

Supporting Information

Gold-catalyzed cyclization/nucleophilic addition reaction of *o*-alkynylanilines with ynamides: stereoselective synthesis of 3-vinylindoles

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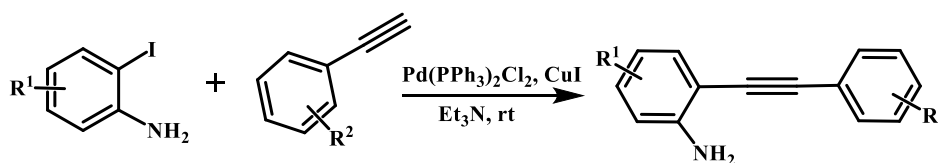
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1. General Information

All reactions were carried out in an air environment unless otherwise noted. All the reactions were monitored by thin layer chromatography (TLC), carried out on 0.25 mm silica gel plates using UV light as visualizing agent. Column chromatography was carried out on silica gel (particle size 300-400 mesh). Unless stated otherwise, all the yields refer to isolated products after flash column chromatography. The solvent mixtures employed in flash column chromatography purifications were reported as volume by volume and in percentages. The melting points were measured with SGW X-4 micro-melting-point apparatus. NMR spectra were recorded with BrukerAvance III HD500 and BrukerAvance III HD600 spectrometer at 500 MHz or 600 MHz. All ^{13}C , ^1H and ^{19}F NMR spectra were recorded using CDCl_3 as solvent. Tetramethylsilane (TMS) signals or residual solvent signals were used [TMS $\delta=0.00$ (^1H NMR), $\text{CDCl}_3=7.26$ ppm (^1H NMR), 77.16 ppm (^{13}C NMR)] as internal standards. Coupling constants (J) are reported in Hz. The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, dd = double doublet, t = triplet, q = quartet, m = multiplet, td = triplet doublet, qd = quartet doublet, ddq = doublet doublet quartet. High-resolution mass spectra were recorded on Agilent 6545 Q-TOF LC/MS. The relative configuration of **3a** was determined by NMR Data, molecular weight compared and X-ray single crystal diffraction.

2. Experiment Section

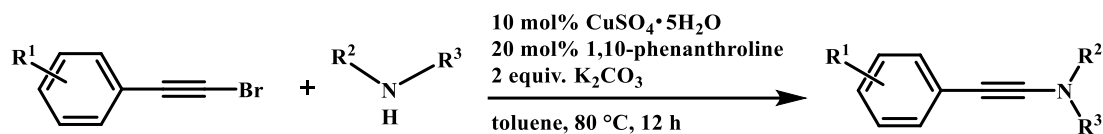
2.1. Preparation for the synthesis of *o*-alkynylaniline¹



Scheme S1. Sonogashira coupling reaction

Under N_2 atmosphere, terminal alkynes (6 mmol) was added to a solution of 2-iodoaniline (5 mmol), $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (0.125 mmol, 87.8 mg) and CuI (0.25 mmol, 47.6 mg) in Et_3N (5 mL) was stirred at room temperature for 4 h. The reaction was monitored by TLC. Upon completion, the solvent was removed under reduced pressure, and the residue was extracted with EtOAc (3 x 5 mL). The combined organic layer was dried over NaSO_4 and concentrated. The residue was purified by a silica gel flash column chromatography (petroleum ether/ethylacetate = 10/1) to afford product in good yields ranging from 95% to 99%.

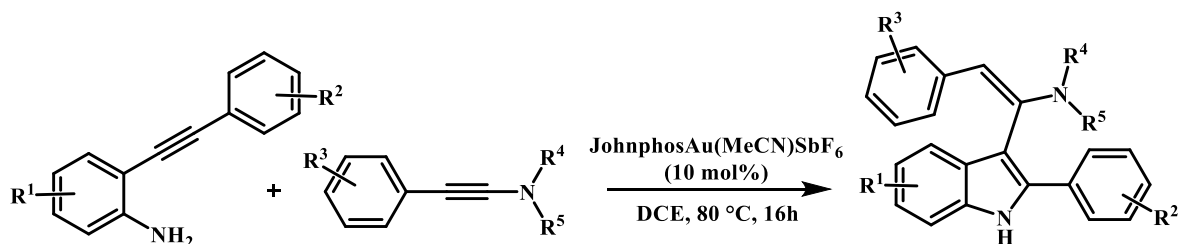
2.2. Preparation for the synthesis of ynamides²



Scheme S2. The alkyne amination reaction

To a dry flask were added sulfonamide (1.09 g, 10 mmol), CuSO₄·5H₂O (249.7 mg, 1.0 mmol), 1,10-phenanthroline (360.4 mg, 2.0 mmol) and K₂CO₃ (2.764 g, 20 mmol). Then toluene (40 mL) and (bromoethynyl)benzene (2.172 g, 12mmol) were added, and the resulting mixture was stirred at 80 °C for 12 h under an atmosphere of argon. When the reaction was complete, the crude mixture was cooled down to room temperature, filtered and washed with ethyl acetate. After solvent evaporation, the residue was purified by column chromatography on silica gel (eluent: petroleum ether: ethyl acetate = 5:1) to afford product (1.82 g, 87%).

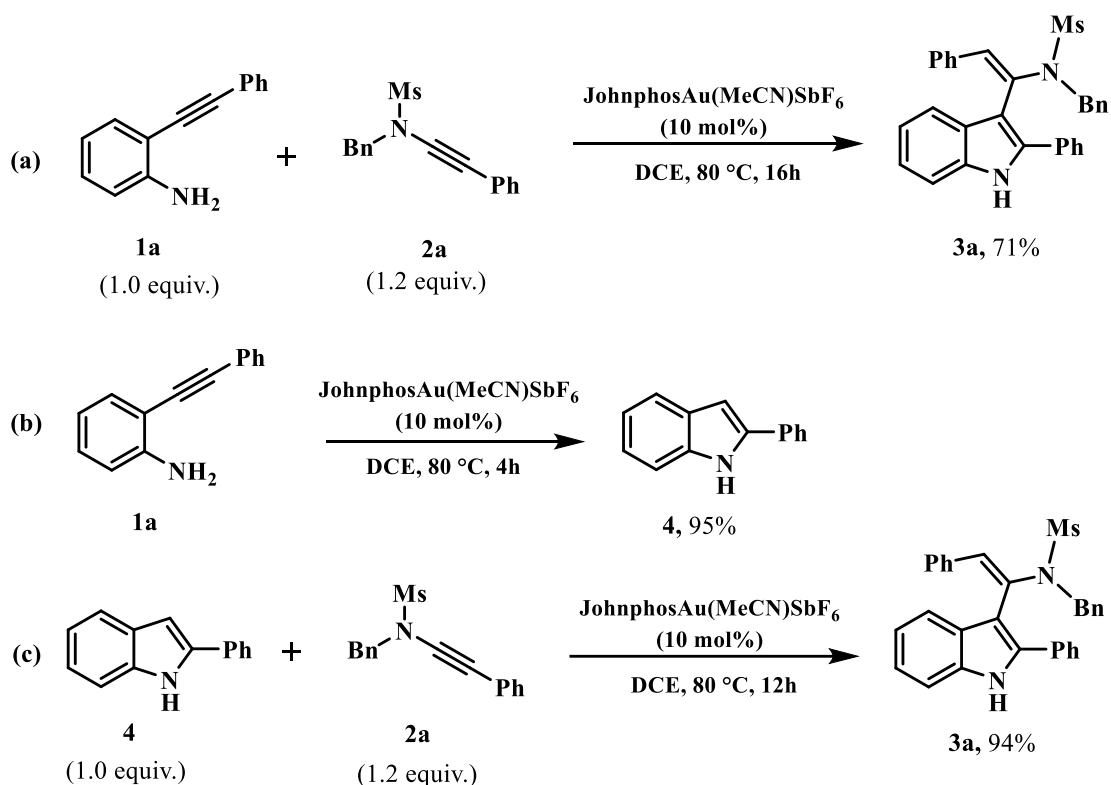
3. Experimental Procedure for the Synthesis of 3-vinylindoles



Scheme S3. The synthesis of 3-vinylindoles from *o*-alkynylanilines and ynamides

To a 10 mL oven-dried reaction vessel was charged with JohnphosAu(MeCN)SbF₆ (10 mol%), *o*-alkynylaniline (0.1 mmol) with anhydrous DCE (1.0 ml) at 80 °C for 4h. Then the resultant mixture was added ynamides (0.12mmol, 1.2 equiv.). The reaction vessel was stirred at 80 °C for 12 h. After the reaction is completed, the solution was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1~ 5:1) to give the pure product as a yellow solid.

4. Control Experiments (Scheme 4)



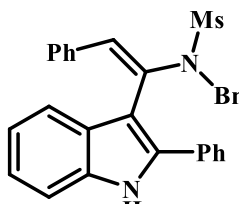
(a) In a 10 mL dried test tube, JohnphosAu(MeCN)SbF₆ (10 mol%), **1a** (0.1 mmol), and **2a** (0.12 mmol, 1.2 equiv.) were added along with anhydrous DCE (1.0 mL). The reaction mixture was heated at 80 °C for 16 hours. After completion of the reaction, the solution was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to obtain a yellow solid (**3a**) as the pure product in 71% yield.

(b) In a 10 mL dried test tube, JohnphosAu(MeCN)SbF₆ (10 mol%), **1a** (0.1 mmol), and anhydrous dichloroethane (1.0 mL) were added. The reaction mixture was heated at 80 °C for 4 hours. After completion of the reaction, the solution was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 8:1) to obtain a white solid(**4**) as the pure product with a yield of 95%. **4** was detected by ¹H NMR, ¹³C NMR and HRMS.

(c) In a 10 mL dried test tube, JohnphosAu(MeCN)SbF₆ (10 mol%), **4** (0.1 mmol), and **2a** (0.12 mmol, 1.2 equiv.) were added along with anhydrous DCE (1.0 mL). The reaction mixture was heated at 80 °C for 12 hours. After completion of the reaction, the solution was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to obtain a yellow solid (**3a**) as the pure product in 94% yield.

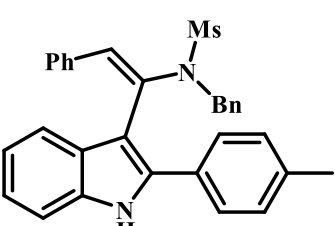
5. Characterization Data for Compounds

(E)-N-Benzyl-N-(2-phenyl-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfonamide(3a).



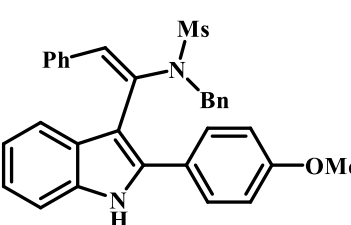
Yellow solid, 44.2 mg, 92% yield; m. p. 200-201 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.30 (s, 1H), 7.40 (m, 2H), 7.23 (m, 9H), 7.12 (m, 2H), 7.06 (m, 1H), 6.94 (m, 3H), 6.88 (m, 2H), 6.84 (s, 1H), 4.45 (m, 2H), 2.67 (s, 3H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 137.56, 137.22, 135.98, 135.81, 132.03, 131.12, 129.97, 128.77, 128.47, 128.37, 128.36, 128.11, 128.03, 127.95, 127.90, 127.34, 126.69, 123.00, 121.00, 120.43, 110.91, 107.40, 51.00, 40.90. HRMS (ESI) m/z calcd for C₃₀H₂₇N₂O₂S [M+H]⁺: 479.1713, found: 479.1784.

(E)-N-Benzyl-N-(2-phenyl-1-(2-(p-tolyl)-1H-indol-3-yl)vinyl)methanesulfonamide



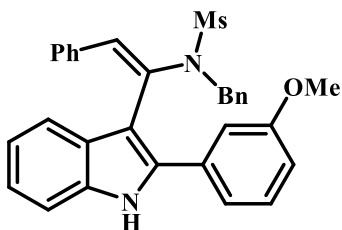
(3b). Yellow solid, 42.7 mg, 86% yield; m. p. 183-184 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.29 (s, 1H), 7.37 (m, 2H), 7.22 (m, 3H), 7.17 (m, 3H), 7.09 (dd, *J* = 6.6, 2.9 Hz, 2H), 7.03 (m, 3H), 6.93 (m, 5H), 6.86 (s, 1H), 4.43 (m, 2H), 2.64 (s, 3H), 2.32 (s, 3H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 138.43, 137.55, 137.19, 135.93, 135.74, 131.00, 130.42, 129.46, 129.15, 128.50, 128.27, 128.11, 128.09, 127.94, 127.74, 127.24, 126.76, 122.82, 120.87, 120.35, 110.83, 107.11, 50.94, 40.77, 21.25. HRMS (ESI) m/z calcd for C₃₁H₂₉N₂O₂S [M+H]⁺: 493.1866, found: 493.1937.

(E)-N-Benzyl-N-(1-(2-(4-methoxyphenyl)-1H-indol-3-yl)-2-phenylvinyl) methanesulfonamide (3c).



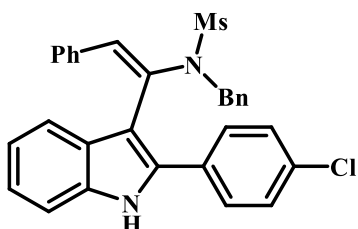
Yellow solid, 47.8 mg, 93% yield; m. p. 174-175 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.29 (s, 1H), 7.38 (m, 2H), 7.21 (m, 4H), 7.12 (m, 4H), 7.03 (m, 1H), 6.95 (m, 3H), 6.90 (dd, *J* = 7.7, 2.1 Hz, 2H), 6.85 (s, 1H), 6.72 (m, 2H), 4.47 (m, 2H), 3.76 (s, 3H), 2.69 (s, 3H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 159.75, 137.50, 137.26, 135.99, 135.71, 131.19, 130.25, 129.14, 128.48, 128.31, 128.15, 128.05, 127.95, 127.26, 126.74, 124.50, 122.69, 120.87, 120.18, 114.18, 110.82, 106.56, 55.32, 50.90, 40.84. HRMS (ESI) m/z calcd for C₃₁H₂₉N₂O₃S [M+H]⁺: 509.1815, found: 509.1888.

(E)-N-Benzyl-N-(1-(2-(3-methoxyphenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3d).



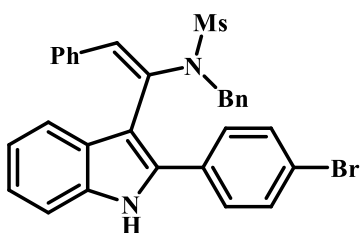
Yellow solid, 40.1 mg, 78% yield; m. p. 189-190 °C. $^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.33 (s, 1H), 7.45 (dd, $J = 8.0, 1.1$ Hz, 1H), 7.41 (m, 1H), 7.20 (m, 5H), 7.07 (m, 3H), 6.97 (m, 3H), 6.93 (m, 4H), 6.80 (m, 2H), 4.41 (m, 2H), 3.48 (s, 3H), 2.64 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 159.84, 137.04, 136.87, 135.77, 135.65, 133.35, 132.47, 130.38, 129.85, 128.58, 128.27, 128.06, 128.00, 127.28, 127.07, 123.15, 121.02, 120.59, 119.76, 115.12, 112.76, 110.94, 107.63, 55.06, 50.95, 40.56. **HRMS** (ESI) m/z calcd for $\text{C}_{31}\text{H}_{29}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 509.1816, found: 509.1891.

(E)-N-Benzyl-N-(1-(2-(4-chlorophenyl)-1H-indol-3-yl)-2-phenylvinyl)ethanesulfonamide (3e).



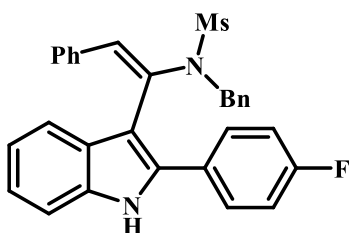
Yellow solid, 39.4 mg, 76% yield; m. p. 151-152 °C. $^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 8.36 (d, $J = 14.8$ Hz, 1H), 7.56 (d, $J = 7.8$ Hz, 1H), 7.40 (d, $J = 8.1$ Hz, 1H), 7.24 (m, 4H), 7.13 (m, 3H), 7.04 (m, 2H), 6.92 (m, 5H), 6.77 (m, 3H), 4.54 (m, 2H), 2.85 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, Chloroform-*d*) δ 137.21, 136.75, 136.03, 135.92, 134.12, 131.46, 130.28, 129.21, 129.33 (d, $J = 2.3$ Hz), 129.01, 128.68, 128.50, 128.38, 127.95, 127.90, 127.43, 126.66, 123.26, 121.25, 120.17, 111.19, 107.12, 50.89, 41.26. **HRMS** (ESI) m/z calcd for $\text{C}_{30}\text{H}_{26}\text{ClN}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 513.1325, found: 513.1393.

(E)-N-Benzyl-N-(1-(2-(4-bromophenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3f).



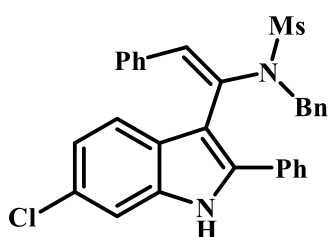
Yellow solid, 36.1 mg, 64% yield; m. p. 173-174 °C. $^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 8.25 (s, 1H), 7.58 (dd, $J = 8.1, 1.1$ Hz, 1H), 7.40 (m, 1H), 7.25 (m, 4H), 7.20 (m, 2H), 7.14 (m, 3H), 6.93 (m, 3H), 6.85 (m, 2H), 6.80 (s, 1H), 6.76 (m, 2H), 4.55 (m, 2H), 2.87 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, Chloroform-*d*) δ 137.23, 136.75, 136.05, 135.91, 131.65, 131.43, 130.71, 130.14 (d, $J = 6.1$ Hz), 129.34, 129.25, 128.71, 128.52, 128.39, 127.96, 127.94, 127.91, 127.43, 126.66, 123.32, 122.41, 121.32, 120.24, 50.88, 41.26. **HRMS** (ESI) m/z calcd for $\text{C}_{30}\text{H}_{26}\text{BrN}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 557.0873, found: 557.0880.

(E)-N-Benzyl-N-(1-(2-(4-fluorophenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3g).



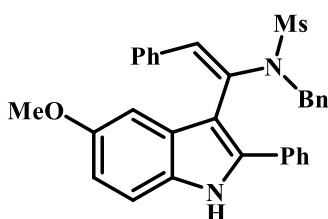
Yellow solid, 26.6 mg, 53% yield; m. p. 168-169 °C. $^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 8.33 (m, 1H), 7.53 (d, $J = 8.0$ Hz, 1H), 7.39 (d, $J = 8.1$ Hz, 1H), 7.24 (m, 4H), 7.13 (m, 3H), 6.99 (m, 2H), 6.91 (m, 3H), 6.78 (m, 5H), 4.50 (m, 2H), 2.83 (d, $J = 1.4$ Hz, 3H). $^{13}\text{C NMR}$ (126 MHz, Chloroform-*d*) δ 162.61 (d, $J = 248.8$ Hz), 137.34, 137.10, 136.15, 135.87, 135.85, 131.67, 129.73, 129.67, 129.06 (t, $J = 2.9$ Hz), 128.72, 128.53, 128.41, 128.01, 127.47, 126.65, 123.12, 121.22, 120.17, 115.57 (d, $J = 21.6$ Hz), 111.15 (d, $J = 3.1$ Hz), 106.86 (d, $J = 2.9$ Hz), 50.97, 41.32. $^{19}\text{F NMR}$ (471 MHz, Chloroform-*d*) δ -112.88. **HRMS** (ESI) m/z calcd for $\text{C}_{30}\text{H}_{26}\text{FN}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 497.1612, found: 497.1682.

(E)-N-Benzyl-N-(1-(6-chloro-2-phenyl-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3h).



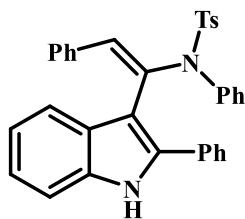
Yellow solid, 19.1 mg, 37% yield; m. p. 145-146 °C. $^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 8.43 (s, 1H), 7.28 (m, 9H), 7.10 (m, 4H), 6.97 (q, $J = 6.7, 6.1$ Hz, 3H), 6.90 (m, 2H), 6.86 (s, 1H), 4.41 (s, 2H), 2.58 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, Chloroform-*d*) δ 138.61, 136.68, 135.63, 134.06, 131.61, 130.69, 130.10, 129.13, 128.93, 128.79, 128.44, 128.39, 128.15, 128.07, 127.92, 127.53, 126.98, 126.52, 123.35, 119.77, 111.96, 107.37, 51.18, 40.64. **HRMS** (ESI) m/z calcd for $\text{C}_{30}\text{H}_{26}\text{ClN}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 513.1324, found: 513.1393.

(E)-N-Benzyl-N-(1-(5-methoxy-2-phenyl-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3i).



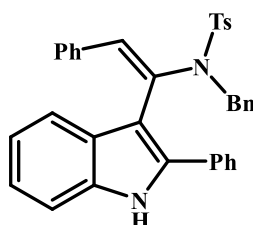
Yellow solid, 21.4 mg, 42% yield; m. p. 184-185 °C. $^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 8.26 (d, $J = 12.2$ Hz, 1H), 7.29 (m, 2H), 7.25 (m, 4H), 7.21 (dd, $J = 5.4, 1.8$ Hz, 3H), 7.10 (m, 2H), 6.96 (d, $J = 1.4$ Hz, 5H), 6.82 (m, 2H), 6.73 (d, $J = 2.4$ Hz, 1H), 4.40 (d, $J = 15.0$ Hz, 2H), 3.60 (s, 3H), 2.60 (d, $J = 1.0$ Hz, 3H). $^{13}\text{C NMR}$ (126 MHz, Chloroform-*d*) δ 154.74, 137.88, 137.09, 135.98, 132.23, 130.96, 130.77 (d, $J = 1.1$ Hz), 130.28, 128.83, 128.62, 128.48, 128.37, 128.32, 128.13, 127.99, 127.88, 127.33, 126.79, 113.56, 111.67 (d, $J = 1.8$ Hz), 107.37 (d, $J = 1.7$ Hz), 101.48, 55.47, 50.82, 40.89. **HRMS** (ESI) m/z calcd for $\text{C}_{31}\text{H}_{29}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 509.1817, found: 509.1890.

(E)-4-Methyl-N-phenyl-N-(2-phenyl-1-(2-phenyl-1H-indol-3-yl)vinyl)benzenesulfo-



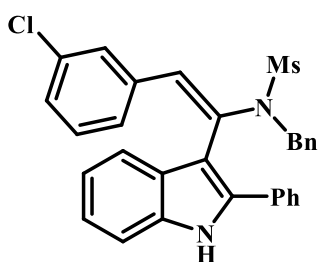
namide (3j). Yellow solid, 41.8mg, 78% yield; m. p. 225-226 °C. $^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 8.03 (s, 1H), 7.62 (m, 1H), 7.45 (m, 2H), 7.22 (m, 4H), 7.13 (m, 5H), 7.01 (m, 2H), 6.96 (m, 7H), 6.88 (m, 3H), 2.39 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, Chloroform-*d*) δ 143.26, 138.79, 138.20, 137.17, 136.20, 135.59, 133.63, 131.96, 130.04, 129.60, 129.27 (d, $J = 5.9$ Hz), 128.40, 128.34, 128.23, 128.15, 128.06, 127.96 (d, $J = 2.5$ Hz), 127.79, 127.76, 127.23, 126.59, 126.34, 122.46, 120.56 (d, $J = 10.3$ Hz), 110.53, 108.63, 21.54. **HRMS** (ESI) m/z calcd for $\text{C}_{35}\text{H}_{29}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 541.1867, found: 541.1937.

(E)-N-Benzyl-4-methyl-N-(2-phenyl-1-(2-phenyl-1H-indol-3-yl)vinyl)benzenesulfon-



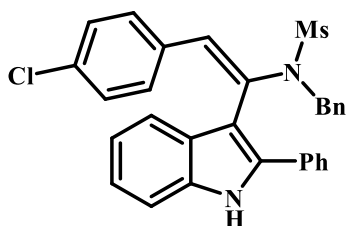
amide (3k). Yellow solid, 48.8mg, 88% yield; m. p. 155-156 °C. $^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 8.16 (s, 1H), 7.52 (m, 2H), 7.26 (d, $J = 30.9$ Hz, 1H), 7.16 (m, 4H), 7.12 (m, 4H), 7.06 (m, 2H), 7.01 (t, $J = 7.7$ Hz, 2H), 6.94 (m, 1H), 6.83 (m, 6H), 6.65 (m, 2H), 4.62 (m, 2H), 2.37 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, Chloroform-*d*) δ 143.19, 138.41, 138.29, 137.94, 136.64, 135.62, 132.34, 131.93, 129.48, 129.29, 128.33, 128.25, 128.25, 128.05, 127.82, 127.77, 127.75, 127.68, 127.66, 127.07, 126.05, 122.56, 120.62, 120.30, 110.72, 106.90, 52.02, 21.48. **HRMS** (ESI) m/z calcd for $\text{C}_{36}\text{H}_{31}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 555.2028, found: 555.2102.

(E)-N-Benzyl-N-(2-(3-chlorophenyl)-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfo-



namide (3m). Yellow solid, 33.9mg, 66% yield; m. p. 169-170 °C. $^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.31 (s, 1H), 7.42 (m, 2H), 7.21 (m, 9H), 7.11 (m, 1H), 7.07 (m, 2H), 6.89 (m, 1H), 6.79 (t, $J = 7.9$ Hz, 1H), 6.72 (t, $J = 1.8$ Hz, 1H), 6.66 (m, 2H), 4.55 (m, 2H), 2.79 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 138.30 (d, $J = 14.8$ Hz), 137.23, 135.82, 133.66, 133.37, 131.73, 130.07, 128.99, 128.94, 128.72, 128.51, 128.43, 128.35, 128.11, 127.82, 127.67, 127.50, 126.32, 126.28, 123.12, 121.26, 120.07, 111.10, 106.43, 51.02, 41.26. **HRMS** (ESI) m/z calcd for $\text{C}_{30}\text{H}_{26}\text{ClN}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 513.1320, found: 513.1389.

(E)-N-Benzyl-N-(2-(4-chlorophenyl)-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfonamide (3n).

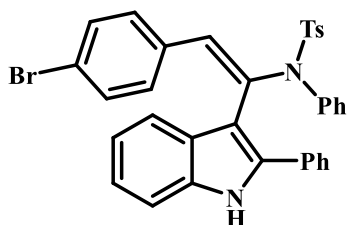


Yellow solid, 40.4mg, 79% yield; m. p. 223-224 °C. $^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.39 (dd, $J = 15.1, 6.8$ Hz, 1H), 7.39 (d, $J = 8.1$ Hz, 2H), 7.22 (m, 7H), 7.14 (m, 4H), 7.07 (dd, $J = 8.2, 6.9$ Hz, 1H), 6.86 (m, 2H), 6.74 (m, 3H), 4.49 (m, 2H), 2.70 (d, $J = 1.2$ Hz, 3H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 137.91, 137.17, 135.88, 134.69,

132.24, 132.17, 131.90, 129.63, 128.78, 128.47, 128.13, 128.08, 127.87, 127.80, 127.72, 127.70, 127.48, 123.15, 121.19, 120.19, 111.15 (d, $J = 2.8$ Hz), 106.74, 51.07, 41.10.

HRMS (ESI) m/z calcd for $\text{C}_{30}\text{H}_{26}\text{ClN}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 513.1324, found: 513.1396.

(E)-N-(2-(4-Bromophenyl)-1-(2-phenyl-1H-indol-3-yl)vinyl)-4-methyl-N-phenylbenzenesulfonamide (3o).

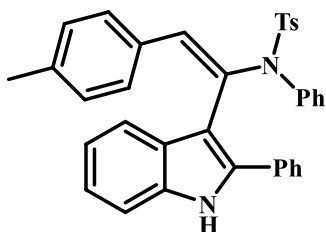


Yellow solid, 38.2mg, 63% yield; m. p. 205-206 °C. $^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.03 (s, 1H), 7.61 (d, $J = 8.0$ Hz, 1H), 7.44 (m, 2H), 7.25 (m, 4H), 7.14 (m, 5H), 7.05 (m, 4H), 6.98 (dd, $J = 8.5, 6.9$ Hz, 2H), 6.89 (m, 2H), 6.78 (m, 3H), 2.40 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 143.42, 138.67, 137.98, 137.35, 135.58,

135.28, 134.54, 131.82, 131.02, 130.04, 129.86, 129.29, 128.45, 128.24, 128.15, 128.07, 128.03, 127.92, 127.71, 124.56, 122.64, 120.74, 120.46, 120.27, 110.64, 108.11, 21.55.

HRMS (ESI) m/z calcd for $\text{C}_{35}\text{H}_{28}\text{BrN}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 619.0958, found: 619.1028.

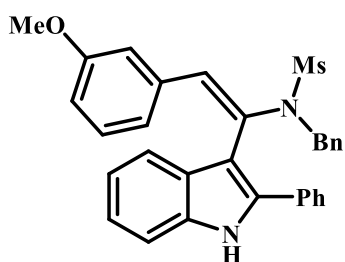
(E)-4-Methyl-N-phenyl-N-(1-(2-phenyl-1H-indol-3-yl)-2-(p-tolyl)vinyl)benzenesulfonamide (3p).



Yellow solid, 36.7mg, 66% yield; m. p. 216-217 °C. $^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.07 (d, $J = 8.6$ Hz, 1H), 7.57 (dd, $J = 7.9, 1.2$ Hz, 1H), 7.42 (m, 2H), 7.21 (m, 3H), 7.15 (dd, $J = 9.7, 7.3$ Hz, 4H), 7.09 (m, 1H), 6.99 (m, 2H), 6.90 (m, 6H), 6.83 (m, 2H), 6.79 (d, $J = 7.9$ Hz, 2H), 2.38 (s, 3H), 2.16 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ

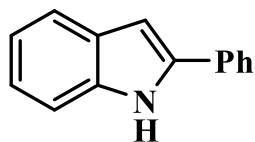
143.44, 139.04, 138.51, 137.17, 136.72, 135.87, 133.44, 132.86, 132.27, 130.31, 129.48, 129.01, 128.58 (d, $J = 2.5$ Hz), 128.52, 128.33, 128.30, 128.18, 128.06, 127.92, 127.00, 122.66, 122.00, 120.88, 120.69, 110.80, 109.13, 21.79, 21.37. **HRMS** (ESI) m/z calcd for $\text{C}_{36}\text{H}_{31}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 555.2024, found: 555.2095.

(E)-N-Benzyl-N-(2-(3-methoxyphenyl)-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfonamide (3q). Yellow solid, 44.8mg, 88% yield; m. p. 215-



216 °C. $^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.40 (dd, $J = 6.7, 3.5$ Hz, 1H), 7.39 (m, 2H), 7.22 (m, 9H), 7.10 (m, 2H), 7.05 (m, 1H), 6.87 (t, $J = 8.0$ Hz, 1H), 6.84 (s, 1H), 6.53 (dd, $J = 8.0, 2.7$ Hz, 2H), 6.40 (t, $J = 2.1$ Hz, 1H), 4.45 (m, 2H), 3.29 (s, 3H), 2.64 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 156.77, 135.06, 134.86, 134.84, 133.46, 129.70, 128.95, 127.86, 126.49, 126.44, 126.05, 126.00, 125.80, 125.73, 125.62, 124.99, 120.70, 119.15, 118.69, 118.09, 111.15, 110.38, 108.58, 105.17, 52.29, 48.69, 38.44. **HRMS** (ESI) m/z calcd for $\text{C}_{31}\text{H}_{29}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 509.1815, found: 509.1886.

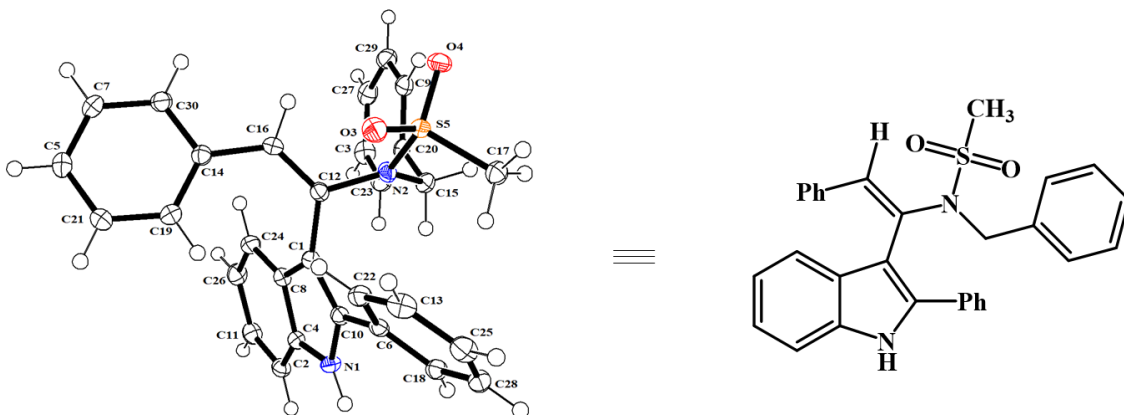
2-Phenyl-1H-indole (4). White solid, 36.7 mg, 95% yield; m. p. 190-191 °C. $^1\text{H NMR}$



(600 MHz, Chloroform-*d*) δ 8.28 (s, 1H), 7.63 (m, 3H), 7.42 (m, 2H), 7.38 (dq, $J = 8.1, 1.0$ Hz, 1H), 7.31 (m, 1H), 7.19 (ddd, $J = 8.2, 7.1, 1.2$ Hz, 1H), 7.12 (ddd, $J = 8.0, 7.0, 1.1$ Hz, 1H), 6.82 (dd, $J = 2.2, 0.9$ Hz, 1H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 137.87, 136.80, 132.36, 129.25, 129.01, 127.70, 125.15, 122.34, 120.66, 120.26, 110.89, 99.97. **HRMS** (ESI) m/z calcd for $\text{C}_{14}\text{H}_{12}\text{N}$ $[\text{M}+\text{H}]^+$: 194.0964, found: 194.1007.

6. Single Crystal X-ray Structure Determinations of Compounds

Single crystal X-ray structure determinations of compound 3a (CCDC: 2284506)

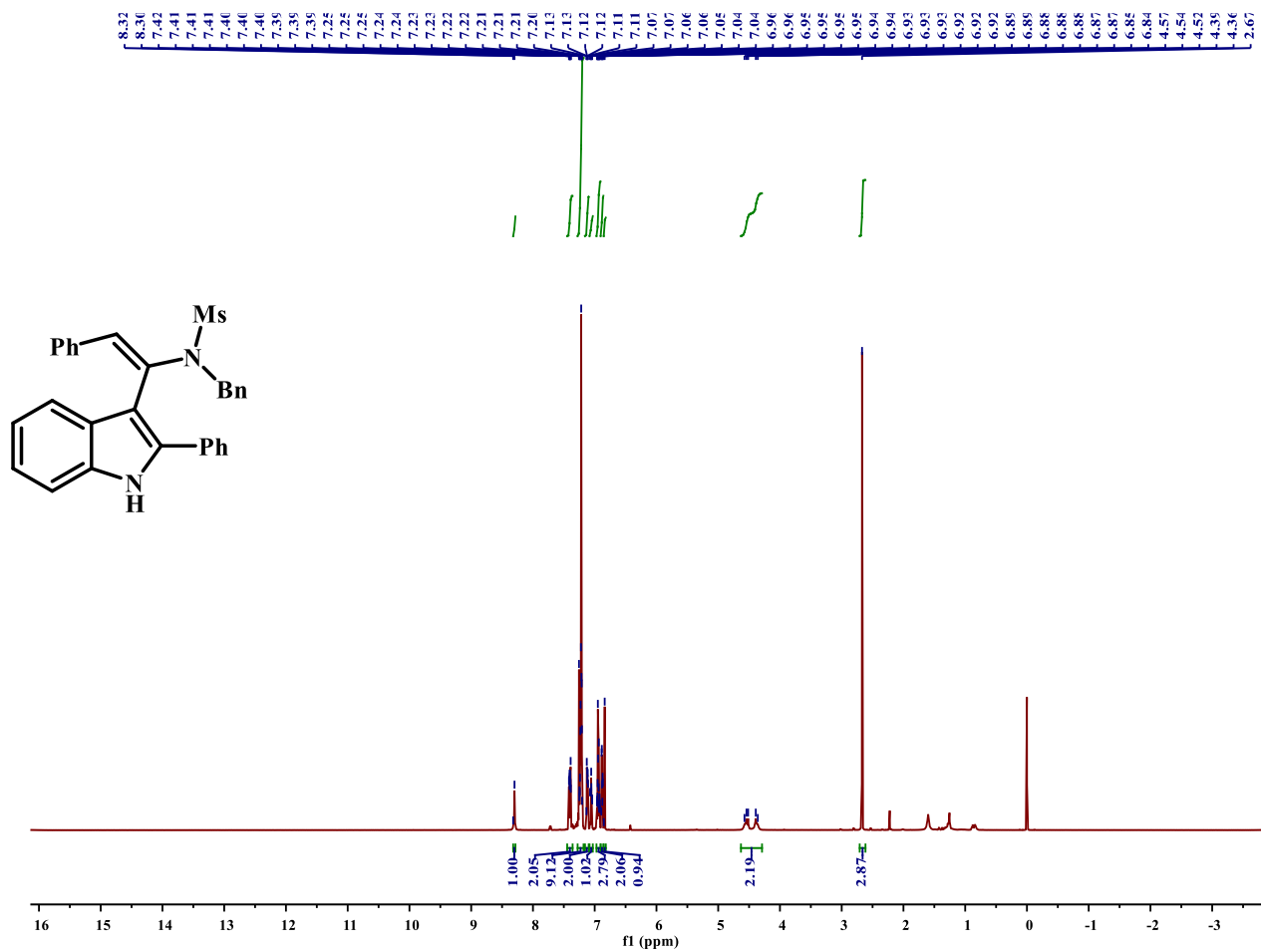


Bond precision:	C-C = 0.0019 Å	Wavelength=1.54184	
Cell:	a=10.6510(1) alpha=90	b=14.5991(1) beta=109.300(1)	c=16.0583(2) gamma=90
Temperature:	100 K		
	Calculated		Reported
Volume	2356.66(4)		2356.66(4)
Space group	P 21/n		P 1 21/n 1
Hall group	-P 2yn		-P 2yn
Moiety formula	C30 H26 N2 O2 S		C30 H26 N2 O2 S
Sum formula	C30 H26 N2 O2 S		C30 H26 N2 O2 S
Mr	478.59		478.59
Dx, g cm ⁻³	1.349		1.349
Z	4		4
Mu (mm ⁻¹)	1.466		1.466
F000	1008.0		1008.0
F000'	1012.00		
h,k,lmax	12,17,19		12,17,19
Nref	4222		4203
Tmin,Tmax	0.768,0.814		0.713,1.000
Tmin'	0.746		
Correction method=	# Reported T Limits: Tmin=0.713 Tmax=1.000		
AbsCorr =	MULTI-SCAN		
Data completeness=	0.995	Theta(max)=	67.076
R(reflections)=	0.0312(3989)		
wR2(reflections)=			0.0815(4203)
S =	1.044	Npar=	317

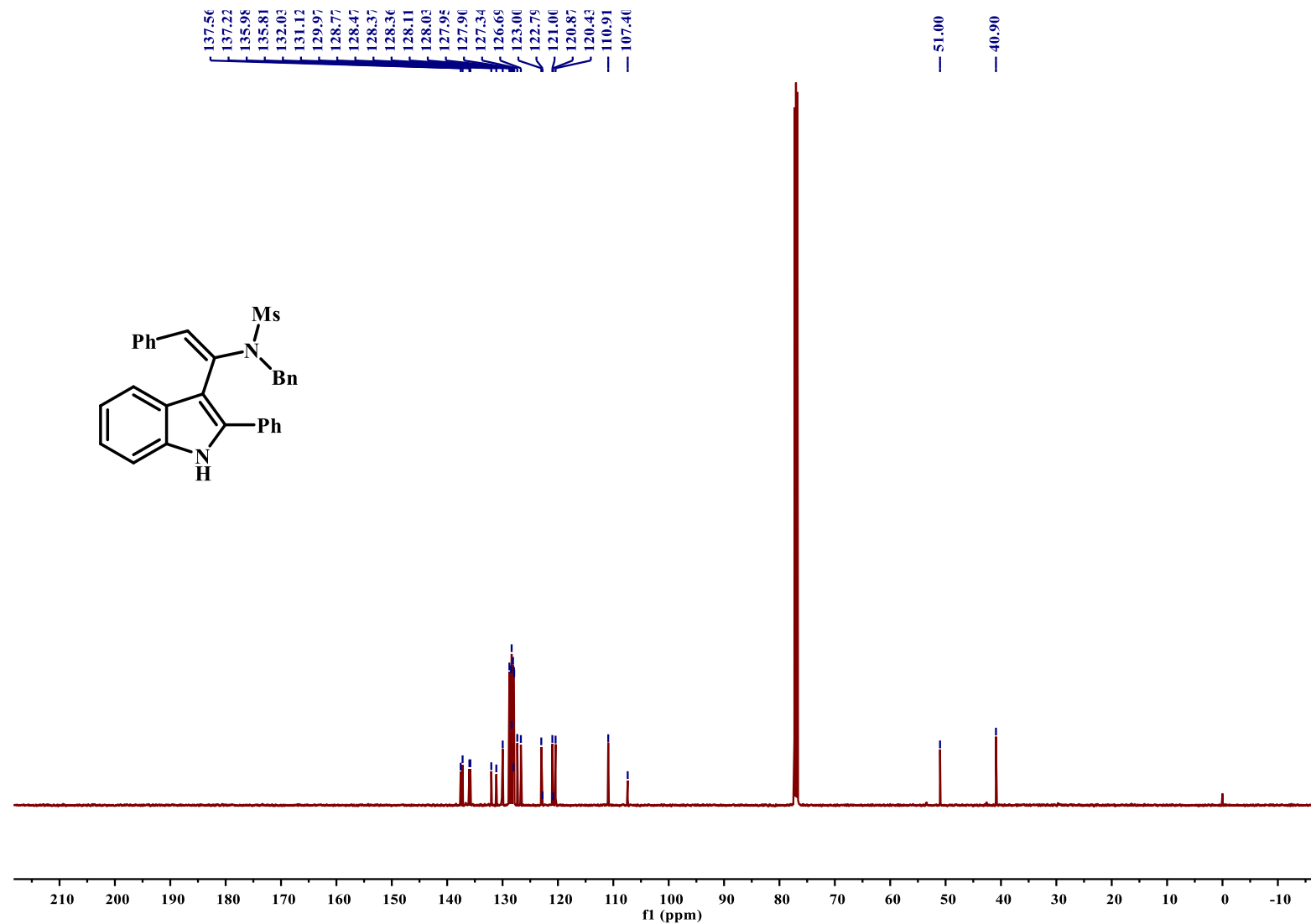
7. Copies of NMR Spectra

^1H NMR, ^{13}C NMR and ^{19}F NMR spectra for compounds:

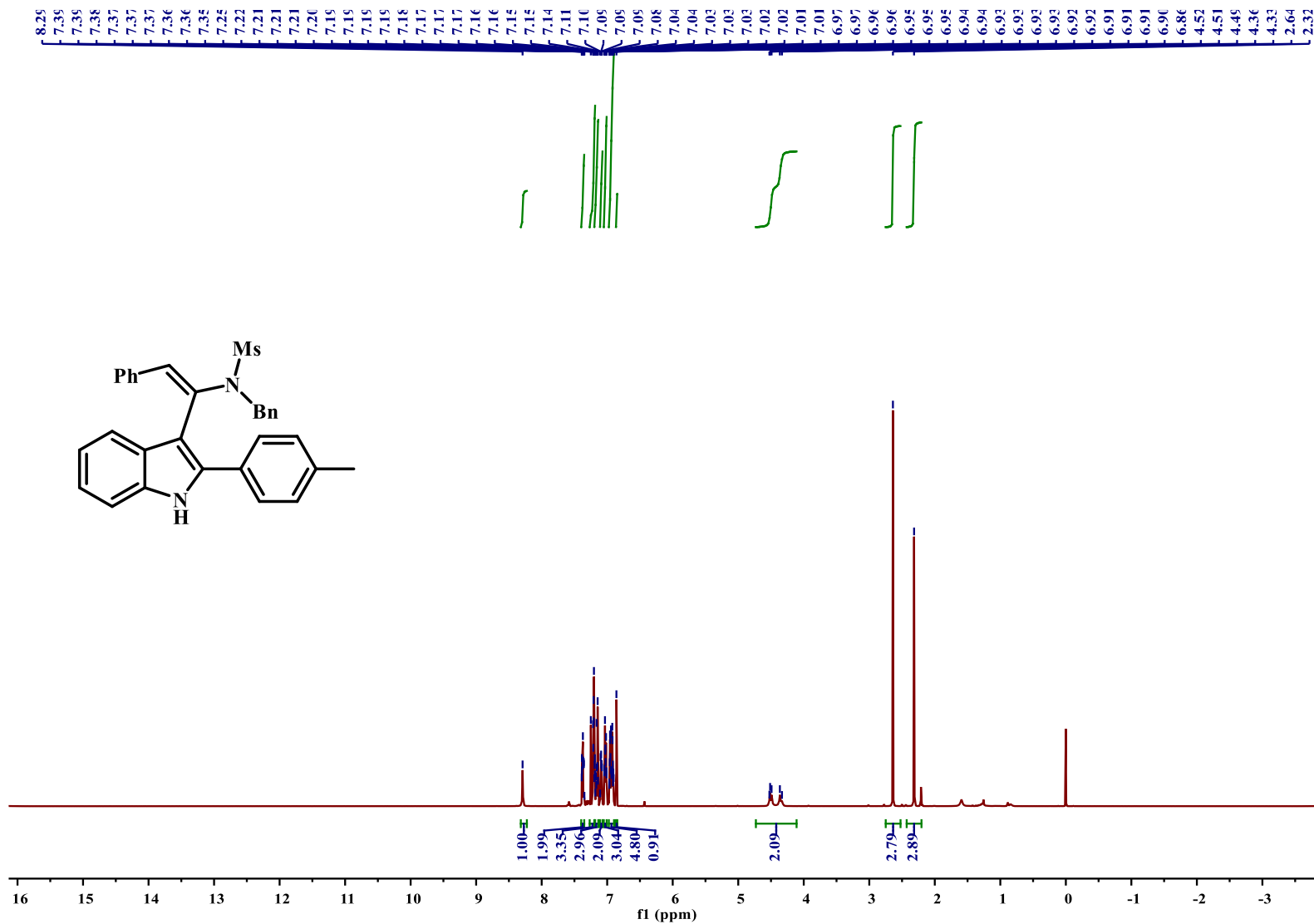
(E)-N-Benzyl-N-(2-phenyl-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfonamide (3a)



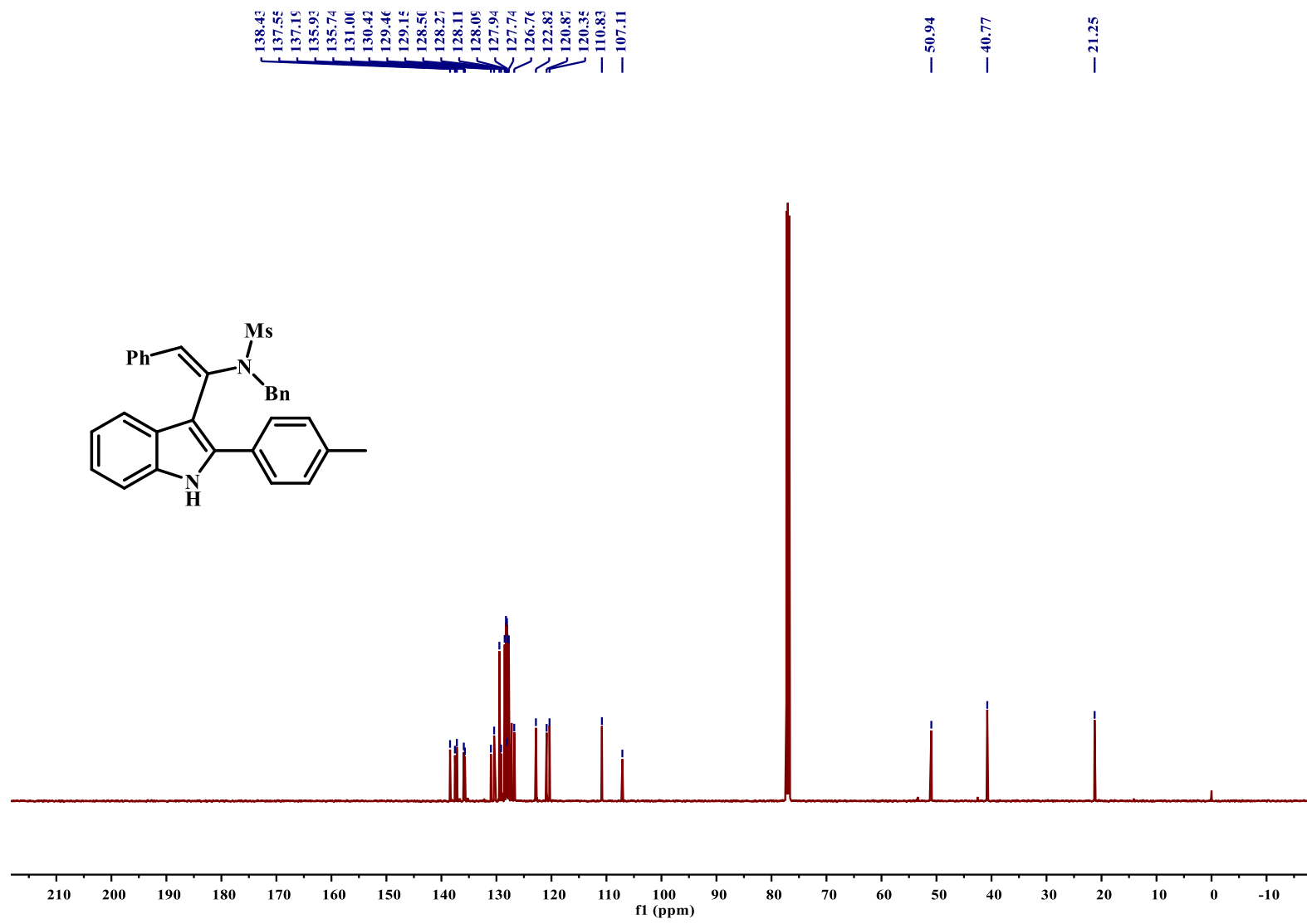
(E)-N-Benzyl-N-(2-phenyl-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfonamide (3a)



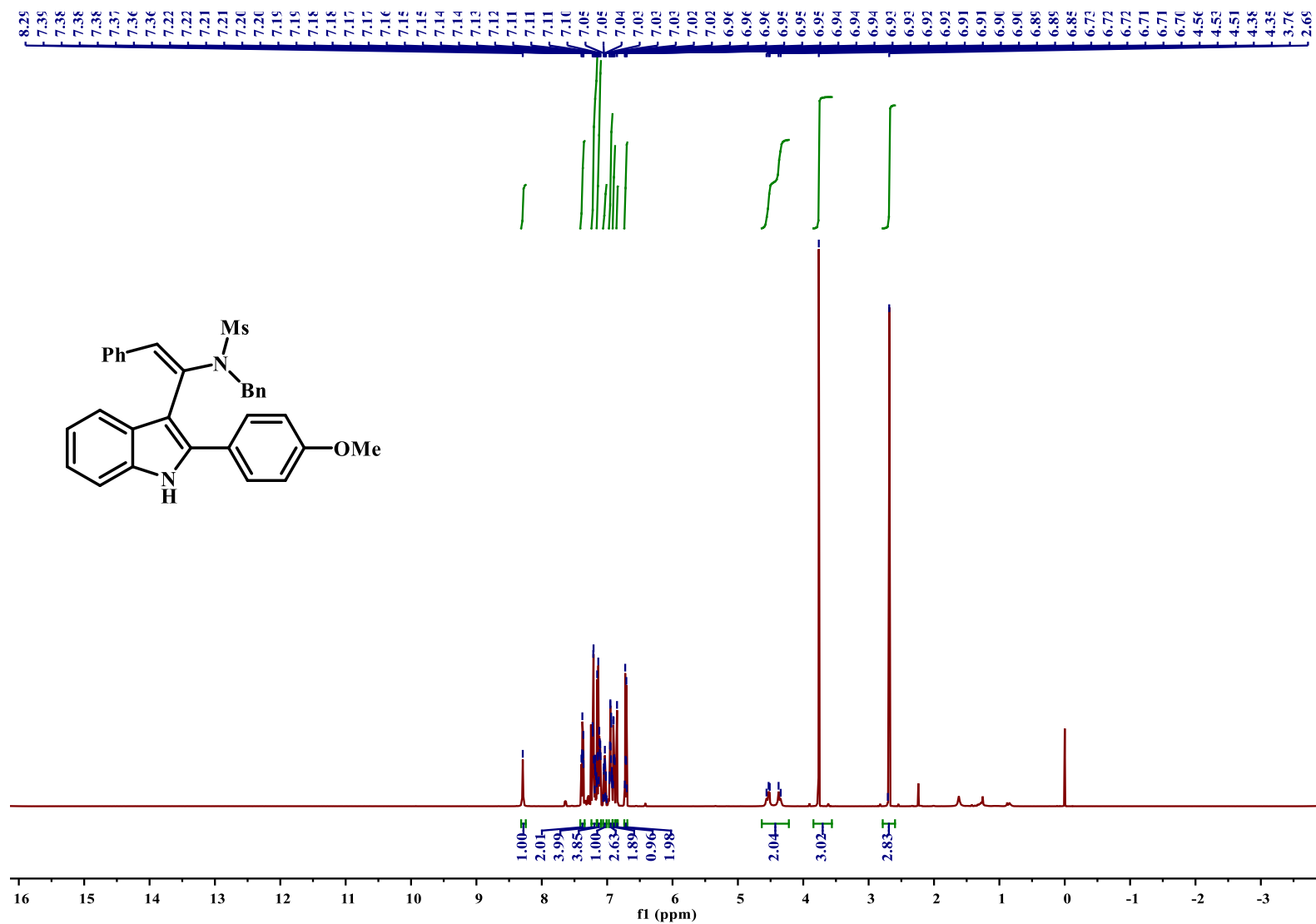
(E)-N-Benzyl-N-(2-phenyl-1-(2-(p-tolyl)-1H-indol-3-yl)vinyl)methanesulfonamide (3b)



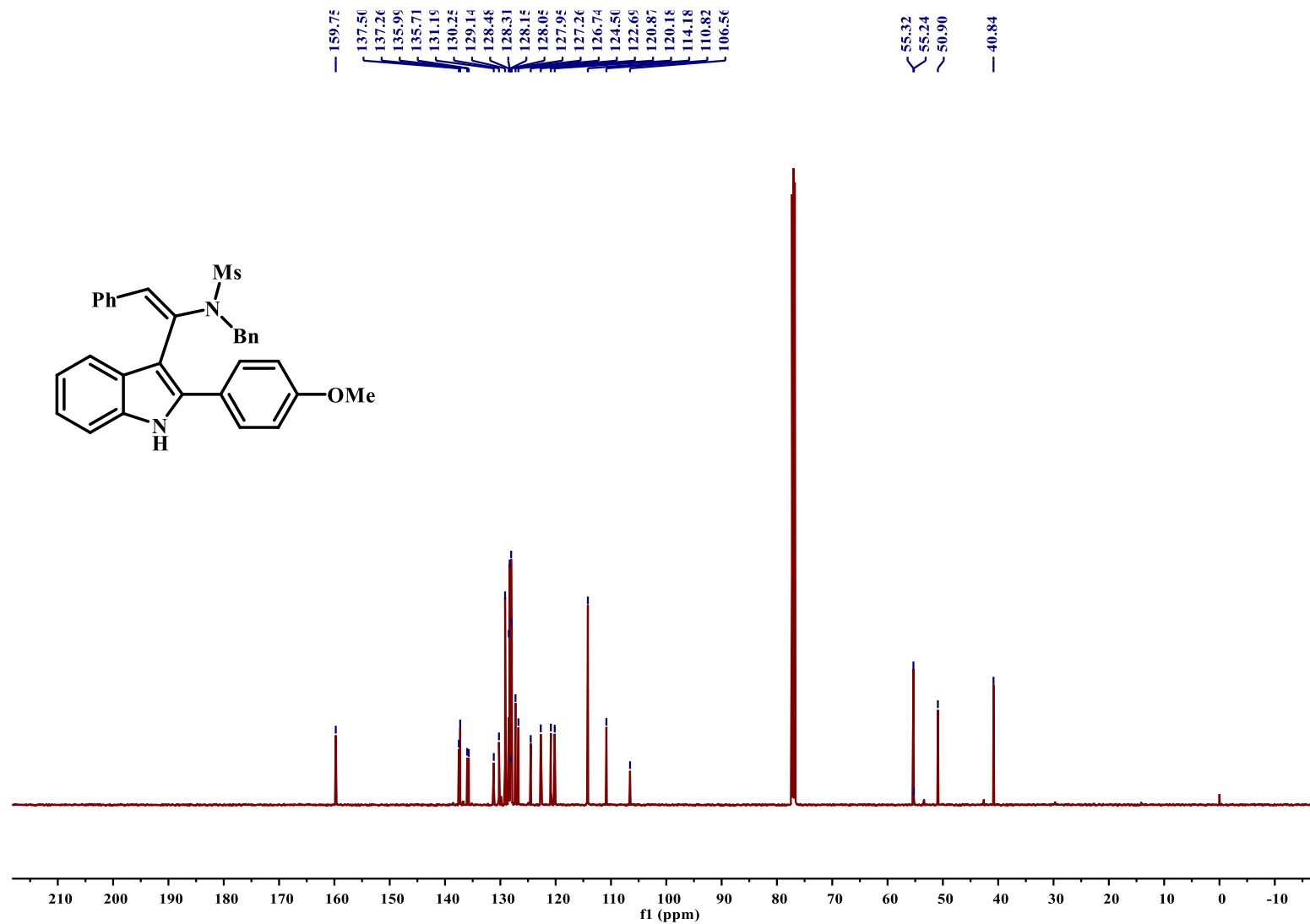
(E)-N-Benzyl-N-(2-phenyl-1-(2-(p-tolyl)-1H-indol-3-yl)vinyl)methanesulfonamide (3b)



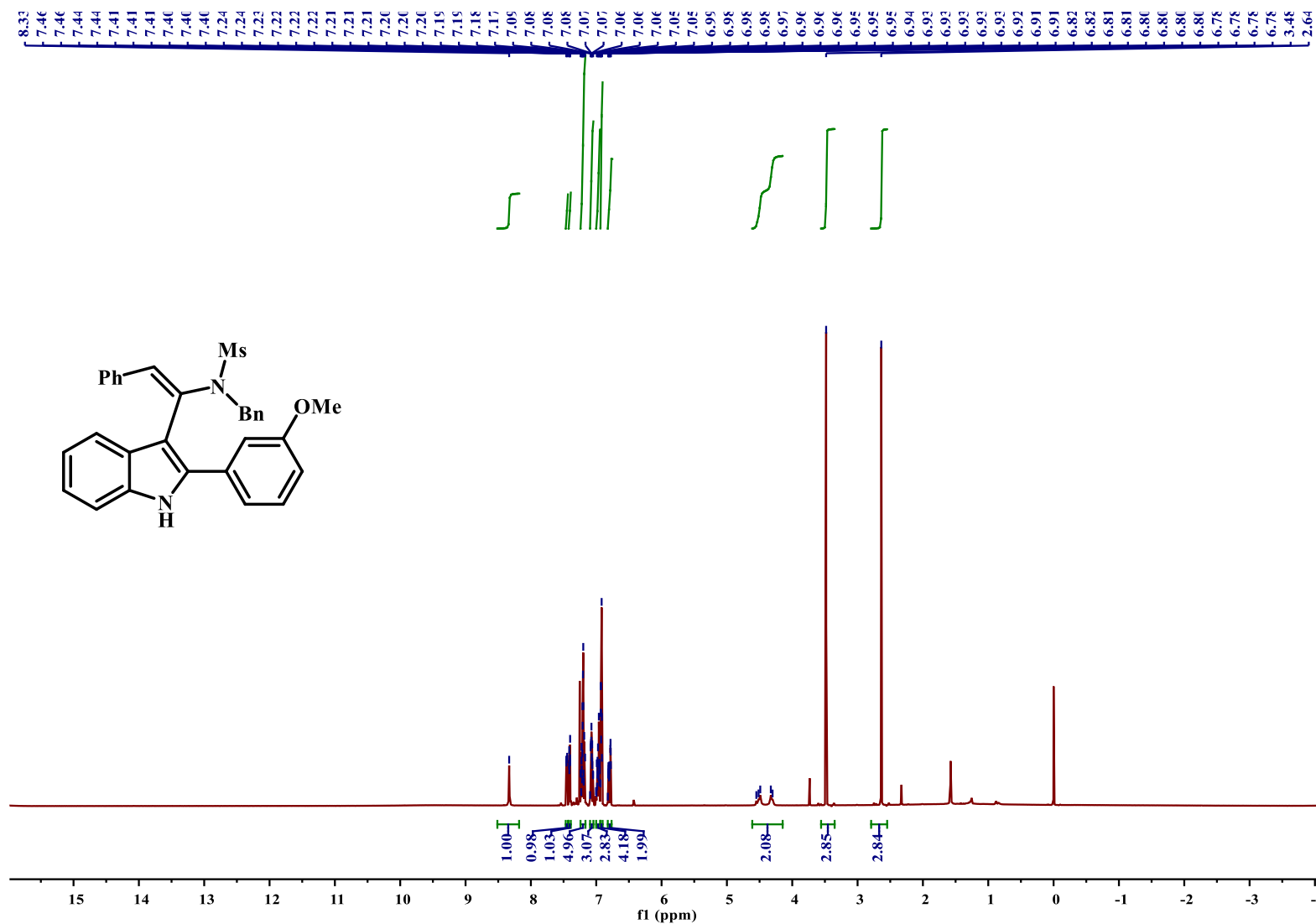
(E)-N-Benzyl-N-(1-(2-(4-methoxyphenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3c)



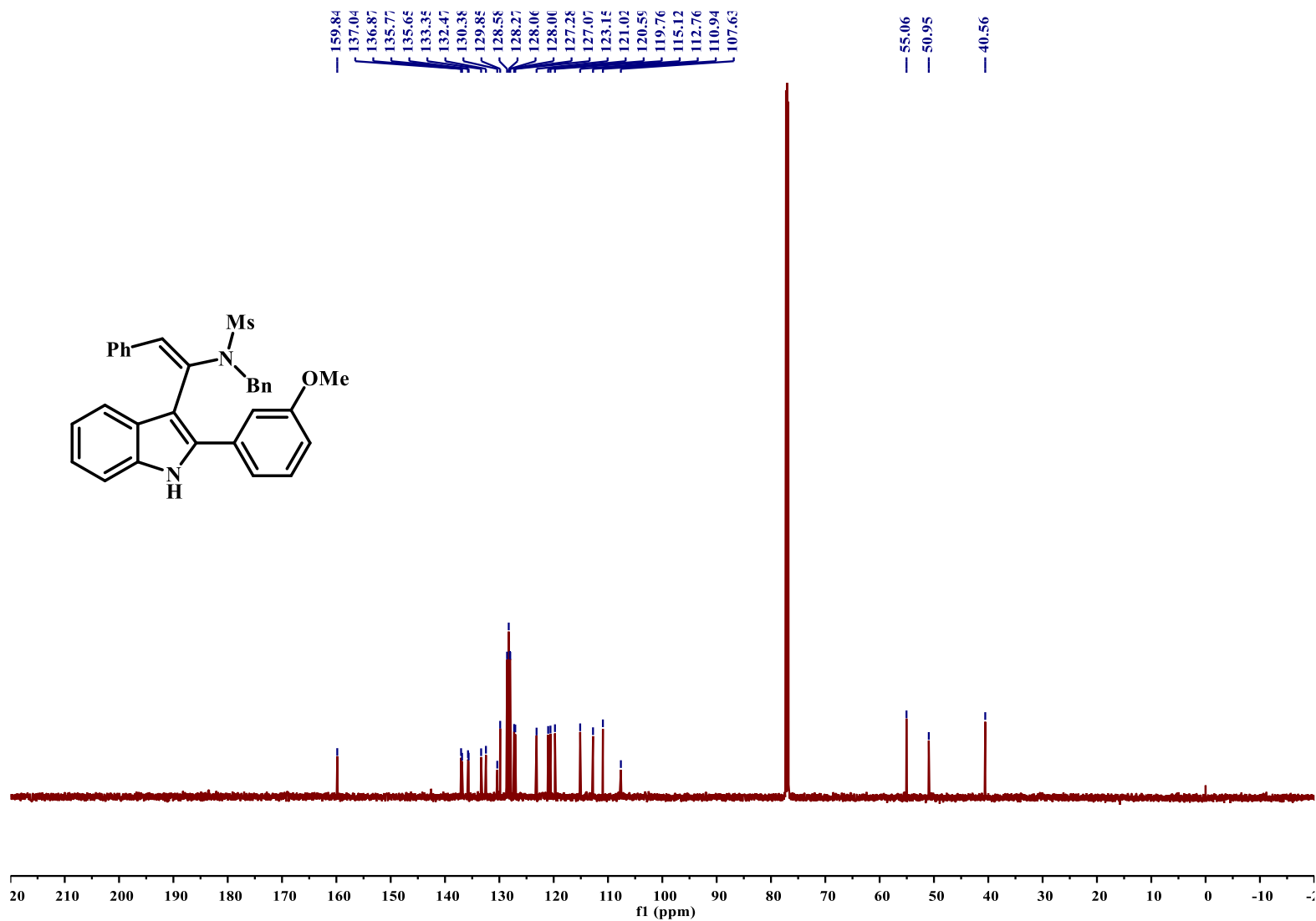
(E)-N-Benzyl-N-(1-(2-(4-methoxyphenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3c)



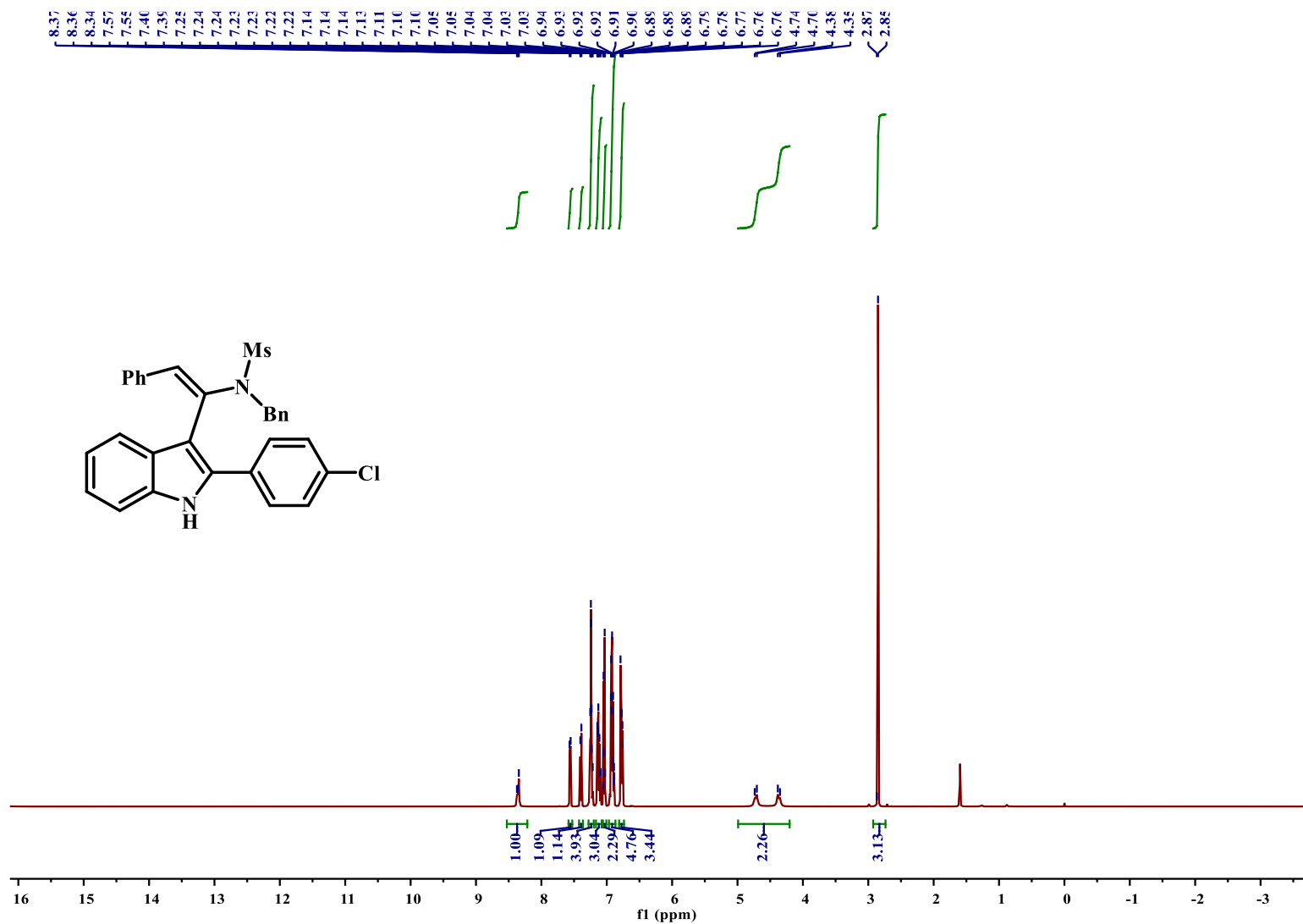
(E)-N-Benzyl-N-(1-(2-(3-methoxyphenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3d)



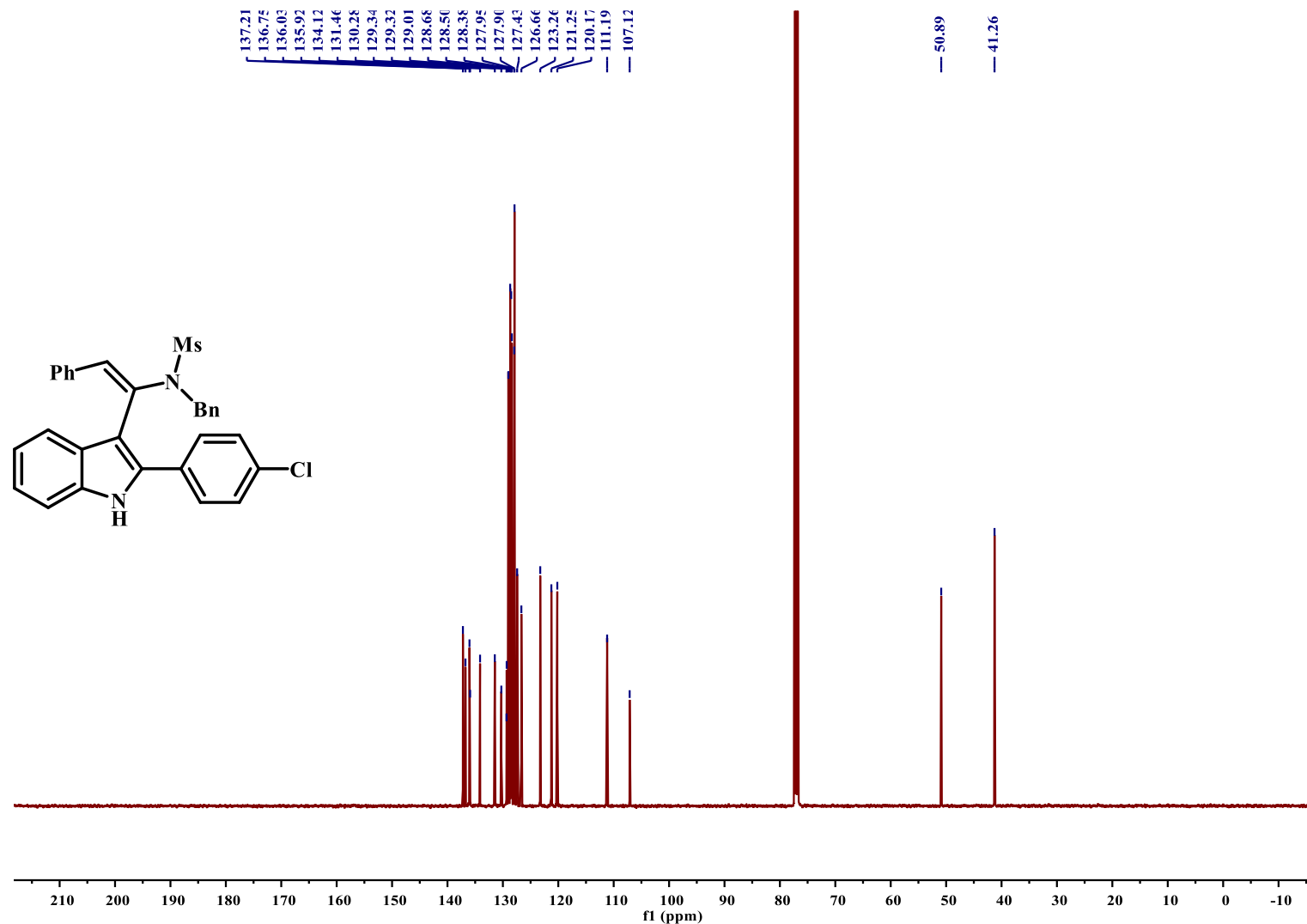
(E)-N-Benzyl-N-(1-(2-(3-methoxyphenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3d)



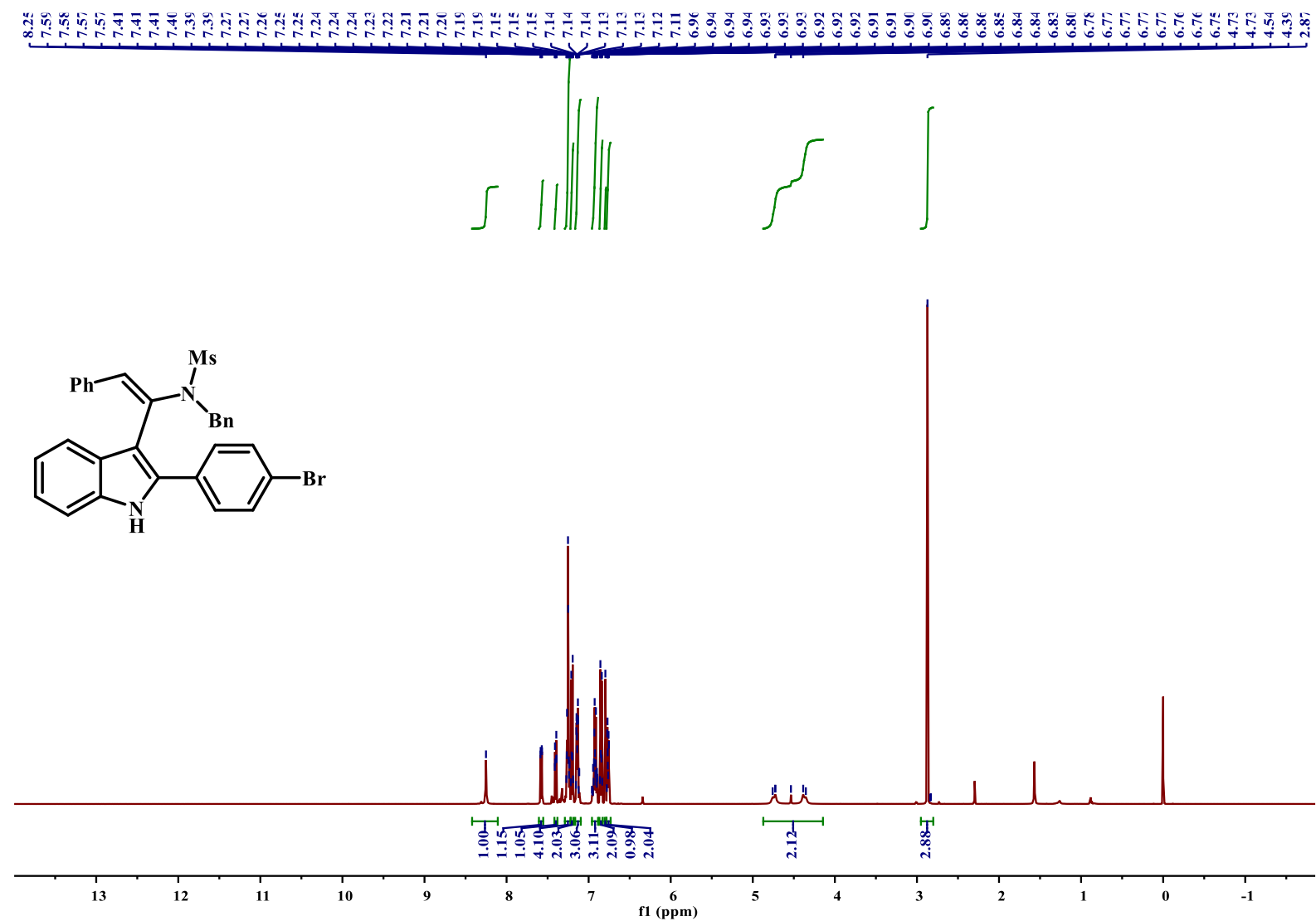
(E)-N-Benzyl-N-(1-(2-(4-chlorophenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3e)



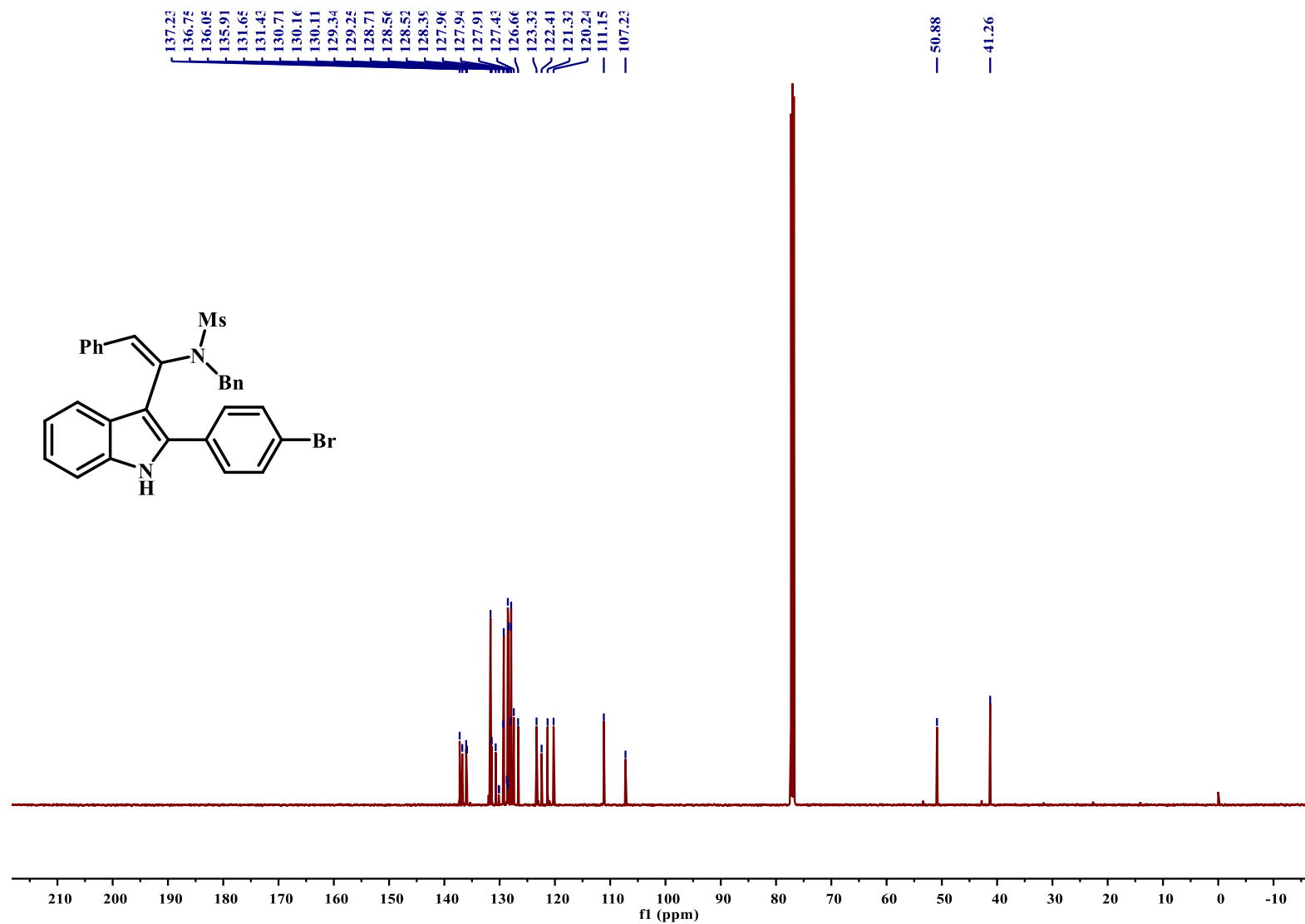
(E)-N-Benzyl-N-(1-(2-(4-chlorophenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3e)



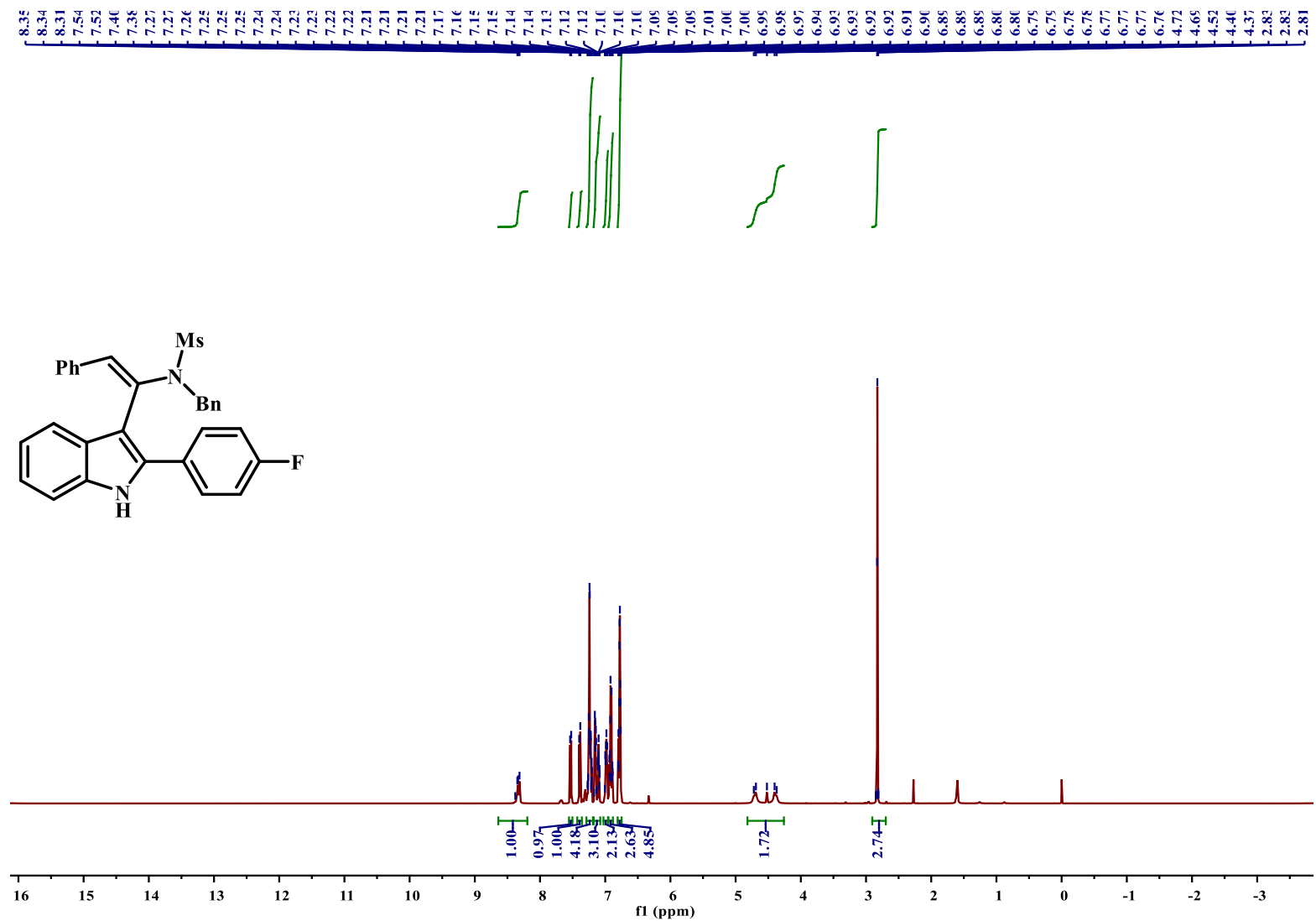
(E)-N-Benzyl-N-(1-(2-(4-bromophenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3f)



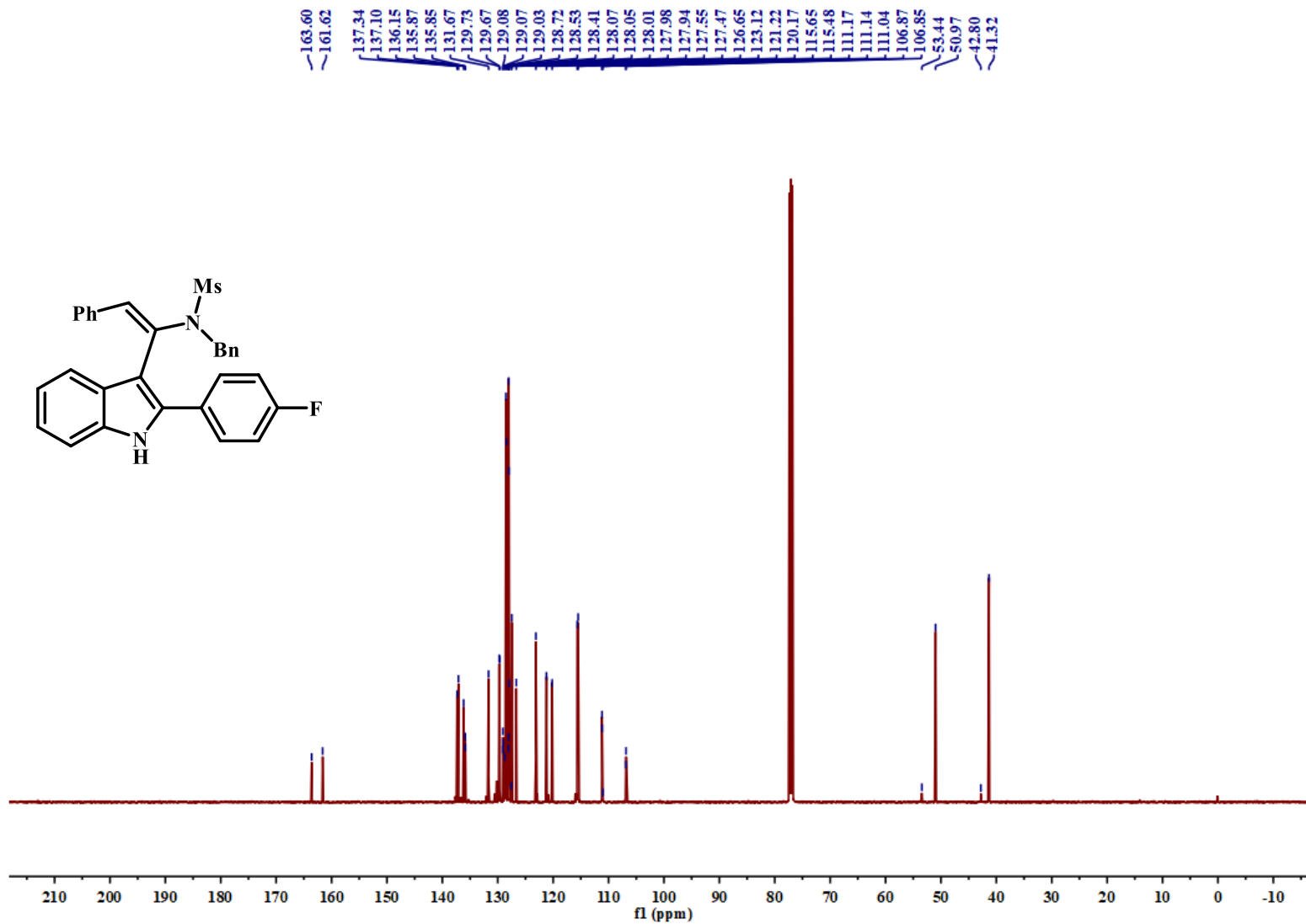
(E)-N-Benzyl-N-(1-(2-(4-bromophenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3f)



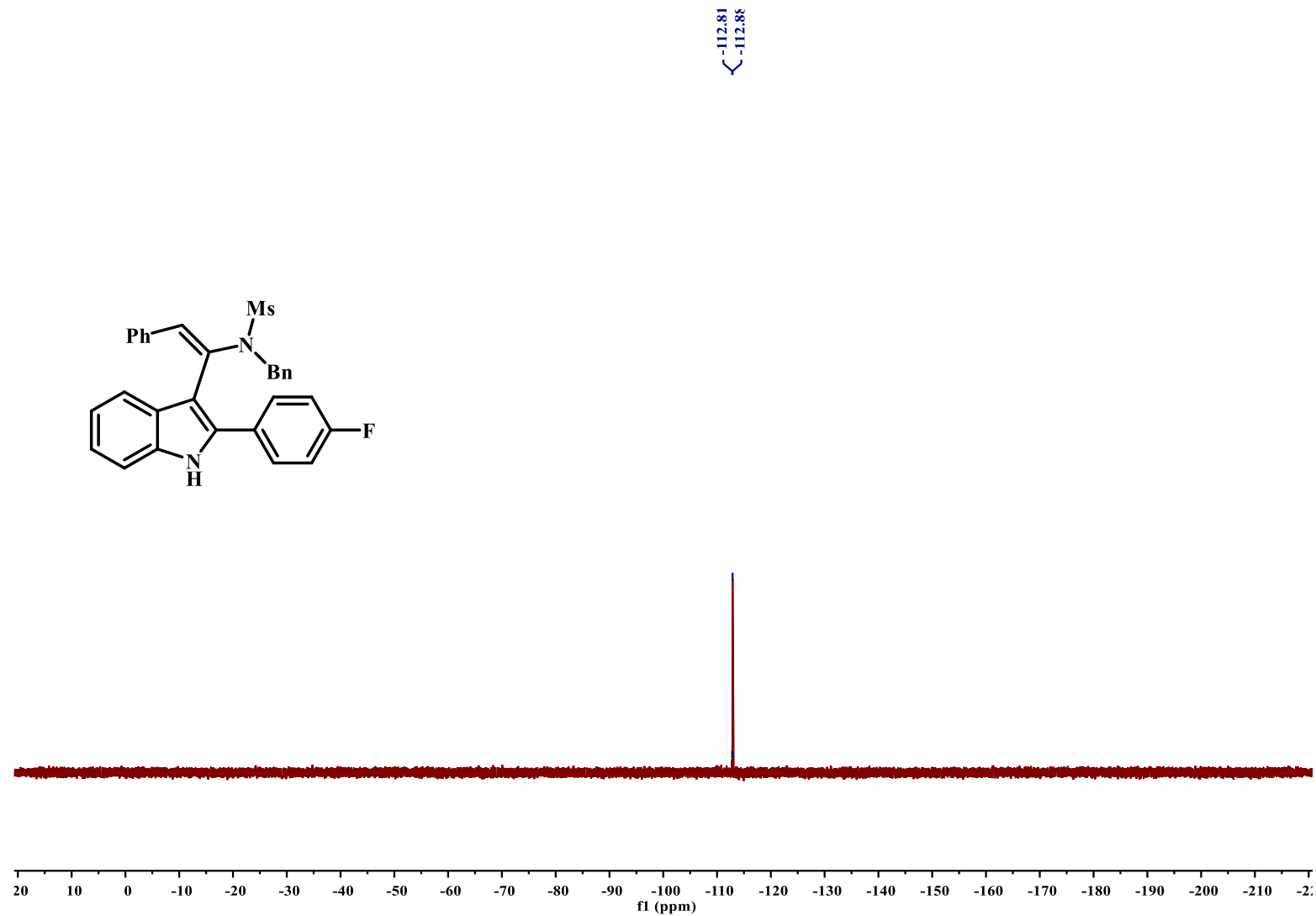
(E)-N-Benzyl-N-(1-(2-(4-fluorophenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3g)



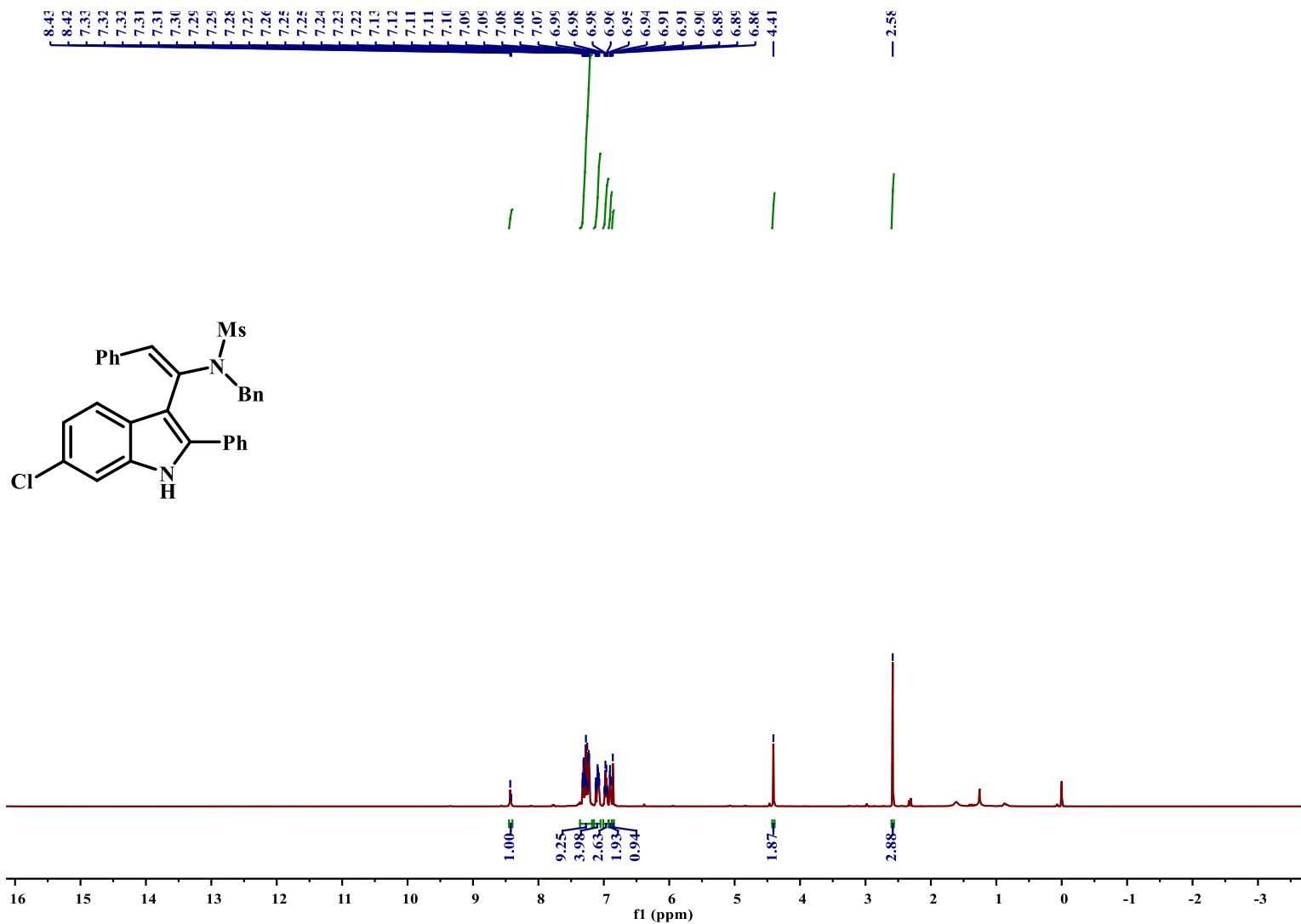
(E)-N-Benzyl-N-(1-(2-(4-fluorophenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3g)



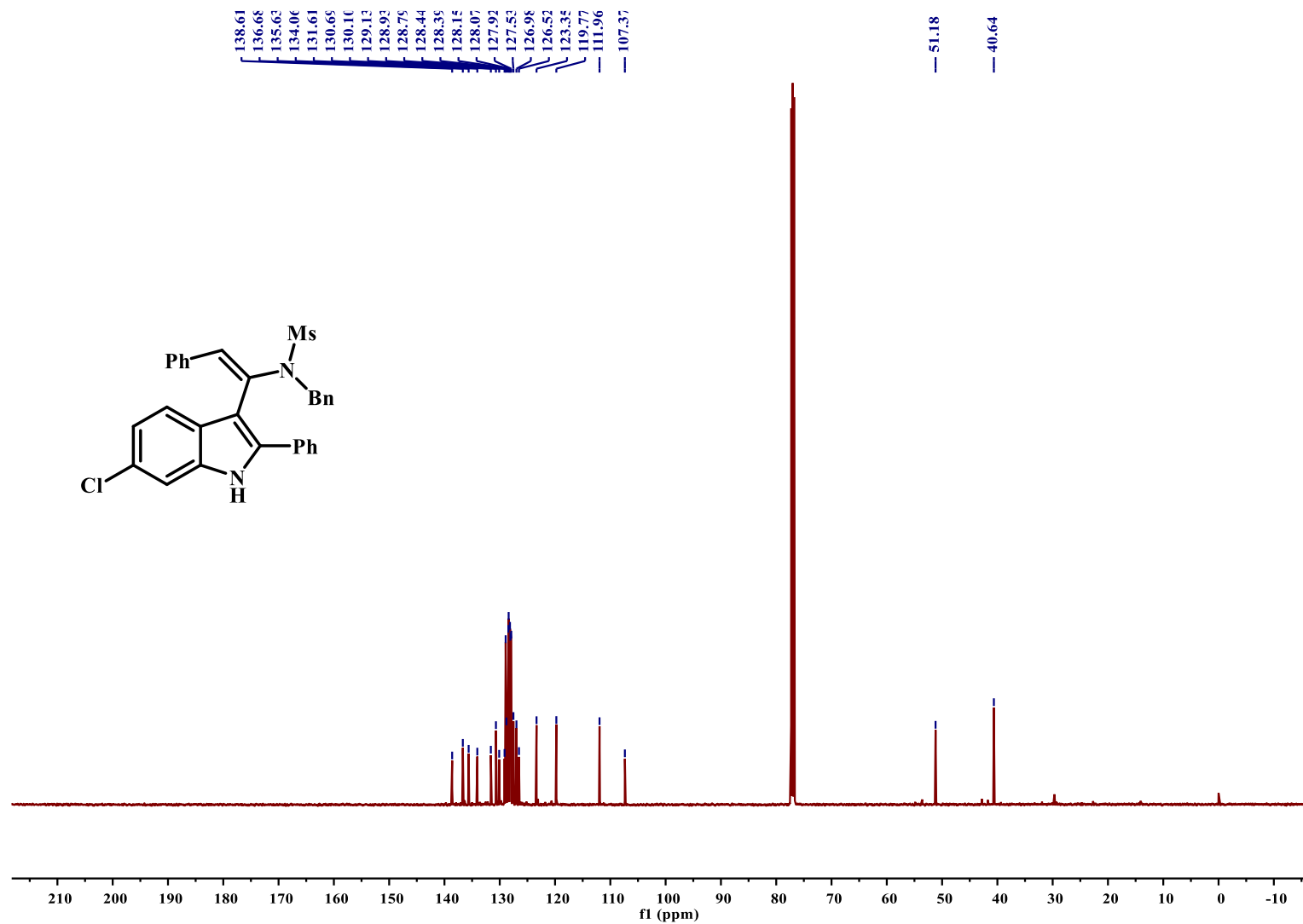
(E)-N-Benzyl-N-(1-(2-(4-fluorophenyl)-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3g)



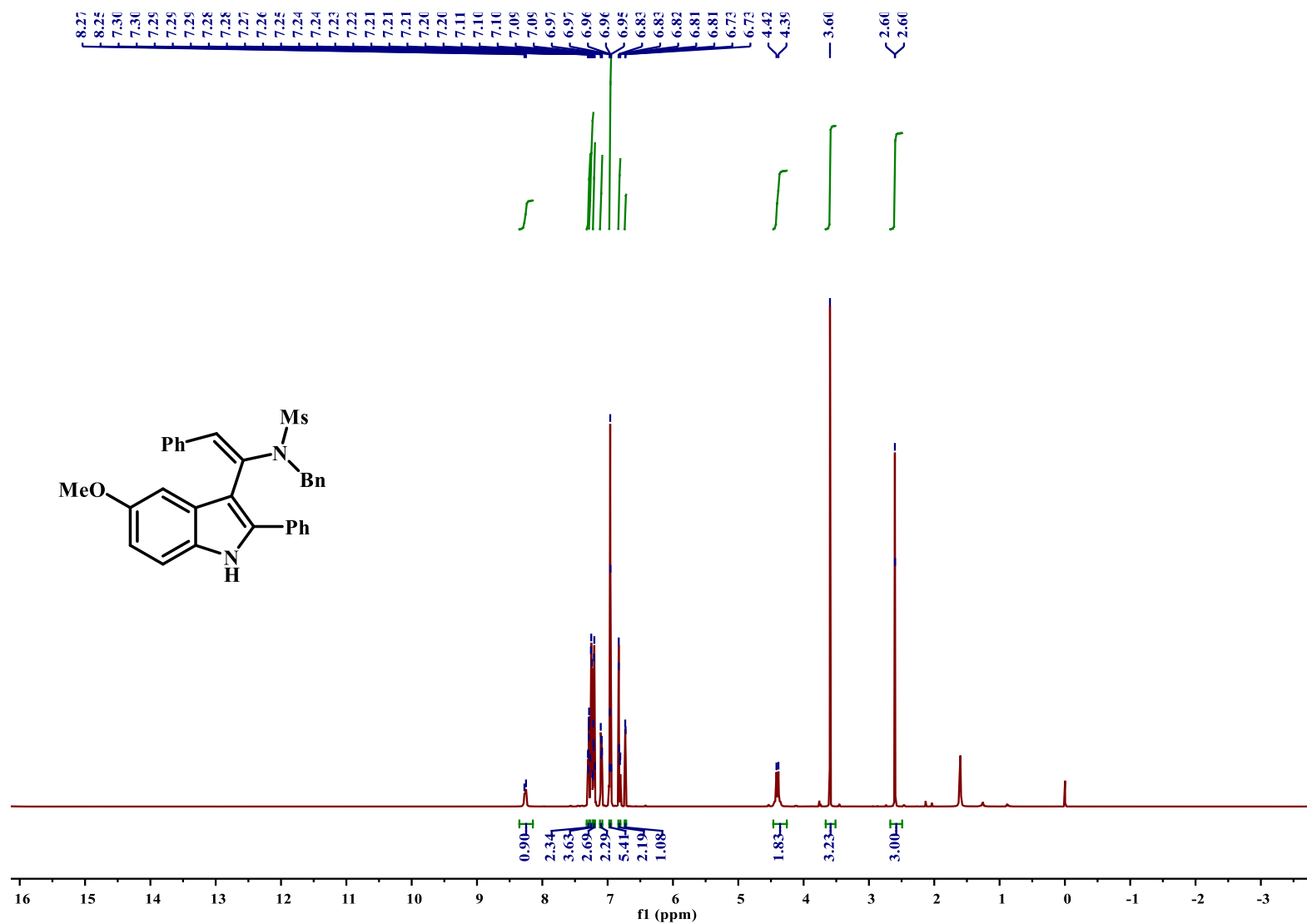
(E)-N-Benzyl-N-(1-(6-chloro-2-phenyl-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3h)



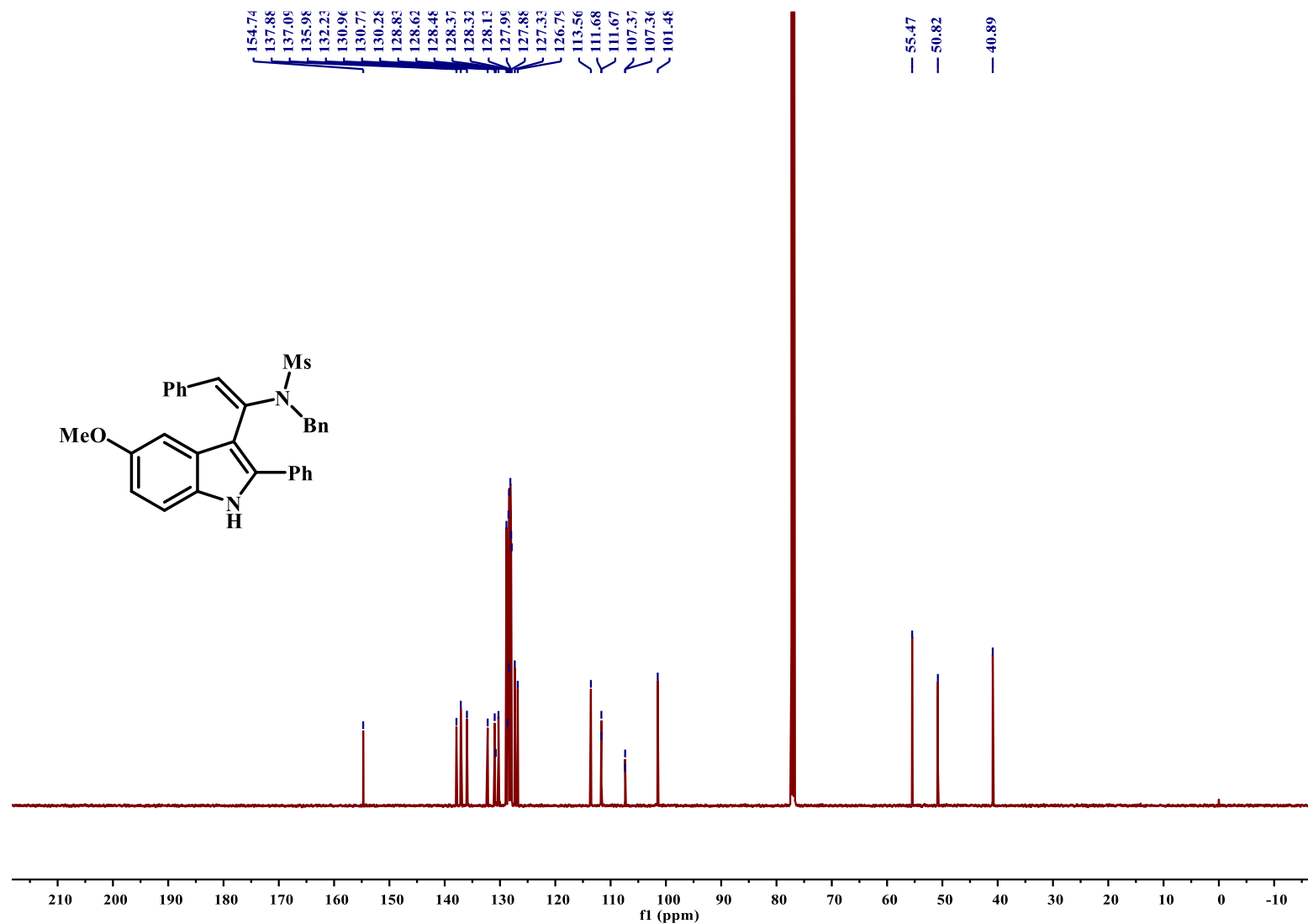
(E)-N-Benzyl-N-(1-(6-chloro-2-phenyl-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3h)



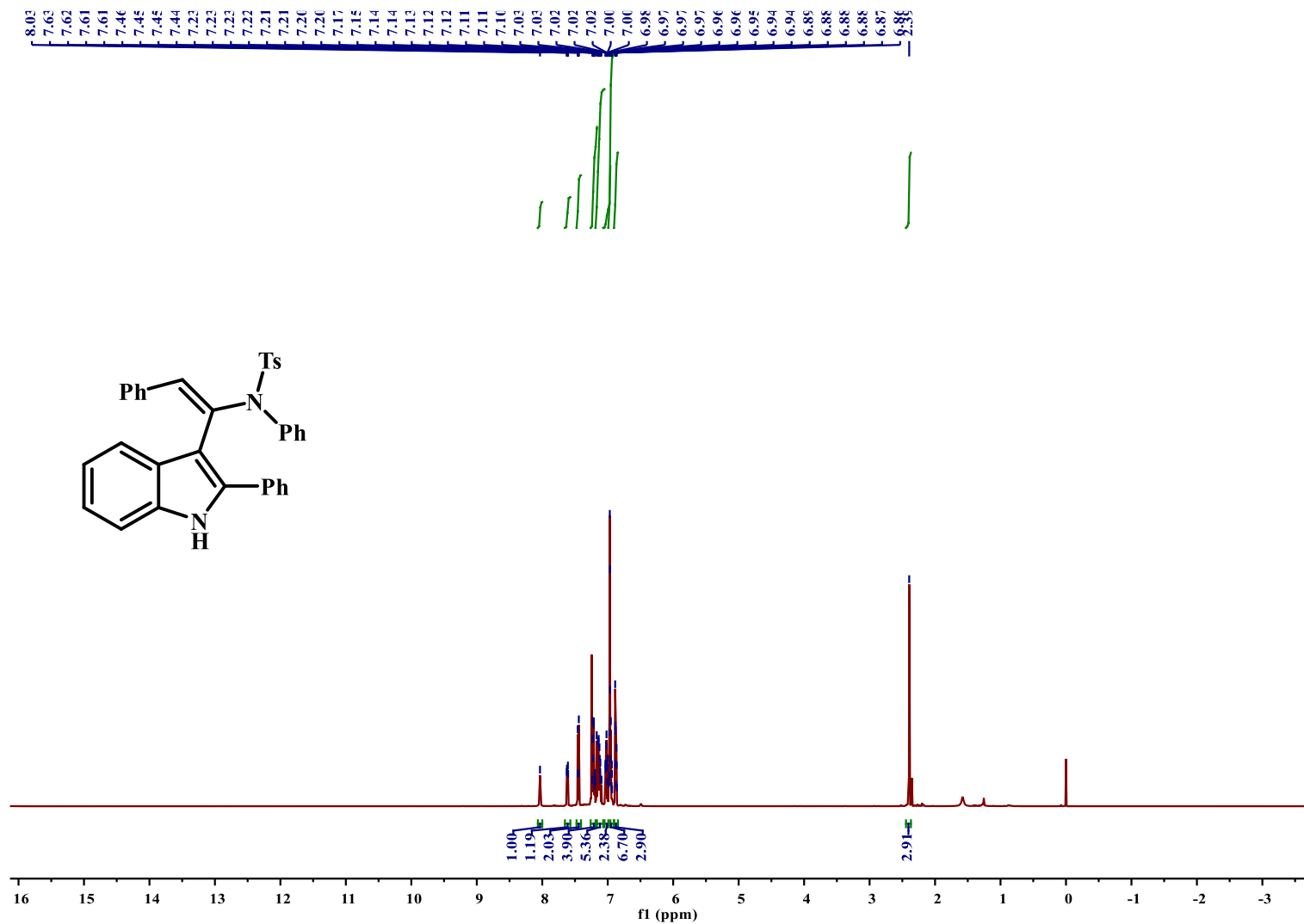
(E)-N-Benzyl-N-(1-(5-methoxy-2-phenyl-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3i)



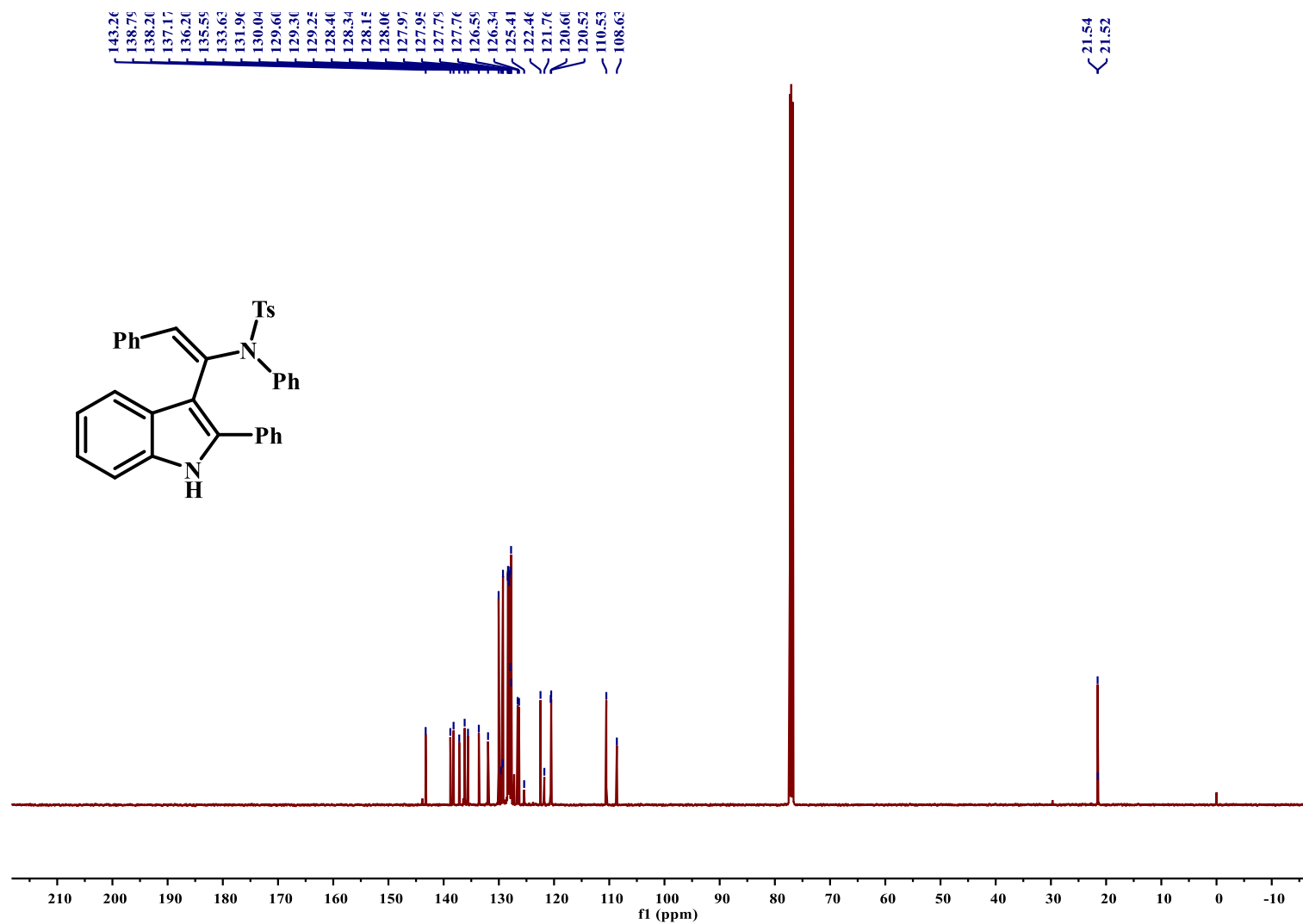
(E)-N-Benzyl-N-(1-(5-methoxy-2-phenyl-1H-indol-3-yl)-2-phenylvinyl)methanesulfonamide (3i)



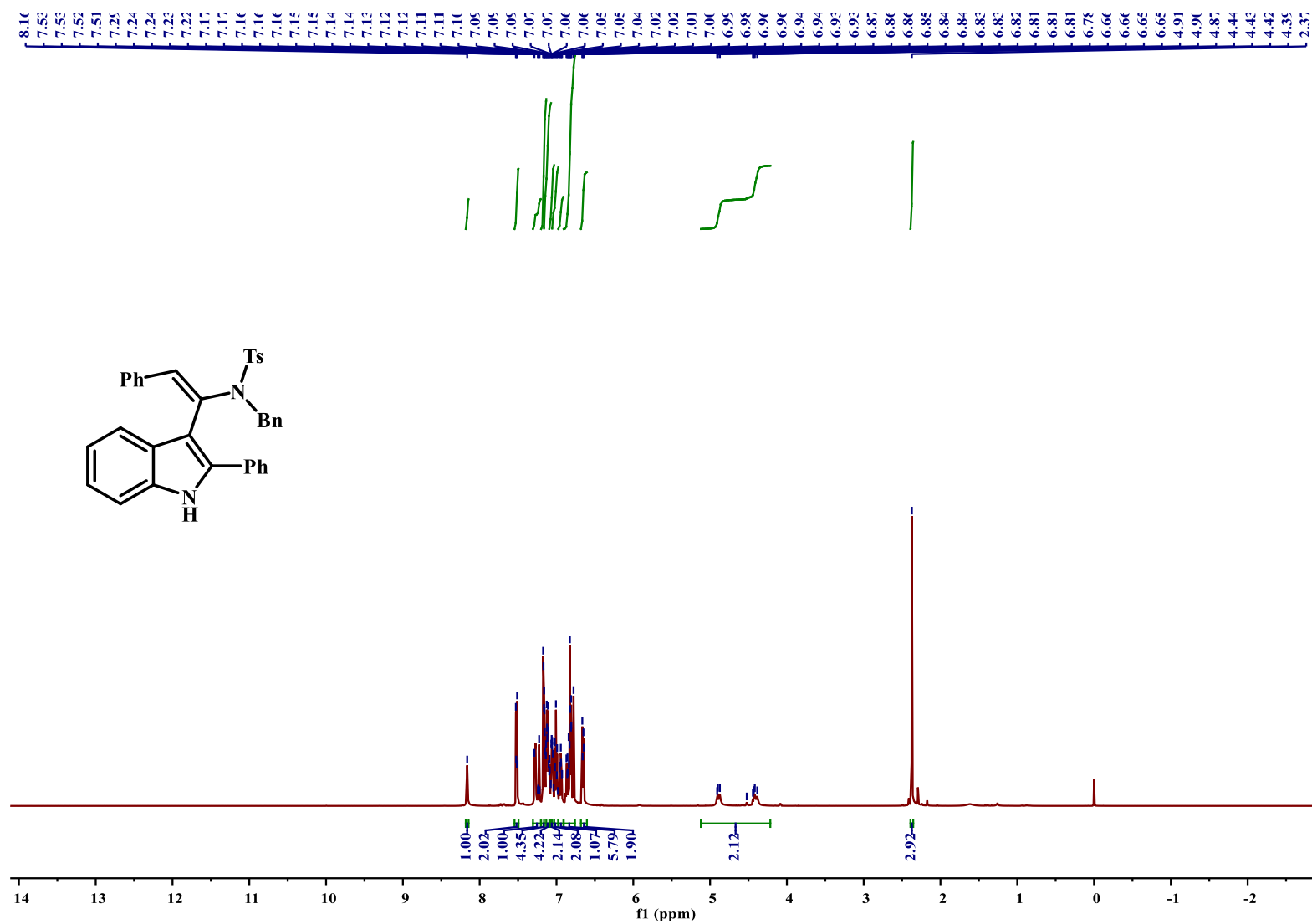
(E)-4-Methyl-N-phenyl-N-(2-phenyl-1-(2-phenyl-1*H*-indol-3-yl)vinyl)benzenesulfonamide (3j)



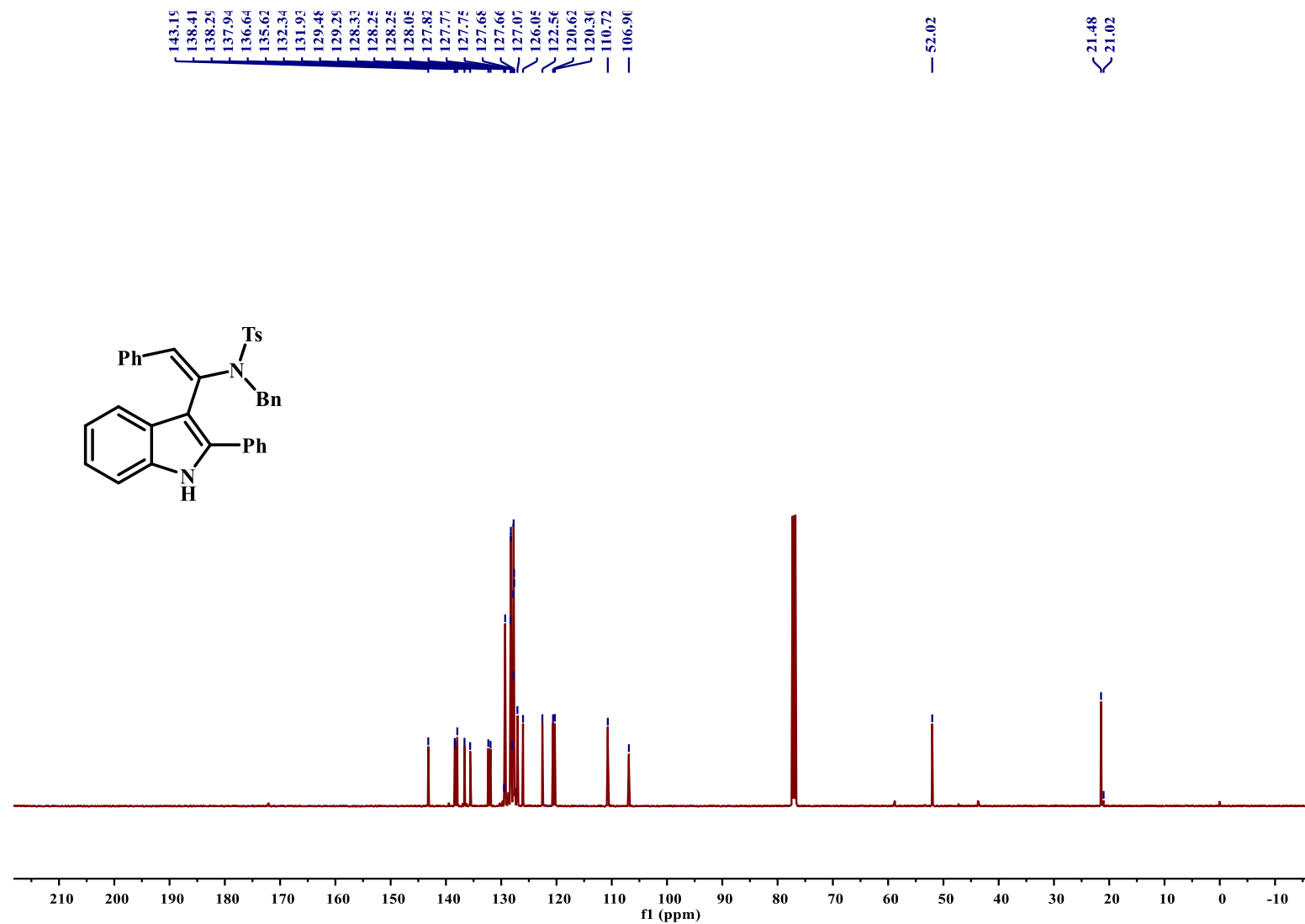
(E)-4-Methyl-N-phenyl-N-(2-phenyl-1-(2-phenyl-1*H*-indol-3-yl)vinyl)benzenesulfonamide (3j)



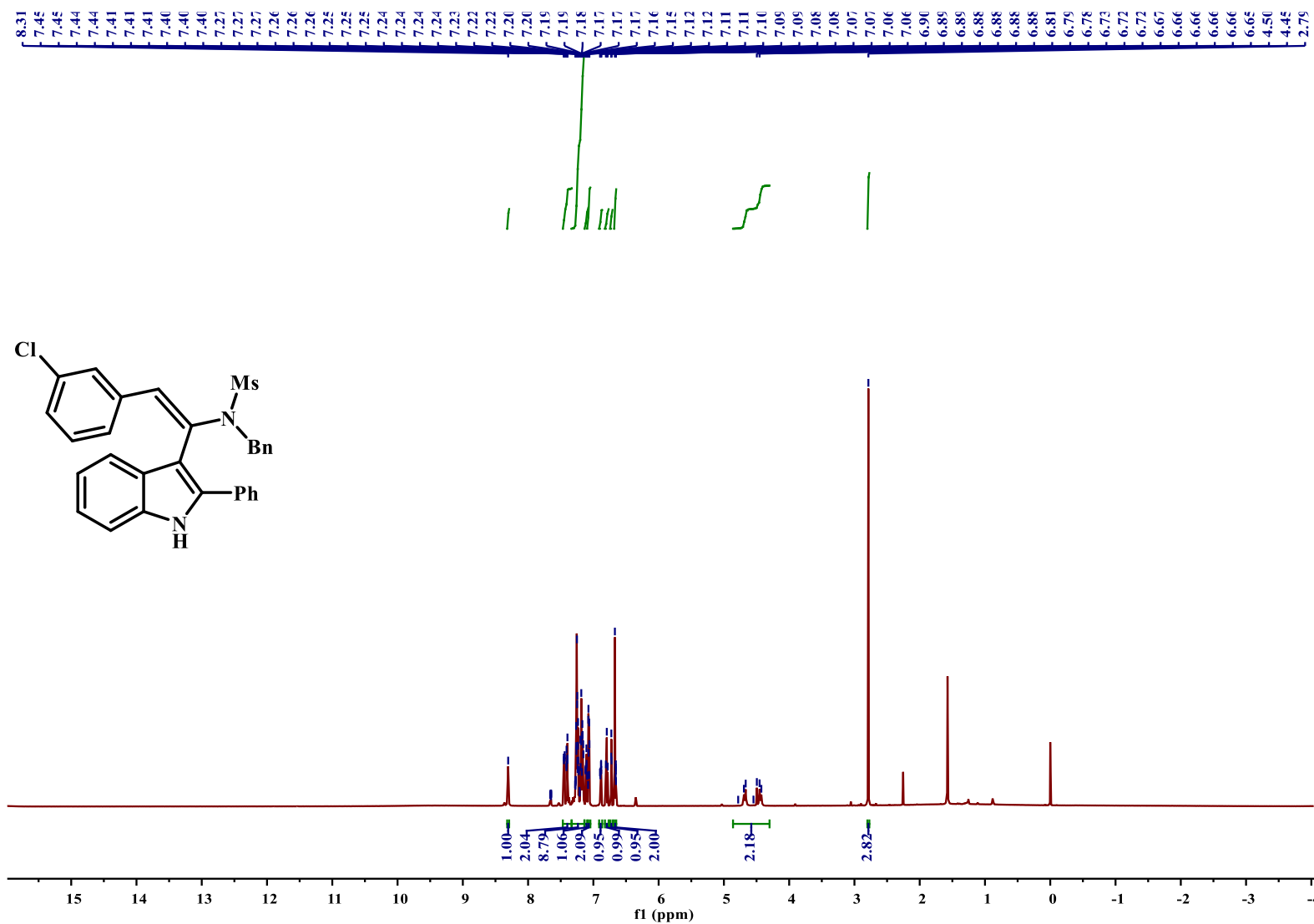
(E)-N-Benzyl-4-methyl-N-(2-phenyl-1-(2-phenyl-1H-indol-3-yl)vinyl)benzenesulfonamide (3k)



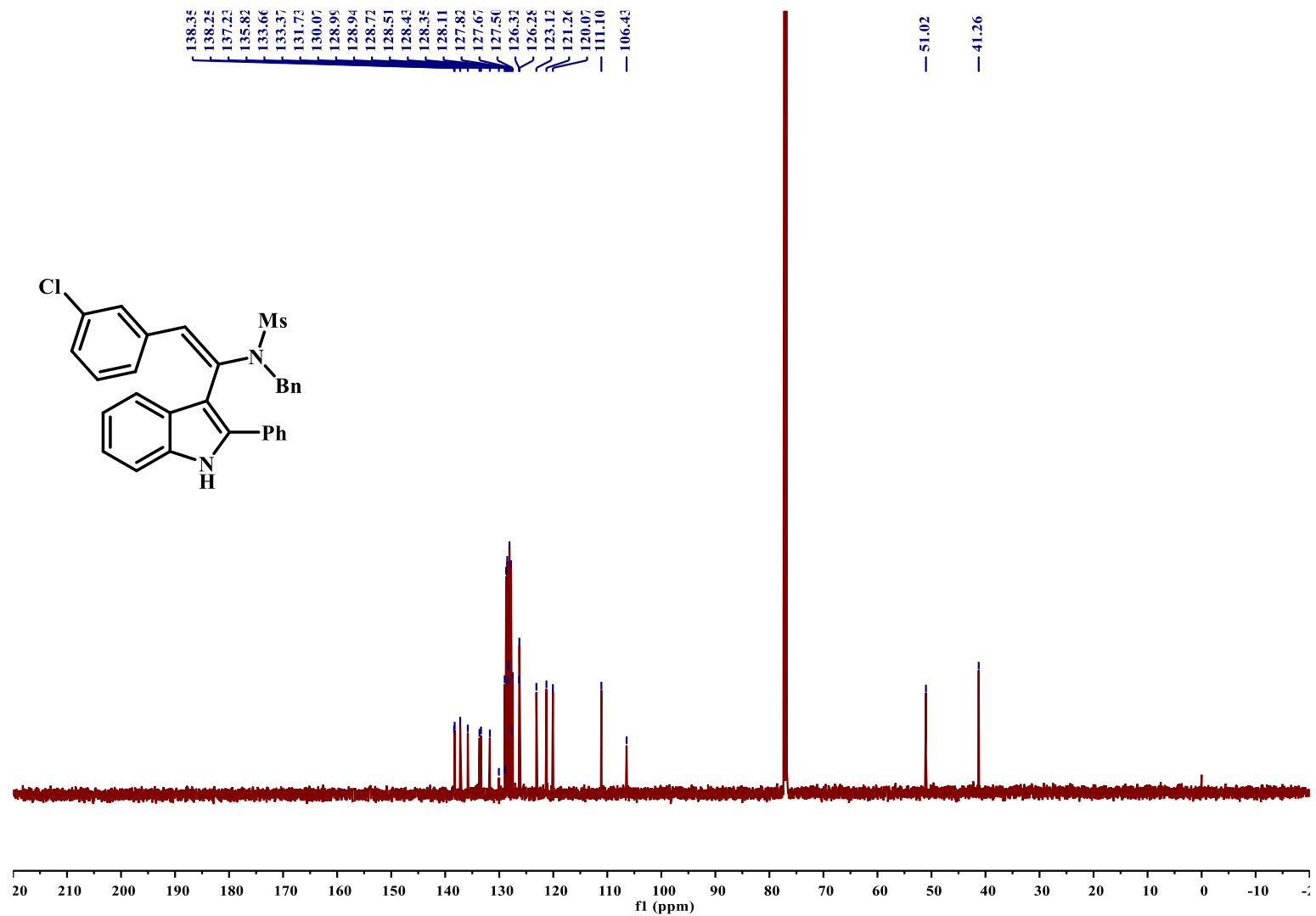
(E)-N-Benzyl-4-methyl-N-(2-phenyl-1-(2-phenyl-1*H*-indol-3-yl)vinyl)benzenesulfonamide (3k)



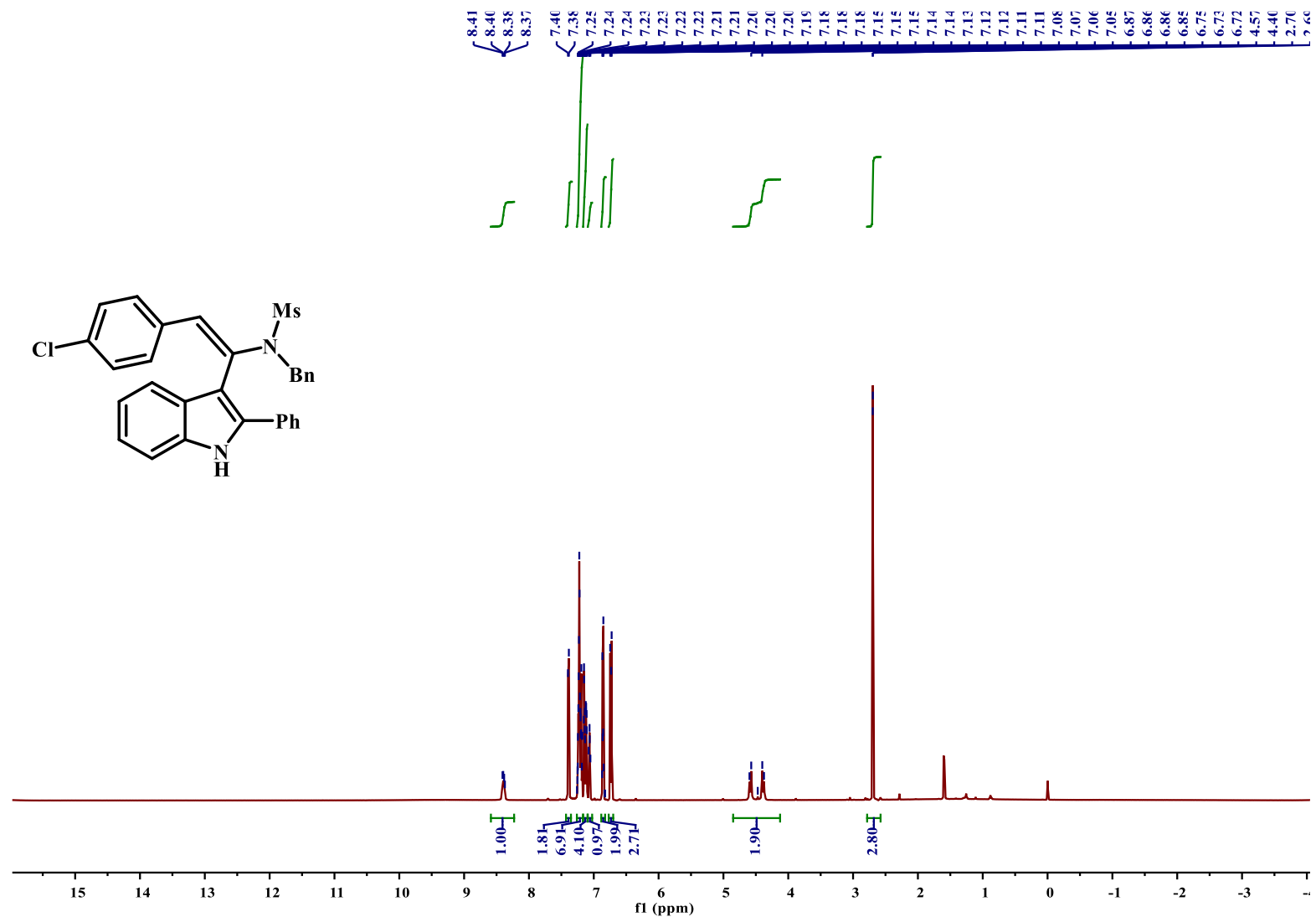
(E)-N-Benzyl-N-(2-(3-chlorophenyl)-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfonamide (3m)



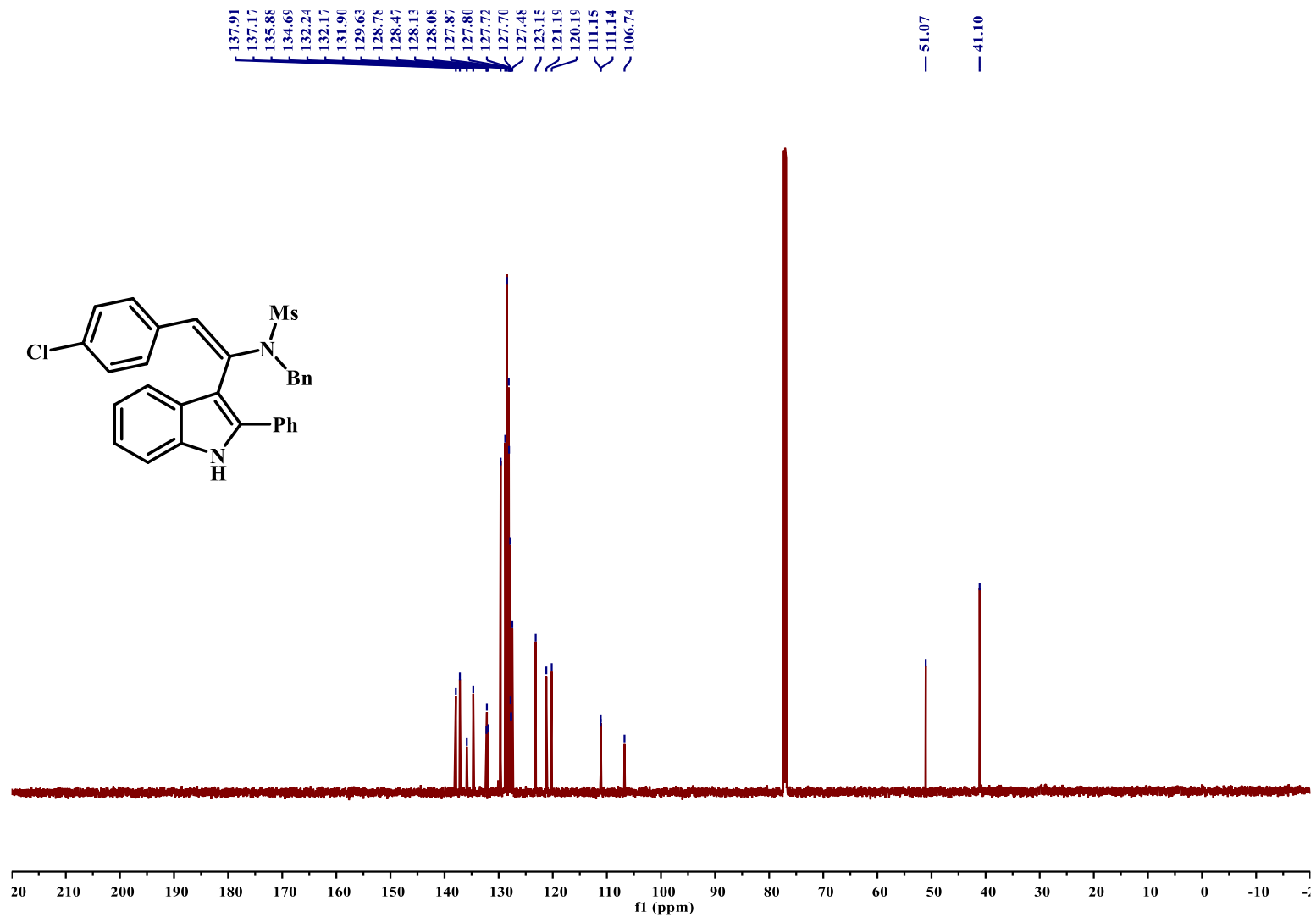
(E)-N-Benzyl-N-(2-(3-chlorophenyl)-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfonamide (3m)



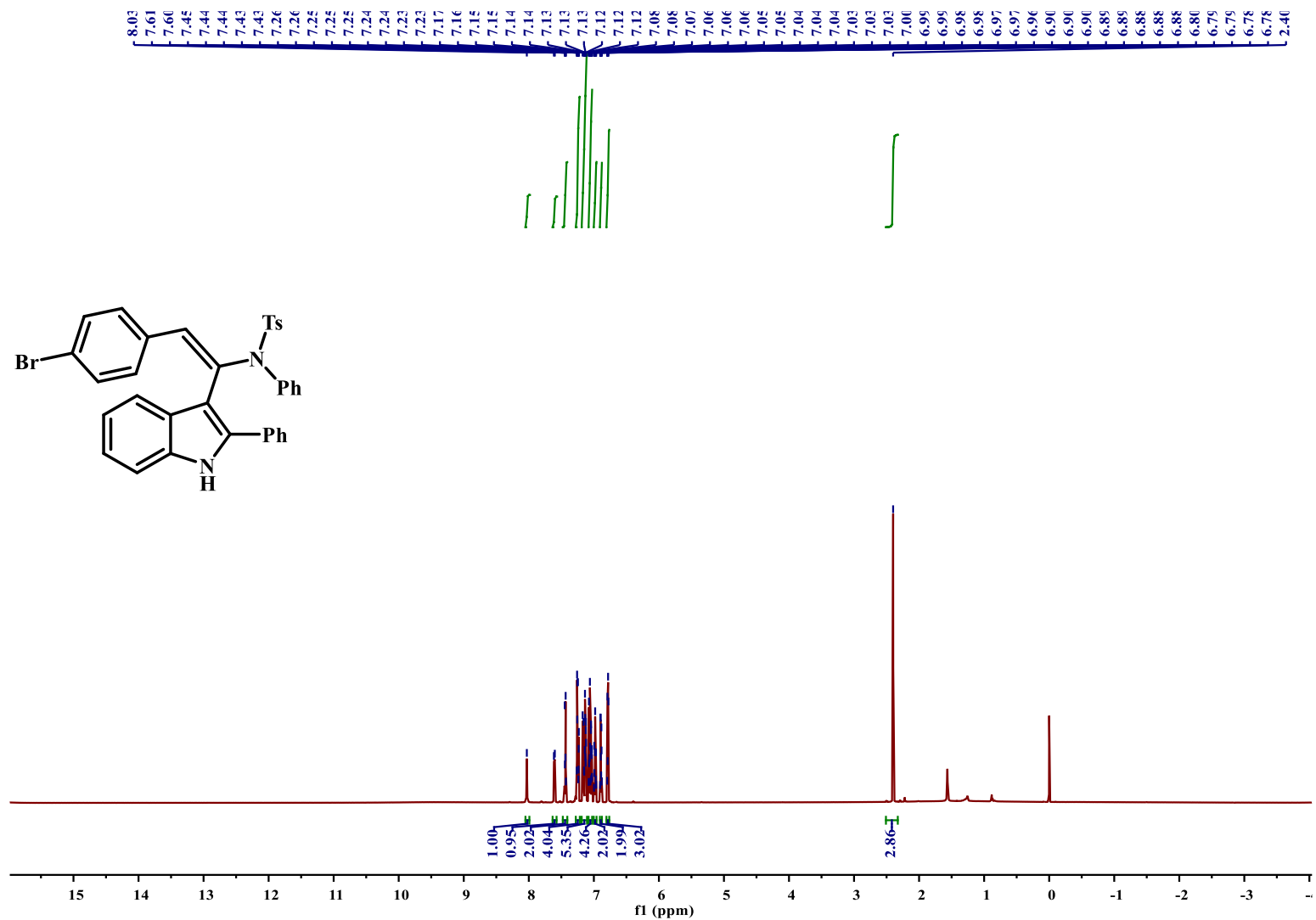
(E)-N-Benzyl-N-(2-(4-chlorophenyl)-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfonamide (3n)



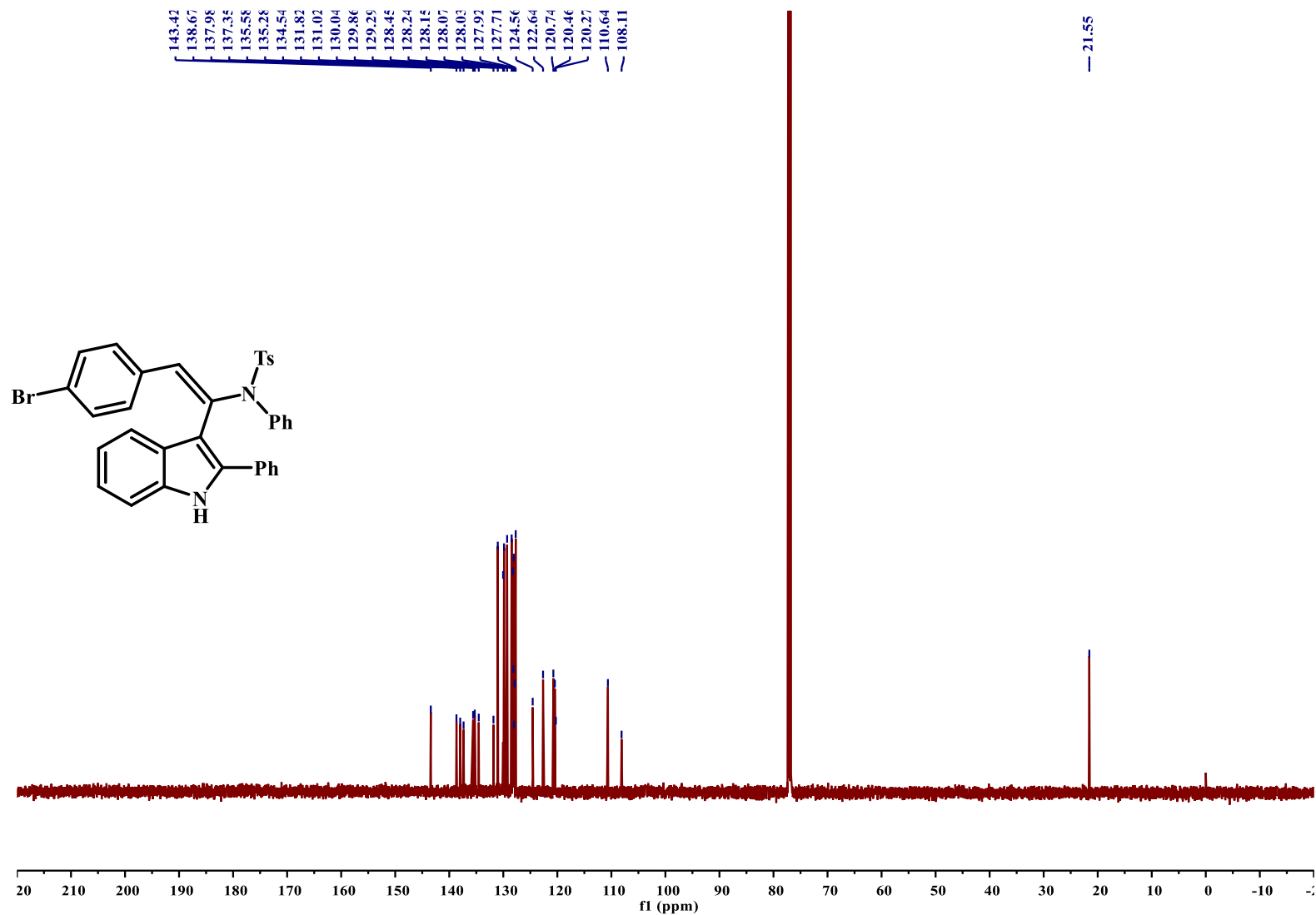
(E)-N-Benzyl-N-(2-(4-chlorophenyl)-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfonamide (3n)



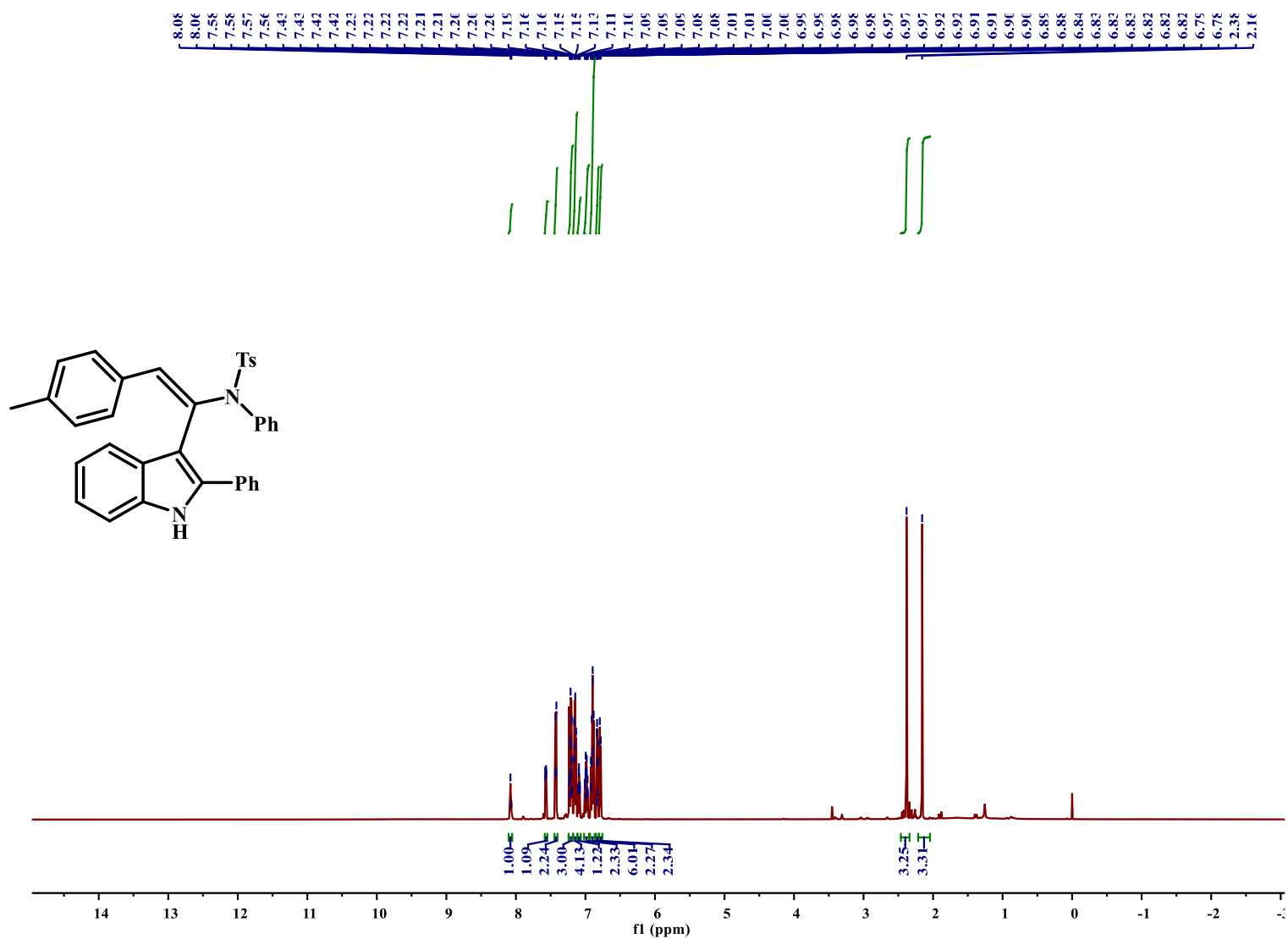
(E)-N-(2-(4-Bromophenyl)-1-(2-phenyl-1H-indol-3-yl)vinyl)-4-methyl-N-phenylbenzenesulfonamide (3o)



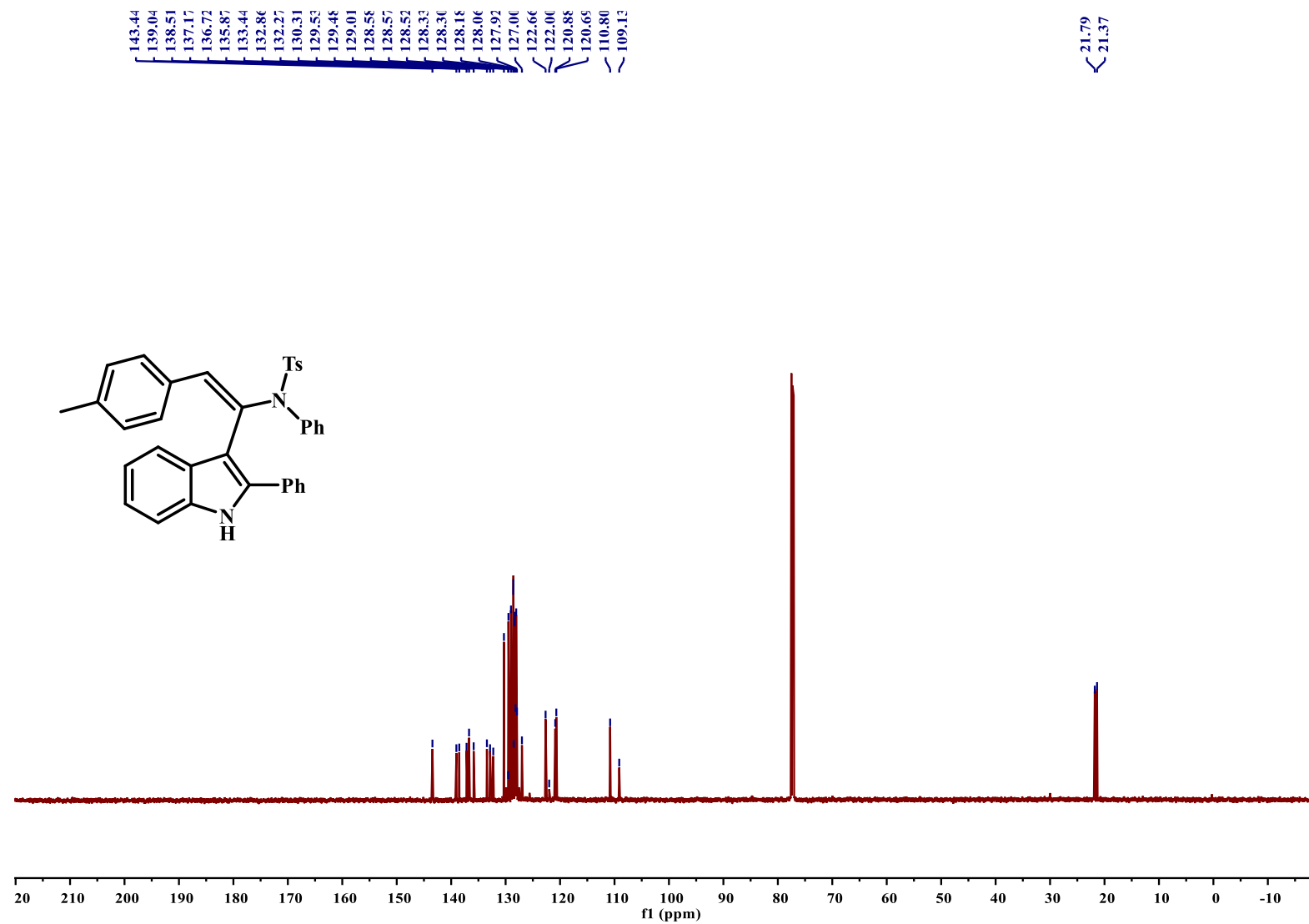
(E)-N-(2-(4-Bromophenyl)-1-(2-phenyl-1*H*-indol-3-yl)vinyl)-4-methyl-*N*-phenylbenzenesulfonamide (3o)



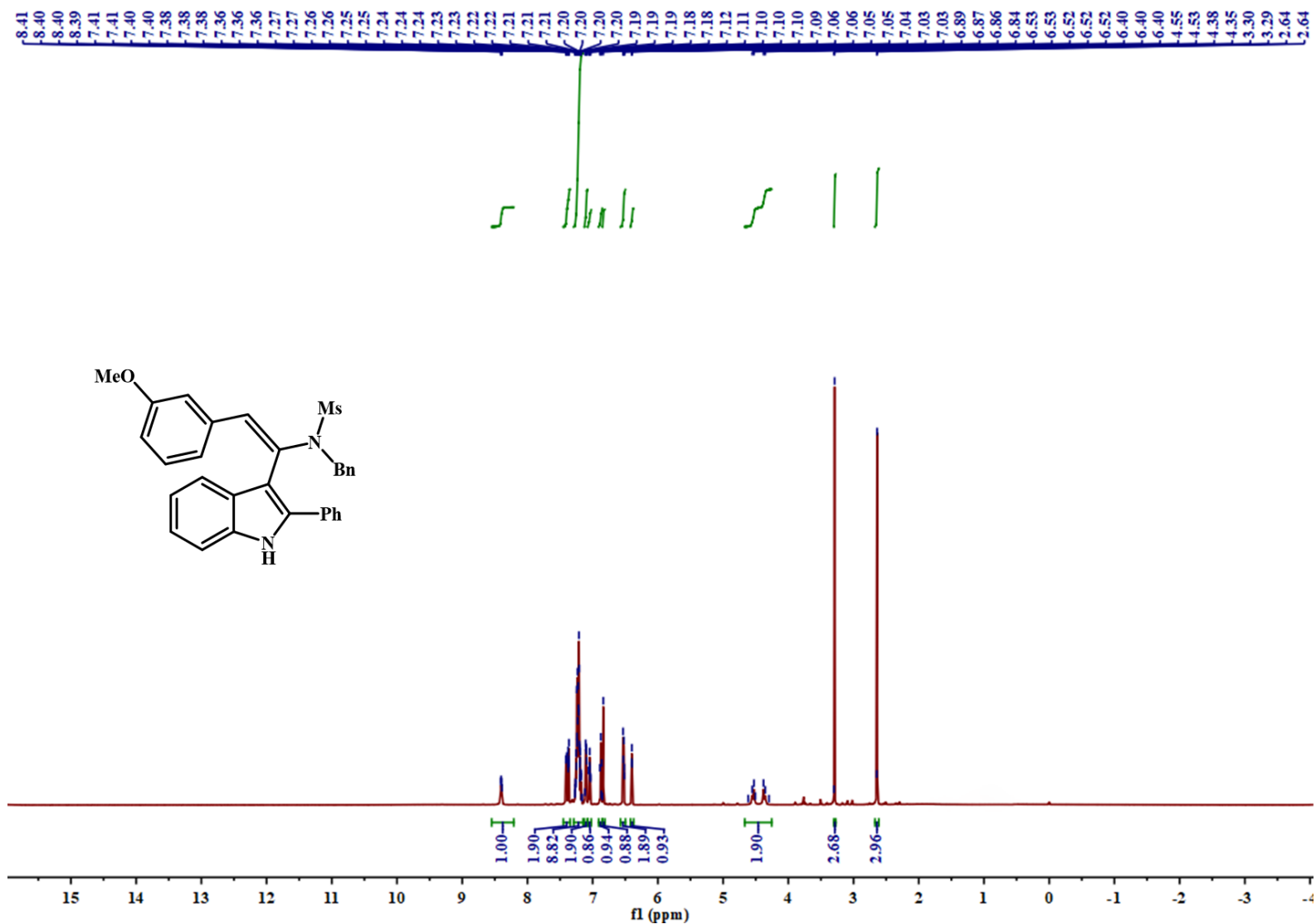
(E)-4-Methyl-N-phenyl-N-(1-(2-phenyl-1H-indol-3-yl)-2-(p-tolyl)vinyl)benzenesulfonamide (3p)



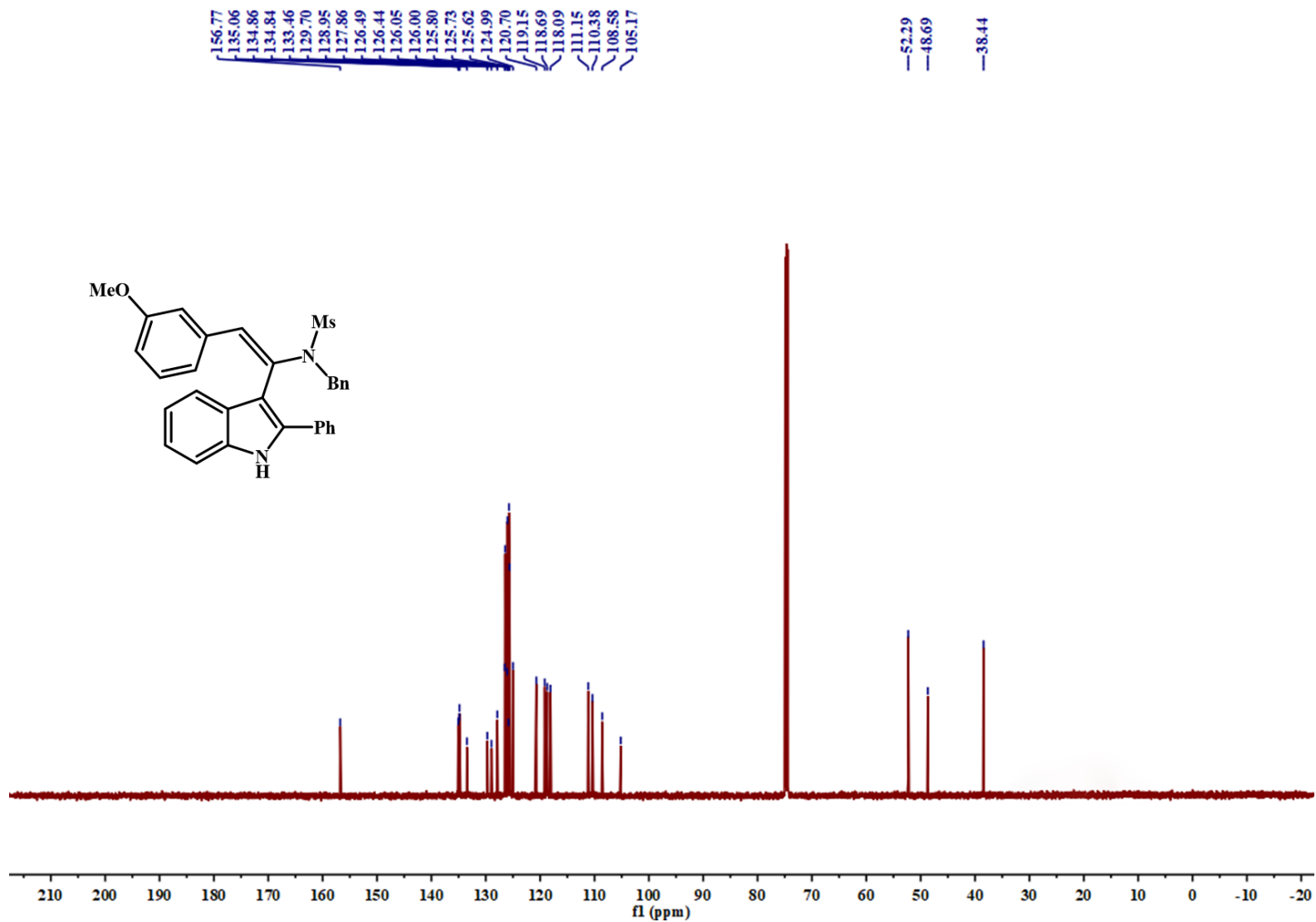
(E)-4-Methyl-N-phenyl-N-(1-(2-phenyl-1H-indol-3-yl)-2-(p-tolyl)vinyl)benzenesulfonamide (3p)



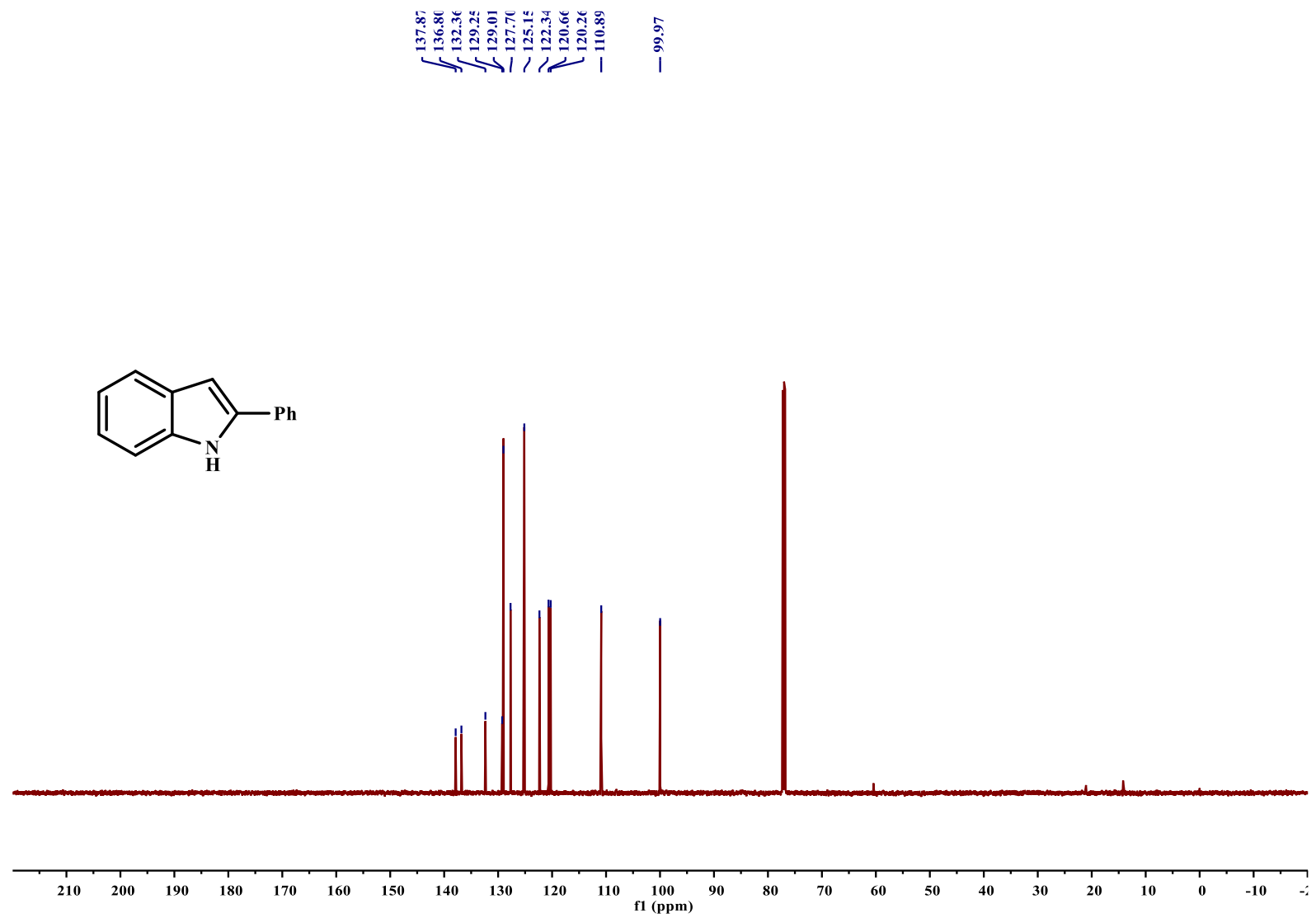
(E)-N-Benzyl-N-(2-(3-methoxyphenyl)-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfonamide (3q)



(E)-N-Benzyl-N-(2-(3-methoxyphenyl)-1-(2-phenyl-1H-indol-3-yl)vinyl)methanesulfonamide (3q)



2-Phenyl-1H-indole (4)



8. DFT calculation details

The DFT calculations were conducted by using the M06/SDD/6-31G(d,p) method in the Gaussian 16 software package.³ The M06 functional⁴ could produce accurate results for noncovalent interactions in organometallic and inorganometallic chemistry. The SDD basis set⁵ was used to describe the heavy elements Au, and the 6-31G(d,p) basis set was used for the other atoms. Frequency analyses were also performed based on the structures obtained to confirm that the transition states had one and only one imaginary frequency. Intrinsic reaction coordinate (IRC) calculations were performed to further verify that the transition states connect the correct reactants and products. The single-point calculations were performed using M06-2x-D3 functional and the SDD basis set for heavy atoms (Au) and the def2tzvpp for other atoms with the IEFPCM model (DCE as solvent). Furthermore, according to the actual reaction temperature, the Gibbs free energies were evaluated at 353.15 K in units of kcal/mol. The 3D structures of the studied species visually were analysed by CYL view.⁶

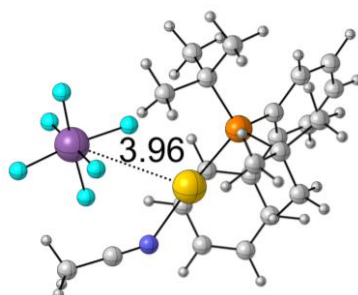


Figure S1. The Optimized JohnphosAu(MeCN)SbF₆ structure

In the structure of JohnphosAu(MeCN)SbF₆, it was obviously that there was strong coordination effect between acetonitrile molecule and gold ion, and weak coordination effect between SbF₆⁻ and gold ion (distance was 3.96 Å). It implies that SbF₆⁻ is prone to dissociation during the reaction, hence it is reasonable to use JohnphosAu⁺(MeCN) as a catalyst to simplify the calculations.

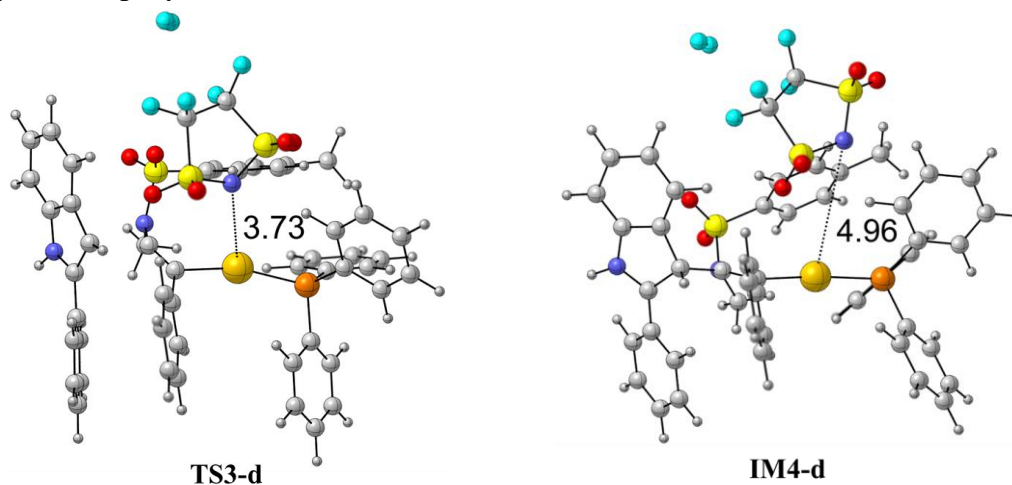
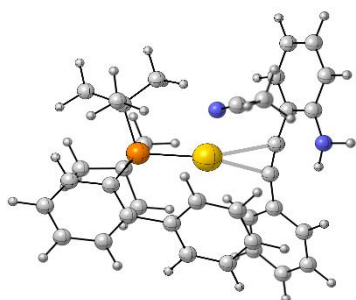


Figure S2. The addition process of indole and ynamide catalyzed by Au(PPh₃)NTf₂

In the structure of TS3-d, the distance between NTf_2^- and gold ion is 3.73 Å, furthermore, it increased to 4.96 Å in IM4-d. It meant that the NTf_2^- would not participate in the addition process of indole and ynamide. Therefore, it was justifiable to simplify following calculations by employing the $\text{Au}^+(\text{PPh}_3)$ as catalyst.

7.1 Coordinates of Optimized Structures in Figure 1

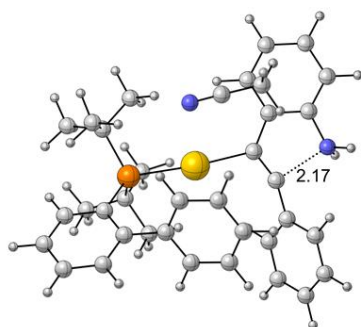
RC:



C	-0.71364900	3.95931300	-3.79163000
C	0.15446100	3.05679000	-3.16445500
C	-0.22154000	1.69430600	-3.11406500
C	-1.45479800	1.28295100	-3.64679400
C	-2.30998500	2.19323600	-4.23706600
C	-1.92414500	3.53397100	-4.31430800
H	-0.42533900	5.00805300	-3.85698700
H	-1.71615100	0.22773000	-3.58721000
H	-3.25978600	1.86797100	-4.65021600
H	-2.57812200	4.25784700	-4.79458300
C	0.66610400	0.74681900	-2.53539800
C	1.53316300	-0.04338200	-2.13648600
C	2.72853000	-0.82440400	-1.98319800
C	2.67706800	-2.18970900	-1.67675200
C	3.97240300	-0.19902000	-2.14838000
C	3.85186600	-2.91024400	-1.51581100
H	1.70915500	-2.67701100	-1.57582800
C	5.14261800	-0.92747900	-1.98937300
H	4.01018400	0.85805400	-2.40418200
C	5.08517100	-2.28044900	-1.66382700
H	3.80556500	-3.97011100	-1.27931700
H	6.10417900	-0.43858400	-2.12253800
H	6.00348300	-2.84769700	-1.53685500
N	1.31286400	3.50879800	-2.55868000
H	1.73257800	4.32965500	-2.97328200
H	1.99009400	2.79951600	-2.30899100
C	2.52940200	-0.28228500	2.14204800
C	1.25736700	0.27474400	2.30834600
C	0.95667200	1.48093300	1.66598700
C	1.90847500	2.11277500	0.86906500
C	3.16959000	1.54641700	0.70647200
C	3.47666000	0.34460800	1.33934000

H	2.77383800	-1.21283400	2.65291900
H	-0.02723900	1.92919100	1.79768900
H	1.65535600	3.04732600	0.36945200
H	3.92012200	2.04488900	0.09557000
H	4.45894600	-0.10471600	1.20998400
C	0.28658000	-0.33748600	3.25406000
C	-0.93783100	-0.94358000	2.89995500
C	0.63171000	-0.26256200	4.60976500
C	-1.77936400	-1.40332100	3.92564800
C	-0.20886900	-0.73203000	5.60784400
H	1.58071100	0.20141000	4.87201400
C	-1.43218000	-1.29443400	5.26422800
H	-2.73010000	-1.86713600	3.67650400
H	0.08644400	-0.64940200	6.65059000
H	-2.11180400	-1.65581700	6.03130300
P	-1.42527600	-1.31940900	1.16839900
C	-1.13670500	-3.18751300	1.00657400
C	0.36538200	-3.39838000	1.21938500
C	-1.87485000	-4.05342700	2.02751300
C	-1.52426100	-3.61955300	-0.40792900
H	0.97939100	-2.80113600	0.53365400
H	0.66603000	-3.15198900	2.24531500
H	0.60073000	-4.45776900	1.05060600
H	-2.96292400	-3.99532000	1.93976300
H	-1.59173800	-5.09994500	1.85329100
H	-1.58984200	-3.81103000	3.05664800
H	-1.24554300	-4.67220300	-0.54917400
H	-2.60387400	-3.54470500	-0.58594600
H	-1.00960500	-3.02959900	-1.17829300
C	-3.23833800	-0.79634300	0.91953600
C	-3.43384400	-0.51079600	-0.57492600
C	-4.28285300	-1.82761700	1.34719700
C	-3.45236200	0.50627900	1.69382100
H	-2.82836300	0.34249800	-0.90403800
H	-3.19883600	-1.37759600	-1.20545900
H	-4.48835100	-0.25548600	-0.74608400
H	-4.22737200	-2.10120100	2.40575800
H	-5.27617000	-1.38787000	1.18695800
H	-4.23891600	-2.74348100	0.74706900
H	-4.43570100	0.91148200	1.42034400
H	-3.44213400	0.35640600	2.77823000
H	-2.70391600	1.26381300	1.43315000
N	-1.51233300	2.57019600	-0.26426200
C	-1.34667200	3.71175600	-0.39631500
C	-1.11897200	5.13428200	-0.55879800
H	-1.21983500	5.65073700	0.39994200
H	-0.10667600	5.29088200	-0.94704300
H	-1.84094100	5.55428600	-1.26497600
Au	-0.10248900	-0.29664500	-0.51876300

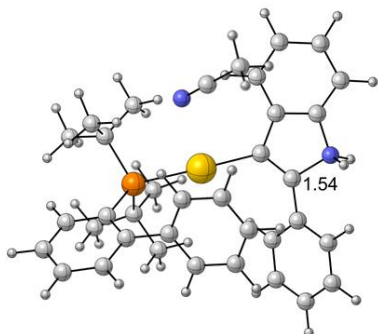
TS1:



C	-1.01145200	2.44621100	-3.28875700
C	-0.44721700	1.61046800	-2.33620400
C	-1.22463300	1.09089300	-1.28266400
C	-2.58851600	1.37772000	-1.23449900
C	-3.15718000	2.20094800	-2.20164000
C	-2.37140000	2.74480700	-3.21517500
H	-0.40106600	2.84738300	-4.09547800
H	-3.19158100	0.96366200	-0.42957100
H	-4.22017600	2.42402900	-2.16217600
H	-2.82044400	3.39115000	-3.96465100
C	-0.47264200	0.31511100	-0.30438300
C	0.79388900	0.12809300	-0.44103600
C	2.05781600	-0.50172100	-0.24484600
C	2.10319400	-1.89330300	-0.05822000
C	3.24856600	0.24041900	-0.21443800
C	3.31643000	-2.52103900	0.18581900
H	1.17543300	-2.46066500	-0.09775800
C	4.45944200	-0.39725300	0.00320900
H	3.20563800	1.31772200	-0.36149600
C	4.49311100	-1.77638600	0.21172300
H	3.34778900	-3.59637000	0.33955400
H	5.38127800	0.17814100	0.01825600
H	5.44394700	-2.27282900	0.38821600
N	0.92514900	1.21770000	-2.31466000
H	1.57320000	1.97970800	-2.49728400
H	1.12811000	0.46139600	-2.96571400
C	1.60460100	-0.91796700	3.88582800
C	0.33163400	-0.47378300	4.25843300
C	-0.06119400	0.82376900	3.91209100
C	0.80977000	1.66135000	3.22100500
C	2.07554000	1.21176600	2.85925600
C	2.46777300	-0.08373000	3.18397300
H	1.91867400	-1.92334100	4.16475700
H	-1.04362800	1.18906900	4.20867200
H	0.49512600	2.67559000	2.98269700
H	2.76306000	1.87283600	2.33529200
H	3.45458700	-0.44241500	2.89735000
C	-0.51872200	-1.30953800	5.14543000
C	-1.77536800	-1.85482900	4.81063900
C	-0.01672500	-1.51734900	6.43756100

C	-2.49425600	-2.53641900	5.80598300
C	-0.73613400	-2.20614100	7.40176500
H	0.95566100	-1.09497600	6.68384200
C	-1.99410600	-2.70653100	7.08839500
H	-3.46916600	-2.95586500	5.57520800
H	-0.32161900	-2.33954500	8.39768100
H	-2.58289200	-3.23444700	7.83383200
P	-2.45905300	-1.84295100	3.10347600
C	-2.31863900	-3.64950500	2.53689100
C	-0.81621200	-3.93498000	2.44337800
C	-2.93508600	-4.69014500	3.47111400
C	-2.94616800	-3.77512500	1.14807000
H	-0.31055700	-3.26337800	1.73716900
H	-0.32209200	-3.83934800	3.41877600
H	-0.67132200	-4.96685200	2.09612300
H	-4.01127400	-4.55818300	3.61610900
H	-2.78844200	-5.68191800	3.02284200
H	-2.44720800	-4.70442700	4.45113800
H	-2.74244800	-4.77991500	0.75431100
H	-4.03568500	-3.65163400	1.16988100
H	-2.52979500	-3.04712700	0.43891600
C	-4.25212900	-1.21431900	3.20140500
C	-4.62551300	-0.65747400	1.82228600
C	-5.29903100	-2.25587000	3.59574400
C	-4.27068700	-0.05467300	4.20045500
H	-4.01344200	0.21920000	1.57722100
H	-4.52692900	-1.39839800	1.01941100
H	-5.67451000	-0.33259700	1.84728700
H	-5.13104300	-2.69670700	4.58345500
H	-6.27648300	-1.75702100	3.63734400
H	-5.38435300	-3.06502300	2.86149000
H	-5.26332400	0.41410200	4.16873900
H	-4.08852100	-0.38311000	5.22906100
H	-3.54017800	0.72057100	3.93765900
N	-2.52252800	2.36414600	2.15582800
C	-2.02113200	3.14268200	1.45476300
C	-1.37357400	4.09332000	0.57093900
H	-1.41757900	5.10273600	0.98937400
H	-0.32407200	3.81025600	0.43287700
H	-1.86746500	4.08877700	-0.40720700
Au	-1.28342300	-0.57824900	1.44768000

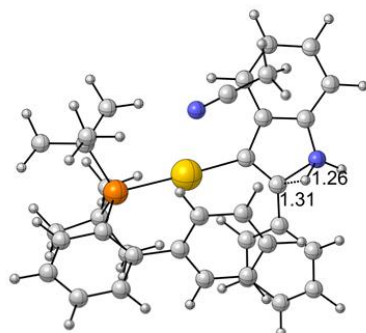
IM1:



C	0.31794900	3.33677400	-4.70307200
C	0.64280600	2.35361200	-3.79350200
C	-0.23469700	1.79962600	-2.86219100
C	-1.55074600	2.25833900	-2.85901400
C	-1.92095800	3.24494300	-3.77116800
C	-1.00500500	3.78419100	-4.67710300
H	1.03622600	3.74035600	-5.41297700
H	-2.26462000	1.84850600	-2.14861400
H	-2.94759100	3.60293200	-3.78185400
H	-1.32303500	4.55067800	-5.37806000
C	0.43595100	0.78288200	-2.04631200
C	1.70544000	0.68078100	-2.49175900
C	2.84182300	-0.17746400	-2.18555300
C	2.61010700	-1.47642300	-1.71262900
C	4.16718900	0.24899700	-2.34486400
C	3.66870200	-2.30537100	-1.37323600
H	1.58163200	-1.82304100	-1.62384400
C	5.22746200	-0.58807800	-2.01793200
H	4.39486500	1.25713300	-2.69513100
C	4.98199600	-1.86553400	-1.52403900
H	3.46752200	-3.30897900	-1.00508800
H	6.24879100	-0.23780900	-2.14336700
H	5.81143300	-2.51939200	-1.26805300
N	1.94130700	1.69082000	-3.62663300
H	2.67936100	2.35657600	-3.37529700
H	2.25148400	1.20807000	-4.47768200
C	2.51727400	-0.22233000	1.99624900
C	1.24306100	0.23299300	2.34949500
C	0.81767800	1.48208000	1.88418800
C	1.65700400	2.25910700	1.09151700
C	2.92233900	1.79695500	0.74477000
C	3.34792100	0.54916900	1.19050400
H	2.85801900	-1.18915100	2.36580800
H	-0.17032800	1.85257500	2.15511100
H	1.31247800	3.23295400	0.74655300
H	3.58383200	2.41005400	0.13464300
H	4.33310000	0.17749200	0.91541300
C	0.42308400	-0.52605300	3.33183200
C	-0.79847300	-1.17921200	3.06444800
C	0.92413700	-0.54184700	4.64080100

C	-1.48276300	-1.77494200	4.13596200
C	0.23700300	-1.14567500	5.68259300
H	1.87045600	-0.03959000	4.83317200
C	-0.98586900	-1.75533200	5.43083300
H	-2.42830600	-2.27834200	3.95675200
H	0.64995000	-1.13042800	6.68798200
H	-1.54896500	-2.22268000	6.23438000
P	-1.46154500	-1.41995800	1.36292400
C	-1.13695700	-3.25908600	1.01937000
C	0.38711800	-3.41316600	1.00507200
C	-1.69389600	-4.23970900	2.05009200
C	-1.69433900	-3.59860800	-0.36351900
H	0.86534400	-2.75324100	0.27047900
H	0.82492000	-3.20095800	1.98872700
H	0.63732400	-4.45109900	0.74615800
H	-2.78424200	-4.21066800	2.12983500
H	-1.41914500	-5.25688300	1.73970700
H	-1.26476900	-4.07978100	3.04479600
H	-1.39307400	-4.62056400	-0.63040200
H	-2.79051600	-3.56823100	-0.38880100
H	-1.31325200	-2.92162600	-1.14021400
C	-3.31195500	-0.97516200	1.39151100
C	-3.72472500	-0.63611400	-0.04608500
C	-4.26403000	-2.05420500	1.90671400
C	-3.45151000	0.29194000	2.23863600
H	-3.17502900	0.23428600	-0.42390000
H	-3.57063900	-1.46968600	-0.74153000
H	-4.79487400	-0.38822000	-0.05573600
H	-4.06578000	-2.36618900	2.93678000
H	-5.28288900	-1.64410600	1.89361600
H	-4.27067700	-2.94498100	1.26812300
H	-4.48026800	0.66439300	2.14151600
H	-3.26195500	0.10813500	3.30143500
H	-2.78270600	1.09090300	1.89321900
N	-1.80757800	2.94604300	0.43454600
C	-1.46748000	3.93863600	-0.06266100
C	-1.03462800	5.16826600	-0.70002300
H	-1.86025600	5.88402700	-0.74904700
H	-0.21516800	5.62384900	-0.13622700
H	-0.69437100	4.95617900	-1.72039700
Au	-0.40607300	-0.18514700	-0.40589500

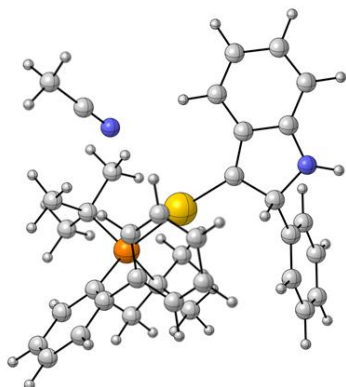
TS2:



C	0.36194100	3.33321900	-4.70382700
C	0.71238200	2.35280000	-3.77475500
C	-0.21845100	1.75213300	-2.89939100
C	-1.57257200	2.12374800	-2.99736800
C	-1.94065400	3.05246300	-3.94906700
C	-0.98146600	3.65129100	-4.79231800
H	1.09946200	3.79668700	-5.35359600
H	-2.30093200	1.66755700	-2.33091300
H	-2.98530100	3.33244000	-4.05691900
H	-1.30647500	4.37679300	-5.53365100
C	0.42955000	0.83292800	-2.00960700
C	1.77347600	0.81006400	-2.35573700
C	2.86889500	-0.14235200	-2.13610800
C	2.56475100	-1.47637200	-1.85153600
C	4.21021000	0.25321100	-2.19779100
C	3.58263200	-2.38825500	-1.60207200
H	1.52147200	-1.78721000	-1.82852200
C	5.22609600	-0.66660200	-1.97305600
H	4.47274400	1.29520300	-2.38933900
C	4.91398700	-1.98813800	-1.66405500
H	3.33247200	-3.42200800	-1.37507100
H	6.26387300	-0.34769100	-2.02405300
H	5.70899000	-2.70543000	-1.47834000
N	1.97428600	1.86498100	-3.46315700
H	2.21703900	2.03322800	-2.23816300
H	2.76339400	1.80613000	-4.10149000
C	2.50751800	-0.18436100	1.94377500
C	1.24230000	0.25590000	2.34668800
C	0.81193400	1.52849800	1.95398200
C	1.64068300	2.34683400	1.19177700
C	2.89939100	1.90110100	0.80001400
C	3.32646100	0.62700400	1.16627200
H	2.85251700	-1.16919000	2.25700800
H	-0.16870200	1.88666400	2.26484900
H	1.29766500	3.34253300	0.91513300
H	3.55998400	2.55241200	0.22836000
H	4.30599700	0.26762900	0.85679000
C	0.44939500	-0.54299300	3.32094100
C	-0.76925200	-1.20353700	3.06112400
C	0.97772300	-0.58822600	4.61849900

C	-1.42523500	-1.83641200	4.12907800
C	0.31929700	-1.22923100	5.65668600
H	1.92193800	-0.08023500	4.80603900
C	-0.90146900	-1.84661800	5.41334700
H	-2.36931400	-2.34457300	3.95499100
H	0.75293800	-1.23677300	6.65337600
H	-1.44208900	-2.34249900	6.21518300
P	-1.46836600	-1.39420400	1.36963400
C	-1.17313200	-3.22469100	0.96241500
C	0.34851400	-3.39376400	0.90514100
C	-1.71654100	-4.23050300	1.97599800
C	-1.76804300	-3.51539000	-0.41604400
H	0.81520300	-2.72214700	0.17332500
H	0.81389000	-3.20949300	1.88179400
H	0.58052400	-4.42803900	0.61636200
H	-2.80344900	-4.18599900	2.08976500
H	-1.46927100	-5.24085200	1.62331400
H	-1.25491500	-4.11211600	2.96187200
H	-1.48377800	-4.53133300	-0.72154000
H	-2.86410300	-3.47412100	-0.41342800
H	-1.39886100	-2.81869200	-1.18098100
C	-3.30928900	-0.92126700	1.44501000
C	-3.74277800	-0.53476500	0.02559000
C	-4.26408800	-2.00154700	1.95170500
C	-3.41339900	0.32308000	2.33030000
H	-3.19137200	0.34295500	-0.33252500
H	-3.61000100	-1.34877400	-0.69697000
H	-4.81030600	-0.27626300	0.04221300
H	-4.04821300	-2.33973700	2.97008700
H	-5.27804800	-1.57978500	1.96930100
H	-4.29388600	-2.87641300	1.29215200
H	-4.43886500	0.71116700	2.26579300
H	-3.20348600	0.10686500	3.38316100
H	-2.74203100	1.12220100	1.99081200
N	-1.81973000	2.86864200	0.32909200
C	-1.56379000	3.86463600	-0.21026800
C	-1.23379600	5.10026200	-0.89567000
H	-2.08119300	5.79113500	-0.86593700
H	-0.37612000	5.58449900	-0.41940500
H	-0.99085200	4.88932700	-1.94372400
Au	-0.41326800	-0.13017000	-0.37399300

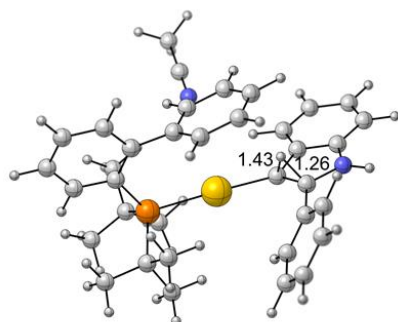
IM2:



C	1.08097400	2.87912700	-4.98696300
C	1.30005000	2.05116600	-3.87172600
C	0.25922800	1.82523200	-2.90479300
C	-1.01201100	2.43783700	-3.07343700
C	-1.21528700	3.23602700	-4.16534000
C	-0.16864400	3.44426200	-5.10668900
H	1.85840000	3.05943400	-5.72389300
H	-1.77995900	2.26490500	-2.32157200
H	-2.17298500	3.72107400	-4.32858200
H	-0.36772100	4.08373200	-5.96428900
C	0.72037200	0.96316800	-1.91819300
C	2.15077800	0.66979000	-2.24631300
C	2.50994800	-0.79693200	-2.27033400
C	1.88113900	-1.64956700	-3.18007800
C	3.43085000	-1.31286300	-1.36254900
C	2.17615700	-3.00678500	-3.17991300
H	1.15687600	-1.24382300	-3.88686500
C	3.72850700	-2.67346200	-1.36531200
H	3.90900900	-0.64686200	-0.64453300
C	3.10168500	-3.52018700	-2.27251400
H	1.68586000	-3.66717100	-3.89090500
H	4.45355600	-3.06984900	-0.65876700
H	3.33617400	-4.58173600	-2.27791600
N	2.39292700	1.36539700	-3.50925200
H	2.72815700	1.16530000	-1.43893000
H	3.26571100	1.34032000	-4.01576400
C	2.54569900	0.43852800	2.25151000
C	1.18986100	0.67269100	2.50086100
C	0.59985400	1.82955400	1.97541900
C	1.35018900	2.73027200	1.22325900
C	2.70124700	2.49081500	0.98855600
C	3.29564400	1.33913500	1.49959900
H	3.01486400	-0.45285100	2.66654400
H	-0.45146500	2.03657100	2.17296600
H	0.86894200	3.61993000	0.82265300
H	3.29325300	3.20741500	0.42281600
H	4.35550500	1.15271800	1.33550400
C	0.43972700	-0.21747100	3.42717000

C	-0.67449500	-1.01761500	3.09163200
C	0.88987700	-0.21218400	4.75478200
C	-1.31022300	-1.73614500	4.11647700
C	0.25215600	-0.93764500	5.74942600
H	1.75202800	0.40450900	5.00206700
C	-0.86733900	-1.69604700	5.43050400
H	-2.17069100	-2.35665500	3.88316600
H	0.62266200	-0.90220600	6.77068200
H	-1.39007700	-2.26304500	6.19626500
P	-1.25332600	-1.26701900	1.36056500
C	-0.74927400	-3.04813800	0.94624100
C	0.78253600	-3.03919300	0.90461100
C	-1.19447900	-4.11096000	1.94875400
C	-1.28303200	-3.39569200	-0.44438800
H	1.17521600	-2.36417500	0.13211700
H	1.21618500	-2.75137200	1.87154200
H	1.13675300	-4.05266700	0.67018700
H	-2.28150400	-4.17088700	2.06197600
H	-0.85223900	-5.08984500	1.58704800
H	-0.74682800	-3.95781100	2.93643800
H	-0.85436300	-4.35767000	-0.75680100
H	-2.37414700	-3.50677700	-0.45835900
H	-0.99718100	-2.64665900	-1.19517200
C	-3.13189600	-0.98170700	1.32740500
C	-3.51914600	-0.64675900	-0.11858300
C	-3.99884800	-2.14997400	1.79490700
C	-3.41041400	0.24879900	2.19335200
H	-3.02150500	0.26625700	-0.46938000
H	-3.28398600	-1.45701400	-0.81813200
H	-4.60373400	-0.47703500	-0.16166600
H	-3.81729300	-2.44270300	2.83401700
H	-5.05187700	-1.84352300	1.73392200
H	-3.88648100	-3.03481300	1.15823800
H	-4.46587600	0.52893700	2.07439600
H	-3.23012700	0.06262700	3.25760300
H	-2.80564200	1.10952800	1.87858500
N	-2.08871600	3.04154900	0.18889200
C	-2.55532700	4.02058100	0.60454200
C	-3.14254300	5.24267300	1.12146400
H	-2.83012900	5.40608500	2.15671800
H	-2.82495500	6.09984200	0.52117400
H	-4.23394500	5.17998000	1.09156900
Au	-0.20543000	0.09716600	-0.30856100

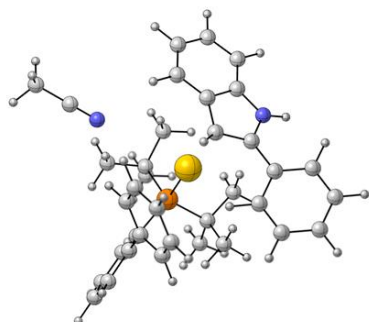
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C	1.47642400	3.36571200	-4.51297500
C	1.48874000	2.21567500	-3.72056000
C	0.45030900	1.92825400	-2.80486600
C	-0.62912200	2.81321100	-2.66641800
C	-0.65299600	3.94362000	-3.45797700
C	0.38847500	4.20837400	-4.36964700
H	2.27667700	3.58694500	-5.21398900
H	-1.41212200	2.60085100	-1.93980400
H	-1.47988000	4.64432800	-3.38126400
H	0.33797900	5.10774800	-4.97878200
C	0.73131800	0.68406400	-2.14212800
C	2.02208100	0.29807500	-2.65130500
C	2.72641900	-0.99337300	-2.50487400
C	2.00736800	-2.18976000	-2.48921000
C	4.11841800	-1.01773400	-2.38513500
C	2.67746300	-3.39976900	-2.34890300
H	0.92470400	-2.16151600	-2.59728200
C	4.78505000	-2.22909700	-2.25130700
H	4.67805600	-0.08196900	-2.37786200
C	4.06386900	-3.42045900	-2.23033200
H	2.11302000	-4.32953900	-2.33887200
H	5.86752800	-2.24484400	-2.15591900
H	4.58618300	-4.36773200	-2.12388100
N	2.42670800	1.21919500	-3.61923700
H	2.00719400	0.87191600	-1.53516500
H	3.26595500	1.12775200	-4.17313000
C	2.50228000	0.32022600	1.64949400
C	1.20175500	0.65518300	2.03878500
C	0.62836900	1.83222400	1.53878600
C	1.34140400	2.65819200	0.67631900
C	2.63606100	2.31470800	0.29040800
C	3.21208100	1.13990000	0.77446100
H	2.96163400	-0.58357500	2.04766100
H	-0.38341500	2.10707600	1.83348300
H	0.87341500	3.56500400	0.29894200
H	3.19978000	2.96855500	-0.37374600
H	4.22715000	0.87010500	0.48996400
C	0.49982600	-0.13145300	3.09122800
C	-0.65184300	-0.92703800	2.90812200
C	1.03157300	-0.00328300	4.38138100

C	-1.24754900	-1.50829100	4.03858500
C	0.43655400	-0.60027400	5.48270900
H	1.92387700	0.60652100	4.51101300
C	-0.72382400	-1.34525800	5.31286100
H	-2.14219200	-2.11399900	3.92299500
H	0.87109200	-0.47298800	6.47085200
H	-1.21614000	-1.80709300	6.16458300
P	-1.32859000	-1.35368900	1.25030800
C	-0.91439800	-3.19220800	1.03859800
C	0.61615200	-3.26410600	0.99928100
C	-1.40165500	-4.12212500	2.14840700
C	-1.48023000	-3.65989000	-0.30322800
H	1.04704600	-2.65413000	0.19411900
H	1.06166000	-2.94311200	1.94956000
H	0.91776400	-4.30675000	0.82785600
H	-2.48935300	-4.12188100	2.26699000
H	-1.10417600	-5.14779800	1.89203400
H	-0.94221400	-3.88679400	3.11401500
H	-1.10639800	-4.67082000	-0.51553100
H	-2.57570400	-3.71552000	-0.29661800
H	-1.17477800	-3.00710000	-1.13181900
C	-3.18792700	-0.97349700	1.25643500
C	-3.62040300	-0.77784100	-0.20172600
C	-4.08631300	-2.03694900	1.88561300
C	-3.36297400	0.35681200	1.99168500
H	-3.10042300	0.06893600	-0.66847100
H	-3.44827800	-1.66732400	-0.81900700
H	-4.69739200	-0.56316300	-0.22453900
H	-3.85917100	-2.23436400	2.93840500
H	-5.12343400	-1.67737000	1.84857500
H	-4.05775200	-2.98574100	1.33767800
H	-4.40514600	0.68428400	1.87663400
H	-3.15348900	0.27267500	3.06362700
H	-2.72561100	1.14526200	1.56880800
N	-2.18334400	3.32969700	0.37042900
C	-2.75578100	4.29841400	0.65683400
C	-3.47318900	5.50716700	1.01567900
H	-3.71274600	5.50255500	2.08275100
H	-2.86455400	6.38937000	0.79834300
H	-4.40582900	5.57654700	0.44873000
Au	-0.27743600	-0.21545900	-0.56116600

IM3:

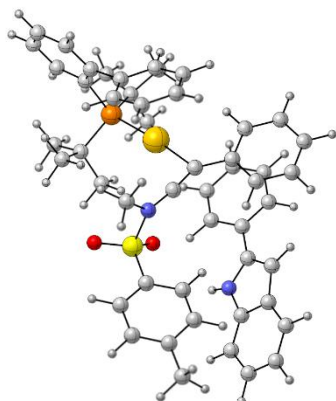


C	-1.22478300	1.07280500	-4.50328400
C	-0.14479000	0.88819400	-3.64604000
C	0.17261500	1.79274700	-2.61484800
C	-0.59732900	2.94743200	-2.45483100
C	-1.66481700	3.15013400	-3.31505400
C	-1.97966000	2.22242200	-4.32080200
H	-1.45968500	0.35899800	-5.28900700
H	-0.37339200	3.64862800	-1.65413600
H	-2.27543300	4.04334100	-3.21069900
H	-2.82607100	2.41203000	-4.97550300
C	1.29700200	1.22559400	-1.87616700
C	1.66056900	0.04092700	-2.57065100
C	2.79379500	-0.84992500	-2.34698800
C	3.39349400	-0.92192600	-1.08206600
C	3.31536500	-1.62297300	-3.39157600
C	4.47944000	-1.75637200	-0.86748300
H	2.98736200	-0.33602700	-0.25710600
C	4.40070000	-2.46127300	-3.17042400
H	2.90309000	-1.53989400	-4.39587800
C	4.98333100	-2.53277000	-1.90902400
H	4.92924500	-1.80784100	0.12147500
H	4.80073400	-3.05143700	-3.99055800
H	5.83187900	-3.19009600	-1.73846500
N	0.78997700	-0.14128300	-3.59648300
H	2.02197900	1.80887000	-1.31128100
H	0.74561200	-0.98344000	-4.15398300
C	2.53405900	0.01398300	2.72702600
C	1.19534900	0.41713800	2.76282300
C	0.84934300	1.65673800	2.20926400
C	1.82149200	2.46960900	1.63038400
C	3.15136900	2.05770300	1.59779700
C	3.50426500	0.82701900	2.14664700
H	2.81275600	-0.94217000	3.16904300
H	-0.18156000	2.00669700	2.25049200
H	1.52455500	3.42891400	1.20975700
H	3.91312200	2.69800300	1.15896400
H	4.54323600	0.50403100	2.13536200
C	0.19075100	-0.39605300	3.49724600
C	-0.95900300	-0.99639700	2.93739600
C	0.41467500	-0.53181400	4.87414200

C	-1.85118400	-1.66096100	3.79386100
C	-0.47402000	-1.20206600	5.70089300
H	1.30402000	-0.06831900	5.29696900
C	-1.62554200	-1.75951100	5.15898000
H	-2.74431600	-2.12575500	3.38573700
H	-0.27280900	-1.27838200	6.76630500
H	-2.34237700	-2.27688000	5.79098400
P	-1.28051300	-1.07796000	1.12937000
C	-0.95882700	-2.88653000	0.66149400
C	0.54160000	-3.11078300	0.87714600
C	-1.71960700	-3.91849000	1.49340800
C	-1.28685000	-3.07814800	-0.81985600
H	1.15558400	-2.46905800	0.23121800
H	0.83599500	-2.93522100	1.91995500
H	0.78113600	-4.15530300	0.63714200
H	-2.80669000	-3.81929800	1.41635600
H	-1.45829900	-4.91894900	1.12395900
H	-1.43739900	-3.88149100	2.55076000
H	-0.96389000	-4.08188900	-1.12670000
H	-2.36187600	-3.00616500	-1.02435200
H	-0.76258800	-2.34895500	-1.45461800
C	-3.06199100	-0.49986800	0.80392200
C	-3.15066500	-0.03591600	-0.65660300
C	-4.14821200	-1.54957300	1.03854400
C	-3.30547500	0.71176400	1.70611000
H	-2.50265100	0.82861400	-0.85408600
H	-2.89443400	-0.82622400	-1.37229700
H	-4.18484100	0.27193000	-0.86216800
H	-4.17992600	-1.92564100	2.06610600
H	-5.12345300	-1.08364700	0.84425400
H	-4.06063400	-2.40299000	0.35657100
H	-4.27509600	1.15384800	1.44022600
H	-3.33855500	0.44432400	2.76777600
H	-2.54253500	1.48845800	1.56116800
N	-1.36397100	3.63625300	0.78376600
C	-1.84591200	4.65555600	1.06169200
C	-2.44866200	5.92837900	1.40976400
H	-2.75395800	5.92763300	2.45992000
H	-1.73405200	6.74158400	1.25467600
H	-3.32994000	6.11338900	0.78923900
Au	0.13923600	0.20679600	-0.24998300

7.2 Coordinates of Optimized Structures in Figure 2

IM3:

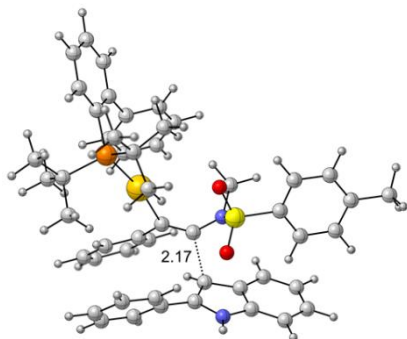


C	0.58581300	-5.93211400	-3.52843500
C	-0.14209700	-5.30102500	-2.52017600
C	-1.55531900	-5.19735100	-2.55528600
C	-2.24725600	-5.74099500	-3.64910300
C	-1.52859000	-6.37200200	-4.65095400
C	-0.12571300	-6.46804000	-4.58986200
H	1.66998900	-6.00614100	-3.48087900
H	-3.33263600	-5.68231200	-3.69805700
H	-2.05469600	-6.81307700	-5.49449000
H	0.40918100	-6.97955700	-5.38675300
C	-1.94847200	-4.51608600	-1.36311200
C	-0.80692300	-4.23523800	-0.64458800
C	-0.65536900	-3.63164400	0.67558500
C	0.55088500	-3.04495600	1.07631000
C	-1.71914100	-3.66376800	1.58759000
C	0.68478300	-2.50273600	2.34819200
H	1.38389200	-2.97836700	0.38139800
C	-1.58572300	-3.11120500	2.85372400
H	-2.65105000	-4.14855400	1.30337900
C	-0.38227900	-2.52616500	3.24241200
H	1.64173300	-2.07547800	2.64227400
H	-2.42227500	-3.15345300	3.54768000
H	-0.27060400	-2.11121500	4.24302600
N	0.28619200	-4.68269900	-1.36802200
H	-2.95860400	-4.26880700	-1.05846400
H	1.23259700	-4.69827100	-1.02016200
C	-4.27057100	-0.87974600	2.15141000
C	-3.06369700	-0.33681000	1.73031800
C	-2.59769700	-0.56818500	0.43111300
C	-3.35464400	-1.37111500	-0.43444800
C	-4.55649000	-1.91751700	-0.00883300
C	-5.01844600	-1.66963300	1.28306900
H	-4.62691200	-0.69106400	3.16105900
H	-2.46522300	0.27601400	2.40466300
H	-2.98131500	-1.57328600	-1.43792800

H	-5.13953000	-2.53610700	-0.68748500
H	-5.96388100	-2.09377900	1.61194300
C	-1.36300500	0.03610000	-0.03184000
C	-0.70783700	0.17534500	-1.11001600
N	0.00894300	0.43075300	-2.15470700
S	1.47780800	-0.53005000	-2.47798300
O	2.50857600	0.46054800	-2.72826700
O	1.54504500	-1.45421300	-1.36413100
C	1.02364800	-1.34968700	-3.95961100
C	1.67589800	-1.03447100	-5.14866600
C	0.01585100	-2.31309300	-3.89420800
C	1.31164500	-1.72156600	-6.29942600
H	2.46065400	-0.28216200	-5.15894100
C	-0.33513000	-2.97447600	-5.05779200
H	-0.47401000	-2.55190000	-2.94883200
C	0.30991900	-2.69587900	-6.26980100
H	1.81990500	-1.50526200	-7.23701500
H	-1.10492300	-3.74499200	-5.02385800
C	-0.08510700	-3.43997100	-7.50586600
H	0.68351600	-3.37988100	-8.28194600
H	-0.27222700	-4.49586700	-7.27986700
H	-1.01304300	-3.03268000	-7.92627300
C	-0.15265200	1.63954700	-2.97717200
H	-0.01016600	1.37830800	-4.03061100
H	-1.16436800	2.01920800	-2.82594700
H	0.58220700	2.39507000	-2.68161800
C	-0.93455600	4.36271500	-0.31810500
C	-0.74306900	4.23166300	1.06073200
C	-1.75463800	3.63908000	1.82631000
C	-2.92195300	3.17890200	1.22379400
C	-3.09799000	3.30553400	-0.15149400
C	-2.10285800	3.90220100	-0.91945400
H	-0.16233100	4.84856300	-0.91451400
H	-1.63576900	3.56834300	2.90677400
H	-3.70404900	2.73092100	1.83275200
H	-4.01640100	2.95609900	-0.61698100
H	-2.24850600	4.03946900	-1.98949400
C	0.44424500	4.86271600	1.69588200
C	1.49126600	4.19188900	2.36577200
C	0.48664100	6.26123600	1.61037600
C	2.51434900	4.96485500	2.94097300
C	1.51018200	7.00339500	2.17891600
H	-0.32645100	6.76747800	1.09359600
C	2.52965400	6.34932900	2.85842800
H	3.32908200	4.47667700	3.46505100
H	1.50651700	8.08719500	2.09708800
H	3.33881500	6.90966200	3.31913300
P	1.68044800	2.35993100	2.40037300
Au	0.01799900	1.16733000	1.20042900
C	3.29361300	1.98381300	1.46279800

C	3.18114900	2.74358400	0.13653800
C	4.58142700	2.38696300	2.17839200
C	3.36081000	0.48370300	1.15476500
H	2.26917800	2.47108800	-0.41540800
H	3.19301600	3.83099700	0.27483100
H	4.03273600	2.47095600	-0.50012400
H	4.71021600	1.86579000	3.13441300
H	5.43202000	2.10527300	1.54374900
H	4.65775000	3.46533400	2.34649400
H	4.23416500	0.30285400	0.51411600
H	3.48341400	-0.12674400	2.05586700
H	2.47925200	0.11912900	0.61135400
C	1.66928900	1.84605100	4.22242500
C	2.04044600	0.36798000	4.31611700
C	2.57674900	2.65431300	5.14833300
C	0.22162600	2.02441900	4.69026500
H	1.44928100	-0.24239400	3.62286300
H	3.10531900	0.19319400	4.12235900
H	1.83380700	0.01372400	5.33512000
H	2.26122600	3.69920700	5.23081300
H	2.51444300	2.21723800	6.15376800
H	3.63067300	2.62461100	4.85012300
H	0.15423800	1.74902200	5.75113600
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H	-0.47304800	1.38079400	4.13211100

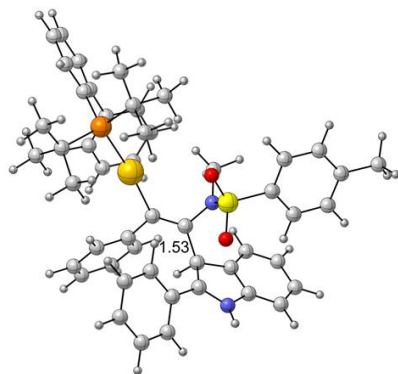
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C	4.02946300	-5.66265800	-7.00667000
C	4.30077000	-6.42600400	-8.13473900
C	5.30640800	-7.40364500	-8.12425400
H	6.86523600	-8.38202600	-6.98270900
H	3.24110200	-4.91174100	-7.01825000
H	3.71828200	-6.27349500	-9.03973500
H	5.48432000	-7.99743700	-9.01750800
C	4.77123100	-5.29974800	-4.52799500
C	5.75964300	-5.98579500	-3.79418300
C	6.16474500	-5.81540900	-2.39858100
C	7.50405200	-5.55312300	-2.08283600

C	5.21360500	-5.90205500	-1.37875400
C	7.87880500	-5.37603400	-0.75658200
H	8.23067600	-5.44171300	-2.88593800
C	5.60066000	-5.74925100	-0.05275300
H	4.17045400	-6.09274400	-1.62914500
C	6.93033000	-5.48095400	0.25936600
H	8.91677300	-5.15750100	-0.51429700
H	4.85805000	-5.83047000	0.73750500
H	7.23066000	-5.35538400	1.29722600
N	6.37761200	-6.87023400	-4.60769100
H	3.90003100	-4.85445700	-4.05763400
H	7.19044800	-7.40783700	-4.33868000
C	3.12994700	-2.96911200	-0.33839500
C	4.25146500	-2.86040700	-1.14814200
C	4.12679700	-2.86524300	-2.54425500
C	2.84135900	-2.94525000	-3.10197100
C	1.71775800	-3.04020700	-2.28743800
C	1.85835900	-3.05637200	-0.90354000
H	3.24701500	-2.98314100	0.74306900
H	5.24634400	-2.80139000	-0.70634200
H	2.73166700	-2.90519400	-4.18636100
H	0.72927700	-3.09690700	-2.73673800
H	0.98100500	-3.12984900	-0.26617200
C	5.27610000	-2.68037000	-3.42480400
C	5.69428700	-3.33998000	-4.47332300
N	6.26896600	-3.09107500	-5.66604200
S	7.97423700	-3.38010000	-5.83337200
O	8.66004300	-2.15216600	-5.45151200
O	8.22626100	-4.62010000	-5.11813200
C	8.15447100	-3.58669800	-7.57615500
C	8.87927100	-2.64146600	-8.29803300
C	7.57445700	-4.69117100	-8.19226700
C	9.02371600	-2.82025300	-9.66685600
H	9.31744600	-1.78775000	-7.78805500
C	7.72579800	-4.84525100	-9.56085500
H	7.01625500	-5.41903300	-7.60986400
C	8.45396600	-3.91945900	-10.31681500
H	9.58844400	-2.09255000	-10.24661400
H	7.27030100	-5.70291800	-10.05412600
C	8.63902300	-4.11645900	-11.78872500
H	8.79861500	-3.16597000	-12.30702300
H	9.51567000	-4.74589100	-11.98664400
H	7.77534000	-4.61493800	-12.24015900
C	5.77541300	-1.91247300	-6.39666100
H	6.15311100	-1.93125300	-7.42325100
H	4.68338900	-1.96880800	-6.41955300
H	6.07990100	-0.98561600	-5.88985900
C	5.60135700	1.80803800	-4.52814800
C	5.75128100	1.80070400	-3.13793200
C	4.75630400	1.19974200	-2.35724100

C	3.64571800	0.60866000	-2.95274100
C	3.51033700	0.61739800	-4.33803600
C	4.48928500	1.21889700	-5.12357200
H	6.36248100	2.29161900	-5.13974800
H	4.84508900	1.21547400	-1.27219000
H	2.88434300	0.14186300	-2.33005800
H	2.63592400	0.16554400	-4.80200900
H	4.38123100	1.24428800	-6.20632300
C	6.87401900	2.55341600	-2.51562300
C	7.94217000	1.99854600	-1.77594000
C	6.82313300	3.94381600	-2.68393100
C	8.88420600	2.87310900	-1.20907600
C	7.77119100	4.78792500	-2.12614200
H	5.99696400	4.36028300	-3.25722300
C	8.80542300	4.24857200	-1.37209600
H	9.70855400	2.47297100	-0.62758300
H	7.69620800	5.86234400	-2.27289900
H	9.55361800	4.89145700	-0.91593300
P	8.23690900	0.18663200	-1.62701400
Au	6.66246300	-1.20479800	-2.75134900
C	9.92579900	-0.15064600	-2.42700600
C	9.82458900	0.47378600	-3.82367400
C	11.15155400	0.41111900	-1.71010900
C	10.10920600	-1.66660200	-2.56536900
H	8.95386200	0.10258100	-4.37983500
H	9.77939700	1.56856100	-3.78039100
H	10.71743000	0.19382800	-4.39856000
H	11.28656300	-0.01710500	-0.71018100
H	12.04154700	0.14090700	-2.29432000
H	11.14401600	1.50255800	-1.63512100
H	10.99332400	-1.85037600	-3.19049100
H	10.28409200	-2.15273000	-1.59934200
H	9.25969800	-2.15337500	-3.05764400
C	8.13653400	-0.21766600	0.22298200
C	8.45426100	-1.70117000	0.42116100
C	9.03577000	0.61483500	1.13617500
C	6.68271300	0.04286800	0.62920300
H	7.90469700	-2.34754100	-0.27735600
H	9.52514300	-1.90950100	0.31257900
H	8.17021900	-1.99120500	1.44234800
H	8.75079400	1.67182700	1.14371300
H	8.92108900	0.24369300	2.16358100
H	10.09822900	0.53786900	0.88256500
H	6.56465700	-0.19509400	1.69492700
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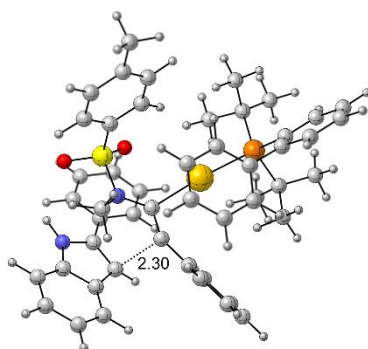
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C	-2.65664300	-2.56308500	-3.41016800
C	-2.86207000	-3.24310900	-4.61026700
C	-2.48851600	-4.58121900	-4.75619400
H	-1.60009800	-6.32255100	-3.81486400
H	-2.93741600	-1.51704800	-3.30211600
H	-3.31798500	-2.72429300	-5.44919100
H	-2.66145200	-5.08628300	-5.70259000
C	-1.70970400	-2.82183200	-0.97020800
C	-1.00688900	-4.04104500	-0.43274800
C	-0.49705700	-4.29073400	0.90106000
C	0.22284000	-3.31766700	1.61230300
C	-0.73168000	-5.54537700	1.49040900
C	0.70094900	-3.60911000	2.88104100
H	0.43985400	-2.35673800	1.15425400
C	-0.25959500	-5.82092000	2.76349300
H	-1.33448900	-6.28926600	0.97169300
C	0.46171800	-4.85310900	3.45832500
H	1.27457900	-2.85884900	3.42000600
H	-0.46125400	-6.78658800	3.21846200
H	0.83699300	-5.07056700	4.45507700
N	-1.10705700	-5.01044800	-1.32422600
H	-2.62704700	-2.77954000	-0.34901800
H	-0.67729100	-5.91993700	-1.19495200
C	-3.49257800	-1.12499100	3.29922000
C	-2.36278600	-0.98488100	2.50380700
C	-2.47062000	-0.86982800	1.10925400
C	-3.75971900	-0.87923200	0.54953100
C	-4.89191900	-1.00873000	1.34804800
C	-4.76364600	-1.13290700	2.72738900
H	-3.38222400	-1.21898800	4.37725200
H	-1.37446900	-0.95625400	2.96276100
H	-3.86326300	-0.74707000	-0.52879700
H	-5.87852500	-1.00212800	0.88993400
H	-5.64624300	-1.22739000	3.35466300
C	-1.29738300	-0.64397600	0.24652700
C	-1.03734400	-1.46199400	-0.79351100

N	-0.15034800	-1.10666500	-1.86692200
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C	2.73751300	-1.10011100	-4.16832100
C	0.99180600	-2.76861100	-4.41209800
C	2.99755100	-1.19169900	-5.53015000
H	3.30092000	-0.42737700	-3.52643300
C	1.26301400	-2.84221900	-5.76872300
H	0.21429800	-3.38451500	-3.96578800
C	2.26967300	-2.05993400	-6.34737800
H	3.78066800	-0.57716100	-5.97052100
H	0.68535400	-3.52015600	-6.39591900
C	2.57569800	-2.17288000	-7.80856600
H	3.01951800	-1.25252800	-8.20053000
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H	1.67705900	-2.39689900	-8.39248700
C	-0.23574800	0.24155600	-2.42649700
H	0.18168500	0.24121200	-3.44039500
H	-1.29414400	0.51523000	-2.47574300
H	0.27923300	0.99695200	-1.81756500
C	-1.33826000	3.87027800	-0.70643900
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C	-2.09116900	3.15794900	1.46797400
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C	-3.34271800	2.54351700	-0.49807800
C	-2.42179600	3.22038000	-1.29167800
H	-0.62825500	4.42149800	-1.32235200
H	-1.97238400	3.15503000	2.55107100
H	-3.89055900	1.98100600	1.50998600
H	-4.19859500	2.04827800	-0.95214600
H	-2.55578700	3.26186200	-2.37080700
C	-0.08817300	4.66144400	1.30889100
C	1.06909600	4.16899000	1.95052500
C	-0.30434800	6.04563700	1.27141700
C	1.92835300	5.09420800	2.56652100
C	0.56386200	6.94113100	1.87650900
H	-1.19699000	6.41066100	0.76671800
C	1.68383600	6.45951500	2.54229700
H	2.82538900	4.74564700	3.06738400
H	0.36093300	8.00830500	1.83606900
H	2.37261900	7.14115100	3.03456500
P	1.53758300	2.38425600	1.94179400
Au	-0.02388700	0.88533300	0.90822700
C	3.17745500	2.29481300	0.99381200
C	2.79802000	2.52997000	-0.47270700
C	4.24479800	3.31666300	1.38154300
C	3.75388700	0.88556200	1.13891100
H	2.18968100	1.70698200	-0.86600800

H	2.25892800	3.47705000	-0.61307100
H	3.71730000	2.57882700	-1.07240200
H	4.52909500	3.26743200	2.43855100
H	5.14865200	3.10243400	0.79535900
H	3.94211800	4.34214000	1.14607300
H	4.55573400	0.75703100	0.39919600
H	4.19709000	0.72432700	2.12931400
H	3.01091300	0.10391100	0.93767700
C	1.68402000	1.85626500	3.76360900
C	1.75377600	0.32639400	3.83363500
C	2.87561200	2.42436800	4.53203200
C	0.38291900	2.30275600	4.43623200
H	0.90061400	-0.14136000	3.32511300
H	2.67190100	-0.07630700	3.39371100
H	1.72963700	0.02337600	4.88971900
H	2.84899300	3.51528900	4.61359500
H	2.84944200	2.03149800	5.55764900
H	3.83594200	2.12343400	4.09788400
H	0.38057600	1.95166200	5.47693600
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TS4-a:

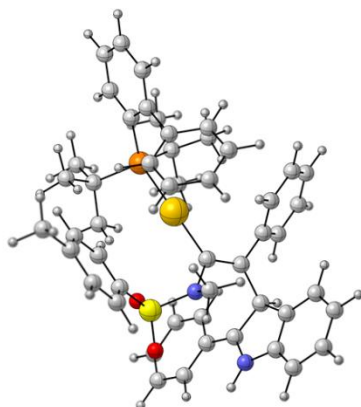


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C	3.56206500	-6.07791300	-5.24714800
C	2.22879200	-5.71811400	-5.46426300
C	1.54074400	-6.32043300	-6.50854600
C	2.15690500	-7.27729200	-7.32954200
H	3.95437800	-8.40618500	-7.75470500
H	1.74370700	-4.98065200	-4.82698500
H	0.50245100	-6.05521400	-6.69124100
H	1.58809500	-7.73447400	-8.13502600
C	4.58604100	-5.62030800	-4.33754700
C	5.74273000	-6.37032900	-4.62383000
C	7.04204500	-6.32199400	-3.97740900
C	7.99169900	-7.33327100	-4.17604500
C	7.37584700	-5.23862700	-3.15195400
C	9.24260800	-7.25179400	-3.58229300
H	7.74703600	-8.20239800	-4.78305100
C	8.62442600	-5.16166400	-2.55641200

H	6.65958200	-4.43212500	-3.01228300
C	9.56484300	-6.16550700	-2.77417800
H	9.96780000	-8.04451900	-3.74529600
H	8.86769500	-4.31249000	-1.92123500
H	10.54555400	-6.10538400	-2.30919800
N	5.47075800	-7.21769100	-5.65720900
H	4.39475500	-5.18333100	-3.36547900
H	6.20123500	-7.61240100	-6.24019300
C	3.28052000	-1.78439800	-2.22074300
C	4.21047700	-2.58642200	-2.86413100
C	4.20288900	-2.69169400	-4.26477600
C	3.22584800	-2.00017100	-5.00088600
C	2.29207300	-1.20589600	-4.35057600
C	2.32030100	-1.09537100	-2.96210600
H	3.29684500	-1.69824000	-1.13738200
H	4.96067100	-3.12527300	-2.28705200
H	3.23340900	-2.08902200	-6.08640300
H	1.54082000	-0.67036400	-4.92611000
H	1.58809500	-0.47377700	-2.45286100
C	5.16303300	-3.48591500	-4.98109300
C	6.02455300	-3.48184800	-5.95025800
N	6.32197300	-4.49508000	-6.85565800
S	7.92969000	-4.92211200	-7.19846800
O	8.72016100	-4.44033800	-6.07938700
O	7.84552100	-6.33734100	-7.54217500
C	8.40383600	-4.03963600	-8.65938900
C	9.05715000	-2.81696000	-8.52659700
C	8.11317700	-4.56750400	-9.91605800
C	9.41141400	-2.11324800	-9.66968900
H	9.29791000	-2.44117300	-7.53372700
C	8.46590900	-3.84415300	-11.04696800
H	7.63902200	-5.54206500	-10.00181600
C	9.11968000	-2.61128800	-10.94374400
H	9.93817800	-1.16338200	-9.57776000
H	8.24614000	-4.24839900	-12.03347200
C	9.53556000	-1.86438000	-12.17235000
H	8.83834400	-2.03000000	-12.99969400
H	9.60217700	-0.78761500	-11.98812900
H	10.52404500	-2.19869400	-12.51119700
C	5.34453600	-4.72227400	-7.92515000
H	5.41941500	-3.95246600	-8.70732700
H	5.51038200	-5.71151000	-8.36066500
H	4.34043400	-4.70175100	-7.49013000
C	4.82070800	0.92120500	-7.24990900
C	6.20808900	0.90843100	-7.41528600
C	6.77753500	-0.05964200	-8.24980600
C	5.98028300	-0.99956100	-8.89684700
C	4.59895900	-0.98202100	-8.71885500
C	4.02282300	-0.02005900	-7.89403100
H	4.36672100	1.68453000	-6.61882900

H	7.85542100	-0.05882100	-8.41115200
H	6.44859200	-1.73655900	-9.54961900
H	3.97081400	-1.70509600	-9.23544500
H	2.94254700	0.01110800	-7.76406300
C	7.04216400	1.99485300	-6.83342500
C	7.98525600	1.84992900	-5.79236300
C	6.86732600	3.25858500	-7.41304300
C	8.73473000	2.97452900	-5.41142700
C	7.61539600	4.35736400	-7.01815400
H	6.13297400	3.35956700	-8.21009000
C	8.56698400	4.21151700	-6.01645600
H	9.46252000	2.89009800	-4.60990400
H	7.46024900	5.32116000	-7.49613600
H	9.17074200	5.05689800	-5.69731300
P	8.17886600	0.29994700	-4.81879400
Au	7.04733400	-1.63130700	-5.62576200
C	10.03116700	-0.10848000	-4.69526500
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C	10.83595400	0.69495400	-3.67326200
C	10.16471300	-1.59341700	-4.33129100
H	10.04043100	-0.42422100	-6.86293300
H	10.65021500	1.16851400	-6.37169200
H	11.64027900	-0.28206700	-6.11641500
H	10.50019000	0.51471800	-2.64589200
H	11.88295400	0.36801300	-3.72825100
H	10.83490000	1.77360000	-3.85736500
H	11.23264000	-1.84630300	-4.28752600
H	9.73409100	-1.82429900	-3.35031600
H	9.69444900	-2.26219000	-5.06258200
C	7.37157700	0.68985600	-3.14664200
C	7.56585300	-0.50535100	-2.21216500
C	7.87553900	1.96151000	-2.46618500
C	5.87746100	0.86276600	-3.43883700
H	7.26321800	-1.45163600	-2.68256300
H	8.60364900	-0.60410500	-1.87132600
H	6.94209100	-0.36086700	-1.31914600
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H	7.34488200	2.07534100	-1.51144500
H	8.94602400	1.93486200	-2.23983000
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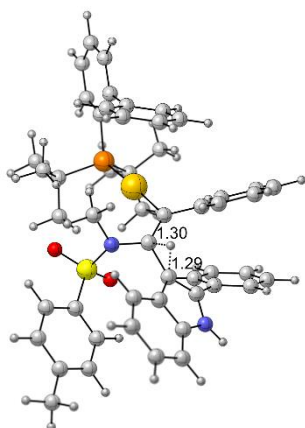


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H	2.61652400	-6.81521800	0.67918200
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H	3.81451600	-5.36209300	2.29382800
N	-1.96863400	-5.05706200	0.28136200
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H	-2.85757600	0.34423900	-0.31835800
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P	1.24595600	2.74500700	1.06493200
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H	3.30272700	2.22338800	-0.85674500
H	3.74424100	3.85411200	-0.31771800
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H	3.71156800	4.44548000	2.21661000
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C	0.34789600	3.12670800	2.69533000
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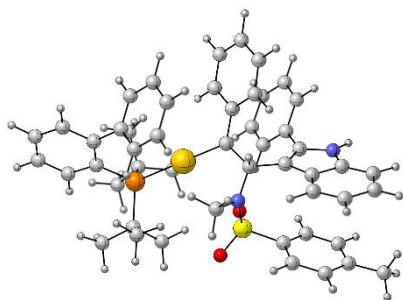
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H	-0.29484700	-4.20135400	4.56918000
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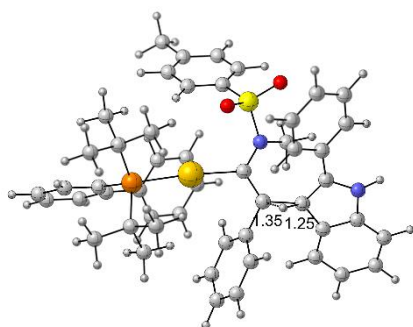
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H	-1.85451000	-6.11170000	-3.96348600
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H	1.74708400	2.55151300	-1.08215800
H	1.75268800	4.22444700	-0.43792900
H	3.12706800	3.61055700	-1.37467600

H	4.55916400	3.69348800	2.02709600
H	4.81826000	4.03916200	0.31757500
H	3.55828200	4.91027900	1.19312000
H	4.50416700	1.76180400	-0.54177900
H	4.49966700	1.26832100	1.15590500
H	3.20623900	0.72816600	0.04939600
C	2.28814100	1.52084200	3.41646800
C	2.46900000	0.03701200	3.07550100
C	3.58979100	2.04195000	4.02205000
C	1.15850100	1.64289900	4.44331500
H	1.52825200	-0.41788300	2.73779600
H	3.22131000	-0.13866000	2.29950000
H	2.79412000	-0.49255500	3.98211900
H	3.52400000	3.08500700	4.34676300
H	3.82008400	1.44724800	4.91633000
H	4.44008700	1.93584900	3.33888500
H	1.38916000	0.99844700	5.30208300
H	1.03842900	2.66704700	4.81376200
H	0.19362900	1.31365800	4.03038300

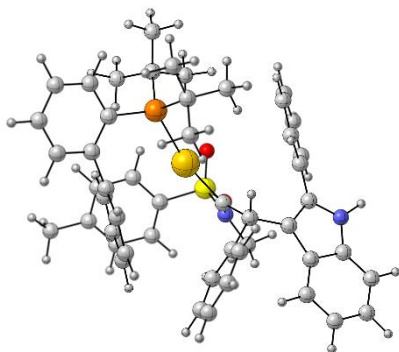
TS5-a:



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C	-4.63125000	-2.70354200	0.69381300
C	-5.82449800	-3.40894600	0.62758600
C	-5.85164000	-4.80905300	0.66828800
H	-4.68836200	-6.63072300	0.78456000
H	-4.63265700	-1.61731500	0.66749300
H	-6.76016300	-2.86254000	0.54477800
H	-6.80498400	-5.32814400	0.61874400
C	-2.02273400	-3.05464300	0.86549800
C	-1.29128700	-4.28068300	0.93966300
C	0.12319800	-4.58172600	1.13470600
C	0.64415900	-5.78095600	0.62458300
C	0.96619100	-3.73308600	1.86281900
C	1.96850900	-6.12453000	0.84636100
H	0.02009100	-6.42743100	0.00843000
C	2.28889500	-4.08463700	2.08746800
H	0.59609000	-2.79037800	2.26458600
C	2.79227900	-5.27954100	1.58353000

H	2.36313400	-7.04731200	0.43029400
H	2.93193600	-3.41234300	2.64837000
H	3.83169900	-5.54639100	1.75422000
N	-2.18774800	-5.29721800	0.89926500
H	-1.42146300	-2.43954500	1.77517000
H	-1.93456000	-6.25725200	1.09086900
C	-3.66516600	0.32128500	3.14570000
C	-2.76675100	-0.61083100	2.64165800
C	-2.37321400	-0.57787400	1.29803800
C	-2.88874800	0.43076200	0.47764000
C	-3.78401200	1.36917500	0.98274600
C	-4.18385100	1.31150900	2.31396400
H	-3.96359800	0.27349800	4.19003900
H	-2.37833800	-1.38639400	3.30455300
H	-2.59679500	0.46395200	-0.57098300
H	-4.17480800	2.14401800	0.32593800
H	-4.89433500	2.03551500	2.70503500
C	-1.48196900	-1.61811900	0.70981500
C	-0.31350800	-1.25022200	0.02422900
N	0.21355500	-2.15656000	-0.87190800
S	1.90249400	-2.27097000	-1.20460700
O	2.58742400	-1.63157400	-0.09507900
O	2.09267500	-3.67266900	-1.53566700
C	2.21230400	-1.33297800	-2.67405500
C	2.69384500	-0.03238200	-2.55941000
C	2.03648100	-1.92818200	-3.92274900
C	2.97790500	0.68681500	-3.71186200
H	2.85585000	0.39101300	-1.57015200
C	2.31124500	-1.18738700	-5.06402100
H	1.72667200	-2.96795500	-3.99424600
C	2.78530600	0.12616500	-4.97851900
H	3.36394400	1.70301600	-3.63124100
H	2.17710200	-1.64144100	-6.04415500
C	3.12347200	0.89830700	-6.21527700
H	4.17445800	0.74587800	-6.49085400
H	2.51571900	0.58018600	-7.06799300
H	2.97887000	1.97364900	-6.07113300
C	-0.62796400	-2.98697500	-1.73416300
H	-1.65183600	-2.60647200	-1.68810800
H	-0.28398800	-2.88960700	-2.76977600
H	-0.60440800	-4.04807900	-1.46111600
C	-1.96220000	3.26921400	-1.68410100
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H	1.21268100	2.20595600	-2.21218300
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H	-2.47823800	0.53937900	-3.64368200
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C	1.06320300	4.29293800	0.13057200
C	-0.08347600	5.62244800	-1.53794200
C	1.70834500	5.47250800	0.53626100
C	0.56127700	6.77382100	-1.11503700
H	-0.78088800	5.67034800	-2.37207100
C	1.47735000	6.69626800	-0.07424500
H	2.40506200	5.44255700	1.36774100
H	0.35625100	7.72310700	-1.60321900
H	2.00455100	7.58191100	0.27049200
P	1.34253400	2.77856800	1.15271800
Au	0.47875900	0.66300400	0.38674300
C	3.22469800	2.59765000	1.40725800
C	3.88986000	2.89690700	0.06176700
C	3.86023400	3.46690500	2.49384100
C	3.50294000	1.13431000	1.77507200
H	3.43432700	2.32417100	-0.75796300
H	3.84163000	3.95811700	-0.20439300
H	4.94783800	2.60796700	0.11496300
H	3.47628900	3.22845500	3.49198300
H	4.93846100	3.25781300	2.50935700
H	3.75395700	4.54309800	2.32876200
H	4.58390400	1.01317200	1.92930400
H	3.00403500	0.83613900	2.70473500
H	3.19657500	0.43072100	0.99289300
C	0.41477600	3.15684800	2.76474500
C	0.65107400	2.00783200	3.74640300
C	0.75795400	4.48510200	3.43574200
C	-1.06582900	3.18317400	2.37807900
H	0.42353200	1.03067300	3.29829300
H	1.67980700	1.98582900	4.12629500
H	-0.01299600	2.13978900	4.61156400
H	0.51557700	5.34263100	2.79916700
H	0.14885600	4.57581300	4.34523100
H	1.80609500	4.56012200	3.74064700
H	-1.66645800	3.37835000	3.27738100
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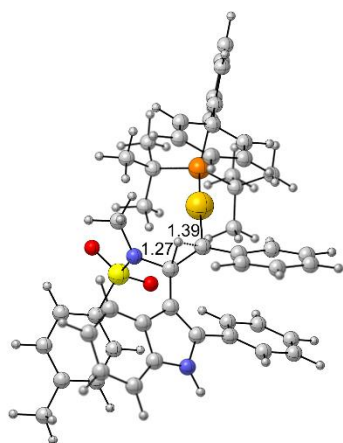
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C	-4.71519900	-3.25854500	0.51882400
C	-5.66838900	-4.26121200	0.53735300
C	-5.38176100	-5.54097400	1.03910400
H	-3.88781800	-6.83054100	1.91851600
H	-4.97916600	-2.27843400	0.13411000
H	-6.66593700	-4.05112600	0.15954400
H	-6.15725100	-6.30252200	1.04328300
C	-2.19928500	-2.77679400	1.17019700
C	-1.27543000	-3.63280900	1.73809400
C	0.14072600	-3.44017000	2.06933400
C	1.10653100	-4.31692800	1.55919600
C	0.54697400	-2.40246300	2.91451700
C	2.45049000	-4.14559700	1.86892800
H	0.80045900	-5.12982200	0.90091000
C	1.88971900	-2.24559500	3.23647600
H	-0.20576800	-1.74775600	3.35336800
C	2.84532000	-3.10837300	2.70753100
H	3.19051600	-4.82430800	1.45291500
H	2.18969100	-1.45624000	3.92354900
H	3.89548000	-2.97808500	2.95795300
N	-1.84944500	-4.87424200	1.90048000
H	-1.57923000	-0.79825900	1.60319600
H	-1.41748900	-5.62825700	2.41450800
C	-5.04072200	0.66985400	0.50823200
C	-3.87298300	0.07923200	0.97489700
C	-3.02609600	-0.61515300	0.10685300
C	-3.34873700	-0.66548200	-1.24920800
C	-4.52676500	-0.08875100	-1.71644800
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H	-5.69681100	1.19133300	1.20057400
H	-3.63022600	0.11830500	2.03650600
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H	-4.77856900	-0.15857600	-2.77265800
H	-6.30437100	1.01282900	-1.20432800
C	-1.85519300	-1.37594300	0.70688000
C	-0.60053300	-1.24363200	-0.16041500

N	-0.28798800	-2.18694400	-1.01257000
S	1.41508300	-2.30762800	-1.65374800
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C	1.49709100	-1.21130300	-3.03106200
C	2.29142400	-0.07290800	-2.92994100
C	0.86519700	-1.55926200	-4.22406400
C	2.44265300	0.73673700	-4.04688800
H	2.79594000	0.15061300	-1.99273200
C	1.01686900	-0.72719500	-5.32296500
H	0.29244200	-2.48029500	-4.30277500
C	1.80958400	0.42601300	-5.25483300
H	3.06940500	1.62576100	-3.98523400
H	0.53100600	-0.98382600	-6.26224900
C	2.00369700	1.28869100	-6.46146700
H	2.88023000	0.95853300	-7.03276800
H	1.14207100	1.24177000	-7.13427600
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C	-1.11182600	-3.34478800	-1.42723100
H	-2.16027600	-3.14074600	-1.22024400
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H	-0.80342500	-4.25342000	-0.90398800
C	-1.80325600	3.53152300	-0.97381200
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H	-2.23520200	4.20072600	-0.23062700
H	1.21484900	2.60971300	-2.22576000
H	-0.25157700	1.23639900	-3.67560700
H	-2.71984500	1.35760500	-3.41346100
H	-3.70673600	2.80110100	-1.65585000
C	0.44544800	4.43688100	-0.38077900
C	1.41800300	4.10005300	0.58203500
C	0.27034500	5.78500600	-0.72413700
C	2.19916600	5.13377500	1.12448900
C	1.04907500	6.78977100	-0.17244700
H	-0.48786300	6.02957900	-1.46562200
C	2.03282600	6.45900800	0.75142400
H	2.94855200	4.90655900	1.87513400
H	0.89392700	7.82407800	-0.46839500
H	2.66235500	7.22778000	1.19159600
P	1.60121200	2.40702000	1.28663400
Au	0.47506700	0.52982600	0.25127000
C	3.46465000	2.01362400	1.35677500
C	4.04927400	2.44966900	0.01087800
C	4.26089300	2.65233100	2.49624900
C	3.62111800	0.49497100	1.48927500
H	3.48109400	2.03545100	-0.83433200

H	4.07497100	3.53850100	-0.10402200
H	5.07845200	2.07551800	-0.06869200
H	3.91314000	2.32231700	3.48157100
H	5.30606800	2.32804000	2.40309800
H	4.27298800	3.74559500	2.47955800
H	4.69278600	0.25330300	1.50123300
H	3.18860400	0.10925000	2.41934500
H	3.16484300	-0.05755900	0.66059500
C	0.80282800	2.56443700	3.00286700
C	1.03273000	1.26919800	3.77914200
C	1.28352600	3.74993500	3.83816100
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H	0.73304300	0.38491100	3.20063500
H	2.08086300	1.14610300	4.07941600
H	0.43213300	1.29221100	4.69859700
H	1.04888600	4.70981900	3.36684400
H	0.75951500	3.72490700	4.80297400
H	2.35641000	3.71868200	4.05296300
H	-1.21408000	2.83685900	3.70972400
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TS6:

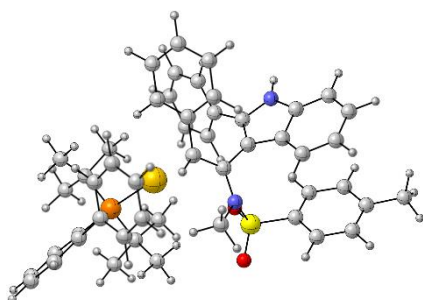


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C	-1.57855600	-1.95050900	-4.31357200
C	-1.95239900	-2.63396100	-5.45918300
C	-2.21368100	-4.01304100	-5.43337000
H	-2.32263900	-5.80554100	-4.22777800
H	-1.36118000	-0.88476600	-4.35482800
H	-2.04365900	-2.09441600	-6.39858300
H	-2.50964100	-4.51846500	-6.34928000
C	-1.10904600	-2.30609400	-1.75800700
C	-1.18084700	-3.46887200	-0.99401800
C	-0.90961000	-3.73922200	0.41949100
C	0.23938100	-3.24356700	1.04691700
C	-1.80536300	-4.53060800	1.14901200

C	0.48154400	-3.54185100	2.38294000
H	0.94954500	-2.63861000	0.48506800
C	-1.55970600	-4.81804800	2.48576600
H	-2.71740300	-4.88902700	0.67308900
C	-0.41380300	-4.32660700	3.10469500
H	1.38628400	-3.16882100	2.85824700
H	-2.26568100	-5.42607700	3.04586200
H	-0.21672000	-4.56017700	4.14809200
N	-1.56705800	-4.49164300	-1.81423600
H	-1.70978000	-0.11056600	-1.23511900
H	-1.59107700	-5.45786100	-1.51982500
C	-3.21589100	-1.48176200	2.90661500
C	-2.15781400	-1.00804400	2.14071500
C	-2.25539500	-0.94509100	0.74507700
C	-3.46677100	-1.31748000	0.14122800
C	-4.53714500	-1.74789000	0.91135900
C	-4.41250000	-1.84321700	2.29635900
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H	-1.23179800	-0.69486300	2.62245900
H	-3.58260700	-1.25016500	-0.94101700
H	-5.47582700	-2.00837900	0.42873900
H	-5.25156800	-2.18489500	2.89698300
C	-1.10775500	-0.41531900	-0.01835400
C	-0.76924500	-0.96954600	-1.28792300
N	0.14536400	-0.25018800	-2.14395300
S	1.77541900	-0.72902300	-2.12230800
O	2.51087100	0.42714200	-2.61095800
O	2.05001600	-1.29224100	-0.80488600
C	1.85959200	-2.03041300	-3.31216100
C	1.81785900	-1.69870000	-4.66396800
C	1.86861800	-3.35447800	-2.88685300
C	1.76001300	-2.71886800	-5.60035700
H	1.83655900	-0.65554000	-4.97327300
C	1.80665000	-4.36039700	-3.84091300
H	1.92164400	-3.58557300	-1.82557100
C	1.73187100	-4.06007700	-5.20387700
H	1.72551800	-2.47625500	-6.66096200
H	1.81151900	-5.40252800	-3.52510200
C	1.58548000	-5.14989900	-6.21848100
H	2.03926500	-4.87689000	-7.17636700
H	2.03822200	-6.08629500	-5.87761200
H	0.52132200	-5.34810700	-6.40569100
C	-0.18649000	1.08369600	-2.64305400
H	0.49424700	1.33918100	-3.45766900
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H	-0.12390200	1.86665100	-1.87360000
C	-1.56081400	4.07466000	-0.10380300
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H	-0.91323100	4.79295200	-0.60565500
H	-2.09671700	2.73046700	2.96761600
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C	-0.36480000	4.59863300	2.03306800
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C	1.71651600	5.03999400	3.18007600
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H	-1.78457200	6.19973800	2.10748700
C	1.27103100	6.29696800	3.56150900
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Au	0.08390500	1.09749600	0.81753000
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H	1.84266100	2.64892500	-1.03380600
H	1.79208500	4.30825300	-0.36557700
H	3.22553900	3.72868100	-1.23402900
H	4.51171900	3.73319100	2.21640900
H	4.85256200	4.08810300	0.52238700
H	3.57005800	4.97300000	1.35239700
H	4.52400400	1.81257600	-0.36915800
H	4.43820400	1.30706000	1.32219200
H	3.17630200	0.80720900	0.16269400
C	2.14616700	1.63834000	3.50799200
C	2.32094700	0.14853800	3.18429000
C	3.43118400	2.13819300	4.16625600
C	0.97704100	1.78579900	4.48499300
H	1.39654900	-0.29960200	2.79662000
H	3.11273100	-0.04086300	2.45196700
H	2.58923900	-0.37939200	4.10989400
H	3.37292600	3.18271700	4.48766000
H	3.61355100	1.54109300	5.06989500
H	4.30689300	2.01548400	3.51914600
H	1.17439800	1.16865700	5.37167000
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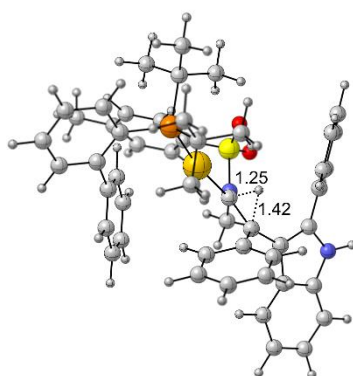


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C	-2.11373000	-4.76858900	-4.43656700
H	-1.74537700	-6.26419600	-2.92018500
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C	1.41565400	-2.80399100	1.11851500
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C	1.96830400	-2.96745800	2.38407300
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C	-0.15732800	-3.73216900	3.22950300
H	-1.75880400	-3.83676100	1.78312900
C	1.18691500	-3.43439100	3.43756200
H	3.02114900	-2.74163000	2.54410400
H	-0.77147900	-4.09076800	4.05191600
H	1.62666300	-3.56650200	4.42373200
N	-0.81901000	-4.38305100	-0.98631600
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H	-0.66943400	-5.25410500	-0.49730200
C	-3.81864400	-1.58860200	2.34813400
C	-2.82326900	-0.86891200	1.69293700
C	-2.68558200	-0.92751100	0.30304000
C	-3.58591200	-1.72350700	-0.41653400
C	-4.57264700	-2.45300400	0.23520200
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H	-3.90328400	-1.52838500	3.43077800
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H	-3.50601500	-1.77670000	-1.50181200
H	-5.25737600	-3.06756500	-0.34431200
H	-5.46968000	-2.95416700	2.13024200
C	-1.65005500	-0.12837000	-0.42626900
C	-0.76954100	-0.74624400	-1.33359300
N	-0.13664500	-0.03065300	-2.32793800

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O	2.12653500	-0.94500700	-1.47589900
C	1.53467200	-1.58268800	-3.96739700
C	1.27850800	-1.15652600	-5.26820000
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C	1.20837000	-2.10565200	-6.27700800
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C	1.67018700	-3.85498200	-4.68625700
H	1.94781500	-3.22624900	-2.63694500
C	1.38577500	-3.46447700	-5.99921500
H	1.01205200	-1.79091700	-7.30004500
H	1.82349300	-4.91020600	-4.46676700
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H	1.33371600	-4.05489000	-8.07405400
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C	3.07648200	1.94774700	1.36114200
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C	3.49993600	0.47778600	1.35728900
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H	2.39872200	3.42141400	-0.12091700

H	3.73895000	2.38414200	-0.64499300
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H	5.12757700	2.54739800	1.35038300
H	4.04361600	3.86877800	1.78047200
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H	3.85904200	0.15254700	2.34192100
H	2.69424500	-0.19120300	1.02844200
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C	1.30787700	-0.10792700	3.96495300
C	2.56624600	1.81781300	4.89238700
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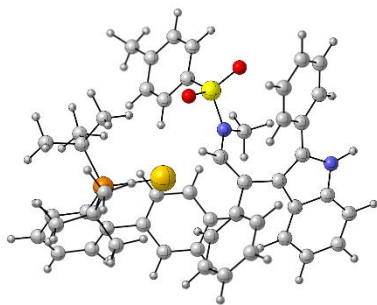


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C	-5.83458100	-3.71255900	-0.24957900
C	-5.77085800	-5.10652400	-0.08780400
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C	0.35413500	-3.32137300	2.60590200
C	2.15973800	-5.08702000	1.43774400
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C	1.67534100	-3.34513100	3.03198300

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C	-2.97085000	0.53542500	0.64937700
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C	-0.60435400	-1.22934000	-0.08113500
N	-0.13972500	-2.13892900	-1.03764600
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H	1.87811200	-1.65177400	-6.16367700
C	2.91652700	0.85398900	-6.27136200
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H	2.85623500	1.93172300	-6.09041700
C	-1.05821600	-2.85665100	-1.92268200
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C	0.06169200	4.39055600	-0.88551700
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H	1.97871800	7.53110100	0.40992000
P	1.29664800	2.69730300	1.10113200
Au	0.27390900	0.69312400	0.27630300
C	3.18210700	2.43346300	1.18028600
C	3.73416400	2.75958500	-0.20932900
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C	3.43739500	0.95051800	1.47775800
H	3.19401100	2.22495900	-1.00232800
H	3.69085700	3.83030800	-0.43626700
H	4.78473800	2.44436100	-0.25816700
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H	3.03185800	0.64213600	2.44817000
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C	0.52547500	2.99926100	2.80948000
C	0.84250000	1.80520200	3.71237000
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H	0.25826600	1.89961900	4.63768500
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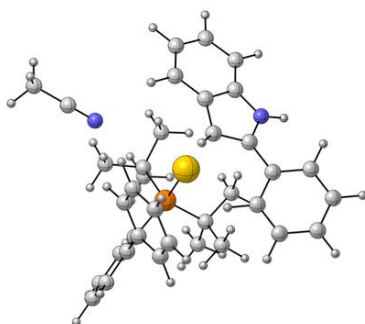
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C	-5.71858600	-2.15832400	-0.65853900
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C	-2.17589200	-2.95843300	0.49025000
C	-1.75746400	-4.27971500	0.35293700
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H	-0.57166000	-6.33958200	-0.90740700
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H	1.87179300	-4.92399400	3.16459900
H	2.68851700	-6.85082300	1.83168800
N	-2.77973200	-4.99905900	-0.21700700
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S	2.15287900	-2.38143200	-0.44270200

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H	-0.93257400	0.11388800	-3.04607200
H	-3.28719300	-0.26117100	-2.29938700
H	-4.41469600	1.45042600	-0.90651900
C	-0.69761100	4.24755800	-0.92443900
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H	3.45590300	1.42135900	1.97254400
H	3.09280500	0.80667800	0.35740200
C	0.86003200	3.61038800	2.68225800
C	1.54071600	2.61527300	3.62300000
C	1.27860800	5.03426200	3.04811100
C	-0.65675400	3.50092300	2.84828400
H	1.28621200	1.57444300	3.38243800
H	2.63239500	2.71551000	3.62144100
H	1.19893500	2.80986900	4.64803900
H	0.71721800	5.78621400	2.48412600
H	1.04883300	5.19020400	4.11038100
H	2.34863600	5.22202300	2.91975400
H	-0.92880200	3.83589400	3.85825700
H	-1.19926800	4.13286600	2.13179300
H	-1.00138700	2.46682400	2.73859800

7.3 Coordinates of Optimized Structures in Figure 3

IM3:

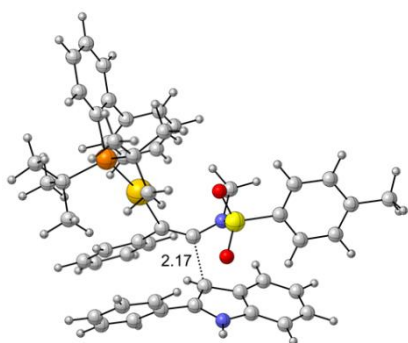


C	-1.22478300	1.07280500	-4.50328400
C	-0.14479000	0.88819400	-3.64604000
C	0.17261500	1.79274700	-2.61484800
C	-0.59732900	2.94743200	-2.45483100
C	-1.66481700	3.15013400	-3.31505400
C	-1.97966000	2.22242200	-4.32080200
H	-1.45968500	0.35899800	-5.28900700
H	-0.37339200	3.64862800	-1.65413600
H	-2.27543300	4.04334100	-3.21069900
H	-2.82607100	2.41203000	-4.97550300
C	1.29700200	1.22559400	-1.87616700
C	1.66056900	0.04092700	-2.57065100
C	2.79379500	-0.84992500	-2.34698800
C	3.39349400	-0.92192600	-1.08206600
C	3.31536500	-1.62297300	-3.39157600
C	4.47944000	-1.75637200	-0.86748300
H	2.98736200	-0.33602700	-0.25710600
C	4.40070000	-2.46127300	-3.17042400
H	2.90309000	-1.53989400	-4.39587800

C	4.98333100	-2.53277000	-1.90902400
H	4.92924500	-1.80784100	0.12147500
H	4.80073400	-3.05143700	-3.99055800
H	5.83187900	-3.19009600	-1.73846500
N	0.78997700	-0.14128300	-3.59648300
H	2.02197900	1.80887000	-1.31128100
H	0.74561200	-0.98344000	-4.15398300
C	2.53405900	0.01398300	2.72702600
C	1.19534900	0.41713800	2.76282300
C	0.84934300	1.65673800	2.20926400
C	1.82149200	2.46960900	1.63038400
C	3.15136900	2.05770300	1.59779700
C	3.50426500	0.82701900	2.14664700
H	2.81275600	-0.94217000	3.16904300
H	-0.18156000	2.00669700	2.25049200
H	1.52455500	3.42891400	1.20975700
H	3.91312200	2.69800300	1.15896400
H	4.54323600	0.50403100	2.13536200
C	0.19075100	-0.39605300	3.49724600
C	-0.95900300	-0.99639700	2.93739600
C	0.41467500	-0.53181400	4.87414200
C	-1.85118400	-1.66096100	3.79386100
C	-0.47402000	-1.20206600	5.70089300
H	1.30402000	-0.06831900	5.29696900
C	-1.62554200	-1.75951100	5.15898000
H	-2.74431600	-2.12575500	3.38573700
H	-0.27280900	-1.27838200	6.76630500
H	-2.34237700	-2.27688000	5.79098400
P	-1.28051300	-1.07796000	1.12937000
C	-0.95882700	-2.88653000	0.66149400
C	0.54160000	-3.11078300	0.87714600
C	-1.71960700	-3.91849000	1.49340800
C	-1.28685000	-3.07814800	-0.81985600
H	1.15558400	-2.46905800	0.23121800
H	0.83599500	-2.93522100	1.91995500
H	0.78113600	-4.15530300	0.63714200
H	-2.80669000	-3.81929800	1.41635600
H	-1.45829900	-4.91894900	1.12395900
H	-1.43739900	-3.88149100	2.55076000
H	-0.96389000	-4.08188900	-1.12670000
H	-2.36187600	-3.00616500	-1.02435200
H	-0.76258800	-2.34895500	-1.45461800
C	-3.06199100	-0.49986800	0.80392200
C	-3.15066500	-0.03591600	-0.65660300
C	-4.14821200	-1.54957300	1.03854400
C	-3.30547500	0.71176400	1.70611000
H	-2.50265100	0.82861400	-0.85408600
H	-2.89443400	-0.82622400	-1.37229700
H	-4.18484100	0.27193000	-0.86216800
H	-4.17992600	-1.92564100	2.06610600

H	-5.12345300	-1.08364700	0.84425400
H	-4.06063400	-2.40299000	0.35657100
H	-4.27509600	1.15384800	1.44022600
H	-3.33855500	0.44432400	2.76777600
H	-2.54253500	1.48845800	1.56116800
N	-1.36397100	3.63625300	0.78376600
C	-1.84591200	4.65555600	1.06169200
C	-2.44866200	5.92837900	1.40976400
H	-2.75395800	5.92763300	2.45992000
H	-1.73405200	6.74158400	1.25467600
H	-3.32994000	6.11338900	0.78923900
Au	0.13923600	0.20679600	-0.24998300

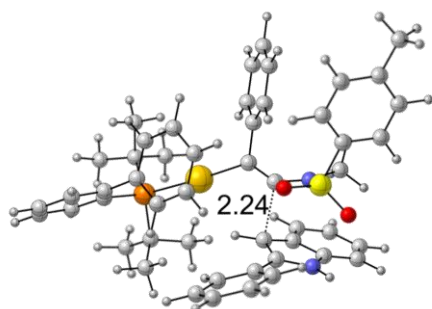
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C	5.80044800	-6.85413800	-5.87254900
C	4.77441100	-5.88855500	-5.84830600
C	4.02946300	-5.66265800	-7.00667000
C	4.30077000	-6.42600400	-8.13473900
C	5.30640800	-7.40364500	-8.12425400
H	6.86523600	-8.38202600	-6.98270900
H	3.24110200	-4.91174100	-7.01825000
H	3.71828200	-6.27349500	-9.03973500
H	5.48432000	-7.99743700	-9.01750800
C	4.77123100	-5.29974800	-4.52799500
C	5.75964300	-5.98579500	-3.79418300
C	6.16474500	-5.81540900	-2.39858100
C	7.50405200	-5.55312300	-2.08283600
C	5.21360500	-5.90205500	-1.37875400
C	7.87880500	-5.37603400	-0.75658200
H	8.23067600	-5.44171300	-2.88593800
C	5.60066000	-5.74925100	-0.05275300
H	4.17045400	-6.09274400	-1.62914500
C	6.93033000	-5.48095400	0.25936600
H	8.91677300	-5.15750100	-0.51429700
H	4.85805000	-5.83047000	0.73750500
H	7.23066000	-5.35538400	1.29722600
N	6.37761200	-6.87023400	-4.60769100
H	3.90003100	-4.85445700	-4.05763400
H	7.19044800	-7.40783700	-4.33868000
C	3.12994700	-2.96911200	-0.33839500

C	4.25146500	-2.86040700	-1.14814200
C	4.12679700	-2.86524300	-2.54425500
C	2.84135900	-2.94525000	-3.10197100
C	1.71775800	-3.04020700	-2.28743800
C	1.85835900	-3.05637200	-0.90354000
H	3.24701500	-2.98314100	0.74306900
H	5.24634400	-2.80139000	-0.70634200
H	2.73166700	-2.90519400	-4.18636100
H	0.72927700	-3.09690700	-2.73673800
H	0.98100500	-3.12984900	-0.26617200
C	5.27610000	-2.68037000	-3.42480400
C	5.69428700	-3.33998000	-4.47332300
N	6.26896600	-3.09107500	-5.66604200
S	7.97423700	-3.38010000	-5.83337200
O	8.66004300	-2.15216600	-5.45151200
O	8.22626100	-4.62010000	-5.11813200
C	8.15447100	-3.58669800	-7.57615500
C	8.87927100	-2.64146600	-8.29803300
C	7.57445700	-4.69117100	-8.19226700
C	9.02371600	-2.82025300	-9.66685600
H	9.31744600	-1.78775000	-7.78805500
C	7.72579800	-4.84525100	-9.56085500
H	7.01625500	-5.41903300	-7.60986400
C	8.45396600	-3.91945900	-10.31681500
H	9.58844400	-2.09255000	-10.24661400
H	7.27030100	-5.70291800	-10.05412600
C	8.63902300	-4.11645900	-11.78872500
H	8.79861500	-3.16597000	-12.30702300
H	9.51567000	-4.74589100	-11.98664400
H	7.77534000	-4.61493800	-12.24015900
C	5.77541300	-1.91247300	-6.39666100
H	6.15311100	-1.93125300	-7.42325100
H	4.68338900	-1.96880800	-6.41955300
H	6.07990100	-0.98561600	-5.88985900
C	5.60135700	1.80803800	-4.52814800
C	5.75128100	1.80070400	-3.13793200
C	4.75630400	1.19974200	-2.35724100
C	3.64571800	0.60866000	-2.95274100
C	3.51033700	0.61739800	-4.33803600
C	4.48928500	1.21889700	-5.12357200
H	6.36248100	2.29161900	-5.13974800
H	4.84508900	1.21547400	-1.27219000
H	2.88434300	0.14186300	-2.33005800
H	2.63592400	0.16554400	-4.80200900
H	4.38123100	1.24428800	-6.20632300
C	6.87401900	2.55341600	-2.51562300
C	7.94217000	1.99854600	-1.77594000
C	6.82313300	3.94381600	-2.68393100
C	8.88420600	2.87310900	-1.20907600
C	7.77119100	4.78792500	-2.12614200

H	5.99696400	4.36028300	-3.25722300
C	8.80542300	4.24857200	-1.37209600
H	9.70855400	2.47297100	-0.62758300
H	7.69620800	5.86234400	-2.27289900
H	9.55361800	4.89145700	-0.91593300
P	8.23690900	0.18663200	-1.62701400
Au	6.66246300	-1.20479800	-2.75134900
C	9.92579900	-0.15064600	-2.42700600
C	9.82458900	0.47378600	-3.82367400
C	11.15155400	0.41111900	-1.71010900
C	10.10920600	-1.66660200	-2.56536900
H	8.95386200	0.10258100	-4.37983500
H	9.77939700	1.56856100	-3.78039100
H	10.71743000	0.19382800	-4.39856000
H	11.28656300	-0.01710500	-0.71018100
H	12.04154700	0.14090700	-2.29432000
H	11.14401600	1.50255800	-1.63512100
H	10.99332400	-1.85037600	-3.19049100
H	10.28409200	-2.15273000	-1.59934200
H	9.25969800	-2.15337500	-3.05764400
C	8.13653400	-0.21766600	0.22298200
C	8.45426100	-1.70117000	0.42116100
C	9.03577000	0.61483500	1.13617500
C	6.68271300	0.04286800	0.62920300
H	7.90469700	-2.34754100	-0.27735600
H	9.52514300	-1.90950100	0.31257900
H	8.17021900	-1.99120500	1.44234800
H	8.75079400	1.67182700	1.14371300
H	8.92108900	0.24369300	2.16358100
H	10.09822900	0.53786900	0.88256500
H	6.56465700	-0.19509400	1.69492700
H	6.40689000	1.09699600	0.49655300
H	5.97391900	-0.57720300	0.06479600

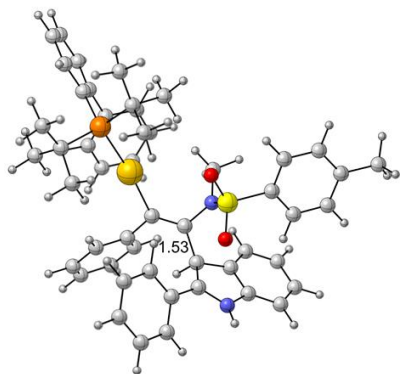
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C	9.18261800	-6.38111400	-6.17555800
C	8.66189400	-5.09257300	-6.10470900
C	8.79890900	-4.27449200	-4.96681100
C	9.49134800	-4.76387200	-3.85504200
C	10.02938300	-6.04151800	-3.91971100
C	9.87383400	-6.84139100	-5.06344100
H	9.06296200	-6.99516000	-7.06500500
H	9.60150600	-4.15278700	-2.96028900
H	10.58461700	-6.43357300	-3.07135200
H	10.30894300	-7.83717400	-5.08066900
C	8.05518700	-3.06513900	-5.24262800
C	7.65830400	-3.12786500	-6.58851100
C	7.05638600	-2.09546200	-7.42054900
C	6.19725000	-2.41251200	-8.48016900
C	7.38030400	-0.75418400	-7.18114400
C	5.66702900	-1.40529000	-9.27394200
H	5.90347800	-3.44642200	-8.65517700
C	6.85548700	0.24931900	-7.98426500
H	8.07003600	-0.50598200	-6.37601500
C	5.99511500	-0.07392300	-9.02999200
H	4.98994900	-1.65964400	-10.08499600
H	7.12543400	1.28671000	-7.80005200
H	5.58293500	0.71141800	-9.65833600
N	7.95770500	-4.36404300	-7.05529600
H	8.10857600	-2.13730100	-4.68630600
H	7.66477200	-4.72244000	-7.95456500
C	4.48038600	-4.24055200	0.11584300
C	5.42517400	-3.76667600	-0.78673900
C	5.09824800	-3.60330300	-2.13972400
C	3.79569300	-3.89725900	-2.55304000
C	2.84678400	-4.35311900	-1.64612200
C	3.18690700	-4.53239300	-0.30882100
H	4.75414300	-4.37452600	1.15969400
H	6.43499900	-3.52825800	-0.45281200
H	3.52689700	-3.72516600	-3.59157200
H	1.83648200	-4.56968600	-1.98845800
H	2.44627700	-4.88995700	0.40195200
C	6.14547800	-3.13313100	-3.08793100
C	6.20814100	-3.80320500	-4.22020100
N	5.83016800	-4.92309900	-4.81190700
S	4.68283500	-4.89386100	-6.15028300

O	4.27941300	-3.50418600	-6.26224800
O	5.34032700	-5.59923900	-7.24279200
C	3.31592700	-5.87705100	-5.61545700
C	2.15111400	-5.24077600	-5.19305500
C	3.38955400	-7.26803800	-5.70540100
C	1.06087900	-6.01549100	-4.82193700
H	2.09339000	-4.15501900	-5.18647200
C	2.29282400	-8.02168700	-5.32025500
H	4.28413600	-7.74836200	-6.09327900
C	1.11610300	-7.41087600	-4.87036000
H	0.14216700	-5.52871900	-4.49970900
H	2.33888200	-9.10744000	-5.38192400
C	-0.06639600	-8.24391500	-4.48825800
H	-0.81163100	-7.66331700	-3.93705100
H	-0.55760200	-8.65078300	-5.38066800
H	0.23076000	-9.09782300	-3.87010900
C	6.23054800	-6.24934300	-4.31571600
H	6.52600200	-6.89241500	-5.15043400
H	7.08980200	-6.11633800	-3.65502300
H	5.40196500	-6.69809600	-3.75425100
C	5.61314200	0.69382600	-4.53941400
C	5.53813800	1.09795800	-3.20253000
C	4.55555900	0.53675600	-2.38022300
C	3.67349200	-0.41501000	-2.88444900
C	3.76450900	-0.81553400	-4.21415500
C	4.73908000	-0.26649500	-5.04094400
H	6.36357400	1.14525600	-5.18938400
H	4.47435700	0.86374200	-1.34435900
H	2.91533400	-0.84560300	-2.23349200
H	3.08074700	-1.56098900	-4.61567800
H	4.81718200	-0.58717300	-6.07874300
C	6.38883600	2.21935900	-2.71341500
C	7.57882800	2.09394700	-1.96588300
C	5.92947900	3.50212400	-3.03969400
C	8.24397700	3.26578400	-1.56767300
C	6.60386900	4.64640900	-2.64173700
H	5.01091800	3.58486800	-3.61776800
C	7.76992000	4.52730800	-1.89525400
H	9.15887700	3.19660300	-0.98723200
H	6.21862300	5.62664100	-2.91074800
H	8.31248100	5.41088900	-1.56946200
P	8.33452100	0.46602400	-1.55732700
Au	7.18402500	-1.42666500	-2.43758200
C	10.08687600	0.48900300	-2.29600400
C	9.94288100	1.05908400	-3.70967200
C	11.13416700	1.28818200	-1.52238200
C	10.58118400	-0.95750700	-2.41233100
H	9.16276900	0.53384200	-4.27996800
H	9.70074000	2.12731700	-3.70733200
H	10.89214500	0.92706400	-4.24563800

H	11.32408800	0.87093200	-0.52679100
H	12.08265100	1.24301500	-2.07440900
H	10.88157800	2.34771000	-1.41831200
H	11.58942600	-0.95112700	-2.84784200
H	10.64313000	-1.46695700	-1.44426800
H	9.93726700	-1.55532100	-3.06892700
C	8.30185200	0.32743900	0.33037400
C	9.04928900	-0.94188000	0.74092100
C	8.87182200	1.52298500	1.09230200
C	6.82320900	0.18515900	0.70604700
H	8.69498500	-1.82647300	0.19429300
H	10.13245400	-0.85265800	0.59400200
H	8.88256300	-1.12160300	1.81139000
H	8.28741400	2.43345200	0.92386400
H	8.82198700	1.30198500	2.16691600
H	9.92042100	1.72827500	0.85335400
H	6.74178100	0.09049600	1.79717500
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H	6.35984400	-0.70192700	0.25380500

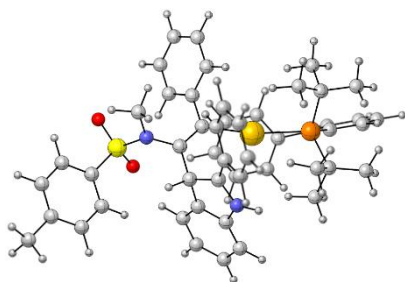
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C	-1.89687700	-5.28257800	-3.70718000
C	-1.70444000	-4.57970100	-2.52973800
C	-2.07342500	-3.24840800	-2.35788700
C	-2.65664300	-2.56308500	-3.41016800
C	-2.86207000	-3.24310900	-4.61026700
C	-2.48851600	-4.58121900	-4.75619400
H	-1.60009800	-6.32255100	-3.81486400
H	-2.93741600	-1.51704800	-3.30211600
H	-3.31798500	-2.72429300	-5.44919100
H	-2.66145200	-5.08628300	-5.70259000
C	-1.70970400	-2.82183200	-0.97020800
C	-1.00688900	-4.04104500	-0.43274800
C	-0.49705700	-4.29073400	0.90106000
C	0.22284000	-3.31766700	1.61230300
C	-0.73168000	-5.54537700	1.49040900
C	0.70094900	-3.60911000	2.88104100
H	0.43985400	-2.35673800	1.15425400
C	-0.25959500	-5.82092000	2.76349300

H	-1.33448900	-6.28926600	0.97169300
C	0.46171800	-4.85310900	3.45832500
H	1.27457900	-2.85884900	3.42000600
H	-0.46125400	-6.78658800	3.21846200
H	0.83699300	-5.07056700	4.45507700
N	-1.10705700	-5.01044800	-1.32422600
H	-2.62704700	-2.77954000	-0.34901800
H	-0.67729100	-5.91993700	-1.19495200
C	-3.49257800	-1.12499100	3.29922000
C	-2.36278600	-0.98488100	2.50380700
C	-2.47062000	-0.86982800	1.10925400
C	-3.75971900	-0.87923200	0.54953100
C	-4.89191900	-1.00873000	1.34804800
C	-4.76364600	-1.13290700	2.72738900
H	-3.38222400	-1.21898800	4.37725200
H	-1.37446900	-0.95625400	2.96276100
H	-3.86326300	-0.74707000	-0.52879700
H	-5.87852500	-1.00212800	0.88993400
H	-5.64624300	-1.22739000	3.35466300
C	-1.29738300	-0.64397600	0.24652700
C	-1.03734400	-1.46199400	-0.79351100
N	-0.15034800	-1.10666500	-1.86692200
S	1.38229000	-1.78931300	-1.88994200
O	2.37437700	-0.90791600	-1.28070000
O	1.19882300	-3.14012500	-1.35018200
C	1.73369100	-1.89246700	-3.62270500
C	2.73751300	-1.10011100	-4.16832100
C	0.99180600	-2.76861100	-4.41209800
C	2.99755100	-1.19169900	-5.53015000
H	3.30092000	-0.42737700	-3.52643300
C	1.26301400	-2.84221900	-5.76872300
H	0.21429800	-3.38451500	-3.96578800
C	2.26967300	-2.05993400	-6.34737800
H	3.78066800	-0.57716100	-5.97052100
H	0.68535400	-3.52015600	-6.39591900
C	2.57569800	-2.17288000	-7.80856600
H	3.01951800	-1.25252800	-8.20053000
H	3.29176400	-2.98339300	-7.99347000
H	1.67705900	-2.39689900	-8.39248700
C	-0.23574800	0.24155600	-2.42649700
H	0.18168500	0.24121200	-3.44039500
H	-1.29414400	0.51523000	-2.47574300
H	0.27923300	0.99695200	-1.81756500
C	-1.33826000	3.87027800	-0.70643900
C	-1.15807500	3.84117700	0.67871400
C	-2.09116900	3.15794900	1.46797400
C	-3.17591400	2.51237600	0.88383400
C	-3.34271800	2.54351700	-0.49807800
C	-2.42179600	3.22038000	-1.29167800
H	-0.62825500	4.42149800	-1.32235200

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H	-3.89055900	1.98100600	1.50998600
H	-4.19859500	2.04827800	-0.95214600
H	-2.55578700	3.26186200	-2.37080700
C	-0.08817300	4.66144400	1.30889100
C	1.06909600	4.16899000	1.95052500
C	-0.30434800	6.04563700	1.27141700
C	1.92835300	5.09420800	2.56652100
C	0.56386200	6.94113100	1.87650900
H	-1.19699000	6.41066100	0.76671800
C	1.68383600	6.45951500	2.54229700
H	2.82538900	4.74564700	3.06738400
H	0.36093300	8.00830500	1.83606900
H	2.37261900	7.14115100	3.03456500
P	1.53758300	2.38425600	1.94179400
Au	-0.02388700	0.88533300	0.90822700
C	3.17745500	2.29481300	0.99381200
C	2.79802000	2.52997000	-0.47270700
C	4.24479800	3.31666300	1.38154300
C	3.75388700	0.88556200	1.13891100
H	2.18968100	1.70698200	-0.86600800
H	2.25892800	3.47705000	-0.61307100
H	3.71730000	2.57882700	-1.07240200
H	4.52909500	3.26743200	2.43855100
H	5.14865200	3.10243400	0.79535900
H	3.94211800	4.34214000	1.14607300
H	4.55573400	0.75703100	0.39919600
H	4.19709000	0.72432700	2.12931400
H	3.01091300	0.10391100	0.93767700
C	1.68402000	1.85626500	3.76360900
C	1.75377600	0.32639400	3.83363500
C	2.87561200	2.42436800	4.53203200
C	0.38291900	2.30275600	4.43623200
H	0.90061400	-0.14136000	3.32511300
H	2.67190100	-0.07630700	3.39371100
H	1.72963700	0.02337600	4.88971900
H	2.84899300	3.51528900	4.61359500
H	2.84944200	2.03149800	5.55764900
H	3.83594200	2.12343400	4.09788400
H	0.38057600	1.95166200	5.47693600
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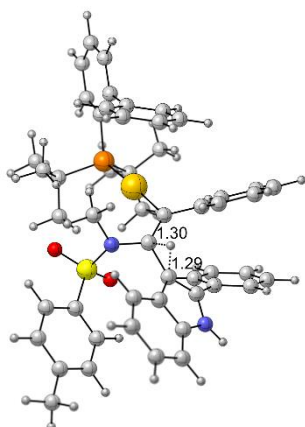
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C	2.28416200	-0.34167100	-2.92348400
C	3.59130200	-0.83106000	-2.87819500
C	3.92809100	-1.95984600	-2.12924200
H	3.19957400	-3.52776400	-0.81499200
H	2.03901600	0.56115300	-3.47754900
H	4.36853300	-0.31119400	-3.43272400
H	4.95645300	-2.30994300	-2.11206100
C	-0.19171100	-0.82584800	-2.08286500
C	-0.56365800	-1.90778300	-1.09565000
C	-1.87108400	-2.31978900	-0.61355800
C	-2.12203800	-3.68912600	-0.40847500
C	-2.88588000	-1.39131600	-0.33041100
C	-3.34679600	-4.11442500	0.08072400
H	-1.37350800	-4.43207100	-0.68001200
C	-4.10911800	-1.82568400	0.15850300
H	-2.68456000	-0.33130300	-0.44816300
C	-4.34115500	-3.18221600	0.37016800
H	-3.53363200	-5.17545200	0.22079000
H	-4.88274000	-1.09736500	0.38668900
H	-5.30162900	-3.51622200	0.75400600
N	0.50717800	-2.64306000	-0.85341800
H	-0.66351300	-1.17221700	-3.02548200
H	0.51181400	-3.41649800	-0.19479200
C	-1.27798800	4.87432200	-0.90893500
C	-0.75369700	3.60795700	-1.14213800
C	-1.16199400	2.51180500	-0.37142700
C	-2.09265100	2.73331400	0.65596700
C	-2.62359600	3.99761500	0.88147700
C	-2.21639200	5.07474600	0.09865800
H	-0.95348800	5.70771700	-1.52747200
H	-0.00340500	3.46633400	-1.91677100
H	-2.40709100	1.89403700	1.27831000
H	-3.35421100	4.14359400	1.67401800
H	-2.62690300	6.06566500	0.27585800
C	-0.62693400	1.15555200	-0.60433300
C	-0.73571800	0.57631300	-1.81960500
N	-1.48366700	1.14402100	-2.90560600
S	-0.77706700	2.03873500	-4.13604400

O	-1.52308200	3.27349700	-4.31537200
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C	-1.03807500	1.04604400	-5.58601100
C	-2.03688500	1.39964700	-6.48633500
C	-0.25149500	-0.08571300	-5.79375500
C	-2.25449200	0.59891500	-7.60130900
H	-2.61965100	2.30155400	-6.31571000
C	-0.48214500	-0.87177200	-6.91251400
H	0.55135800	-0.33318700	-5.09987900
C	-1.48466200	-0.54263700	-7.83216000
H	-3.03284900	0.86924900	-8.31280600
H	0.13248100	-1.75310400	-7.08963100
C	-1.69995500	-1.37793900	-9.05629800
H	-1.46159200	-2.43088700	-8.87383200
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C	-2.93657900	1.21284700	-2.80114900
H	-3.36409800	1.56408000	-3.74437000
H	-3.34072300	0.21158000	-2.60315100
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C	3.27001300	0.97501900	1.29268900
C	2.62334000	1.71634200	2.28682400
C	2.03056900	2.93584400	1.94483500
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C	3.30057000	1.43336900	-0.02012800
H	3.76482000	0.04061100	1.55648900
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H	1.58158900	4.33413000	0.37624500
H	2.70145600	2.98681200	-1.38800900
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C	2.68113000	1.28402000	3.70816500
C	1.94305200	0.21959200	4.26851200
C	3.57022200	1.99431600	4.52485300
C	2.16624200	-0.10971200	5.61628900
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H	4.12712300	2.81728900	4.08082800
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H	1.62231800	-0.93190000	6.07006800
H	4.46355100	2.23307800	6.46345200
H	3.21154400	0.30969800	7.44324000
P	0.60290100	-0.63642800	3.34005600
Au	0.11190700	0.24808700	1.13285100
C	1.10436800	-2.46295000	3.26051000
C	2.29673900	-2.50695100	2.30020500
C	1.53583400	-3.11392300	4.57344400
C	-0.05976700	-3.25970800	2.66908100
H	2.07103100	-2.04319100	1.33055600
H	3.16717500	-1.98656500	2.71925900
H	2.59140900	-3.55424400	2.13524400

H	0.75699200	-3.08743500	5.34258400
H	1.76468100	-4.17117200	4.37991400
H	2.44422100	-2.65698400	4.97845700
H	0.29743500	-4.25743400	2.36994400
H	-0.86300000	-3.42007300	3.39800300
H	-0.50375300	-2.76415100	1.79490400
C	-0.98747500	-0.33767900	4.34592700
C	-2.19794200	-0.70852500	3.48053500
C	-1.11221000	-1.08379400	5.67270100
C	-1.02177500	1.17309700	4.60309600
H	-2.20409600	-0.16725900	2.52621100
H	-2.25176500	-1.78065600	3.25850500
H	-3.11241200	-0.44154000	4.02749800
H	-0.32135300	-0.83147900	6.38482700
H	-2.06216300	-0.79638100	6.14347500
H	-1.13919800	-2.17195100	5.54101700
H	-1.99255600	1.43641100	5.04379500
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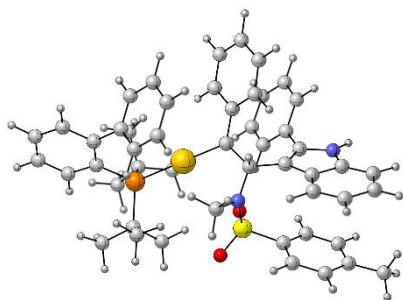
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C	-1.60104500	-3.21745500	-5.23438400
C	-1.75656200	-4.60470000	-5.08680700
H	-1.85731400	-6.27148100	-3.71147900
H	-1.27085200	-1.31971100	-4.26964600
H	-1.62982200	-2.78321100	-6.23088600
H	-1.91182600	-5.22234000	-5.96766900
C	-1.15529200	-2.45962500	-1.51765200
C	-1.20141600	-3.56131700	-0.64496600
C	-0.97882900	-3.68255100	0.79429400
C	0.17361100	-3.13843200	1.37475800
C	-1.88442700	-4.40405700	1.57874900
C	0.41339800	-3.33474300	2.72883900
H	0.88191500	-2.58585300	0.75739500
C	-1.64250200	-4.58094300	2.93611000

H	-2.79370000	-4.79958500	1.12739500
C	-0.49112900	-4.05130400	3.51037800
H	1.32162400	-2.93514800	3.17487000
H	-2.35250900	-5.13532300	3.54440500
H	-0.29484700	-4.20135400	4.56918000
N	-1.44753200	-4.66931300	-1.39213800
H	-1.97235200	-1.45991400	-1.49058100
H	-1.44211500	-5.60289500	-1.00272700
C	-3.34243600	-1.31212500	2.98460600
C	-2.23539300	-0.93107600	2.24163800
C	-2.31305100	-0.80319400	0.84439900
C	-3.56517100	-0.99578800	0.23442800
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H	-3.25078500	-1.43202200	4.06154600
H	-1.28032700	-0.75234400	2.73428200
H	-3.68665300	-0.79715100	-0.83240700
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H	-5.44231800	-1.80147400	2.94637400
C	-1.14010500	-0.39777800	0.07166000
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H	2.73488300	-5.03042400	-6.97026600
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C	-0.21559900	4.67042200	2.02625200
C	1.04632800	4.18237200	2.42620200
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C	1.87336300	5.02459300	3.18771500
C	0.25351500	6.79157700	3.13118400
H	-1.55304400	6.34207500	2.05899700
C	1.48849700	6.30819600	3.54531000
H	2.85240300	4.67724200	3.50248100
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P	1.67619800	2.51902300	1.94563100
Au	0.09028300	1.09286300	0.85854700
C	3.13222500	2.84256800	0.78157300
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H	3.30592600	3.62535900	-1.21614400
H	4.62213700	3.57957400	2.22892200
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H	3.72774800	4.86363800	1.37983200
H	4.53099600	1.66698900	-0.34883300
H	4.42016200	1.16105600	1.34189400
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C	2.16924900	1.62276500	3.54921700
C	2.27466900	0.12134500	3.25088400
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H	1.32150700	-0.29213000	2.89654600
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H	2.54556200	-0.39998000	4.17986800
H	3.47907100	3.12292300	4.49253200
H	3.63897200	1.48320100	5.10587400
H	4.34578400	1.89148700	3.54230100
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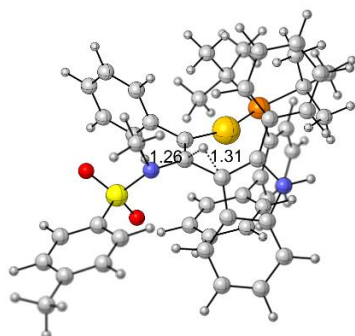
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C	-1.64157300	-2.20584700	-4.31877500
C	-1.95100800	-3.00667300	-5.40491700
C	-2.02094000	-4.40460400	-5.27931400
H	-1.85451000	-6.11170000	-3.96348600
H	-1.56352300	-1.12500800	-4.43418100
H	-2.13759300	-2.55079700	-6.37409200
H	-2.26624200	-5.00657000	-6.15108500
C	-1.08007600	-2.30860400	-1.77164600
C	-1.00201200	-3.39495300	-0.92130000
C	-0.82521600	-3.52180900	0.53254200
C	0.27730500	-2.98282100	1.20381300
C	-1.80267600	-4.20981100	1.26456000
C	0.39140500	-3.13419000	2.58370200
H	1.04804600	-2.46108900	0.64096000
C	-1.68865400	-4.34523100	2.64216400
H	-2.67178000	-4.61355600	0.74614700
C	-0.58766000	-3.80794600	3.30602800
H	1.26554300	-2.73557000	3.09451200
H	-2.45815400	-4.87436000	3.19931500
H	-0.48920900	-3.92650800	4.38237100
N	-1.26282300	-4.53547500	-1.65366900
H	-1.91215300	-0.40387000	-1.98064700
H	-1.19254100	-5.46763300	-1.27300000
C	-3.62680000	-1.02043900	2.70301800
C	-2.48887400	-0.64983300	2.00620800
C	-2.40460200	-0.80433200	0.60242000
C	-3.54066100	-1.31309500	-0.07920400
C	-4.69338000	-1.62751500	0.61185200
C	-4.73346300	-1.49426400	2.00402100
H	-3.66172400	-0.92198600	3.78440800
H	-1.62028900	-0.25756200	2.53407300
H	-3.52070700	-1.44346800	-1.15887300
H	-5.56725400	-1.98825700	0.07624900
H	-5.64024300	-1.75997600	2.54266100
C	-1.19413200	-0.41676700	-0.05785600
C	-1.01046600	-0.83217400	-1.48882400
N	0.07537900	-0.14975100	-2.20770500
S	1.67137200	-0.66509300	-2.13536900

O	2.45910300	0.45650900	-2.63112700
O	1.92578800	-1.20052400	-0.79972600
C	1.80077000	-2.00228500	-3.28508900
C	1.70391500	-1.71955100	-4.64508600
C	1.95380500	-3.30431100	-2.82367600
C	1.73194700	-2.76786200	-5.55074300
H	1.60838700	-0.69028800	-4.98628100
C	1.97723500	-4.34079000	-3.74679300
H	2.04361300	-3.49498100	-1.75710500
C	1.84923500	-4.09215400	-5.11562300
H	1.65037500	-2.56287900	-6.61678800
H	2.09079200	-5.36715200	-3.40082500
C	1.79553300	-5.22165800	-6.09556800
H	2.21311300	-4.93734300	-7.06669600
H	2.33674400	-6.10110500	-5.73251100
H	0.75265400	-5.52324500	-6.26405000
C	-0.22943600	1.14887200	-2.79433200
H	0.60492900	1.48169500	-3.41337000
H	-1.12574800	1.06580400	-3.42493400
H	-0.40916000	1.91267600	-2.02246800
C	-1.46479800	3.59953700	0.18780600
C	-1.43853900	3.59793700	1.58708500
C	-2.51282100	3.02519900	2.27677200
C	-3.58321900	2.46242600	1.58803400
C	-3.60361300	2.47592300	0.19616200
C	-2.54194000	3.04447400	-0.50129800
H	-0.65262300	4.07593900	-0.36074900
H	-2.50822200	3.04109400	3.36644000
H	-4.41434800	2.02916200	2.14041600
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H	-2.56269300	3.08345100	-1.58902800
C	-0.39707200	4.34682700	2.34231100
C	0.97009500	4.01095900	2.45279400
C	-0.86040300	5.50672000	2.97933400
C	1.80829500	4.87636100	3.17591300
C	-0.01598000	6.34178300	3.69421100
H	-1.91581400	5.75588300	2.88632600
C	1.33386500	6.02797100	3.78607800
H	2.86313100	4.64344000	3.27623500
H	-0.41012700	7.23564700	4.17071600
H	2.01728400	6.67027600	4.33513200
P	1.68596500	2.42145100	1.85290300
Au	0.12228400	0.92392500	0.80450600
C	3.07332300	2.84622400	0.63738000
C	2.36780300	3.33477100	-0.63100200
C	4.04507300	3.93477800	1.09023800
C	3.85412100	1.56954500	0.32186900
H	1.74708400	2.55151300	-1.08215800
H	1.75268800	4.22444700	-0.43792900
H	3.12706800	3.61055700	-1.37467600

H	4.55916400	3.69348800	2.02709600
H	4.81826000	4.03916200	0.31757500
H	3.55828200	4.91027900	1.19312000
H	4.50416700	1.76180400	-0.54177900
H	4.49966700	1.26832100	1.15590500
H	3.20623900	0.72816600	0.04939600
C	2.28814100	1.52084200	3.41646800
C	2.46900000	0.03701200	3.07550100
C	3.58979100	2.04195000	4.02205000
C	1.15850100	1.64289900	4.44331500
H	1.52825200	-0.41788300	2.73779600
H	3.22131000	-0.13866000	2.29950000
H	2.79412000	-0.49255500	3.98211900
H	3.52400000	3.08500700	4.34676300
H	3.82008400	1.44724800	4.91633000
H	4.44008700	1.93584900	3.33888500
H	1.38916000	0.99844700	5.30208300
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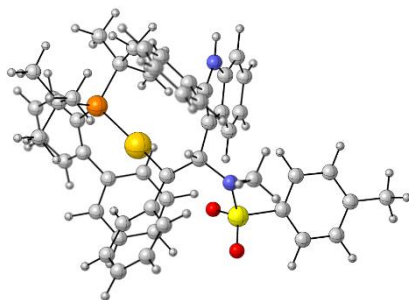
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C	2.00702400	-2.30108600	-3.24157900
C	3.15191200	-2.71911000	-3.90154400
C	3.71900300	-3.97946800	-3.66039500
H	3.61990700	-5.80589600	-2.50474500
H	1.61632800	-1.30079000	-3.39583700
H	3.62830000	-2.04905600	-4.61232300
H	4.61752100	-4.27421000	-4.19570800
C	0.29341700	-3.06739200	-1.40202300
C	0.27022200	-4.26065900	-0.63980000
C	-0.67823500	-4.83045900	0.32568400
C	-0.21219800	-5.76465400	1.26108200
C	-2.05267400	-4.55708100	0.28899400
C	-1.08931600	-6.40875500	2.12414000
H	0.85462600	-5.97106000	1.33765700
C	-2.92576600	-5.19144800	1.16076900
H	-2.46343700	-3.86006000	-0.43999600
C	-2.44929600	-6.12471500	2.07830800

H	-0.70380000	-7.13063700	2.84042900
H	-3.98873500	-4.97162600	1.10797700
H	-3.13747100	-6.62895400	2.75157800
N	1.31435500	-5.02926000	-1.05146600
H	-1.01787800	-3.00421300	-1.45268800
H	1.42738500	-5.99627400	-0.78047300
C	-2.08044300	2.17805500	0.83339700
C	-1.20695100	1.12691000	0.59655600
C	-1.70265200	-0.13289900	0.23213400
C	-3.08873700	-0.32757700	0.17038700
C	-3.95795500	0.72336200	0.44170200
C	-3.45749000	1.98078600	0.76041200
H	-1.68405300	3.15972400	1.08109500
H	-0.12888000	1.27399600	0.65612500
H	-3.48447000	-1.31904900	-0.04904100
H	-5.03177100	0.55727300	0.40062700
H	-4.13831400	2.80454500	0.95805000
C	-0.78436900	-1.26782900	0.05072900
C	-0.63227800	-1.83049300	-1.20551500
N	-1.12131200	-1.26466000	-2.44835600
S	-0.66795000	0.31738000	-2.86900300
O	-1.73400800	1.25887100	-2.56604300
O	0.65814100	0.50422300	-2.28979100
C	-0.57465000	0.21758000	-4.64595000
C	-0.80776300	1.40765200	-5.33475700
C	-0.24373400	-0.94924100	-5.33058400
C	-0.68310400	1.42550900	-6.71569300
H	-1.09737300	2.30191800	-4.78916600
C	-0.13602100	-0.91307000	-6.71473000
H	-0.09476900	-1.88189000	-4.79200700
C	-0.34193900	0.27112400	-7.42671500
H	-0.86462800	2.35169700	-7.25821000
H	0.10781800	-1.82537600	-7.25632600
C	-0.19430200	0.31174500	-8.91587600
H	-0.25826600	-0.68752400	-9.35709900
H	-0.96333400	0.94012300	-9.37729000
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H	-2.63200600	-1.29894900	-3.91510100
H	-2.54698500	-2.73453200	-2.89602100
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C	3.28447200	-1.76119100	1.58273600
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C	3.25465600	-1.71285700	0.19088800
H	3.52598300	-2.69150100	2.09635000
H	2.59588800	1.49514300	2.25545100
H	2.49073300	1.56546300	-0.23421900

H	2.93557400	-0.47652500	-1.54525700
H	3.46610300	-2.61012600	-0.39118500
C	3.20465500	-0.60035600	3.81250100
C	2.27343800	-1.10307400	4.74421000
C	4.39154500	-0.02457300	4.28402600
C	2.58571900	-1.01564600	6.11143600
C	4.68104100	0.05158100	5.63775700
H	5.09804900	0.36398100	3.55290000
C	3.77153200	-0.45248600	6.55947900
H	1.88495800	-1.38764100	6.85155800
H	5.61224700	0.50261100	5.97099500
H	3.97755100	-0.40282500	7.62549900
P	0.62022000	-1.74072800	4.24507100
Au	0.08967100	-1.69970600	1.89335600
C	0.51261800	-3.51169400	4.90276100
C	1.49761100	-4.30895000	4.04255200
C	0.88307500	-3.73116100	6.36911100
C	-0.90967900	-4.02033400	4.66813200
H	1.26535900	-4.22560200	2.97261200
H	2.53092900	-3.97365200	4.20064000
H	1.44611200	-5.37055400	4.32431900
H	0.27047800	-3.14530200	7.06240200
H	0.71831200	-4.79051600	6.60887600
H	1.93882400	-3.51924900	6.56486100
H	-0.93958100	-5.10081000	4.86677400
H	-1.62928600	-3.54872800	5.34814400
H	-1.24855400	-3.86223000	3.63517400
C	-0.63910300	-0.54628200	5.03117200
C	-2.00403800	-0.73119500	4.35667200
C	-0.82663300	-0.68798500	6.54020900
C	-0.13435600	0.86297600	4.70568500
H	-1.96858700	-0.52149500	3.27994700
H	-2.41618300	-1.73649800	4.49501300
H	-2.71088300	-0.02150400	4.80741000
H	0.09672800	-0.52768500	7.10532000
H	-1.53865000	0.07834500	6.87501000
H	-1.25016000	-1.66014800	6.81865400
H	-0.90192600	1.58950800	5.00392000
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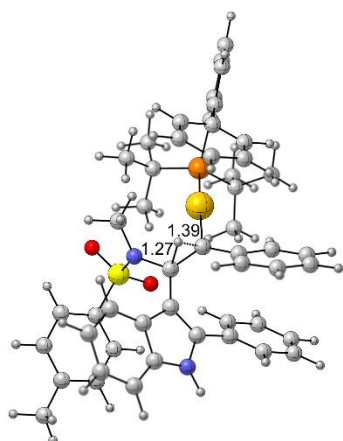
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C	2.81569400	-1.59323800	-2.22308600
C	3.05799500	-2.95082600	-1.95277900
H	2.22764200	-4.82958400	-1.27798000
H	1.37378100	0.00800600	-2.28984800
H	3.63467800	-0.96421500	-2.56505300
H	4.05748000	-3.35494300	-2.09295800
C	-0.90151000	-1.65590800	-1.36345800
C	-1.39963900	-2.85436600	-0.88444100
C	-2.70550400	-3.20300800	-0.31110800
C	-2.75257700	-3.83164800	0.94133600
C	-3.90965600	-2.93278200	-0.97131600
C	-3.96969800	-4.16278800	1.52264400
H	-1.82143100	-4.04151500	1.46752400
C	-5.12705800	-3.26006300	-0.38472700
H	-3.88914000	-2.49978500	-1.96893700
C	-5.16107600	-3.87290300	0.86336100
H	-3.98927000	-4.64669900	2.49610700
H	-6.05335000	-3.05113600	-0.91409300
H	-6.11353400	-4.13247400	1.31798100
N	-0.38087500	-3.78398700	-0.86119800
H	-2.71466300	-0.66529100	-1.08138500
H	-0.51819700	-4.76198000	-0.65220900
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C	-1.77808200	2.86881900	0.55051700
C	-2.18127500	1.84277800	-0.33561200
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C	-4.19636600	3.12254300	-0.80377000
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H	-2.20779200	4.78862800	1.40608300
H	-0.83072700	2.75920500	1.07652900
H	-3.76289300	1.24209100	-1.70425800
H	-5.14531800	3.22576000	-1.32204400
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C	-1.32628500	0.69601900	-0.47775400
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N	-1.92195200	0.06239500	-2.84087500
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C	0.12749500	-0.49274700	-5.04761200
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H	1.16685400	-1.88827000	-6.29978100
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H	2.23965900	-1.24547300	-8.41240700
C	-2.94395900	-0.58205400	-3.64357700
H	-2.96901100	-0.13885400	-4.64312800
H	-2.72249300	-1.65290000	-3.75471100
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C	2.61763000	1.82495200	0.65200700
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C	1.72464200	3.67557200	1.90941100
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C	2.23251600	2.44947200	-0.53208000
H	3.15513300	0.87769600	0.61498100
H	1.53835400	4.15853100	2.86818500
H	0.84942100	5.26699500	0.75710200
H	1.28267000	4.15702100	-1.42795300
H	2.43137800	1.96772200	-1.48651300
C	2.86821400	1.85807300	3.16271400
C	2.50085800	0.61182100	3.71693900
C	3.79273400	2.65528100	3.85289900
C	3.09614000	0.22318400	4.92901200
C	4.36612300	2.25216700	5.04853200
H	4.07323200	3.61041000	3.41325000
C	4.01871400	1.02114000	5.58950100
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H	4.45703400	0.68121000	6.52409800
P	1.17387300	-0.46231200	3.02106100
Au	0.07121500	0.26091200	0.99369500
C	1.96356500	-2.15655300	2.71065300
C	2.92533900	-1.93702100	1.53911600
C	2.75379600	-2.77665200	3.86240100
C	0.86109300	-3.12846700	2.28800700
H	2.41072500	-1.59711300	0.63051500
H	3.71222000	-1.21439200	1.79301200
H	3.41884800	-2.88854500	1.29915000

H	2.16613200	-2.89638100	4.77906700
H	3.07592000	-3.77979200	3.55182300
H	3.66022900	-2.20898600	4.09415000
H	1.32729300	-4.03418200	1.87384400
H	0.24325300	-3.43957600	3.14010000
H	0.20858000	-2.70731900	1.51093600
C	-0.20276600	-0.46168600	4.33824400
C	-1.48125200	-1.05738000	3.73836900
C	0.10937500	-1.20946700	5.63260900
C	-0.46088200	1.01590300	4.65212200
H	-1.80606600	-0.52484900	2.83556000
H	-1.37759500	-2.11816100	3.48557900
H	-2.28484600	-0.97500900	4.48259100
H	0.97407900	-0.80183500	6.16455300
H	-0.75186200	-1.11037800	6.30704500
H	0.26404400	-2.28234300	5.46845700
H	-1.33373000	1.09035300	5.31424100
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H	-0.68441300	1.59371800	3.74375600

TS6:

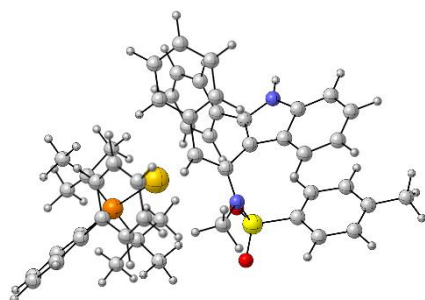


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C	-1.45801100	-2.66031400	-3.11314600
C	-1.57855600	-1.95050900	-4.31357200
C	-1.95239900	-2.63396100	-5.45918300
C	-2.21368100	-4.01304100	-5.43337000
H	-2.32263900	-5.80554100	-4.22777800
H	-1.36118000	-0.88476600	-4.35482800
H	-2.04365900	-2.09441600	-6.39858300
H	-2.50964100	-4.51846500	-6.34928000
C	-1.10904600	-2.30609400	-1.75800700
C	-1.18084700	-3.46887200	-0.99401800
C	-0.90961000	-3.73922200	0.41949100
C	0.23938100	-3.24356700	1.04691700
C	-1.80536300	-4.53060800	1.14901200
C	0.48154400	-3.54185100	2.38294000
H	0.94954500	-2.63861000	0.48506800

C	-1.55970600	-4.81804800	2.48576600
H	-2.71740300	-4.88902700	0.67308900
C	-0.41380300	-4.32660700	3.10469500
H	1.38628400	-3.16882100	2.85824700
H	-2.26568100	-5.42607700	3.04586200
H	-0.21672000	-4.56017700	4.14809200
N	-1.56705800	-4.49164300	-1.81423600
H	-1.70978000	-0.11056600	-1.23511900
H	-1.59107700	-5.45786100	-1.51982500
C	-3.21589100	-1.48176200	2.90661500
C	-2.15781400	-1.00804400	2.14071500
C	-2.25539500	-0.94509100	0.74507700
C	-3.46677100	-1.31748000	0.14122800
C	-4.53714500	-1.74789000	0.91135900
C	-4.41250000	-1.84321700	2.29635900
H	-3.11054100	-1.54721900	3.98663600
H	-1.23179800	-0.69486300	2.62245900
H	-3.58260700	-1.25016500	-0.94101700
H	-5.47582700	-2.00837900	0.42873900
H	-5.25156800	-2.18489500	2.89698300
C	-1.10775500	-0.41531900	-0.01835400
C	-0.76924500	-0.96954600	-1.28792300
N	0.14536400	-0.25018800	-2.14395300
S	1.77541900	-0.72902300	-2.12230800
O	2.51087100	0.42714200	-2.61095800
O	2.05001600	-1.29224100	-0.80488600
C	1.85959200	-2.03041300	-3.31216100
C	1.81785900	-1.69870000	-4.66396800
C	1.86861800	-3.35447800	-2.88685300
C	1.76001300	-2.71886800	-5.60035700
H	1.83655900	-0.65554000	-4.97327300
C	1.80665000	-4.36039700	-3.84091300
H	1.92164400	-3.58557300	-1.82557100
C	1.73187100	-4.06007700	-5.20387700
H	1.72551800	-2.47625500	-6.66096200
H	1.81151900	-5.40252800	-3.52510200
C	1.58548000	-5.14989900	-6.21848100
H	2.03926500	-4.87689000	-7.17636700
H	2.03822200	-6.08629500	-5.87761200
H	0.52132200	-5.34810700	-6.40569100
C	-0.18649000	1.08369600	-2.64305400
H	0.49424700	1.33918100	-3.45766900
H	-1.21045300	1.06178500	-3.03967600
H	-0.12390200	1.86665100	-1.87360000
C	-1.56081400	4.07466000	-0.10380300
C	-1.36485500	3.81238800	1.25508800
C	-2.22827400	2.91980900	1.90221500
C	-3.25663900	2.29495300	1.20273000
C	-3.43653800	2.55538600	-0.15340700
C	-2.58623700	3.44481700	-0.80509000

H	-0.91323100	4.79295200	-0.60565500
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H	-2.73452200	3.66983800	-1.85943700
C	-0.36480000	4.59863300	2.03306800
C	0.92469400	4.16880700	2.41360000
C	-0.79065100	5.87804800	2.41316700
C	1.71651600	5.03999400	3.18007600
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C	1.27103100	6.29696800	3.56150900
H	2.71478300	4.73702900	3.48043000
H	-0.35536500	7.70728100	3.45121400
H	1.91279100	6.94062000	4.15731300
P	1.62782300	2.54060000	1.91805300
Au	0.08390500	1.09749600	0.81753000
C	3.07218200	2.92455300	0.75716900
C	2.43020300	3.43104100	-0.53794000
C	4.04463100	3.99041400	1.25958100
C	3.83432700	1.63117700	0.46588400
H	1.84266100	2.64892500	-1.03380600
H	1.79208500	4.30825300	-0.36557700
H	3.22553900	3.72868100	-1.23402900
H	4.51171900	3.73319100	2.21640900
H	4.85256200	4.08810300	0.52238700
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H	4.52400400	1.81257600	-0.36915800
H	4.43820400	1.30706000	1.32219200
H	3.17630200	0.80720900	0.16269400
C	2.14616700	1.63834000	3.50799200
C	2.32094700	0.14853800	3.18429000
C	3.43118400	2.13819300	4.16625600
C	0.97704100	1.78579900	4.48499300
H	1.39654900	-0.29960200	2.79662000
H	3.11273100	-0.04086300	2.45196700
H	2.58923900	-0.37939200	4.10989400
H	3.37292600	3.18271700	4.48766000
H	3.61355100	1.54109300	5.06989500
H	4.30689300	2.01548400	3.51914600
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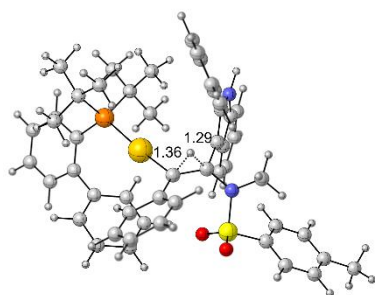


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H	-1.61748300	-1.39846700	-4.13478500
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H	-2.47441100	-5.48801200	-5.16752700
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C	1.41565400	-2.80399100	1.11851500
C	-0.71104800	-3.59471800	1.96154000
C	1.96830400	-2.96745800	2.38407300
H	2.02039500	-2.45486400	0.28327500
C	-0.15732800	-3.73216900	3.22950300
H	-1.75880400	-3.83676100	1.78312900
C	1.18691500	-3.43439100	3.43756200
H	3.02114900	-2.74163000	2.54410400
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H	1.62666300	-3.56650200	4.42373200
N	-0.81901000	-4.38305100	-0.98631600
H	-1.98668200	0.88269200	-0.69561400
H	-0.66943400	-5.25410500	-0.49730200
C	-3.81864400	-1.58860200	2.34813400
C	-2.82326900	-0.86891200	1.69293700
C	-2.68558200	-0.92751100	0.30304000
C	-3.58591200	-1.72350700	-0.41653400
C	-4.57264700	-2.45300400	0.23520200
C	-4.69312200	-2.38844800	1.62139500
H	-3.90328400	-1.52838500	3.43077800
H	-2.13011100	-0.25792000	2.27493100
H	-3.50601500	-1.77670000	-1.50181200
H	-5.25737600	-3.06756500	-0.34431200
H	-5.46968000	-2.95416700	2.13024200
C	-1.65005500	-0.12837000	-0.42626900
C	-0.76954100	-0.74624400	-1.33359300
N	-0.13664500	-0.03065300	-2.32793800

S	1.55303200	-0.37783600	-2.68548700
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O	2.12653500	-0.94500700	-1.47589900
C	1.53467200	-1.58268800	-3.96739700
C	1.27850800	-1.15652600	-5.26820000
C	1.74166300	-2.92496600	-3.66167700
C	1.20837000	-2.10565200	-6.27700800
H	1.15346900	-0.09803500	-5.48549400
C	1.67018700	-3.85498200	-4.68625700
H	1.94781500	-3.22624900	-2.63694500
C	1.38577500	-3.46447700	-5.99921500
H	1.01205200	-1.79091700	-7.30004500
H	1.82349300	-4.91020600	-4.46676700
C	1.24509200	-4.49340800	-7.07578000
H	1.33371600	-4.05489000	-8.07405400
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C	-0.58154800	1.31733500	-2.67262600
H	-0.10553200	1.62496700	-3.60408100
H	-1.66700400	1.29266800	-2.81362200
H	-0.33264500	2.05448900	-1.89461600
C	-1.39920200	4.13655100	-0.30946600
C	-1.17910500	3.87426600	1.04612200
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C	-3.28740500	2.67476100	1.12032600
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C	-2.54493200	3.66597600	-0.94538900
H	-0.66889200	4.72957100	-0.85969700
H	-1.99946600	2.97096500	2.82072800
H	-4.02790100	2.11417600	1.68618300
H	-4.39570400	2.58084600	-0.72425700
H	-2.70732000	3.88999800	-1.99792300
C	-0.04720400	4.53353100	1.75038100
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C	1.96683100	4.68515500	3.07741000
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H	2.57680900	6.63975400	3.71968500
P	1.40455900	2.08794700	2.24890600
Au	-0.11315100	0.83617000	0.90913600
C	3.07648200	1.94774700	1.36114200
C	2.79920300	2.39934300	-0.07725900
C	4.21983500	2.79713000	1.91536400
C	3.49993600	0.47778600	1.35728900
H	2.10433000	1.72676300	-0.59293800
H	2.39872200	3.42141400	-0.12091700

H	3.73895000	2.38414200	-0.64499300
H	4.43525300	2.60305100	2.97169700
H	5.12757700	2.54739800	1.35038300
H	4.04361600	3.86877800	1.78047200
H	4.32872400	0.35487400	0.64741000
H	3.85904200	0.15254700	2.34192100
H	2.69424500	-0.19120300	1.02844200
C	1.37425900	1.41731100	4.02461300
C	1.30787700	-0.10792700	3.96495300
C	2.56624600	1.81781300	4.89238700
C	0.08178500	1.93061900	4.66248900
H	0.45067900	-0.46988800	3.38042600
H	2.21101300	-0.55140000	3.53467000
H	1.20295600	-0.49894200	4.98658100
H	2.63603600	2.89813800	5.05253600
H	2.44159100	1.35944000	5.88254400
H	3.51794800	1.45389300	4.48895200
H	-0.00099300	1.51273800	5.67441900
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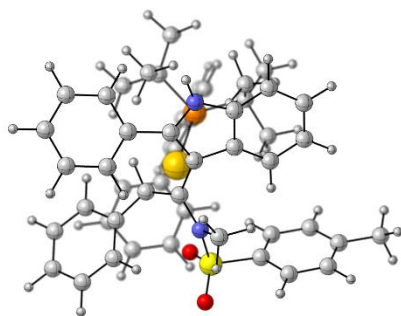


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H	2.28335800	-4.75352700	-1.25731300
H	1.52293700	0.08824700	-2.35441800
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C	-0.75608400	-1.50528800	-1.40988600
C	-1.29941500	-2.65957400	-0.87401900
C	-2.59820400	-2.90826700	-0.24362600
C	-2.67135600	-3.74066500	0.88342400
C	-3.77888500	-2.30623700	-0.70088100
C	-3.87986100	-3.95446300	1.53313200
H	-1.76549400	-4.20235200	1.27372700
C	-4.98485100	-2.51299500	-0.04180600
H	-3.76900300	-1.70354900	-1.60604800
C	-5.04053000	-3.33613500	1.07787800

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H	-5.98520300	-3.50122600	1.58883900
N	-0.31400300	-3.62650700	-0.85339100
H	-2.30139400	-0.23203600	-0.67375000
H	-0.48361600	-4.59614600	-0.63007700
C	-2.49306600	4.24770500	0.31060700
C	-1.75539300	3.07363800	0.25152200
C	-2.20293200	1.98363300	-0.50466600
C	-3.44965700	2.07645600	-1.14147800
C	-4.20592700	3.23365200	-1.04603100
C	-3.72258500	4.32919600	-0.33463400
H	-2.11619100	5.09135300	0.88411300
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H	-5.17349400	3.28577100	-1.53780200
H	-4.31340100	5.23949800	-0.27211000
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C	-1.39187400	-0.17446300	-1.58771300
N	-1.75828100	0.15310200	-2.90474600
S	-1.21742400	1.62172000	-3.62302500
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H	1.63966900	-1.02108600	-6.60163600
C	0.87644000	-0.09291700	-9.03481400
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H	0.14822700	0.08296100	-9.83230200
H	1.77179200	0.49384000	-9.27532400
C	-2.62163700	-0.71367100	-3.69685600
H	-2.42714300	-0.56592600	-4.76264200
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C	2.43487600	1.85250200	0.72504200
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H	1.52917900	4.29726600	2.89650100
H	0.93981000	5.42296800	0.76838800

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C	2.30387300	0.70690500	3.82426300
C	3.66860700	2.70344600	3.90221300
C	2.89670600	0.32683600	5.04082200
C	4.23661300	2.31070600	5.10335600
H	3.98214600	3.63583800	3.43713300
C	3.85086000	1.10627000	5.67699900
H	2.60293300	-0.60299900	5.51520900
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H	4.28425700	0.77279700	6.61617900
P	0.94609800	-0.35801400	3.17746500
Au	-0.19222500	0.30232600	1.17279900
C	1.72347900	-2.05837900	2.85508200
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C	2.53718300	-2.66983700	3.99473200
C	0.61170800	-3.02993500	2.46041100
H	2.11650700	-1.52944700	0.75829700
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H	1.96574200	-2.78587500	4.92211800
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H	1.06922100	-3.94336000	2.05179500
H	-0.00262300	-3.32715100	3.31978800
H	-0.04480500	-2.61094600	1.68570300
C	-0.39961600	-0.34395500	4.52442900
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H	-2.03938400	-0.35325100	3.06065800
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H	-2.48213500	-0.84506600	4.70470900
H	0.79510500	-0.72020700	6.33358800
H	-0.93303500	-1.00039800	6.49427500
H	0.05205400	-2.18205700	5.63271900
H	-1.49804200	1.22610100	5.50943400
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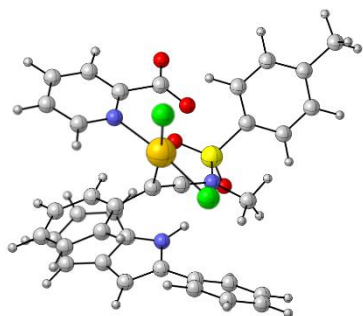
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C	0.55141900	-2.68435100	-2.44314500
C	1.43213600	-3.72954100	-2.67180900
C	1.22214100	-4.99619300	-2.10326000
H	-0.02778900	-6.21529800	-0.82877400
H	0.73722500	-1.70744000	-2.88430700
H	2.29974600	-3.56434100	-3.30761000
H	1.92517600	-5.79934600	-2.30825700
C	-1.64307400	-2.07493700	-1.14457800
C	-2.43474700	-2.87097800	-0.32068300
C	-3.68417400	-2.58533800	0.38517500
C	-3.90802000	-3.11926200	1.66038400
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C	-5.09201100	-2.85094900	2.33745700
H	-3.13659100	-3.72476300	2.13528400
C	-5.84871900	-1.50922700	0.48387900
H	-4.51798500	-1.37525100	-1.19753100
C	-6.06208000	-2.04340100	1.75289500
H	-5.25347600	-3.26783400	3.32828400
H	-6.60624800	-0.88265500	0.02045200
H	-6.98595800	-1.83074400	2.28430900
N	-1.87479900	-4.12153500	-0.25789200
H	-2.32612700	-0.40319700	0.58153500
H	-2.34264900	-4.91802200	0.15117200
C	-4.01042100	3.13068900	1.09419200
C	-3.18043900	2.02685500	0.94994500
C	-2.98115300	1.42688200	-0.30073800
C	-3.65979500	1.95651400	-1.40483600
C	-4.48838400	3.06155900	-1.26074300
C	-4.66326800	3.65867900	-0.01482600
H	-4.15067200	3.57647900	2.07662800
H	-2.66972400	1.61348000	1.82203300
H	-3.55704900	1.50253700	-2.38762500
H	-5.00510500	3.45703300	-2.13173600
H	-5.31300000	4.52377200	0.09110000
C	-2.17390600	0.19033300	-0.32773200
C	-1.82661300	-0.64972600	-1.39107700
N	-1.73275200	-0.26796900	-2.73261400
S	-0.99523000	1.17969100	-3.29934700

O	-1.84917900	1.66747000	-4.36618200
O	-0.68250800	1.96613300	-2.12057000
C	0.52833100	0.61739400	-4.00106300
C	0.55195200	0.08805600	-5.29046400
C	1.68358600	0.69159300	-3.22614300
C	1.74785200	-0.41108400	-5.78538100
H	-0.34915200	0.08403400	-5.89879900
C	2.87198300	0.19502100	-3.74513800
H	1.64161800	1.13922300	-2.23373800
C	2.92100400	-0.37028400	-5.02302900
H	1.77999700	-0.83142600	-6.78894600
H	3.78381900	0.25297100	-3.15216400
C	4.20737500	-0.88854600	-5.58609600
H	4.93352600	-1.11290500	-4.79880400
H	4.04904200	-1.79557500	-6.17891700
H	4.66543500	-0.14683600	-6.25204400
C	-2.13448500	-1.19870900	-3.79692200
H	-1.28839400	-1.76963900	-4.19954200
H	-2.86704600	-1.89919500	-3.39188400
H	-2.61133400	-0.62309900	-4.59439400
C	1.54908200	3.21995400	0.33154300
C	1.39282900	3.10542500	1.71642800
C	0.26671700	3.66884300	2.32237100
C	-0.70270200	4.30434400	1.55234000
C	-0.54623000	4.40473400	0.17411100
C	0.59037300	3.87787600	-0.43204600
H	2.44937900	2.82080900	-0.13697800
H	0.16345400	3.61513700	3.40601800
H	-1.58091300	4.73069100	2.03182700
H	-1.30927400	4.89126100	-0.42916000
H	0.72221200	3.96541300	-1.50632200
C	2.47624600	2.54049500	2.56095100
C	2.77821000	1.16995000	2.70694200
C	3.23257200	3.47968600	3.27369600
C	3.83207400	0.80915200	3.56478900
C	4.27435500	3.10334000	4.10732600
H	2.98473400	4.53233800	3.15191800
C	4.57836400	1.75560300	4.25132700
H	4.07527300	-0.23577000	3.71791800
H	4.84347200	3.85864800	4.64315900
H	5.38748800	1.43571700	4.90261200
P	1.71603600	-0.15922100	2.00545200
Au	-0.02718000	0.41432500	0.47877300
C	2.82249500	-1.42397100	1.11769100
C	3.16973400	-0.78557700	-0.22999800
C	4.13026200	-1.80698800	1.81043400
C	2.00814800	-2.69381200	0.87095200
H	2.27779000	-0.65283900	-0.85552800
H	3.66641600	0.18800400	-0.11024200
H	3.85687300	-1.44971200	-0.77355100

H	3.98406600	-2.21951200	2.81493500
H	4.61026800	-2.59125400	1.20992100
H	4.83234800	-0.96921600	1.86633500
H	2.54874800	-3.32849300	0.15533800
H	1.87057700	-3.28003100	1.78725400
H	1.02491300	-2.48433900	0.43004500
C	0.82151500	-0.88314800	3.52591900
C	-0.36518700	-1.74826000	3.08759500
C	1.72314000	-1.70955300	4.44121900
C	0.26864200	0.31534000	4.30324300
H	-1.09857400	-1.17487200	2.50497900
H	-0.07003800	-2.62148500	2.49708000
H	-0.87655500	-2.11394700	3.98852100
H	2.55964100	-1.12881700	4.84276000
H	1.13139500	-2.05000800	5.30146900
H	2.11681800	-2.60520200	3.94646300
H	-0.34906300	-0.05699600	5.13113100
H	1.06171200	0.93905800	4.73159500
H	-0.36883000	0.95178800	3.67352600

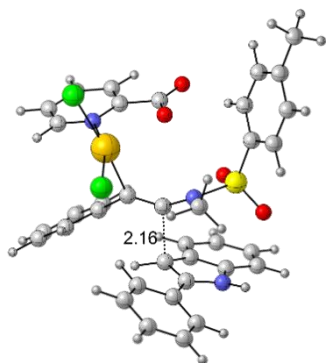
7.4 Coordinates of Optimized Structures in Figure 4

IM3-c:



C	-0.52314000	-4.27691900	-2.74084900
C	-1.07998900	-4.07992000	-1.47706600
C	-2.47993300	-4.05363400	-1.25930900
C	-3.33706200	-4.29017400	-2.34359100
C	-2.79020300	-4.50649500	-3.59639400
C	-1.39679800	-4.48710300	-3.79509800
H	0.55485700	-4.25877900	-2.88726700
H	-4.41648500	-4.28448100	-2.19970000
H	-3.44436500	-4.69048000	-4.44606700
H	-0.99837000	-4.64745600	-4.79427800
C	-2.67745800	-3.74882300	0.12091800
C	-1.43505200	-3.63475900	0.69738700
C	-1.07464900	-3.37962400	2.09011300
C	-0.02008800	-4.07291000	2.69953600
C	-1.79319000	-2.44365200	2.84505700
C	0.29530200	-3.84540000	4.03438700
H	0.53376200	-4.81516500	2.12611500
C	-1.46923900	-2.21171000	4.17691700
H	-2.59716700	-1.88446800	2.36681500
C	-0.42597300	-2.91369700	4.77692600
H	1.10437500	-4.40444800	4.49974700
H	-2.02747500	-1.47101400	4.74462500
H	-0.17672400	-2.73433200	5.81998300
N	-0.46693700	-3.84608500	-0.26934700
H	-3.62210500	-3.66152100	0.64470000
H	0.53518300	-3.77850200	-0.12055000
C	-4.66366600	-0.20525300	-0.45332000
C	-3.47139500	0.09765500	0.19042400
C	-2.25597100	-0.20478800	-0.43584700
C	-2.23858400	-0.78265900	-1.71060800
C	-3.43896000	-1.05078700	-2.35617900
C	-4.64881100	-0.77097700	-1.72771600
H	-5.60994300	0.01510500	0.03486800
H	-3.46410100	0.56915400	1.17269000
H	-1.28279000	-1.00749100	-2.18412900
H	-3.42274800	-1.50850800	-3.34207300
H	-5.58613900	-0.99223300	-2.23304200
C	-0.98621700	0.19358800	0.15586500

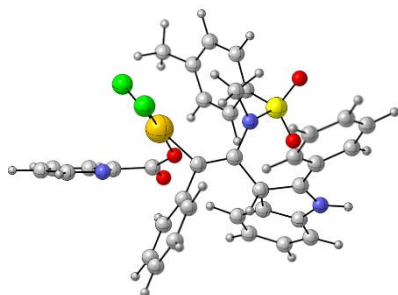
C	0.09693900	-0.42457600	0.43738700
N	1.17689600	-0.94518800	0.84654800
S	2.33692600	-1.63072300	-0.38209500
O	2.41162100	-3.01746800	0.07270000
O	1.74651700	-1.28465000	-1.65339600
C	3.86418200	-0.83843000	-0.06454600
C	4.70390300	-1.39778900	0.90490500
C	4.20930800	0.29979000	-0.79133500
C	5.91428100	-0.77897700	1.16131800
H	4.41837400	-2.30965500	1.42275500
C	5.43500800	0.88954000	-0.51105800
H	3.55411200	0.72842300	-1.55617900
C	6.29193900	0.37648800	0.46432600
H	6.58691600	-1.19913600	1.90681500
H	5.72670400	1.77746800	-1.06855000
C	7.58763200	1.05806400	0.77422700
H	7.44414600	1.82073400	1.55009900
H	8.33792700	0.35243200	1.14549100
H	7.99416200	1.56585700	-0.10603000
Au	-0.74430700	2.24548200	0.52933800
Cl	-0.78718000	1.77904700	2.82576200
Cl	-0.77757500	4.58073800	0.86068500
O	1.56445400	1.79564400	-0.57729600
O	2.36531400	1.85654900	-2.68642400
N	-0.93461500	2.56661100	-1.55419400
C	0.10395300	2.36563800	-2.37430700
C	-0.06913800	2.50598400	-3.74940000
C	-1.31086100	2.85172600	-4.25535300
C	-2.36939900	3.06956200	-3.37656400
C	-2.14328000	2.92130100	-2.02136600
C	1.48908700	1.97010700	-1.81810300
H	0.80507500	2.33116500	-4.36858400
H	-1.45792100	2.95783600	-5.32743000
H	-3.35625300	3.35349700	-3.72778400
H	-2.92377000	3.08533300	-1.28203900
C	1.52520200	-1.08596200	2.27097100
H	2.30917400	-0.35780500	2.50180400
H	0.63211500	-0.86435700	2.86180100
H	1.85727400	-2.10947000	2.46045200

TS4-c:

C	7.08760700	-5.96079300	-8.36733600
C	6.40018500	-5.18587700	-7.44361100
C	5.46940000	-4.19999800	-7.80389100
C	5.16000300	-4.02829400	-9.15396600
C	5.81787000	-4.81233800	-10.08902400
C	6.78205000	-5.75443800	-9.70372600
H	7.83634200	-6.68416700	-8.05530900
H	4.41239900	-3.30211700	-9.46283000
H	5.58862000	-4.69071300	-11.14464600
H	7.29463200	-6.33649800	-10.46506700
C	5.04744200	-3.55151300	-6.57295200
C	5.60800800	-4.30966200	-5.51528500
C	5.39618400	-4.18422600	-4.08449200
C	5.78359800	-5.20675100	-3.20573400
C	4.80219800	-3.02815500	-3.55965500
C	5.59722600	-5.06564600	-1.83857300
H	6.20317400	-6.13316900	-3.59437300
C	4.62409100	-2.88874600	-2.19137400
H	4.52701800	-2.21067200	-4.22264600
C	5.02188000	-3.90483900	-1.32692000
H	5.89716000	-5.86734700	-1.16844100
H	4.18906700	-1.97166800	-1.80212500
H	4.88411200	-3.79301100	-0.25444400
N	6.45547100	-5.21502000	-6.05060300
H	4.10132100	-3.03528100	-6.45822000
H	7.19219000	-5.68185500	-5.53788800
C	1.75884000	-0.30243900	-6.69506100
C	3.04201700	-0.41930800	-6.17156100
C	4.11221400	-0.74255900	-7.01467200
C	3.88582800	-0.90369100	-8.38797600
C	2.60184500	-0.77758100	-8.90336100
C	1.53502300	-0.48184600	-8.05772400
H	0.92995900	-0.06030100	-6.03421600
H	3.23128000	-0.24331500	-5.11300000
H	4.73782000	-1.11011500	-9.03611600
H	2.43543700	-0.90339800	-9.97104000
H	0.53046400	-0.38296700	-8.46177900
C	5.48932000	-0.80589100	-6.52644900
C	6.32101200	-1.81276400	-6.38320300

N	7.55937700	-2.10252200	-6.01500300
S	8.74480700	-2.73082500	-7.17818900
O	9.04965100	-4.05693800	-6.64398100
O	8.13547400	-2.54747300	-8.47743300
C	10.20216000	-1.76122500	-6.98119300
C	11.08037400	-2.07593700	-5.94070400
C	10.49168600	-0.77142200	-7.91422500
C	12.24852800	-1.34362200	-5.81111100
H	10.86107000	-2.89815000	-5.26458500
C	11.67613800	-0.06145100	-7.76586000
H	9.81628600	-0.53974500	-8.73664000
C	12.55594200	-0.31876300	-6.71417200
H	12.94290700	-1.57350700	-5.00460700
H	11.91006000	0.72001900	-8.48680600
C	13.80158300	0.49481500	-6.54518000
H	14.58900600	-0.07017300	-6.03510000
H	14.19088500	0.83713000	-7.50957700
H	13.59860600	1.38940500	-5.94289500
Au	6.10428900	1.12460200	-6.00039200
Cl	5.91026000	0.47914900	-3.73311900
Cl	6.56115100	3.38662000	-5.41985500
O	8.07027800	0.63710500	-7.51580000
O	8.57895300	0.79715800	-9.71205300
N	5.65237000	1.83234700	-8.00032100
C	6.51268000	1.63410000	-8.99910600
C	6.18956700	2.04103000	-10.29174700
C	4.97421600	2.66337100	-10.52479700
C	4.10300800	2.88108400	-9.45926000
C	4.47927300	2.45057300	-8.19976300
C	7.86200000	0.95220700	-8.71459100
H	6.92585300	1.84766000	-11.06563800
H	4.70473900	2.98724200	-11.52747300
H	3.14769000	3.37850000	-9.59489400
H	3.84723500	2.59325400	-7.32560600
C	7.98193300	-2.15952100	-4.61015200
H	8.86281200	-1.51857300	-4.48872500
H	7.18293000	-1.75325700	-3.98785200
H	8.22285500	-3.18721500	-4.31583800

IM4-c:

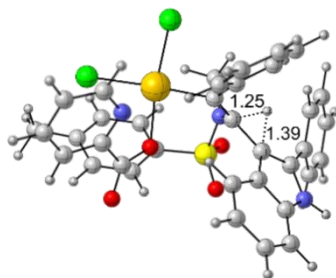


C	-0.18178500	-5.15220900	-2.03081200
C	-0.54404100	-4.38358700	-0.93944500
C	-0.71165400	-3.00208800	-0.98916000

C	-0.45322300	-2.32379100	-2.16582600
C	-0.06088100	-3.07140600	-3.27720200
C	0.05281500	-4.46160600	-3.21805600
H	-0.05421100	-6.22958900	-1.96259200
H	-0.47812200	-1.23758900	-2.20264100
H	0.18409900	-2.54665200	-4.19704900
H	0.35759400	-5.01403700	-4.10286000
C	-1.12154800	-2.52630700	0.38061000
C	-0.92861400	-3.75182900	1.20657900
C	-0.98058000	-3.85317200	2.64379000
C	-0.21779600	-4.82147500	3.31289500
C	-1.74981900	-2.93999400	3.37872700
C	-0.24484400	-4.88681600	4.69673700
H	0.45616800	-5.46750300	2.75252700
C	-1.78373800	-3.02167300	4.76103800
H	-2.32152300	-2.17423500	2.85735500
C	-1.03312000	-3.99416000	5.41906300
H	0.36709300	-5.61899500	5.21579700
H	-2.38640700	-2.31885900	5.32949500
H	-1.04796700	-4.04414300	6.50485200
N	-0.71284100	-4.77679900	0.40635300
H	-2.22305000	-2.38068700	0.34889200
H	-0.57507700	-5.72315200	0.74271800
C	-4.90186800	-0.16178300	0.37522800
C	-3.58091500	-0.19820900	0.80553100
C	-2.52250200	-0.01428800	-0.09977200
C	-2.82850300	0.24545000	-1.44288400
C	-4.14906400	0.27721100	-1.86925100
C	-5.18913000	0.06871500	-0.96641800
H	-5.70823100	-0.29983900	1.09200500
H	-3.34678100	-0.32716900	1.86278700
H	-2.01943500	0.44115700	-2.14137100
H	-4.36856200	0.47341400	-2.91617800
H	-6.22163900	0.10063400	-1.30623100
C	-1.14882600	-0.07029300	0.41076500
C	-0.55150700	-1.19395700	0.85755800
N	0.53440100	-1.23491400	1.76572100
S	1.99050800	-2.03976300	1.44273900
O	2.56121000	-2.35936700	2.74352800
O	1.64169800	-3.11867000	0.51950400
C	3.01356600	-0.86234500	0.63242700
C	3.79602600	-0.00772400	1.41348100
C	2.92013400	-0.70685100	-0.74724700
C	4.47306100	1.02740800	0.79168500
H	3.86761400	-0.16568000	2.48680000
C	3.61506600	0.33282400	-1.34843100
H	2.29101000	-1.36462800	-1.34270900
C	4.37071300	1.22680000	-0.58998400
H	5.07312800	1.71394400	1.38624000
H	3.50549000	0.48290900	-2.42151700

C	4.99897900	2.42194500	-1.23155900
H	5.89542500	2.75135600	-0.69541700
H	5.26500700	2.22994800	-2.27626500
H	4.27758800	3.25069100	-1.21653100
Au	-0.07009900	1.66641100	0.21361700
Cl	-1.07617800	2.57819700	2.11795000
Cl	1.51344900	3.48555700	-0.03178800
O	0.56804100	0.68301600	-1.51485200
O	1.21457400	0.62118300	-3.62098400
N	-0.96393700	2.93832200	-2.14970900
C	0.04708100	2.56771100	-2.93944000
C	0.54407600	3.36547500	-3.96527000
C	-0.00162700	4.63030500	-4.13580300
C	-1.03608500	5.03465100	-3.30007700
C	-1.49192500	4.14595100	-2.33106600
C	0.66550200	1.21631100	-2.70022200
H	1.34769300	2.98476800	-4.58838400
H	0.37728200	5.29569100	-4.90826200
H	-1.48506800	6.01967900	-3.39349500
H	-2.30711800	4.41971600	-1.66135700
C	0.60781300	-0.27610900	2.87190900
H	1.20608300	0.61292300	2.62713800
H	-0.40623400	0.06374000	3.09568900
H	1.03476600	-0.78125000	3.74306400

TS5-c:

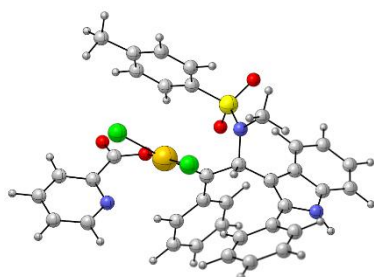


C	-1.21978700	-5.00615900	-2.60053900
C	-1.10253500	-4.32206800	-1.39651700
C	-1.14543700	-2.91798900	-1.31219700
C	-1.25075500	-2.16591700	-2.48345900
C	-1.35503300	-2.83901700	-3.69088400
C	-1.35662400	-4.23985800	-3.74839400
H	-1.18340800	-6.09211300	-2.64203200
H	-1.22206200	-1.07999100	-2.45040000
H	-1.42851700	-2.26880300	-4.61306500
H	-1.44634500	-4.73482700	-4.71200600
C	-0.94617500	-2.59407700	0.08103000
C	-0.79721000	-3.80287900	0.78304300
C	-0.51133300	-4.06386700	2.18819300
C	0.44255300	-5.03168100	2.52451300
C	-1.14011500	-3.34134900	3.20778600

C	0.76303500	-5.26519200	3.85399700
H	0.98384500	-5.54662600	1.73270700
C	-0.81289200	-3.57316900	4.53584100
H	-1.90864600	-2.60724000	2.96393000
C	0.13941200	-4.53533000	4.86057800
H	1.52180000	-6.00190300	4.10396500
H	-1.30729400	-3.00633700	5.32072900
H	0.39910600	-4.71193400	5.90125900
N	-0.88461000	-4.81380900	-0.11788500
H	-1.62675800	-1.81527800	1.00712900
H	-0.84150000	-5.79015400	0.13622600
C	-4.93489000	-0.47428700	0.39279700
C	-3.57724400	-0.52682800	0.67342800
C	-2.63056400	-0.03022400	-0.24305500
C	-3.09524400	0.58439100	-1.42025900
C	-4.45164700	0.62111700	-1.69879900
C	-5.37513500	0.08801400	-0.80064300
H	-5.65102000	-0.84988400	1.11927900
H	-3.24632900	-0.88635000	1.64893200
H	-2.36842700	1.01982800	-2.10682800
H	-4.79549000	1.08180800	-2.62189700
H	-6.43908300	0.13625700	-1.01917700
C	-1.21535200	-0.09064900	0.06609800
C	-0.59593000	-1.21127100	0.62499900
N	0.47542500	-1.12171700	1.52654800
S	2.01173600	-1.86046500	1.28665000
O	2.39487300	-2.33435500	2.60921500
O	1.86393900	-2.77873600	0.16933500
C	3.07947100	-0.53072100	0.84046300
C	3.59715100	0.28864500	1.84557300
C	3.34826700	-0.29371300	-0.50456400
C	4.35767600	1.38893600	1.48271200
H	3.41777900	0.05188600	2.89153600
C	4.11724000	0.81076500	-0.84096200
H	2.94165800	-0.93566500	-1.27983100
C	4.60604700	1.67802000	0.13686800
H	4.75975800	2.04464400	2.25312300
H	4.30314600	1.01874200	-1.89354800
C	5.33697100	2.92257300	-0.25406500
H	5.98830000	3.28440300	0.54843800
H	5.94291300	2.77035600	-1.15362400
H	4.61022200	3.71497400	-0.47754000
Au	-0.05182600	1.55084500	-0.26120100
Cl	-1.20660300	2.69223000	1.41982400
Cl	1.45255200	3.37455400	-0.63866800
O	0.85964600	0.32306800	-1.65994900
O	2.11785500	0.15199700	-3.46807900
N	-0.68580200	2.22001900	-3.03140400
C	0.53737900	1.90797300	-3.46694600
C	1.19182000	2.62443200	-4.46439500

C	0.56732200	3.74796900	-4.98672700
C	-0.69391000	4.09711100	-4.51720800
C	-1.28380400	3.29096300	-3.55014400
C	1.23899000	0.72792900	-2.84665300
H	2.17342800	2.29472600	-4.79022800
H	1.05926300	4.34889800	-5.74796400
H	-1.21429300	4.97406800	-4.89182700
H	-2.27998300	3.51859100	-3.16621000
C	0.37785200	-0.22656800	2.68130400
H	0.91695200	0.71782800	2.52830800
H	-0.67668000	0.02105000	2.83893100
H	0.76712100	-0.74077400	3.56586000

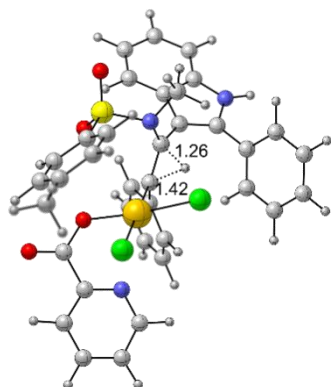
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C	-1.88927500	-6.51998800	0.00156900
C	-1.73579000	-5.21775400	0.47084400
C	-0.88326800	-4.27020600	-0.14447200
C	-0.15400700	-4.67243800	-1.27617900
C	-0.29867000	-5.96822900	-1.74317400
C	-1.15531100	-6.88466200	-1.11451600
H	-2.55752800	-7.22091700	0.49736300
H	0.50117600	-3.98133100	-1.79721200
H	0.26556600	-6.28068400	-2.61829000
H	-1.24464700	-7.89415500	-1.50857100
C	-1.01459200	-3.04273400	0.60555600
C	-1.90699700	-3.29689400	1.63543400
C	-2.36296000	-2.46496800	2.75082900
C	-2.42418300	-3.01211900	4.04082300
C	-2.74463400	-1.13135900	2.56848500
C	-2.84210100	-2.24116000	5.11633900
H	-2.10606600	-4.04142400	4.19998500
C	-3.14994500	-0.35791700	3.64925000
H	-2.74558700	-0.70175100	1.56817900
C	-3.20068700	-0.90921300	4.92435700
H	-2.87377600	-2.67654300	6.11228200
H	-3.42721800	0.68117400	3.49011200
H	-3.51671300	-0.30227100	5.76911700
N	-2.32807900	-4.60489100	1.55128000
H	-0.35855500	-1.30844100	1.55490600
H	-3.06605100	-4.99511300	2.11736100
C	-3.35879800	-1.57828000	-2.58756700
C	-2.23810900	-1.65401300	-1.78589300
C	-1.83336300	-0.53126600	-1.01894400
C	-2.59511000	0.65912000	-1.10042900

C	-3.74634300	0.70317600	-1.86599200
C	-4.12337200	-0.40962400	-2.61441600
H	-3.64303600	-2.43078900	-3.19803300
H	-1.63173800	-2.55264400	-1.78790100
H	-2.27030200	1.54384200	-0.55353200
H	-4.33434500	1.61603600	-1.90404700
H	-5.01351600	-0.36417300	-3.23823900
C	-0.66658400	-0.57020700	-0.20831600
C	-0.20951700	-1.77275900	0.54507100
N	1.22972000	-1.96674300	0.47425200
S	2.01488500	-1.88938600	-1.00808400
O	2.90425600	-3.03963200	-1.09156400
O	0.93578400	-1.69877600	-1.98105800
C	3.00005100	-0.41974900	-0.98877700
C	3.90853600	-0.20930700	0.04903300
C	2.89014400	0.47108200	-2.05174900
C	4.68643500	0.93550500	0.03136700
H	3.99745100	-0.92157000	0.86660100
C	3.68356600	1.61093600	-2.04917600
H	2.16289500	0.30216300	-2.83987900
C	4.57427200	1.86642300	-1.00763300
H	5.38231200	1.12665300	0.84630600
H	3.57185100	2.33264000	-2.85656300
C	5.35057500	3.14441400	-0.96535000
H	6.30838000	3.02270000	-0.44817400
H	5.54465700	3.53378800	-1.97007600
H	4.77662000	3.90633000	-0.42162500
Au	0.35299800	1.18770400	0.21922800
Cl	0.45348500	0.69168200	2.50862600
Cl	1.70955000	3.10732400	0.63162100
O	0.22841000	1.58870000	-1.79047200
O	0.62276500	3.04268900	-3.39718700
N	-1.32987400	3.56738900	-0.50373100
C	-0.51595900	3.89625700	-1.51172700
C	-0.26189700	5.21453000	-1.88042100
C	-0.83705400	6.23337100	-1.13526400
C	-1.66100200	5.89997000	-0.06684100
C	-1.88641700	4.55355300	0.19726100
C	0.17177300	2.80323500	-2.29160900
H	0.38998800	5.40382700	-2.72743300
H	-0.64152600	7.27472700	-1.38004900
H	-2.12504300	6.66400200	0.55061500
H	-2.53934100	4.25485000	1.01772900
C	1.86035200	-2.63026000	1.60731100
H	2.81684300	-3.05500800	1.29493700
H	2.01205600	-1.91797100	2.42875700
H	1.22708700	-3.45864400	1.95076000

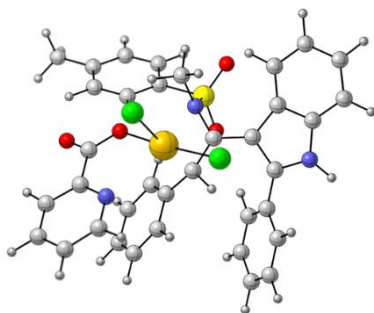
TS6-c:



C	-1.71011100	-6.58684600	-0.25013900
C	-1.53973700	-5.29755800	0.24845400
C	-0.74572800	-4.32709900	-0.40387100
C	-0.08088800	-4.67811600	-1.58812000
C	-0.23918800	-5.96306400	-2.07997300
C	-1.04589500	-6.90565300	-1.42313900
H	-2.33491700	-7.31327400	0.26473700
H	0.54100000	-3.95530200	-2.11174000
H	0.27256000	-6.24786500	-2.99575800
H	-1.15017200	-7.90409500	-1.84083100
C	-0.83966600	-3.12291900	0.38374600
C	-1.64293000	-3.40716800	1.47173100
C	-1.96943300	-2.58830900	2.64713900
C	-1.51049500	-2.97792700	3.91155500
C	-2.70912300	-1.41000000	2.52045700
C	-1.76636800	-2.18484700	5.02234600
H	-0.92863300	-3.89411200	4.00762300
C	-2.95976300	-0.61653300	3.63428800
H	-3.09716500	-1.12589800	1.54397600
C	-2.48487800	-0.99951000	4.88356700
H	-1.39430200	-2.48507900	5.99881900
H	-3.52559500	0.30537300	3.52258500
H	-2.67305200	-0.37405900	5.75255500
N	-2.05276200	-4.71539400	1.38916100
H	-0.42101500	-1.13805900	1.16951300
H	-2.70677400	-5.13971300	2.02944300
C	-3.35550000	-1.12470900	-2.46248400
C	-2.13994300	-1.31697500	-1.82235200
C	-1.76908100	-0.47538500	-0.76251200
C	-2.62577300	0.56050600	-0.36231800
C	-3.85610700	0.71924100	-0.98043300
C	-4.21721200	-0.11771100	-2.03495800
H	-3.63275900	-1.76435800	-3.29609600
H	-1.45539000	-2.09521200	-2.15240000
H	-2.31477800	1.22556000	0.44151500
H	-4.52490400	1.51366700	-0.65813900
H	-5.17309200	0.02366700	-2.53397800
C	-0.45419100	-0.63907200	-0.16249100
C	0.01268200	-1.91145500	0.26769000

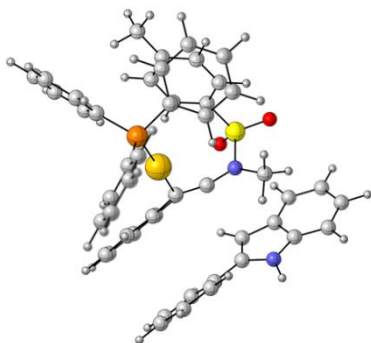
N	1.39303700	-2.10240700	0.45891400
S	2.40501400	-2.02433800	-0.93954000
O	3.28489500	-3.17485300	-0.80436700
O	1.50397800	-1.89256000	-2.07708400
C	3.34595400	-0.54096600	-0.78167900
C	4.07344100	-0.30474000	0.38574900
C	3.40262300	0.32683500	-1.86813500
C	4.84039400	0.84327600	0.46926500
H	4.02263400	-0.99448800	1.22540900
C	4.18377800	1.46951400	-1.76140700
H	2.80833400	0.13825900	-2.75669600
C	4.89487200	1.75070800	-0.59556600
H	5.39143000	1.05853700	1.38279700
H	4.20132300	2.17554100	-2.58957300
C	5.64981800	3.03379200	-0.45540700
H	6.51763100	2.92652900	0.20412800
H	5.99230600	3.41071600	-1.42450900
H	4.99349300	3.79705300	-0.01685200
Au	0.64368300	1.08395500	0.18974100
Cl	0.54525700	0.58471800	2.48812200
Cl	1.90981600	3.05942400	0.59781300
O	0.72991700	1.31660800	-1.84641400
O	1.17886900	2.68670100	-3.51072500
N	-1.08785400	3.19606800	-0.84624300
C	-0.27617200	3.53348000	-1.85097600
C	-0.22905400	4.81702100	-2.38874600
C	-1.03993300	5.79704000	-1.83442800
C	-1.87827900	5.45662600	-0.77930700
C	-1.86913700	4.14038100	-0.32945500
C	0.61935000	2.47813200	-2.44876900
H	0.44297400	5.01093300	-3.21892500
H	-1.01834100	6.81430000	-2.21834200
H	-2.52701000	6.19203500	-0.31136700
H	-2.52023400	3.83454000	0.49247200
C	1.79985000	-3.01839200	1.52788600
H	2.88038600	-2.95761000	1.66295700
H	1.31482300	-2.69030400	2.45353300
H	1.53781400	-4.06068300	1.30766100

PD-c:



C	-0.81170200	-5.71017700	2.15900600
C	-1.05535900	-4.53379400	1.46770500
C	-0.05466700	-3.76731100	0.84408300
C	1.26043300	-4.23012300	0.91051100
C	1.52350600	-5.40929100	1.59602600
C	0.50693700	-6.14004000	2.21808800
H	-1.61629100	-6.26654000	2.63342700
H	2.06306900	-3.71703200	0.39415900
H	2.54515100	-5.77732200	1.63728200
H	0.74881300	-7.05836900	2.74635600
C	-0.71975300	-2.58300100	0.29969600
C	-2.11642900	-2.77695500	0.53007200
C	-3.26563700	-2.05315300	-0.00140900
C	-4.35916400	-1.75766300	0.82149600
C	-3.27378800	-1.66502700	-1.34872400
C	-5.44737000	-1.06951400	0.30128800
H	-4.32453700	-2.01937700	1.87843600
C	-4.36801000	-0.97952500	-1.85755400
H	-2.42103100	-1.90322900	-1.98408200
C	-5.45241100	-0.68135700	-1.03664500
H	-6.28773800	-0.82276900	0.94505900
H	-4.36466000	-0.66522100	-2.89839000
H	-6.30311400	-0.13651200	-1.43847500
N	-2.27934100	-3.90182200	1.23933900
H	-1.79909600	-0.34753500	0.64678700
H	-3.18581400	-4.30396800	1.43948600
C	-1.26221200	1.91218500	-3.18310700
C	-0.80369900	0.93616300	-2.30520400
C	-1.30700400	0.86145200	-1.00443700
C	-2.31730000	1.76101000	-0.62726300
C	-2.77698400	2.73134200	-1.50309900
C	-2.23955200	2.81835200	-2.78603600
H	-0.84840700	1.95777300	-4.18764900
H	-0.07206500	0.21577400	-2.64974500
H	-2.73271900	1.69185800	0.37918500
H	-3.55044600	3.42589600	-1.18198500
H	-2.58962100	3.58271300	-3.47591800
C	-0.93888800	-0.15135500	0.00995300
C	-0.18409300	-1.37797000	-0.17216000
N	1.13461000	-1.38419700	-0.71333900

S	1.35969000	-2.18534600	-2.18310800
O	2.09630300	-3.43198900	-2.01024000
O	0.02929700	-2.22868200	-2.78541400
C	2.43383200	-1.06383000	-3.04665000
C	3.17880600	-1.60145600	-4.09565800
C	2.50309900	0.29188200	-2.73343100
C	3.98274400	-0.75691100	-4.84760700
H	3.13131700	-2.66609300	-4.31098800
C	3.32167200	1.11665700	-3.49235700
H	1.95767400	0.71936800	-1.89534000
C	4.06730700	0.60892600	-4.55848100
H	4.56407300	-1.16488600	-5.67316900
H	3.36669200	2.17175000	-3.22495600
C	4.96626500	1.50618100	-5.35272800
H	5.17405100	1.09541300	-6.34623300
H	4.52763100	2.50202900	-5.47538300
H	5.92983300	1.64101600	-4.84521600
Au	0.29396800	0.79491800	1.57416000
Cl	-0.91609000	-0.46282100	3.14206300
Cl	1.75462300	1.70291800	3.23920700
O	1.40218500	1.68626700	0.05255000
O	1.88979300	3.29062600	-1.37691800
N	-0.50192300	3.34923200	1.23794900
C	0.25287500	3.81767100	0.24416200
C	0.13654700	5.11947500	-0.23730200
C	-0.79856100	5.95950400	0.35100800
C	-1.57792100	5.47522700	1.39630000
C	-1.39061800	4.15902400	1.80598800
C	1.25102700	2.89478100	-0.41118000
H	0.77691800	5.43201900	-1.05621900
H	-0.91754000	6.98262000	0.00178000
H	-2.31615400	6.10246000	1.88861100
H	-1.97669500	3.73321000	2.62136300
C	2.32173900	-1.18093600	0.14319300
H	2.62695200	-0.13061400	0.15243400
H	2.10752500	-1.51234300	1.16602600
H	3.14002200	-1.79540100	-0.24847300

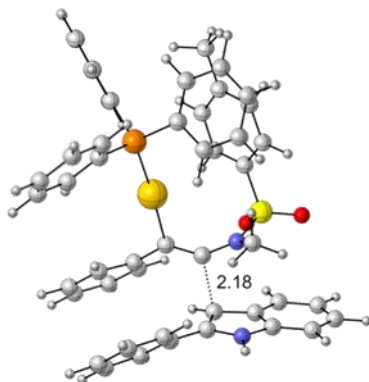
IM3-d:

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C	-4.77501400	1.36168800	-2.17215300
C	-4.62487800	2.42431300	-3.07443000
C	-4.77206300	2.17556000	-4.42897600
C	-5.07327700	0.88717200	-4.90341500
H	-5.43490000	-1.18560300	-4.40382300
H	-4.38916800	3.42332200	-2.71337900
H	-4.65474600	2.98894200	-5.14024100
H	-5.19669300	0.72805900	-5.97179000
C	-4.66235500	1.24075000	-0.75150700
C	-4.82982300	-0.08509900	-0.43212200
C	-4.76210600	-0.75578100	0.86181500
C	-4.21266600	-2.03965900	0.97394000
C	-5.23111100	-0.11691800	2.01514300
C	-4.14158300	-2.67169500	2.21011500
H	-3.81912000	-2.53448800	0.08581600
C	-5.15543400	-0.74944100	3.24848200
H	-5.67484700	0.87329000	1.92979200
C	-4.61425900	-2.02886800	3.35086900
H	-3.71834400	-3.67109200	2.28208800
H	-5.53073500	-0.24396100	4.13548200
H	-4.56765100	-2.52631100	4.31670500
N	-5.03089500	-0.80529900	-1.60260200
H	-4.44597800	2.03339400	-0.04454000
H	-5.41839200	-1.73765600	-1.61596300
C	-2.36486400	0.86444200	4.25044800
C	-1.81218000	0.40104900	3.06417800
C	-1.94064500	1.15343400	1.89222700
C	-2.59424900	2.39359900	1.93030000
C	-3.12515600	2.85965900	3.12589000
C	-3.01745400	2.09405000	4.28462400
H	-2.28123500	0.26563300	5.15410100
H	-1.29929500	-0.55972400	3.02950700
H	-2.65107600	2.99218700	1.02161100
H	-3.62220300	3.82603300	3.15407600
H	-3.43605500	2.46108900	5.21842100
C	-1.34017100	0.71114200	0.64211000
C	-1.60949500	0.75952400	-0.60373100

N	-1.57768900	0.91816400	-1.88043600
S	-0.96097600	2.49591600	-2.46020800
O	-1.12467400	2.42010800	-3.89519500
O	-1.62016200	3.47059400	-1.61649500
C	0.74569100	2.40120000	-2.02846300
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C	1.18535700	2.98440200	-0.83972200
C	2.96513500	1.67921300	-2.55244800
H	1.25674500	1.31400200	-3.82171100
C	2.53748500	2.91943000	-0.53184100
H	0.47969300	3.50240200	-0.19383800
C	3.44494300	2.27383400	-1.38110000
H	3.66173000	1.17069400	-3.21720600
H	2.90595100	3.39609800	0.37623800
C	4.90289400	2.24512300	-1.04131700
H	5.48415100	1.71042200	-1.79879400
H	5.30531100	3.26197400	-0.96330600
H	5.07418400	1.76053900	-0.06961800
C	-1.84081600	-0.14686500	-2.85868800
H	-0.88507500	-0.55194100	-3.21618100
H	-2.41423700	-0.92480500	-2.34752500
H	-2.42089400	0.25085800	-3.69447000
P	2.64514900	-1.36731500	0.58498800
C	3.89196500	-0.51577300	1.59396200
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C	3.63222600	0.77418400	2.06468800
C	6.06839200	-0.45098800	2.63804000
H	5.30488000	-2.15309100	1.56547700
C	4.59134700	1.45137900	2.81149300
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C	5.81070800	0.84179800	3.08989900
H	7.01533900	-0.93090200	2.87080400
H	4.38368600	2.45319700	3.17979000
H	6.56080000	1.37035000	3.67262700
C	3.29162100	-1.50975800	-1.11257600
C	2.40204300	-1.93962500	-2.10502600
C	4.61529500	-1.22464800	-1.44975500
C	2.83332600	-2.08428500	-3.41710400
H	1.36691700	-2.16524400	-1.84346100
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H	5.31554000	-0.88537000	-0.68823000
C	4.15572000	-1.79522500	-3.75004900
H	2.13948600	-2.42437000	-4.18209200
H	6.07617000	-1.14528100	-3.02507600
H	4.49433300	-1.90784200	-4.77686900
C	2.55365200	-3.06519400	1.22845600
C	1.80735700	-3.28442100	2.39141300
C	3.23340700	-4.12567600	0.62504500
C	1.74939400	-4.55452500	2.94983000
H	1.27271100	-2.45618100	2.85913900

C	3.16598800	-5.39713600	1.18641700
H	3.81220100	-3.96134900	-0.28281300
C	2.42732400	-5.61072800	2.34555600
H	1.17031100	-4.72321300	3.85399600
H	3.69292600	-6.22295600	0.71548500
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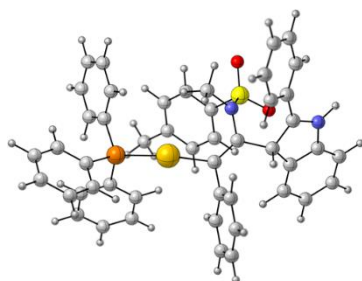


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H	2.26086700	-3.94088800	-8.42950300
H	3.27166100	0.16751600	-5.73306800
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H	2.28189400	-1.68782100	-9.48627200
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C	3.00752100	-4.77501500	-3.25069300
C	3.47119500	-6.08761800	-3.40704400
C	2.47799900	-4.37571800	-2.01965500
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H	3.90928000	-6.40040400	-4.35492000
C	2.39976200	-5.27950300	-0.96855700
H	2.11722400	-3.35631900	-1.89441700
C	2.86363600	-6.58150700	-1.12957100
H	3.77326900	-7.99871500	-2.47484600
H	1.97860700	-4.96212200	-0.01794200
H	2.80154700	-7.28713900	-0.30496900
N	2.78347000	-4.22209700	-5.63600100
H	3.34310700	-1.84286900	-3.46765500
H	2.48341400	-5.15453100	-5.88492000
C	4.87675300	-3.22848200	0.42845700
C	5.40337000	-3.56805900	-0.81039900
C	5.38877700	-2.64333600	-1.86147000
C	4.88604200	-1.35534900	-1.63007800
C	4.37043000	-1.01724600	-0.38353900

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H	4.87328100	-3.96244500	1.23128600
H	5.80327700	-4.56727500	-0.98709500
H	4.92634100	-0.61994600	-2.43393000
H	3.98551000	-0.01464400	-0.21381300
H	3.95242400	-1.68854400	1.61914900
C	5.96497600	-2.96955700	-3.16585000
C	5.44962900	-2.92131900	-4.37008400
N	5.81433100	-2.93544500	-5.65131900
S	6.45471600	-1.46058300	-6.32665500
O	6.22126600	-1.59166300	-7.75176400
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C	9.02275600	-2.22250900	-6.90509900
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H	12.62888100	-1.98159300	-4.26101400
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H	7.02969300	-4.36326900	-6.62194500
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P	10.00624800	-4.89243400	-3.12668700
C	11.34132900	-3.99271300	-2.28347700
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H	10.17116600	-2.19419900	-2.10014700
C	13.37673600	-2.56025500	-1.02984900
H	14.53214900	-4.37332700	-1.17203300
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C	10.57325600	-5.28712000	-4.81443300
C	9.62708800	-5.83283200	-5.69079000
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C	9.98121400	-6.15758000	-6.99364600
H	8.60718300	-6.00695400	-5.34297000
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H	9.24151400	-6.58486600	-7.66676400
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C	9.73111600	-8.86917600	-0.82167200
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H	10.90604700	-9.73346800	-2.40480300
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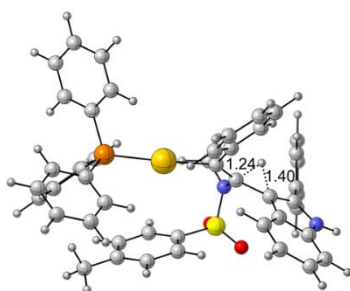


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H	-5.55932200	-3.30219600	-4.02788600
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H	6.83182100	1.74655100	2.49785900
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C	3.77674700	-3.59188500	4.55696800
H	2.25994400	-2.47514200	5.60352400
H	5.22587000	-4.53242400	3.27243400
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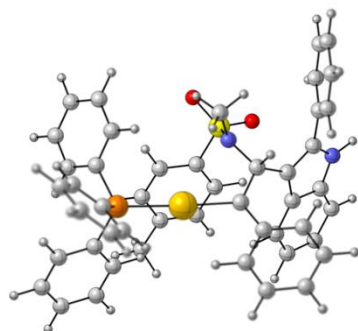


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N	-5.52717900	-0.07169400	-1.62917800
H	-3.52551700	-1.82523100	0.32833100
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C	-1.60571300	-1.39118300	0.81991400
C	-2.46480700	-1.58763400	-0.26115300
N	-2.14343700	-2.44769400	-1.34376200
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C	2.26807200	-1.43281000	-3.00246700
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C	-1.72144400	-3.82450200	-1.09618200
H	-0.62742100	-3.93984000	-1.06701000
H	-2.12328000	-4.12657500	-0.12424900
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C	4.94399100	-0.77109200	1.79500200
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H	6.64160700	0.42187300	2.35166700
H	3.25319800	2.57983800	0.82346100
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C	3.53753700	-3.17788900	-0.39986300
C	2.89194100	-4.30548200	-0.91997500
C	4.74436900	-2.75526500	-0.95872700
C	3.44512500	-4.99797200	-1.98910300
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C	5.29262700	-3.44706700	-2.03602000
H	5.25720500	-1.88095300	-0.56137200
C	4.64459700	-4.56466000	-2.55199100
H	2.94057200	-5.87483300	-2.38699800
H	6.23123400	-3.11128200	-2.47017700
H	5.07508200	-5.10294700	-3.39261200
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H	1.59511500	-2.32696000	3.63075500
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H	4.65244400	-4.54449400	1.55382400
C	3.62502600	-4.79748700	4.78298200
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H	5.11253900	-5.82949700	3.61843300
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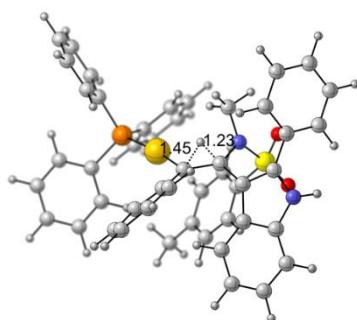


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C	-5.46159500	-2.84511700	-3.07767200
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H	-1.40220200	2.36075700	-2.80478700
C	1.93337100	2.82931900	-2.23715100
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H	0.27825700	4.16963800	-2.55828500
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H	7.21192600	1.13433400	2.38955500
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C	3.57345900	-3.66612500	4.62212200
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H	4.78575800	-4.82250900	3.27039800
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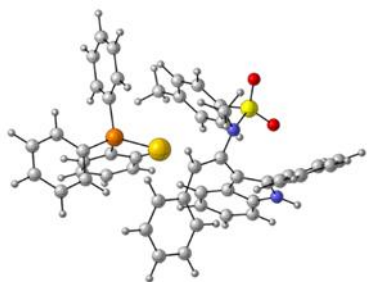


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C	-4.96582700	-2.04522000	-0.28031500
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C	-5.23805800	-3.39769900	-0.44986700
H	-4.79706500	-1.63992500	0.71789500
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H	0.29845200	2.08441900	1.91379600
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C	-1.32990900	0.40275700	0.68954800
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C	4.21621300	1.79952000	1.94910100
C	2.53155400	2.34164000	0.29907400
C	4.63212700	3.12641600	1.95145100
H	4.70581800	1.07313000	2.59670800
C	2.95782300	3.66516200	0.29933300
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H	5.44639900	3.43513800	2.60178400
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C	3.05332300	-1.08018500	2.63009100
C	2.15400400	-0.89979000	3.68726100
C	4.24282500	-1.78294100	2.83738900
C	2.44719500	-1.41670000	4.94249300
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C	4.52753000	-2.30204000	4.09672500
H	4.94470600	-1.92727900	2.01723400
C	3.63255100	-2.11953200	5.14607900
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Au	0.35589700	-0.63231000	0.59316100

9. Reference

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