Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information

Rhodium-Catalysed Direct C-H Allylation of *N*-Sulfonyl Ketimines with Allyl Carbonates

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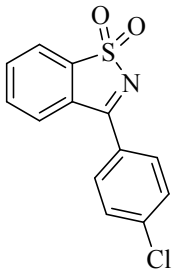
Materials and Methods

General. All reactions dealing with air- and moisture-sensitive compounds were carried out in dry reaction vessels under a nitrogen atmosphere. ^{1}H and^{13}C nuclear magnetic resonance (NMR) spectra were recorded on Agilent 600 MHz NMR spectrometer. ^{1}H and ^{13}C NMR spectra are reported in parts per million (ppm) downfield from an internal standard, tetramethylsilane (0 ppm) and $CHCl_3$ (77.0 ppm), respectively. ESI high-resolution mass spectra (HRMS) were recorded on a Waters SYNPAT G2. Melting points were determined using a capillary melting point apparatus and are uncorrected.

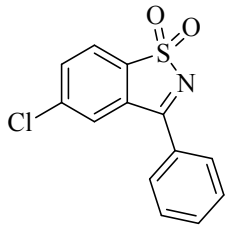
Materials. Unless otherwise noted, materials were purchased from commercial suppliers and were used as received. Anhydrous DCM was distilled over CaH_2 and stored under N_2.

Preparation of Substrates

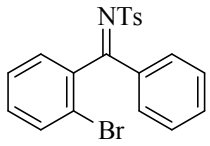
All *N*-sulfonyl ketimines[1] were synthesized according to the literature procedures, and the yields were not optimized. Allyl carbonates were synthesized from the corresponding allyl alcohols and methyl chloroformate.[2] Below are summaried characterization data for newly synthesized ketimines and allyl carbonates. ^{1}H and ^{13}C NMR spectra data for the rest of the ketimines and allyl carbonates showed good agreement with the literature data.



3-(4-Chlorophenyl)benzo[d]isothiazole 1,1-dioxide (1f): Brown solid; Mp = 210–211 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.03 (d, *J* = 7.4 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.81 (t, *J* = 7.4 Hz, 1H), 7.76 (t, *J* = 7.5 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 2H); **^{13}C NMR** (150 MHz $CDCl_3$): δ 169.9, 141.1, 140.0, 133.7, 133.5, 130.8, 130.2, 129.6, 128.8, 126.2, 123.2; **HRMS** (ESI) Calcd for $C_{13}H_8ClNO_2S$ $[M + Na]^+$ 299.9862 , found 299.9863.



5-Chloro-3-phenylbenzo[d]isothiazole 1,1-dioxide (1o): Yellow solid; Mp = 156–157 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.96–7.94 (m, 3H), 7.85 (d, *J* = 1.0 Hz, 1H), 7.77–7.70 (m, 2H), 7.64 (t, *J* = 7.7 Hz, 2H); **^{13}C NMR** (150 MHz $CDCl_3$): δ 169.7, 140.2, 139.3, 133.7, 133.2, 132.4, 129.9, 129.4, 129.4, 126.7, 123.9; **HRMS** (ESI) Calcd for $C_{13}H_8ClNO_2S$ $[M + H]^+$ 299.9862, found 299.9863.



N-((2-Bromophenyl)(phenyl)methylene)-4-methylbenzenesulfonamide (1u): White solid; Mp = 93–95 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.85 (d, *J* = 8.1 Hz, 2H), 7.67 (d, *J* = 7.7 Hz, 2H), 7.61 (d, *J* = 8.1 Hz, 1H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.43–7.35 (m, 4H), 7.29 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H); **^{13}C NMR** (150 MHz $CDCl_3$): δ 175.3, 143.8, 137.5, 136.8, 135.7, 133.8, 132.5, 131.0, 130.1, 129.4 (two signals are overlapped), 128.7, 127.7, 127.0, 120.1, 21.6;

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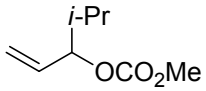
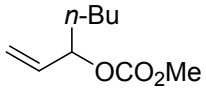
1 (a) G. Yang and W. Zhang, *Angew. Chem., Int. Ed.*, 2013, **52**, 7540; (b) T. Nishimura, A. Noishiki, G. C. Tsui and T. Hayashi, *J. Am. Chem. Soc.*, 2012, **134**, 5056; (c) D. Hellwinkel and R. Karle, *Synthesis*, 1989, 394.

2 D. C. Vrieze, G. S. Hoge, P. Z. Hoerter, J. T. V. Haitsma and B. M. Sames, *Org. Lett.*, 2009, **11**, 3140.

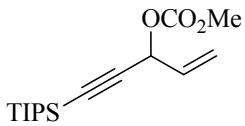
HRMS (ESI) Calcd for $C_{20}H_{16}BrNO_2S$ $[M + H]^+$ 435.9983, found 435.9980.



Methyl (4-methylpent-1-en-3-yl) carbonate (2g): Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$): 5.80–5.75 (m, 1H), 5.28 (d, J = 16.8 Hz, 1H), 5.25 (d, J = 10.2 Hz, 1H), 4.84 (t, J = 6.5 Hz, 1H), 3.77 (s, 3H), 1.94–1.89 (m, 1H), 0.93 (dd, J = 13.8, 7.2 Hz, 6H); **^{13}C NMR** (150 MHz $CDCl_3$): δ 155.4, 134.2, 118.3, 83.8, 54.6, 31.8, 17.9; **HRMS** (ESI) Calcd for $C_8H_{14}O_3$ $[M + Na]^+$ 181.0841, found 181.0841.



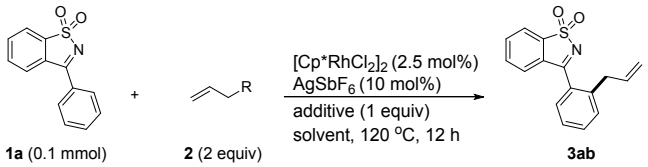
Hept-1-en-3-yl methyl carbonate (2h): Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 5.79–5.76 (m, 1H), 5.29 (d, J = 17.2 Hz, 1H), 5.20 (d, J = 10.5 Hz, 1H), 5.04 (m, 1H), 3.77 (s, 3H), 1.64–1.55 (m, 2H), 1.35–1.31 (m, 4H), 0.89 (t, J = 6.8 Hz, 3H); **^{13}C NMR** (150 MHz $CDCl_3$): δ 155.3, 136.0, 117.3, 79.2, 54.6, 33.9, 27.0, 22.4, 13.9; **HRMS** (ESI) Calcd for $C_9H_{16}O_3$ $[M + H]^+$ 195.0997, found 195.1000.



Methyl (5-(triisopropylsilyl)pent-1-en-4-yn-3-yl) carbonate (2i) : Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 5.96–5.92 (m, 1H), 5.76 (d, J = 5.6 Hz, 1H), 5.62 (d, J = 16.8 Hz, 1H), 5.34 (d, J = 10.1 Hz, 1H), 3.80 (s, 3H), 1.07 (s, 18H), 1.05–0.96 (m, 3H); **^{13}C NMR** (150 MHz $CDCl_3$): δ 154.7, 132.5, 119.5, 101.2, 89.9, 68.7, 54.9, 18.5, 11.0; **HRMS** (ESI) Calcd for $C_{16}H_{28}O_3Si$ $[M + H]^+$ 319.1705, found 319.1699.

Rh-Catalysed Direct Aryl C-H Allylation

Table S1. Reaction optimization



2a (R = OAc), **2b** (R = OCO_2Me)
2c (R = OCOPh), **2d** (R =OCO^tBu)
2e (R = OTs)

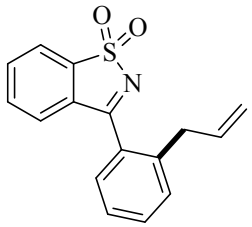
Entry	**2**	Additive	Solvent[a]	Yield (%)[b]
1	**2a**	none	dioxane	41
2	**2a**	K_2CO_3	dioxane	0
3	**2a**	NaOAc	dioxane	0
4	**2a**	HOAc	dioxane	30
5	**2a**	EtCOOH	dioxane	54
6	**2a**	PhCOOH	dioxane	51
7	**2a**	*p*-MeO-C_6H_4COOH	dioxane	40
8	**2a**	*p*-NO_2-C_6H_4COOH	dioxane	62
9	**2a**	*p*-NO_2-C_6H_4COOH	toluene	0
10	**2a**	*p*-NO_2-C_6H_4COOH	PhCl	74
11	**2a**	*p*-NO_2-C_6H_4COOH	DCM	60
12	**2a**	*p*-NO_2-C_6H_4COOH	PhCl/DCM	85
13	**2b**	*p*-NO_2-C_6H_4COOH	PhCl/DCM	89
14	**2c**	*p*-NO_2-C_6H_4COOH	PhCl/DCM	55
15	**2d**	*p*-NO_2-C_6H_4COOH	PhCl/DCM	31
16	**2e**	*p*-NO_2-C_6H_4COOH	PhCl/DCM	30
17[c]	**2b**	*p*-NO_2-C_6H_4COOH	PhCl/DCM	89

[a]The ratio of mixed solvents is 1:9. [b]Isolated yields. [c]Reaction was run at 80 °C.

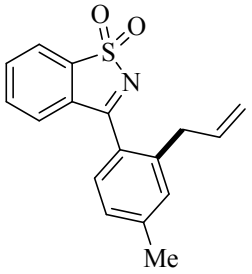
N-sulfonyl ketimine **1a**, a readily accessible derivative of saccharin, and allyl acetate **2a** were chosen as model substrates to optimize the reaction conditions (Table S1). Pleasingly, the reaction took place in the presence of $[Cp^*RhCl_2]_2$ (2.5 mol%) and $AgSbF_6$ (10 mol%) at 120 °C in dioxane, affording the desirable **3ab** in 41% yield (entry 1). Next, we tested the effect of various additives on the reaction. Whereas the reaction did not occur at all with K_2CO_3 or NaOAc as a base (entries 2 and 3), the addition of 1 equiv of acid, such as propionic acid, benzoic acid, 4-methoxybenzoic acid or 4-nitrobenzoic acid, improved the yield up to 62% (entries 5-8) while acetic acid gave a lower yield (entry 4). A screening of different solvents showed that mixed solvents of PhCl and DCM gave an 85% yield of **3ab** (entries 9-12). Among other allyl electrophiles with different leaving groups, allyl carbonate **2b** slightly improved the yield (entries 13-16). Note that, with **2b** as the allyl electrophile, the allylation reaction was also performed excellently at 80 °C (entry 17).

A General Procedure

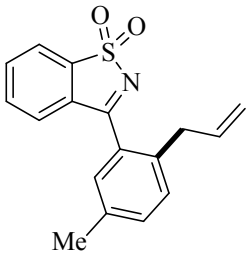
A 10 mL of Schlenk tube equipped with a stirrer bar was charged with ketimine (0.2 mmol), 4-nitrobenzoic acid (1 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol%), and $AgSbF_6$ (10 mol%) under air. Then, the Schlenk tube was quickly evacuated and refilled with N_2 for three times, followed by the addition of allyl carbonate (2 equiv), chlorobenzene (0.2 mL), and dichloromethane (1.8 mL). The Schlenk tube was sealed with a Teflon screwcap and the reaction mixture was stirred at 80 °C for 12 h. Upon cooling to room temperature, the reaction mixture was diluted with 10 mL of ethyl acetate, filtered through a pad of silica gel, followed by washing the pad of the silica gel with ethyl acetate (20 mL). Subsequently, the filtrate was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel to afford the allylated product.



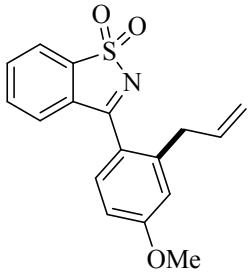
3-(2-Allylphenyl)benzo[d]isothiazole 1,1-dioxide (3ab): Following the general procedure; White solid (89% yield, eluent = petroleum ether/EtOAc (13:1)); Mp = 89–90 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.99 (d, *J* = 7.5 Hz, 1H), 7.77 (t, *J* = 7.5 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.50–7.48 (m, 2H), 7.46 (d, *J* = 7.7 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 5.85 (ddt, *J* = 17.1, 13.2, 6.65 Hz, 1H), 4.96–4.91 (m, 2H), 3.62 (d, *J* = 6.5 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 172.0, 140.1, 140.0, 136.2, 133.7, 133.4, 131.7, 131.7, 131.2, 129.1, 129.0, 126.4, 126.4, 122.7, 116.9, 37.4; **HRMS** (ESI) Calcd for $C_{16}H_{13}NO_2S$ $[M + Na]^+$ 306.0565, found 306.0565.



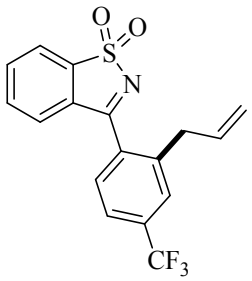
3-(2-Allyl-4-methylphenyl)benzo[d]isothiazole 1,1-dioxide (3bb): Following the general procedure; Yellow oil (97% yield, eluent = petroleum ether/EtOAc (13:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.97 (d, *J* = 7.4 Hz, 1H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.26 (s, 1H), 7.22 (d, *J* = 7.8 Hz, 1H), 5.84 (ddt, *J* = 17.1, 12.6, 6.6 Hz, 1H), 4.99–4.86 (m, 2H), 3.61 (d, *J* = 6.4 Hz, 2H), 2.44 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 171.9, 142.4, 140.2, 136.4, 133.6, 133.2, 132.0, 131.9, 129.3, 127.0, 126.5, 126.2, 122.6, 116.7 (two signals are overlapped), 37.4, 21.5; **HRMS** (ESI) Calcd for $C_{17}H_{15}NO_2S$ $[M + Na]^+$ 320.0721, found 320.0720.



3-(2-Allyl-5-methylphenyl)benzo[d]isothiazole 1,1-dioxide (3cb): Following the general procedure but the reaction was run at 120 °C; Yellow oil (92% yield, eluent = petroleum ether/EtOAc (13:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.98 (d, *J* = 7.5 Hz, 1H), 7.76 (t, *J* = 7.5 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.36–7.32 (m, 2H), 7.29 (s, 1H), 5.81 (ddt, *J* = 17.7, 12.6, 6.6 Hz, 1H), 4.93–4.90 (m, 2H), 3.55 (d, *J* = 6.5 Hz, 2H), 2.41 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 172.3, 140.1, 136.8, 136.4, 136.2, 133.7, 133.3, 132.5, 131.8, 131.1, 129.3, 129.0, 126.4, 122.6, 116.6, 37.0, 20.9; **HRMS** (ESI) Calcd for $C_{17}H_{15}NO_2S$ $[M + Na]^+$ 320.0721, found 320.0719.

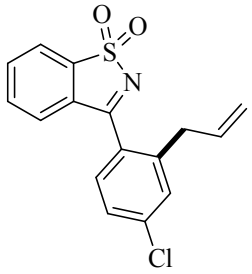


3-(2-Allyl-4-methoxyphenyl)benzo[d]isothiazole 1,1-dioxide (3db): Following the general procedure; Yellow solid (88% yield, eluent = petroleum ether/EtOAc (13:1)); Mp = 73–74 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.98 (d, *J* = 7.4 Hz, 1H), 7.74 (t, *J* = 7.5 Hz, 1H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 8.5 Hz, 1H), 6.98 (d, *J* = 2.4 Hz, 1H), 6.92 (dd, *J* = 8.5, 2.5 Hz, 1H), 5.86 (ddt, *J* = 17.7, 12.6, 6.6 Hz, 1H), 5.01–4.95 (m, 2H), 3.89 (s, 3H), 3.67 (d, *J* = 6.6 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 171.1, 162.4, 143.2, 140.3, 136.2, 133.5, 133.1, 132.0, 131.5, 126.5, 122.6, 121.3, 117.0, 116.9, 111.6, 55.5, 37.6; **HRMS** (ESI) Calcd for $C_{17}H_{15}NO_3S$ $[M + Na]^+$ 336.0670, found 336.0668.

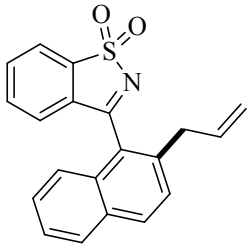


3-(2-Allyl-4-(trifluoromethyl)phenyl)benzo[d]isothiazole 1,1-dioxide (3eb): Following the general procedure; White solid (84% yield, eluent = petroleum ether/EtOAc (9:1)); Mp = 74–75 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.02 (d, *J* = 7.5 Hz, 1H), 7.81 (t, *J* = 7.5 Hz, 1H), 7.72–7.69 (m, 3H), 7.61 (d, *J* = 7.9 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 5.81 (ddt, *J* = 16.5, 12.6, 6.6 Hz, 1H), 4.99–4.96 (m, 2H), 3.64 (d, *J* = 6.4 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 171.0, 141.1, 140.0,

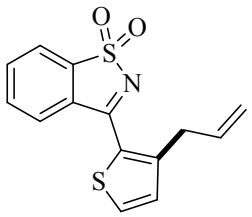
134.9, 133.9, 133.8, 133.4 (q, $^{2}J_{C\text{-}F}$ = 33 Hz), 132.7, 131.2, 129.3, 127.8 (q, $^{3}J_{C\text{-}F}$ = 4 Hz), 126.0, 125.2 (q, $^{1}J_{C\text{-}F}$ = 272 Hz), 123.4 (q, $^{3}J_{C\text{-}F}$ = 4 Hz), 123.0, 118.0, 37.3; **HRMS** (ESI) Calcd for $C_{17}H_{12}F_3NO_2S$ $[M + H]^+$ 352.0619, found 352.0621.



3-(2-Allyl-4-chlorophenyl)benzo[d]isothiazole 1,1-dioxide (3fb): Following the general procedure but the reaction was run at 120 °C; White solid (65% yield, eluent = petroleum ether/EtOAc (13:1)); Mp = 87–88 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.00 (d, *J* = 7.4 Hz, 1H), 7.78 (t, *J* = 7.4 Hz, 1H), 7.70 (t, *J* = 7.5 Hz, 1H), 7.48–7.44 (m, 3H), 7.41 (d, *J* = 8.0 Hz, 1H), 5.81 (ddt, *J* = 17.1, 13.8, 6.6 Hz, 1H), 4.98 (d, *J* = 12.6 Hz, 2H), 3.60 (d, *J* = 6.3 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 171.0, 142.3, 140.1, 138.0, 135.3, 133.8, 133.6, 131.4, 131.3, 130.3, 127.5, 126.7, 126.1, 122.9, 117.7, 37.2; **HRMS** (ESI) Calcd for $C_{16}H_{12}ClNO_2S$ $[M + Na]^+$ 340.0175, found 340.0170.

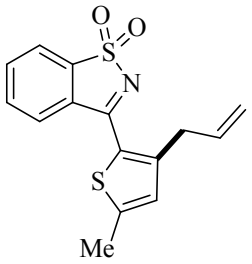


3-(2-Allylnaphthalen-1-yl)benzo[d]isothiazole 1,1-dioxide (3gb): Following the general procedure and using 20 mol% of $Cu(OAc)_2$ as an additive; Brown oil (83% yield, eluent = petroleum ether/EtOAc (13:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.04 (d, *J* = 7.6 Hz, 1H), 8.01 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.56–7.50 (m, 3H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.45–7.41 (m, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 5.83 (ddt, *J* = 16.5, 13.2, 6.6 Hz, 1H), 4.98–4.94 (m, 2H), 3.56 (dd, *J* = 15.6, 7.2 Hz, 1H), 3.44 (dd, *J* = 15.0, 5.4 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 173.4, 139.6, 136.8, 135.5, 133.9, 133.7, 132.5, 132.0, 131.0, 130.7, 128.4, 127.8, 127.4, 126.3, 126.2, 125.5, 124.6, 122.6, 117.2, 38.0; **HRMS** (ESI) Calcd for $C_{20}H_{15}NO_2S$ $[M + H]^+$ 334.0902, found 334.0903.

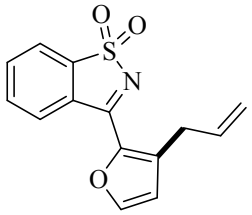


3-(3-Allylthiophen-2-yl)benzo[d]isothiazole 1,1-dioxide (3hb): Following the general procedure but the reaction was run in the presence of $AgSbF_6$ (40 mol%) and $Cu(OAc)_2$ (50 mol%) at 120 °C;

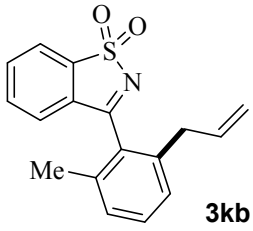
Yellow solid (55% yield, eluent = petroleum ether/EtOAc (8:1)); Mp = 124–125 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.28–8.26 (m, 1H), 7.99–7.98 (m, 1H), 7.77–7.74 (m, 3H), 7.24 (d, *J* = 5.0 Hz, 1H), 6.02 (ddt, *J* = 16.8, 13.8, 6.6 Hz, 1H), 5.17–5.10 (m, 2H), 3.92 (d, *J* = 6.7 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 163.5, 151.3, 140.4, 135.3, 133.5, 133.1, 132.8, 131.9, 131.5, 126.5, 125.6, 122.8, 117.0, 35.5; **HRMS** (ESI) Calcd for $C_{14}H_{11}NO_2S_2$ $[M + Na]^+$ 312.0129, found 312.0125.



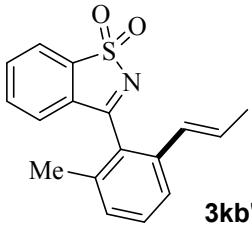
3-(3-Allyl-5-methylthiophen-2-yl)benzo[d]isothiazole 1,1-dioxide (3ib): Following the general procedure but the reaction was run in the presence of $AgSbF_6$ (40 mol%) and $Cu(OAc)_2$ (50 mol%); Yellow solid (57% yield, eluent = petroleum ether/EtOAc (11:1)); Mp = 130–131 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.31–8.27 (m, 1H), 7.99–7.95 (m, 1H), 7.76–7.71 (m, 2H), 6.93 (s, 1H), 6.02 (ddt, *J* = 16.5, 13.2, 6.6 Hz, 1H), 5.16 (d, *J* = 17.0 Hz, 1H), 5.11 (d, *J* = 9.9 Hz, 1H), 3.89 (d, *J* = 6.8 Hz, 2H), 2.61 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 162.7, 152.8, 149.3, 140.5, 135.4, 133.3, 132.9, 131.8, 131.0, 126.4, 123.5, 122.7, 116.9, 35.9, 15.8; **HRMS** (ESI) Calcd for $C_{15}H_{13}NO_2S_2$ $[M + Na]^+$ 326.0285, found 326.0280.



3-(3-Allylfuran-2-yl)benzo[d]isothiazole 1,1-dioxide (3jb): Following the general procedure but the reaction was run in the presence of $AgSbF_6$ (40 mol%) and $Cu(OAc)_2$ (50 mol%) at 120 °C; Yellow solid (41% yield, eluent = petroleum ether/EtOAc (7:1)); Mp = 143–144 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.55–8.54 (m, 1H), 7.98–7.97 (m, 1H), 7.81 (s, 1H), 7.77–7.72 (m, 2H), 6.70 (s, 1H), 6.01 (ddt, *J* = 16.5, 13.2, 6.6 Hz, 1H), 5.22 (d, *J* = 16.8 Hz, 1H), 5.16 (d, *J* = 10.2 Hz, 1H), 3.87 (d, *J* = 6.7 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 158.1, 148.2, 143.4, 140.3, 140.1, 134.0, 133.6, 133.1, 130.6, 127.9, 122.4, 117.4, 115.8, 31.4; **HRMS** (ESI) Calcd for $C_{14}H_{11}NO_3S$ $[M + Na]^+$ 296.0357, found 296.0353.



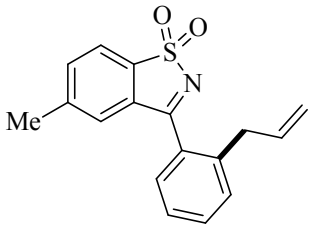
3kb



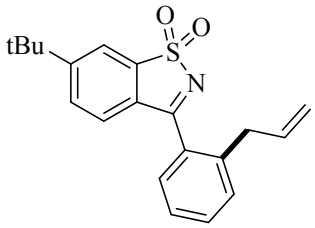
3kb'

Following the general procedure and using 20 mol% of $Cu(OAc)_2$ as an additive. The reaction gave an inseparable mixture containing **3kb** and **3kb'** with a ratio of 2:1 determined by ^{1}H NMR. **3-(2-Allyl-6-methylphenyl)benzo[d]isothiazole 1,1-dioxide (3kb):** 43% yield (eluent = petroleum ether/EtOAc (19:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.00 (d, *J* = 7.5 Hz, 1H), 7.77–7.34 (m, 1H), 7.65–7.61 (m, 1H), 7.46–7.37 (m, 1H), 7.25–7.18 (m, 3H), 5.73 (ddt, *J* = 16.8, 13.2, 6.6 Hz, 1H, 1H), 4.90–4.86 (m, 2H), 3.35 (dd, *J* = 15.6, 7.2 Hz,1H), 3.24 (dd, *J* = 15.6, 6.0 Hz, 1H), 2.19 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 173.9, 139.6, 138.1, 135.7, 134.0, 133.6, 132.0, 130.5, 129.2, 128.6, 127.5, 125.7, 123.6, 122.7, 117.0, 37.7, 19.7; **HRMS** (ESI) Calcd for $C_{17}H_{15}NO_2S$ $[M + Na]^+$ 320.0721, found 320.0720.

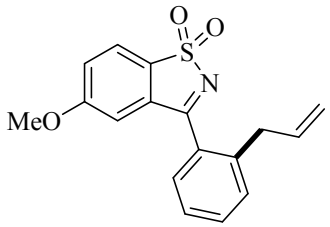
(*E*)-3-(2-methyl-6-(prop-1-en-1-yl)phenyl)benzo[d]isothiazole 1,1-dioxide (3kb'): 22% yield (eluent = petroleum ether/EtOAc (19:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.00 (d, *J* = 7.5 Hz, 1H), 7.77–7.34 (m, 1H), 7.65–7.61 (m, 1H), 7.46–7.37 (m, 1H), 7.25–7.18 (m, 3H), 6.21–6.13 (m, 2H), 2.22 (s, 3H), 1.69 (d, *J* = 5.1 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 174.0, 139.7, 138.1, 135.8, 133.9, 133.5, 131.9, 130.4, 129.2, 129.0, 127.5, 126.1, 123.6, 122.6, 117.0, 19.6, 18.6; **HRMS** (ESI) Calcd for $C_{17}H_{15}NO_2S$ $[M + Na]^+$ 320.0721, found 320.0720.



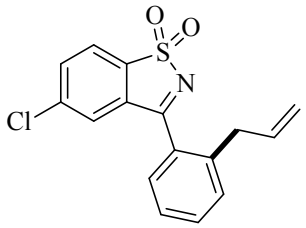
3-(2-Allylphenyl)-5-methylbenzo[d]isothiazole 1,1-dioxide (3lb): Following the general procedure; Yellow solid (78% yield, eluent = petroleum ether/EtOAc (15:1)); Mp = 101–102 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.86 (d, *J* = 7.7 Hz, 1H), 7.56–7.54 (m, 2H), 7.49–7.38 (m, 3H), 7.24 (s, 1H), 5.83 (ddt, *J* = 17.1, 13.2, 6.6 Hz, 1H), 4.97–4.93 (m, 2H), 3.61 (d, *J* = 6.5 Hz, 2H), 2.46 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 172.1, 145.0, 139.9, 137.4, 136.2, 133.9, 132.3, 131.6, 131.1, 129.2, 129.0, 126.8, 126.3, 122.5, 116.8, 37.4, 21.7; **HRMS** (ESI) Calcd for $C_{17}H_{15}NO_2S$ $[M + H]^+$ 298.0902, found 298.0906.



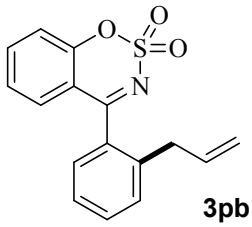
3-(2-Allylphenyl)-6-(tert-butyl)benzo[d]isothiazole 1,1-dioxide (3mb): Following the general procedure but the reaction was run at 120 °C; Yellow solid (66% yield, eluent = petroleum ether/EtOAc (19:1)); Mp = 91–92 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.01 (s, 1H), 7.67 (d, *J* = 8.1 Hz, 1H), 7.53 (tf, *J* = 7.5 Hz, 1H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.45 (d, *J* = 7.7 Hz, 1H), 7.42–7.39 (m, 2H), 5.85 (m, 1H), 5.00–4.89 (m, 2H), 3.63 (d, *J* = 6.2 Hz, 2H), 1.39 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 172.0, 158.4, 140.5, 140.0, 136.3, 131.6, 131.1, 130.8, 129.3, 129.3, 129.0, 126.3, 126.0, 119.9, 116.8, 37.4, 35.8, 31.0; **HRMS** (ESI) Calcd for $C_{20}H_{21}NO_2S$ $[M + Na]^+$ 362.1191, found 362.1185.



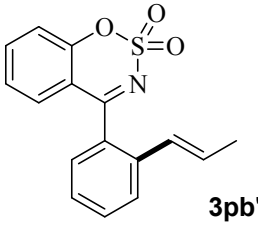
3-(2-Allylphenyl)-5-methoxybenzo[d]isothiazole 1,1-dioxide (3nb): Following the general procedure but the reaction was stirred at 120 °C; Yellow solid (72% yield, eluent = petroleum ether/EtOAc (13:1)); Mp = 87–88 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.3 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.46 (t, *J* = 9.2 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.19 (d, *J* = 8.3 Hz, 1H), 6.88 (s, 1H), 5.84 (ddt, *J* = 16.5, 13.2, 6.6 Hz, 1H), 5.00–4.90 (m, 2H), 3.84 (d, *J* = 18.7 Hz, 3H), 3.61 (d, *J* = 6.3 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 171.5, 164.1, 139.9, 136.2, 134.3, 131.6, 131.5, 131.2, 129.1, 128.9, 126.4, 124.0, 117.7, 116.9, 112.1, 56.2, 37.4; **HRMS** (ESI) Calcd for $C_{17}H_{15}NO_3S$ $[M + H]^+$ 314.0851, found 314.0857.



3-(2-Allylphenyl)-5-chlorobenzo[d]isothiazole 1,1-dioxide (3ob): Following the general procedure but the reaction was stirred at 120 °C; Yellow solid (81% yield, eluent = petroleum ether/EtOAc (19:1)); Mp = 110–111 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.92 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.49–7.42 (m, 4H), 5.87–5.80 (m, 1H), 4.97–4.91 (m, 2H), 3.62 (d, *J* = 6.0 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 170.7, 140.3, 140.2, 138.4, 136.1, 133.6, 133.3, 132.0, 131.4, 128.9, 128.5, 126.6, 126.4, 123.6, 117.0, 37.4; **HRMS** (ESI) Calcd for $C_{16}H_{12}ClNO_2S$ $[M + H]^+$ 318.0356, found 318.0353.



3pb

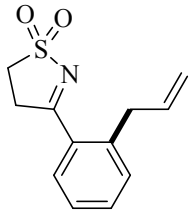


3pb'

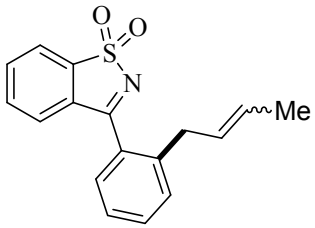
Following the general procedure and using 50 mol% of $Cu(OAc)_2$ as an additive. The reaction gave an inseparable mixture containing **3pb** and **3pb'** with a ratio of 1.45:1 determined by ^{1}H NMR. **4-(2-Allylphenyl)benzo[e][1,2,3]oxathiazine 2,2-dioxide (3pb)**: 51% yield (eluent = petroleum ether/EtOAc (39:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.74–7.69 (m, 1H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.42-7.35 (m, 3H), 7.31–7.24 (m, 3H), 5.81 (ddt, *J* = 16.8, 13.2, 6.6 Hz, 1H), 4.96–4.92 (m, 2H), 3.47 (d, *J* = 6.0 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 177.6, 154.2, 139.3, 137.2, 133.1, 131.7, 131.4, 130.7, 129.5, 127.5, 126.6, 125.7, 119.0, 117.2, 117.1, 37.4; **HRMS** (ESI) Calcd for $C_{16}H_{13}NO_3S$ $[M + Na]^+$ 322.0514, found 322.0507.

(*E*)-4-(2-(prop-1-en-1-yl)phenyl)benzo[e][1,2,3]oxathiazine 2,2-dioxide (3pb'): 36% yield

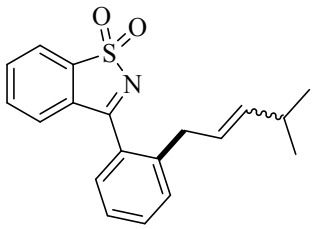
(eluent = petroleum ether/EtOAc (39:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): δ7.74–7.69 (m, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.42-7.35 (m, 3H), 7.31–7.24 (m, 3H), 6.27 (d, *J* = 15.6 Hz, 1H), 6.19–6.13 (m, 1H), 1.72 (d, *J* = 6.6 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 178.0, 154.0, 137.5, 137.1, 135.9, 131.5, 131.5, 130.7, 129.4, 127.5, 126.8, 126.3, 118.9, 117.2, 117.1, 18.7; **HRMS** (ESI) Calcd for $C_{16}H_{13}NO_3S$ $[M + Na]^+$ 322.0514, found 322.0507.



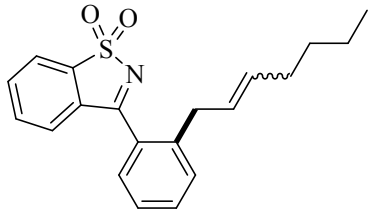
3-(2-Allylphenyl)-4,5-dihydroisothiazole 1,1-dioxide (3qb): Following the general procedure, and using 50 mol% of $Cu(OAc)_2$ as an additive; Yellow solid (74% yield, eluent = petroleum ether/EtOAc (5:1)); Mp = 120–121 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.58 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.40–7.33 (m, 2H), 6.01–5.91 (m, 1H), 5.06–5.00 (m, 2H), 3.82 (d, *J* = 6.4 Hz, 2H), 3.62–3.59 (m, 2H), 3.36 (t, *J* = 7.2 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 177.0, 141.9, 136.8, 132.8, 131.7, 130.6, 129.2, 126.7, 116.4, 43.7, 38.4, 36.6; **HRMS** (ESI) Calcd for $C_{12}H_{13}NO_2S$ $[M + Na]^+$ 258.0565, found 258.0561.



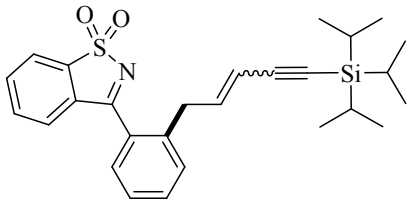
(*E*)-3-(2-(But-2-en-1-yl)phenyl)benzo[d]isothiazole 1,1-dioxide and (*Z*)- 3-(2-(but-2-en-1-yl)phenyl)benzo[d]isothiazole 1,1-dioxide (3af): Following the general procedure and the reaction was run in the presence of $[Cp^*RhCl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%) and $Cu(OAc)_2$ (20 mol%); Colorless oil (75% yield, eluent = petroleum ether/EtOAc (13:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): ***E* isomer**: δ 8.00 (d, *J* = 7.5 Hz, 1H), 7.78–7.76 (m, 1H), 7.70–7.68 (m, 1H), 7.54–7.44 (m, 4H), 7.40 (t, *J* = 7.2 Hz, 1H), 5.52–5.31 (m, 2H), 3.58 (d, *J* = 7.0 Hz, 2H), 1.55 (d, *J* = 6.6 Hz, 3H). ***Z* isomer**: δ8.00 (d, *J* = 7.5 Hz, 1H), 7.78–7.76 (m, 1H), 7.70–7.68 (m, 1H), 7.54–7.44 (m, 4H), 7.40 (t, *J* = 7.2 Hz, 1H), 5.52–5.31 (m, 2H), 3.52 (d, *J* = 5.5 Hz, 2H), 1.40 (d, *J* = 5.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): ***E* isomer**: δ 172.3, 141.1, 140.1, 133.7, 133.4, 131.8, 131.7, 130.8, 129.0, 128.9, 127.8, 126.4, 126.2, 126.1, 122.7, 30.9, 12.9. ***Z* isomer**: δ 172.4, 141.0, 140.0, 133.6, 133.3, 132.0, 131.5, 131.0, 128.7, 128.6, 127.9, 126.3, 126.2, 126.1, 122.6, 36.5, 17.6; **HRMS** (ESI) Calcd for $C_{17}H_{15}NO_2S$ $[M + Na]^+$ 320.0721, found 320.0719.



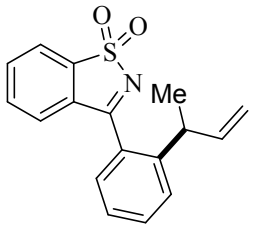
(*E*)-3-(2-(4-Methylpent-2-en-1-yl)phenyl)benzo[d]isothiazole 1,1-dioxide and (*Z*)- 3-(2-(4-methylpent-2-en-1-yl)phenyl)benzo[d]isothiazole 1,1-dioxide (3ag): Following the general procedure and the reaction was run in the presence of $[Cp^*RhCl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%) and $Cu(OAc)_2$ (20 mol%); Yellow solid (70% yield, eluent = petroleum ether/EtOAc (15:1)); Mp = 92–93 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): ***E* isomer**: δ 7.98 (d, *J* = 7.2 Hz, 1H), 7.77–7.74 (m, 1H), 7.69–7.65 (m, 1H), 7.55–7.40 (m, 4H), 7.38 (t, *J* = 7.5 Hz, 1H), 5.36–5.18 (m, 2H), 3.58–3.55 (m, 2H), 2.57–2.53 (m, 1H), 0.87 (d, *J* = 6.6 Hz, 6H); ***Z* isomer**: δ 7.96 (d, *J* = 7.8 Hz, 1H), 7.77–7.74 (m, 1H), 7.69–7.65 (m, 1H), 7.55–7.40 (m, 4H), 7.38 (t, *J* = 7.5 Hz, 1H), 5.36–5.18 (m, 2H), 3.58–3.55 (m, 2H), 2.57–2.53 (m, 1H), 0.65 (d, *J* = 6.7 Hz, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$): ***E* isomer**: δ 172.2, 141.3, 140.2, 139.5, 133.7, 133.4, 131.7, 131.5, 130.7, 128.9, 128.8, 126.5, 126.1, 124.4, 122.7, 31.0, 26.6, 22.9. ***Z* isomer**: δ 172.2, 141.3, 140.2, 140.0, 133.6, 133.3, 131.9, 131.7, 131.0, 129.2, 128.8, 126.3, 126.1, 124.7, 122.6, 36.3, 30.8, 22.0; **HRMS** (ESI) Calcd for $C_{19}H_{19}NO_2S$ $[M + Na]^+$ 348.1034, found 348.1031.



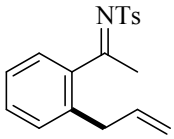
(*E*)-3-(2-(Hept-2-en-1-yl)phenyl)benzo[d]isothiazole 1,1-dioxide and (*Z*)- 3-(2-(hept-2-en-1-yl)phenyl)benzo[d]isothiazole 1,1-dioxide (i): Following the general procedure and the reaction was run in the presence of $[Cp^*RhCl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%) and $Cu(OAc)_2$ (20 mol%); Yellow oil (47% yield, eluent = petroleum ether/EtOAc (15:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): ***E* isomer**: δ 8.00 (d, *J* = 7.4 Hz, 1H), 7.77 (t, *J* = 7.5 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.54–7.45 (m, 4H), 7.39 (t, *J* = 7.4 Hz, 1H), 5.46–5.38 (m, 2H), 3.58 (d, *J* = 5.5 Hz, 2H), 1.97–1.93 (m, 2H), 1.26 (m, 4H), 0.88–0.84 (m, 2H). ***Z* isomer**: δ 8.00 (d, *J* = 7.4 Hz, 1H), 7.77 (t, *J* = 7.5 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 7.4 Hz, 1H), 7.51–7.43 (m, 3H), 7.39 (t, *J* = 7.4 Hz, 1H), 5.38–5.35 (m, 2H), 3.58 (d, *J* = 5.5 Hz, 2H), 1.97–1.93 (m, 2H), 1.26 (m, 4H), 0.88–0.84 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): ***E* isomer**: δ 172.2, 141.3, 140.2, 133.7, 133.4, 132.2, 131.8, 131.7, 130.7, 129.0, 128.9, 126.7, 126.4, 126.1, 122.7, 31.6, 31.1, 27.0, 22.3, 13.9. ***Z* isomer**: δ 172.2, 141.2, 140.2, 133.6, 133.3, 132.2, 131.8, 131.5, 131.0, 129.1, 128.8, 127.5, 126.3, 126.1, 122.6, 32.0, 31.2, 29.7, 22.1, 13.9; **HRMS** (ESI) Calcd for $C_{20}H_{21}NO_2S$ $[M + Na]^+$ 362.1191, found 362.1187.



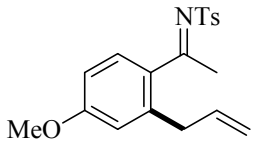
(*E*)-3-(2-(5-(Triisopropylsilyl)pent-2-en-4-yn-1-yl)phenyl)benzo[d]isothiazole 1,1-dioxide and (*Z*)- 3-(2-(5-(triisopropylsilyl)pent-2-en-4-yn-1-yl)phenyl)benzo[d]isothiazole 1,1-dioxide (3ai): Following the general procedure and using 20 mol% of $Cu(OAc)_2$ as an additive; Yellow solid (60% yield, eluent = petroleum ether/EtOAc (24:1)); Mp = 99–100 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): ***E* isomer**: δ 8.02–7.99 (m, 1H), 7.79–7.74 (m, 1H), 7.72–7.65 (m, 1H), 7.59–7.47 (m, 4H), 7.46–7.41 (m, 1H), 6.17–6.09 (m, 1H), 5.61 (d, *J* = 10.8 Hz, 1H), 3.86 (d, *J* = 7.2 Hz, 1H), 1.08–1.02 (m, 21H). ***Z* isomer**: δ 8.02–7.98 (m, 1H), 7.77 (dd, *J* = 15.0, 7.4 Hz, 1H), 7.72–7.65 (m, 1H), 7.59–7.47 (m, 4H), 7.46–7.41 (m, 1H), 6.17–6.09 (m, 1H), 5.45 (d, *J* = 16.2 Hz, 1H), 3.66 (d, *J* = 6.6 Hz, 1H), 1.08–1.02 (m, 21H); **^{13}C NMR** (150 MHz, $CDCl_3$): ***E* isomer**: δ 171.8, 141.6, 139.8, 139.1, 133.7, 133.4, 131.9, 131.6, 131.3, 129.0, 128.8, 126.5, 126.4, 122.8, 112.2, 103.4, 95.9, 34.1, 18.6, 11.3. ***Z* isomer**: δ 171.8, 142.0, 140.2, 139.1, 133.7, 133.4, 131.8, 131.6, 131.4, 129.2, 128.8, 126.6, 126.3, 122.7, 112.4, 105.1, 90.5, 36.3, 18.5, 11.2; **HRMS** (ESI) Calcd for $C_{27}H_{33}NO_2SSi$ $[M + Na]^+$ 486.1899, found 486.1895.



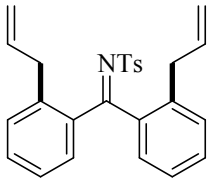
3-(2-(But-3-en-2-yl)phenyl)benzo[d]isothiazole 1,1-dioxide (3aj): Following the general procedure and the reaction was run in the presence of $[Cp^*RhCl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%) and $Cu(OAc)_2$ (20 mol%); Yellow solid (28% yield, eluent = petroleum ether/EtOAc (13:1)); Mp = 77–78 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.00 (d, *J* = 7.5 Hz, 1H), 7.77 (t, *J* = 7.5 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 7.9 Hz, 1H), 7.46–7.42 (m, 2H), 7.39 (t, *J* = 7.4 Hz, 1H), 5.93–5.86 (m, 1H), 4.96–4.94 (m, 2H), 3.96–3.88 (m, 1H), 1.37 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 172.3, 145.2, 141.9, 140.1, 133.7, 133.4, 132.0, 131.6, 128.7, 128.6, 128.2, 126.4, 126.1, 122.7, 114.3, 38.7, 20.8; **HRMS** (ESI) Calcd for $C_{17}H_{15}NO_2S$ $[M + Na]^+$ 320.0721, found 320.0715.



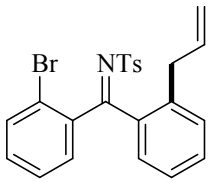
***N*-(1-(2-Allylphenyl)ethylidene)-4-methylbenzenesulfonamide (3rb)**: Following the general procedure and using 50 mol% of $Cu(OAc)_2$ as an additive; Yellow solid (32% yield, eluent = petroleum ether/EtOAc (79:1)); Mp = 79–80 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.2 Hz, 2H), 7.37–7.30 (m, 4H), 7.27–7.25 (m, 1H), 7.23 (d, *J* = 7.7 Hz, 1H), 5.80 (ddt, *J* = 16.8, 12.6, 6.6 Hz, 1H), 4.99–4.93 (m, 2H), 3.47 (d, *J* = 6.3 Hz, 2H), 2.91 (s, 3H), 2.43 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 184.2, 143.7, 139.7, 138.2, 137.7, 136.9, 130.9, 130.5, 129.4, 127.7, 127.2, 126.4, 116.2, 37.4, 25.5, 21.6; **HRMS** (ESI) Calcd for $C_{18}H_{19}NO_2S$ $[M + Na]^+$ 336.1034, found 336.1028.



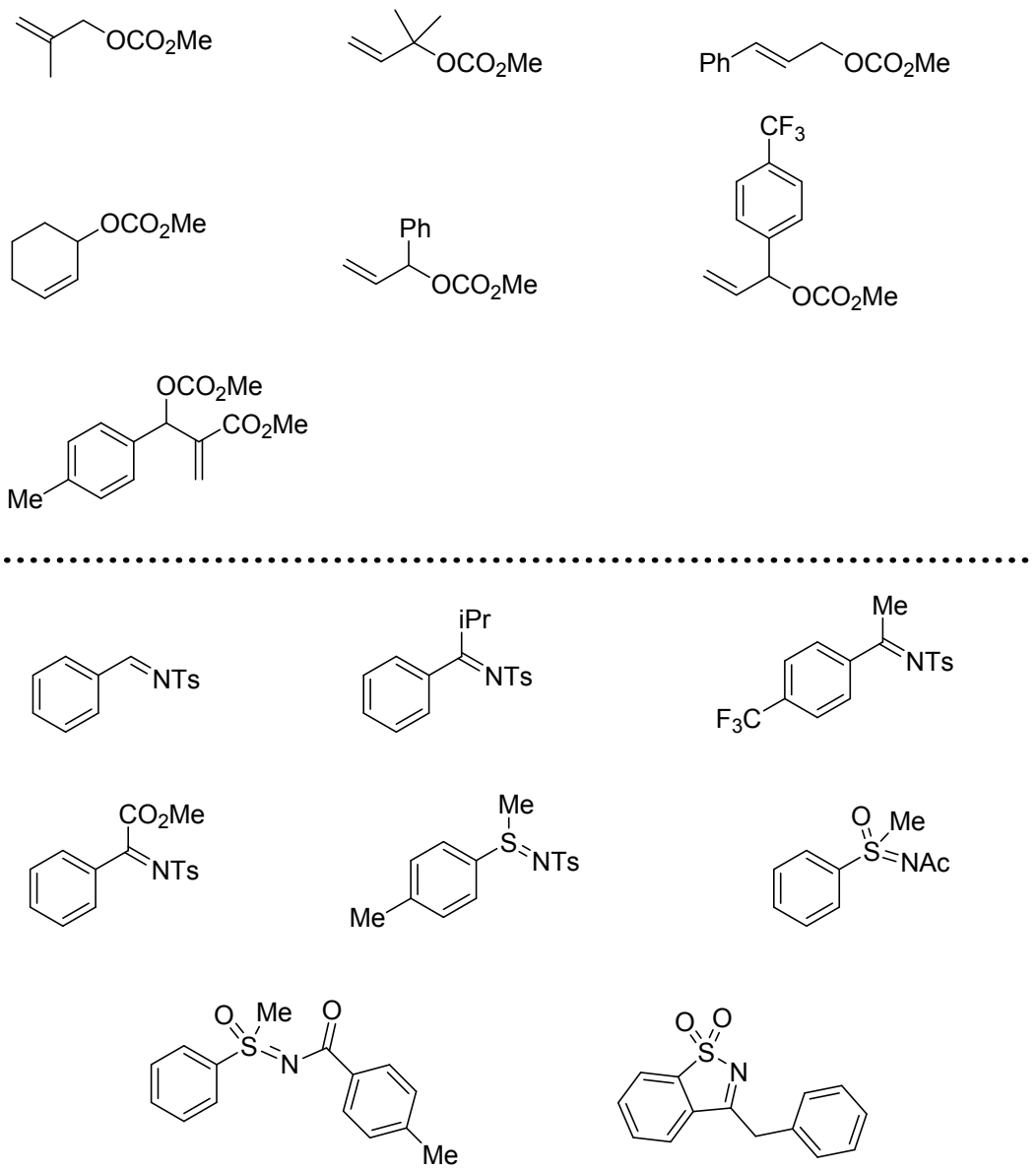
***N*-(1-(2-Allyl-4-methoxyphenyl)ethylidene)-4-methylbenzenesulfonamide (3sb)**: Following the general procedure and using 50 mol% of $Cu(OAc)_2$ as an additive; Yellow oil (50% yield, eluent = petroleum ether/EtOAc (15:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.1 Hz, 2H), 7.45 (d, *J* = 8.6 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 6.78–6.74 (m, 2H), 5.75 (ddt, *J* = 16.8, 12.6, 6.6 Hz, 1H), 4.96–4.90 (m, 2H), 3.81 (s, 3H), 3.49 (d, *J* = 6.3 Hz, 2H), 2.91 (s, 3H), 2.43 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 182.5, 161.6, 143.4, 141.5, 138.5, 136.9, 131.5, 130.8, 129.4, 127.1, 116.7, 116.0, 111.4, 55.3, 38.1, 24.9, 21.5; **HRMS** (ESI) Calcd for $C_{19}H_{21}NO_3S$ $[M + Na]^+$ 366.1140, found 366.1137.



***N*-(Bis(2-allylphenyl)methylene)-4-methylbenzenesulfonamide (3tb)**: Following the general procedure and using 20 mol% of $Cu(OAc)_2$ as an additive in the presence of 6 equiv of **2b**; White solid (80% yield, eluent = petroleum ether/EtOAc (39:1)); Mp = 80–81 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.1 Hz, 2H), 7.46–7.31 (m, 4H), 7.28 (d, *J* = 7.8 Hz, 4H), 7.14–7.04 (m, 2H), 5.78–5.67 (m, 2H), 4.93–4.83 (m, 4H), 3.60 (s, 2H), 3.10 (d, *J* = 75.2 Hz, 2H), 2.43 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 180.1, 143.5, 141.4, 138.1, 137.1, 137.0, 136.8, 136.2, 135.8, 133.2, 132.1, 131.7, 130.2, 129.4, 129.3, 128.7, 127.5, 126.2, 125.7, 116.6, 115.6, 38.3, 37.7, 21.6; **HRMS** (ESI) Calcd for $C_{26}H_{25}NO_2S$ $[M + Na]^+$ 438.1504, found 438.1501.



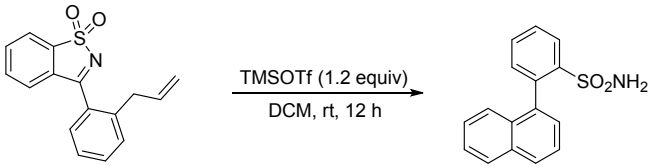
***N*-((2-Allylphenyl)(2-bromophenyl)methylene)-4-methylbenzenesulfonamide (3ub)**: Following the general procedure; Yellow oil (67% yield, eluent = petroleum ether/EtOAc (39:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.84 (d, *J* = 8.2 Hz, 2H), 7.62–7.53 (m, 2H), 7.49 (t, *J* = 7.3 Hz, 1H), 7.42–7.34 (m, 2H), 7.29 (d, *J* = 7.8 Hz, 3H), 7.13 (t, *J* = 7.3 Hz, 1H), 7.07 (d, *J* = 7.8 Hz, 1H), k9 (m, 1H), 4.92–4.86 (m, 2H), 3.61–3.56 (m, 2H), 2.43 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 176.8 143.8, 142.0, 138.3, 137.6, 137.1, 135.2, 132.7, 132.3, 132.1, 131.6, 131.2, 130.1, 129.4, 127.6, 126.9, 126.0, 120.1, 115.6, 38.3, 21.6; **HRMS** (ESI) Calcd for $C_{23}H_{20}BrNO_2S$ $[M + Na]^+$ 476.0296, found 476.0295.



Scheme S1. Unreactive substrates with respect to the allyl carbonates and aromatics.

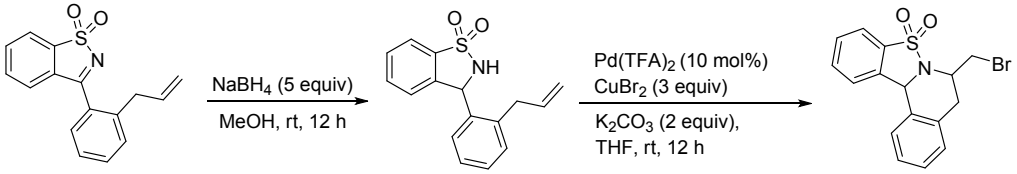
We tried to explore the substrate scope with respect to the allyl carbonates and aromatics, however, no desired products were obtained after considerable experimentation.

Synthetic Transformations



3ab **4a**

To a solutionof **3ab** (0.035mmol, 10 mg) in 1 ml of dry dichloromethane was added trimethylsilyl trifluoromethanesulfonate (1.2 equiv, 0.042mmol, 8 μl). The mixture was stirred at room temperature for 12h and then concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel to afford the product **4a**. Yellow solid (90% yield, eluent = petroleum ether/EtOAc (17:3)); Mp = 131-132 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.26 (d, *J* = 7.9 Hz, 1H), 7.96–7.90 (m, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.63–7.57 (m, 3H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.42–7.39 (m, 2H), 7.35 (d, *J* = 8.4 Hz, 1H), 3.96 (s, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 141.6, 138.1, 135.5, 133.4, 133.0, 132.1, 131.8, 129.0, 128.5, 128.5, 128.2, 127.9, 126.7, 126.2, 125.6, 125.1; **HRMS** (ESI) Calcd for $C_{16}H_{13}NO_2S$ $[M + Na]^+$ 306.0565, found 306.0560.



3ab **4f** **4b**

$NaBH_4$ (5 equiv) was added portionwise to a solution of **3ab** (0.035 mmol, 10 mg) in MeOH (1 mL) at 0 °C. The resulting suspension was stirred for 12h at room temperature and then concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel to afford **4f** in quantitative yield. Yellow solid (eluent = petroleum ether/EtOAc (13:1)); Mp = 152-153 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.85–7.84 (m, 1H), 7.57–7.55 (m, 2H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.26 (d, *J* = 7.8 Hz, 1H), 7.22 (t, *J* = 7.8 Hz, 1H), 7.10–7.07 (m, 2H), 6.09–6.03 (m, 1H), 6.01 (d, *J* = 4.2 Hz, 1H), 5.14 (d, *J* = 10.2 Hz, 1H), 5.00 (d, *J* = 16.8 Hz, 1H), 4.78 (s, 1H), 3.63–3.55 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 140.3, 138.4, 137.2, 136.6, 135.7, 133.3, 130.8, 129.4, 129.3, 128.4, 127.8, 125.4, 121.2, 116.6, 57.4, 37.0; **HRMS** (ESI) Calcd for $C_{16}H_{14}BrNO_2S$ $[M + Na]^+$ 308.0721, found 308.0720.

To a solution of the **4f** (0.035 mmol, 10 mg) in dry tetrahydrofuran (1 mL) was added K_2CO_3 (2 equiv, 0.07 mmol, 9.6 mg), $CuBr_2$ (3 equiv, 0.1 mmol, 22.3 mg) and $Pd(TFA)_2$ (10 mol%, 1.5 mg) at 0 °C. Then the mixture was stirred at rt for 12 h. Volatile materials were removed and the residue was purified by flash chromatography on silica gel to afford the final product **4b**. Yellow solid (79% yield, eluent = petroleum ether/EtOAc (13:1)); Mp = 159-160 °C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.87 (d, *J* = 7.8 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.62–7.58 (m, 2H), 7.33–7.27 (m, 3H), 7.19 (d, *J* = 7.5 Hz, 1H), 5.71 (s, 1H), 4.34–4.26 (m, 1H), 3.72 (dd, *J* = 10.5, 4.1 Hz, 1H), 3.62–3.59 (m, 1H), 3.21 (dfd, *J* = 15.3, 4.9 Hz, 1H), 3.07 (dd, *J* = 15.3, 7.7 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 135.7, 135.4, 133.6, 133.3, 132.7, 129.6, 128.9, 128.6, 127.2, 125.7, 124.8, 121.8, 58.7, 51.0, 35.4, 32.0; **HRMS** (ESI) Calcd for $C_{16}H_{14}BrNO_2S$ $[M + Na]^+$ 385.9826, found 385.9828.

Deuteration and Competition Experiments

(A) H-D exchange experiment (Scheme S2a)

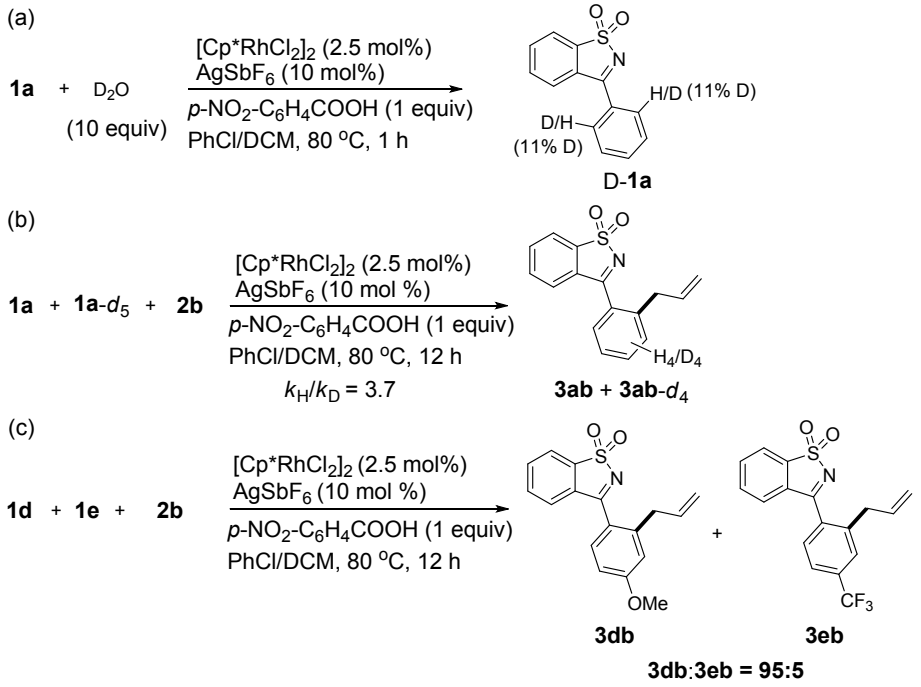
The reaction between **1a** (0.2 mmol) and D_2O (10 equiv) was performed in the presence of $[Cp^*RhCl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), and 4-nitrobenzoic acid (1 equiv) with PhCl/DCM as the solvent at 80 °C for 1 h. After standard workup and purification, a mixture of **1a** and D-**1a** was obtained. ^{1}H NMR analysis of the mixture showed 11% D was incorporated into the two *ortho* positions of the ketimine aryl ring (see the attached spectrum).

(B) Intermolecular Competition (Scheme S2b)

A mixture of **1a** and **1a**-d_5 (0.2 mmol each) was subjected to the standard reaction conditions for 12 h. After standard workup and purification, a mixture of **3ab** and **3ab**-d_4 was obtained**.** ^{1}H NMR analysis of the mixture showed a large value of $k_H/k_D = 3.7$ (see the attached spectrum).

(C) Intermolecular Competition (Scheme S2c)

A mixture of **1d** and **1e** (0.2 mmol each) was subjected to the standard reaction conditions for 12 h. GC results showed a ratio of 95:5 of **3db** and **3eb**.



Scheme S2. Deuteration and competition experiments.

The result of H/D exchange experiment between **1a** and 10 equiv of deuterium oxide showed that 11% D was introduced into the two ortho positions of the ketimine aryl ring (Scheme S2a). An intermolecular competition reaction between **1a** and **1a**-*d*5 was performed, giving a primary kinetic isotope effect of 3.7 (Scheme S2b). These results suggested that the reaction involved a Rh-mediated reversible C-H activation process, which was consistent with our previous observation in the Rh-catalysed aryl C-H olefination. Furthermore, an intermolecular competition reaction of **1d** and **1e** with **2b** was also carried out (Scheme S2c). GC analysis of the resulting mixture revealed that **3db** was the major product, indicating that the more electron-rich ketimine is significantly kinetically favored.

Computational Studies

Computational method

All calculations were performed with the Gaussian 09 program suite.[3] Density functional theory (DFT) method was used, employing B3LYP hybrid functional.[4] Geometry optimization was done using a combined basis set where LANL2DZ[5] was used for Rh atom and 6-31+G(d) for the rest. Frequency calculations were carried out at the same level of theory for thermochemical analysis and to confirm that the number of imaginary frequencies of intermediate and transition states was 0 and 1, respectively. For transition states, intrinsic reaction coordinate analysis (IRC)[6] was done to verify that they connect the right reactants and products on the potential energy surface.

To take solvent effects into account, solution-phase single-point calculations were performed on the gas-phase geometries.[7] The M06-L functional was used, and this method has been frequently employed in describing the energetics of Rh-catalysed reactions.[8]In the solution-phase single-point calculations, the Lanl2DZ ECP with an additional polarization function Rh(ζ(f)=1.350) was used for the Rh atom,[9] and 6-311++G(d,p) was used for C, H, O, N, and S atoms. The self-consistent reaction field (SCRF) with CPCM solvation model was used for all these calculations.[10] DMC was used as solvent, because this reaction also can be carried out in the DMC with 40% yield. Solution-phase single-point energies corrected by the gas-phase Gibbs free energy corrections were used to describe all the reaction energetics. All of these energies correspond to the reference state of 1 mol L^{-1}, 298 K.

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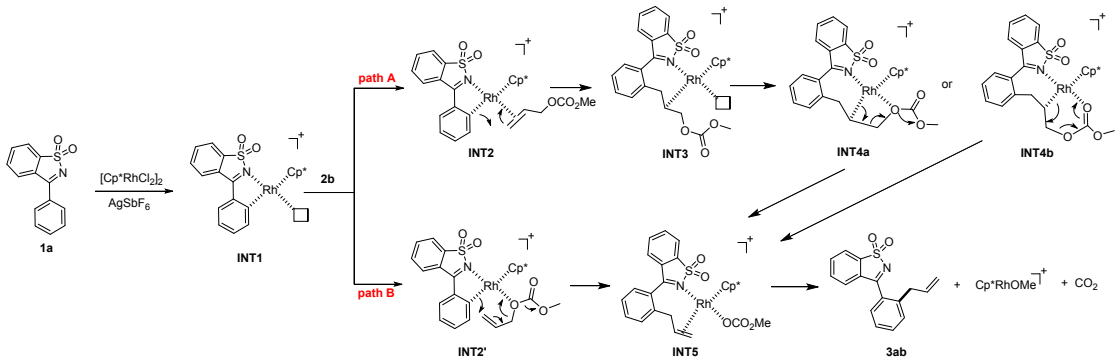
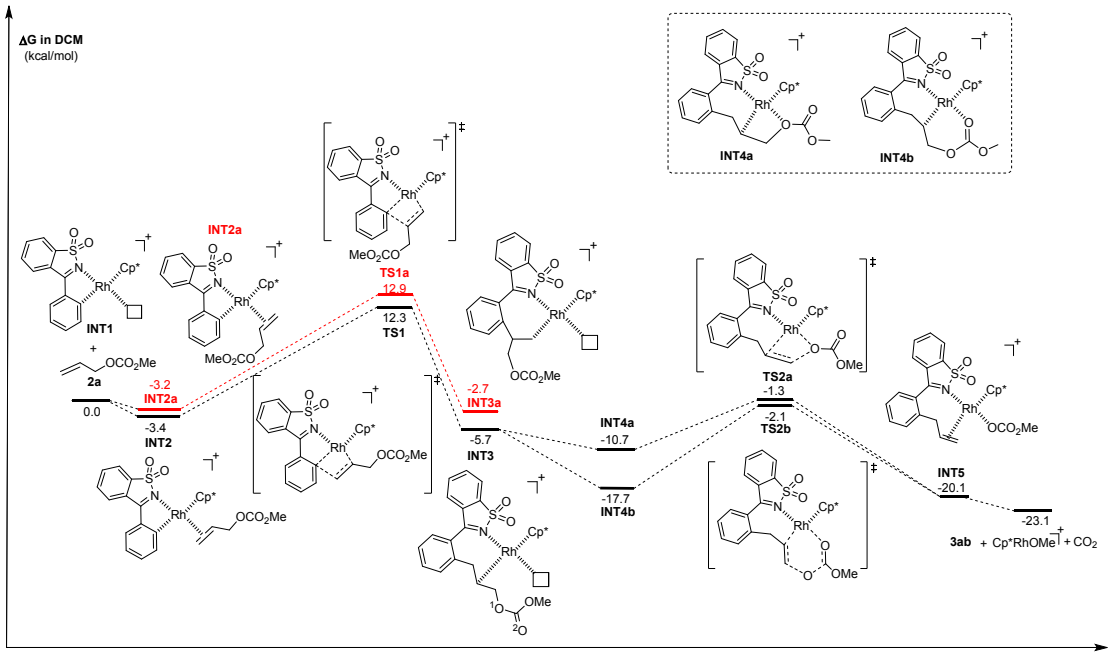
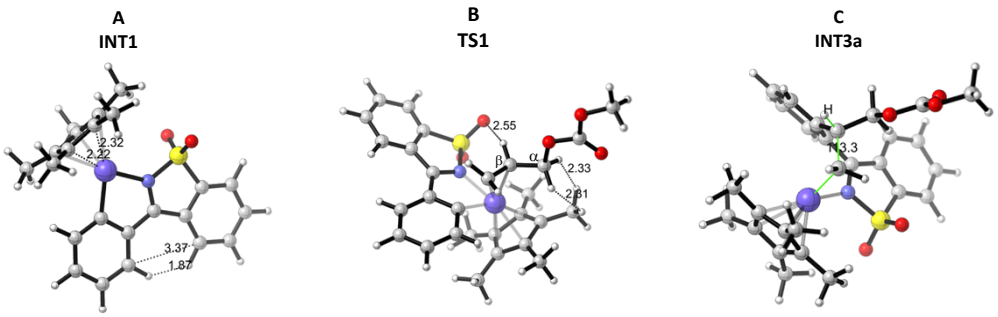
Computational Results and Discuss



Scheme S3. Two Plausible Pathways.



Scheme S4. Energy profile of olefin insertion and allylarene formation with relative Gibbs free energies [kcal/mol].



Scheme S5. Optimized structure of intermediates **INT1** (A)**, TS1** (B), and **INT3a** (C). The bond distances of the optimized structures are in angstroms.

On the basis of the literatures and our experiments, a coordinatively unsaturated cationic species (**INT1**) was postulated to be formed by the reaction of **1a** and $[Cp^*RhCl_2]_2$ through C-H cleavage. (Scheme S3).

It was interesting to note that the bond length between the rhodium metal center and carbon atom in a pentamethylcyclopentadienyl (Cp*) ligand is not equivalent depending on the relative position to 3-phenylbenzo[d]isothiazole 1,1-dioxide (**1a**). For example, the Rh−C_a distance (2.32 Å) was calculated to be longer than that of Rh−C_b (2.22 Å), presumably due to the discrepancy in the degree of trans-influence between the thiazole and phenyl moieties of **1a** in **INT1** (Scheme S5). As a result, this mode of metal−ligand bonding was revealed to provide more open space around the thiazole than the phenyl side. Such perturbation results in the directional preference in the coordination of Rh metal with an allyl methyl carbonate **2b** to form **INT2,** which showed a 0.2 kcal/mol lower energy than **INT2a** (Scheme S4). Moreover, the proposed intermediate **INT3a** generated through **TS1a** had a higher energy value (-2.7 kcal/mol) than that of **INT2a** (-3.2 kcal/mol). The energy barrier for olefin insertion through **TS1a** (16.2 kcal/mol) was higher than **TS1** (15.7 kcal/mol). As reported by Chang group,[11] these results indicated that the **INT1** may prefer to coordinate with **2b** as **INT2**. While, as shown in Scheme S5 (**INT3a**), the dihedral angle between *β*-H, α-C, β-C, and Rh(III) atoms was 113.3. The coordinative model of **INT3a** may prohibit the hydrogen atom from approaching a coplanar configuration to occur *β*-hydride elimination. Indeed, we didn't observe olefin by-product derived from *β*-hydride elimination during the reaction even though adding $Cu(OAc)_2$ as an oxidant.

DFT calculations allowed us to validate our proposed stepwise olefin insertion and the allyl formation process from **INT2** to **INT5** through the path **A** as shown in Scheme S3.[12] In addition, pathway B involving a concerted process to directly produce **INT5** was also considered as shown in Scheme S3. However, we failed to identify any reasonable TS in this mechanism. Thus, our calculated results indicated that the reaction might prefer to occur via the olefin insertion mechanism. The coordinatively saturated species **INT5** can release one CO_2 to give final product **3a** and unsaturated species $[Cp^*RhOMe]^+$ that could react with **1a** to generate **INT1** to fulfill the catalytic cycle. Although the reaction of Rh-catalysed decarboxylation is important for catalytic cycle, the processes of decarboxylation of **INT5** and formation of **INT1** were not included because the current DFT calculations were only focused on the allylation process. Importantly, the process of releasing CO_2 from HOC(O)OMe has been calculated.[13]

In addition, a pathway involving a π-allyl rhodium (V) complex generated by oxidative addition of allyl carbonate to a Rh(III) species seems to be less likely owing to the excellent *γ*-selectivity of reactions involving the branched allyl carbonates **1f-1j**.

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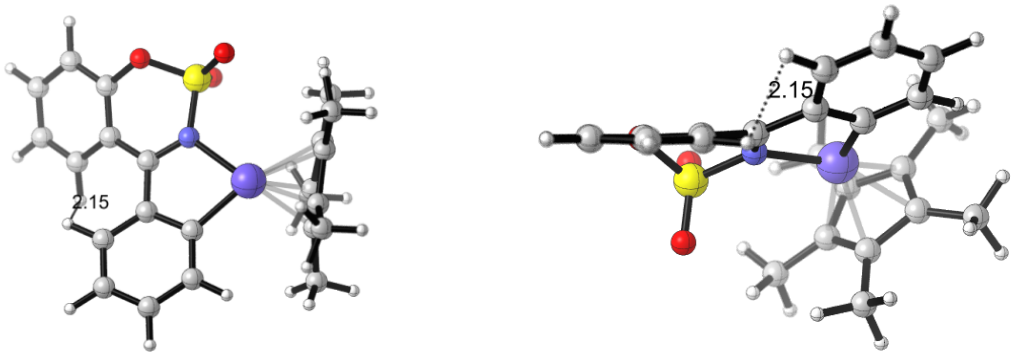
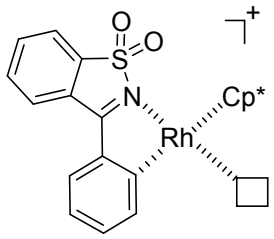
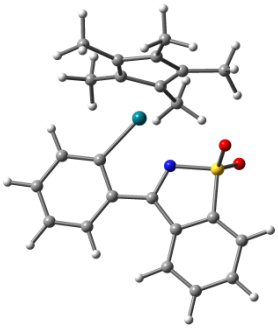


Scheme S6. Optimized structure of intermediate **1p-INT1**. The bond distances of the optimized structures are in angstroms.

INT1





Thermal correction to Gibbs Free Energy= 0.347012 A.U.

E(sov) = -1603.22528394 A.U.

Standard orientation:

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4	6	0	3.176433	0.399182	-0.054059
5	6	0	3.347108	-0.995727	-0.041341
6	6	0	4.578730	-1.625664	-0.046355
7	6	0	1.735889	0.761837	-0.047435
8	7	0	0.920016	-0.276327	-0.048027
9	16	0	1.748306	-1.791218	0.001085
10	8	0	1.448033	-2.527545	-1.225564
11	8	0	1.488066	-2.408530	1.302831
12	6	0	1.056222	2.055856	-0.038997
13	6	0	-0.370910	1.970071	-0.048503
14	45	0	-1.135036	0.074083	-0.183502
15	6	0	1.697213	3.306959	-0.033380
16	6	0	0.943815	4.481566	-0.039733
17	6	0	-0.449144	4.409097	-0.060645
18	6	0	-1.094846	3.161637	-0.064997
19	1	0	6.704014	-1.260295	-0.077862
20	1	0	6.475963	1.206632	-0.107632
21	1	0	4.278138	2.276602	-0.095967
22	1	0	4.661649	-2.708021	-0.033696
23	1	0	2.775502	3.389182	-0.026202
24	1	0	1.444803	5.444733	-0.031575
25	1	0	-1.039514	5.321778	-0.069054
26	1	0	-2.179950	3.144562	-0.080507
27	6	0	-2.240368	-1.929958	0.311928

28	6	0	-2.748041	-1.428643	-0.896675
29	6	0	-3.294375	-0.071100	-0.660552
30	6	0	-3.142274	0.231662	0.716069
31	6	0	-2.375681	-0.867437	1.307754
32	6	0	-1.684716	-3.298332	0.570831
33	6	0	-2.771647	-2.117864	-2.223048
34	6	0	-4.035868	0.724706	-1.690199
35	6	0	-3.737946	1.373439	1.480790
36	6	0	-2.004431	-0.990447	2.748873
37	1	0	-1.286218	-3.754946	-0.338368
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41	1	0	-2.066254	-2.950755	-2.262516
42	1	0	-3.777303	-2.515904	-2.420395
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47	1	0	-4.634341	1.025158	2.012001
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49	1	0	-2.802669	-1.524280	3.286162
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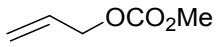
Allyl methyl carbonate (2a)



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Standard orientation:

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5	6	0	-1.001901	-0.609850	-0.091590
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7	8	0	-1.106998	0.690864	0.268676
8	6	0	-2.392941	1.292421	0.019802

9	1	0	3.773092	1.076648	-1.175818
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12	1	0	1.924915	-1.065364	1.228396
13	1	0	0.808147	0.272869	1.601589
14	1	0	-2.297443	2.322670	0.364064
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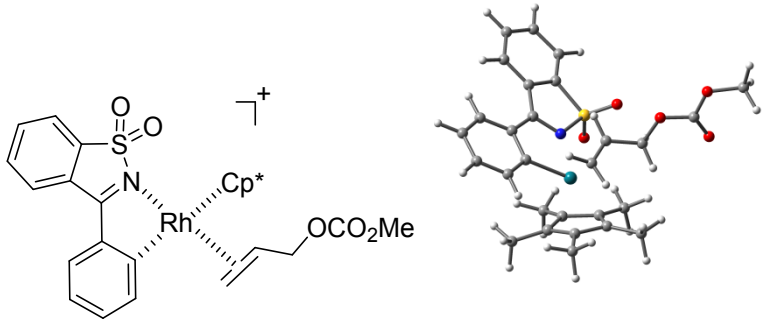
INT2



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14	6	0	-1.629340	-1.126548	1.367366
15	6	0	-3.592676	0.119099	2.167734
16	6	0	-3.901854	-0.912889	3.043312

17	6	0	-3.068004	-2.036087	3.109245
18	6	0	-1.945389	-2.135766	2.281690
19	6	0	1.233425	-1.165002	1.948613
20	6	0	1.431182	0.054113	1.334369
21	6	0	2.679490	0.395169	0.561239
22	8	0	3.458743	1.228691	1.448625
23	6	0	4.659760	1.595862	0.950529
24	8	0	5.108282	1.235639	-0.119206
25	8	0	5.249326	2.398482	1.834280
26	6	0	6.559230	2.879865	1.459618
27	6	0	-0.687666	-2.116526	-1.945408
28	6	0	0.745426	-1.840803	-2.118373
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48	1	0	3.257422	-0.495781	0.310982
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53	1	0	-1.831058	-2.316917	-3.730176
54	1	0	-1.583530	-0.634582	-3.235046
55	1	0	-2.750619	-1.654339	-2.374575
56	1	0	1.503482	-1.657938	-4.108111
57	1	0	2.325182	-0.617074	-2.940305
58	1	0	0.710446	-0.191112	-3.517990
59	1	0	3.262569	-2.894676	-0.024819
60	1	0	3.475962	-1.957474	-1.515842

61	1	0	3.209082	-3.701474	-1.586490
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63	1	0	-0.011683	-4.651124	1.303473
64	1	0	1.697956	-4.206736	1.195201
65	1	0	-2.174017	-4.740089	-1.301151
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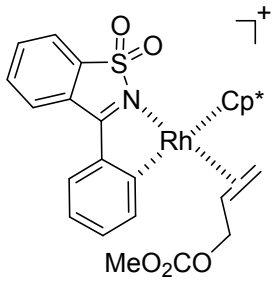
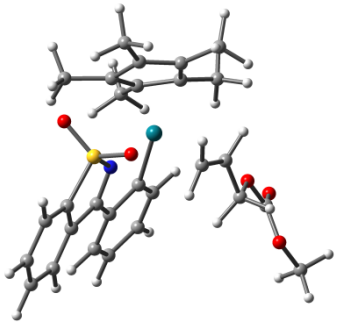
INT2a





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6	6	0	-3.953255	1.118959	-0.550859
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12	8	0	-2.902832	-0.695119	-2.265047
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14	6	0	0.557786	0.869650	0.927965
15	6	0	-0.442990	2.966369	1.754826
16	6	0	0.759529	3.314695	2.353927
17	6	0	1.863595	2.461133	2.230526
18	6	0	1.761170	1.256751	1.526728

19	6	0	-0.340579	-2.514432	1.451573
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21	6	0	0.867697	-3.171154	-0.413360
22	6	0	1.774759	-2.474476	0.515348
23	6	0	1.032320	-2.173585	1.703434
24	6	0	-1.454795	-2.445260	2.450929
25	6	0	-1.603386	-3.951639	-0.373608
26	6	0	1.284280	-3.830204	-1.693809
27	6	0	3.269210	-2.437408	0.391556
28	6	0	1.595639	-1.715197	3.013788
29	6	0	0.279431	-0.173964	-2.214114
30	6	0	1.614572	-0.203681	-1.887018
31	6	0	2.467404	1.023001	-1.747627
32	8	0	3.576465	0.678862	-0.896088
33	6	0	4.605289	1.536921	-0.721140
34	8	0	5.482647	1.307557	0.076876
35	8	0	4.511037	2.613873	-1.514403
36	6	0	5.596935	3.566748	-1.405328
37	1	0	-6.656073	3.099621	-0.885082
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39	1	0	-2.862826	3.985164	0.914167
40	1	0	-5.888015	0.783570	-1.450389
41	1	0	-1.293647	3.622783	1.879026
42	1	0	0.839217	4.239587	2.917045
43	1	0	2.810656	2.728944	2.692830
44	1	0	2.641515	0.630296	1.445846
45	1	0	-1.493768	-3.384497	3.021207
46	1	0	-2.425093	-2.308440	1.968764
47	1	0	-1.305857	-1.632394	3.166864
48	1	0	-1.566623	-4.994525	-0.027699
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50	1	0	-2.546076	-3.519943	-0.035650
51	1	0	1.653993	-4.843824	-1.484264
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56	1	0	3.599988	-2.419110	-0.649236
57	1	0	1.784799	-2.592961	3.647562
58	1	0	0.908321	-1.059861	3.554533
59	1	0	2.545282	-1.189452	2.894874
60	1	0	-0.208022	-1.013784	-2.697567
61	1	0	-0.256028	0.769905	-2.260243
62	1	0	2.180124	-1.115088	-2.055708

63	1	0	2.844383	1.299893	-2.740007
64	1	0	1.921137	1.874905	-1.334504
65	1	0	5.349750	4.358596	-2.111554
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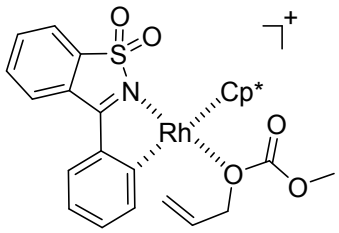
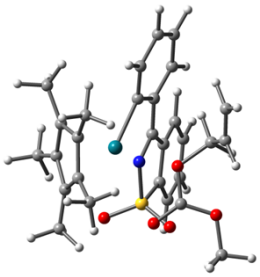
67	1	0	6.540730	3.086531	-1.671512

INT2'



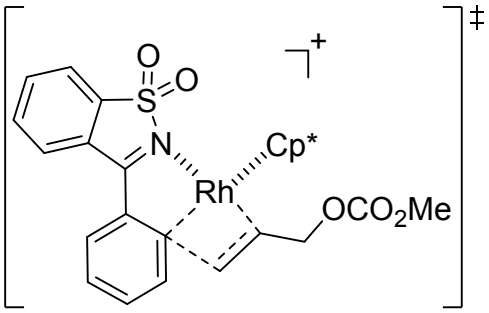


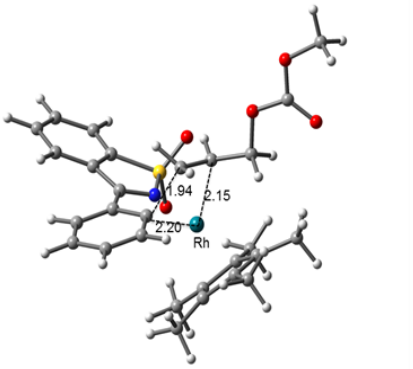
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.948955	0.271510	0.527720
2	6	0	-5.998788	-0.293338	0.115911
3	6	0	-5.748267	1.026492	-0.272822
4	6	0	-4.441405	1.511980	-0.399878
5	6	0	-3.364563	0.654587	-0.139329
6	6	0	-3.654093	-0.652362	0.275011
7	6	0	-4.935591	-1.158560	0.407889
8	6	0	-1.894734	0.892375	-0.164309
9	7	0	-1.162751	-0.114817	0.270153
10	16	0	-2.127994	-1.505436	0.638927
11	8	0	-2.012281	-1.801180	2.067997
12	8	0	-1.843667	-2.546298	-0.348261
13	6	0	-1.135288	2.056282	-0.602099
14	6	0	0.269129	1.968252	-0.372915
15	6	0	-1.680652	3.159362	-1.291889
16	6	0	-0.854677	4.185903	-1.739448
17	6	0	0.523815	4.109326	-1.515278
18	6	0	1.074903	3.008162	-0.846625
19	6	0	1.145591	0.313622	2.690442
20	6	0	1.693096	-1.016032	2.398394
21	6	0	2.805044	-0.832749	1.567314
22	6	0	2.989683	0.608566	1.322681
23	6	0	2.037352	1.311712	2.123566
24	6	0	0.033139	0.585019	3.654188

25	6	0	1.182828	-2.315558	2.946211
26	6	0	3.724073	-1.881987	1.031789
27	6	0	4.177950	1.190820	0.616050
28	6	0	2.025037	2.775087	2.444910
29	6	0	2.975388	0.714915	-4.282444
30	6	0	2.214457	-0.311955	-3.890933
31	6	0	0.991699	-0.142542	-3.043206
32	8	0	1.145346	-0.804094	-1.727545
33	6	0	1.015880	-2.158892	-1.622965
34	8	0	1.269423	-2.724003	-0.586055
35	8	0	0.598832	-2.718933	-2.754660
36	6	0	0.350222	-4.148707	-2.690149
37	1	0	-7.021153	-0.647664	0.206884
38	1	0	-6.580962	1.693485	-0.474684
39	1	0	-4.295420	2.548382	-0.672165
40	1	0	-5.110755	-2.179358	0.733384
41	1	0	-2.737224	3.211163	-1.518735
42	1	0	-1.279590	5.031876	-2.271073
43	1	0	1.174712	4.905229	-1.869315
44	1	0	2.152119	2.969494	-0.713905
45	1	0	0.424505	0.540773	4.680947
46	1	0	-0.762110	-0.159036	3.568559
47	1	0	-0.399407	1.578460	3.508508
48	1	0	0.107465	-2.285639	3.131076
49	1	0	1.683383	-2.544878	3.897459
50	1	0	1.376949	-3.140462	2.255977
51	1	0	4.669529	-1.853028	1.592860
52	1	0	3.967389	-1.707720	-0.020779
53	1	0	3.300079	-2.882321	1.119819
54	1	0	5.071226	1.114670	1.252003
55	1	0	4.037842	2.249030	0.380113
56	1	0	4.395588	0.660665	-0.316014
57	1	0	2.591344	2.940908	3.372064
58	1	0	1.012962	3.156139	2.602613
59	1	0	2.493198	3.376028	1.662521
60	1	0	3.834973	0.571190	-4.931388
61	1	0	2.755068	1.738485	-3.984487
62	1	0	2.446469	-1.324234	-4.217142
63	1	0	0.825753	0.902268	-2.784876
64	1	0	0.097431	-0.555034	-3.514617
65	1	0	0.013251	-4.418075	-3.690317
66	1	0	1.272767	-4.673258	-2.433654
67	1	0	-0.421796	-4.347434	-1.945141

TS1



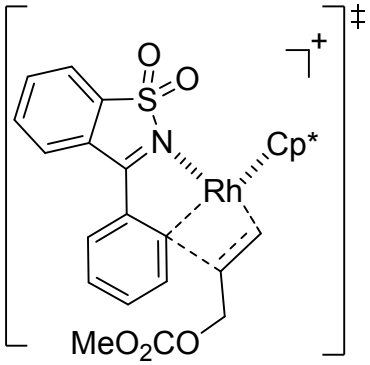


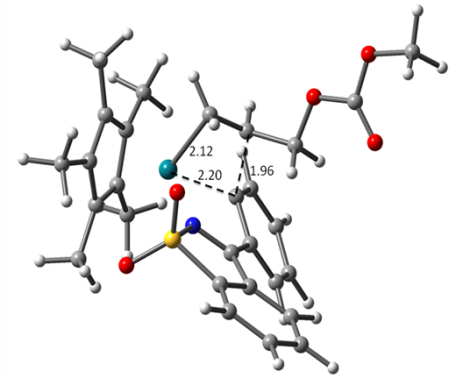
Imaginary frequency: -315.75
Thermal correction to Gibbs Free Energy= 0.470473 A.U.
E(sov) = -2024.30335553 A.U.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.333903	-0.861712	-0.166943
2	6	0	-5.250397	3.327011	-0.302100
3	6	0	-5.262528	2.801116	0.994355
4	6	0	-4.319586	1.848860	1.399828
5	6	0	-3.360087	1.412259	0.479304
6	6	0	-3.357860	1.977910	-0.802878
7	6	0	-4.275587	2.923530	-1.226571
8	6	0	-2.238701	0.456225	0.645426
9	7	0	-1.433286	0.348455	-0.388872
10	16	0	-1.964623	1.334353	-1.723624
11	8	0	-2.391663	0.437103	-2.798264
12	8	0	-0.957166	2.360596	-1.983787
13	6	0	-1.876669	-0.348498	1.801457
14	6	0	-0.509379	-0.762974	1.858433
15	6	0	-2.797372	-0.794281	2.766600
16	6	0	-2.383653	-1.633952	3.798296
17	6	0	-1.041283	-2.026332	3.875223
18	6	0	-0.118424	-1.589440	2.923204
19	6	0	0.823970	0.628554	1.625343
20	6	0	1.297550	0.996488	0.306103
21	6	0	2.780455	1.022783	0.068262
22	8	0	3.285196	2.217164	0.720595
23	6	0	4.602404	2.442457	0.526454

24	8	0	5.347791	1.714778	-0.099826
25	8	0	4.927824	3.579991	1.137609
26	6	0	6.313057	3.975350	1.020967
27	6	0	-0.275604	-2.639208	-1.473152
28	6	0	0.699021	-1.792361	-2.185914
29	6	0	1.940311	-1.880920	-1.494775
30	6	0	1.715844	-2.643242	-0.288243
31	6	0	0.364172	-3.188255	-0.339754
32	6	0	-1.654828	-2.943810	-1.973856
33	6	0	0.487992	-1.192864	-3.544190
34	6	0	3.270076	-1.426461	-2.016943
35	6	0	2.782040	-3.077410	0.674216
36	6	0	-0.194241	-4.207280	0.605410
37	1	0	-5.991062	4.065640	-0.593334
38	1	0	-6.009826	3.142629	1.704164
39	1	0	-4.332102	1.486038	2.420586
40	1	0	-4.239600	3.342682	-2.227341
41	1	0	-3.846263	-0.531909	2.684559
42	1	0	-3.100389	-1.983507	4.534872
43	1	0	-0.711646	-2.672899	4.684329
44	1	0	0.924100	-1.879008	3.024339
45	1	0	1.579826	0.246360	2.307326
46	1	0	0.149037	1.333116	2.103776
47	1	0	0.766569	1.803195	-0.193123
48	1	0	3.285922	0.153840	0.499612
49	1	0	3.024768	1.083814	-0.993163
50	1	0	6.385315	4.911344	1.573709
51	1	0	6.961494	3.213545	1.460112
52	1	0	6.574802	4.123897	-0.029290
53	1	0	-1.600903	-3.714325	-2.755918
54	1	0	-2.129032	-2.063224	-2.414279
55	1	0	-2.303543	-3.326226	-1.181117
56	1	0	0.692849	-1.949893	-4.315220
57	1	0	1.159568	-0.349021	-3.724320
58	1	0	-0.536342	-0.843125	-3.684628
59	1	0	3.993008	-1.212529	-1.227082
60	1	0	3.188364	-0.543125	-2.654984
61	1	0	3.694723	-2.231214	-2.634103
62	1	0	3.280302	-3.981372	0.295927
63	1	0	2.371733	-3.325192	1.657076
64	1	0	3.555391	-2.315278	0.807089
65	1	0	0.179437	-5.205658	0.339441
66	1	0	-1.285928	-4.243835	0.569161
67	1	0	0.100710	-4.015117	1.640711

TS1a





Imaginary frequency: 318.015

Thermal correction to Gibbs Free Energy= 0.469757

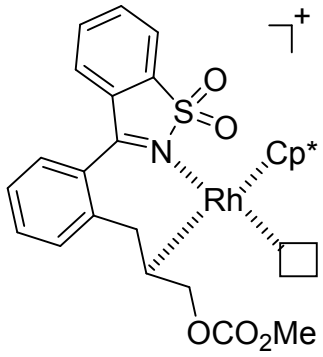
E(sov) = -2024.301717 A.U.

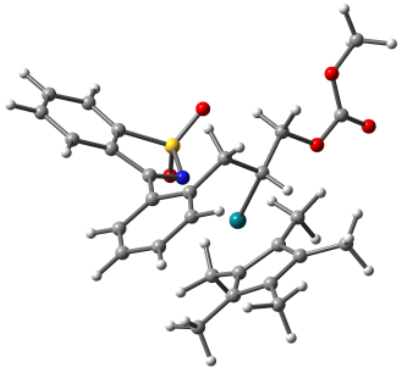
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.093974	0.882062	-0.171647
2	6	0	5.715118	-2.779852	-1.358673
3	6	0	5.654965	-2.699509	0.036774
4	6	0	4.646278	-1.970686	0.678288
5	6	0	3.694468	-1.304382	-0.101289
6	6	0	3.763896	-1.428397	-1.495555
7	6	0	4.747940	-2.146198	-2.153104
8	6	0	2.517655	-0.501703	0.306463
9	7	0	1.736454	-0.105142	-0.672400
10	16	0	2.355882	-0.599010	-2.226456
11	8	0	2.746309	0.609581	-2.953204
12	8	0	1.419185	-1.545993	-2.827951
13	6	0	2.082527	-0.108815	1.639941
14	6	0	0.695713	0.216343	1.769208
15	6	0	2.967331	0.085040	2.715546
16	6	0	2.500770	0.591113	3.926559
17	6	0	1.141641	0.897172	4.072549
18	6	0	0.254751	0.699929	3.013408
19	6	0	-0.993286	-1.030282	-0.263823
20	6	0	-0.633970	-1.077439	1.139873
21	6	0	0.089475	-2.332227	1.626909
22	8	0	-0.890927	-3.379823	1.528735
23	6	0	-0.413756	-4.621677	1.781291

24	8	0	0.743047	-4.878108	2.045771
25	8	0	-1.424096	-5.480143	1.683344
26	6	0	-1.089275	-6.867662	1.915427
27	6	0	0.273457	3.005260	-0.989930
28	6	0	-0.607807	2.231591	-1.886807
29	6	0	-1.817590	1.966466	-1.183792
30	6	0	-1.654383	2.449680	0.168406
31	6	0	-0.385865	3.166175	0.248375
32	6	0	1.583315	3.602040	-1.406955
33	6	0	-0.365624	2.007614	-3.349811
34	6	0	-3.064214	1.360680	-1.756620
35	6	0	-2.729911	2.479789	1.214363
36	6	0	0.081340	3.968642	1.424965
37	1	0	6.506375	-3.351801	-1.833853
38	1	0	6.395968	-3.219637	0.636055
39	1	0	4.601076	-1.958067	1.760741
40	1	0	4.768091	-2.224316	-3.235702
41	1	0	4.028132	-0.102912	2.592429
42	1	0	3.190155	0.750456	4.749966
43	1	0	0.772046	1.285645	5.017925
44	1	0	-0.800434	0.911329	3.165166
45	1	0	-0.482718	-1.704257	-0.947741
46	1	0	-2.041999	-0.870389	-0.499082
47	1	0	-1.434909	-0.779766	1.813031
48	1	0	0.945840	-2.581057	0.996079
49	1	0	0.421662	-2.244565	2.664305
50	1	0	-2.027394	-7.406856	1.789951
51	1	0	-0.348049	-7.202398	1.186083
52	1	0	-0.699471	-6.996211	2.927801
53	1	0	1.402689	4.512046	-1.996512
54	1	0	2.160379	2.916498	-2.033070
55	1	0	2.197159	3.883805	-0.547344
56	1	0	-0.715075	2.880918	-3.919295
57	1	0	-0.906047	1.132723	-3.721314
58	1	0	0.693680	1.866915	-3.573259
59	1	0	-3.663459	0.849750	-0.997196
60	1	0	-2.845464	0.647922	-2.556306
61	1	0	-3.694552	2.151983	-2.185272
62	1	0	-3.389767	3.342777	1.047114
63	1	0	-2.318238	2.581623	2.222177
64	1	0	-3.358646	1.584525	1.188304
65	1	0	-0.435472	4.937700	1.451562
66	1	0	1.154779	4.169115	1.379749
67	1	0	-0.124207	3.464131	2.373995

INT3





Thermal correction to Gibbs Free Energy= 0.469535

E(sov) = -2024.33114223 A.U.

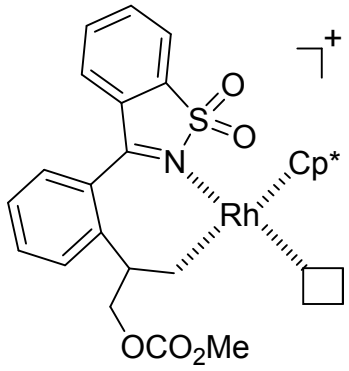
Standard orientation:

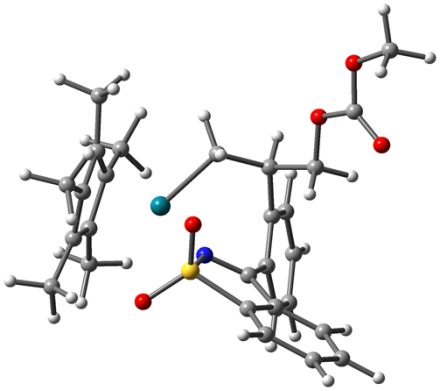
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.605301	-0.896518	0.192815
2	6	0	5.024980	3.218776	0.697522
3	6	0	5.457845	2.191836	-0.149498
4	6	0	4.595288	1.155397	-0.528011
5	6	0	3.289594	1.159060	-0.029599
6	6	0	2.878612	2.203760	0.805980
7	6	0	3.708408	3.243967	1.185816
8	6	0	2.190189	0.207378	-0.297207
9	7	0	1.048926	0.477684	0.273830
10	16	0	1.146976	1.971066	1.204213
11	8	0	0.944809	1.640905	2.613171
12	8	0	0.300561	2.965125	0.548628
13	6	0	2.293002	-0.991135	-1.157015
14	6	0	1.355222	-1.196237	-2.202374
15	6	0	3.303698	-1.935938	-0.903456
16	6	0	3.379546	-3.105802	-1.657595
17	6	0	2.458268	-3.322357	-2.687174
18	6	0	1.470265	-2.372259	-2.956330
19	6	0	-1.070193	-1.578955	2.434586
20	6	0	-2.164365	-0.903199	1.713997
21	6	0	-2.596683	-1.760442	0.618537
22	6	0	-1.635005	-2.802771	0.528965

23	6	0	-0.723312	-2.709850	1.697324
24	6	0	-0.495869	-1.108439	3.735416
25	6	0	-2.882963	0.300454	2.225607
26	6	0	-3.865577	-1.638372	-0.167609
27	6	0	-1.653919	-3.953175	-0.429258
28	6	0	0.346070	-3.713930	1.994758
29	6	0	0.313798	-0.149721	-2.568012
30	6	0	-0.999539	-0.171397	-1.746376
31	6	0	-1.634192	1.209934	-1.830645
32	8	0	-2.862657	1.199220	-1.072435
33	6	0	-3.655441	2.283967	-1.014035
34	8	0	-4.639661	2.299254	-0.306823
35	8	0	-3.231703	3.281732	-1.800425
36	6	0	-4.037943	4.483366	-1.774302
37	1	0	5.711108	4.013017	0.975992
38	1	0	6.476591	2.201622	-0.524895
39	1	0	4.933347	0.374298	-1.201160
40	1	0	3.361804	4.046275	1.829710
41	1	0	4.010874	-1.765993	-0.095971
42	1	0	4.155520	-3.836625	-1.449721
43	1	0	2.520335	-4.222546	-3.292418
44	1	0	0.783579	-2.533522	-3.783941
45	1	0	-1.204278	-1.316139	4.549243
46	1	0	-0.301368	-0.033605	3.730517
47	1	0	0.441109	-1.617657	3.975198
48	1	0	-3.586640	-0.015683	3.011500
49	1	0	-3.458175	0.805056	1.447522
50	1	0	-2.192240	1.016983	2.680098
51	1	0	-4.630972	-2.282213	0.287913
52	1	0	-3.740128	-1.965527	-1.204240
53	1	0	-4.242234	-0.615786	-0.180510
54	1	0	-2.224151	-3.719541	-1.331850
55	1	0	-2.126837	-4.825260	0.044743
56	1	0	-0.644025	-4.252170	-0.726931
57	1	0	-0.103684	-4.648449	2.358343
58	1	0	1.039579	-3.358880	2.760756
59	1	0	0.924838	-3.966430	1.099468
60	1	0	0.069256	-0.273528	-3.632114
61	1	0	0.771510	0.843743	-2.483438
62	1	0	-1.687045	-0.914995	-2.166640
63	1	0	-0.976876	1.985757	-1.428169
64	1	0	-1.866612	1.463675	-2.874263
65	1	0	-3.542271	5.170750	-2.459107
66	1	0	-5.052388	4.259988	-2.111389

67	1	0	-4.064597	4.892460	-0.762157

INT3a





Thermal correction to Gibbs Free Energy= 0.467879

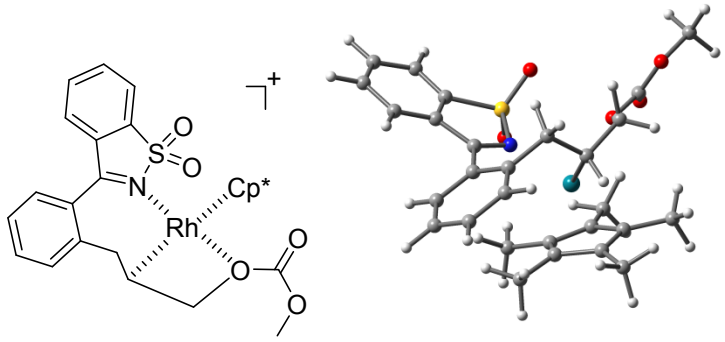
E(sov) = -2024.32468 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.565333	-0.392159	-0.133591
2	6	0	3.681080	4.201712	-0.439625
3	6	0	3.742891	3.745091	0.881960
4	6	0	2.819028	2.811293	1.367395
5	6	0	1.822952	2.349345	0.503441
6	6	0	1.788906	2.814136	-0.816409
7	6	0	2.694356	3.730456	-1.321226
8	6	0	0.764888	1.349467	0.756387
9	7	0	-0.014692	1.074655	-0.248302
10	16	0	0.458549	1.982546	-1.682568
11	8	0	-0.639578	2.889875	-2.013526
12	8	0	0.957011	1.035797	-2.676270
13	6	0	0.511499	0.673663	2.047460
14	6	0	0.432387	-0.741521	2.145765
15	6	0	0.268322	1.487655	3.168972
16	6	0	-0.083578	0.924942	4.393975
17	6	0	-0.177289	-0.464289	4.505919
18	6	0	0.088471	-1.273881	3.399928
19	6	0	0.025053	-1.713338	-0.283421
20	6	0	0.844867	-1.725552	1.035077
21	6	0	2.354362	-1.576804	0.779546
22	8	0	2.756059	-2.691961	-0.031533
23	6	0	4.037287	-2.657040	-0.455637

24	8	0	4.826450	-1.764822	-0.219378
25	8	0	4.268757	-3.759211	-1.167630
26	6	0	5.605357	-3.885456	-1.700918
27	6	0	-3.603572	0.642164	-0.860187
28	6	0	-2.966862	-0.335833	-1.765752
29	6	0	-3.046503	-1.654231	-1.149264
30	6	0	-3.480762	-1.444086	0.186426
31	6	0	-3.881339	-0.020981	0.332665
32	6	0	-3.873477	2.072765	-1.217118
33	6	0	-2.615636	-0.062741	-3.193483
34	6	0	-2.773011	-2.958579	-1.832520
35	6	0	-3.740714	-2.494991	1.223114
36	6	0	-4.484562	0.539607	1.583189
37	1	0	4.410914	4.922922	-0.794978
38	1	0	4.524252	4.113569	1.539516
39	1	0	2.885704	2.447170	2.387580
40	1	0	2.651859	4.069275	-2.351611
41	1	0	0.324450	2.568163	3.067597
42	1	0	-0.280288	1.564086	5.249589
43	1	0	-0.440598	-0.919819	5.456429
44	1	0	0.048618	-2.354350	3.513984
45	1	0	0.632441	-1.391108	-1.133644
46	1	0	-0.362708	-2.710742	-0.498569
47	1	0	0.712042	-2.718273	1.479407
48	1	0	2.593121	-0.647549	0.252018
49	1	0	2.919132	-1.593488	1.718479
50	1	0	5.606105	-4.834559	-2.235879
51	1	0	5.820254	-3.057023	-2.380132
52	1	0	6.336003	-3.897437	-0.888735
53	1	0	-4.671394	2.127958	-1.970031
54	1	0	-2.989147	2.559162	-1.638452
55	1	0	-4.197998	2.652193	-0.349046
56	1	0	-3.514329	-0.186457	-3.816518
57	1	0	-1.854758	-0.752646	-3.567350
58	1	0	-2.254399	0.958665	-3.335386
59	1	0	-2.530370	-3.752140	-1.120920
60	1	0	-1.949061	-2.881326	-2.547629
61	1	0	-3.664701	-3.277072	-2.389591
62	1	0	-4.803692	-2.775074	1.216771
63	1	0	-3.506444	-2.136968	2.230450
64	1	0	-3.159067	-3.402190	1.039687
65	1	0	-5.496057	0.137497	1.731764
66	1	0	-4.559367	1.628861	1.548946
67	1	0	-3.900466	0.267250	2.469794

INT4a



Thermal correction to Gibbs Free Energy= 0.471834

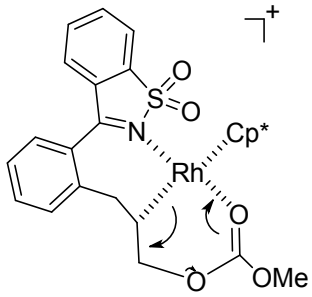
E(sov) = -2024.34131236 A.U.

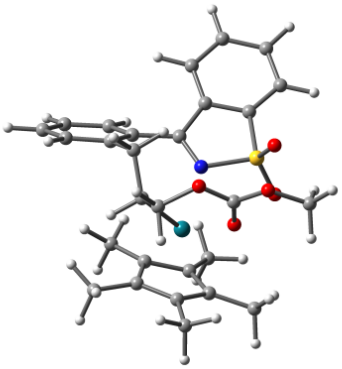
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.977492	0.552780	0.165855
2	6	0	-4.877636	-3.234307	0.621715
3	6	0	-5.399483	-2.060118	0.066239
4	6	0	-4.570712	-0.973836	-0.239411
5	6	0	-3.203005	-1.074532	0.036366
6	6	0	-2.707290	-2.266121	0.572719
7	6	0	-3.502813	-3.358920	0.872813
8	6	0	-2.122258	-0.088251	-0.223913
9	7	0	-0.911695	-0.486111	0.062449
10	16	0	-0.927525	-2.147600	0.679468
11	8	0	-0.449827	-2.109682	2.059708
12	8	0	-0.289674	-3.013600	-0.308324
13	6	0	-2.374308	1.244572	-0.801310
14	6	0	-1.616244	1.703252	-1.905945
15	6	0	-3.388381	2.051389	-0.250733
16	6	0	-3.643332	3.320596	-0.766102
17	6	0	-2.902929	3.779650	-1.859337
18	6	0	-1.910361	2.972402	-2.420730
19	6	0	0.934251	1.190594	2.437254
20	6	0	2.175790	0.590758	2.203163
21	6	0	2.828726	1.322869	1.098538
22	6	0	2.003190	2.426248	0.729414
23	6	0	0.759694	2.279916	1.458235
24	6	0	-0.068865	0.835347	3.491001
25	6	0	2.788997	-0.578444	2.911273

26	6	0	4.221698	1.041437	0.623597
27	6	0	2.363163	3.560141	-0.181526
28	6	0	-0.348056	3.287955	1.494328
29	6	0	-0.556803	0.844226	-2.558905
30	6	0	0.841173	0.933403	-1.922907
31	6	0	1.766385	-0.178277	-2.414984
32	8	0	1.926000	-1.033661	-1.218607
33	6	0	2.794696	-2.075844	-1.157201
34	8	0	3.151801	-2.539579	-0.101488
35	8	0	3.162424	-2.465189	-2.377953
36	6	0	4.069394	-3.596564	-2.428579
37	1	0	-5.539201	-4.065154	0.848081
38	1	0	-6.463292	-1.992511	-0.140532
39	1	0	-4.985053	-0.081458	-0.695566
40	1	0	-3.083949	-4.274578	1.278547
41	1	0	-3.955957	1.695882	0.604766
42	1	0	-4.416881	3.941466	-0.323812
43	1	0	-3.106019	4.759519	-2.282626
44	1	0	-1.359957	3.326932	-3.289197
45	1	0	0.010770	1.539220	4.331195
46	1	0	0.082281	-0.174914	3.873929
47	1	0	-1.094174	0.897986	3.113741
48	1	0	3.650197	-0.250306	3.509426
49	1	0	3.143226	-1.333416	2.201605
50	1	0	2.075723	-1.061947	3.581800
51	1	0	4.947712	1.489799	1.316502
52	1	0	4.411594	1.461998	-0.367953
53	1	0	4.422967	-0.033134	0.592104
54	1	0	2.799044	4.381246	0.404020
55	1	0	1.487601	3.958520	-0.702034
56	1	0	3.103321	3.266714	-0.931539
57	1	0	-0.104307	4.081518	2.215711
58	1	0	-1.293733	2.840520	1.808778
59	1	0	-0.505965	3.759846	0.520921
60	1	0	-0.480480	1.140328	-3.616379
61	1	0	-0.879290	-0.203161	-2.564457
62	1	0	1.275855	1.919166	-2.108149
63	1	0	1.353901	-0.793144	-3.219858
64	1	0	2.760436	0.173300	-2.703078
65	1	0	4.251174	-3.762791	-3.489507
66	1	0	4.996741	-3.354283	-1.905367
67	1	0	3.596958	-4.467448	-1.970276

INT4b





Thermal correction to Gibbs Free Energy= 0.475614

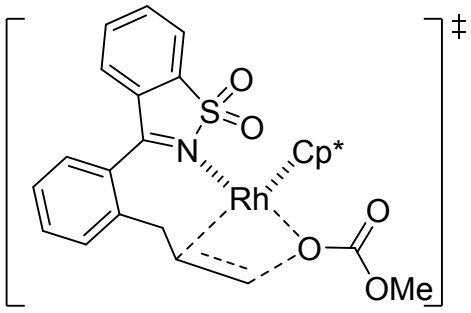
E(sov) = -2024.35632412

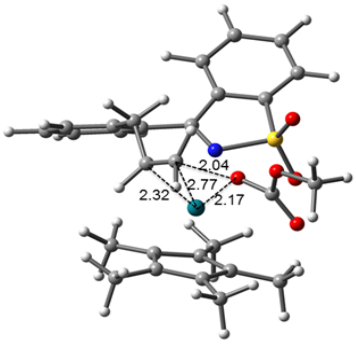
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.210058	0.208309	-0.150051
2	6	0	5.395430	-2.097904	-0.704833
3	6	0	5.641434	-0.793403	-0.260823
4	6	0	4.589572	0.080998	0.037887
5	6	0	3.274543	-0.365864	-0.132538
6	6	0	3.061022	-1.680192	-0.553798
7	6	0	4.081793	-2.570225	-0.842354
8	6	0	1.995771	0.345471	0.140009
9	7	0	0.904209	-0.358223	-0.022123
10	16	0	1.308901	-2.011276	-0.496134
11	8	0	0.727753	-2.266825	-1.812446
12	8	0	1.009732	-2.903041	0.625678
13	6	0	1.951567	1.742599	0.597906
14	6	0	1.134145	2.118447	1.690729
15	6	0	2.754572	2.702777	-0.050980
16	6	0	2.745356	4.032915	0.358650
17	6	0	1.951092	4.410160	1.446179
18	6	0	1.164568	3.459406	2.099137
19	6	0	-1.308083	0.605848	-2.493428
20	6	0	-2.415188	-0.174171	-2.149001
21	6	0	-3.166096	0.545877	-1.102914
22	6	0	-2.551177	1.822148	-0.903244
23	6	0	-1.322087	1.819228	-1.654154
24	6	0	-0.277616	0.322774	-3.543122
25	6	0	-2.812958	-1.511631	-2.694061

26	6	0	-4.487094	0.091601	-0.559761
27	6	0	-3.114034	2.976642	-0.131274
28	6	0	-0.423389	3.001284	-1.861060
29	6	0	0.259817	1.135667	2.433926
30	6	0	-1.142629	0.981984	1.814290
31	6	0	-2.064119	0.176237	2.715261
32	8	0	-1.640320	-1.196850	2.967240
33	6	0	-1.717283	-2.055855	1.964280
34	8	0	-1.807505	-1.751949	0.765663
35	8	0	-1.710937	-3.289120	2.416420
36	6	0	-1.756157	-4.369153	1.447859
37	1	0	6.227518	-2.758812	-0.928397
38	1	0	6.665508	-0.454945	-0.135331
39	1	0	4.799505	1.077082	0.410791
40	1	0	3.878200	-3.589733	-1.154733
41	1	0	3.360198	2.410836	-0.904039
42	1	0	3.355584	4.766239	-0.160293
43	1	0	1.950690	5.440753	1.790297
44	1	0	0.565618	3.759126	2.955975
45	1	0	-0.483171	0.925942	-4.438453
46	1	0	-0.267680	-0.728832	-3.833563
47	1	0	0.729953	0.582536	-3.203895
48	1	0	-3.720806	-1.424391	-3.306297
49	1	0	-3.028912	-2.219076	-1.885814
50	1	0	-2.026102	-1.946494	-3.313928
51	1	0	-5.279603	0.270603	-1.299824
52	1	0	-4.763589	0.628505	0.351929
53	1	0	-4.482139	-0.979993	-0.339296
54	1	0	-3.752021	3.581584	-0.790098
55	1	0	-2.330394	3.634240	0.255432
56	1	0	-3.734148	2.651664	0.709462
57	1	0	-0.819081	3.634067	-2.668747
58	1	0	0.585586	2.698002	-2.150406
59	1	0	-0.342267	3.620199	-0.963743
60	1	0	0.144291	1.499902	3.466791
61	1	0	0.745740	0.158194	2.513468
62	1	0	-1.596464	1.976996	1.741315
63	1	0	-2.093733	0.591234	3.729292
64	1	0	-3.086625	0.144846	2.325902
65	1	0	-1.733024	-5.275350	2.051375
66	1	0	-2.685050	-4.310912	0.876158
67	1	0	-0.889248	-4.309661	0.790908

TS2a





Imaginary frequency -300.51

Thermal correction to Gibbs Free Energy= 0.470227 A.U.

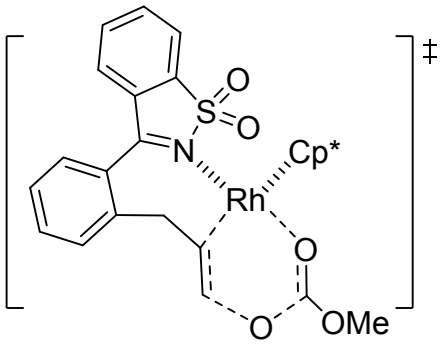
E(sov) = -2024.32480847 A.U.

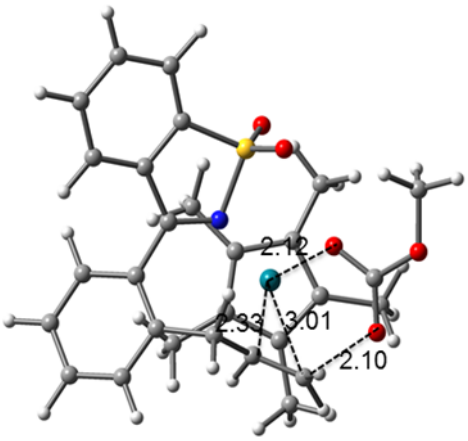
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.030008	0.522843	-0.070564
2	6	0	4.843168	-3.306134	-0.518787
3	6	0	5.381095	-2.091044	-0.077550
4	6	0	4.558402	-0.989640	0.185854
5	6	0	3.179554	-1.119583	-0.014680
6	6	0	2.669457	-2.348428	-0.436201
7	6	0	3.459166	-3.456810	-0.692291
8	6	0	2.104797	-0.119716	0.216604
9	7	0	0.882200	-0.543577	0.049276
10	16	0	0.884731	-2.258616	-0.452551
11	8	0	0.338390	-2.289053	-1.808576
12	8	0	0.335222	-3.100618	0.600431
13	6	0	2.408289	1.270440	0.615264
14	6	0	1.775904	1.868576	1.729836
15	6	0	3.372938	1.986051	-0.120382
16	6	0	3.700986	3.296757	0.221036
17	6	0	3.085616	3.892910	1.325013
18	6	0	2.142647	3.178382	2.067552
19	6	0	-0.813891	1.157133	-2.236538
20	6	0	-2.031026	0.416272	-2.116228
21	6	0	-2.884117	1.127970	-1.172951
22	6	0	-2.190773	2.299774	-0.733989
23	6	0	-0.876829	2.302214	-1.351449
24	6	0	0.312652	0.836419	-3.167884

25	6	0	-2.440429	-0.784711	-2.907635
26	6	0	-4.299319	0.760677	-0.859393
27	6	0	-2.761803	3.394132	0.115284
28	6	0	0.099467	3.437589	-1.307887
29	6	0	0.772563	1.128707	2.589807
30	6	0	-0.679211	1.211672	2.116122
31	6	0	-1.593608	0.284765	2.635687
32	8	0	-1.765279	-1.110894	1.162442
33	6	0	-2.785511	-1.919337	1.001411
34	8	0	-3.326505	-2.201703	-0.060573
35	8	0	-3.177567	-2.422395	2.195364
36	6	0	-4.233160	-3.402960	2.151197
37	1	0	5.500559	-4.147957	-0.714804
38	1	0	6.452871	-2.003026	0.072573
39	1	0	4.986159	-0.063243	0.553303
40	1	0	3.029094	-4.402738	-1.006537
41	1	0	3.850501	1.520174	-0.977920
42	1	0	4.437708	3.841859	-0.361782
43	1	0	3.348166	4.906254	1.615879
44	1	0	1.691144	3.640128	2.942736
45	1	0	0.090121	1.256409	-4.158885
46	1	0	0.447642	-0.241128	-3.282578
47	1	0	1.256051	1.275486	-2.832780
48	1	0	-3.098003	-0.468752	-3.730905
49	1	0	-2.985451	-1.497522	-2.284362
50	1	0	-1.579496	-1.299257	-3.337469
51	1	0	-4.943871	1.078150	-1.691685
52	1	0	-4.662529	1.257849	0.044148
53	1	0	-4.408856	-0.320006	-0.740338
54	1	0	-3.314412	4.098349	-0.522196
55	1	0	-1.985356	3.965879	0.630312
56	1	0	-3.464171	3.014414	0.862665
57	1	0	-0.157792	4.178646	-2.078007
58	1	0	1.122184	3.105499	-1.496358
59	1	0	0.089568	3.948074	-0.341756
60	1	0	0.831287	1.549533	3.603672
61	1	0	1.053341	0.074016	2.683050
62	1	0	-1.063348	2.219059	1.959279
63	1	0	-1.280813	-0.520150	3.291974
64	1	0	-2.656569	0.502765	2.647751
65	1	0	-4.399700	-3.690461	3.189795
66	1	0	-5.140713	-2.971785	1.720403
67	1	0	-3.922288	-4.266710	1.558463

TS2b





Imaginary frequency -230.40

Thermal correction to Gibbs Free Energy= 0.472103

E(sov) = -2024.32792925 A.U.

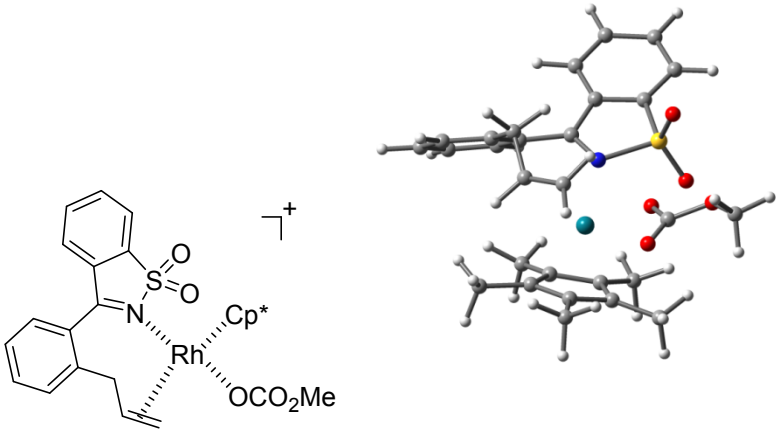
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.154948	0.247094	0.143952
2	6	0	-5.346067	-2.499312	0.362896
3	6	0	-5.661884	-1.175819	0.032528
4	6	0	-4.658197	-0.222281	-0.173061
5	6	0	-3.321733	-0.611610	-0.024777
6	6	0	-3.037453	-1.942126	0.281376
7	6	0	-4.009486	-2.909600	0.474445
8	6	0	-2.083244	0.192393	-0.207750
9	7	0	-0.952003	-0.454251	-0.108875
10	16	0	-1.270418	-2.182960	0.196241
11	8	0	-0.680955	-2.502892	1.496345
12	8	0	-0.960694	-2.977871	-0.986123
13	6	0	-2.144568	1.633669	-0.513383
14	6	0	-1.407690	2.180337	-1.588732
15	6	0	-2.998913	2.455715	0.250115
16	6	0	-3.124429	3.812826	-0.034494
17	6	0	-2.422127	4.354537	-1.115567
18	6	0	-1.580667	3.542155	-1.877115
19	6	0	0.958378	0.690253	2.352146
20	6	0	1.984004	-0.299885	2.173868
21	6	0	3.022676	0.293116	1.353642
22	6	0	2.640295	1.642079	1.049115

23	6	0	1.335058	1.885275	1.634310
24	6	0	-0.266902	0.530470	3.195965
25	6	0	2.066806	-1.648276	2.817998
26	6	0	4.324579	-0.358806	1.007653
27	6	0	3.506663	2.658408	0.371509
28	6	0	0.638303	3.211712	1.700180
29	6	0	-0.423259	1.377644	-2.411516
30	6	0	0.990650	1.487579	-1.817819
31	6	0	2.087302	1.092675	-2.593015
32	8	0	3.229859	-0.620471	-2.149369
33	6	0	2.579282	-1.601209	-1.709396
34	8	0	1.587661	-1.541757	-0.903209
35	8	0	2.974815	-2.810977	-2.131158
36	6	0	2.288291	-3.977988	-1.629539
37	1	0	-6.141734	-3.222343	0.515873
38	1	0	-6.702300	-0.885049	-0.076986
39	1	0	-4.919404	0.790458	-0.458575
40	1	0	-3.751767	-3.940855	0.694773
41	1	0	-3.549028	2.031044	1.085021
42	1	0	-3.773912	4.437847	0.571373
43	1	0	-2.532010	5.405807	-1.366822
44	1	0	-1.043773	3.970461	-2.720312
45	1	0	-0.024178	0.785905	4.237038
46	1	0	-0.636005	-0.497430	3.181031
47	1	0	-1.069787	1.199434	2.875454
48	1	0	2.809871	-1.624779	3.627312
49	1	0	2.378080	-2.415102	2.102781
50	1	0	1.110192	-1.960287	3.237276
51	1	0	5.075787	-0.098151	1.766653
52	1	0	4.699170	-0.040383	0.032443
53	1	0	4.235921	-1.447813	0.994452
54	1	0	4.080815	3.205627	1.132459
55	1	0	2.927416	3.399720	-0.186047
56	1	0	4.224700	2.192006	-0.307049
57	1	0	0.953175	3.758764	2.599948
58	1	0	-0.448237	3.102366	1.741552
59	1	0	0.875619	3.840235	0.837753
60	1	0	-0.417876	1.793429	-3.427936
61	1	0	-0.725708	0.331243	-2.507012
62	1	0	1.157886	2.411630	-1.265188
63	1	0	1.946819	0.571440	-3.534421
64	1	0	3.048999	1.573464	-2.472359
65	1	0	2.756344	-4.816846	-2.145245
66	1	0	2.431412	-4.070677	-0.549132

67	1	0	1.222040	-3.925125	-1.853087

INT5



Thermal correction to Gibbs Free Energy= 0.471090

E(sov) = -2024.35564955 A.U.

Standard orientation:

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1	45	0	1.103891	0.447624	-0.023999
2	6	0	-4.918702	-3.284171	0.503620
3	6	0	-5.450241	-2.022077	0.209972
4	6	0	-4.615454	-0.923908	-0.023375
5	6	0	-3.228957	-1.105716	0.057277
6	6	0	-2.728363	-2.377611	0.328127
7	6	0	-3.531477	-3.483853	0.551010
8	6	0	-2.141363	-0.115266	-0.158423
9	7	0	-0.918351	-0.566678	-0.103480
10	16	0	-0.947168	-2.351259	0.183223
11	8	0	-0.307255	-2.604240	1.469864
12	8	0	-0.581476	-3.048078	-1.042341
13	6	0	-2.464472	1.302232	-0.444034
14	6	0	-1.935268	1.960245	-1.576005
15	6	0	-3.369368	1.974232	0.399414
16	6	0	-3.730639	3.296832	0.150684
17	6	0	-3.212545	3.952093	-0.969819
18	6	0	-2.331984	3.281845	-1.822015
19	6	0	1.353161	0.726460	2.183618
20	6	0	2.657094	0.578573	1.602544
21	6	0	2.844173	1.636239	0.638011

22	6	0	1.688537	2.521566	0.734745
23	6	0	0.773533	1.959484	1.668296
24	6	0	0.791317	-0.122846	3.280421
25	6	0	3.641280	-0.482135	1.967517
26	6	0	4.105825	1.908331	-0.121686
27	6	0	1.569114	3.867031	0.088239
28	6	0	-0.466786	2.610920	2.191297
29	6	0	-0.981442	1.275232	-2.534259
30	6	0	0.477457	1.459664	-2.183719
31	6	0	1.434090	0.499402	-2.368211
32	8	0	1.723531	-1.508744	-0.381164
33	6	0	2.883169	-1.834881	-0.884831
34	8	0	3.774177	-1.071052	-1.262510
35	8	0	3.001001	-3.178943	-0.935889
36	6	0	4.226333	-3.686338	-1.493647
37	1	0	-5.585713	-4.122757	0.680400
38	1	0	-6.527016	-1.894148	0.153475
39	1	0	-5.042315	0.040844	-0.274125
40	1	0	-3.107942	-4.463993	0.747243
41	1	0	-3.772596	1.463875	1.269355
42	1	0	-4.419723	3.806153	0.818027
43	1	0	-3.504233	4.975394	-1.189000
44	1	0	-1.957825	3.788140	-2.709042
45	1	0	1.215358	0.192325	4.244503
46	1	0	1.027121	-1.178418	3.130956
47	1	0	-0.295302	-0.033467	3.350190
48	1	0	4.119841	-0.204283	2.917816
49	1	0	4.418096	-0.594988	1.210663
50	1	0	3.150991	-1.448658	2.114923
51	1	0	4.838744	2.393984	0.537679
52	1	0	3.934824	2.578448	-0.968957
53	1	0	4.535749	0.979675	-0.504104
54	1	0	1.998639	4.625018	0.758463
55	1	0	0.528856	4.146009	-0.099550
56	1	0	2.123530	3.925872	-0.852129
57	1	0	-0.211282	3.203049	3.081891
58	1	0	-1.217700	1.878386	2.495220
59	1	0	-0.920290	3.285421	1.462706
60	1	0	-1.119342	1.718329	-3.531386
61	1	0	-1.204469	0.209796	-2.638443
62	1	0	0.785652	2.487945	-2.012372
63	1	0	1.154052	-0.500110	-2.688590
64	1	0	2.493740	0.725502	-2.381817
65	1	0	4.124268	-4.771595	-1.459841

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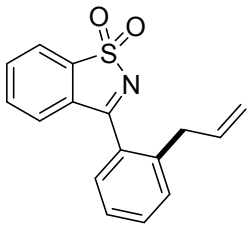
3a



Thermal correction to Gibbs Free Energy= 0.207522

E(sov) = -1220.95241658 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.778850	-1.861796	-0.750979
2	6	0	2.658302	-2.693285	-0.863347
3	6	0	1.376073	-2.222499	-0.554264
4	6	0	1.235436	-0.902174	-0.120384
5	6	0	2.364879	-0.088263	-0.032755
6	6	0	3.641789	-0.529305	-0.336082
7	6	0	-0.001892	-0.137557	0.240818
8	7	0	0.145701	1.110105	0.550032
9	16	0	1.812396	1.552703	0.461869
10	8	0	2.286673	1.888244	1.805280
11	8	0	1.985294	2.504585	-0.639251
12	6	0	-1.343990	-0.770376	0.254941
13	6	0	-2.452852	-0.224800	-0.431993
14	6	0	-1.492196	-1.957216	0.998382
15	6	0	-2.721823	-2.604081	1.084902
16	6	0	-3.817967	-2.082125	0.393259
17	6	0	-3.672394	-0.916132	-0.356514
18	6	0	-2.395991	1.050579	-1.261182
19	6	0	-3.109816	2.212003	-0.600427
20	6	0	-2.541585	3.381601	-0.298359
21	1	0	4.764192	-2.247820	-0.996805
22	1	0	2.783327	-3.718405	-1.200642
23	1	0	0.511597	-2.870032	-0.660117
24	1	0	4.501420	0.129914	-0.261426
25	1	0	-0.638515	-2.354819	1.540564

26	1	0	-2.821664	-3.506433	1.681717
27	1	0	-4.781759	-2.582970	0.434733
28	1	0	-4.528089	-0.524061	-0.902097
29	1	0	-2.883128	0.842585	-2.225697
30	1	0	-1.365591	1.337802	-1.478601
31	1	0	-4.165201	2.053923	-0.372562
32	1	0	-1.487920	3.572638	-0.487817
33	1	0	-3.111588	4.183607	0.164304

Thermal correction to Gibbs Free Energy= 0.217783

SCF Done: E(RM06L) = -614.723159263 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.486831	0.000957	-0.586173
2	6	0	0.794035	1.204047	0.710496
3	6	0	0.146796	0.148072	1.468433
4	6	0	0.604873	-1.116726	0.924959
5	6	0	1.544078	-0.830765	-0.141851
6	6	0	1.661014	0.588667	-0.269287
7	6	0	0.655704	2.671177	0.961059
8	6	0	-0.734111	0.331296	2.662056
9	6	0	0.250848	-2.474018	1.441041
10	6	0	2.266683	-1.858122	-0.955787
11	6	0	2.523341	1.323855	-1.247923
12	8	0	-2.257494	0.004043	-1.158265
13	6	0	-3.611154	0.001906	-0.758826
14	1	0	1.432800	2.994160	1.668676
15	1	0	-0.313567	2.923063	1.398531
16	1	0	0.782039	3.256407	0.046617
17	1	0	-0.113780	0.380811	3.568314
18	1	0	-1.432598	-0.499987	2.786168
19	1	0	-1.309429	1.258964	2.606590
20	1	0	0.980460	-2.773856	2.206990
21	1	0	0.274237	-3.230533	0.652524
22	1	0	-0.739048	-2.490750	1.903845
23	1	0	3.189494	-2.156275	-0.438781
24	1	0	2.550576	-1.476103	-1.939416
25	1	0	1.667055	-2.760996	-1.100401
26	1	0	3.495980	1.549125	-0.788906

27	1	0	2.077205	2.274865	-1.551444
28	1	0	2.714399	0.735061	-2.148557
29	1	0	-4.234234	0.141486	-1.649902
30	1	0	-3.864293	-0.957492	-0.290004
31	1	0	-3.802607	0.820323	-0.053136

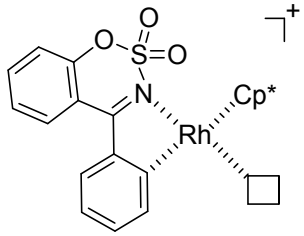
CO_2

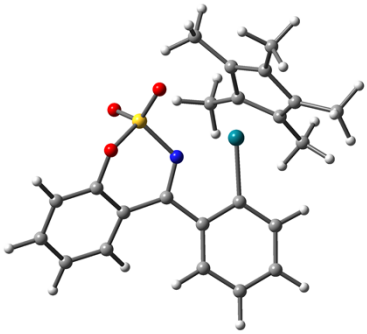
Sum of electronic and thermal Free Energies= -188.596028

Thermal correction to Gibbs Free Energy= -0.005636

SCF Done: E(RM06L) = -188.633399100 A.U

1p-INT1





Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.846446	0.363119	-0.334048
2	6	0	-5.351842	-0.829895	-0.879559
3	6	0	-4.006940	-1.154010	-0.747365
4	6	0	-3.119652	-0.288670	-0.067189
5	6	0	-3.640920	0.940375	0.395543
6	6	0	-4.986946	1.263350	0.297834
7	6	0	-1.703673	-0.580024	0.136892
8	7	0	-0.816512	0.396954	0.320720
9	16	0	-1.314889	2.014249	0.307297
10	8	0	-1.478929	2.466033	-1.065566
11	8	0	-0.502000	2.741677	1.257353
12	6	0	-1.104794	-1.916123	0.201896
13	6	0	0.320549	-1.952421	0.163644
14	45	0	1.240164	-0.133115	0.185315
15	6	0	-1.845790	-3.091783	0.426214
16	6	0	-1.191719	-4.318769	0.548089
17	6	0	0.199930	-4.371166	0.464001

18	6	0	0.944911	-3.194327	0.280868
19	6	0	2.442917	1.735440	-0.594810
20	6	0	2.396170	0.572324	-1.491446
21	6	0	3.129033	-0.523069	-0.868673
22	6	0	3.427733	-0.106722	0.457390
23	6	0	3.024879	1.313286	0.605675
24	6	0	1.975554	3.112859	-0.953837
25	6	0	1.908807	0.602000	-2.902897
26	6	0	3.570023	-1.776081	-1.562204
27	6	0	4.186764	-0.870403	1.496703
28	6	0	3.239905	2.119282	1.847144
29	8	0	-2.800301	1.854816	1.017162
30	1	0	-6.899582	0.609737	-0.431198
31	1	0	-6.016937	-1.499857	-1.415174
32	1	0	-3.626836	-2.057383	-1.209074
33	1	0	-5.336616	2.212316	0.690607
34	1	0	-2.921356	-3.054970	0.554984
35	1	0	-1.766657	-5.222830	0.724068
36	1	0	0.713917	-5.324022	0.561412
37	1	0	2.027315	-3.270082	0.253123
38	1	0	1.089418	3.096211	-1.593705
39	1	0	1.736501	3.706213	-0.069253
40	1	0	2.770246	3.632959	-1.506642
41	1	0	1.681428	-0.399671	-3.275706
42	1	0	1.017419	1.226267	-3.010006
43	1	0	2.689788	1.030677	-3.548773
44	1	0	4.430374	-1.550305	-2.206675
45	1	0	3.889257	-2.545801	-0.855695
46	1	0	2.784014	-2.197732	-2.194310
47	1	0	4.179269	-1.945897	1.304793
48	1	0	5.235251	-0.540200	1.508574
49	1	0	3.783414	-0.700388	2.499735
50	1	0	4.294642	2.418588	1.924989
51	1	0	2.629230	3.024468	1.854418
52	1	0	3.002059	1.543584	2.747752

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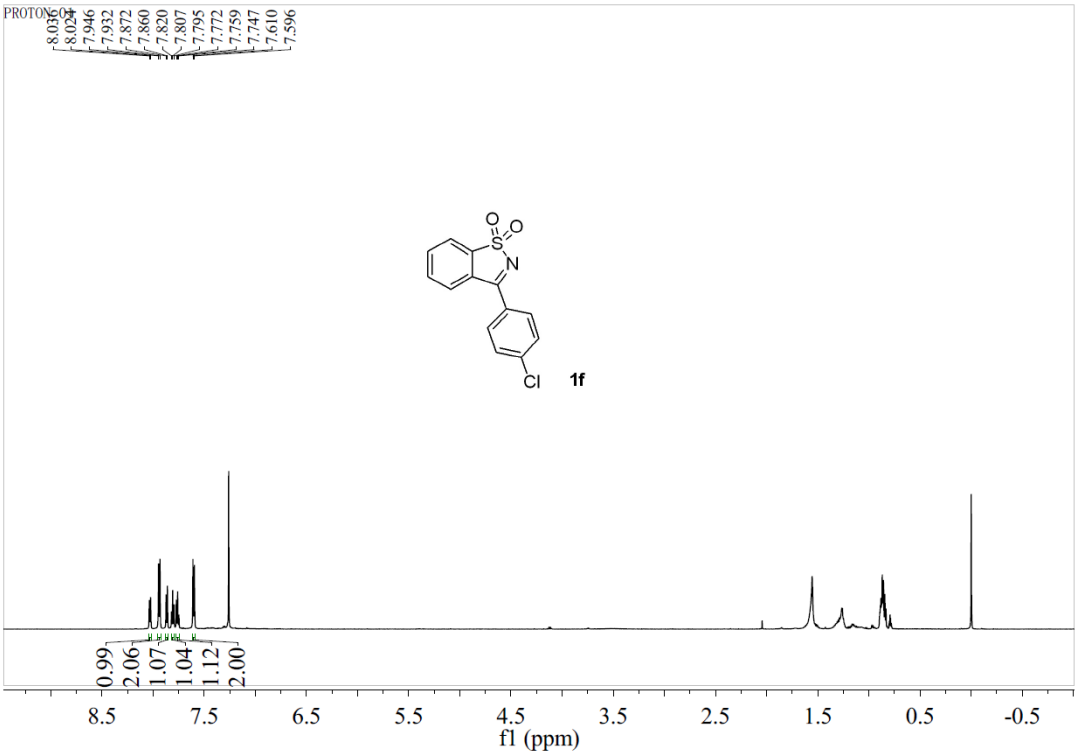
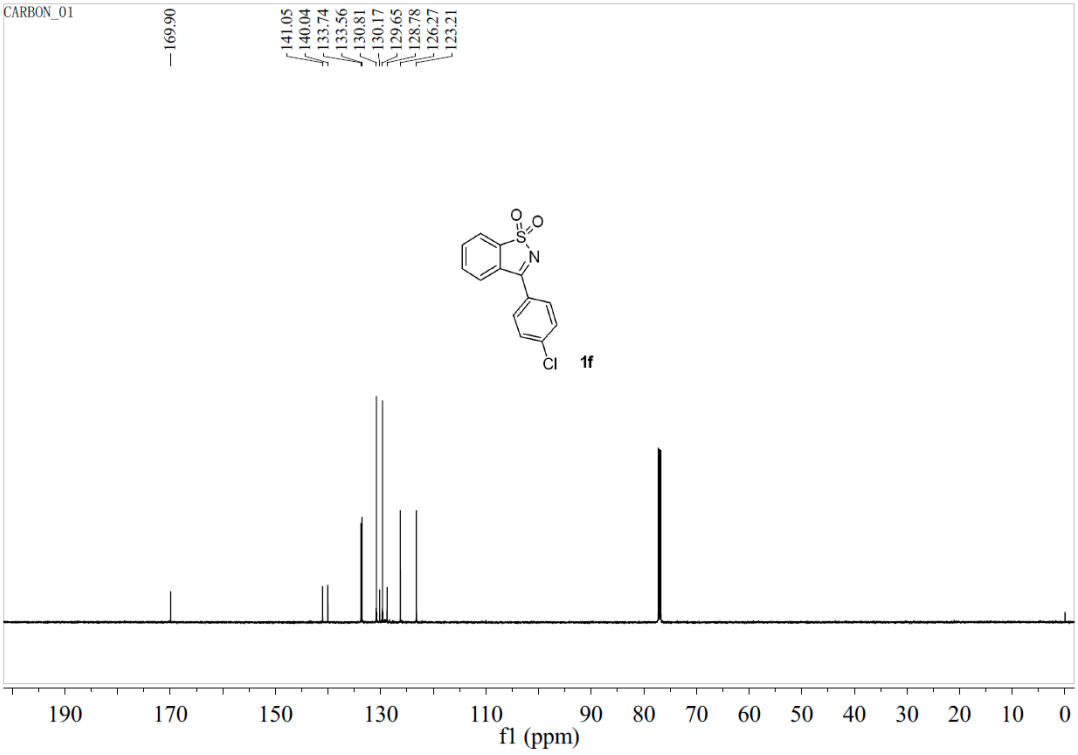
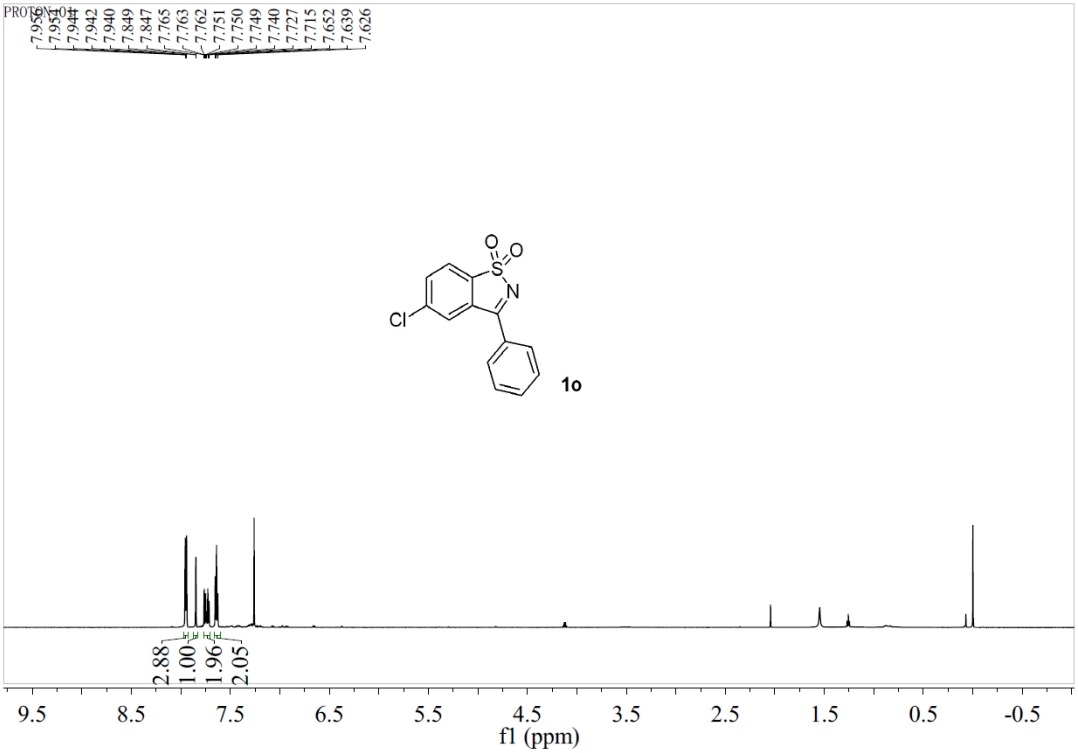
^{1}H and ^{13}C NMR Spectra



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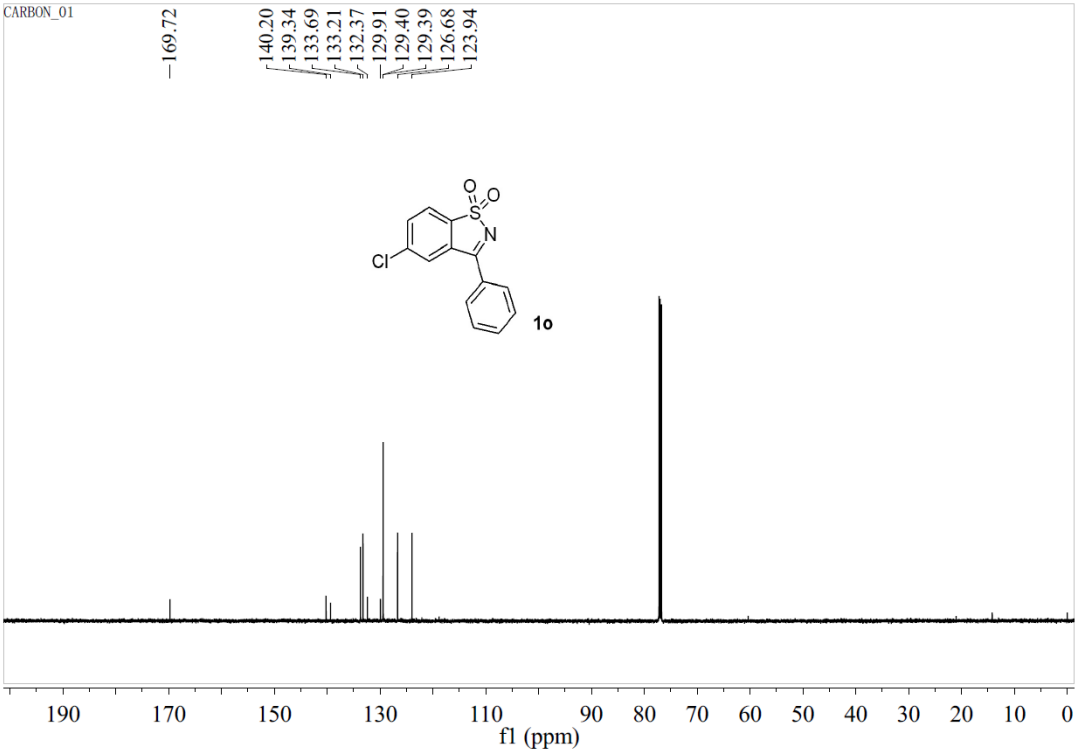
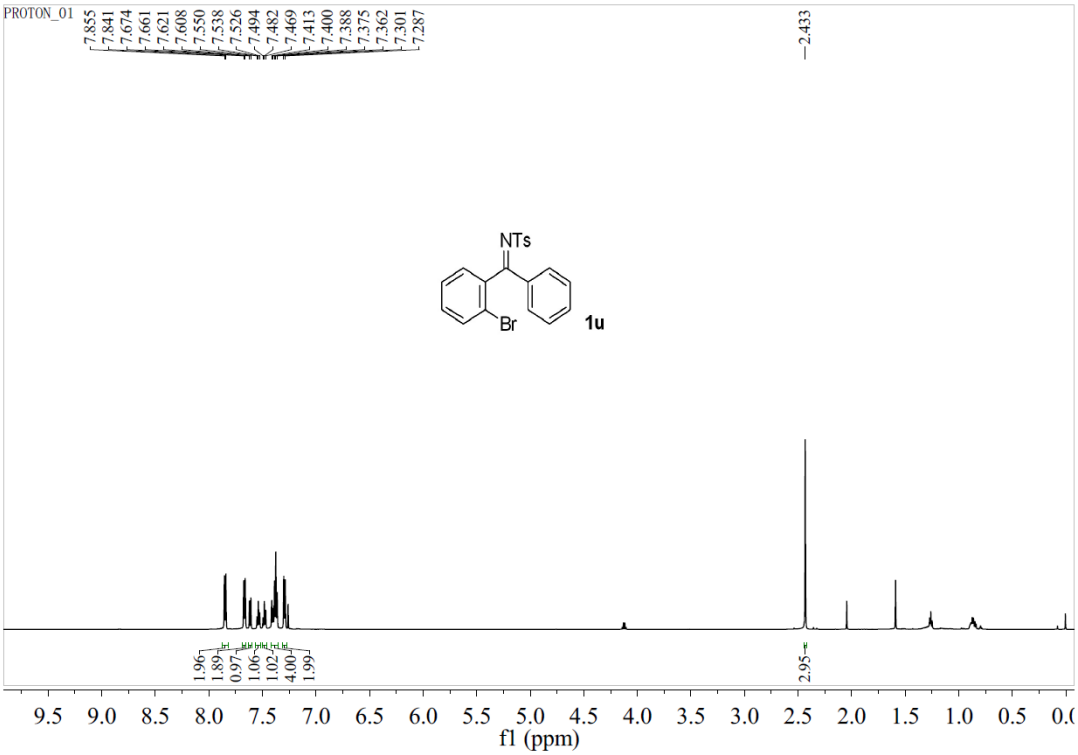
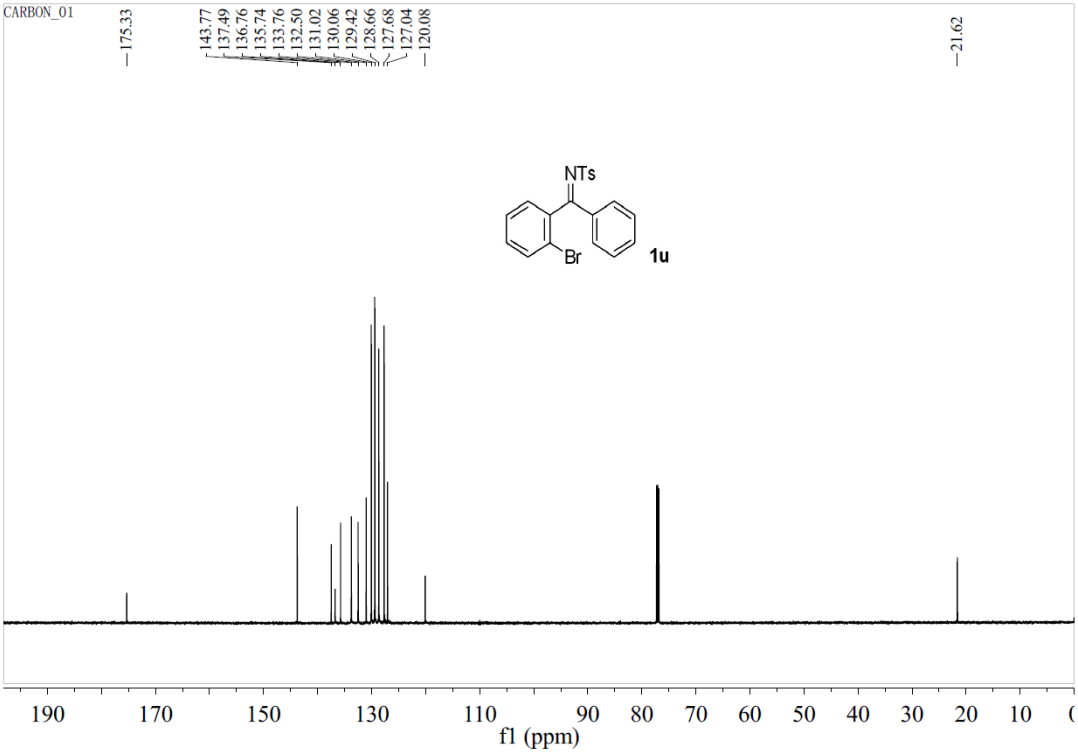
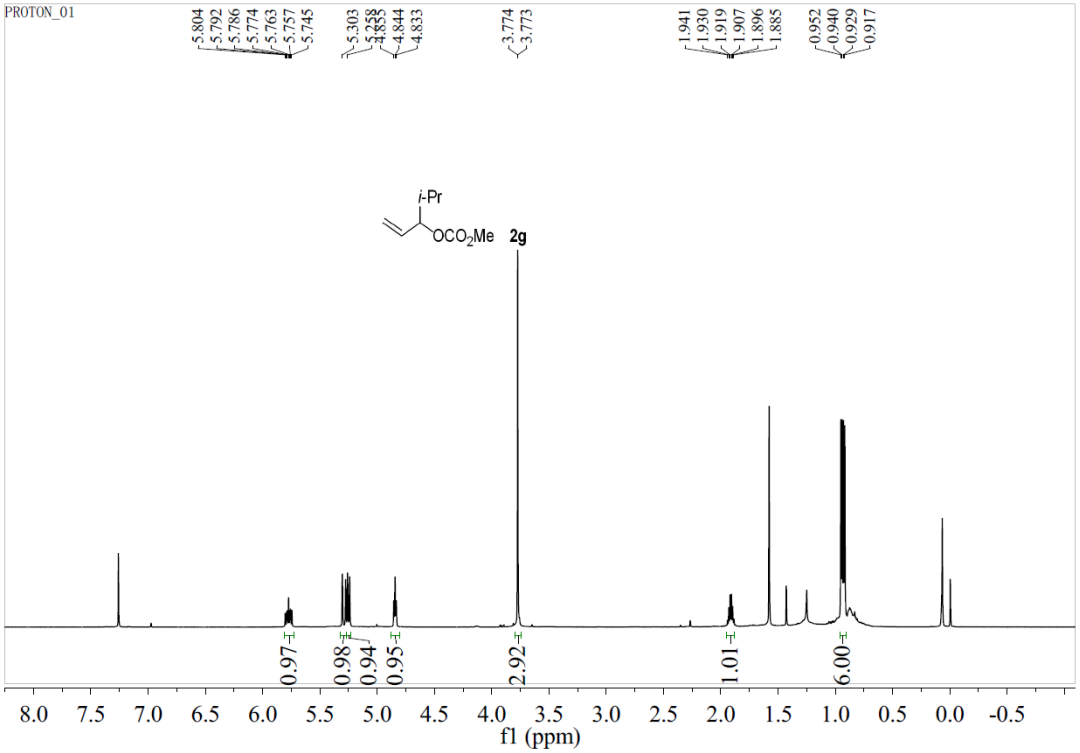
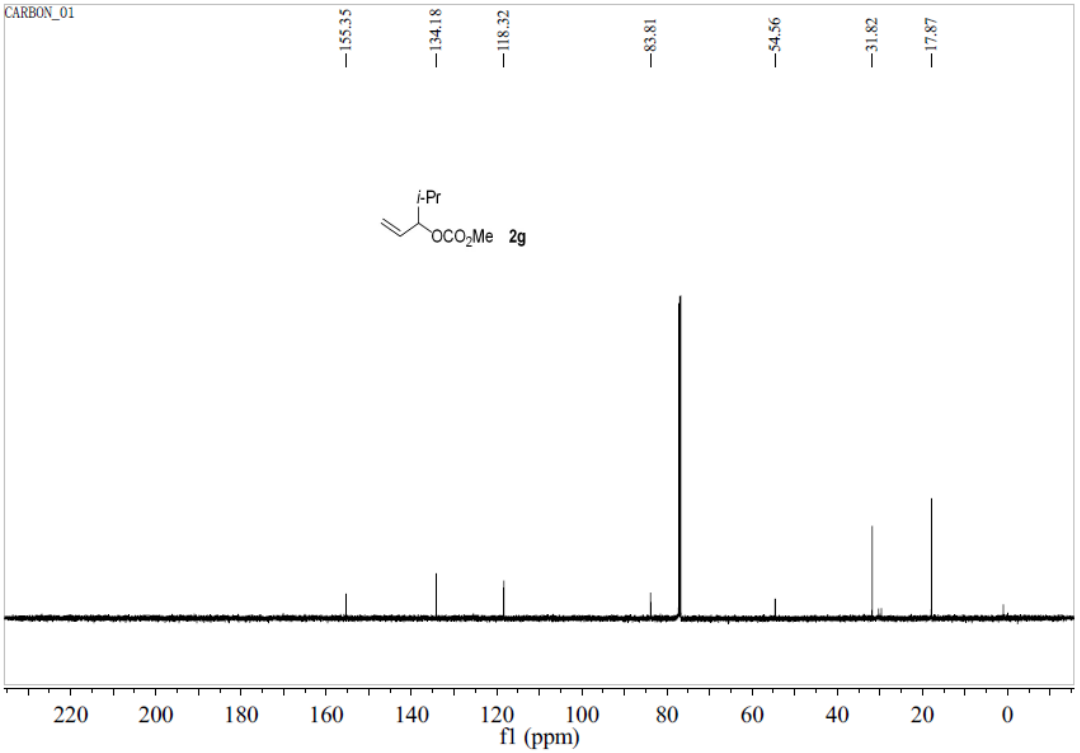
f1 (ppm)

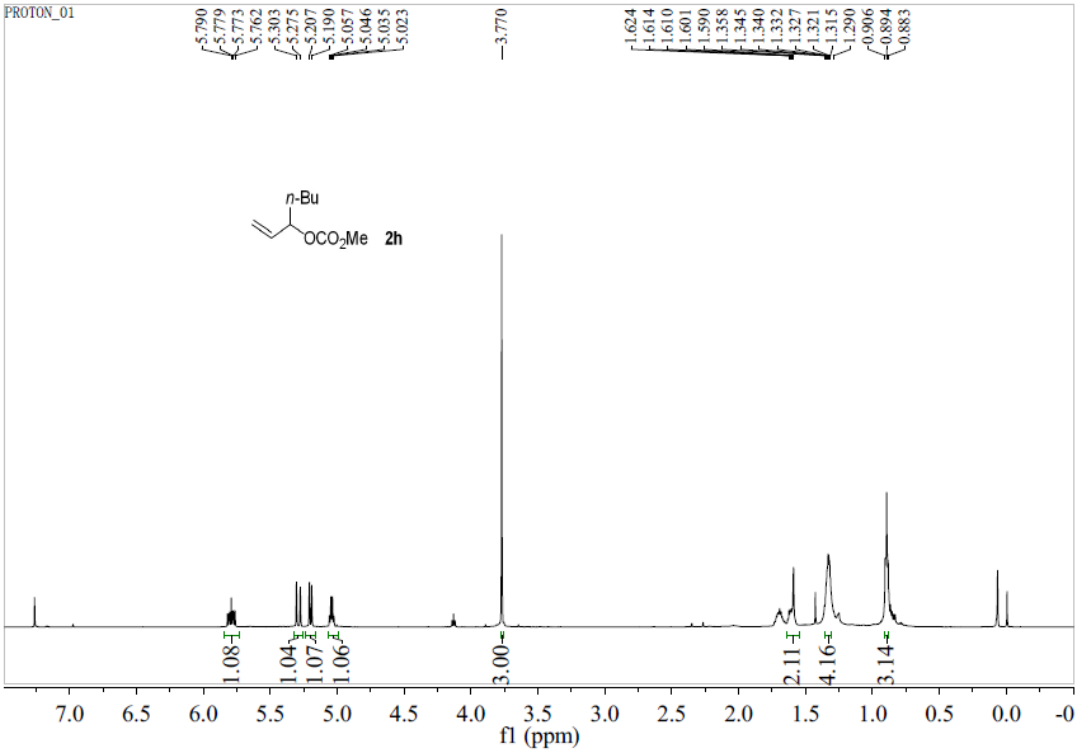

CARBON_01
169.72
140.20
139.34
133.69
133.21
132.37
129.91
129.40
129.39
126.68
123.94
Cl
1o
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

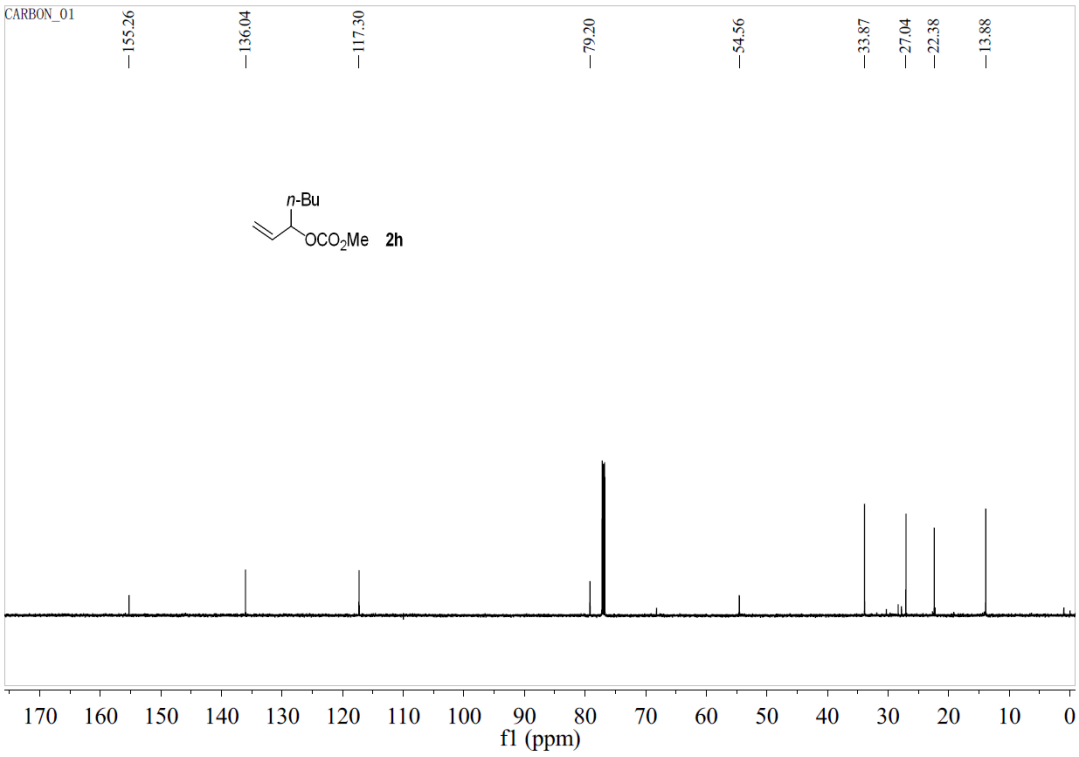

PROTON_01
7.855
7.841
7.674
7.661
7.621
7.608
7.550
7.538
7.526
7.494
7.482
7.469
7.413
7.400
7.388
7.375
7.362
7.301
7.287
2.433
NTs
Br
1u
1.96
1.89
0.97
1.06
1.02
4.00
1.99
2.95
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

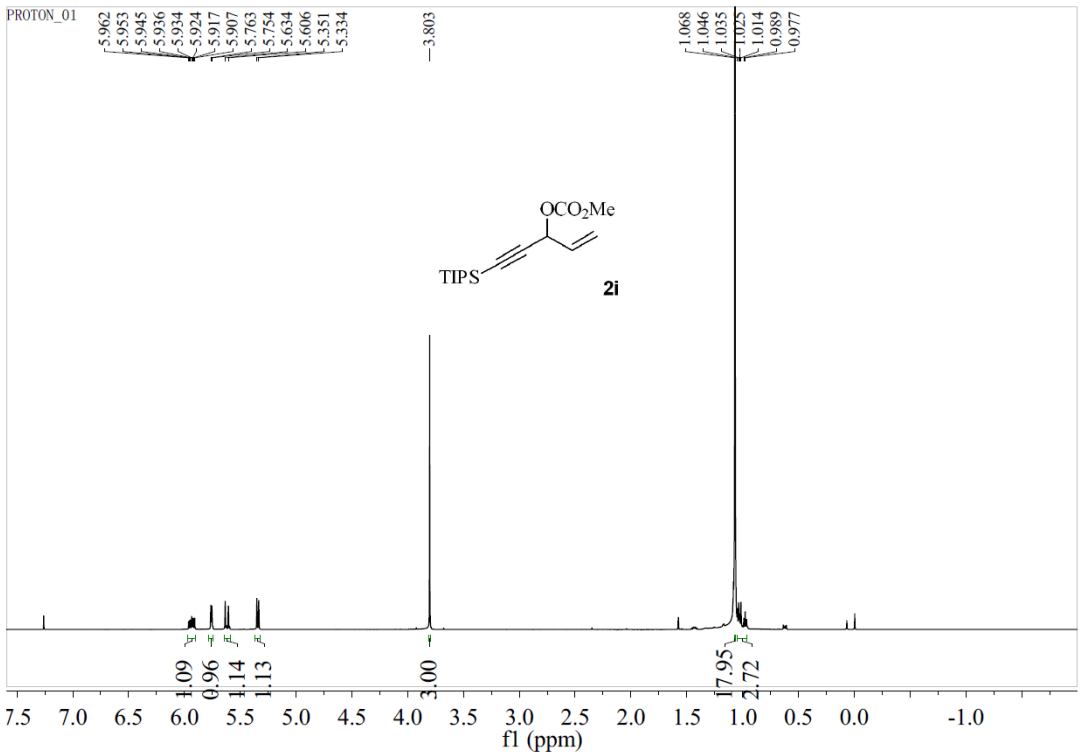

CARBON_01
175.33
143.77
137.49
136.76
135.74
133.76
132.50
131.02
130.06
129.42
128.66
127.68
127.04
120.08
21.62
NTs
Br
1u
190 170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

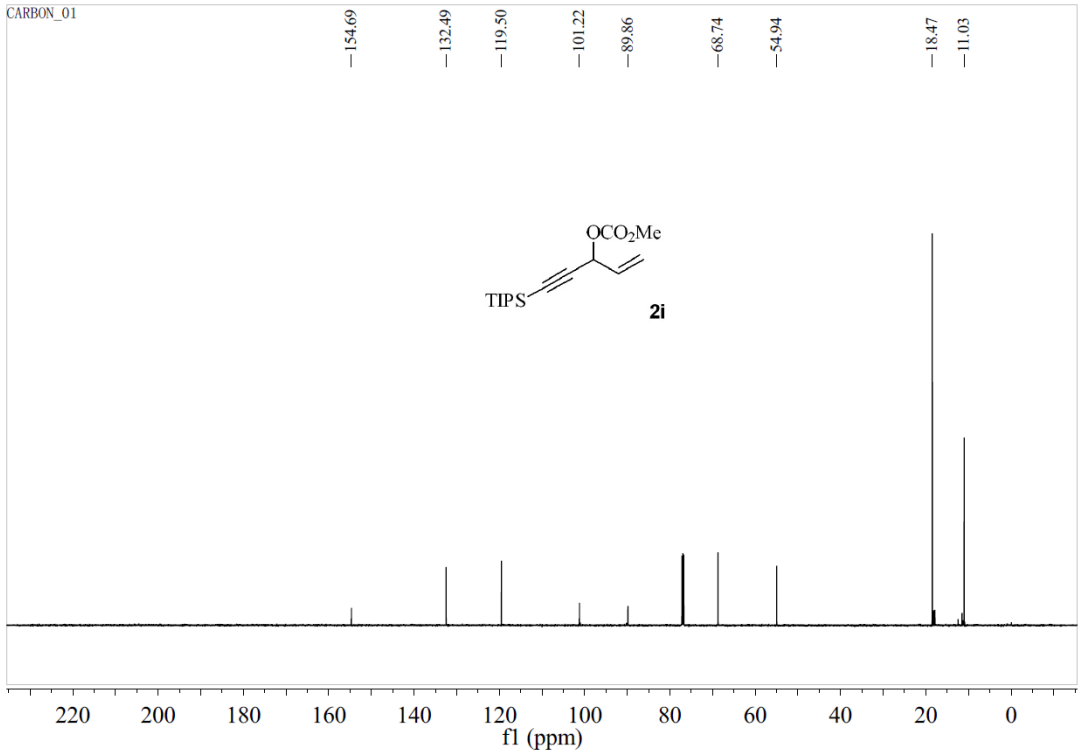

PROTON_01
5.804
5.792
5.786
5.774
5.763
5.757
5.745
5.303
5.298
4.855
4.844
4.833
3.774
3.773
1.941
1.930
1.919
1.907
1.896
1.885
0.952
0.940
0.929
0.917
i-Pr
OCO2Me 2g
0.97
0.98
0.94
0.95
2.92
1.01
6.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

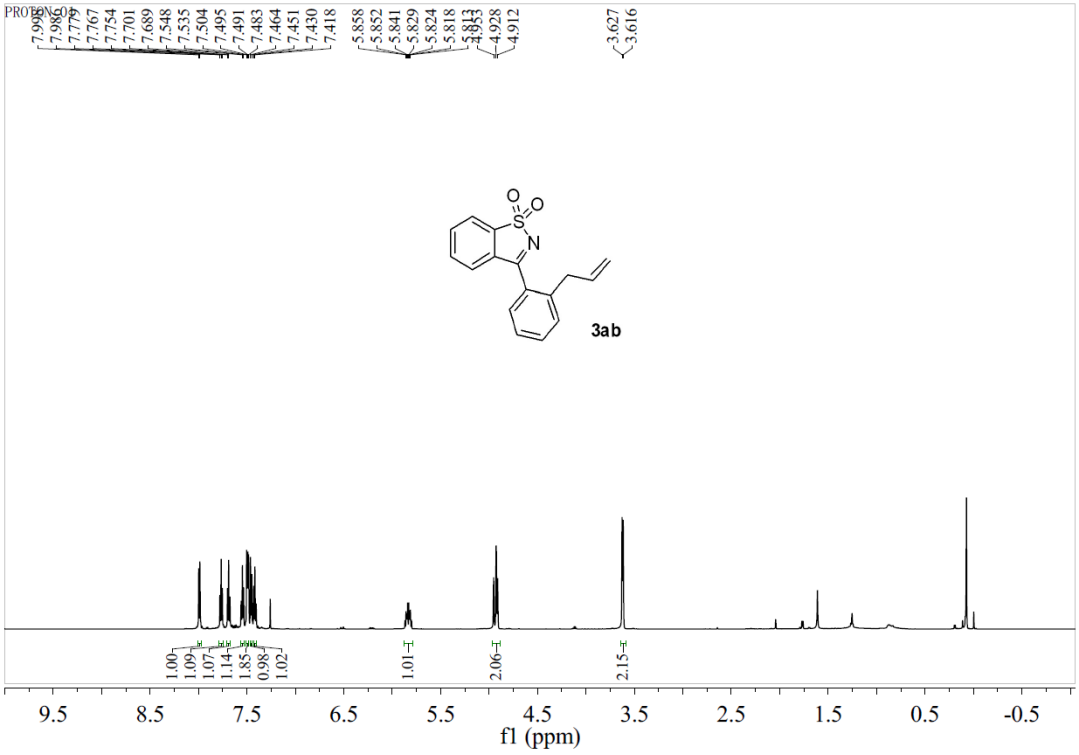

CARBON_01
155.35
134.18
118.32
83.81
54.56
31.82
17.87
i-Pr
OCO2Me 2g
220 200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

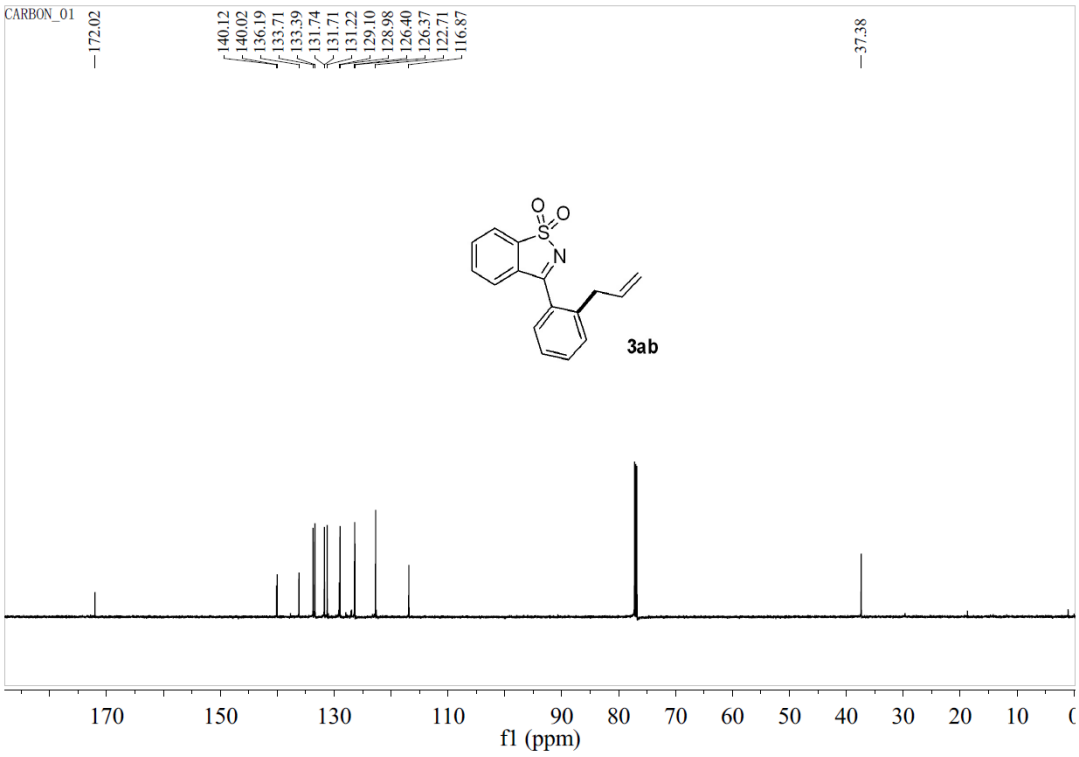

PROTON_01
5.790
5.779
5.773
5.762
5.303
5.275
5.207
5.190
5.057
5.046
5.035
5.023
3.770
1.624
1.614
1.610
1.601
1.590
1.358
1.345
1.340
1.332
1.327
1.321
1.315
1.290
0.906
0.894
0.883
n-Bu
OCO2Me 2h
1.08
1.04
1.07
1.06
3.00
2.11
4.16
3.14
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

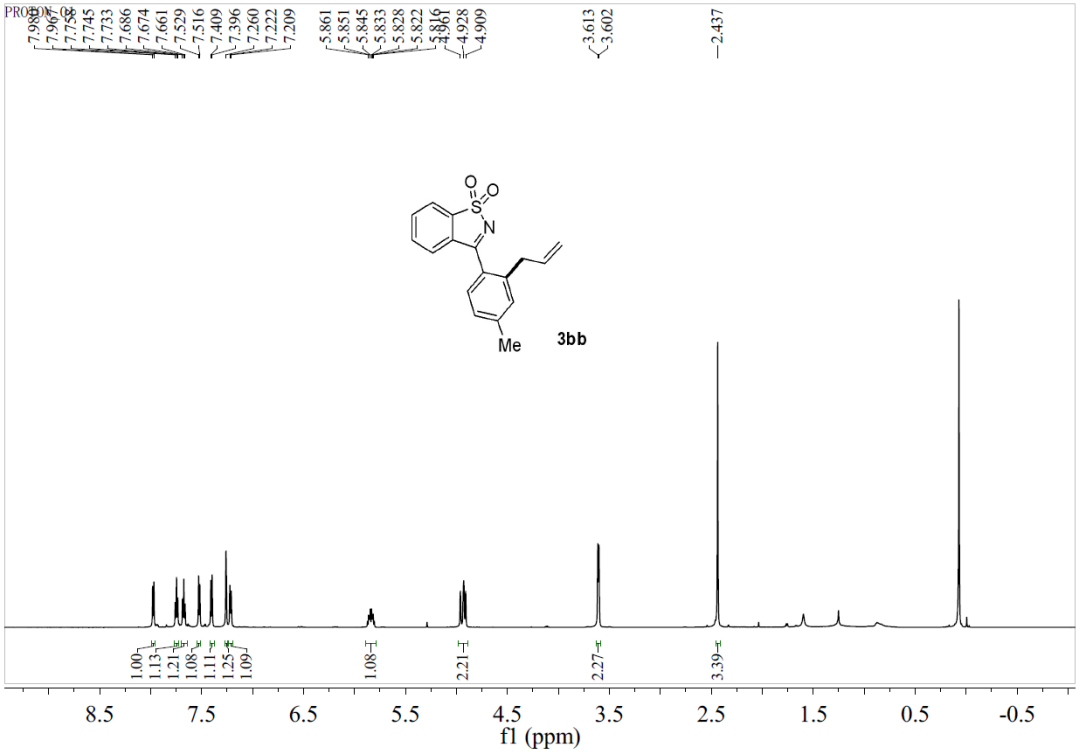

CARBON_01
155.26
136.04
117.30
79.20
54.56
33.87
27.04
22.38
13.88
n-Bu
OCO2Me 2h
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


PROTON_01
5.962
5.953
5.945
5.936
5.934
5.924
5.917
5.907
5.763
5.754
5.634
5.606
5.351
5.334
3.803
1.068
1.046
1.035
1.025
1.014
0.989
0.977
OCO2Me
TIPS
2i
1.09
0.96
1.14
1.13
3.00
17.95
2.72
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)


CARBON_01
154.69
132.49
119.50
101.22
89.86
68.74
54.94
18.47
11.03
OCO2Me
TIPS
2i
220 200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)


PROTON_01
7.998
7.986
7.779
7.767
7.754
7.701
7.689
7.548
7.535
7.504
7.495
7.491
7.483
7.464
7.451
7.430
7.418
5.858
5.852
5.841
5.829
5.824
5.818
5.813
4.953
4.928
4.912
3.627
3.616
3ab
1.00
1.09
1.07
1.14
1.85
0.98
1.02
1.01
2.06
2.15
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


CARBON_01
172.02
140.12
140.02
136.19
133.71
133.39
131.74
131.71
131.22
129.10
128.98
126.40
126.37
122.71
116.87
37.38
3ab
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)


PROTON_01
7.988
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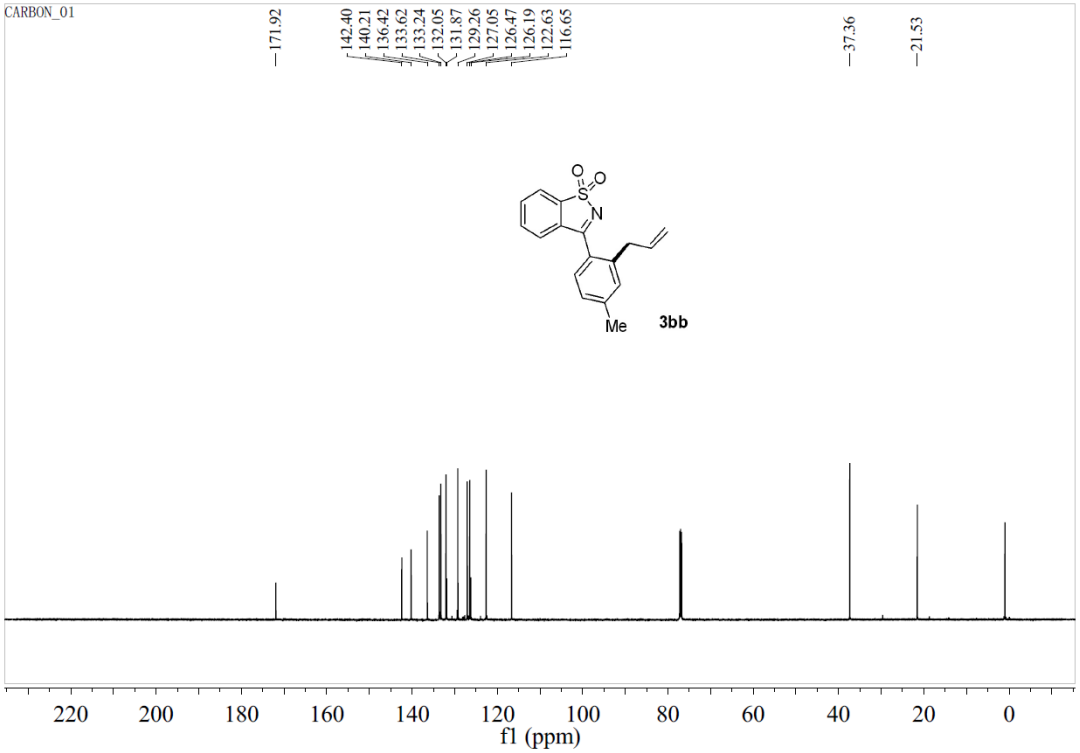
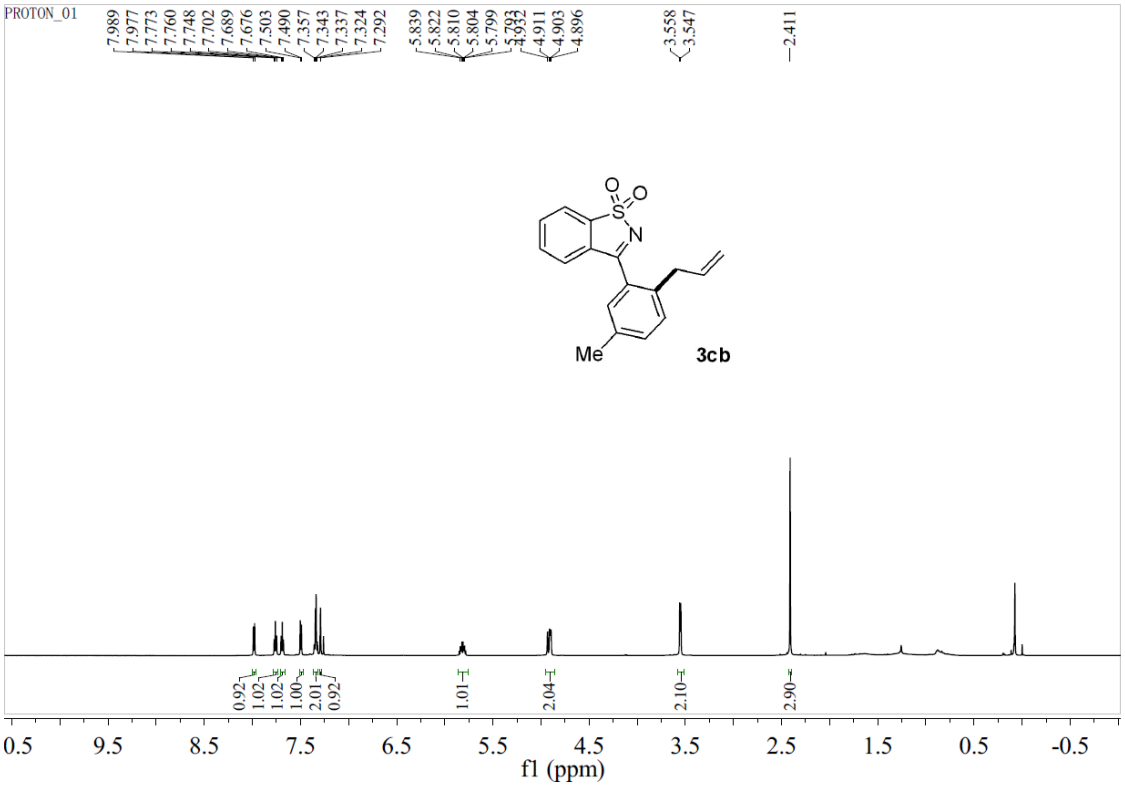
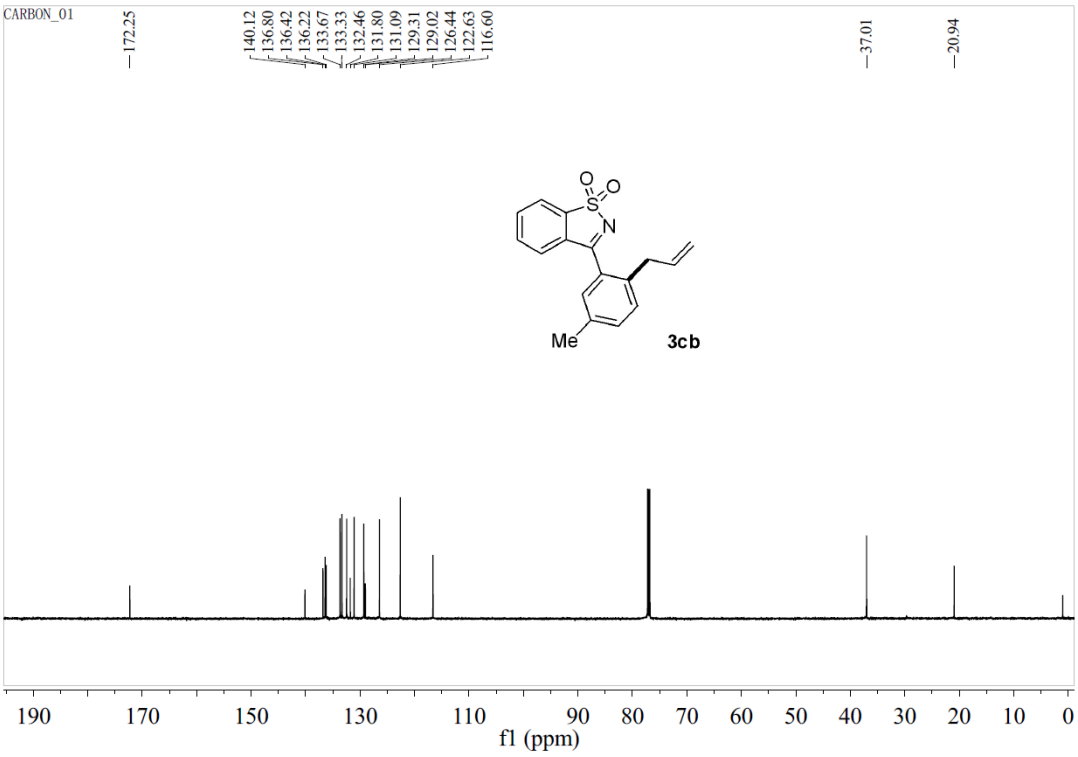
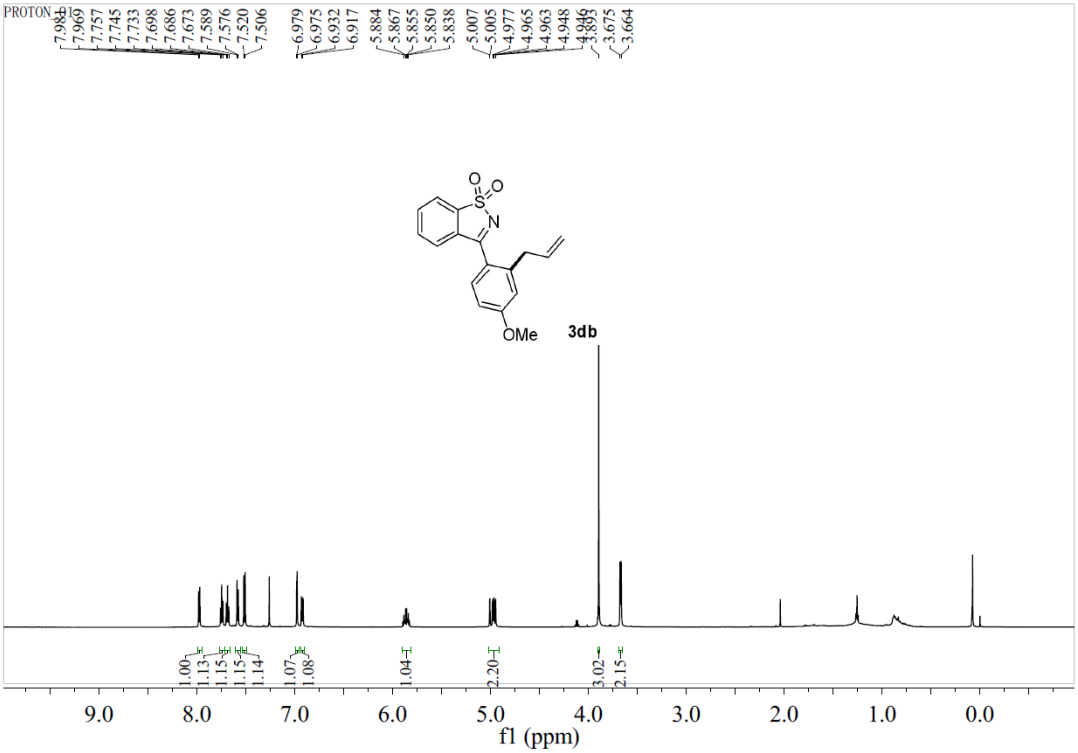
7.745
7.733
7.686
7.674
7.661
7.529
7.516
7.409
7.396
7.260
7.222
7.209
5.861
5.851
5.845
5.833
5.828
5.822
4.928
4.909
3.613
3.602
2.437
Me
3bb
1.00
1.13
1.21
1.08
1.11
1.25
1.09
1.08
2.21
2.27
3.39
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


CARBON_01
171.92
142.40
140.21
136.42
133.62
133.24
132.05
131.87
129.26
127.05
126.47
126.19
122.63
116.65
37.36
21.53
Me
3bb
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


PROTON_01
7.989
7.977
7.773
7.760
7.748
7.702
7.689
7.676
7.503
7.490
7.357
7.343
7.337
7.324
7.292
5.839
5.822
5.810
5.804
5.799
5.793
4.932
4.911
4.903
4.896
3.558
3.547
2.411
O
O
S
N
Me
3cb
0.92
1.02
1.02
1.00
2.01
0.92
1.01
2.04
2.10
2.90
0.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


CARBON_01
172.25
140.12
136.80
136.42
136.22
133.67
133.33
132.46
131.80
131.09
129.31
129.02
126.44
122.63
116.60
37.01
20.94
O
O
S
N
Me
3cb
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


PROTON_1
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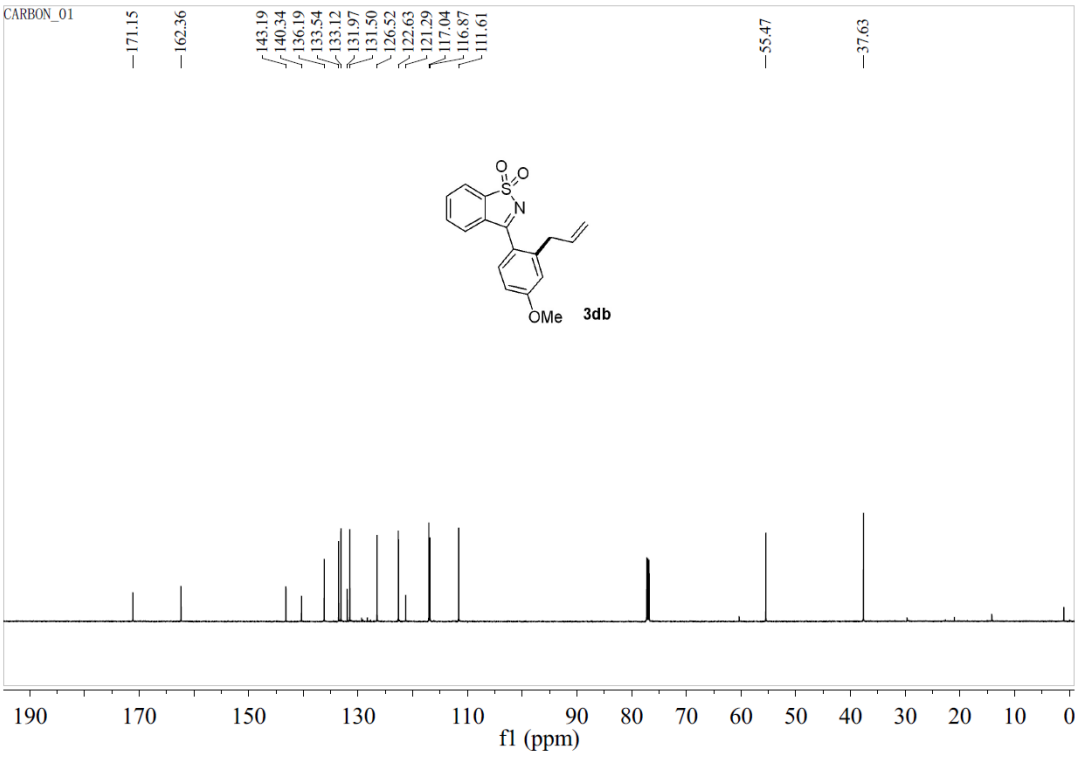
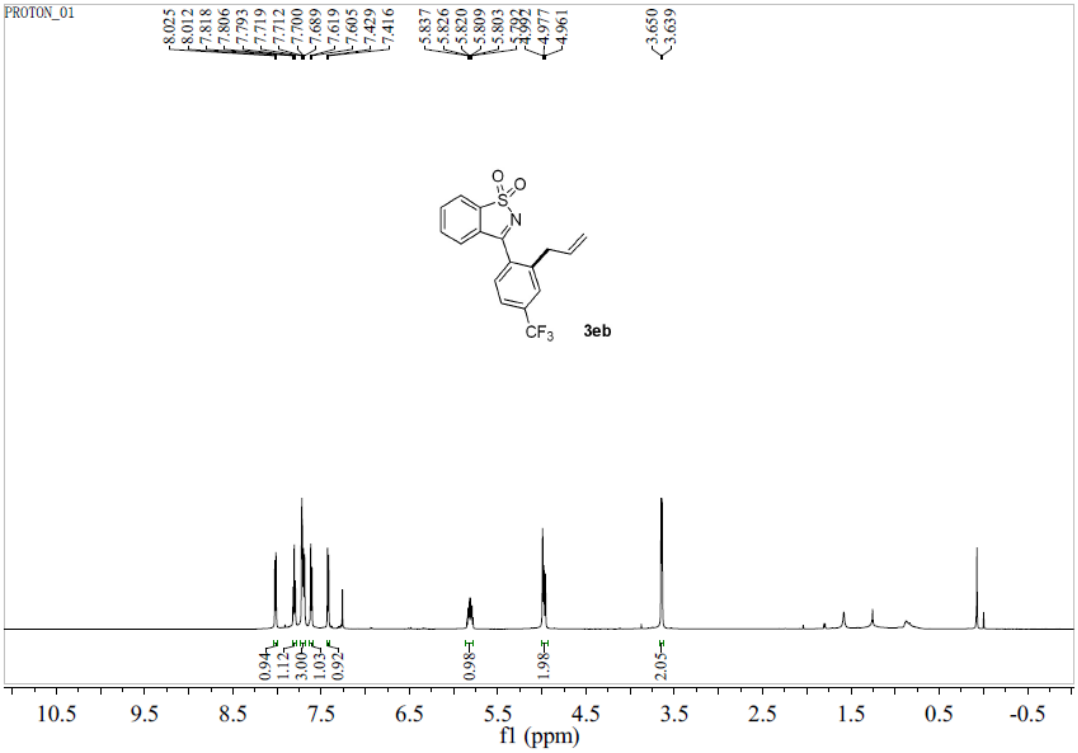
7.969
7.757
7.745
7.733
7.698
7.686
7.673
7.589
7.576
7.520
7.506
6.979
6.975
6.932
6.917
5.884
5.867
5.855
5.850
5.838
5.007
5.005
4.977
4.965
4.963
4.948
4.946
3.893
3.675
3.664
OMe
3db
1.00
1.13
1.15
1.15
1.14
1.07
1.08
1.04
2.20
3.02
2.15
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


CARBON_01
171.15
162.36
143.19
140.34
136.19
133.54
133.12
131.97
131.50
126.52
122.63
121.29
117.04
116.87
111.61
55.47
37.63
OMe
3db
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


PROTON_01
8.025
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7.793
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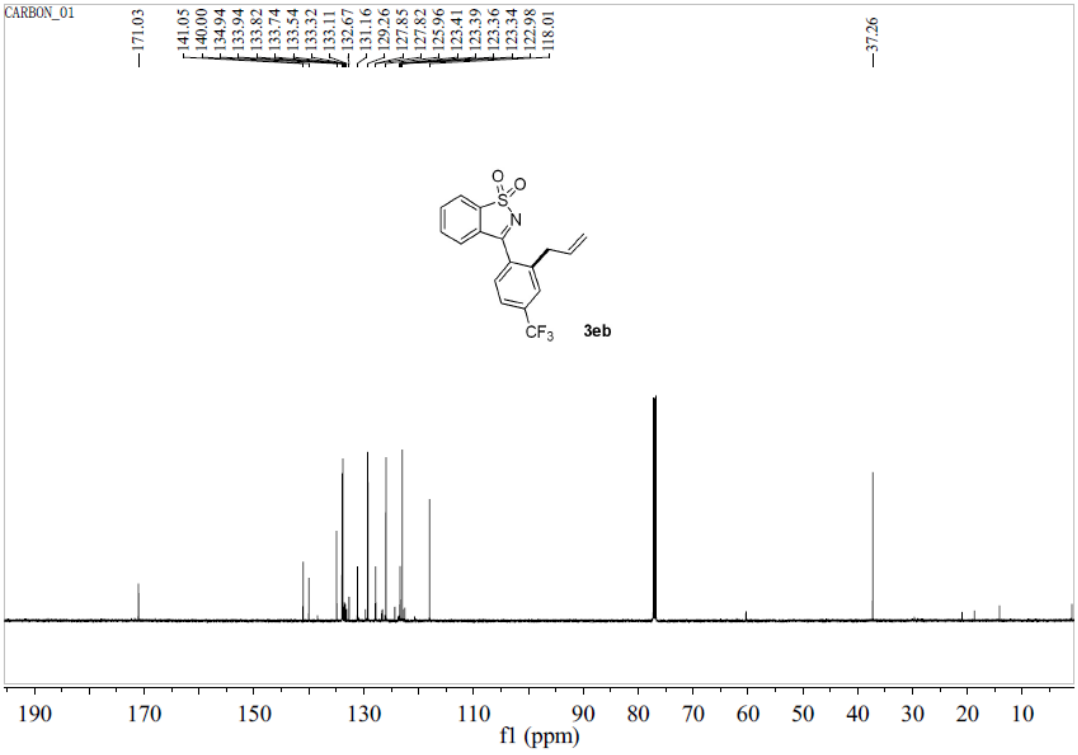
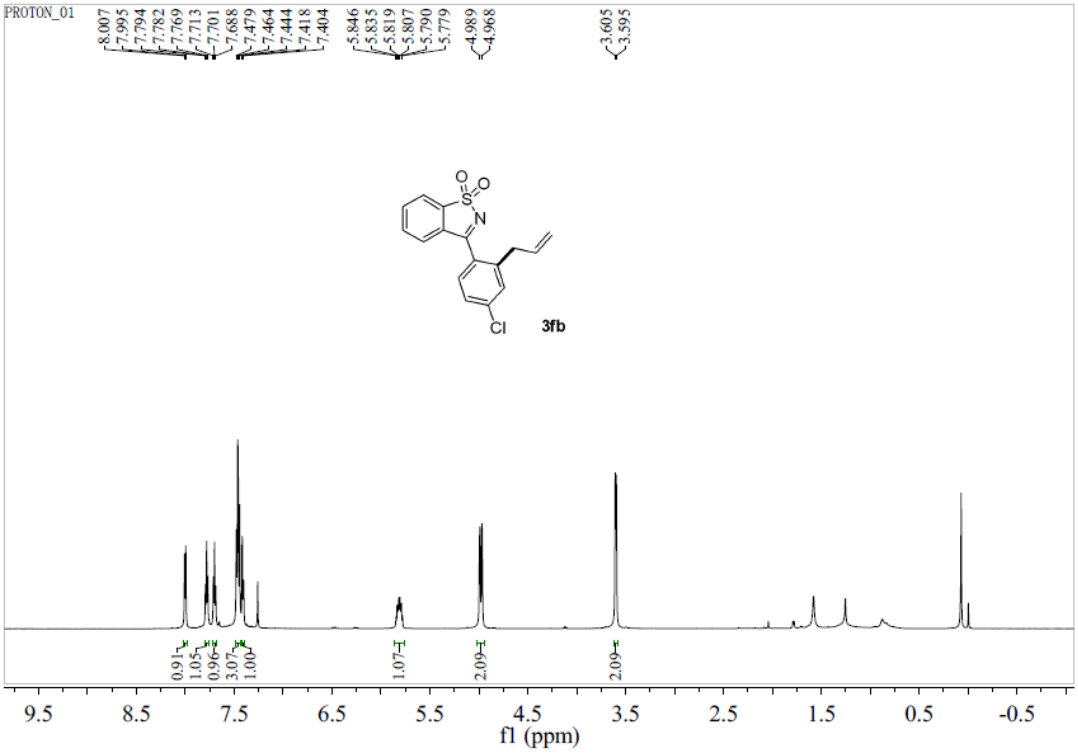
7.712
7.700
7.689
7.619
7.605
7.429
7.416
5.837
5.826
5.820
5.809
5.803
4.977
4.961
3.650
3.639
3eb
0.94
1.12
3.00
1.03
0.92
0.98
1.98
2.05
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


CARBON_01
171.03
141.05
140.00
134.94
133.94
133.82
133.74
133.54
133.32
133.11
132.67
131.16
129.26
127.85
127.82
125.96
123.41
123.39
123.36
123.34
122.98
118.01
37.26
3eb
190
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)


PROTON_01
8.007
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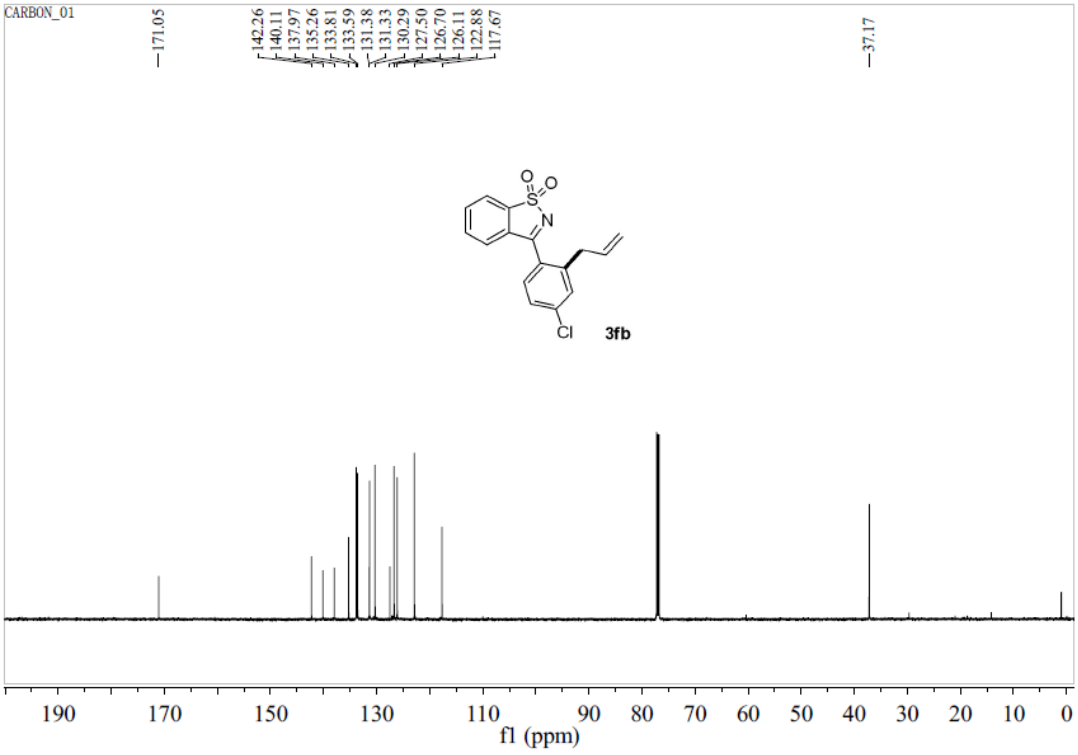
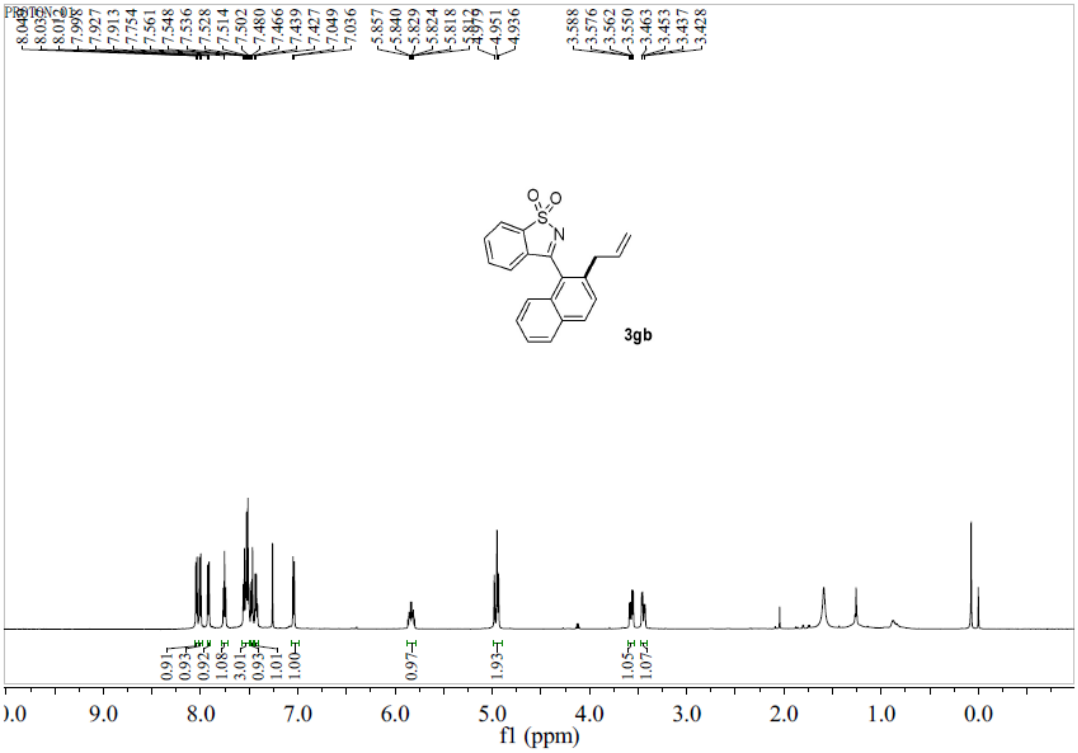
7.713
7.701
7.688
7.479
7.464
7.444
7.418
7.404
5.846
5.835
5.819
5.807
5.790
5.779
4.989
4.968
3.605
3.595
3fb
0.91
1.05
0.96
3.07
1.00
1.07
2.09
2.09
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


CARBON_01
171.05
142.26
140.11
137.97
135.26
133.81
133.59
131.38
131.33
130.29
127.50
126.70
126.11
122.88
117.67
37.17
3fb
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


PROTON-1
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8.039
8.017
7.998
7.927
7.913
7.754
7.561
7.548
7.536
7.528
7.514
7.502
7.480
7.466
7.439
7.427
7.049
7.036
5.857
5.840
5.829
5.824
5.818
5.812
4.979
4.951
4.936
3.588
3.576
3.562
3.550
3.463
3.453
3.437
3.428
3gb
0.91
0.93
0.92
1.08
3.01
0.93
1.01
1.00
0.97
1.93
1.05
1.07
0.0
9.0
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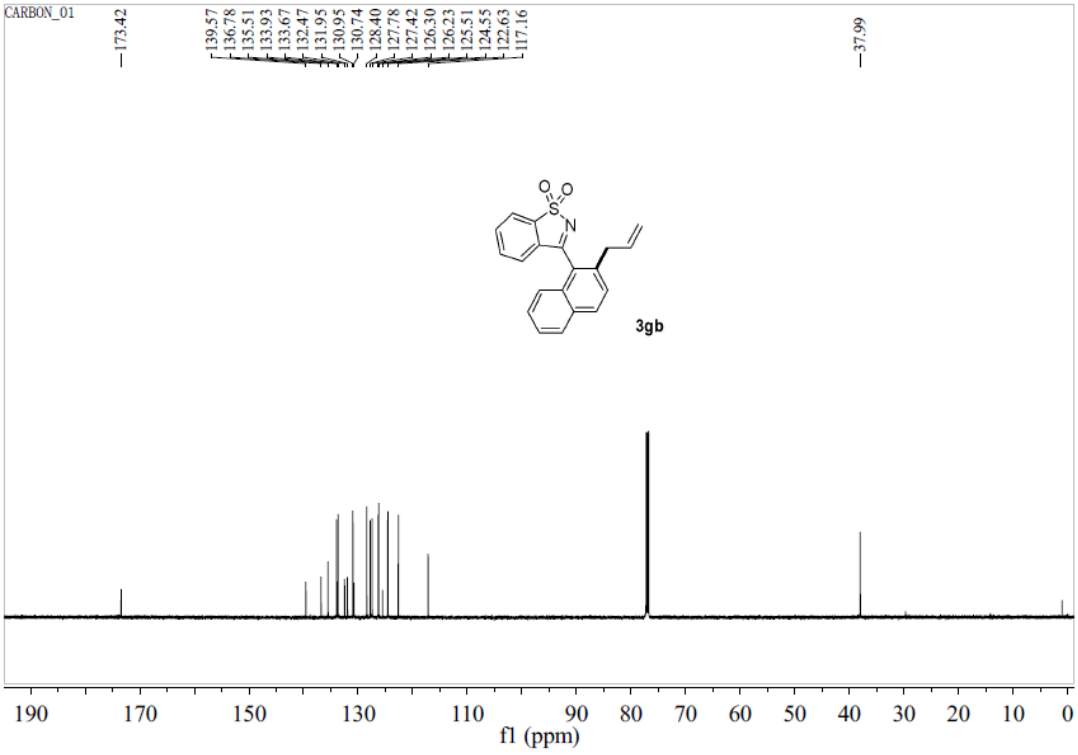
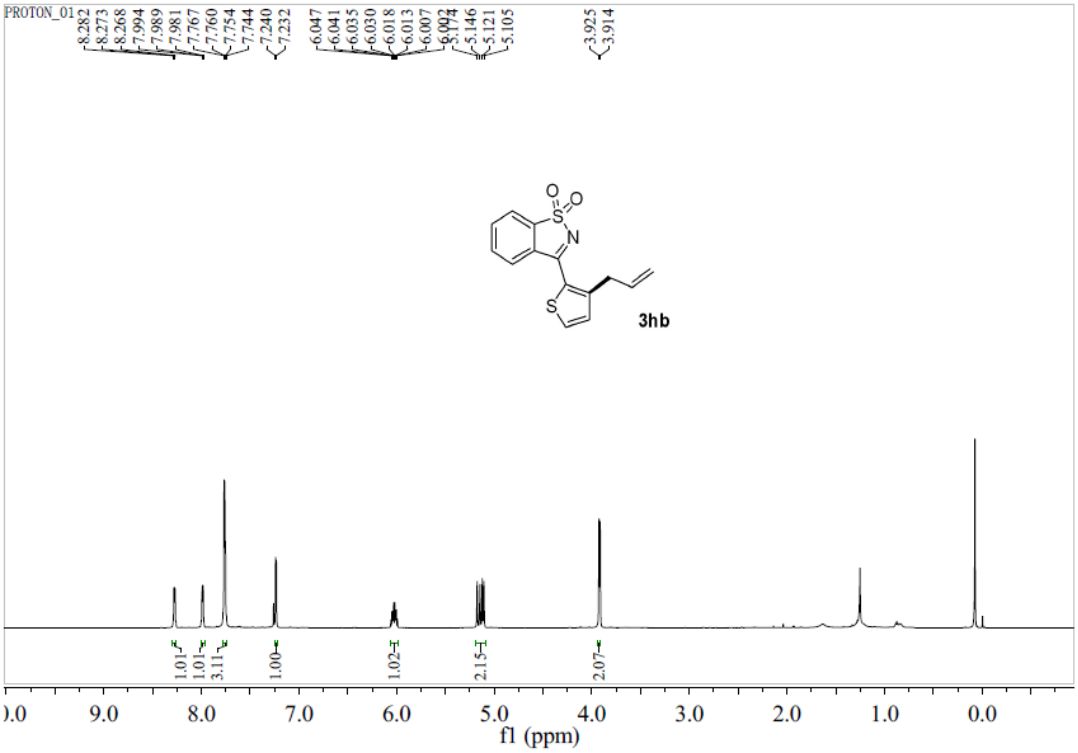
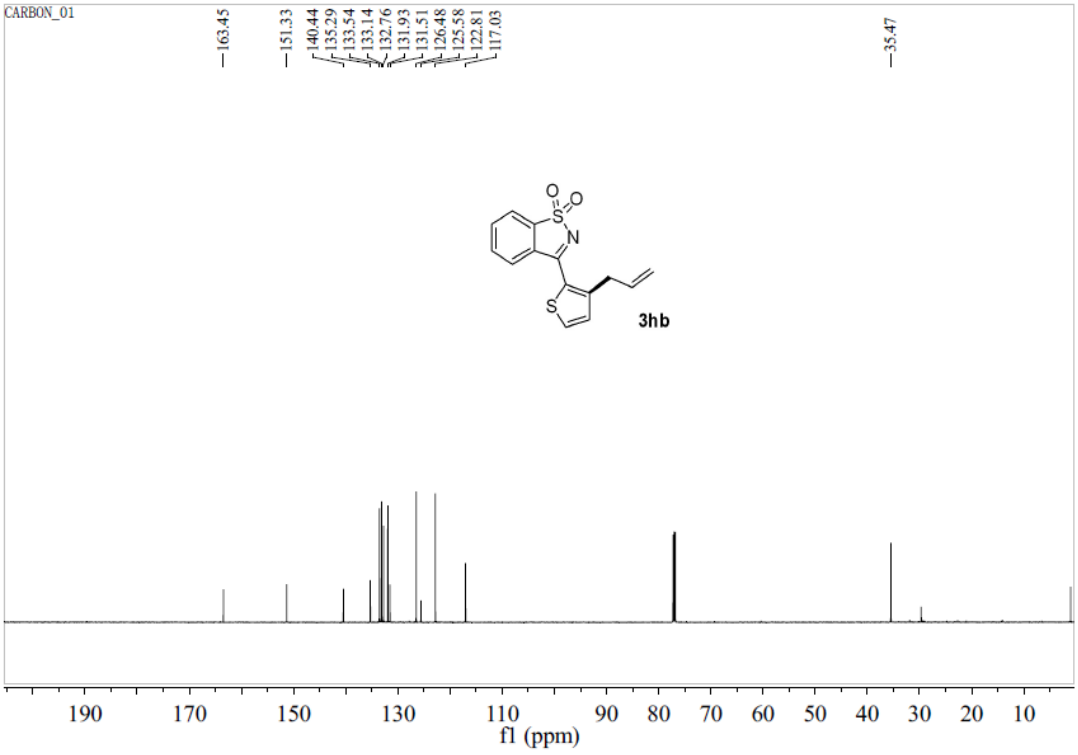
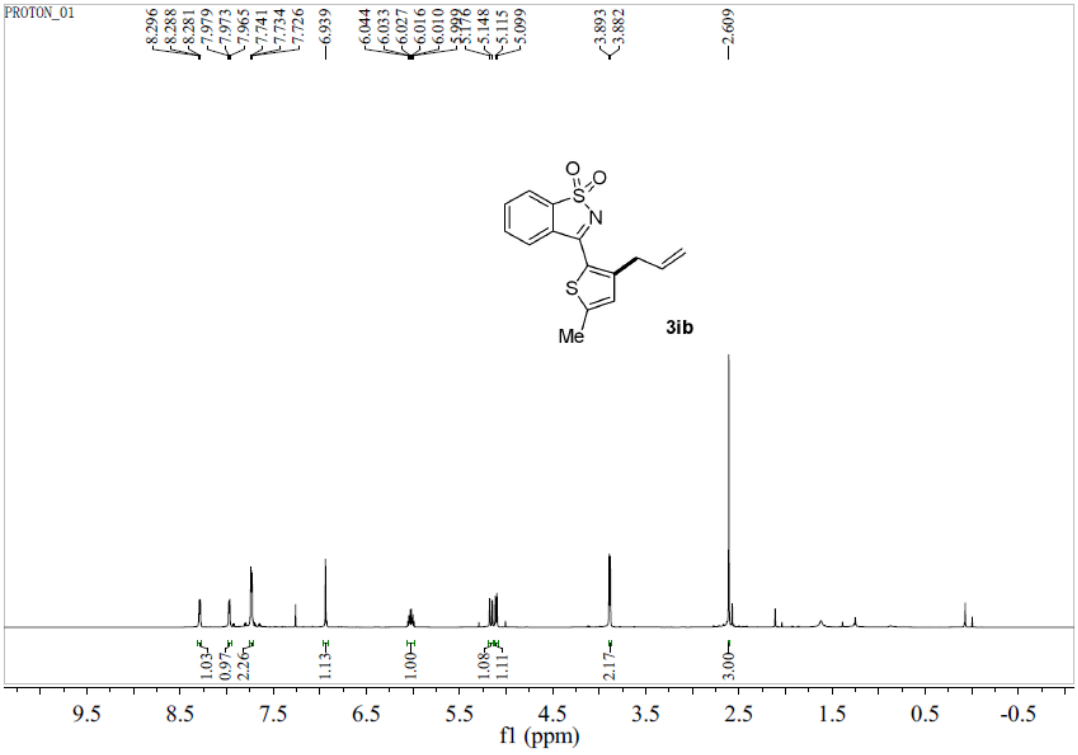
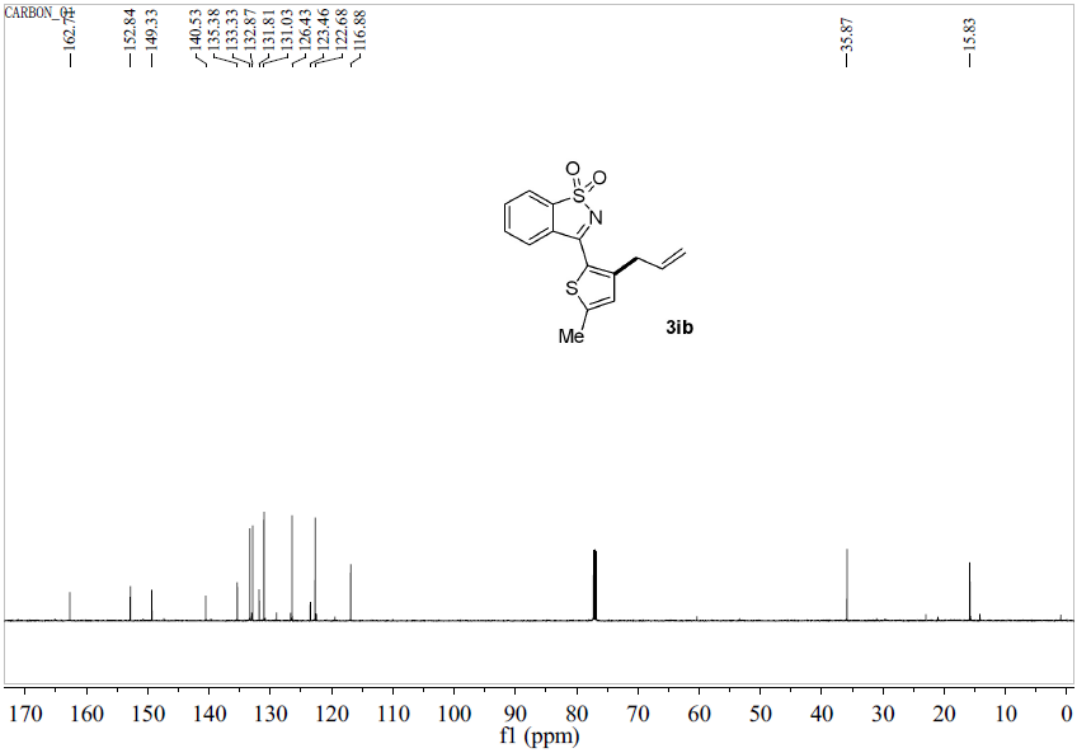
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

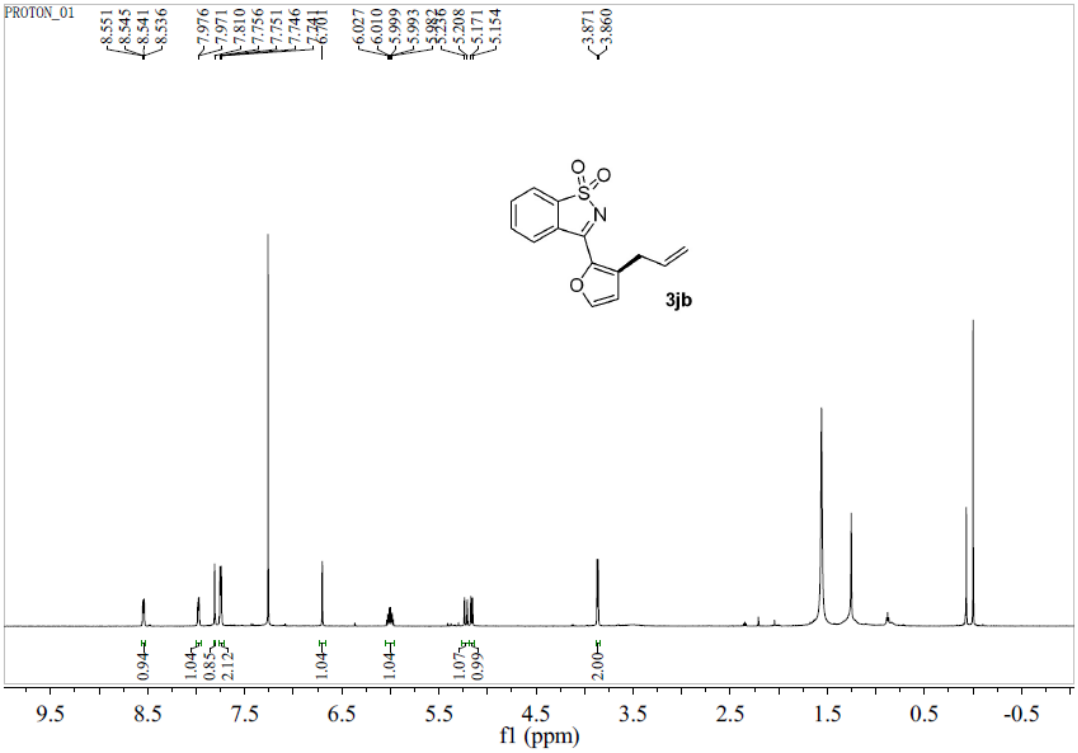

CARBON_01
173.42
139.57
136.78
135.51
133.93
133.67
132.47
131.95
130.95
130.74
128.40
127.78
127.42
126.30
126.23
125.51
124.55
122.63
117.16
37.99
3gb
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

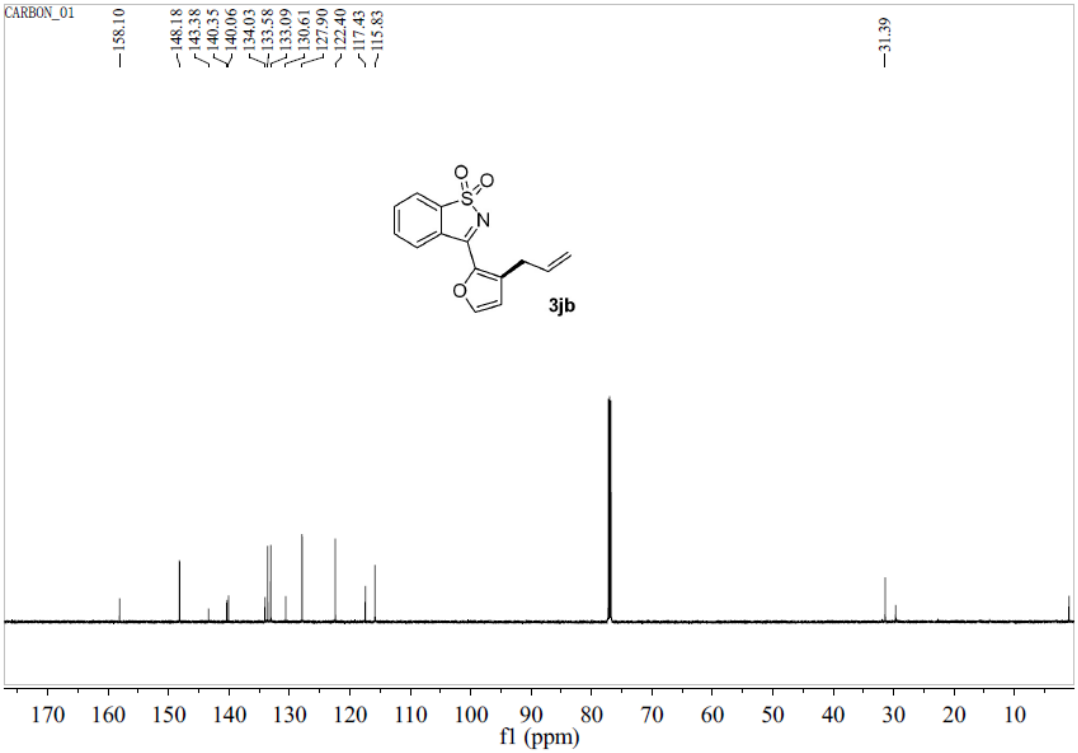

PROTON_01
8.282
8.273
8.268
7.994
7.989
7.981
7.767
7.760
7.754
7.744
7.240
7.232
6.047
6.041
6.035
6.030
6.018
6.013
6.007
5.146
5.121
5.105
3.925
3.914
3hb
1.01
1.01
3.11
1.00
1.02
2.15
2.07
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

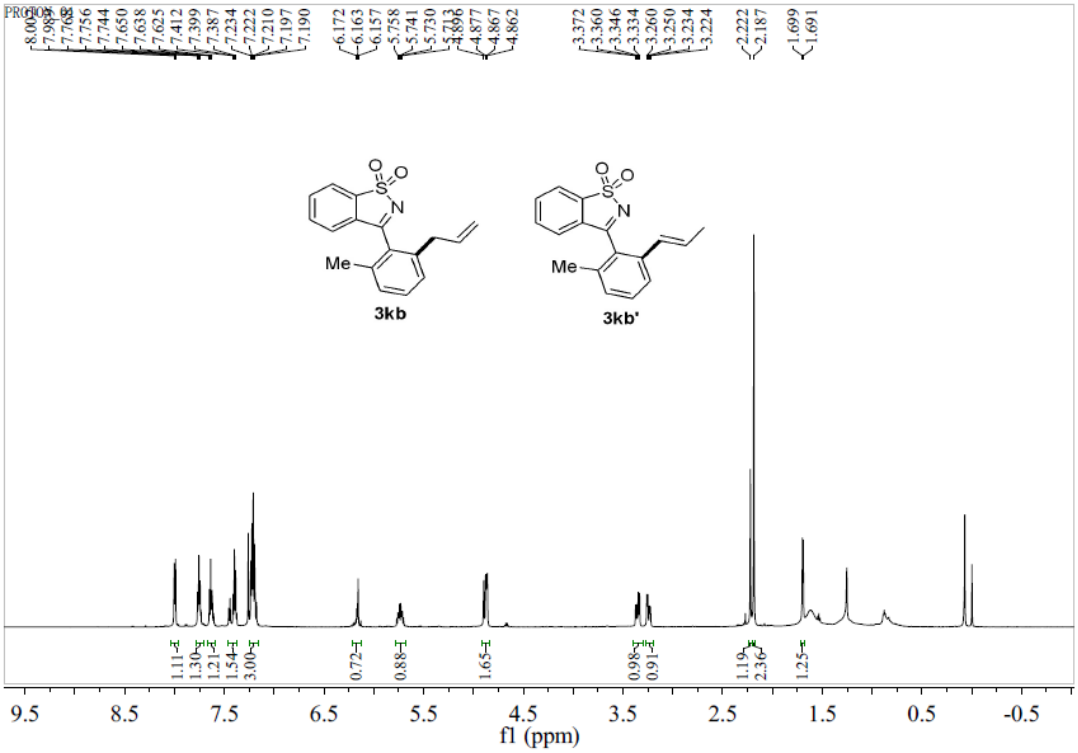

CARBON_01
163.45
151.33
140.44
135.29
133.54
133.14
132.76
131.93
131.51
126.48
125.58
122.81
117.03
35.47
3hb
190
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

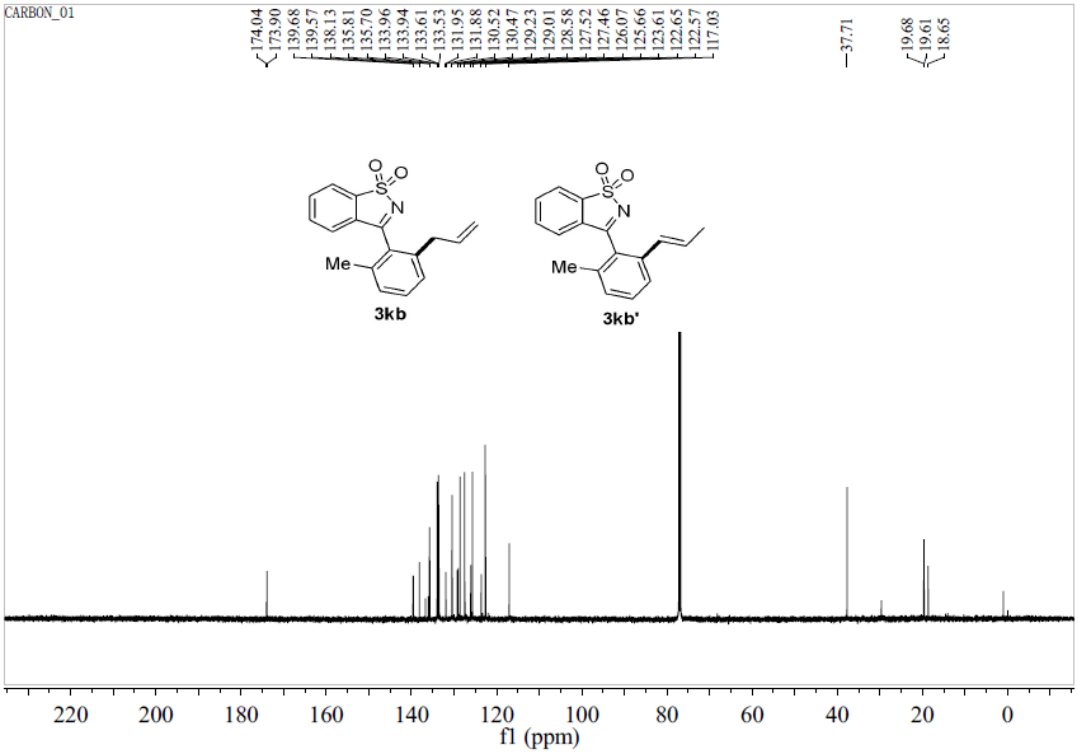

PROTON_01
8.296
8.288
8.281
7.979
7.973
7.965
7.741
7.734
7.726
6.939
6.044
6.033
6.027
6.016
6.010
5.999
5.178
5.148
5.115
5.099
3.893
3.882
2.609
1.03
0.97
2.26
1.13
1.00
1.08
1.11
2.17
3.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)
O
O
S
N
S
Me
3ib

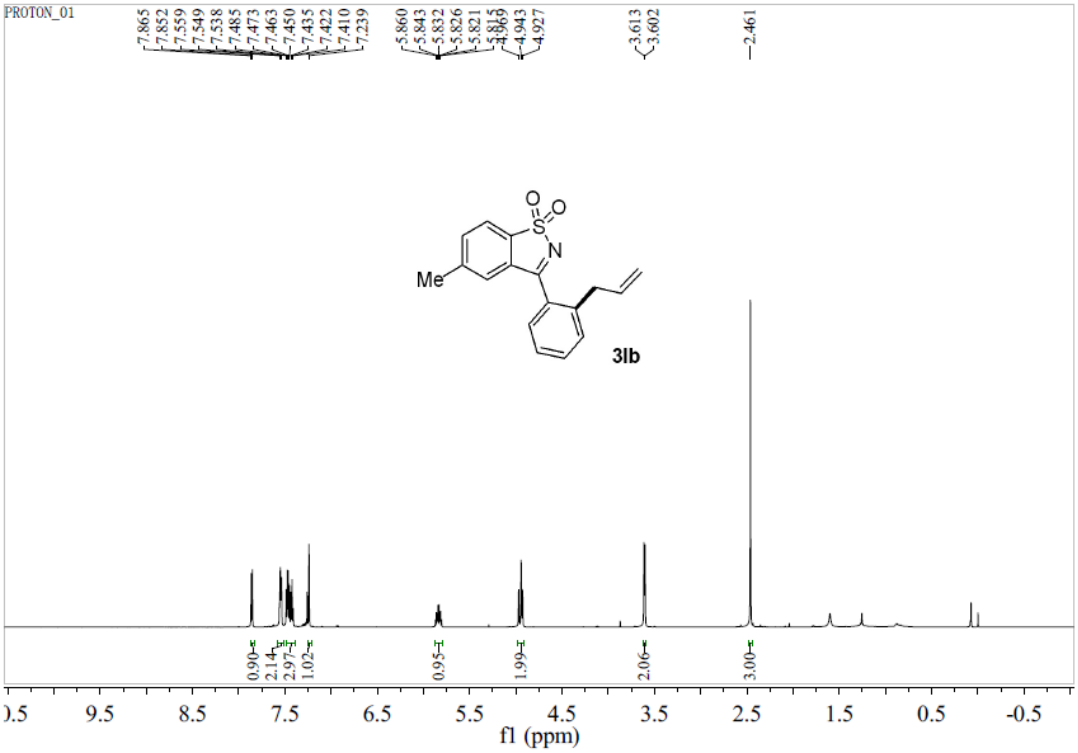

CARBON_01
162.74
152.84
149.33
140.53
135.38
133.33
132.87
131.81
131.03
126.43
123.46
122.68
116.88
35.87
15.83
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
O
S
N
S
Me
3ib

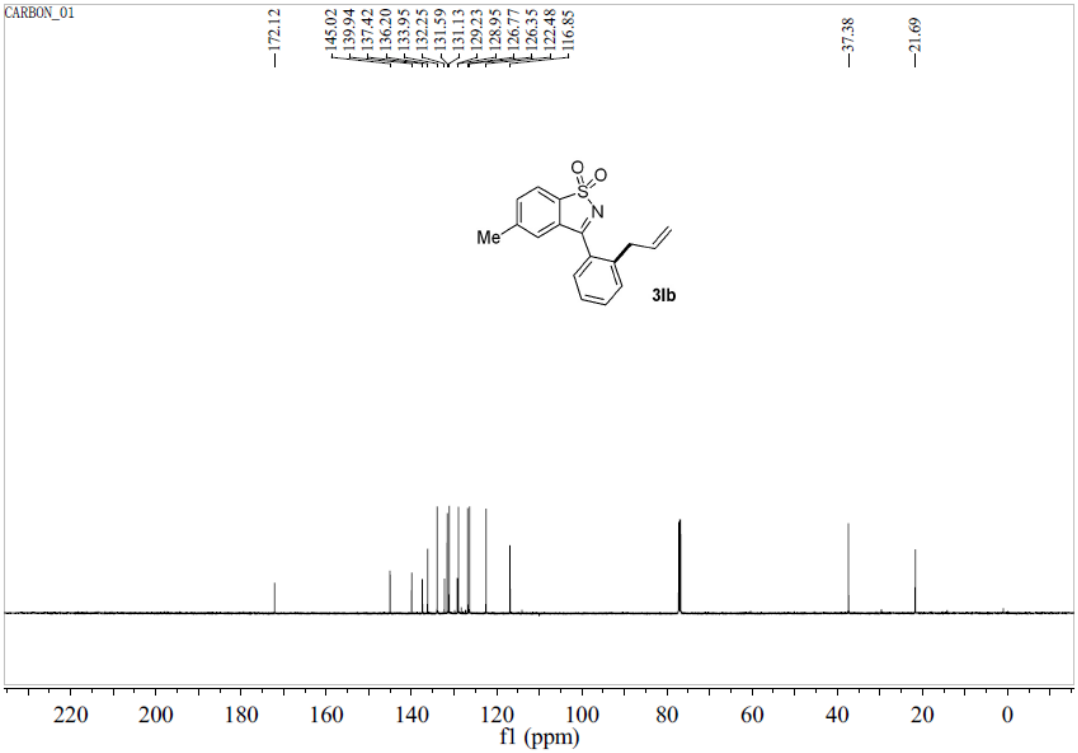

PROTON_01
8.551
8.545
8.541
8.536
7.976
7.971
7.810
7.756
7.751
7.746
7.741
6.701
6.027
6.010
5.999
5.993
5.208
5.171
5.154
3.871
3.860
0.94
1.04
0.85
2.12
1.04
1.04
1.07
0.99
2.00
3jb
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

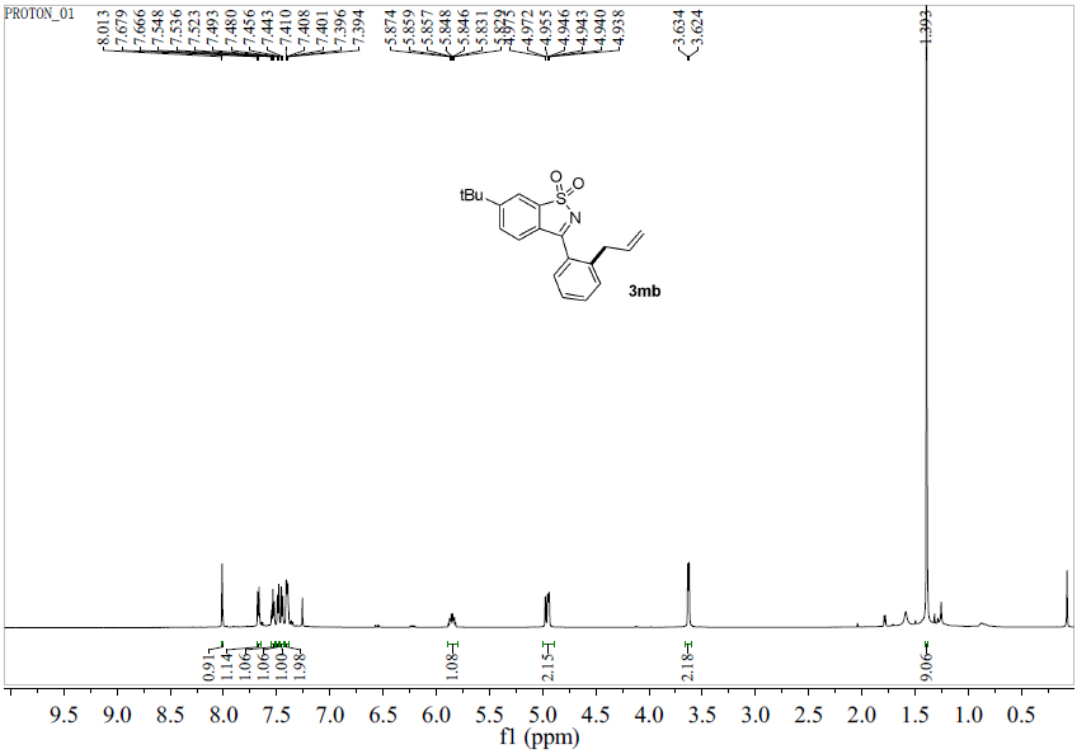

CARBON_01
158.10
148.18
143.38
140.35
140.06
134.03
133.58
133.09
130.61
127.90
122.40
117.43
115.83
31.39
3jb
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

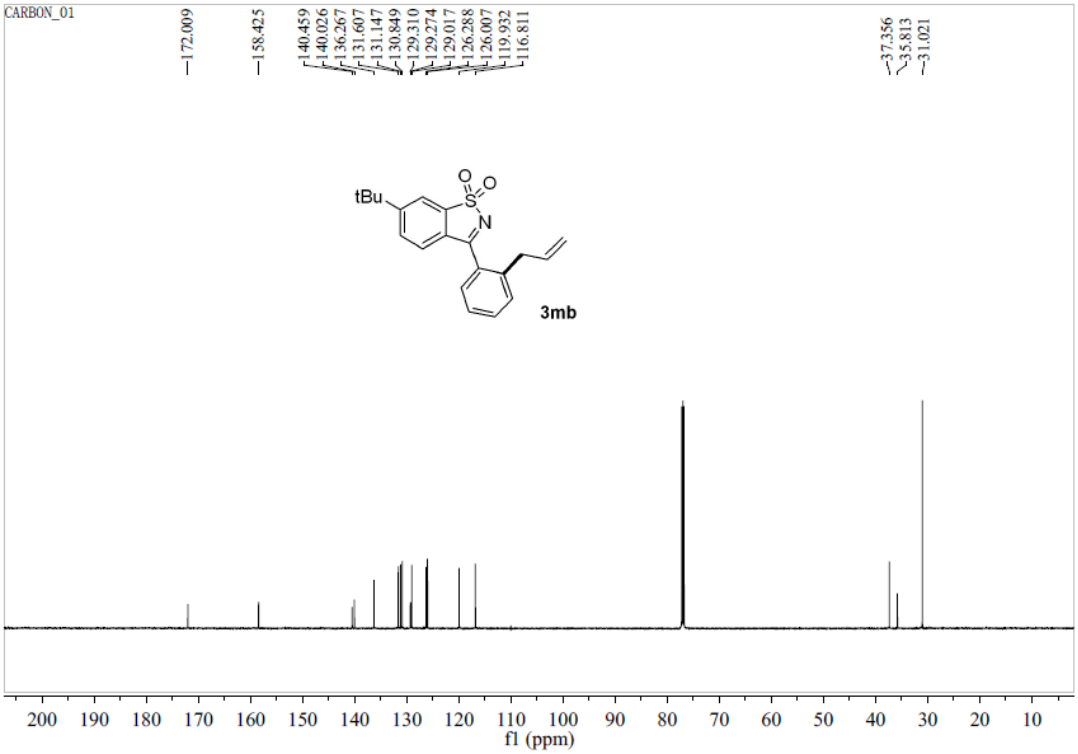

PROTON_01
8.002
7.988
7.762
7.756
7.744
7.650
7.638
7.625
7.412
7.399
7.387
7.234
7.222
7.210
7.197
7.190
6.172
6.163
6.157
5.758
5.741
5.730
5.713
5.696
4.877
4.867
4.862
3.372
3.360
3.346
3.334
3.260
3.250
3.234
3.224
2.222
2.187
1.699
1.691
Me
3kb
Me
3kb'
1.11
1.30
1.21
1.54
3.00
0.72
0.88
1.65
0.98
0.91
1.19
2.36
1.25
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

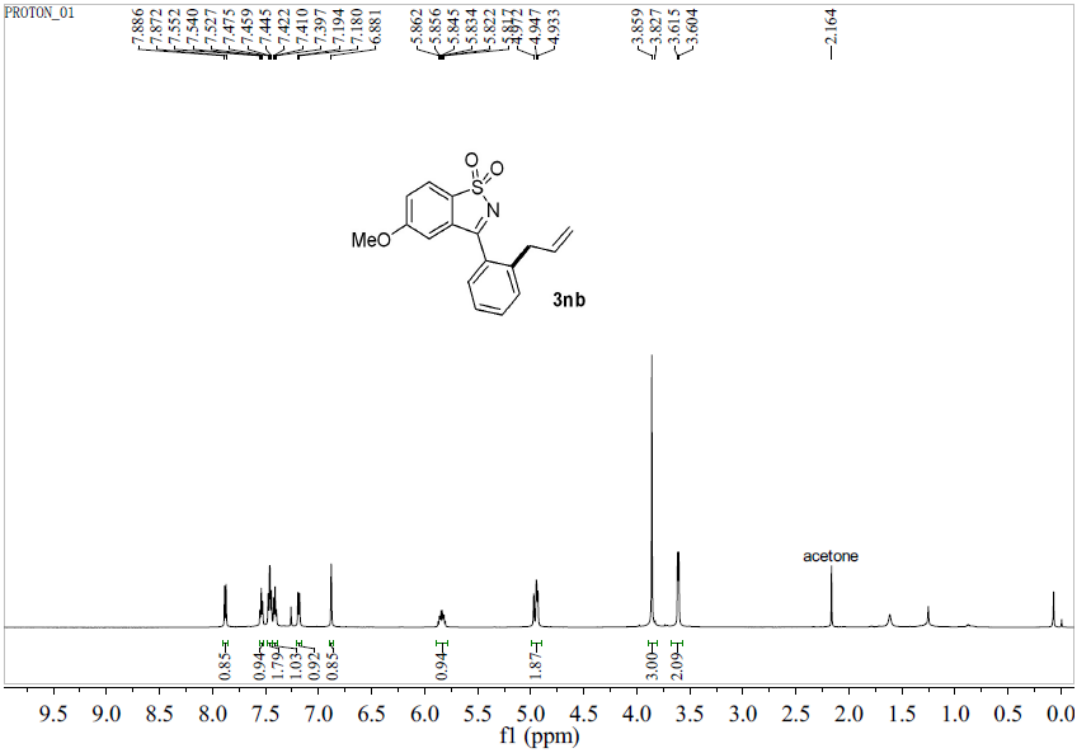

CARBON_01
174.04
173.90
139.68
139.57
138.13
135.81
135.70
133.96
133.94
133.61
133.53
131.95
131.88
130.52
130.47
129.23
129.01
128.58
127.52
127.46
126.07
125.66
123.61
122.65
122.57
117.03
37.71
19.68
19.61
18.65
Me
3kb
Me
3kb'
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

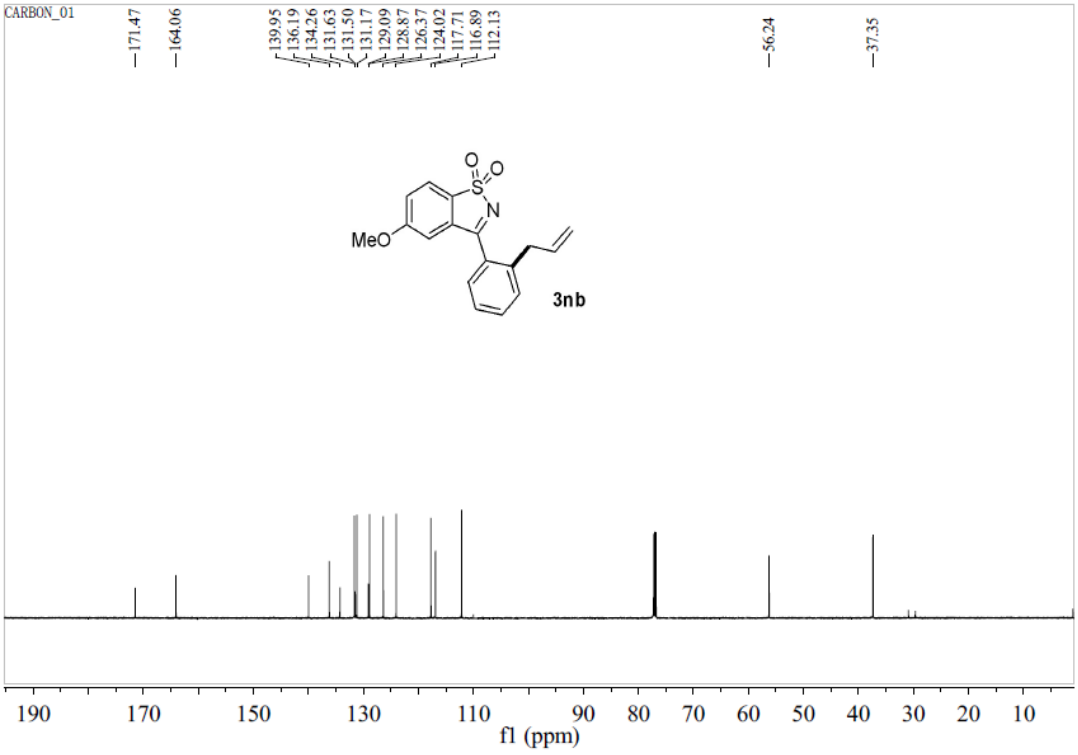

PROTON_01
7.865
7.852
7.559
7.549
7.538
7.485
7.473
7.463
7.450
7.435
7.422
7.410
7.239
5.860
5.843
5.832
5.826
5.821
4.969
4.943
4.927
3.613
3.602
2.461
Me
3Ib
0.90
2.14
2.97
1.02
0.95
1.99
2.06
3.00
0.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

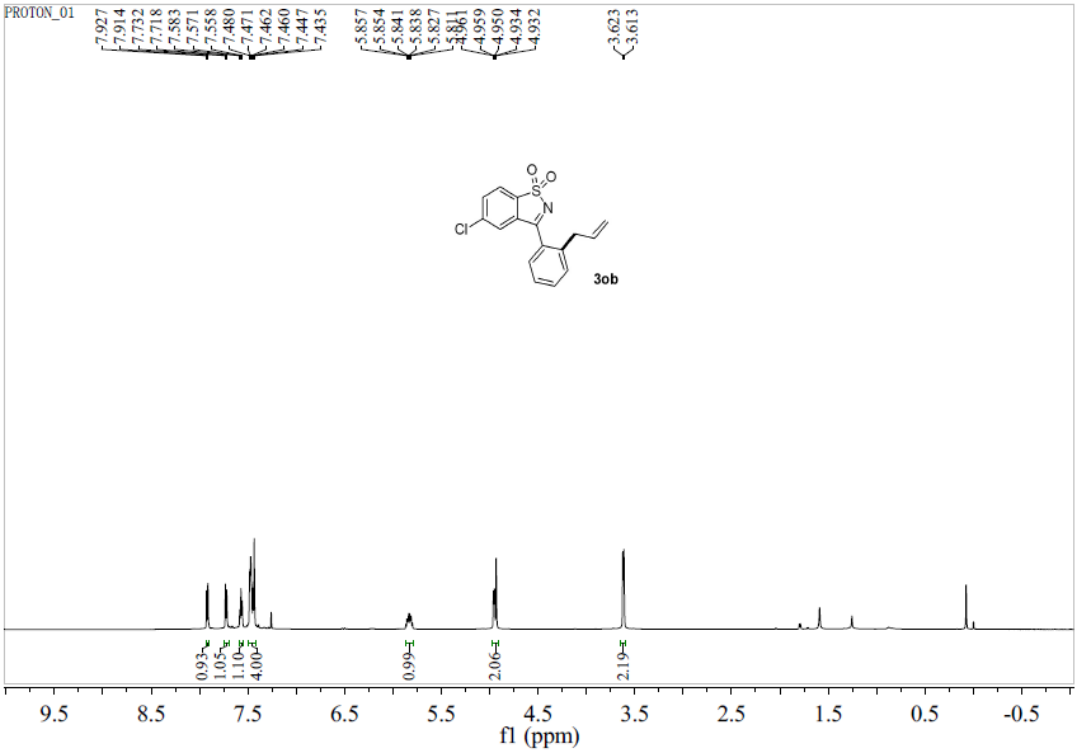

CARBON_01
172.12
145.02
139.94
137.42
136.20
133.95
132.25
131.59
131.13
129.23
128.95
126.77
126.35
122.48
116.85
37.38
21.69
Me
3Ib
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

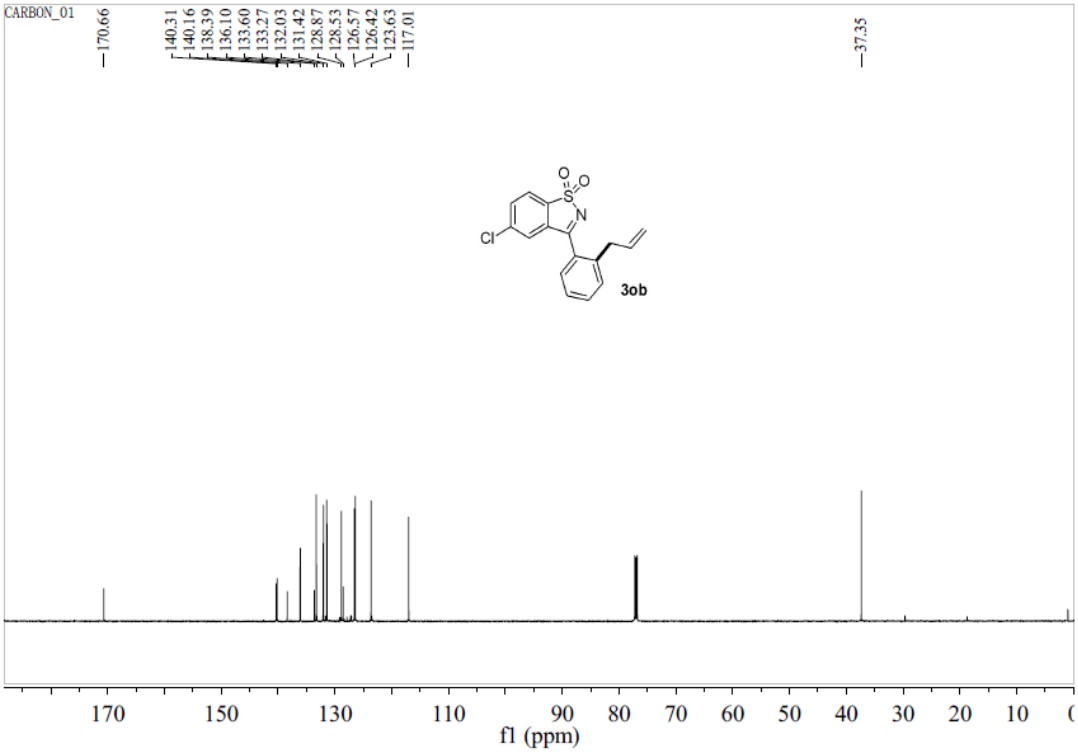

PROTON_01
8.013
7.679
7.666
7.548
7.536
7.523
7.493
7.480
7.456
7.443
7.410
7.408
7.401
7.396
7.394
5.874
5.859
5.857
5.848
5.846
5.831
5.829
4.972
4.955
4.946
4.943
4.940
4.938
3.634
3.624
1.393
tBu
3mb
0.91
1.14
1.06
1.06
1.00
1.98
1.08
2.15
2.18
9.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

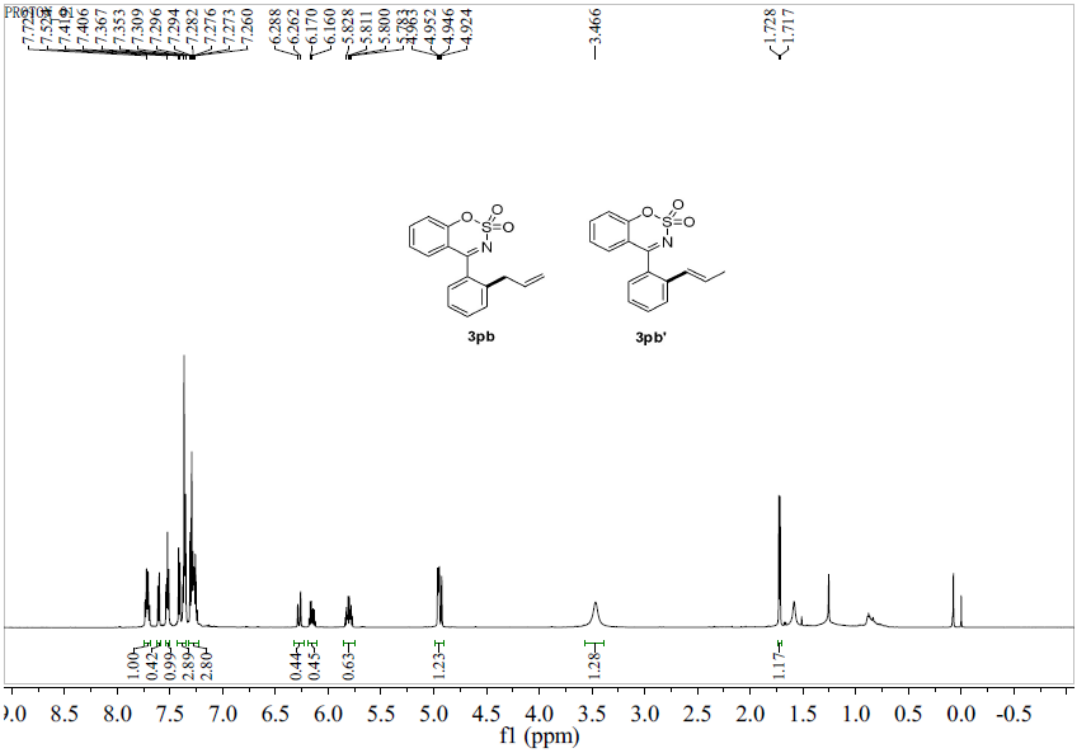

CARBON_01
172.009
158.425
140.459
140.026
136.267
131.607
131.147
130.849
129.310
129.274
129.017
126.288
126.007
119.932
116.811
37.356
35.813
31.021
tBu
3mb
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

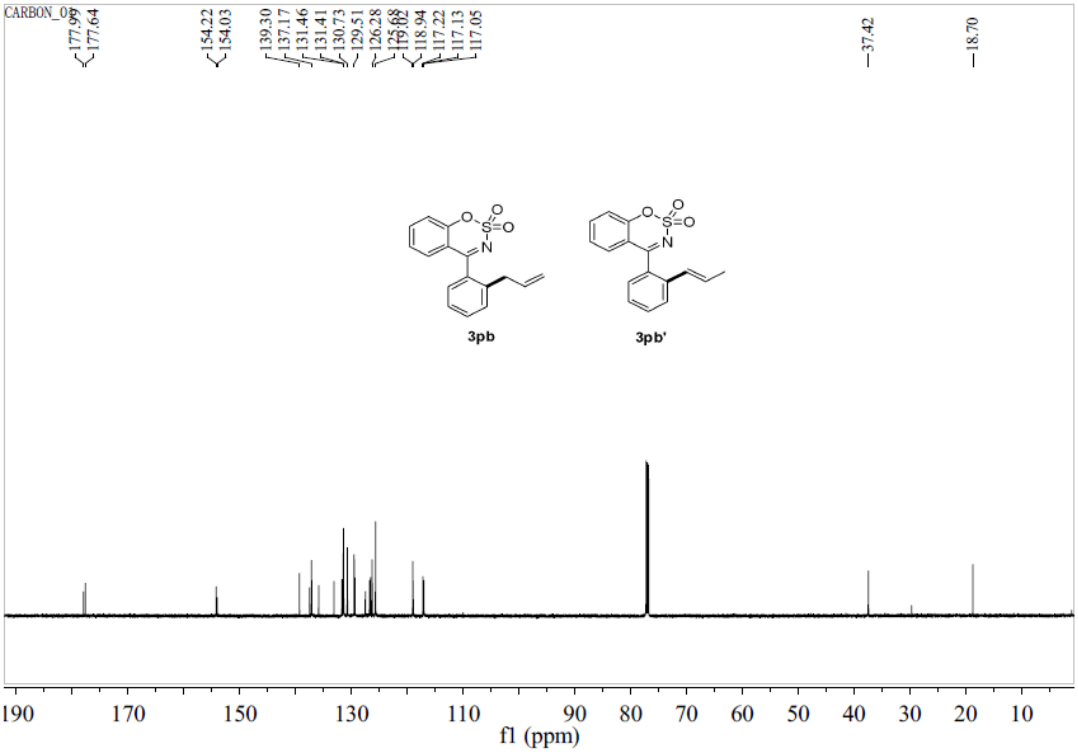

PROTON_01
7.886
7.872
7.552
7.540
7.527
7.475
7.459
7.445
7.422
7.410
7.397
7.194
7.180
6.881
5.862
5.856
5.845
5.834
5.822
4.972
4.947
4.933
3.859
3.827
3.615
3.604
2.164
MeO
3nb
acetone
0.85
0.94
1.79
1.03
0.92
0.85
0.94
1.87
3.00
2.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

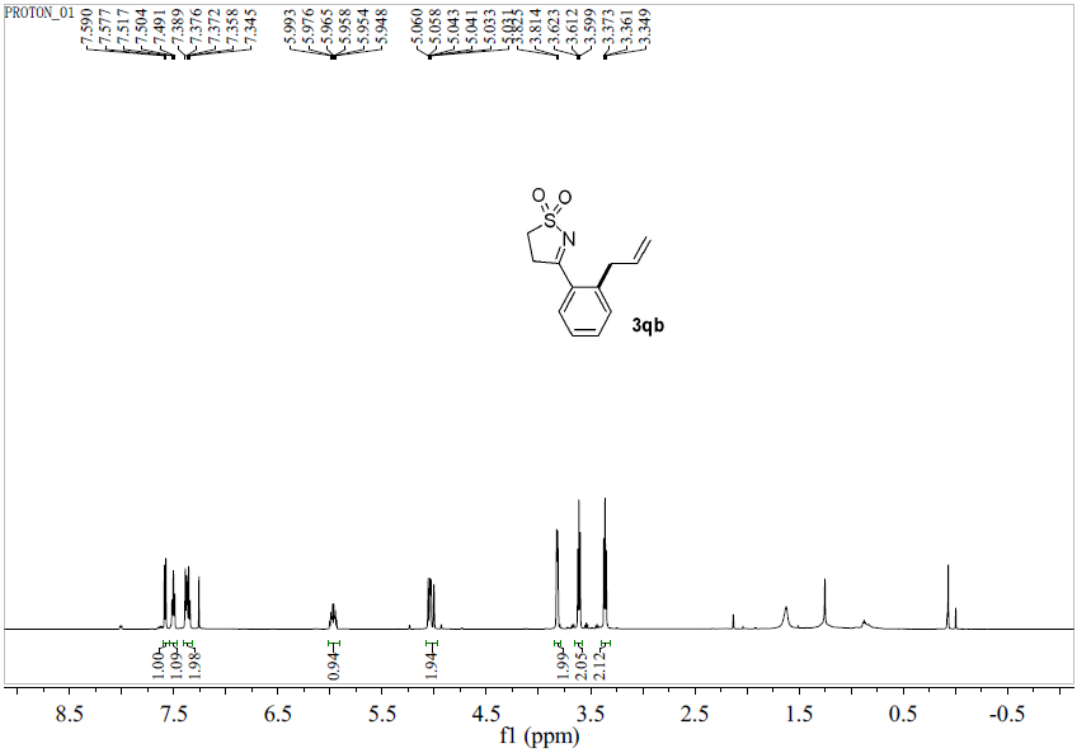

CARBON_01
171.47
164.06
139.95
136.19
134.26
131.63
131.50
131.17
129.09
128.87
126.37
124.02
117.71
116.89
112.13
56.24
37.35
MeO
3nb
190 170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

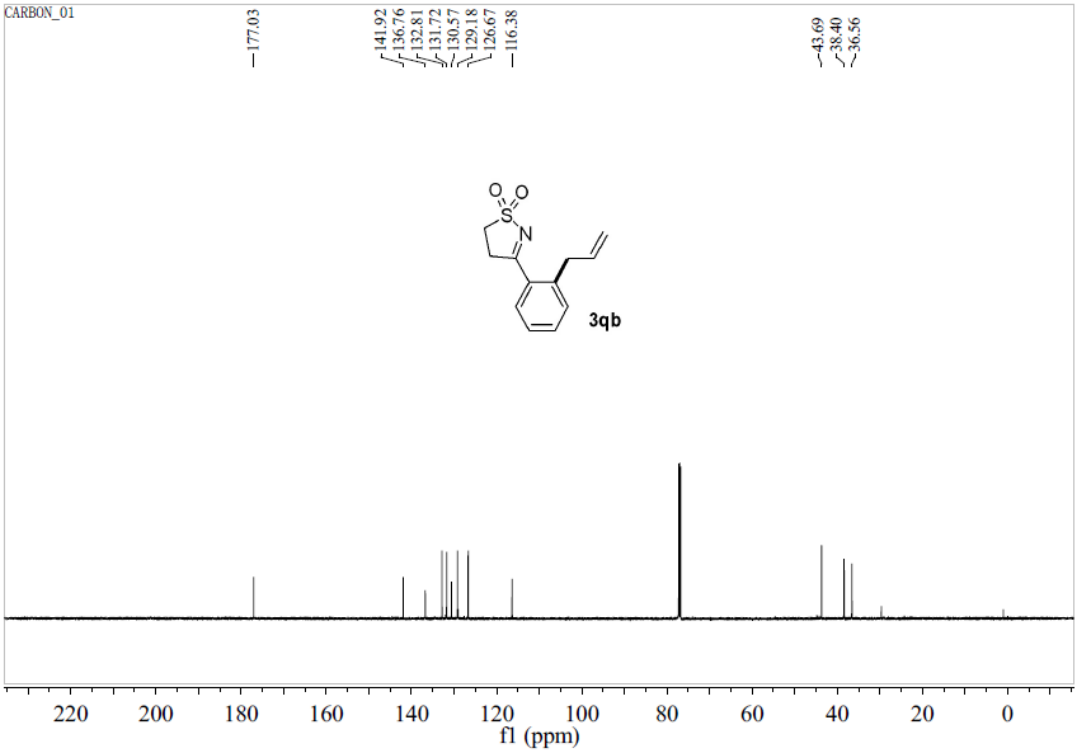

PROTON_01
7.927
7.914
7.732
7.718
7.583
7.571
7.558
7.480
7.471
7.462
7.460
7.447
7.435
5.857
5.854
5.841
5.838
5.827
4.961
4.959
4.950
4.934
4.932
3.623
3.613
3ob
0.93
1.05
1.10
4.00
0.99
2.06
2.19
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

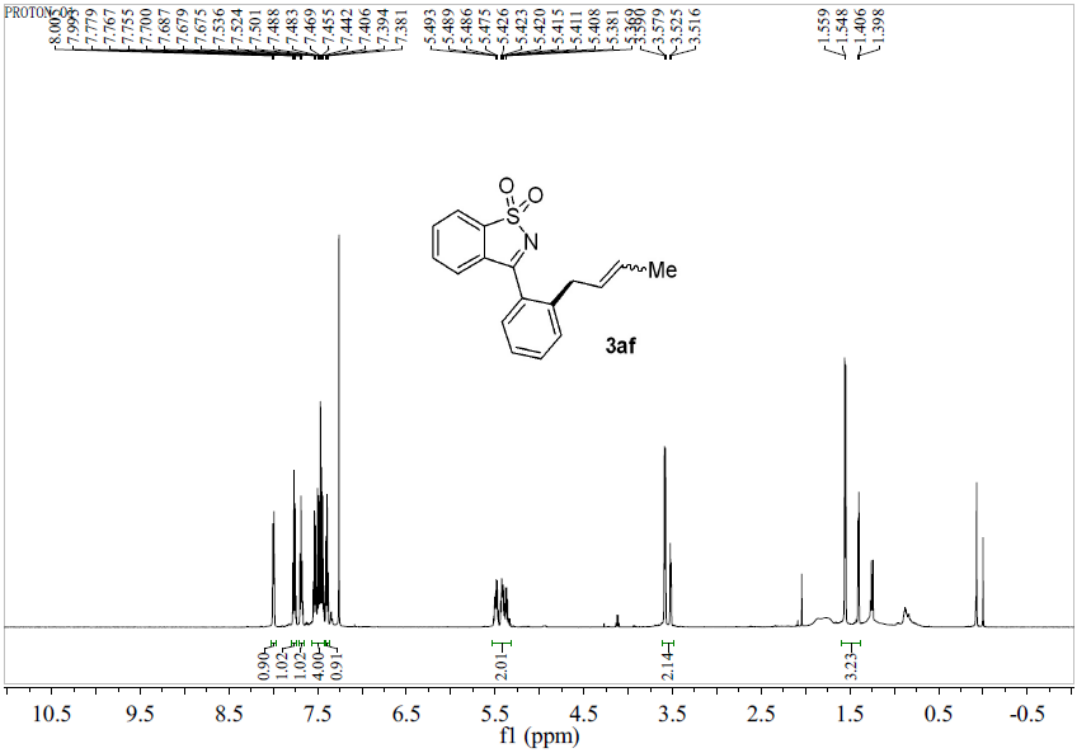

CARBON_01
170.66
140.31
140.16
138.39
136.10
133.60
133.27
132.03
131.42
128.87
128.53
126.57
126.42
123.63
117.01
37.35
3ob
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.728
7.526
7.419
7.406
7.367
7.353
7.309
7.296
7.294
7.282
7.276
7.273
7.260
6.288
6.262
6.170
6.160
5.828
5.811
5.800
5.783
4.963
4.952
4.946
4.924
3.466
1.728
1.717
3pb
3pb'
1.00
0.42
0.99
2.89
2.80
0.44
0.45
0.63
1.23
1.28
1.17
f1 (ppm)


CARBON_07
177.99
177.64
154.22
154.03
139.30
137.17
131.46
131.41
130.73
129.51
126.28
118.94
117.22
117.13
117.05
37.42
18.70
3pb
3pb'
f1 (ppm)


PROTON_01
7.590
7.577
7.517
7.504
7.491
7.389
7.376
7.372
7.358
7.345
5.993
5.976
5.965
5.958
5.954
5.948
5.060
5.058
5.043
5.041
5.033
3.825
3.814
3.623
3.612
3.599
3.373
3.361
3.349
3qb
1.00
1.09
1.98
0.94
1.94
1.99
2.05
2.12
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


CARBON_01
177.03
141.92
136.76
132.81
131.72
130.57
129.18
126.67
116.38
43.69
38.40
36.56
3qb
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


PROTON_01
8.005
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7.755
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7.687
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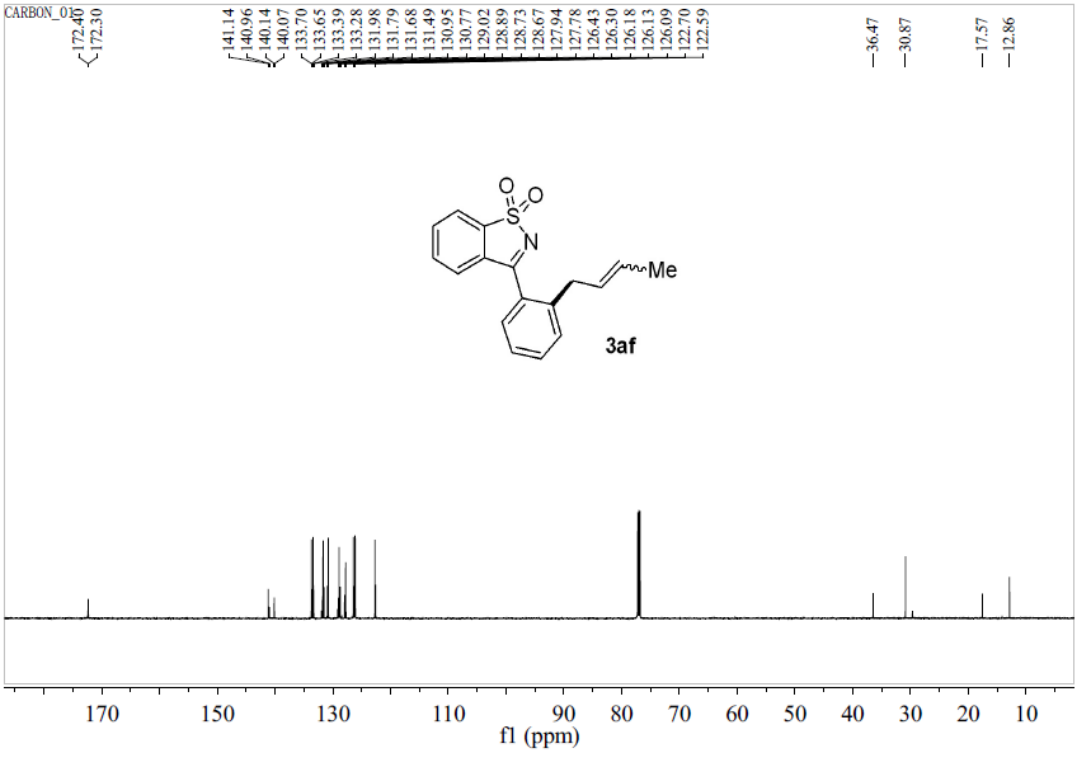
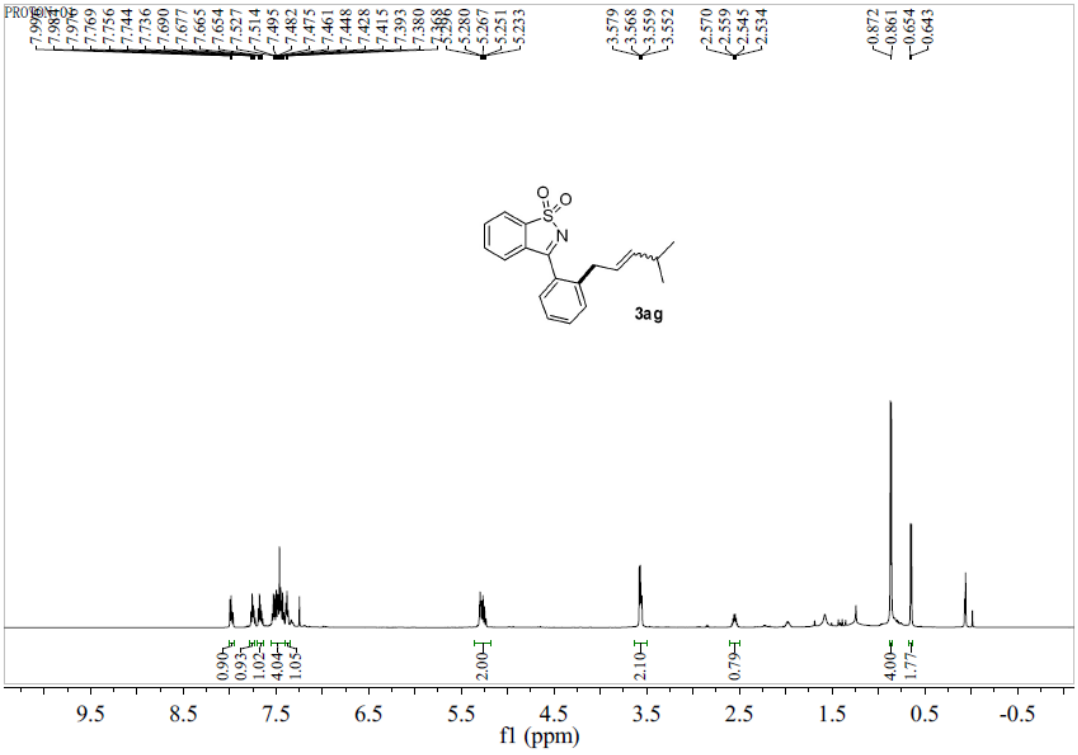
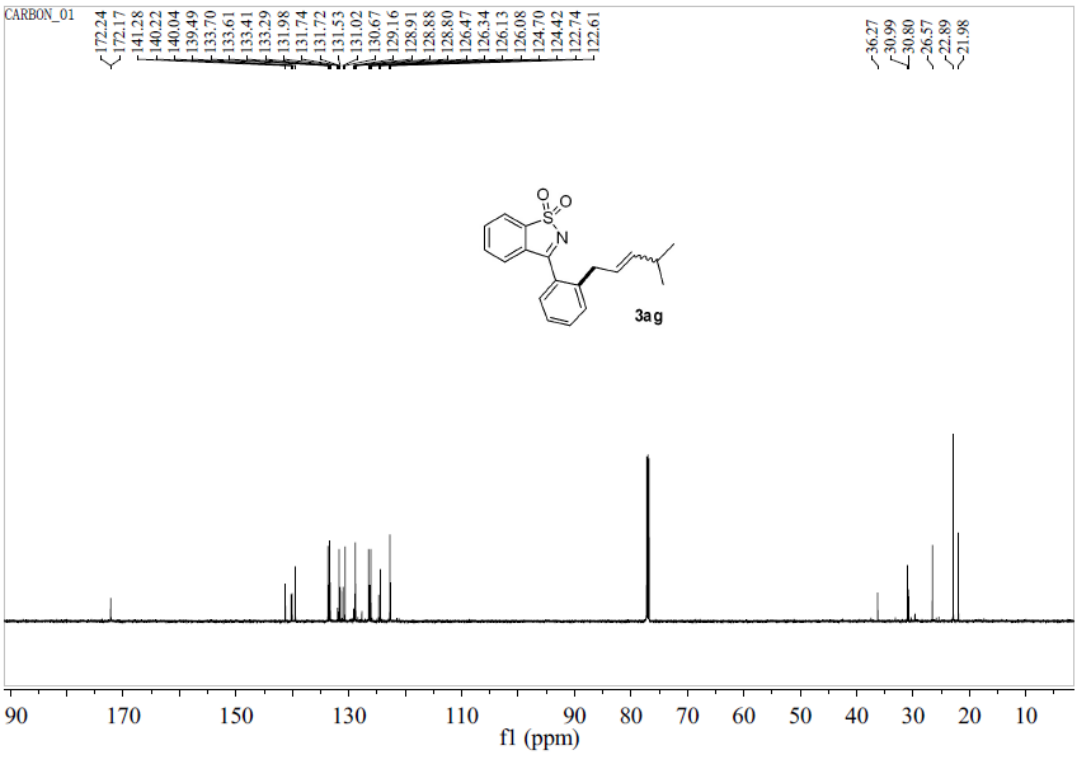
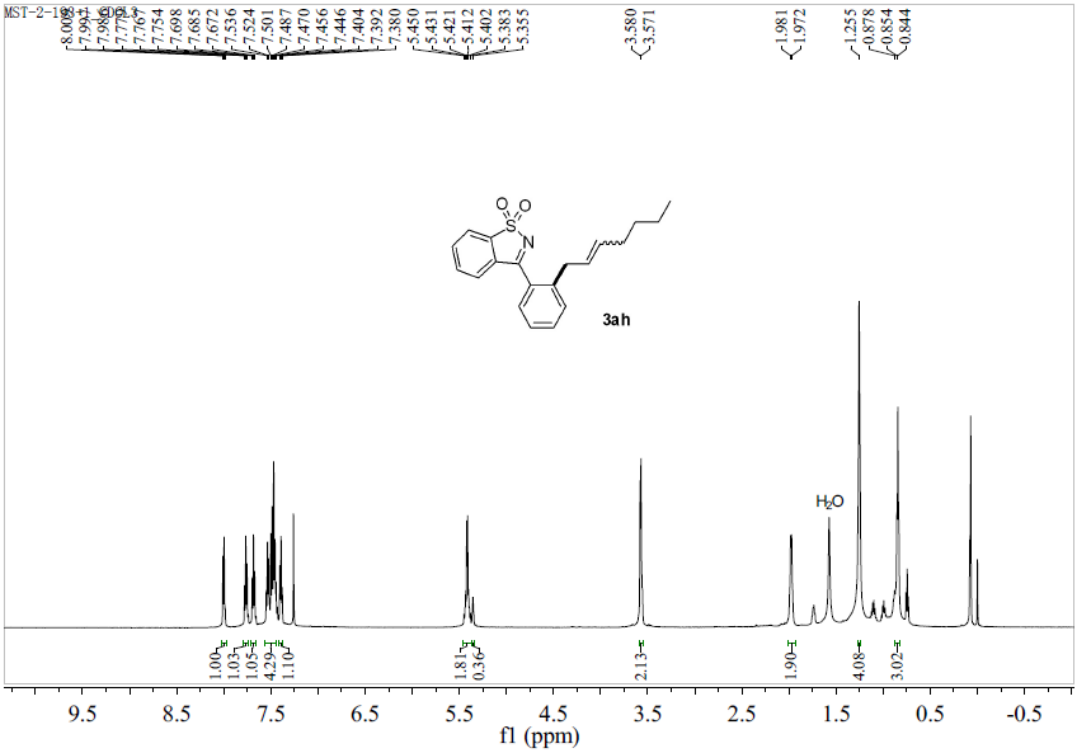
7.675
7.536
7.524
7.501
7.488
7.483
7.469
7.455
7.442
7.406
7.394
7.381
5.493
5.489
5.486
5.475
5.426
5.423
5.420
5.415
5.411
5.408
5.381
3.579
3.525
3.516
1.559
1.548
1.406
1.398
O
S
O
N
Me
3af
0.90
1.02
1.02
4.00
0.91
2.01
2.14
3.23
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


CARBON_01
172.40
172.30
141.14
140.96
140.14
140.07
133.70
133.65
133.39
133.28
131.98
131.79
131.68
131.49
130.95
130.77
129.02
128.89
128.73
128.67
127.94
127.78
126.43
126.30
126.18
126.13
126.09
122.70
122.59
36.47
30.87
17.57
12.86
O
S
O
N
Me
3af
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)


PROTON_01
7.996
7.983
7.976
7.769
7.756
7.744
7.736
7.690
7.677
7.665
7.654
7.527
7.514
7.495
7.482
7.475
7.461
7.448
7.428
7.415
7.393
7.380
7.368
7.366
5.280
5.267
5.251
5.233
3.579
3.568
3.559
3.552
2.570
2.559
2.545
2.534
0.872
0.861
0.654
0.643
3ag
0.90
0.93
1.02
4.04
1.05
2.00
2.10
0.79
4.00
1.77
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


CARBON_01
172.24
172.17
141.28
140.22
140.04
139.49
133.70
133.61
133.41
133.29
131.98
131.74
131.72
131.53
131.02
130.67
129.16
128.91
128.88
128.80
126.47
126.34
126.13
126.08
124.70
124.42
122.74
122.61
36.27
30.99
30.80
26.57
22.89
21.98
3ag
90
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.008
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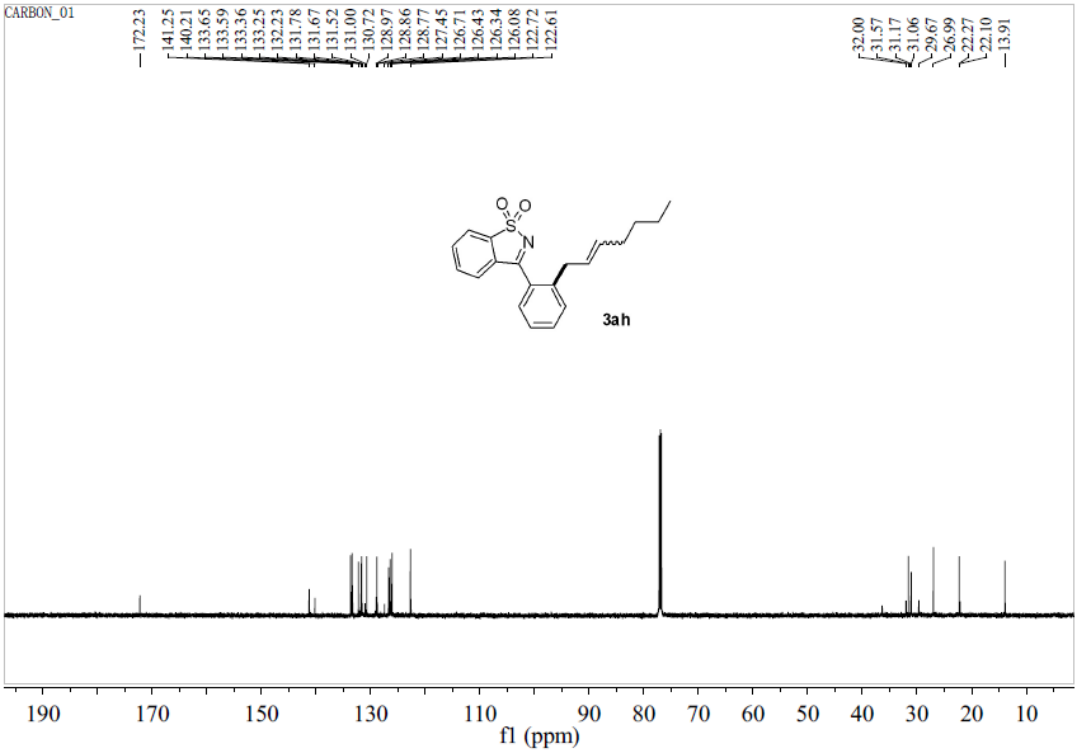
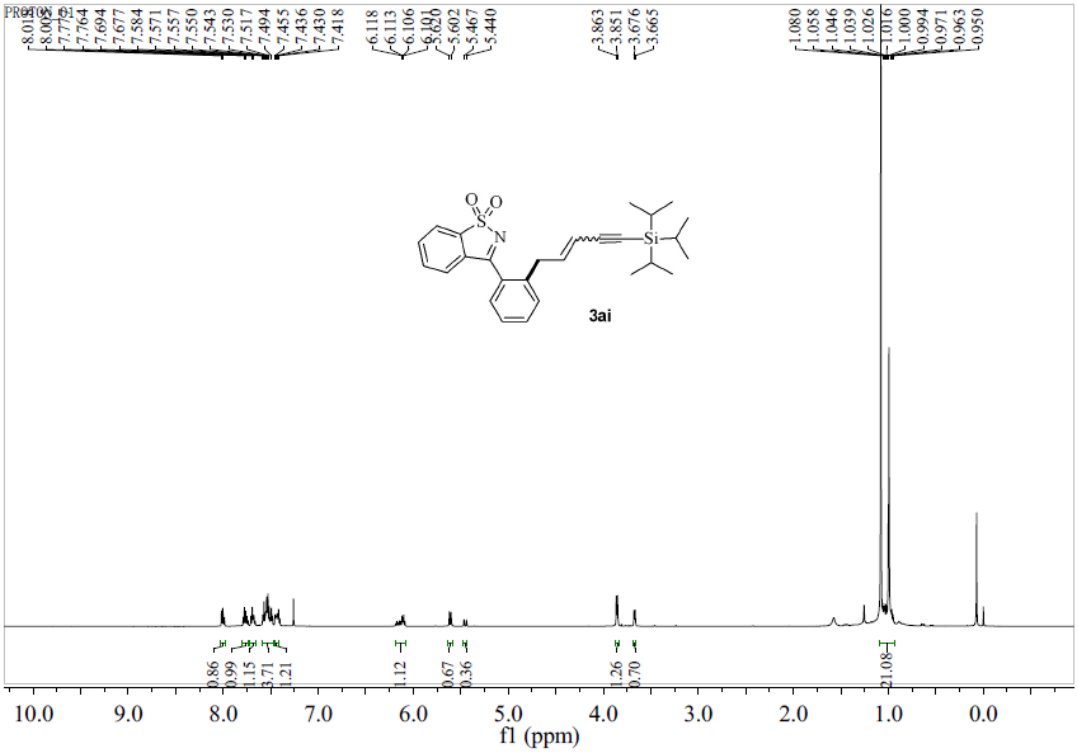
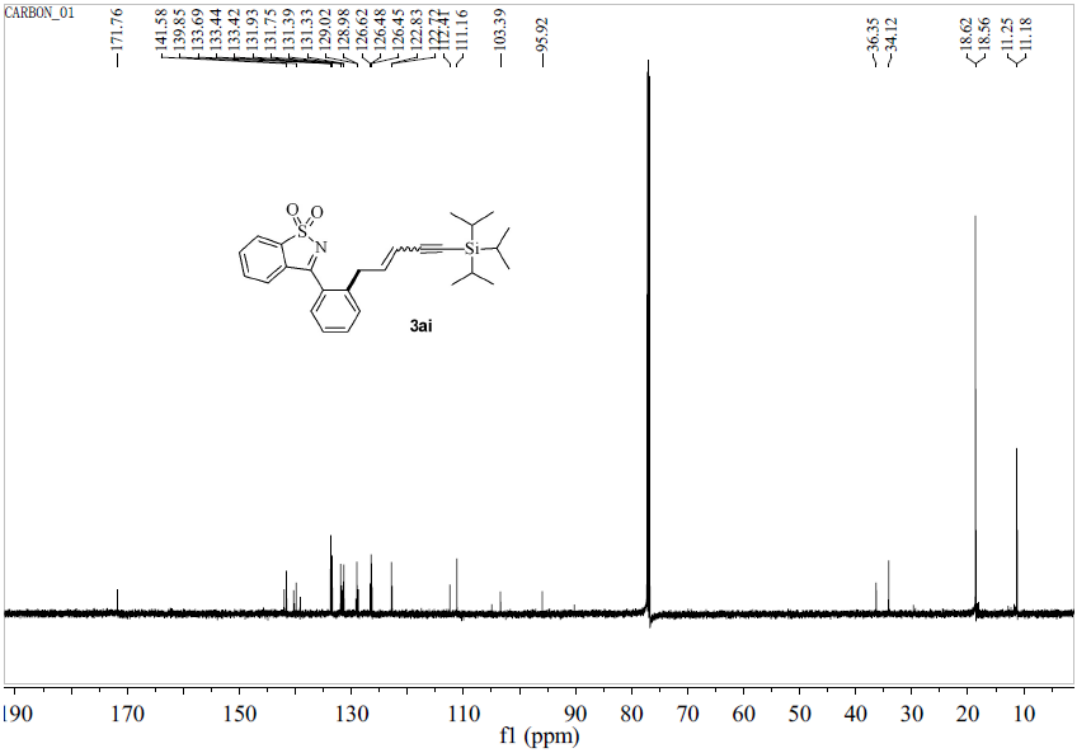
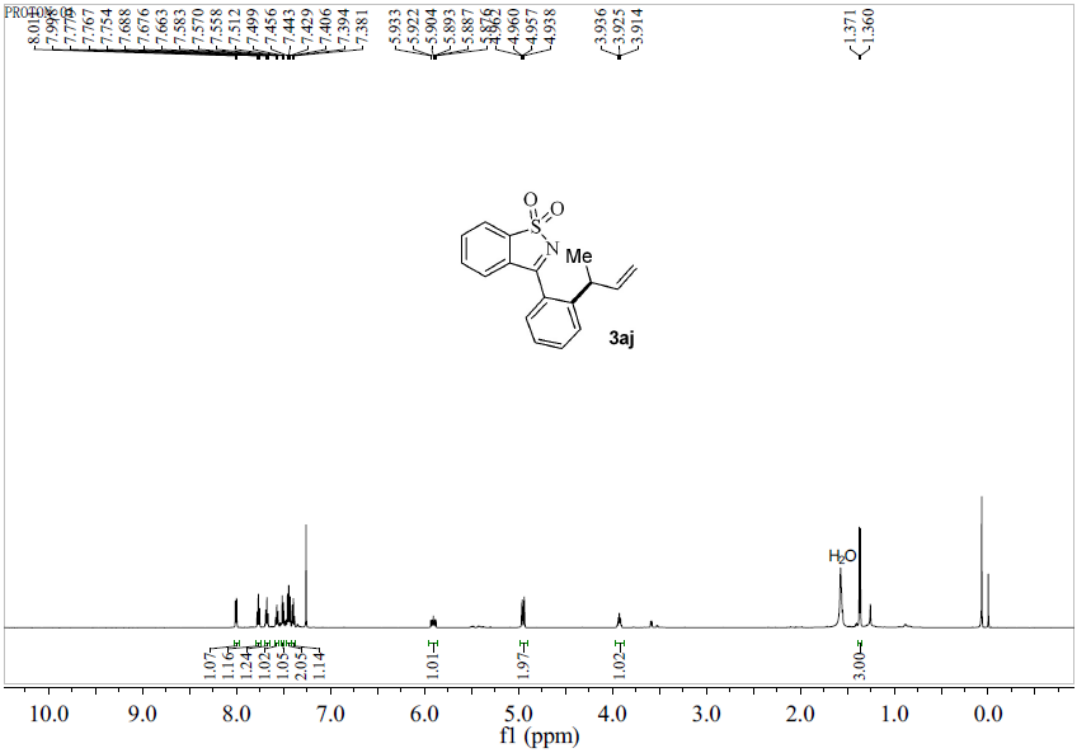
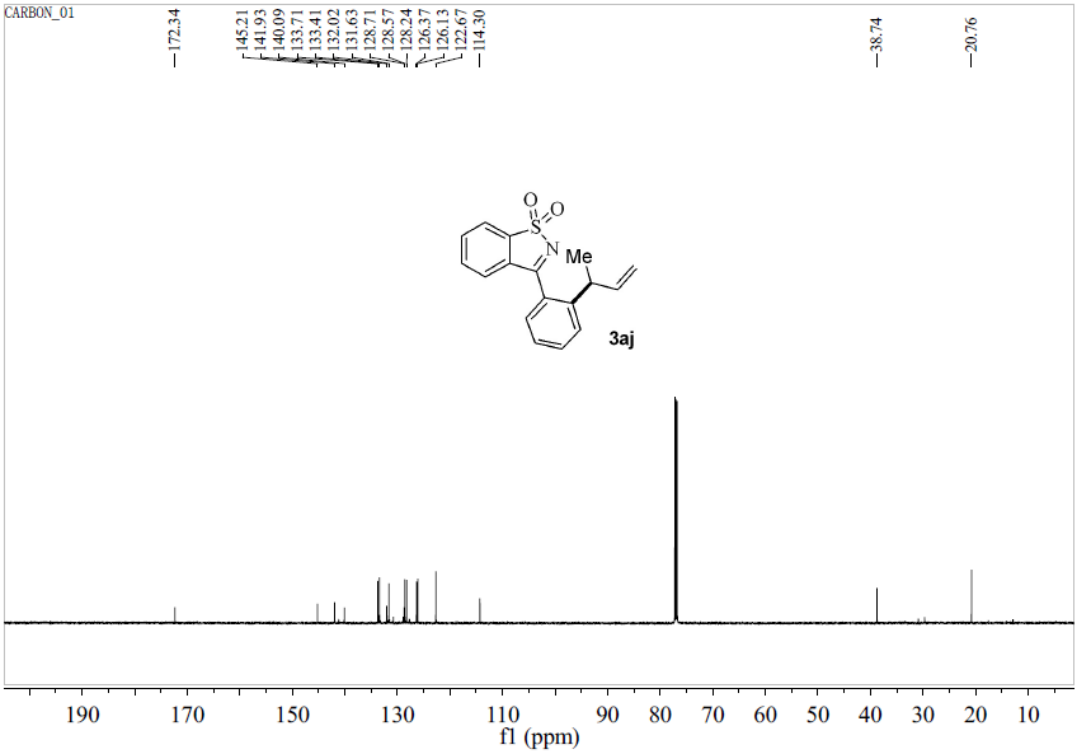
7.754
7.698
7.685
7.672
7.536
7.524
7.501
7.487
7.470
7.456
7.446
7.404
7.392
7.380
5.450
5.431
5.421
5.412
5.402
5.383
5.355
3.580
3.571
1.981
1.972
1.255
0.878
0.854
0.844
3ah
H2O
1.00
1.03
1.05
4.29
1.10
1.81
0.36
2.13
1.90
4.08
3.02
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

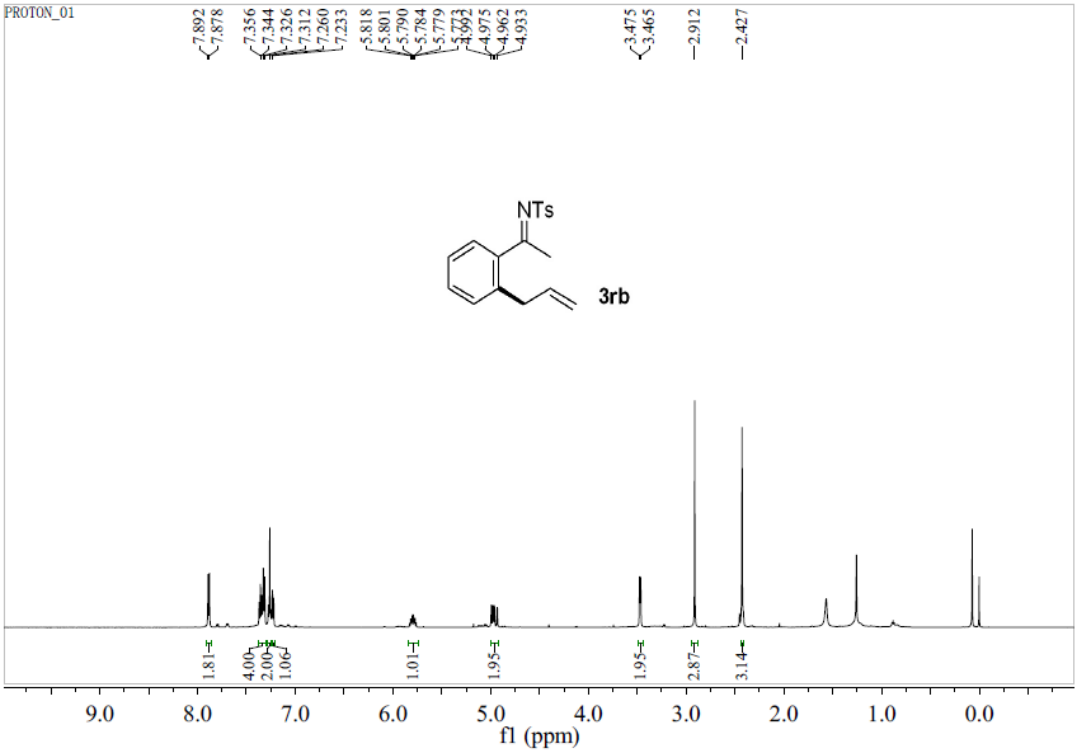

CARBON_01
172.23
141.25
140.21
133.65
133.59
133.36
133.25
132.23
131.78
131.67
131.52
131.00
130.72
128.97
128.86
128.77
127.45
126.71
126.43
126.34
126.08
122.72
122.61
32.00
31.57
31.17
31.06
29.67
26.99
22.27
22.10
13.91
3ah
190
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

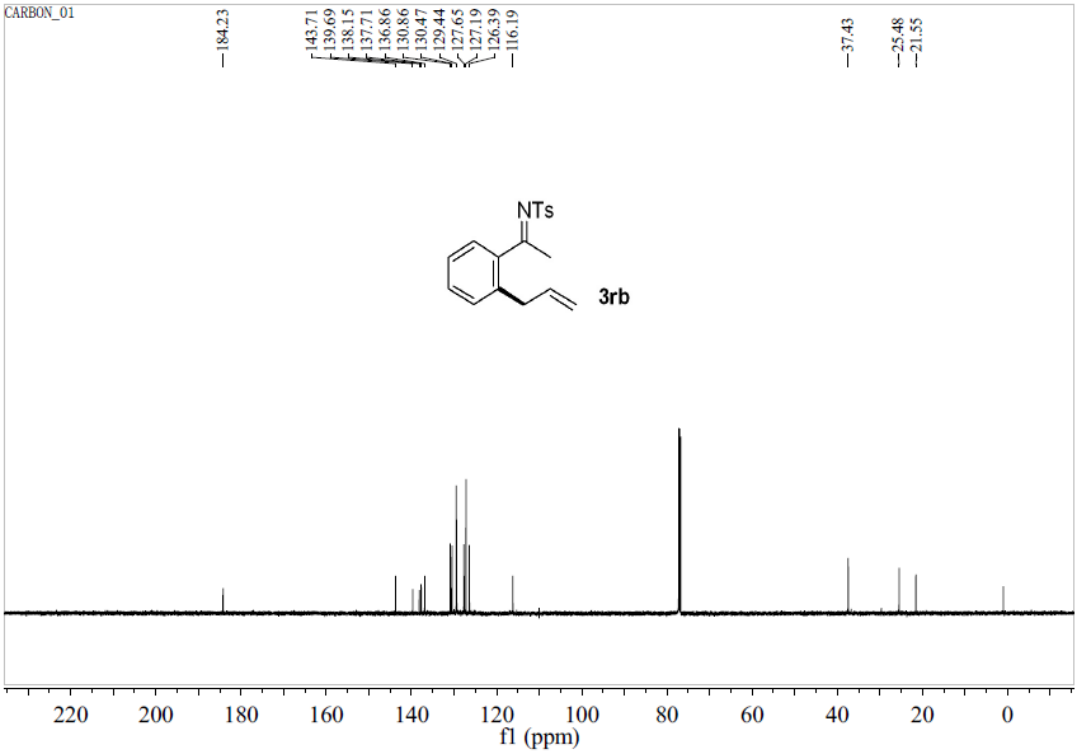

PROTON_01
8.019
8.002
7.775
7.764
7.694
7.677
7.584
7.571
7.557
7.550
7.543
7.530
7.517
7.494
7.455
7.436
7.430
7.418
6.118
6.113
6.106
6.101
5.620
5.602
5.467
5.440
3.863
3.851
3.676
3.665
1.080
1.058
1.046
1.039
1.026
1.016
1.000
0.994
0.971
0.963
0.950
3ai
0.86
0.99
1.15
3.71
1.21
1.12
0.67
0.36
1.26
0.70
21.08
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

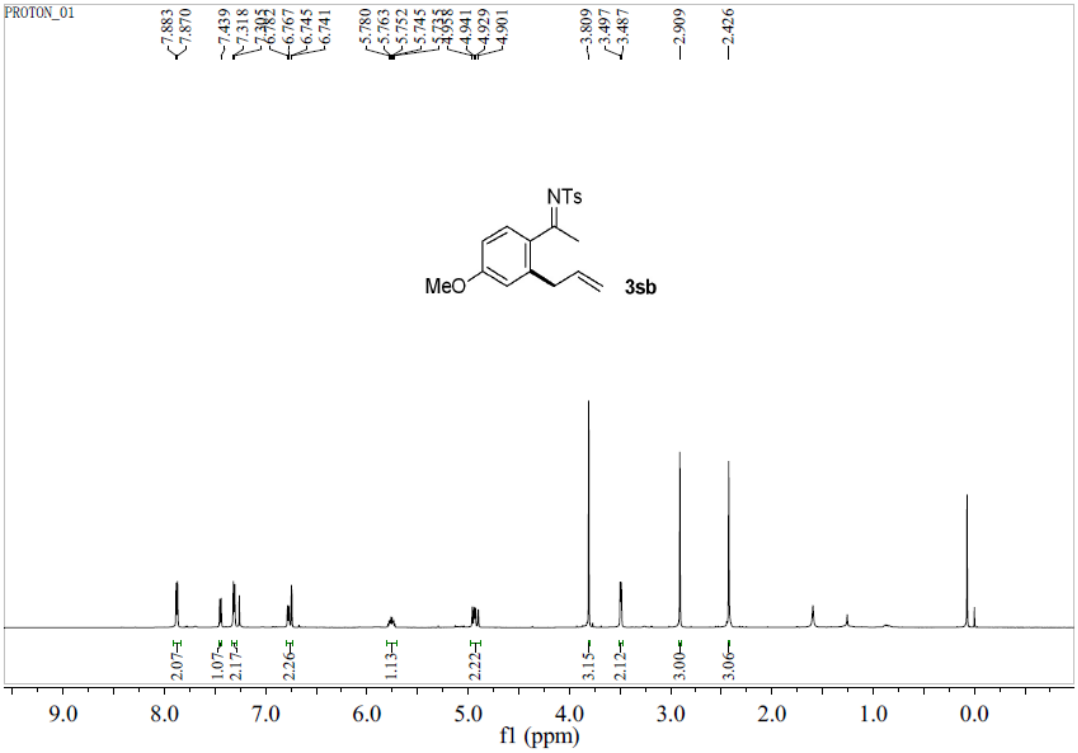

CARBON_01
171.76
141.58
139.85
133.69
133.44
133.42
131.93
131.75
131.39
131.33
129.02
128.98
126.62
126.48
126.45
122.83
122.47
122.41
111.16
103.39
95.92
36.35
34.12
18.62
18.56
11.25
11.18
3ai
190
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

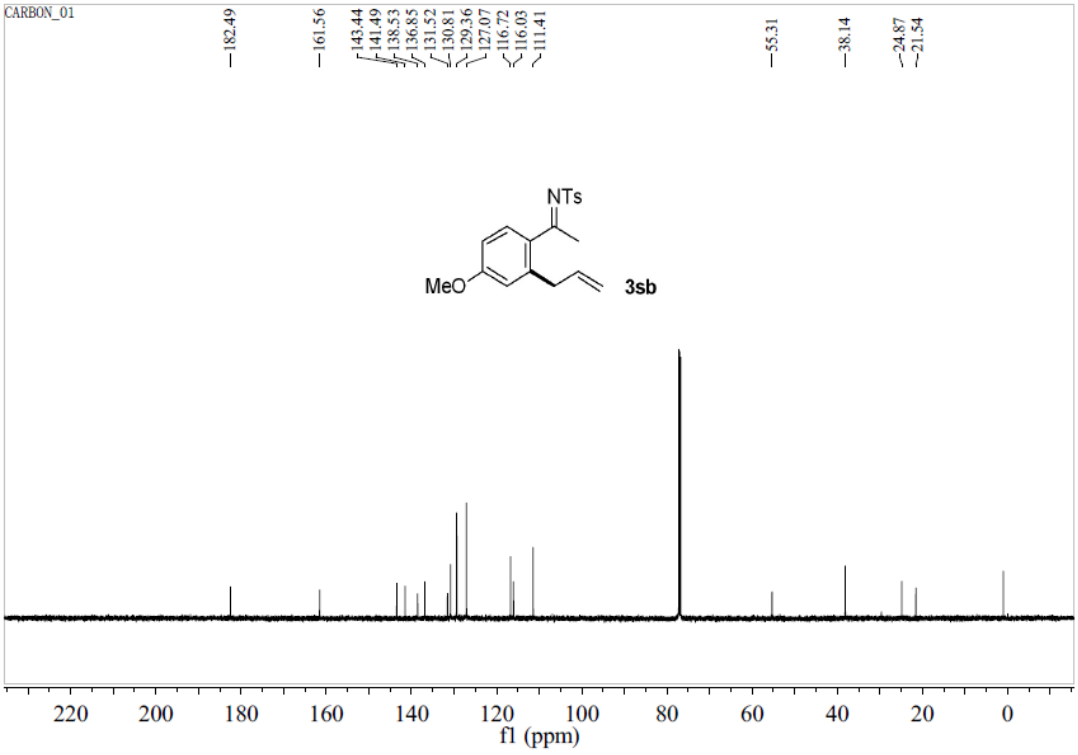

PROTON_01
8.011
7.999
7.779
7.767
7.754
7.688
7.676
7.663
7.583
7.570
7.558
7.512
7.499
7.456
7.443
7.429
7.406
7.394
7.381
5.933
5.922
5.904
5.893
5.887
5.876
4.962
4.960
4.957
4.938
3.936
3.925
3.914
1.371
1.360
O
O
S
N
Me
3aj
H2O
1.07
1.16
1.24
1.02
1.05
2.05
1.14
1.01
1.97
1.02
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

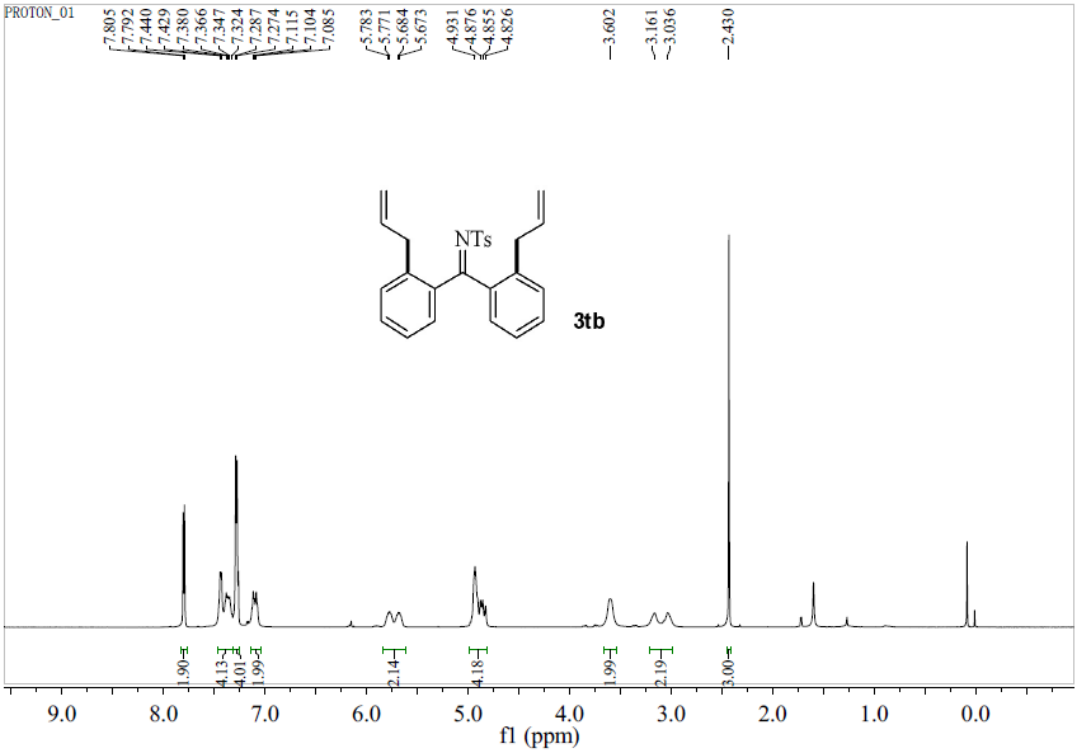

CARBON_01
172.34
145.21
141.93
140.09
133.71
133.41
132.02
131.63
128.71
128.57
128.24
126.37
126.13
122.67
114.30
38.74
20.76
O
O
S
N
Me
3aj
190
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

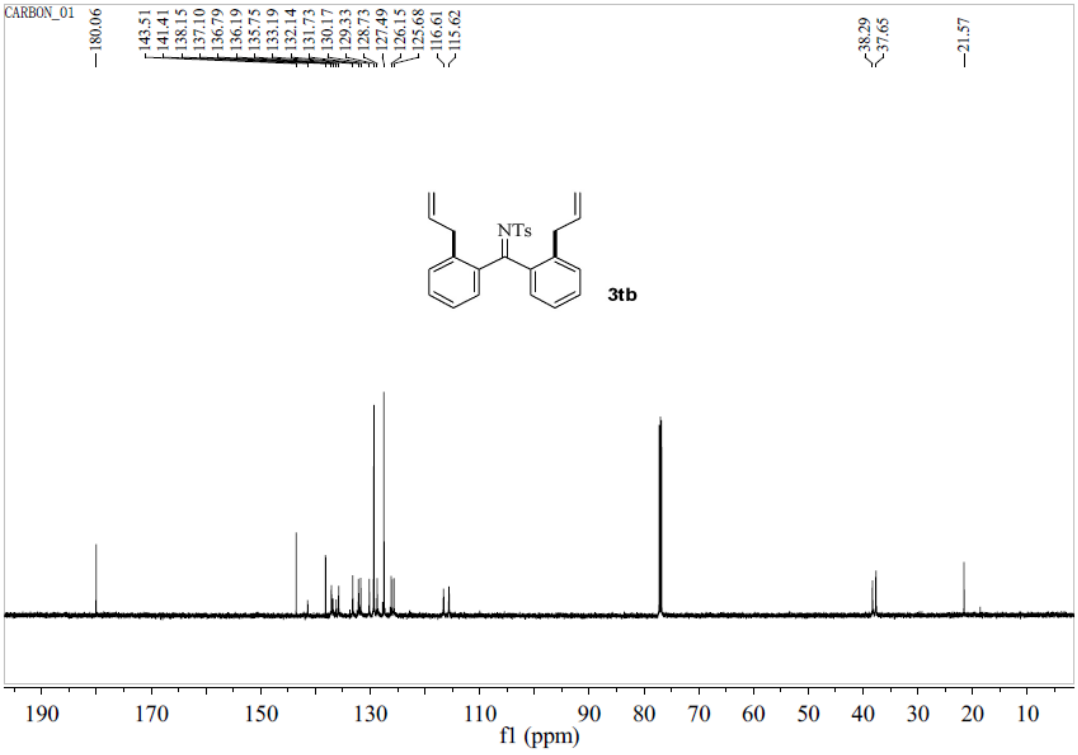

PROTON_01
7.892
7.878
7.356
7.344
7.326
7.312
7.260
7.233
5.818
5.801
5.790
5.784
5.779
5.773
4.992
4.975
4.962
4.933
3.475
3.465
2.912
2.427
NTs
3rb
1.81
4.00
2.00
1.06
1.01
1.95
1.95
2.87
3.14
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

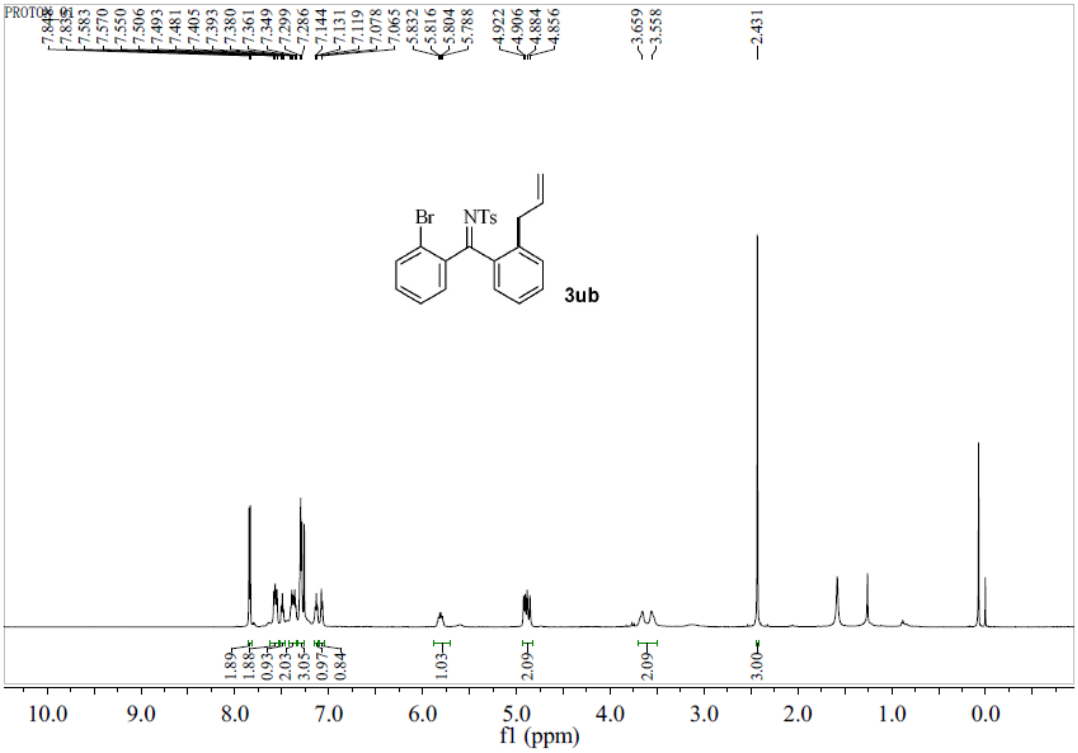

CARBON_01
184.23
143.71
139.69
138.15
137.71
136.86
130.86
130.47
129.44
127.65
127.19
126.39
116.19
37.43
25.48
21.55
NTs
3rb
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

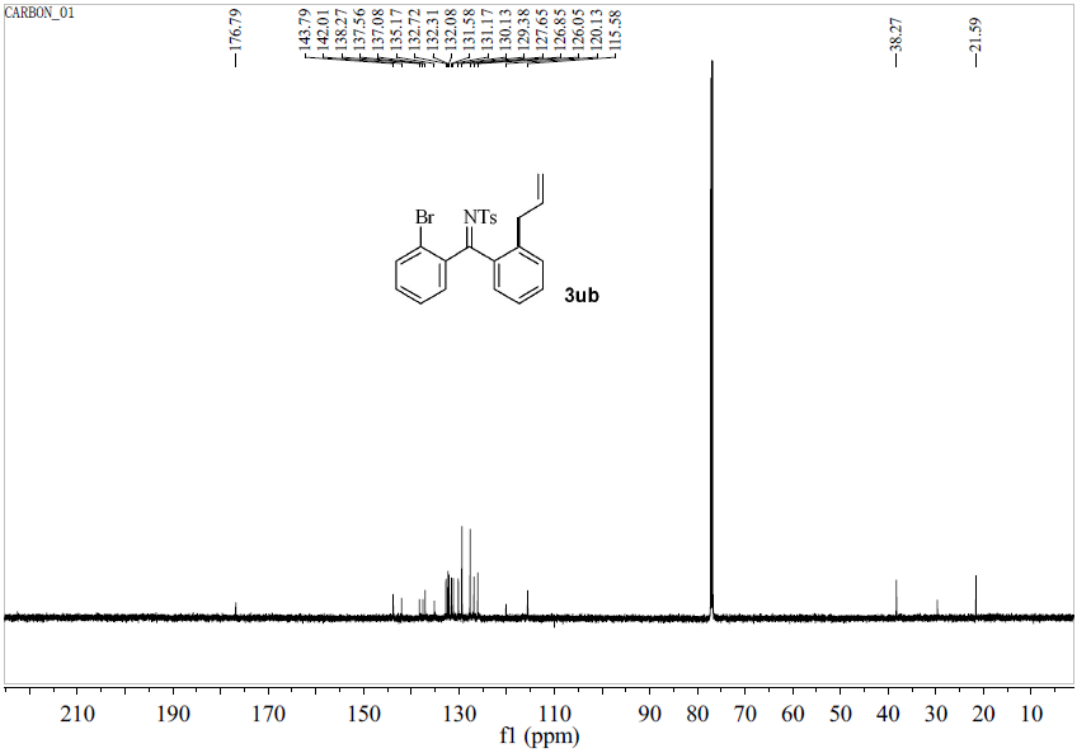

PROTON_01
7.883
7.870
7.439
7.318
7.305
6.782
6.767
6.745
6.741
5.780
5.763
5.752
5.745
5.735
4.958
4.941
4.929
4.901
3.809
3.497
3.487
2.909
2.426
NTs
MeO
3sb
2.07
1.07
2.17
2.26
1.13
2.22
3.15
2.12
3.00
3.06
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

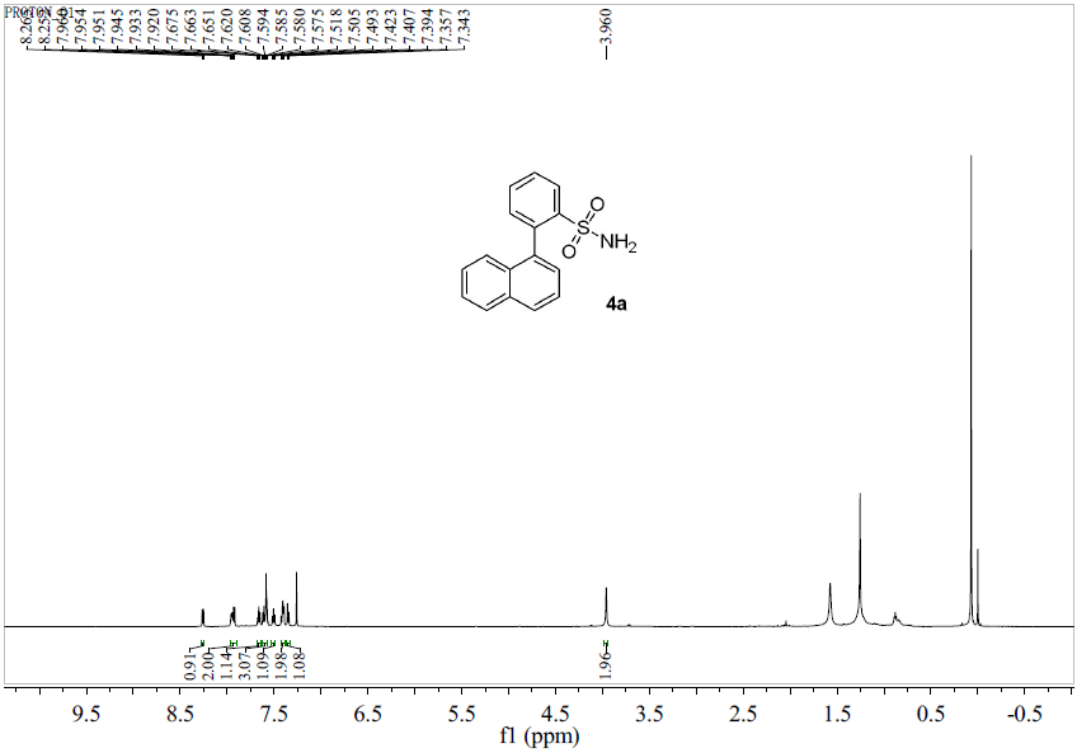

CARBON_01
182.49
161.56
143.44
141.49
138.53
136.85
131.52
130.81
129.36
127.07
116.72
116.03
111.41
55.31
38.14
24.87
21.54
NTs
MeO
3sb
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

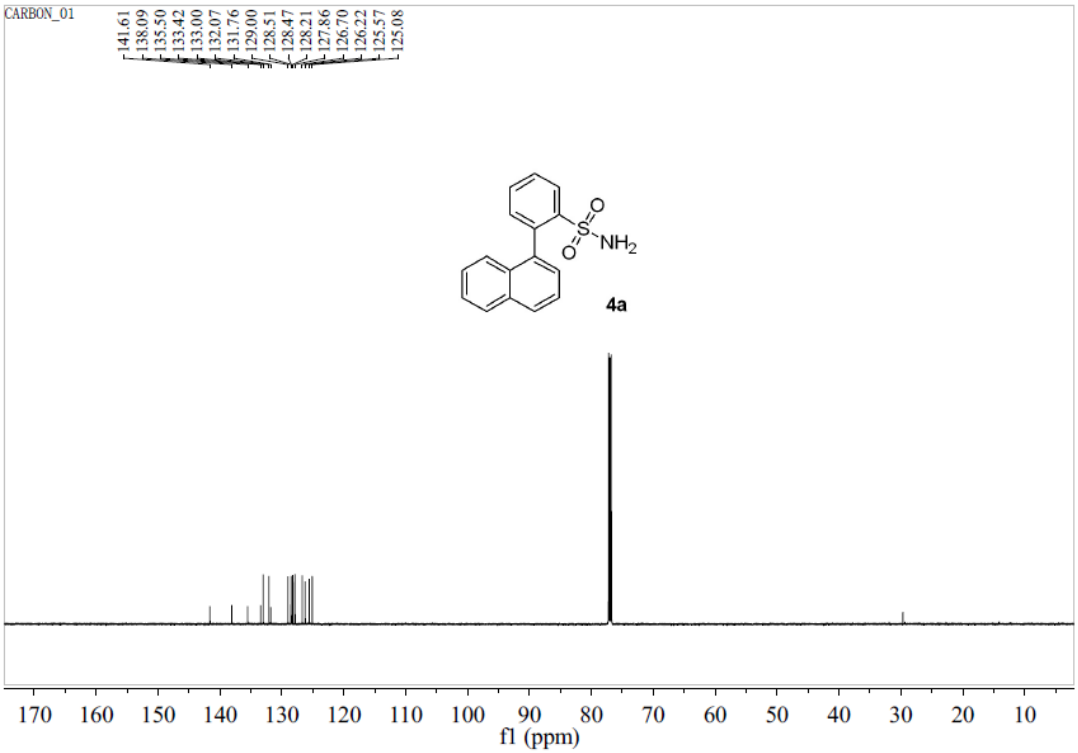

PROTON_01
7.805
7.792
7.440
7.429
7.380
7.366
7.347
7.324
7.287
7.274
7.115
7.104
7.085
5.783
5.771
5.684
5.673
4.931
4.876
4.855
4.826
3.602
3.161
3.036
2.430
NTs
3tb
1.90
4.13
4.01
1.99
2.14
4.18
1.99
2.19
3.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

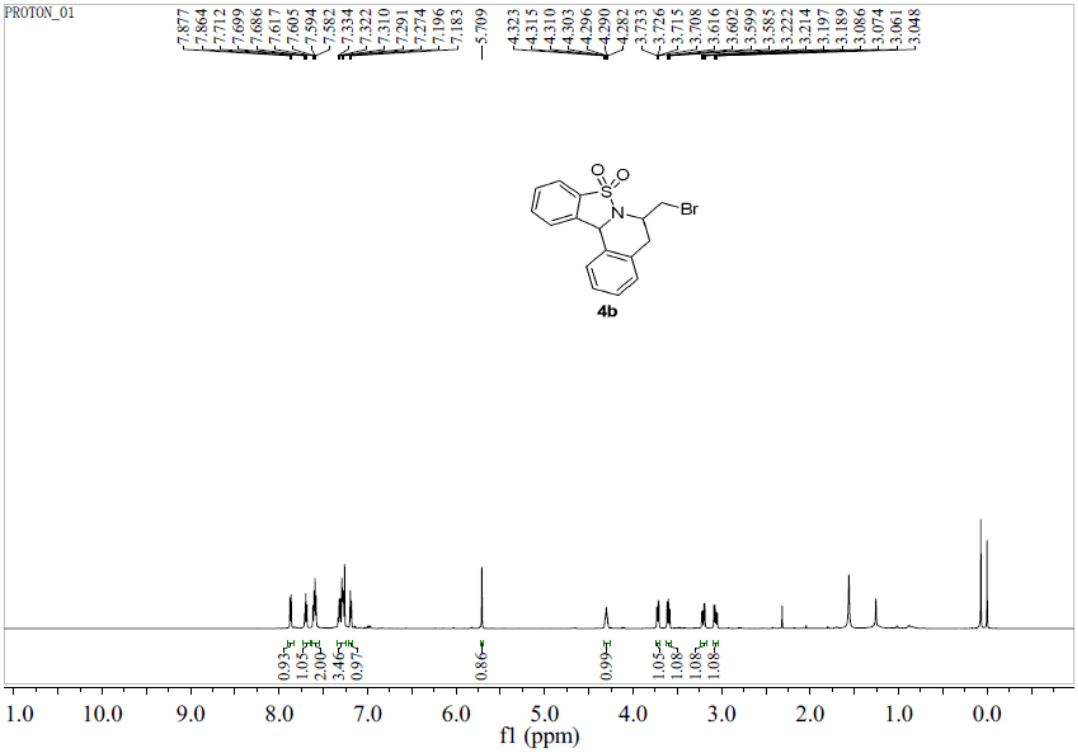

CARBON_01
180.06
143.51
141.41
138.15
137.10
136.79
136.19
135.75
133.19
132.14
131.73
130.17
129.33
128.73
127.49
126.15
125.68
116.61
115.62
38.29
37.65
21.57
NTs
3tb
190
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

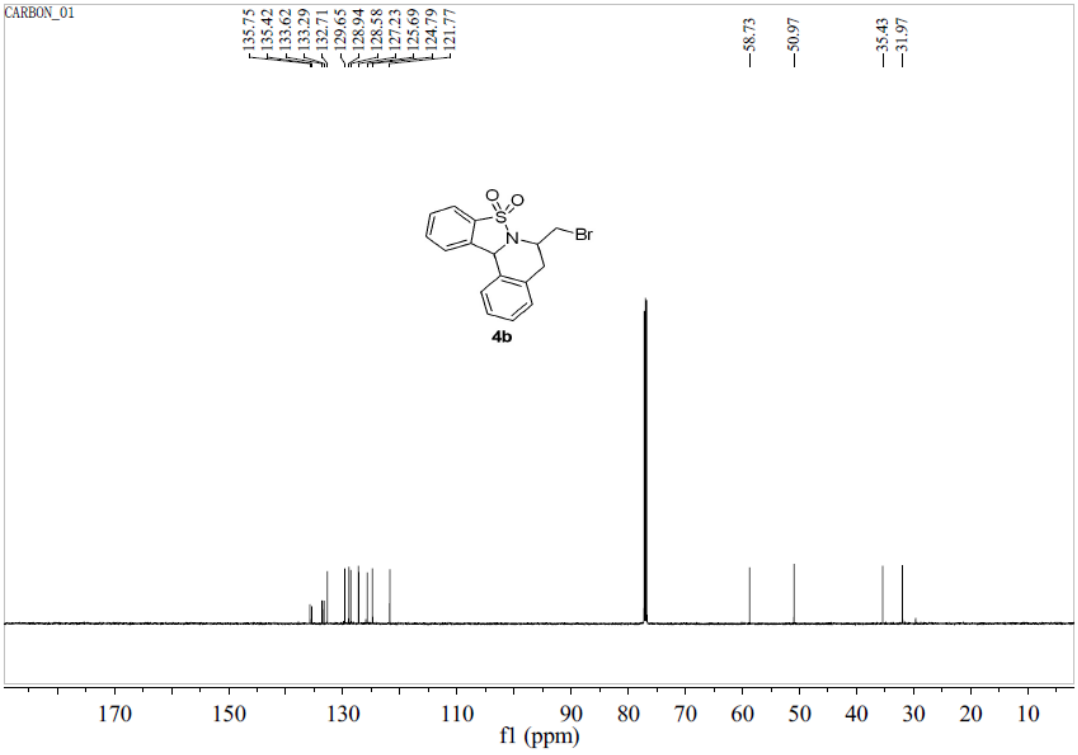

PROTON_01
7.848
7.832
7.583
7.570
7.550
7.506
7.493
7.481
7.405
7.393
7.380
7.361
7.349
7.299
7.286
7.144
7.131
7.119
7.078
7.065
5.832
5.816
5.804
5.788
4.922
4.906
4.884
4.856
3.659
3.558
2.431
Br
NTs
3ub
1.89
1.88
0.93
2.03
3.05
0.97
0.84
1.03
2.09
2.09
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

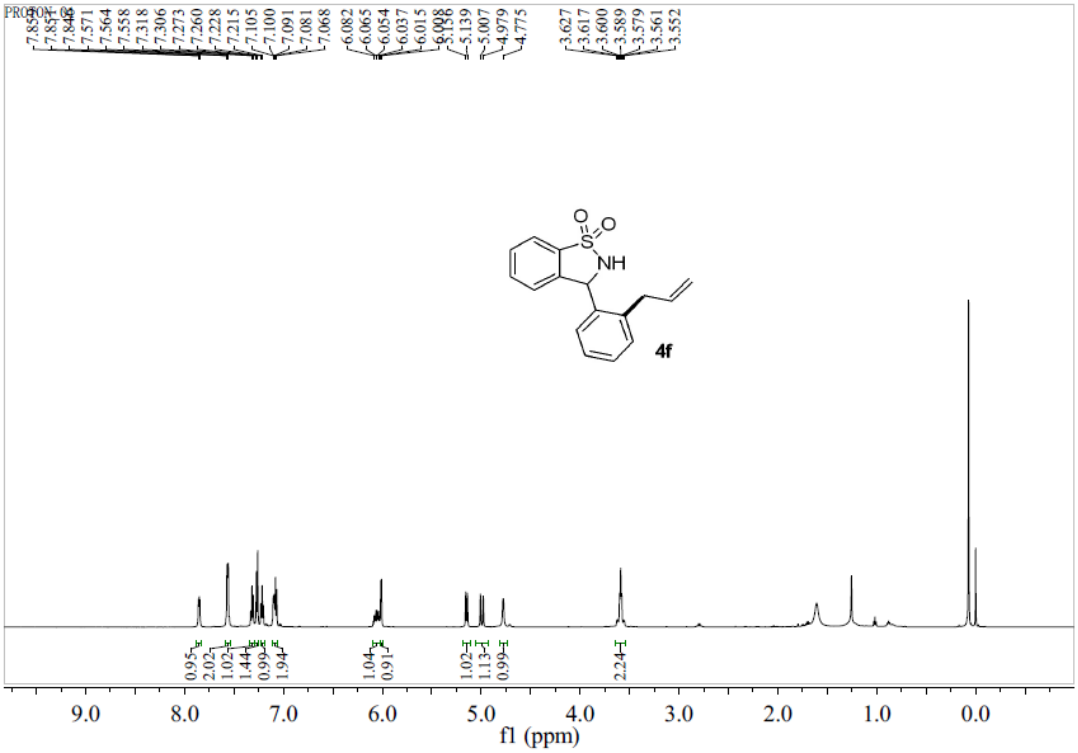

CARBON_01
176.79
143.79
142.01
138.27
137.56
137.08
135.17
132.72
132.31
132.08
131.58
131.17
130.13
129.38
127.65
126.85
126.05
120.13
115.58
38.27
21.59
Br
NTs
3ub
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

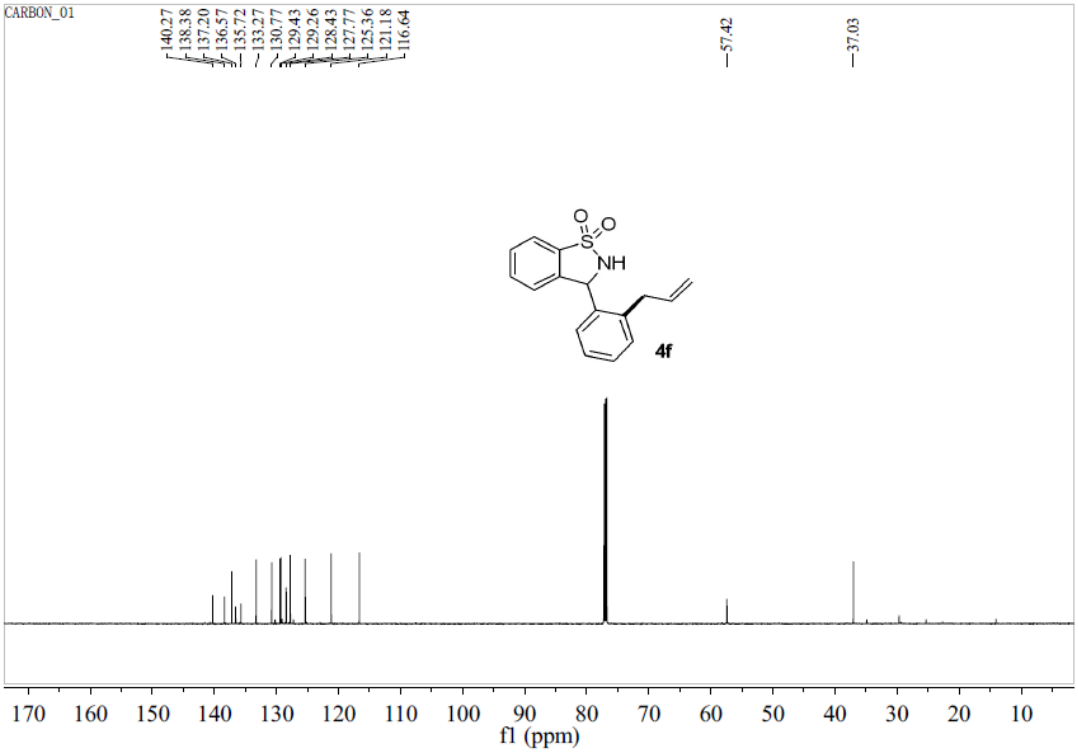

PROTON
8.267
8.252
7.964
7.954
7.951
7.945
7.933
7.920
7.675
7.663
7.651
7.620
7.608
7.594
7.585
7.580
7.575
7.518
7.505
7.493
7.423
7.407
7.394
7.357
7.343
3.960
NH2
4a
0.91
2.00
1.14
3.07
1.09
1.98
1.08
1.96
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

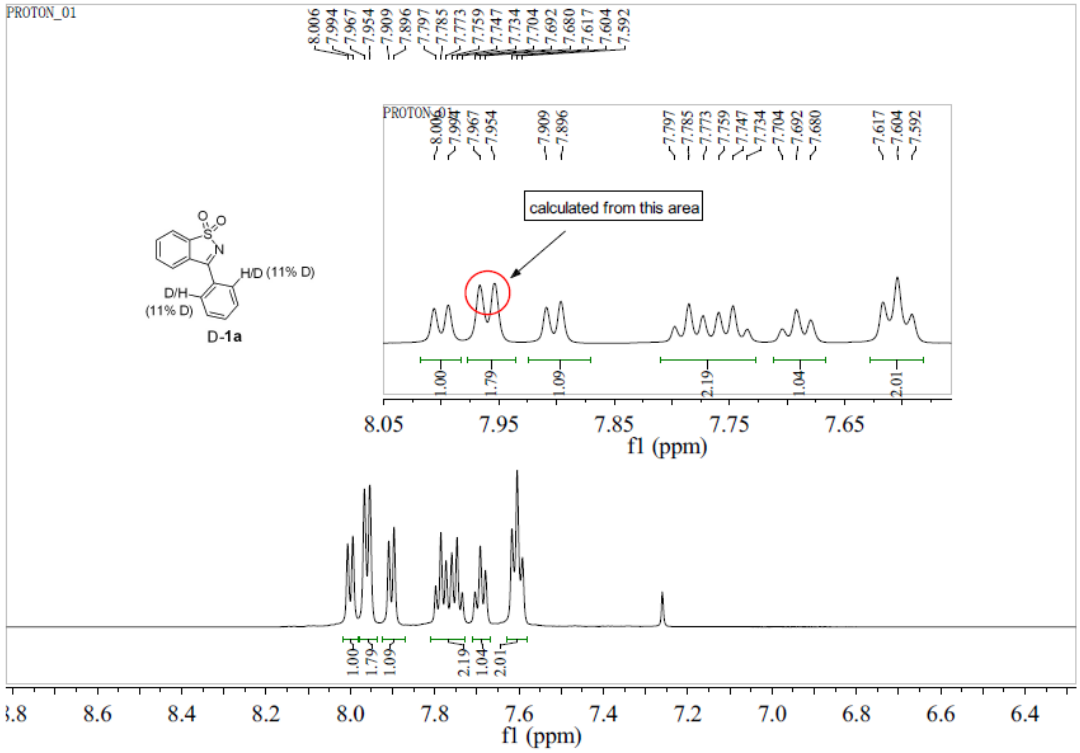

CARBON_01
141.61
138.09
135.50
133.42
133.00
132.07
131.76
129.00
128.51
128.47
128.21
127.86
126.70
126.22
125.57
125.08
NH2
4a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

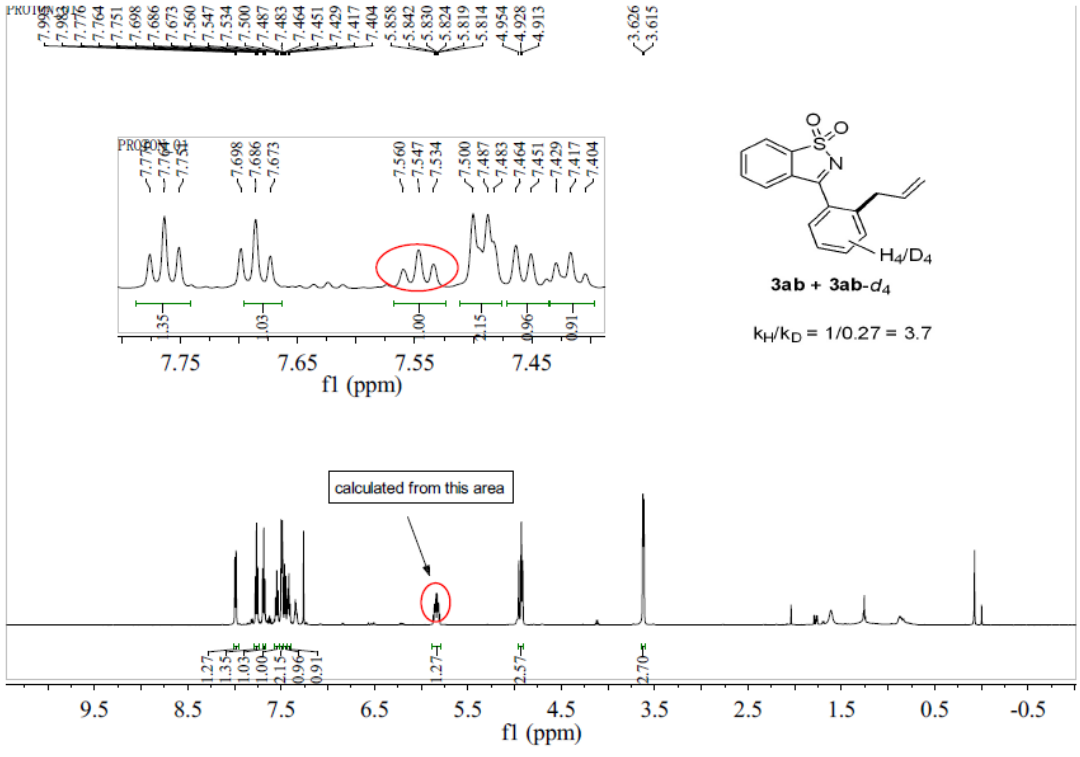

PROTON_01
7.877
7.864
7.712
7.699
7.686
7.617
7.605
7.594
7.582
7.334
7.322
7.310
7.291
7.274
7.196
7.183
5.709
4.323
4.315
4.310
4.303
4.296
4.290
4.282
3.733
3.726
3.715
3.708
3.616
3.602
3.599
3.585
3.222
3.214
3.197
3.189
3.086
3.074
3.061
3.048
Br
4b
0.93
1.05
2.00
3.46
0.97
0.86
0.99
1.05
1.08
1.08
1.08
1.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


CARBON_01
135.75
135.42
133.62
133.29
132.71
129.65
128.94
128.58
127.23
125.69
124.79
121.77
58.73
50.97
35.43
31.97
Br
4b
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)


PROTON_1
7.859
7.857
7.848
7.571
7.564
7.558
7.318
7.306
7.273
7.260
7.228
7.215
7.105
7.100
7.091
7.081
7.068
6.082
6.065
6.054
6.037
6.015
6.008
5.156
5.139
5.007
4.979
4.775
3.627
3.617
3.600
3.589
3.579
3.561
3.552
NH
4f
0.95
2.02
1.02
1.44
0.99
1.94
1.04
0.91
1.02
1.13
0.99
2.24
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


CARBON_01
140.27
138.38
137.20
136.57
135.72
133.27
130.77
129.43
129.26
128.43
127.77
125.36
121.18
116.64
57.42
37.03
NH
4f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


PROTON_01
calculated from this area
H/D (11% D)
D/H
(11% D)
D-1a
fl (ppm)


calculated from this area
H4/D4
3ab + 3ab-d4
kH/kD = 1/0.27 = 3.7
fl (ppm)