Supporting Information for

Ru(II)-catalyzed spirocyclization of aryl *N*-sulfonyl ketimines with aryl isocyanates through an aromatic C-H bond activation

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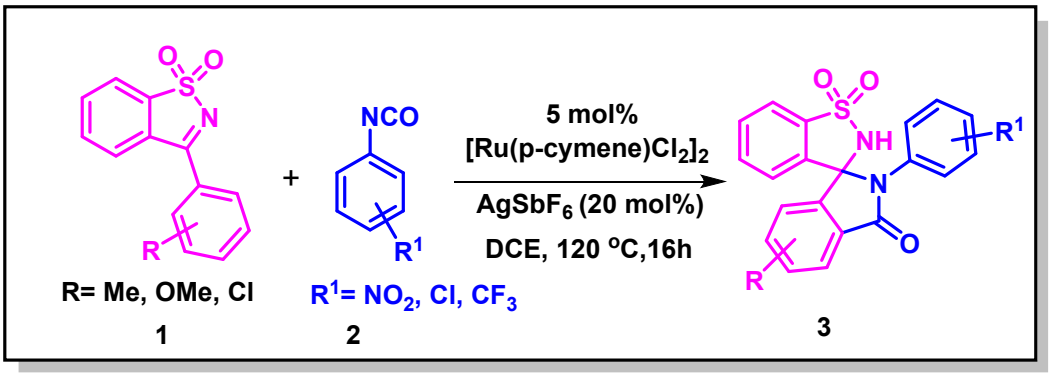

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Experimental section

1. General remarks

^{1}HNMR spectra were recorded at 300, 400 and 500 MHz and ^{13}C NMR at 126, 75 MHz. For 1H NMR, tetramethylsilane (TMS) was used as internal standard (δ = 0) and the values are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t= triplet, q =quartet, m = multiplet), and the coupling constants in Hz. For ^{13}C NMR, $CDCl_3$ (δ = 77.00) was used as internal standard and spectra were obtained with complete proton decoupling. HRMS data were obtained using ESI ionization. Melting points were measured on micro melting point apparatus.

2. Typical procedure for the synthesis of spiroisoindolinone-benzosultams:

To an oven-dried sealed tube charged with 3-phenylbenzo[*d*]isthiazole1,1-dioxide (**1a**) (0.1 mmol%), [Ru(p-cymene)Cl_2]$_2$ (5 mol%), aryl isocyanate (**2a**) (0.1 mmol) was added $AgSbF_6$ (20 mol%) in DCE (2 mL) under N_2 atm at room temperature. The reaction mixture was allowed to stir at 120 ^{o}C for 16h and cooled to room temperature. The reaction mixture was diluted with dichloromethane and concentrated in vacuum. The residue was purified by flash column chromatography (n-hexane/EtOAc = 3:1) to afford the product **3a**.

3. Characterization data for the products (3a-q):

2'-(3,5-Bis(trifluoromethyl)phenyl)-6'-methoxy-2H-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3a): White solid, yield 85%, mp 225-227 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 – 7.81 (m, 3H), 7.64 (s, 1H), 7.63 – 7.57 (m, 2H), 7.56 – 7.52 (m, 1H), 7.10 (d, J = 8.4 Hz, 1H), 7.00 (d, J = 7.5 Hz, 1H), 6.94 (d, J = 8.4 Hz, 1H), 6.02 (s, 1H), 4.00 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.4, 157.4, 147.1, 136.2, 136.1, 135.9, 135.2, 134.3, 132.3, 132.0, 131.7, 127.3, 123.8, 121.8, 121.1, 115.8, 114.4, 113.0, 80.8, 56.0 ppm. HRMS (*m/z*) calcd for $C_{23}H_{15}O_4N_2F_6S$ $[M+H]^+$ 529.0651, found 529.0672.

6'-Methoxy-2'-tosyl-2H-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3b): White solid, yield 88%, mp 265-267 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$+DMSO) δ 9.05 (s, 1H), 8.04 (d, J = 8.2 Hz, 2H), 7.94 (d, J = 7.9 Hz, 1H), 7.76 – 7.64 (m, 3H), 7.34 (d, J = 8.1 Hz, 2H), 7.22 (d, J = 7.2 Hz, 1H), 7.05 (dd, J = 8.5, 2.1 Hz, 1H), 6.70 (s, 1H), 3.77 (s, 3H), 2.43 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$+DMSO) δ 164.7, 163.9, 147.9, 144.32, 136.5, 135.5, 134.9, 133.2, 130.3, 128.6, 128.1, 125.3, 123.0, 120.4, 118.7, 117.1, 106.3, 80.3, 55.3, 20.9 ppm. HRMS (*m/z*) calcd for $C_{22}H_{18}O_6N_2NaS_2$ $[M+Na]^+$ 493.0498, found 493.0514.

6'-Methoxy-2'-(4-nitrophenyl)-2H-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3c): White solid, yield 82%, mp 210-211 °C. ^{1}H NMR (300 MHz, $CDCl_3$+DMSO) δ 9.41 (s, 1H), 8.10 (d, J = 9.1 Hz, 2H), 7.87 (dd, J = 11.2, 8.4 Hz, 2H), 7.64 (dd, J = 11.1, 4.2 Hz, 4H), 7.14 (dd, J = 13.5, 5.0 Hz, 2H), 6.89 (d, J = 1.9 Hz, 1H), 3.83 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.6, 163.7, 147.1, 144.5, 140.7, 135.3, 135.13, 133.3, 130.5, 125.4, 124.8, 123.2, 123.0, 120.5, 116.4, 106.3, 80.3, 55.0 ppm. HRMS (*m/z*) calcd for $C_{21}H_{16}O_6N_3S$ $[M+H]^+$ 438.0754, found 438.0769.

2'-(4-Chlorophenyl)-6'-methoxy-2H-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3d): White solid, yield 80%, mp 200-202 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.81 (dd, J = 6.8, 2.5 Hz, 1H), 7.63 – 7.58 (m, 2H), 7.23 (d, J = 1.7 Hz, 4H), 7.15 – 7.13 (m, 1H), 7.09 (dd, J = 8.5, 2.2 Hz, 1H), 6.88 (d, J = 2.1 Hz, 1H), 5.53 (s, 2H), 3.81 (s, 6H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.0, 164.7, 147.2, 135.9, 135.8, 134.3, 133.6, 132.9, 131.4, 129.3, 128.8, 126.0, 124.3, 122.1, 121.6, 117.7, 106.7, 81.3, 56.0 ppm. HRMS (*m/z*) calcd for $C_{21}H_{15}O_4N_2ClNaS$ $[M+Na]^+$ 449.0333, found 449.0351.

2'-(4-Nitrophenyl)-2*H*-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3e): White solid, yield 78%, mp 275-277 °C. ^{1}H NMR (300 MHz, $CDCl_3$+DMSO) δ 9.40 (s, 0.7H), 8.13 (d, J = 9.1 Hz, 2H), 7.99 (dd, J = 5.6, 2.7 Hz, 1H), 7.87 – 7.82 (m, 1H), 7.68 – 7.57 (m, 6H), 7.48 – 7.44 (m, 1H), 7.18 – 7.12 (m, 1H), 5.37 (s, 0.2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$+DMSO) δ 166.2, 145.1, 144.9, 140.7, 135.8, 135.2, 133.5, 130.8, 130.0, 128.7, 126.2, 123.5, 123.3, 122.3, 120.8, 117.3, 81.1 ppm. HRMS (*m/z*) calcd for $C_{20}H_{14}O_5N_3S$ $[M+H]^+$ 408.0648, found 408.0646.

5'-Methyl-2'-tosyl-2*H*-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3f): White solid, yield 86%, mp 220-222 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 8.4 Hz, 2H), 7.98 (dd, J = 7.0, 1.2 Hz, 1H), 7.87 (d, J = 7.2 Hz, 1H), 7.75 – 7.55 (m, 4H), 7.34 (dd, J = 7.8, 4.3 Hz, 3H), 7.26 – 7.23 (m, 1H), 3.70 (s, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 150.5, 150.3, 146.0, 141.1, 140.6, 138.9, 136.2, 135.3, 134.1, 131.6, 128.9, 128.6, 127.7, 126.2, 122.6, 86.5 ppm. HRMS (*m/z*) calcd for $C_{21}H_{16}O_5N_2NaS_2$ $[M+Na]^+$ 463.0392, found 463.0399.

2'-(4-Chlorophenyl)-2*H*-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3g): White solid, yield 78%, mp 262-264 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (ddd, J = 3.8, 2.3, 0.6 Hz, 1H), 7.83 – 7.80 (m, 1H), 7.65 – 7.58 (m, 4H), 7.46 – 7.44 (m, 1H), 7.28 – 7.23 (m, 4H), 7.13 – 7.11 (m, 1H), 5.30 (s, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7, 144.8, 135.9, 135.8, 134.2, 134.1, 133.9, 132.6, 131.4, 131.0, 130.0, 129.4, 128.9, 124.5,

124.3, 122.5, 121.7, 81.7 ppm. HRMS (*m/z*) calcd for $C_{20}H_{14}O_3N_2ClS[M+H]^+$ 397.0408, found 397.0400.

5'-Chloro-2'-tosyl-2*H*-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3h): White solid, yield 75%, mp 280-282 °C. ^{1}H NMR (300 MHz, $CDCl_3$+DMSO) δ 9.14 (s, 1H), 8.04 (d, J = 8.3 Hz, 2H), 7.95 (d, J = 7.4 Hz, 1H), 7.78 – 7.64 (m, 2H), 7.61 – 7.58 (m, 1H), 7.35 (d, J = 8.2 Hz, 2H), 7.24 (t, J = 7.1 Hz, 2H), 2.44 (s, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.6, 145.2, 144.0, 136.7, 136.4, 135.7, 135.6, 135.1, 133.8, 131.1, 129.2, 128.8, 124.5, 124.0, 123.5, 121.1, 21.5 ppm. HRMS (*m/z*) calcd for $C_{21}H_{15}O_5N_2ClNaS_2[M+Na]^+$ 497.0003, found 497.0020.

2'-(4-Chlorophenyl)-5'-methoxy-2H-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3i): White solid, yield 82%, mp 190-191 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (dd, J = 6.0, 2.8 Hz, 1H), 7.60 – 7.58 (m, 2H), 7.41 (d, J = 2.4 Hz, 1H), 7.31 (d, J = 8.4 Hz, 1H), 7.24 (d, J = 7.2 Hz, 4H), 7.15 – 7.10 (m, 2H), 5.53 (s, 1H), 3.90 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$+DMSO) δ 166.1, 160.9, 136.7, 135. 7, 133.0, 132.7, 132.5, 131.0, 130.4, 128.8, 128.3, 123.3, 120.4, 106.2, 80.8, 55.2 ppm. HRMS (*m/z*) calcd for $C_{21}H_{15}O_4N_2ClNaS$ $[M+Na]^+$ 449.0333, found 449.0351.

5'-Methoxy-2'-(4-nitrophenyl)-2H-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3j): White solid, yield 84%, mp 210-211 °C. ^{1}H NMR (300 MHz, $CDCl_3$+DMSO) δ 9.17 (s, 1H), 8.12 (d, J = 9.1 Hz, 2H), 7.83 (dd, J = 6.4, 2.1 Hz, 1H), 7.66 – 7.57 (m, 4H), 7.44 (d, J = 2.3 Hz, 1H), 7.34 (d, J = 8.5 Hz, 1H), 7.15 (ddd, J = 8.3, 7.3, 2.0 Hz, 2H), 3.92 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7, 161.59, 145.6, 141.2, 137.3, 136.2, 136.1, 133.9, 131.2, 130.8, 126.6, 124.0, 123.9, 123.7, 121.7, 121.3, 106.8, 81.4, 55.8 ppm. HRMS (*m/z*) calcd for $C_{21}H_{16}O_6N_3S$ $[M+H]^+$ 438.07543, found 438.0769.

2'-(3,5-Bis(trifluoromethyl)phenyl)-5'-methoxy-2H-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3k): White solid, yield 86%, mp 230-232 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.78 (m, 3H), 7.70 (s, 1H), 7.64 – 7.60 (m, 2H), 7.41 (s, 1H), 7.33 (d, J = 8.5 Hz, 1H), 7.16 (d, J = 8.5 Hz, 1H), 7.13 – 7.09 (m, 1H), 5.85 (s, 1H), 3.90 (s, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.60 162.2, 136.3, 136.1, 136.0, 135.6, 134.5, 132.5, 132.2, 131.7, 131.0, 127.1, 123.9, 123.8, 123.7, 122.4, 121.8, 121.6, 121.3, 107.5, 81.6, 56.0 ppm. HRMS (*m/z*) calcd for $C_{23}H_{15}O_4N_2F_6S$ $[M+H]^+$ 529.0651, found 529.0672.

2'-(4-Chlorophenyl)-5'-methyl-2H-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3l): White solid, yield 80%, mp 190-192 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 – 7.78 (m, 1H), 7.72 (s, 1H), 7.61 – 7.56 (m, 2H), 7.42 (d, J = 7.9 Hz, 1H), 7.31 (d, J = 7.8 Hz, 1H), 7.24 – 7.20 (m, 4H), 7.11 – 7.08 (m, 1H), 5.69 (s, 1H), 2.47 (s, 3H) ppm. ^{13}C NMR (126

MHz, $CDCl_3$) δ 167.0, 142.1, 141.5, 136.0, 135.9, 134.9, 134.2, 133.8, 132.7, 131.3, 130.1, 129.3, 128.9, 124.6, 124.2, 122.3, 121.6, 81.7, 21.5 ppm. HRMS (*m/z*) calcd for $C_{21}H_{16}O_3N_2ClS$ $[M+H]^+$ 411.0564, found 411.0581.

5'-Methyl-2'-tosyl-2H-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3m): White solid, yield 88%, mp 120-122 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 8.3 Hz, 2H), 7.96 (d, J = 7.4 Hz, 1H), 7.68 (m, 3H), 7.42 (d, J = 7.9 Hz, 1H), 7.32 (d, J = 8.2 Hz, 2H), 7.22 (dd, J = 11.9, 7.6 Hz, 2H), 5.19 (s, 1H), 2.42 (d, J = 2.8 Hz, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.9, 145.5, 142.8, 142.0, 137.2, 136.7, 135.9, 134.93, 134.5, 131.2, 129.7, 129.5, 129.0, 127.6, 126.4, 124.9, 123.9, 122.5, 121.5, 81.3, 77.3, 77.0, 76.7, 21.7, 21.4 ppm. HRMS (*m/z*) calcd for $C_{22}H_{18}O_5N_2NaS_2$ $[M+Na]^+$ 477.0549, found 477.0563.

3'-Oxo-N,2-ditosyl-1,1'-spirobi[isoindoline]-7-carboxamide (3n): White solid, yield 88%, mp 140-141 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 11.28 (s, 1H), 8.07 (d, J = 7.5 Hz, 1H), 7.88 – 7.82 (m, 3H), 7.66 (d, J = 7.5 Hz, 1H), 7.63 – 7.57 (m, 3H), 7.53 – 7.46 (m, 2H), 7.24 (s, 1H), 7.13 (d, J = 8.1 Hz, 2H), 6.97 (d, J = 7.6 Hz, 1H), 6.88 – 6.85 (m, 1H), 5.29 (s, 1H), 2.39 (d, J = 10.6 Hz, 6H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.0, 165.0, 145.5, 144.8, 143.3, 143.0, 135.7, 135.0, 134.9, 131.2, 130.6, 129.6, 129.4, 129.0, 128.7, 128.5, 128.2, 125.6, 125.2, 122.6, 121.0, 82.7, 21.7, 21.7 ppm. HRMS (*m/z*) calcd for $C_{30}H_{24}O_7N_3S_2$ $[M+H]^+$ 602.1050, found 602.1062.

5'-Methyl-2'-(4-nitrophenyl)-2*H*-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3o): White solid, yield 80%, mp 230-232 °C. ^1H NMR (300 MHz, $CDCl_3$+DMSO) δ 8.11 (d, J = 9.0 Hz, 2H), 7.83 (d, J = 6.8 Hz, 1H), 7.78 (s, 1H), 7.62 (dd, J = 11.0, 7.8 Hz, 4H), 7.47 (d, J = 7.8 Hz, 1H), 7.33 (d, J = 7.8 Hz, 1H), 7.13 (d, J = 7.3 Hz, 1H), 2.51 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCL_3$+DMSO) δ 171.7, 150.4, 147.6, 146.2, 145.8, 141.1, 140.9, 139.8, 138.8, 136.1, 134.2, 131.5, 128.9, 128.6, 127.4, 126.1, 86.4, 26.2 ppm. HRMS (*m/z*) calcd for $C_{21}H_{16}O_5N_3S$ $[M+H]^+$ 422.0805, found 422.0808.

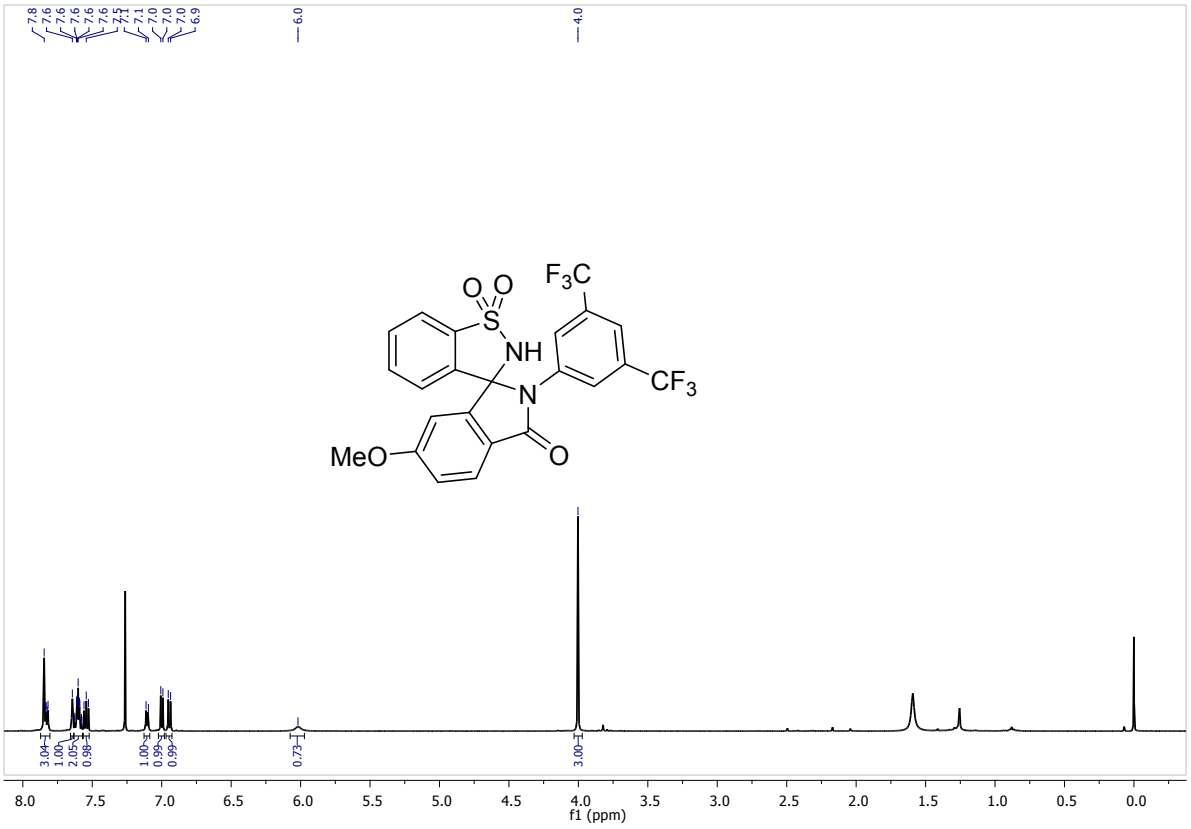
6'-Methyl-2'-tosyl-2*H*-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3p): White solid, yield 85%, mp 125-127 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.4 Hz, 2H), 7.97 (d, J = 8.2 Hz, 1H), 7.75 – 7.65 (m, 3H), 7.34 (dd, J = 15.8, 8.0 Hz, 3H), 7.24 (d, J = 6.0 Hz, 1H), 7.10 (s, 1H), 5.19 (s, 1H), 2.42 (s, 3H), 2.37 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.6, 147.5, 145.8, 145.4, 137.2, 136.0, 134.9, 134.5, 132.3, 131.2, 129.5, 129.0, 124.9, 124.8, 123.9, 122.9, 121.6, 81.2, 22.1, 21.7 ppm. HRMS (*m/z*) calcd for $C_{22}H_{18}O_5N_2NaS_2$ $[M+Na]^+$ 477.0549, found 477.0563.

5'-Methoxy-2'-tosyl-2*H*-spiro[benzo[d]isothiazole-3,1'-isoindolin]-3'-one-1,1-dioxide (3q): White solid, yield 90%, mp 140-141 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.4

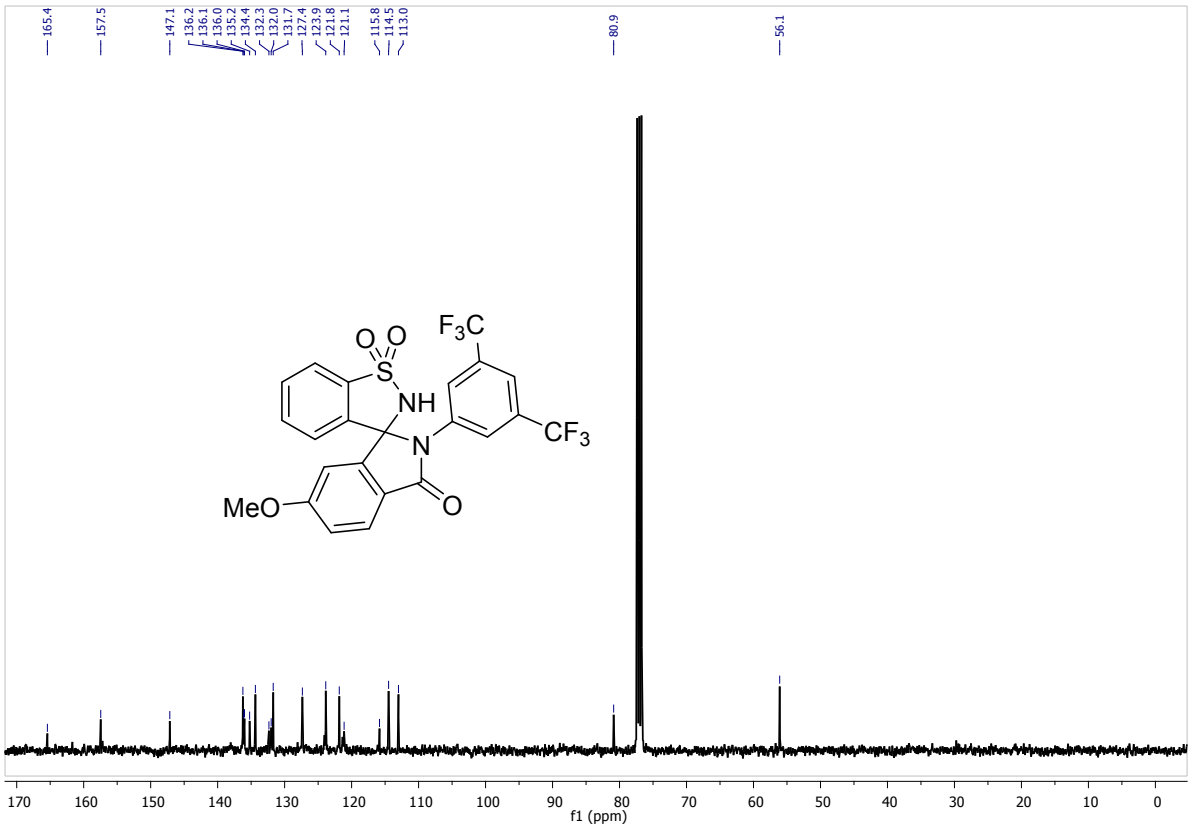
Hz, 2H), 7.93 (d, J = 7.8 Hz, 1H), 7.72 – 7.63 (m, 2H), 7.31 (d, J = 8.1 Hz, 2H), 7.26 – 7.18 (m, 3H), 7.11 (dd, J = 8.6, 2.4 Hz, 1H), 3.82 (s, 3H), 2.40 (s, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.1, 161.9, 145.4, 137.0, 135.9, 135.0, 134.4, 131.2, 129.5, 129.3, 128.9, 124.1, 123.8, 123.5, 121.5, 107.4, 56.0, 21.7 ppm. HRMS (*m/z*) calcd for $C_{22}H_{18}O_6N_2NaS_2$ $[M+Na]^+$ 493.0498, found 493.0514.

2. NMR spectra of products (3a-q)

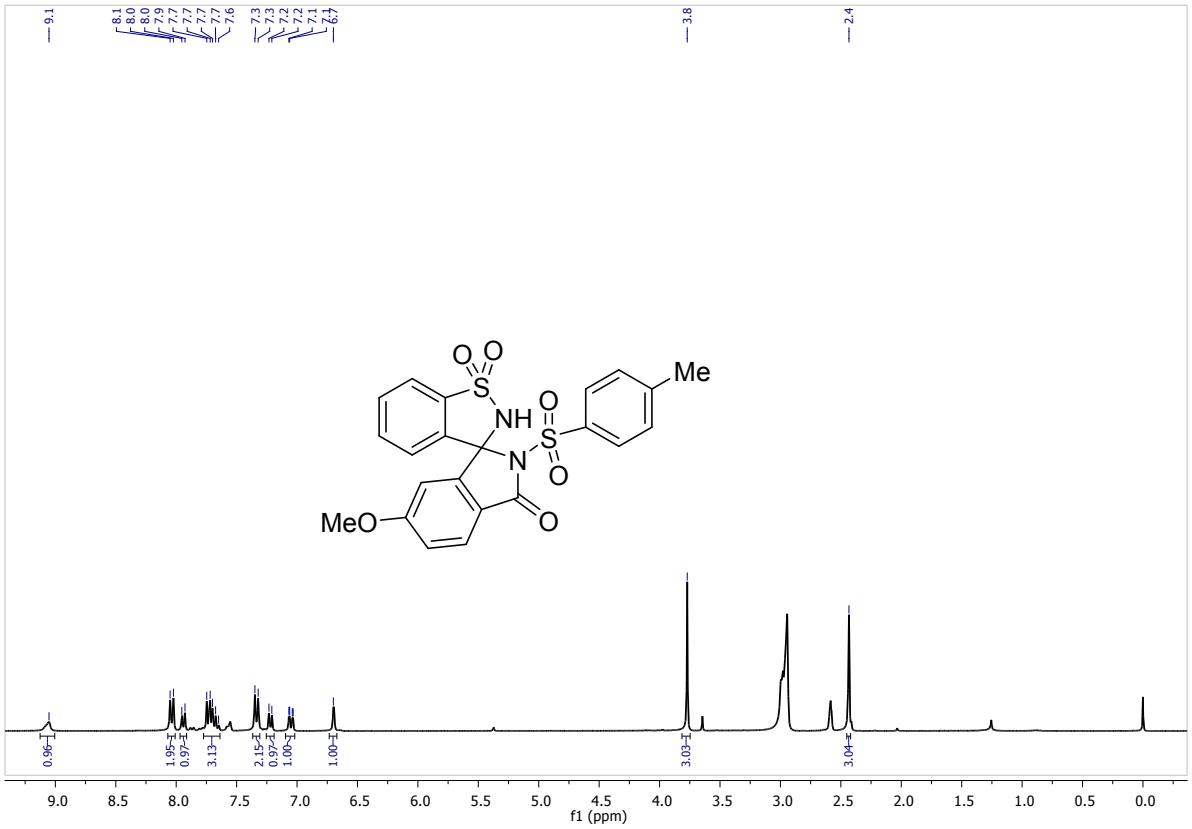
^{1}H NMR (500 MHz,$CDCl_3$) spectrum of compound (3a)



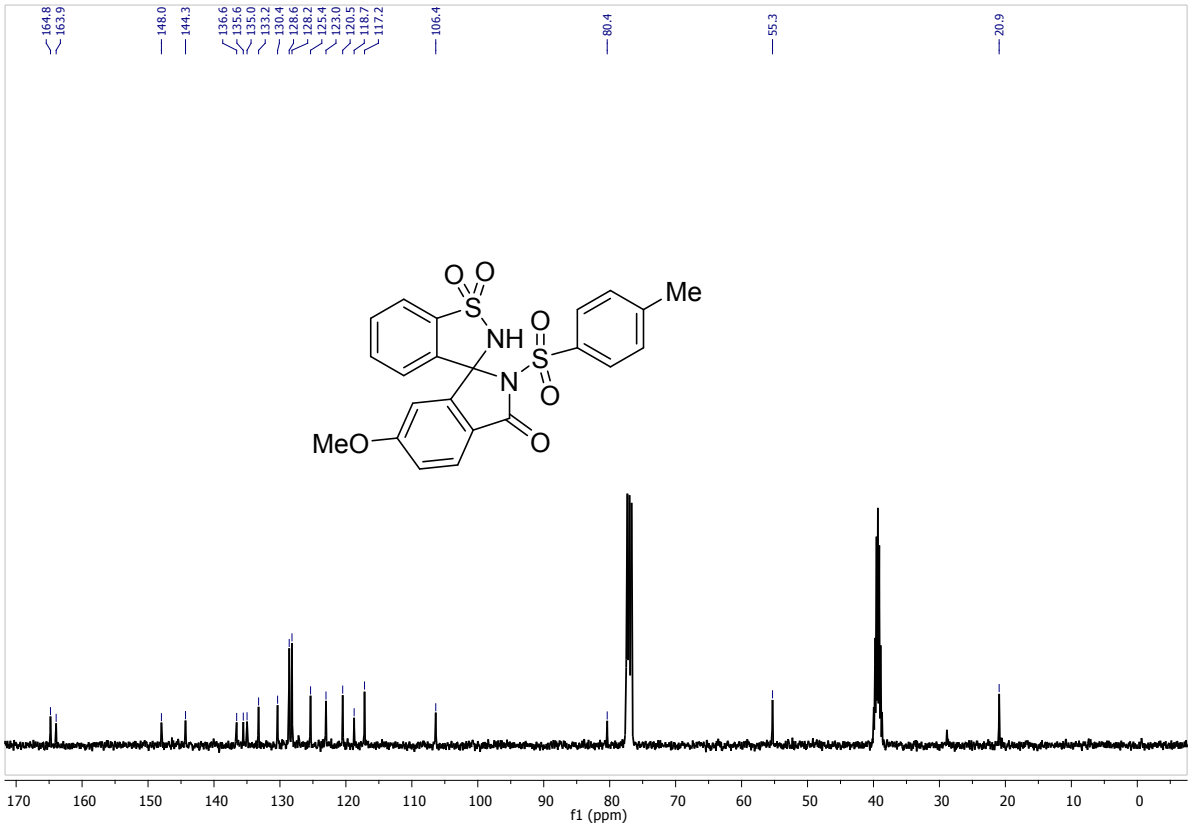
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound (3a)



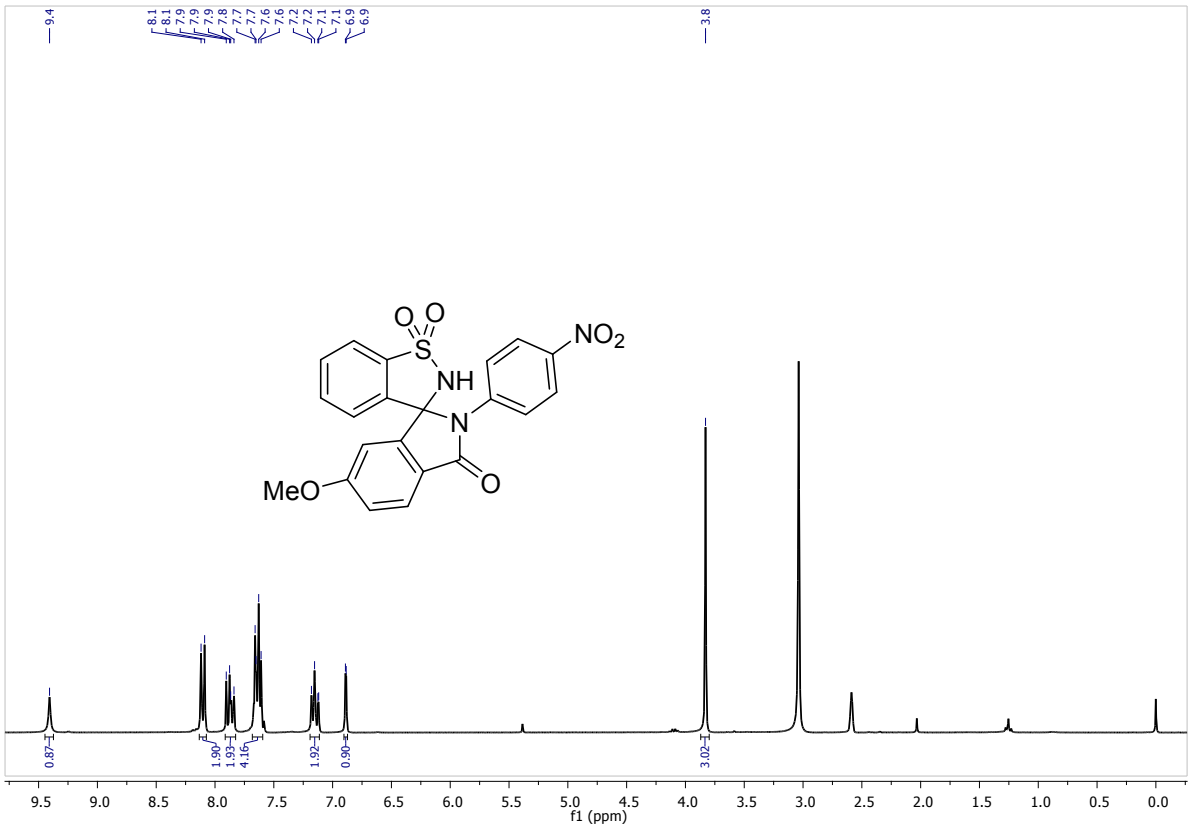
^{1}H NMR (300 MHz,$CDCl_3$ + DMSO) spectrum of compound (3b)



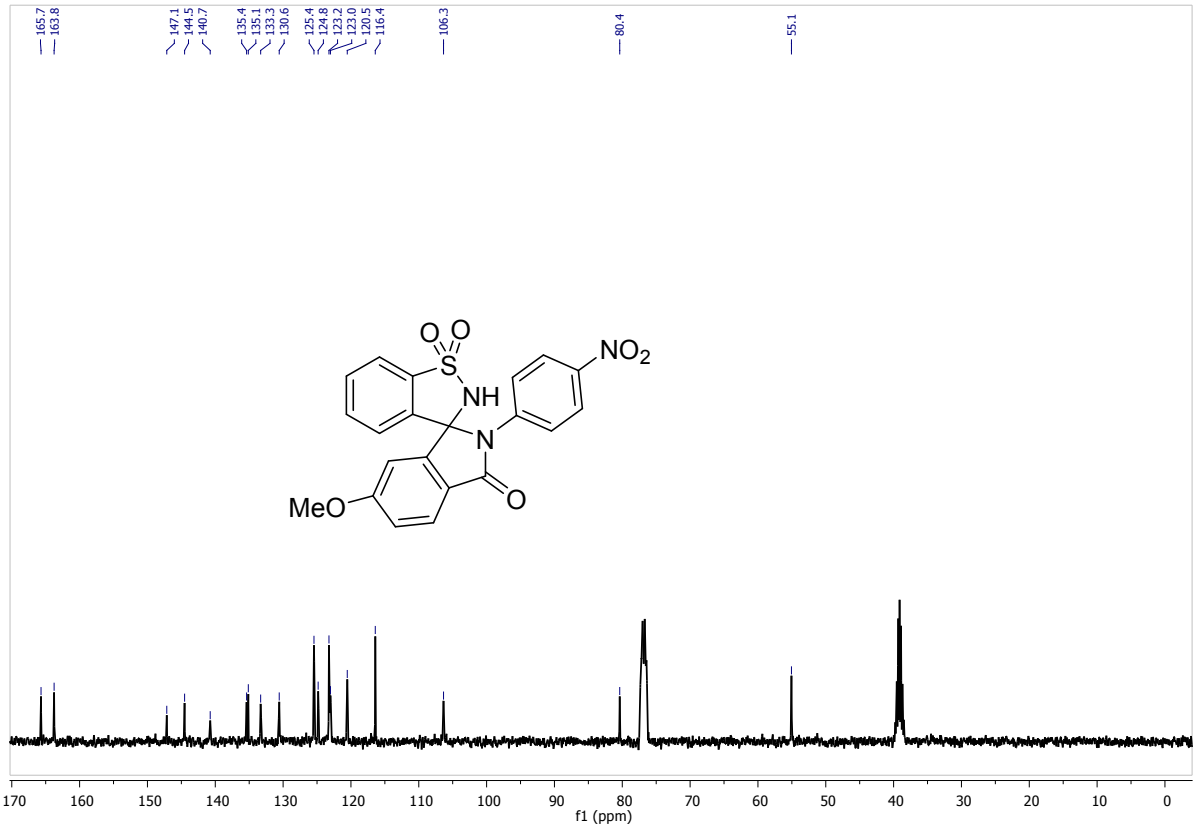
^{13}C NMR (101 MHz, $CDCl_3$+DMSO) spectrum of compound (3b)



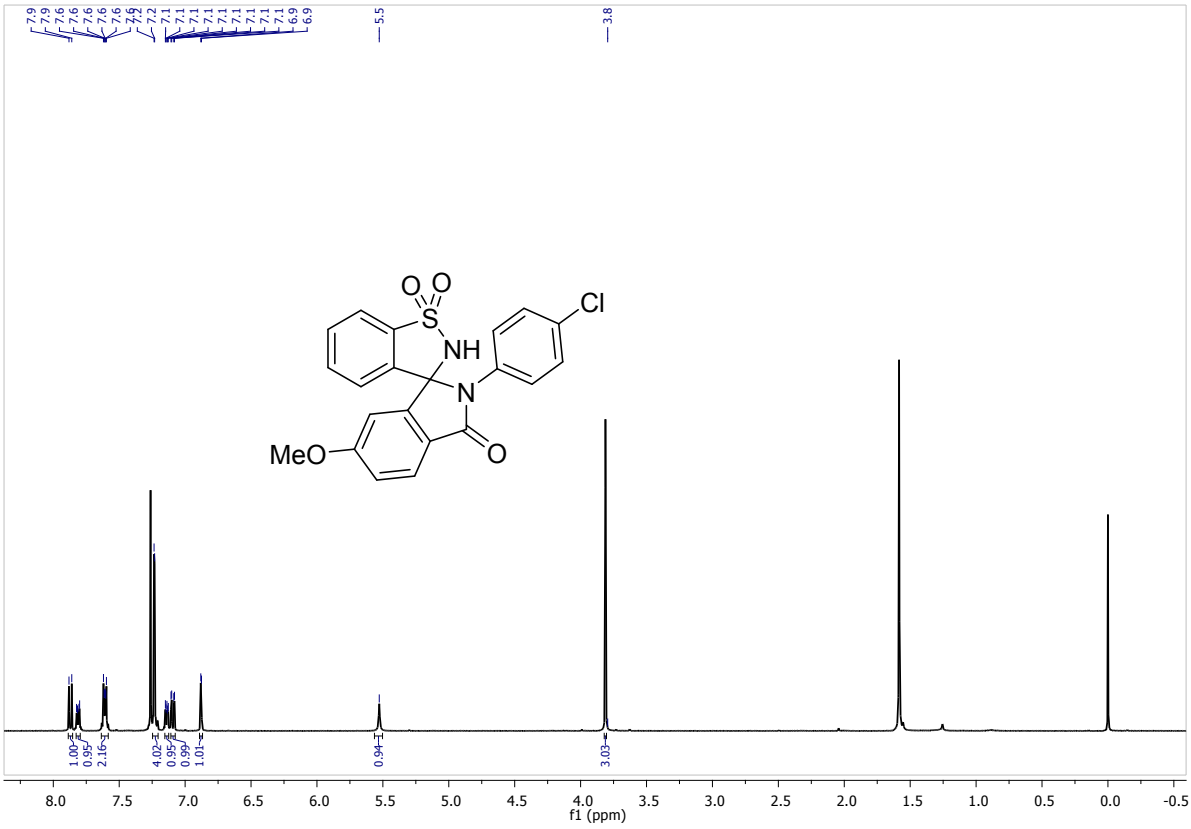
^{1}H NMR (300 MHz,$CDCl_3$ + DMSO) spectrum of compound (3c)



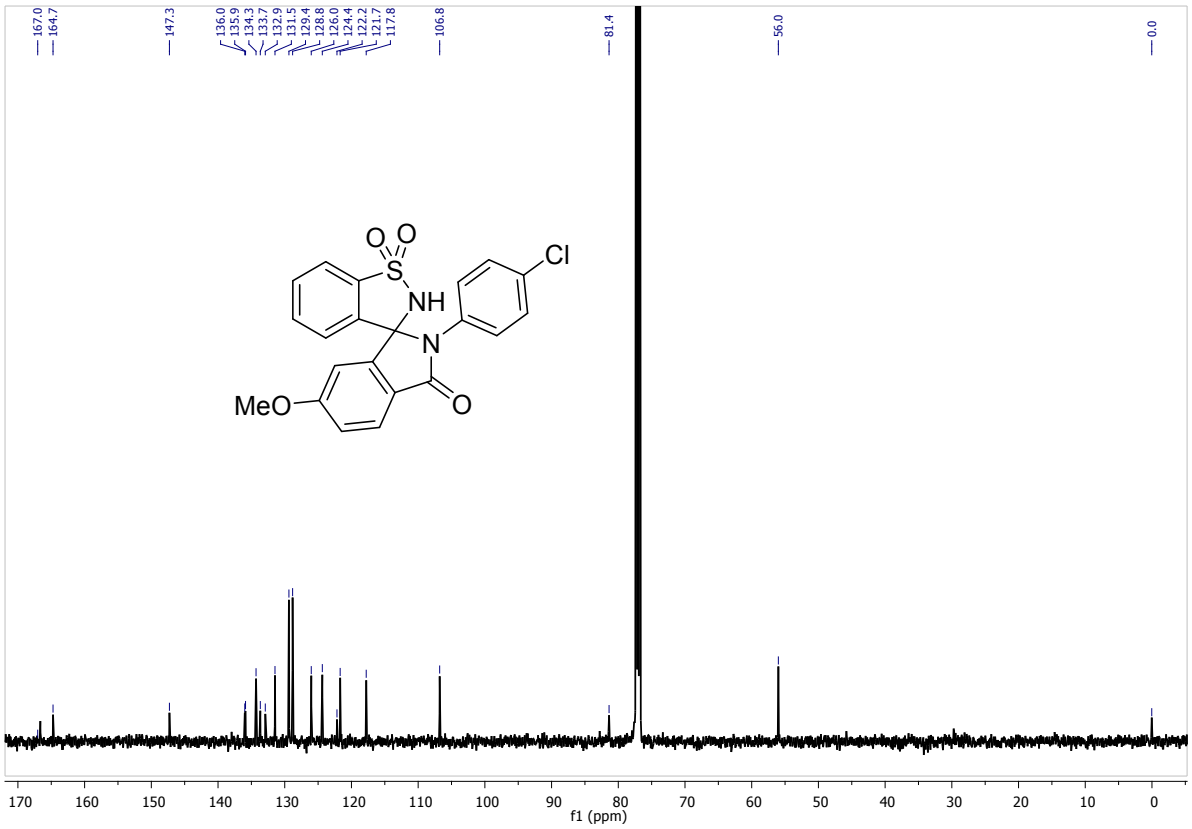
^{13}C NMR (101 MHz, $CDCl_3$ + DMSO) spectrum of compound (3c)



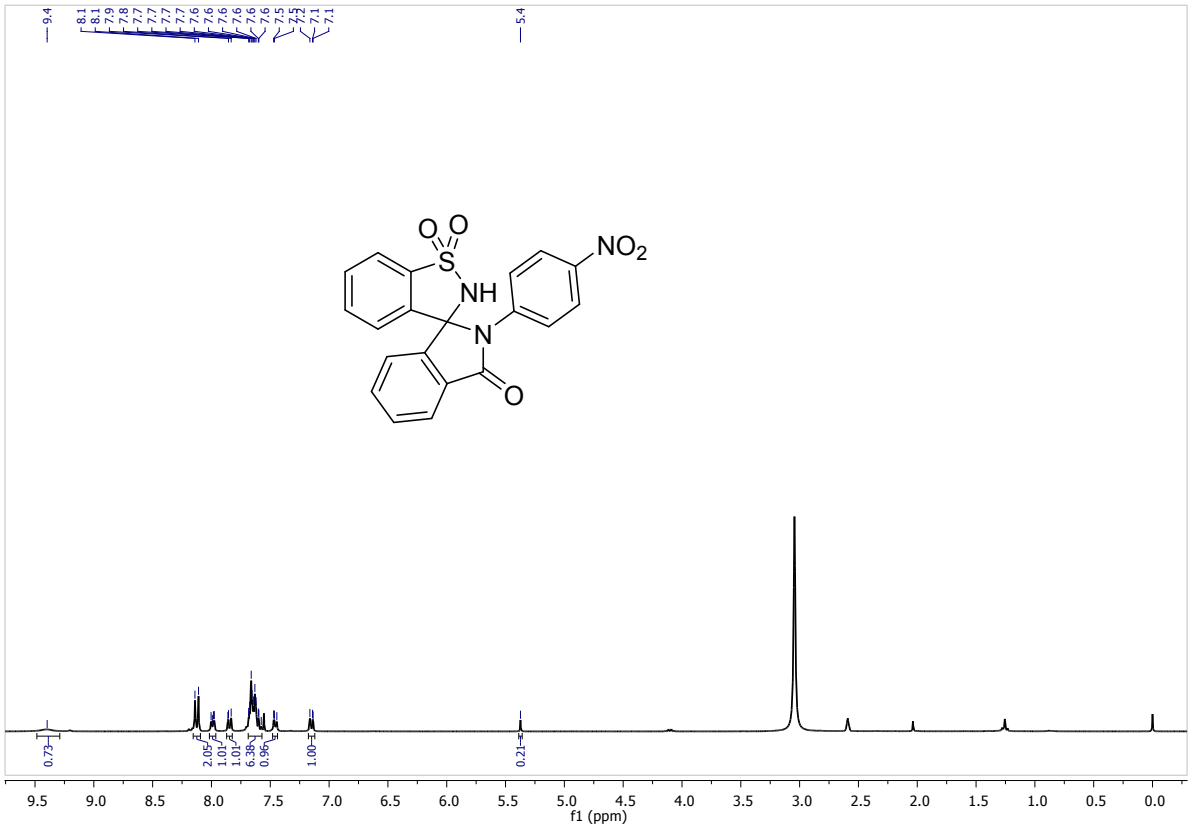
^{1}H NMR (400 MHz,$CDCl_3$) spectrum of compound (3d)



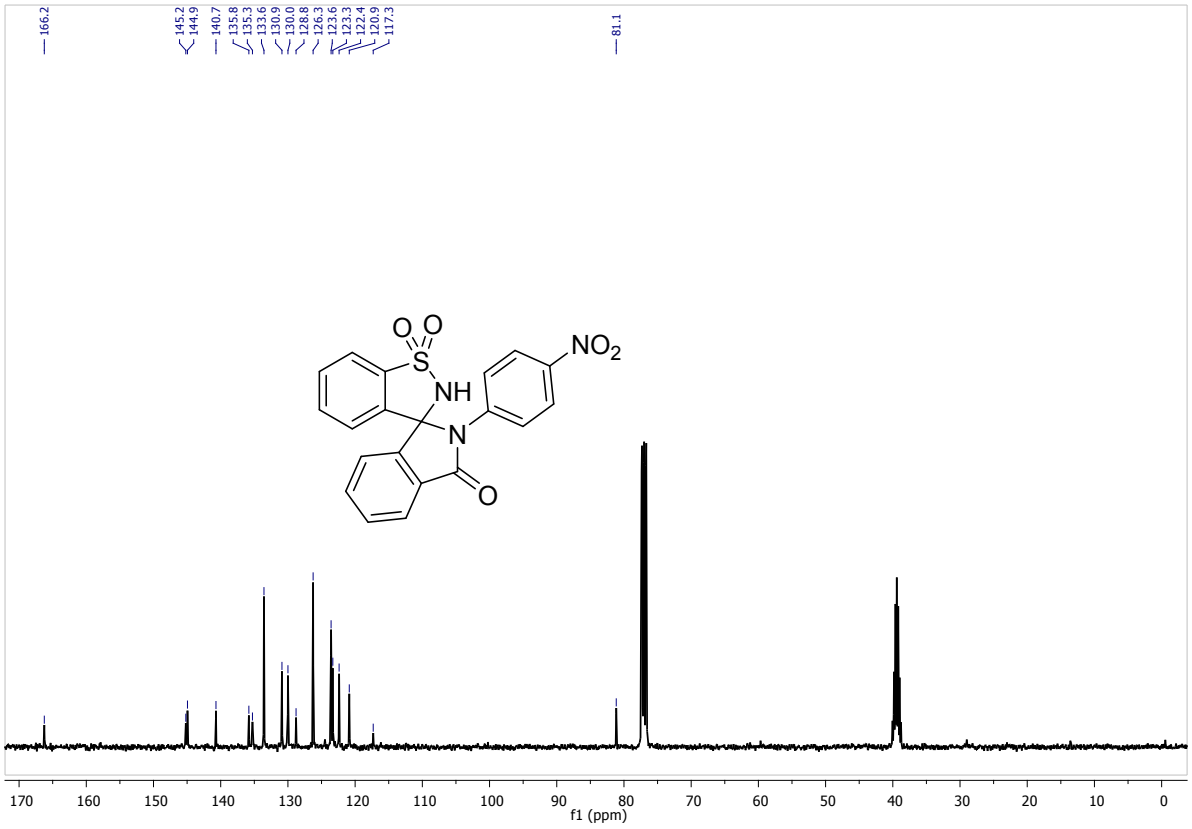
^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound (3d)



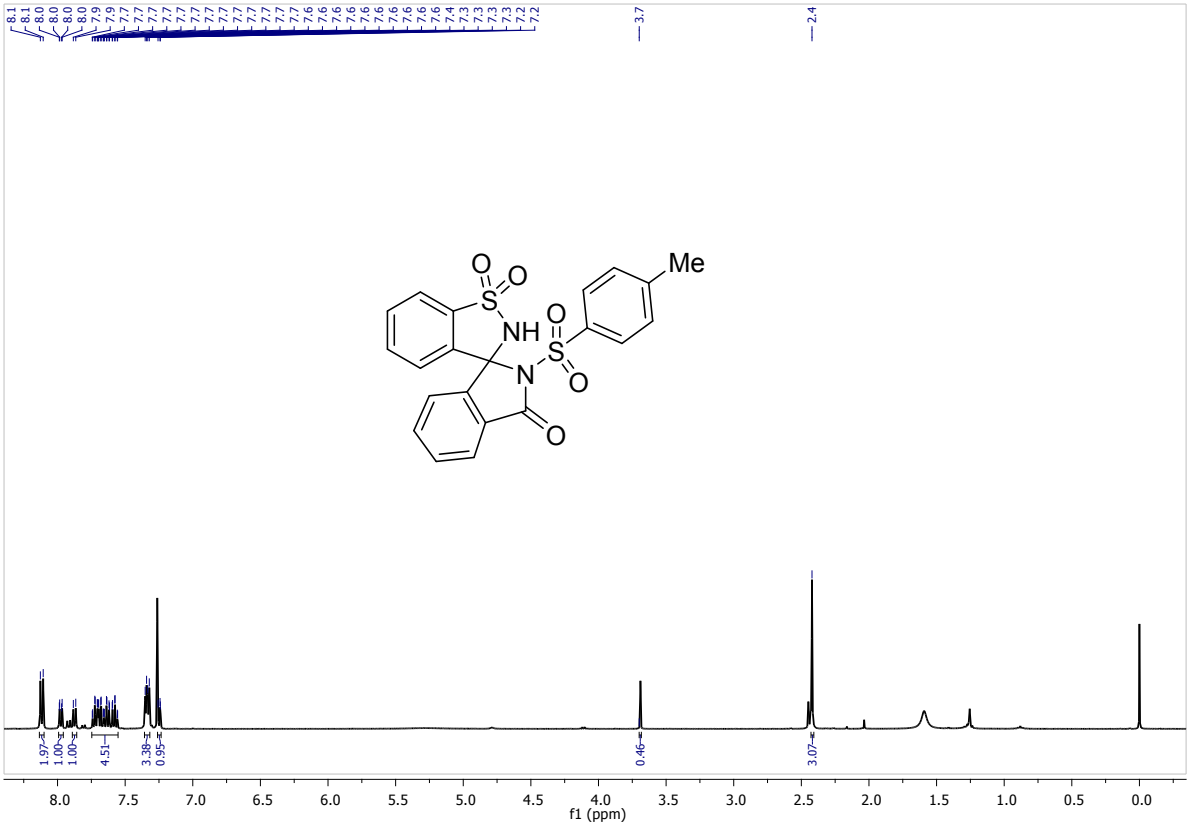
^{1}H NMR (300 MHz, $CDCl_3$ + DMSO) spectrum of compound (3e)



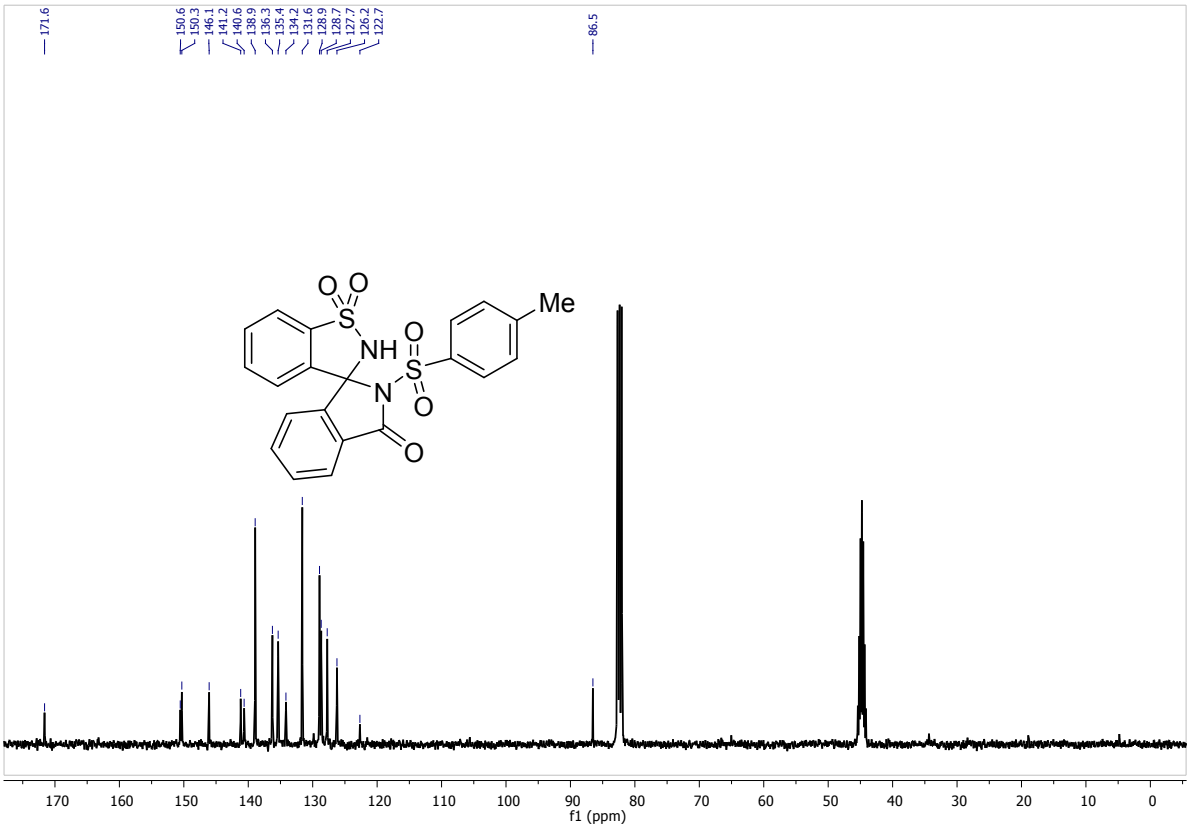
^{13}C NMR (101 MHz, $CDCl_3$ + DMSO) spectrum of compound (3e)



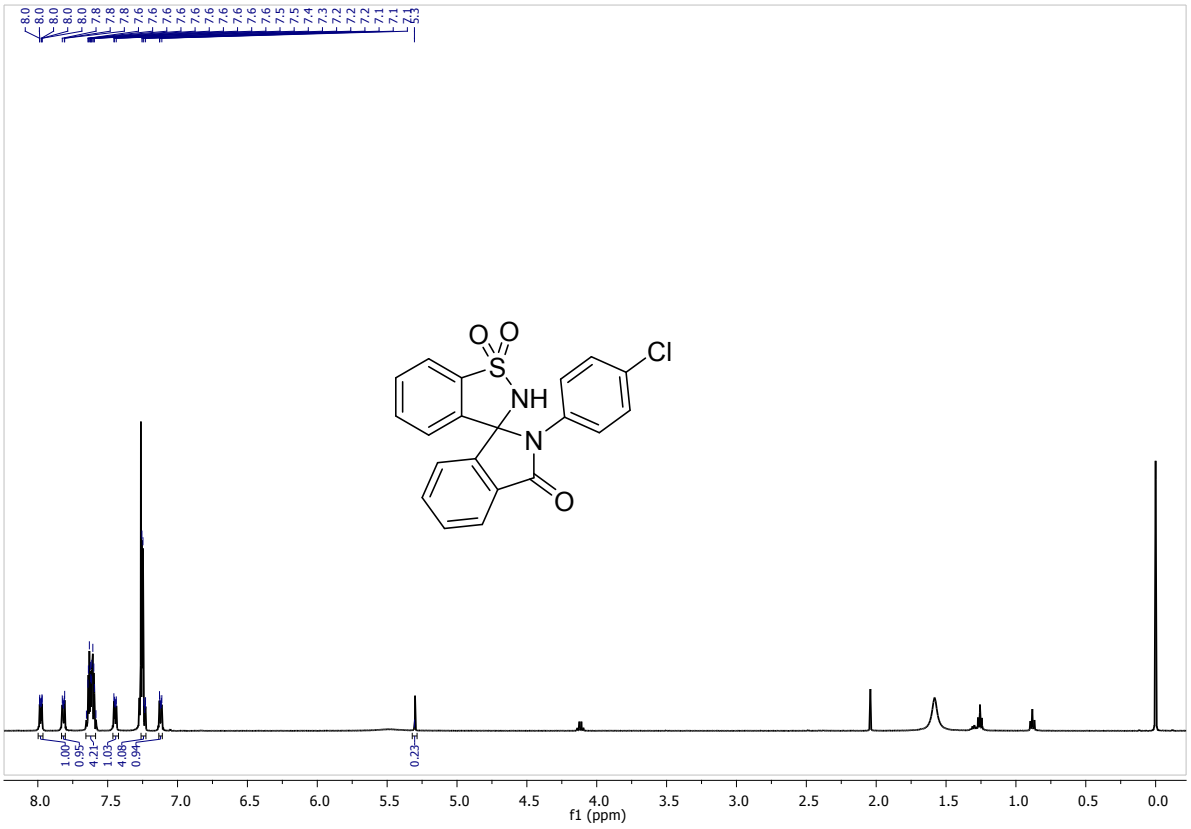
^{1}H NMR (400 MHz,$CDCl_3$ + DMSO) spectrum of compound (3f)



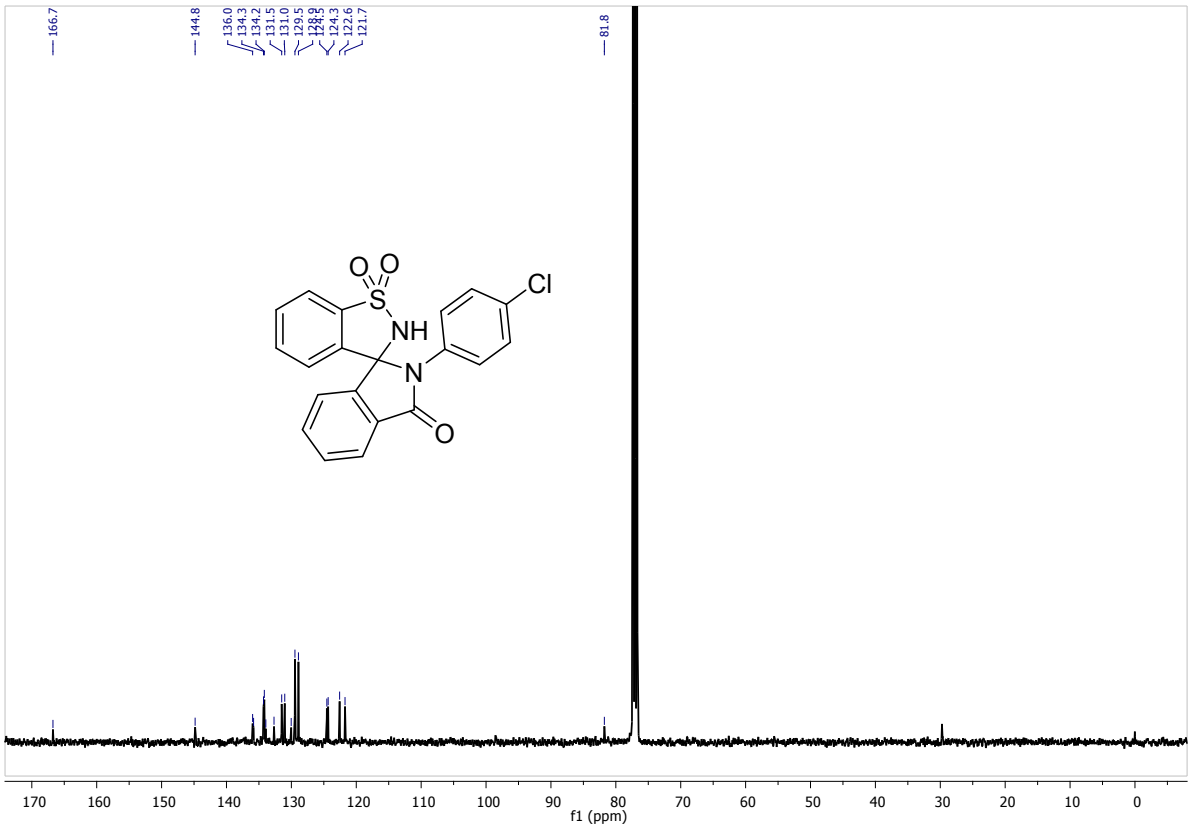
^{13}C NMR (101 MHz, $CDCl_3$ + DMSO) spectrum of compound (3f)



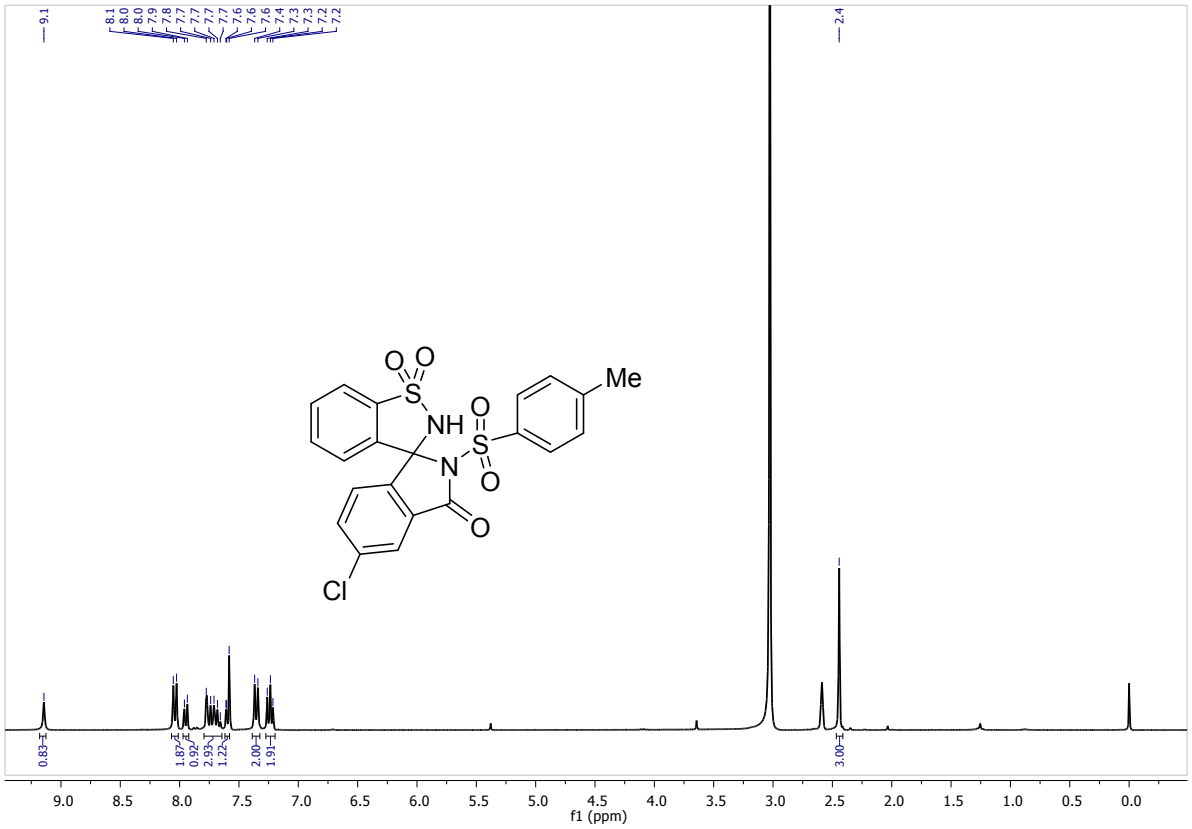
^{1}H NMR (500 MHz,$CDCl_3$) spectrum of compound (3g)



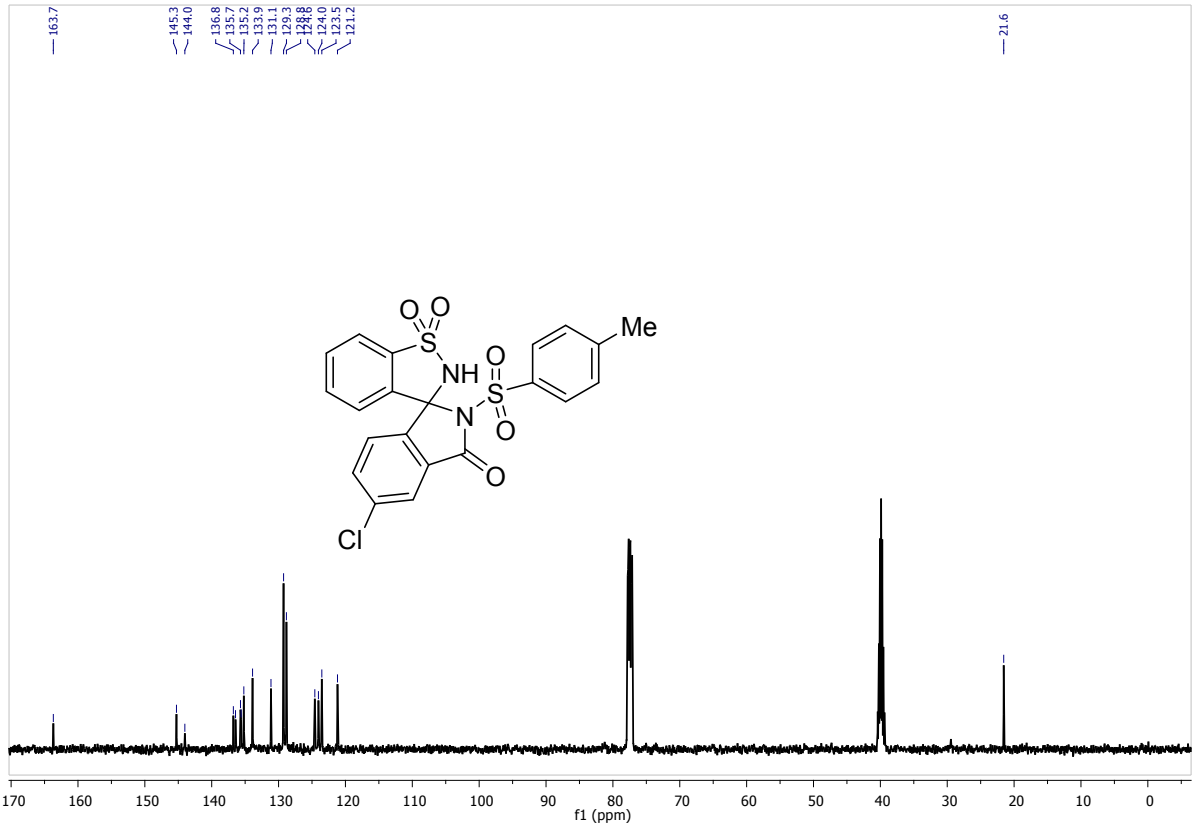
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound (3g)



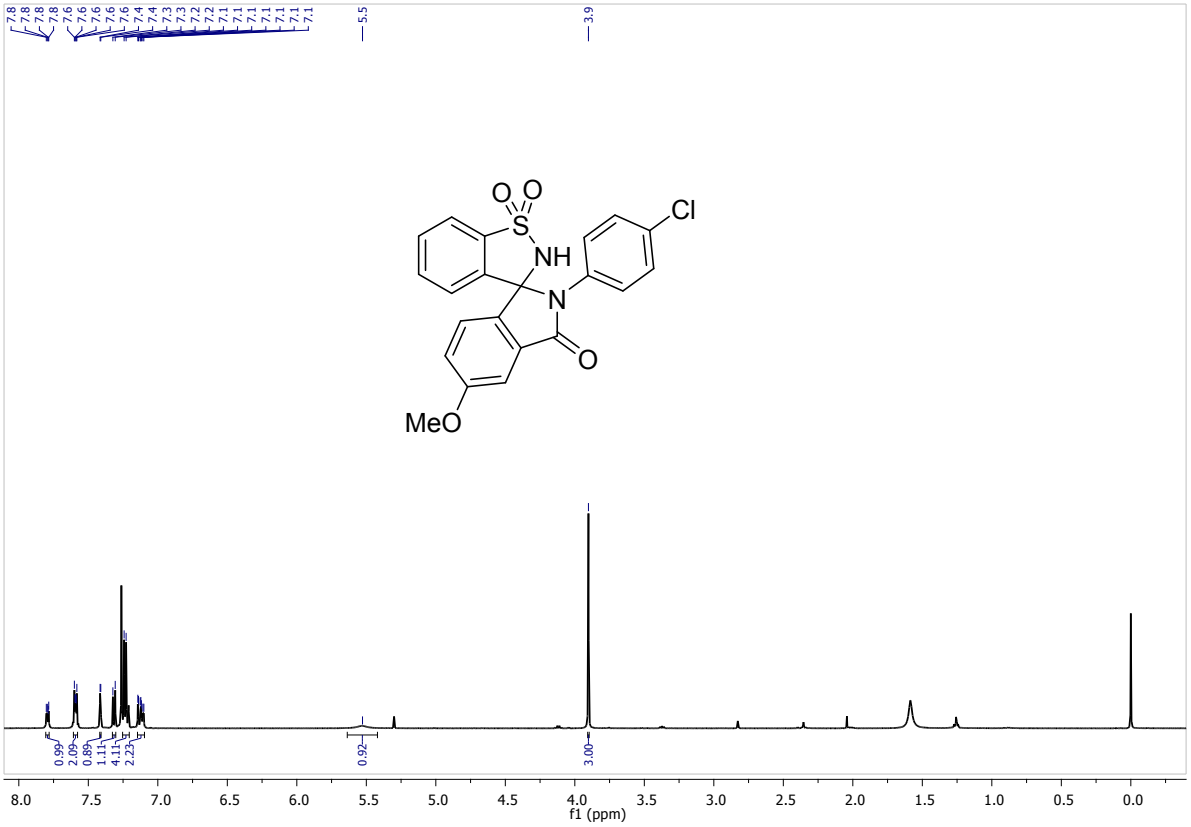
^{1}H NMR (300 MHz,$CDCl_3$ + DMSO) spectrum of compound (3h)



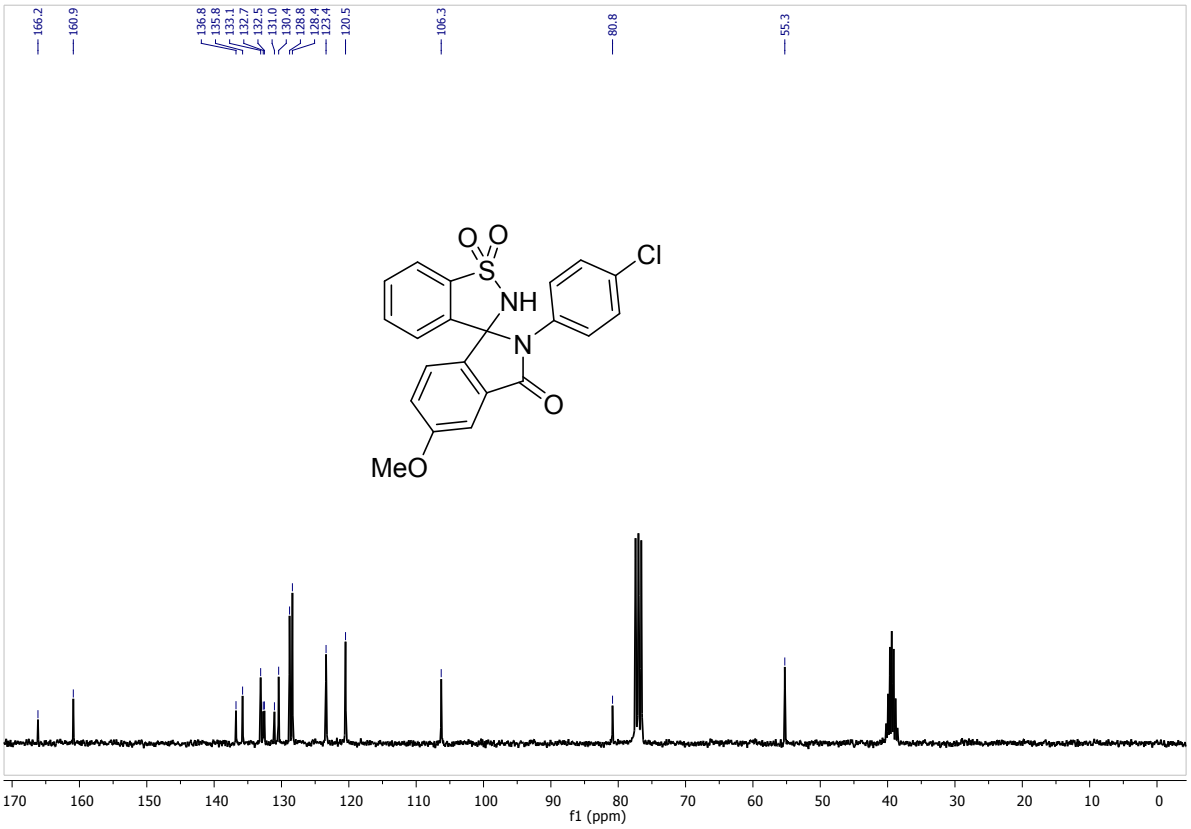
^{13}C NMR (126 MHz, $CDCl_3$ + DMSO) spectrum of compound (3h)



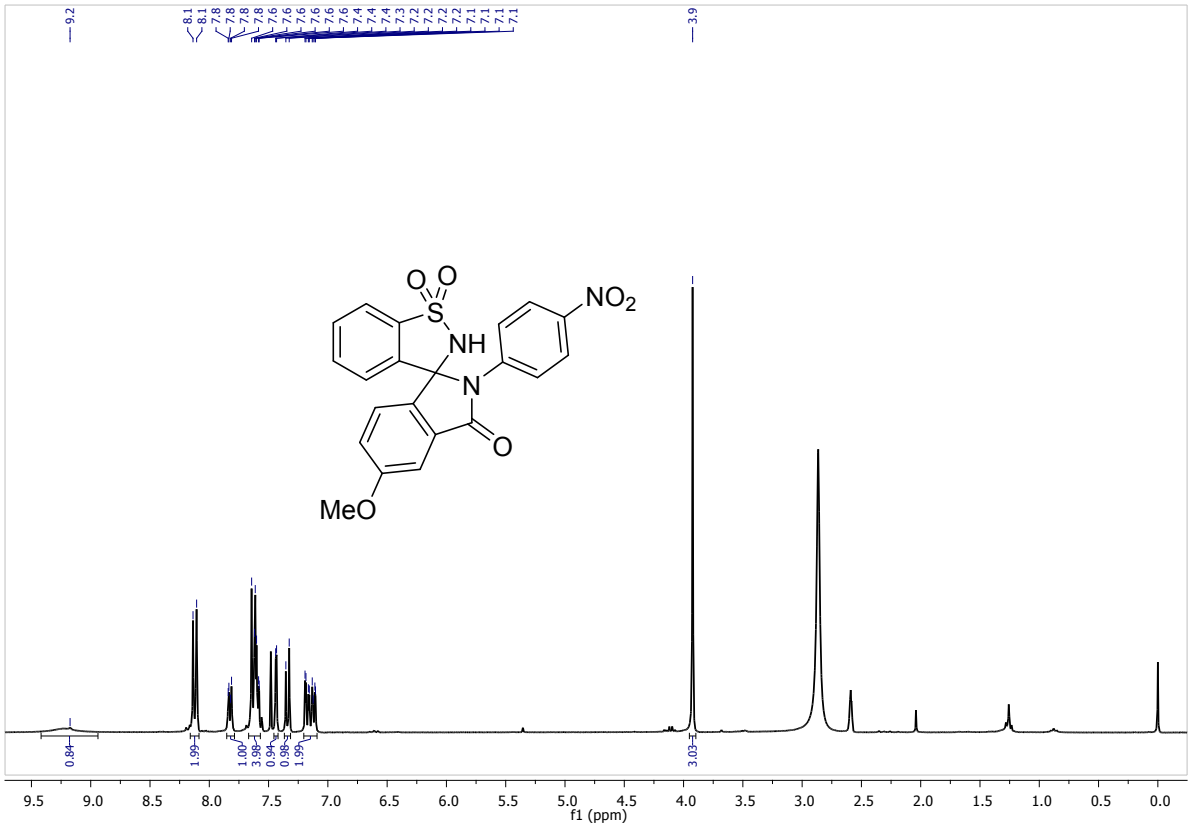
^{1}H NMR (500 MHz,$CDCl_3$) spectrum of compound (3i)



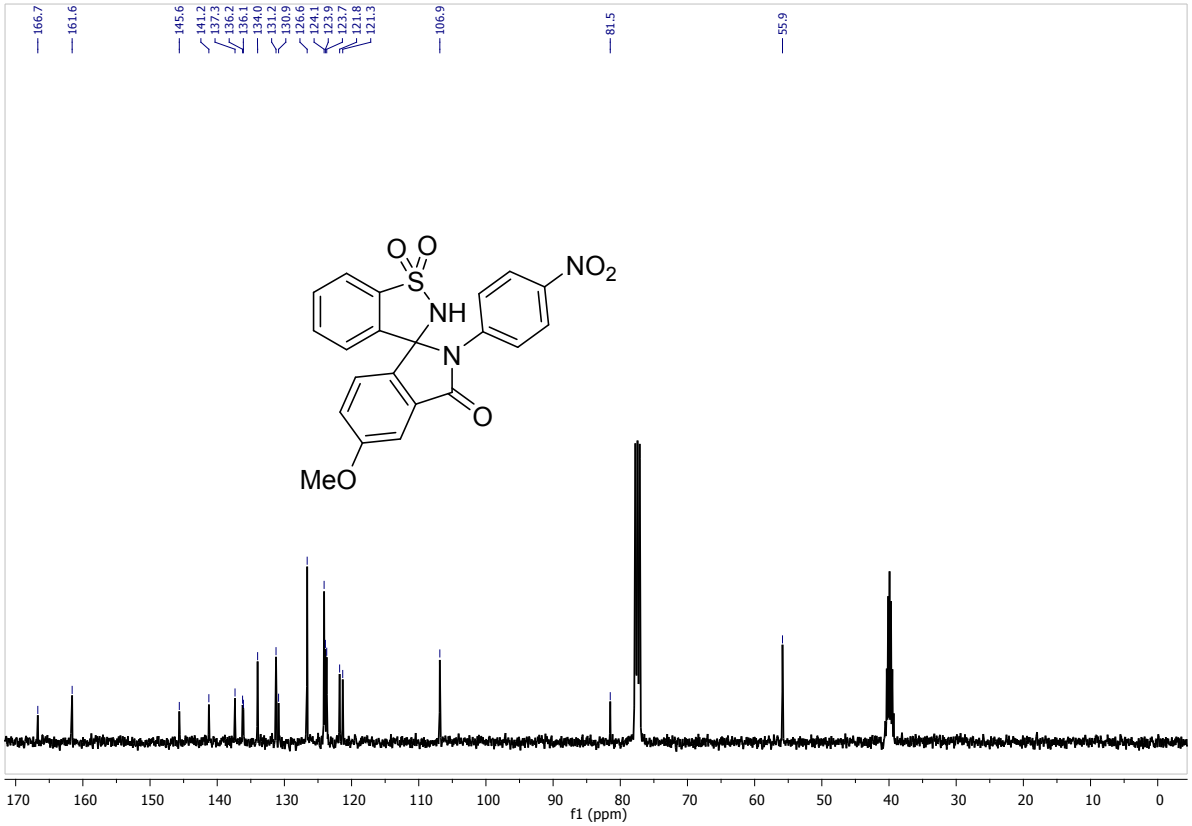
^{13}C NMR (75 MHz, $CDCl_3$ + DMSO) spectrum of compound (3i)



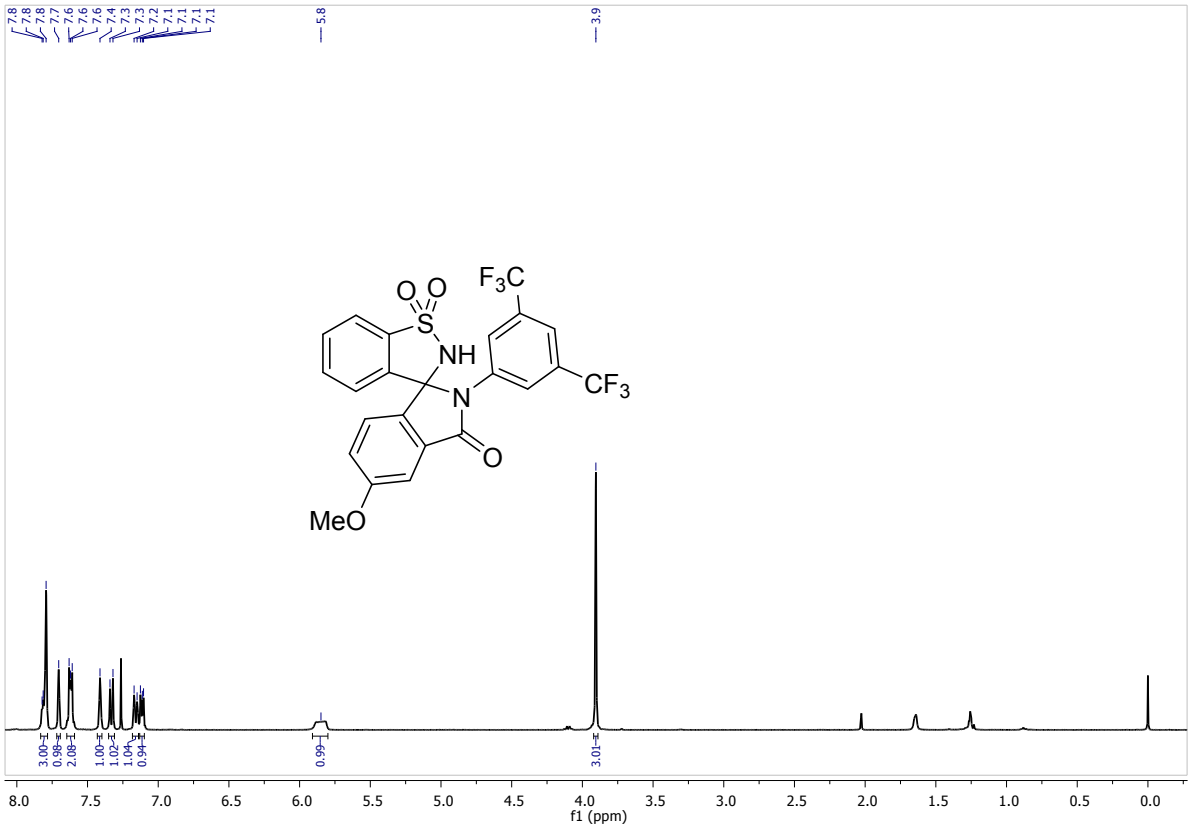
^{1}H NMR (300 MHz,$CDCl_3$ + DMSO) spectrum of compound (3j)



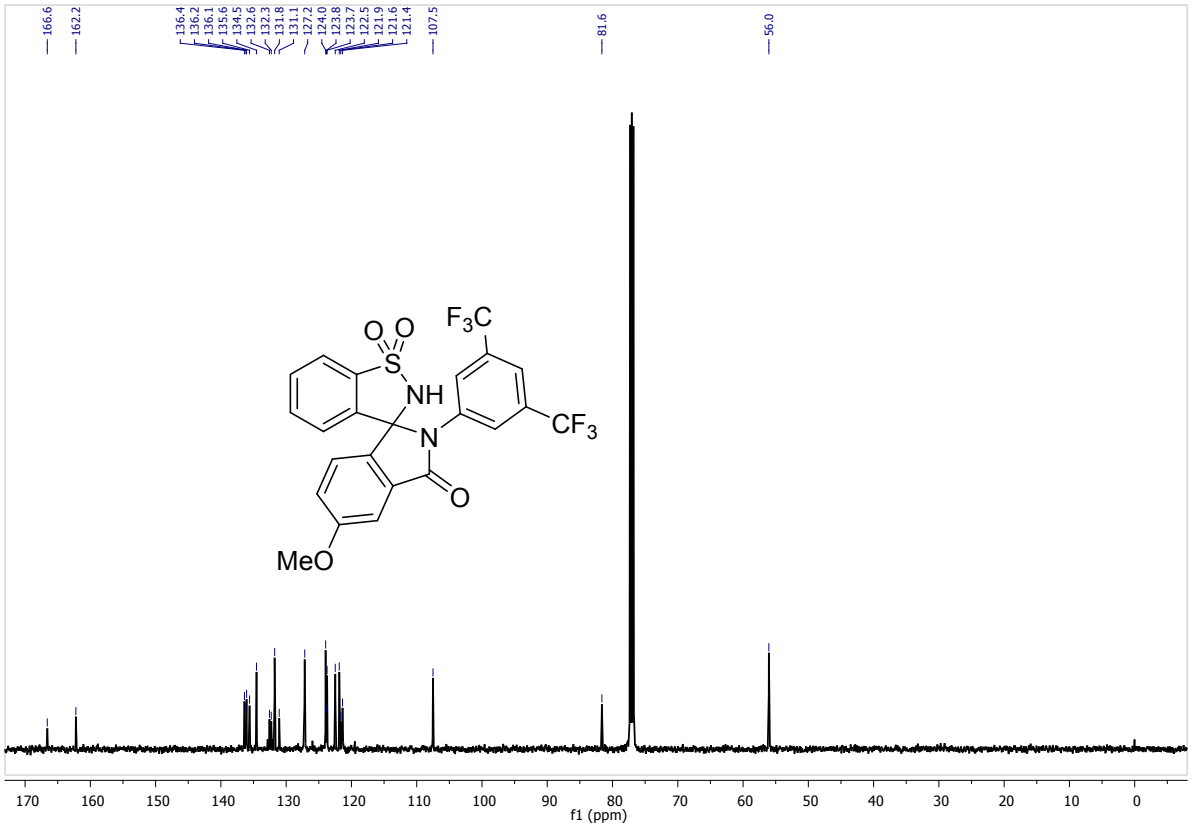
^{13}C NMR (101 MHz, $CDCl_3$ + DMSO) spectrum of compound (3j)



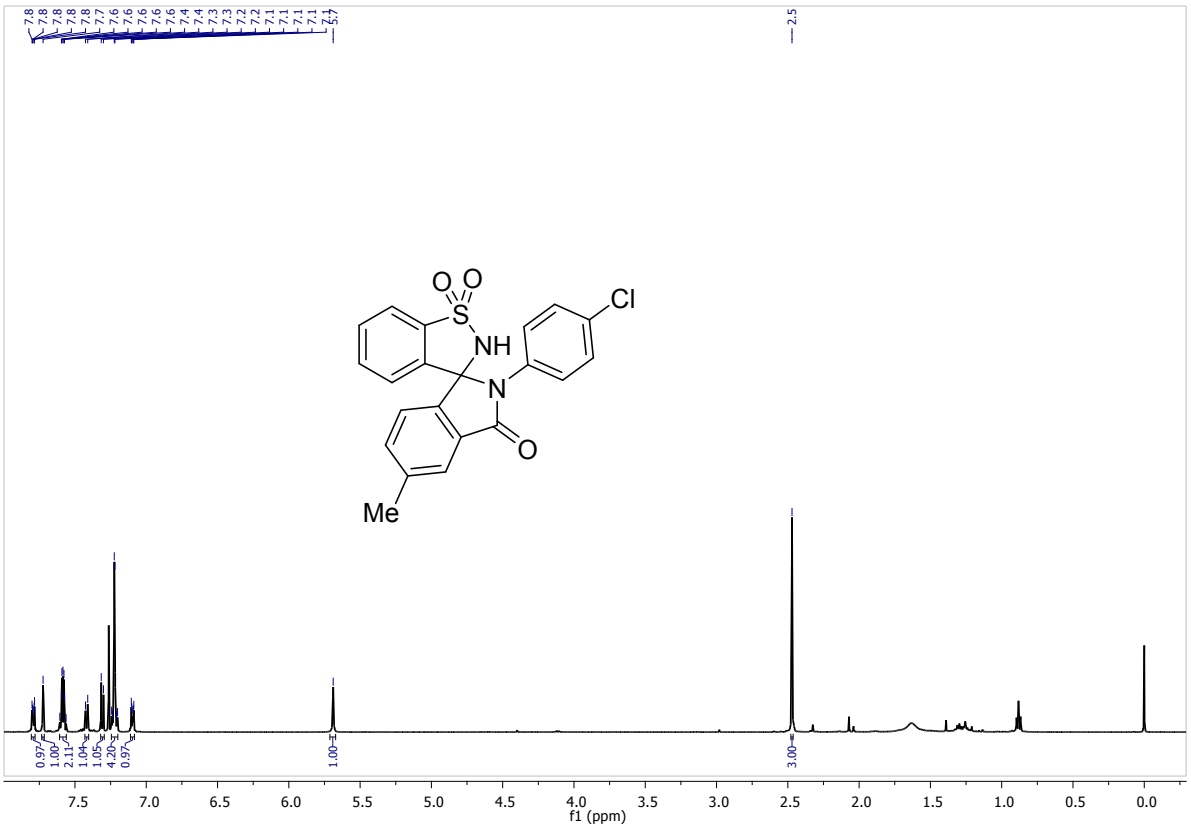
^{1}H NMR (400 MHz,$CDCl_3$) spectrum of compound (3k)



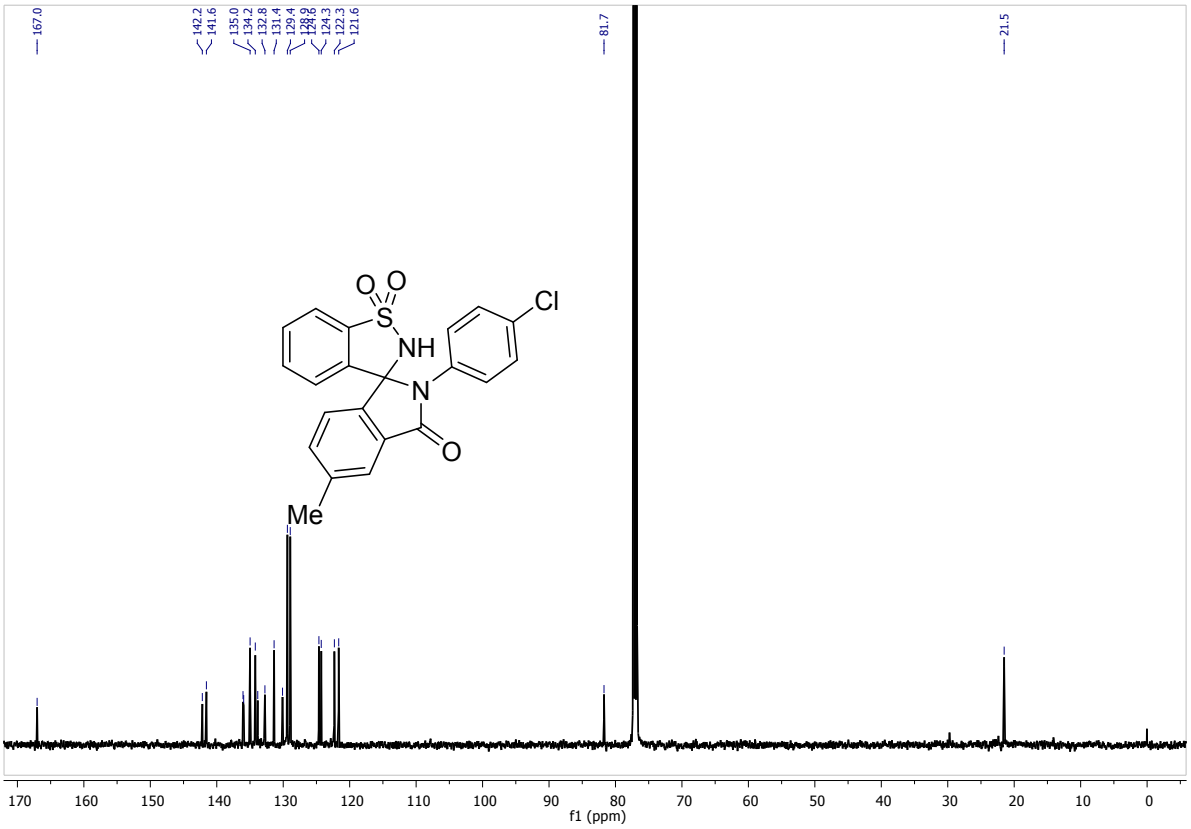
^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound (3k)



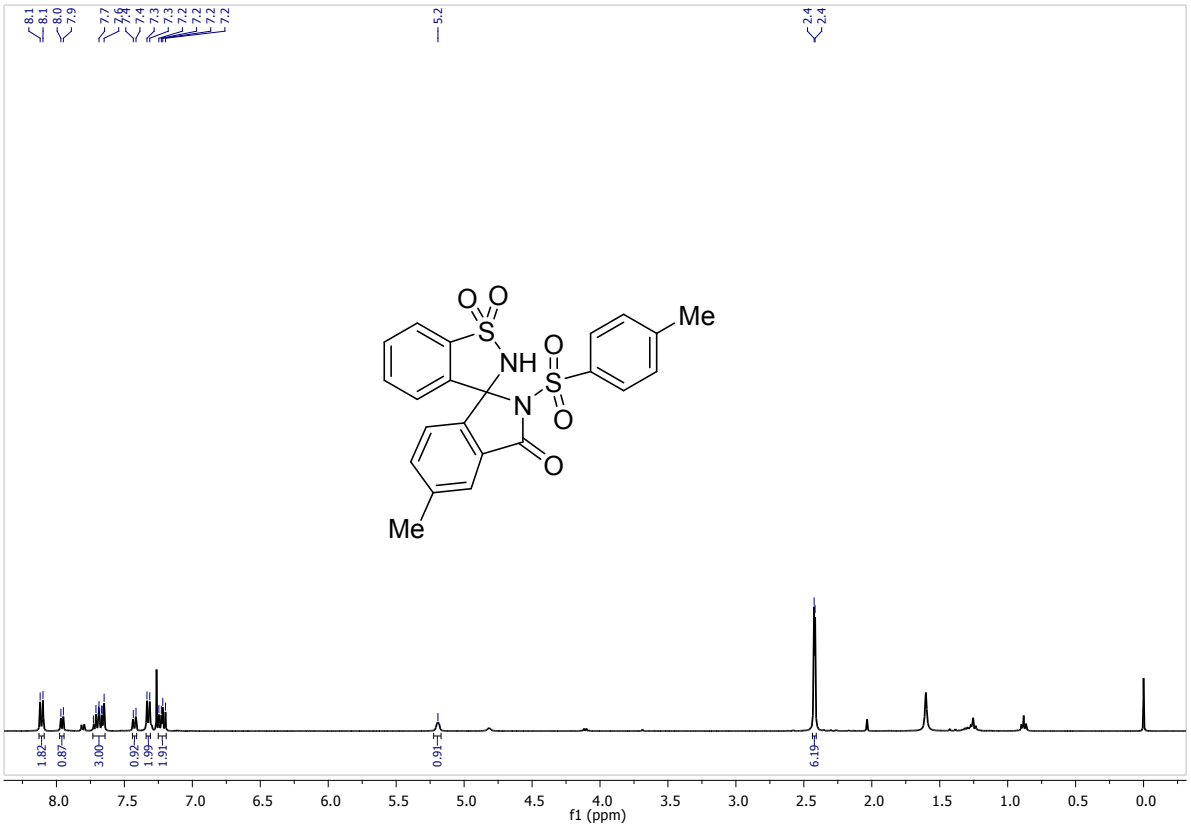
^{1}H NMR (500 MHz,$CDCl_3$) spectrum of compound (3l)



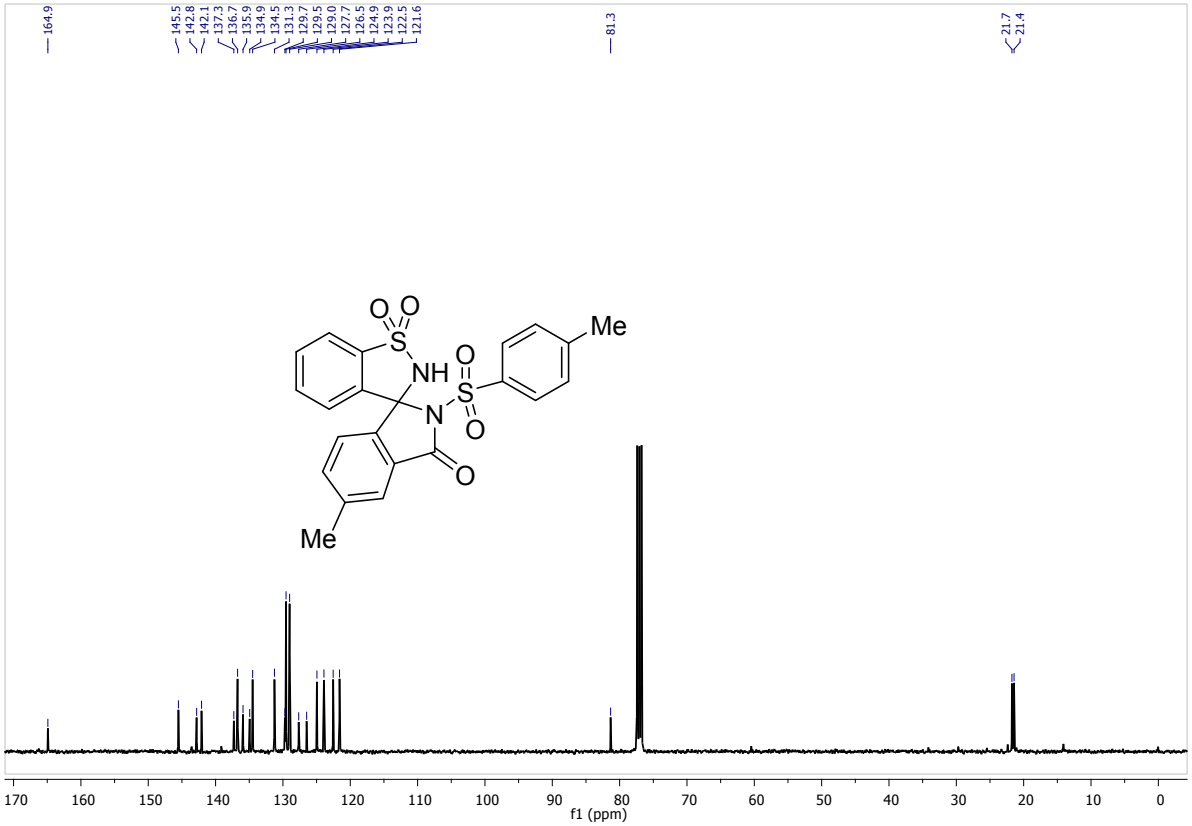
^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound (3l)



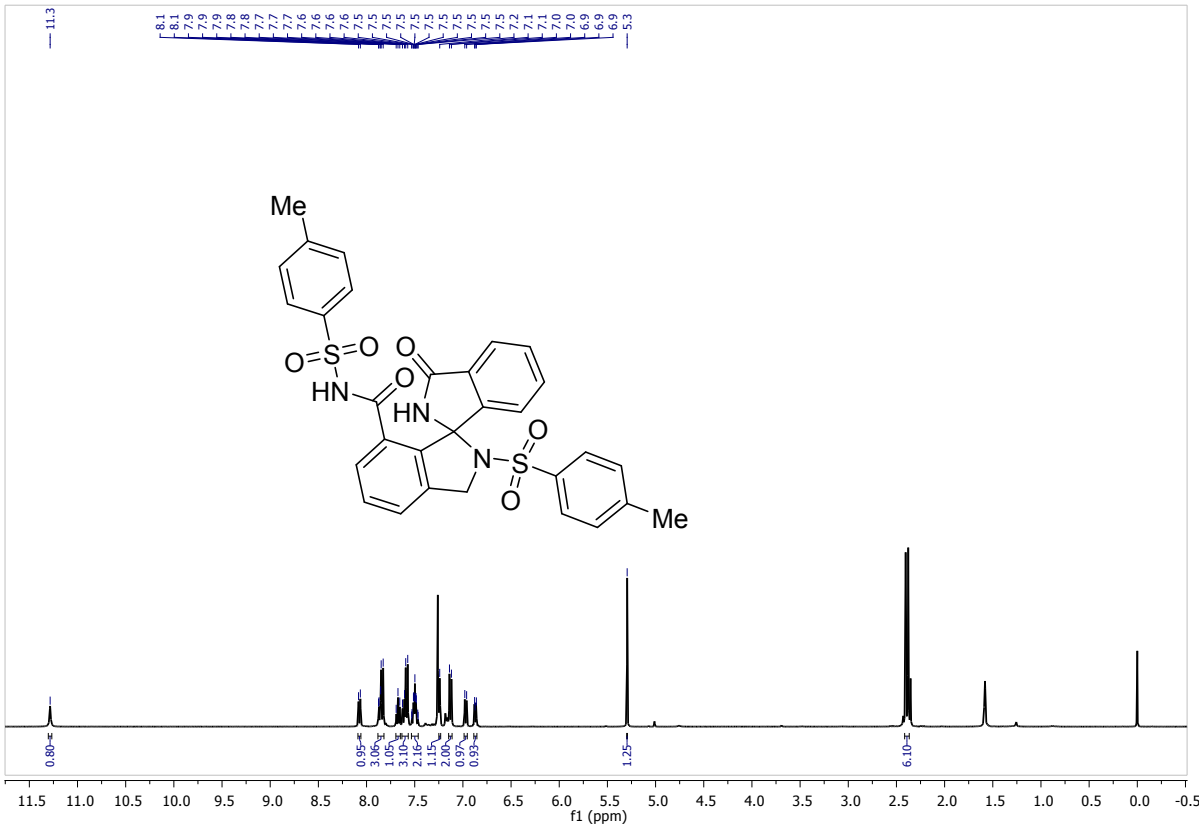
^{1}H NMR (400 MHz,$CDCl_3$) spectrum of compound (3m)



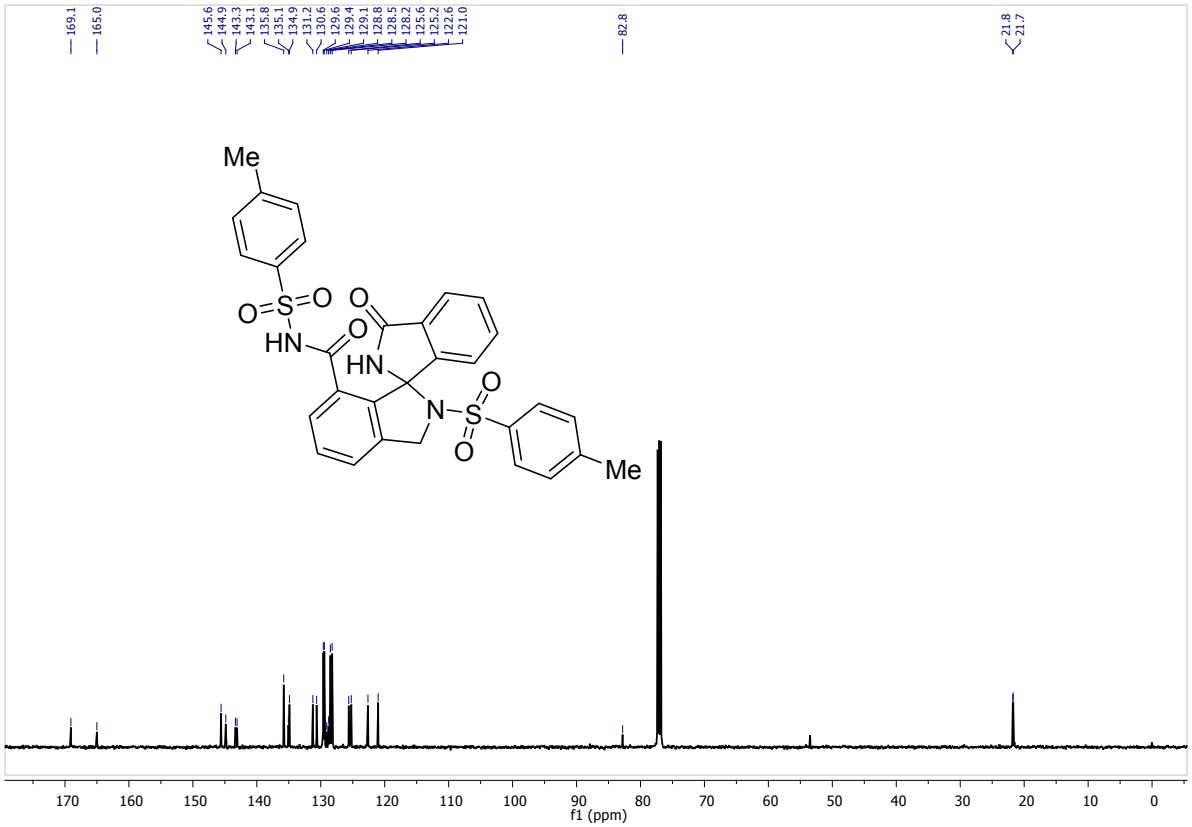
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound (3m)



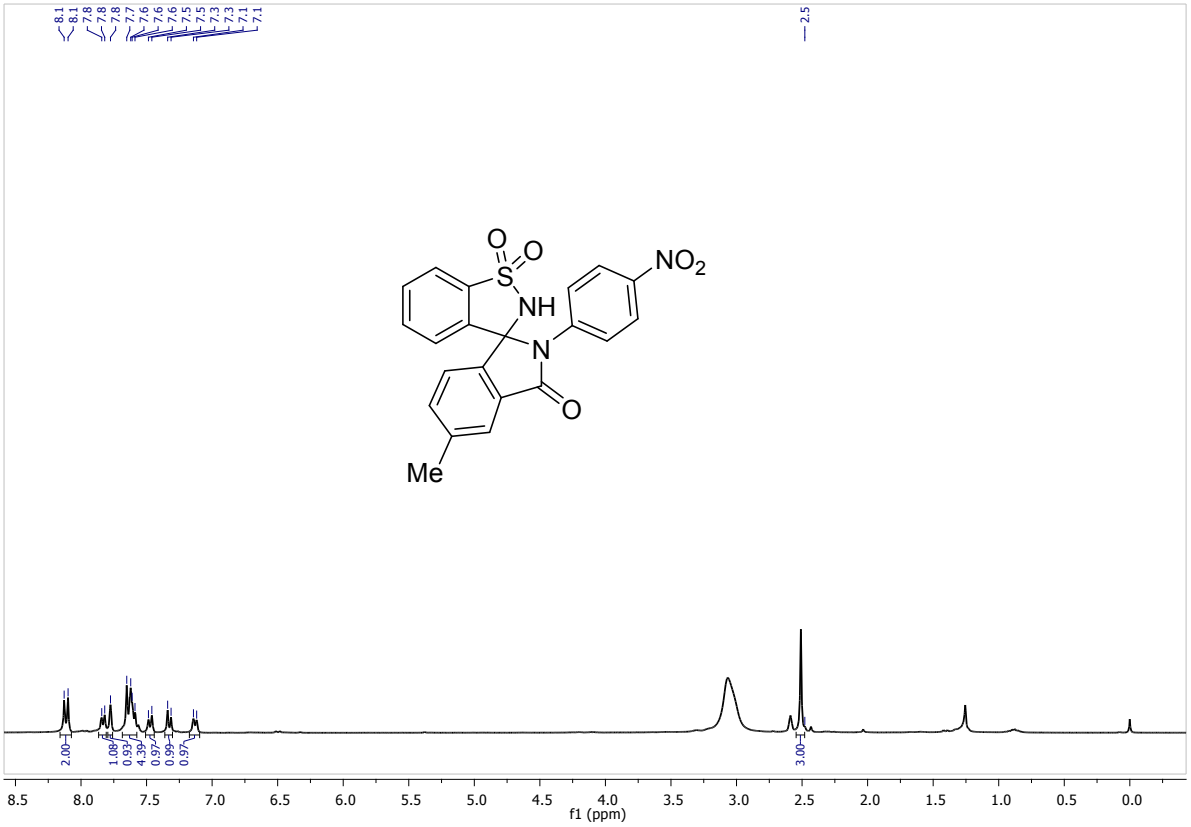
^{1}H NMR (400 MHz,$CDCl_3$) spectrum of compound (3n)



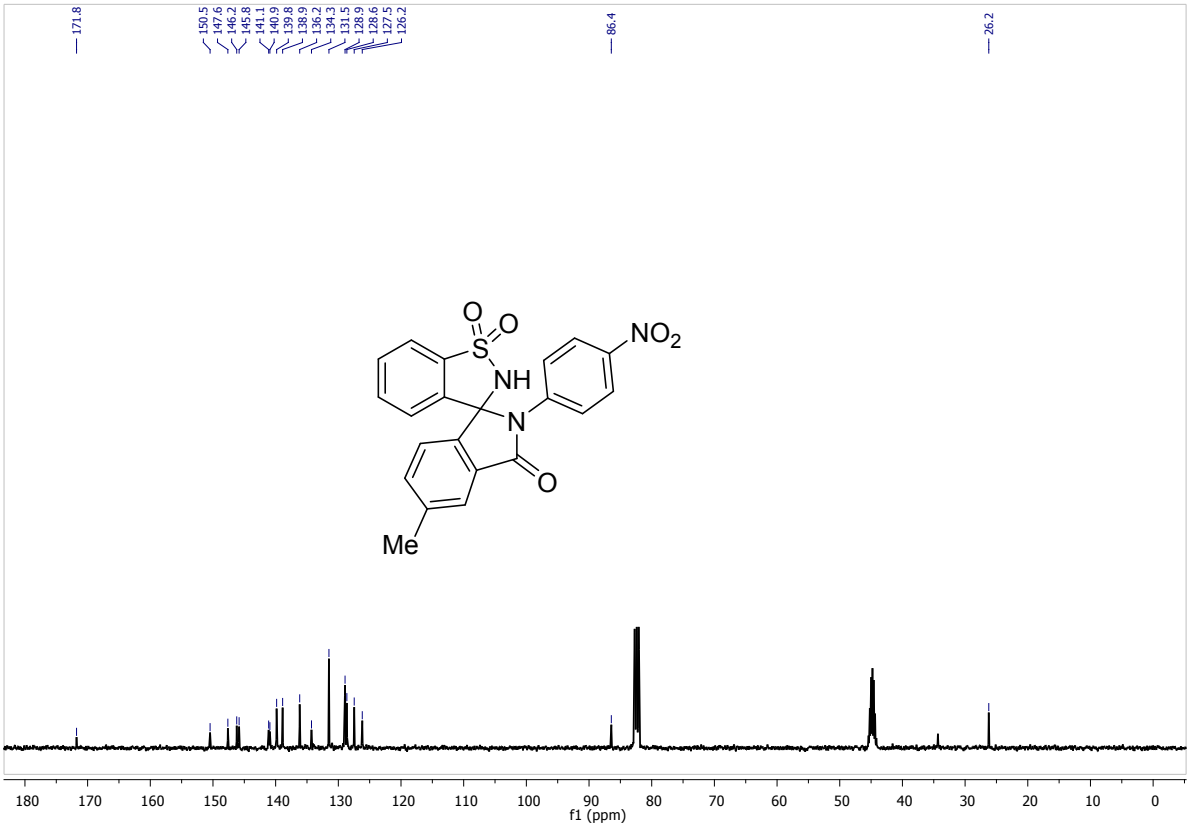
^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound (3n)



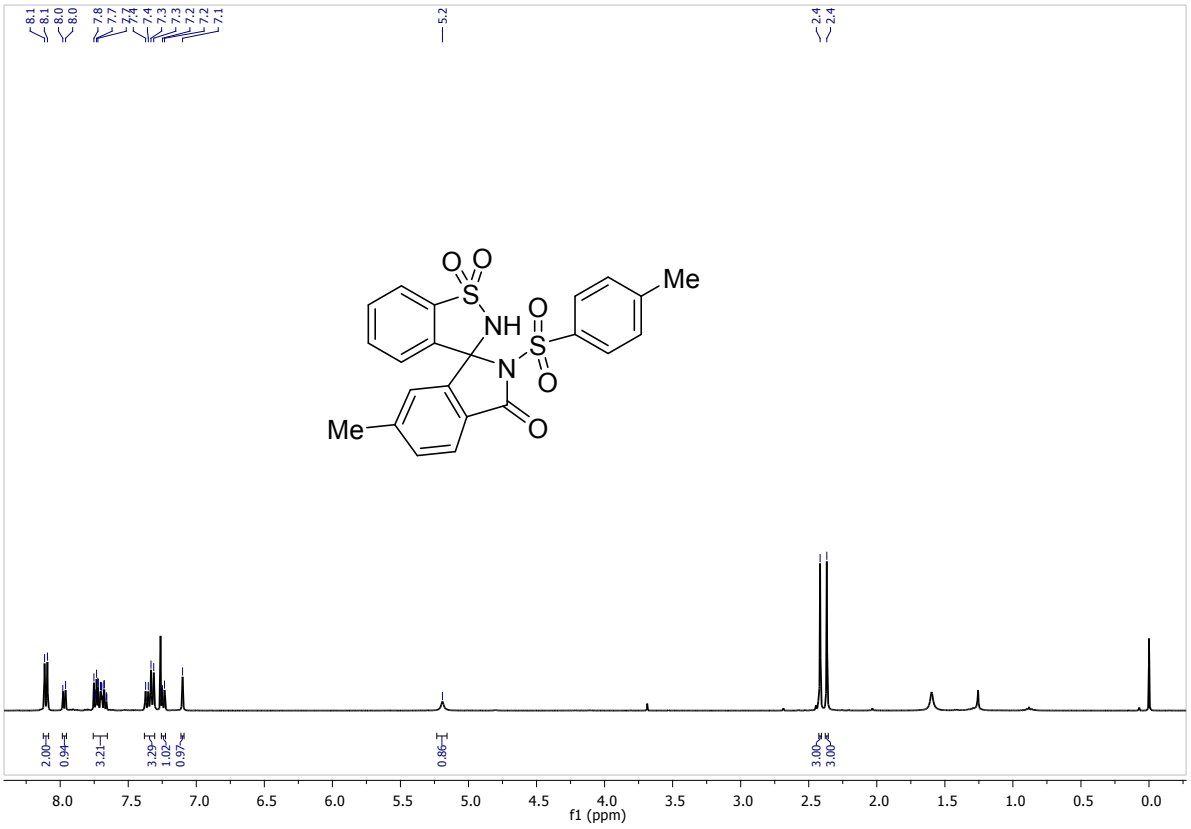
^{1}H NMR (300 MHz, $CDCl_3$ + DMSO) spectrum of compound (3o)



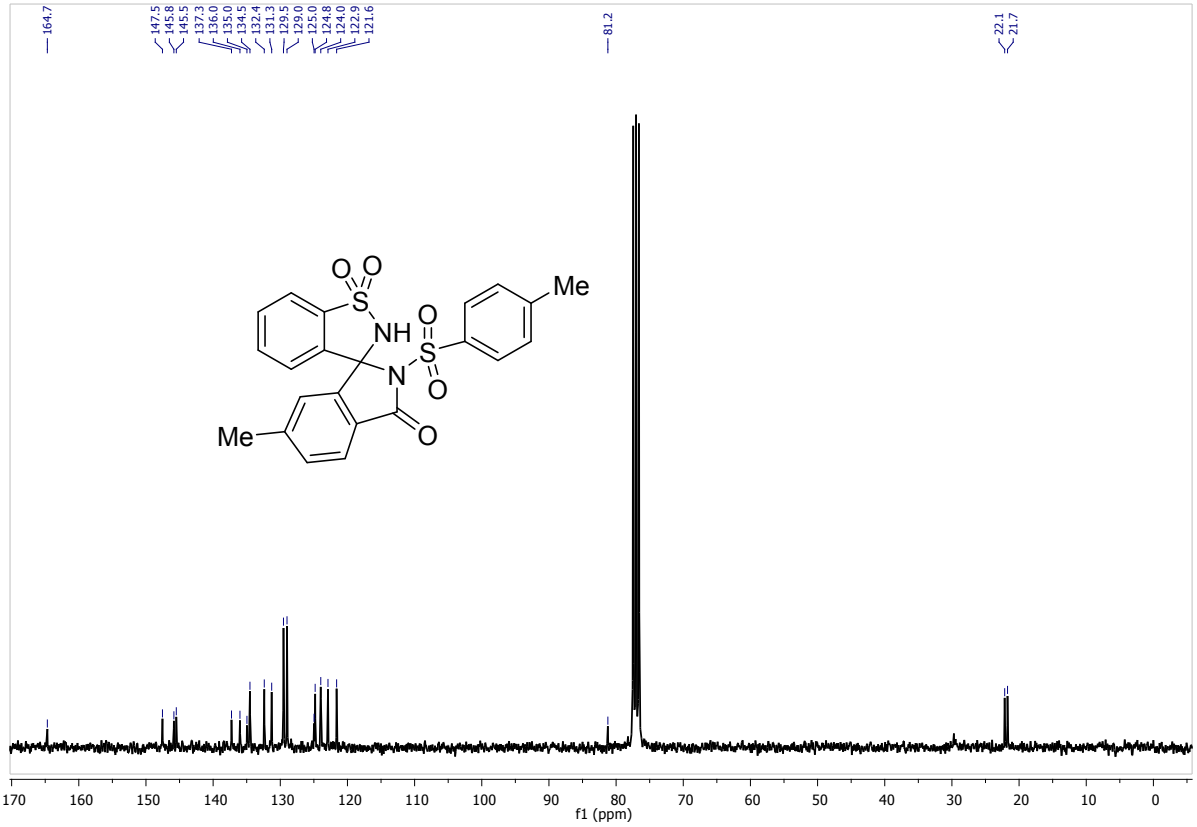
^{13}C NMR (101 MHz, $CDCl_3$ + DMSO) spectrum of compound (3o)



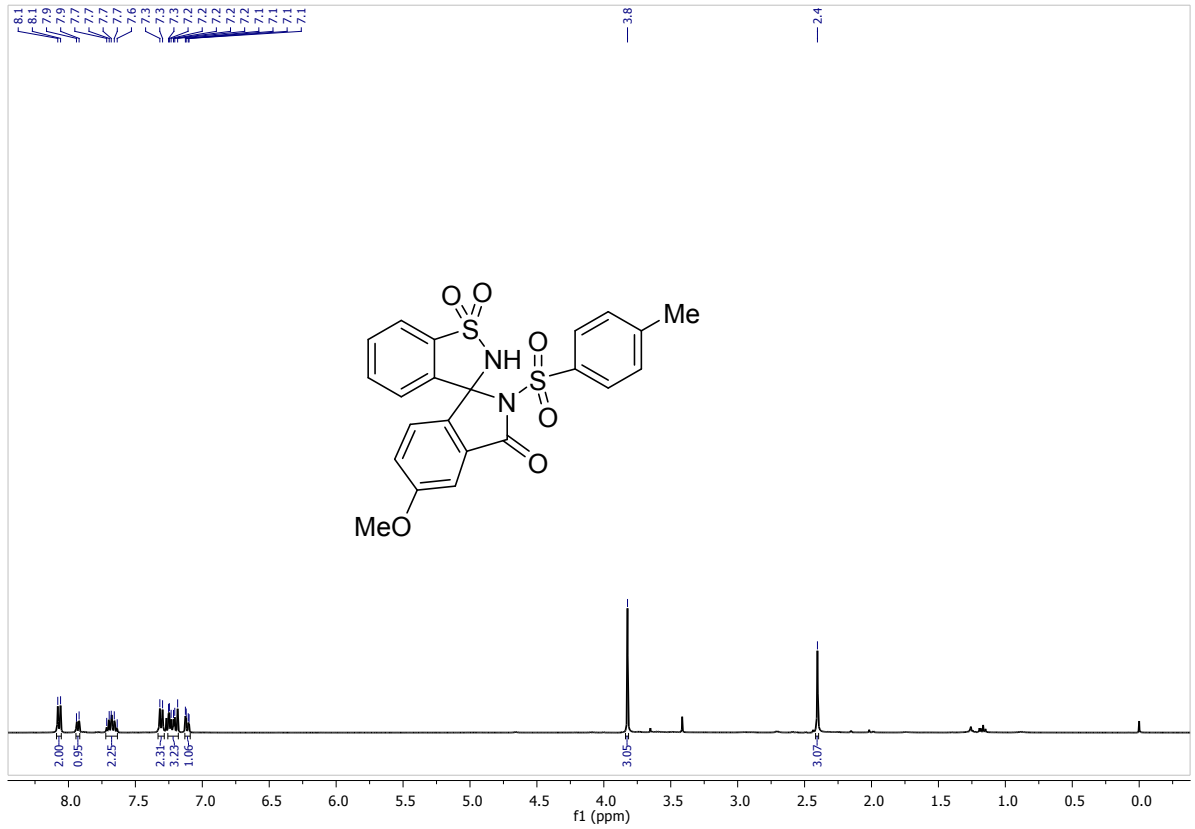
^{1}H NMR (400 MHz, CDCl3) spectrum of compound (3p)



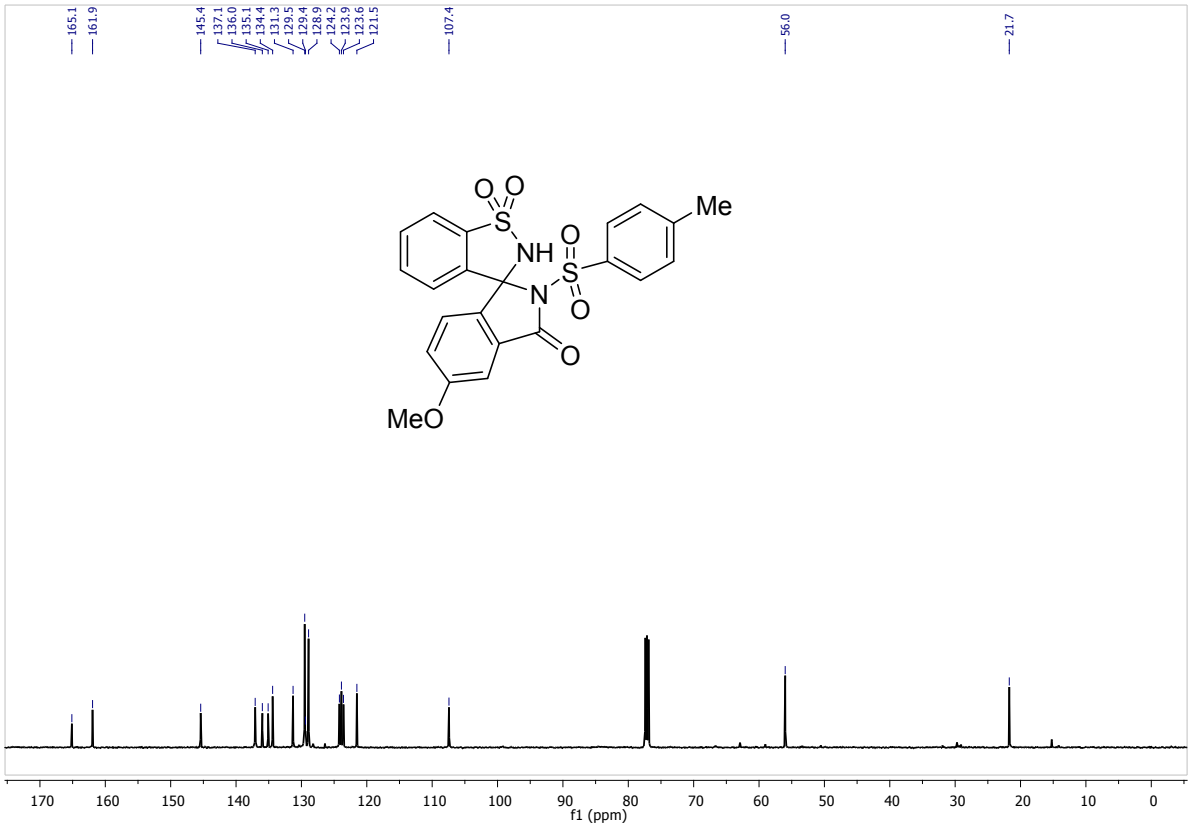
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound (3p)



[1]H NMR (400 MHz, CDCl3) spectrum of compound (3q)



^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound (3q)



3. X-ray Crystallography

X-ray data for the compound KA238 was collected at room temperature on a Bruker D8 QUEST instrument with an IμS Mo microsource (λ = 0.7107 A) and a PHOTON-100 detector. The raw data frames were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs [1]. The structure was solved using intrinsic phasing method [2] and further refined with the SHELXL [2] program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms. All C bound H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 Å, and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H or $1.2U_{eq}(C)$ for other H atoms].

Crystal Data for **3c**: $C_{21}H_{15}N_3O_6S$ (M =437.42 g/mol): monoclinic, space group $P2_1$ (no. 4), a = 8.26140(10) Å, b = 11.3690(2) Å, c = 10.8661(2) Å, β = 106.2970(4)°, V = 979.58(3) Å^3, Z = 2, T = 294.15 K, μ(MoKα) = 0.212 mm^{-1}, $Dcalc$ = 1.483 g/cm^3, 28348 reflections measured (5.138° ≤ 2Θ ≤ 61.14°), 5995 unique (R_{int} = 0.0350, R_{sigma} = 0.0283) which were used in all calculations. The final R_1 was 0.0363 (I > 2σ(I)) and wR_2 was 0.1015 (all data).

CCDC 1578857 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [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].

1. Bruker (2016). APEX3, SAINT and SADABS. Bruker AXS, Inc., Madison, Wisconsin, USA.
2. Sheldrick G. M. (2015**)** Acta Crystallogr C71: 3-8.