz, 4H, ArH), 7.48 (d,  $J = 8.0$  Hz, 2H, ArH), 7.37 (t,  $J = 7.2$  Hz, 2H, ArH), 7.31 (t,  $J = 6.8$  Hz, 2H, ArH), 7.24 (s, 1H, ArH), 7.08 (d,  $J = 8.0$  Hz, 2H, ArH), 3.44 (s, 2H,  $\text{CH}_2$ );

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 184.8, 158.7, 139.6, 137.2, 135.4, 132.9, 130.8, 129.5, 129.2, 128.8, 128.1, 127.61, 126.5, 120.4, 76.7, 44.9.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{22}\text{H}_{16}\text{BrClN}_2\text{NaO}$ : 461.0010  $[\text{M}+\text{Na}]^+$ , found:461.0031.

#### 4-(3-Chlorophenyl)-2-(4-chlorophenyl)-4-(2,4-dichlorobenzyl)-4H-imidazol-5-ol (3f)



White solid, mp: 222-223 °C;

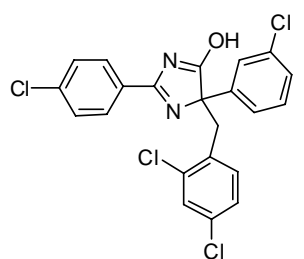
IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3212, 3098, 1725, 1627, 1474, 1265, 1183, 1091, 840, 729, 685  $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 9.83 (s, 1H, OH), 7.86 (d,  $J = 8.0$  Hz, 2H, ArH), 7.75 (s, 1H, ArH), 7.65 (s, 1H, ArH), 7.27 (s, 1H, ArH), 7.52 (d,  $J = 8.4$  Hz, 2H, ArH), 7.28 (d,  $J = 4.0$  Hz, 2H, ArH), 7.10 (d,  $J = 8.0$  Hz, 1H, ArH), 7.00 (d,  $J = 7.6$  Hz, 1H, ArH), 3.65-3.50 (m, 2H,  $\text{CH}_2$ );

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 184.5, 159.1, 141.4, 137.5, 135.9, 133.7, 133.4, 132.7, 132.7, 130.7, 129.5, 129.3, 128.9, 128.2, 127.4, 127.1, 126.4, 125.3, 75.8, 41.6.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{22}\text{H}_{14}\text{Cl}_2\text{N}_2\text{NaO}$ : 484.9758  $[\text{M}+\text{Na}]^+$ , found:484.9770.

#### 4-(3-Chlorophenyl)-2-(4-chlorophenyl)-4-(2,4-dichlorobenzyl)-4H-imidazol-5-ol (3g)



White solid, mp: 227-228 °C;

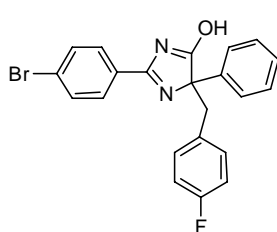
IR (KBr): 3159, 3072, 1717, 1662, 1430, 1307, 1266, 1093, 888, 729, 693 $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 10.59 (s, 1H, OH), 7.87 (d,  $J = 8.4$  Hz, 2H, ArH), 7.78 (s, 1H, ArH), 7.65 (s, 1H, ArH), 7.69 (d,  $J = 6.4$  Hz, 1H, ArH), 7.50 (d,  $J = 8.0$  Hz, 2H, ArH), 7.26 (t,  $J = 7.6$  Hz, 3H, ArH), 7.18 (d,  $J = 7.6$  Hz, 2H, ArH), 7.05 (d,  $J = 8.0$  Hz, 1H, ArH), 3.90-3.78 (m, 2H,  $\text{CH}_2$ );

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{22}\text{H}_{14}\text{Cl}_4\text{N}_2\text{NaO}$ : 484.9758  $[\text{M}+\text{Na}]^+$ , found: 484.9771

$[\text{M}+\text{Na}]^+$ .

#### 2-(4-Bromophenyl)-4-(4-fluorobenzyl)-4-phenyl-4H-imidazol-5-ol (3h)



White solid, mp: 253-254 °C;

IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3164, 3058, 2846, 1682, 1495, 1299, 1165, 1018, 830, 730, 694 $\text{cm}^{-1}$ ;

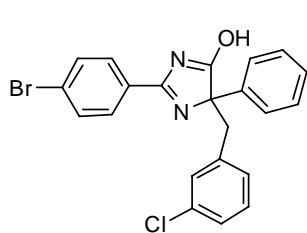
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 8.76 (s, 1H, OH), 7.76 (d,  $J = 7.6$  Hz, 2H, ArH), 7.67-7.62 (m, ArH), 7.42-7.29 (m, 3H, ArH), 7.17-7.14 (m, 2H, ArH), 6.80 (t,  $J = 8.4$  Hz, 2H, ArH), 3.47-3.39 (m, 2H,  $\text{CH}_2$ ).

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{22}\text{H}_{16}\text{BrFN}_2\text{NaO}$ : 445.0328  $[\text{M}+\text{Na}]^+$ , found:445.0345.

#### 2-(4-bromophenyl)-4-(3-chlorobenzyl)-4-phenyl-4H-imidazol-5-ol (3i)

White solid, mp: 216-217 °C;

IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3157, 3044, 1678, 1523, 1423, 1249, 1014, 835, 739, 699 $\text{cm}^{-1}$ ;



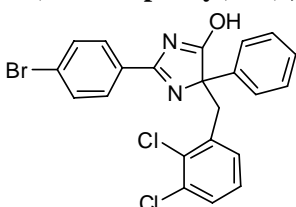
$^1\text{H}$  NMR (400MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 8.86 (s, 1H, OH), 7.76 (d,  $J$  = 7.6 Hz, 2H, ArH), 7.69-7.63 (m, 4H, ArH), 7.38 (t,  $J$  = 8.0 Hz, 2H, ArH), 7.31 (t,  $J$  = 7.2 Hz, 1H, ArH), 7.22 (s, 1H, ArH), 7.06-7.00 (m, 3H, ArH), 3.43 (s, 2H, CH $_2$ );

$^{13}\text{C}$  NMR (100 MHz, CDCl $_3$ ) ( $\delta$ , ppm) 184.8, 158.9, 139.5, 138.4, 132.5, 132.4, 130.6, 129.7, 129.5, 129.3, 128.8, 128.1, 127.9, 127.1, 126.5, 126.2, 76.7, 45..

HRMS (ESI)  $m/z$ : calc. for C $_{22}$ H $_{16}$ BrClN $_2$ NaO: 461.0010 [M+Na] $^+$ ,

found:461.0018.

#### 2-(4-bromophenyl)-4-(2,3-dichlorobenzyl)-4-phenyl-4H-imidazol-5-ol (3j)



Pale white solid, mp: 222-223 °C;

IR(KBr,  $\nu$ , cm $^{-1}$ ): 3164, 3077, 2877, 1719, 1624, 1433, 1307, 1261, 1011, 837, 720, 698cm $^{-1}$ ;

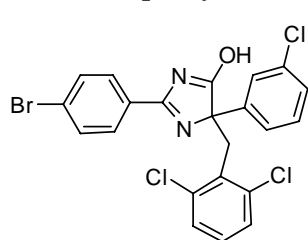
$^1\text{H}$  NMR (400MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 9.69 (s, 1H, OH), 7.75 (d,  $J$  = 8.0 Hz, 4H, ArH), 7.66 (d,  $J$  = 8.4 Hz, 2H, ArH), 7.38-7.29 (m, 3H, ArH), 7.22 (d,  $J$  = 7.6 Hz, 1H, ArH), 7.06 (d,  $J$  = 7.6 Hz, 1H, ArH), 6.90 (t,  $J$  = 8.0 Hz, 1H, ArH), 3.77-3.64 (m,

2H, CH $_2$ );

$^{13}\text{C}$  NMR (100 MHz, CDCl $_3$ ) ( $\delta$ , ppm) 184.9, 158.8, 139.2, 136.6, 133.0, 132.4, 132.0, 130.7, 129.48, 129.3, 128.8, 128.2, 127.9, 127.5, 126.5, 126.2, 76.6, 42.8.

HRMS (ESI)  $m/z$ : calc. for C $_{22}$ H $_{15}$ BrCl $_2$ N $_2$ NaO: 494.9621 [M+Na] $^+$ , found:494.9615.

#### 2-(4-bromophenyl)-4-(3-chlorophenyl)-4-(2,6-dichlorobenzyl)-4H-imidazol-5-ol (3k)



Pale white solid, mp: 217-218 °C;

IR(KBr,  $\nu$ , cm $^{-1}$ ): 3162, 3058, 2941, 1719, 1626, 1493, 1235, 1057, 835, 761, 694cm $^{-1}$ ;

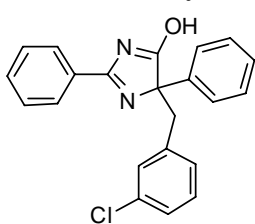
$^1\text{H}$  NMR (400MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 10.55 (s, 1H, OH), 7.80 (d,  $J$  = 8.4 Hz, 3H, ArH), 7.67 (t,  $J$  = 8.4 Hz, 3H, ArH), 7.26 (t,  $J$  = 7.6 Hz, 2H, ArH), 7.18 (d,  $J$  = 8.0 Hz, 2H, ArH), 7.05 (t,  $J$  = 8.0 Hz, 1H, ArH), 3.88 (d,  $J$  = 13.6 Hz, 1H, CH $_2$ ),

3.79 (d,  $J$  = 13.6 Hz, 1H, CH $_2$ );

$^{13}\text{C}$  NMR (100 MHz, CDCl $_3$ ) ( $\delta$ , ppm) 184.8, 159.0, 142.0, 136.7, 133.3, 132.4, 132.2, 130.5, 129.84, 129.4, 128.6, 128.1, 127.8, 126.6, 126.3, 125.4, 74.2, 41.0.

HRMS (ESI)  $m/z$ : calc. for C $_{22}$ H $_{14}$ BrCl $_3$ N $_2$ NaO: 528.9231 [M+Na] $^+$ , found:528.9231.

#### 4-(3-chlorobenzyl)-2,4-diphenyl-4H-imidazol-5-ol (3l)



Pale white solid, mp: 200-201 °C;

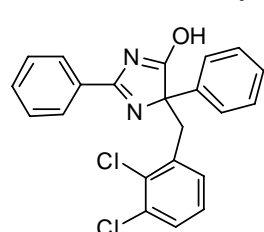
IR(KBr,  $\nu$ , cm $^{-1}$ ): 3173, 3063, 1679, 1535, 1474, 1249, 1016, 840, 759, 688cm $^{-1}$ ;

$^1\text{H}$  NMR (400MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 8.34 (s, 1H, OH), 7.78 (d,  $J$  = 8.0 Hz, 4H, ArH), 7.56 (t,  $J$  = 7.2 Hz, 1H, ArH), 7.49 (t,  $J$  = 7.6 Hz, 2H, ArH), 7.38 (t,  $J$  = 7.2 Hz, 2H, ArH), 7.31 (t,  $J$  = 7.2 Hz, 2H, ArH), 7.12-7.02 (m, 3H, ArH), 3.49-3.42 (m, 2H, CH $_2$ );

$^{13}\text{C}$  NMR (100 MHz, CDCl $_3$ ) ( $\delta$ , ppm) 184.9, 159.6, 139.8, 138.5, 132.4(5), 132.3(7), 130.6, 129.7, 129.5, 129.2, 128.8, 128.0, 127.3, 127.0, 126.5, 126.0, 76.6, 45.0.

HRMS (ESI)  $m/z$ : calc. for C $_{22}$ H $_{17}$ ClN $_2$ NaO: 383.0927 [M+Na] $^+$ , found:383.0940.

#### 4-(2,3-dichlorobenzyl)-2,4-diphenyl-4H-imidazol-5-ol (3m)



White solid, mp: 215-216 °C;

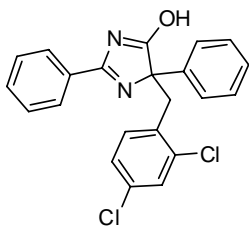
IR (KBr): 3167, 3061, 2888, 1665, 1507, 1453, 1314, 1182, 1046, 835, 720, 699cm $^{-1}$ ;

$^1\text{H}$  NMR (400MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 9.76 (s, 1H, OH), 7.91 (d,  $J$  = 7.6Hz, 2H, ArH), 7.76 (d,  $J$  = 6.8 Hz, 2H, ArH), 7.60-7.50 (m, 3H, ArH), 7.38-7.29 (m, 3H, ArH), 7.25 (s, 1H, ArH), 7.15 (d,  $J$  = 7.6 Hz, 1H, ArH), 6.98 (d,  $J$  = 7.6 Hz, 1H, ArH), 3.69 (d,

$J = 13.6$  Hz, 1H, CH<sub>2</sub>), 3.59 (d,  $J = 14.0$  Hz, 1H, CH<sub>2</sub>);

HRMS (ESI)  $m/z$ : calc. for C<sub>22</sub>H<sub>16</sub>Cl<sub>2</sub>N<sub>2</sub>NaO: 417.0537 [M+Na]<sup>+</sup>, found: 417.0550 [M+Na]<sup>+</sup>.

#### 4-(2,4-Dichlorobenzyl)-2,4-diphenyl-4H-imidazol-5-ol (3n)



Pale white solid, mp: 219-220 °C;

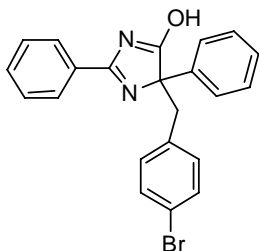
IR(KBr,  $\nu$ , cm<sup>-1</sup>): 3158, 3110, 1718, 1628, 1440, 1236, 1015, 838, 782, 694cm<sup>-1</sup>;

<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) ( $\delta$ , ppm): 11.58 (s, 1H, OH), 7.97 (d,  $J = 5.2$  Hz, 2H, ArH), 7.70–7.45 (m, 6H, ArH), 7.36-7.25 (m, 5H, ArH), 3.60 (d,  $J = 13.6$  Hz, 1H, CH<sub>2</sub>), 3.46 (d,  $J = 14.0$  Hz, 1H, CH<sub>2</sub>).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) ( $\delta$ , ppm) 185.1, 159.5, 139.4, 135.9, 133.5, 133.2, 132.5, 132.4, 129.3, 128.9, 128.8, 128.1, 127.4, 127.0, 126.5, 76.3, 41.3.

HRMS (ESI)  $m/z$ : calc. for C<sub>22</sub>H<sub>16</sub>Cl<sub>2</sub>N<sub>2</sub>NaO: 417.0537 [M+Na]<sup>+</sup>, found:417.0545.

#### 4-(4-Bromobenzyl)-2,4-diphenyl-4H-imidazol-5-ol (3o)



White solid, mp: 240-242 °C;

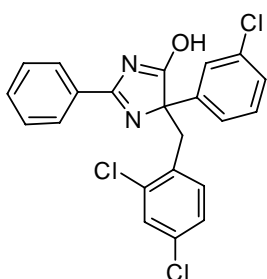
IR(KBr,  $\nu$ , cm<sup>-1</sup>): 3191, 3068, 1676, 1477, 1226, 1369, 1094, 839, 720, 693cm<sup>-1</sup>;

<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) ( $\delta$ , ppm): 8.39 (s, 1H, OH), 7.78 (d,  $J = 7.2$  Hz, 4H, ArH), 7.57 (d,  $J = 6.4$  Hz, 1H, ArH), 7.50 (t,  $J = 7.6$  Hz, 2H, ArH), 7.41–7.30 (m, 4H, ArH), 7.25 (s, 1H, ArH), 7.12 (d,  $J = 7.6$  Hz, 2H, ArH), 3.44 (s, 2H, CH<sub>2</sub>).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) ( $\delta$ , ppm) 184.9, 159.5, 139.9, 135.5, 133.0, 132.4, 130.8, 129.3, 128.8, 128.8, 128.0, 127.4, 126.5, 120.4, 76.5, 44.9.

HRMS (ESI)  $m/z$ : calc. for C<sub>22</sub>H<sub>17</sub>BrN<sub>2</sub>NaO: 427.0400 [M+Na]<sup>+</sup>, found:427.0422.

#### 4-(3-Chlorophenyl)-4-(2,4-dichlorobenzyl)-2-phenyl-4H-imidazol-5-ol (3p)



Pale white solid, mp: 213-214 °C;

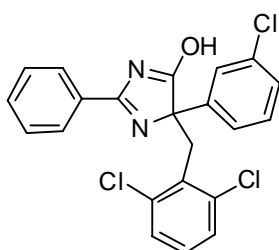
IR(KBr,  $\nu$ , cm<sup>-1</sup>): 3170, 3067, 2885, 1726, 1629, 1473, 1263, 1185, 1046, 864, 785, 696cm<sup>-1</sup>;

<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) ( $\delta$ , ppm): 9.43 (s, 1H, OH), 7.89 (d,  $J = 7.6$ Hz, 2H, ArH), 7.77 (s, 1H, ArH), 7.67 (s, 1H, ArH), 7.60 (t,  $J = 6.8$  Hz, 1H, ArH), 7.53 (t,  $J = 7.2$  Hz, 2H, ArH), 7.28 (t,  $J = 4.4$  Hz, 3H, ArH), 7.16 (d,  $J = 8.4$  Hz, 1H, ArH), 7.01(d,  $J = 8.0$  Hz, 1H, ArH), 3.65 (d,  $J = 13.6$  Hz, 1H, CH<sub>2</sub>), 3.53 (d,  $J = 13.6$  Hz, 1H, CH<sub>2</sub>);

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) ( $\delta$ , ppm) 184.6, 160.0, 141.6, 135.9, 133.7, 133.4, 132.8, 132.6, 132.6, 130.7, 129.3, 128.9, 128.6, 128.2, 127.5, 127.0, 126.4, 125.4, 75.7, 41.5.

HRMS (ESI)  $m/z$ : calc. for C<sub>22</sub>H<sub>15</sub>Cl<sub>3</sub>N<sub>2</sub>NaO: 451.0148 [M+Na]<sup>+</sup>, found:451.0160.

#### 4-(3-Chlorophenyl)-4-(2,6-dichlorobenzyl)-2-phenyl-4H-imidazol-5-ol (3q)



White solid, mp: 188-189 °C;

IR(KBr,  $\nu$ , cm<sup>-1</sup>): 3169, 3059, 2937, 1719, 1633, 1453, 1270, 1162, 886, 769, 694cm<sup>-1</sup>;

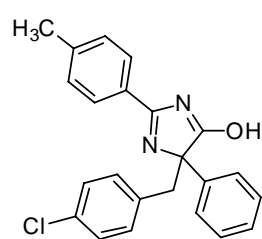
<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) ( $\delta$ , ppm): 10.17 (s, 1H, OH), 7.90 (d,  $J = 7.2$  Hz, 2H, ArH), 7.80 (s, 1H, ArH), 7.71 (d,  $J = 6.4$  Hz, 1H, ArH), 7.57 (t,  $J = 7.2$  Hz, 1H, ArH), 7.51 (t,  $J = 7.6$  Hz, 2H, ArH), 7.26 (s, 2H, ArH), 7.19 (d,  $J = 8.0$  Hz, 2H, ArH), 7.04 (t,  $J = 8.0$  Hz, 1H, ArH), 3.90 (d,  $J = 13.2$  Hz, 1H, CH<sub>2</sub>), 3.80 (d,  $J = 13.6$  Hz, 1H,

CH<sub>2</sub>);

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) ( $\delta$ , ppm) 184.9, 159.6, 142.3, 136.7, 133.2, 132.5, 132.3, 130.5, 129.8, 129.2, 128.7, 128.6, 128.0, 127.4, 126.5, 125.5, 74.0, 41.0.

HRMS (ESI)  $m/z$ : calc. for C<sub>22</sub>H<sub>15</sub>Cl<sub>3</sub>N<sub>2</sub>NaO: 451.0159 [M+Na]<sup>+</sup>, found:451.0159.

#### 4-(4-Chlorobenzyl)-4-phenyl-2-(p-tolyl)-4H-imidazol-5-ol (3r)



Pale white solid, mp: 248-249 °C;

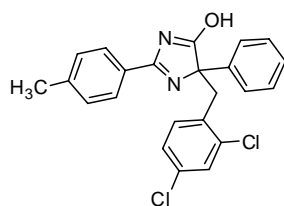
IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3159, 3057, 1681, 1549, 1464, 1290, 1093, 836, 700, 641 $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 11.36 (s, 1H, OH), 7.82 (d,  $J = 7.6$  Hz, 2H, ArH), 7.67 (d,  $J = 7.6$  Hz, 2H, ArH), 7.39–7.30 (m, 5H, ArH), 7.22–7.17 (m, 4H, ArH), 3.37–3.34 (m, 2H,  $\text{CH}_2$ ), 2.37 (s, 3H,  $\text{CH}_3$ ).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 184.9, 159.4, 142.4, 140.0, 135.1, 132.6, 131.7, 129.8, 128.7, 128.0, 127.9, 127.3, 126.5, 126.1, 76.5, 44.9, 21.5

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{23}\text{H}_{19}\text{ClN}_2\text{NaO}$ : 397.1084  $[\text{M}+\text{Na}]^+$ , found:397.1092.

#### 4-(2,4-Dichlorobenzyl)-4-phenyl-2-(p-tolyl)-4H-imidazol-5-ol (3s)



Pale white solid, mp: 222-224 °C;

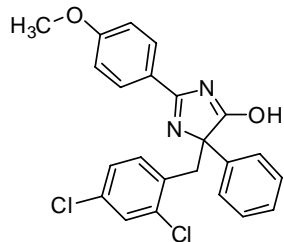
IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3112, 3058, 1721, 1542, 1436, 1262, 1092, 839, 705, 670 $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 11.55 (s, 1H, OH), 7.85 (d,  $J = 7.6$  Hz, 2H, ArH), 7.64 (d,  $J = 8.0$  Hz, 2H, ArH), 7.48 (s, 1H, ArH), 7.38–7.23 (m, 7H, ArH), 3.56 (s, 1H,  $\text{CH}_2$ ), 3.46 (s, 1H,  $\text{CH}_2$ ).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 184.7, 158.9, 142.1, 139.0, 135.4, 133.0, 132.7, 131.9, 129.3, 128.4, 128.3, 127.6, 126.9, 126.5, 126.0, 125.5, 75.8, 40.8, 21.0.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{23}\text{H}_{18}\text{Cl}_2\text{N}_2\text{NaO}$ : 431.0694  $[\text{M}+\text{Na}]^+$ , found:431.0676.

#### 4-(2,4-Dichlorobenzyl)-2-(4-methoxyphenyl)-4-phenyl-4H-imidazol-5-ol (3t)



White solid, mp: 218-220 °C;

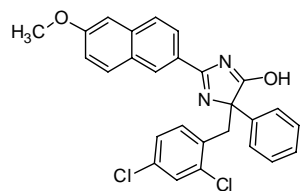
IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3172, 3069, 1676, 1467, 1333, 1048, 836, 700, 654 $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 11.49 (s, 1H, OH), 7.91 (d,  $J = 8.0$  Hz, 2H, ArH), 7.64 (d,  $J = 7.6$  Hz, 2H, ArH), 7.46 (s, 1H, ArH), 7.35 (t,  $J = 7.2$  Hz, 2H, ArH), 7.30 (d,  $J = 7.2$  Hz, 2H, ArH), 7.23 (d,  $J = 8.4$  Hz, 1H, ArH), 7.07 (d,  $J = 8.4$  Hz, 2H, ArH), 3.83 (s, 3H,  $\text{CH}_3$ ), 3.57 (d,  $J = 14.0$  Hz, 1H,  $\text{CH}_2$ ), 3.43 (d,  $J = 14.0$  Hz, 1H,  $\text{CH}_2$ ).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 185.1, 159.3, 142.5, 139.5, 135.9, 133.5, 133.2, 132.4, 129.8, 128.8, 128.7, 128.1, 127.4, 126.9, 126.5, 126.1, 76.2, 41.3, 21.6.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{23}\text{H}_{18}\text{Cl}_2\text{N}_2\text{NaO}_2$ : 447.0643  $[\text{M}+\text{Na}]^+$ , found:447.0655.

#### 4-(2,4-Dichlorobenzyl)-2-(6-methoxynaphthalen-2-yl)-4-phenyl-4H-imidazol-5-ol (3u)



Pale white solid, mp: 224-226 °C;

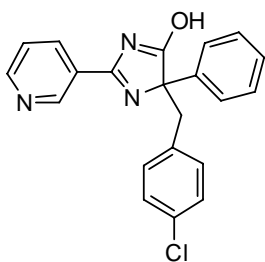
IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3144, 3012, 1670, 1557, 1457, 1256, 1031, 846, 757, 693 $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 8.44 (s, 1H, ArH), 8.15 (d,  $J = 8.4$  Hz, 1H, ArH), 7.83 (d,  $J = 8.0$  Hz, 2H, ArH), 7.77 (d,  $J = 6.0$  Hz, 2H, ArH), 7.61 (s, 1H, ArH), 7.36-7.28 (m, 5H, ArH), 7.20 (s, 2H, ArH), 7.02 (d,  $J = 8.0$  Hz, 1H, ArH), 3.96 (s, 3H,  $\text{CH}_3$ ), 3.70 (d,  $J = 14.0$  Hz, 1H,  $\text{CH}_2$ ), 3.59 (d,  $J = 13.2$  Hz, 1H,  $\text{CH}_2$ ).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 185.0, 159.6, 159.3, 139.5, 136.6, 135.9, 133.6, 133.3, 132.4, 130.8, 128.9, 128.8, 128.1, 128.0, 127.9, 127.8, 127.0, 126.6, 124.3, 123.9, 120.1, 106.7, 76.4, 55.9, 41.3.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{27}\text{H}_{20}\text{Cl}_2\text{N}_2\text{NaO}_2$ : 497.0800  $[\text{M}+\text{Na}]^+$ , found:497.0826.

#### 4-(4-Chlorobenzyl)-4-phenyl-2-(pyridin-3-yl)-4H-imidazol-5-ol (3v)



White solid, mp: 237-239 °C;

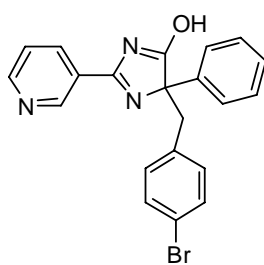
IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3174, 3056, 1716, 1675, 1593, 1434, 1183, 1077, 811, 759, 669 $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 9.51 (s, 1H, OH), 9.10 (s, 1H, Pyridine H) 8.80 (d,  $J$  = 4.0 Hz, 1H, Pyridine H), 8.26 (d,  $J$  = 7.6 Hz, 1H), 7.77 (d,  $J$  = 8.0 Hz, 2H, Pyridine H), 7.52-7.49 (m, 1H ArH), 7.40-7.32 (m, 3H, ArH), 7.15-7.09 (m, 4H, ArH), 3.42 (s, 2H,  $\text{CH}_2$ );

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 184.7, 158.0, 153.0, 148.3, 139.4, 134.9, 134.8, 132.6, 131.9, 128.8, 128.1, 127.9, 126.5, 124.7, 124.4, 76.7, 44.8.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{21}\text{H}_{16}\text{BrIN}_3\text{NaO}$ : 428.0352  $[\text{M}+\text{Na}]^+$ , found: 428.0367.

#### 4-(4-Bromobenzyl)-4-phenyl-2-(pyridin-3-yl)-4H-imidazol-5-ol (3w)



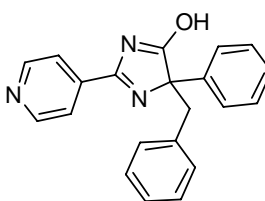
White solid, mp: 249-250 °C;

IR (KBr): 3174, 3056, 1716, 1675, 1593, 1434, 1183, 1077, 811, 759, 669 $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.92 (s, 1H, OH), 9.09 (s, 1H, Pyridine H), 8.79 (d,  $J$  = 4.0 Hz, 1H, Pyridine H), 8.24 (d,  $J$  = 8.0 Hz, 1H, ArH), 7.76 (d,  $J$  = 7.6 Hz, 2H, ArH), 7.50-7.47 (m, 1H, ArH), 7.38 (d,  $J$  = 7.2 Hz, 2H, ArH), 7.31 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.25 (d,  $J$  = 8.4 Hz, 2H, Pyridine H), 7.07 (d,  $J$  = 8.4 Hz, 2H, ArH), 3.43 (s, 2H).

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{21}\text{H}_{16}\text{BrIN}_3\text{NaO}$ : 428.0374  $[\text{M}+\text{Na}]^+$ , found: 428.0367.

#### 4-Benzyl-4-phenyl-2-(pyridin-4-yl)-4H-imidazol-5-ol (3x)



White solid, mp: 195-196 °C;

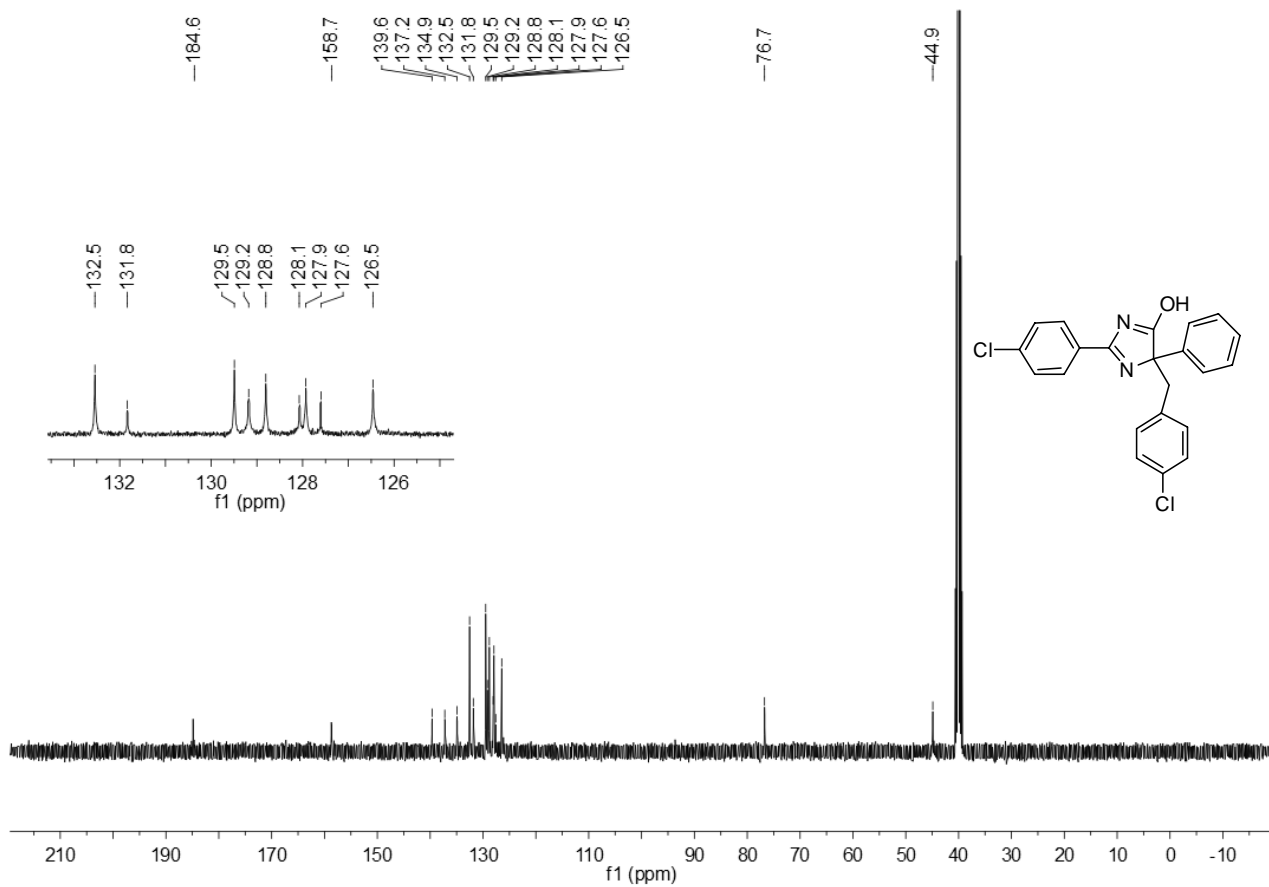
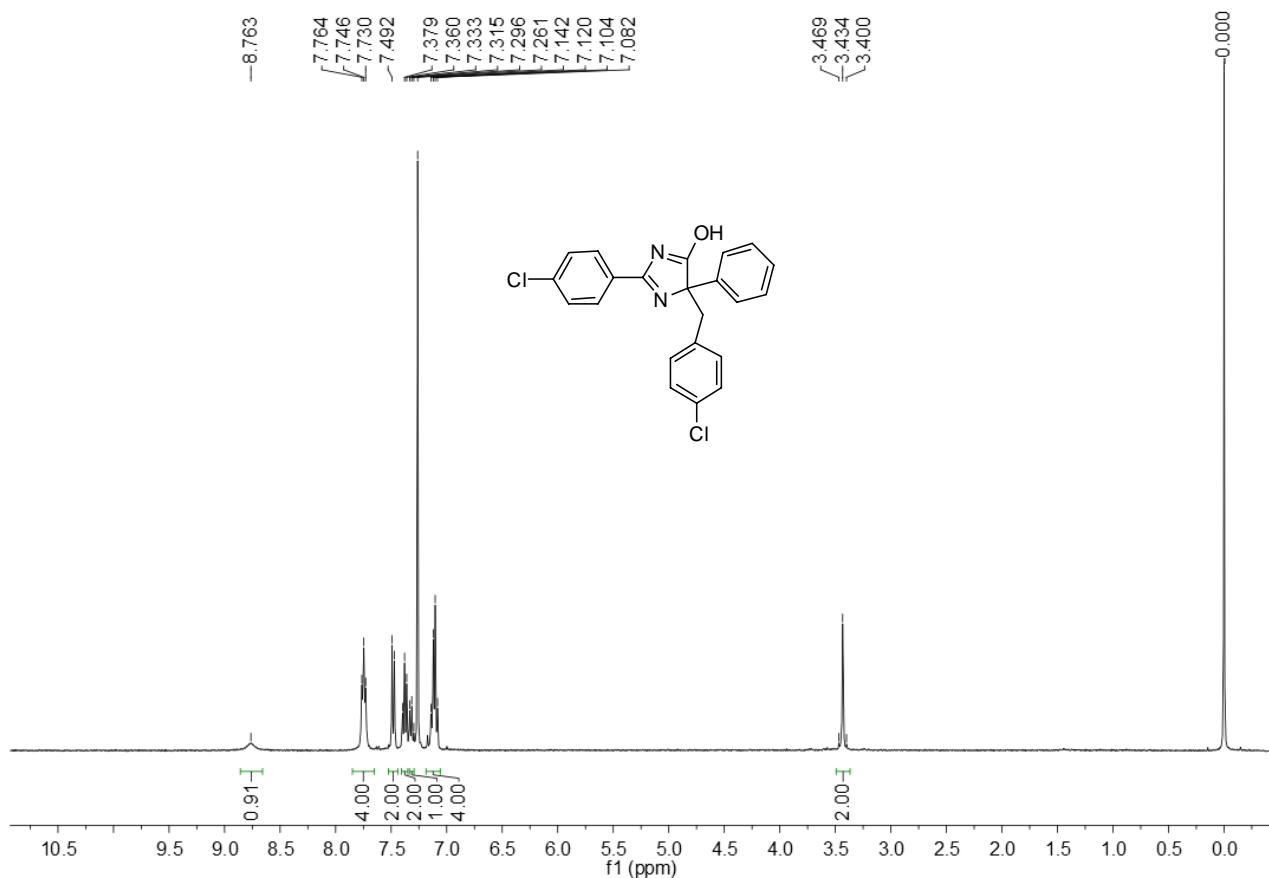
IR(KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3184, 3033, 1734, 1685, 1559, 1406, 1202, 859, 751, 696 $\text{cm}^{-1}$ ;

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 10.24 (s, 1H, OH), 8.77 (s, 2H, Pyridine H), 7.77-7.72 (m, 4H, ArH), 7.38 (t,  $J$  = 7.2 Hz, 2H, ArH), 7.32 (d,  $J$  = 7.2 Hz, 1H, ArH), 7.16-7.14 (m, 2H, Pyridine H), 7.09-7.04 (m, 3H, ArH), 3.49 (s, 2H,  $\text{CH}_2$ ).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm) 185.0, 151.0, 139.5, 135.9, 135.6, 130.7, 129.5, 128.9, 128.1, 128.0, 127.2, 126.5, 121.2, 77.2, 45.8.

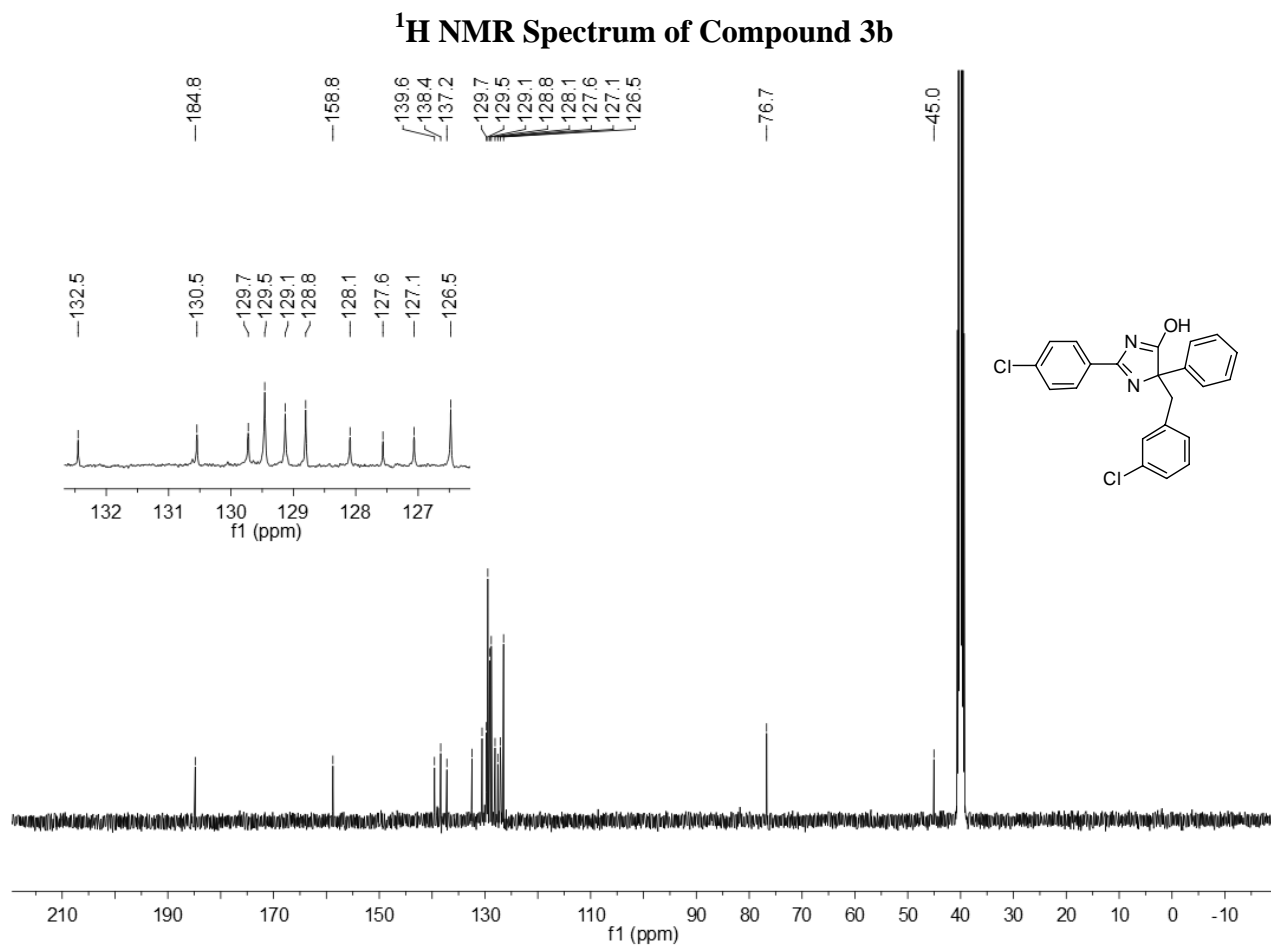
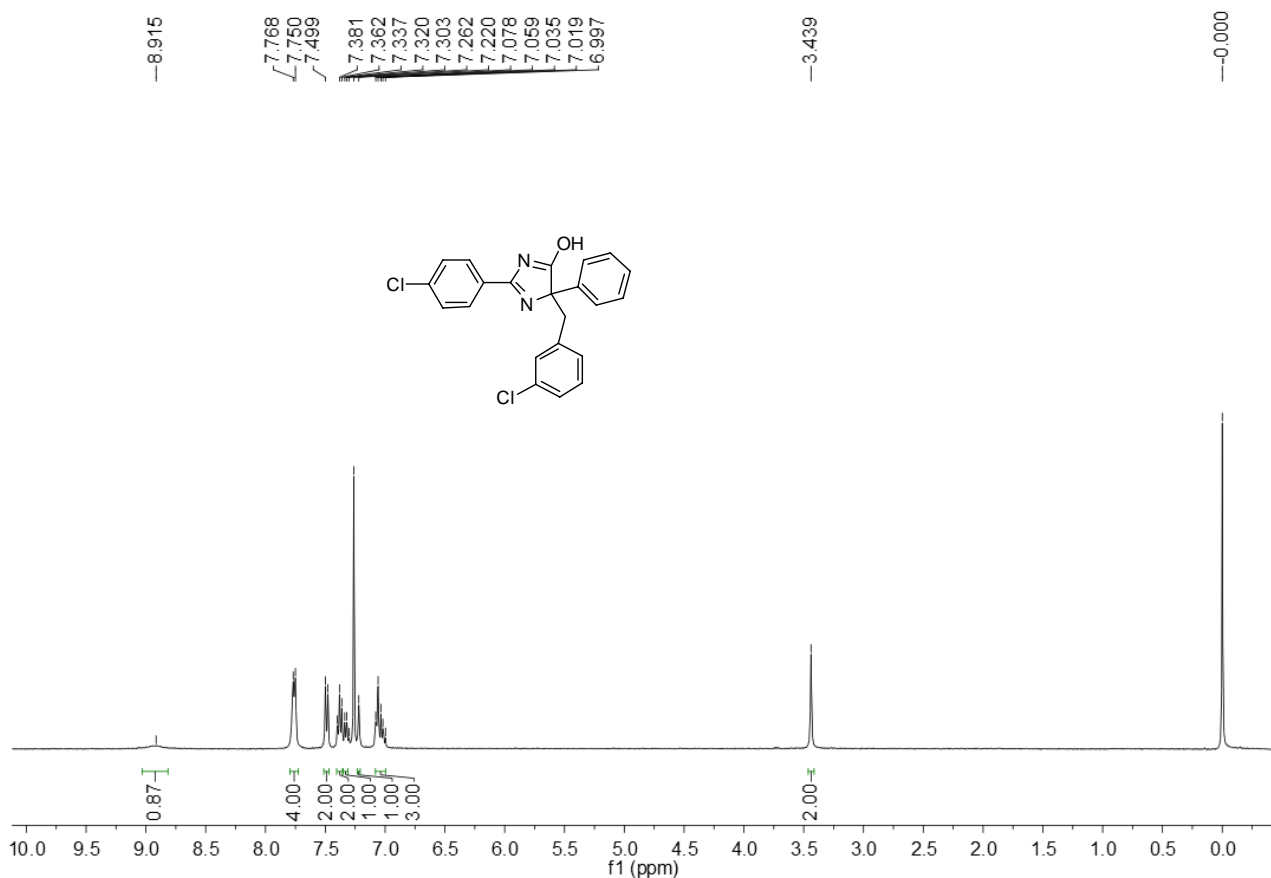
HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{21}\text{H}_{17}\text{N}_3\text{NaO}$ : 350.1269  $[\text{M}+\text{Na}]^+$ , found: 350.1277.



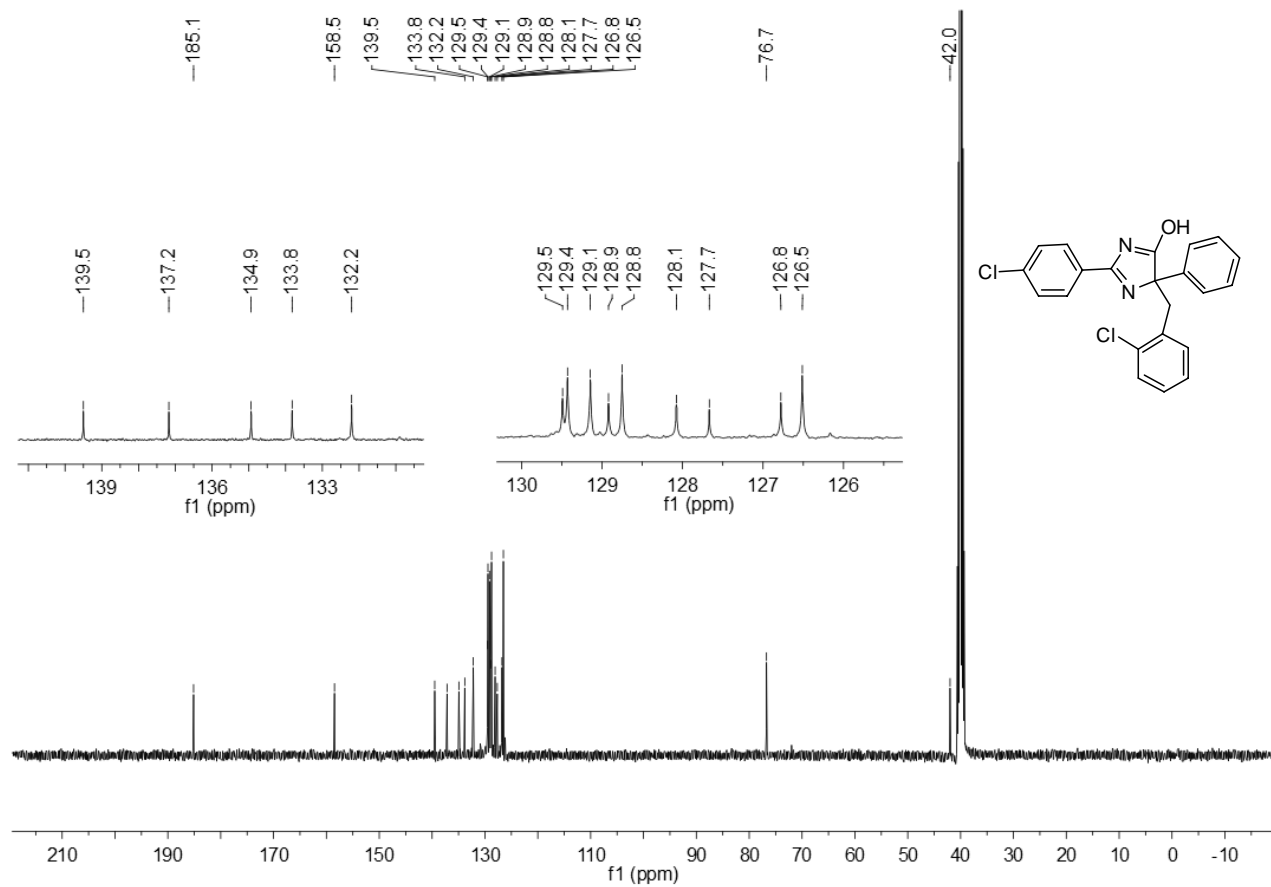
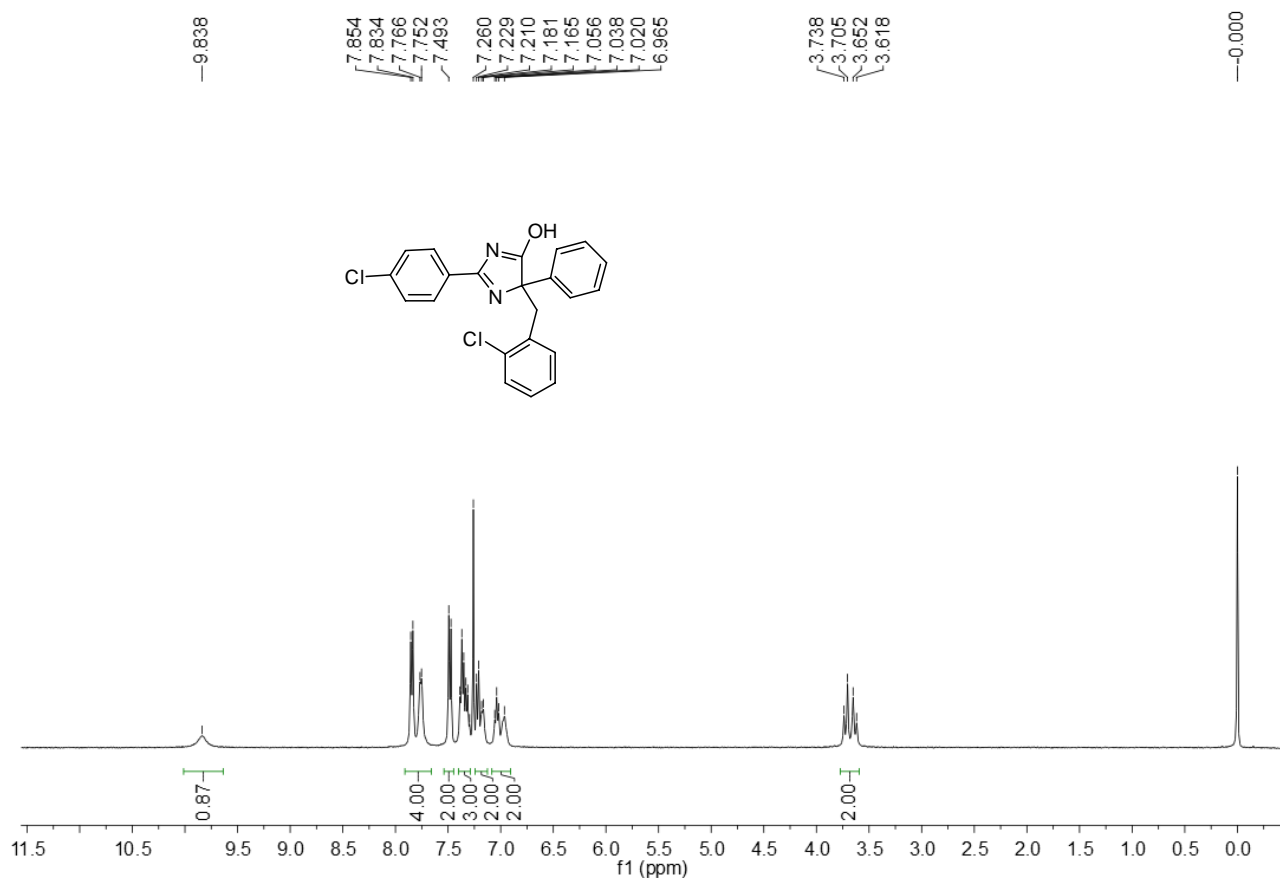


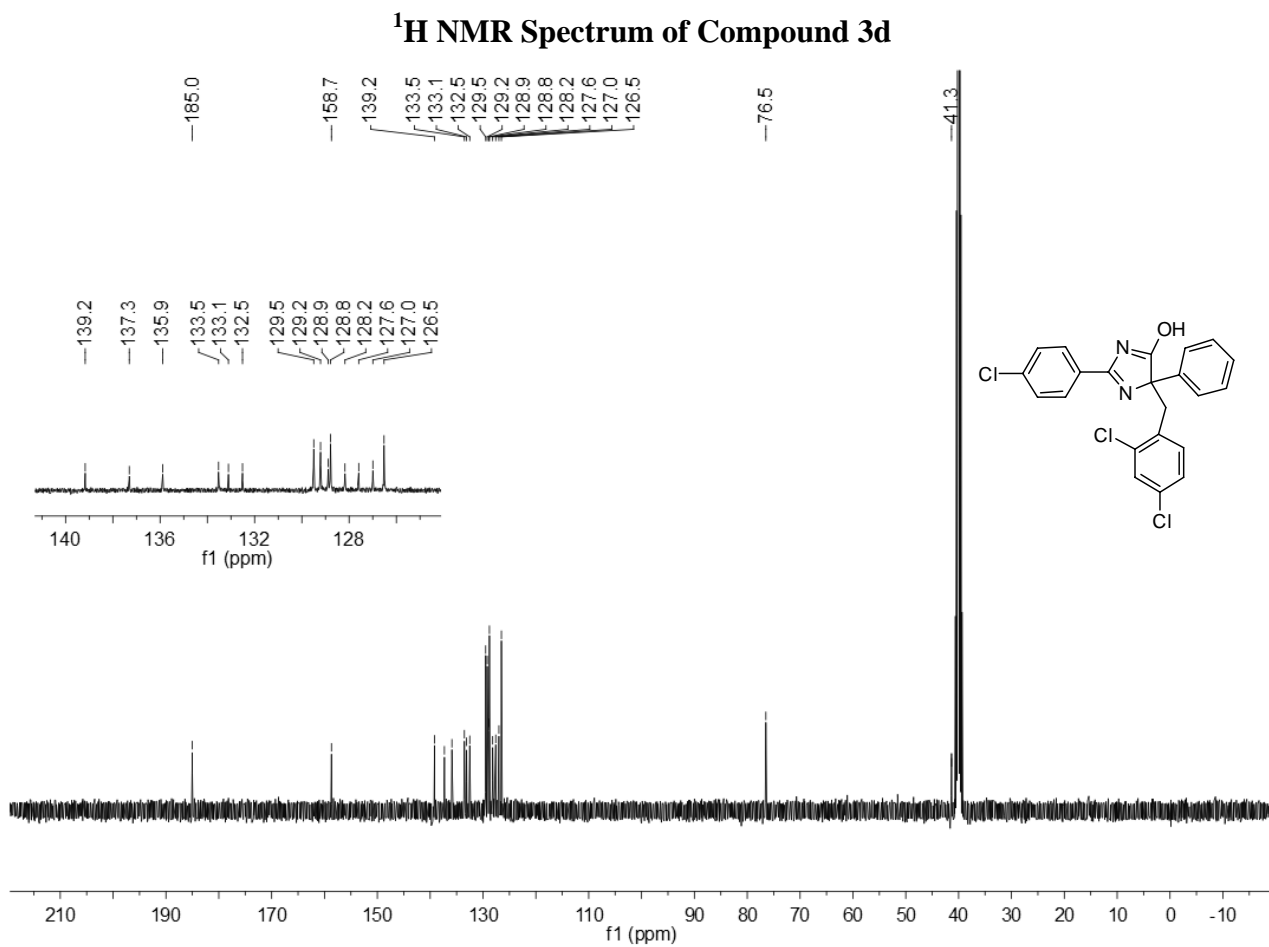
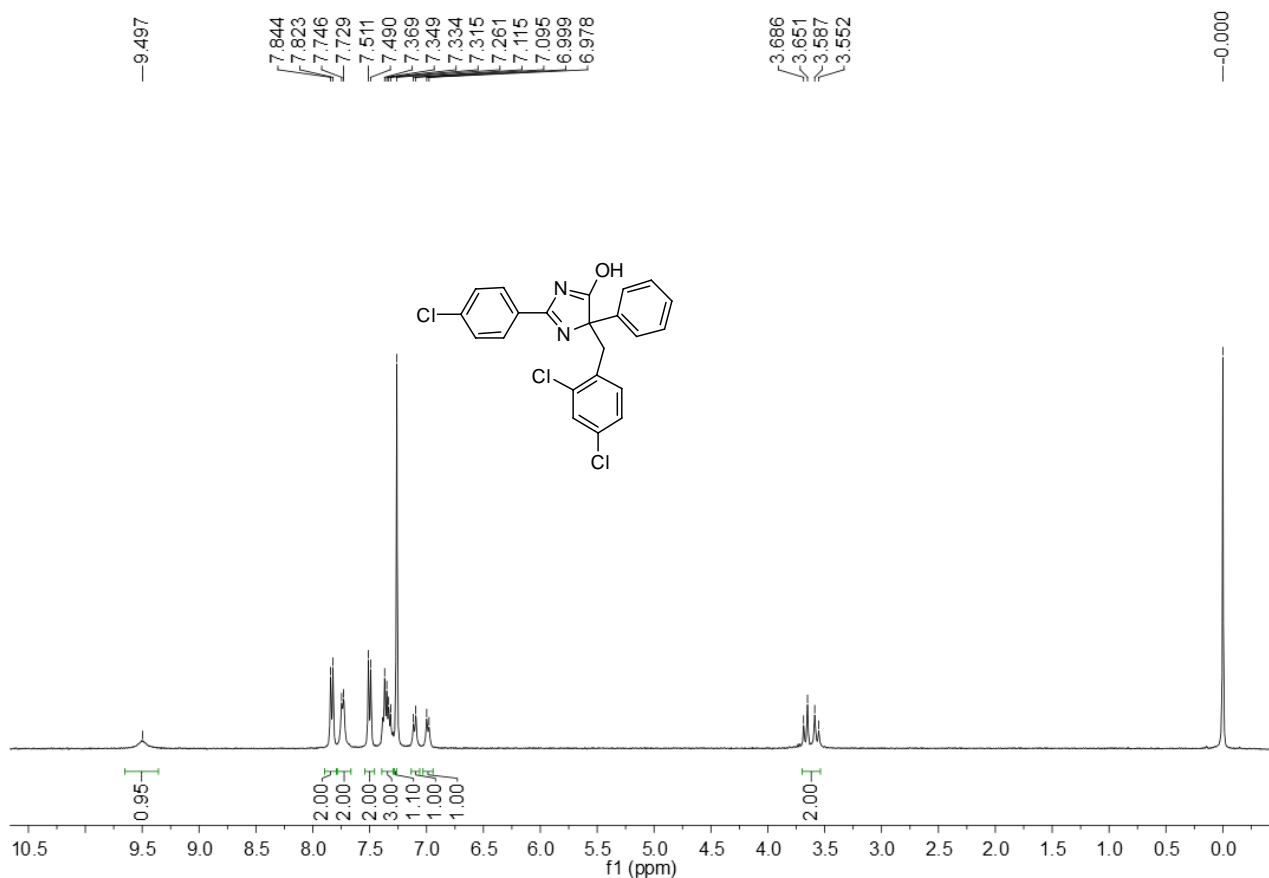
**<sup>13</sup>C NMR Spectrum of Compound 3a**



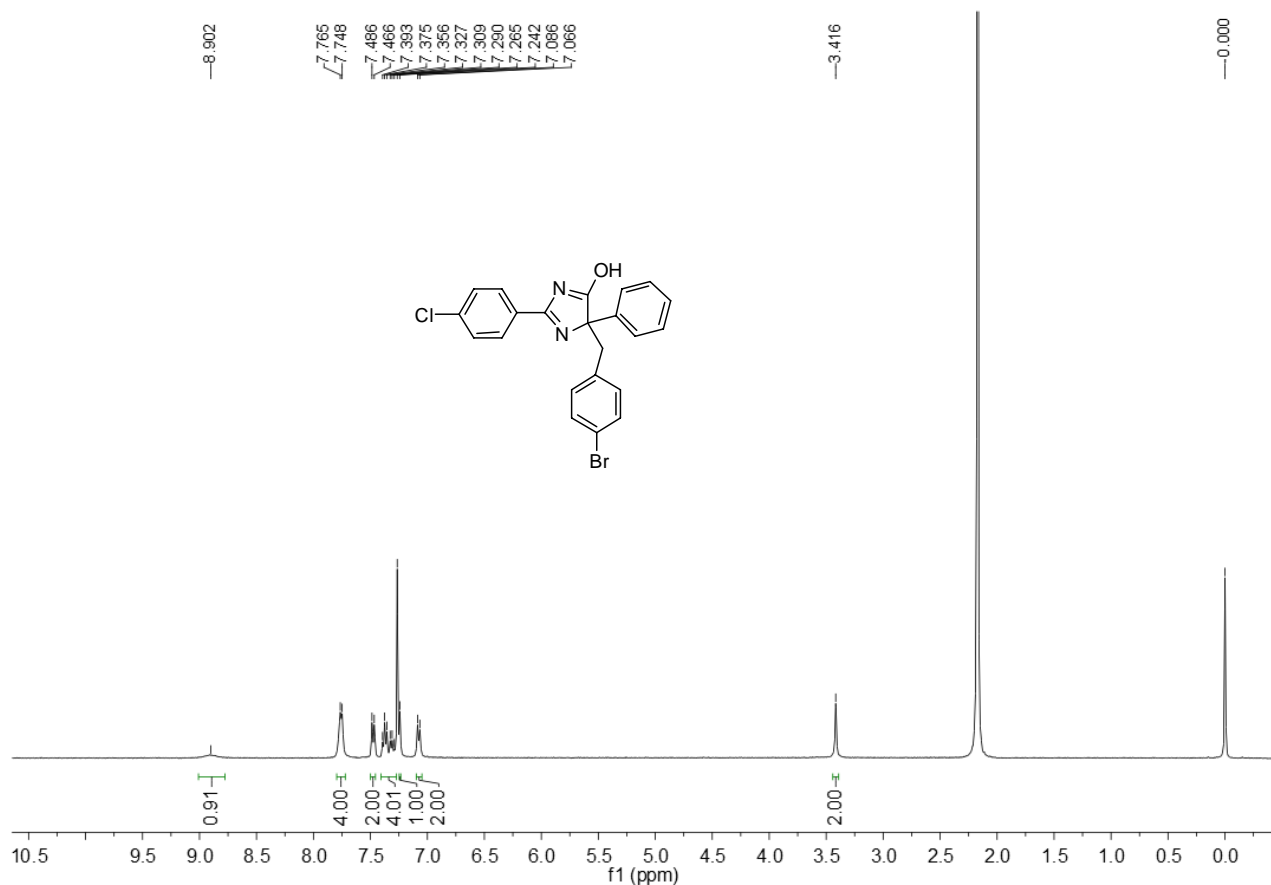


**<sup>13</sup>C NMR Spectrum of Compound 3b**

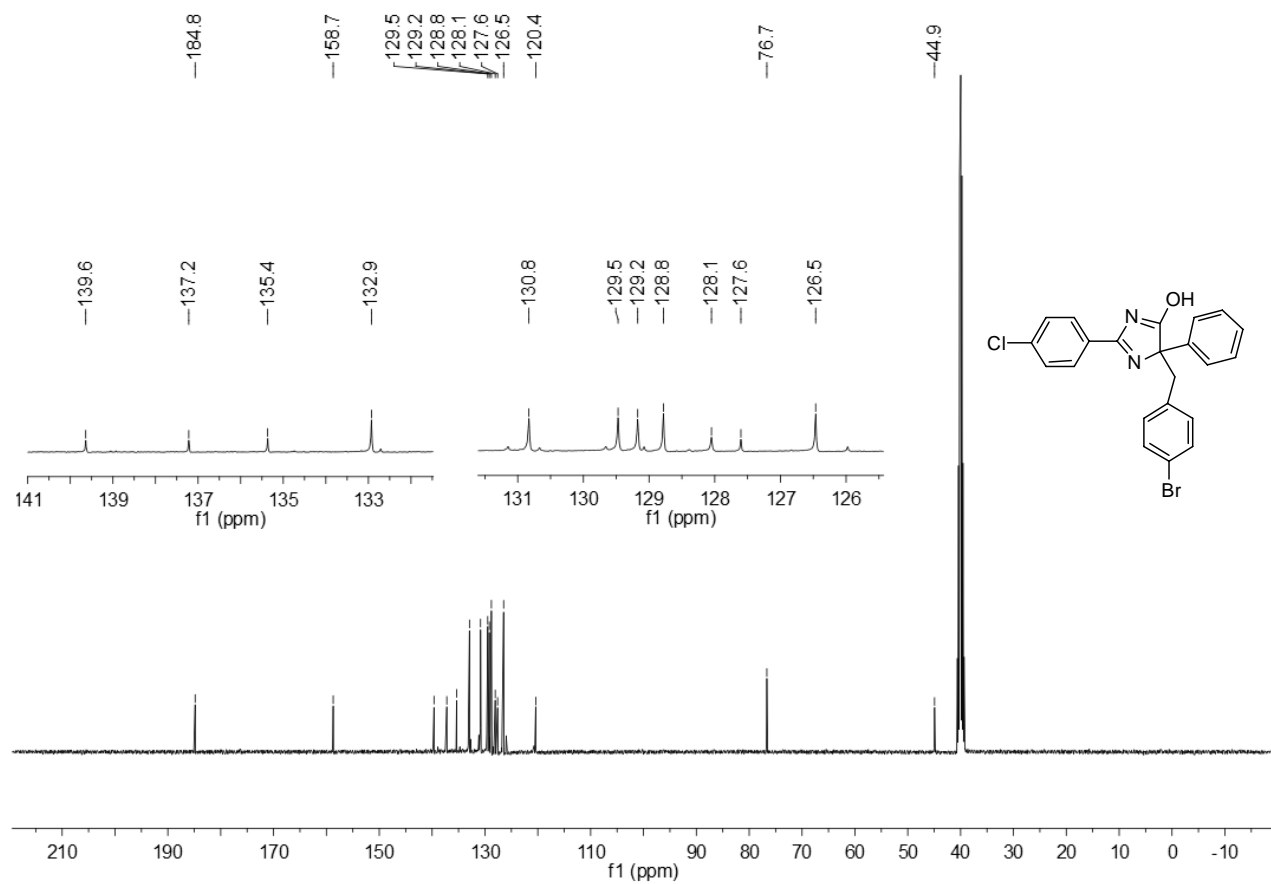




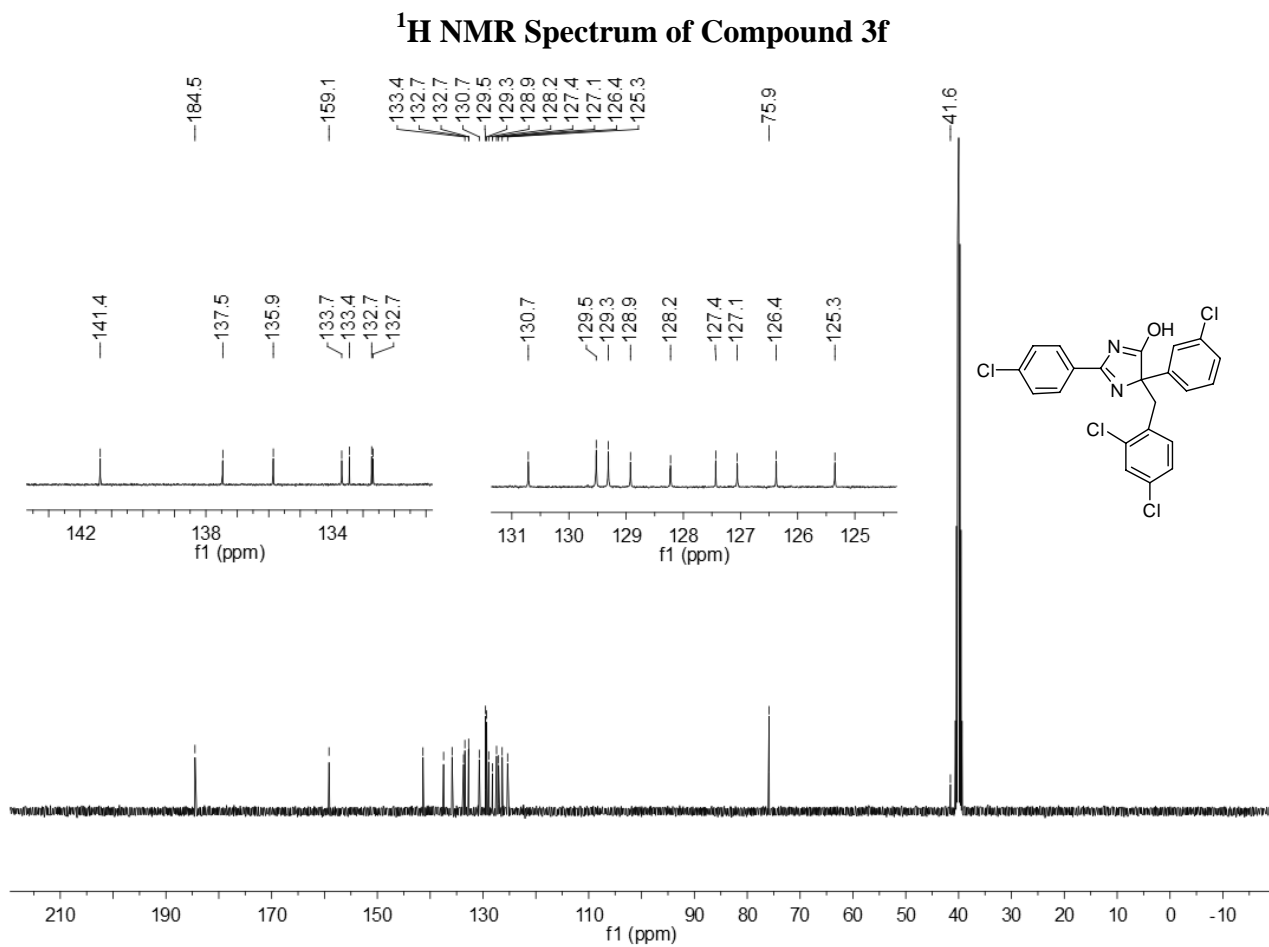
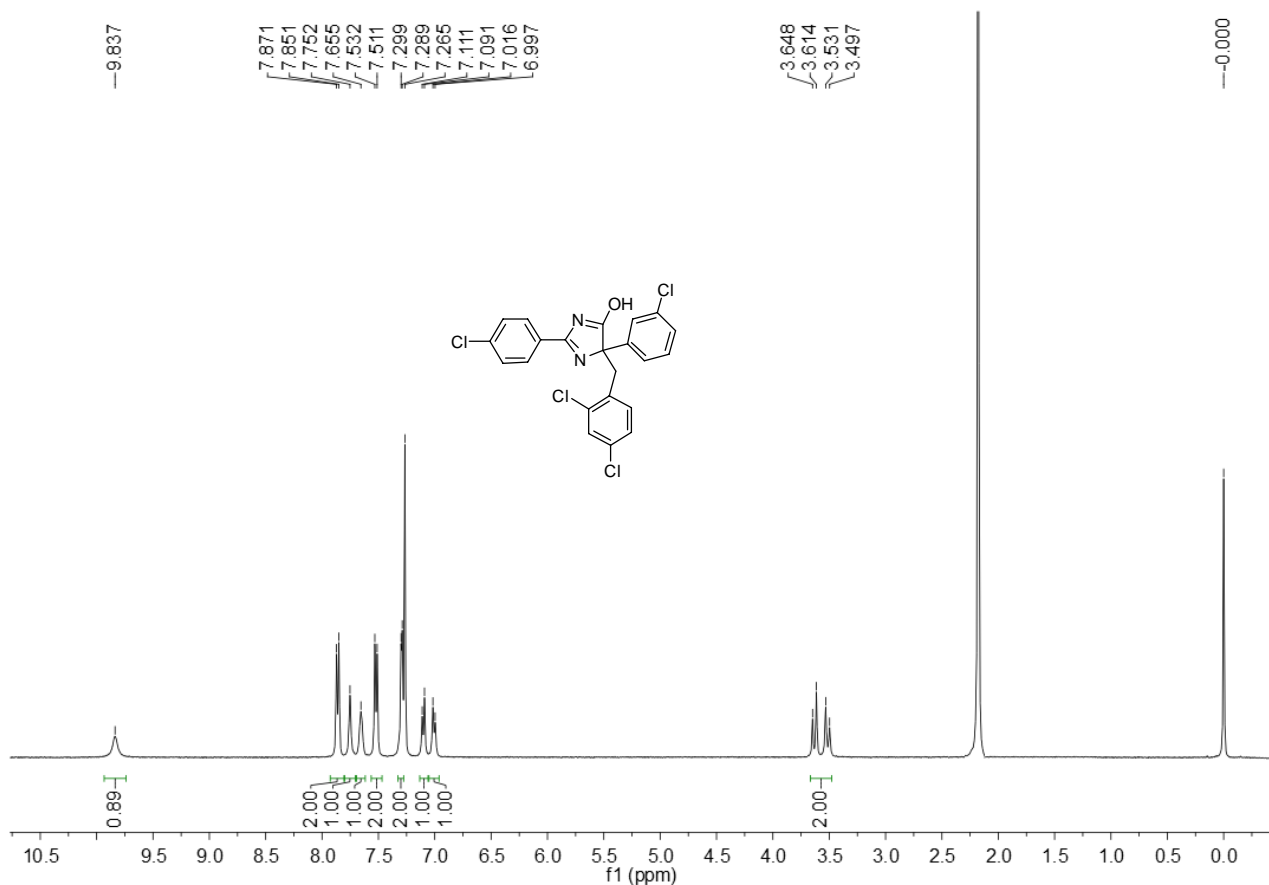
**<sup>13</sup>C NMR Spectrum of Compound 3d**

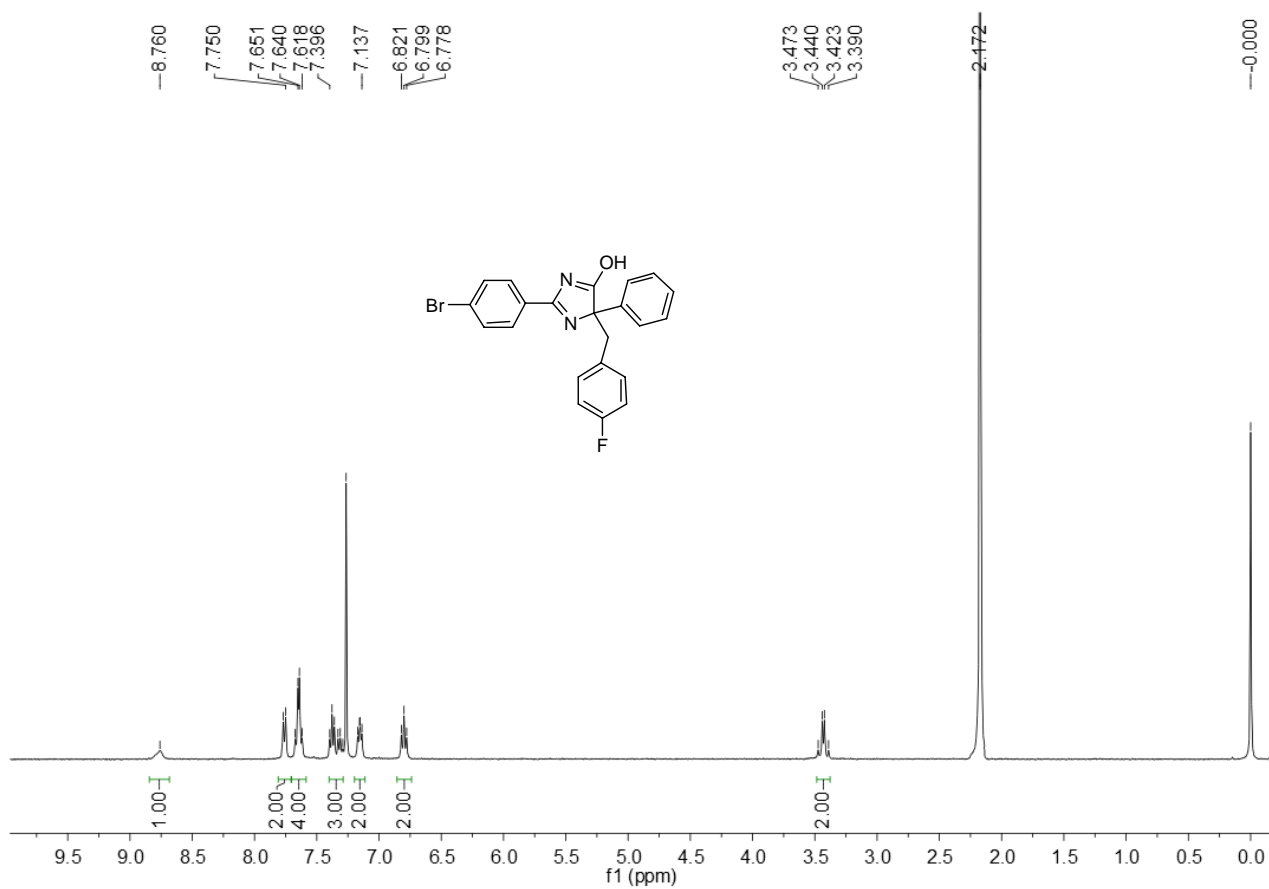
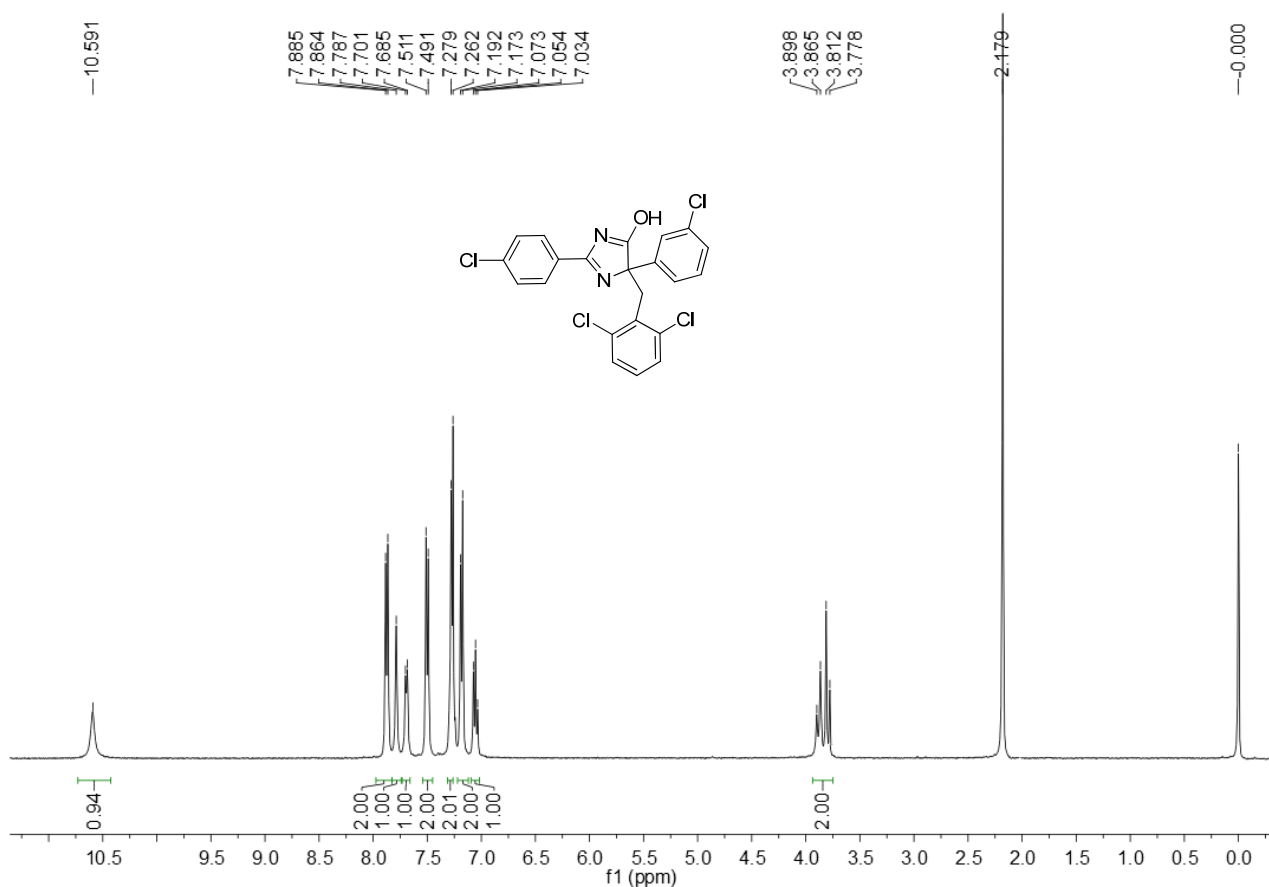


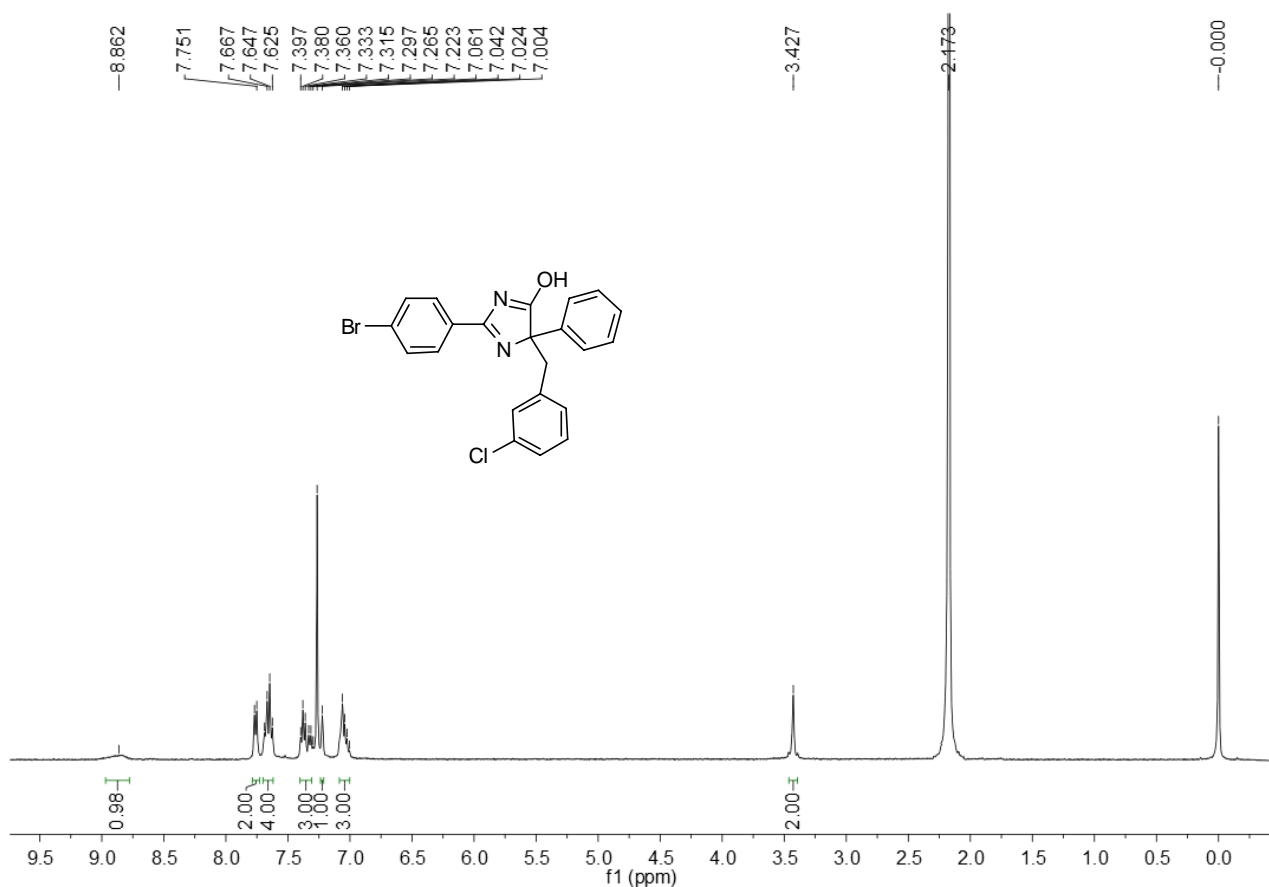
<sup>1</sup>H NMR Spectrum of Compound 3e



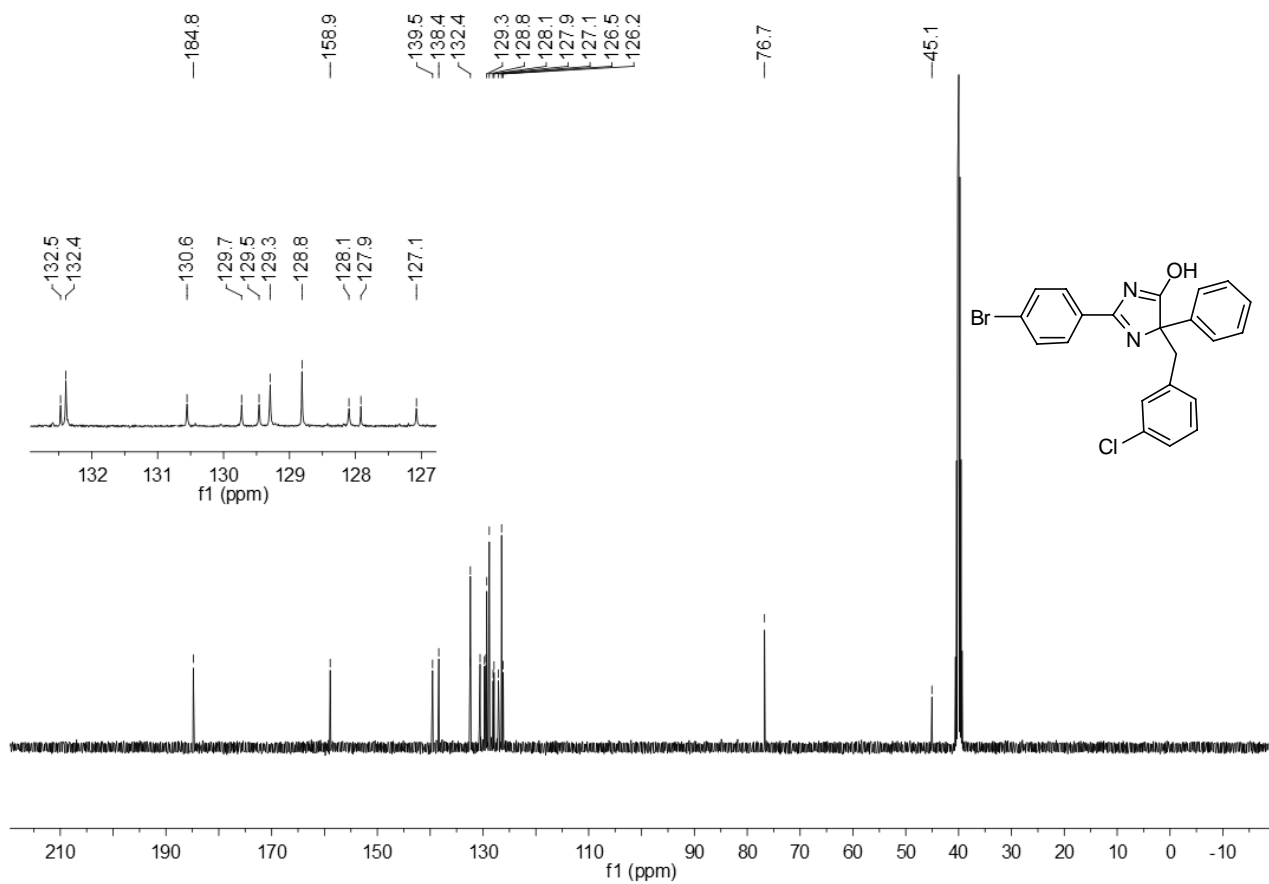
<sup>13</sup>C NMR Spectrum of Compound 3e





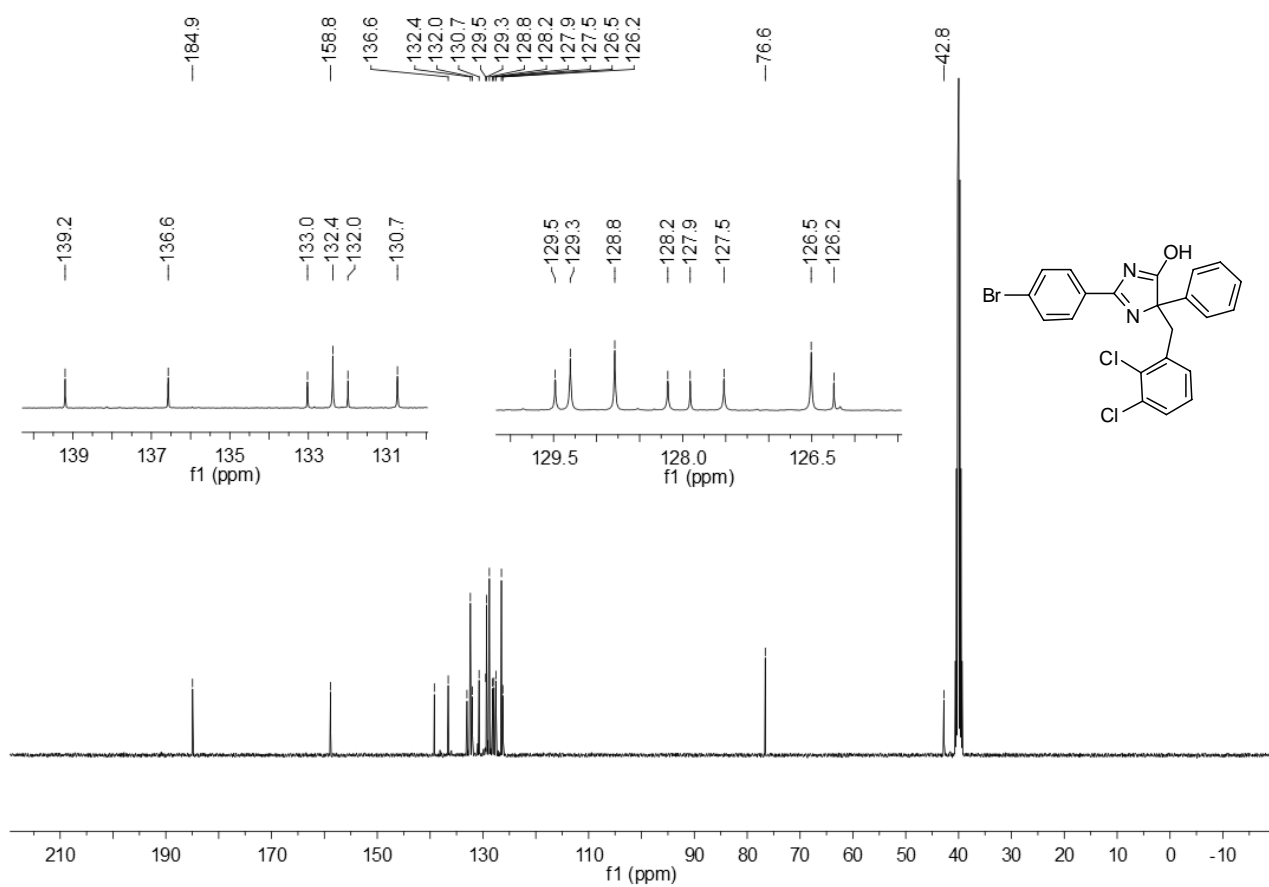
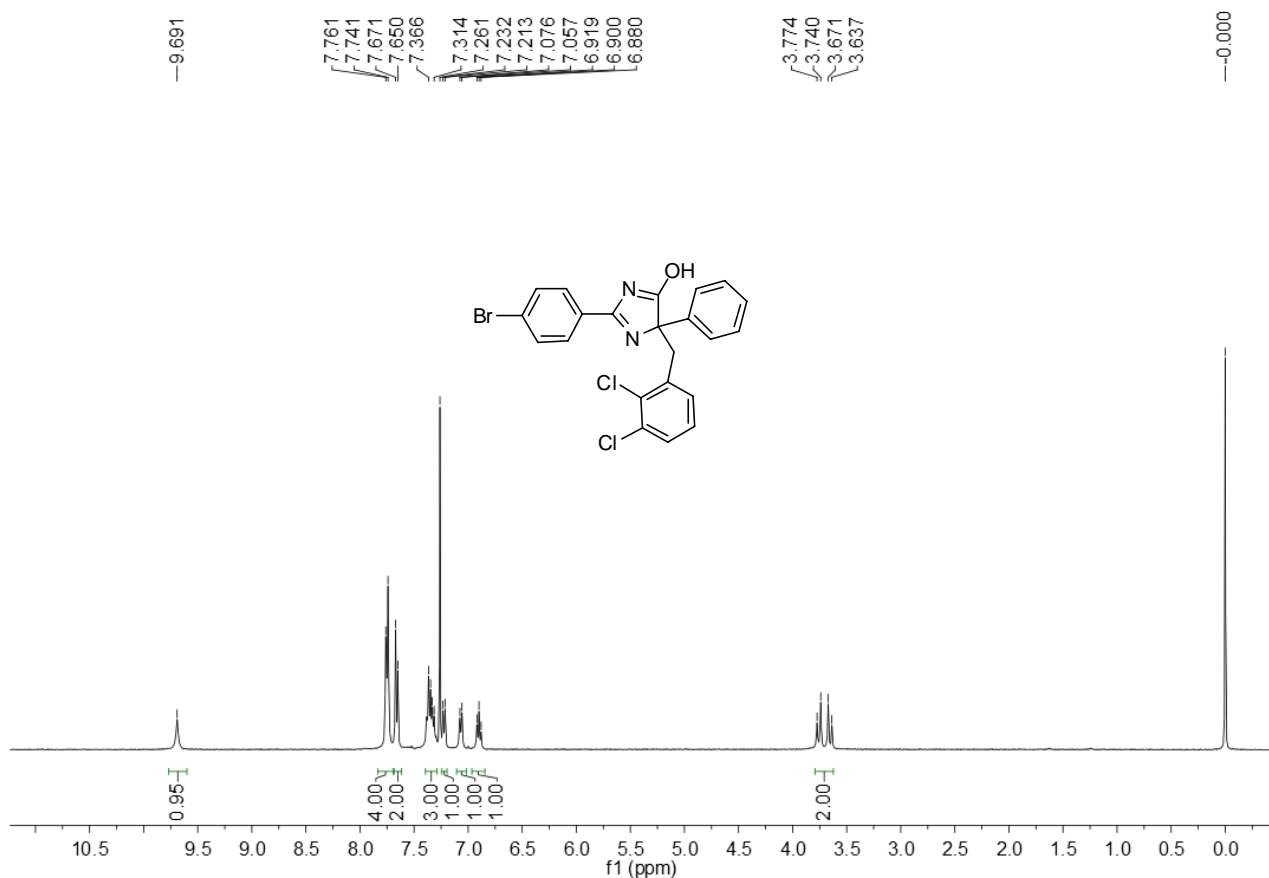


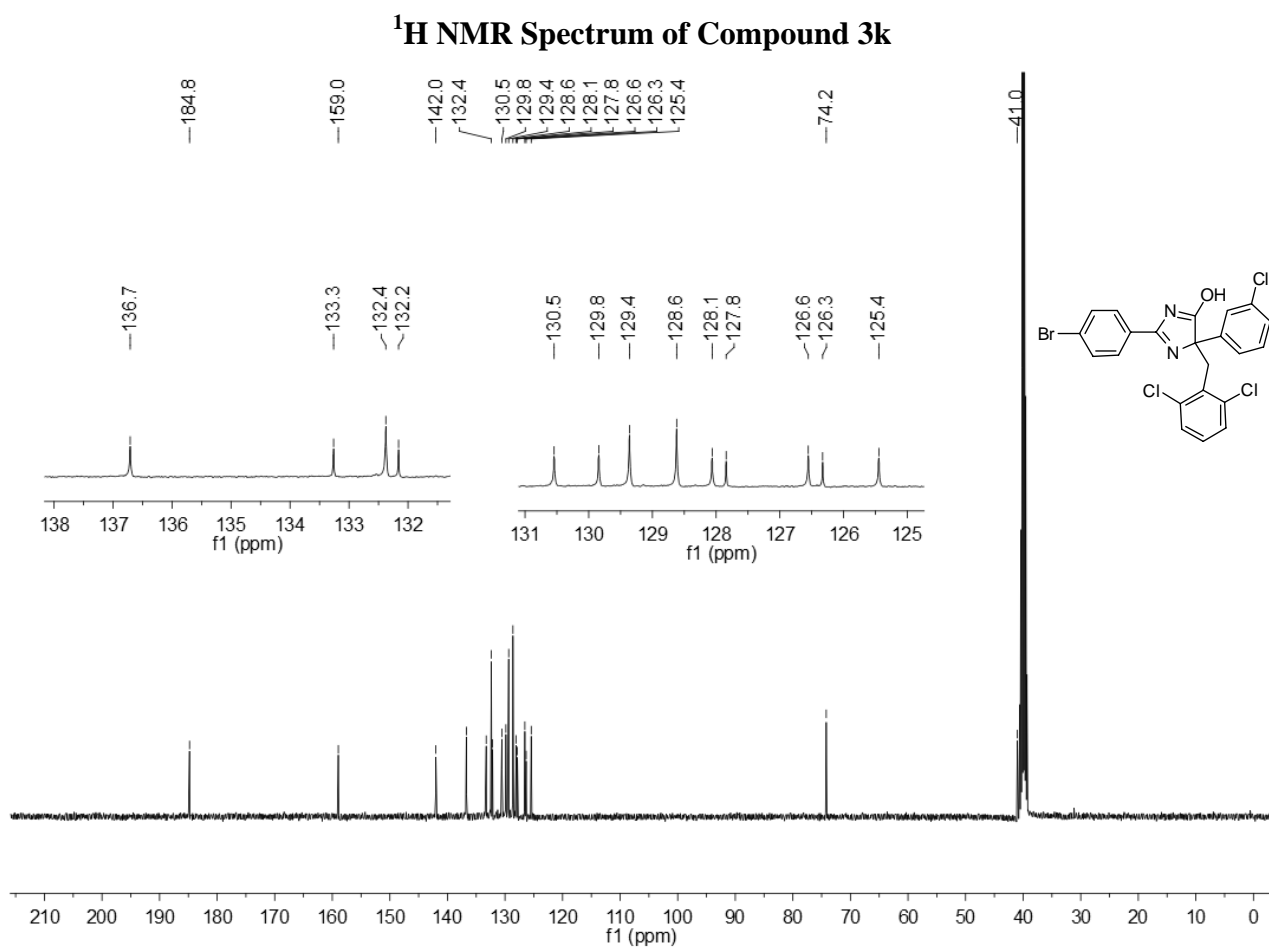
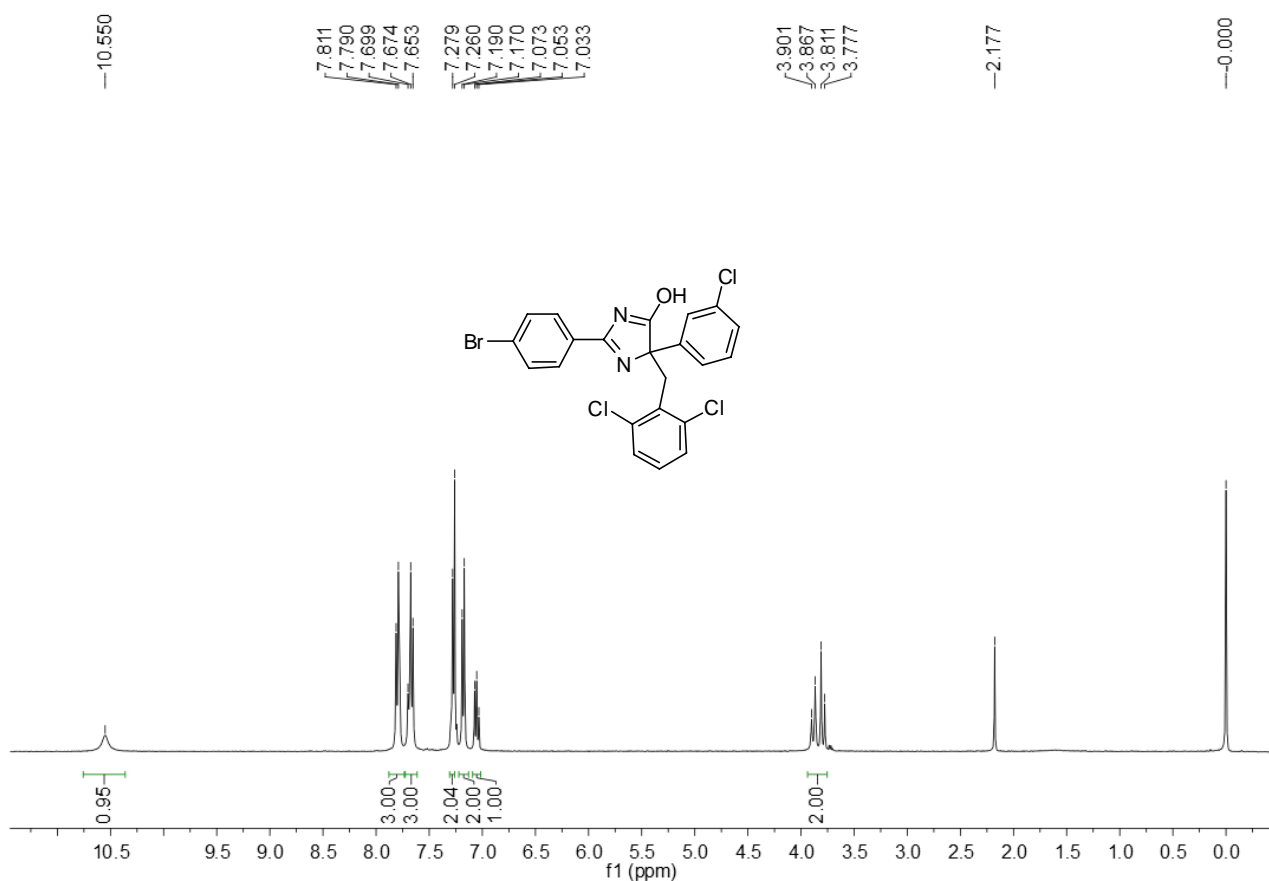
<sup>1</sup>H NMR Spectrum of Compound 3i

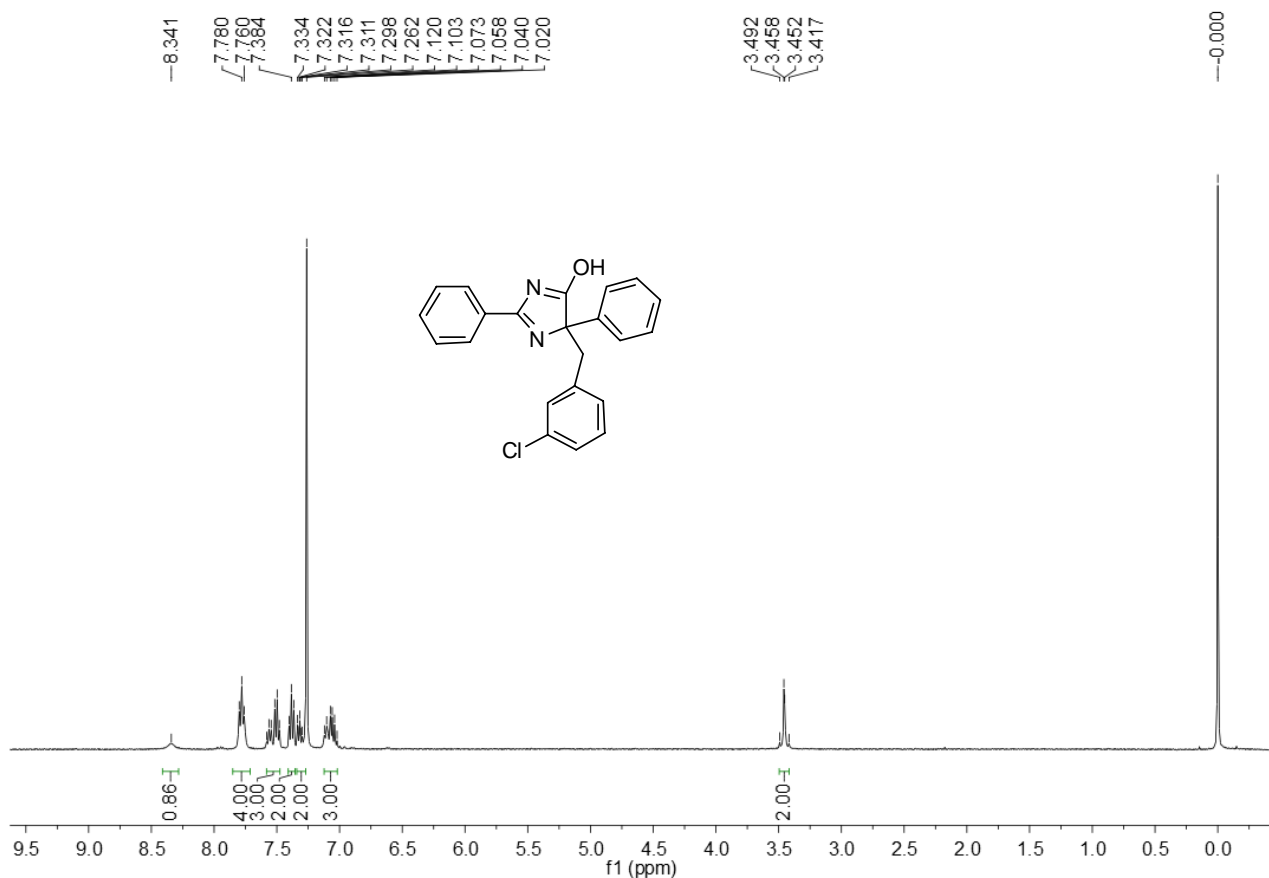


<sup>13</sup>C NMR Spectrum of Compound 3i

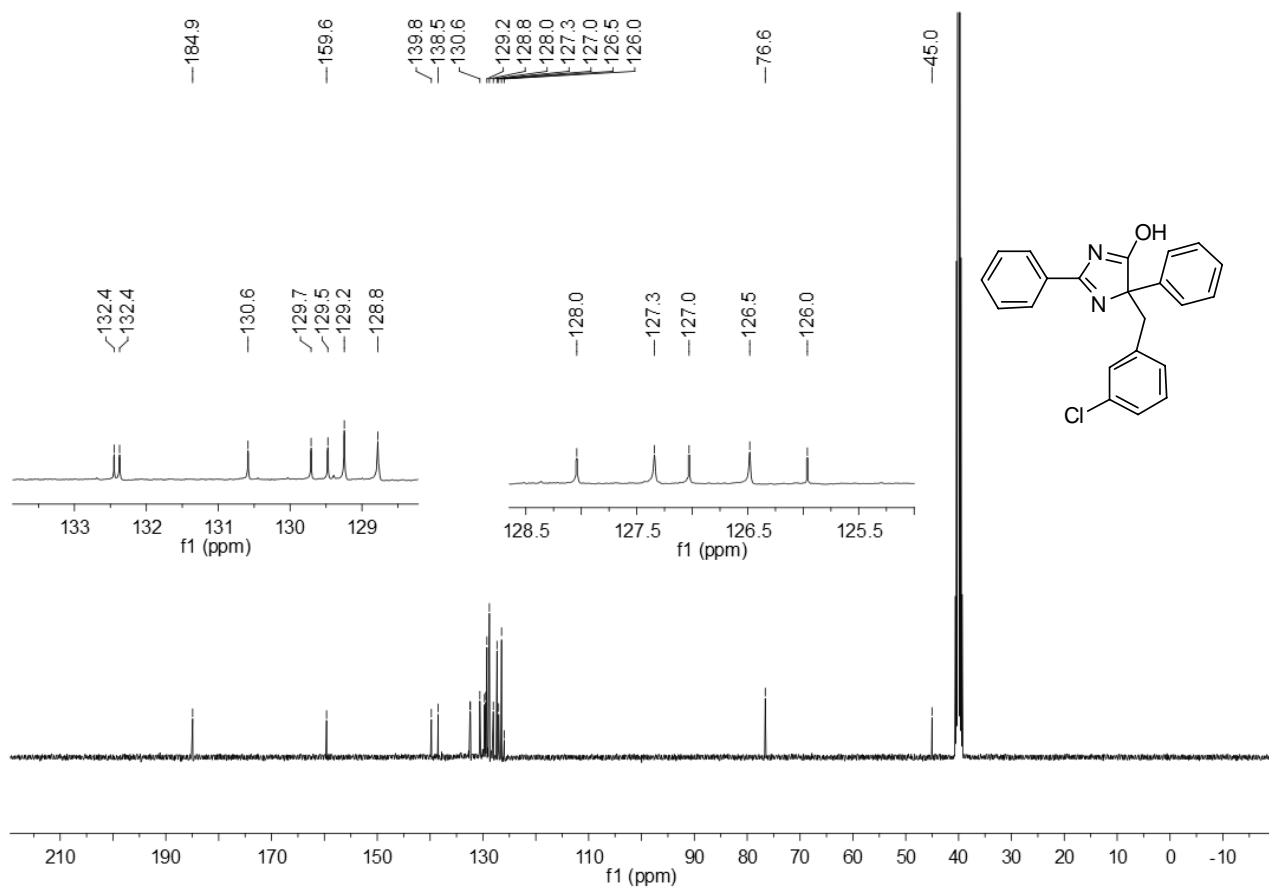




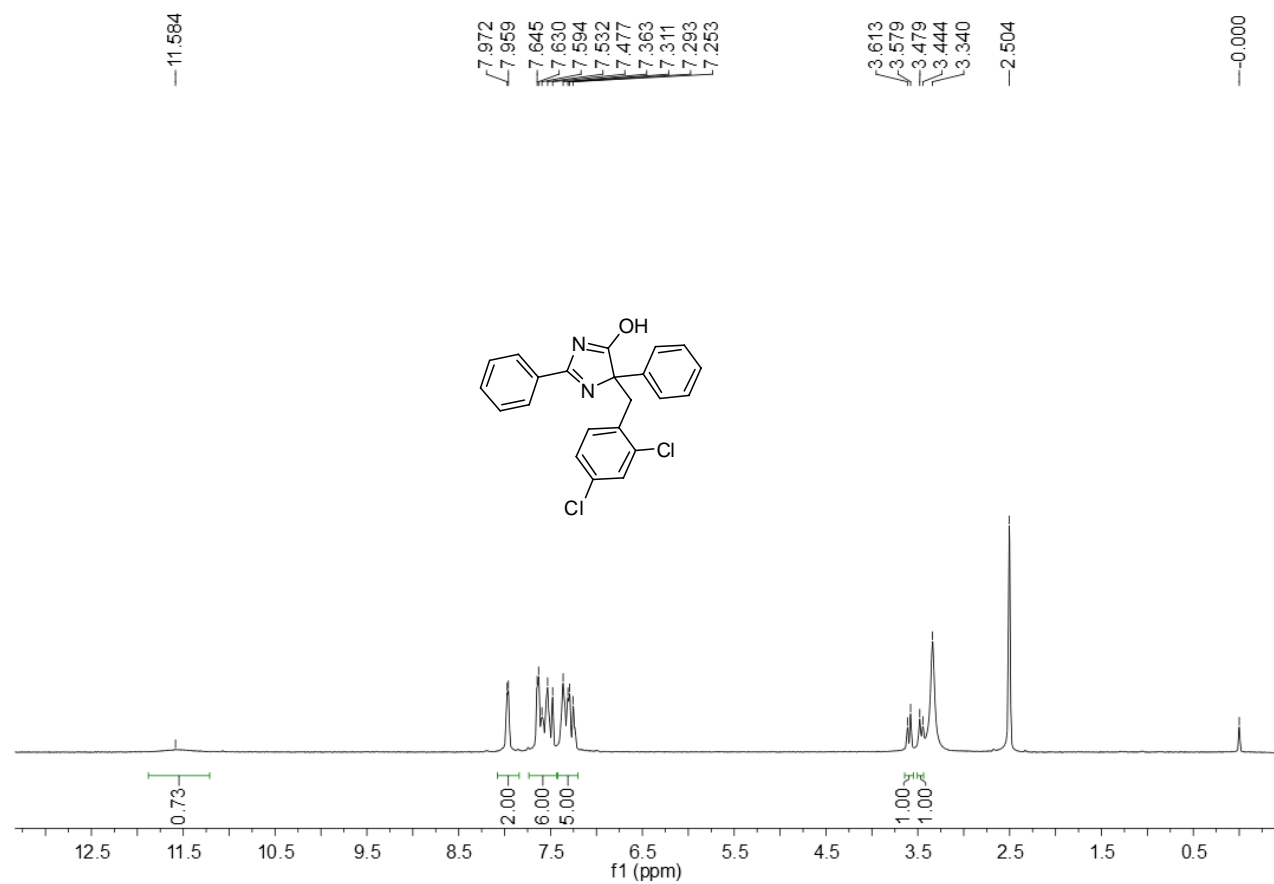
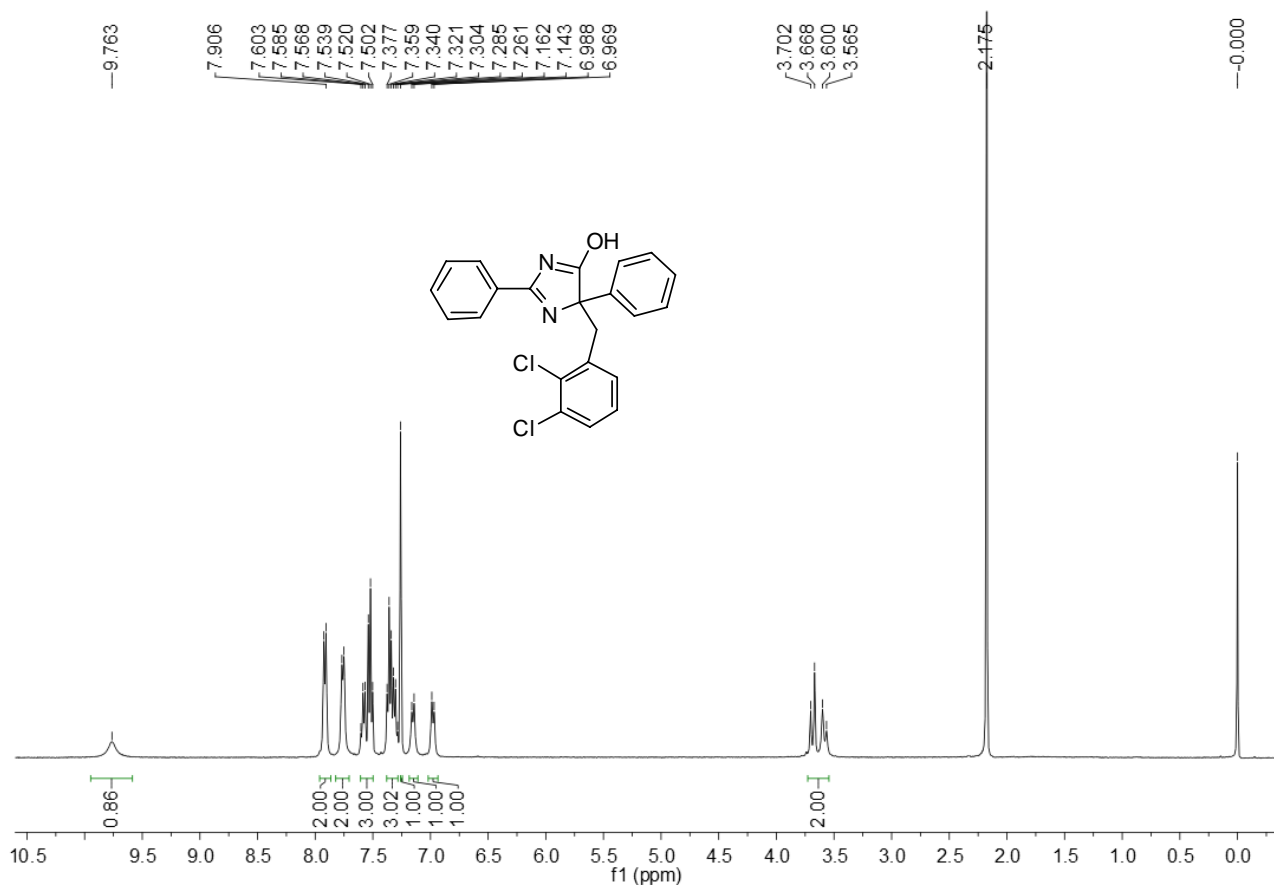


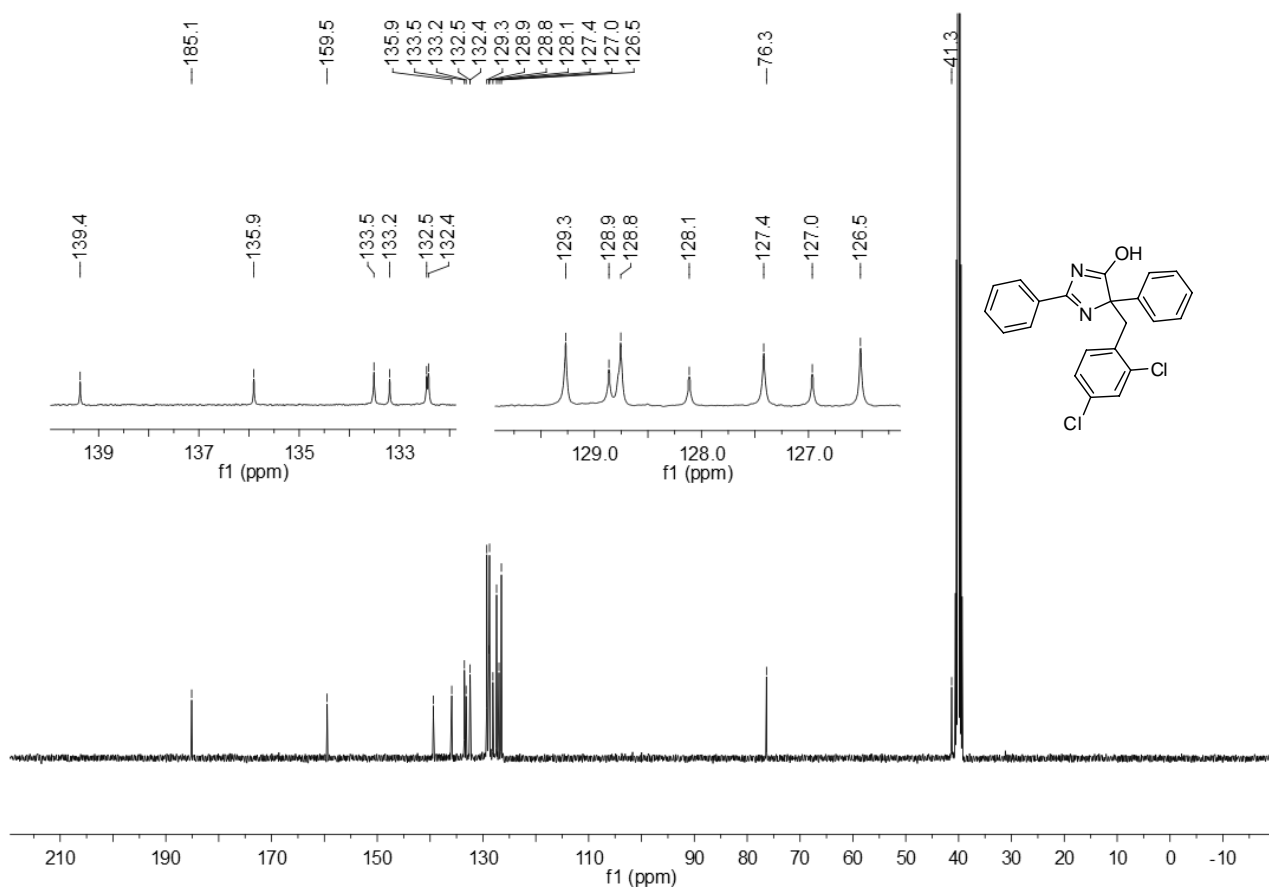


**<sup>1</sup>H NMR Spectrum of Compound 31**

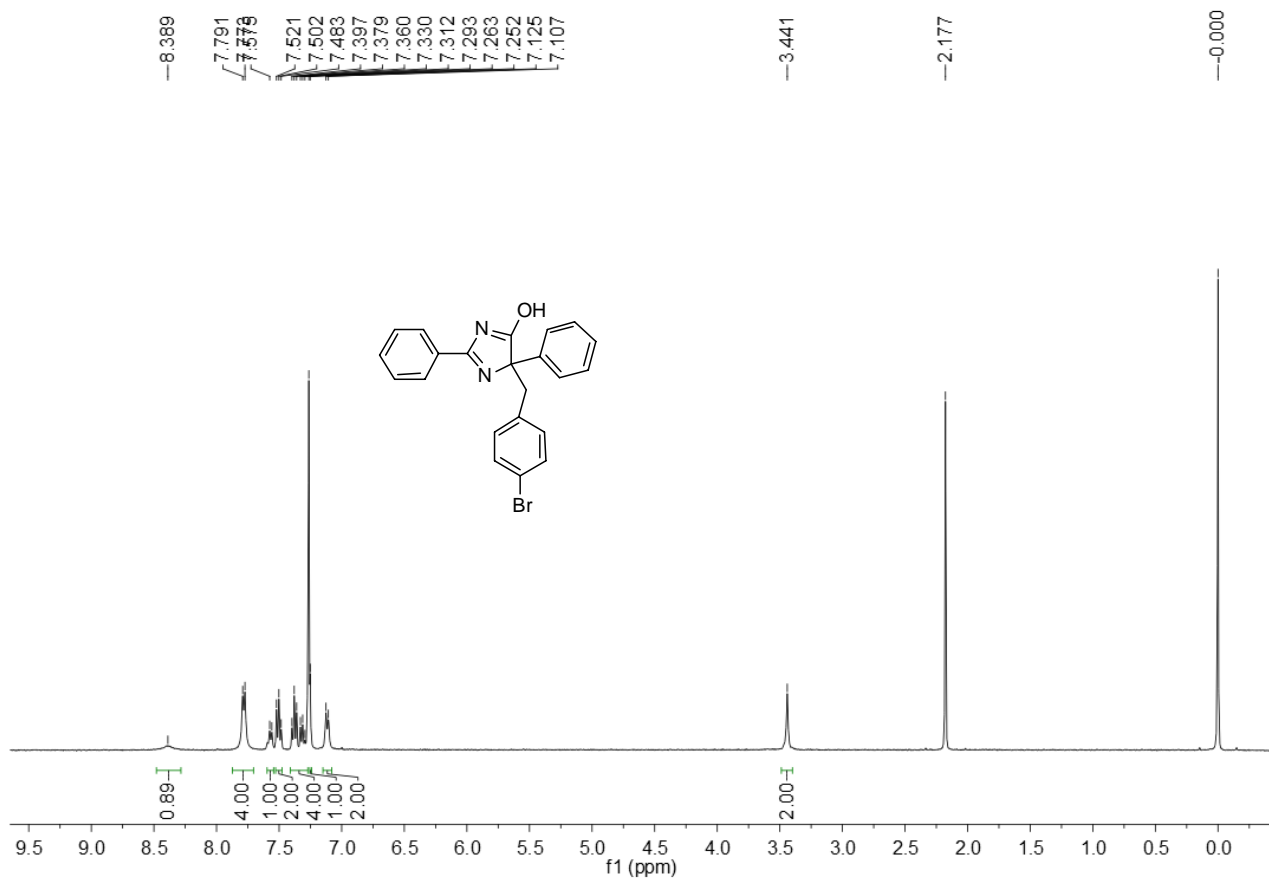


**<sup>13</sup>C NMR Spectrum of Compound 31**

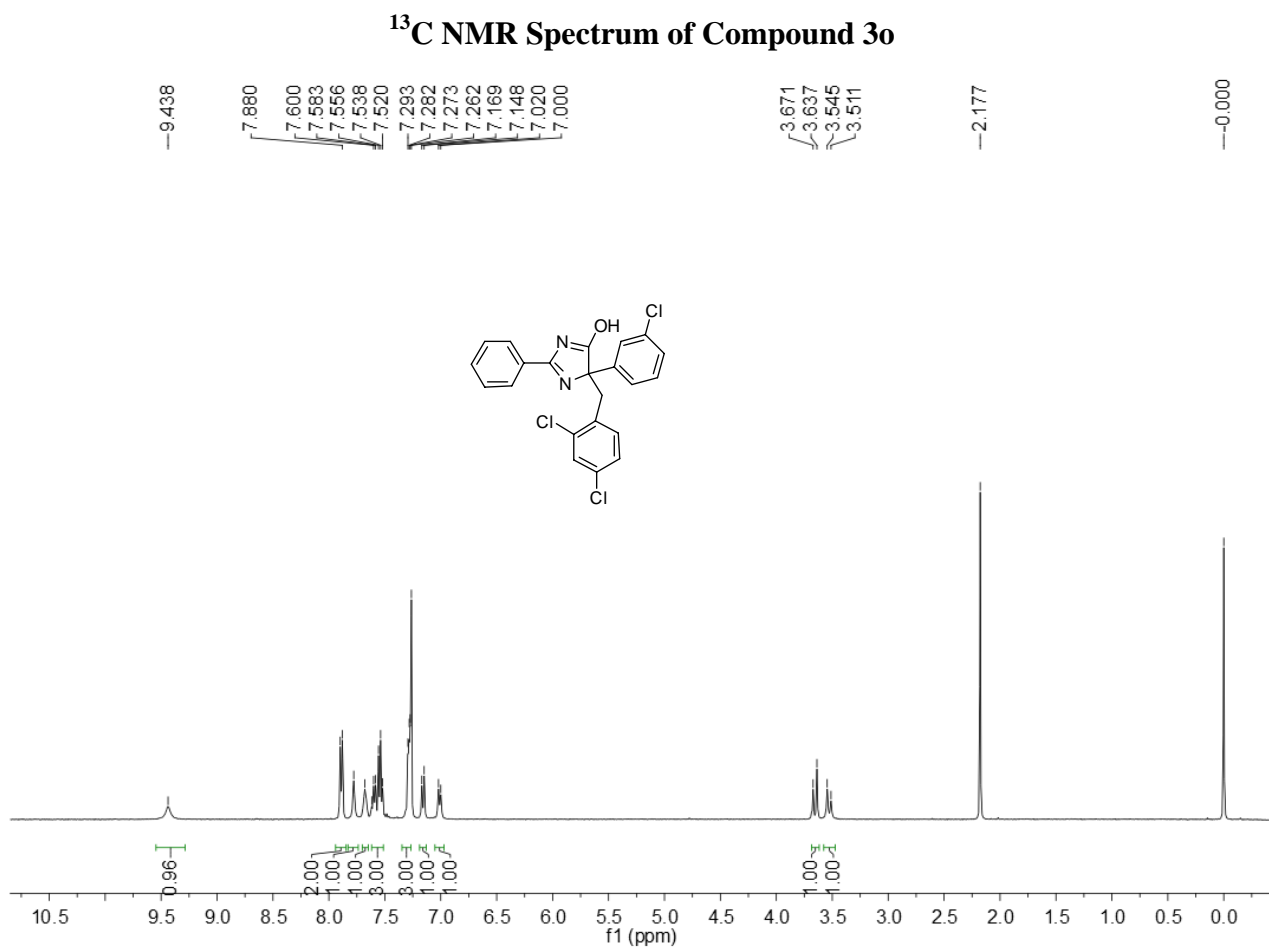
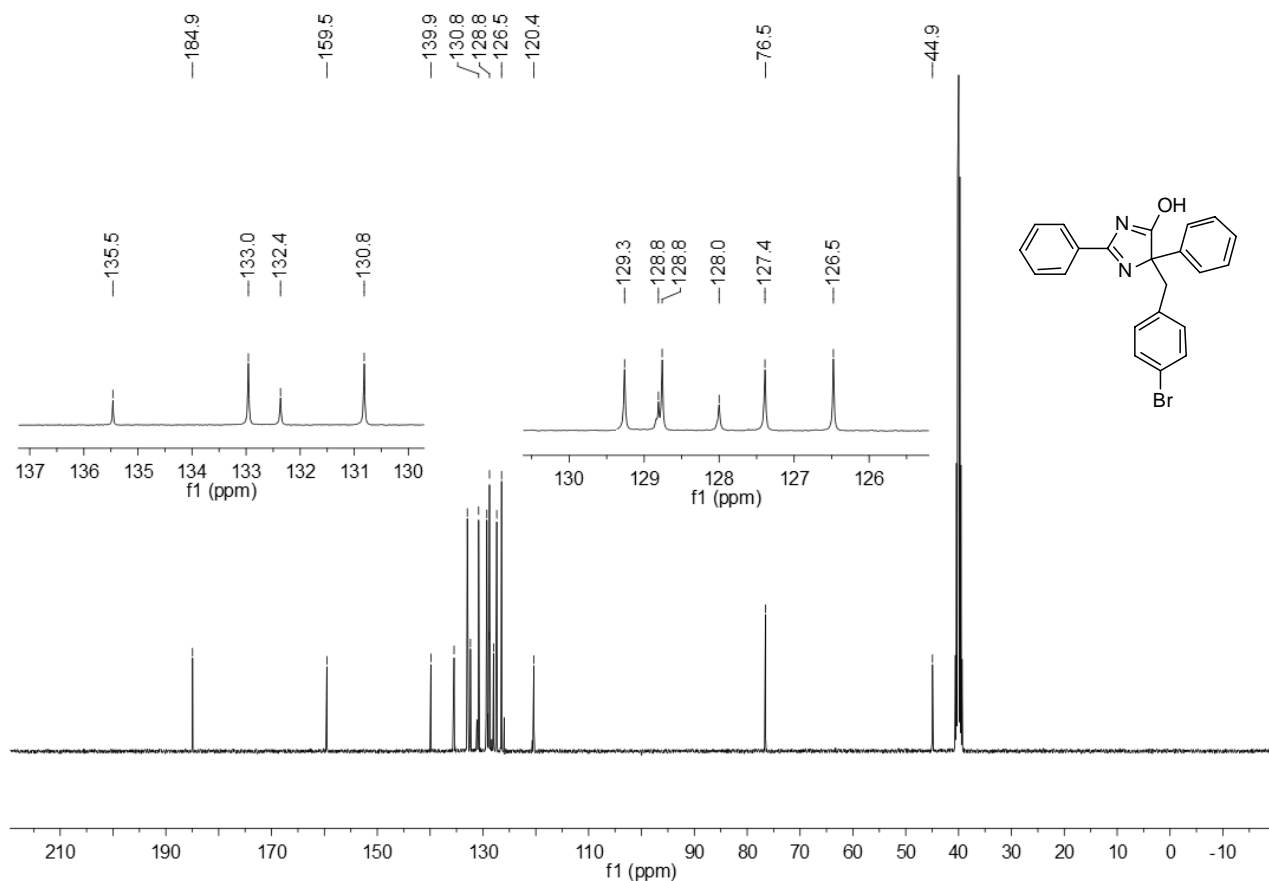


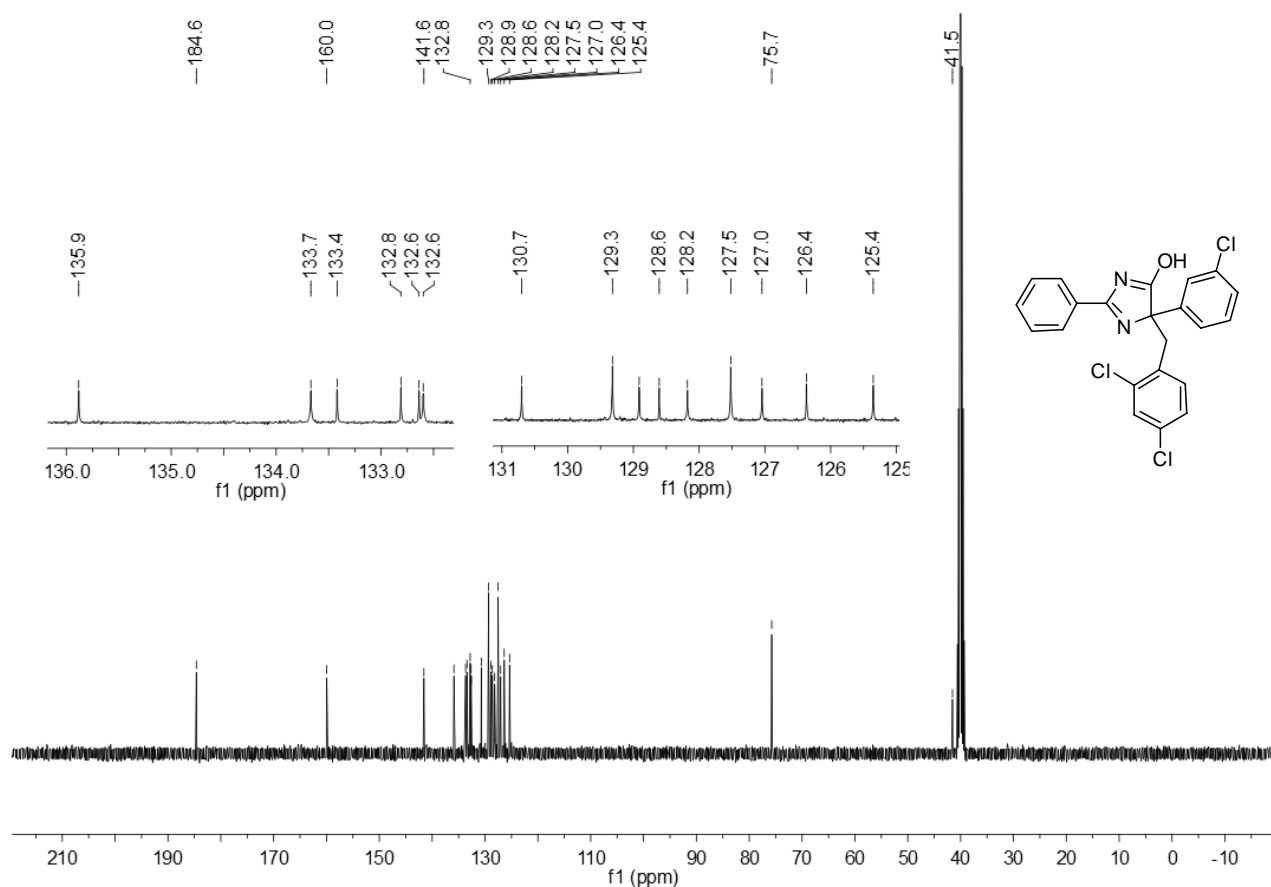


**<sup>13</sup>C NMR Spectrum of Compound 3n**

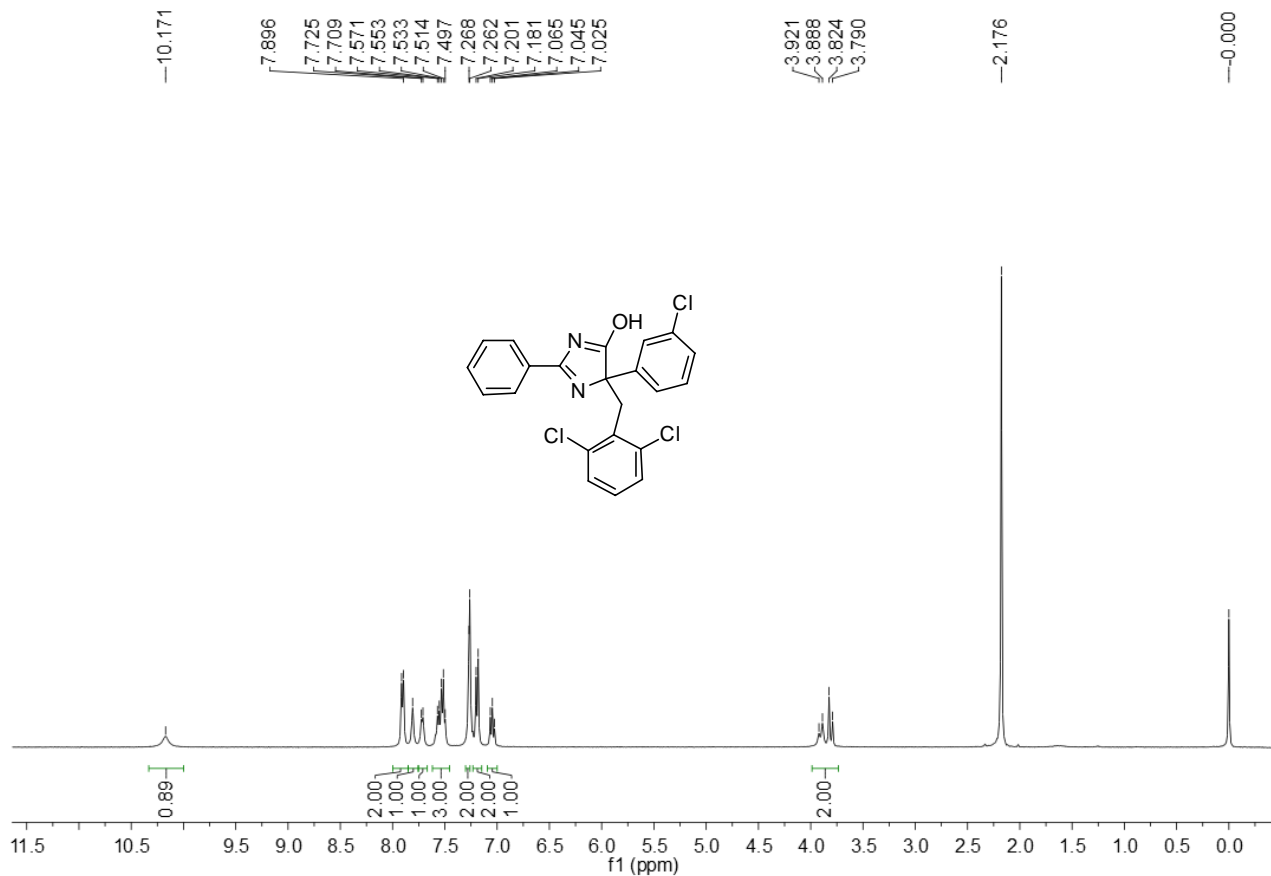


**<sup>1</sup>H NMR Spectrum of Compound 3o**



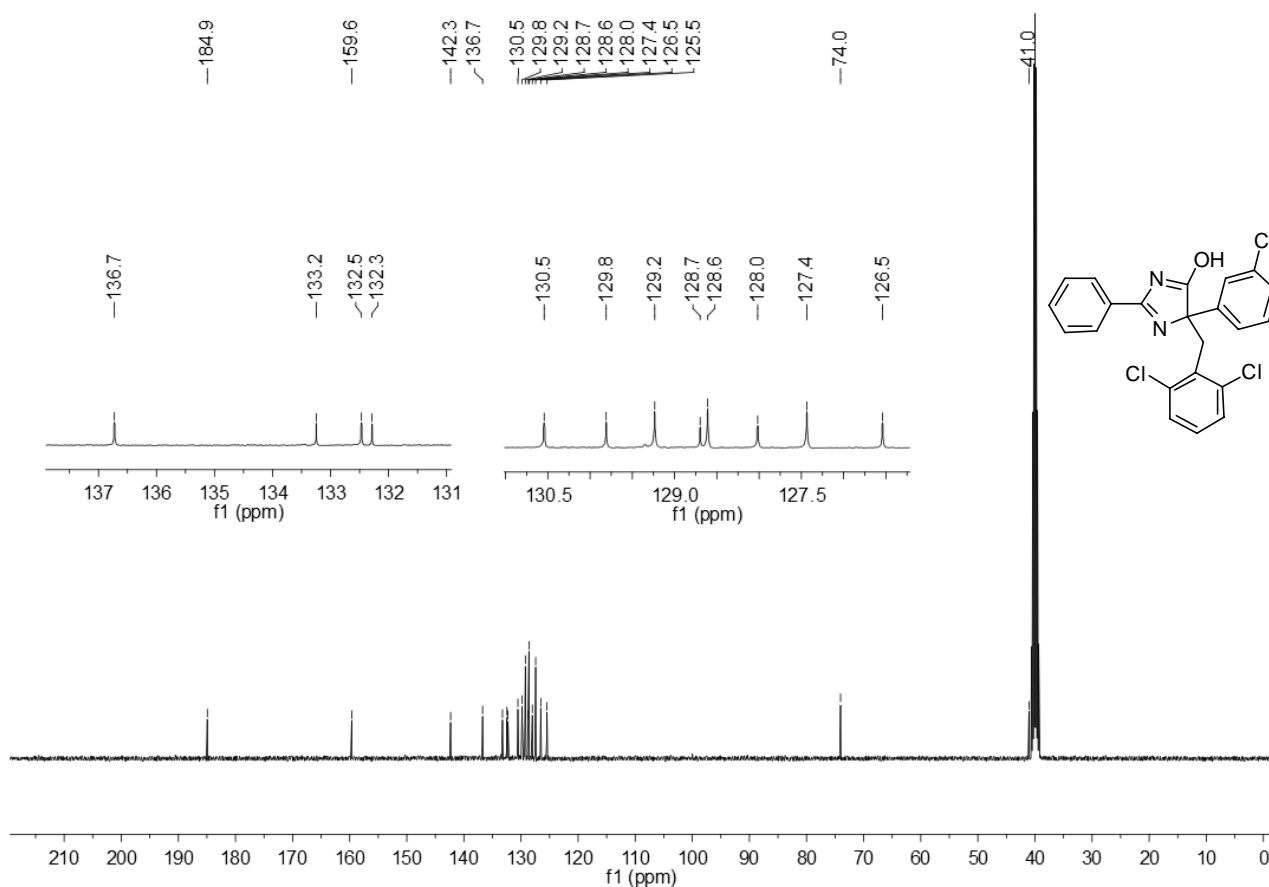


**<sup>13</sup>C NMR Spectrum of Compound 3p**

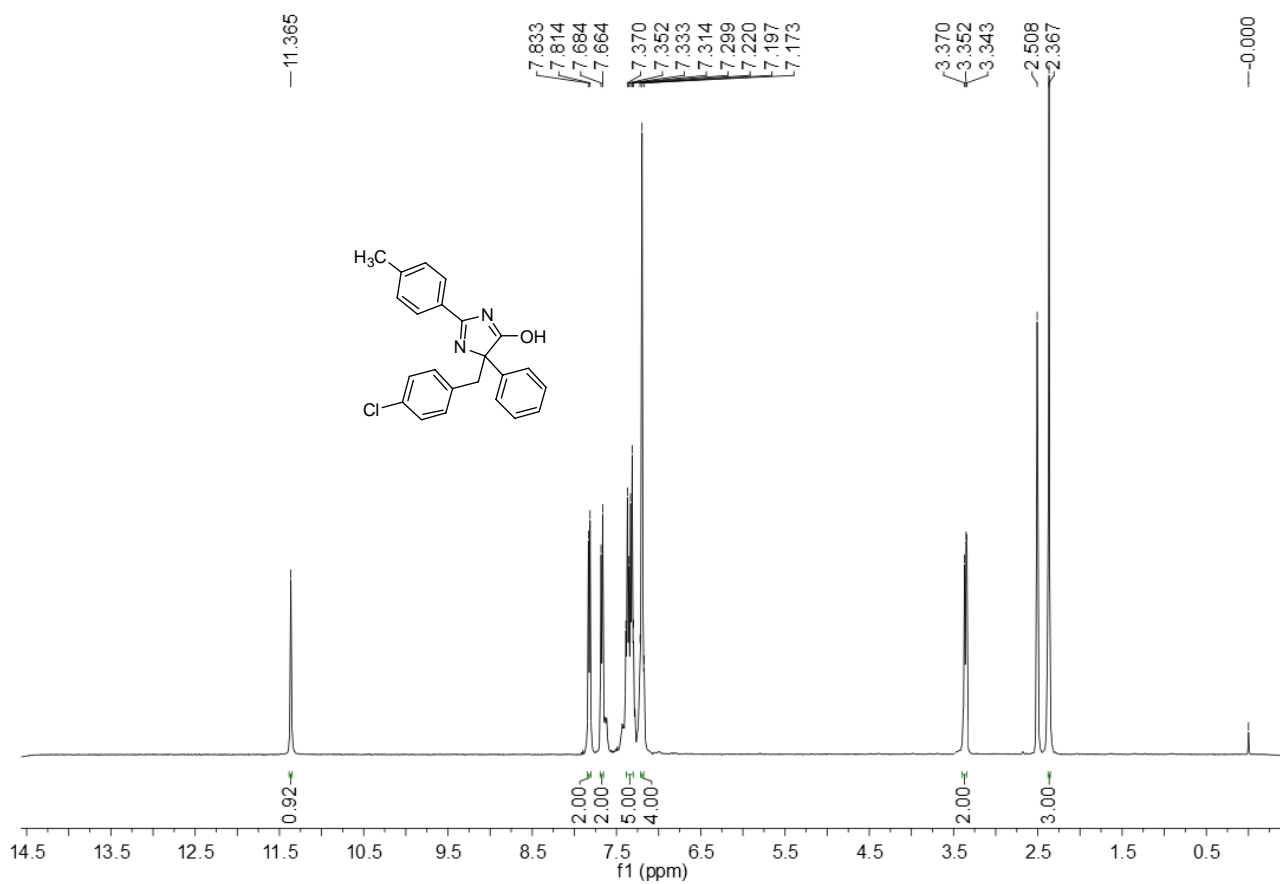


**<sup>1</sup>H NMR Spectrum of Compound 3p**

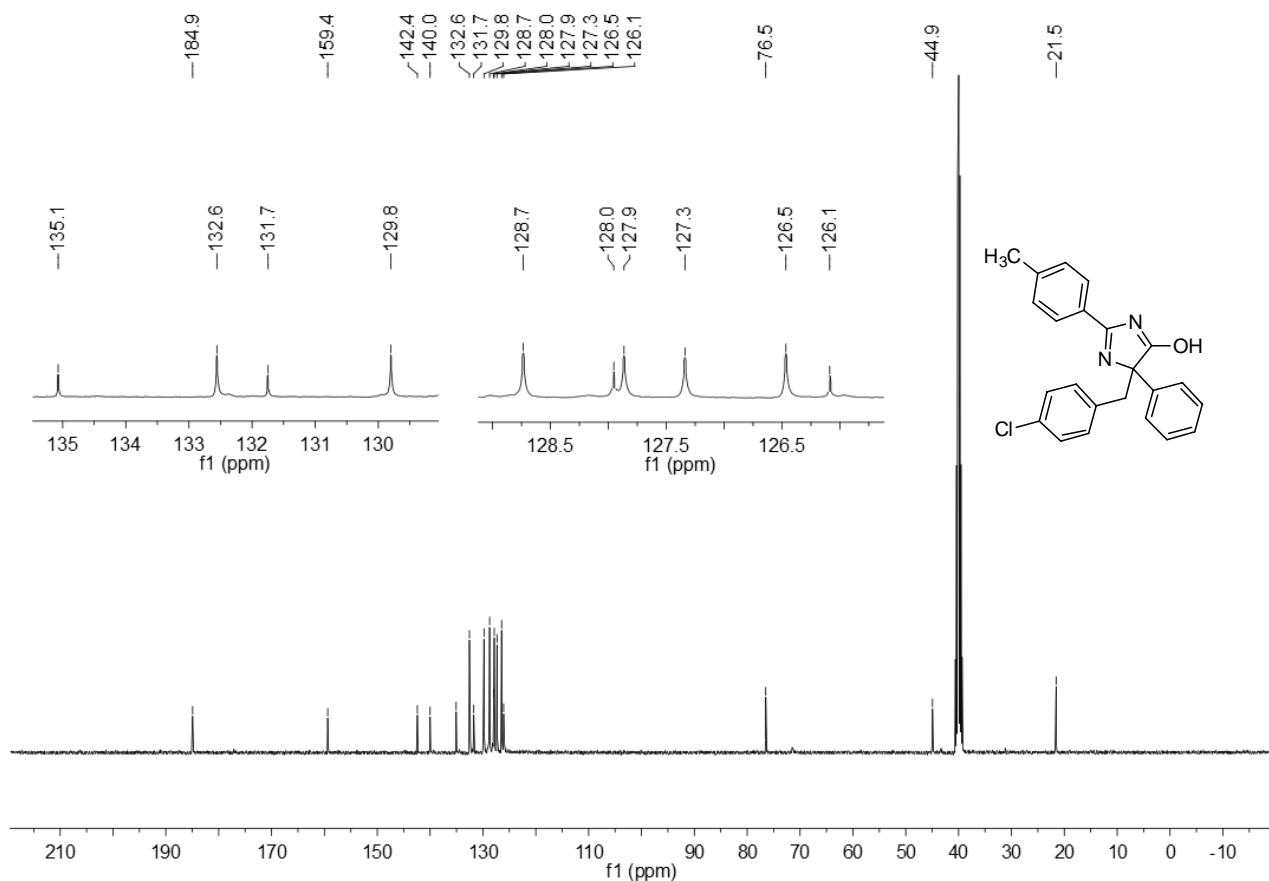




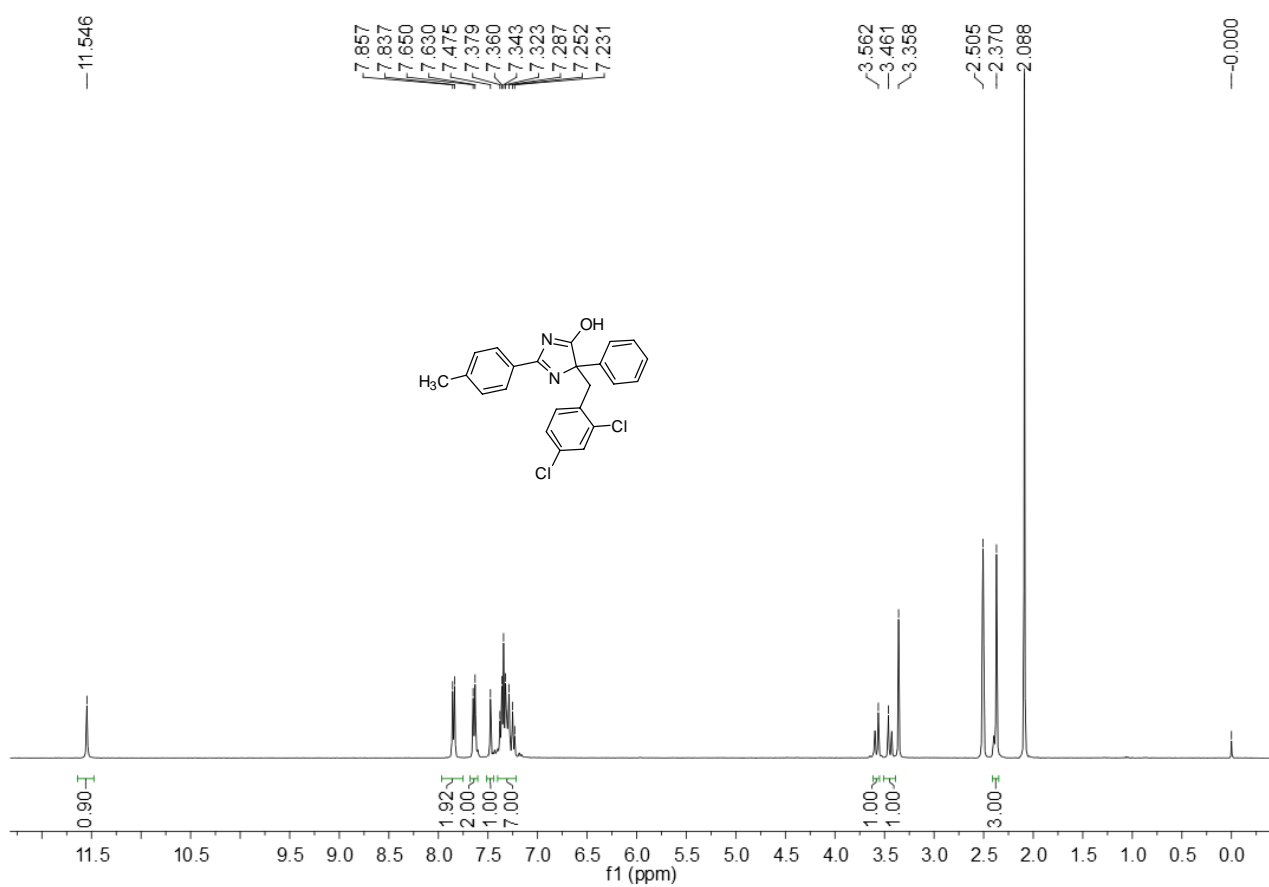
**<sup>13</sup>C NMR Spectrum of Compound 3q**



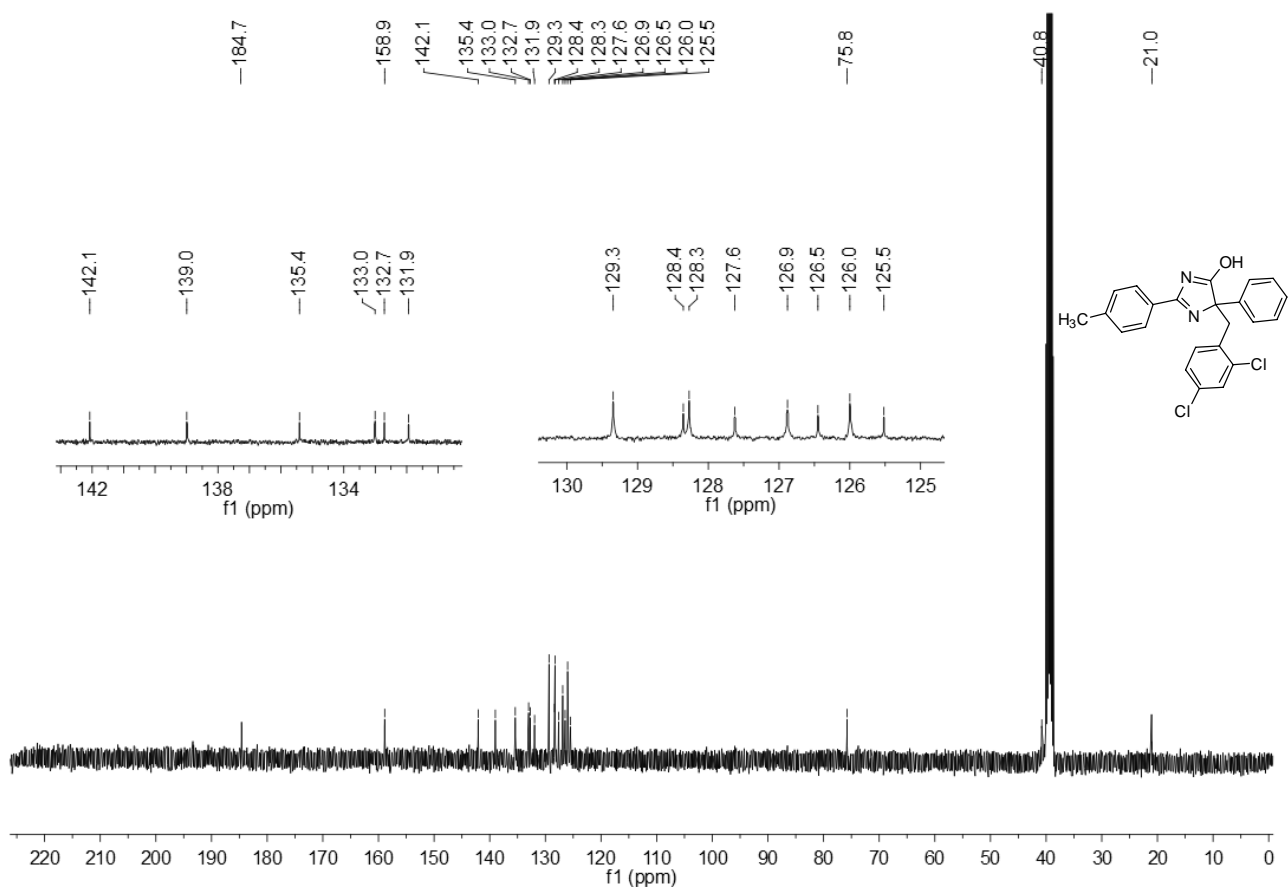
**<sup>1</sup>H NMR Spectrum of Compound 3r**



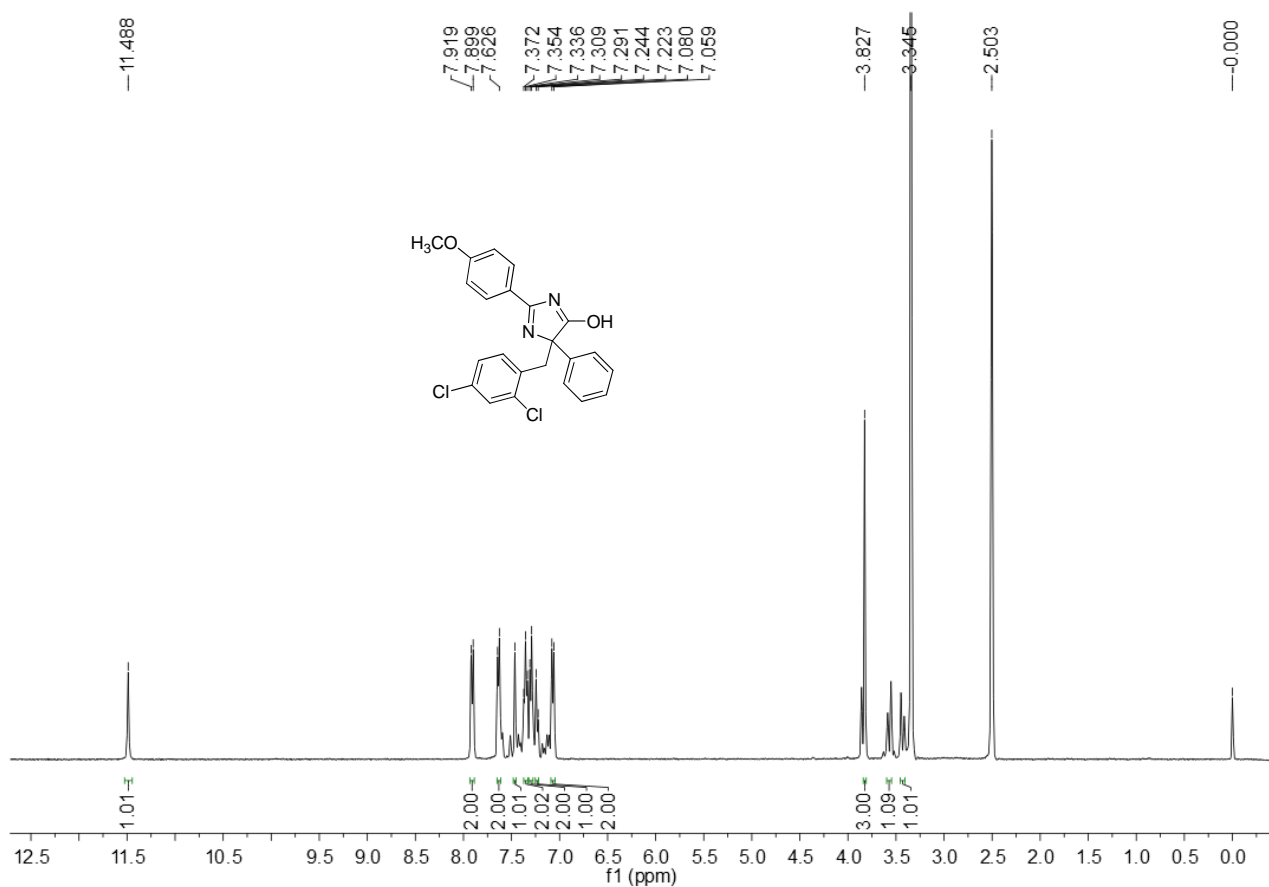
**<sup>13</sup>C NMR Spectrum of Compound 3r**



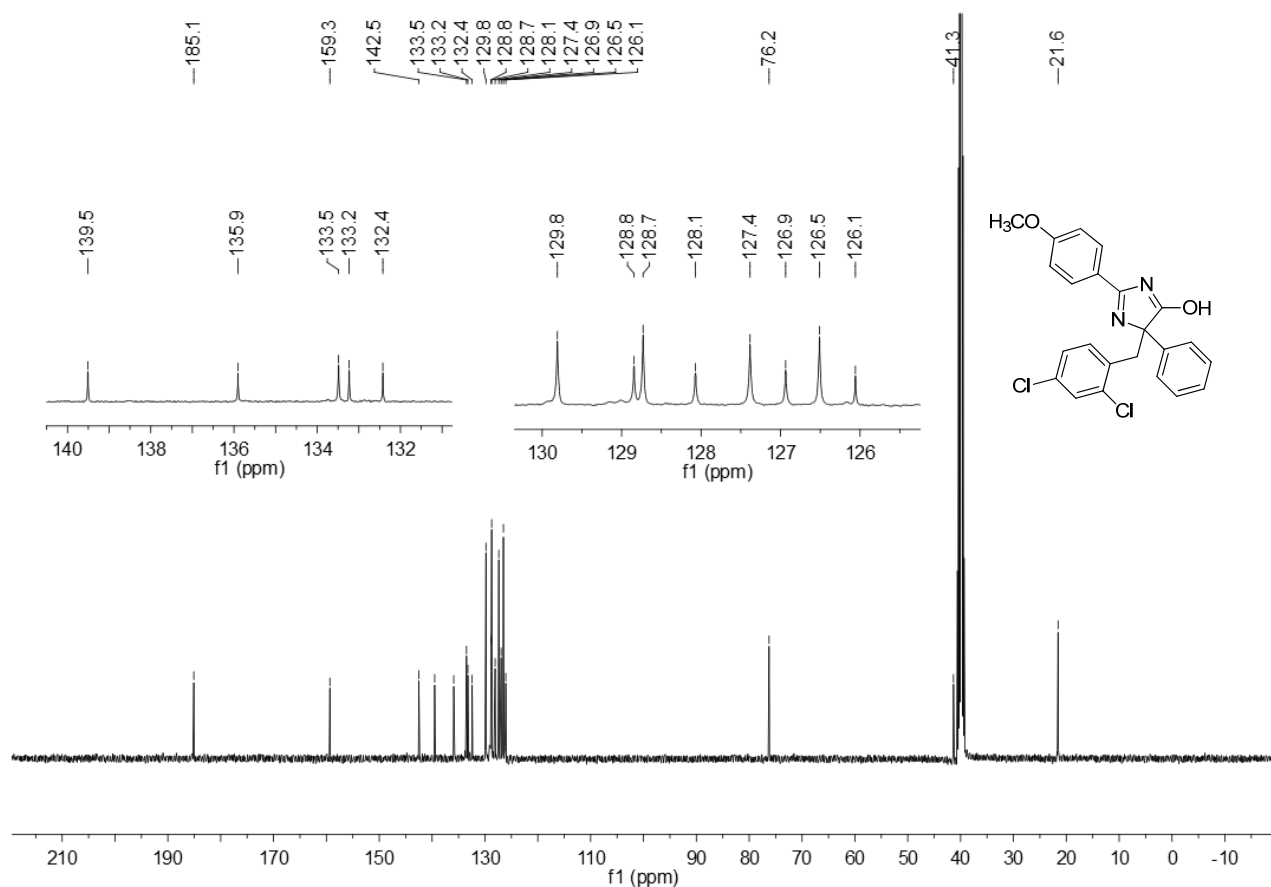
**<sup>1</sup>H NMR Spectrum of Compound 3s**



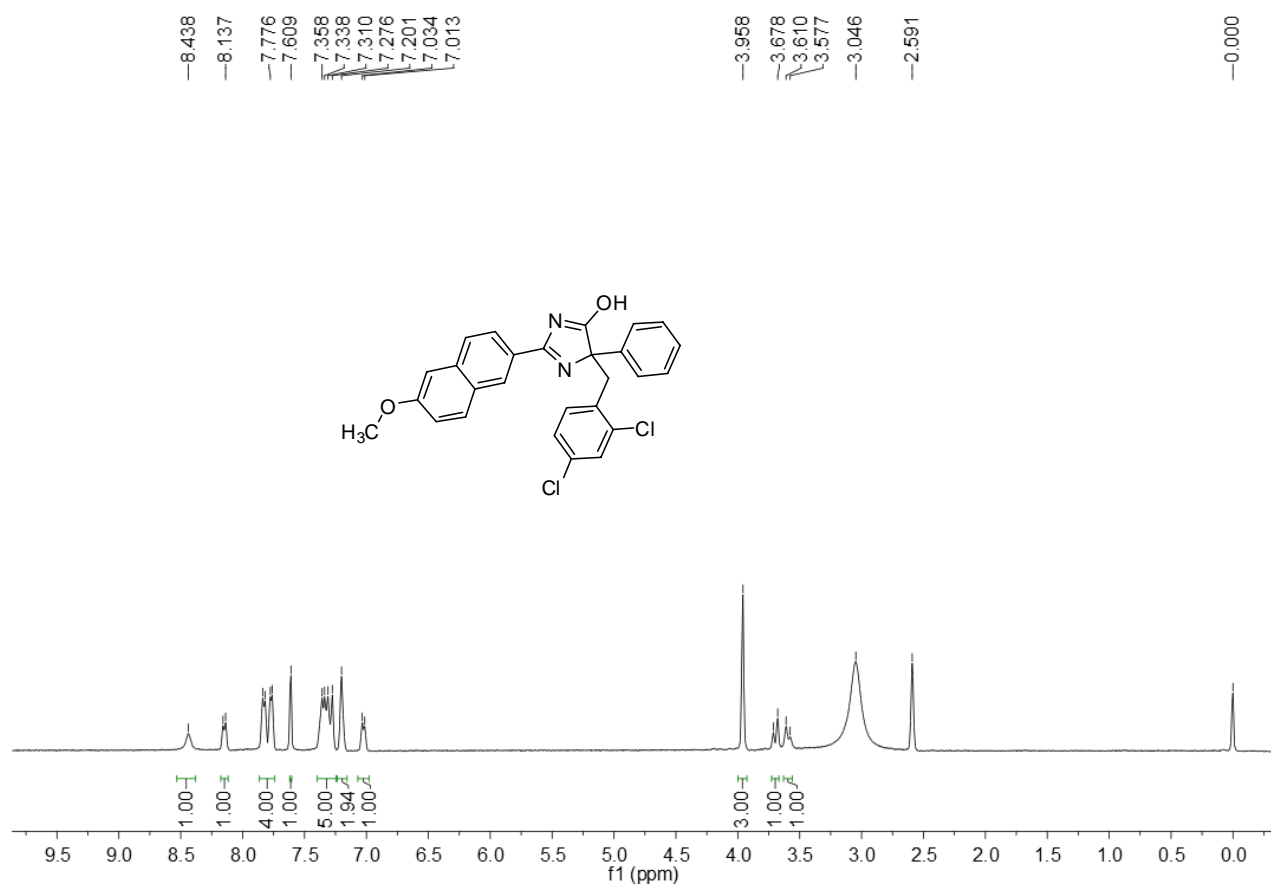
**<sup>13</sup>C NMR Spectrum of Compound 3s**



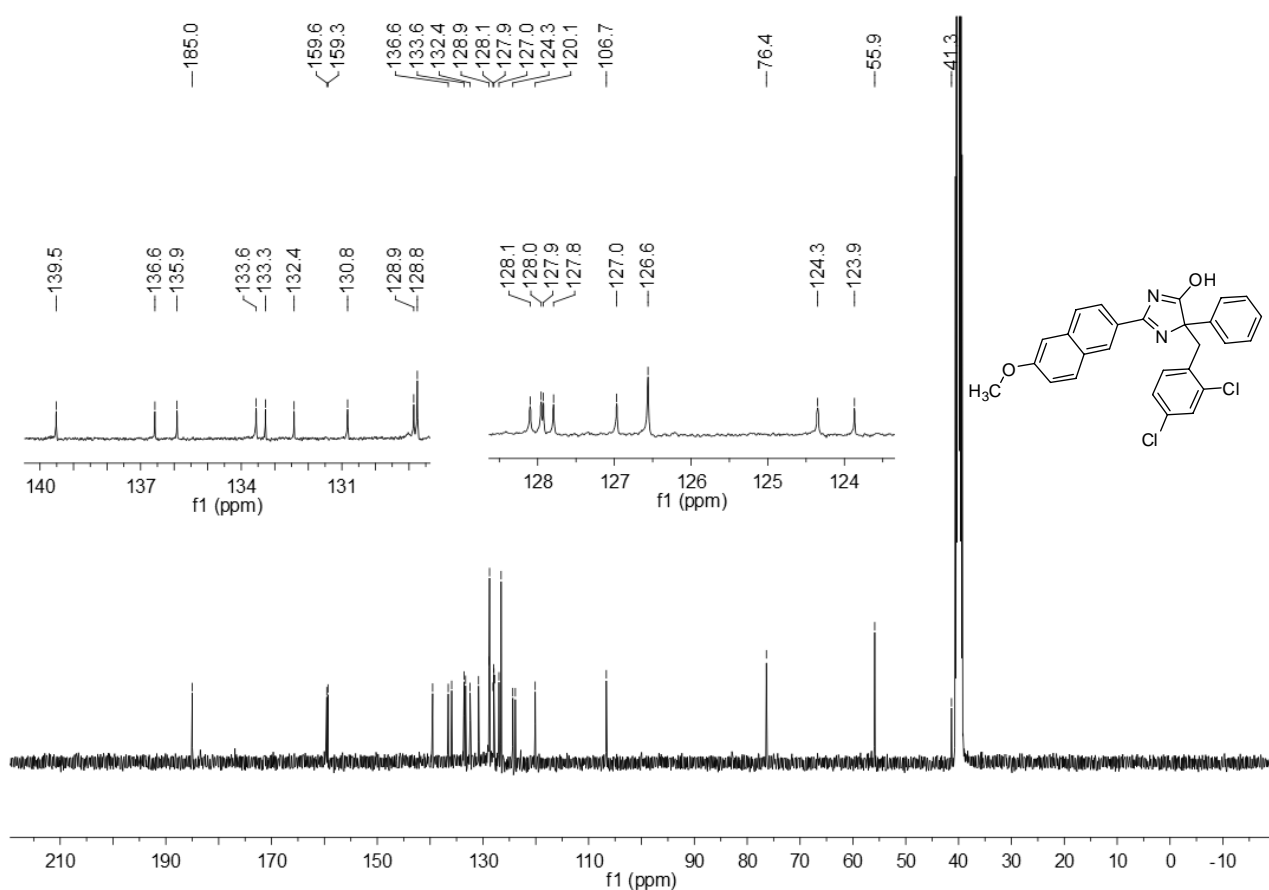
**<sup>1</sup>H NMR Spectrum of Compound 3t**



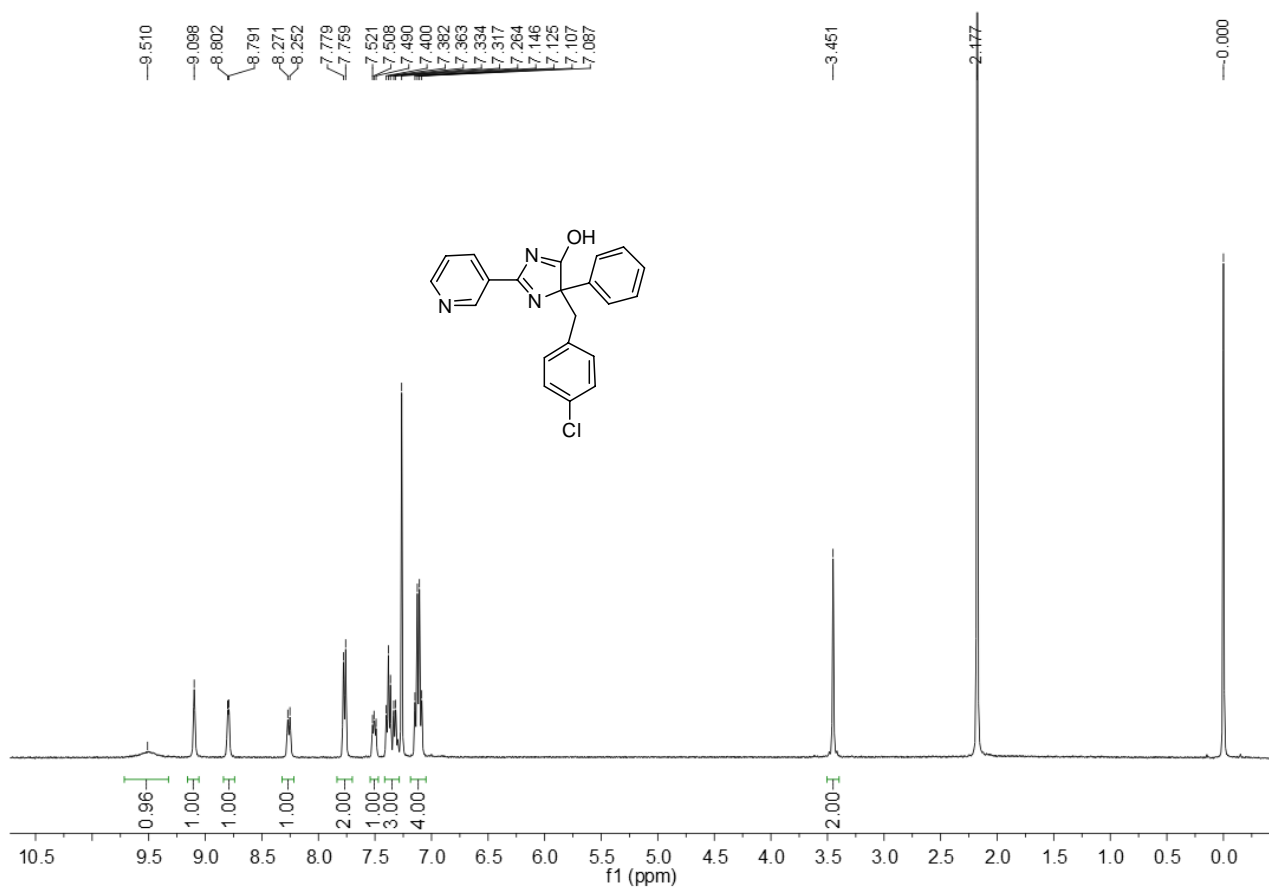
**<sup>13</sup>C NMR Spectrum of Compound 3t**



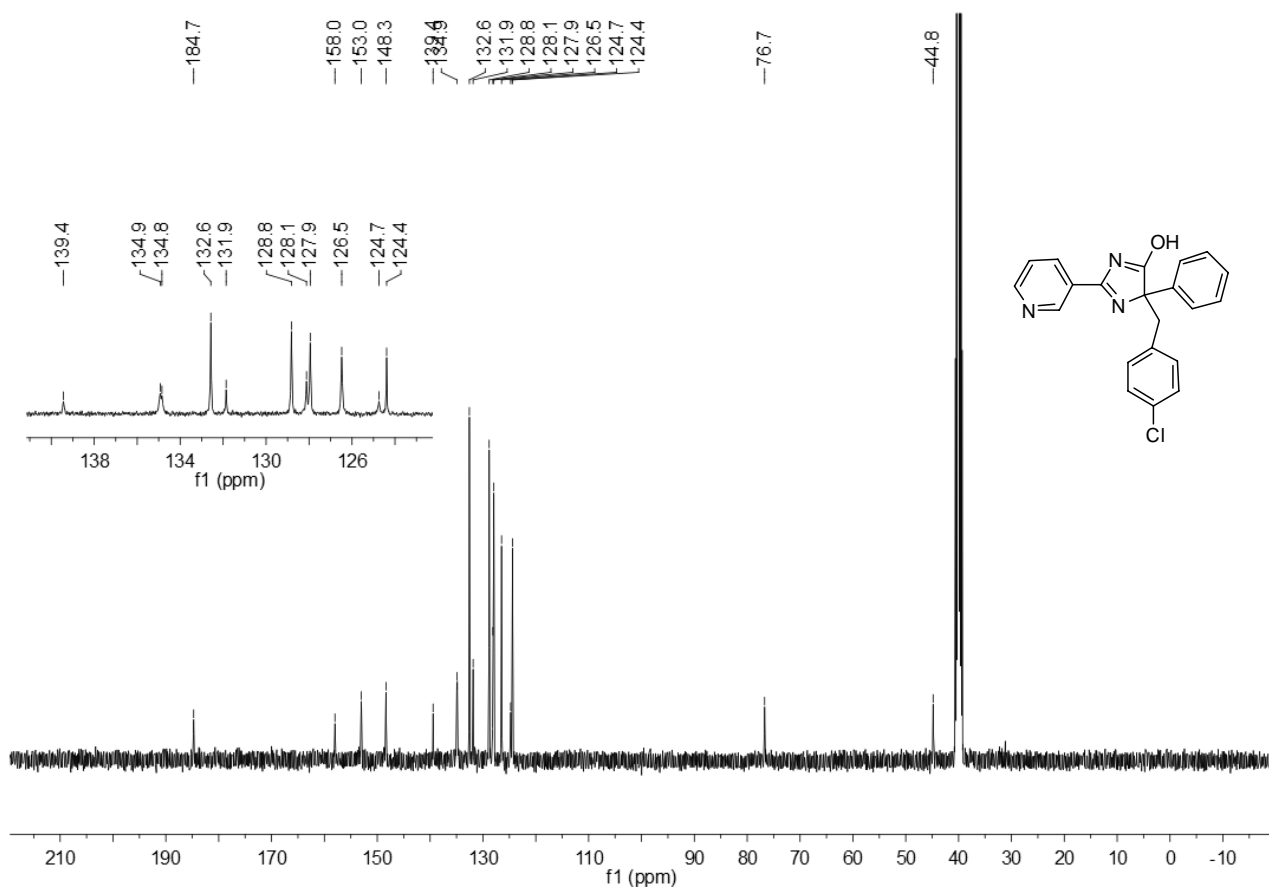
**<sup>1</sup>H NMR Spectrum of Compound 3u**



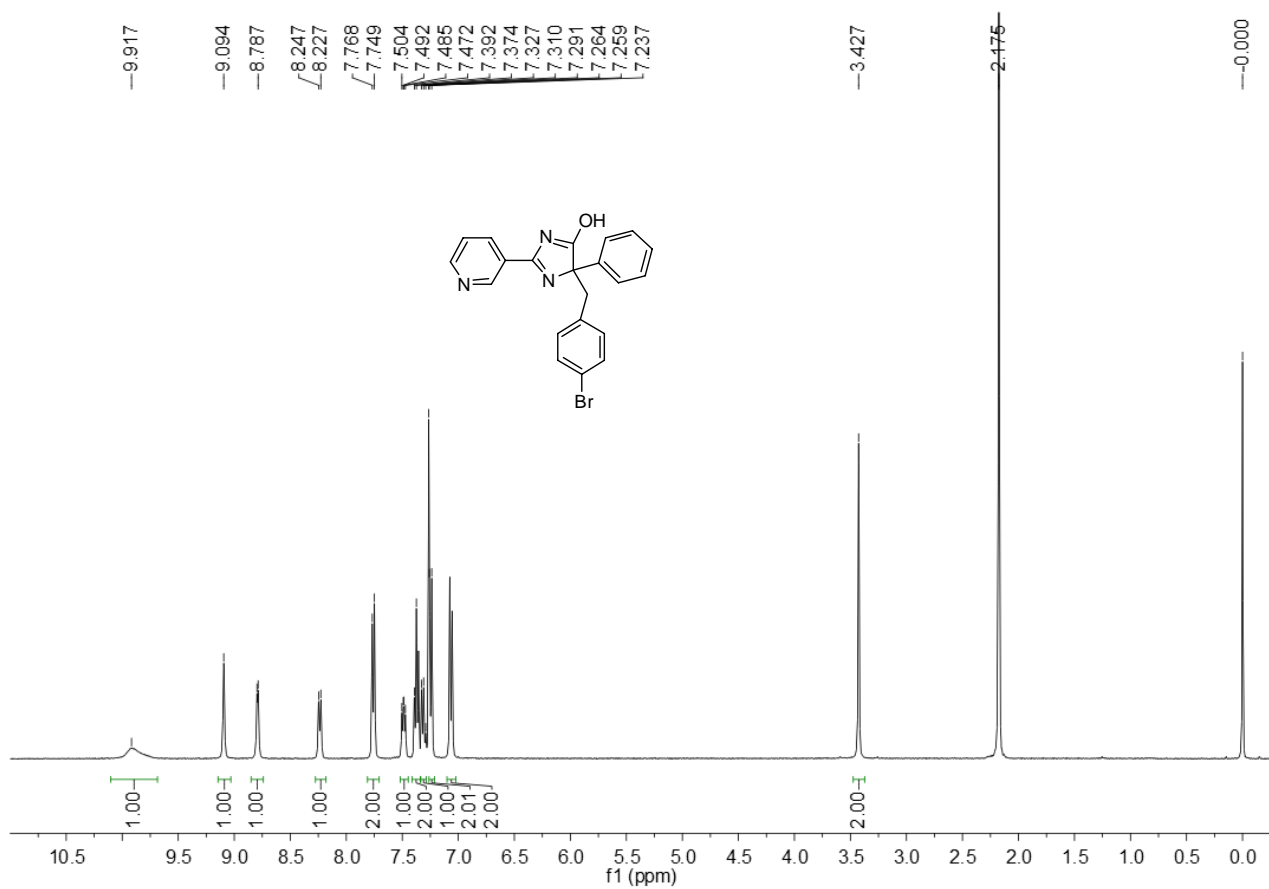
**<sup>13</sup>C NMR Spectrum of Compound 3u**



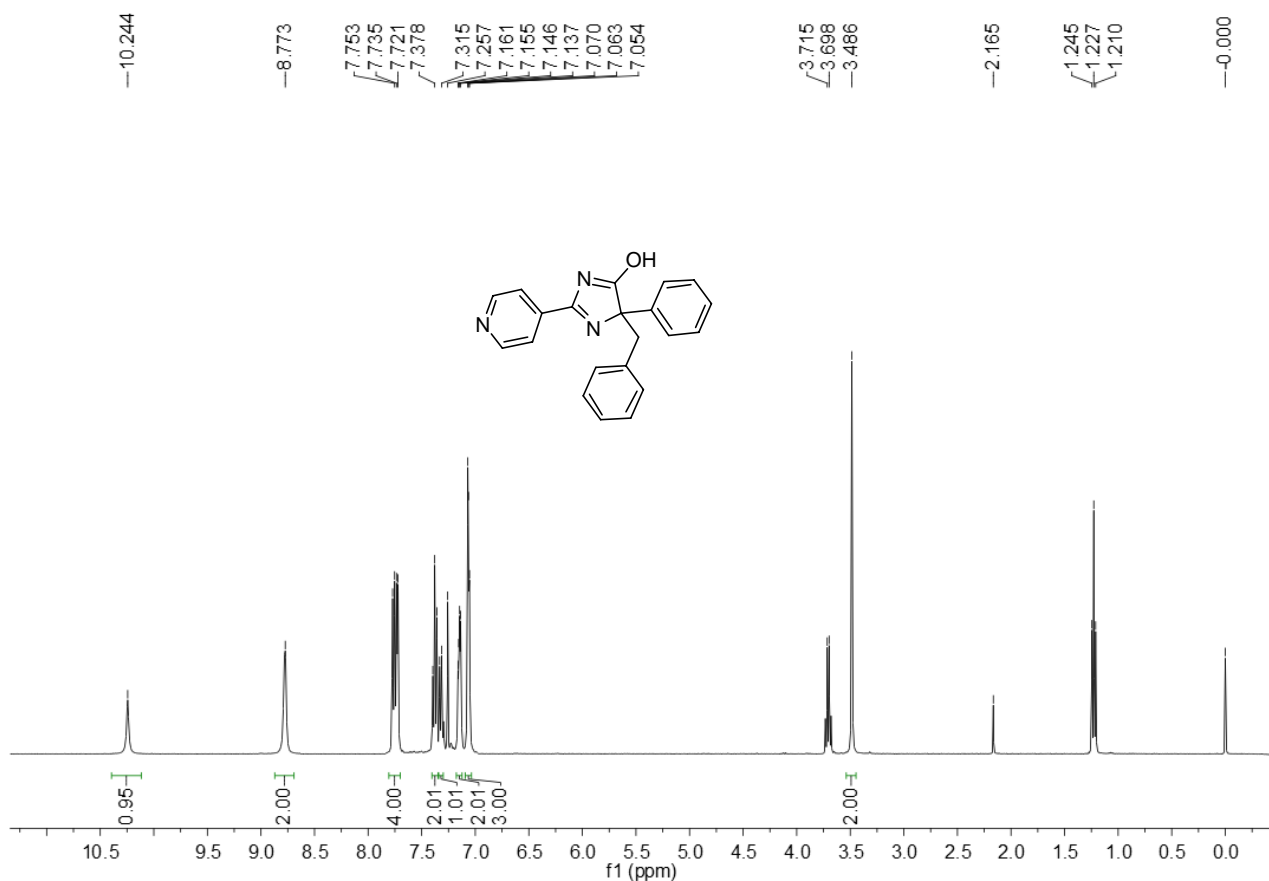
**<sup>1</sup>H NMR Spectrum of Compound 3v**



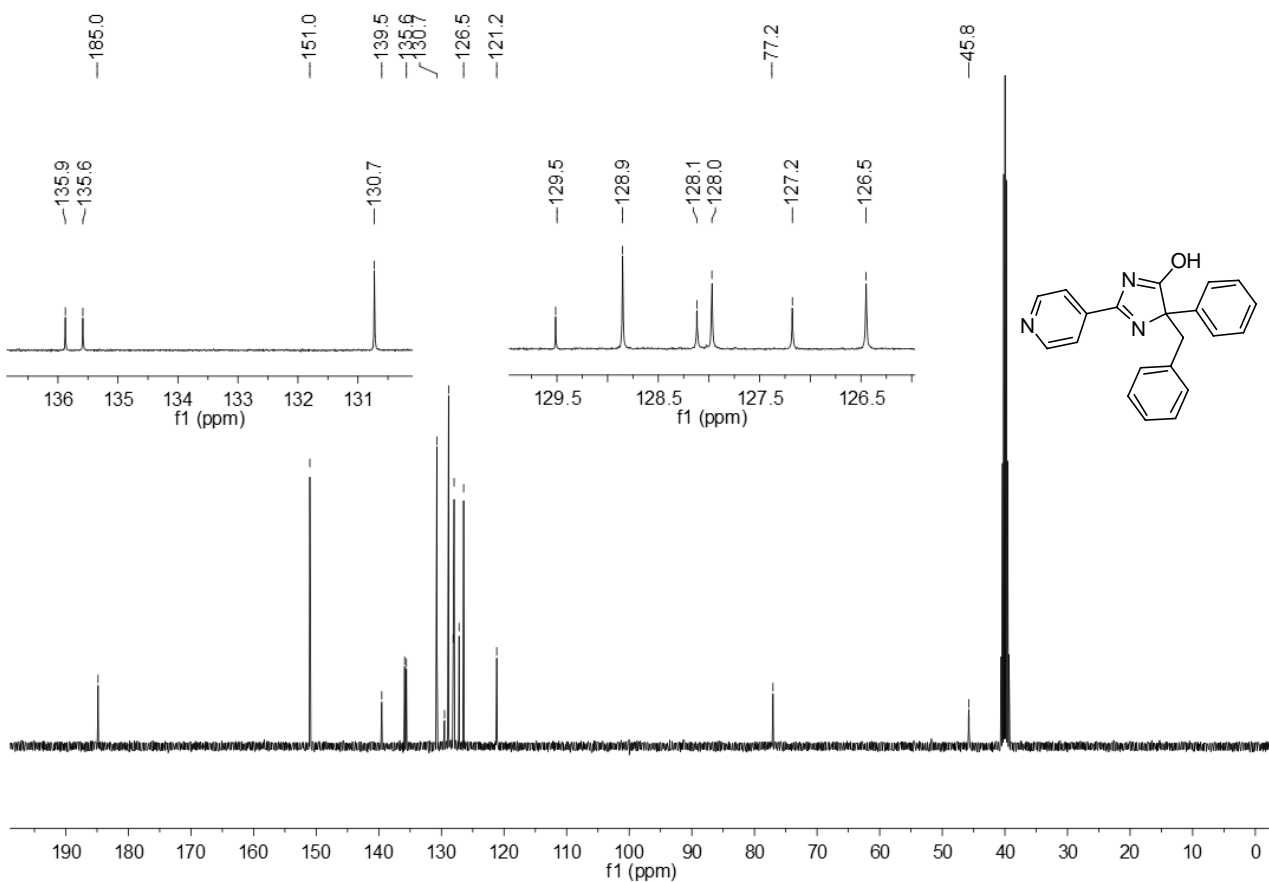
**<sup>13</sup>C NMR Spectrum of Compound 3v**



**<sup>1</sup>H NMR Spectrum of Compound 3w**



**<sup>1</sup>H NMR Spectrum of Compound 3x**



**<sup>13</sup>C NMR Spectrum of Compound 3x**