Supporting Information

Iridium-Catalyzed Direct C–H Arylation of Cyclic *N*-sulfonyl Ketimines with Arylsiloxanes at Ambient Temperature

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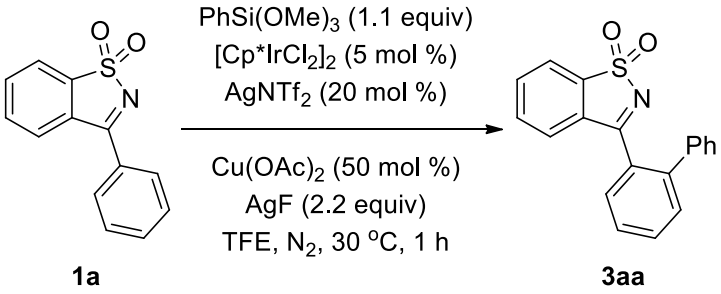
Table of contents

General information:

All reactions were carried out in oven-dried reaction vessels under nitrogen atmosphere unless otherwise mentioned. TLC analysis was performed on silica gel TLC plates. Column chromatography was done using 230-400 mesh silica gel by applying pressure through an air pump. ^{1}H and ^{13}C NMR spectra were recorded on 400 and 600 MHz spectrometers and are reported as chemical shifts (δ) in parts per million (ppm), and multiplicities are abbreviated as s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, comp = complex. Internal standards or residual solvent signals were used as reference. HRMS (m/z) was recorded using ESI (Q-Tof, Orbitrap, positive ion) and EI (magnetic sector, positive ion) mode. Melting points were determined in a capillary melting point apparatus and are uncorrected. Single-crystal X-ray data were recorded in a diffractometer with Mo Kα radiation. The CIF file was submitted to CCDC (1891261, 1891262, and 2014574) and can be obtained at https://summary.ccdc.cam.ac.uk/structure-summary-form. Ketimines (**1a**−**1p**),[1] ketimines (**4a**−**4f**)[2] were prepared following a literature method.

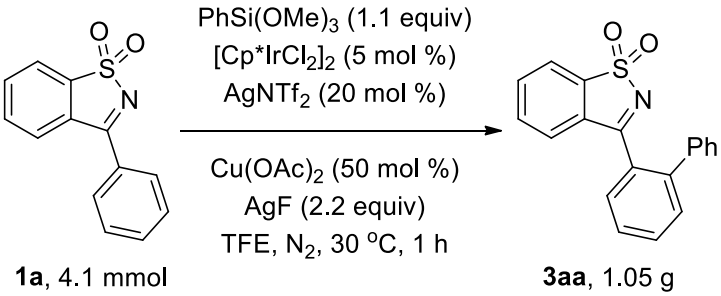
General procedure for arylation:

(milligram scale)



An oven dried 10 mL Schlenk tube was charged with 3-phenylbenzo[*d*]isothiazole 1,1-dioxide (**1a**) (48.7 mg, 0.2 mmol), trimethoxy(phenyl)silane (41 µL, 0.22 mmol), silver (bistrifluoromethanesulfonyl)imide (15.5 mg, 20 mol %), copper acetate (18.1 mg, 50 mol %), silver fluoride (55.8 mg, 2.2 equiv) and catalyst $[Cp^*IrCl_2]_2$ (8.0 mg, 5 mol %). The tube was evacuated and backfilled with nitrogen and to it was added TFE (2.0 mL, 0.1 M) under nitrogen atmosphere. The reaction mixture was degassed and backfilled with nitrogen 3 times. It was then closed with teflon-lined cap and kept at 30℃ while stirring for 1 h. After completion of the reaction, the reaction mixture was filtered through a short pad of celite, the solvent was removed under reduced pressure and the crude reaction mixture was directly purified through column chromatography on silica gel using petroleum ether:ethylacetate (7:3) as eluent to obtain 3-([1,1'-biphenyl]-2-yl)benzo[d]isothiazole 1,1-dioxide (**3aa**) in 83% (53.0 mg). Cases where the mono- and bis-arylated products were obtained as an inseparable mixture, the ratio was calculated from ^{1}H NMR.

(gram scale)

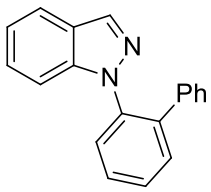


An oven dried 100 mL two-neck round bottom flask was charged with 3-phenylbenzo[*d*]isothiazole-1,1-dioxide (**1a**) (1.0 g, 4.1 mmol), trimethoxy(phenyl)silane (0.84 mL, 4.5 mmol), silver (bistrifluoromethanesulfonyl)imide (318.9 mg, 20 mol %),

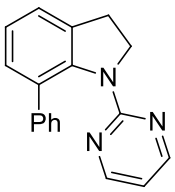
copper acetate (372.3 mg, 50 mol %), silver fluoride (1.14 g, 2.2 equiv) and catalyst $[Cp^*IrCl_2]_2$ (163.3 mg, 5 mol %). The flask was evacuated and backfilled with nitrogen and to it was added TFE (41 mL, 0.1 M) under nitrogen atmosphere. The reaction mixture was degassed and backfilled with nitrogen 3 times. It was then closed with a stopper and kept at 30℃ while stirring for 1 h. After completion of the reaction, the reaction mixture was filtered through a short pad of celite, the solvent was removed under reduced pressure and the crude reaction mixture was directly purified through column chromatography on silica gel using petroleum ether:ethylacetate (7:3) as eluent to obtain3-([1,1'-biphenyl]-2-yl)benzo[d]isothiazole 1,1-dioxide (**3aa**) in 80% (1.05 g) yield.

The ratio of mono and bis products was determined by ^{1}H NMR. The characterization data for all the mono-arylated products are given below. Compounds **3ma, 5ea, 5fa, 5ab, 5ac** were recrystallized from EtOH to get mono-arylated product exclusively.

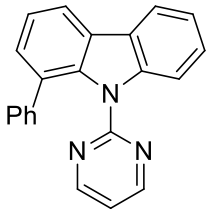
Table S1: Scope of other substrates



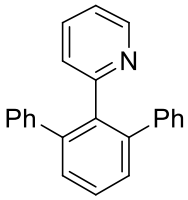
6, 94%, m:b = 1.5:1



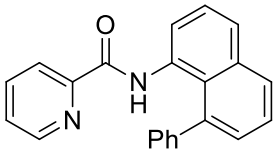
7, 82%



17%

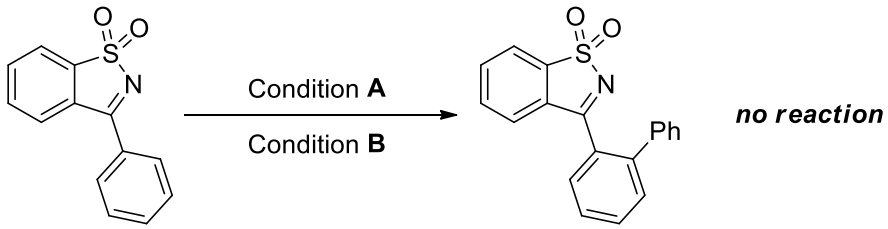


23%



0%

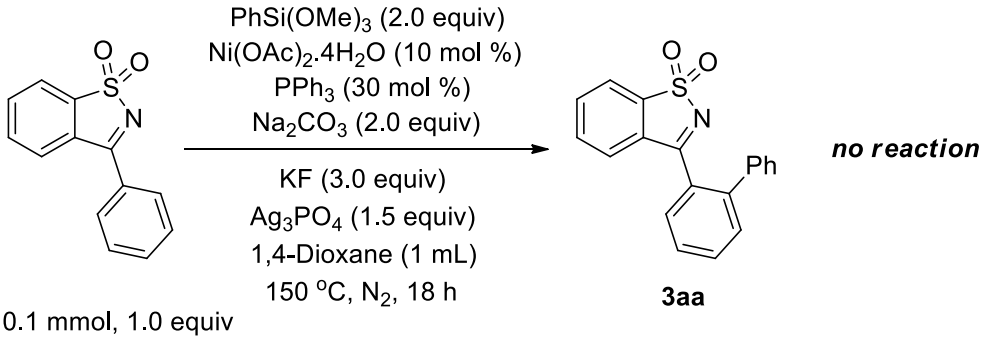
Arylation under Pd and Ni catalysis:



1a **3aa**

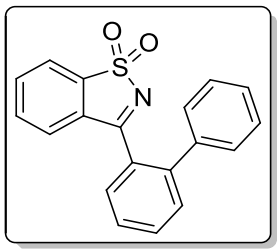
Condition **A**: **1a** (0.1 mmol, 1.0 equiv), $PhSi(OMe)_3$ (2.0 equiv), $Pd(OAc)_2$ (10 mol %), *p*-BQ (1.0 equiv), AgF (2.0 equiv), 1,4-Dioxane (1 mL), 110 ^oC, N_2, 24 h

Condition **B**: **1a** (0.1 mmol, 1.0 equiv), $PhSi(OMe)_3$ (2.0 equiv), $Pd(OAc)_2$ (5 mol %), $Cu(OTf)_2$ (2.0 equiv), AgF (2.0 equiv), 1,4-Dioxane (2.5 mL), 110 ^oC, N_2, 48 h



1a, 0.1 mmol, 1.0 equiv **3aa**

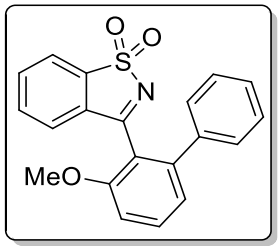
Characterization data for arylated products:



3-([1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3aa):

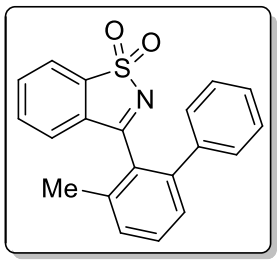
Combined Yield 83% (55 mg); **mono**:**bis** 5:1; colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 130-132 ^oC; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.92 (d, *J* = 7.6 Hz, 1H), 7.15-7.19 (m, 1H), 7.22-7.25 (comp, 2H), 7.29 (dd, *J* = 7.8 Hz, 2.2 Hz, 1H), 7.37 (app d, *J* = 8.0 Hz, 2H), 7.50 (td, *J* = 7.6 Hz, 2.0 Hz, 1H), 7.55-7.59 (m, 1H), 7.65-7.67 (m, 1H), 7.70-7.74 (comp, 2H), 7.80 (d, *J* = 7.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 122.3, 126.5, 128.1, 128.4, 129.0, 129.2, 129.8, 130.1,

130.6, 131.0, 132.3, 132.9, 133.1, 139.6, 139.7, 141.5, 174.4; **HRMS** (ESI, m/z) calcd for $C_{19}H_{13}NO_2S$ $[M+H]^+$ 320.0745, found 320.0737.



3-(3-methoxy-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3ba):

Yield 82% (57 mg); colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 112-114 ^oC; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.81 (s, 3H), 7.07 (d, *J* = 8.4 Hz, 1H), 7.16 (d, *J* = 7.8 Hz, 2H), 7.18-7.26 (comp, 5H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.57-7.61 (comp, 2H), 7.82 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 56.3, 110.3, 118.4, 122.3, 122.8, 125.9, 128.1, 128.6, 129.1, 132.3, 132.4, 133.0, 133.5, 139.1, 139.4, 143.3, 157.8, 172.0; **HRMS** (ESI, m/z) calcd for $C_{20}H_{15}NO_3S$ $[M+H]^+$ 350.0851, found 350.0851.



3-(3-methyl-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3ca):

Yield 60% (40 mg); colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 150-152 ^oC (crystallization from $CDCl_3$ and hexane); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.39 (s, 3H), 6.91 (d, *J* = 7.6 Hz, 1H), 7.10-7.13 (m, 1H), 7.20 (t, *J* = 7.4 Hz, 2H), 7.32-7.43 (comp, 5H), 7.50-7.56 (comp, 2H), 7.79 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 20.1, 122.3 (x 2), 126.0, 127.9, 128.1, 128.6, 128.7, 129.3, 130.2, 130.9, 131.5, 133.1, 133.3, 137.3, 139.5, 139.8, 141.3; **HRMS** (ESI, m/z) calcd for $C_{20}H_{15}NO_2S$ $[M+H]^+$ 334.0902, found 334.0886.

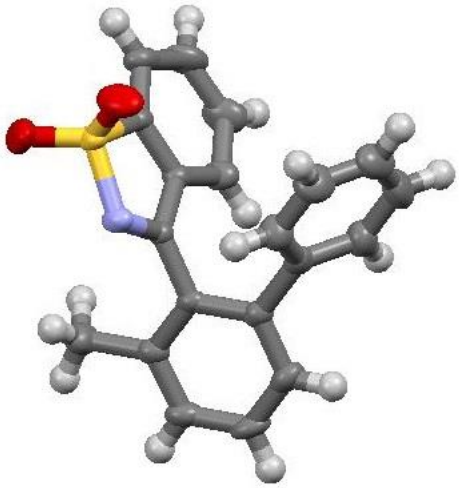
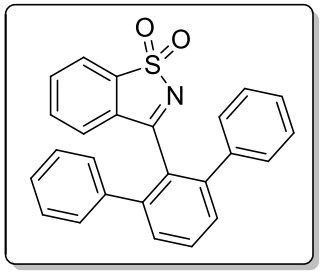


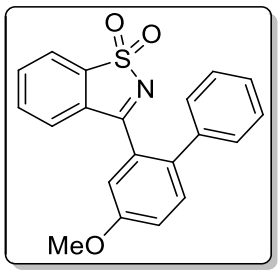
Figure S1. X-ray crystal structure of **3ca** (ellipsoid contour at 50% probability level)

Empirical formula	$C_{20}H_{15}NO_2S$
Formula weight	333.39
Temperature/K	273.15
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	7.4364(5)
b/Å	26.4068(16)
c/Å	8.4485(5)
α/°	90
β/°	94.973(2)
γ/°	90
Volume/Å^3	1652.80(18)
Z	4
ρ_{calc}g/cm^3	1.340
μ/mm^{-1}	0.207
F(000)	696.0
Crystal size/mm^3	0.74 × 0.52 × 0.41
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.08 to 49.998
Index ranges	$-8 \le h \le 8$, $-31 \le k \le 31$, $-10 \le l \le 10$
Reflections collected	19836
Independent reflections	2892 [R_{int} = 0.0318, R_{sigma} = 0.0167]
Data/restraints/parameters	2892/0/218
Goodness-of-fit on F^2	1.086
Final R indexes [I>=2σ (I)]	R_1 = 0.0461, wR_2 = 0.1078
Final R indexes [all data]	R_1 = 0.0477, wR_2 = 0.1089
Largest diff. peak/hole / e Å^{-3}	0.36/-0.50



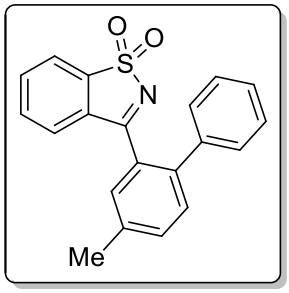
3-([1,1':3',1''-terphenyl]-2'-yl)benzo[*d*]isothiazole 1,1-dioxide (3da):

Yield 80% (63 mg); colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 180-182 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.00 (d, *J* = 7.8 Hz, 1H), 7.19-7.22 (comp, 2H), 7.24 (app d, *J* = 7.8 Hz, 3H), 7.26-7.28 (comp, 5H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 2H), 7.69-7.73 (comp, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 122.3, 125.7, 128.1, 128.3, 128.6, 129.2, 129.7, 130.9, 132.2, 132.8, 133.2, 139.4, 139.5, 142.3, 173.6; **HRMS** (ESI, m/z) calcd for $C_{25}H_{17}NO_2S$ $[M+H]^+$ 396.1058; found 396.1057.



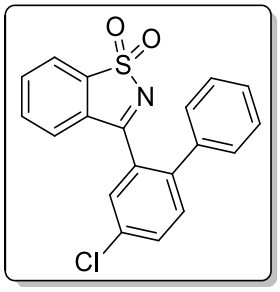
3-(4-methoxy-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3ea):

Combined Yield 77% (55 mg); **mono**:**bis** 7:1; colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.94 (s, 3H), 6.95 (d, *J* = 8.0 Hz, 1H), 7.13-7.17 (m, 1H) 7.23 (d, *J* = 7.6 Hz, 2H), 7.28-7.30 (comp, 2H), 7.32-7.36 (comp, 3H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.82 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.9, 114.3, 119.0, 122.3, 126.6, 127.9, 128.9, 129.2, 130.7, 130.9, 131.9, 132.9, 133.0, 133.9, 139.5, 139.7, 159.4, 174.3; **HRMS**(ESI, m/z) calcd for $C_{20}H_{15}NO_3S$ $[M+H]^+$ 350.0851, found 350.0852.



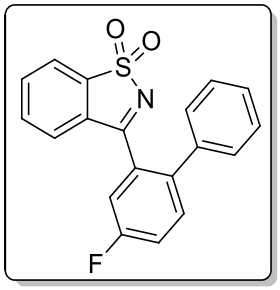
3-(4-methyl-[1,1'-biphenyl]-2 yl)benzo[*d*]isothiazole 1,1-dioxide (3fa):

Yield 87% (58 mg); colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 110-112 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.48 (s, 3H), 6.90 (d, *J* = 8.0 Hz, 1H), 7.12-7.17 (m, 1H), 7.23 (t, *J* = 7.6 Hz, 2H), 7.27 (td, *J* = 7.6 Hz, 0.8 Hz, 1H), 7.34-7.36 (comp, 2H), 7.49 (td, *J* = 7.9 Hz, 0.7 Hz, 1H), 7.52-7.56 (comp, 3H), 7.80 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 21.1, 122.3, 126.6, 128.1, 129.0, 129.2, 129.7, 130.5, 130.6, 131.1, 132.8, 133.0, 133.1, 138.3, 138.7, 139.7, 139.8, 174.6; **HRMS** (ESI, m/z) calcd for $C_{20}H_{15}NO_2S$ $[M+Na]^+$ 356.0721, found 356.0720.



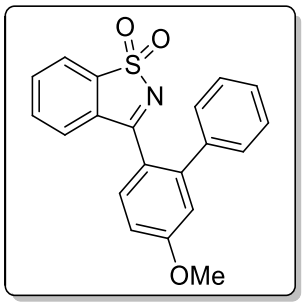
3-(4-chloro-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3ga):

Yield 73% (52 mg); colourless solid; $\mathbf{R_f}$ 0.4 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 120-122 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.89 (d, *J* = 7.6 Hz, 1H), 7.18 (app t, *J* = 7.2 Hz, 1H), 7.23 (app s, 1H), 7.25 (app s, 1H), 7.29-7.34 (comp, 3H), 7.52 (app t, *J* = 7.4 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.68 (dd, *J* = 8.4 Hz, 2.0 Hz, 1H), 7.73 (m, 1H), 7.81 (d, *J* = 7.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 122.5, 126.3, 128.7, 129.1, 129.9, 130.5, 131.2, 131.9, 132.3, 133.2, 134.4, 136.7, 138.6, 138.6, 139.7, 140.0, 173.0; **HRMS** (ESI, m/z) calcd for $C_{19}H_{12}ClNO_2S$ $[M+H]^+$ 354.0356; found 354.0346.



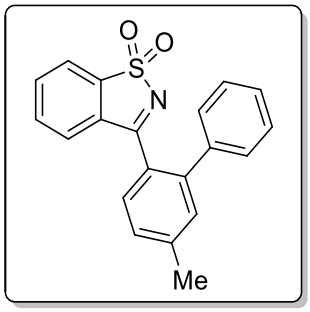
3-(4-fluoro-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3ha):

Combined Yield 73% (50 mg); **mono**:**bis** 14:1; colourless solid; $\mathbf{R_f}$ 0.4 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 6.99 (d, *J* = 7.8 Hz, 1H), 7.18 (app t, *J* = 7.5 Hz, 1H), 7.25 (app t, *J* = 7.5 Hz, 2H), 7.34 (dd, *J* = 7.2 Hz, 0.9 Hz, 1H), 7.36 (app s, 1H), 7.37 (app s, 1H), 7.45 (td, *J* = 8.1 Hz, 1.2 Hz, 1H), 7.51-7.56 (comp, 3H), 7.79 (d, *J* = 7.2 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 119.6 (d, $^2J_{F–C}$ = 23.1 Hz), 122.4, 125.6 (d, $^4J_{F–C}$ = 3.6 Hz), 126.3, 128.7, 128.9, 129.0 (d, $^3J_{F–C}$ = 6.75 Hz), 129.2 (d, $^3J_{F–C}$ = 6.6 Hz), 130.0, 130.0, 130.5, 130.5 (d, $^2J_{F–C}$ = 20.8 Hz), 132.6, 133.1, 133.1, 139.6, 159.7 (d, $^1J_{F–C}$ = 247.9 Hz), 172.9 (d, *J* = 3.0 Hz); **HRMS** (ESI, m/z) calcd for $C_{19}H_{12}FNO_2S$ $[M+H]^+$ 338.0651, found 338.0650.



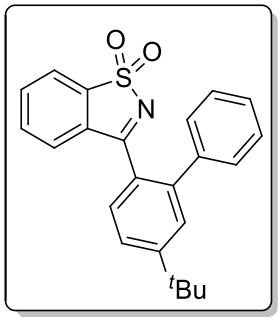
3-(5-methoxy-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3ia):

Yield 70% (49 mg); colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 88-90 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.99 (s, 3H), 6.96 (d, *J* = 7.6 Hz, 1H), 7.11 (dd, *J* = 8.6 Hz, 2.6 Hz, 1H), 7.18 (d, *J* = 2.4 Hz, 1H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.28 (s, 1H), 7.29-7.32 (comp, 2H), 7.40 (d, *J* = 7.2 Hz, 2H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.9, 113.6, 116.3, 122.2 (x 2), 122.4, 126.6, 128.5, 129.0, 129.2, 131.4, 132.4, 132.6, 132.8, 139.9, 143.7, 162.8, 173.8; **HRMS** (ESI, m/z) calcd for $C_{20}H_{15}NO_3S$ $[M+H]^+$ 350.0851, found 350.0840.



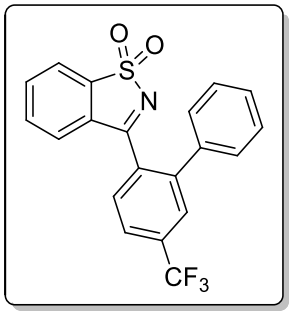
3-(5-methyl-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3ja):

Combined Yield 88% (59 mg); **mono**:**bis** 12:1; colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.56 (s, 3H), 6.95 (d, *J* = 7.6 Hz, 1H), 7.16-7.20 (m,1H), 7.24 (app s, 1H), 7.28 (m, 1H), 7.31 (dd, *J* = 7.6 Hz, 0.8 Hz, 1H), 7.37 (app s, 1H), 7.39 (app s, 1H), 7.41-7.42 (m, 1H), 7.49 (app s, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.81 (d, *J* = 6.8 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 21.8, 122.2, 126.6, 127.1, 128.3, 128.9, 128.9, 129.2, 130.3, 131.2, 131.4, 132.7, 132.9, 139.8, 139.9, 141.6, 142.9, 174.3; **HRMS** (ESI, m/z) calcd for $C_{20}H_{15}NO_2S$ $[M+H]^+$ 334.0902, found 334.0904.



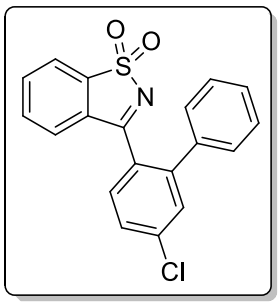
3-(5-(tert-butyl)-4'-methoxy-[1,1'-biphenyl]-2yl)benzo[*d*] isothiazole 1,1-dioxide (3ka):

Combined Yield 66% (50 mg); **mono**:**bis** 32:1; colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 160-162 ^oC; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 1.44 (s, 9H), 6.97 (d, *J* = 8.0 Hz, 1H), 7.14-7.19 (m, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.26-7.27 (m, 1H), 7.28 (app t, *J* = 7.2 Hz, 1H), 7.36-7.39 (comp, 2H), 7.49 (td, *J* = 7.4 Hz, 0.8 Hz, 1H), 7.59 (dd, *J* = 8.2 Hz, 1.8 Hz, 1H), 7.65 (d, *J* = 2.0 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 31.4, 35.4, 122.2, 125.3, 126.7, 127.1, 127.8, 128.2, 128.9, 129.3, 130.1, 131.2, 132.8, 132.9, 139.8, 140.4, 141.4, 156.1, 174.3; **HRMS** (ESI, m/z) calcd for $C_{23}H_{21}NO_2S$ $[M+H]^+$ 376.1371, found 376.1373.



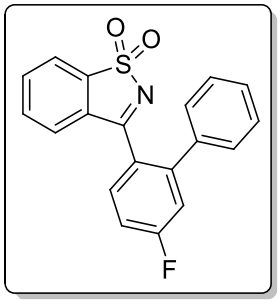
3-(5-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole1,1-dioxide (3la):

Combined Yield 74% (58 mg); **mono**:**bis** 6:1; colourless solid; $\mathbf{R_f}$ 0.3 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 6.90 (d, *J* = 7.8 Hz, 1H), 7.22 (app t, *J* = 7.5 Hz, 1H), 7.27-7.30 (comp, 2H), 7.33 (app t, *J* = 7.8 Hz, 1H), 7.38-7.40 (comp, 2H), 7.54 (app t, *J* = 7.5 Hz, 1H), 7.82-7.84 (comp, 2H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.92 (app s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 122.6, 124.9 (q, *J* = 3.5 Hz), 126.1, 127.4 (q, *J* = 3.5 Hz), 128.8, 128.9, 129.2, 129.3, 130.4, 130.7, 133.2, 133.3, 133.3, 134.1 (q, *J* = 32.8 Hz), 139.0 (q, *J* = 207.5 Hz), 142.4, 173.1; **HRMS** (ESI, m/z) calcd for $C_{20}H_{12}F_3NO_2S$ $[M+H]^+$ 388.0619, found 388.0618.



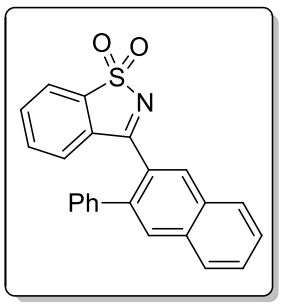
3-(5-chloro-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3ma):

Combined Yield 73% (54 mg); **mono**:**bis** 3:1; colourless solid; $\mathbf{R_f}$ 0.4 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 98-100 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 6.89 (d, *J* = 7.8 Hz, 1H), 7.19-7.22 (m, 1H), 7.25-7.27 (comp, 2H), 7.30 (td, *J* = 7.5 Hz, 0.8 Hz, 1H), 7.35-7.36 (comp, 2H), 7.52 (td, *J* = 7.5 Hz, 0.8 Hz, 1H), 7.56 (dd, *J* = 8.1 Hz, 2.1 Hz, 1H), 7.66 (d, *J* = 1.8 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.81 (d, *J* = 7.8 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 122.5, 126.3, 128.3, 128.4, 129.0, 129.1, 129.2, 130.7, 130.7, 131.6, 133.1, 133.1, 138.5, 138.5, 139.7, 143.2, 173.3; **HRMS** (ESI, m/z) calcd for $C_{19}H_{12}ClNO_2S$ $[M+H]^+$ 354.0356, found 354.0358.



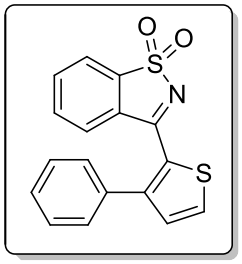
3-(5-fluoro-[1,1'-biphenyl]-2-yl)benzo[d]isothiazole 1,1-dioxide (3na):

Combined Yield 72% (50 mg); **mono**:**bis** 13:1; colourless solid; $\mathbf{R_f}$ 0.4 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.90 (d, *J* = 8.0 Hz, 1H), 7.18-7.22 (m, 1H), 7.24 (app s, 1H), 7.26-7.29 (comp, 2H), 7.30 (app t, *J* = 7.6 Hz, 1H), 7.34-7.38 (comp, 3H), 7.51 (app t, *J* = 7.6 Hz, 1H), 7.75 (dd, *J* = 8.4 Hz, 5.6 Hz, 1H), 7.80 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 115.4 (d, $^2J_{F–C}$ = 21.7 Hz), 117.6 (d, $^2J_{F–C}$ = 22.2 Hz), 122.4, 125.9, 126.3, 129.0, 129.0, 129.1, 130.8, 132.6 (d, $^3J_{F–C}$ = 9.1 Hz), 133.0, 133.1, 138.6 (d, $^4J_{F–C}$ = 1.5 Hz), 139.7, 144.3 (d, $^3J_{F–C}$ = 8.5 Hz), 164.8 (d, $^1J_{F–C}$ = 252.3 Hz), 173.3; **HRMS** (ESI, m/z) calcd for $C_{19}H_{12}FNO_2S$ $[M+H]^+$ 338.0651, found 338.0635.



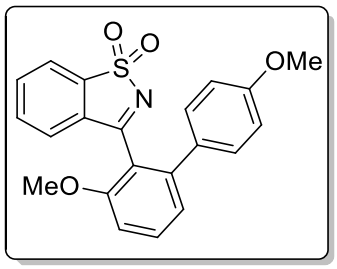
3-(3-phenylnaphthalen-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3oa):

Yield 84% (62 mg); colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 122-124 ^oC; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.98 (d, *J* = 7.6 Hz, 1H), 7.19 (app t, *J* = 7.4 Hz, 1H), 7.28-7.33 (comp, 3H), 7.47 (d, *J* = 7.6 Hz, 2H), 7.51 (app t, *J* = 7.6 Hz, 1H), 7.61 (td, *J* = 7.5 Hz, 0.9 Hz, 1H), 7.68 (td, *J* = 7.5 Hz, 0.9 Hz, 1H), 7.82 (d, *J* = 7.6 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 2H), 8.10 (s, 1H), 8.30 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 122.3, 126.7, 127.5, 128.2, 128.2 (x 2), 128.8, 128.9, 129.0, 129.3, 129.9, 131.0, 131.3, 132.0, 132.9, 133.1, 134.9, 137.6, 139.7, 139.9, 174.2; **HRMS** (ESI, m/z) calcd for $C_{23}H_{15}NO_2S$ $[M+H]^+$ 370.0902, found 370.0893.



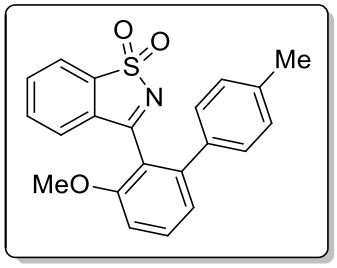
3-(3-phenylthiophen-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3pa):

Yield 80% (52 mg); colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 114-116 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.93 (d, *J* = 8.0 Hz, 1H), 7.23 (td, *J* = 7.8 Hz, 0.8 Hz, 1H), 7.28-7.31 (comp, 3H), 7.35-7.38 (comp, 2H), 7.39 (d, *J* = 5.2 Hz, 1H), 7.54 (td, *J* = 7.6 Hz, 0.8 Hz, 1H), 7.76 (d, *J* = 5.2 Hz, 1H), 7.86 (d, *J* = 7.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 122.5, 127.4, 127.7, 129.0, 129.2, 129.4, 130.2, 131.3, 132.3, 132.9, 133.0, 135.5, 140.7, 147.8, 166.6; **HRMS** (ESI, m/z) calcd for $C_{17}H_{11}NO_2S_2$ $[M+H]^+$ 326.0310, found 326.0309.



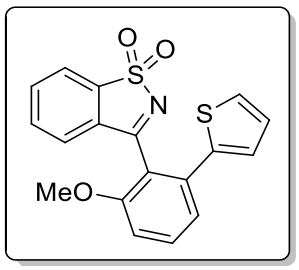
3-(3,4'-dimethoxy-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole1,1-dioxide (3bb):

Yield 70% (53 mg); colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 120-122 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.70 (s, 3H), 3.80 (s, 3H), 6.74-6.77 (comp, 2H), 7.03 (d, *J* = 8.0 Hz, 1H), 7.10 (d, *J* = 7.6 Hz, 1H), 7.13 (dd, *J* = 8.0 Hz, 0.4 Hz, 1H), 7.18-7.22 (comp, 2H), 7.46 (td, *J* = 7.6, 0.8 Hz, 1H), 7.55 (d,*J* = 8.0 Hz, 1H), 7.58-7.60 (m, 1H), 7.83 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.4, 56.3, 110.0, 114.1, 118.3, 122.3, 122.8, 125.9, 130.4, 131.5, 132.2, 132.5, 132.9, 133.5, 139.5, 142.9, 157.8, 159.5, 172.1; **HRMS** (ESI, m/z) calcd for $C_{21}H_{17}NO_4S$ $[M+H]^+$ 380.0957, found 380.0959.



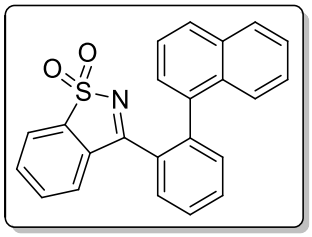
3-(3-methoxy-4'-methyl-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3bc):

Yield 84% (61 mg); colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 162-164 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.24 (s, 3H), 3.80 (s, 3H), 7.02-7.06 (comp, 3H), 7.14-7.16 (comp, 4H), 7.48 (app t, *J* = 7.6 Hz, 1H), 7.55-7.60 (comp, 2H), 7.83 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 21.2. 56.3, 110.1, 118.3, 122.3, 122.9, 125.9, 129.0, 129.4, 132.2, 132.5, 132.9, 133.5, 136.2, 137.9, 139.5, 143.3, 157.8, 172.1; **HRMS** (ESI, m/z) calcd for $C_{21}H_{17}NO_3S$ $[M+H]^+$ 364.1007, found 364.0997.



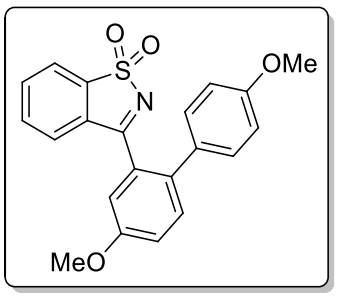
3-(2-methoxy-6-(thiophen-2-yl)phenyl)benzo[*d*]isothiazole1,1-dioxide (3bd):

Yield 76% (54 mg); colourless solid; $\mathbf{R_f}$ 0.4 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 88-90 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.78 (s, 3H), 6.84 (dd, *J* = 4.8 Hz, 3.6 Hz, 1H), 6.96 (dd, *J* = 3.6 Hz, 0.8 Hz, 1H), 7.03 (d, *J* = 8.4 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 7.17 (dd, *J* = 5.0 Hz, 0.6 Hz, 1H), 7.24-7.25 (m, 1H), 7.48 (app t, *J* = 7.6 Hz, 1H), 7.54 (app t, *J* = 8.0 Hz, 1H), 7.60 (app t, *J* = 7.4 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 56.4, 110.8, 118.1, 122.4, 122.8, 125.4, 127.0, 128.0, 128.2, 132.3, 132.3, 133.1, 133.7, 135.4, 139.4, 140.2, 157.9, 171.8; **HRMS** (ESI, m/z) calcd for $C_{18}H_{13}NO_3S_2$ $[M+H]^+$ 356.0415, found 356.0406.



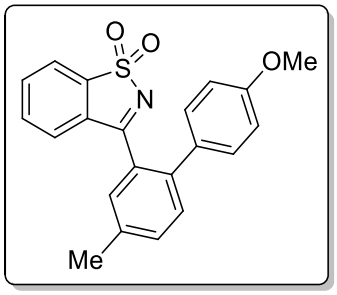
3-(2-(naphthalen-1-yl)phenyl)benzo[*d*]isothiazole1,1-dioxide (3be):

Yield 65% (48 mg); colourless solid; $\mathbf{R_f}$ 0.4 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 152-154 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.00-7.06 (comp, 2H), 7.31 (app t, *J* = 7.4 Hz, 1H), 7.34-7.39 (comp, 2H), 7.44-7.50 (comp, 2H), 7.63-7.68 (comp, 3H), 7.73-7.79 (comp, 3H), 7.82 (d, *J* = 7.6 Hz, 1H), 7.94 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 122.2, 125.2, 125.4, 125.6, 126.2, 127.0, 128.3, 128.7, 129.0, 129.1, 130.0, 130.8, 131.4, 131.4, 131.6, 132.4, 132.6, 132.9, 133.8, 136.8, 139.4, 139.9, 173.7; **HRMS** (ESI, m/z) calcd for $C_{23}H_{15}NO_2S$ $[M+H]^+$ 370.0902, found 370.0888.



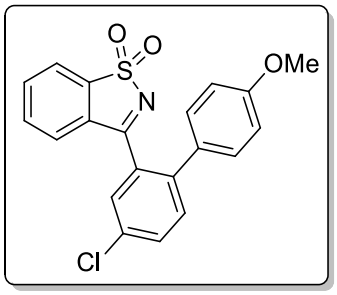
3-(4,4'-dimethoxy-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3db):

Yield 65% (49 mg); colourless solid; $\mathbf{R_f}$ 0.7 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 140-142 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.68 (s, 3H), 3.90 (s, 3H), 6.73-6.76 (comp, 2H), 6.91 (d, *J* = 7.6 Hz, 1H), 7.20-7.25 (comp, 4H), 7.30 (d, *J* = 7.6 Hz, 1H), 7.49 (dd, *J* = 7.6 Hz, 0.4 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.4, 55.9, 114.1, 114.4, 119.2, 122.3, 126.7, 130.3, 130.5, 131.0, 131.8. 132.0, 132.9, 133.1, 133.7, 139.7, 159.1, 159.5, 174.5; **HRMS** (ESI, m/z) calcd for $C_{21}H_{17}NO_4S$ $[M+H]^+$ 380.0957, found 380.0946.



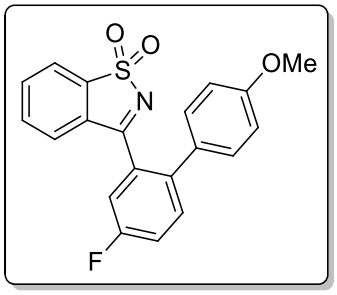
3-(4'-methoxy-4-methyl-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole1,1-dioxide (3eb):

Yield 86% (63 mg); colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 126-128 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.46 (s, 3H), 3.68, (s, 3H), 6.74-6.77 (comp, 2H), 6.89 (d, *J* = 8.0 Hz, 1H), 7.25-7.26 (m, 1H), 7.26-7.27 (m, 1H), 7.29 (dd, *J* = 7.6 Hz, 0.8 Hz, 1H), 7.47-7.51 (comp, 3H), 7.53 (m, 1H), 7.80 (dd, *J* = 7.6 Hz, 0.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 21.1, 55.4, 114.4, 122.2, 126.7, 129.5, 130.3 (x 2), 130.5, 131.1, 132.2, 132.8, 133.1, 133.1, 137.8, 138.3, 139.7, 159.6, 174.8; **HRMS** (ESI, m/z) calcd for $C_{21}H_{17}NO_3S$ $[M+H]^+$ 364.1007, found 364.0995.



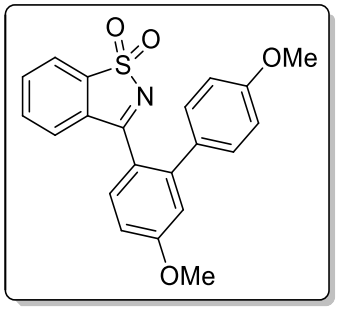
3-(4-chloro-4'-methoxy-[1,1'-biphenyl]-2yl)benzo[*d*]isothiazole1,1-dioxide (3fb):

Combined Yield 68% (54 mg); **mono**:**bis** 10:1; colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.71 (s, 3H), 6.77-6.80 (comp, 2H), 6.89 (d, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 2.0 Hz, 1H), 7.33 (td, *J* = 8.0 Hz, 0.9 Hz, 1H), 7.53 (dd, *J* = 7.6 Hz, 0.8 Hz, 1H), 7.56-7.60 (comp, 2H), 7.66 (dd, *J* = 8.4 Hz, 2.4 Hz, 1H), 7.72 (d, *J* = 2.0 Hz, 1H), 7.83 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.4, 114.6, 122.5, 126.4, 129.8, 130.3, 130.6, 130.9, 131.0, 131.7, 132.2, 133.1, 133.2, 133.9, 139.6, 139.7, 160.1, 173.2; **HRMS** (ESI, m/z) calcd for $C_{20}H_{14}ClNO_3S$ $[M+H]^+$ 384.0461, found 384.0448.



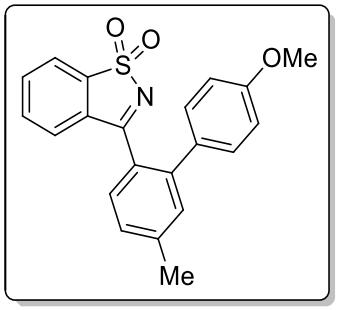
3-(4-fluoro-4'-methoxy-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3gb):

Combined Yield 82% (62 mg); **mono**:**bis** 9:1; colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 3.69 (s, 3H), 6.78 (d, *J* = 9.0 Hz, 2H), 6.96 (d, *J* = 8.0 Hz, 1H), 7.30 (dd, *J* = 8.7 Hz, 1.5 Hz, 2H), 7.34 (td, *J* = 7.6 Hz, 0.8 Hz, 1H), 7.41-7.45 (m, 1H), 7.50-7.52 (comp, 2H), 7.53 (dd, *J* = 7.5 Hz, 0.9 Hz, 1H), 7.80 (d, *J* = 7.8 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 55.4, 114.2, 119.5 (d, $^2J_{F–C}$ = 23.2 Hz), 122.4, 124.8, 125.6 (d, $^3J_{F–C}$ = 3.6 Hz), 126.4, 128.6 (d, $^2J_{F–C}$ = 16.9 Hz), 129.5 (d, $^3J_{F–C}$ = 8.7 Hz), 130.6, 131.7, 131.8, 132.4 (d, $^4J_{F–C}$ = 3.1 Hz), 133.1, 133.2, 139.6, 159.8 (d, $^1J_{F–C}$ = 247.0 Hz), 160.0, 173.2; **HRMS** (ESI, m/z) calcd for $C_{20}H_{15}FNO_3S$ $[M+H]^+$ 368.0757, found 368.0756.



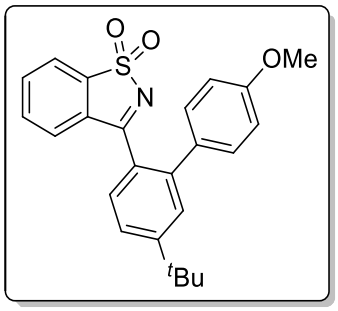
3-(4',5-dimethoxy-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3hb):

Combined Yield 83% (65 mg); **mono**:**bis** 8:1; colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.69 (s, 3H), 3.94 (s, 3H), 6.75-6.79 (comp, 2H), 6.90 (d, *J* = 8.0 Hz, 1H), 7.03 (dd, *J* = 8.6 Hz, 2.6 Hz, 1H), 7.10 (d, *J* = 2.4 Hz, 1H), 7.26-7.30 (comp, 3H), 7.48 (td, *J* = 7.5 Hz, 0.7 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.79 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.4, 55.8, 113.2, 114.1, 114.5, 115.9, 122.2, 122.3, 126.8, 130.4, 131.4, 132.4, 132.6, 132.9, 139.9, 143.4, 160.0, 162.8, 174.0; **HRMS** (ESI, m/z) calcd for $C_{21}H_{17}NO_4S$ $[M+H]^+$ 380.0957, found 380.0948.



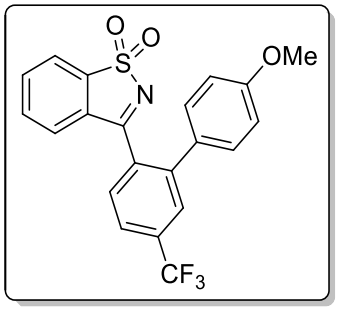
3-(4'-methoxy-5-methyl-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3ib):

Combined Yield 61% (46 mg); **mono**:**bis** 9:1; colourless solid; $\mathbf{R_f}$ 0.7 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 2.52 (s, 3H), 3.69 (s, 3H), 6.76 (d, *J* = 9.0 Hz, 2H), 6.90 (d, *J* = 7.8 Hz, 1H), 7.27-7.29 (comp, 3H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.43 (app s, 1H), 7.49 (app t, *J* = 7.5, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.80 (d, *J* = 7.8 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 21.8, 55.4, 114.4, 122.2, 126.7, 127.0, 128.4, 130.3, 130.4, 131.1, 131.3, 132.4, 132.7, 133.0, 139.8, 141.2, 142.9, 159.7, 174.6; **HRMS** (ESI, m/z) calcd for $C_{21}H_{17}NO_3S$ $[M+H]^+$ 364.1007, found 364.0993.



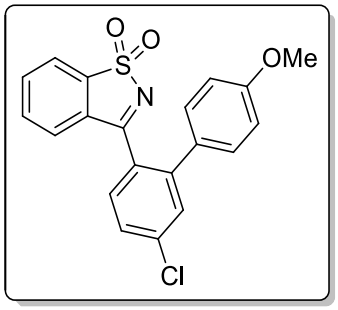
3-(5-(tert-butyl)-4'-methoxy-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3jb):

Combined Yield 60% (50 mg); **mono**:**bis** 8:1; colourless solid; $\mathbf{R_f}$ 0.7 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 1.40 (s, 9H), 3.68 (s, 3H), 6.74-6.78 (comp, 2H), 6.92 (d, *J* = 7.6 Hz, 1H), 7.24-7.25 (m, 1H), 7.26-7.28 (comp, 2H), 7.47 (td, *J* = 7.4 Hz, 0.7 Hz, 1H), 7.52 (dd, *J* = 8.2 Hz, 1.8 Hz, 1H), 7.58 (d, *J* = 2.0 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 31.4, 35.4, 55.4, 114.4, 122.2, 124.9, 126.8, 127.0, 127.6, 130.1, 130.5, 131.3, 132.7, 132.9, 133.0, 139.8, 141.0, 156.0, 159.8, 174.6; **HRMS** (ESI, m/z) calcd for $C_{24}H_{23}NO_3S$ $[M+H]^+$ 406.1477, found 406.1468.



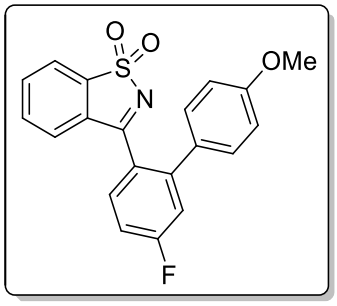
3-(4'-methoxy-5-(trifluoromethyl)-[1,1'-biphenyl]-2yl)benzo[*d*] isothiazole1,1-dioxide (3kb):

Yield 70% (58 mg); colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 102-104 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.71(s, 3H), 6.78-6.82 (comp, 2H), 6.87 (d, *J* = 8.0 Hz, 1H), 7.30-7.32 (comp, 2H), 7.34 (dd, *J* = 7.6 Hz, 0.8 Hz, 1H), 7.55 (td, *J* = 7.4 Hz, 0.5 Hz, 1H), 7.78 (dd, *J* = 8.0 Hz, 1.2 Hz, 1H), 7.83-7.85 (comp, 2H), 7.87 (app s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.5, 114.8 , 122.6, 124.3 (q, *J* = 3.6 Hz), 126.2, 127.2 (q, *J* = 3.6 Hz), 130.5, 130.7, 130.7, 132.9, 133.3, 133.4, 134.1 (q, *J* = 32.4 Hz), 139.7, 140.9 (q, *J* = 227.7 Hz), 142.0, 160.4, 173.4; **HRMS** (ESI, m/z) calcd for $C_{21}H_{14}F_3NO_3S$ $[M+H]^+$ 418.0725, found 418.0714.



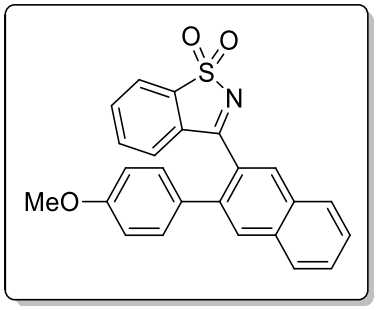
3-(5-chloro-4'-methoxy-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3lb):

Yield 70% (54 mg); colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 136-138 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.68 (s, 3H), 6.73-6.77 (comp, 2H), 6.84 (d, *J* = 7.6 Hz, 1H), 7.23-7.25 (comp, 2H), 7.29 (dd, *J* = 7.6 Hz, 0.8 Hz, 1H), 7.46-7.52 (comp, 2H), 7.59 (d, *J* = 2.0 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.5, 114.6 , 122.4, 126.4, 127.9, 128.1, 130.4 (x 2), 130.8, 130.9, 131.6, 133.0, 133.2, 138.4, 139.8, 142.9, 160.2, 173.6; **HRMS** (ESI, m/z) calcd for $C_{20}H_{14}ClNO_3S$ $[M+H]^+$ 384.0461, found 384.0448.



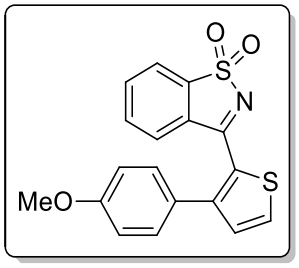
3-(5-fluoro-4'-methoxy-[1,1'-biphenyl]-2-yl)benzo[*d*]isothiazole1,1-dioxide (3mb):

Yield 68% (50 mg); colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 120-122 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.67 (s, 3H), 6.73-6.77 (comp, 2H), 6.85 (d, *J* = 8.0 Hz, 1H), 7.20 (td, *J* = 8.2 Hz, 2.7 Hz, 1H), 7.24-7.26 (comp, 2H), 7.28-7.31 (comp, 2H), 7.49 (td, *J* = 7.6 Hz, 0.8 Hz, 1H), 7.70 (dd, *J* = 8.8 Hz, 5.6 Hz, 1H), 7.79 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.4, 114.6, 115.0 (d, $^{2}J_{F–C}$ = 21.9 Hz), 117.3 (d, $^{2}J_{F–C}$ = 22.1 Hz), 122.4, 125.8 (d, $^{4}J_{F–C}$ = 2.6 Hz), 126.5, 130.3, 130.9, 131.1, 132.6 (d, $^{3}J_{F–C}$ = 9.3 Hz), 133.0, 133.1, 139.8, 144.0 (d, $^{3}J_{F–C}$ = 8.6 Hz), 160.2, 164.9 (d, $^{1}J_{F–C}$ = 252.1 Hz), 173.6; **HRMS** (ESI, m/z) calcd for $C_{20}H_{14}FNO_3S$ $[M+H]^+$ 368.0757, found 368.0763.



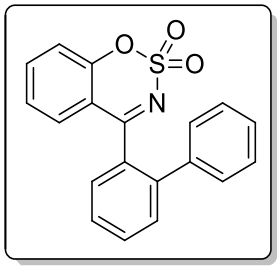
3-(3-(4-methoxyphenyl)naphthalen-2-yl)benzo[*d*]isothiazole 1,1-dioxide (3nb):

Yield 88% (70 mg); colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 80-82 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.71 (s, 3H), 6.81 (d, *J* = 8.8 Hz, 2H), 6.95 (d, *J* = 7.6 Hz, 1H), 7.31 (app t, *J* = 7.6 Hz, 1H), 7.38-7.40 (comp, 2H), 7.52 (app t, *J* = 7.6 Hz, 1H), 7.59 (app t, *J* = 7.6 Hz, 1H), 7.65 (app t, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 7.6 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 2H), 8.04 (s, 1H), 8.27 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.4, 114.5, 122.2, 126.8, 127.3, 128.1, 128.3, 128.8, 128.8, 129.4, 130.4, 130.9, 131.3, 131.8, 132.4, 132.9, 133.1, 135.0, 137.2, 139.7, 159.6, 174.4; **HRMS** (ESI, m/z) calcd for $C_{24}H_{17}NO_3S$ $[M+H]^+$ 400.1007, found 400.1008.



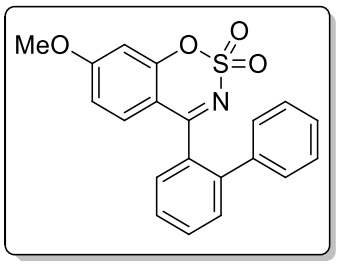
3-(3-(4-methoxyphenyl)thiophen-2-yl)benzo[*d*]isothiazole1,1dioxide (3ob):

Yield 82% (58 mg); colourless solid; $\mathbf{R_f}$ 0.4 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 136-138 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.76 (s, 3H), 6.80-6.84 (comp, 2H), 6.96 (d, *J* = 7.6 Hz, 1H), 7.25 (dd, *J* = 7.6 Hz, 0.8 Hz, 1H), 7.27-7.30 (comp, 2H), 7.34 (d, *J* = 4.8 Hz, 1H), 7.55 (td, *J* = 7.5 Hz, 0.92 Hz, 1H), 7.73 (d, *J* = 4.8 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.5, 114.6, 122.4, 126.8, 127.5, 128.0, 130.3, 130.7, 131.2, 132.2, 133.0, 133.0, 140.7, 147.6, 160.3, 166.7; **HRMS** (ESI, m/z) calcd for $C_{18}H_{13}NO_3S_2$ $[M+H]^+$ 356.0415, found 356.0414.



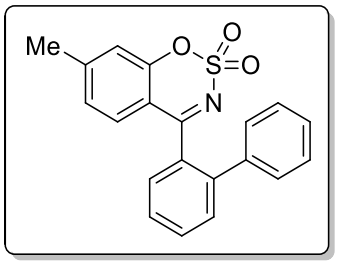
4-([1,1'-biphenyl]-2-yl)benzo[*e*][1,2,3]oxathiazine 2,2-dioxide (5aa):

Yield 95% (64 mg); colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 78-80 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.97-7.01 (m, 1H), 7.10 (dd, *J* = 8.0 Hz, 1.6 Hz, 1H), 7.12-7.15 (comp, 2H), 7.20 (app t, *J* = 7.4 Hz, 2H), 7.23-7.25 (comp, 2H), 7.46 (td, *J* = 7.8 Hz, 1.5 Hz, 1H), 7.54-7.58 (comp, 2H), 7.67-7.72 (comp, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 117.1, 118.7, 125.4, 127.9, 128.0, 128.7, 129.1, 130.4, 130.5, 131.2, 132.1, 133.3, 136.7, 139.5, 142.2, 153.8, 178.7; **HRMS** (ESI, m/z) calcd for $C_{19}H_{13}NO_3S$ $[M+Na]^+$ 358.0514, found 358.0518.



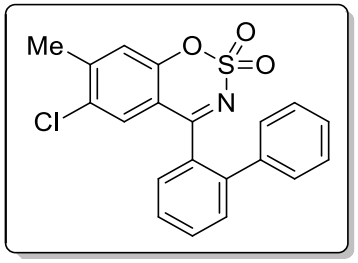
4-([1,1'-biphenyl]-2-yl)-7-methoxybenzo[*e*][1,2,3]oxathiazine2,2-dioxide (5ba):

Yield 74% (54 mg); colourless solid; $\mathbf{R_f}$ 0.7 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 56-58 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.84 (s, 3H), 6.53 (dd, *J* = 9.0 Hz, 2.6 Hz, 1H), 6.63 (d, *J* = 2.4 Hz, 1H), 7.05 (d, *J* = 8.8 Hz, 1H), 7.18-7.22 (m, 1H), 7.24-7.26 (m, 1H), 7.27-7.31 (comp, 3H), 7.56 (td, *J* = 6.6 Hz, 1.2 Hz, 1H), 7.59 (d, *J* = 4.8 Hz, 1H), 7.64-7.66 (m, 1H), 7.70 (td, *J* = 7.6 Hz, 1.5 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 56.3, 102.8, 110.5, 112.9, 127.8, 127.9, 128.7, 129.0, 130.2, 130.5, 131.8, 132.9, 133.5, 139.5, 141.9, 156.3, 166.3, 177.8; **HRMS** (ESI, m/z) calcd for $C_{20}H_{15}NO_4S$ $[M+H]^+$ 366.0800, found 366.0840.



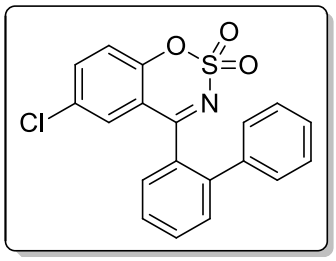
4-([1,1'-biphenyl]-2-yl)-7-methylbenzo[*e*][1,2,3]oxathiazine2,2-dioxide (5ca):

Yield 79% (55 mg); colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 154-156 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.33 (s, 3H), 6.79 (d, *J* = 8.0 Hz, 1H), 6.95 (app s, 1H), 6.98 (d, *J* = 8.0 Hz, 1H), 7.15 (t, *J* = 7.0 Hz, 1H), 7.21 (app t, *J* = 7.4 Hz, 2H), 7.25 (d, *J* = 7.2 Hz, 2H), 7.52-7.57 (comp, 2H), 7.63-7.69 (comp, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 22.2, 114.8, 118.9, 126.4, 127.8, 127.9, 128.7, 129.1, 130.3, 130.5, 131.0, 131.9, 133.4, 139.6, 142.1, 149.2, 153.9, 178.4; **HRMS** (ESI, m/z) calcd for $C_{20}H_{15}NO_3S$ $[M+Na]^+$ 372.0670, found 372.0662.



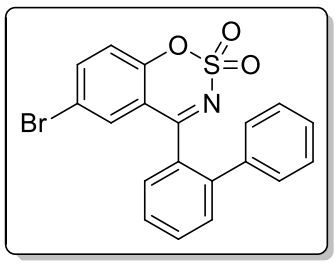
4-([1,1'-biphenyl]-2-yl)-6-chloro-7methylbenzo[*e*][1,2,3] oxathiazine2,2-dioxide (5da):

Yield 51% (39 mg); colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 160-162 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.33 (s, 3H), 7.00 (d, *J* = 8.0 Hz, 2H), 7.15-7.17 (m, 1H), 7.23-7.24 (comp, 4H), 7.58-7.72 (comp, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 21.1, 115.7, 120.6, 128.1, 128.1, 128.8, 129.0, 130.6, 130.6, 130.9, 131.0, 132.4, 132.8, 139.6, 142.3, 146.5, 151.9, 177.5; **HRMS** (ESI, m/z) calcd for $C_{20}H_{15}ClNO_3S$ $[M+Na]^+$ 384.0461, found 384.0481.



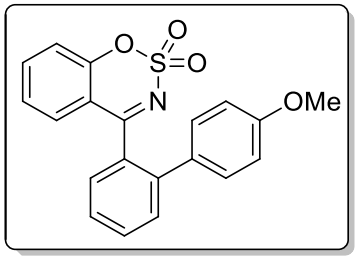
4-([1,1'-biphenyl]-2-yl)-6-chlorobenzo[*e*][1,2,3]oxathiazine 2,2-dioxide (5ea):

Combined Yield 72% (54 mg); **mono**:**bis** 17:1; colourless solid; $\mathbf{R_f}$ 0.4 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 144-146 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.99 (d, *J* = 2.4 Hz, 1H), 7.07 (d, *J* = 8.4 Hz, 1H), 7.12-7.17 (m, 1H), 7.22-7.23 (comp, 4H), 7.36 (dd, *J* = 8.8 Hz, 2.4Hz, 1H), 7.60 (app t, *J* = 7.4 Hz, 2H), 7.72-7.75 (comp, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 117.7, 120.1, 128.2, 128.3, 128.7, 128.9, 129.0, 130.6, 130.6, 130.7, 132.6, 132.7, 136.2, 139.6, 142.4, 152.0, 177.7; **HRMS** (ESI, m/z) calcd for $C_{19}H_{12}ClNO_3S$ $[M+H]^+$ 370.0305, found 370.0292.



4-([1,1'-biphenyl]-2-yl)-6-bromobenzo[*e*][1,2,3]oxathiazine 2,2-dioxide (5fa):

Combined Yield 75% (62 mg); **mono**:**bis** 18:1; colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 120-122 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.00 (d, *J* = 8.8 Hz, 1H), 7.13-7.17 (comp, 2H), 7.22-7.26 (comp, 4H), 7.50 (dd, *J* = 8.8 Hz, 2.0 Hz, 1H), 7.58-7.62 (comp, 2H), 7.72-7.76 (comp, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 118.0, 118.0, 120.3, 128.2, 128.3, 128.9, 129.0, 130.6, 130.8, 132.7, 132.7, 133.6, 139.0, 139.6, 142.4, 152.5, 177.6; **HRMS** (ESI, m/z) calcd for $C_{19}H_{12}BrNO_3S$ $[M+H]^+$ 413.9800, found 413.9820.



4-(4'-methoxy-[1,1'-biphenyl]-2-yl)benzo[*e*][1,2,3]oxathiazine 2,2-dioxide (5ab):

Combined Yield 80% (60 mg); **mono**:**bis** 7:1; colourless solid; $\mathbf{R_f}$ 0.7 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 98-100 ^{o}C (crystallization from $CDCl_3$ and hexane); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.70 (s, 3H), 6.71-6.75 (comp, 2H), 6.99 (td, *J* = 7.6 Hz, 0.93 Hz, 1H), 7.07 (dd, *J* = 8.0 Hz, 1.6 Hz, 1H), 7.13-7.18 (comp, 3H), 7.45-7.49 (m, 1H), 7.50-7.54 (comp, 2H), 7.64-7.69 (comp, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.4, 114.2, 116.9, 118.7, 125.4, 127.5, 130.2, 130.3, 130.4, 131.2, 132.0 (x 2), 133.1, 136.7, 141.7, 153.8, 159.4, 179.0; **HRMS** (ESI, m/z) calcd for $C_{20}H_{15}NO_4S$ $[M+H]^+$ 366.0800, found 366.0811.

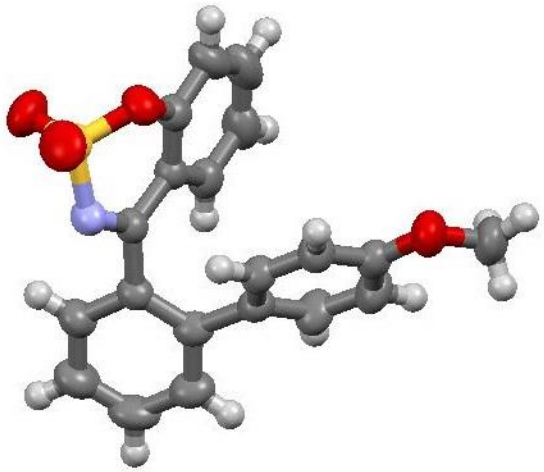
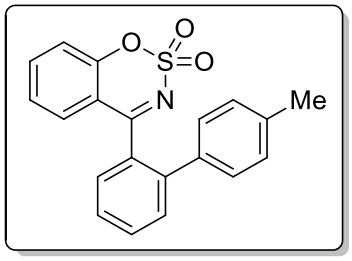


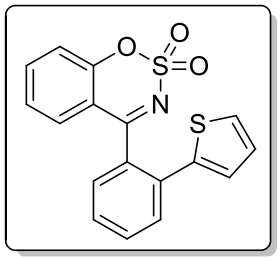
Figure S2. X-ray crystal structure of **5ab** (ellipsoid contour at 50% probability level)

Empirical formula	$C_{20}H_{15}NO_4S$
Formula weight	365.39
Temperature/K	298
Crystal system	Monoclinic
Space group	$P2_1/n$
a/Å	8.107(7)
b/Å	11.495(9)
c/Å	19.194(16)
α/°	90
β/°	93.585(10)
γ/°	90
Volume/$Å^3$	1785(3)
Z	4
$\rho_{calc}g/cm^3$	1.359
μ/mm^{-1}	0.206
F(000)	760.0
Crystal size/mm^3	0.6 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.132 to 52.708
Index ranges	$-10 \leq h \leq 9$, $-14 \leq k \leq 14$, $-23 \leq l \leq 22$
Reflections collected	22553
Independent reflections	3549 [R_{int} = 0.1755, R_{sigma} = 0.1126]
Data/restraints/parameters	3549/0/236
Goodness-of-fit on F^2	0.966
Final R indexes [I>=2σ (I)]	R_1 = 0.0956, wR_2 = 0.2265
Final R indexes [all data]	R_1 = 0.1832, wR_2 = 0.3164
Largest diff. peak/hole / e $Å^{-3}$	0.61/-0.94



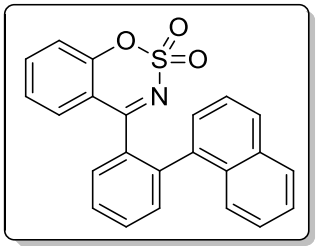
4-(4'-methyl-[1,1'-biphenyl]-2-yl)benzo[*e*][1,2,3]oxathiazine 2,2-dioxide (5ac):

Combined Yield 79% (56 mg); **mono**:**bis** 15:1; colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 100-124 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.21 (s, 3H), 6.97-7.01 (comp, 3H), 7.09 (dd, *J* = 8.0 Hz, 1.6 Hz, 1H), 7.13-7.15 (comp, 3H), 7.47 (td, *J* = 7.8 Hz, 1.6 Hz, 1H), 7.51-7.56 (comp, 2H), 7.63-7.69 (comp, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 21.1, 117.0, 118.6, 125.4, 127.6, 128.9, 129.4, 130.2, 130.5, 131.2, 132.0, 133.1, 136.6, 136.6, 137.8, 142.0, 153.7, 178.9; **HRMS** (ESI, m/z) calcd for $C_{20}H_{15}NO_3S$ $[M+Na]^+$ 372.0670, found 372.0671.



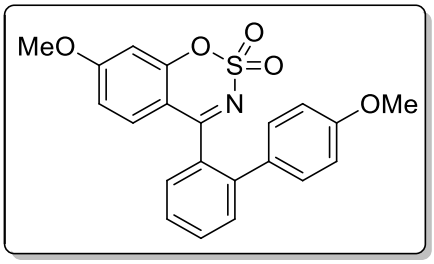
4-(2-(thiophen-2-yl)phenyl)benzo[*e*][1,2,3]oxathiazine 2,2-dioxide (5ad):

Yield 60% (41 mg); colourless solid; $\mathbf{R_f}$ 0.4 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 128-130 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.81 (dd, *J* = 4.8 Hz, 3.6 Hz, 1H), 6.89 (dd, *J* = 3.6 Hz, 1.2 Hz, 1H), 7.05 (td, *J* = 7.6 Hz, 0.8 Hz, 1H), 7.11 (dd, *J* = 7.8 Hz, 1.8 Hz, 1H), 7.16 (dd, *J* = 5.0 Hz, 1.0 Hz, 1H), 7.20 (dd, *J* = 8.4 Hz, 0.8 Hz, 1H), 7.50-7.56 (comp, 2H), 7.63-7.66 (comp, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 117.0, 118.8, 125.6, 127.3, 128.1, 128.1, 128.3, 130.2, 130.5, 130.6, 132.0, 133.2, 134.4, 136.8, 141.0, 153.8, 178.3; **HRMS** (ESI, m/z) calcd for $C_{17}H_{11}NO_3S_2$ $[M+H]^+$ 342.0259, found 342.0293.



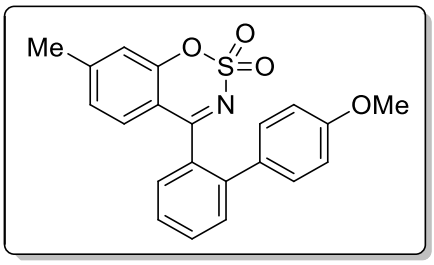
4-(2-(naphthalen-1-yl)phenyl)benzo[e][1,2,3]oxathiazine 2,2-dioxide (5ae):

Yield 45% (35 mg); colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 102-104 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.91 (d, *J* = 8.0 Hz, 1H), 7.13 (d, *J* = 6.8 Hz, 1H), 7.24-7.40 (comp, 4H), 7.42-7.48 (comp, 2H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.66-7.68 (comp, 2H), 7.71-7.74 (m, 1H), 7.75-7.77 (m, 1H), 7.80-7.82 (comp, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 116.8, 118.2, 119.6, 124.6, 125.0, 125.8, 126.2, 126.7, 128.3 (x 2), 128.5, 128.7 (x 2), 129.0, 130.4, 130.7, 131.3, 132.1, 133.6, 134.9, 136.2, 153.1, 178.4; **HRMS** (ESI, m/z) calcd for $C_{23}H_{15}NO_3S$ $[M+H]^+$ 386.0851, found 386.0883.



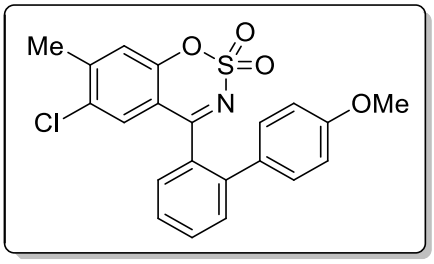
7-methoxy-4-(4'-methoxy-[1,1'-biphenyl]-2-yl)benzo[*e*][1,2,3]oxathiazine 2,2-dioxide (5bb):

Yield 78% (62 mg); colourless solid; $\mathbf{R_f}$ 0.7 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 94-96 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.72 (s, 3H), 3.81 (s, 3H), 6.49 (dd, *J* = 8.8 Hz, 2.4 Hz, 1H), 6.60 (d, *J* = 2.4Hz, 1H), 6.74-6.78 (comp, 2H), 6.98 (d, *J* = 9.2 Hz, 1H), 7.18-7.21 (comp, 2H), 7.47-7.52 (comp, 2H), 7.58 (dd, *J* = 7.8 Hz, 1 Hz, 1H), 7.63 (td, *J* = 7.5 Hz, 1.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.4, 56.3, 102.8, 110.4, 112.9, 114.2, 127.4, 130.2, 130.2, 130.3, 131.7, 132.0, 132.9, 133.3, 141.4, 156.3, 159.4, 166.3, 178.1; **HRMS** (ESI, m/z) calcd for $C_{21}H_{17}NO_5S$ $[M+Na]^+$ 418.0725, found 418.0739.



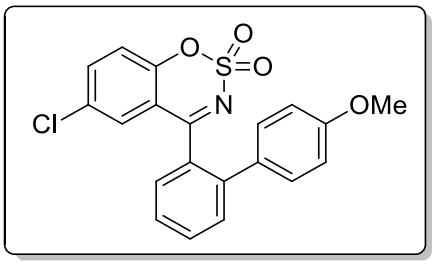
4-(4'-methoxy-[1,1'-biphenyl]-2-yl)-7-methylbenzo[*e*] [1,2,3]oxathiazine2,2-dioxide (5cb):

Yield 75% (55 mg); colourless solid; $\mathbf{R_f}$ 0.7 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 108-110 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.34 (s, 3H), 3.72 (s, 3H), 6.73-6.76 (comp, 2H), 6.79 (dd, *J* = 8.0 Hz, 0.8 Hz, 1H), 6.94-6.96 (comp, 2H), 7.16-7.20 (comp, 2H), 7.48-7.53 (comp, 2H), 7.60-7.67 (comp, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 22.2, 55.4, 114.3, 114.7, 119.0, 126.4, 127.4, 130.2 (x 2), 130.4, 131.0, 131.8, 132.1, 133.2, 141.6, 149.1, 154.0, 159.4, 178.7; **HRMS** (ESI, m/z) calcd for $C_{21}H_{17}NO_4S$ $[M+Na]^+$ 402.0775, found 402.0776.



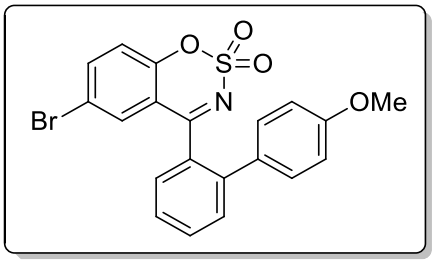
6-chloro-4-(4'-methoxy-[1,1'-biphenyl]-2-yl)-7-methylbenzo[e][1,2,3]oxathiazine-2,2-dioxide (5db):

Yield 52% (45 mg); colourless solid; $\mathbf{R_f}$ 0.6 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 122-124 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.34 (s, 3H), 3.72 (s, 3H), 6.76 (d, *J* = 8.4 Hz, 2H), 6.97 (s, 1H), 7.03 (s, 1H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.52-7.56 (comp, 2H), 7.65-7.70 (comp, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 21.1, 55.5, 114.4, 115.6, 120.7, 127.7, 130.2, 130.5 (x 2), 130.9, 131.0, 132.1, 132.4, 132.7, 141.8, 146.4, 152.0, 159.5, 177.7; **HRMS** (ESI, m/z) calcd for $C_{21}H_{17}ClNO_4S$ $[M+H]^+$ 414.0567, found 414.0601.



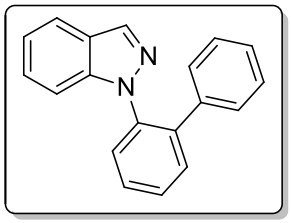
6-chloro-4-(4'-methoxy-[1,1'-biphenyl]-2-yl)benzo[*e*] [1,2,3]oxathiazine 2,2-dioxide (5eb):

Yield 76% (61 mg); colourless solid; $\mathbf{R_f}$ 0.4 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 118-120 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.71 (s, 3H), 6.75-6.78 (comp, 2H), 6.97 (d, *J* = 2.4 Hz, 1H), 7.09 (d, *J* = 8.8 Hz, 1H), 7.14-7.17 (comp, 2H), 7.38 (dd, *J* = 8.8 Hz, 2.4 Hz, 1H), 7.54-7.58 (comp, 2H), 7.69-7.73 (comp, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.5, 114.4, 117.6, 120.1, 127.8, 130.2 , 130.5, 130.6, 130.6, 130.7, 132.0, 132.5, 132.6, 136.2, 141.9, 152.1, 159.5, 177.9; **HRMS** (ESI, m/z) calcd for $C_{20}H_{14}ClNO_4S$ $[M+H]^+$ 400.0410, found 400.0434.



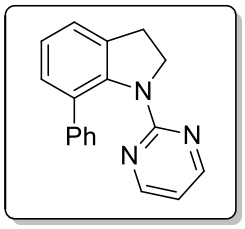
6-bromo-4-(4'-methoxy-[1,1'-biphenyl]-2-yl)benzo[*e*] [1,2,3]oxathiazine 2,2-dioxide (5fb):

Yield 72% (64 mg); colourless solid; $\mathbf{R_f}$ 0.5 (petroleum ether/ethyl acetate = 7:3); **eluent composition** petroleum ether/ethyl acetate = 7:3; **mp** 120-124 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.72 (s, 3H), 6.75-6.78 (comp, 2H), 7.02 (d, *J* = 8.4 Hz, 1H), 7.11-7.16 (comp, 3H), 7.50-7.56 (comp, 3H), 7.71-7.75 (comp, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.5, 114.4, 117.9, 118.0, 120.3, 127.8, 130.2, 130.5, 130.7, 132.1, 132.5, 132.6, 133.6, 139.0, 142.0, 152.6, 159.6, 177.8; **HRMS** (ESI, m/z) calcd for $C_{20}H_{14}BrNO_4S$ $[M+H]^+$ 443.9905, found 443.9901.



1-([1,1'-biphenyl]-2-yl)-1*H*-indazole (6):

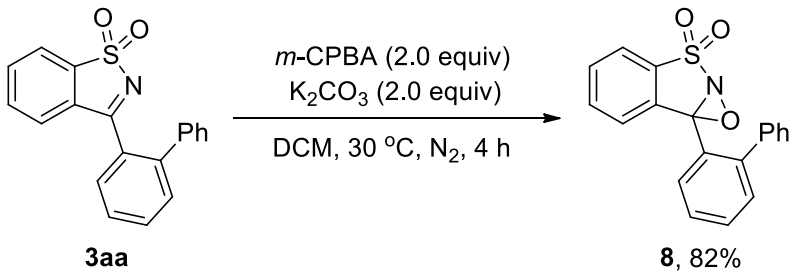
Combined Yield 94% (28 mg, 0.1 mmol scale); **mono**:**bis** 1.5:1; colourless oil; $\mathbf{R_f}$ 0.4 (petroleum ether/ethyl acetate = 19:1); **eluent composition** petroleum ether/ethyl acetate = 19:1; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.01-7.02 (m, 1H), 7.07-7.08 (comp, 3H), 7.09-7.11 (comp, 3H), 7.14-7.18 (m, 1H), 7.56-7.58 (comp, 3H), 7.61 (dd, *J* = 8.0 Hz, 1.6 Hz, 1H), 7.67-7.69 (m, 1H), 8.11 (d, *J* = 0.8 Hz, 1H). The ^{1}H NMR data correspond with that reported in the literature.[3]



7-phenyl-1-(pyrimidin-2-yl)indoline (7):

Yield 82% (45 mg); colourless oil; $\mathbf{R_f}$ 0.2 (petroleum ether/ethyl acetate = 9:1); **eluent composition** petroleum ether/ethyl acetate = 9:1; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.19 (t, *J* = 8.0 Hz, 2H), 4.47 (t, *J* = 8.0 Hz, 2H), 6.38 (t, *J* = 4.8 Hz, 1H), 7.08-7.11 (m, 1H), 7.12-7.18 (comp, 3H), 7.24 (dd, *J* = 7.6 Hz, 1.2 Hz, 1H), 7.28 (dd, *J* = 8.0 Hz, 0.8 Hz, 1H), 7.32-7.35 (comp, 2H), 7.96 (d, *J* = 4.8 Hz, 2H). The ^{1}H NMR data correspond with that reported in the literature.[4]

Synthesis of 7b-([1,1'-biphenyl]-2-yl)-7bH-benzo[d][1,2]oxazireno[2,3-b]isothiazole 3,3-dioxide (8):



3aa **8**, 82%

In an oven-dried 10 mL round bottomed flask, **3aa** (64 mg, 0.2 mmol, 1.0 equiv) was taken and to it *m*-CPBA (69 mg, 0.4 mmol, 2.0 equiv), K_2CO_3 (55 mg, 0.4 mmol, 2.0 equiv) and DCM (10 mL) were added. The reaction mixture was degassed and backfilled with nitrogen. It was then closed with a stopper and kept at 30℃ while stirring for 4 h. After completion of reaction (checked by TLC), the reaction mixture was quenched with saturated NH_4Cl solution and then it was extracted with ethyl acetate. The combined organic layer were given brine wash and concentrated under vacuo. The crude reaction mixture was subjected to column chromatography using ethyl acetate/petroleum ether as eluent to give **8** in 82% yield.

Yield 82% (55 mg); colourless solid; $\mathbf{R_f}$ 0.5 (pet ether/ethyl acetate = 4:1); **eluent composition** petroleum ether/ethyl acetate = 4:1; **mp** 88-90 ^oC (crystallization from $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.04 (d, *J* = 7.6 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 7.18 (app t, *J* = 7.6 Hz, 2H), 7.29 (dd, *J* = 8.0 Hz, 0.8 Hz , 2H), 7.34 (td, *J* = 8.0 Hz, 0.8 Hz, 1H), 7.44 (td, *J* = 8.0 Hz, 0.8 Hz, 1H), 7.49 (dd, *J* = 7.6 Hz, 1.2 Hz, 1H), 7.52-7.56 (comp, 2H), 7.65 (td, *J* = 7.6 Hz, 1.2 Hz, 1H), 7.72 (dd, *J* = 7.6 Hz, 1.2 Hz, 1H); **^{13}C NMR** (100 MHz $CDCl_3$) δ 85.8, 123.3, 126.5, 127.2, 127.8, 128.0, 128.7, 128.8, 129.4, 131.0, 131.4, 132.0, 133.0, 133.2, 135.4, 139.4, 142.8; **HRMS** (EI, m/z) calcd for $C_{19}H_{13}NO_3S$ [M^+] 335.0616, found 335.0608.

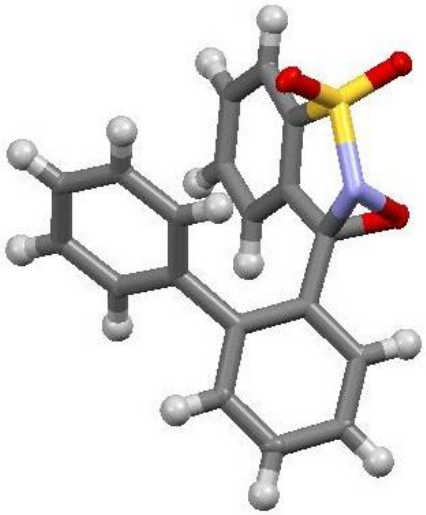


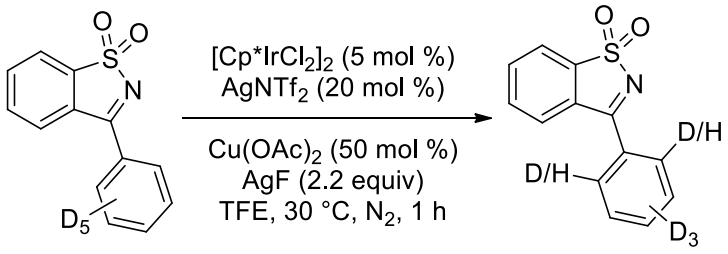
Figure S3. X-ray crystal structure of **8** (ellipsoid contour at 50% probability level)

Empirical formula	$C_{19}H_{13}NO_3S$
Formula weight	335.36
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.9907(2)
b/Å	8.1808(2)
c/Å	19.0908(5)
α/°	90
β/°	90.2160(10)
γ/°	90
Volume/Å^3	1560.32(6)
Z	4
ρ_{calc}g/cm^3	1.428
μ/mm^{-1}	1.992
F(000)	696.0
Crystal size/mm^3	0.35 × 0.25 × 0.18
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.008 to 130.144
Index ranges	$-11 \leq h \leq 11$, $-9 \leq k \leq 9$, $-22 \leq l \leq 22$
Reflections collected	19662
Independent reflections	2642 [R_{int} = 0.0914, R_{sigma} = 0.0507]
Data/restraints/parameters	2642/0/218
Goodness-of-fit on F^2	1.226
Final R indexes [I>=2σ (I)]	R_1 = 0.0589, wR_2 = 0.1253
Final R indexes [all data]	R_1 = 0.0622, wR_2 = 0.1269
Largest diff. peak/hole / e Å^{-3}	0.43/-0.40

Mechanistic experiments:

(a) Procedure for H/D exchange experiments:

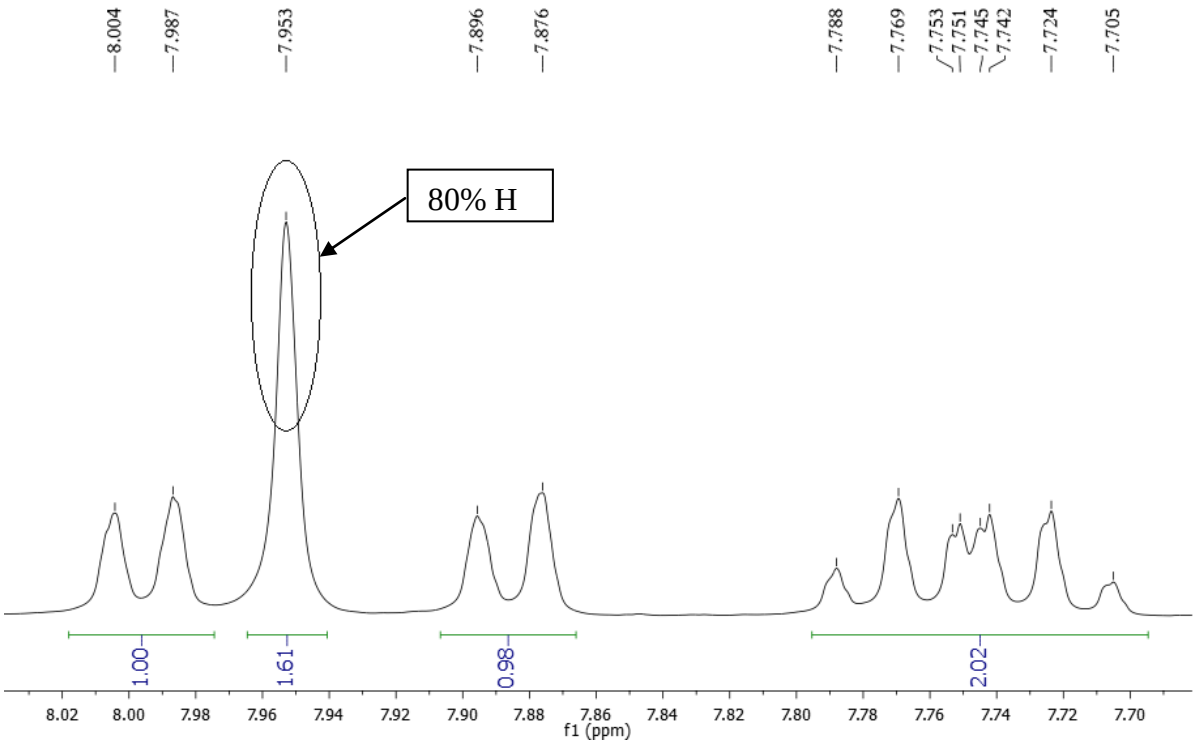
(in absence of arylsiloxane)



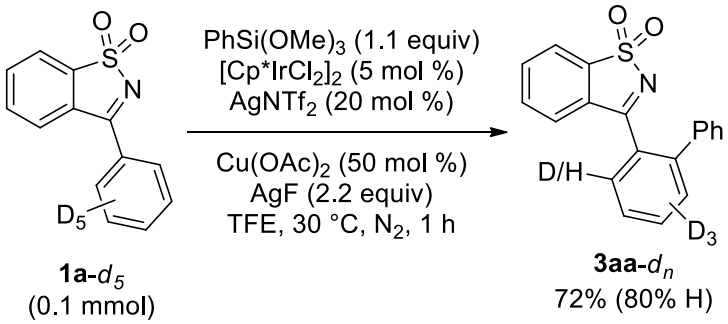
1a-d_5
(0.1 mmol)

1a-d_n
92% (80% H)

An oven dried 10 mL schlenk tube was charged with **1a**-d_5 (24.3 mg, 0.1 mmol), silver (bistrifluoromethanesulfonyl)imide (7.7 mg, 20 mol %), copper acetate (9.0 mg, 50 mol %), silver fluoride (27.9 mg, 2.2 equiv) and catalyst $[Cp^*IrCl_2]_2$ (4.0 mg, 5 mol %). The tube was evacuated and backfilled with nitrogen and to it was added anhydrous TFE (1.0 mL, 0.1 M) under nitrogen atmosphere. The reaction mixture was degassed and backfilled with nitrogen 3 times. It was then closed with teflon-lined cap and kept at 30 ℃ while stirring for 1 h. After completion of the reaction, the reaction mixture was filtered through a short pad of celite, the solvent was removed under reduced pressure and the crude reaction mixture was directly purified through column chromatography on silica gel using petroleum ether/ethyl acetate (7:3) as eluent to recover the starting material **1a**-d_n (92%). The proton incorporation (80%) was determined by ^{1}H NMR spectroscopy.



(in presence of arylsiloxane)

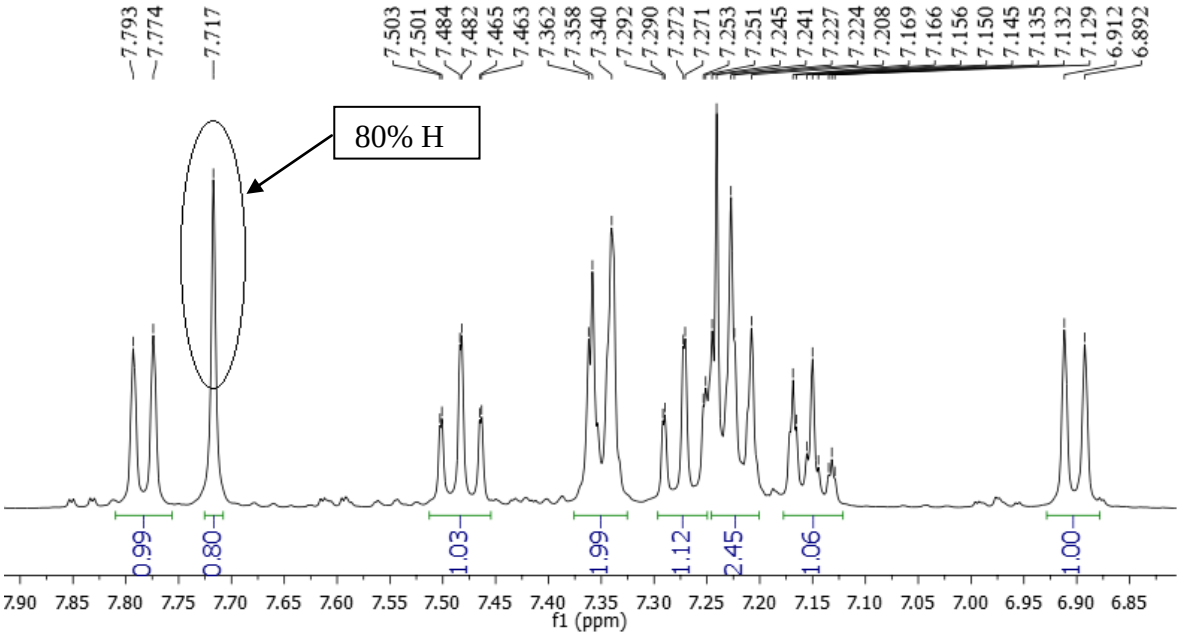


1a-d_5
(0.1 mmol)

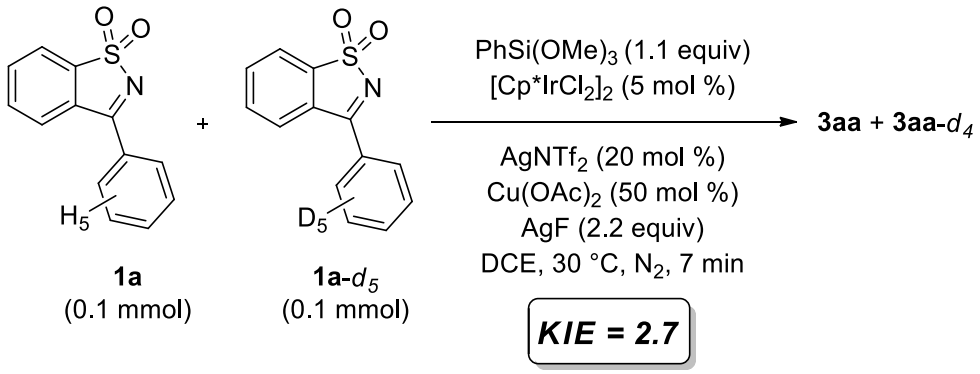
3aa-d_n
72% (80% H)

An oven dried 10 mL schlenk tube was charged with **1a**-d_5 (24.3 mg, 0.1 mmol), trimethoxyphenylsilane (20.5 µL, 1.1 equiv), silver (bistrifluoromethanesulfonyl)imide (15.5 mg, 20 mol %), copper acetate (18.1 mg, 50 mol %), silver fluoride (55.8 mg, 2.2 equiv) and catalyst $[Cp^*IrCl_2]_2$ (8.0 mg, 5 mol %). The tube was evacuated and backfilled with nitrogen and to it was added anhydrous TFE (1.0 mL, 0.1 M) under nitrogen atmosphere. The reaction mixture was degassed and backfilled with nitrogen 3 times. It was then closed with teflon-lined cap and kept at 30℃ while stirring for 1 h. After completion of the reaction, the reaction mixture was filtered through a short pad of celite, the solvent was removed under reduced pressure and the crude reaction mixture was directly purified through column chromatography on silica gel using petroleum ether/ethyl acetate (7:3) as eluent yielding the

product **3aa**-d_n (72%). The proton incorporation (80%) was determined by ^{1}H NMR spectroscopy.

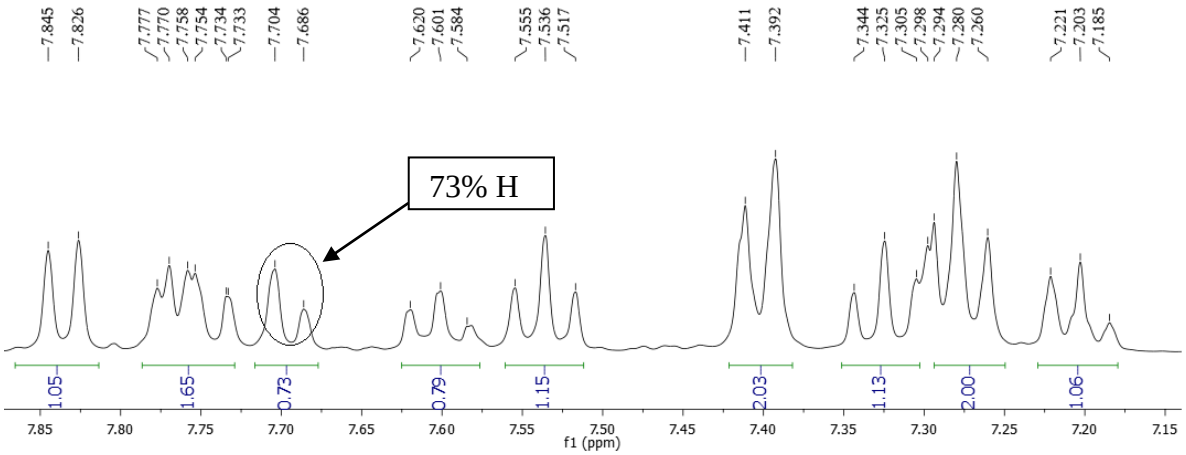


(b) Procedure for competitive experiment between 1a and 1a-d_5:

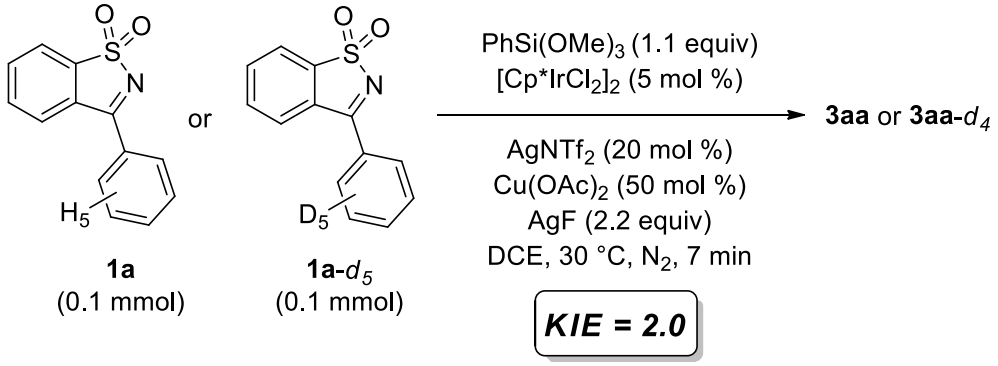


An oven dried 10 mL Schlenk tube was charged with **1a** (24.3 mg, 0.1 mmol), **1a**-d_5 (49.6 mg, 0.1 mmol), trimethoxyphenylsilane (41μL, 1.1 equiv), silver (bistrifluoromethanesulfonyl) imide (15.5 mg, 20 mol %), copper acetate (18.1 mg, 50 mol %), silver fluoride (55.8 mg, 2.2 equiv) and catalyst $[Cp^*IrCl_2]_2$ (8.0 mg, 5 mol %). The tube was evacuated and backfilled with nitrogen and to it was added anhydrous DCE (2.0 mL, 0.1 M) under nitrogen atmosphere. The reaction mixture was degassed and backfilled with nitrogen 3 times and kept for stirring at 30℃. After 7 min, the reaction was quickly quenched by adding ethyl acetate keeping in an ice bath. The reaction mixture was filtered through a short pad of celite and concentrated under vacuo. The crude reaction mixture was directly purified by column chromatography on silica gel using petroleum ether/ethyl acetate (7:3) as

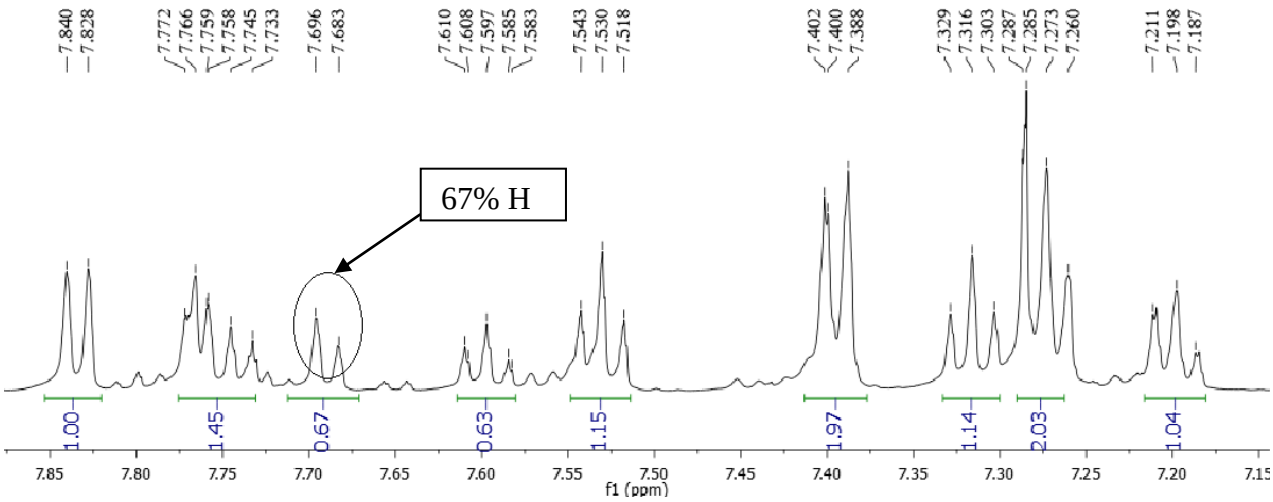
eluent. The ratio of **3aa** and **3aa**-d_4 was determined by ^{1}H NMR spectroscopy. Primary kinetic isotopic effect (KIE) was found be $\boldsymbol{k_H/k_D} \approx 0.73/0.27 \approx 2.7$.



(c) Procedure for parallel experiment between 1a and 1a-d_5:



Two separate oven dried 10 mL Schlenk tubes were charged with **1a** (24.3 mg, 0.1 mmol) and **1a**-d_5 (24.8 mg, 0.1 mmol). To each were added trimethoxyphenylsilane (20.5 µL, 1.1 equiv), silver (bistrifluoromethanesulfonyl) imide (15.5 mg, 20 mol %), copper acetate (18.1 mg, 50 mol %), silver fluoride (55.8 mg, 2.2 equiv) and catalyst $[Cp^*IrCl_2]_2$ (8.0 mg, 5 mol %). The tubes were evacuated and backfilled with nitrogen and to it was added anhydrous DCE (1.0 mL, 0.1 M) under nitrogen atmosphere. The reaction mixtures were degassed and backfilled with nitrogen 3 times and kept for stirring at 30℃. After 7 min, the reactions were quickly quenched by adding ethyl acetate keeping in an ice bath. The reaction mixtures were filtered through a short pad of celite, both the reaction mixtures were combined and concentrated under vacuo. The crude reaction mixture was directly purified by column chromatography on silica gel using petroleum ether/ ethyl acetate (7:3) as eluent. The ratio of **3aa** and **3aa**-d_4 was determined by ^{1}H NMR spectroscopy. Primary kinetic isotopic effect (KIE) was found be $\boldsymbol{k_H/k_D} \approx 0.67/0.33 \approx 2.0$.

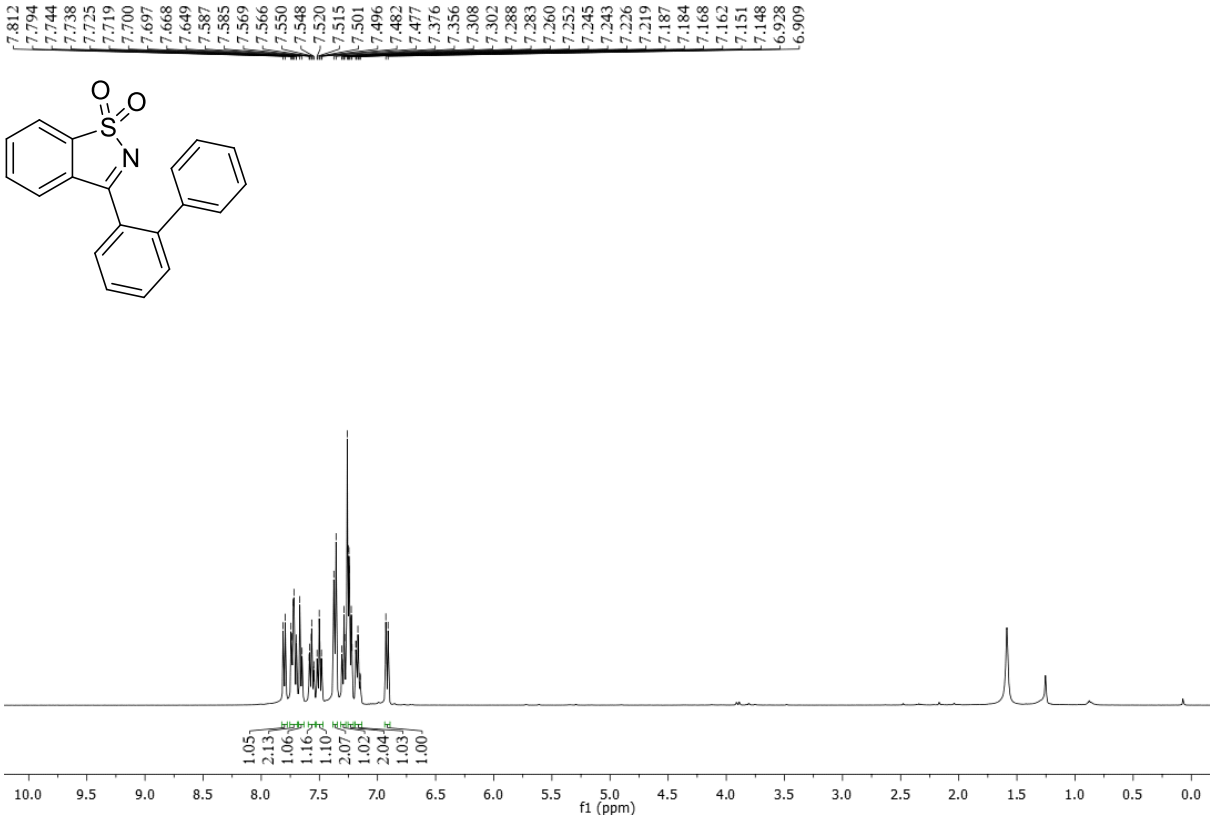


References:

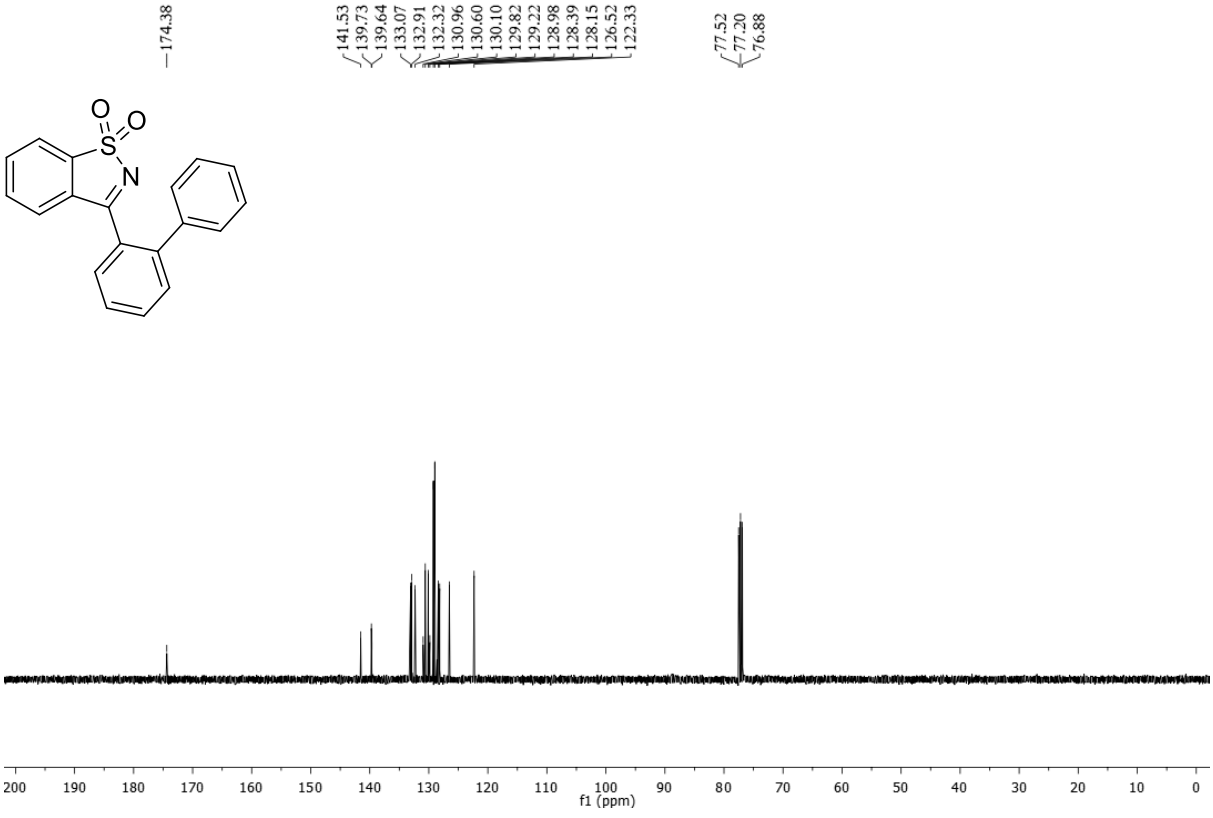
1. T. Nishimura, A. Noishiki, G. C. Tsui and T. Hayashi, *J. Am. Chem. Soc.*, 2012, **134**, 5056.
2. Y.-Q. Wang, C.-B. Yu, D.-W. Wang, X.-B. Wang and Y.-G. Zhou, *Org. Lett.*, 2008, **10**, 2071.
3. M. Moselage, J. Lie, F. Kramm and L. Ackermann *Angew. Chem. Int. Ed.*, 2017, **56**, 5341.
4. P. B. De, S. Pradhan, S. Banerjee and T. Punniyamurthy *Chem. Commun.*, 2018, **54**, 2494.

^{1}H and ^{13}C NMR spectra of compounds:

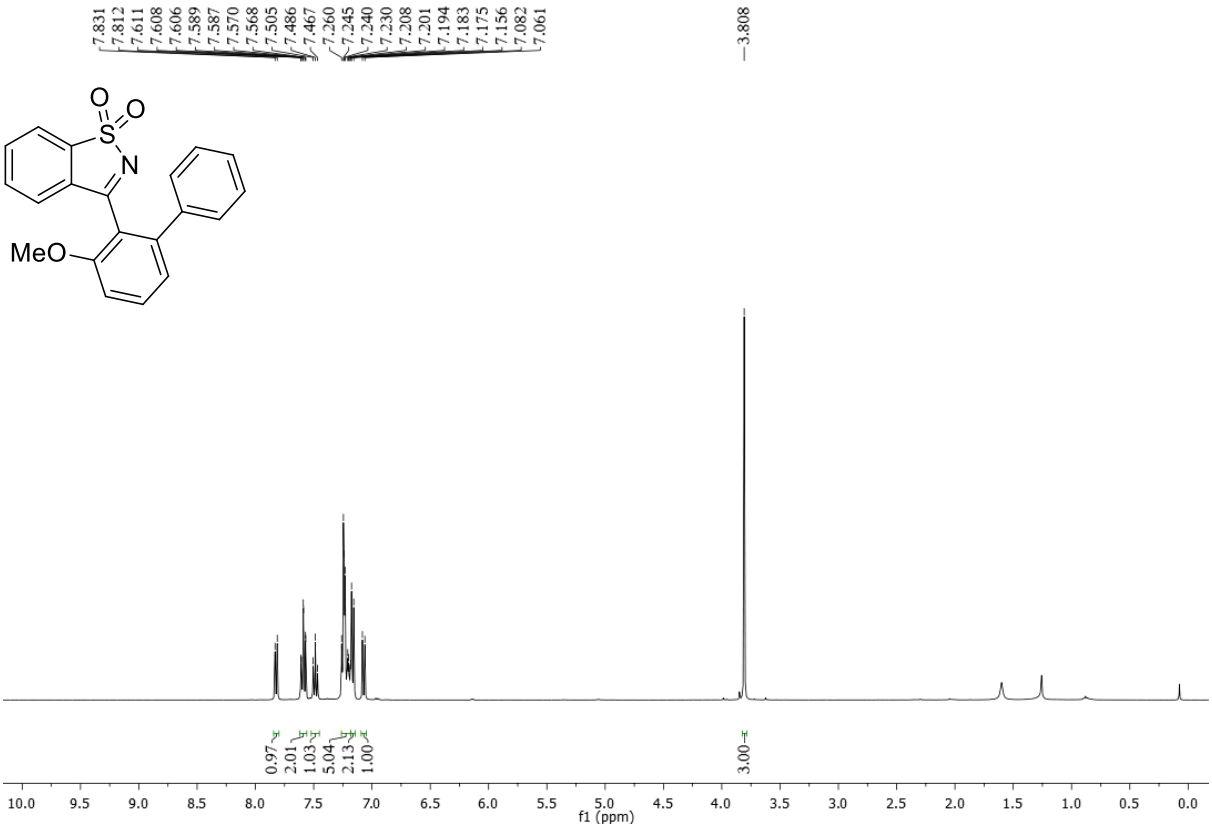
^{1}H NMR of **3aa** (400MHz, $CDCl_3$):



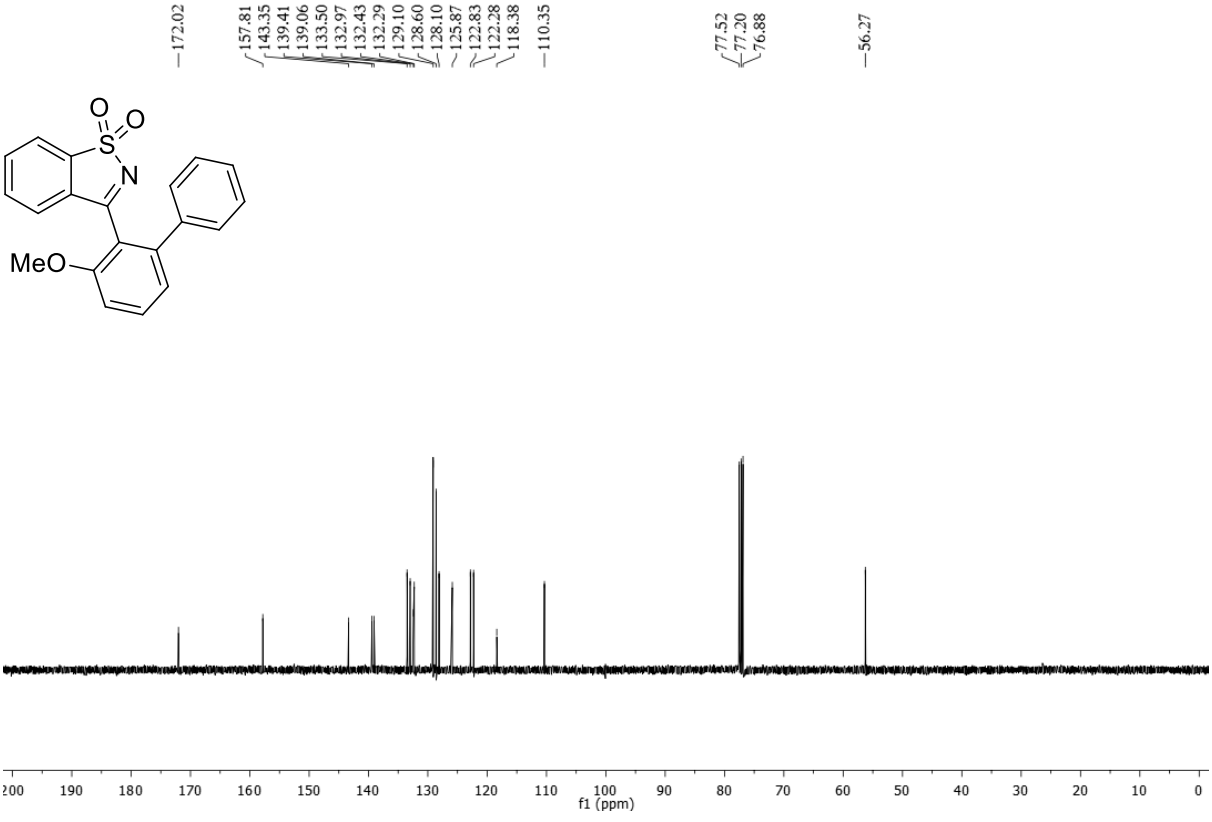
^{13}C NMR of **3aa** (100MHz, $CDCl_3$):



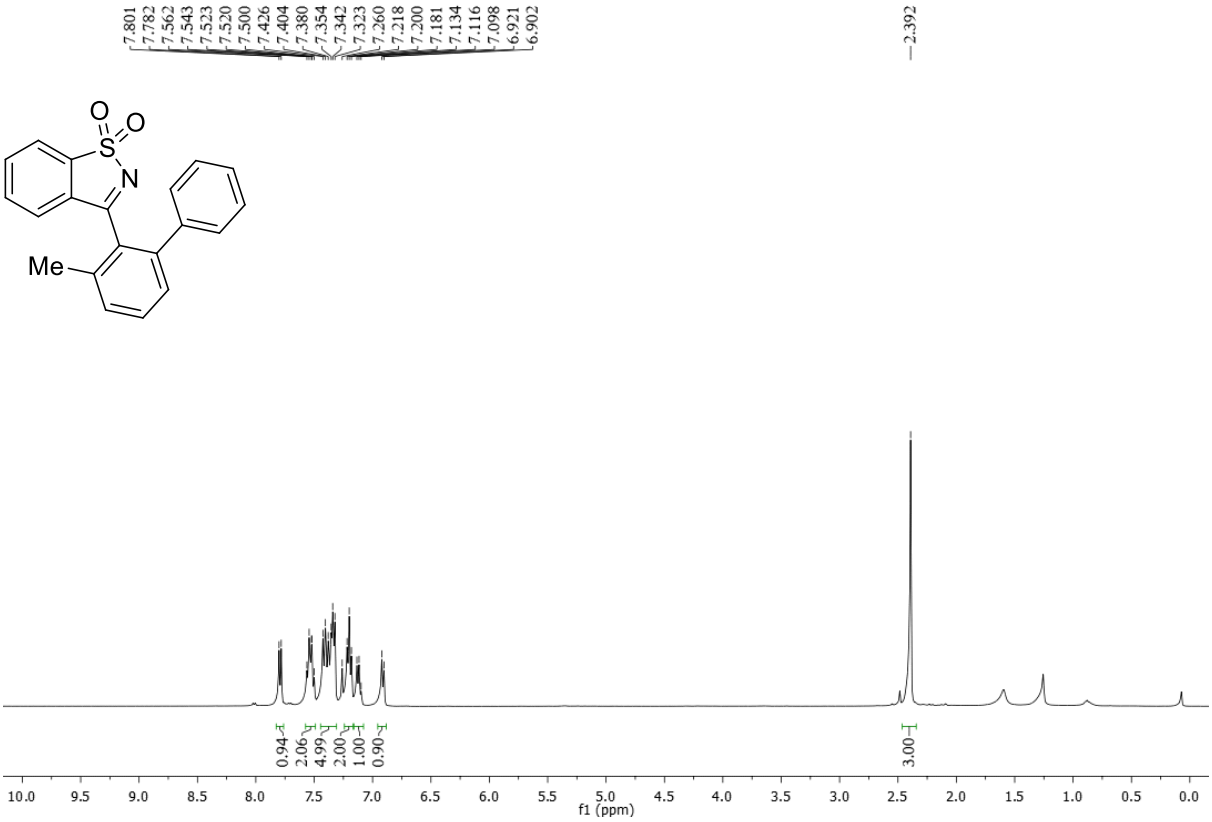
^{1}H NMR of **3ba** (400MHz, $CDCl_3$):



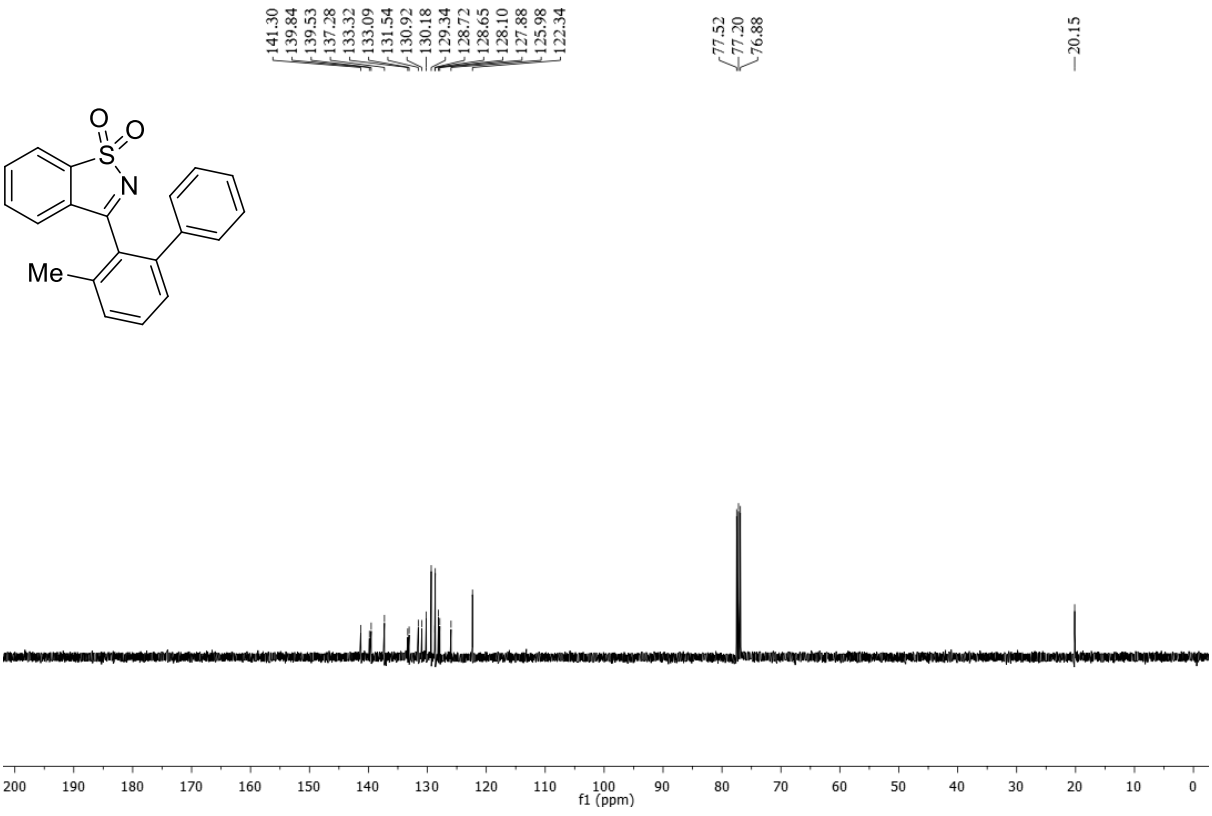
^{13}C NMR of **3ba** (100MHz, $CDCl_3$):



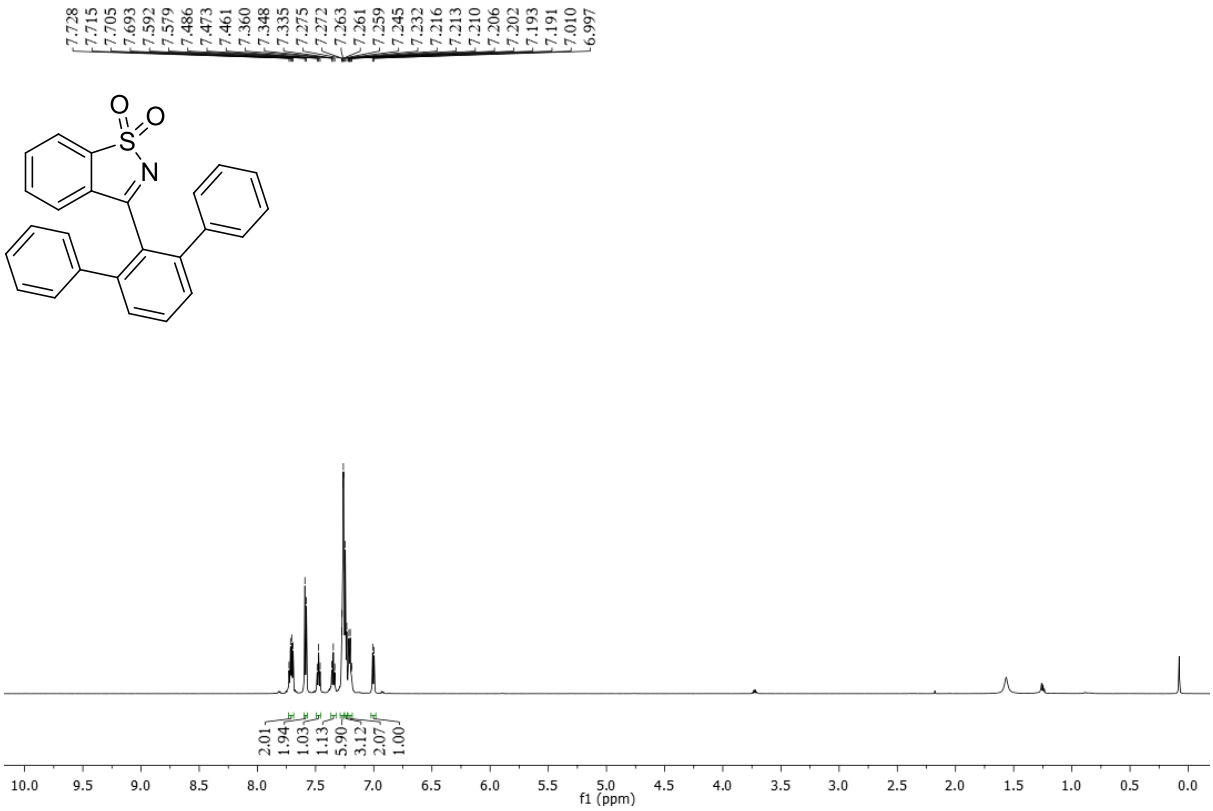
^{1}H NMR of **3ca** (400MHz, $CDCl_3$):



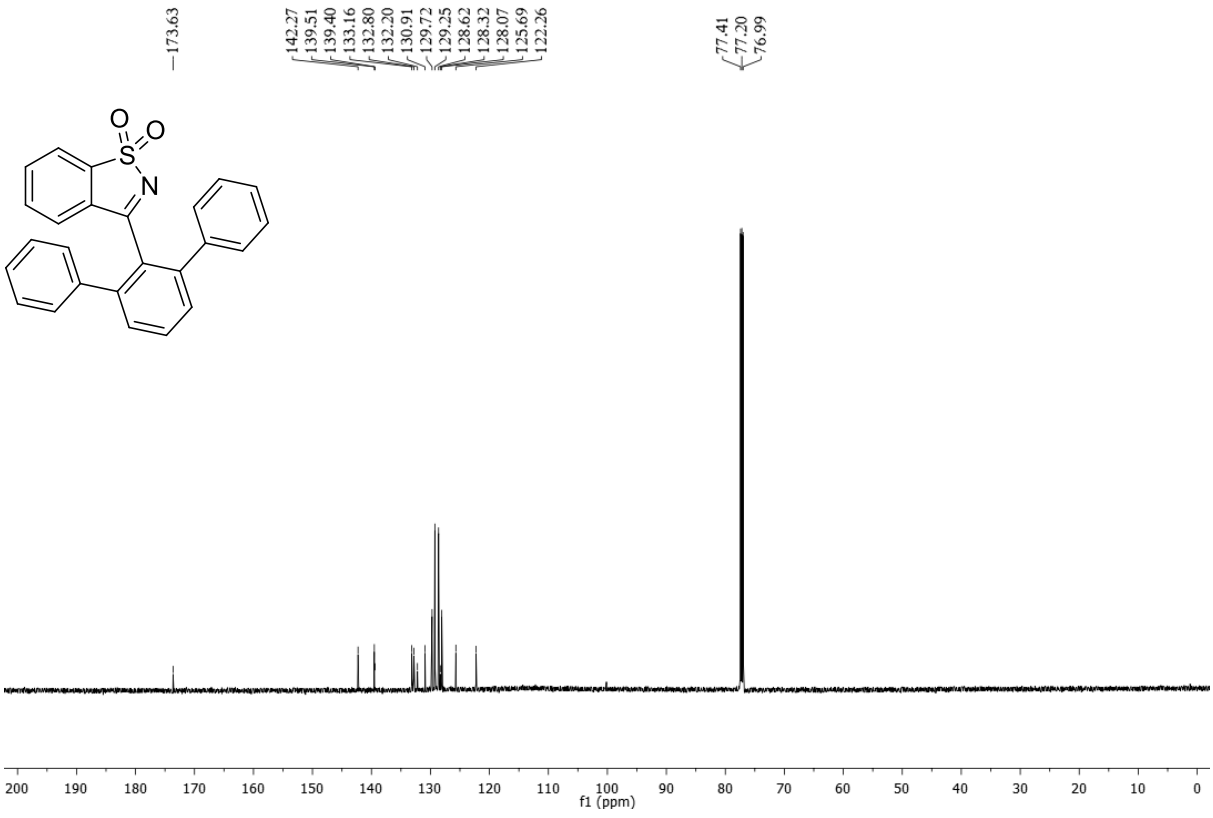
^{13}C NMR of **3ca** (100MHz, $CDCl_3$):



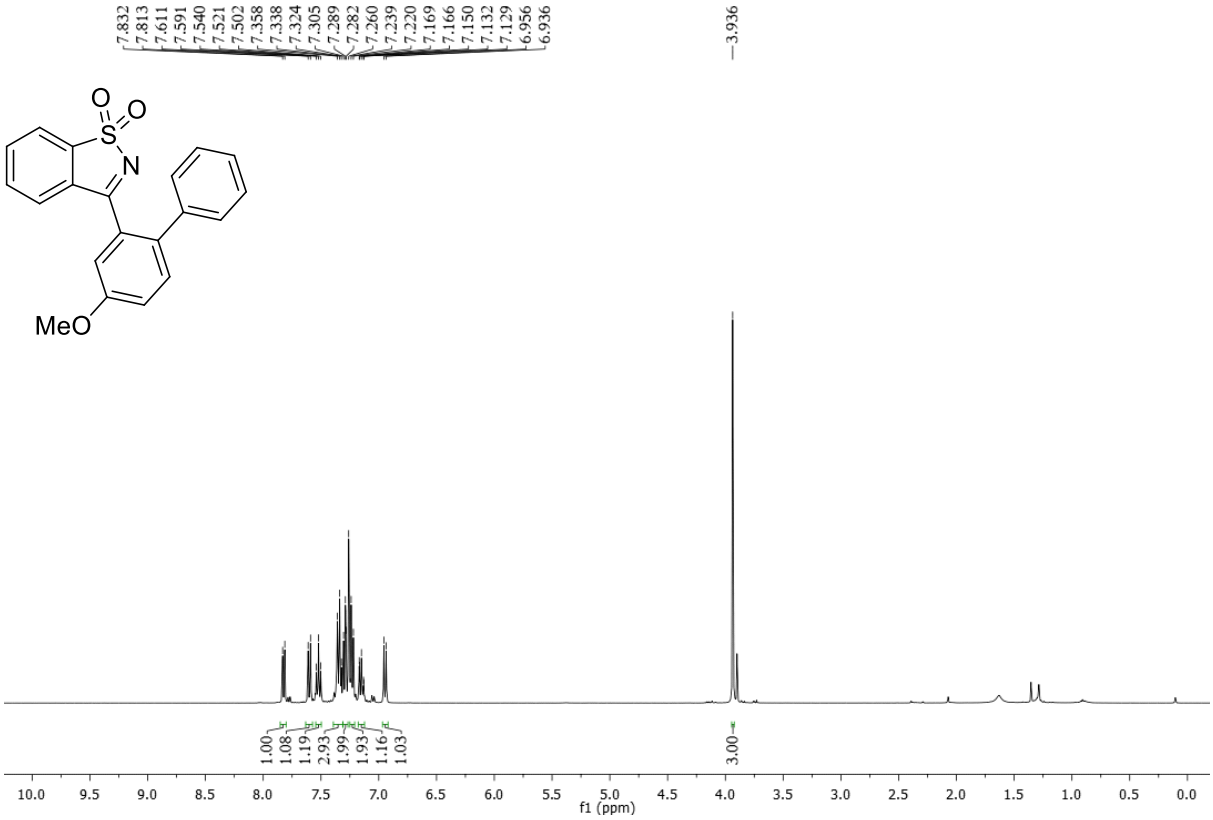
^{1}H NMR of **3da** (600 MHz, $CDCl_3$):



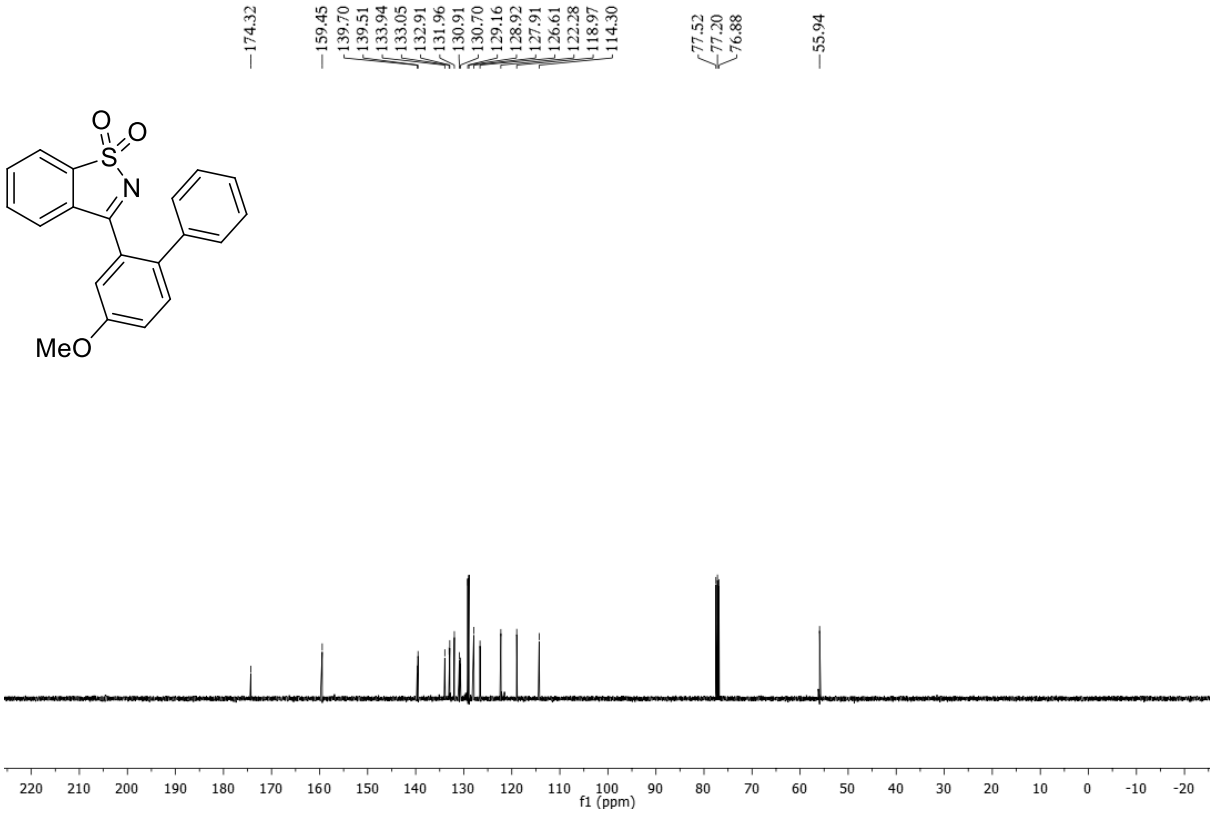
^{13}C NMR of **3da** (150 MHz, $CDCl_3$):



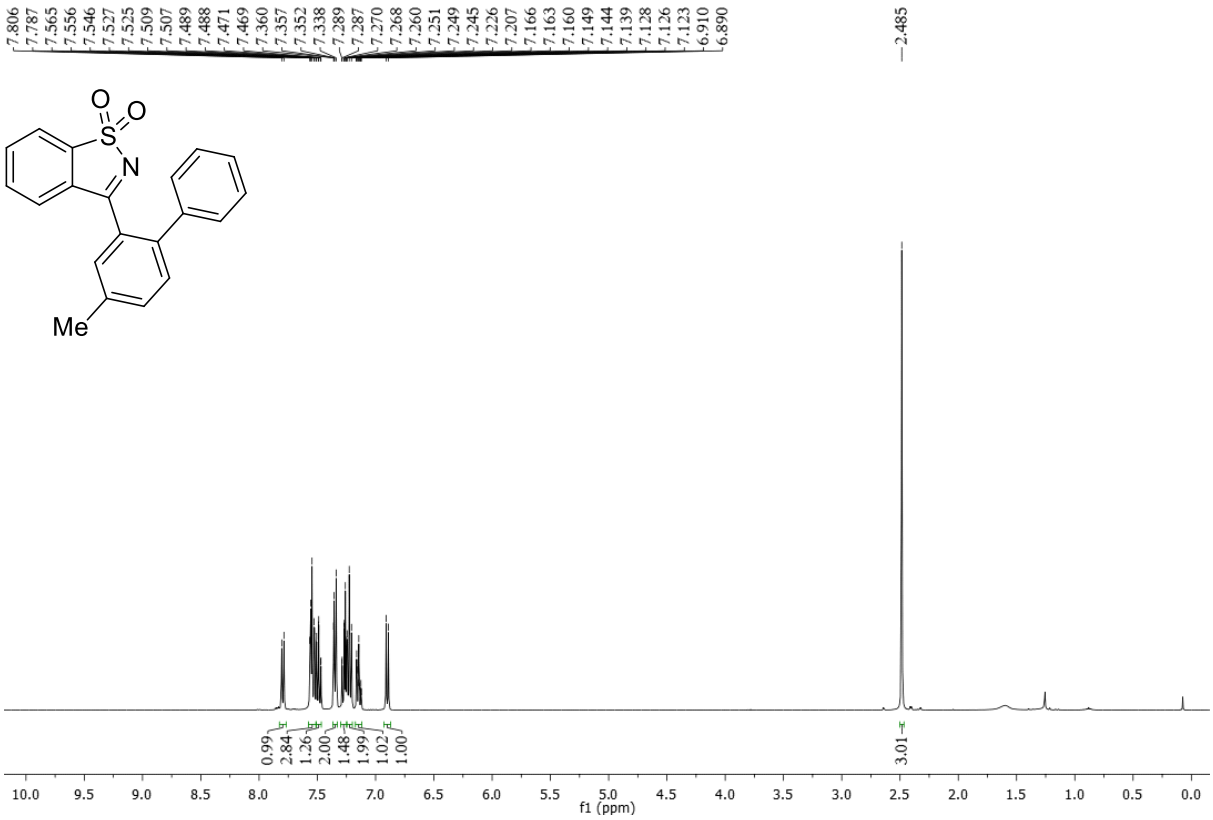
^{1}H NMR of **3ea** (400MHz, $CDCl_3$):



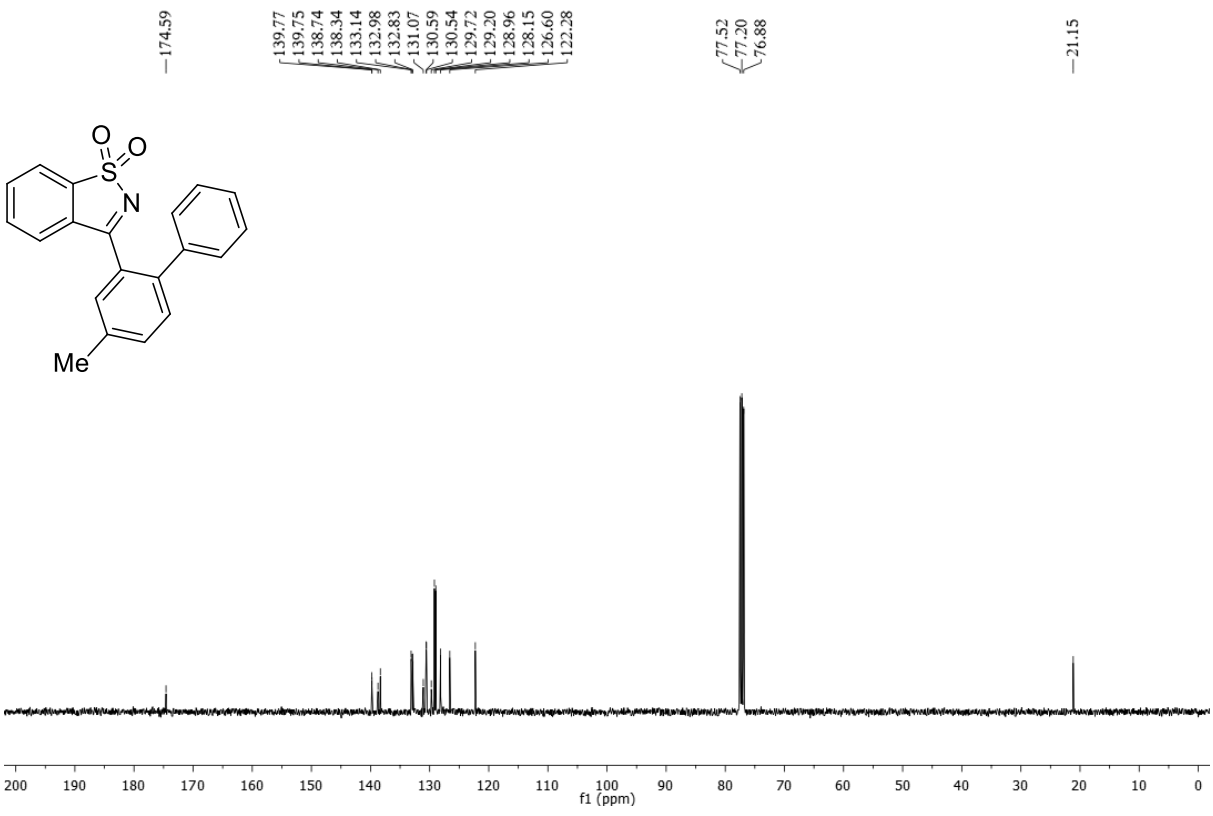
^{13}C NMR of **3ea** (100MHz, $CDCl_3$):



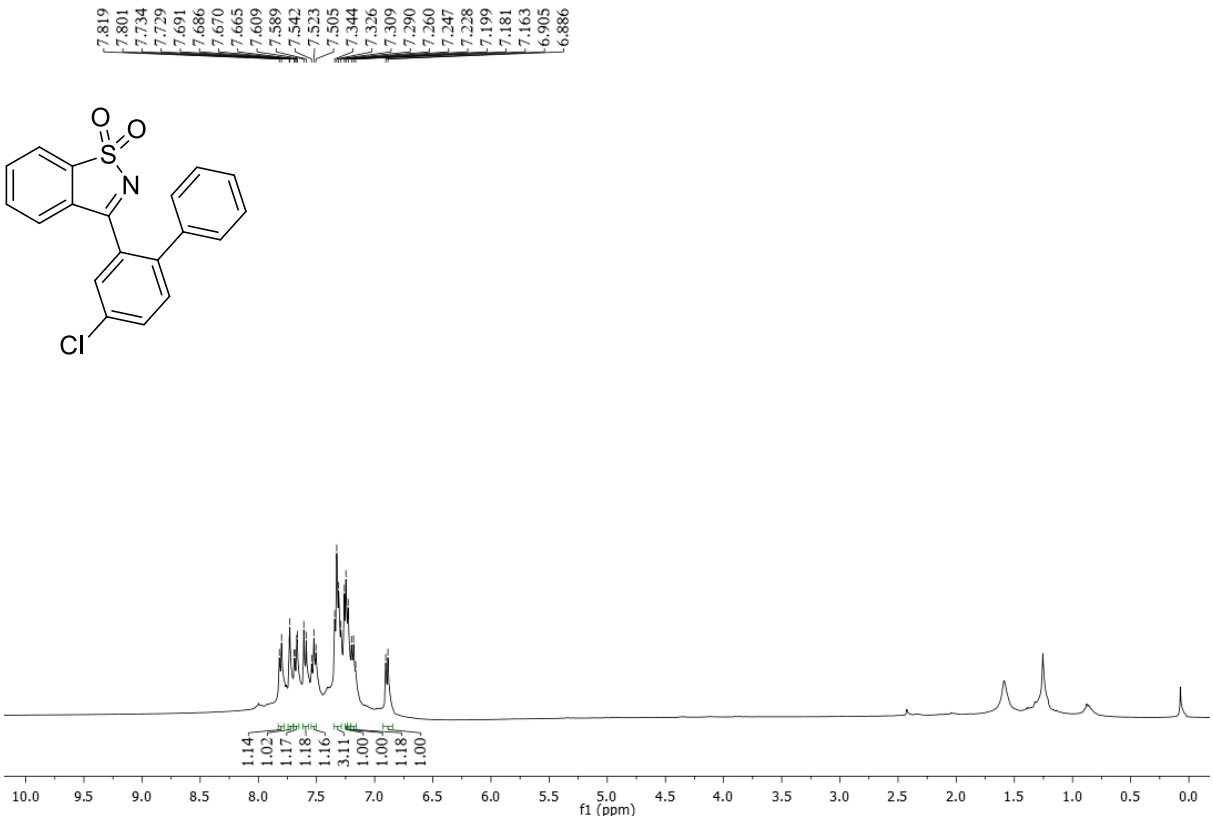
^{1}H NMR of **3fa** (400MHz, $CDCl_3$):



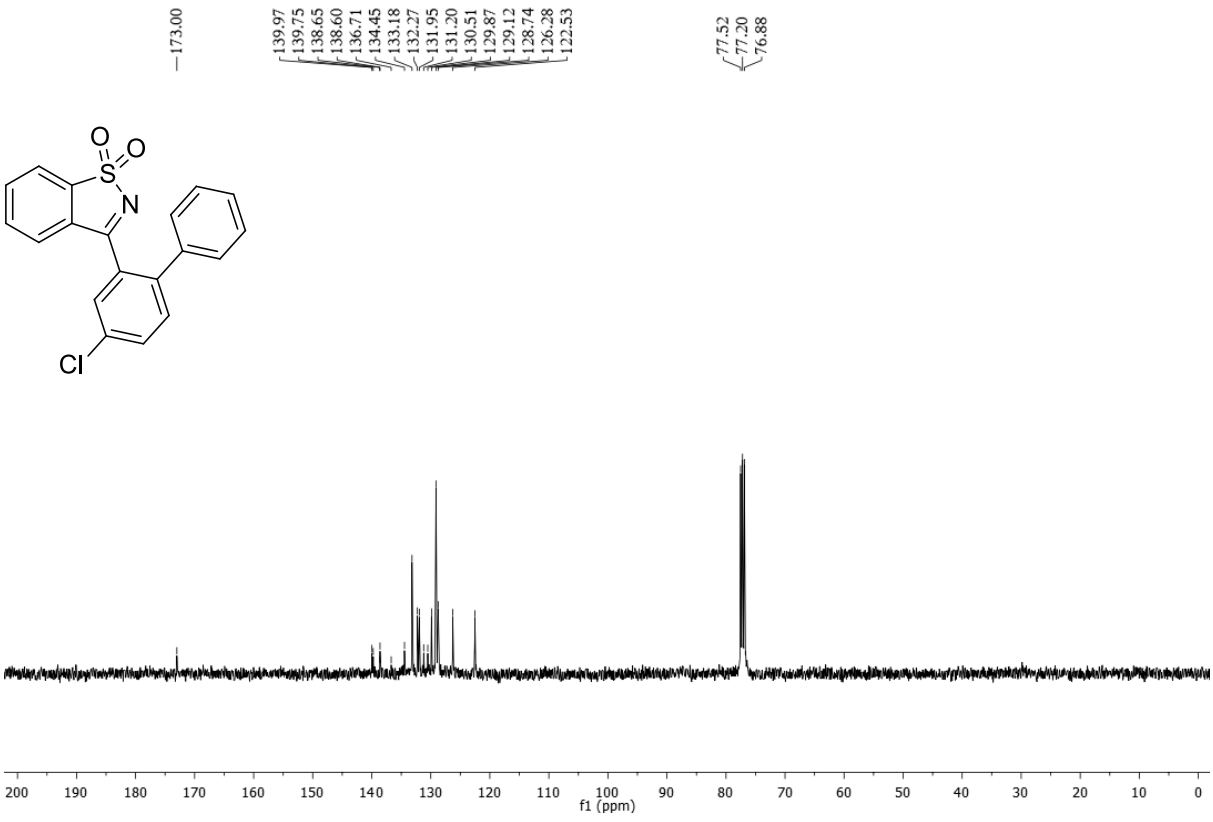
^{13}C NMR of **3fa** (100MHz, $CDCl_3$):



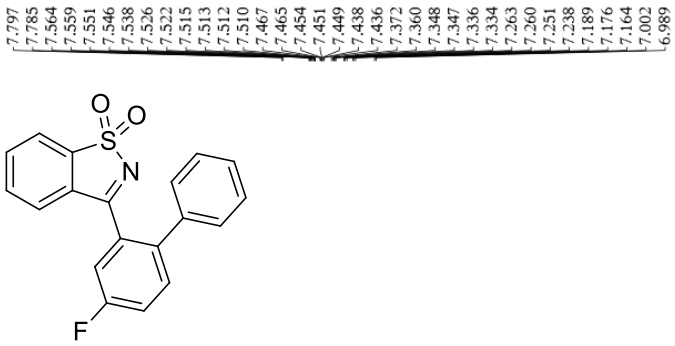
^{1}H NMR of **3ga** (400MHz, $CDCl_3$):

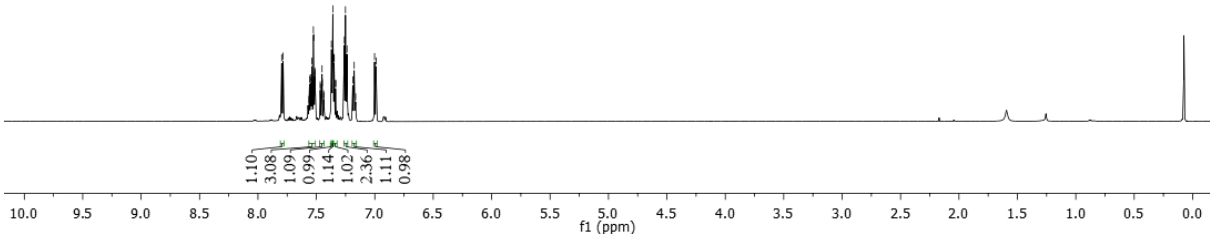


^{13}C NMR of **3ga** (100MHz, $CDCl_3$):

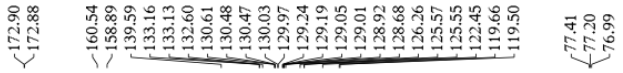


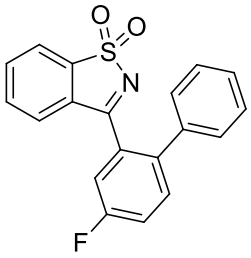
^{1}H NMR of **3ha** (600MHz, $CDCl_3$):



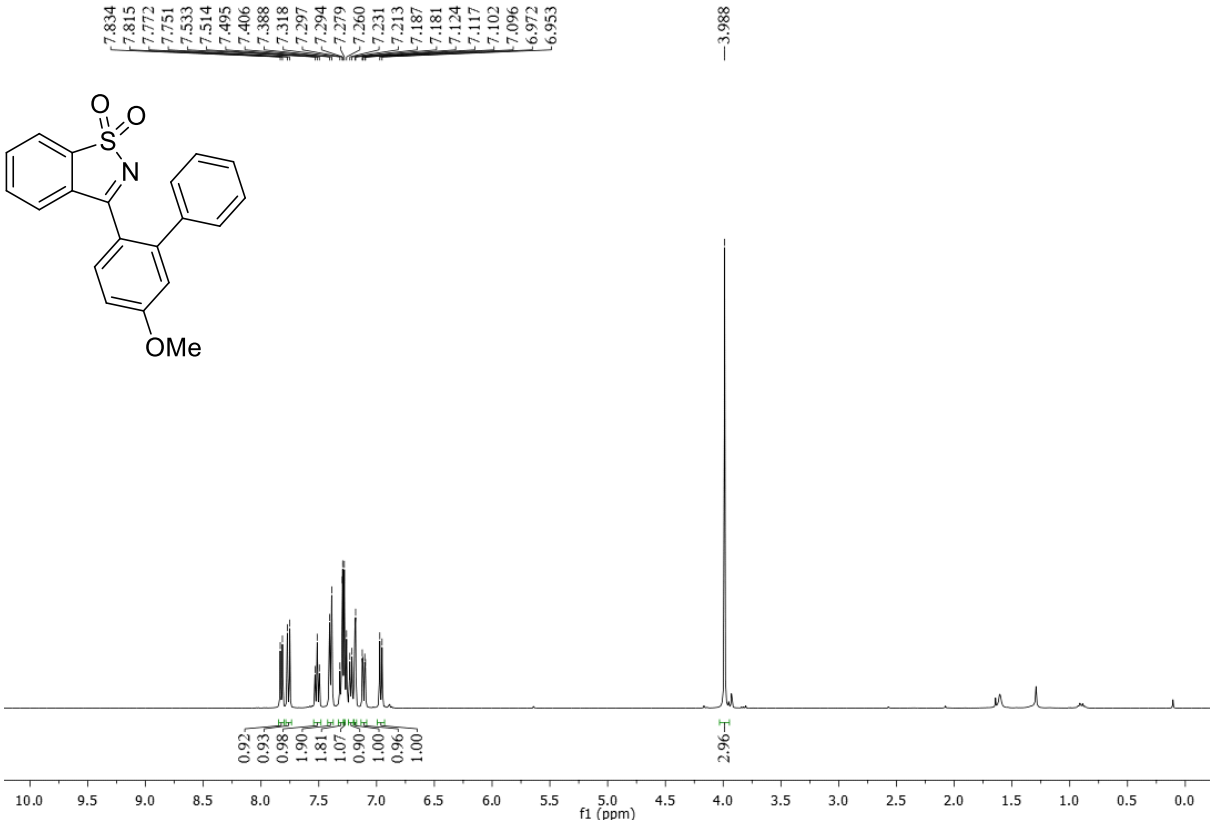


^{13}C NMR of **3ha** (150 MHz, $CDCl_3$):

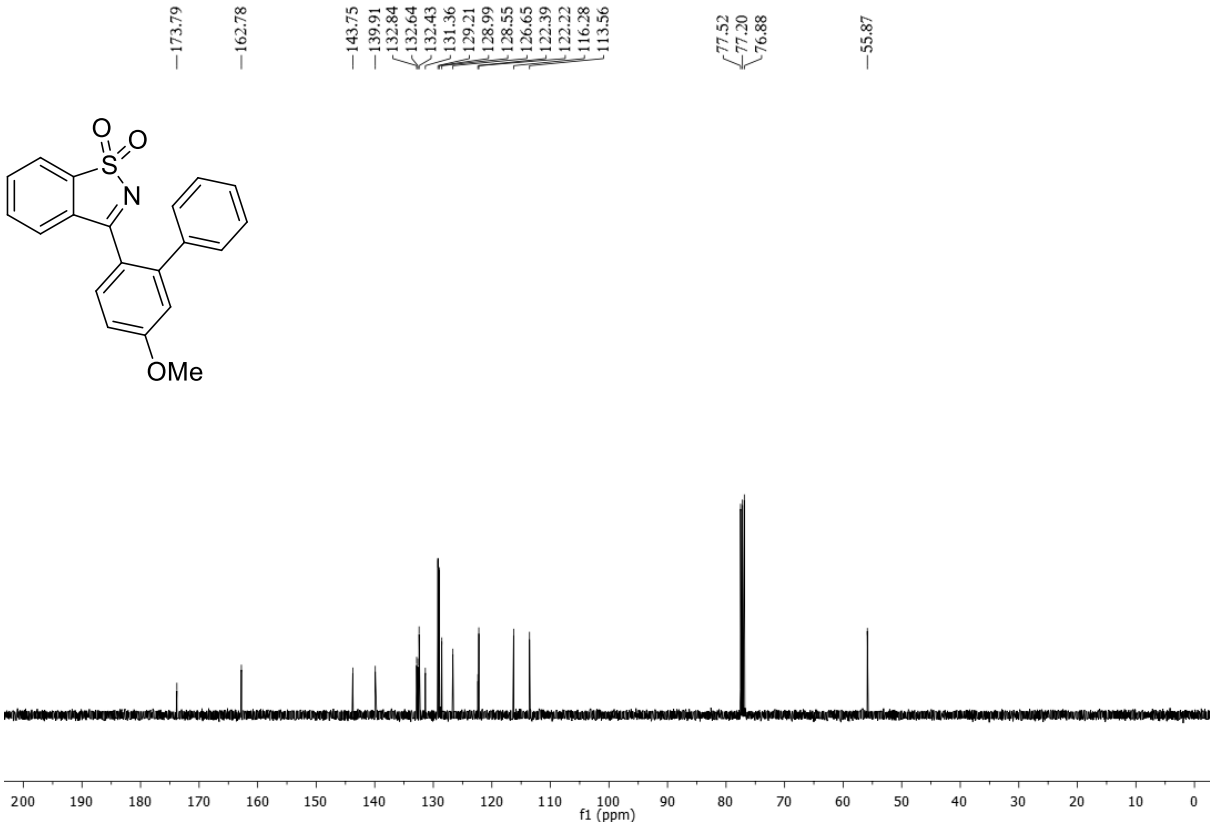




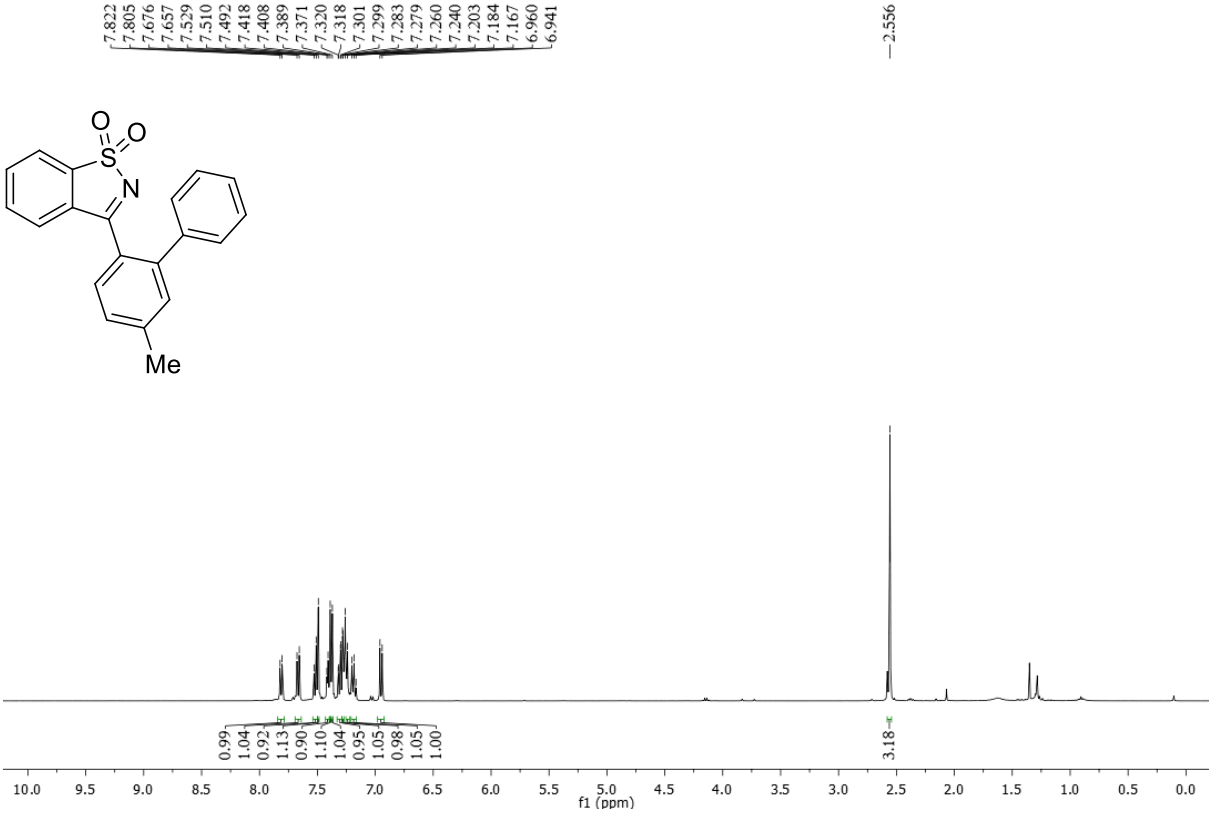
^{1}H NMR of **3ia** (400MHz, $CDCl_3$):



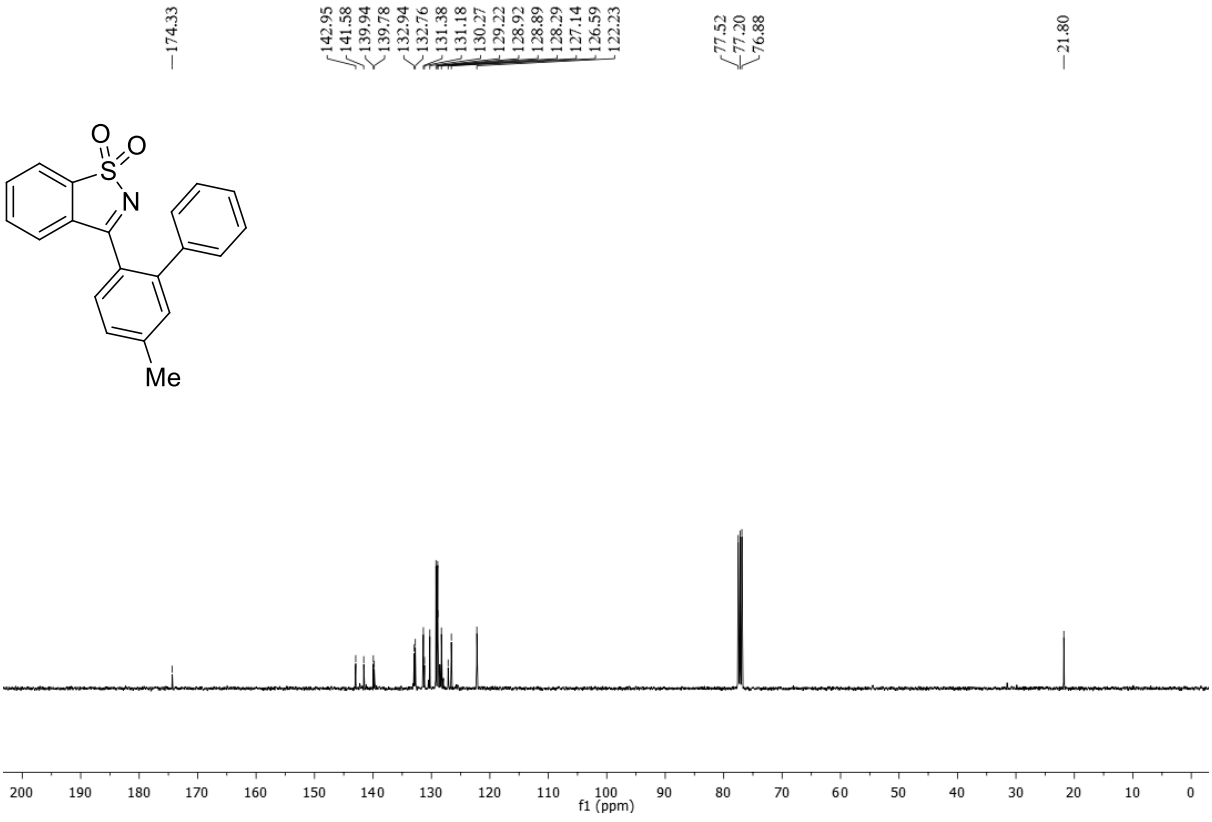
^{13}C NMR of **3ia** (100MHz, $CDCl_3$):



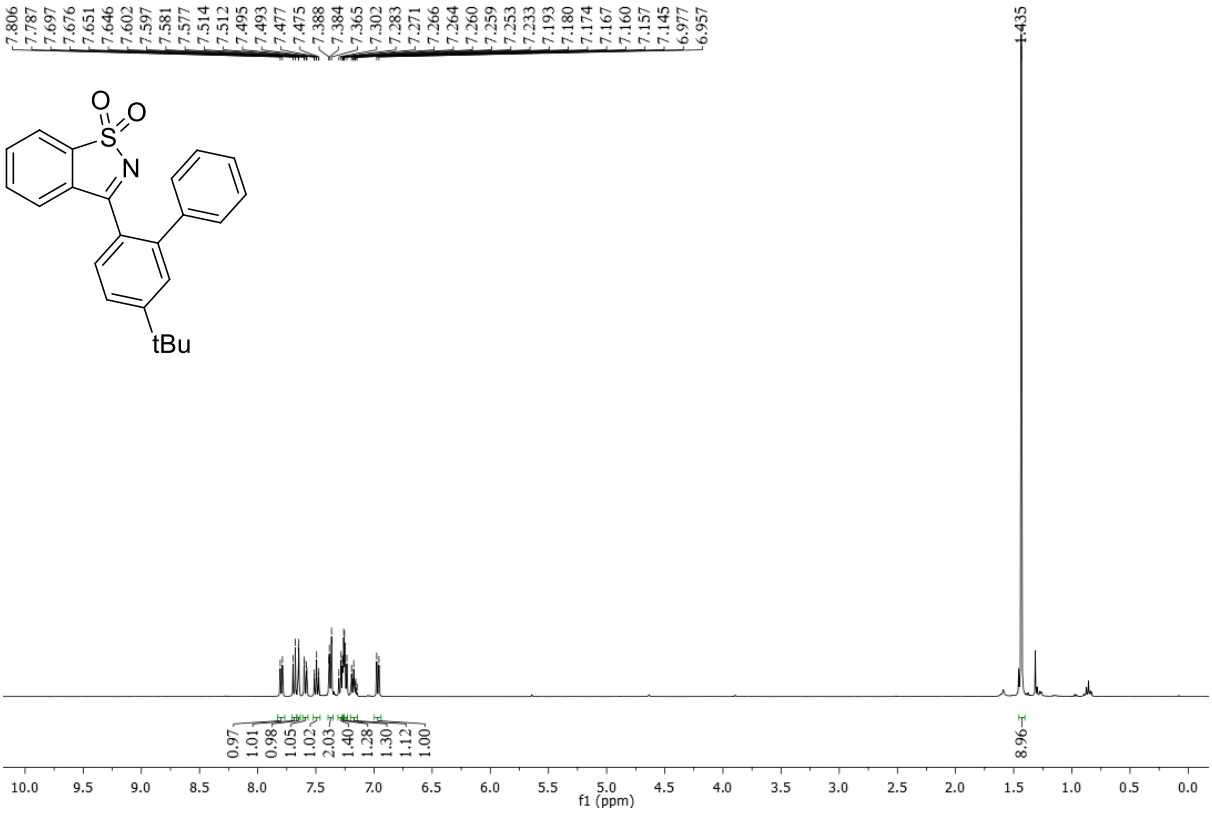
^{1}H NMR of **3ja** (400MHz, $CDCl_3$):



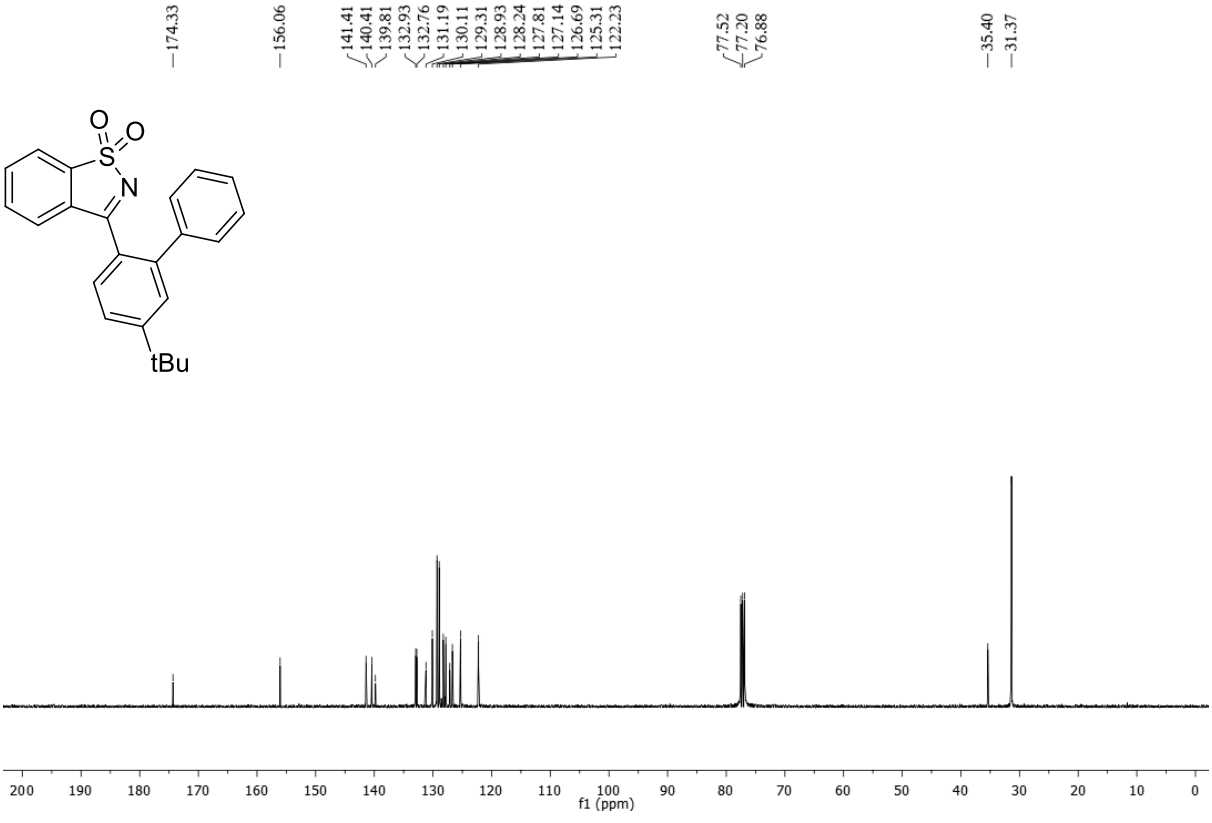
^{13}C NMR of **3ja** (100MHz, $CDCl_3$):



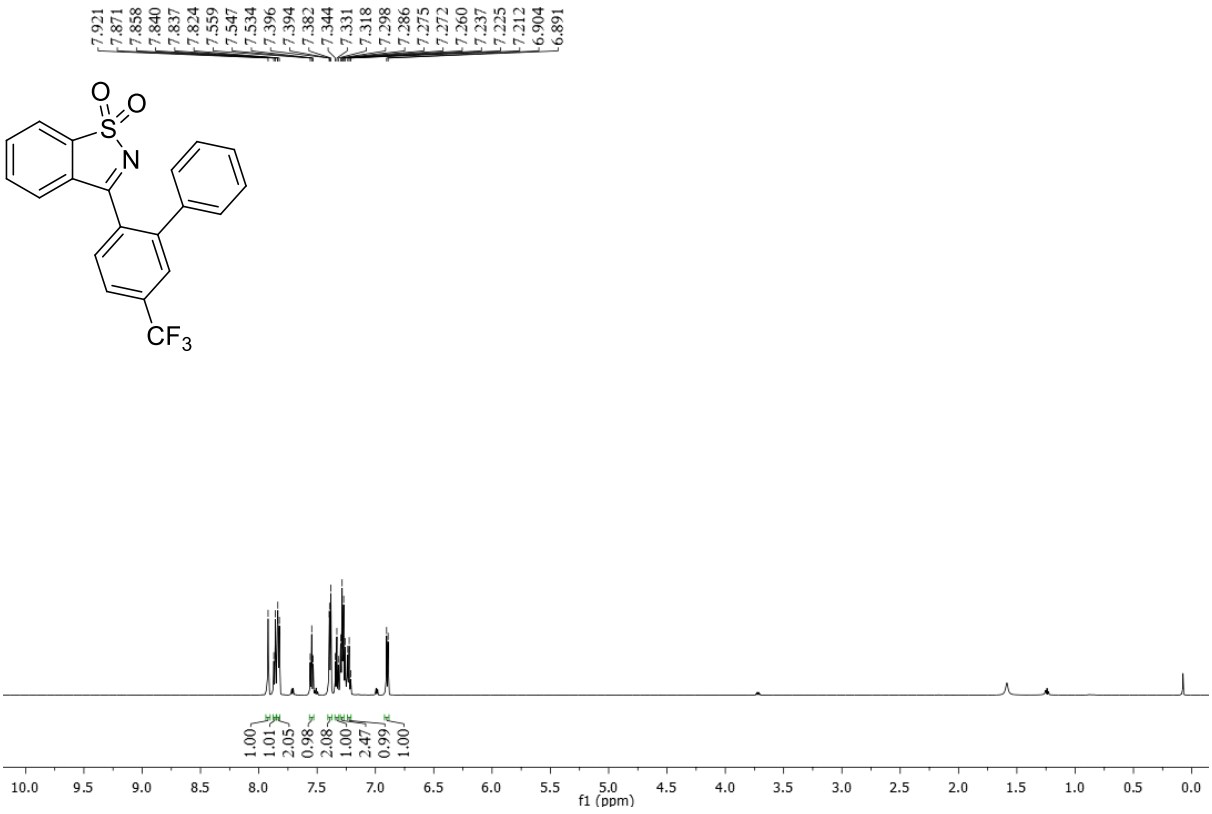
^{1}H NMR of **3ka** (400MHz, $CDCl_3$):



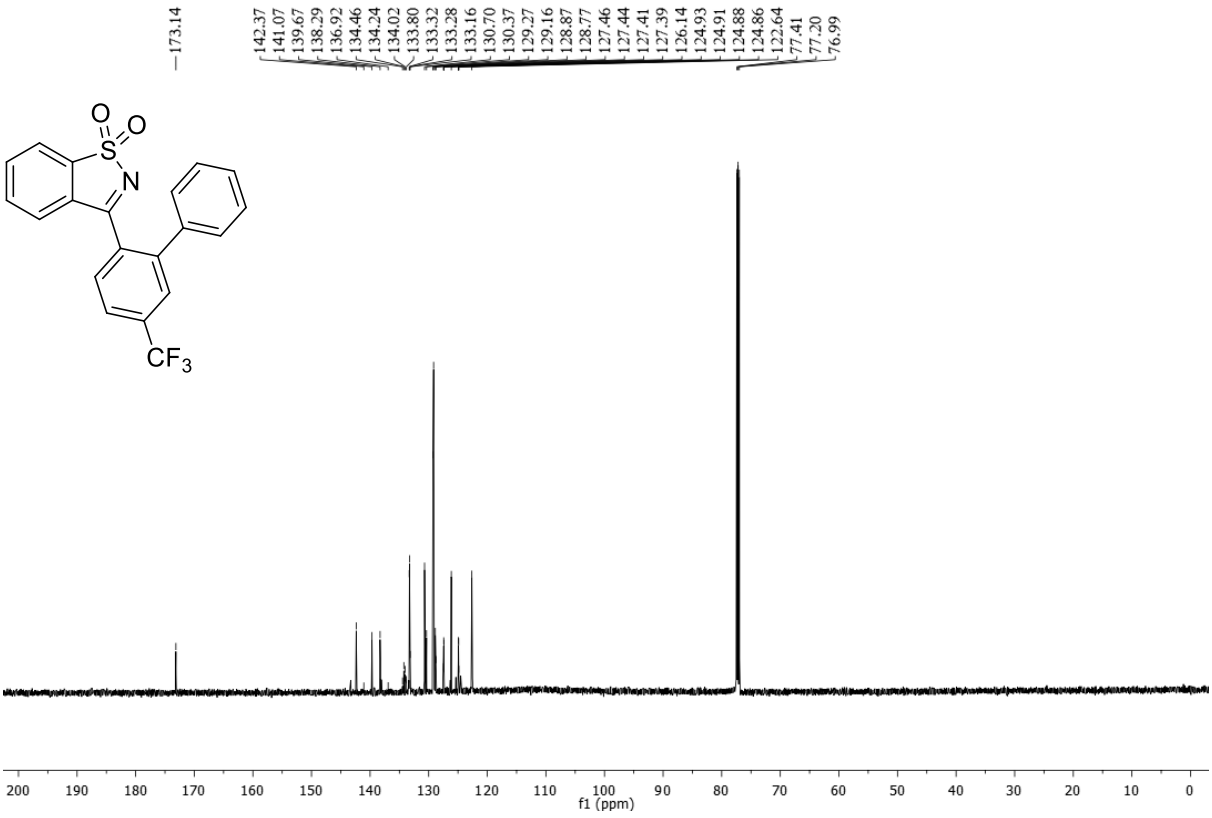
^{13}C NMR of **3ka** (100MHz, $CDCl_3$):



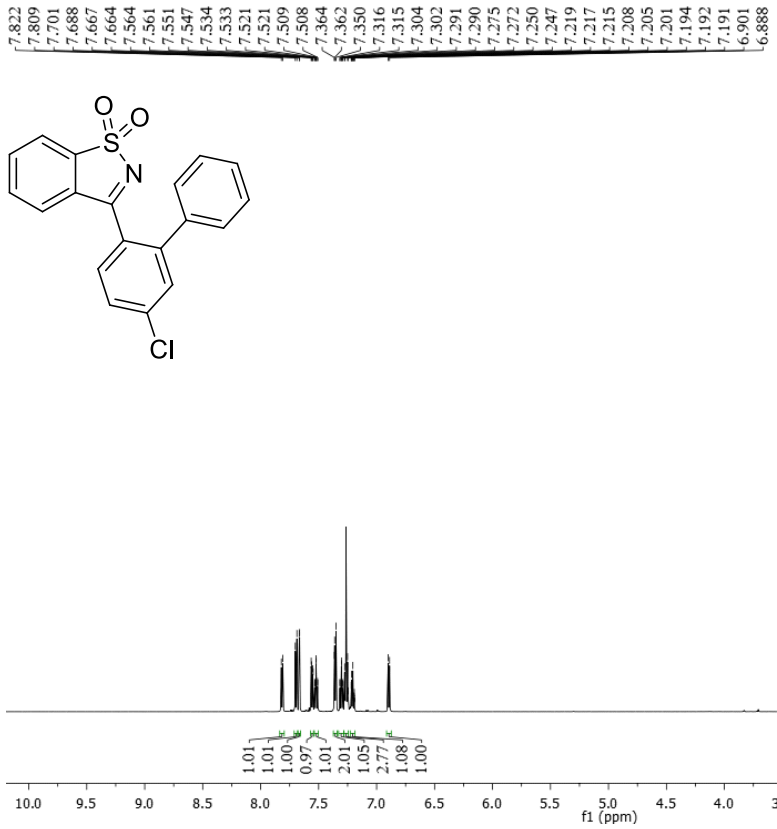
^{1}H NMR of **3la** (600MHz, $CDCl_3$):



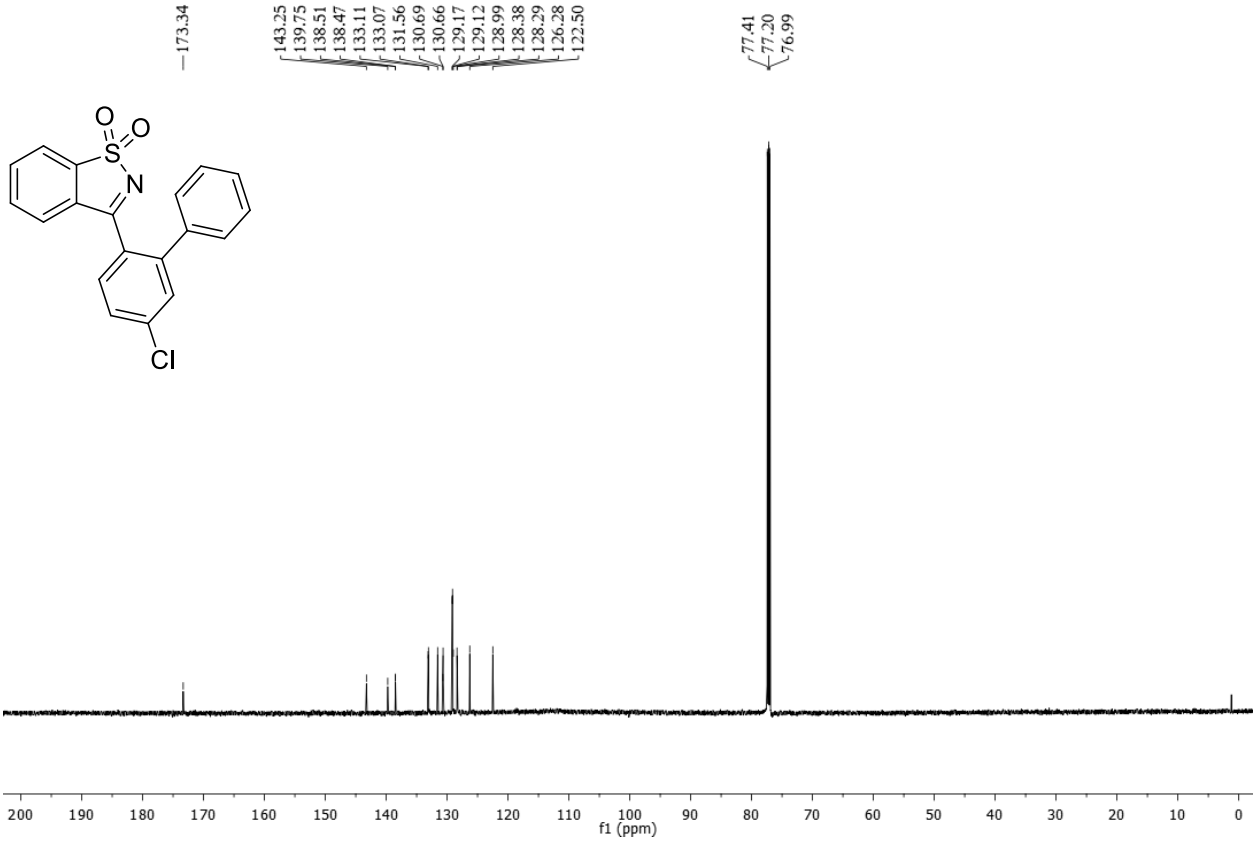
^{13}C NMR of **3la** (150MHz, $CDCl_3$):



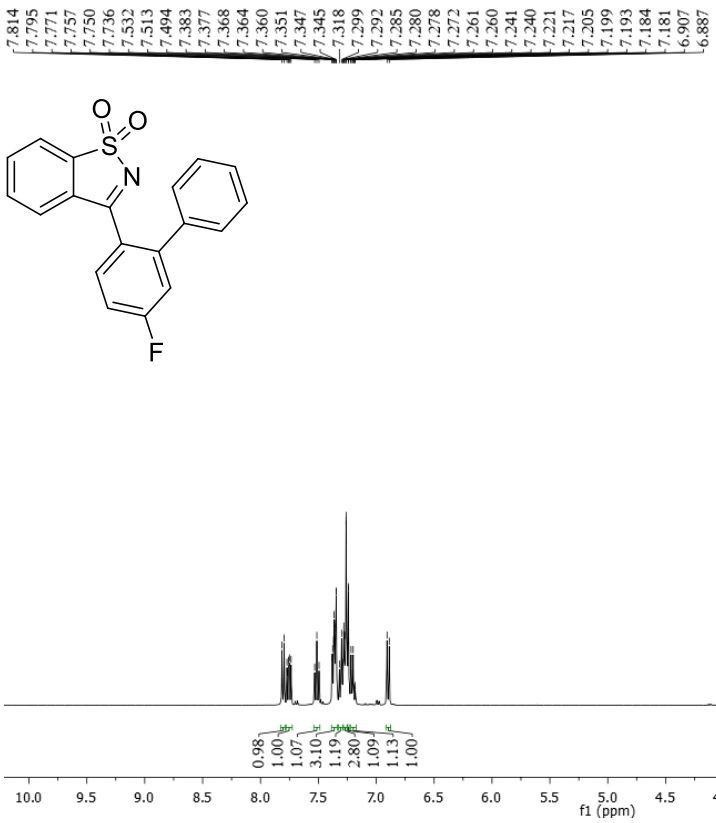
^{1}H NMR of **3ma** (600MHz, $CDCl_3$):



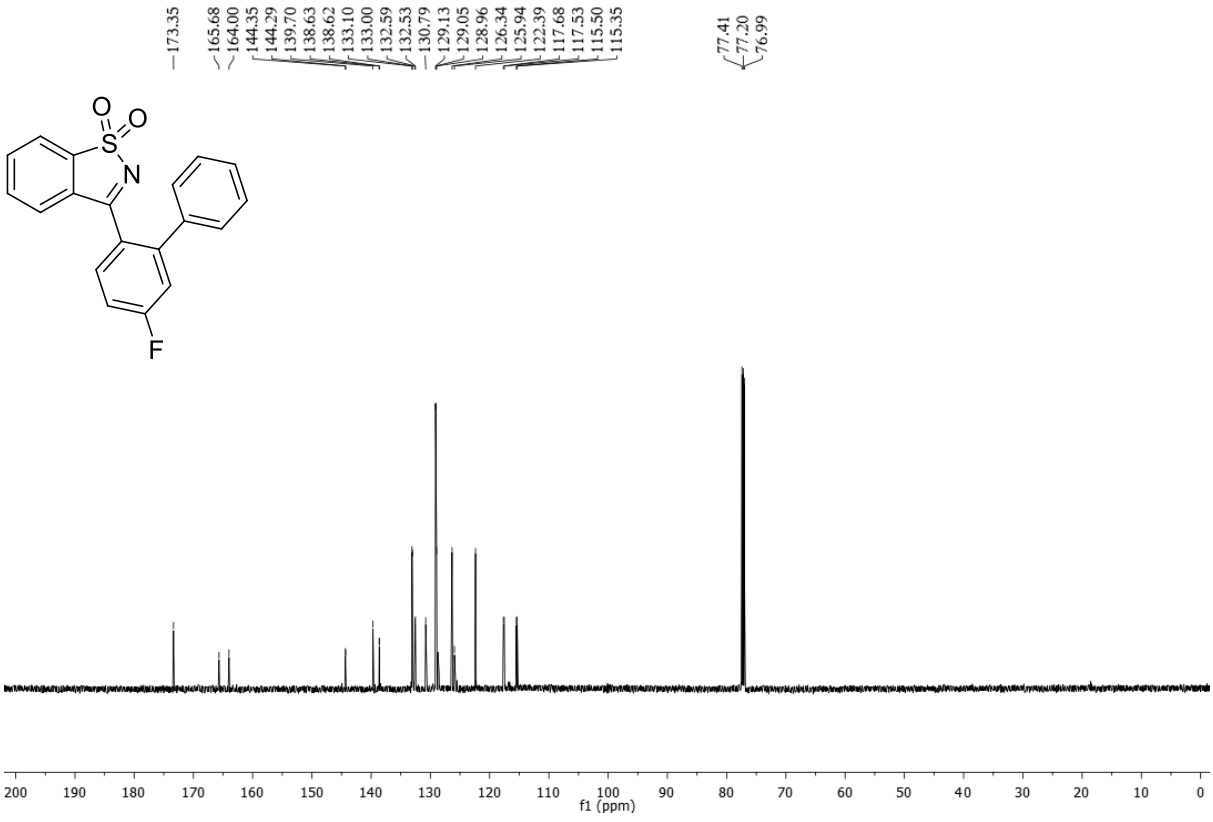
^{13}C NMR of **3ma** (150MHz, $CDCl_3$):



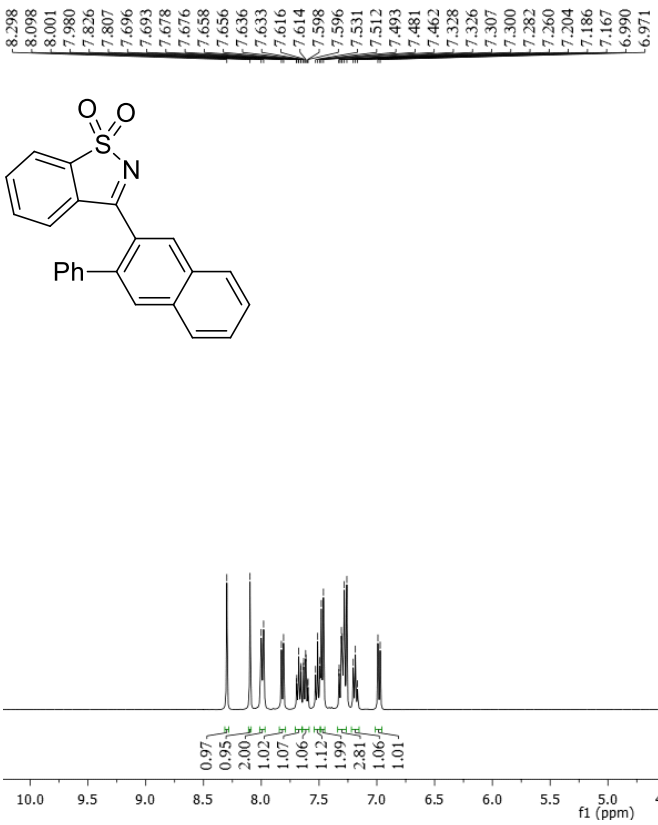
^{1}H NMR of **3na** (400MHz, $CDCl_3$):



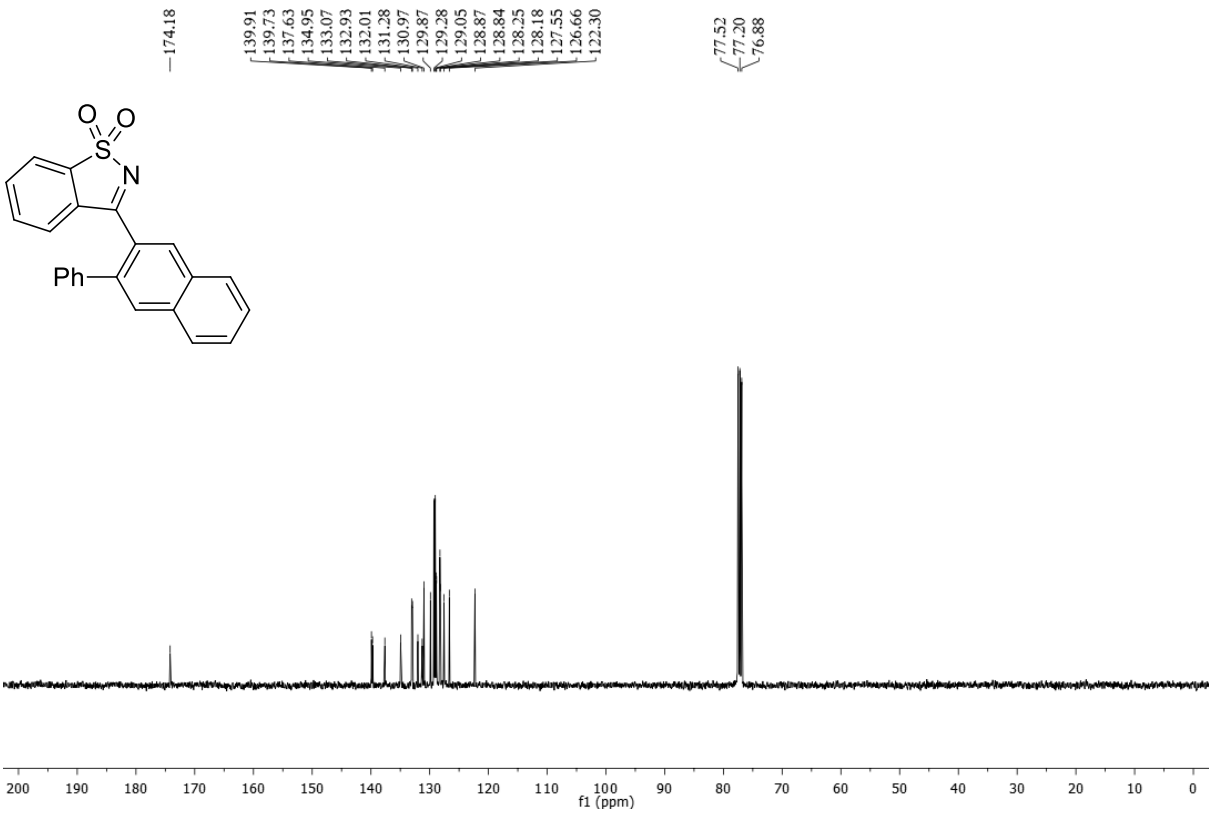
^{13}C NMR of **3na** (600MHz, $CDCl_3$):



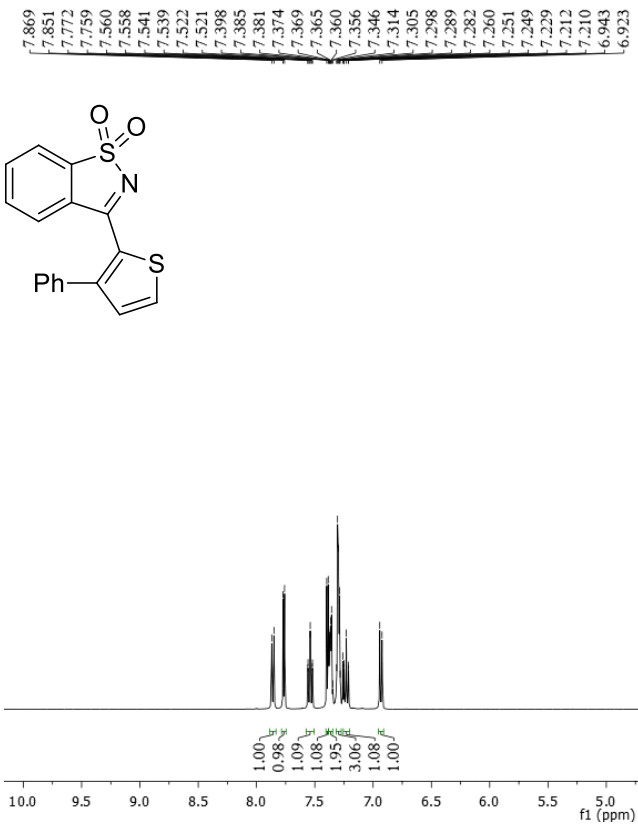
^{1}H NMR of **3oa** (400MHz, $CDCl_3$):



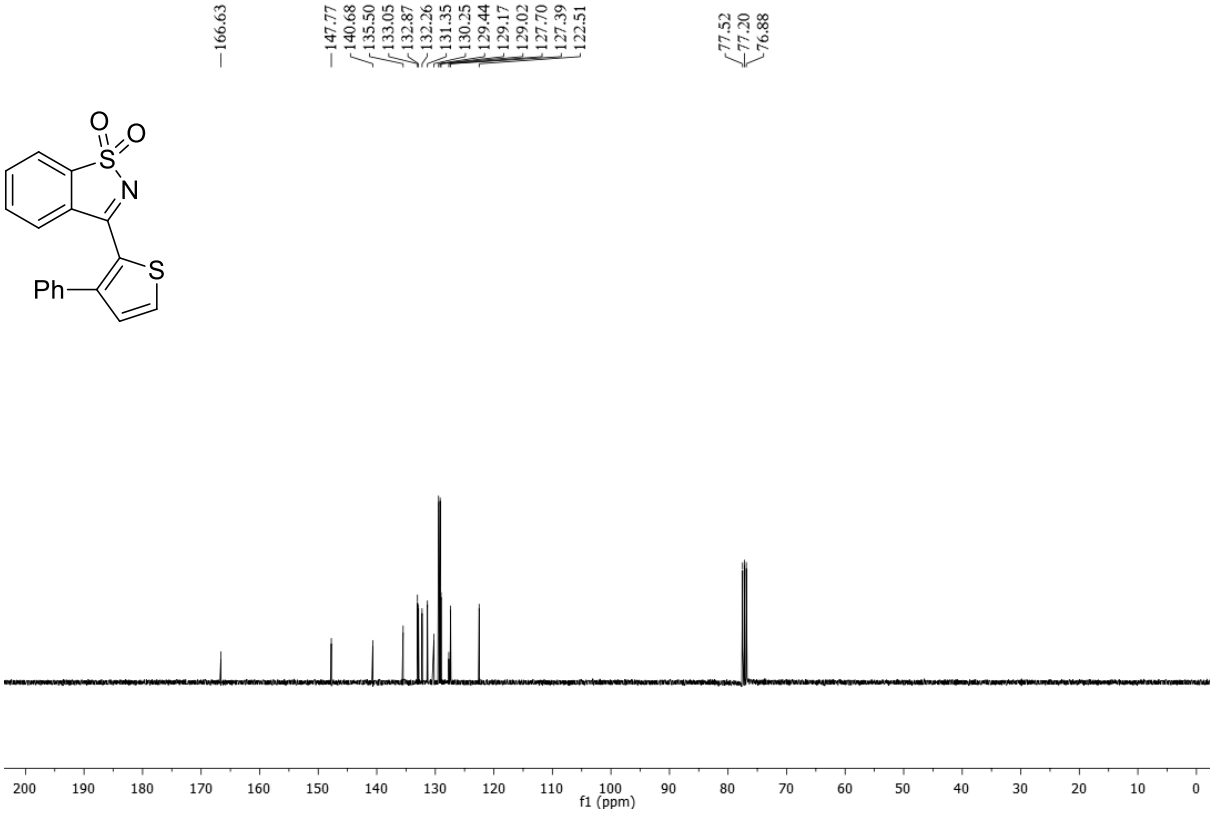
^{13}C NMR of **3oa** (100MHz, $CDCl_3$):



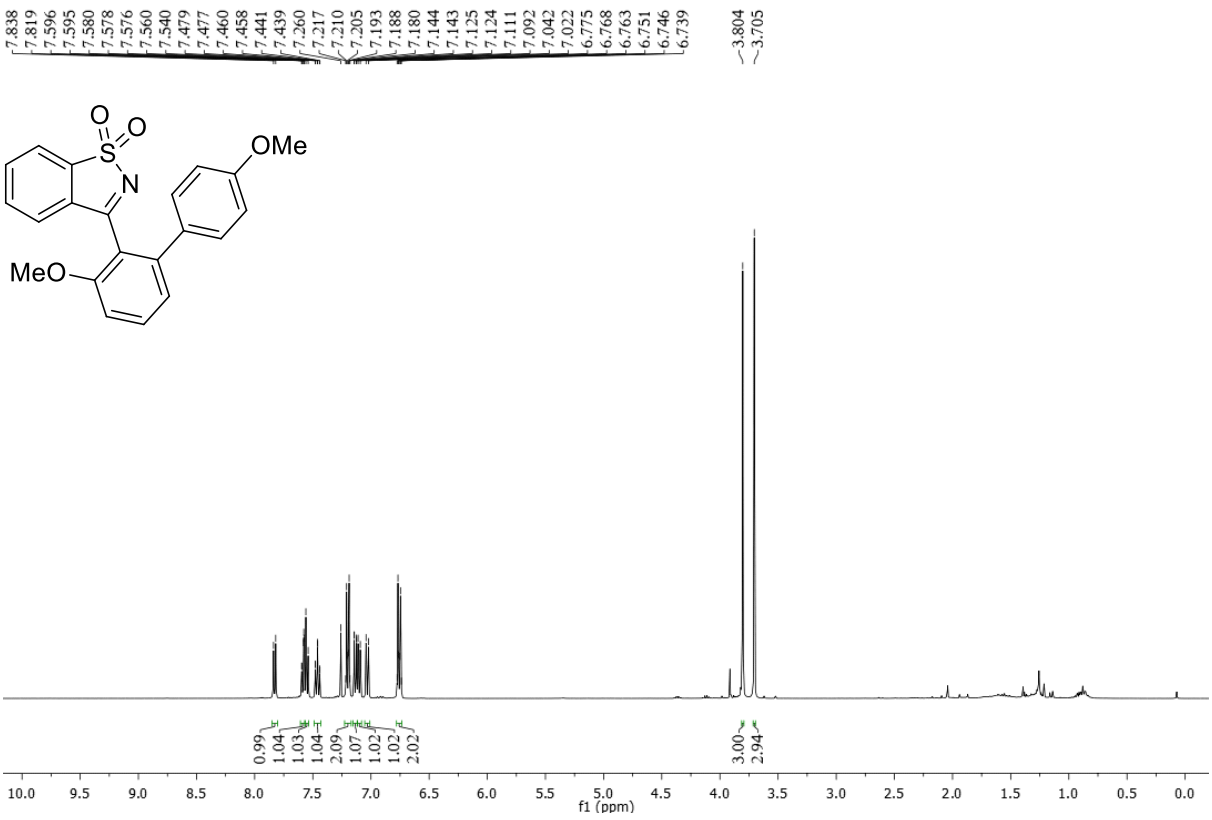
^{1}H NMR of **3pa** (400MHz, $CDCl_3$):



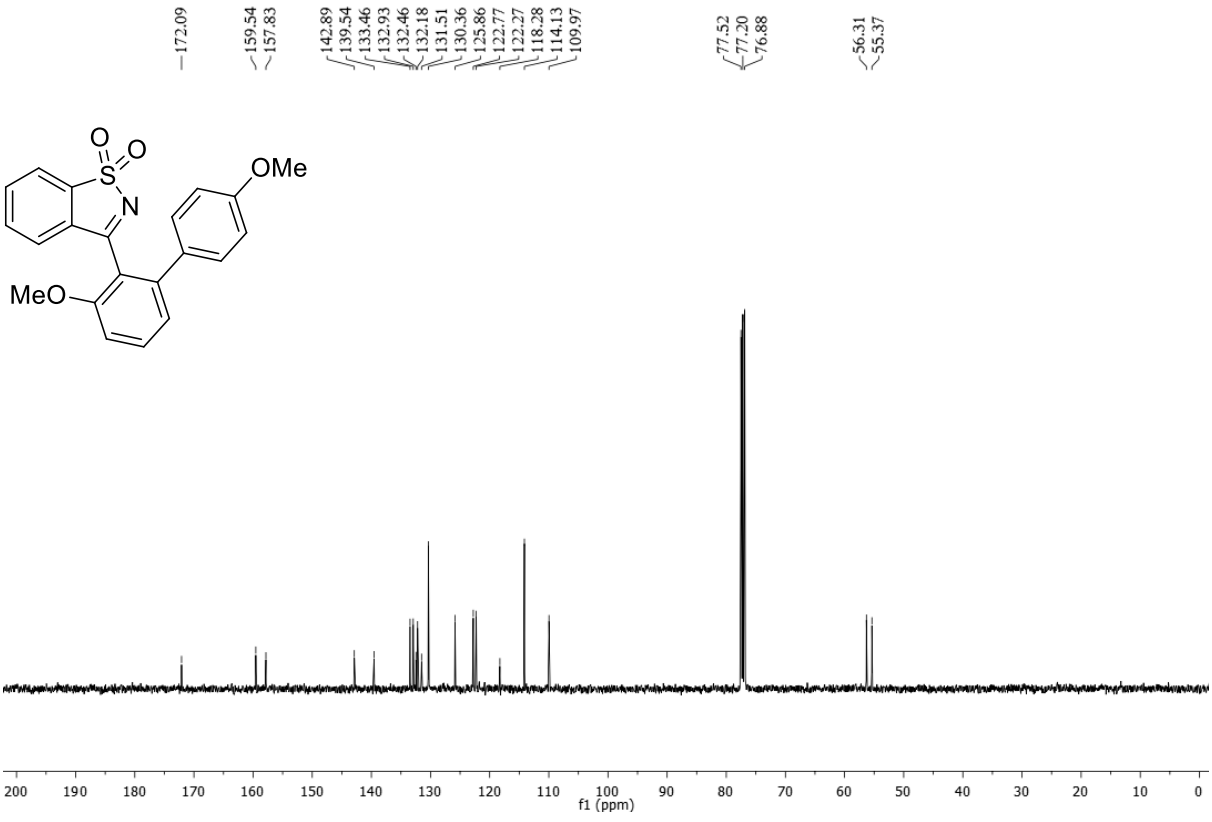
^{13}C NMR of **3pa** (100MHz, $CDCl_3$):



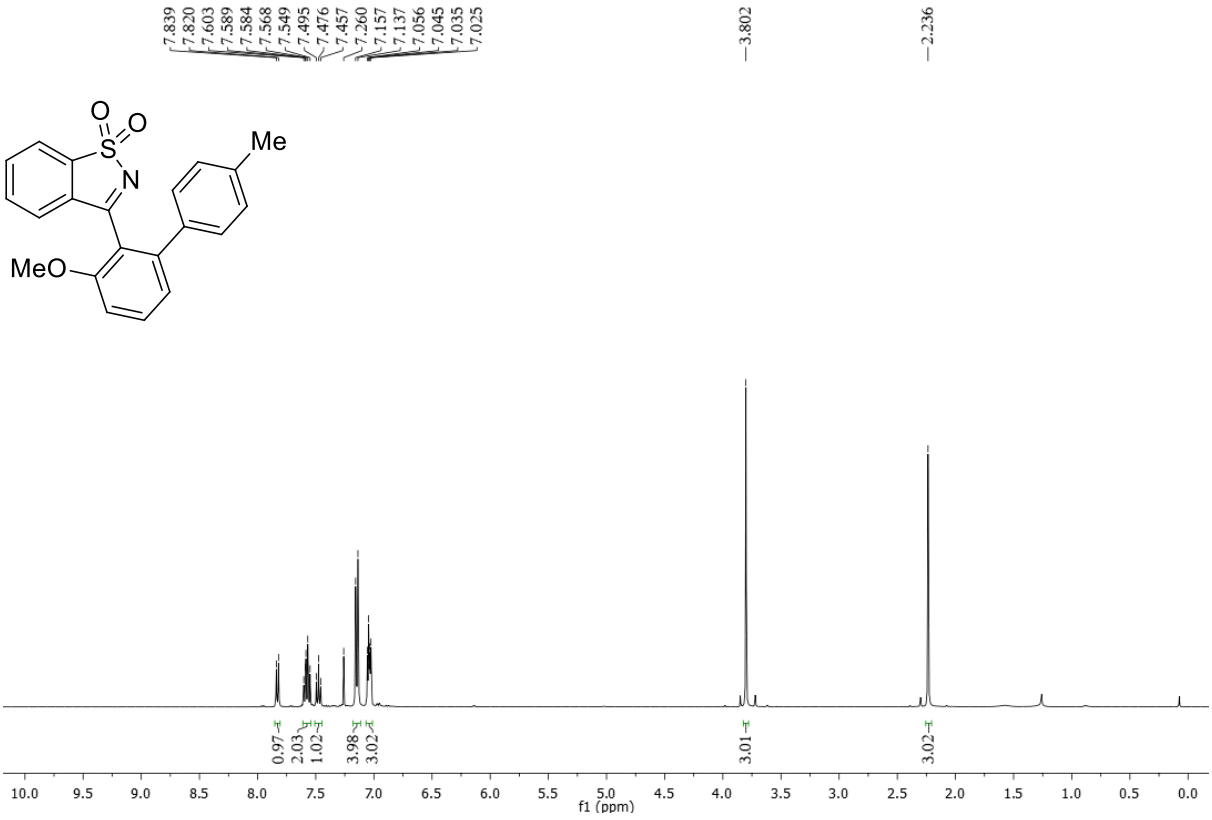
^{1}H NMR of **3bb** (400MHz, $CDCl_3$):



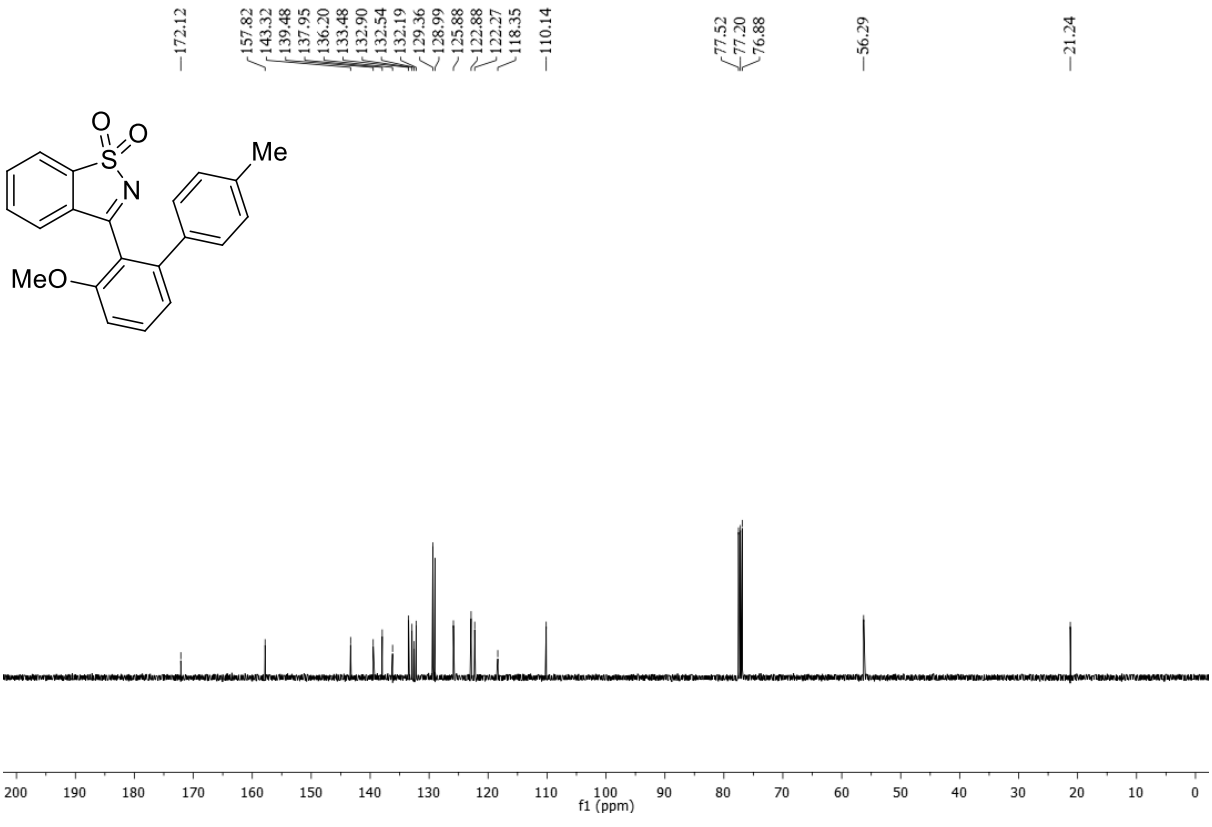
^{13}C NMR of **3bb** (100MHz, $CDCl_3$):



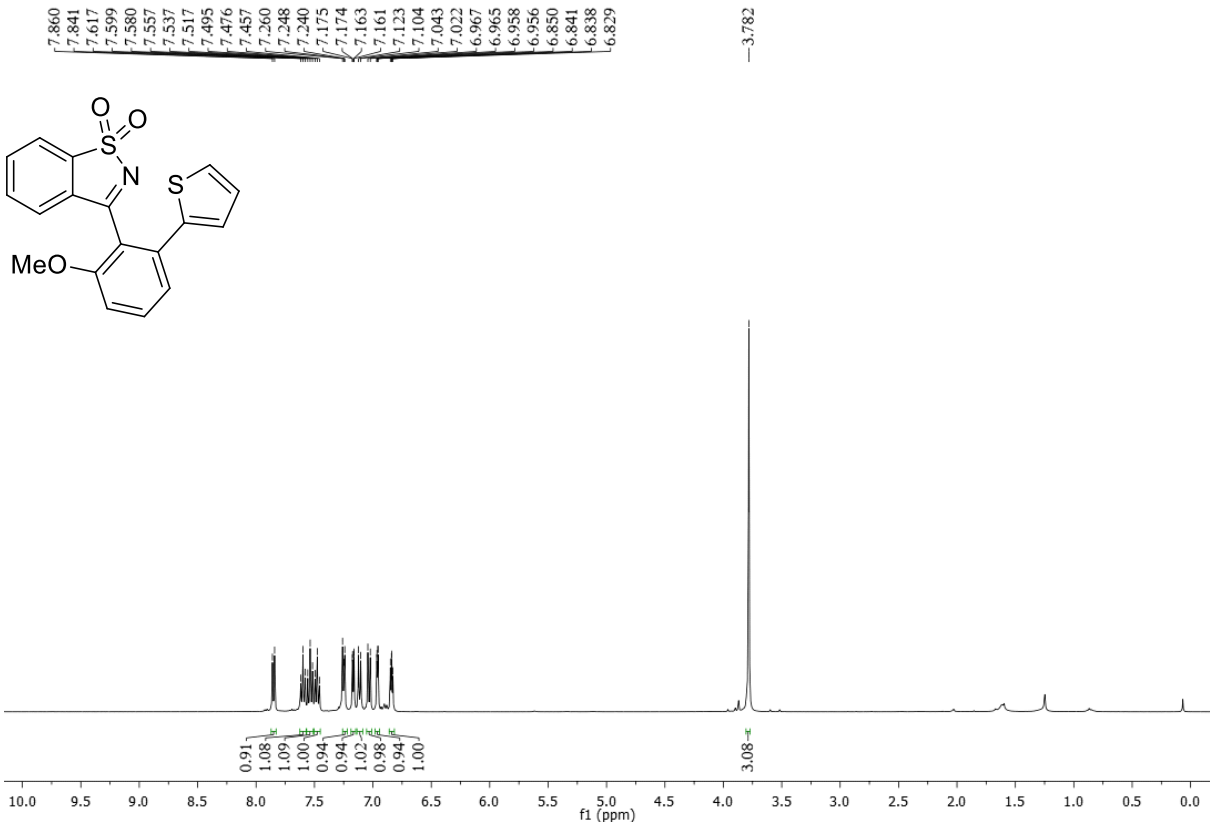
^{1}H NMR of **3bc** (400MHz, $CDCl_3$):



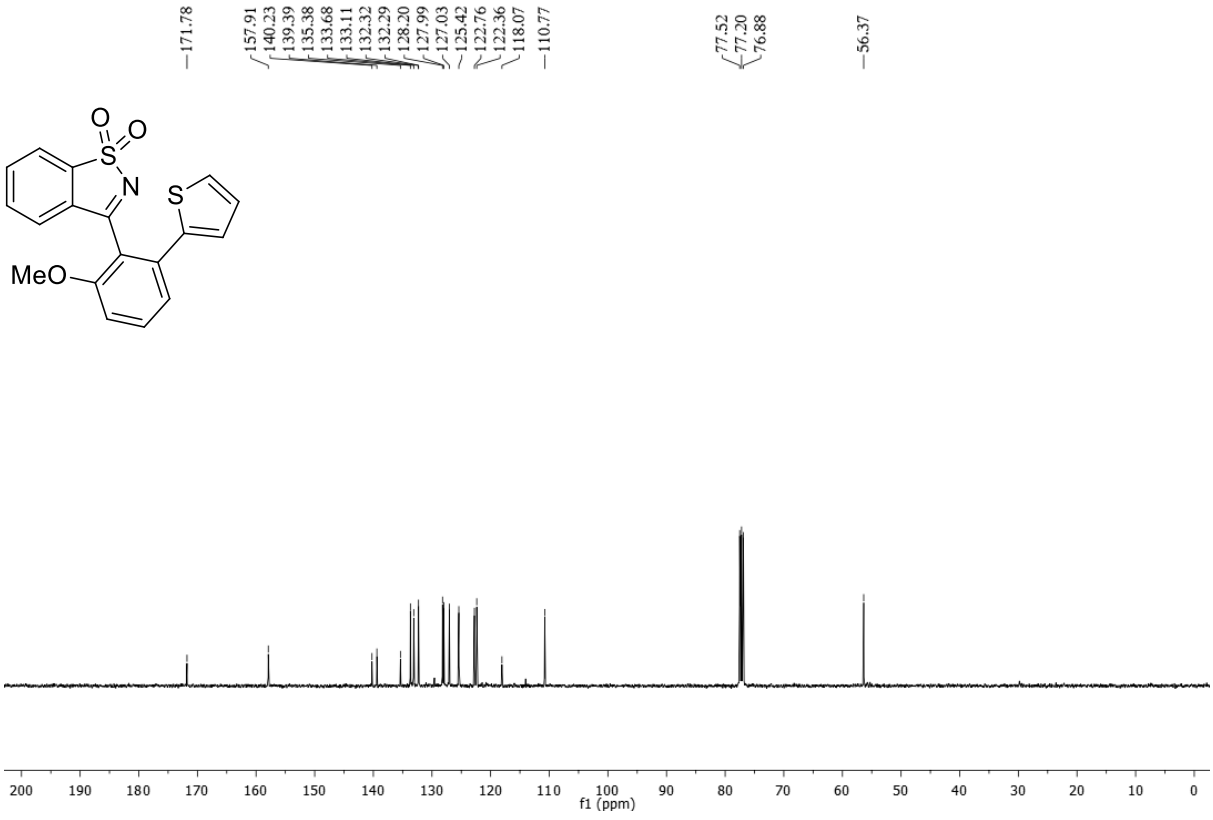
^{13}C NMR of **3bc** (100MHz, $CDCl_3$):



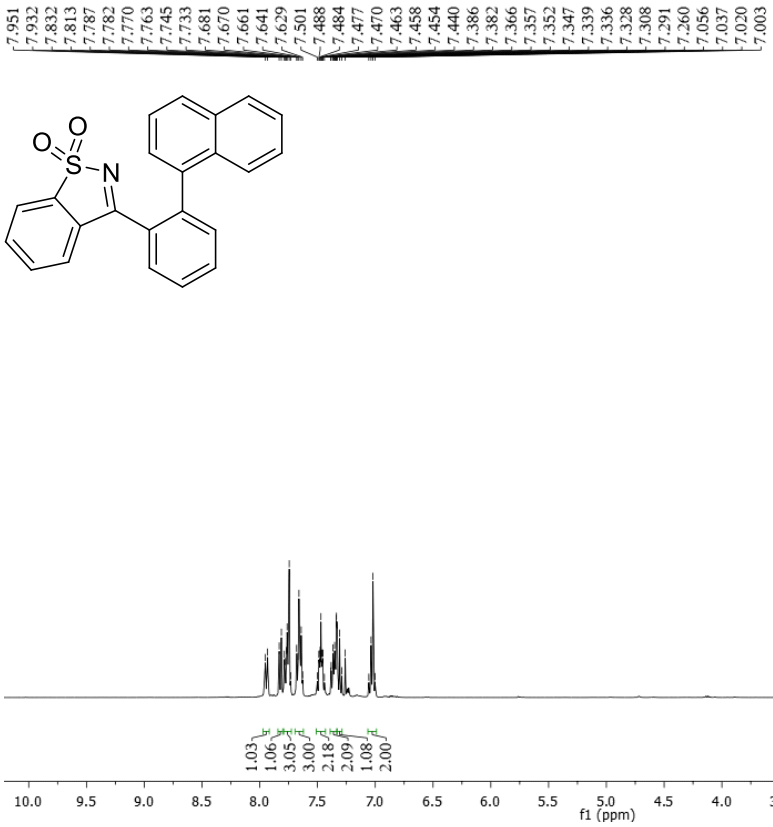
^{1}H NMR of **3bd** (400MHz, $CDCl_3$):



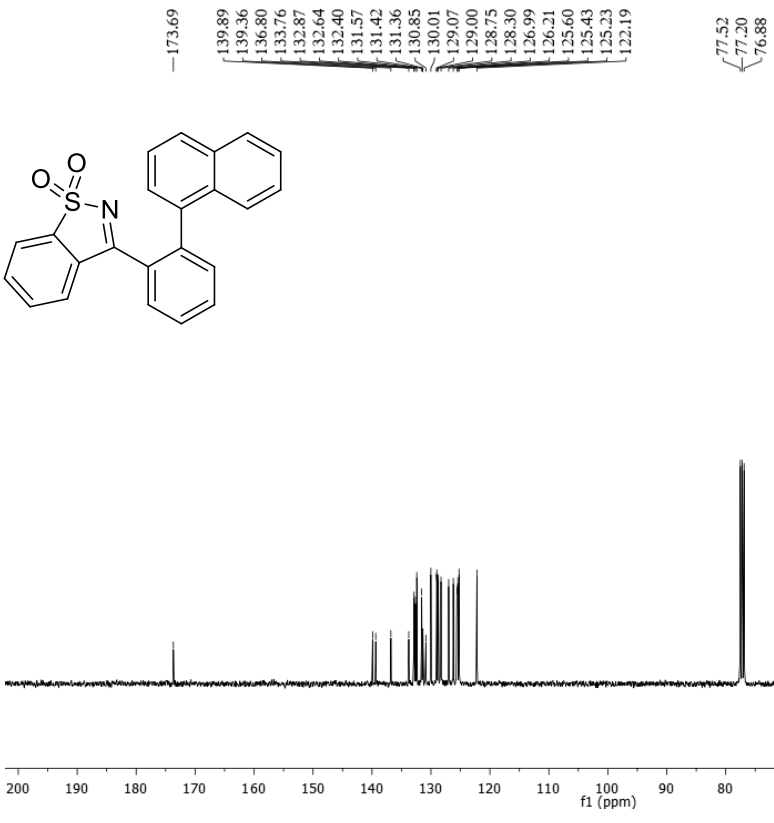
^{13}C NMR of **3bd** (100MHz, $CDCl_3$):



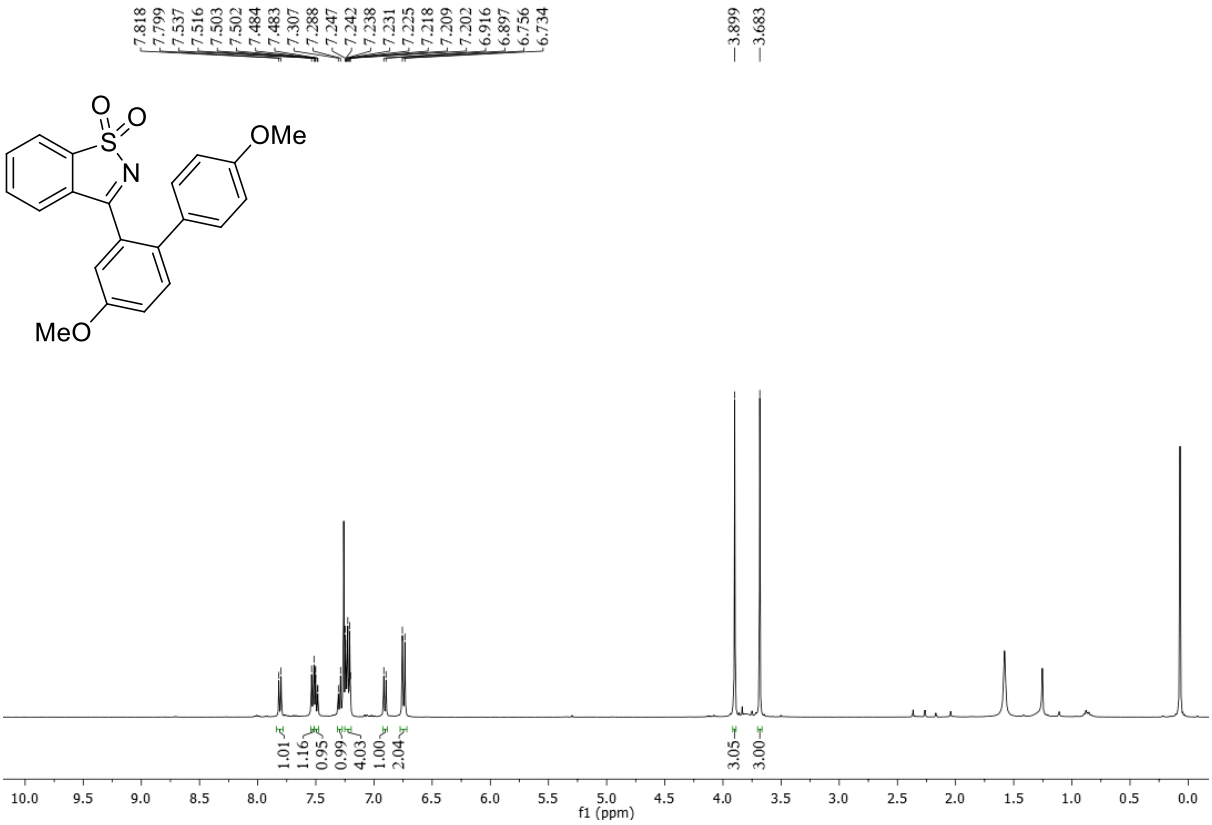
^{1}H NMR of **3be** (400MHz, $CDCl_3$):



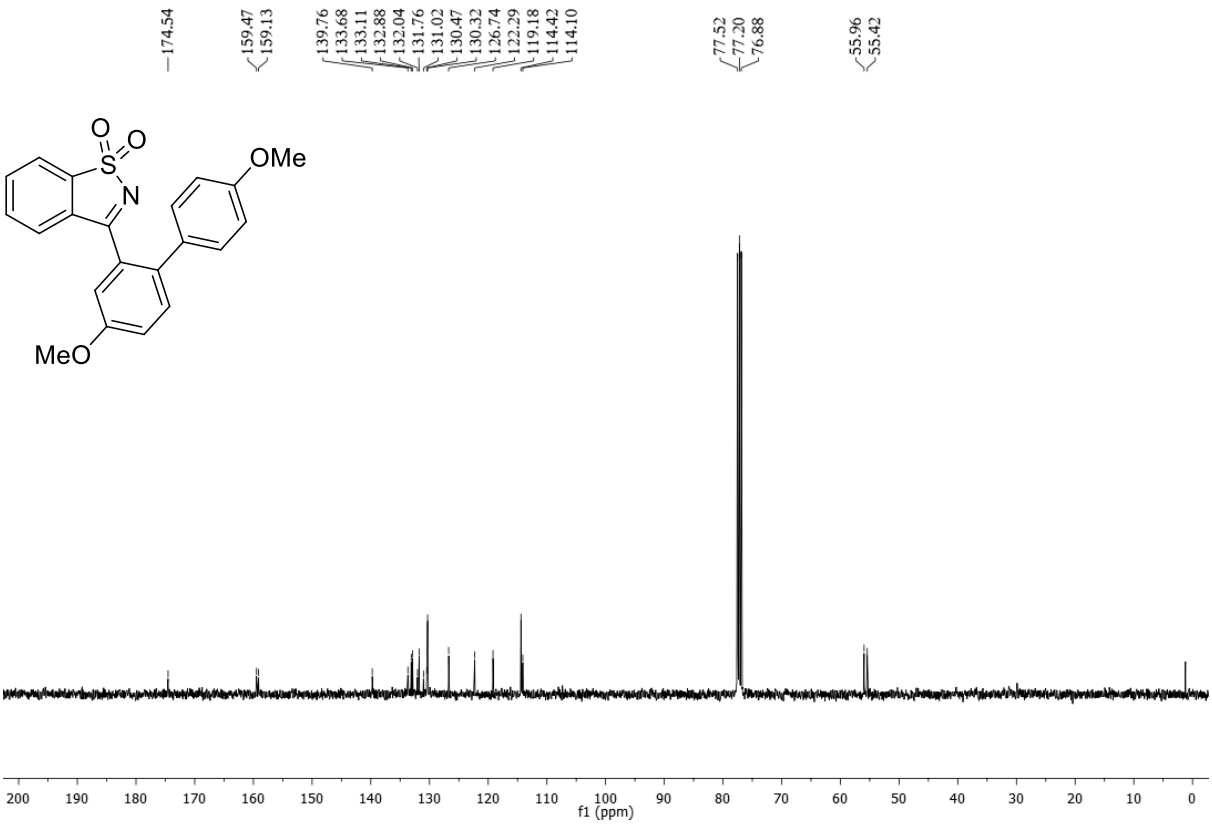
^{13}C NMR of **3be** (100MHz, $CDCl_3$):



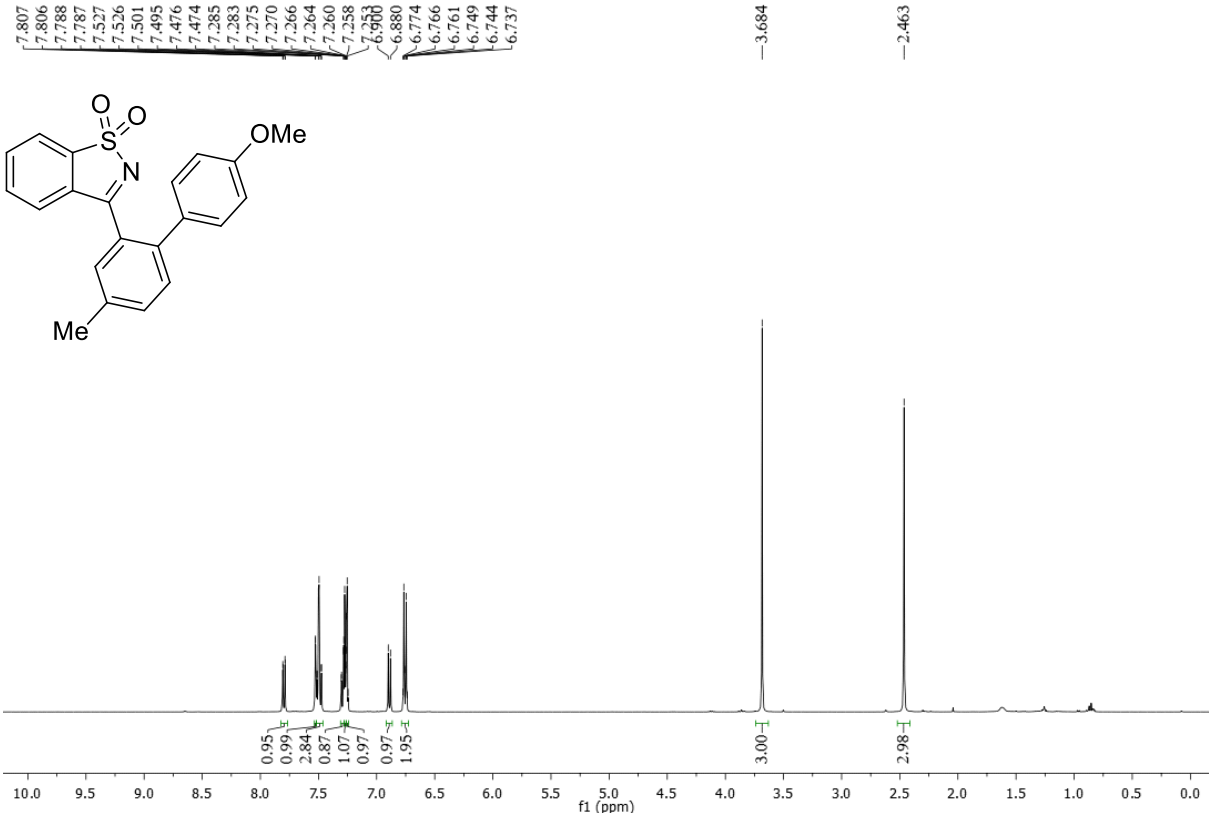
^{1}H NMR of **3db** (400MHz, $CDCl_3$):



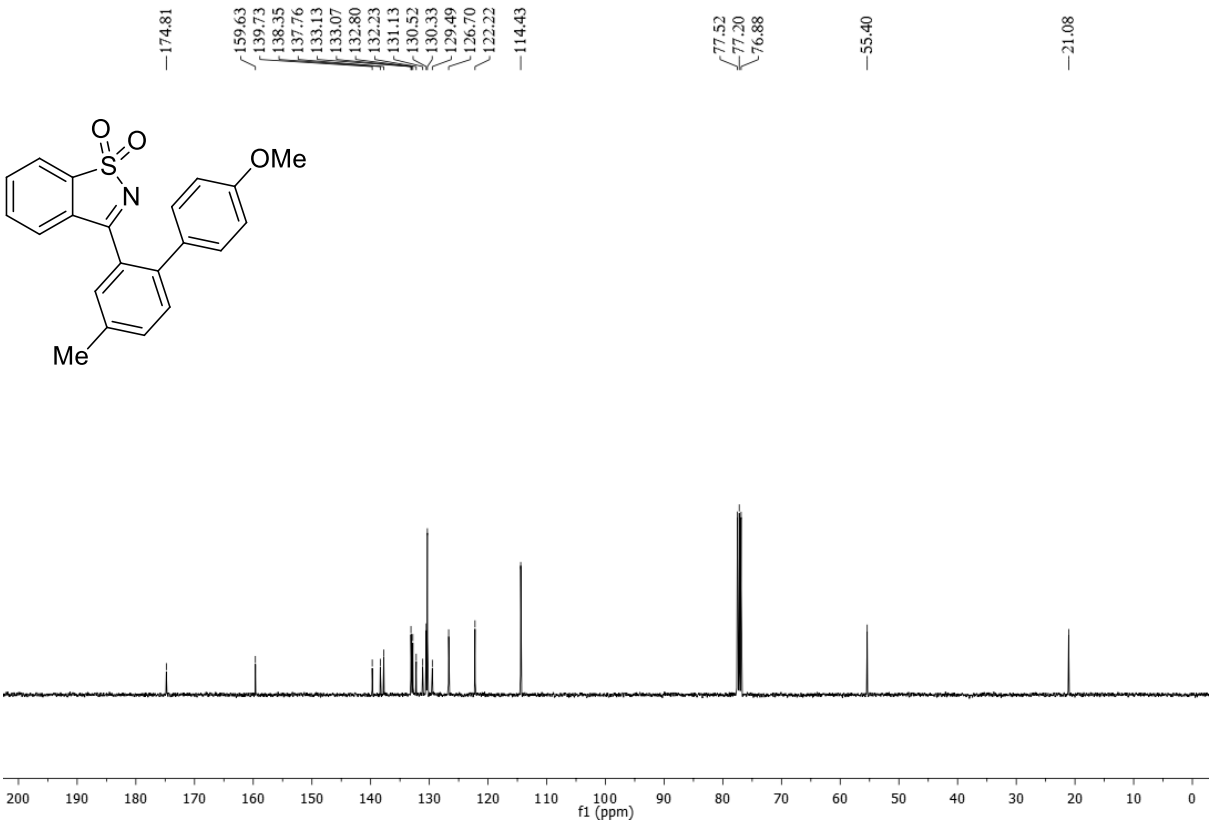
^{13}C NMR of **3db** (100MHz, $CDCl_3$):



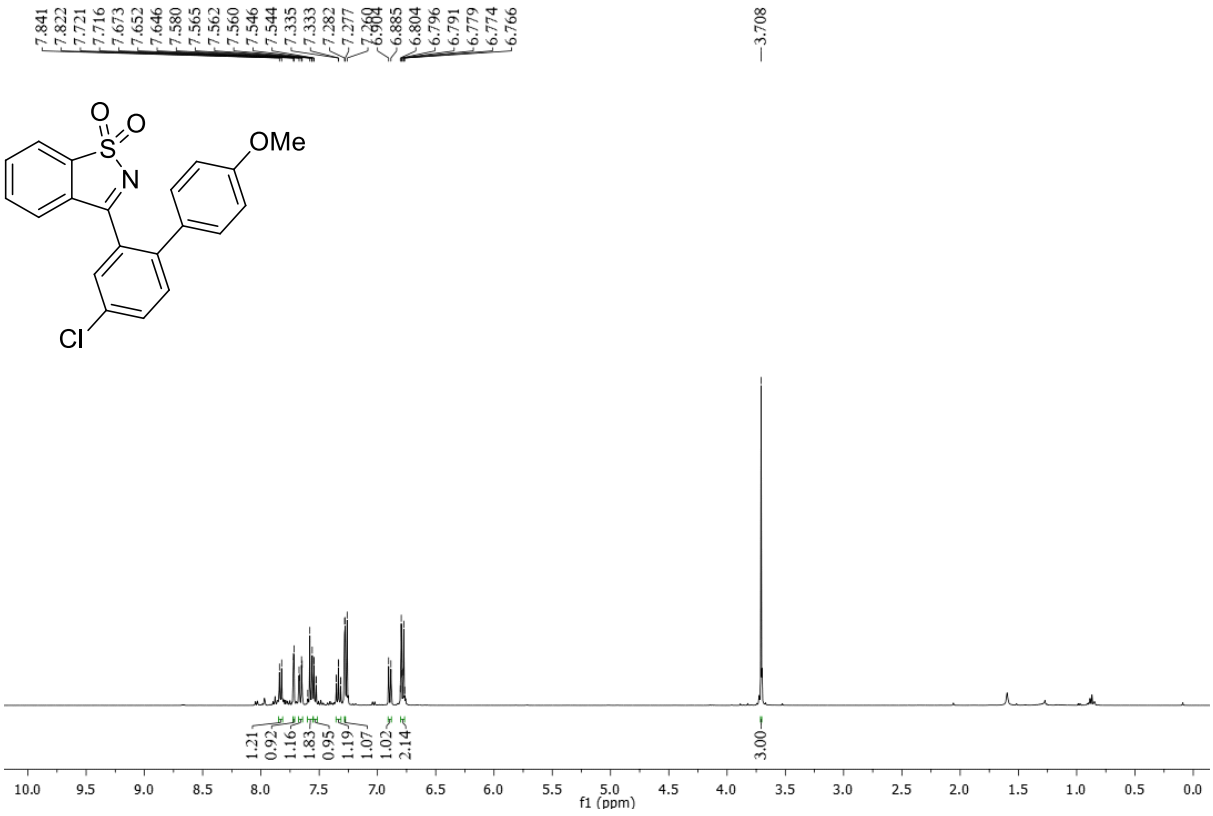
^{1}H NMR of **3eb** (400MHz, $CDCl_3$):



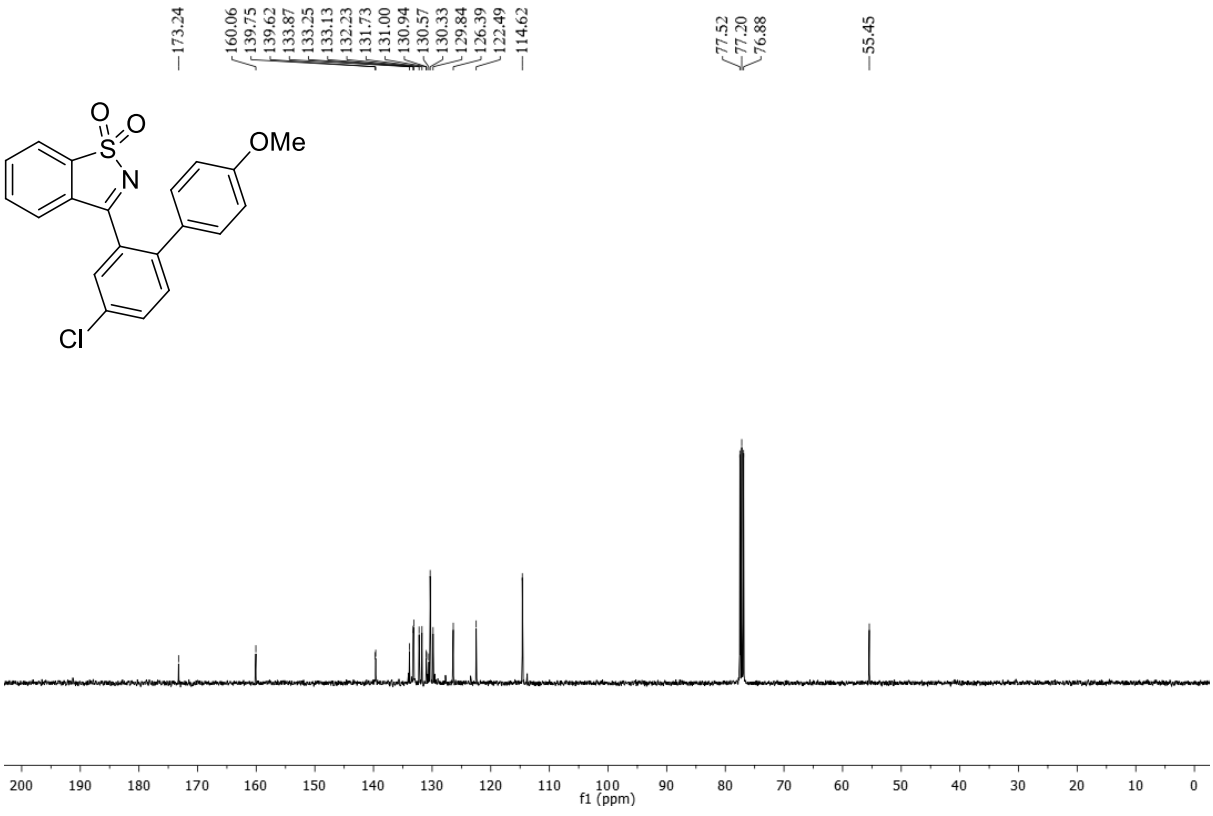
^{13}C NMR of **3eb** (100MHz, $CDCl_3$):



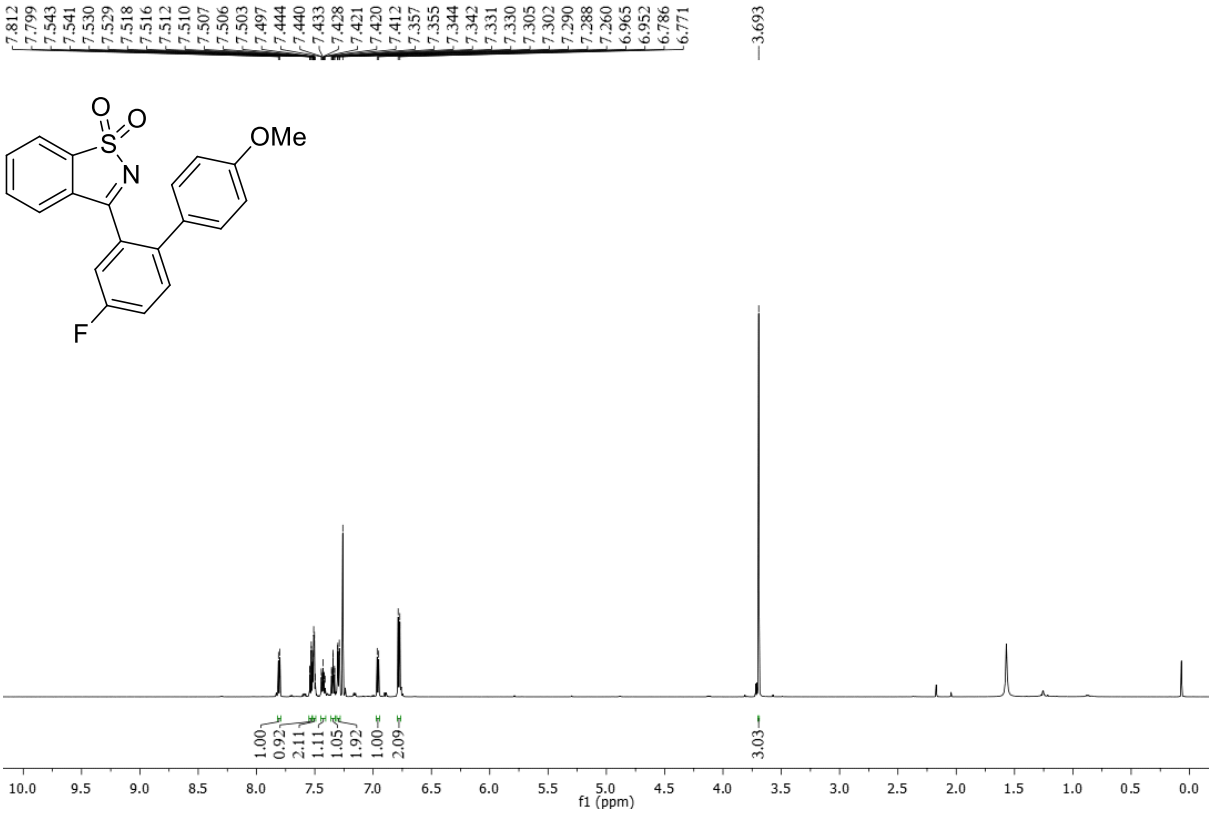
^{1}H NMR of **3fb** (400MHz, $CDCl_3$):



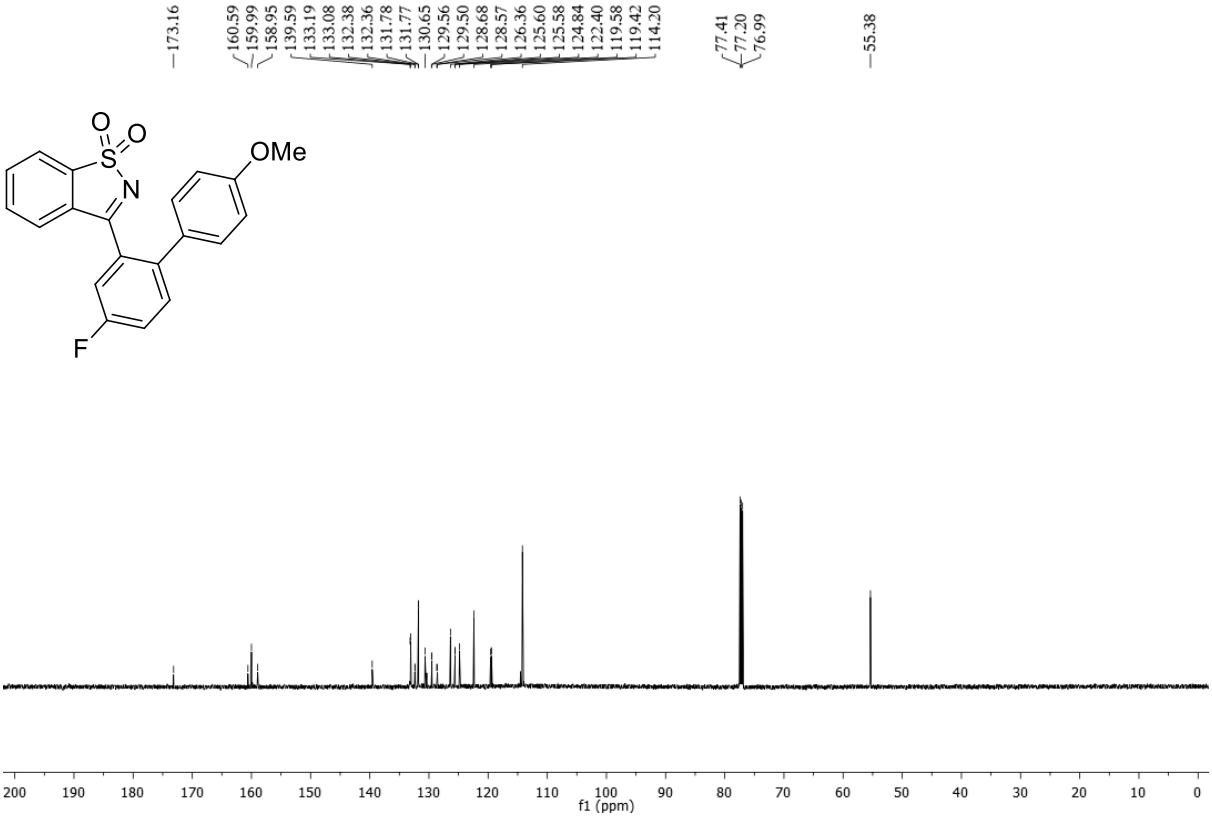
^{13}C NMR of **3fb** (100MHz, $CDCl_3$):



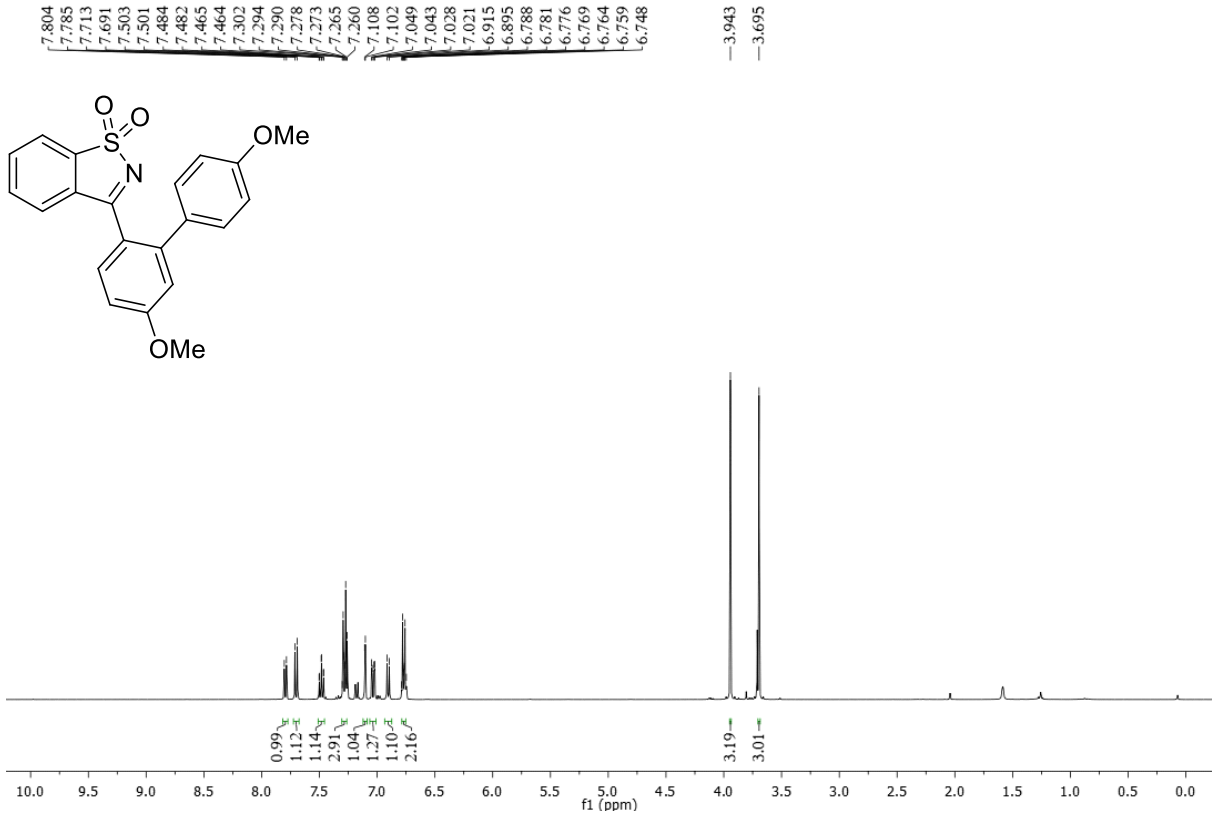
^{1}H NMR of **3gb** (600MHz, $CDCl_3$):



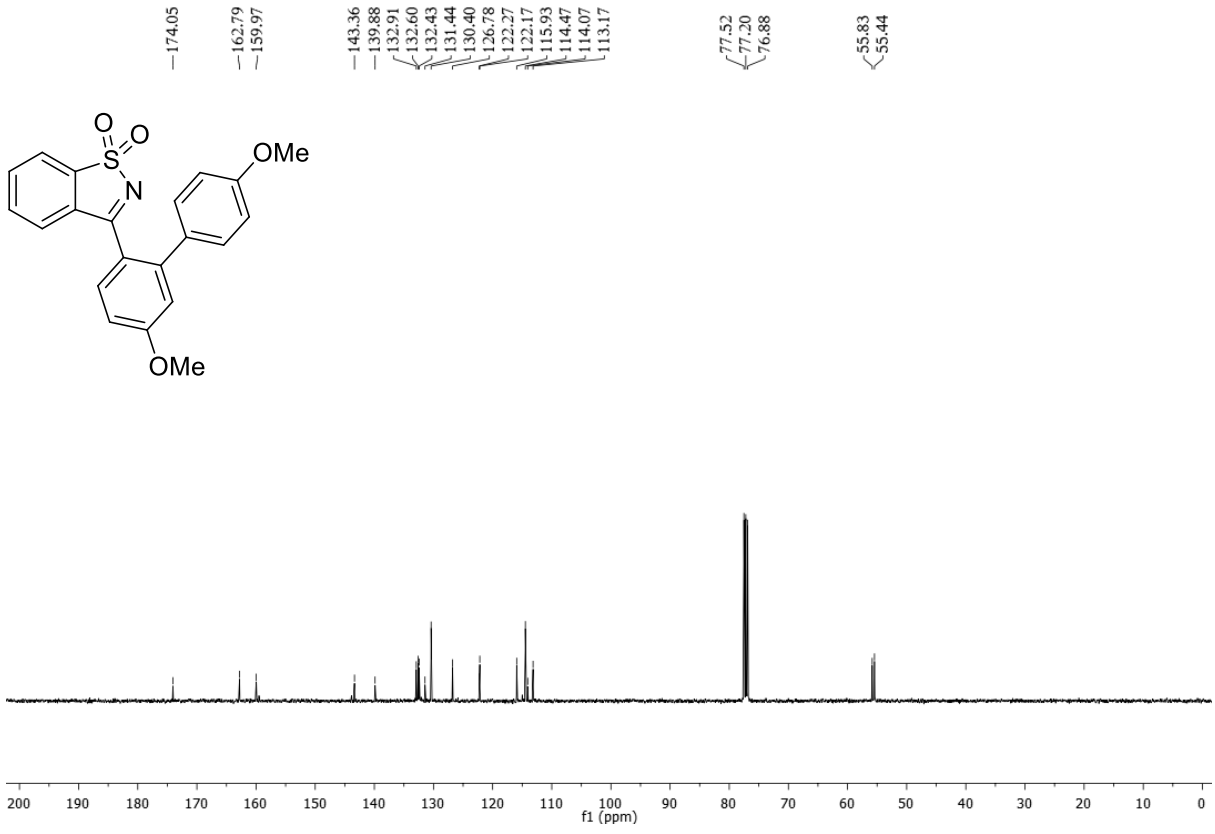
^{13}C NMR of **3gb** (150MHz, $CDCl_3$):



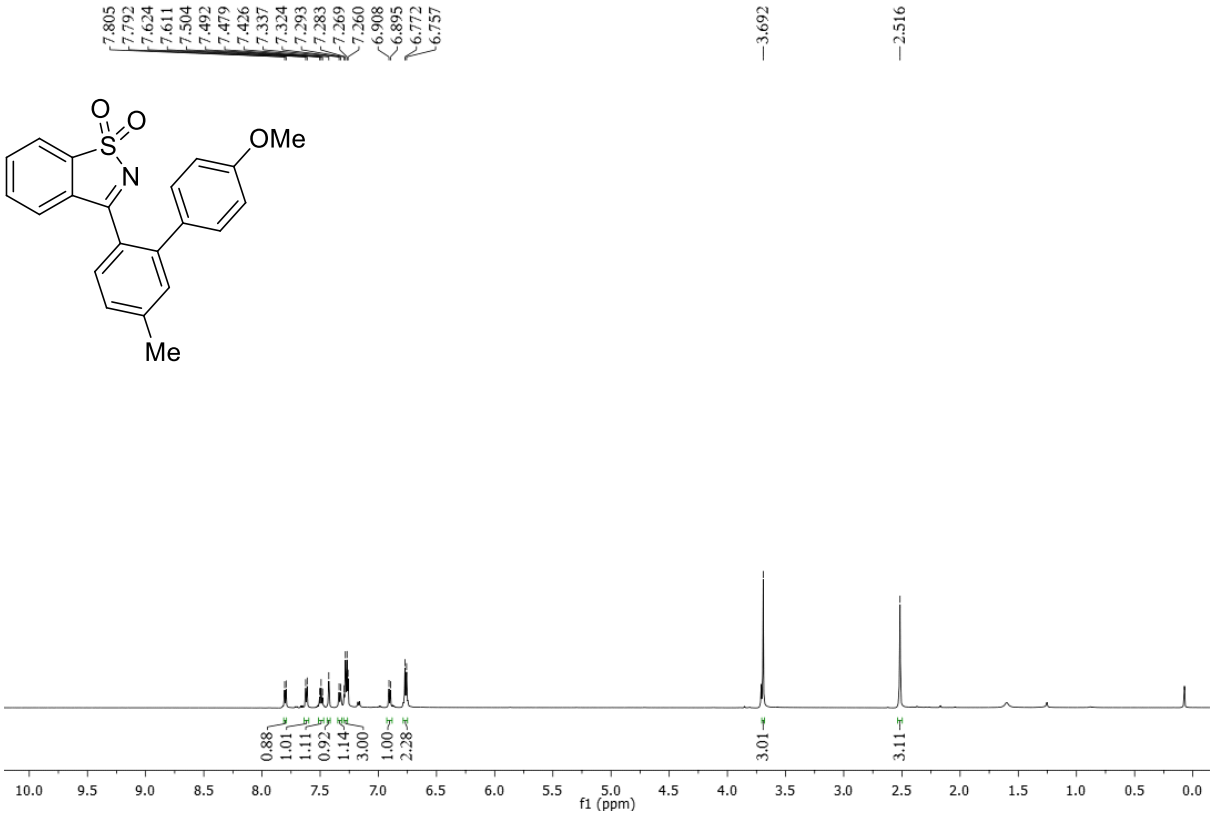
^{1}H NMR of **3hb** (400MHz, $CDCl_3$):



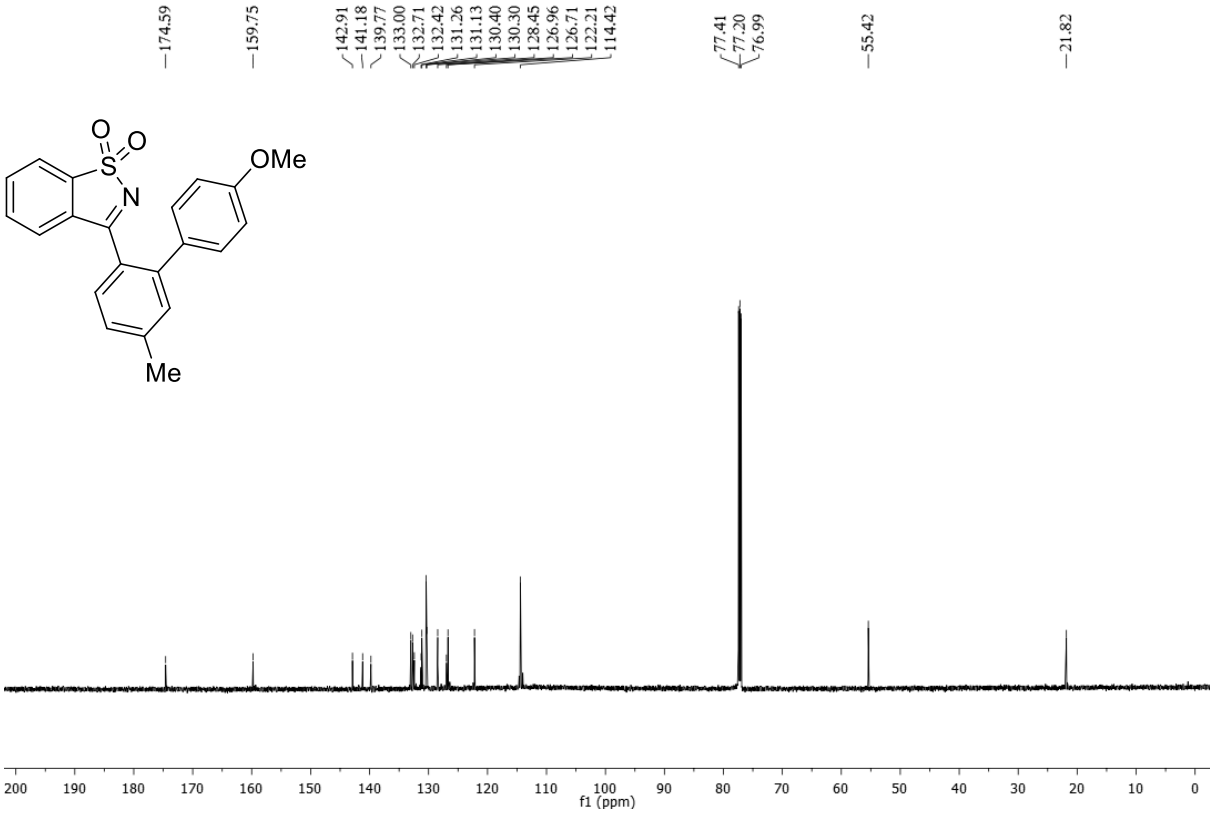
^{13}C NMR of **3hb** (100MHz, $CDCl_3$):



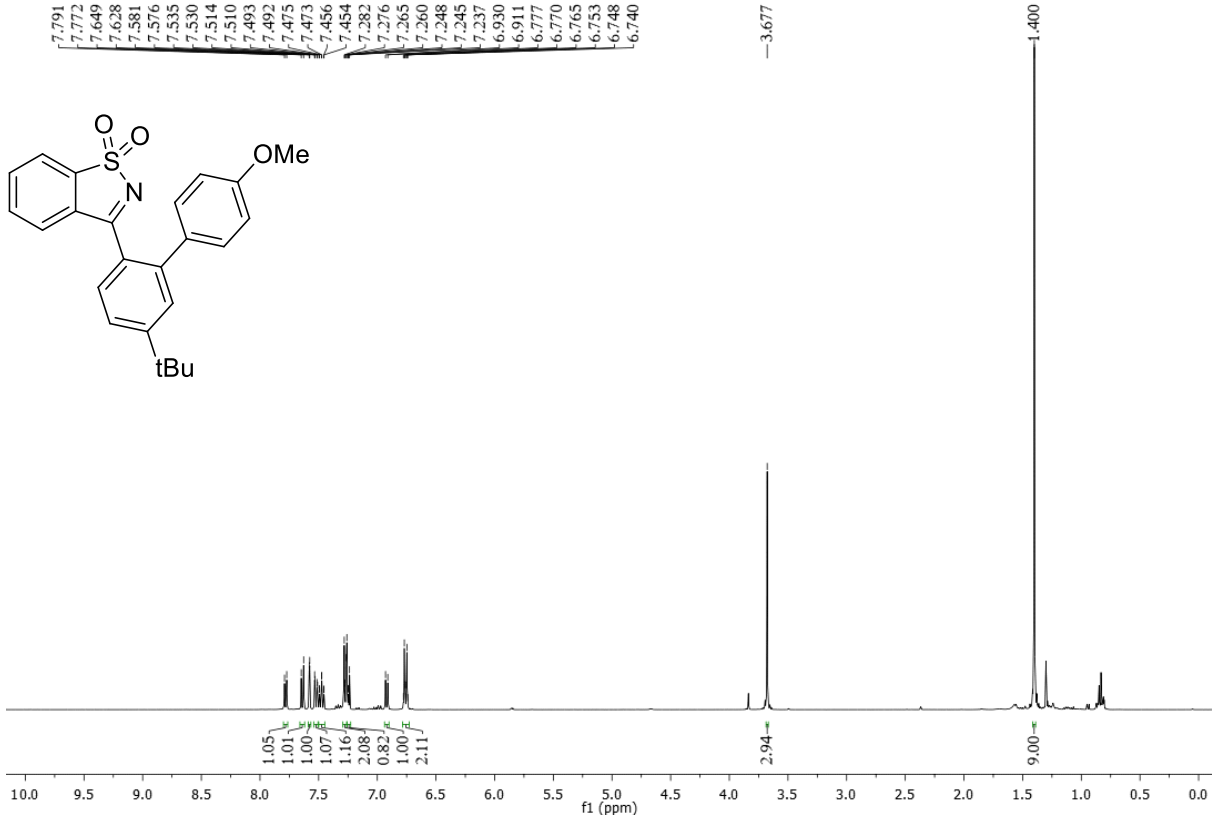
^{1}H NMR of **3ib** (600MHz, $CDCl_3$):



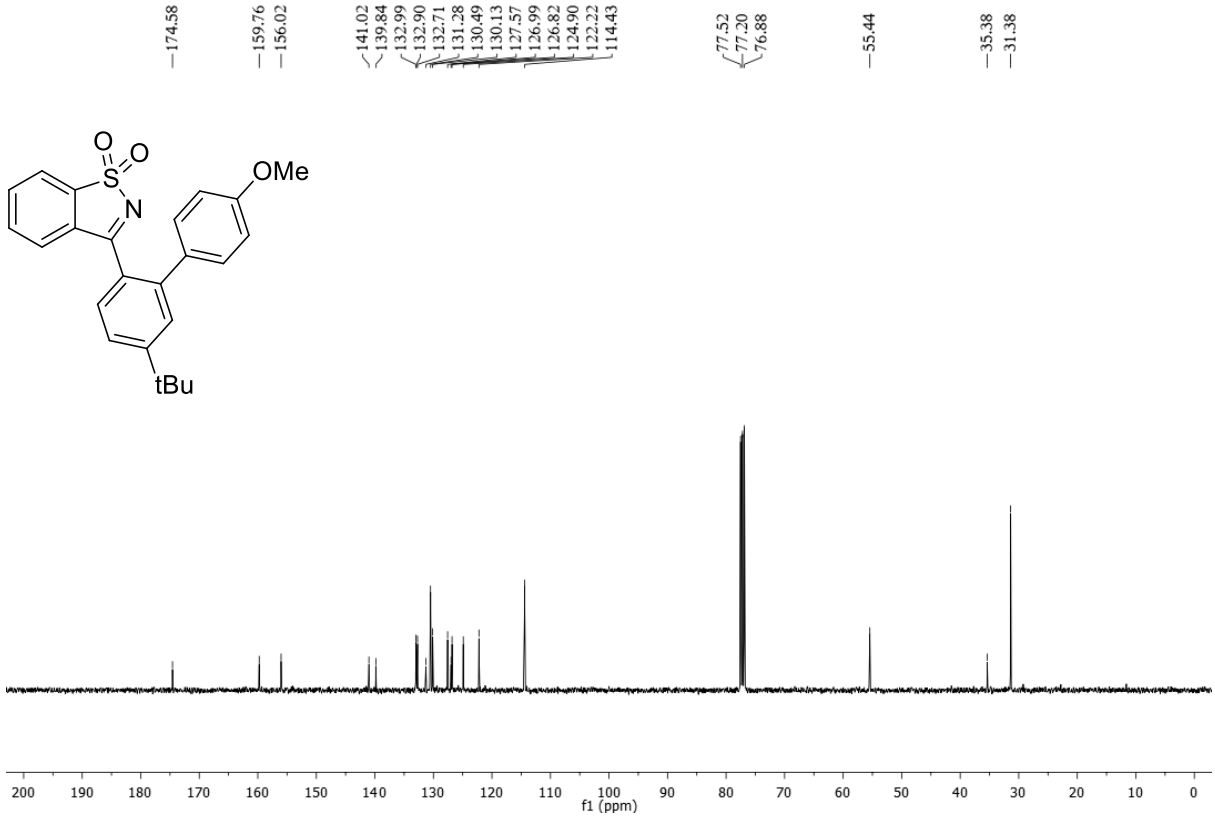
^{13}C NMR of **3ib** (150MHz, $CDCl_3$):



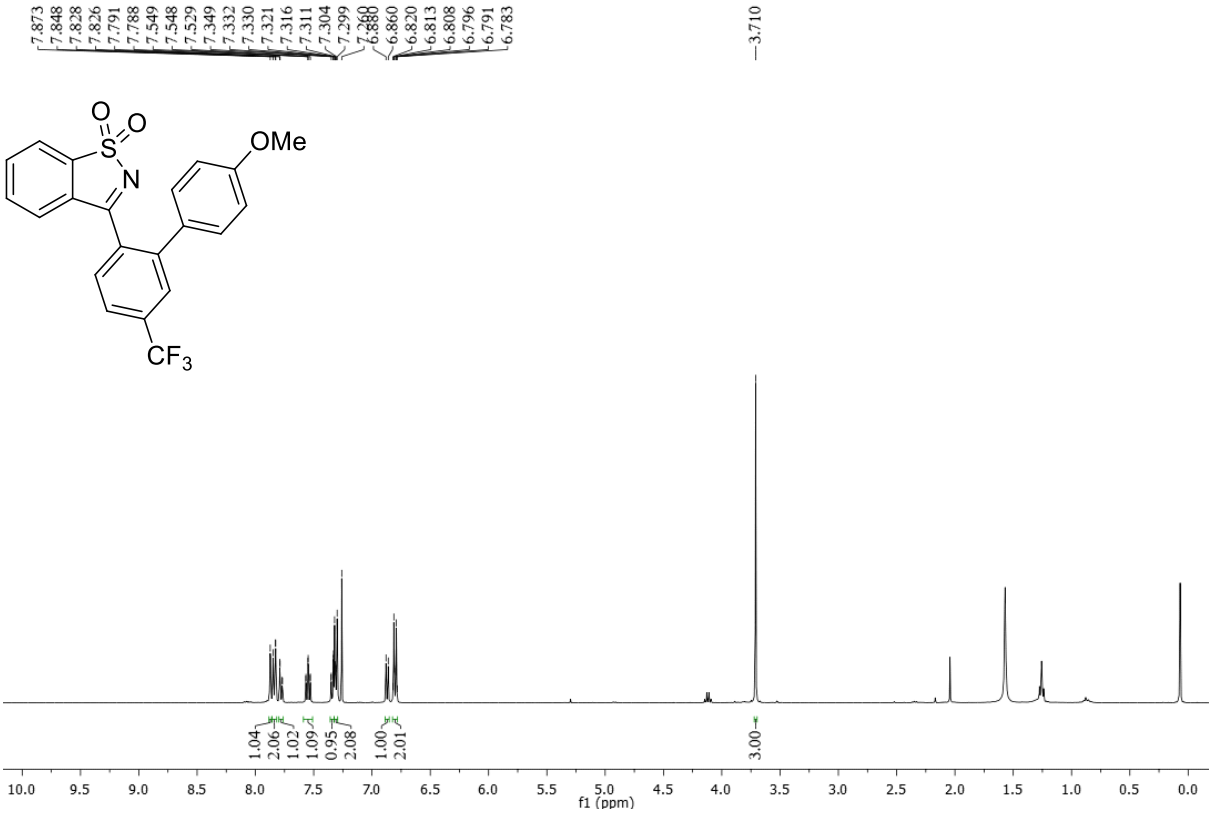
^{1}H NMR of **3jb** (400MHz, $CDCl_3$):



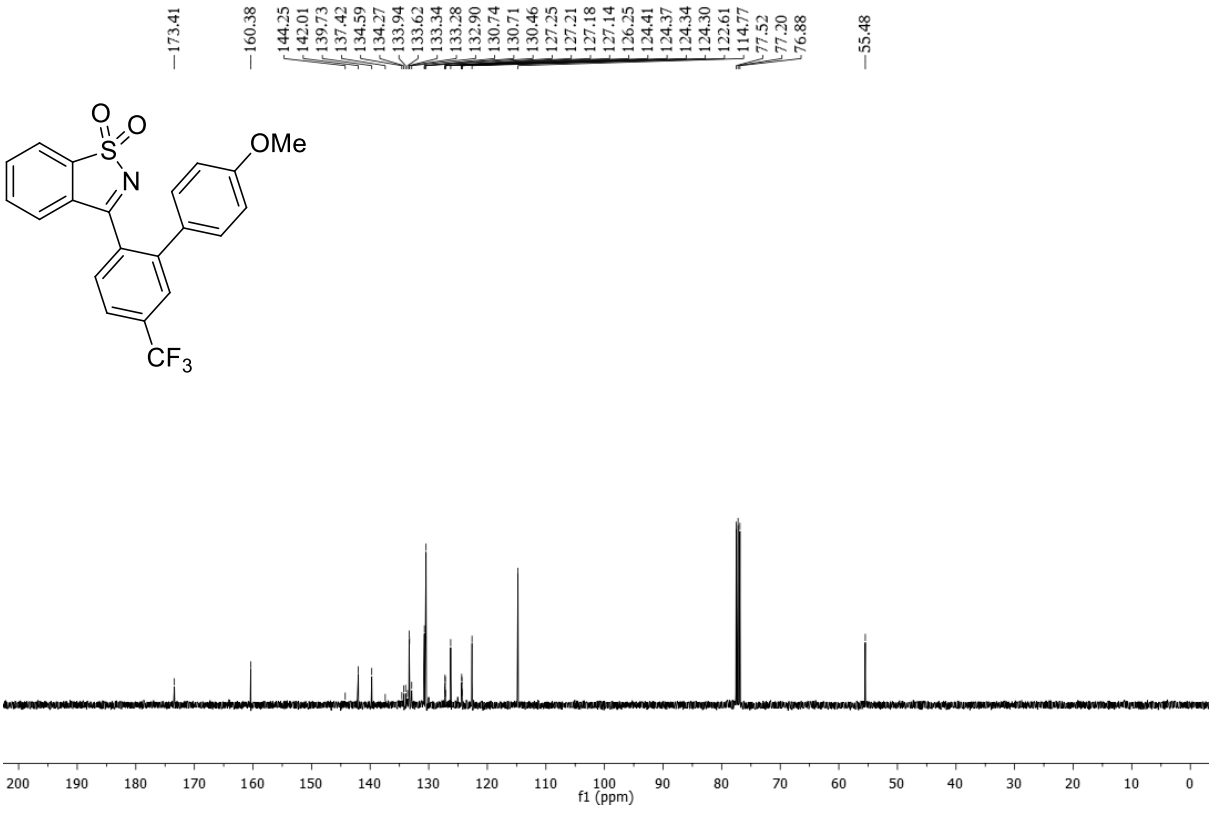
^{13}C NMR of **3jb** (100MHz, $CDCl_3$):



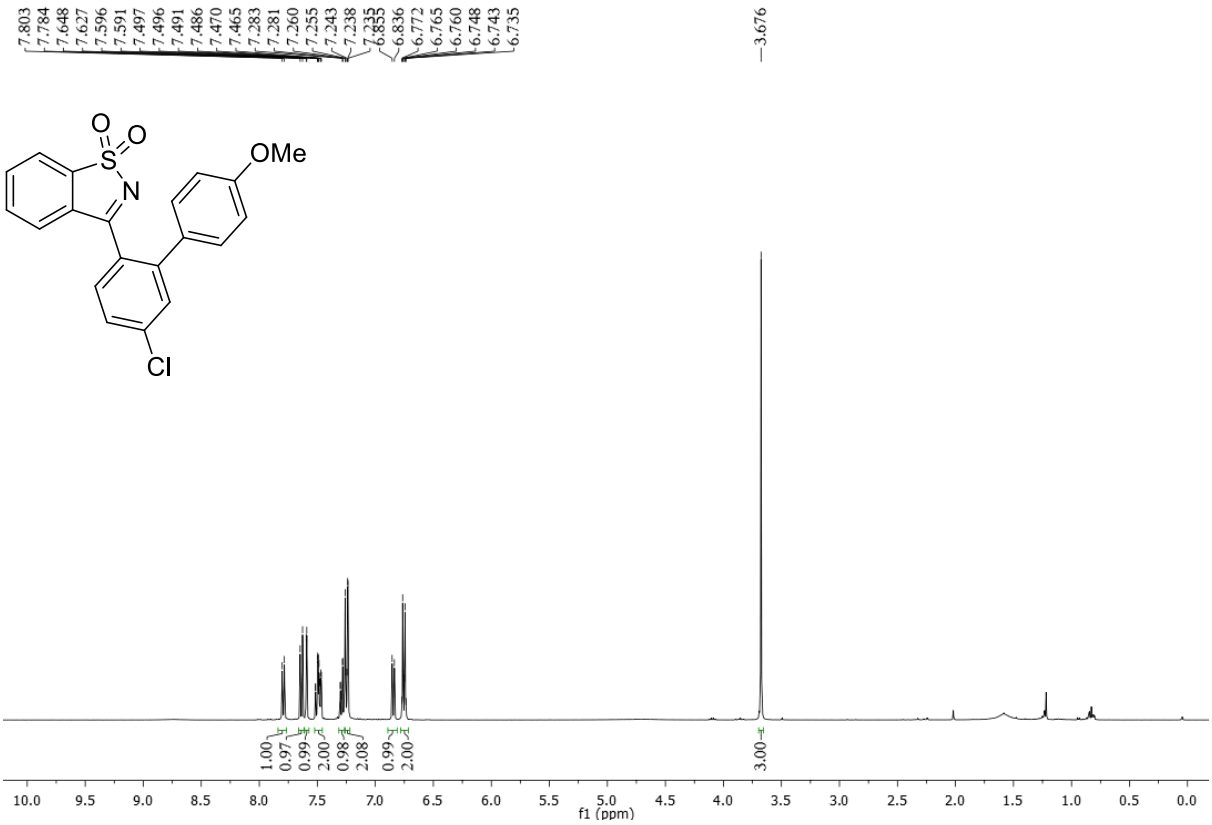
^{1}H NMR of **3kb** (400MHz, $CDCl_3$):



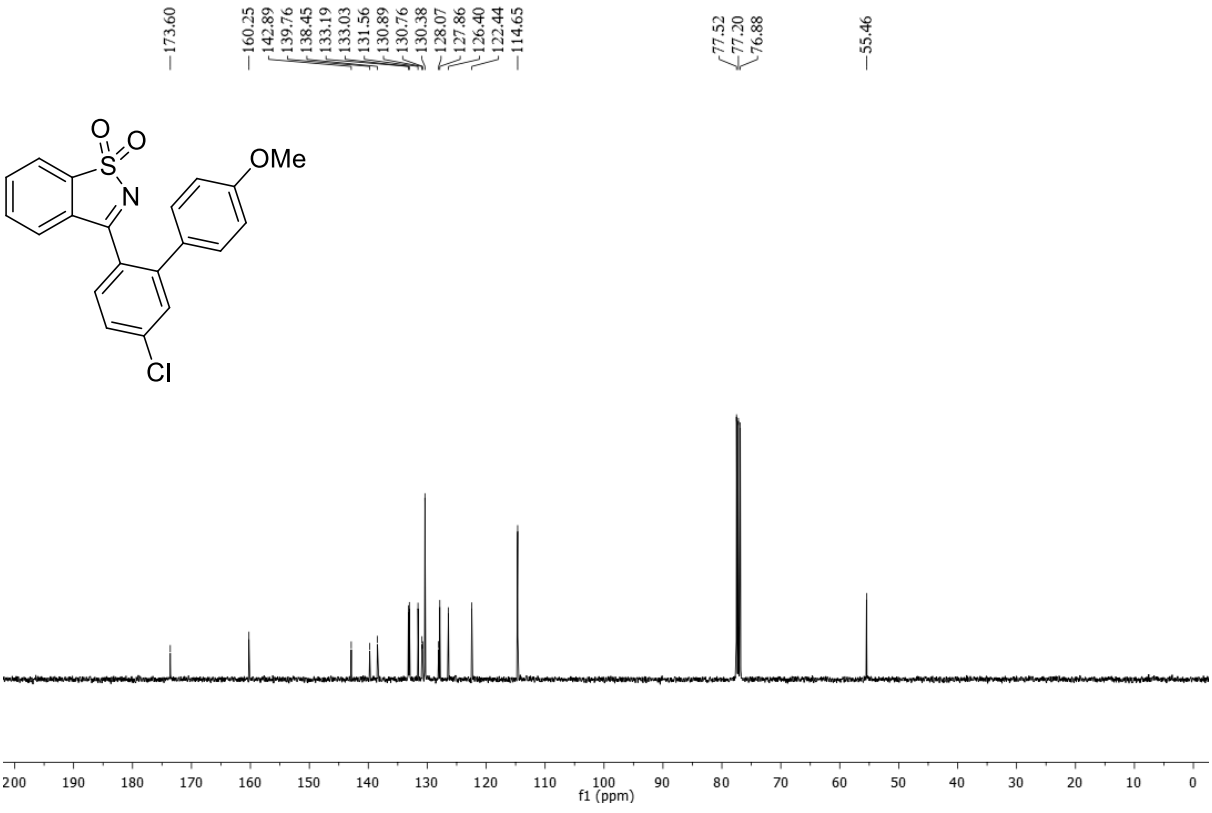
^{13}C NMR of **3kb** (100MHz, $CDCl_3$):



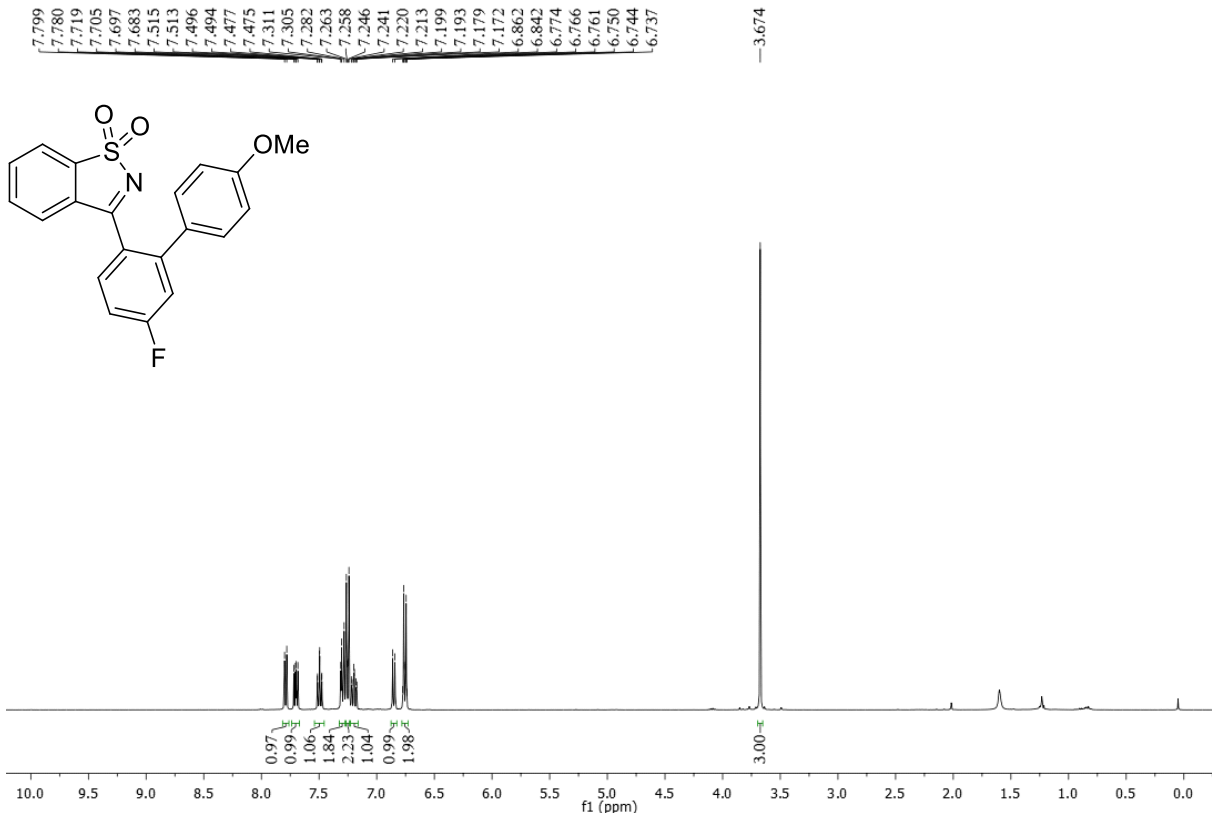
^{1}H NMR of **3lb** (400MHz, $CDCl_3$):



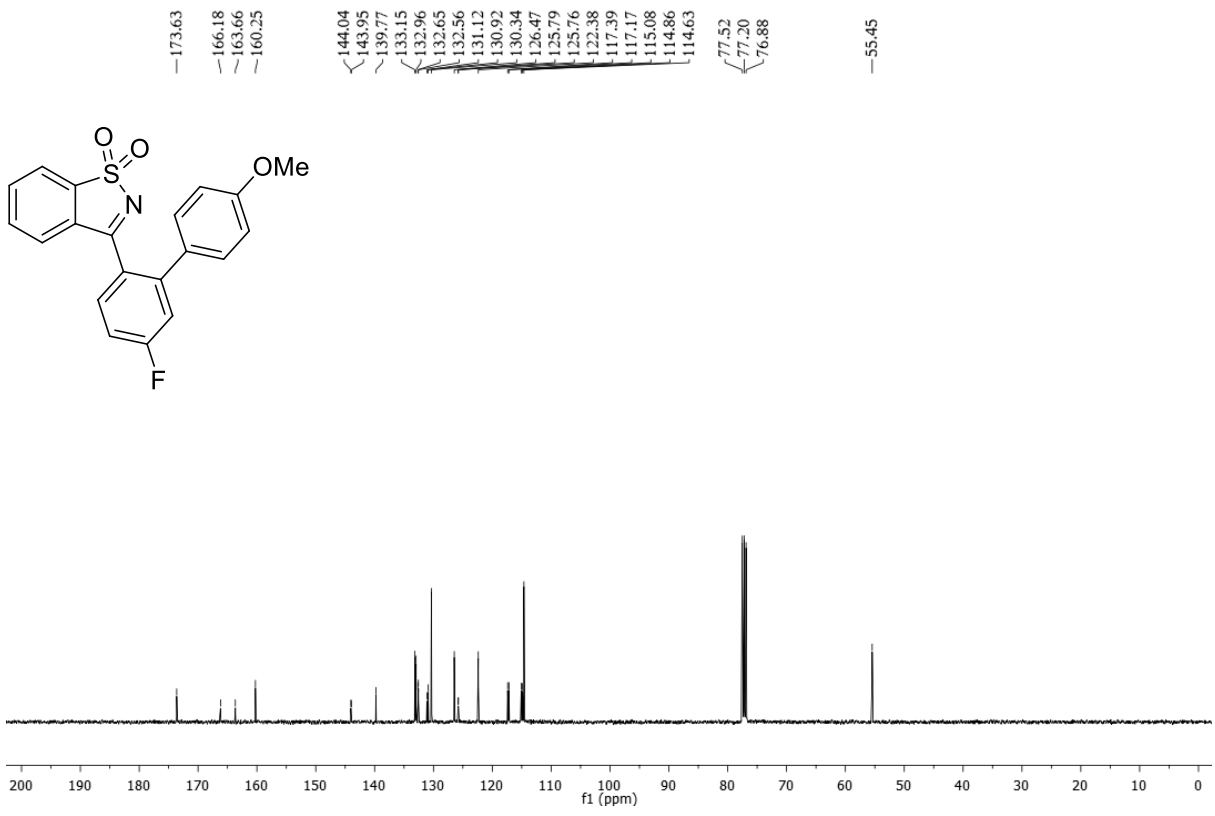
^{13}C NMR of **3lb** (100MHz, $CDCl_3$):



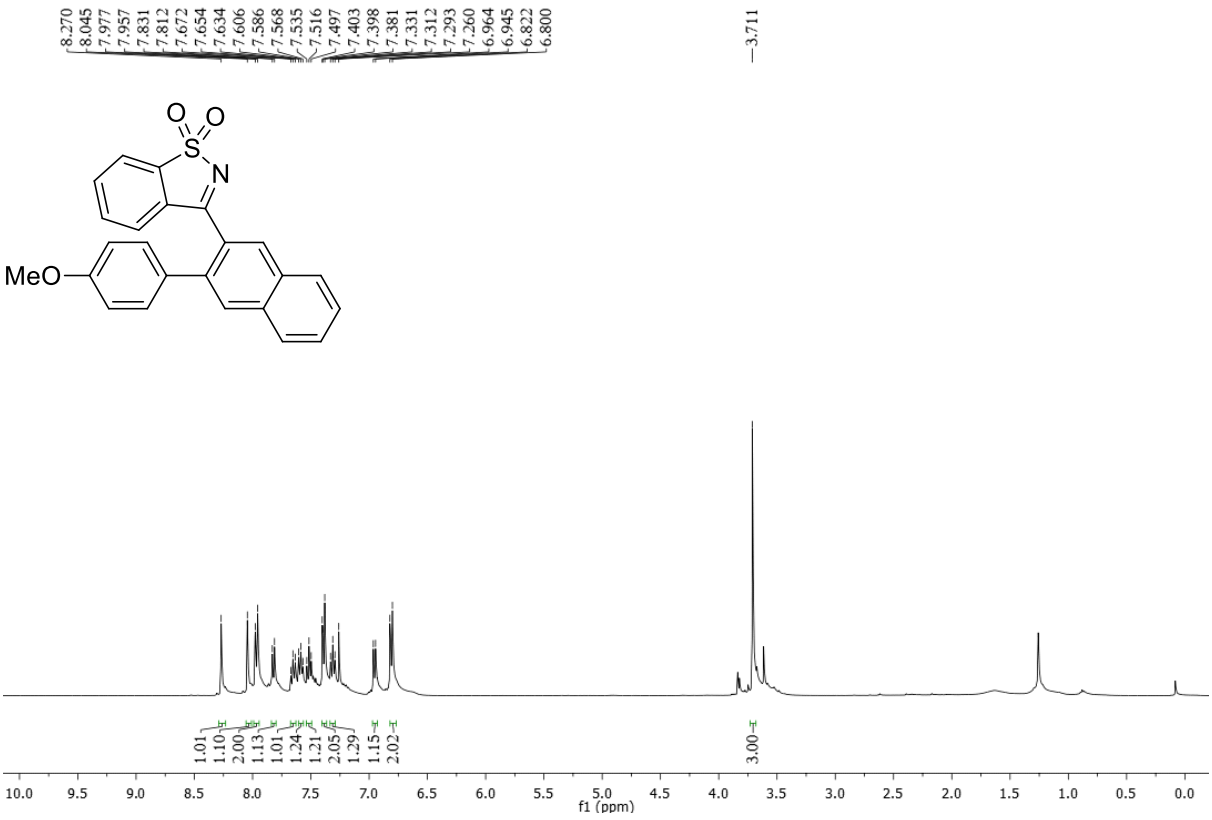
^{1}H NMR of **3mb** (400MHz, $CDCl_3$):



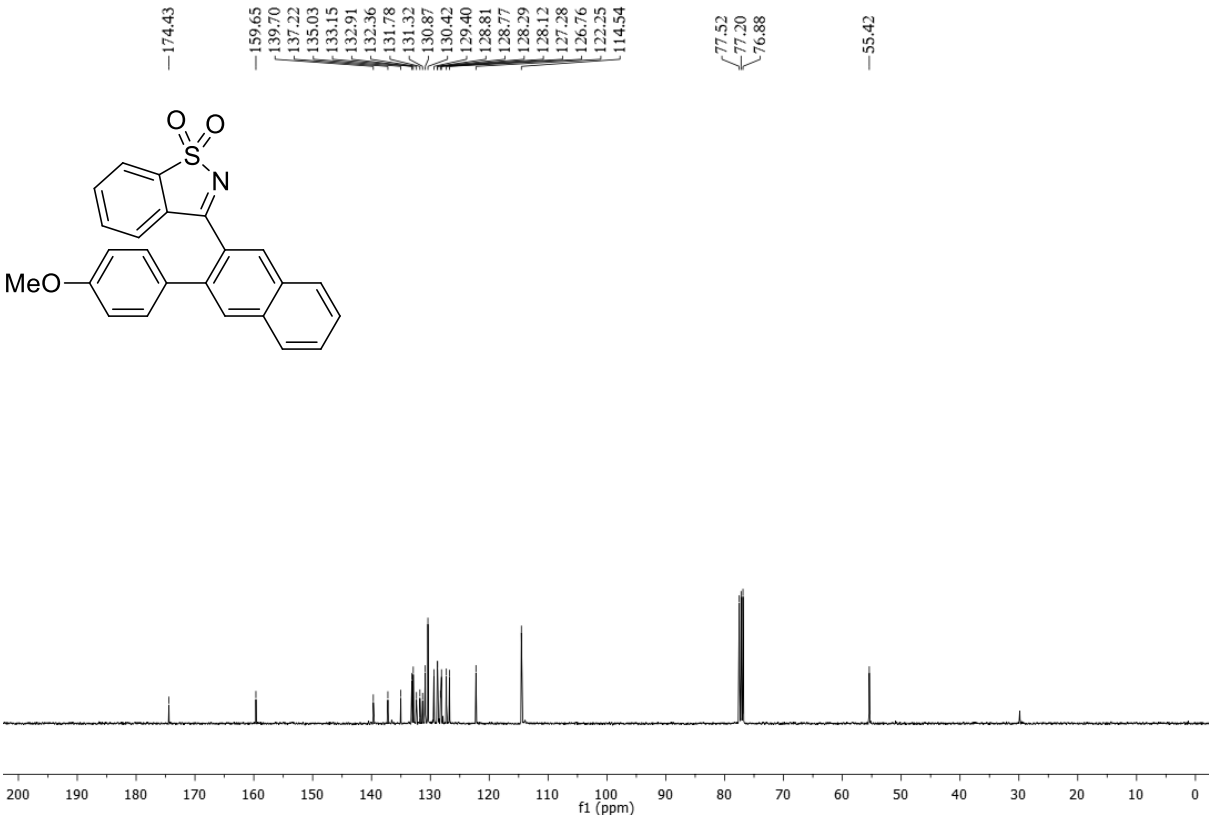
^{13}C NMR of **3mb** (100MHz, $CDCl_3$):



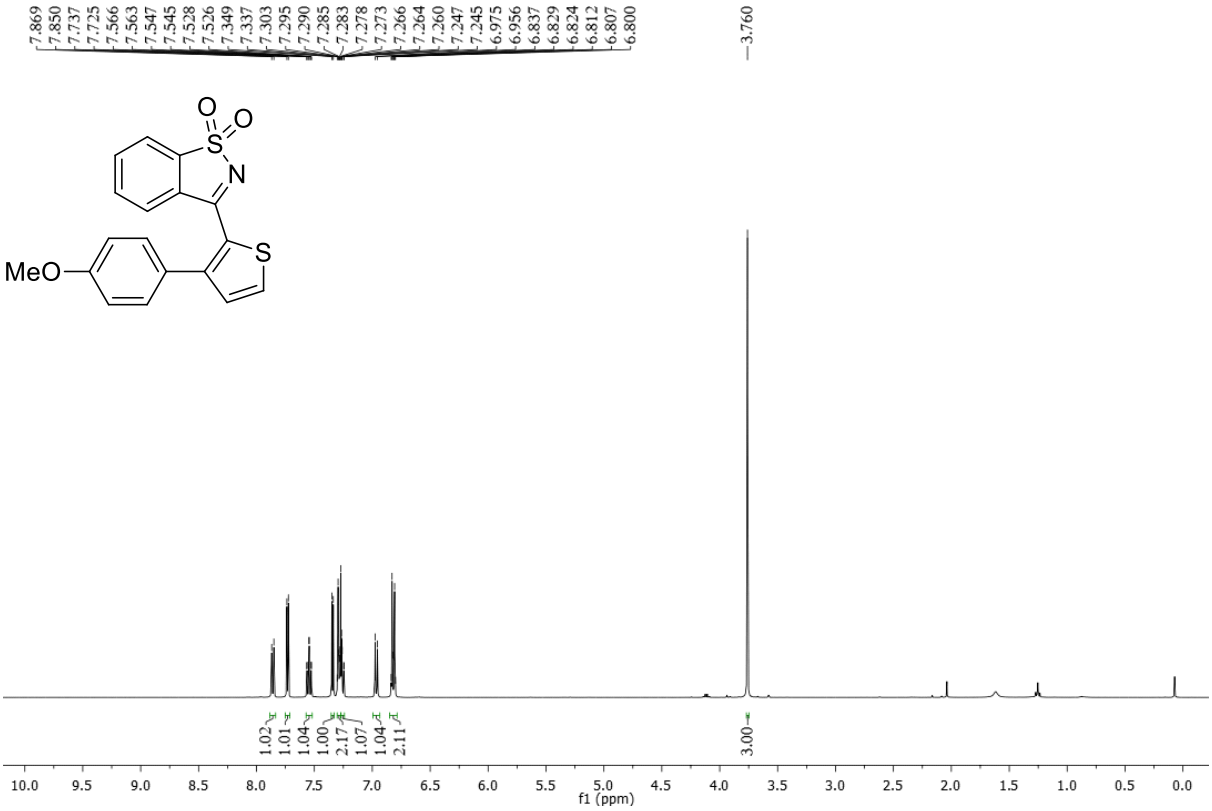
^{1}H NMR of **3nb** (400MHz, $CDCl_3$):



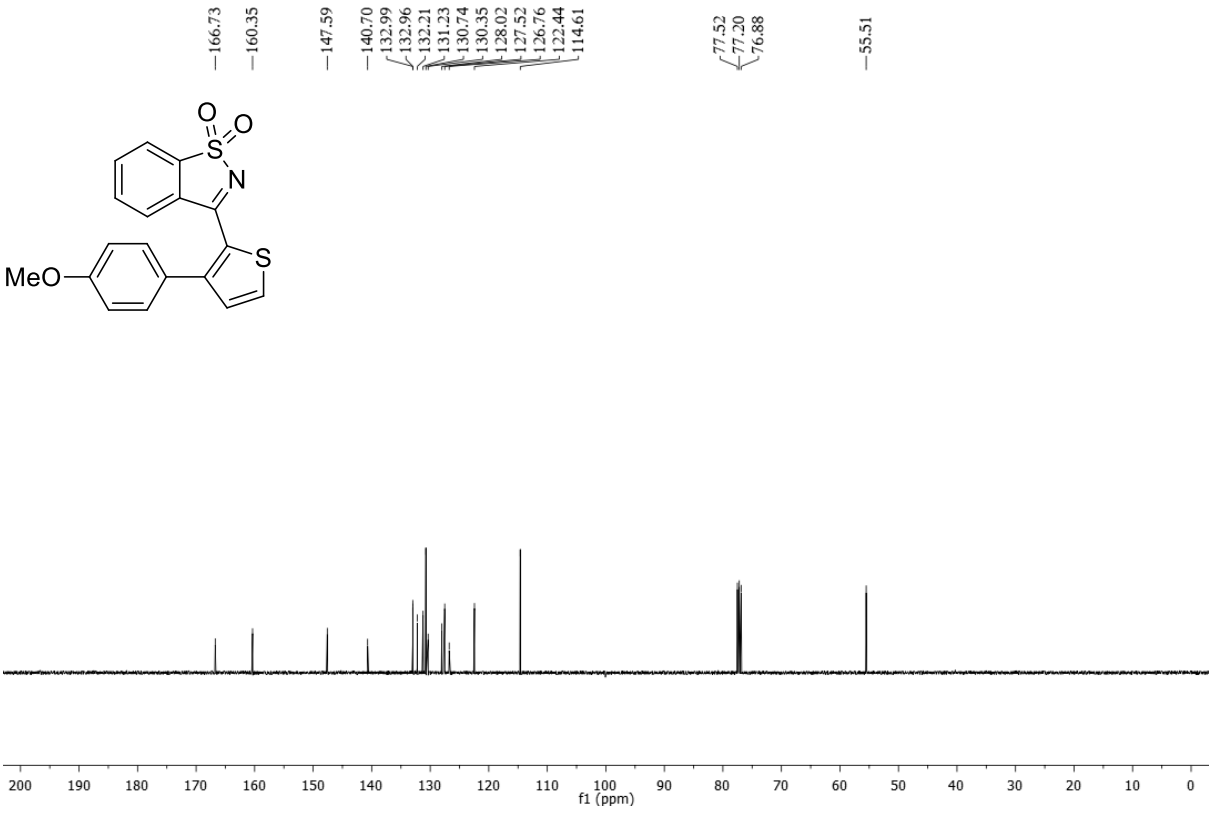
^{13}C NMR of **3nb** (100MHz, $CDCl_3$):



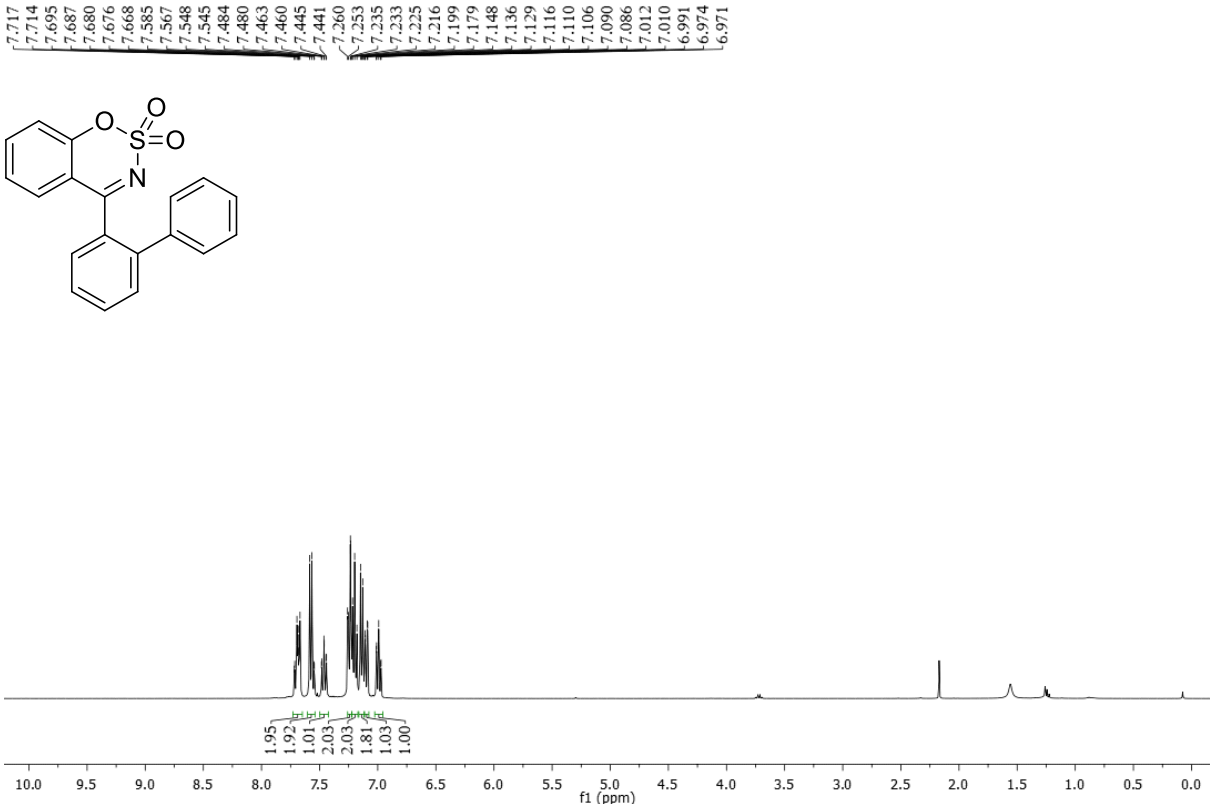
^{1}H NMR of **3ob** (400MHz, $CDCl_3$):



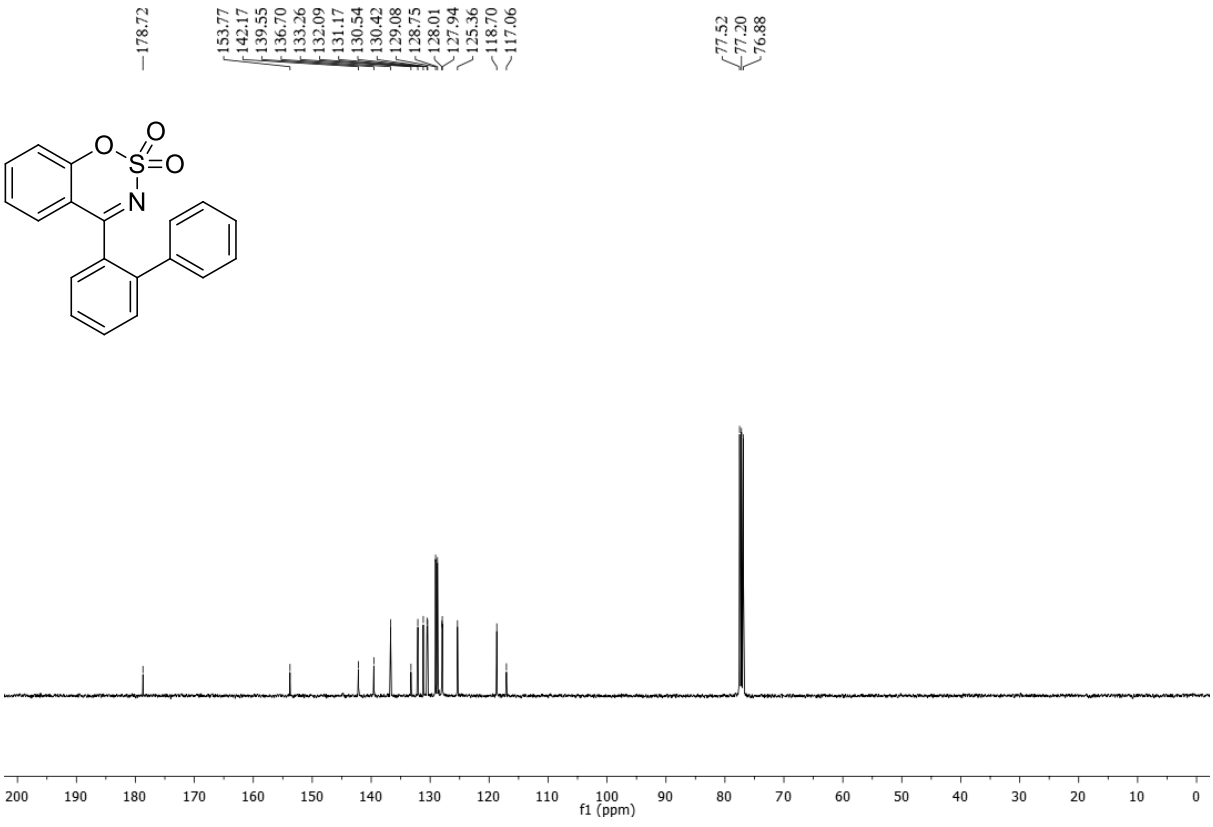
^{13}C NMR of **3ob** (100MHz, $CDCl_3$):



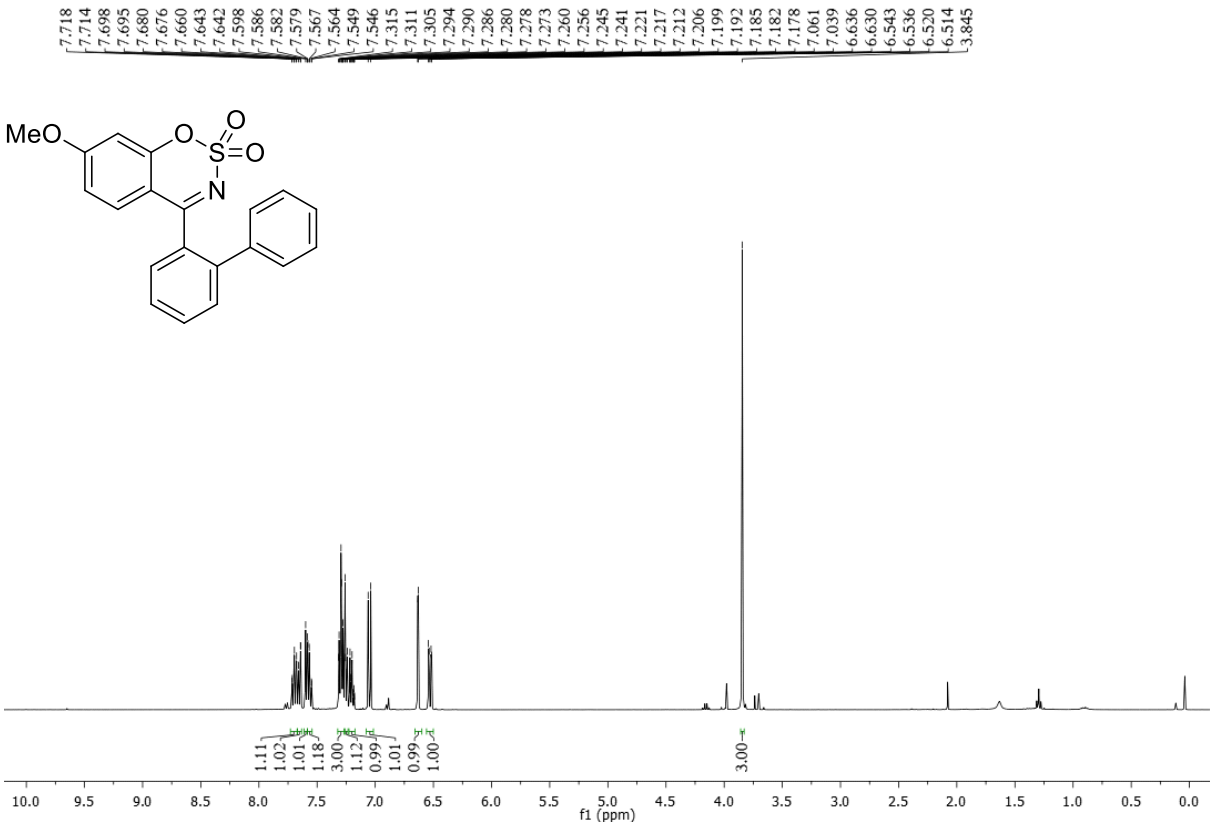
^{1}H NMR of **5aa** (400MHz, $CDCl_3$):



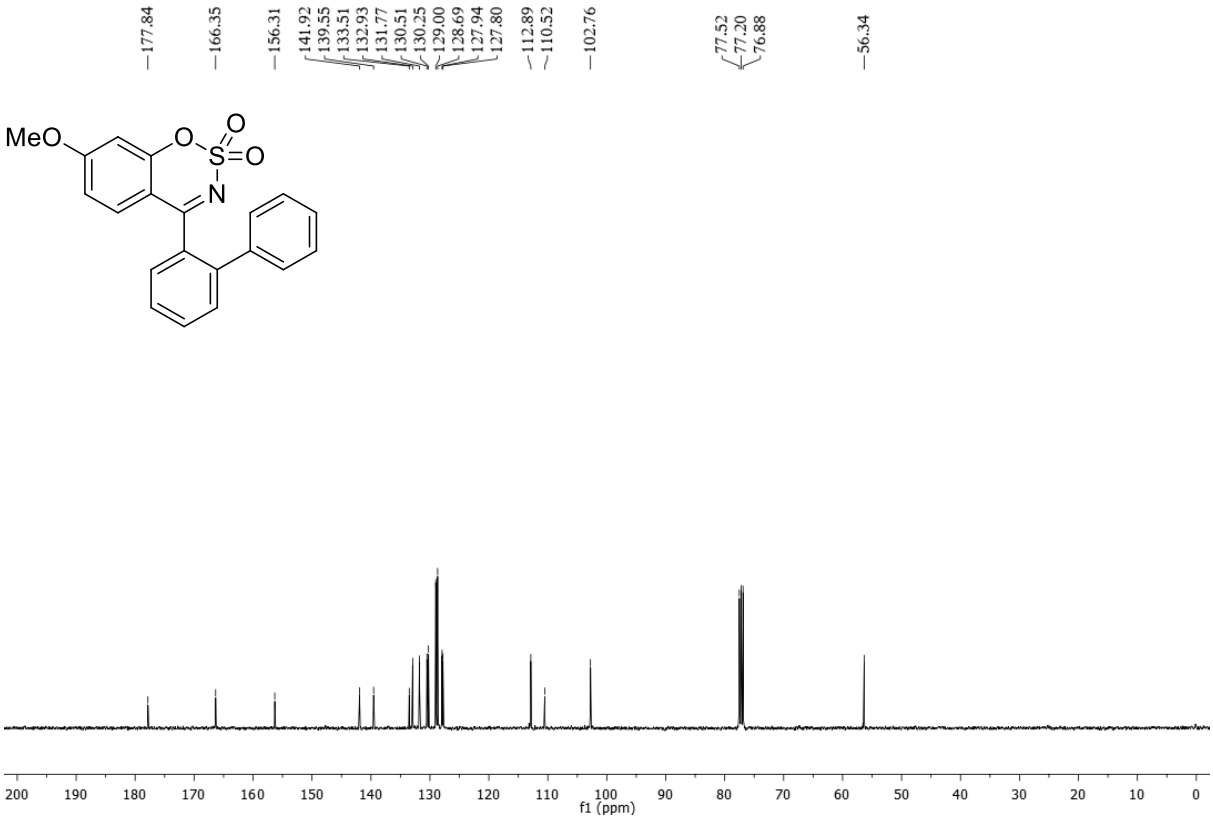
^{13}C NMR of **5aa** (100MHz, $CDCl_3$):



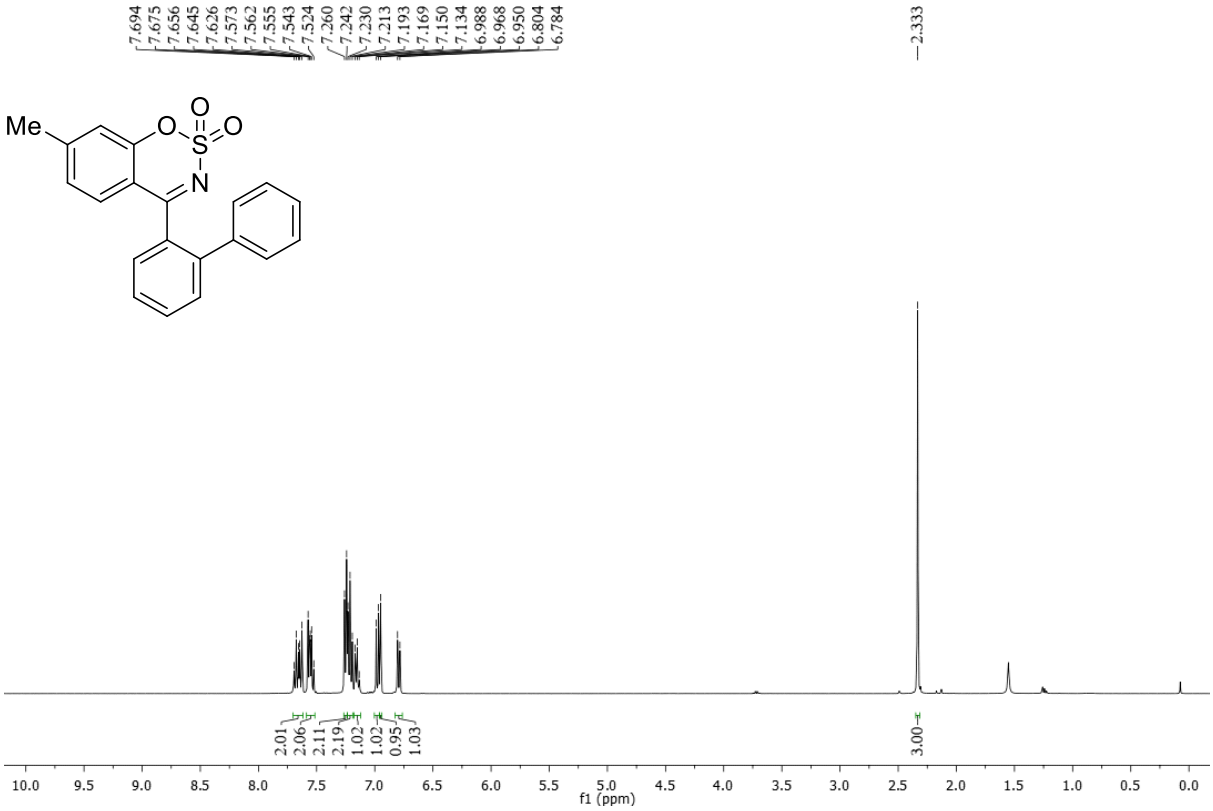
^{1}H NMR of **5ba** (400MHz, $CDCl_3$):



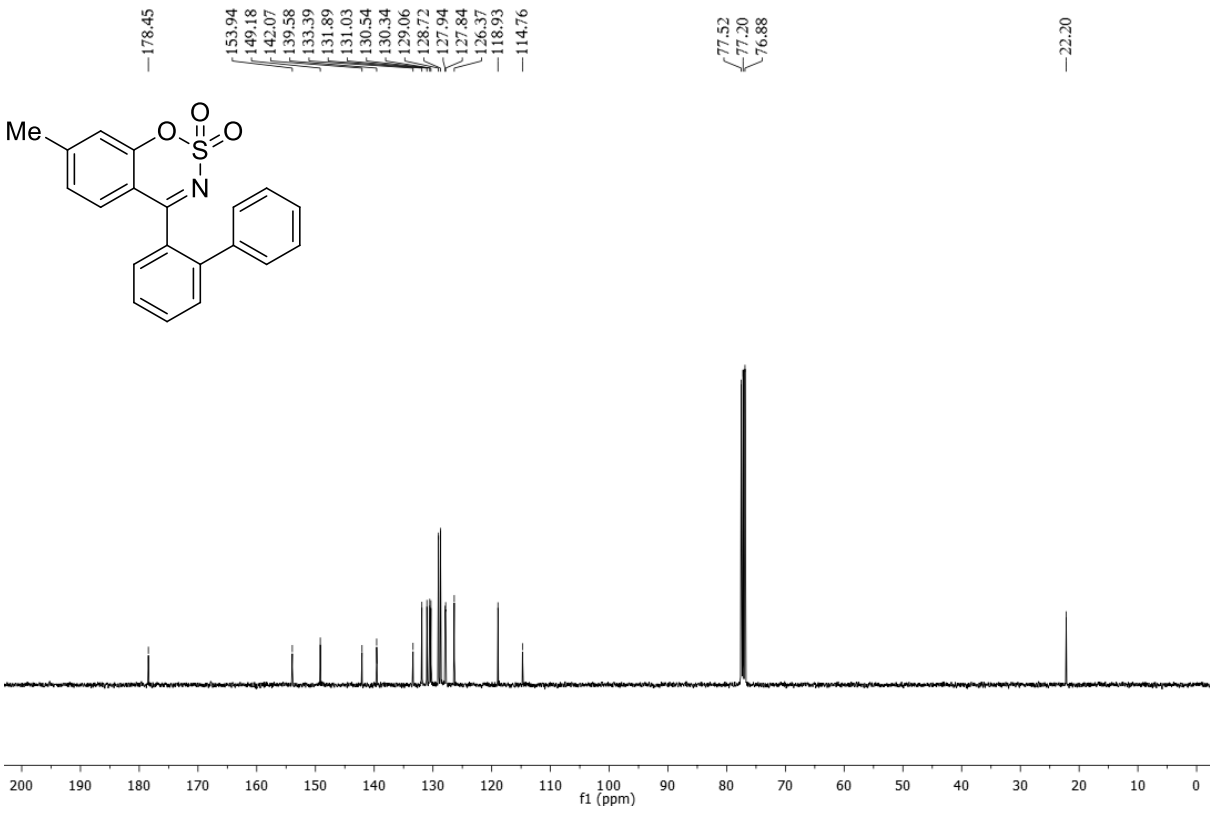
^{13}C NMR of **5ba** (100MHz, $CDCl_3$):



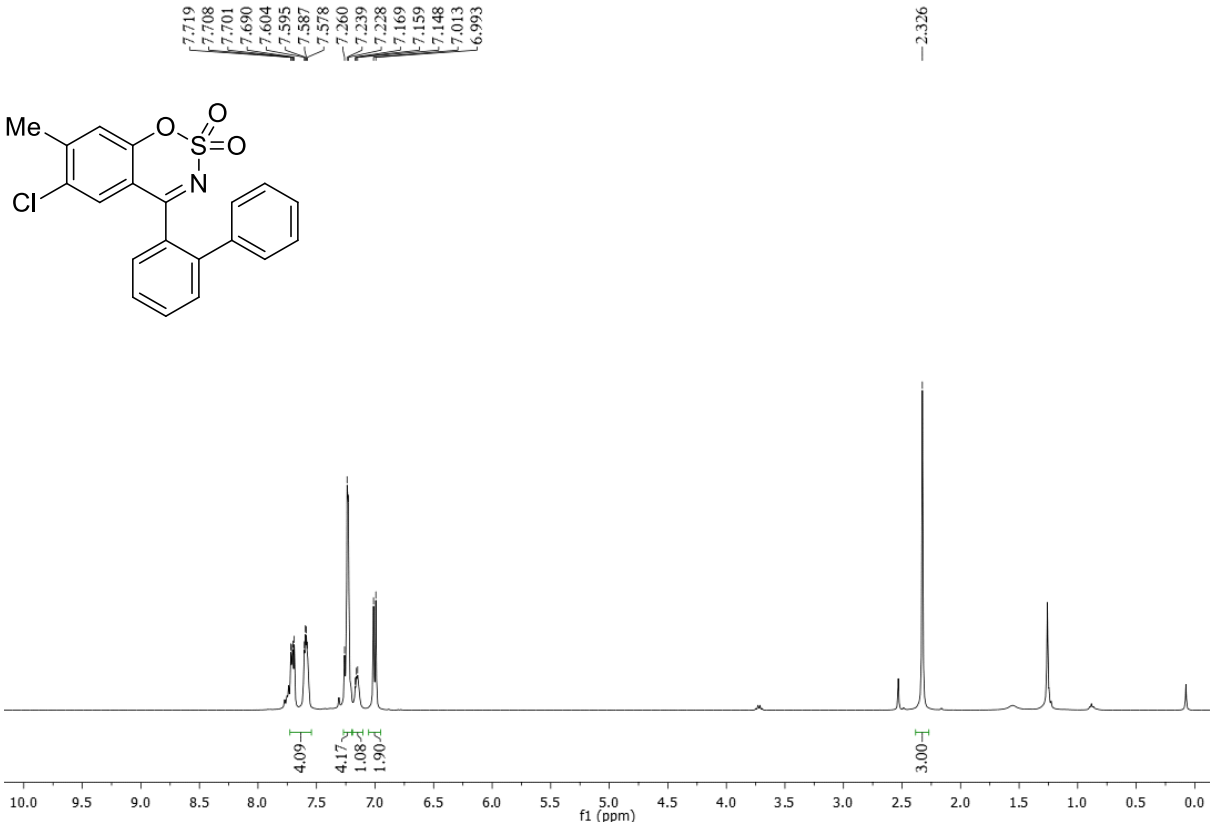
^{1}H NMR of **5ca** (400 MHz, $CDCl_3$):



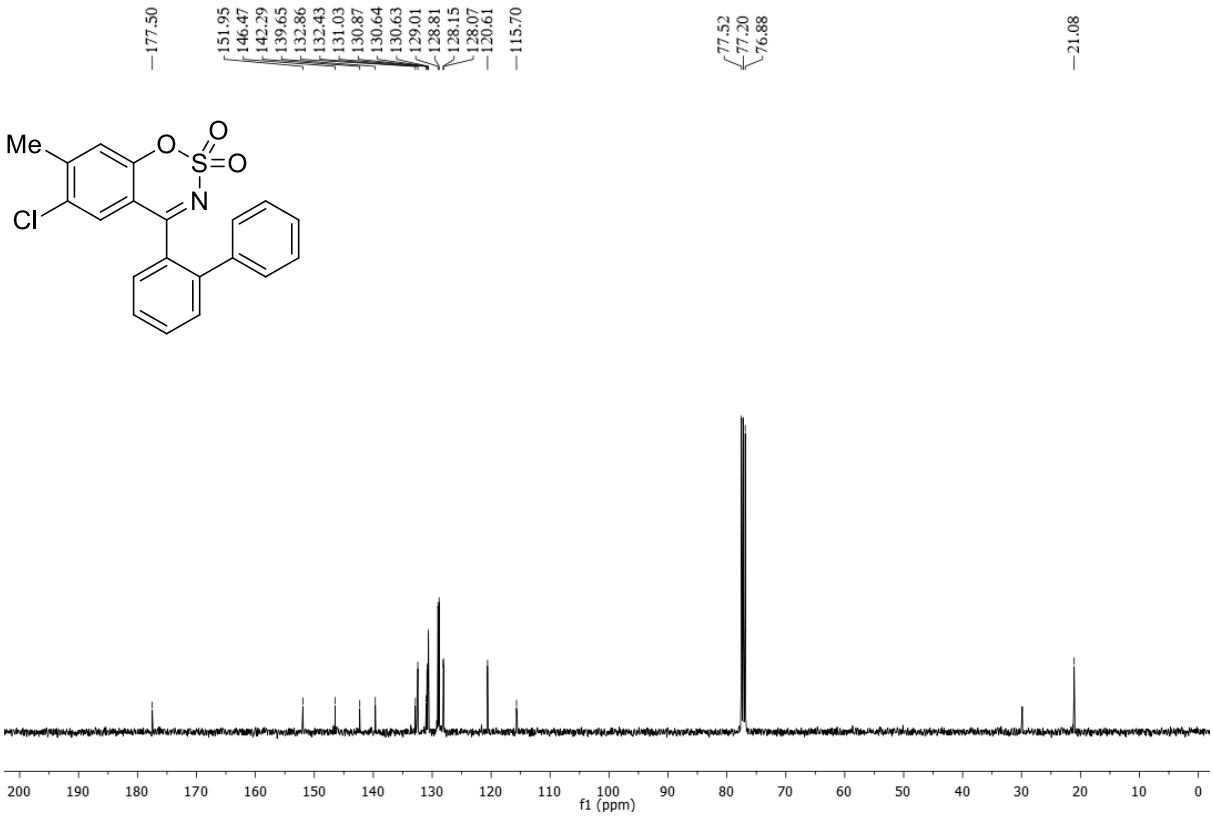
^{13}C NMR of **5ca** (100 MHz, $CDCl_3$):



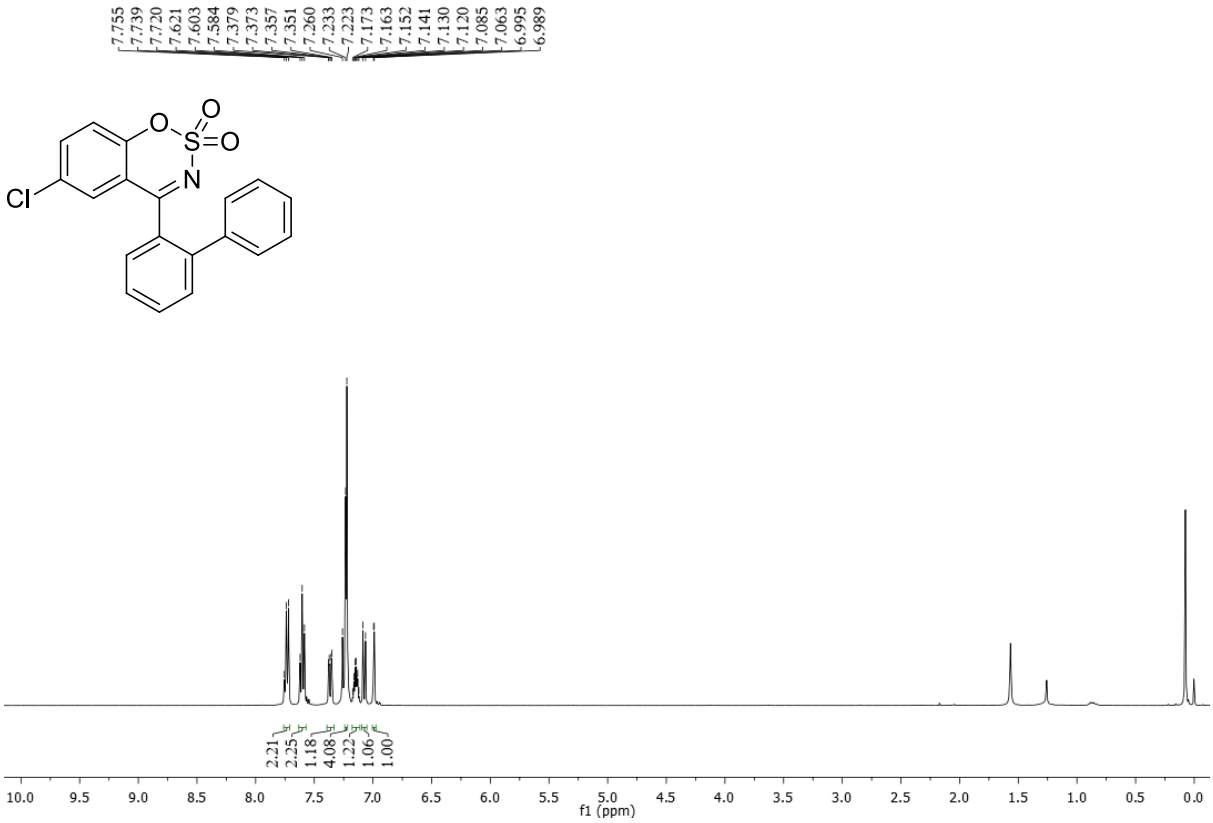
^{1}H NMR of **5da** (400MHz, $CDCl_3$):



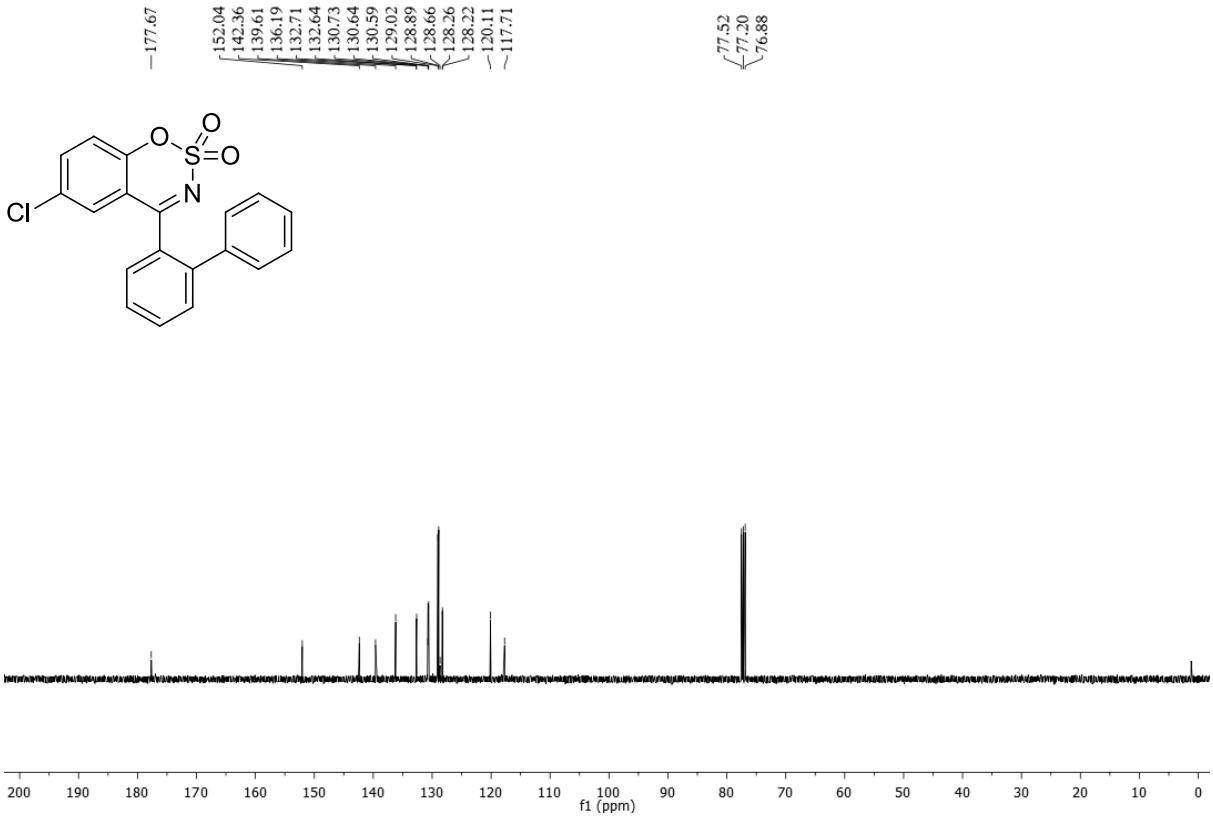
^{13}C NMR of **5da** (100MHz, $CDCl_3$):



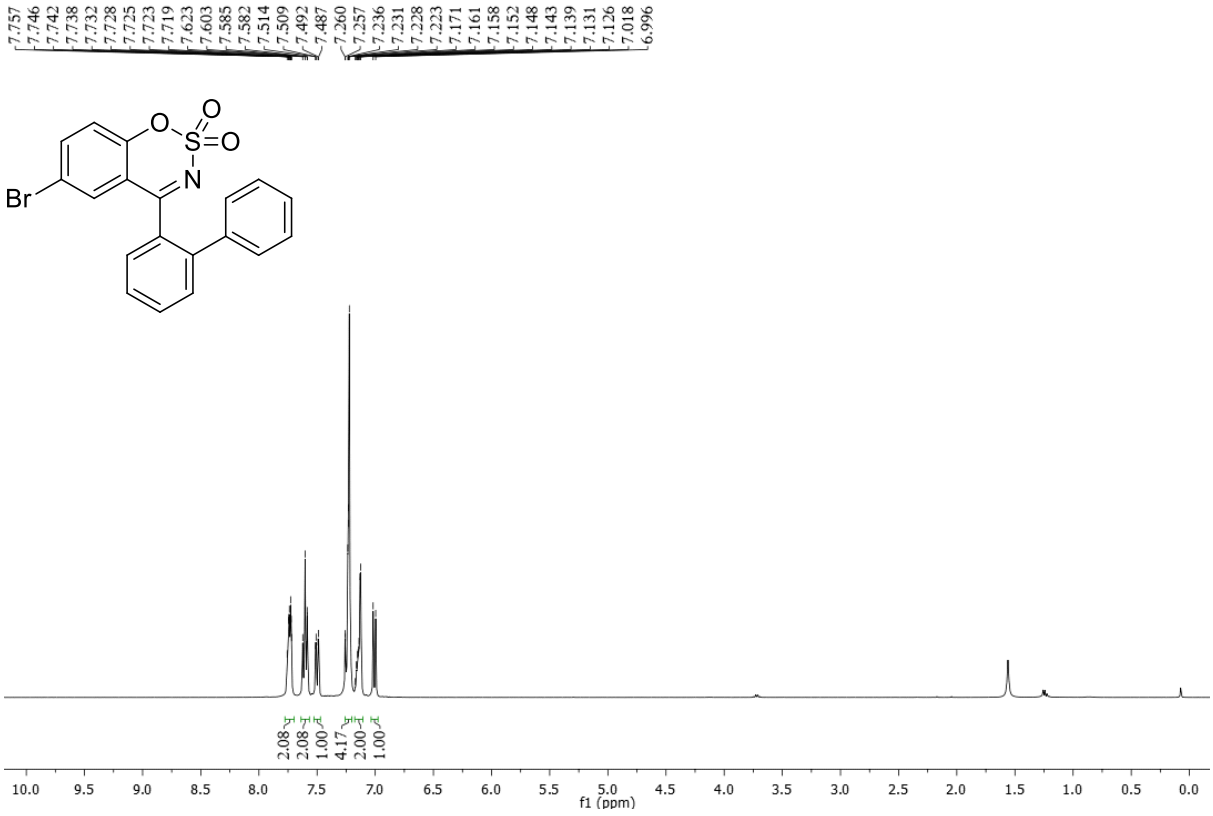
^{1}H NMR of **5ea** (400MHz, $CDCl_3$):



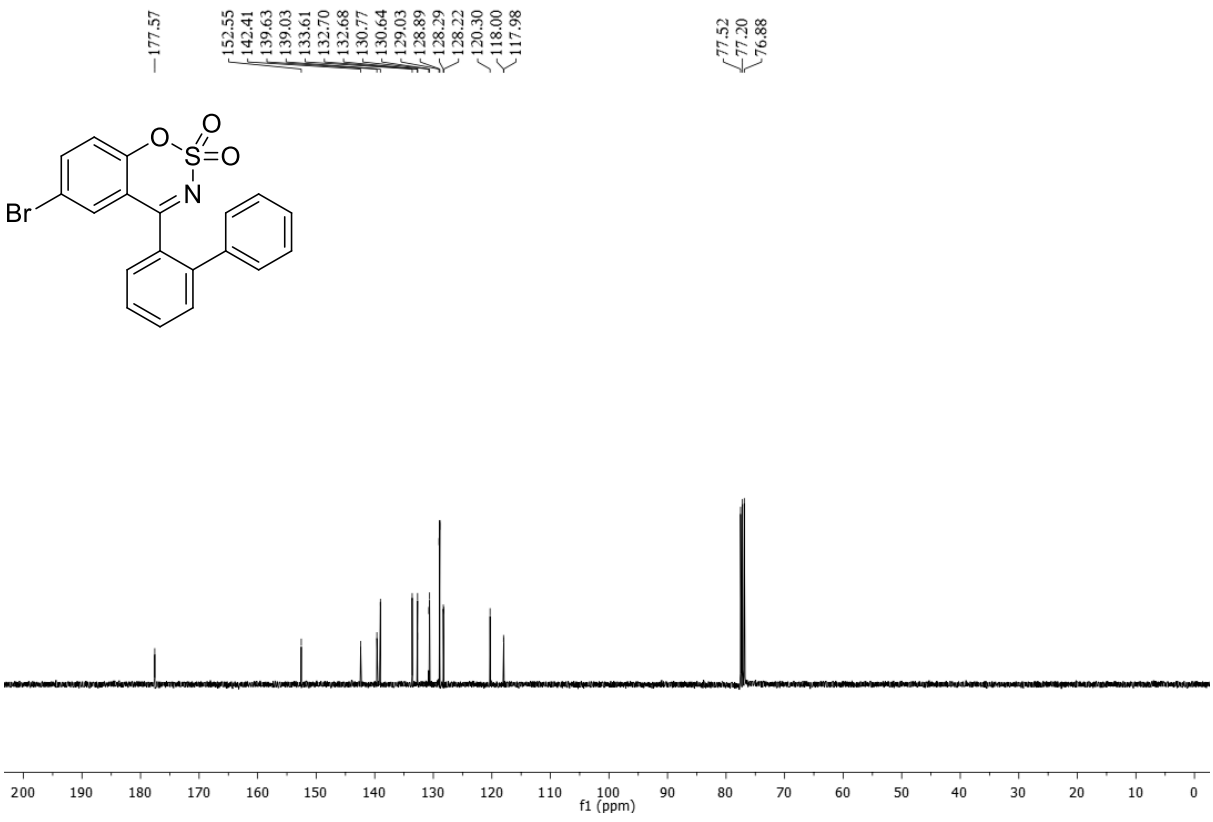
^{13}C NMR of **5ea** (100MHz, $CDCl_3$):



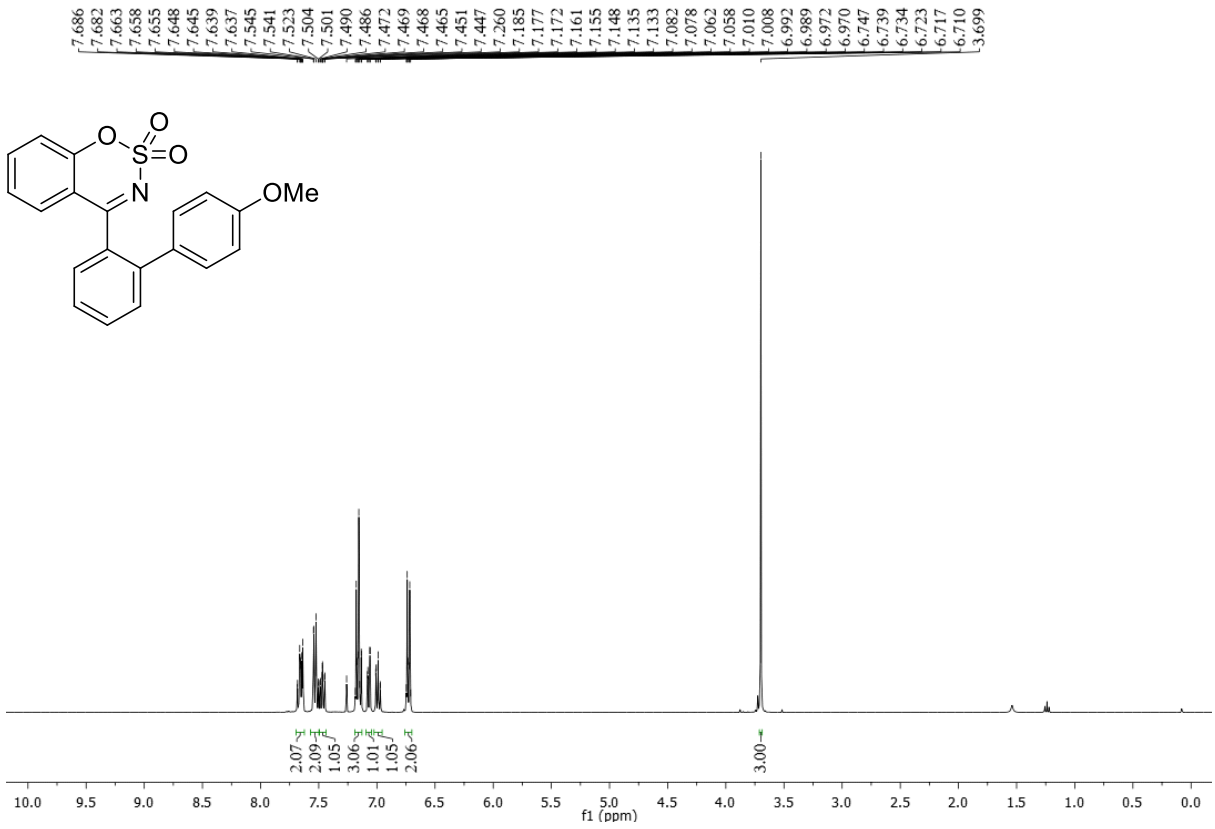
^{1}H NMR of **5fa** (400MHz, $CDCl_3$):



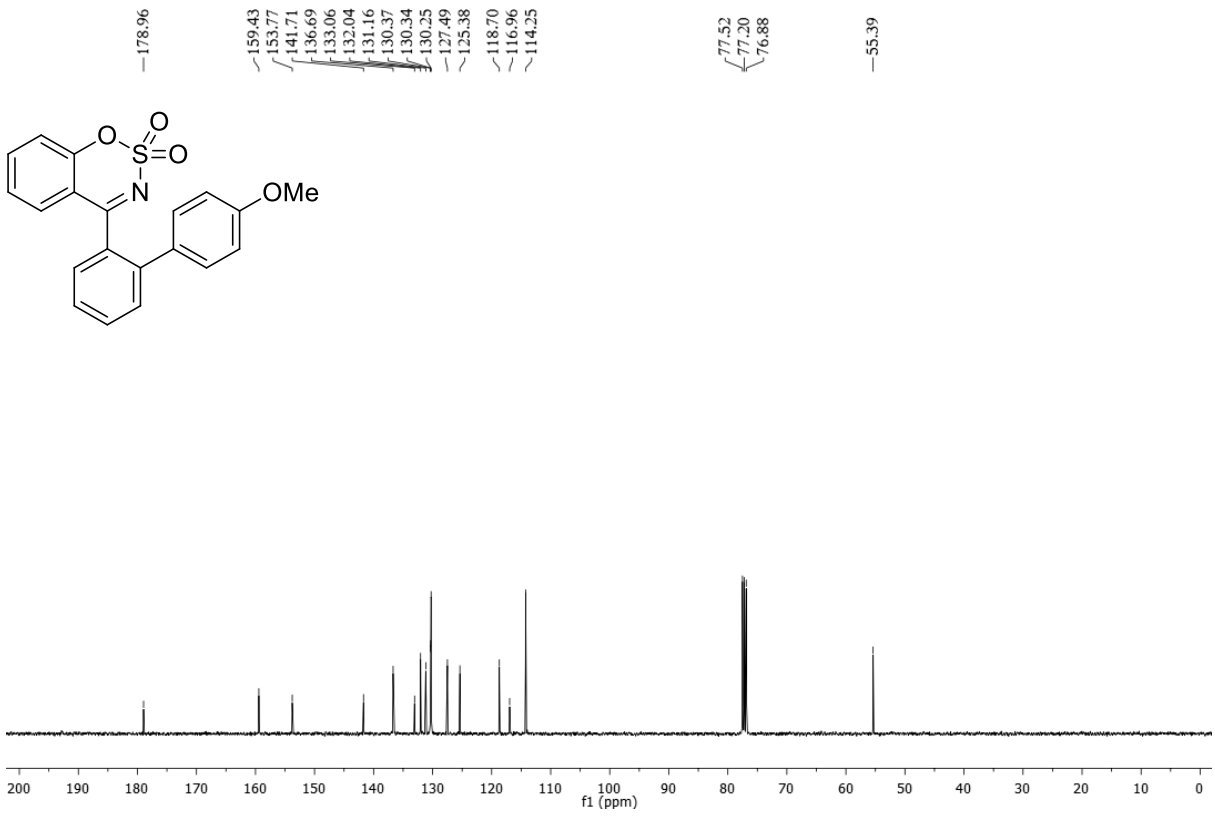
^{13}C NMR of **5fa** (100MHz, $CDCl_3$):



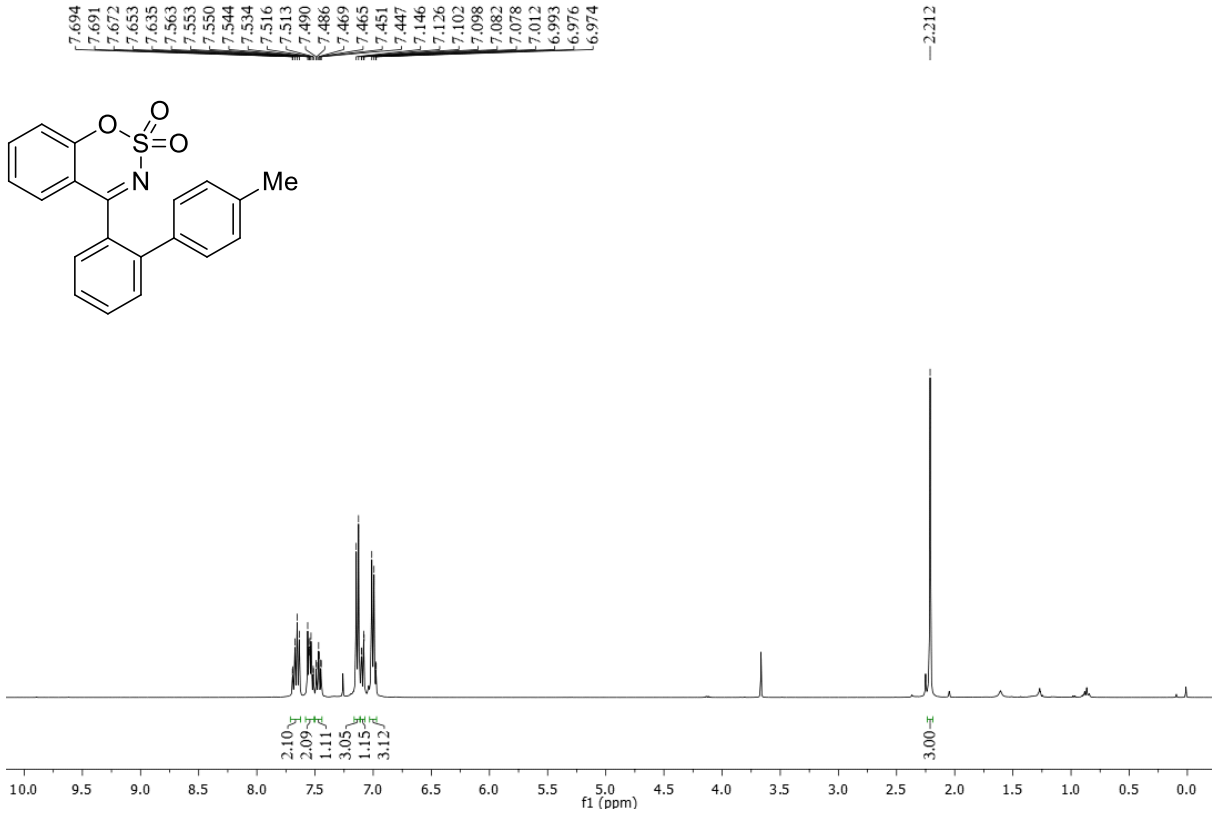
^{1}H NMR of **5ab** (400MHz, $CDCl_3$):



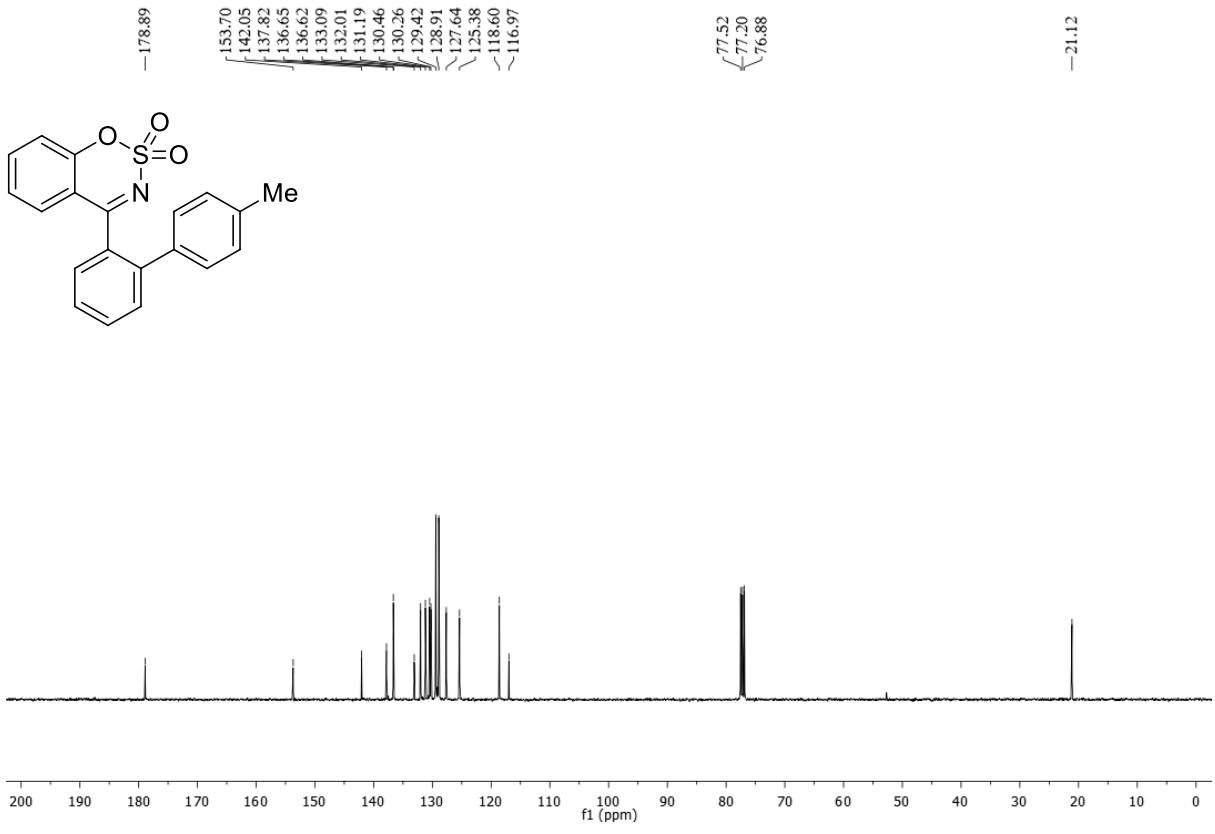
^{13}C NMR of **5ab** (100MHz, $CDCl_3$):



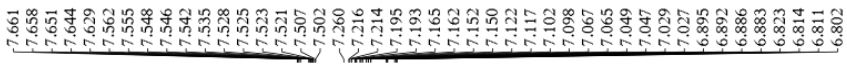
^{1}H NMR of **5ac** (400MHz, $CDCl_3$):

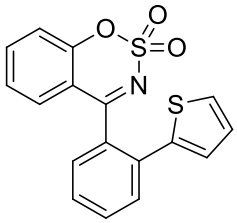


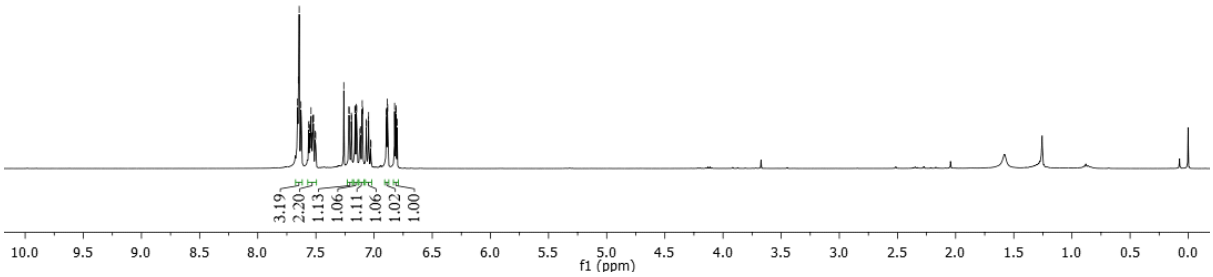
^{13}C NMR of **5ac** (100MHz, $CDCl_3$):



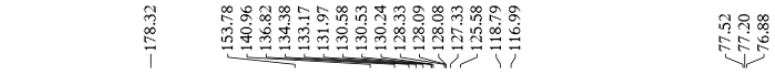
^{1}H NMR of **5ad** (400MHz, $CDCl_3$):

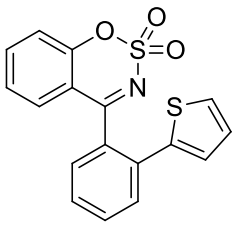


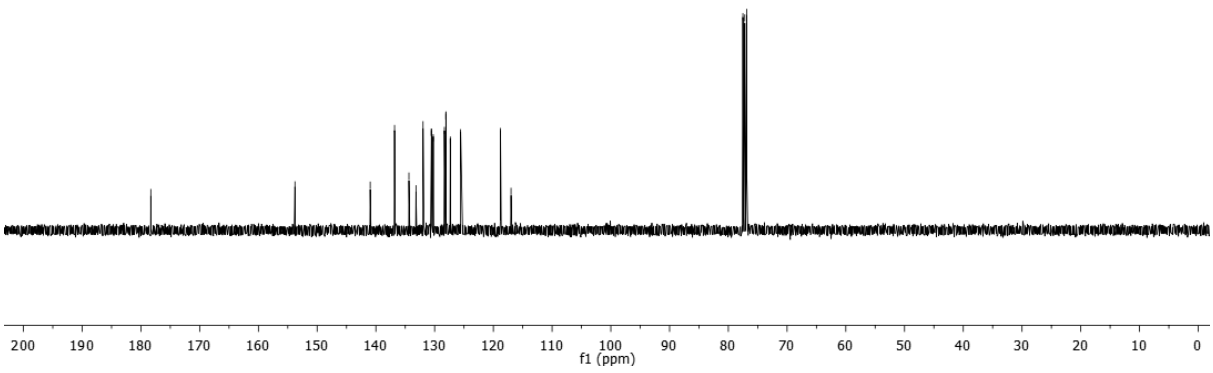




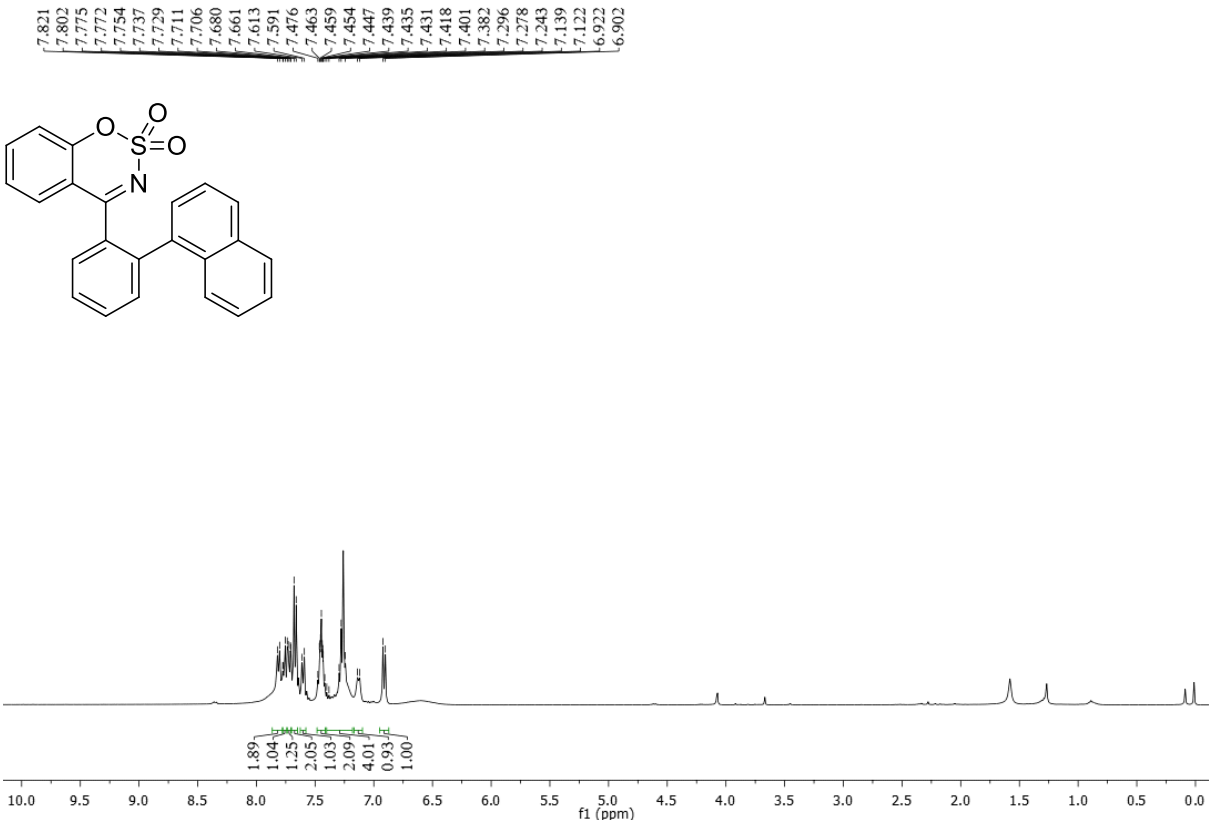
^{13}C NMR of **5ad** (100MHz, $CDCl_3$):



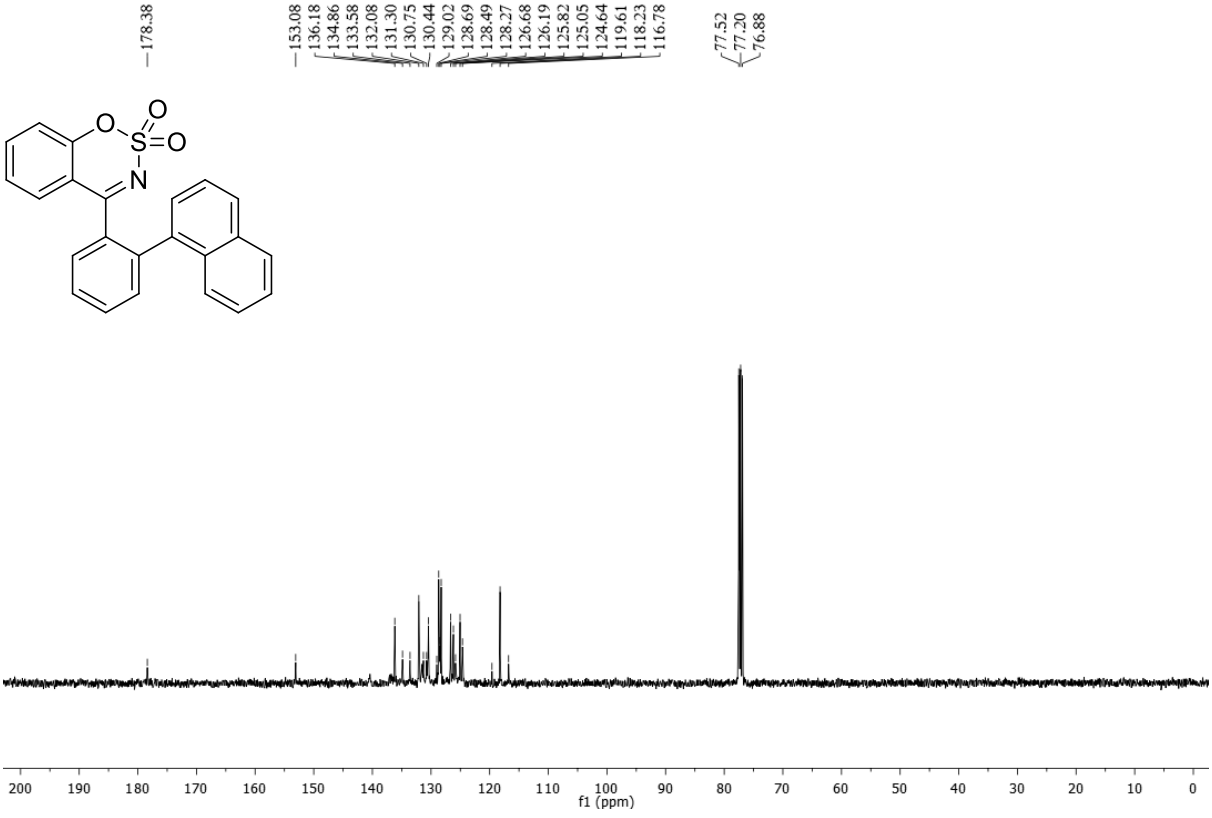




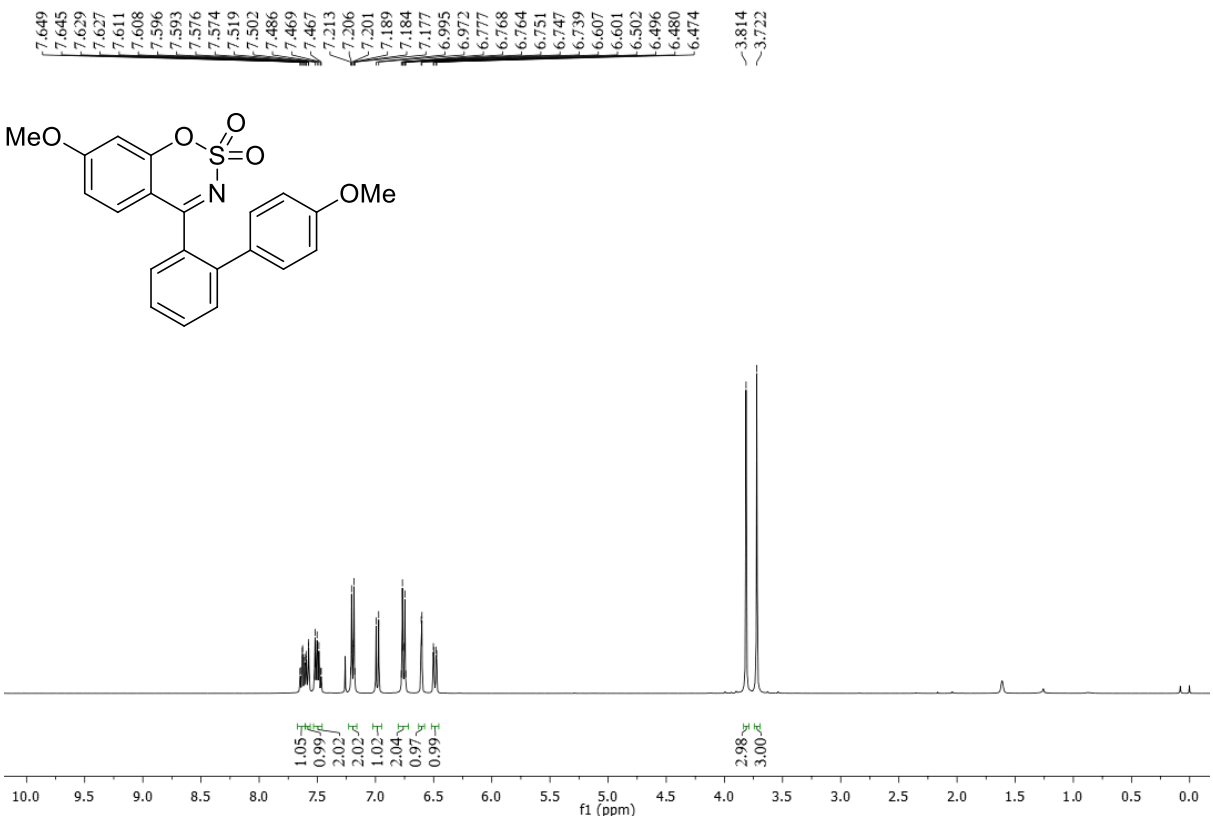
^{1}H NMR of **5ae** (400MHz, $CDCl_3$):



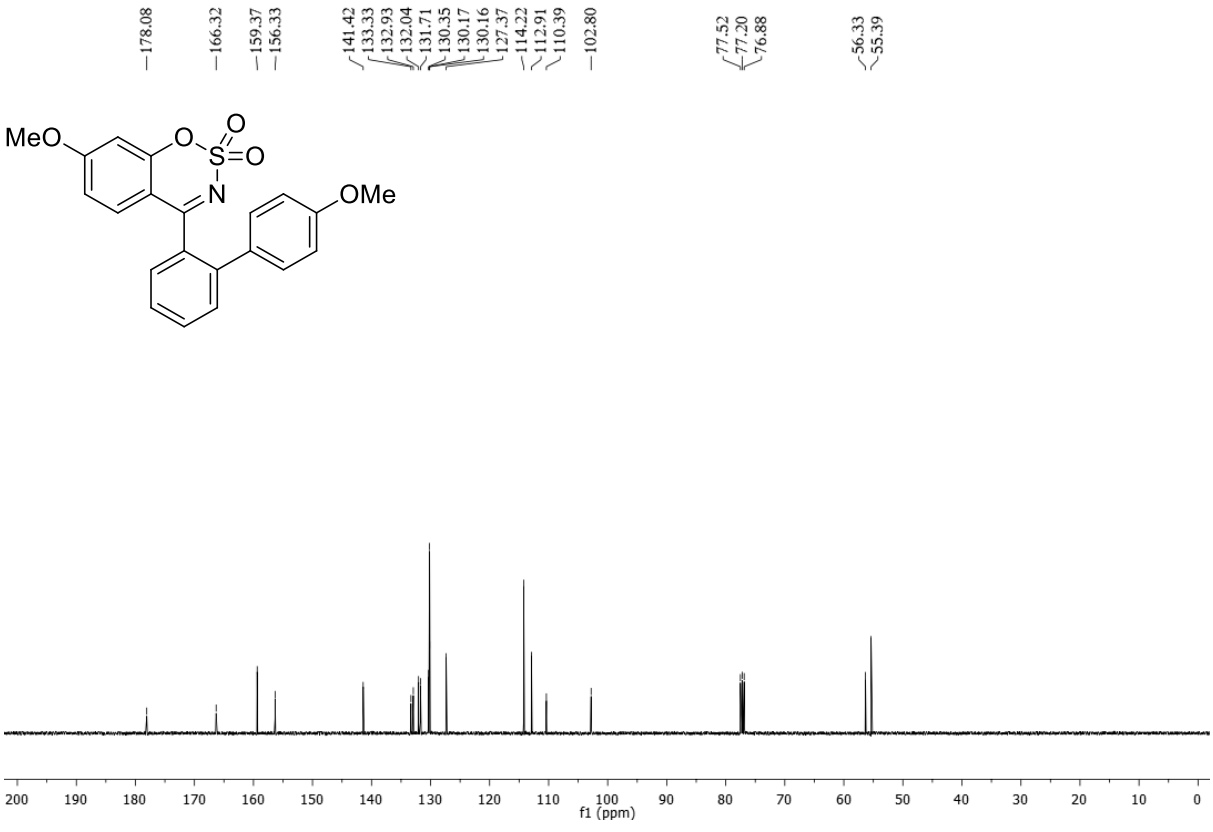
^{13}C NMR of **5ae** (100MHz, $CDCl_3$):



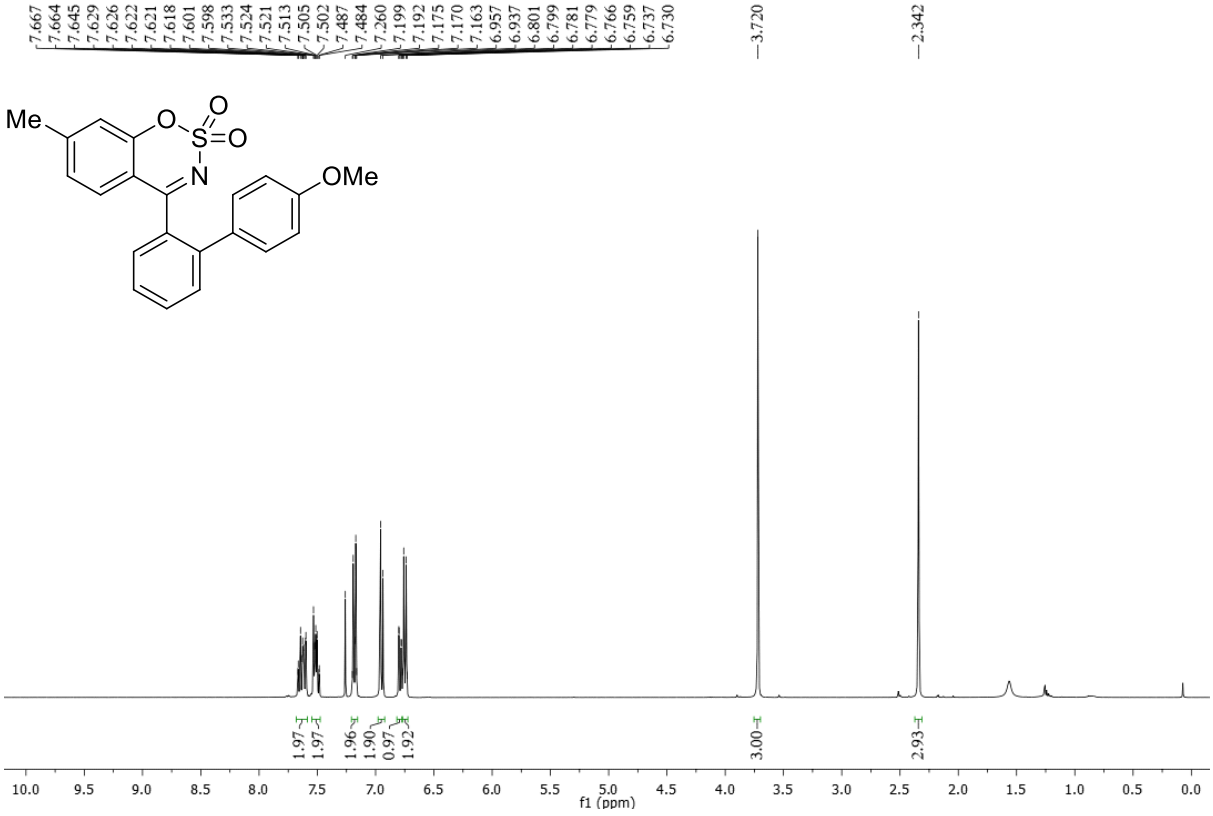
^{1}H NMR of **5bb** (400MHz, $CDCl_3$):



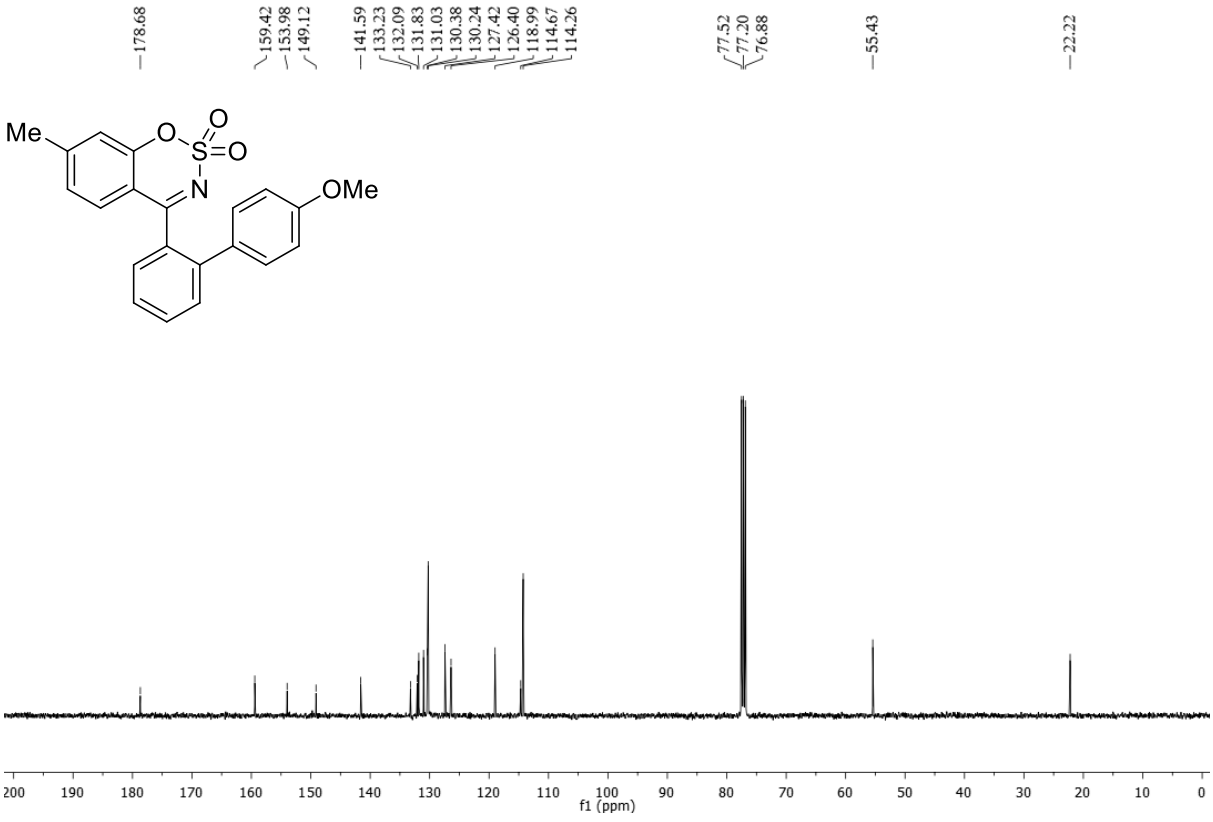
^{13}C NMR of **5bb** (100MHz, $CDCl_3$):



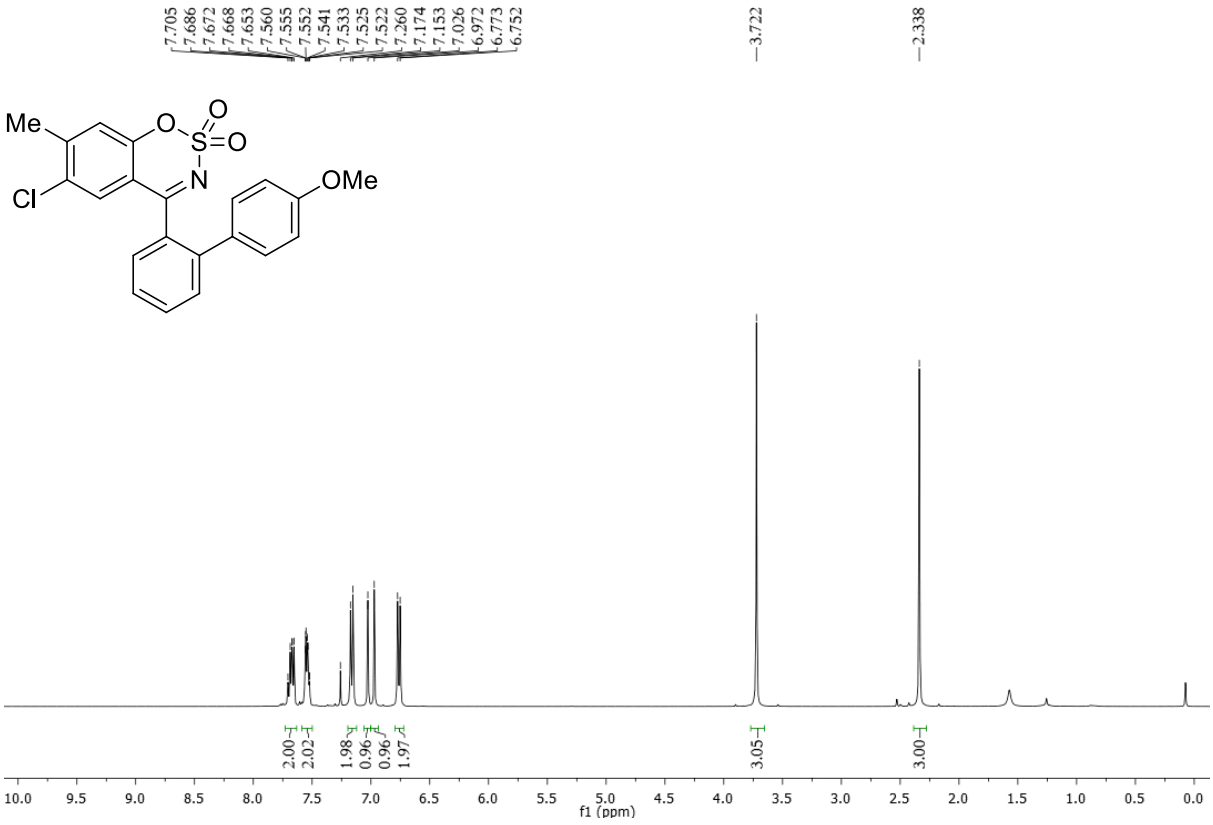
^{1}H NMR of **5cb** (400MHz, $CDCl_3$):



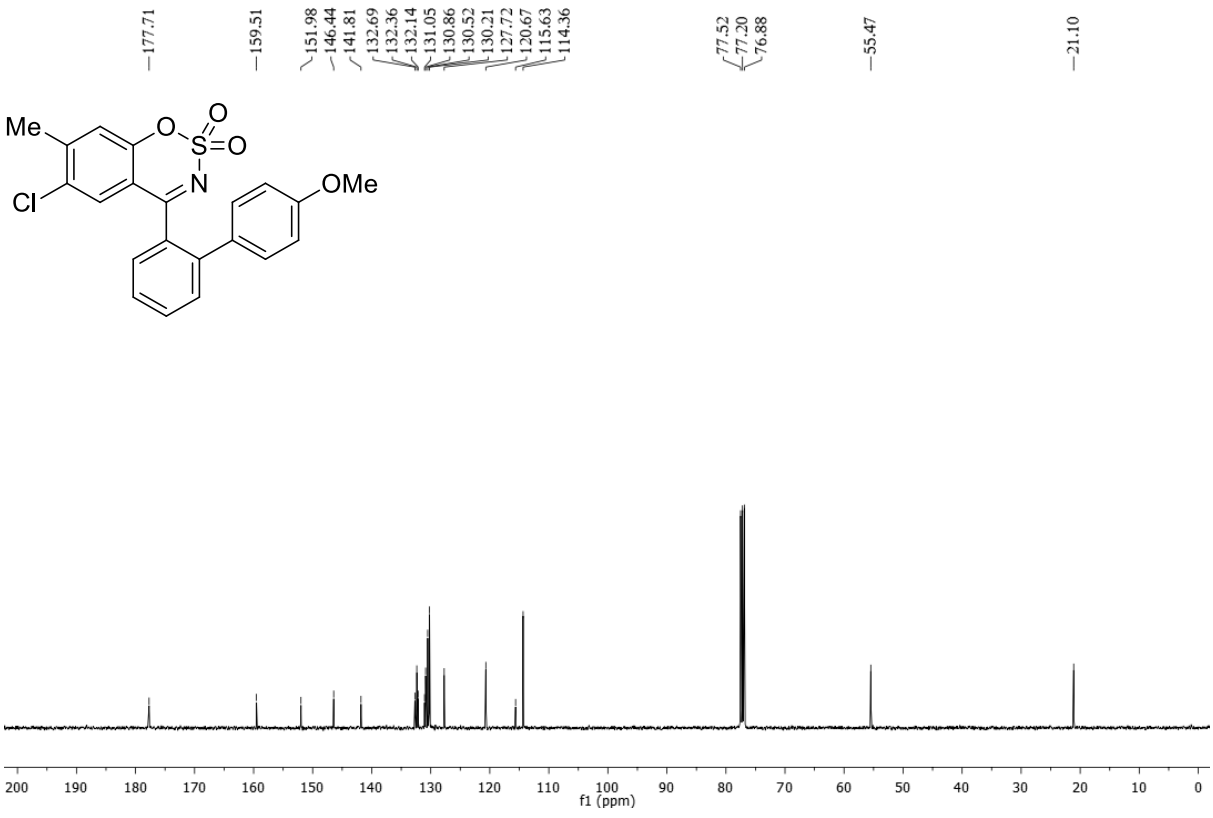
^{13}C NMR of **5cb** (100MHz, $CDCl_3$):



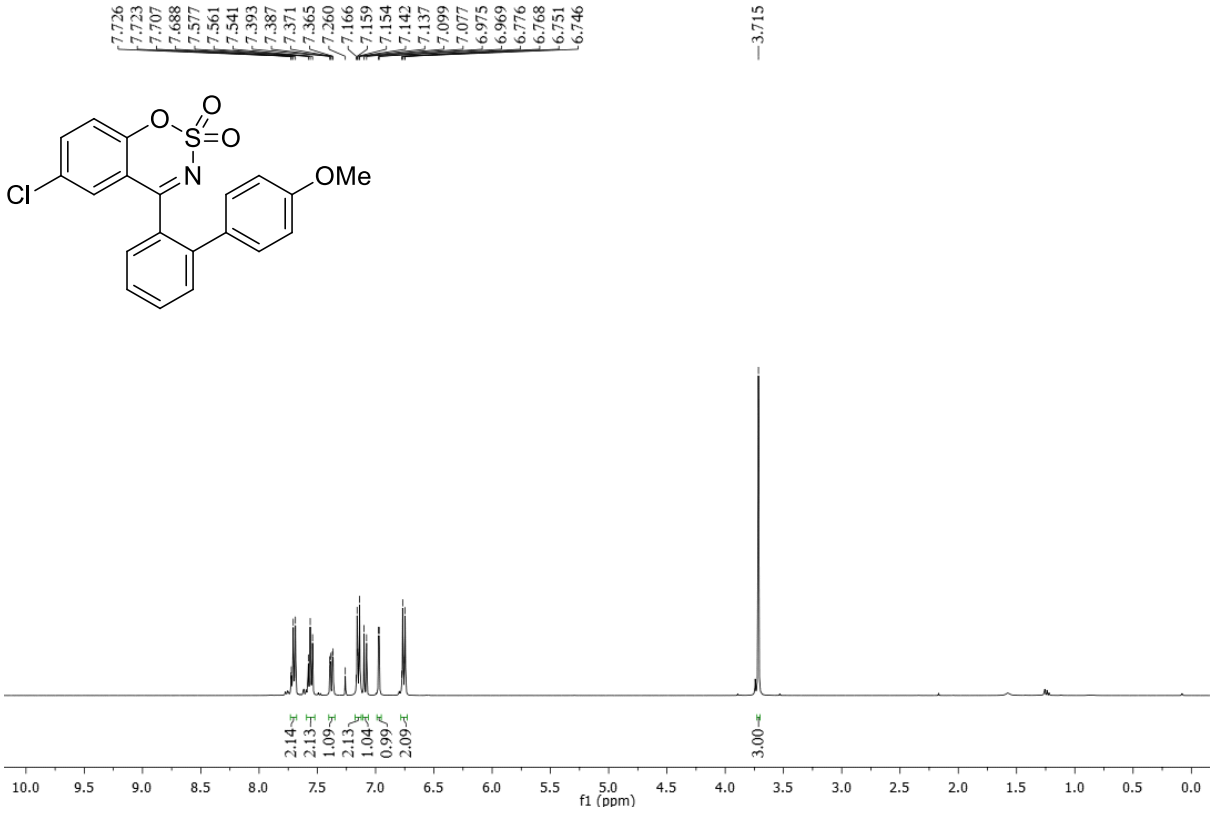
^{1}H NMR of **5db** (400MHz, $CDCl_3$):



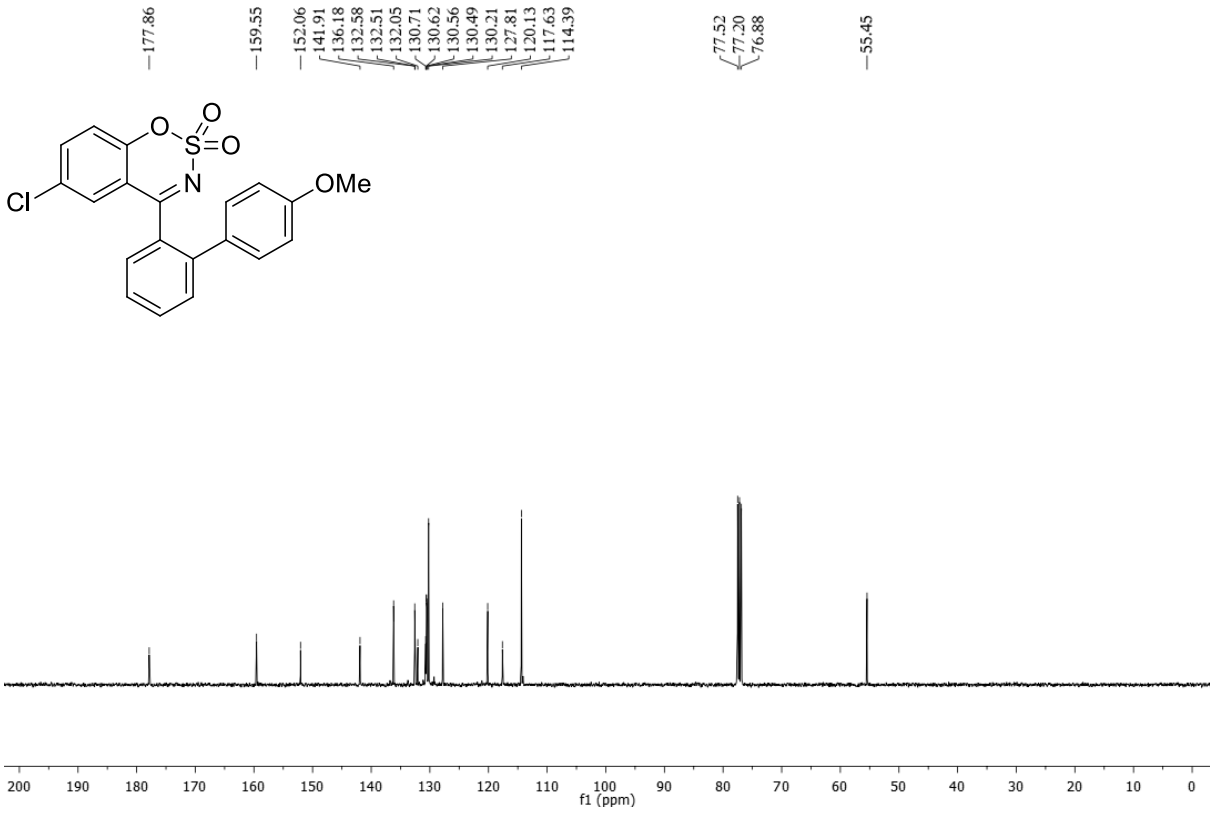
^{13}C NMR of **5db** (100MHz, $CDCl_3$):



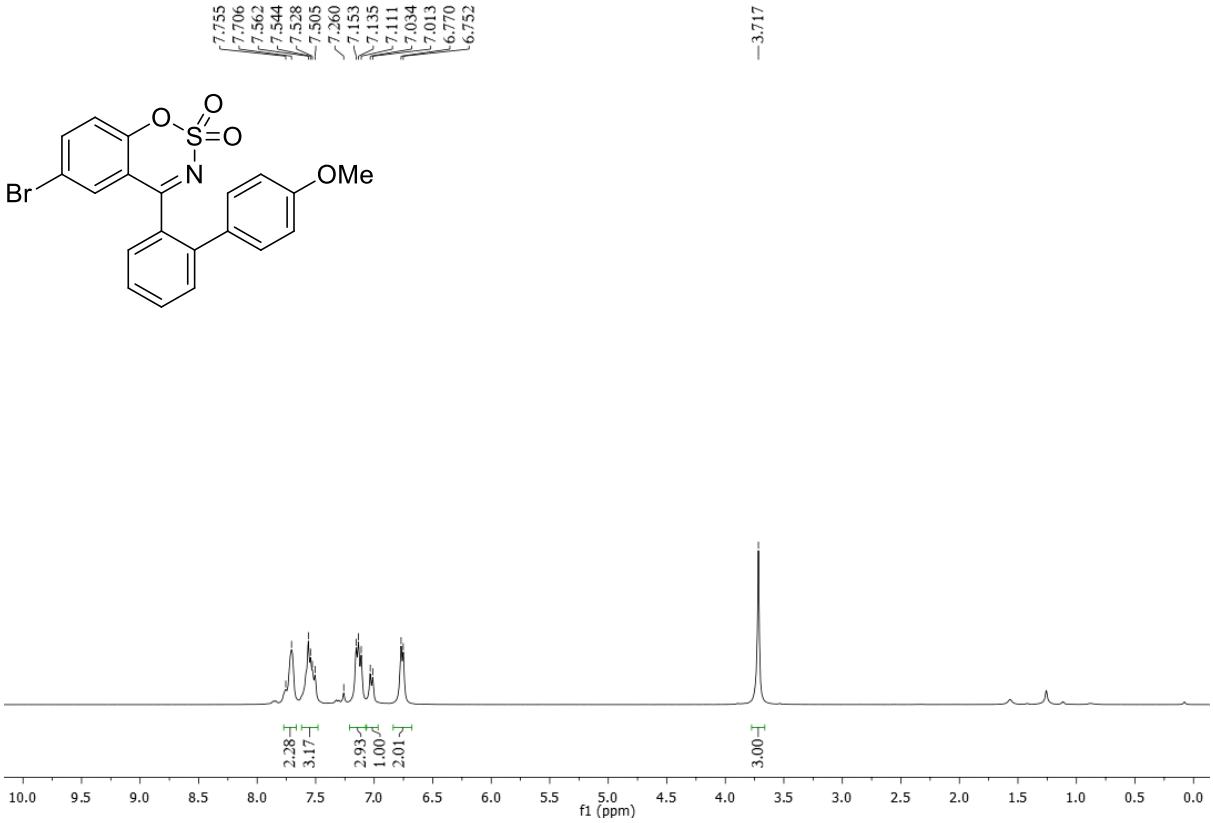
^{1}H NMR of **5eb** (400MHz, $CDCl_3$):



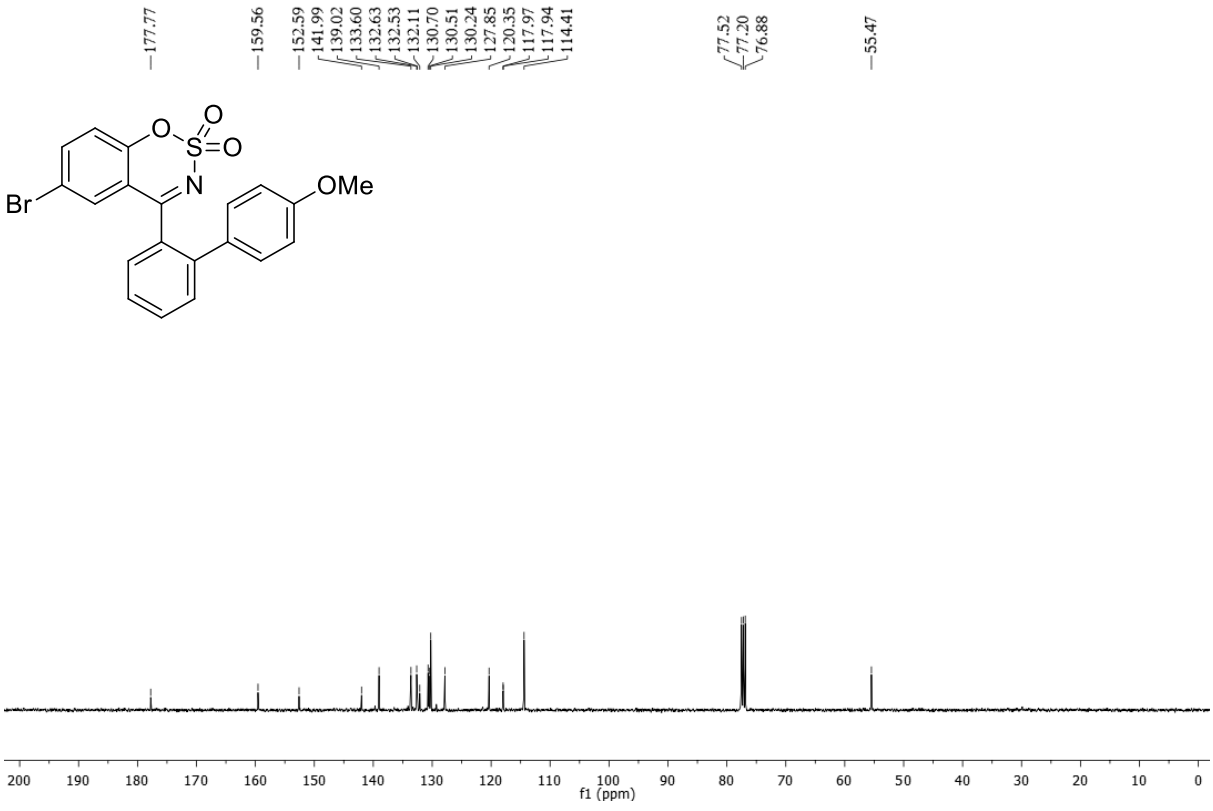
^{13}C NMR of **5eb** (100MHz, $CDCl_3$):



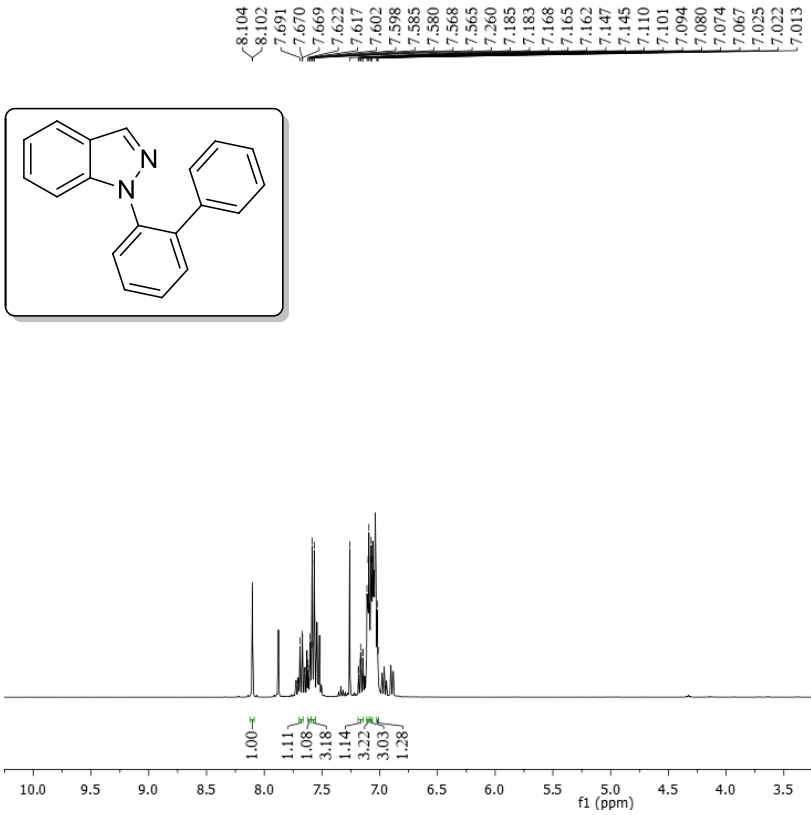
^{1}H NMR of **5fb** (400MHz, $CDCl_3$):



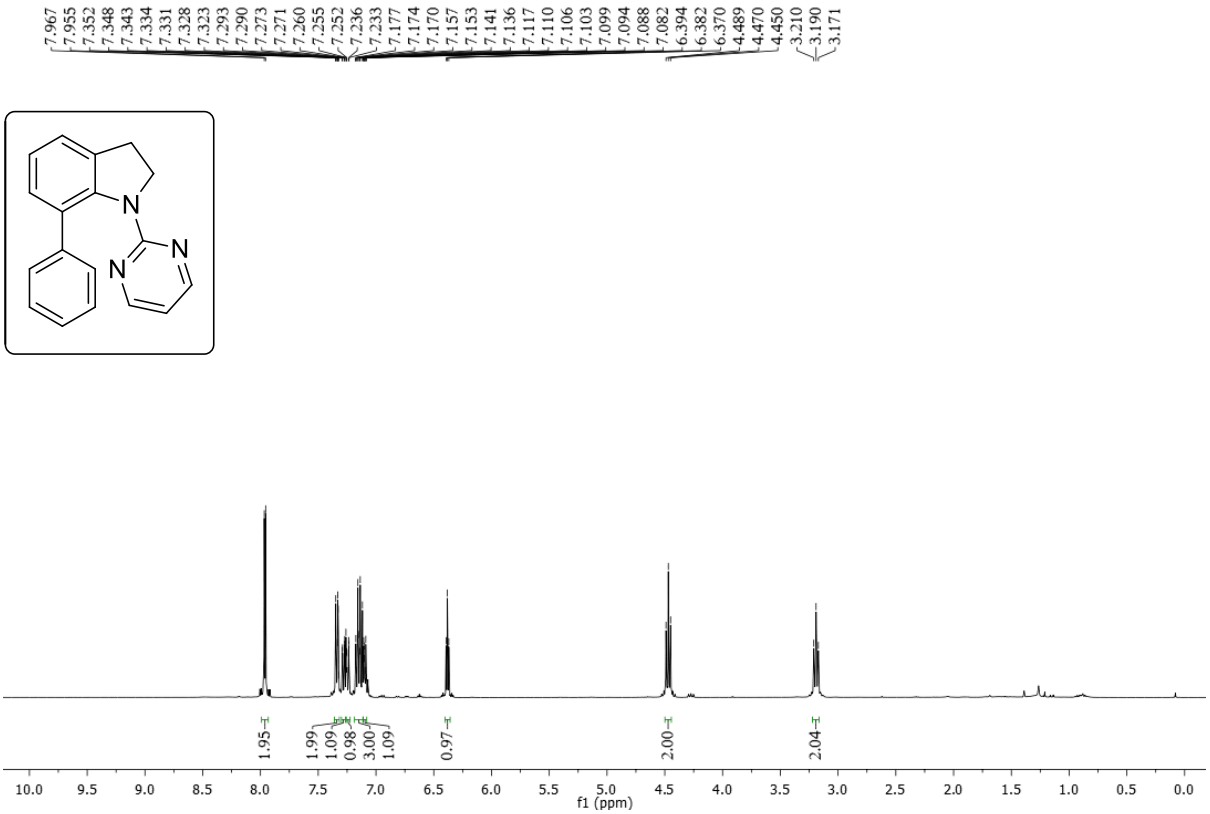
^{13}C NMR of **5fb** (100MHz, $CDCl_3$):



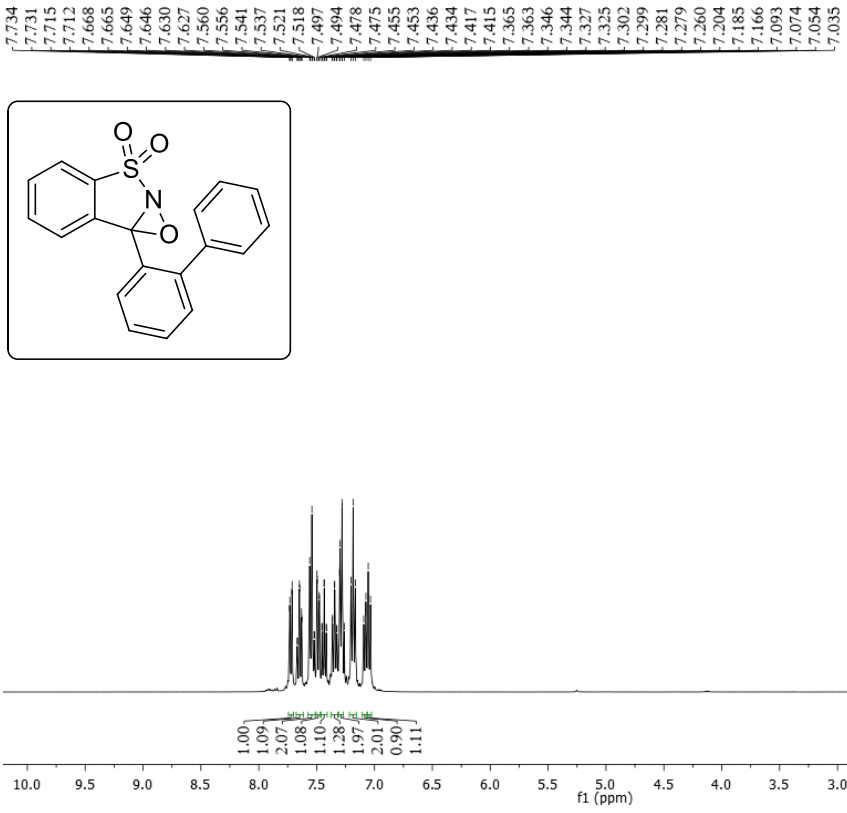
^{1}H NMR of **6** (400MHz, $CDCl_3$):



^{1}H NMR of **7** (400MHz, $CDCl_3$):



^{1}H NMR of **8** (400MHz, $CDCl_3$):



^{13}C NMR of **8** (100MHz, $CDCl_3$):