*Supporting Information*

# Silver-Catalyzed Desulfurizative Annulation of 1,2-Benzisothiazoles with Ynamides to Construct Multi-Substituted Isoquinolines

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## 1. General Information

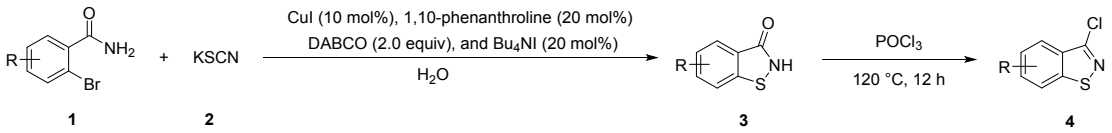
All reactions were carried out under argon atmosphere unless otherwise stated. Commercially available reagents were used without further purification. $^{1}H$ NMR spectra were recorded on a BRUKER AVANCE III HD (400 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$: δ 7.26). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quadruplet, m = multiplet), coupling constants (Hz) and integration. $^{13}C$ NMR spectra were recorded on a BRUKER AVANCE III HD (100 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 77.16). $^{19}F$ NMR spectra were recorded on a BRUKER AVANCE III HD (377 MHz) spectrometer. High resolution mass spectra (HRMS) were measured with a GCT Premier™ and BRUKER micrOTF-Q III. Melting points were measured using INESA WRR melting point instrument and values are uncorrected. X-ray crystal structure analyses were measured on a Bruker D8 Venture instrument. Flash column chromatography was performed using silica gel (300-400 mesh).

## 2. General Procedure and Characterization Data

### 2.1. General procedure for preparation of ynamide


To a solution of phenylacetylene (**S1**) (2.20 mL, 20 mmol) in acetone (60 mL) was added NBS (4.22 g, 24 mmol) and $AgNO_3$ (169.9 mg, 1.0 mmol), the resulting mixture was stirred under Ar at room temperature for 2 hours. After removing excess acetone, the reaction was quenched with saturated $NH_4Cl$ solution, and the organic layer was extracted with petroleum ether (40 mL × 2), dried over anhydrous $NaSO_4$ and concentrated under reduced pressure afford a pure colorless oil of bromoalkyne **S2** (2.94g, 81%).

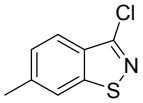
To a dried flask was added *N*-methymethanesulphonamide (2.13 g, 19.5 mmol), $CuSO_4·5H_2O$ (0.50 g, 2.0 mmol), 1,10-phenanthroline (0.74 g, 4.1 mmol) and $K_2CO_3$ (5.54 g, 40 mmol). The resulting mixture was subsequently treated with anhydrous toluene (40 mL) and bromoalkyne (**S2**) (2.94 g, 16.2 mmol, and stirred at 80°C overnight under an atmosphere of Ar. When the reaction is complete, the crude mixture was cooled to room temperature, filtered through Celite, and concentrated in vacuo. The resulting residue was purified by flash column chromatography on silica gel, giving the pure ynamide **1b** as a pale yellow solid (2.86 g, 84%).



**2.2. General Procedure for the Synthesis of Benzisothiazol-3(2*H*)-one (3).** A sealed tube was charged with the mixture of *o*-halobenzamide **1** (5 mmol), potassium thiocyanate **2** (10 mmol), CuI (0.5 mmol), 1,10-phenanthroline (1 mmol), DABCO (10 mmol), and $Bu_4NI$ (0.1 mmol) and then stirred in $H_2O$ (10 mL) at room temperature under nitrogen atmosphere. Half an hour later, the tube was sealed, and the mixture was allowed to stir at 140−160 °C for the indicated time. After completion of the reaction, the mixture was cooled to room temperature, and then $H_2O$ (50 mL) was added and the mixture extracted with EtOAc (50 mL × 3) and dried by anhydrous $Na_2SO_4$. Evaporation of the solvent followed by purification on silica gel (petroleum ether/ethyl acetate = 2/1) provided the corresponding product **3.**

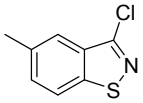
**2.3. General Procedure for the Synthesis of 3-Cl-1,2-Benzisothiazoles (4).** A sealed tube was charged with benzisothiazol-3(2*H*)-one (**3**) (0.5 mmol) and $POCl_3$ (2 mL) and then stirred at 120 °C for 12 h. After completion of the reaction, the mixture was cooled to room temperature, and then $H_2O$ (10 mL) was added and the mixture extracted with EtOAc (10 mL × 3) and dried by anhydrous $Na_2SO_4$. Evaporation of the solvent followed by purification on silica gel (petroleum ether/ethyl acetate = 10/1) provided the corresponding product **4**.

**3-chloro-6-methylbenzo[*d*]isothiazole (1b).**



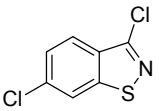

Colourless oil, PE/EA (10:1) as the eluent. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.4 Hz, 1H), 7.61 (m, 1H), 7.27 (m, 1H), 2.51 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.55, 145.80, 139.83, 130.23, 127.74, 123.19, 119.68, 21.80.

**3-chloro-5-methylbenzo[*d*]isothiazole (1c).**



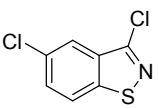

Colourless oil, PE/EA (10:1) as the eluent. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.68 (m, 2H), 7.42 – 7.35 (m, 1H), 2.51 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.55, 145.54, 135.98, 132.44, 130.96, 123.13, 119.74, 21.33.

**3,6-dichlorobenzo[*d*]isothiazole. (1d).**



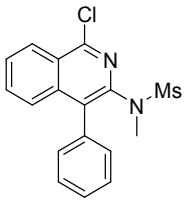

Colourless oil, PE/EA (10:1) as the eluent. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.84 (m, 2H), 7.47 (dd, J = 8.6, 1.7 Hz, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.18, 145.97, 136.33, 130.75, 126.94, 124.63, 119.81.

**3,5-dichlorobenzo[*d*]isothiazole (1e).**



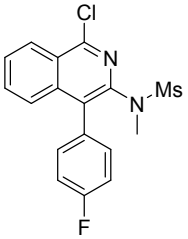
Colourless oil, PE/EA (10:1) as the eluent. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 2.0, 0.6 Hz, 1H), 7.81 (dd, *J* = 8.7, 0.7 Hz, 1H), 7.53 (dd, *J* = 8.7, 1.9 Hz, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.37, 145.21, 133.26, 132.30, 129.68, 123.21, 121.19.

***N*-(1-chloro-4-phenylisoquinolin-3-yl)-*N*-methylmethanesulfonamide (3aa).**



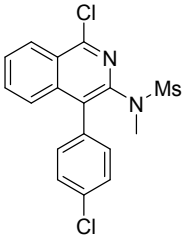

White solid, PE/EA (10:1) as the eluent, 28.4 mg, 82% yield, m.p. 189-190 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.35 (m, 1H), 7.74 – 7.61 (m, 3H), 7.56 – 7.43 (m, 5H), 3.18 (s, 3H), 3.01 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.96, 144.90, 139.03, 133.85, 132.03, 131.60, 130.39, 128.84, 128.52, 128.35, 126.72, 126.57, 126.47, 38.43, 37.80. HRMS (ESI) *m/z*: Calcd for: $C_{17}H_{16}ClN_2O_2S$ $[M + H]^+$ 347.0616, Found: 347.0615.

***N*-(1-chloro-4-(4-fluorophenyl)isoquinolin-3-yl)-*N*-methylmethanesulfonamide (3ab).**




White solid, PE/EA (10:1) as the eluent, 29.1 mg, 80% yield, m.p. 191-192 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.36 (m, 1H), 7.76 – 7.66 (m, 2H), 7.63 – 7.57 (m, 1H), 7.48 – 7.38 (m, 2H), 7.28 – 7.15 (m, 2H), 3.22 (s, 3H), 3.02 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 162.76 (d, *J* = 247.8 Hz), 150.28, 145.05, 139.03, δ 132.20 (d, *J* = 8.0 Hz), 131.77, 131.24, 129.66 (d, *J* = 3.1 Hz), 128.96, 126.62, 126.59, 126.51, 115.67 (d, *J* = 21.5 Hz), 38.21, 37.83. $^{19}$F NMR (377 MHz, $CDCl_3$) δ -113.23. HRMS (ESI) *m/z*: Calcd for: $C_{17}H_{14}ClFN_2O_2SNa$ $[M + Na]^+$ 387.0341, Found: 387.0344.

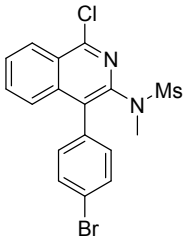
***N*-(1-chloro-4-(4-chlorophenyl)isoquinolin-3-yl)-*N*-methylmethanesulfonamide (3ac).**




White solid, PE/EA (10:1) as the eluent, 28.1 mg, 74% yield, m.p. 205-206 °C. $^{1}$H NMR (400 MHz,

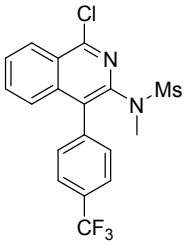
$CDCl_3$) δ 8.47 – 8.33 (m, 1H), 7.76 – 7.66 (m, 2H), 7.63 – 7.57 (m, 1H), 7.54 – 7.47 (m, 2H), 7.43 – 7.34 (m, 2H), 3.22 (s, 3H), 3.03 (s, 3H). $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 150.44, 144.92, 138.81, 134.57, 132.26, 131.84, 131.79, 131.08, 129.03, 128.85, 126.62, 126.44, 38.15, 37.88. HRMS (ESI) *m/z*: Calcd for: $C_{17}H_{15}Cl_2N_2O_2S$ $[M + H]^+$ 381.0226, Found: 381.0215.

**_N_-(4-(4-bromophenyl)-1-chloroisoquinolin-3-yl)-_N_-methylmethanesulfonamide (3dd).**



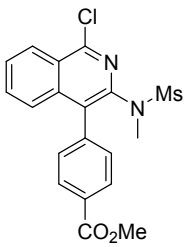

White solid, PE/EA (10:1) as the eluent, 31.8 mg, 75% yield, m.p. 199-200 °C. $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.35 (m, 1H), 7.77 – 7.64 (m, 4H), 7.62 – 7.56 (m, 1H), 7.37 – 7.31 (m, 2H), 3.22 (s, 3H), 3.03 (s, 3H). $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 150.46, 144.85, 138.74, 132.77, 132.08, 131.85, 131.80, 131.08, 129.04, 126.63, 126.43, 122.80, 38.14, 37.89. HRMS (ESI) *m/z*: Calcd for: $C_{17}H_{15}BrClN_2O_2S$ $[M + H]^+$ 424.9721, Found: 424.9729.

**_N_-(1-chloro-4-(4-(trifluoromethyl)phenyl)isoquinolin-3-yl)-_N_-methylmethanesulfon amide (3ae).**



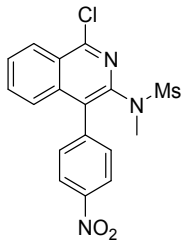

White solid, PE/EA (10:1) as the eluent, 29.0 mg, 70% yield, m.p. 155-156 °C. $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.46 – 8.36 (m, 1H), 7.82 – 7.78 (m, 2H), 7.73 (m, 2H), 7.64 – 7.57 (m, 2H), 7.56 – 7.50 (m, 1H), 3.22 (s, 3H), 3.04 (s, 3H). $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 150.85, 144.84, 138.60, 137.77, 132.03, 130.94, 130.90, 130.57 (q, $J$ = 32.7 Hz), 129.17, 126.71, 126.62, 126.28, 125.49 (q, $J$ = 3.6 Hz), 124.10 (q, $J$ = 272.6 Hz), 115.66 (q, $J$ = 21.2 Hz), 37.99, 37.96. $^{19}F$ NMR (377 MHz, $CDCl_3$) δ -62.54. HRMS (ESI) *m/z*: Calcd for: $C_{18}H_{14}ClF_3N_2O_2SNa$ $[M + Na]^+$ 437.0315, Found: 437.0309.

**Methyl 4-(1-chloro-3-(_N_-methylmethylsulfonamido)isoquinolin-4-yl)benzoate (3af).**



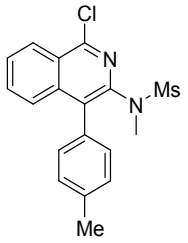
White solid, PE/EA (10:1) as the eluent, 31.5 mg, 78% yield, m.p. 158-159 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.39 (m, 1H), 8.23 – 8.17 (m, 2H), 7.76 –7.67 (m, 2H), 7.58 – 7.51 (m, 3H), 3.98 (s, 3H), 3.20 (s, 3H), 3.02 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 166.79, 150.64, 144.77, 138.77, 138.57, 131.92, 131.30, 130.57, 130.17, 129.74, 129.08, 126.65, 126.58, 126.36, 52.29, 38.13, 37.88. HRMS (ESI) *m/z*: Calcd for: $C_{19}H_{18}ClN_2O_4S$ $[M + H]^+$ 405.0670, Found: 405.0662.

**_N_-(1-chloro-4-(4-nitrophenyl)isoquinolin-3-yl)-_N_-methylmethanesulfonamide (3ag).**



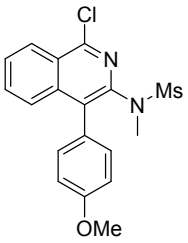

White solid, PE/EA (10:1) as the eluent, 24.2 mg, 62% yield, m.p. 257-258 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.47 – 8.44 (m, 1H), 8.42 – 8.38 (m, 2H), 7.80 – 7.72 (m, 2H), 7.68 – 7.63 (m, 2H), 7.53 – 7.48 (m, 1H), 3.21 (s, 3H), 3.07 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 151.43, 147.91, 144.72, 141.00, 138.22, 132.32, 131.62, 130.43, 129.40, 126.90, 126.65, 126.00, 123.70, 38.02, 37.69. HRMS (ESI) *m/z*: Calcd for: $C_{17}H_{15}ClN_3O_4S$ $[M + H]^+$ 392.0466, Found: 392.0465.

**_N_-(1-chloro-4-(_p_-tolyl)isoquinolin-3-yl)-_N_-methylmethanesulfonamide (3ah).**



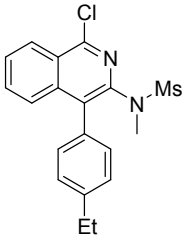

White solid, PE/EA (10:1) as the eluent, 27.4 mg, 76% yield, m.p. 174-175 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.30 (m, 1H), 7.74 – 7.61 (m, 3H), 7.33 (s, 4H), 3.20 (s, 3H), 3.01 (s, 3H), 2.45 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.71, 144.97, 139.18, 138.10, 132.08, 131.47, 130.74, 130.25, 129.24, 128.75, 126.80, 126.57, 126.42, 38.46, 37.79, 21.40. HRMS (ESI) *m/z*: Calcd for: $C_{18}H_{17}ClN_2O_2SNa$ $[M + Na]^+$ 383.0591, Found: 383.0600.

**_N_-(1-chloro-4-(4-methoxyphenyl)isoquinolin-3-yl)-_N_-methylmethanesulfonamide (3ai).**



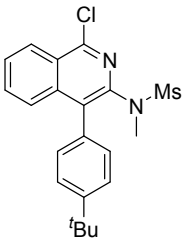

White solid, PE/EA (10:1) as the eluent, 21.4 mg, 57% yield, m.p. 156-157 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.34 (m, 1H), 7.74 – 7.61 (m, 3H), 7.44 – 7.33 (m, 2H), 7.09 – 6.99 (m, 2H), 3.90 (s, 3H), 3.22 (s, 3H), 3.01 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.59, 149.63, 145.11, 139.31, 131.74, 131.62, 131.48, 128.74, 126.79, 126.60, 126.45, 125.75, 114.02, 55.32, 38.50, 37.73. HRMS (ESI) *m/z*: Calcd for: $C_{18}H_{18}ClN_2O_3S$ $[M + H]^+$ 377.0721, Found: 377.0720.

**_N_-(1-chloro-4-(4-ethylphenyl)isoquinolin-3-yl)-_N_-methylmethanesulfonamide (3aj).**



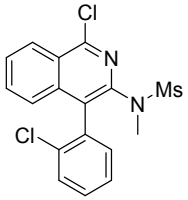

White solid, PE/EA (10:1) as the eluent, 29.5 mg, 79% yield, m.p. 141-142 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.38 (dt, *J* = 8.1, 1.3 Hz, 1H), 7.74 – 7.63 (m, 3H), 7.36 (s, 4H), 3.19 (s, 3H), 3.01 (s, 3H), 2.76 (q, *J* = 7.6 Hz, 2H), 1.33 (t, *J* = 7.6 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.68, 144.96, 144.31, 139.20, 132.05, 131.46, 130.92, 130.31, 128.74, 127.99, 126.85, 126.56, 126.41, 38.49, 37.79, 28.69, 15.34. HRMS (ESI) *m/z*: Calcd for: $C_{19}H_{20}ClN_2O_2S$ $[M + H]^+$ 375.0929, Found: 375.0923.

**_N_-(4-(4-(*tert*-butyl)phenyl)-1-chloroisoquinolin-3-yl)-_N_-methylmethanesulfonamide (3ak).**



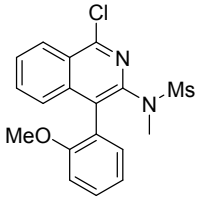

White solid, PE/EA (10:1) as the eluent, 31.4 mg, 78% yield, m.p. 81-82 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.38 (dt, *J* = 8.0, 1.4 Hz, 1H), 7.74 – 7.64 (m, 3H), 7.57 – 7.46 (m, 2H), 7.40 – 7.33 (m, 2H), 3.17 (s, 3H), 3.01 (s, 3H), 1.40 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 151.22, 149.63, 144.97, 139.23, 131.90, 131.43, 130.66, 130.06, 128.71, 126.89, 126.54, 126.40, 125.42, 38.55, 37.81, 34.76, 31.42. HRMS (ESI) *m/z*: Calcd for: $C_{21}H_{24}ClN_2O_2S$ $[M + H]^+$ 403.1242, Found: 403.1251.

**_N_-(1-chloro-4-(2-chlorophenyl)isoquinolin-3-yl)-_N_-methylmethanesulfonamide (3al).**



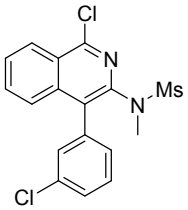

White solid, PE/EA (10:1) as the eluent, 22.4mg, 59% yield, m.p. 171-172 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.41 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.75 – 7.67 (m, 2H), 7.58 – 7.52 (m, 2H), 7.49 – 7.43 (m, 2H), 7.41 – 7.36 (m, 1H), 3.18 (s, 3H), 3.12 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.79, 145.18, 138.55, 133.59, 133.28, 132.97, 131.93, 130.13, 129.66, 129.40, 129.01, 127.25, 126.67, 126.42, 126.24, 37.84, 37.38. HRMS (ESI) *m/z*: Calcd for: $C_{17}H_{15}Cl_2N_2O_2S$ [M + H] $^+$ 381.0226, Found: 381.0216.

***N*-(1-chloro-4-(2-methoxyphenyl)isoquinolin-3-yl)-*N*-methylmethanesulfonamide (3am).**



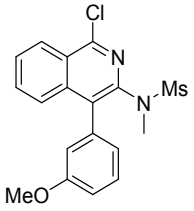

White solid, PE/EA (10:1) as the eluent, 22.9 mg, 61% yield, m.p. 154-155 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.40 – 8.31 (m, 1H), 7.70 – 7.61 (m, 2H), 7.53 – 7.43 (m, 2H), 7.36 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.13 (td, *J* = 7.5, 1.0 Hz, 1H), 7.05 (dd, *J* = 8.4, 1.0 Hz, 1H), 3.70 (s, 3H), 3.15 (s, 3H), 3.06 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 156.92, 149.87, 145.47, 139.24, 132.53, 131.33, 130.11, 129.08, 128.59, 126.65, 126.43, 122.65, 120.98, 110.71, 55.33, 38.04, 37.37. HRMS (ESI) *m/z*: Calcd for: $C_{18}H_{17}ClN_2O_3SNa$ [M + Na] $^+$ 399.0541, Found: 399.0549.

***N*-(1-chloro-4-(3-chlorophenyl)isoquinolin-3-yl)-*N*-methylmethanesulfonamide (3an).**



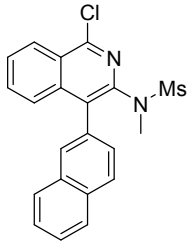

White solid, PE/EA (10:1) as the eluent, 31.5 mg, 83% yield, m.p. 161-162 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.44 – 8.37 (m, 1H), 7.76 – 7.69 (m, 2H), 7.62 – 7.55 (m, 1H), 7.50 – 7.45 (m, 2H), 7.43 – 7.37 (m, 2H), 3.20 (s, 3H), 3.05 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.59, 144.88, 138.73, 135.72, 134.29, 131.93, 130.88, 130.20, 129.93, 129.07, 128.87, 128.62, 126.62, 126.58, 126.44, 38.10, 37.96. HRMS (ESI) *m/z*: Calcd for: $C_{17}H_{14}Cl_2N_2O_2SNa$ [M + Na] $^+$ 403.0045, Found: 403.0039.

***N*-(1-chloro-4-(3-methoxyphenyl)isoquinolin-3-yl)-*N*-methylmethanesulfonamide (3ao).**



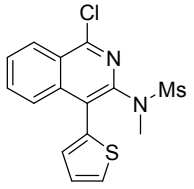

White solid, PE/EA (10:1) as the eluent, 19.9 mg, 53% yield, m.p. 151-152 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.39 (dt, *J* = 7.9, 1.5 Hz, 1H), 7.82 – 7.62 (m, 3H), 7.42 (dd, *J* = 8.3, 7.5 Hz, 1H), 7.10 – 6.90 (m, 3H), 3.85 (s, 3H), 3.22 (s, 3H), 3.01 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.64, 149.95, 144.82, 138.95, 135.03, 131.85, 131.59, 129.41, 128.85, 126.78, 126.56, 126.44, 122.68, 115.80, 114.44, 55.42, 38.53, 37.81. HRMS (ESI) *m/z*: Calcd for: $C_{18}H_{17}ClN_2O_3SNa$ [M + Na] $^{+}$ 399.0541, Found: 399.0548.

***N*-(1-chloro-4-(naphthalen-2-yl)isoquinolin-3-yl)-*N*-methylmethanesulfonamide (3ap).**



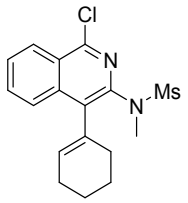

White solid, PE/EA (10:1) as the eluent, 30.5 mg, 77% yield, m.p. 186-187 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.42 (dt, *J* = 8.2, 1.0 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.97 – 7.88 (m, 3H), 7.74 – 7.70 (m, 1H), 7.67 – 7.64 (m, 2H), 7.62 – 7.49 (m, 3H), 3.21 (s, 3H), 3.00 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.07, 145.16, 139.17, 133.11, 133.02, 131.95, 131.66, 131.32, 129.65, 128.88, 128.27, 128.13, 127.90, 126.80, 126.67, 126.60, 126.52, 38.43, 37.88. HRMS (ESI) *m/z*: Calcd for: $C_{21}H_{17}ClN_2O_2SNa$ [M + Na] $^{+}$ 419.0591, Found: 419.0562.

***N*-(1-chloro-4-(thiophen-2-yl)isoquinolin-3-yl)-*N*-methylmethanesulfonamide (3aq).**



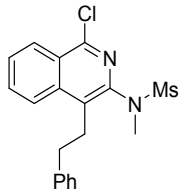

White solid, PE/EA (10:1) as the eluent, 12.3 mg, 35% yield, m.p. 214-215 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.34 (m, 1H), 7.95 – 7.85 (m, 1H), 7.79 – 7.70 (m, 2H), 7.56 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.27 (dd, *J* = 3.6, 1.1 Hz, 1H), 7.22 (dd, *J* = 5.1, 3.5 Hz, 1H), 3.20 (s, 3H), 3.11 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.79, 145.86, 139.57, 133.32, 131.92, 130.42, 129.06, 127.62, 127.29, 126.64, 126.53, 126.48, 125.59, 38.22, 37.76. HRMS (ESI) *m/z*: Calcd for: $C_{15}H_{13}ClN_2O_2S_2Na$ [M + Na] $^{+}$ 374.9999, Found: 375.0002.

***N*-(1-chloro-4-(cyclohex-1-en-1-yl)isoquinolin-3-yl)-*N*-methylmethanesulfonamide (3ar).**



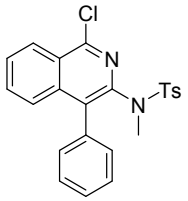

White solid, PE/EA (10:1) as the eluent, 28.0 mg, 80% yield, m.p. 188-189 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.2 Hz, 1H), 8.04 – 7.95 (m, 1H), 7.77 – 7.67 (m, 2H), 5.76 (t, *J* = 1.9 Hz, 1H), 3.28 (s, 3H), 3.26 (s, 3H), 2.58 (d, *J* = 17.1 Hz, 1H), 2.38 – 2.23 (m, 2H), 2.15 (d, *J* = 18.0 Hz, 1H), 1.84 (dt, *J* = 14.8, 9.5 Hz, 4H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 148.88, 144.23, 138.65, 134.63, 132.01, 131.33, 130.06, 128.69, 126.71, 126.49, 126.30, 38.70, 37.86, 29.79, 25.57, 22.95, 22.04. HRMS (ESI) *m/z*: Calcd for: $C_{17}H_{19}ClN_2O_2SNa$ [M + Na] $^+$ 373.0748, Found: 373.0753.

***N*-(1-chloro-4-phenethylisoquinolin-3-yl)-*N*-methylmethanesulfonamide (3as).**



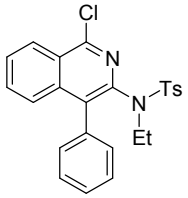

White solid, PE/EA (10:1) as the eluent, 11.6 mg, 31% yield, m.p. 143-144 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 8.5 Hz, 1H), 7.83 – 7.81 (m, 1H), 7.75 – 7.71 (m, 1H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.23 – 7.13 (m, 3H), 3.54 (s, 2H), 3.13 (s, 3H), 3.05 (s, 3H), 3.04 (s, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.02, 145.29, 141.18, 138.37, 131.61, 131.30, 128.72, 128.61, 128.56, 127.22, 126.85, 126.28, 124.87, 37.99, 36.22, 36.17, 29.38. HRMS (ESI) *m/z*: Calcd for: $C_{19}H_{19}ClN_2O_2SNa$ [M + Na] $^+$ 397.0748, Found: 397.0751.

***N*-(1-chloro-4-phenylisoquinolin-3-yl)-*N*,4-dimethylbenzenesulfonamide (3at).**



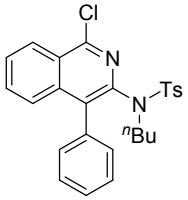

White solid, PE/EA (10:1) as the eluent, 33.8 mg, 80% yield, m.p. 188-189 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.42 – 8.32 (m, 1H), 7.77 – 7.64 (m, 5H), 7.59 – 7.46 (m, 5H), 7.36 – 7.28 (m, 2H), 2.89 (s, 3H), 2.46 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.68, 144.87, 143.52, 139.02, 135.60, 134.19, 132.66, 131.40, 130.49, 129.22, 129.02, 128.73, 128.47, 128.26, 126.81, 126.55, 126.36, 37.46, 21.63. HRMS (ESI) *m/z*: Calcd for: $C_{23}H_{19}ClN_2O_2SNa$ [M + Na] $^+$ 445.0748, Found: 445.0754.

***N*-(1-chloro-4-phenylisoquinolin-3-yl)-*N*-ethyl-4-methylbenzenesulfonamide (3au).**



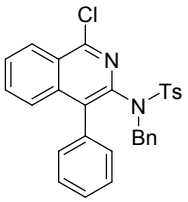

White solid, PE/EA (10:1) as the eluent, 38.4 mg, 88% yield, m.p. 206-207 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.33 (m, 1H), 7.76 – 7.57 (m, 5H), 7.56 – 7.47 (m, 5H), 7.31 (d, *J* = 8.2 Hz, 2H), 3.33 (d, *J* = 7.3 Hz, 2H), 2.45 (s, 3H), 0.79 (t, *J* = 7.2 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.60, 143.47, 142.67, 139.16, 136.17, 134.25, 134.21, 131.36, 131.04, 129.17, 129.07, 128.76, 128.17, 127.05, 126.50, 126.29, 44.94, 21.61, 13.10. HRMS (ESI) *m/z*: Calcd for: $C_{24}H_{21}ClN_2O_2SNa$ [M + Na] $^+$ 459.0904, Found: 459.0901.

***N*-butyl-*N*-(1-chloro-4-phenylisoquinolin-3-yl)-4-methylbenzenesulfonamide (3av).**



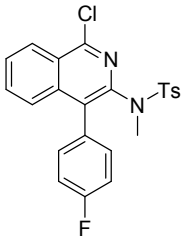

White solid, PE/EA (10:1) as the eluent, 42.7 mg, 92% yield, m.p. 143-144 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.41 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.81 – 7.75 (m, 2H), 7.75 – 7.62 (m, 3H), 7.60 – 7.49 (m, 5H), 7.35 (d, *J* = 8.1 Hz, 2H), 3.56 – 2.97 (m, 2H), 2.49 (s, 3H), 1.18 – 1.08 (m, 2H), 0.99 (m, 2H), 0.69 (t, *J* = 7.3 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.59, 143.46, 143.04, 139.18, 136.16, 134.15, 134.12, 131.33, 131.07, 129.16, 129.12, 128.73, 128.17, 128.15, 127.10, 126.51, 126.27, 50.13, 29.73, 21.62, 19.78, 13.59. HRMS (ESI) *m/z*: Calcd for: $C_{26}H_{25}ClN_2O_2SNa$ [M + Na] $^+$ 487.1217, Found: 487.1207.

***N*-benzyl-*N*-(1-chloro-4-phenylisoquinolin-3-yl)-4-methylbenzenesulfonamide (3aw).**



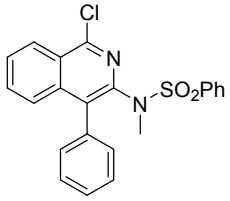

White solid, PE/EA (10:1) as the eluent, 24.9 mg, 50% yield, m.p. 153-154 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, *J* = 8.5, 1.2 Hz, 1H), 7.70 – 7.63 (m, 3H), 7.59 – 7.55 (m, 1H), 7.46 – 7.37 (m, 2H), 7.34 – 7.28 (m, 4H), 7.18 – 7.11 (m, 1H), 7.04 (dd, *J* = 8.3, 6.8 Hz, 2H), 6.91 – 6.75 (m, 4H), 4.48 (s, 2H), 2.47 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.43, 143.74, 142.40, 139.16, 135.84, 134.71, 133.70, 131.20, 130.94, 129.80, 129.28, 129.17, 128.72, 128.20, 127.69, 127.63, 127.17, 126.44, 126.22, 54.03, 21.66. HRMS (ESI) *m/z*: Calcd for: $C_{29}H_{23}ClN_2O_2SNa$ [M + Na] $^+$ 521.1061, Found: 521.1051.

***N*-(1-chloro-4-(4-fluorophenyl)isoquinolin-3-yl)-*N*,4-dimethylbenzenesulfonamide (3ax).**



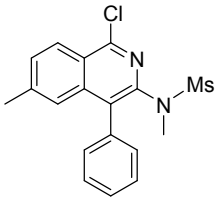
White solid, PE/EA (10:1) as the eluent, 34.8 mg, 79% yield, m.p. 174-175 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.42 – 8.31 (m, 1H), 7.78 – 7.66 (m, 4H), 7.65 – 7.58 (m, 1H), 7.51 – 7.44 (m, 2H), 7.37 – 7.31 (m, 2H), 7.27 (d, *J* = 1.9 Hz, 1H), 7.24 (d, *J* = 8.8 Hz, 1H), 2.90 (s, 3H), 2.47 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 162.76 (d, *J* = 247.8 Hz), 149.94, 145.08, 143.65, 139.01, 135.36, 132.30 (d, *J* = 8.0 Hz), 131.79, 131.57, 130.04 (d, *J* = 3.6 Hz), 129.25, 129.01, 128.84, 126.59, 126.47, 115.60 (d, *J* = 21.7 Hz), 37.47, 21.63. $^{19}$F NMR (377 MHz, $CDCl_3$) δ -113.48. HRMS (ESI) *m/z*: Calcd for: $C_{23}H_{18}ClFN_2O_2SNa$ [M + Na] $^{+}$ 463.0654, Found: 463.0664.

**_N_-(1-chloro-4-phenylisoquinolin-3-yl)-_N_-methylbenzenesulfonamide (3ay).**



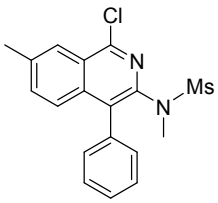
Colourless oil, PE/EA (10:1) as the eluent, 37.9 mg, 93% yield. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.33 (m, 1H), 7.90 – 7.83 (m, 2H), 7.74 – 7.64 (m, 3H), 7.61 – 7.57 (m, 1H), 7.57 – 7.46 (m, 7H), 2.90 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.71, 144.74, 139.02, 138.61, 134.13, 132.75, 132.65, 131.45, 130.49, 128.95, 128.78, 128.57, 128.50, 128.31, 126.81, 126.58, 126.37, 37.55. HRMS (ESI) *m/z*: Calcd for: $C_{22}H_{17}ClN_2O_2SNa$ [M + Na] $^{+}$ 431.0591, Found: 431.0587.

**_N_-(1-chloro-6-methyl-4-phenylisoquinolin-3-yl)-_N_-methylmethanesulfonamide (3ba).**



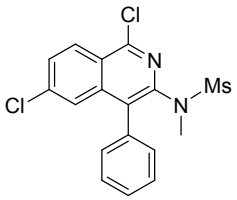
White solid, PE/EA (10:1) as the eluent, 28.8 mg, 80% yield, m.p. 226-227 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.6 Hz, 1H), 7.57 – 7.41 (m, 6H), 7.38 – 7.35 (m, 1H), 3.18 (s, 3H), 3.00 (s, 3H), 2.44 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.71, 145.00, 142.47, 139.28, 134.06, 131.47, 131.03, 130.40, 128.48, 128.24, 126.31, 125.60, 124.93, 38.39, 37.79, 22.13. HRMS (ESI) *m/z*: Calcd for: $C_{18}H_{17}ClN_2O_2SNa$ [M + Na] $^{+}$ 383.0591, Found: 383.0599.

**_N_-(1-chloro-7-methyl-4-phenylisoquinolin-3-yl)-_N_-methylmethanesulfonamide (3ca).**



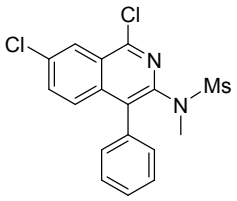
White solid, PE/EA (10:1) as the eluent, 30.6 mg, 85% yield, m.p. 216-217 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.15 (m, 1H), 7.54 – 7.41 (m, 7H), 3.17 (s, 3H), 3.00 (s, 3H), 2.58 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.12, 144.14, 139.30, 137.26, 134.01, 133.79, 131.94, 130.38, 128.45, 128.26, 126.73, 126.57, 125.27, 38.35, 37.83, 21.88. HRMS (ESI) *m/z*: Calcd for: $C_{18}H_{17}ClN_2O_2SNa$ [M + Na] $^+$ 383.0591, Found: 383.0587.

**_N_-(1,6-dichloro-4-phenylisoquinolin-3-yl)-_N_-methylmethanesulfonamide (3da).**



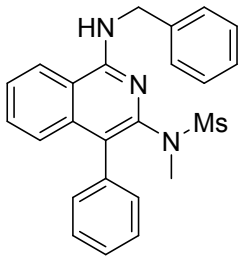

White solid, PE/EA (10:1) as the eluent, 20.9 mg, 55% yield, m.p. 229-230 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 9.0 Hz, 1H), 7.64 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.59 (d, *J* = 2.1 Hz, 1H), 7.58 – 7.47 (m, 3H), 7.46 – 7.40 (m, 2H), 3.16 (s, 3H), 2.99 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.91, 146.08, 139.90, 138.57, 133.18, 131.12, 130.29, 129.82, 128.76, 128.67, 128.23, 125.57, 124.85, 38.54, 37.68. HRMS (ESI) *m/z*: Calcd for: $C_{17}H_{14}Cl_2N_2O_2SNa$ [M + Na] $^+$ 403.0045, Found: 403.0041.

**_N_-(1,7-dichloro-4-phenylisoquinolin-3-yl)-_N_-methylmethanesulfonamide (3ea).**




White solid, PE/EA (10:1) as the eluent, 28.1 mg, 74% yield, m.p. 196-197 °C. $^1$H NMR (400 MHz, Chloroform-*d*) δ 8.36 (dd, *J* = 1.6, 1.0 Hz, 1H), 7.61 – 7.56 (m, 2H), 7.56 – 7.46 (m, 3H), 7.46 – 7.40 (m, 2H), 3.16 (s, 3H), 3.00 (s, 4H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 148.77, 145.28, 137.39, 135.12, 133.32, 132.54, 131.96, 130.31, 128.65, 128.61, 128.52, 127.26, 125.33, 38.45, 37.72. HRMS (ESI) *m/z*: Calcd for: $C_{17}H_{14}Cl_2N_2O_2SNa$ [M + Na] $^+$ 403.0045, Found: 403.0050.

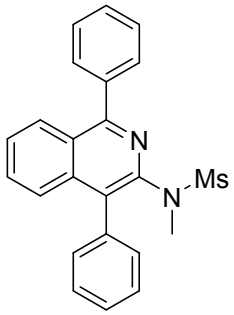
**_N_-(1-(benzylamino)-4-phenylisoquinolin-3-yl)-_N_-methylmethanesulfonamide (4a).**




White solid, PE/EA (10:1) as the eluent, 26.3 mg, 63% yield, m.p. 212-213 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 7.4, 1.5 Hz, 1H), 7.55 – 7.27 (m, 13H), 5.74 (t, *J* = 5.2 Hz, 1H), 4.80 (d, *J* = 5.3 Hz, 2H), 2.97 (s, 3H), 2.92 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 154.26, 144.95, 139.06, 138.49, 135.64, 131.12, 130.13, 128.78, 128.23, 127.56, 127.45, 127.31, 126.82, 126.31, 121.45, 121.25,

117.45, 46.09, 38.06, 37.54. HRMS (ESI) *m/z*: Calcd for: $C_{24}H_{23}N_3O_2SNa$ [M + Na] $^+$ 440.1403, Found: 440.1409.

***N*-(1,4-diphenylisoquinolin-3-yl)-*N*-methylmethanesulfonamide (4b).**




White solid, PE/EA (10:1) as the eluent, 22.9 mg, 59% yield, m.p. 171-172 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.19 (m, *J* = 8.3, 1.4, 0.7 Hz, 1H), 7.78 – 7.73 (m, 2H), 7.69 (m, *J* = 8.4, 1.5, 0.8 Hz, 1H), 7.63 – 7.48 (m, 10H), 3.23 (s, 3H), 3.02 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.98, 146.03, 138.97, 138.46, 134.76, 130.58, 130.41, 130.38, 130.15, 128.94, 128.45, 128.03, 127.58, 127.41, 126.43, 126.23, 38.80, 37.86. HRMS (ESI) *m/z*: Calcd for: $C_{23}H_{20}N_2O_2SNa$ [M + Na] $^+$ 411.1138, Found: 411.1139.

## 3. Computational Studies

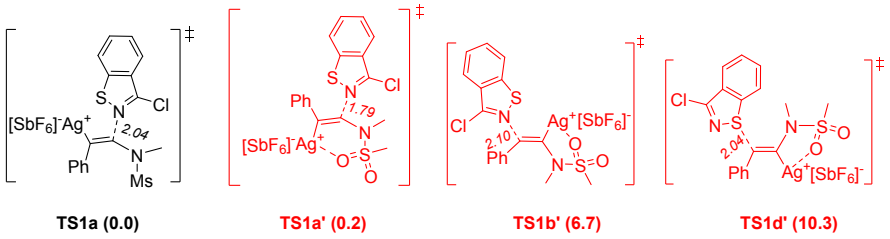



**Figure S1.** The other possible structural conformers of the transition states of nucleophilic addition of **1a**. The relative Gibbs energies (in kcal/mol) are given in parentheses.

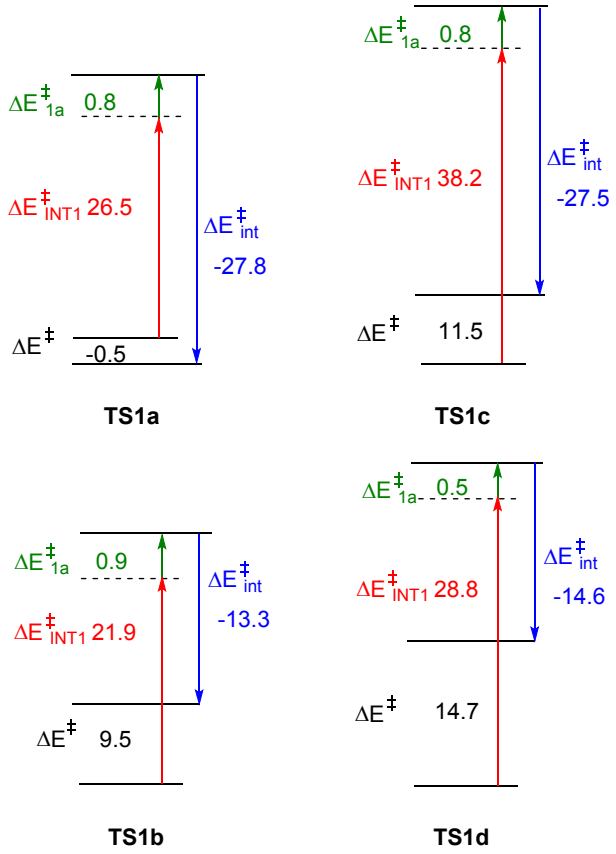



**Figure S2.** Distortion, interaction and activation energies for **TS1a** and **TS1c**, **TS1b** and **TS1d** (green arrow: distortion energy of substrate **1a**; red arrow: distortion energy of **INT1**; blue arrow: interaction energy; black: activation energy, in kcal/mol)

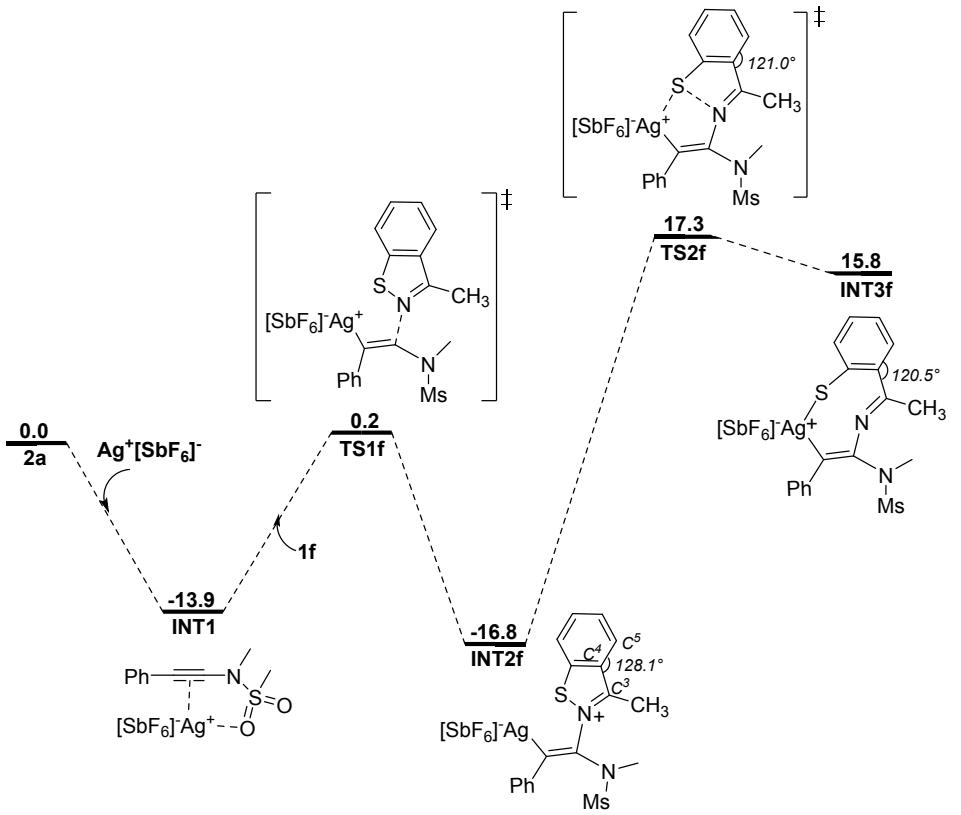



**Figure S3.** Energy profile (in kcal/mol) for the nucleophilic N-attack of **1f** with the silver-activated **2a** and subsequent S-N bond breaking.

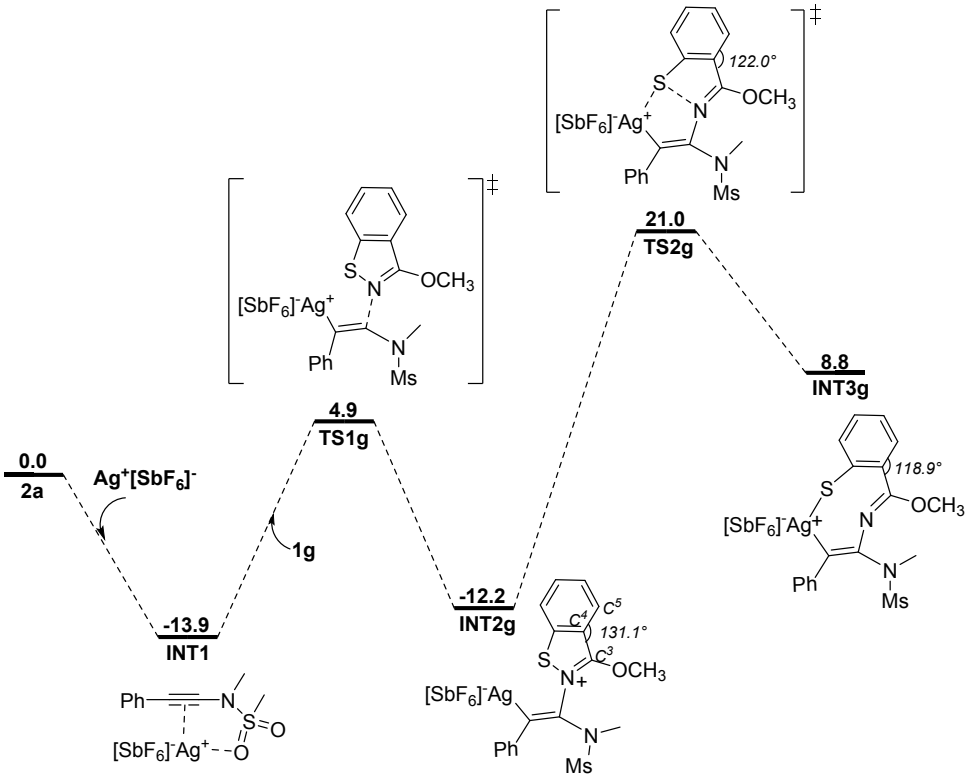



**Figure S4.** Energy profile (in kcal/mol) for the nucleophilic N-attack of **1g** with the silver-activated **2a** and subsequent S-N bond breaking.

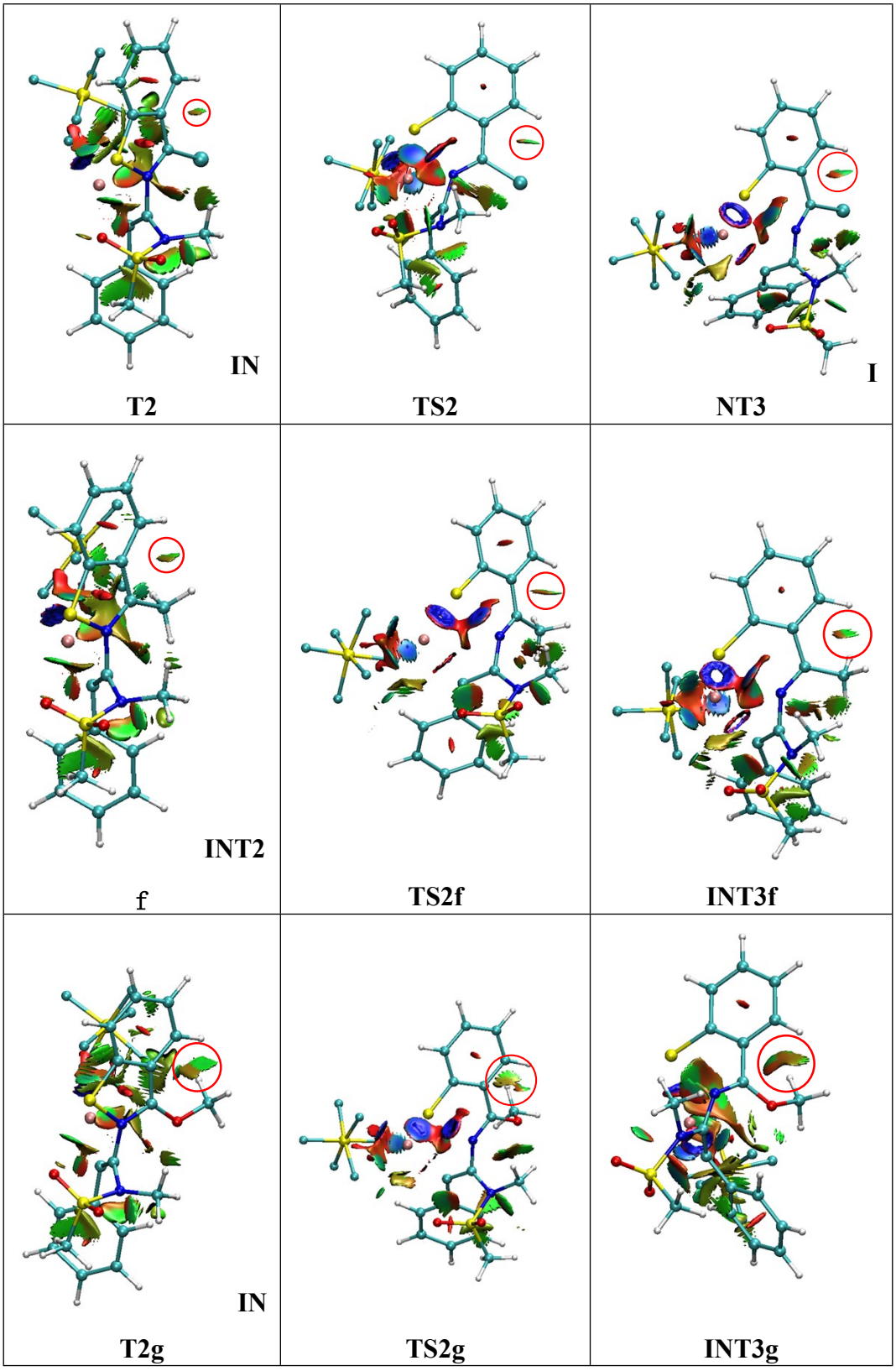
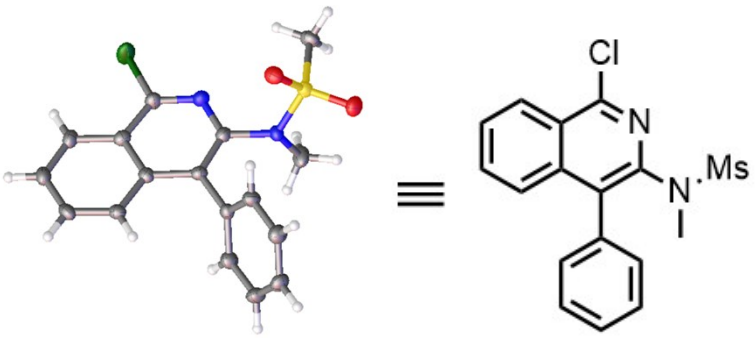



**Figure S5.** Non-covalent interaction analysis for the step of S-N bond cleavage for **INT2**, **INT2f**, and **INT2g**. The key steric repulsive interactions are highlighted by red circles (blue, attraction; green, weak interaction; red, steric effect).

## 4. X-ray Crystallographic Data of 3aa




---

Bond precision: C-C = 0.0043 A Wavelength=0.71073

Cell: a=31.7379(19) b=6.9825(4) c=42.976(3)
alpha=90 beta=92.976(2) gamma=90
Temperature: 120 K

| | Calculated | Reported |
|---|---|---|
| Volume | 9511.1(10) | 9511.0(10) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C17 H15 Cl N2 O2 S | 6(C17 H15 Cl N2 O2 S) |
| Sum formula | C17 H15 Cl N2 O2 S | C102 H90 C16 N12 O12 S6 |
| Mr | 346.82 | 2080.91 |
| Dx,g cm-3 | 1.453 | 1.453 |
| Z | 24 | 4 |
| Mu (mm-1) | 0.383 | 0.383 |
| F000 | 4320.0 | 4320.0 |
| F000' | 4328.08 | |
| h,k,lmax | 41,9,55 | 41,9,55 |
| Nref | 21890 | 21857 |
| Tmin,Tmax | | 0.586,0.746 |
| Tmin' | | |

Correction method= # Reported T Limits: Tmin=0.586 Tmax=0.746
AbsCorr = NONE

Data completeness= 0.998 Theta(max)= 27.538

R(reflections)= 0.0564( 13144) wR2(reflections)= 0.1591( 21857)

S = 1.051 Npar= 1255

---

## 5. X-ray diffraction analysis of $S_8$

Elemental sulfur was isolation by column chromatography (PE/EA, 10:1) as pale-yellow solid, $R_f$ = 0.95 (PE/EA, 10:1).

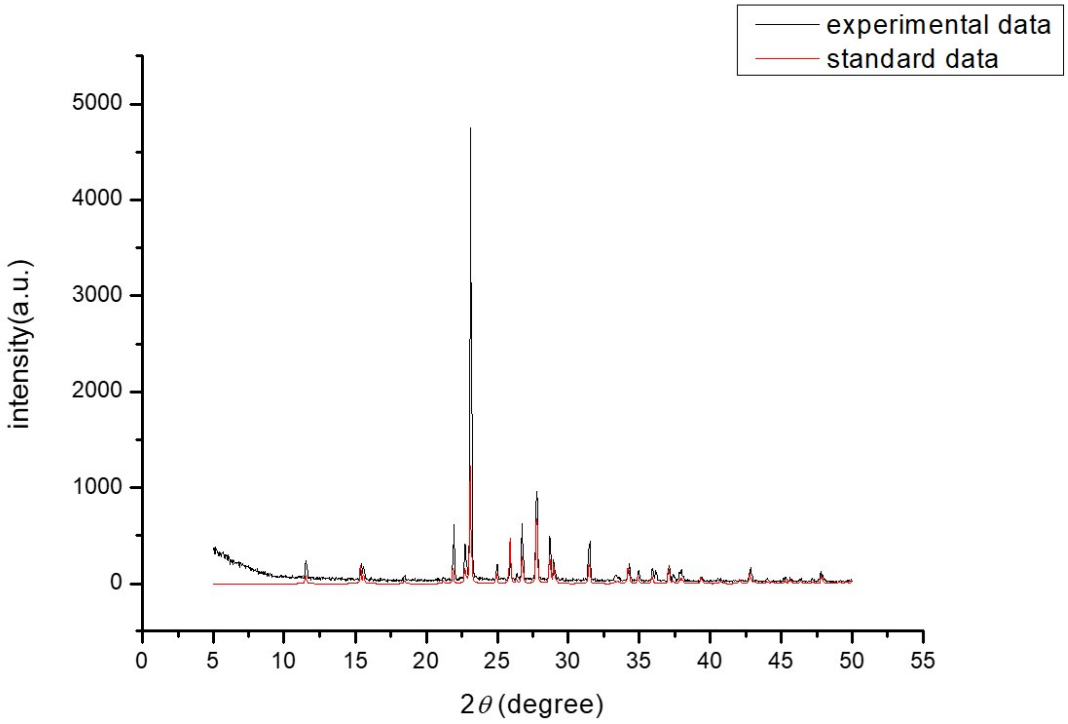
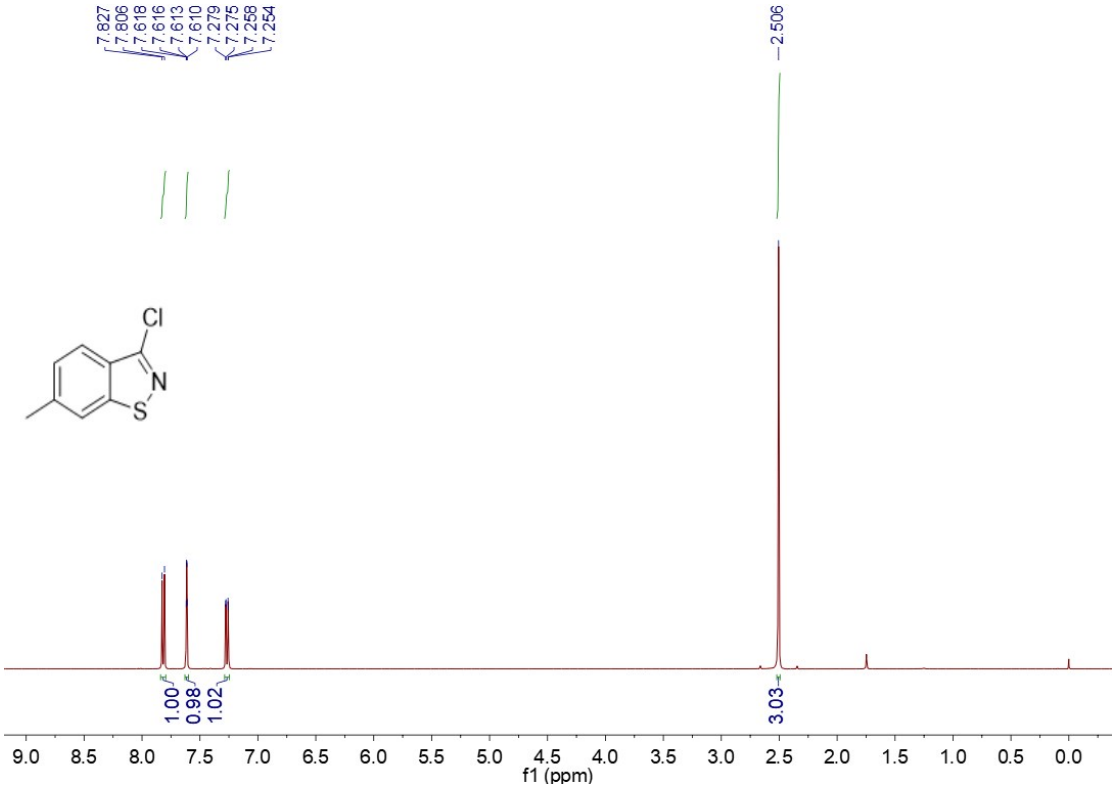
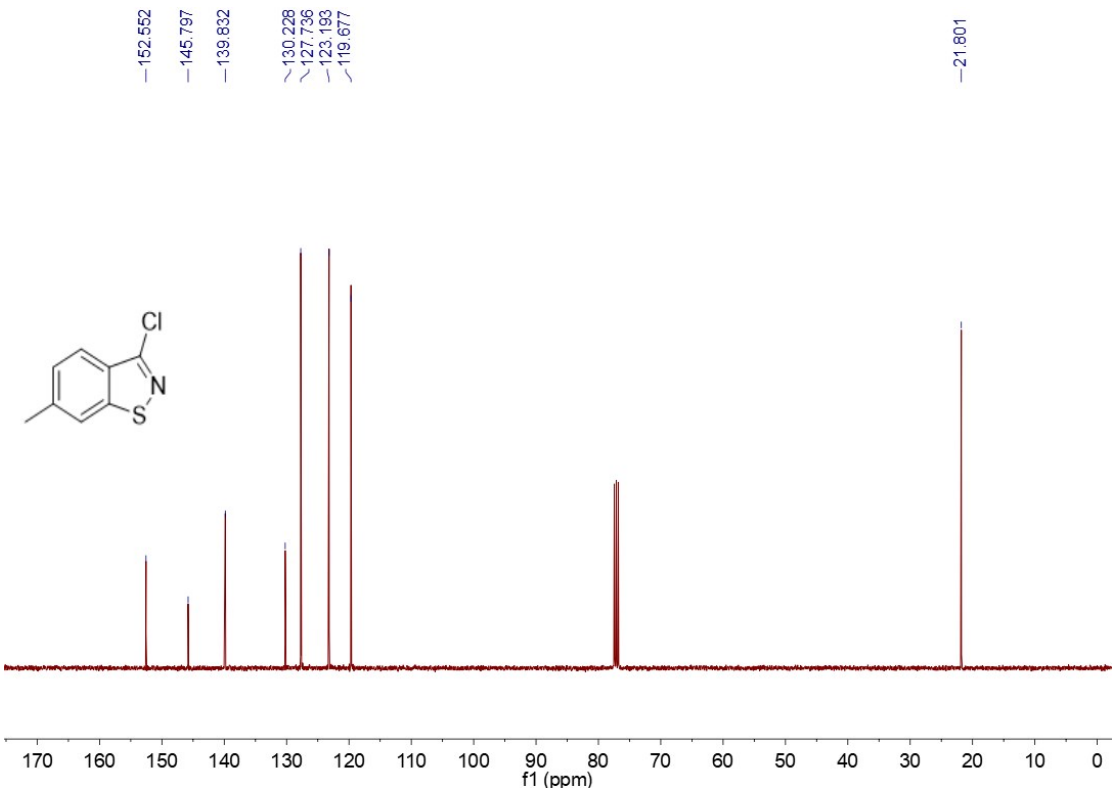
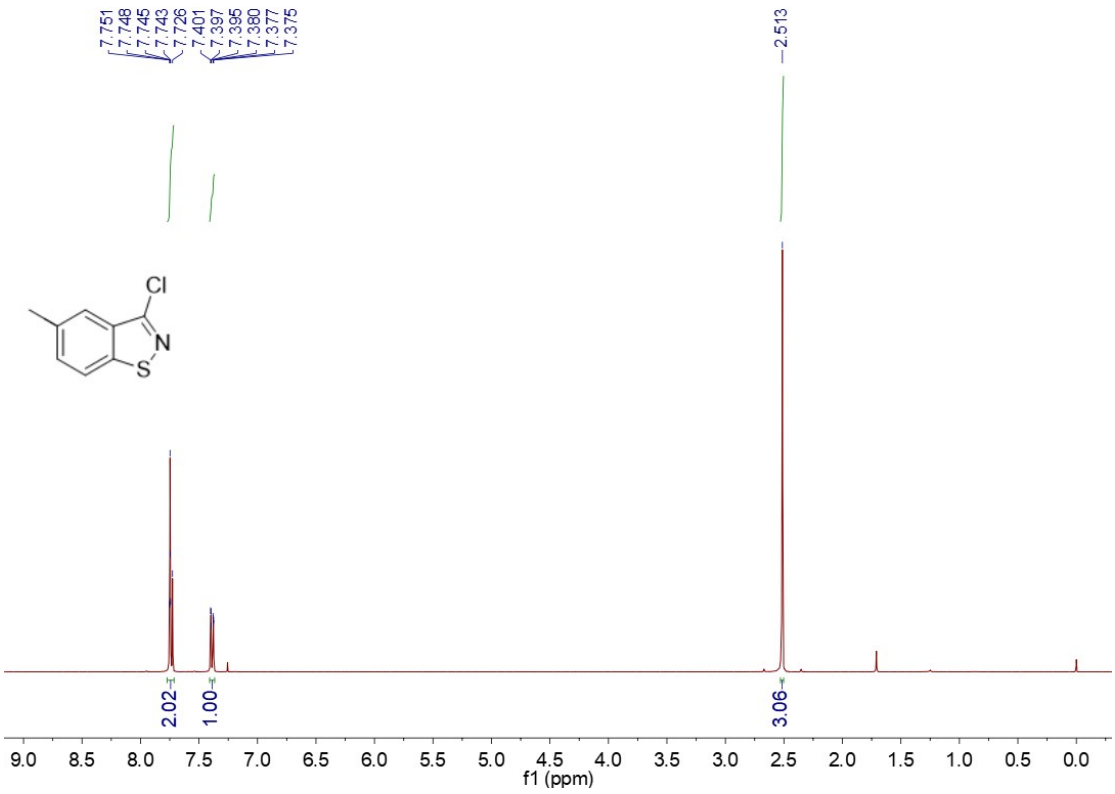


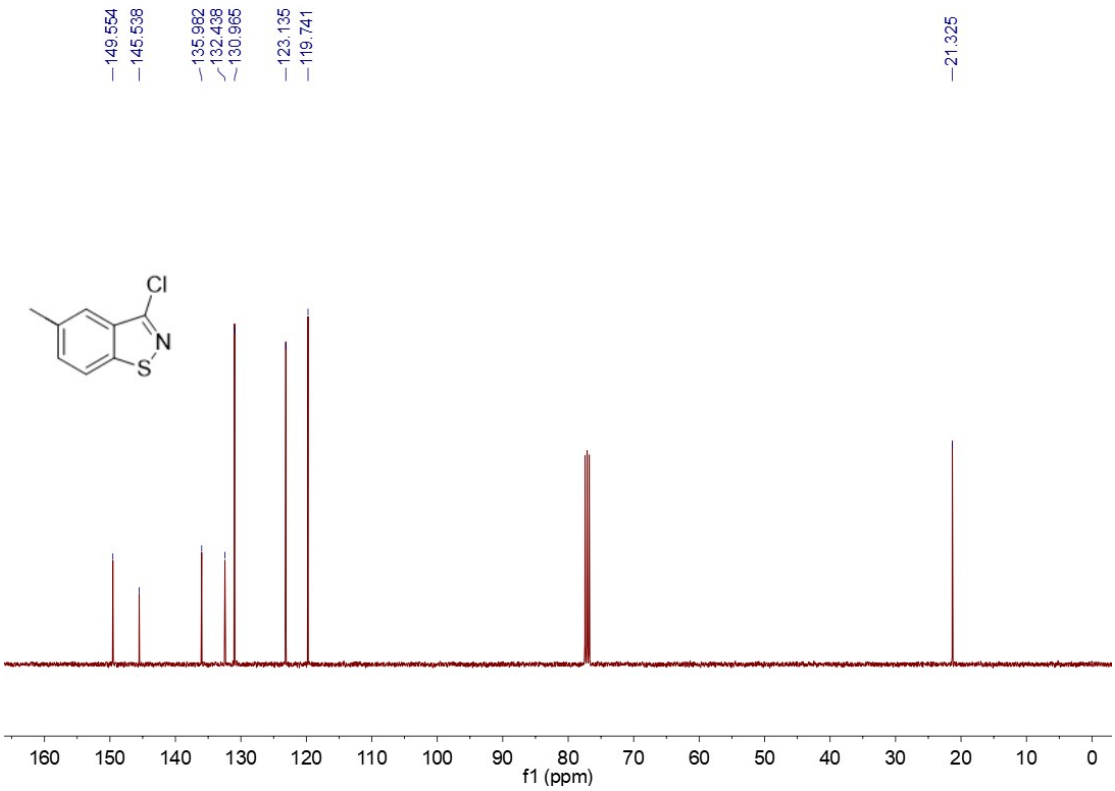

**Figure S6**. X-ray diffraction spectrum of isolated elemental sulfur.

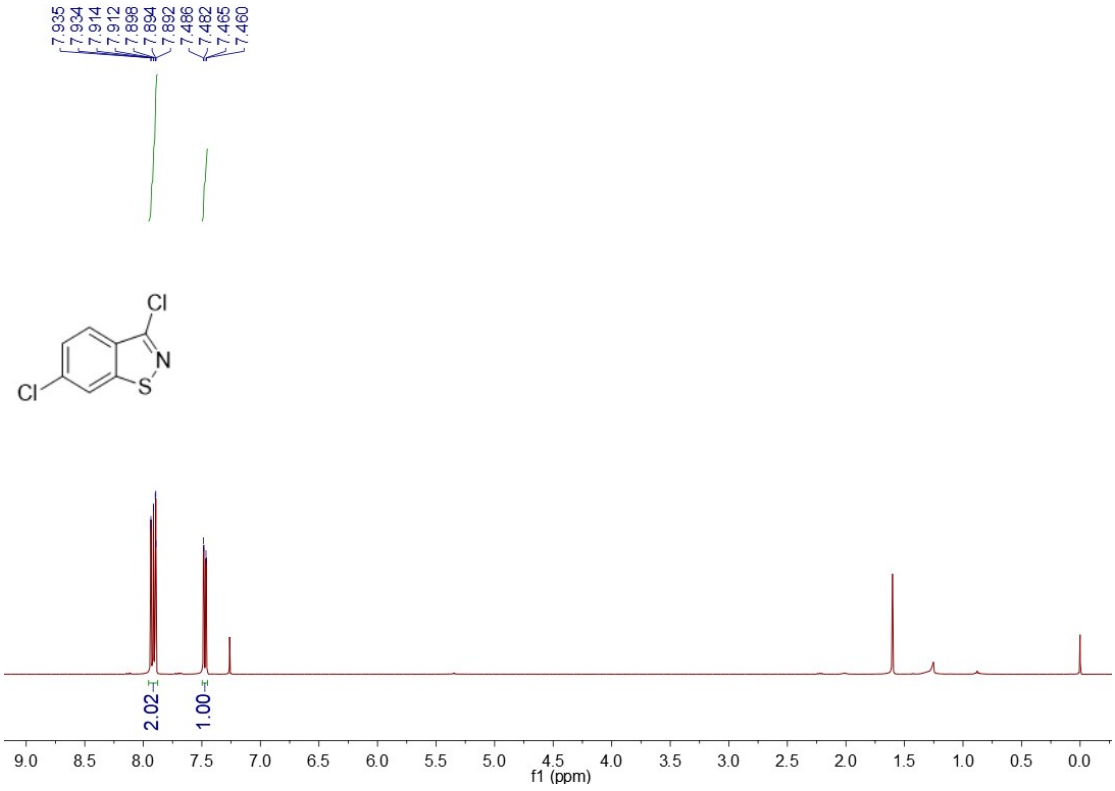
## 6. NMR Spectra




7.751
7.748
7.745
7.743
7.726
7.401
7.397
7.395
7.380
7.377
7.375
2.513
Cl
N
S
2.02
1.00
3.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


149.554
145.538
135.982
132.438
130.965
123.135
119.741
21.325
Cl
N
S
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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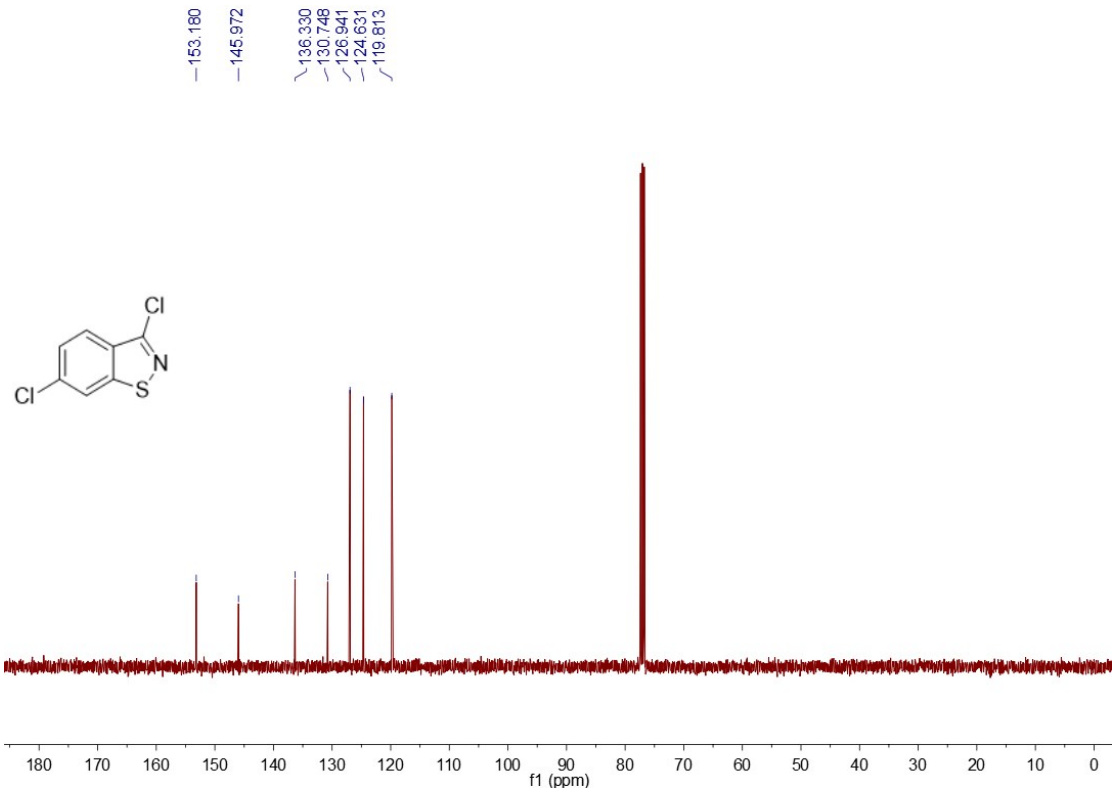
7.934
7.914
7.912
7.898
7.894
7.892
7.486
7.482
7.465
7.460
Cl
N
S
Cl
2.02
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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136.330
130.748
126.941
124.631
119.813
Cl
N
S
Cl
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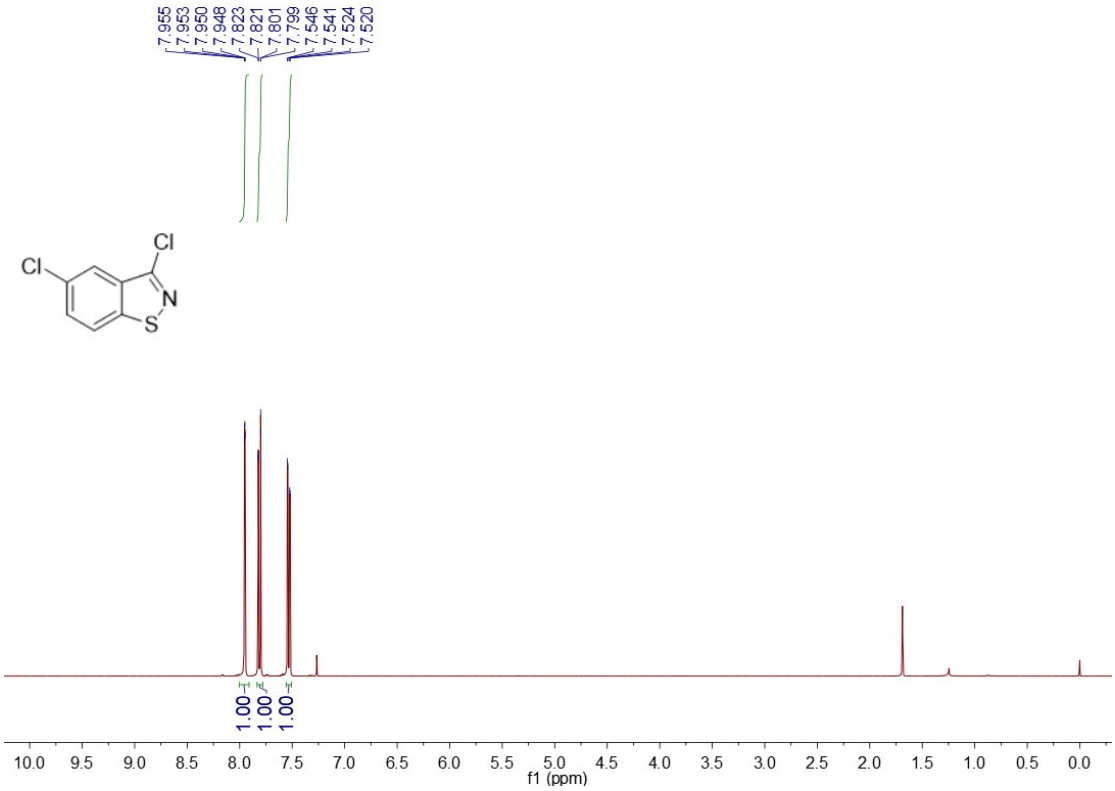
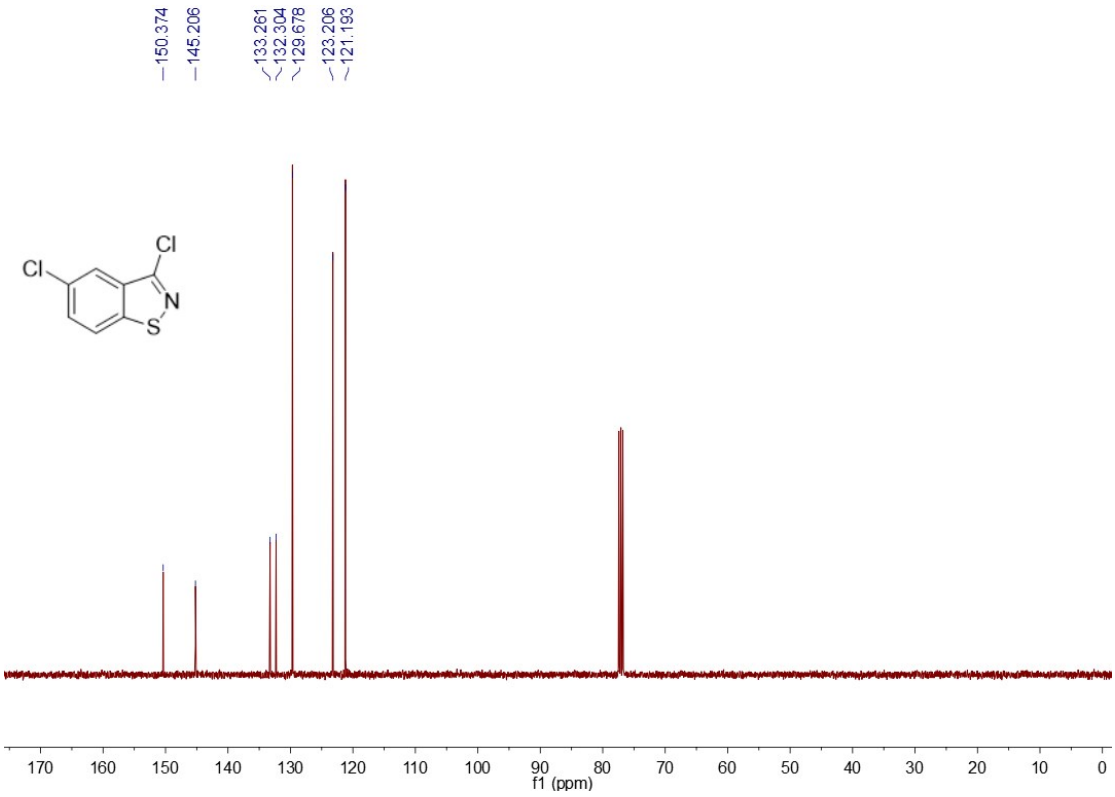
f1 (ppm)


7.955
7.953
7.950
7.948
7.823
7.821
7.801
7.799
7.546
7.541
7.524
7.520
Cl
Cl
N
S
1.00
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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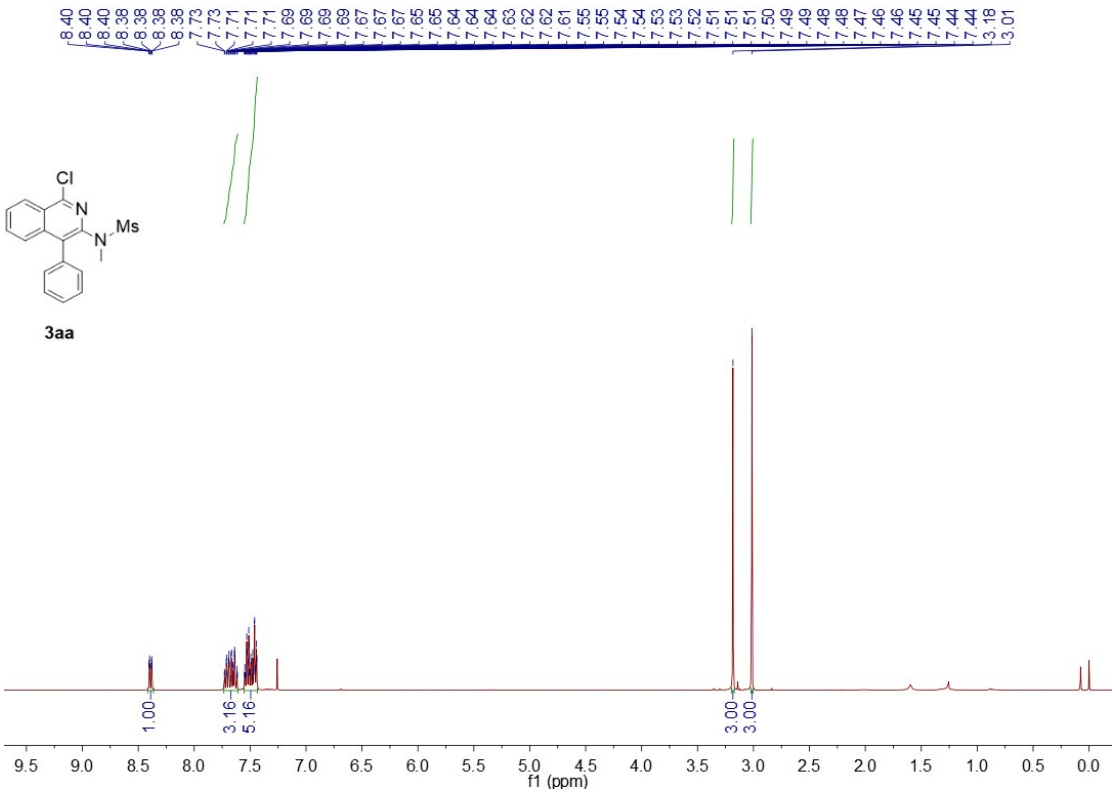
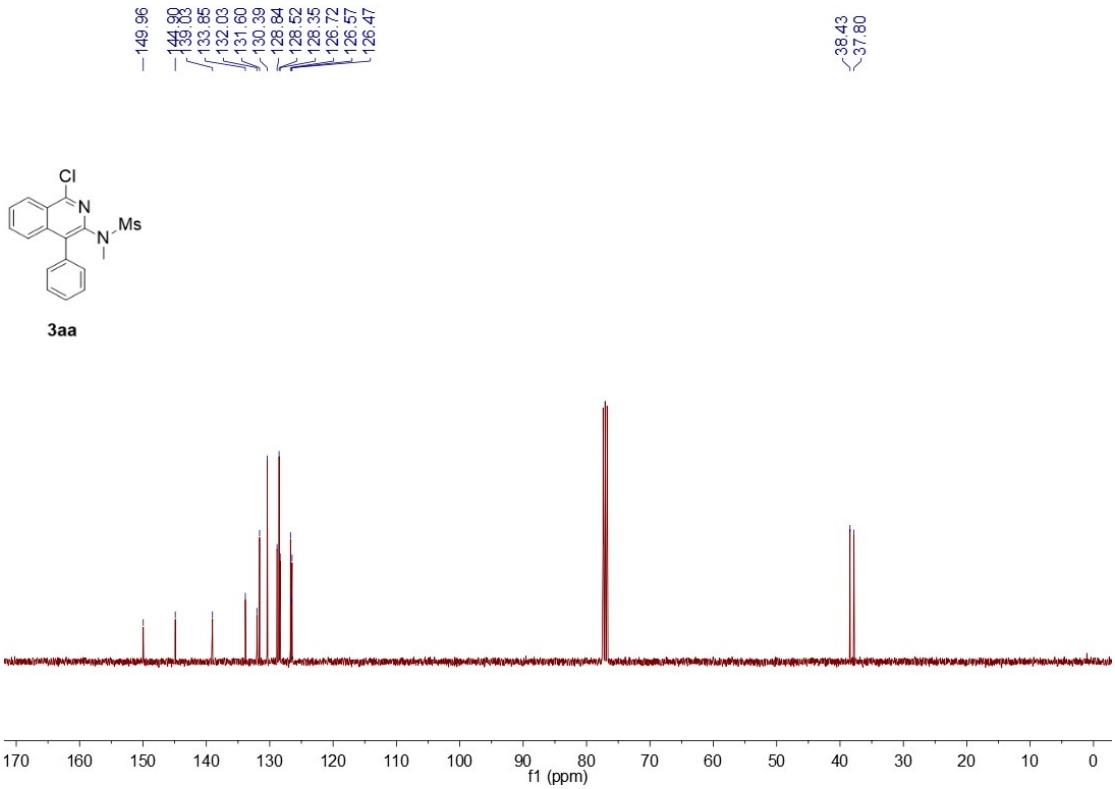
145.206
133.261
132.304
129.678
123.206
121.193
Cl
Cl
N
S
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.40 8.40 8.40 8.38 8.38 8.38 8.38 7.73 7.73 7.71 7.71 7.71 7.69 7.69 7.69 7.69 7.67 7.67 7.67 7.65 7.65 7.64 7.64 7.64 7.63 7.62 7.62 7.61 7.55 7.55 7.54 7.54 7.53 7.53 7.52 7.51 7.51 7.51 7.50 7.49 7.49 7.48 7.48 7.47 7.46 7.46 7.45 7.45 7.44 7.44 3.18 3.01
Cl
N
N
Ms
3aa
1.00
3.16
5.16
3.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.03
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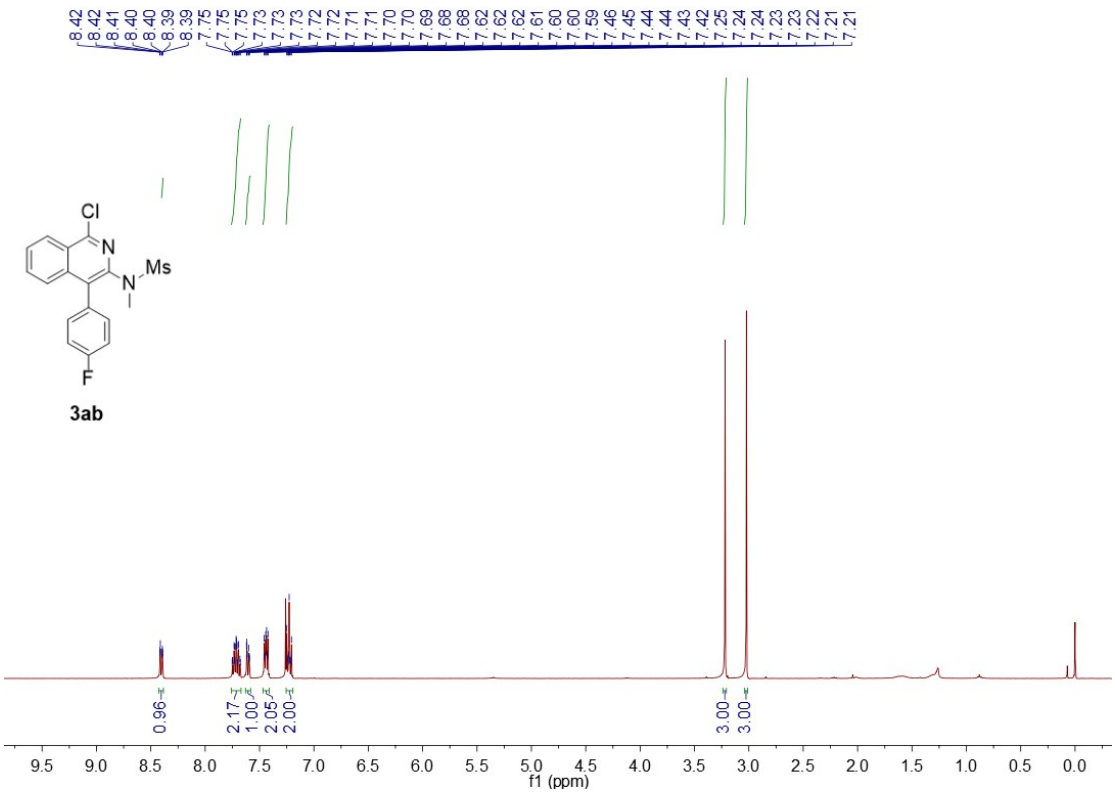
130.39
128.84
128.52
128.35
126.72
126.57
126.47
38.43
37.80
Cl
N
N
Ms
3aa
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.45
7.44
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7.25
7.24
7.24
7.23
7.23
7.22
7.21
7.21
Cl
N
N
Ms
F
3ab
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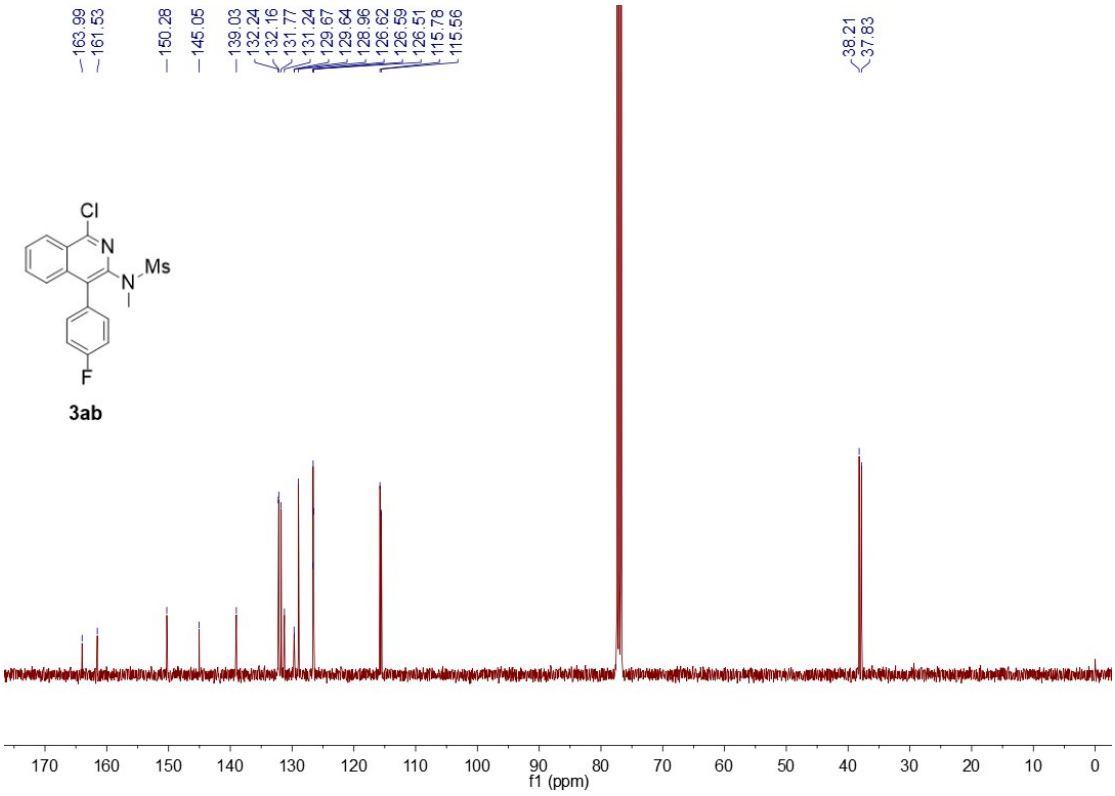
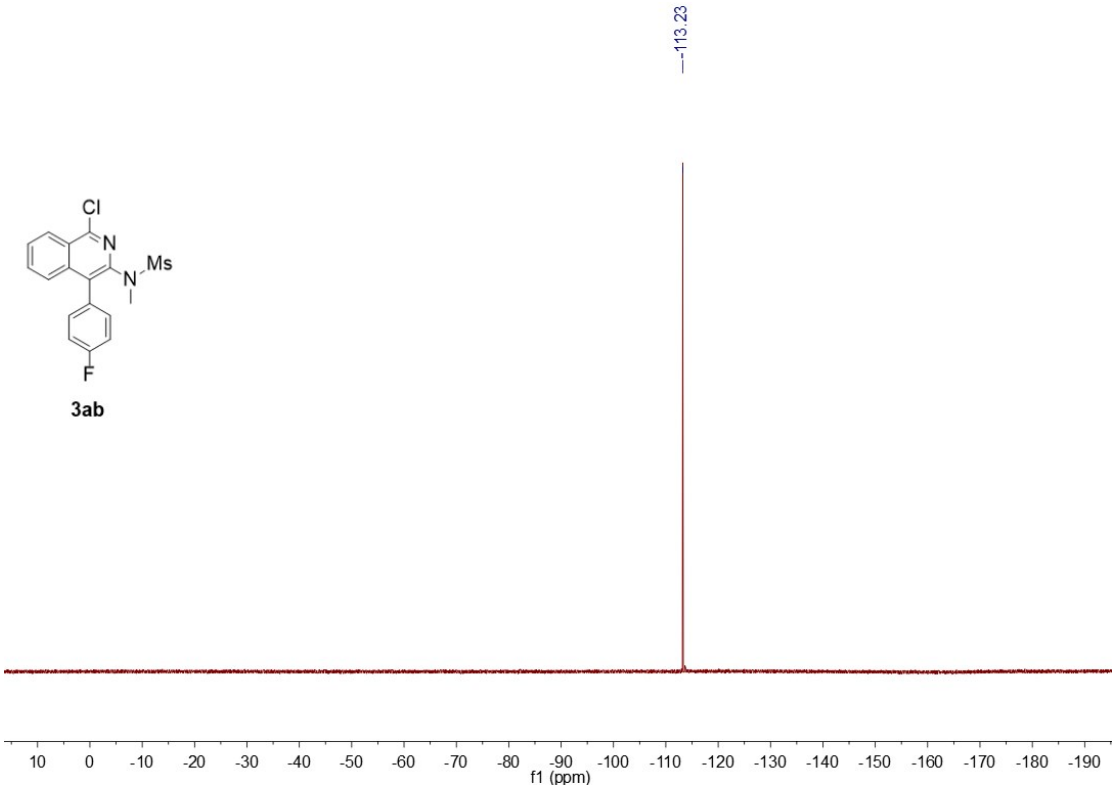
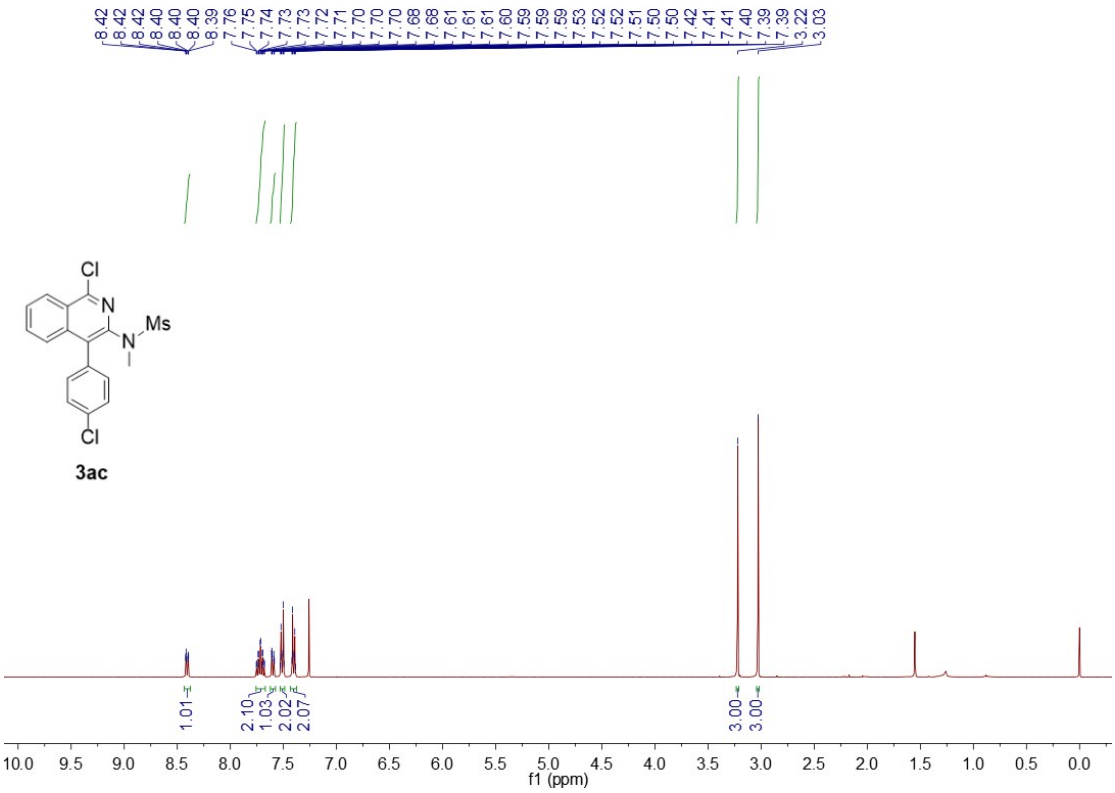
2.17
1.00
2.05
2.00
3.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

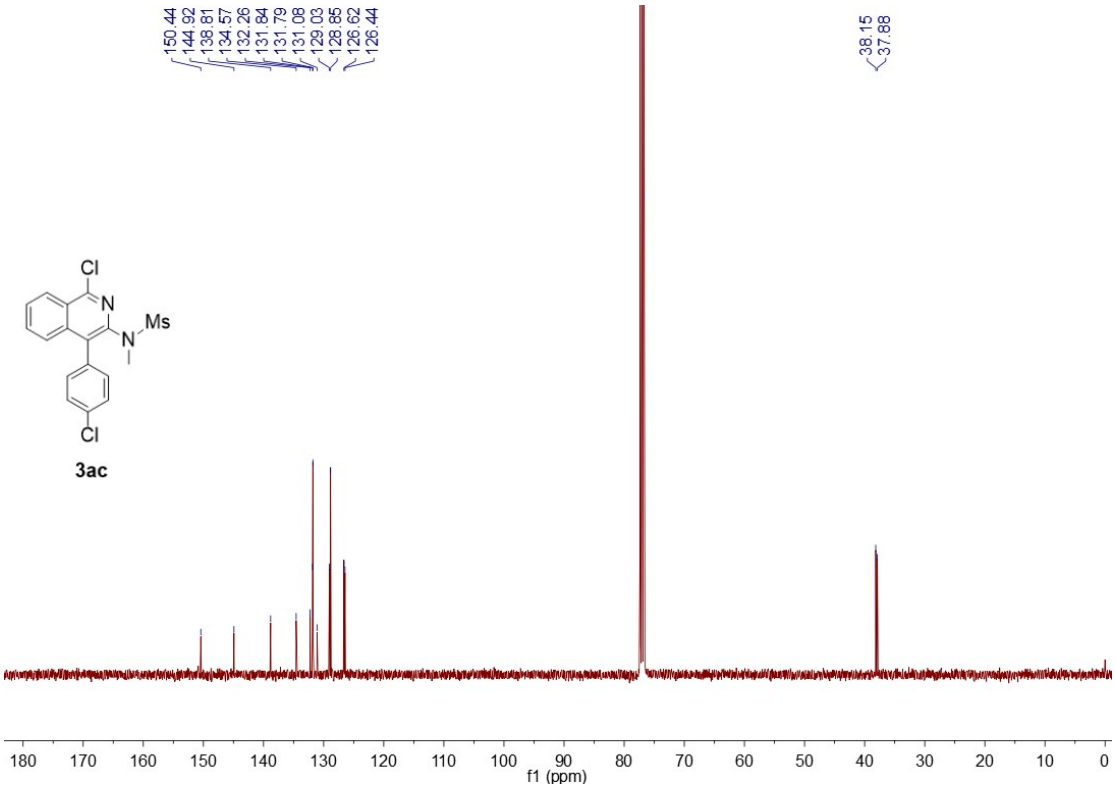

163.99
161.53
150.28
145.05
139.03
132.24
132.16
131.77
131.24
129.67
129.64
128.96
126.62
126.59
126.51
115.78
115.56
38.21
37.83
Cl
N
N
Ms
F
3ab
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-113.23
Cl
N
N
Ms
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

**3ab**


8.42 8.42 8.40 8.40 8.40 8.39 7.76 7.75 7.74 7.73 7.73 7.72 7.71 7.70 7.70 7.70 7.68 7.68 7.61 7.61 7.61 7.60 7.59 7.59 7.59 7.53 7.52 7.52 7.51 7.50 7.50 7.42 7.41 7.41 7.40 7.39 7.39 3.22 3.03
Cl
N
N
Ms
Cl
1.01 2.10 1.03 2.02 2.07 3.00 3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

**3ac**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144.92
138.81
134.57
132.26
131.84
131.79
131.08
129.03
128.85
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126.44
38.15
37.88
Cl
N
N
Ms
Cl
3ac
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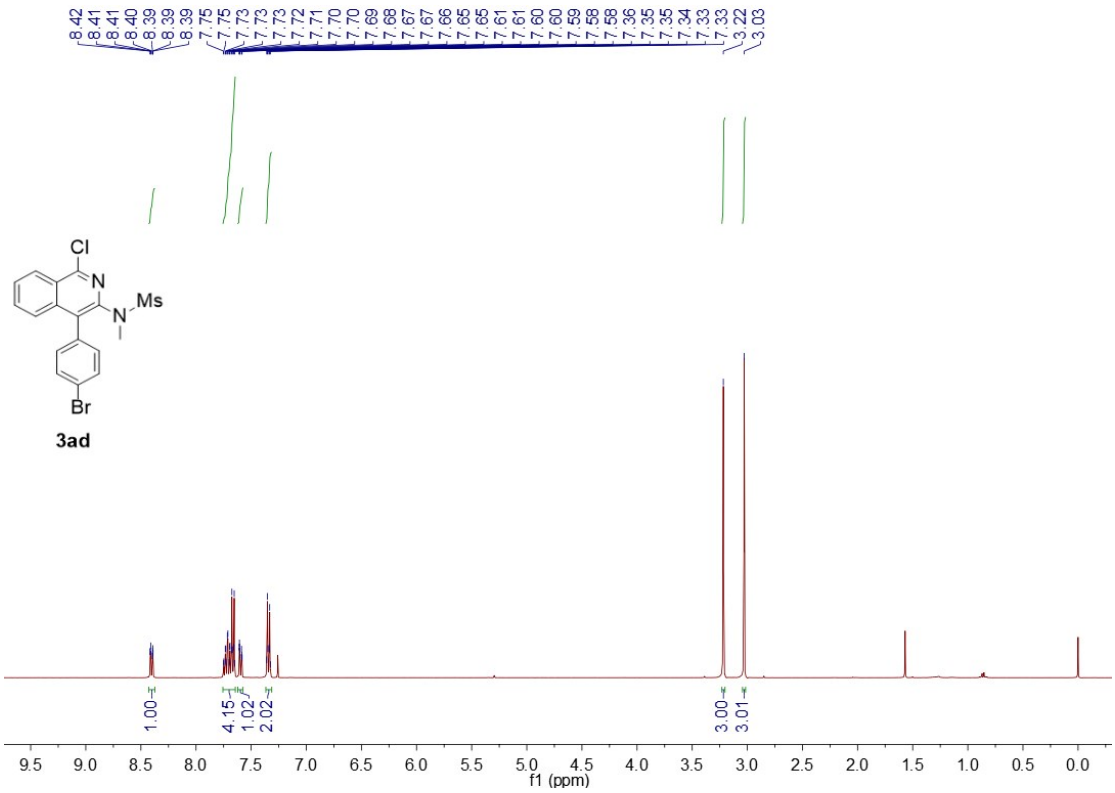
f1 (ppm)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8.39
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8.39
7.75
7.75
7.73
7.73
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7.70
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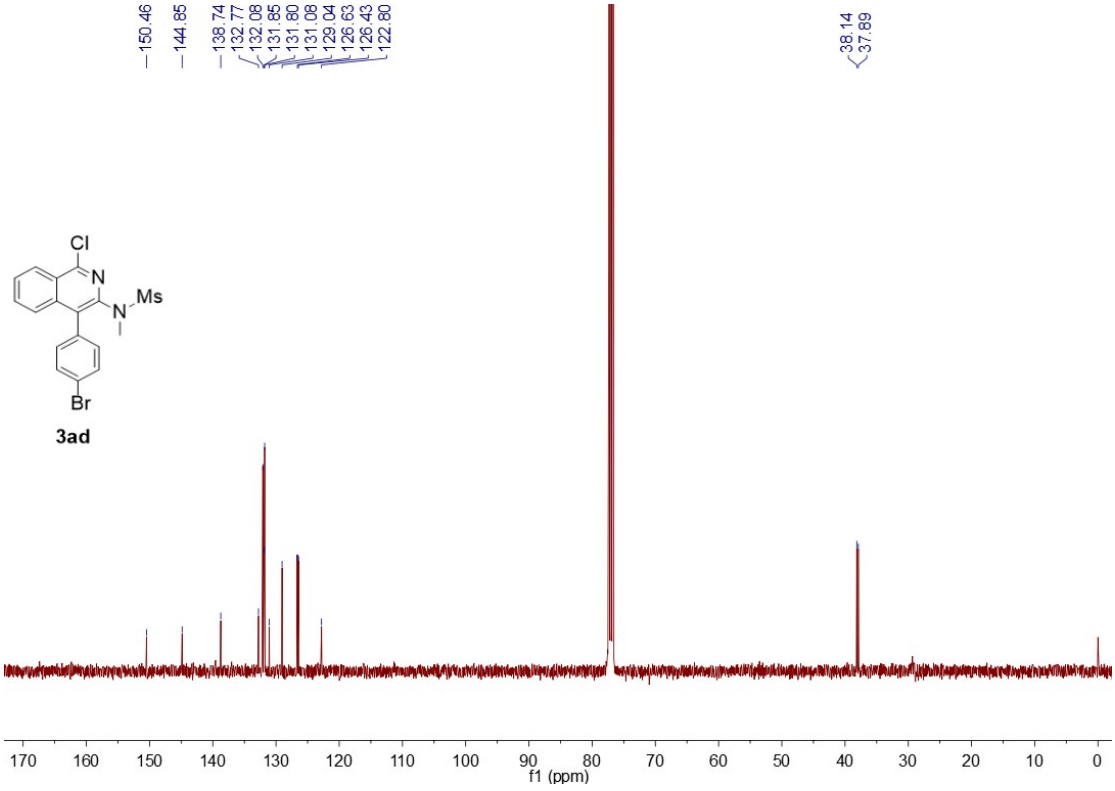
7.61
7.60
7.60
7.59
7.58
7.58
7.36
7.35
7.34
7.33
7.33
3.22
3.03
Cl
N
N
Ms
Br
3ad
1.00
4.15
1.02
2.02
3.00
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


150.46
144.85
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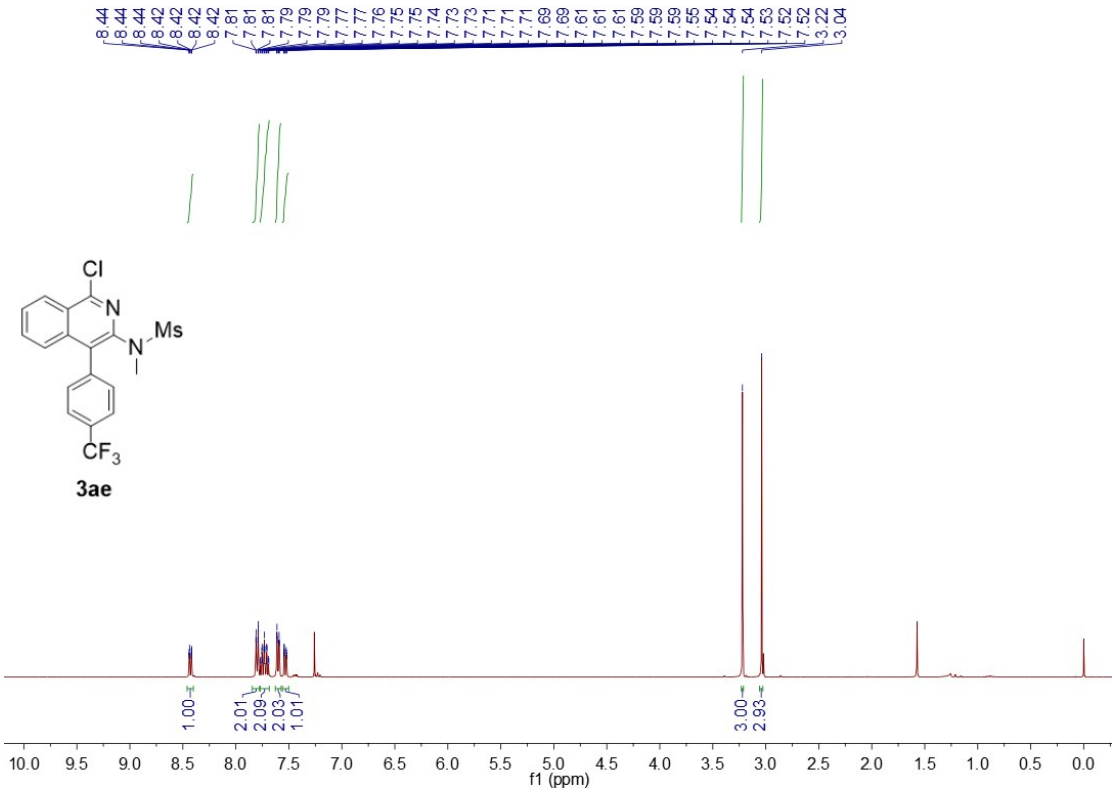
132.77
132.08
131.85
131.80
131.08
129.04
126.63
126.43
122.80
38.14
37.89
Cl
N
Ms
N
Br
3ad
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.44
8.44
8.44
8.42
8.42
8.42
7.81
7.81
7.79
7.79
7.79
7.77
7.77
7.76
7.75
7.75
7.74
7.73
7.73
7.71
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7.55
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7.54
7.54
7.53
7.52
7.52
3.22
3.04
Cl
N
Ms
N
CF3
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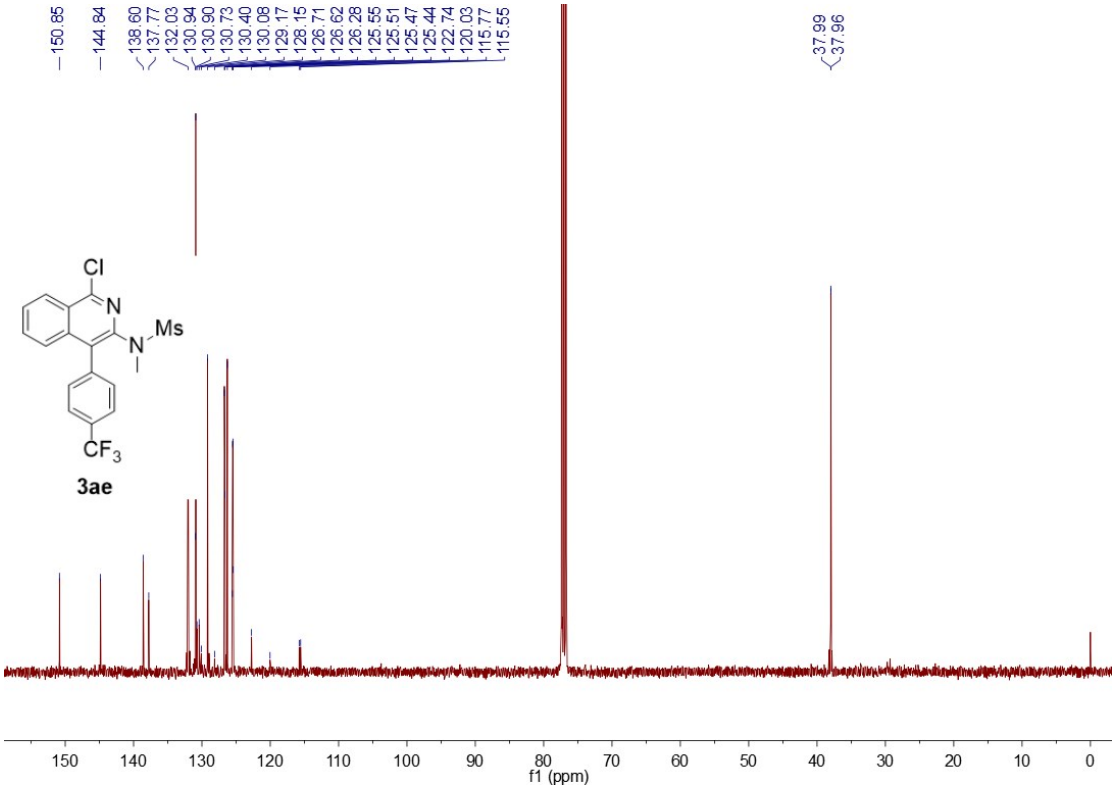
2.01
2.09
2.03
1.01
3.00
2.93
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


150.85
144.84
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137.77
132.03
130.94
130.90
130.73
130.40
130.08
129.17
128.15
126.71
126.62
126.28
125.55
125.51
125.47
125.44
122.74
120.03
115.77
115.55
37.99
37.96
Cl
N
Ms
N
CF3
3ae
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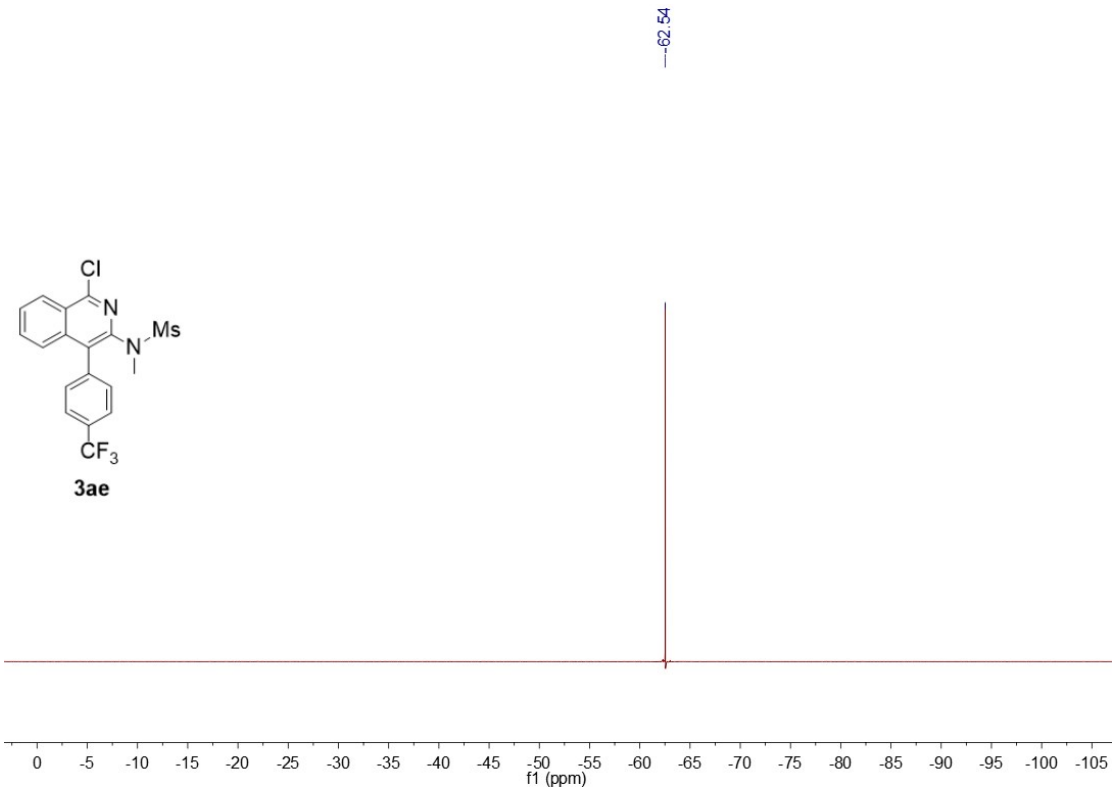
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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Ms
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CF3
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-5
-10
-15
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-25
-30
-35
-40
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-50
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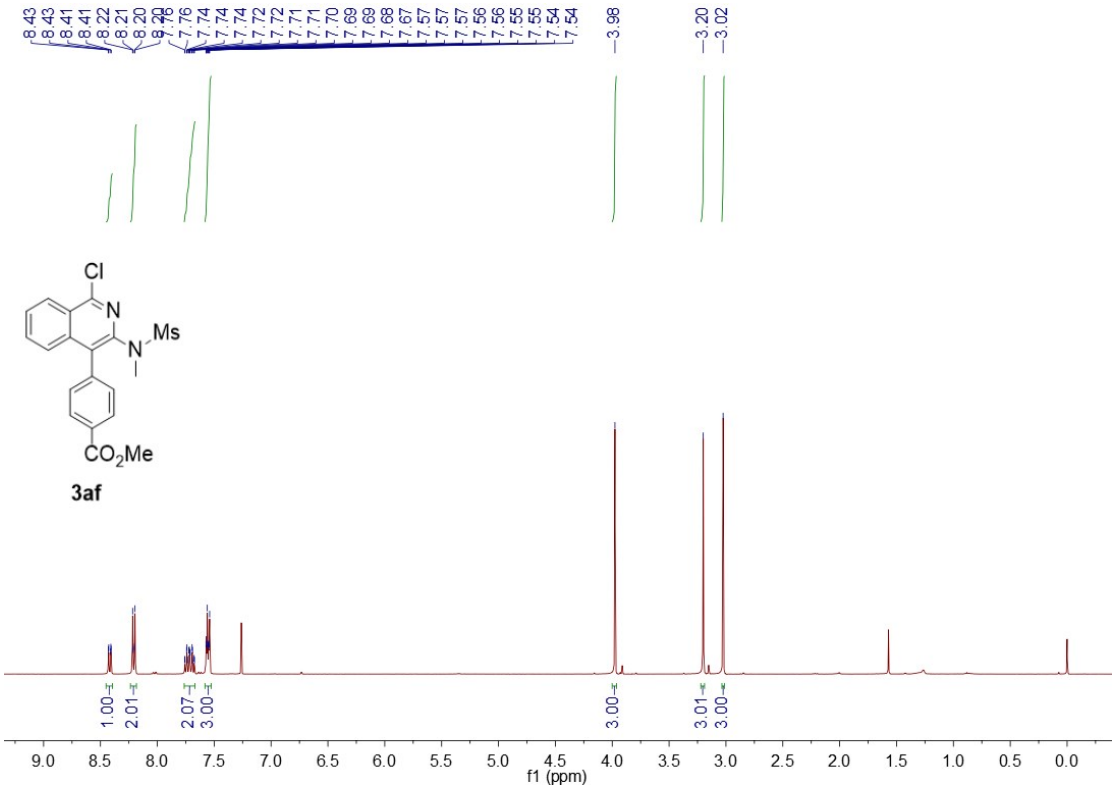
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
f1 (ppm)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7.72
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7.69
7.68
7.67
7.57
7.56
7.55
7.54
3.98
3.20
3.02
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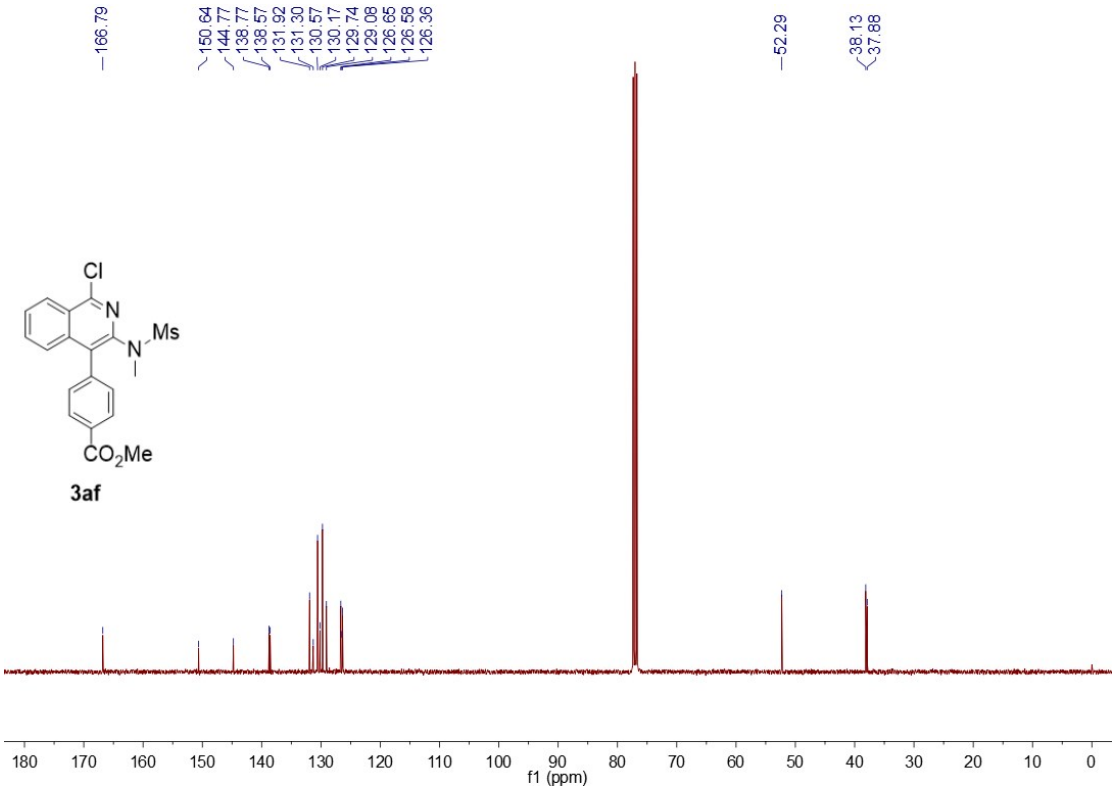
Ms
N
CO2Me
3af
1.00
2.01
2.07
3.00
3.00
3.01
3.00
f1 (ppm)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129.74
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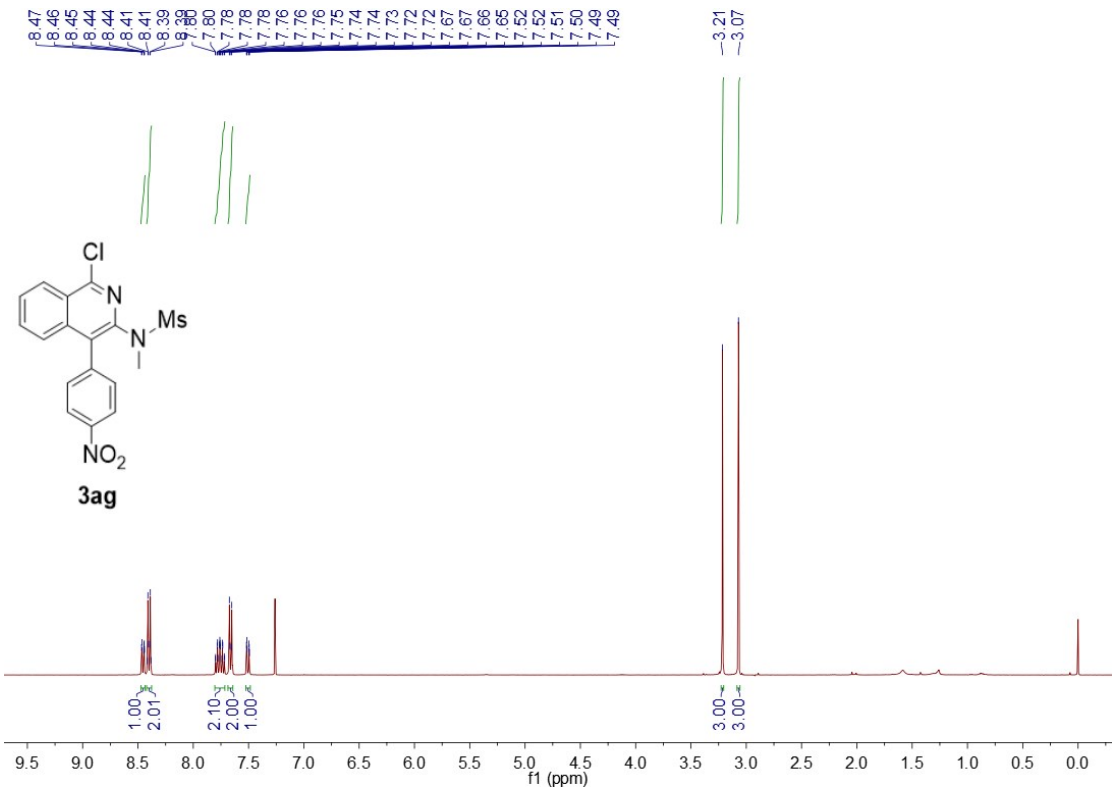
126.36
52.29
38.13
37.88
Cl
N
Ms
N
CO2Me
3af
f1 (ppm)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7.76
7.75
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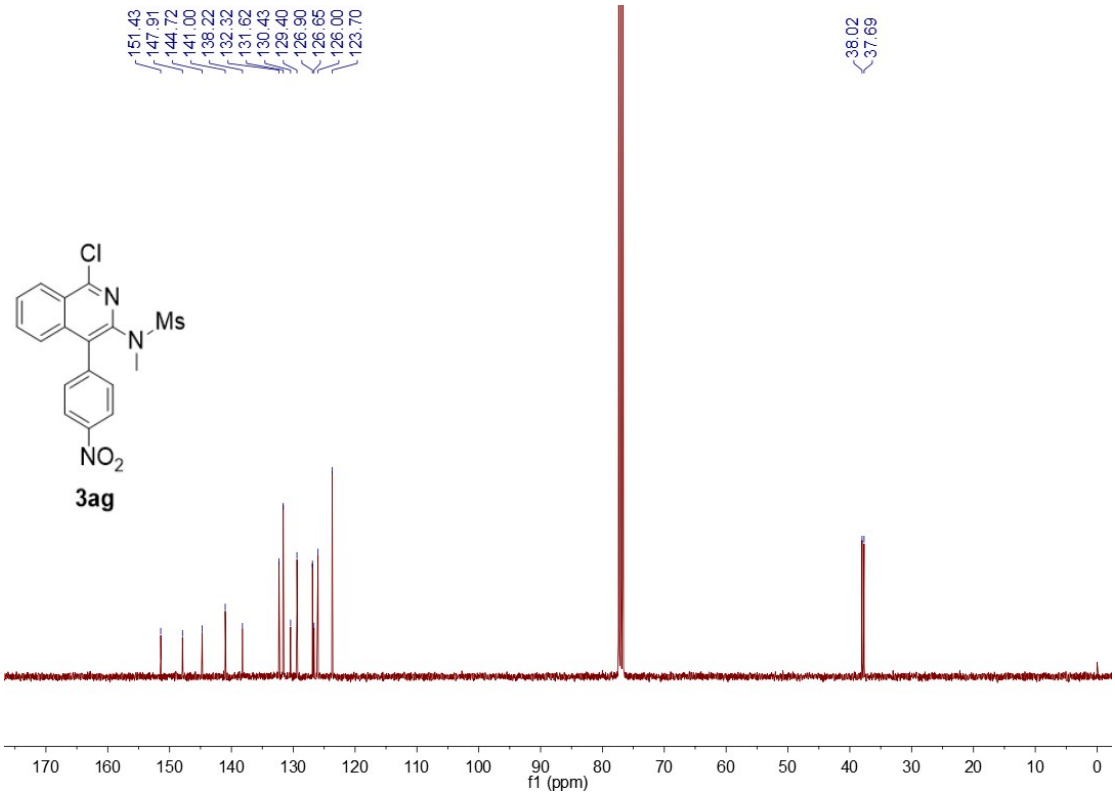
7.73
7.72
7.72
7.67
7.66
7.65
7.52
7.52
7.51
7.50
7.49
7.49
3.21
3.07
Cl
N
N
Ms
NO2
3ag
1.00
2.01
2.10
2.00
1.00
3.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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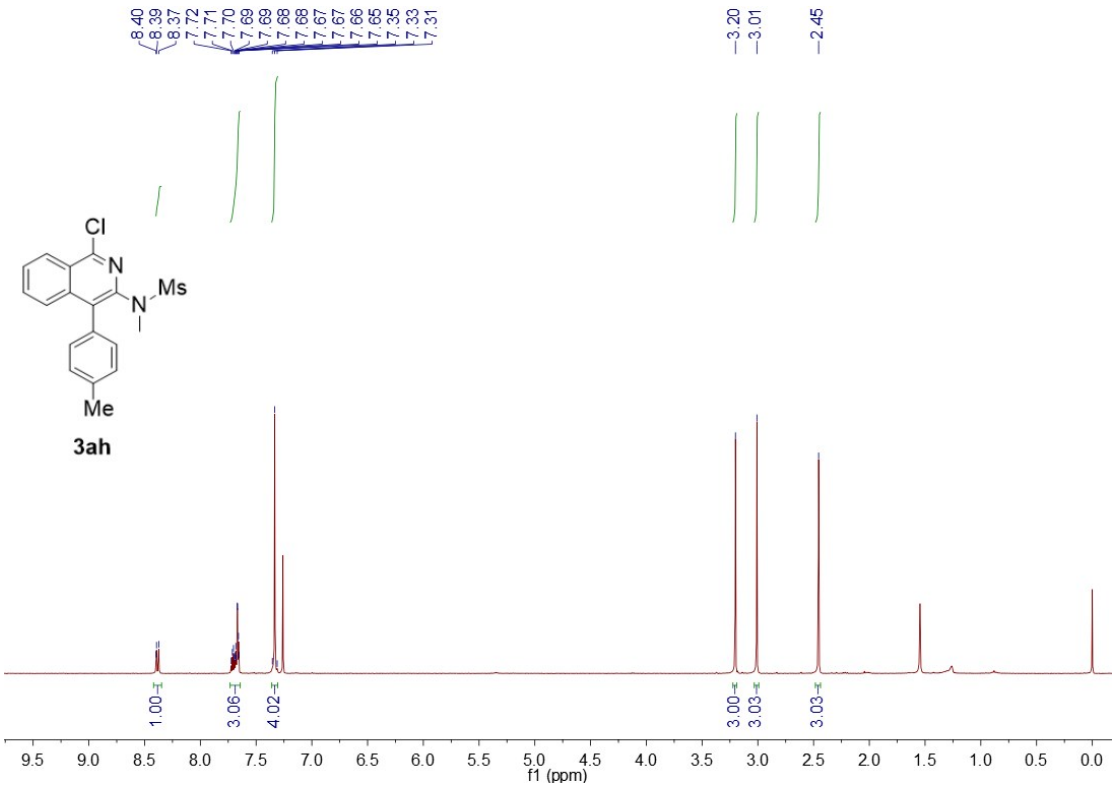
126.90
126.65
126.00
123.70
38.02
37.69
Cl
N
N
Ms
NO2
3ag
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.39
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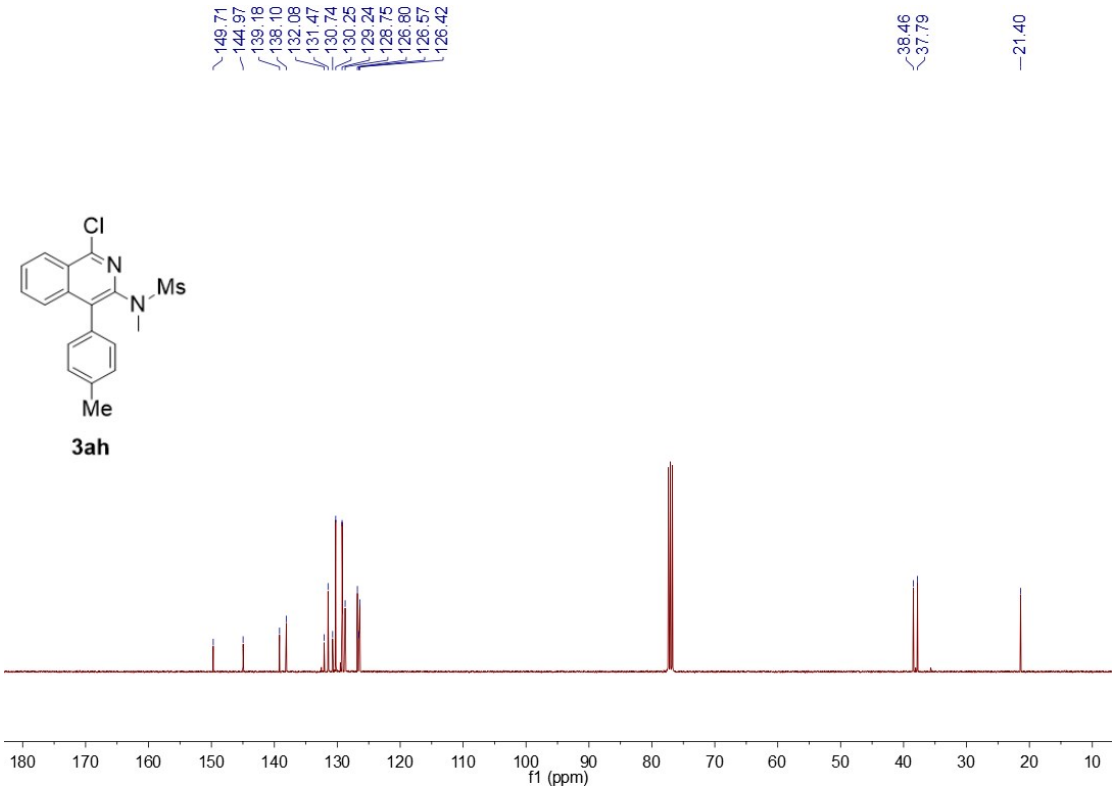
7.69
7.69
7.68
7.68
7.67
7.67
7.66
7.65
7.35
7.33
7.31
3.20
3.01
2.45
Cl
N
Ms
N
Me
1.00
3.06
4.02
3.00
3.03
3.03
f1 (ppm)

**3ah**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38.46
37.79
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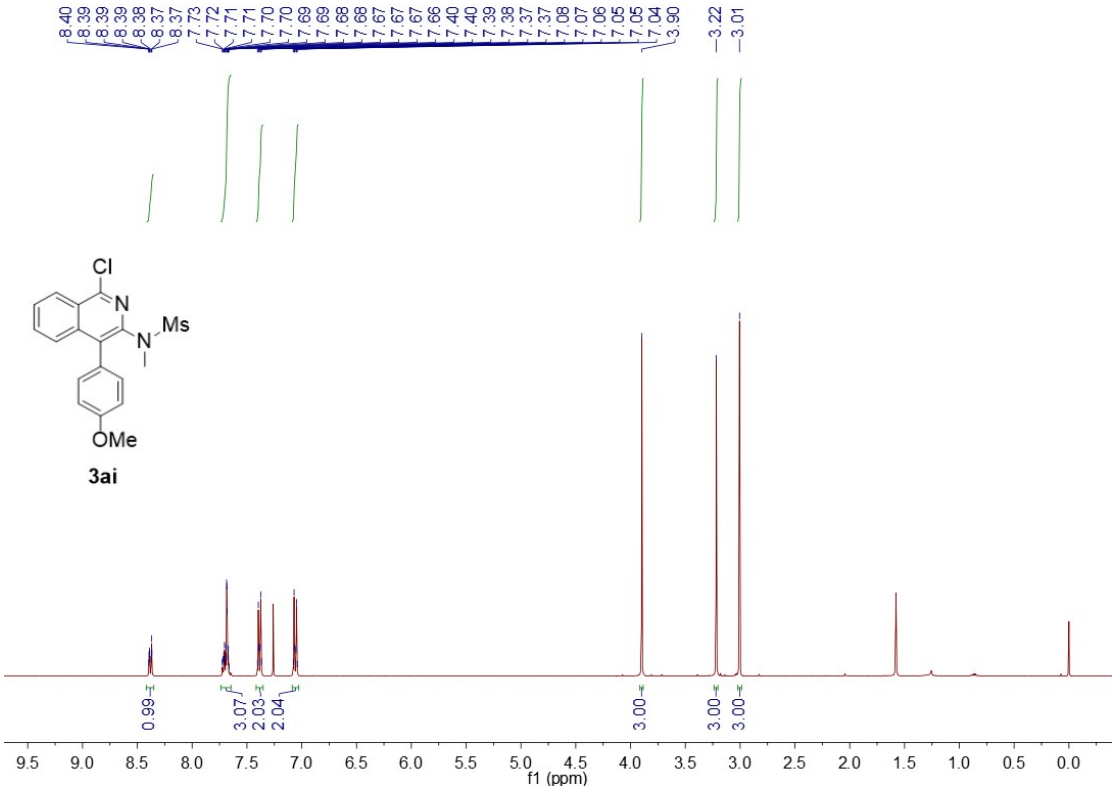
Ms
N
Me
f1 (ppm)

**3ah**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7.71
7.71
7.70
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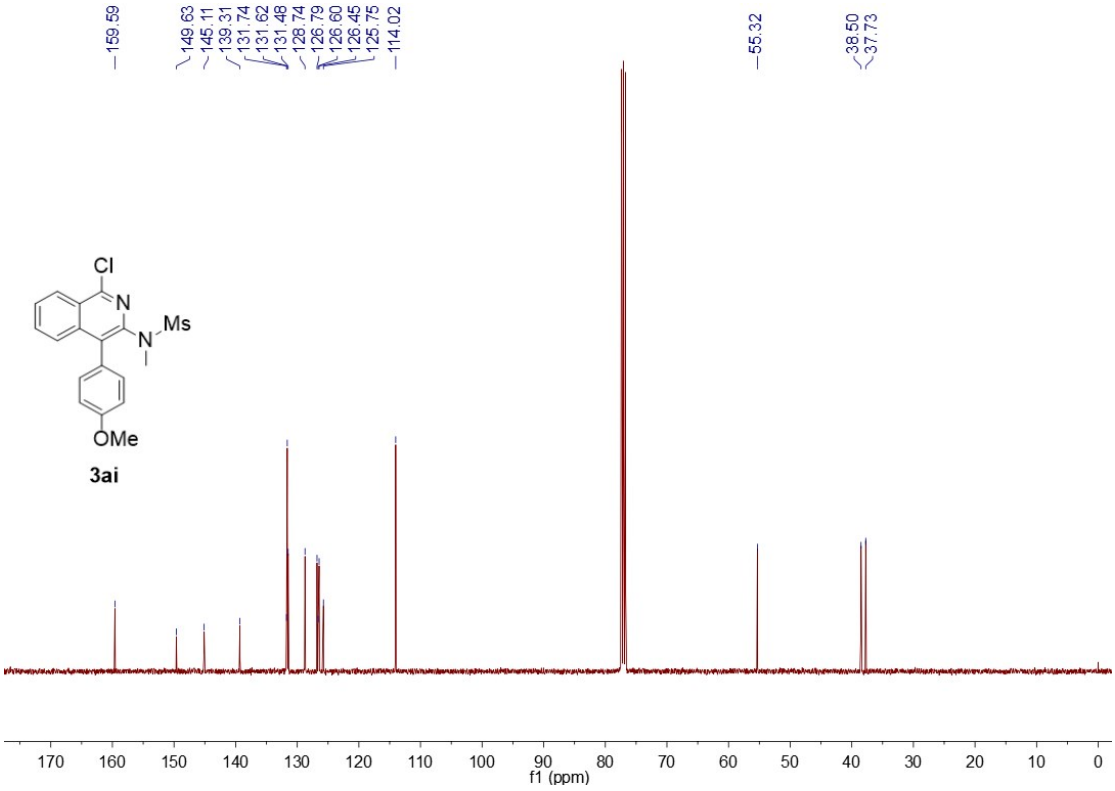
7.69
7.69
7.68
7.68
7.67
7.67
7.67
7.66
7.40
7.40
7.39
7.38
7.37
7.37
7.08
7.07
7.06
7.05
7.05
7.04
3.90
3.22
3.01
Cl
N
N
Ms
OMe
3ai
0.99
3.07
2.03
2.04
3.00
3.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.62
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128.74
126.79
126.60
126.45
125.75
114.02
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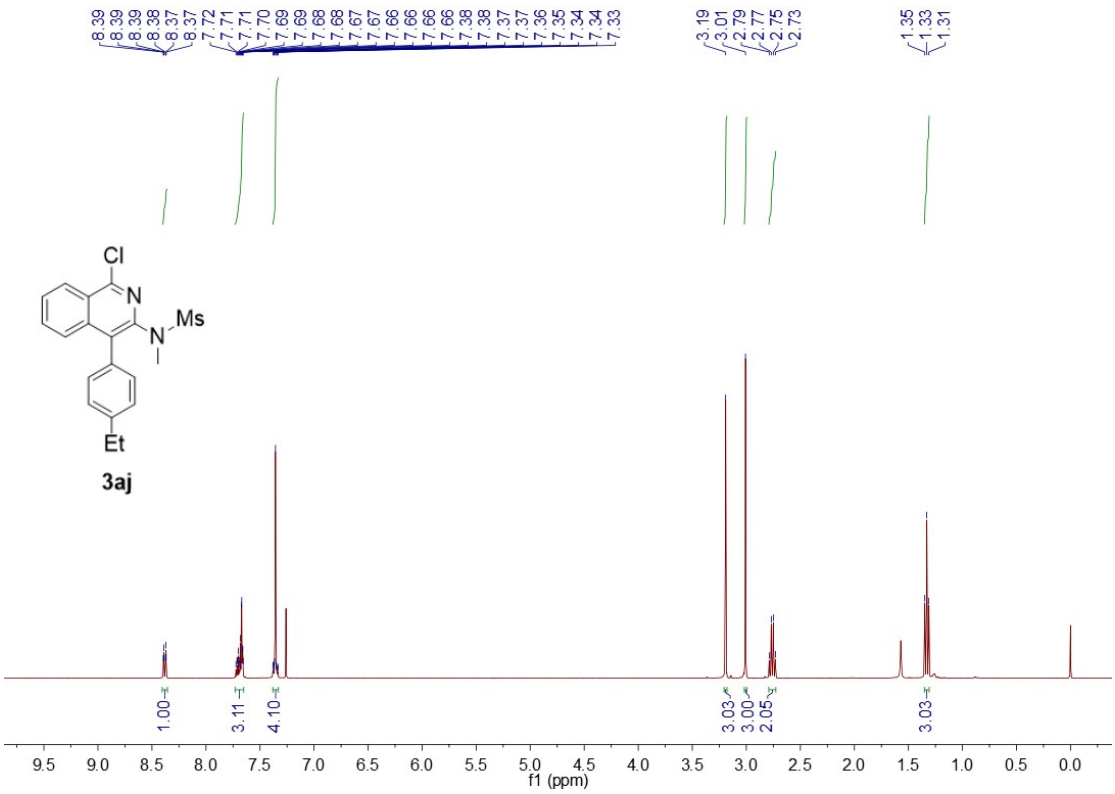
38.50
37.73
Cl
N
N
Ms
OMe
3ai
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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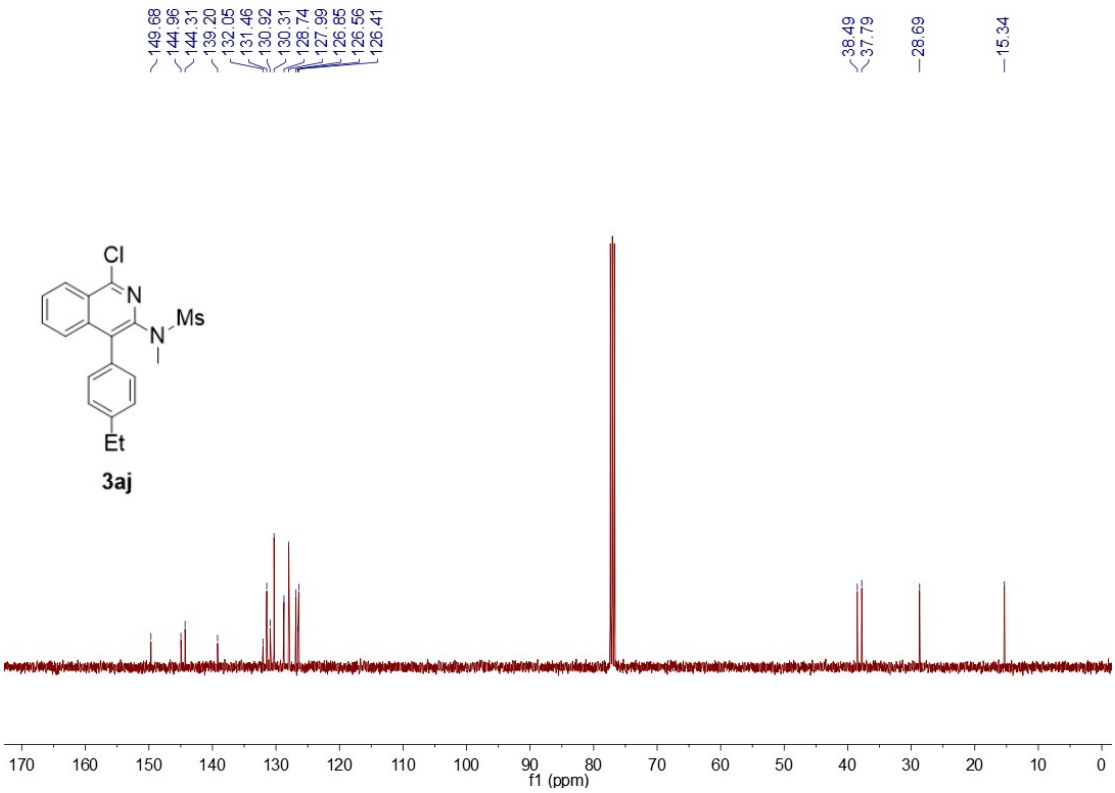
7.35
7.34
7.34
7.33
3.19
3.01
2.79
2.77
2.75
2.73
1.35
1.33
1.31
Cl
N
Ms
N
Et
3aj
1.00
3.11
4.10
3.03
3.00
2.05
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.85
126.56
126.41
38.49
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Cl
N
Ms
N
Et
3aj
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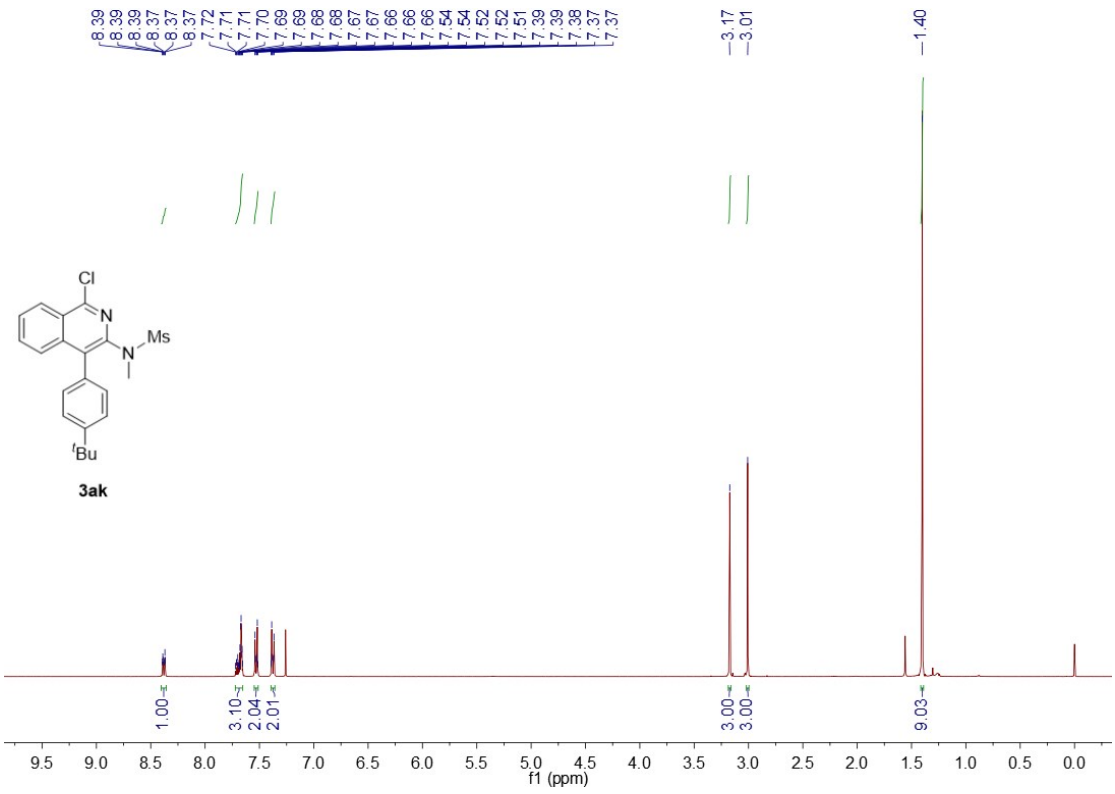
f1 (ppm)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7.52
7.51
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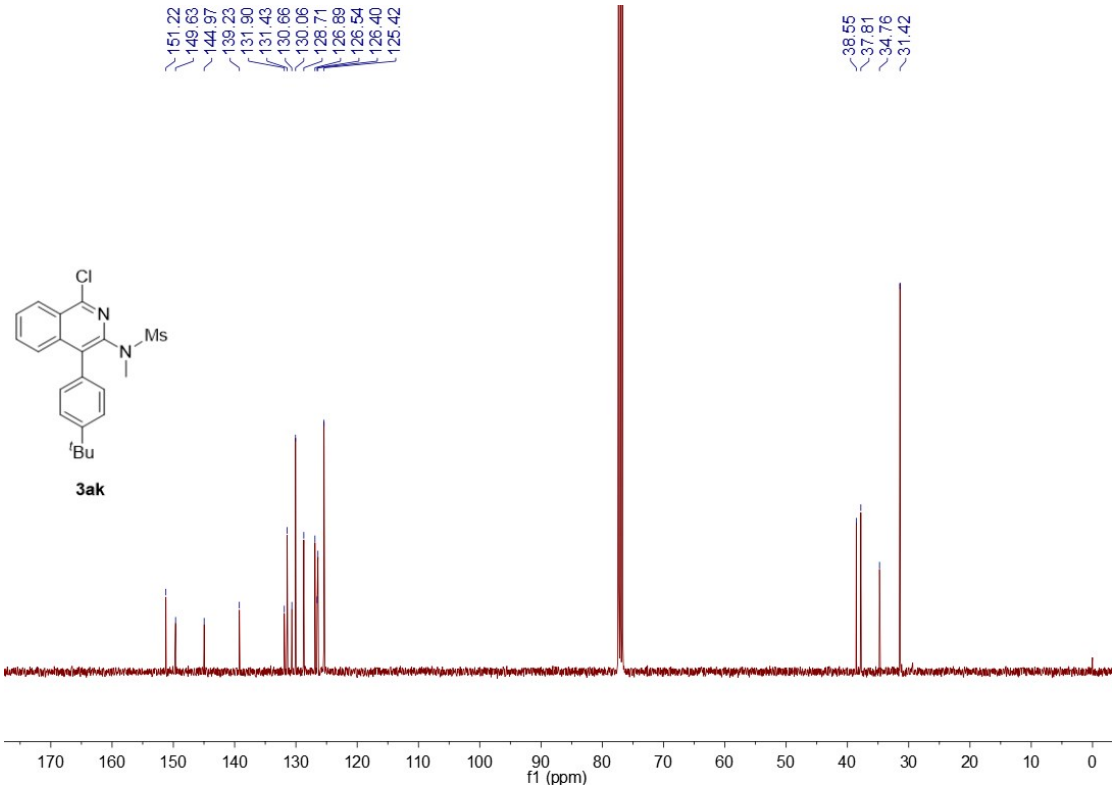
7.39
7.38
7.37
7.37
3.17
3.01
1.40
Cl
N
Ms
N
tBu
3ak
1.00
3.10
2.04
2.01
3.00
3.00
9.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.54
126.40
125.42
38.55
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Cl
N
Ms
N
tBu
3ak
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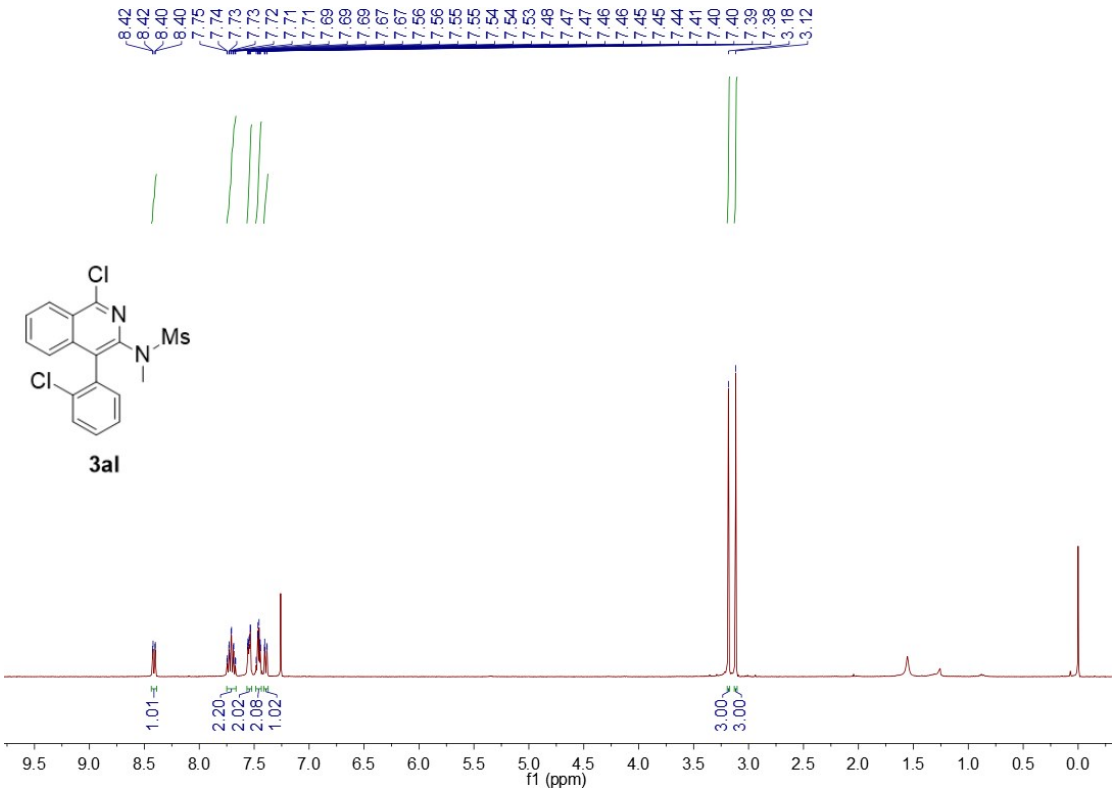
f1 (ppm)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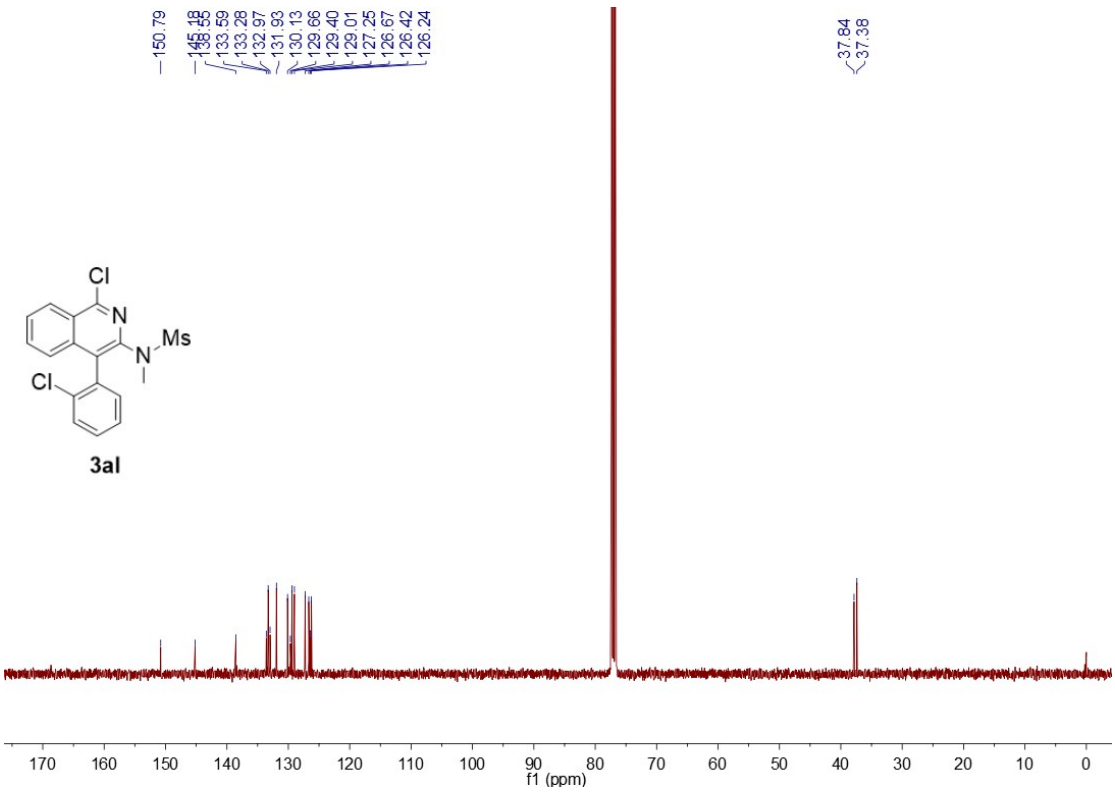
7.46
7.45
7.45
7.44
7.41
7.40
7.40
7.39
7.38
3.18
3.12
Cl
N
Ms
N
Cl
3al
1.01
2.20
2.02
2.08
1.02
3.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.67
126.42
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Cl
N
Ms
N
Cl
3al
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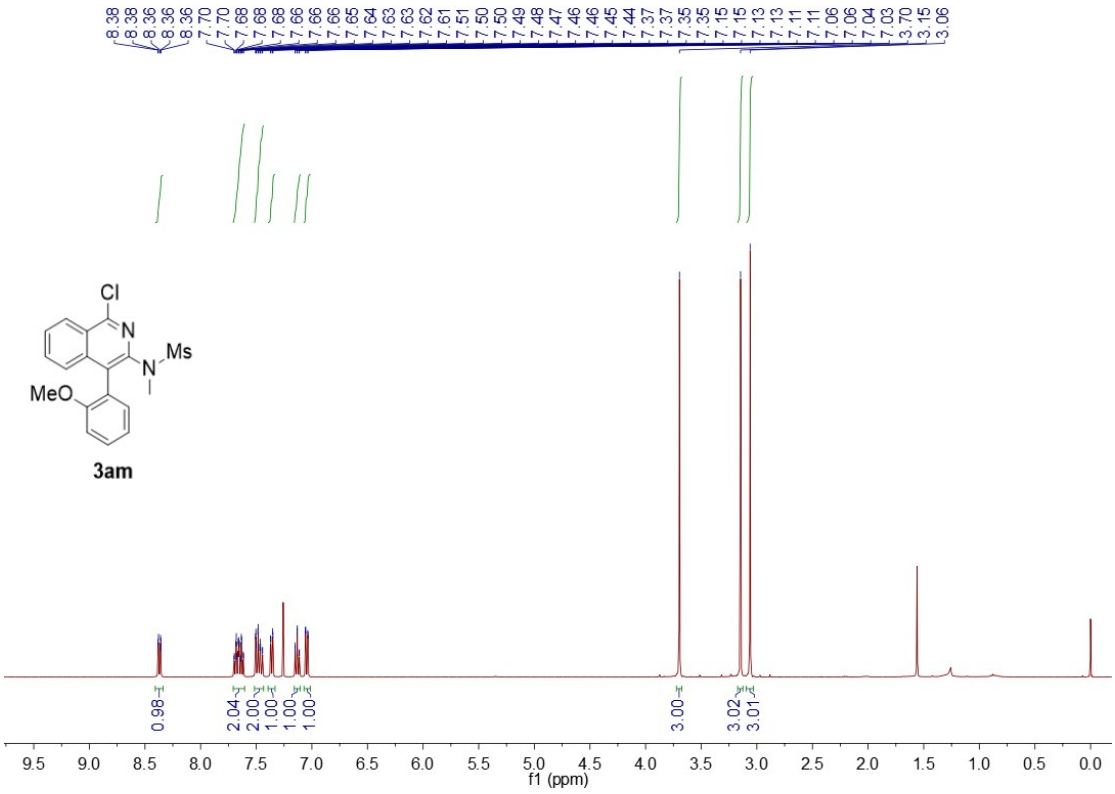
f1 (ppm)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7.48
7.47
7.46
7.45
7.44
7.37
7.35
7.15
7.13
7.11
7.06
7.04
7.03
3.70
3.15
3.06
Cl
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Ms
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MeO
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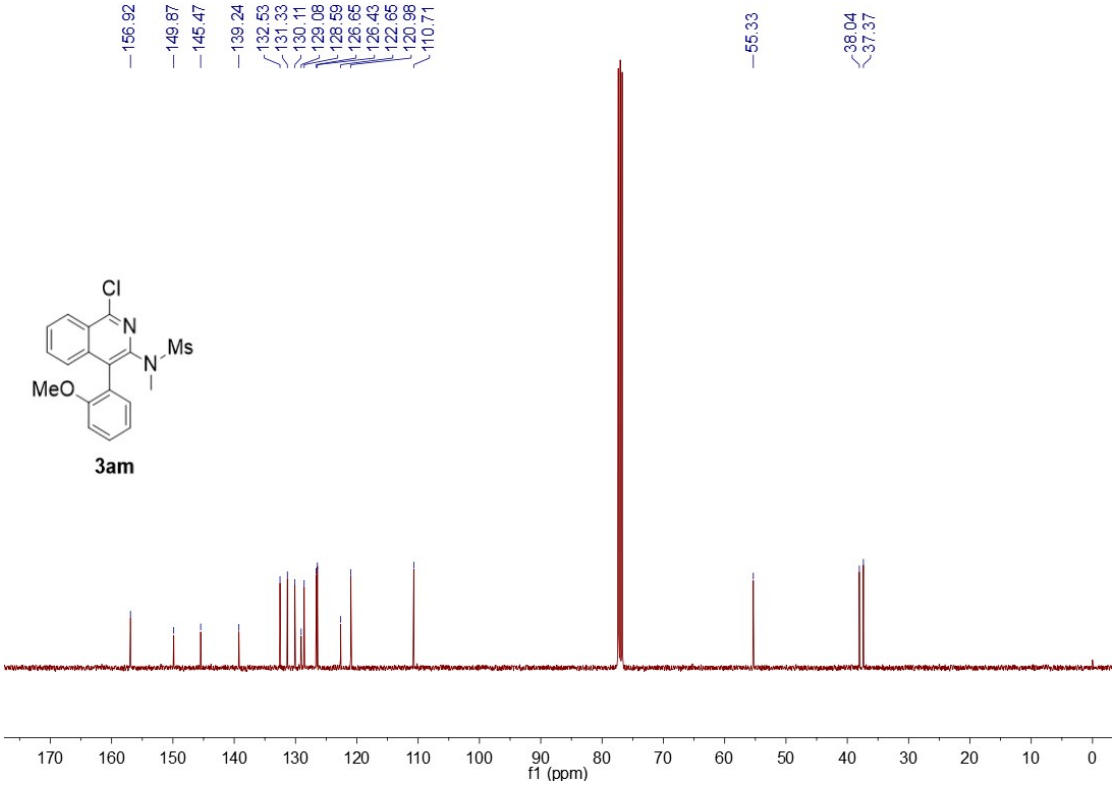
2.00
1.00
1.00
3.00
3.02
3.01
f1 (ppm)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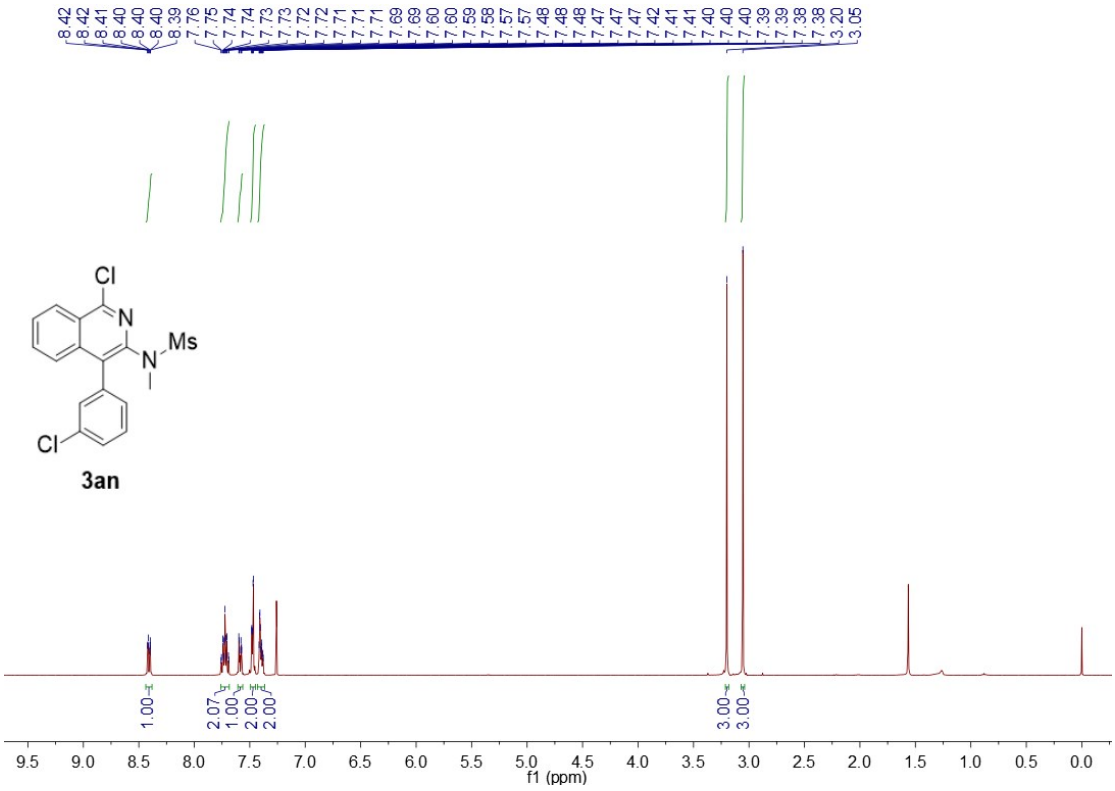
55.33
38.04
37.37
Cl
N
Ms
N
MeO
3am
f1 (ppm)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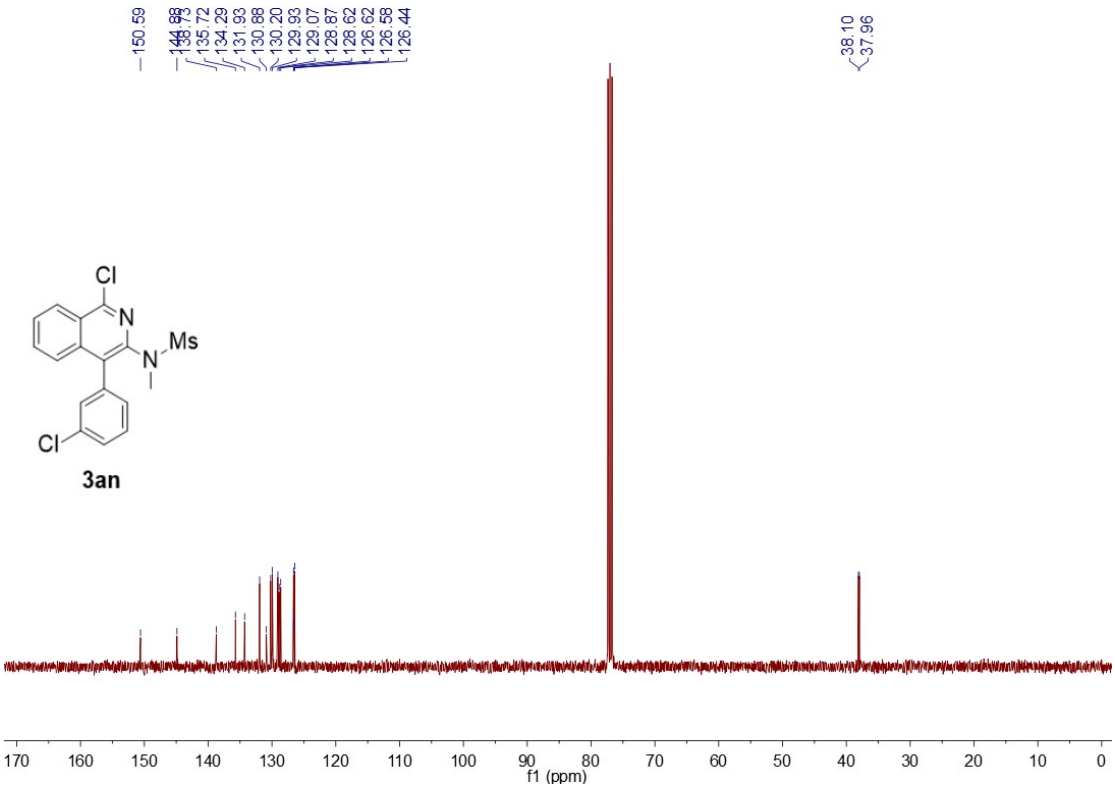
Cl
N
Ms
N
Cl
3an
1.00 2.07 1.00 2.00 2.00 3.00 3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


150.59 144.88 144.73 138.73 135.72 134.29 131.93 130.88 130.20 129.93 129.07 128.87 128.62 126.62 126.58 126.44
38.10 37.96
Cl
N
Ms
N
Cl
3an
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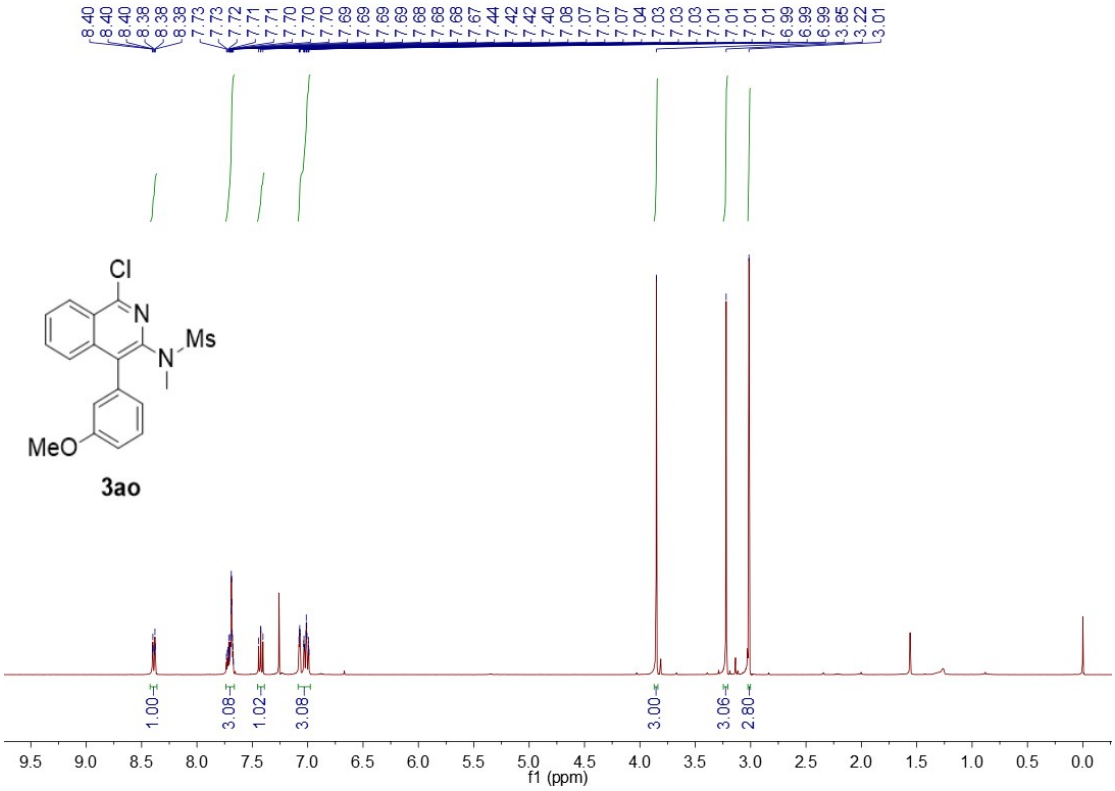
f1 (ppm)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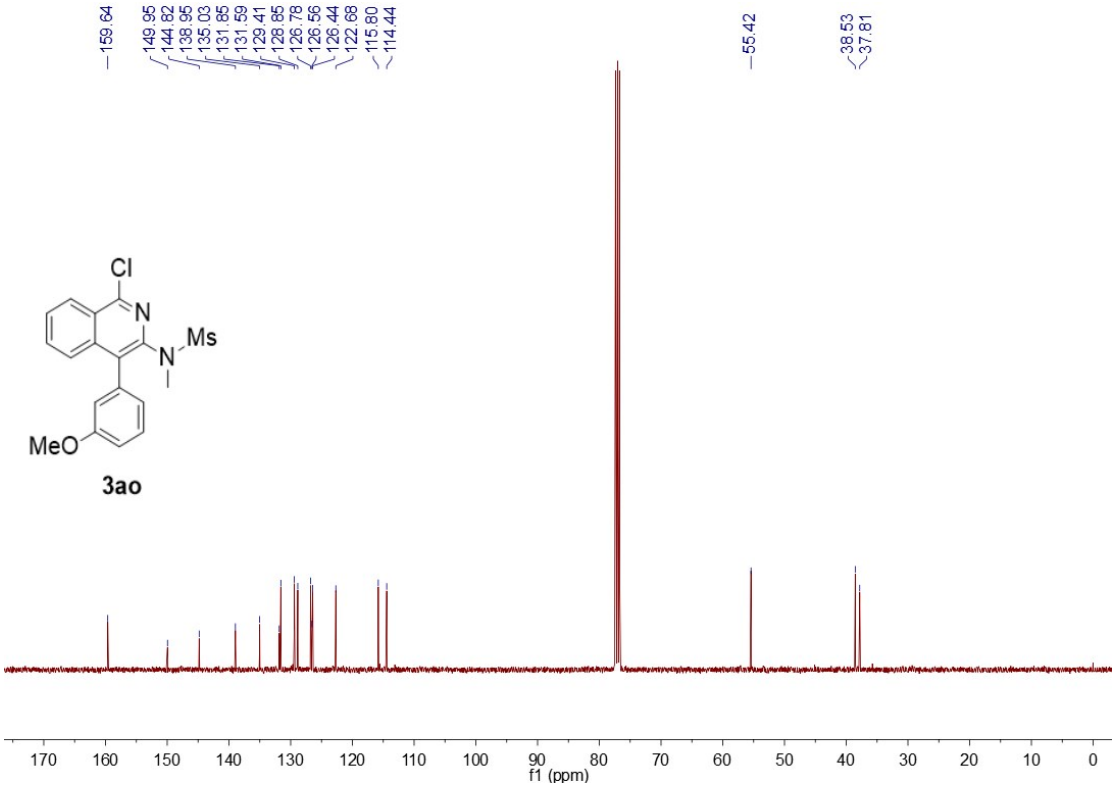
7.01
7.01
7.01
6.99
6.99
6.99
3.85
3.22
3.01
Cl
N
Ms
N
MeO
3ao
1.00
3.08
1.02
3.08
3.00
3.06
2.80
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.78
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126.44
122.68
115.80
114.44
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38.53
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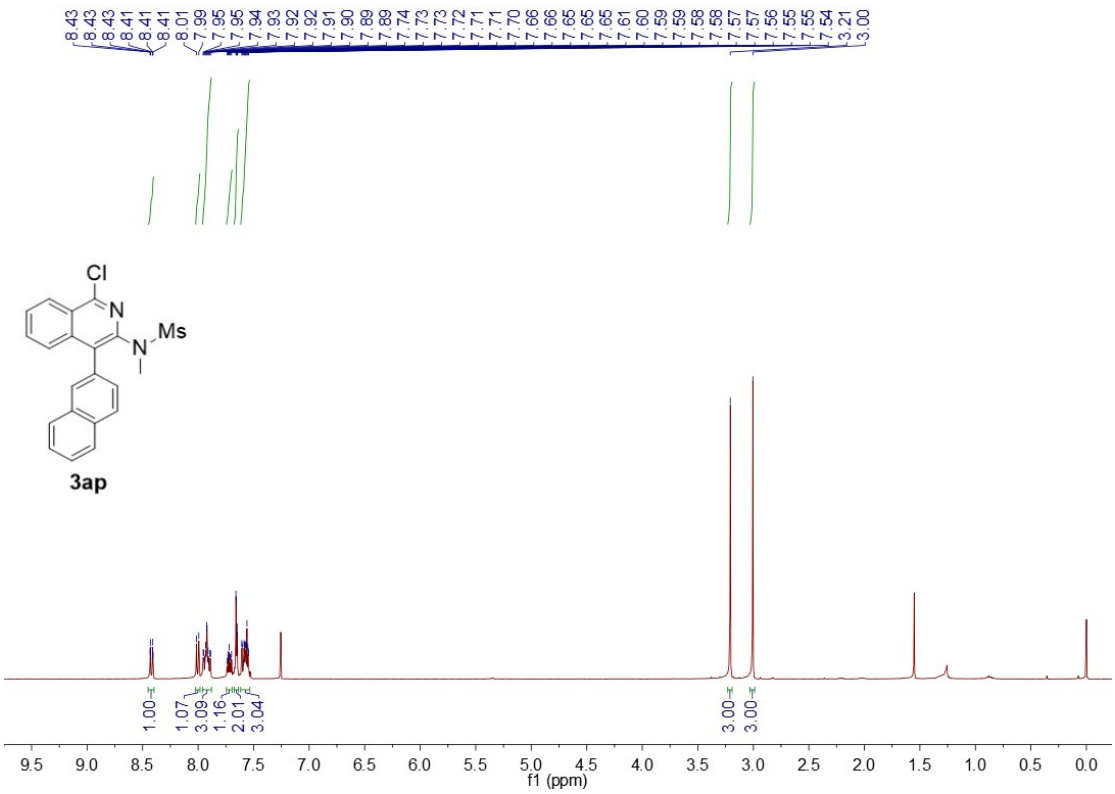
Cl
N
Ms
N
MeO
3ao
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.54
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3.00
Cl
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Ms
N
3ap
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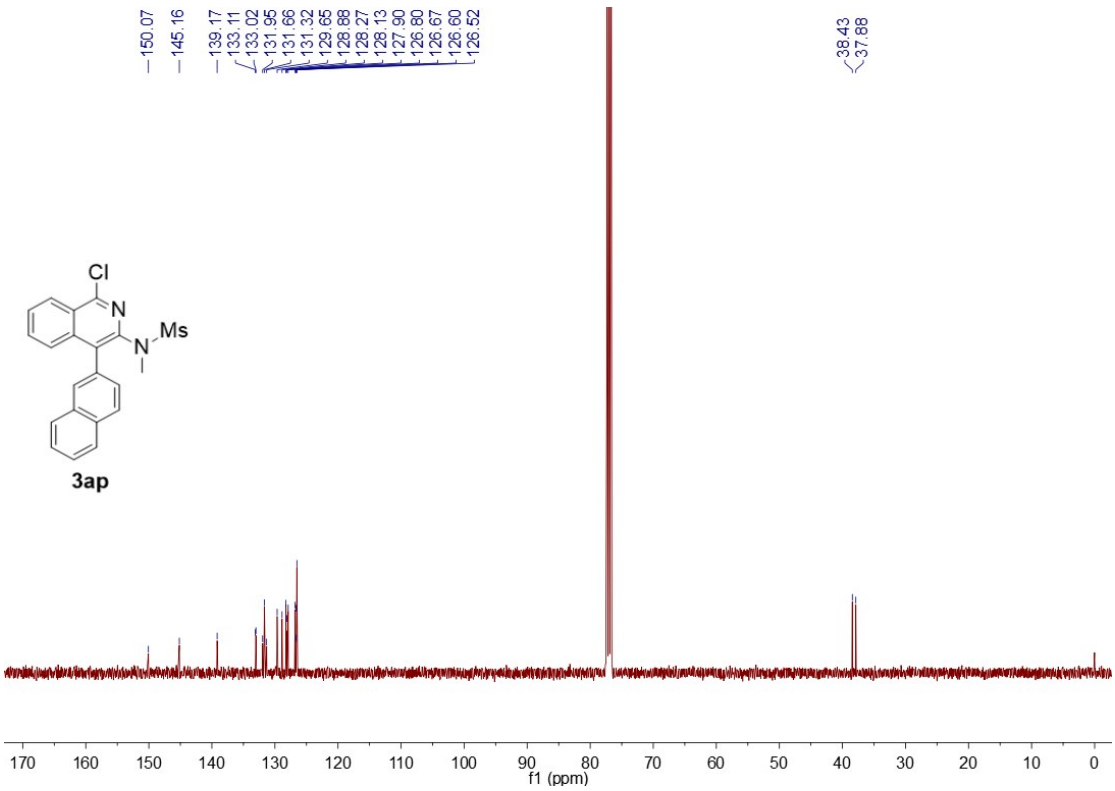
1.07
3.09
1.16
2.01
3.04
3.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.32
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128.13
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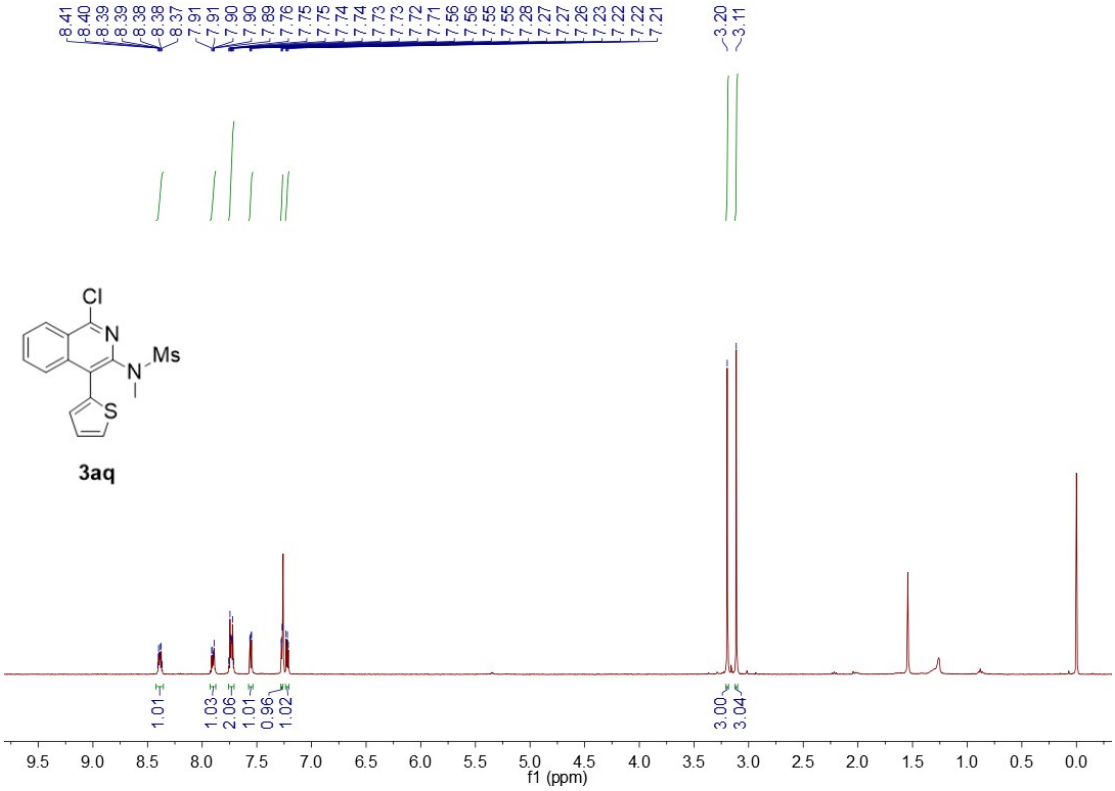
126.80
126.67
126.60
126.52
38.43
37.88
Cl
N
Ms
N
3ap
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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Cl
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Ms
N
S
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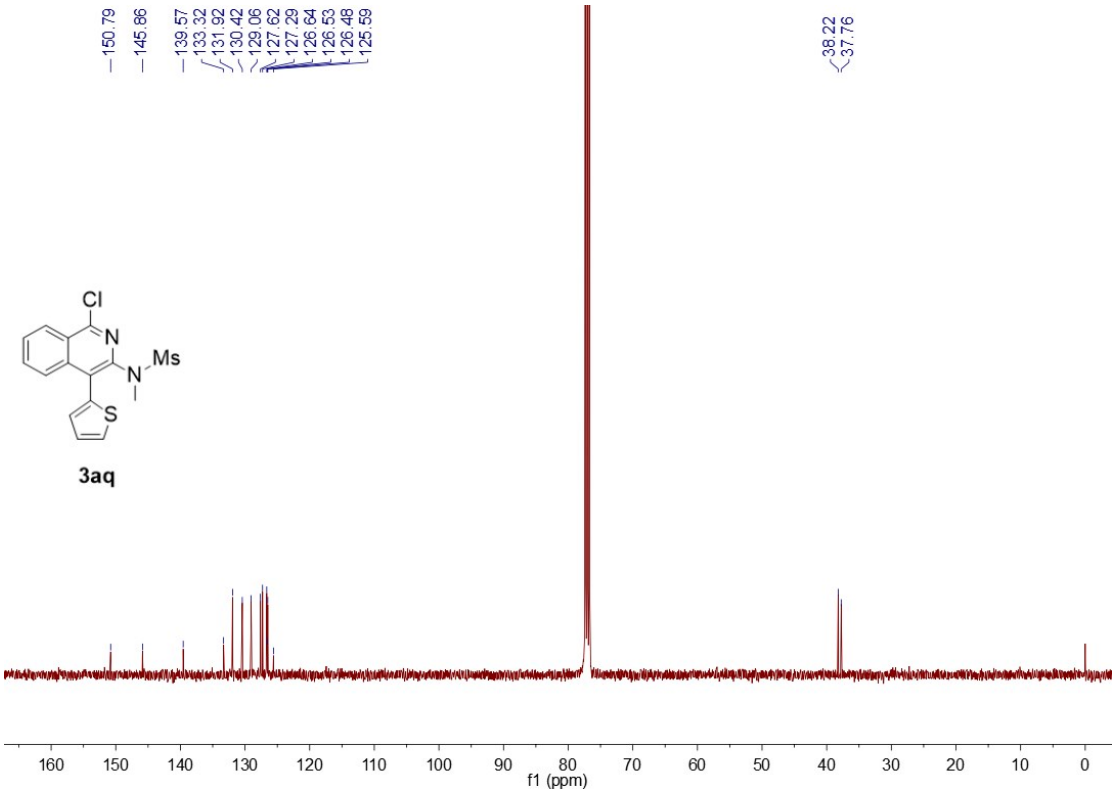
1.03
2.06
1.01
0.96
1.02
3.00
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.62
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126.64
126.53
126.48
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38.22
37.76
Cl
N
Ms
N
S
3aq
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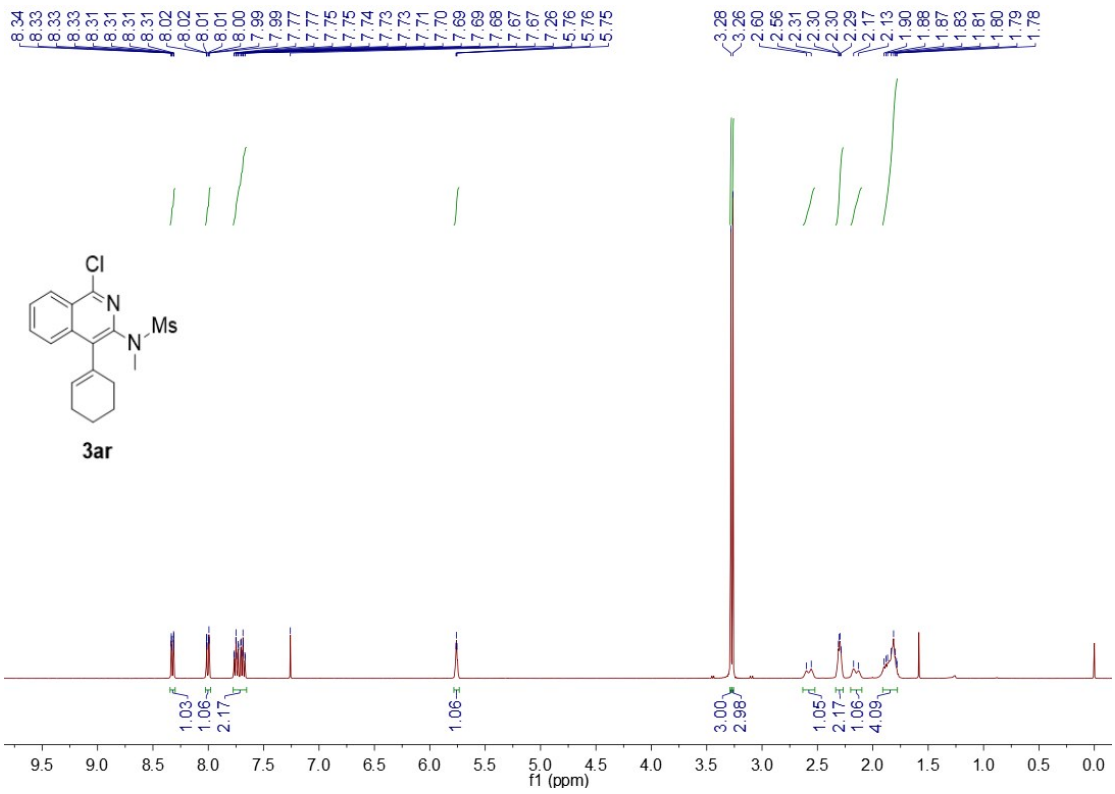
f1 (ppm)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8.01
8.01
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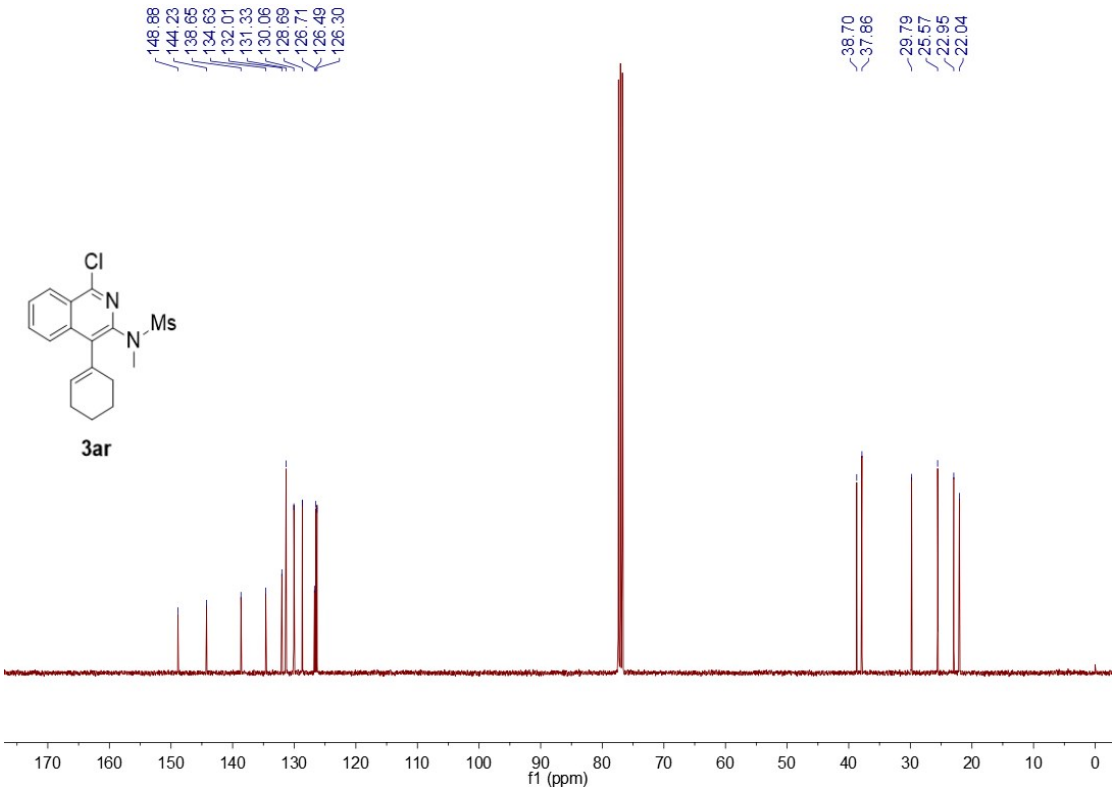
7.99
7.99
7.77
7.77
7.75
7.75
7.74
7.73
7.73
7.71
7.70
7.69
7.69
7.68
7.67
7.67
7.26
5.76
5.76
5.75
3.28
3.26
2.60
2.56
2.31
2.30
2.30
2.29
2.17
2.13
1.90
1.88
1.87
1.83
1.81
1.80
1.79
1.78
Cl
N
N
Ms
3ar
1.03
1.06
2.17
1.06
3.00
2.98
1.05
2.17
1.06
4.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.30
38.70
37.86
29.79
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22.04
Cl
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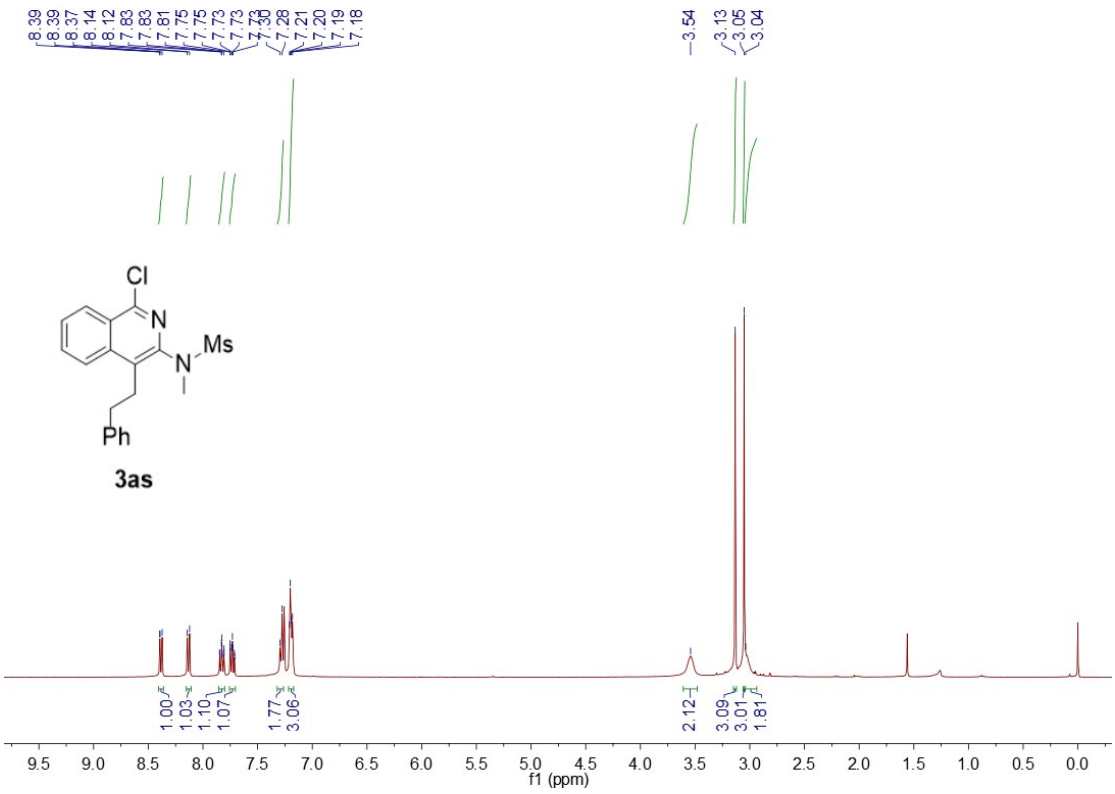
N
Ms
3ar
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.37
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8.12
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7.83
7.81
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7.75
7.73
7.73
7.30
7.28
7.21
7.20
7.19
7.18
3.54
3.13
3.05
3.04
Cl
N
Ms
N
Ph
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1.10
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1.77
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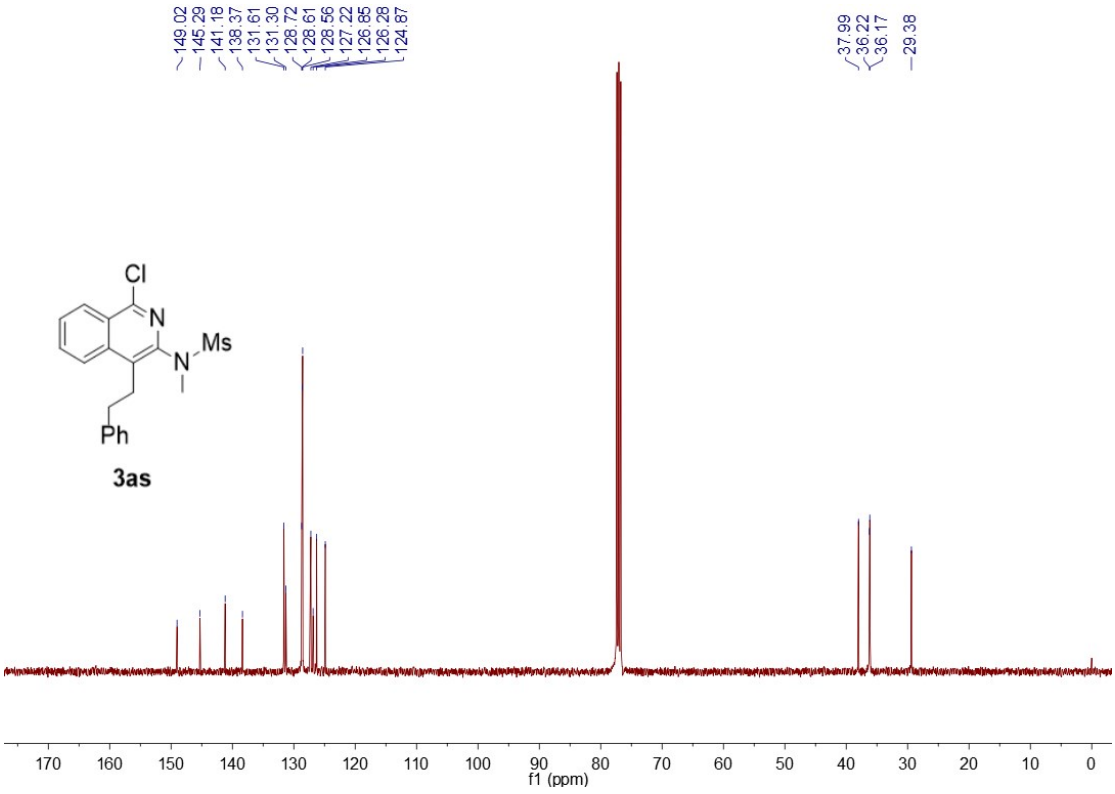
2.12
3.09
3.01
1.81
f1 (ppm)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131.30
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128.61
128.56
127.22
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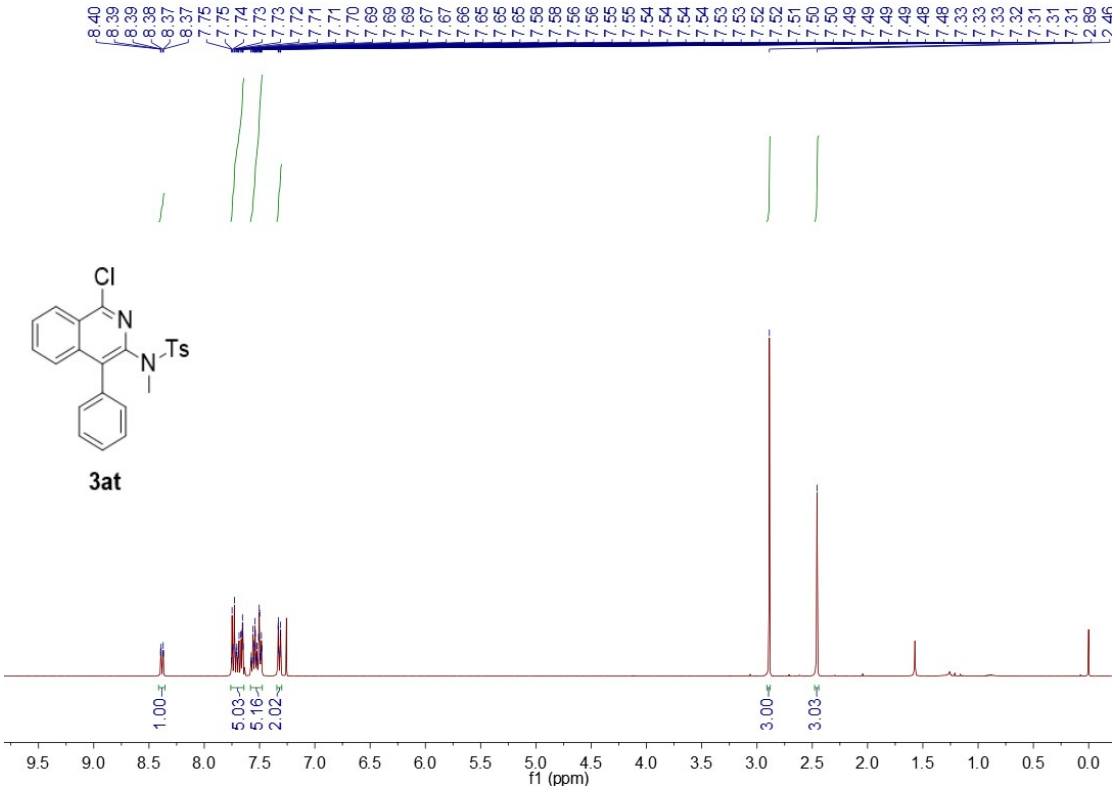
126.28
124.87
37.99
36.22
36.17
29.38
Cl
N
Ms
N
Ph
3as
f1 (ppm)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Ts
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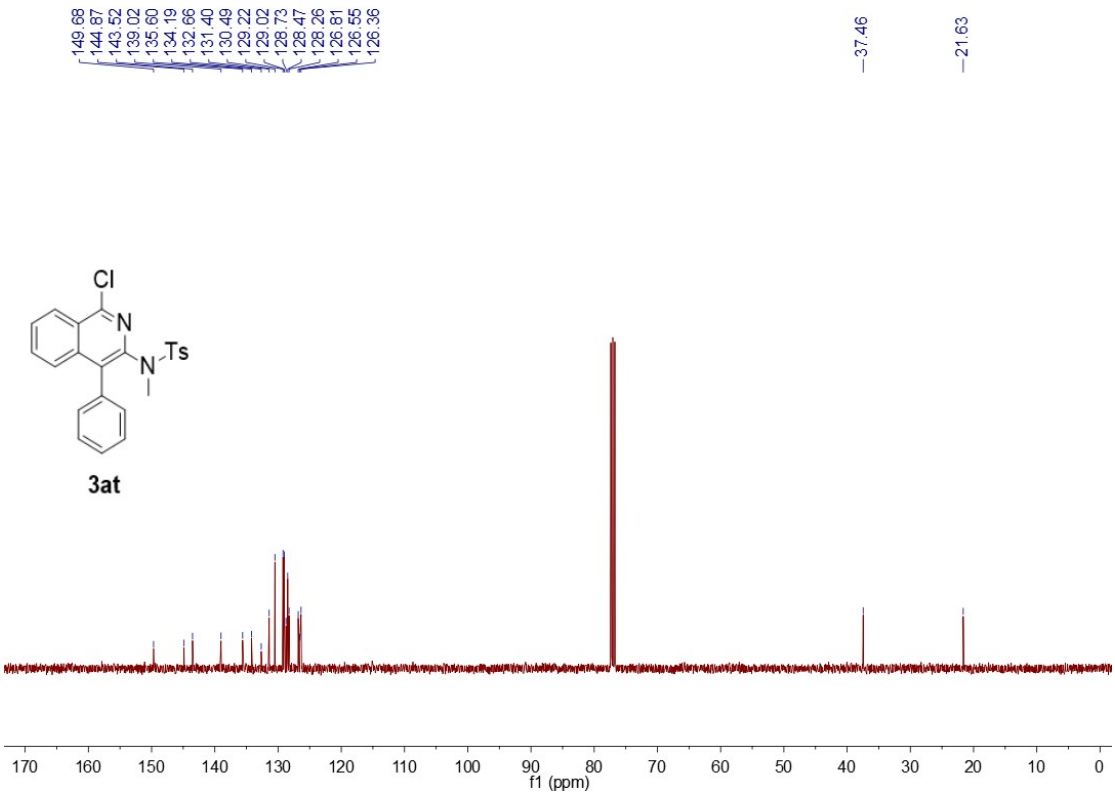
5.16
2.02
3.00
3.03
f1 (ppm)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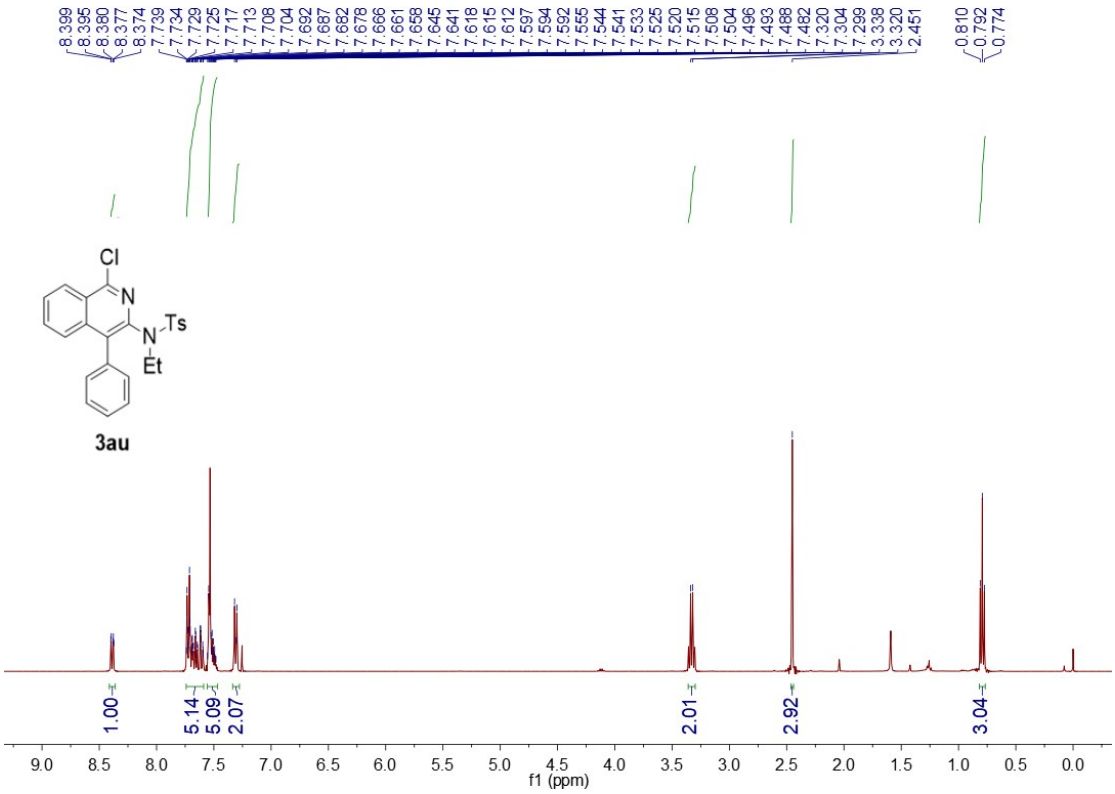
126.55
126.36
37.46
21.63
Cl
N
N
Ts
3at
f1 (ppm)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7.713
7.708
7.704
7.692
7.687
7.682
7.678
7.666
7.661
7.658
7.645
7.641
7.618
7.615
7.612
7.597
7.594
7.592
7.555
7.544
7.541
7.533
7.525
7.520
7.515
7.508
7.504
7.496
7.493
7.488
7.482
7.320
7.304
7.299
3.338
3.320
2.451
0.810
0.792
0.774
Cl
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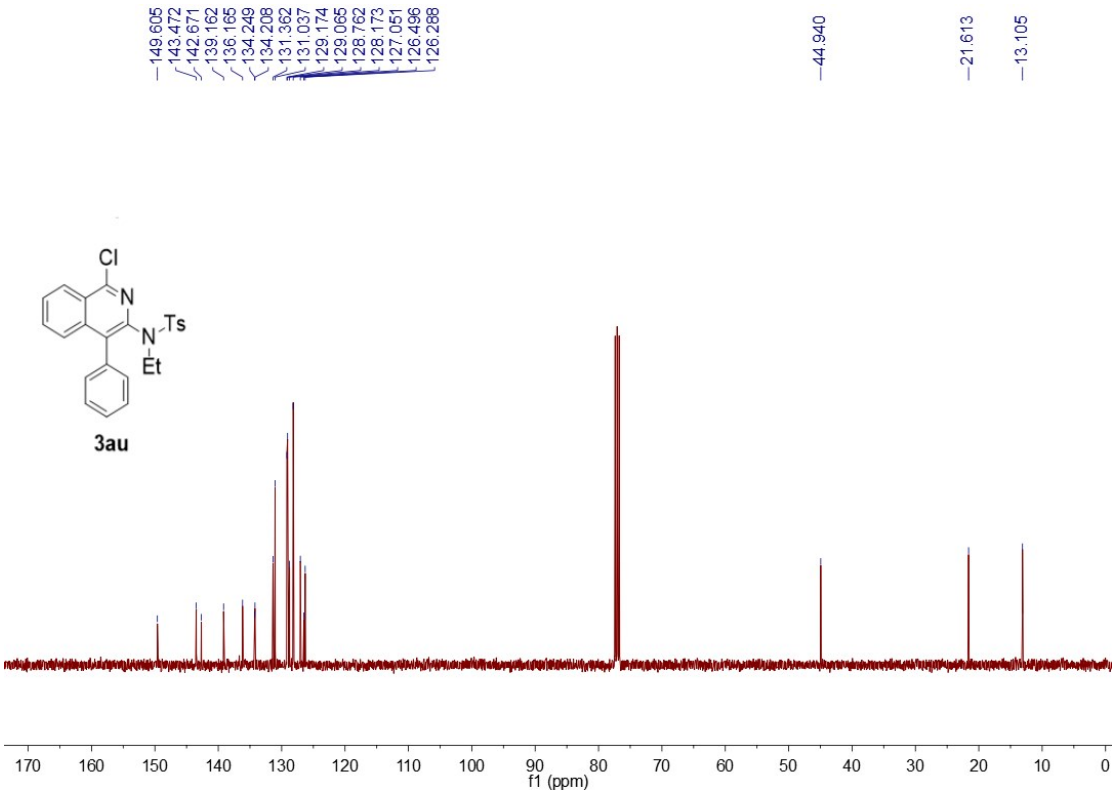
Ts
N
Et
3au
1.00
5.14
5.09
2.07
2.01
2.92
3.04
f1 (ppm)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134.249
134.208
131.362
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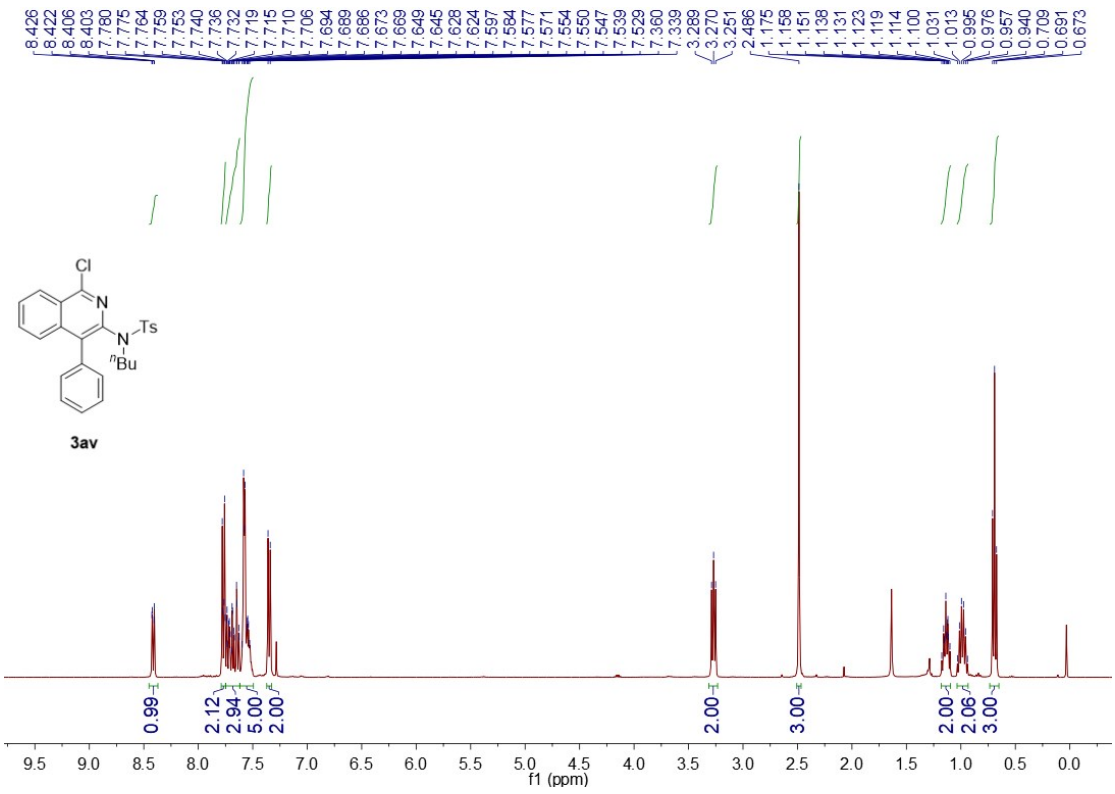
129.174
129.065
128.762
128.173
127.051
126.496
126.288
44.940
21.613
13.105
Cl
N
Ts
N
Et
3au
f1 (ppm)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7.759
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7.740
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7.732
7.719
7.715
7.710
7.706
7.694
7.689
7.686
7.673
7.669
7.649
7.645
7.628
7.624
7.597
7.584
7.577
7.571
7.554
7.550
7.547
7.539
7.529
7.360
7.339
3.289
3.270
3.251
2.486
1.175
1.158
1.151
1.138
1.131
1.123
1.119
1.114
1.100
1.031
1.013
0.995
0.976
0.957
0.940
0.709
0.691
0.673
Cl
N
Ts
N
nBu
3av
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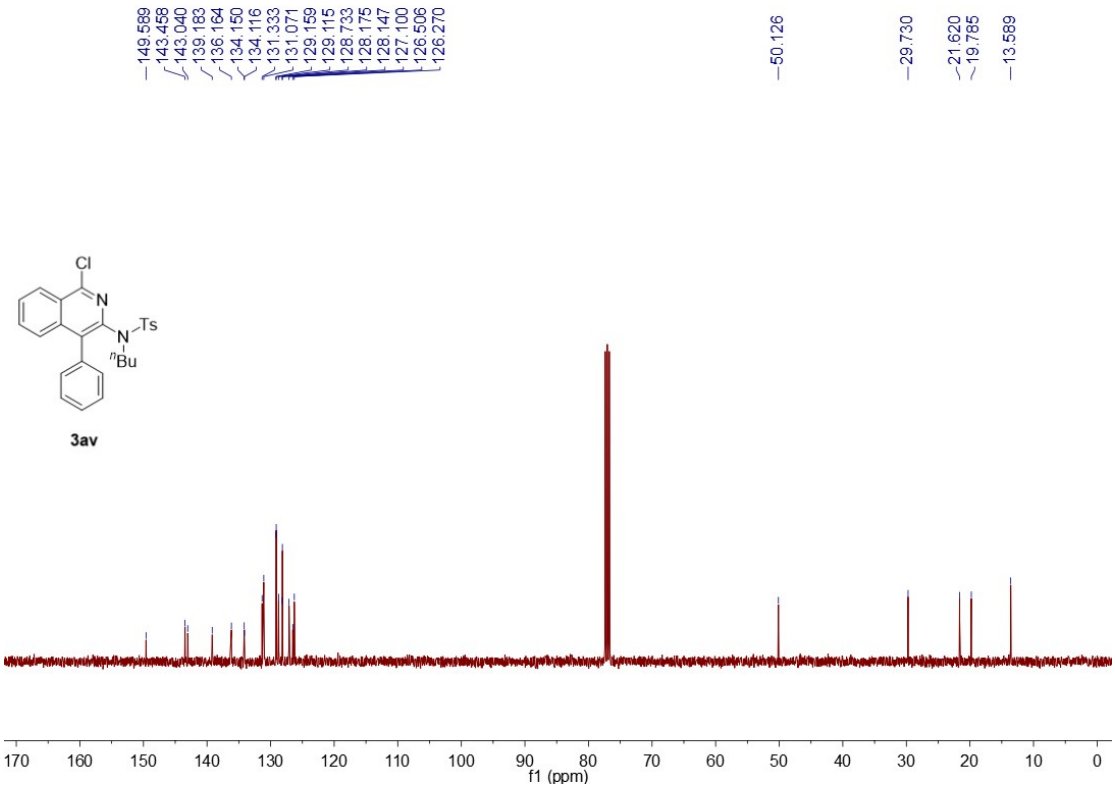
2.94
5.00
2.00
2.00
3.00
2.00
2.06
3.00
f1 (ppm)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131.333
131.071
129.159
129.115
128.733
128.175
128.147
127.100
126.506
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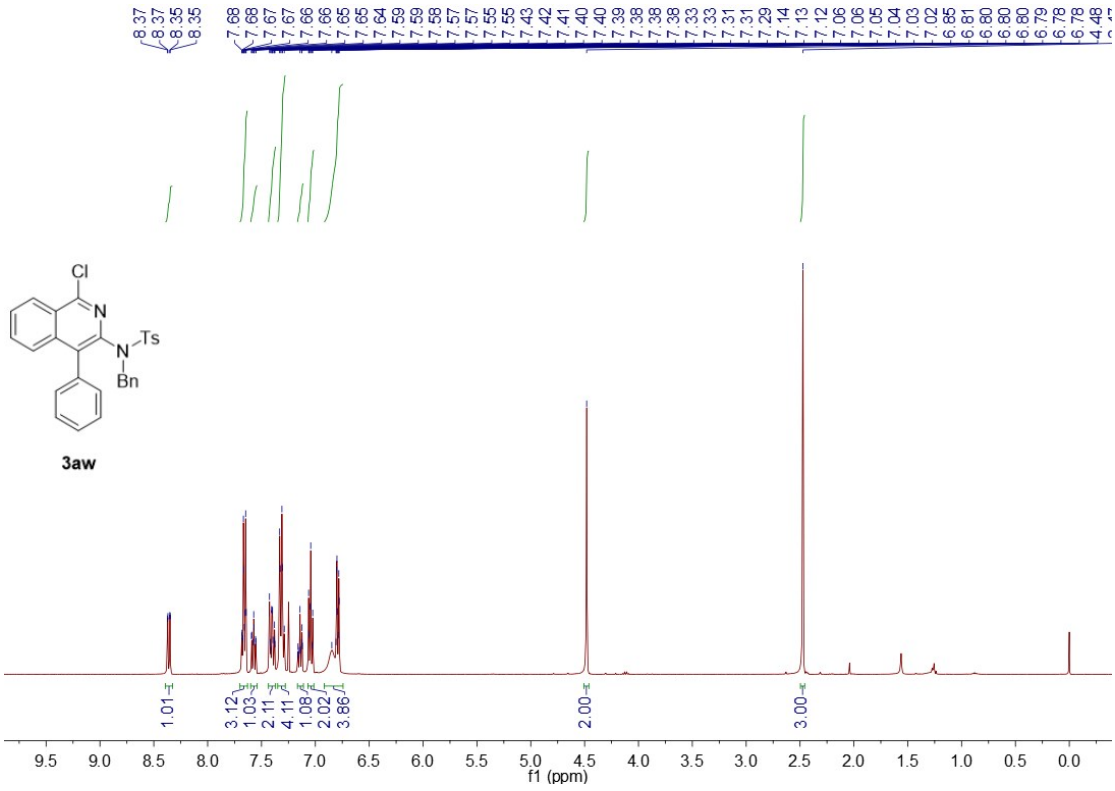
50.126
29.730
21.620
19.785
13.589
Cl
N
Ts
N
nBu
3av
f1 (ppm)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7.40
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7.38
7.38
7.38
7.33
7.31
7.31
7.29
7.14
7.13
7.12
7.06
7.06
7.05
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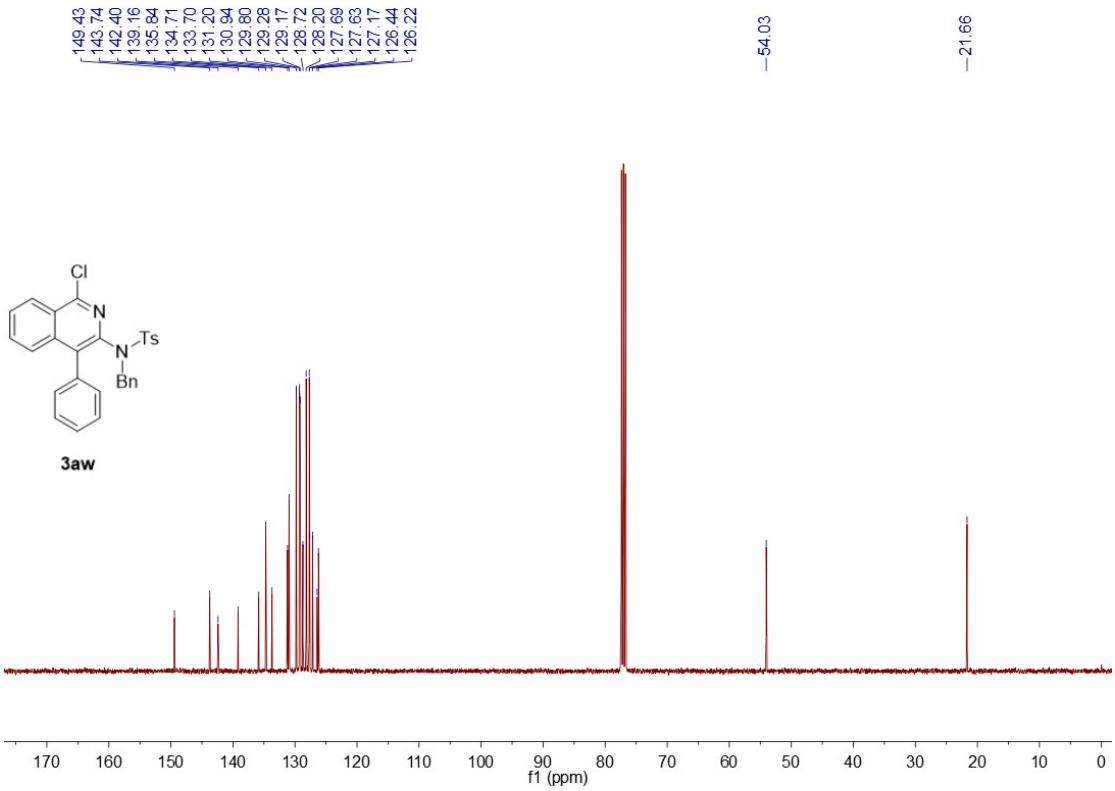
7.03
7.02
6.85
6.81
6.80
6.80
6.80
6.79
6.78
6.78
4.48
Cl
N
Ts
N
Bn
3aw
1.01
3.12
1.03
2.11
4.11
1.08
2.02
3.86
2.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.72
128.20
127.69
127.63
127.17
126.44
126.22
54.03
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Cl
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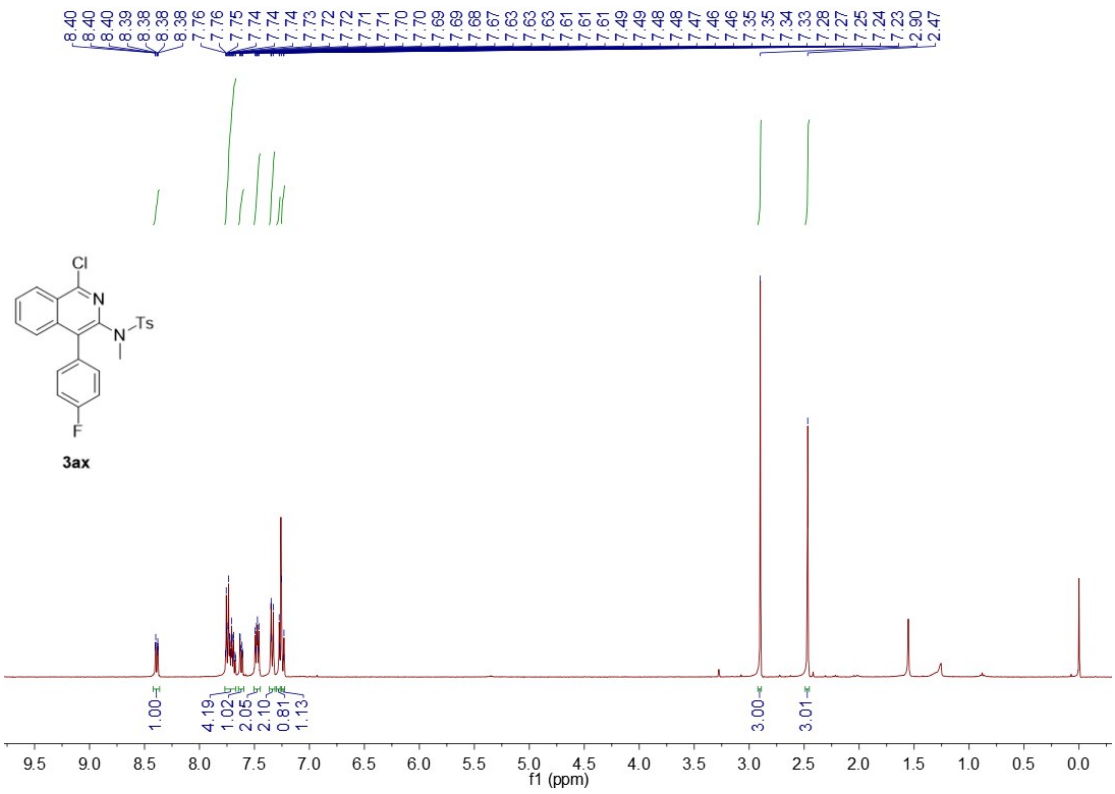
Ts
N
Bn
3aw
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.75
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7.73
7.72
7.72
7.71
7.71
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7.69
7.68
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7.61
7.61
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7.48
7.48
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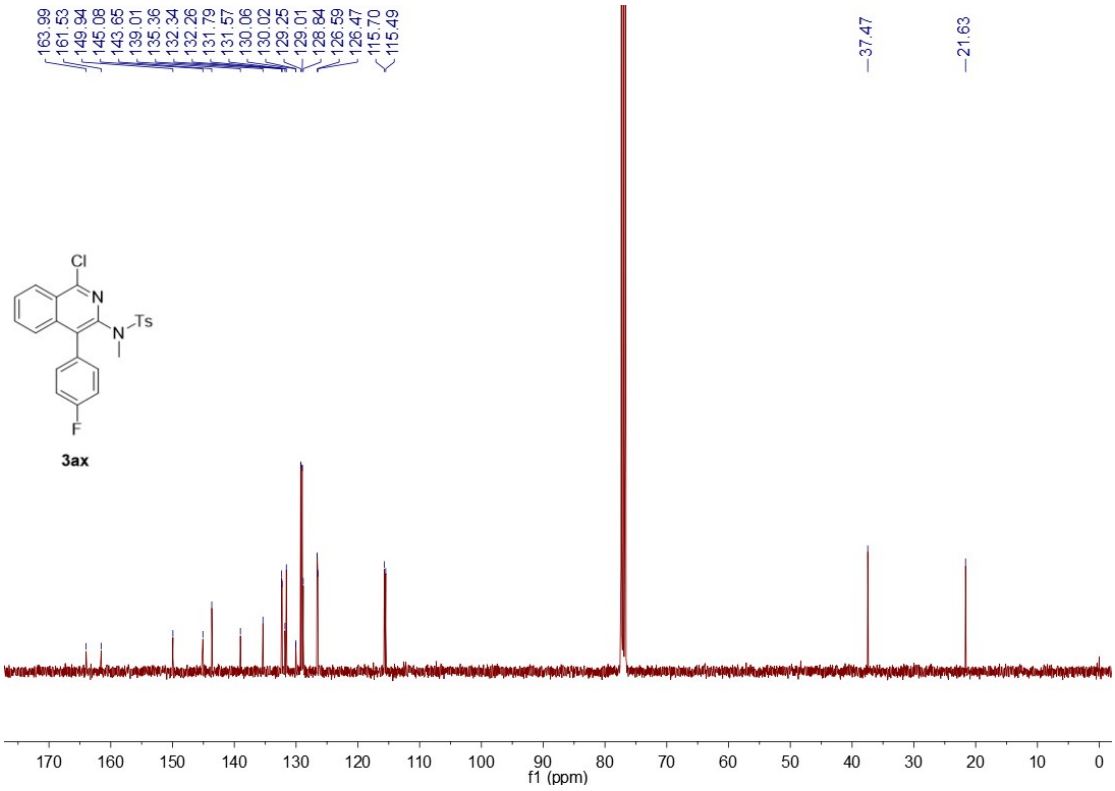
7.46
7.46
7.35
7.34
7.33
7.28
7.27
7.25
7.24
7.23
2.90
2.47
Cl
N
N
Ts
F
3ax
1.00
4.19
1.02
2.05
2.10
0.81
1.13
3.00
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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161.53
149.94
145.08
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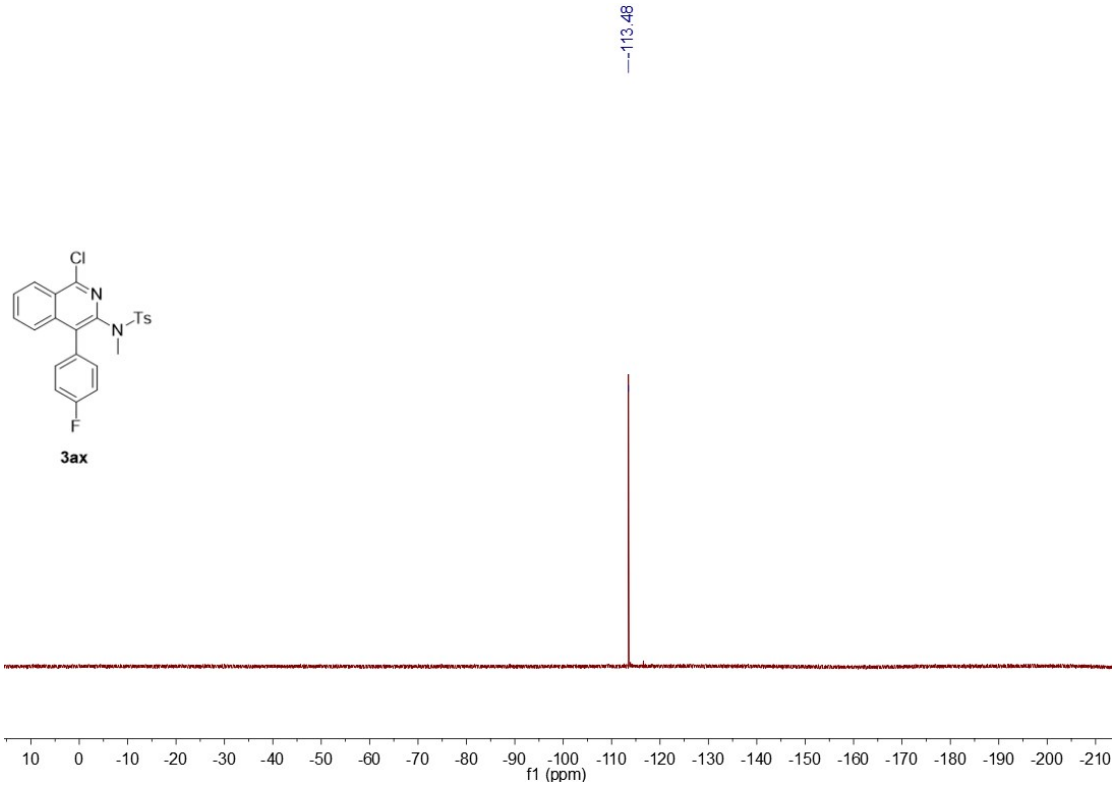
139.01
135.36
132.34
132.26
131.79
131.57
130.06
130.02
129.25
129.01
128.84
126.59
126.47
115.70
115.49
37.47
21.63
Cl
N
N
Ts
F
3ax
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-113.48
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N
Ts
F
3ax
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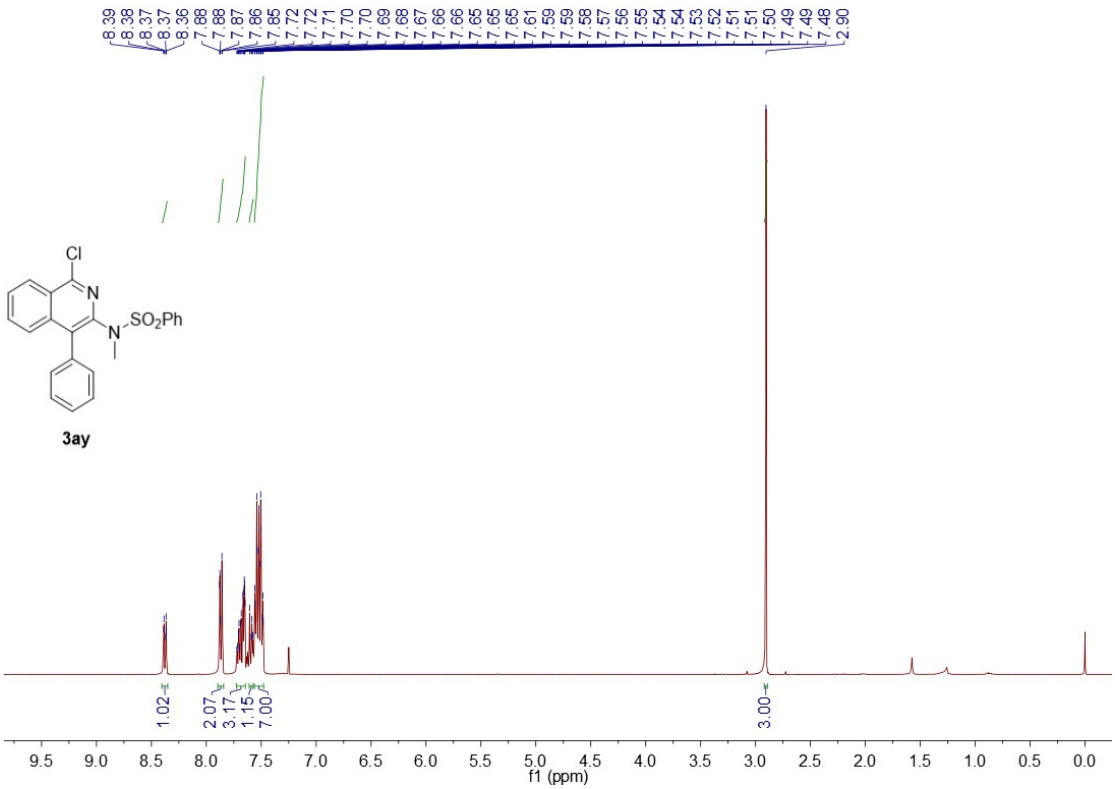
f1 (ppm)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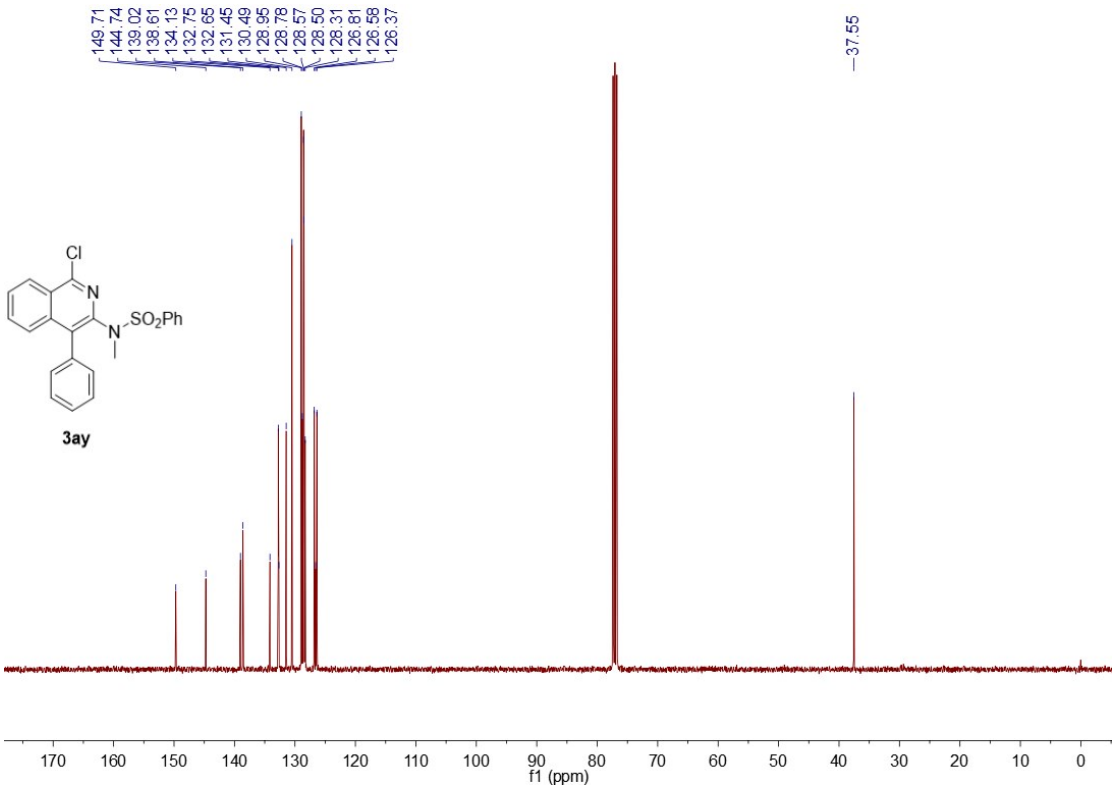
Cl
N
N
SO2Ph
3ay
1.02 2.07 3.17 1.15 7.00 3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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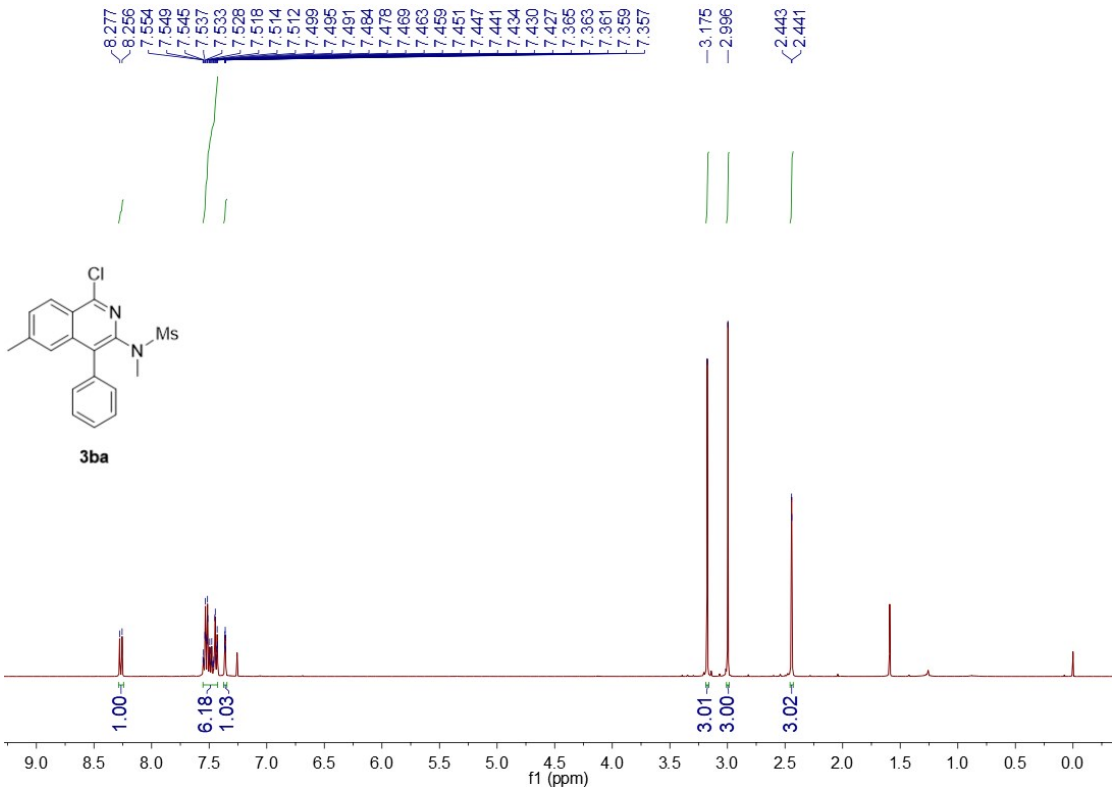
128.95
128.78
128.57
128.50
128.31
126.81
126.58
126.37
37.55
Cl
N
N
SO2Ph
3ay
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.514
7.512
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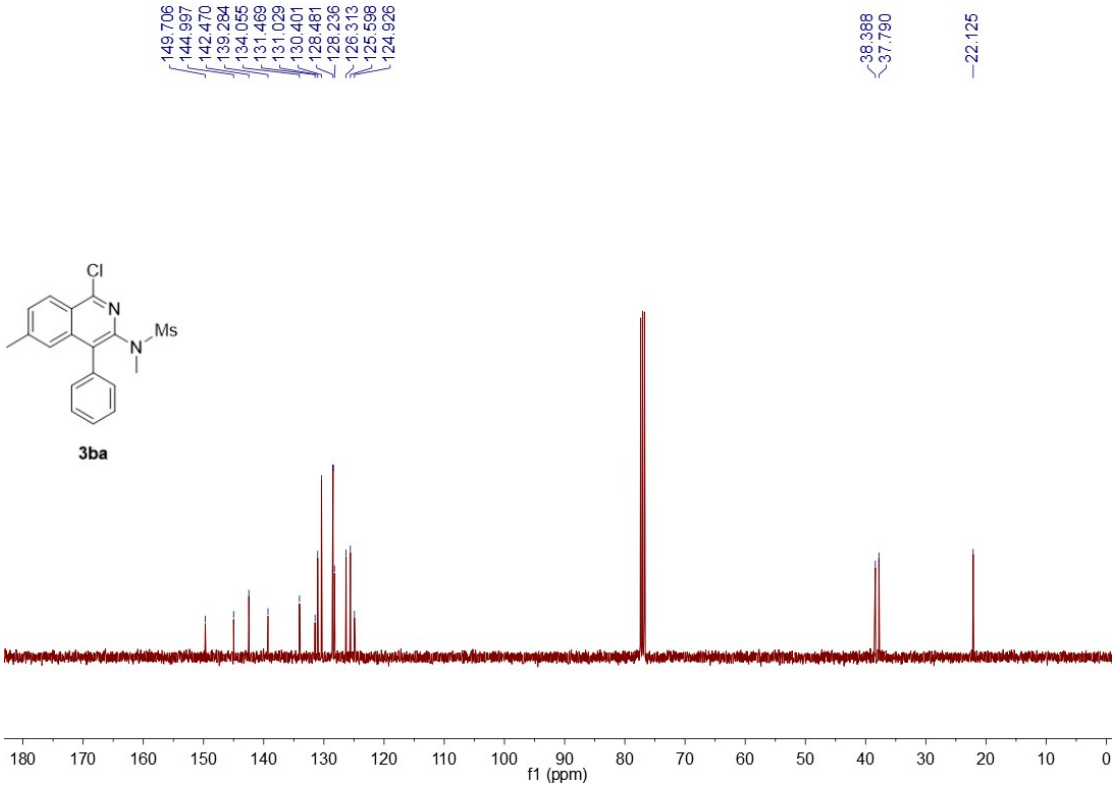
7.495
7.491
7.484
7.478
7.469
7.463
7.459
7.451
7.447
7.441
7.434
7.430
7.427
7.365
7.363
7.361
7.359
7.357
3.175
2.996
2.443
2.441
Cl
N
N
Ms
3ba
1.00
6.18
1.03
3.01
3.00
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.236
126.313
125.598
124.926
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22.125
Cl
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Ms
N
3ba
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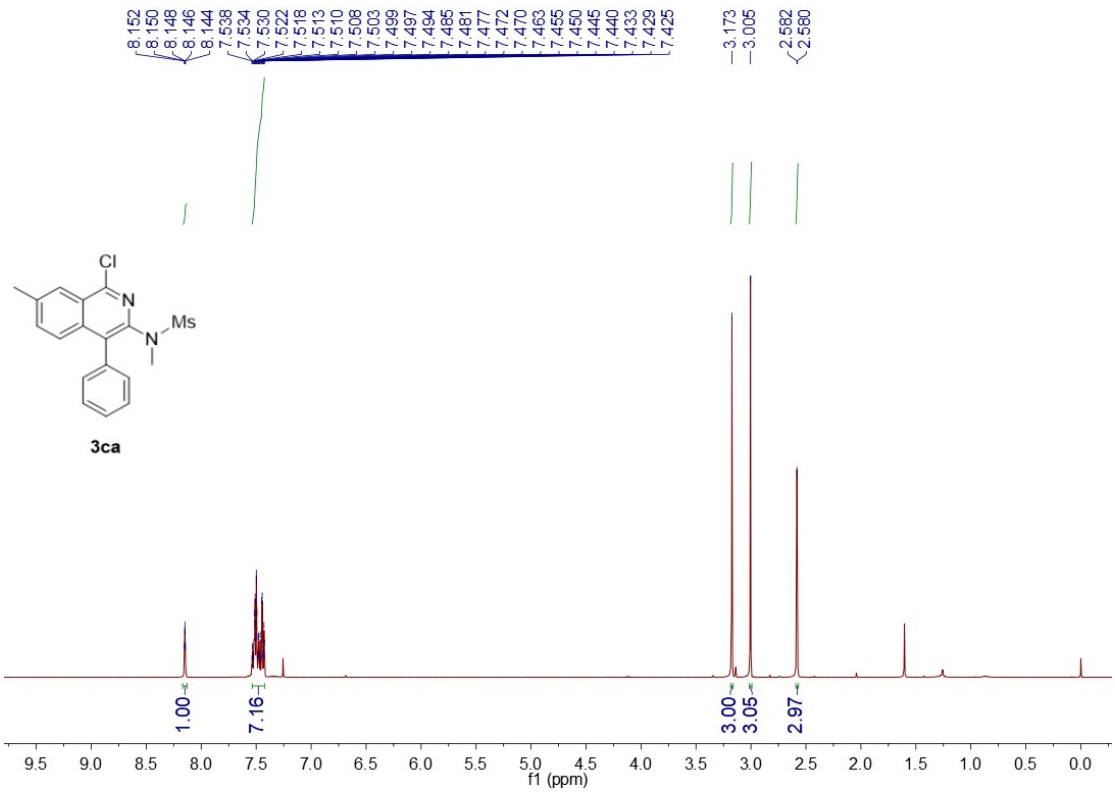
f1 (ppm)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7.530
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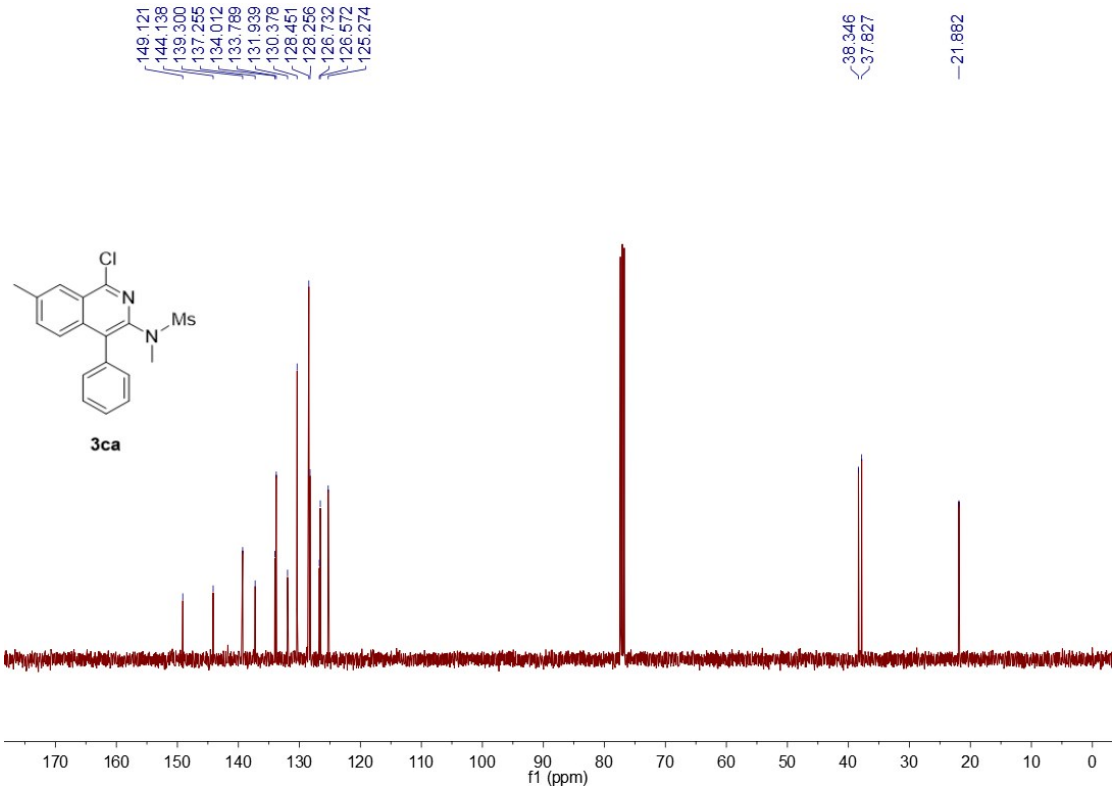
7.518
7.513
7.510
7.508
7.503
7.499
7.497
7.494
7.485
7.481
7.477
7.472
7.470
7.463
7.455
7.450
7.445
7.440
7.433
7.429
7.425
3.173
3.005
2.582
2.580
Cl
N
Ms
N
3ca
1.00
7.16
3.00
3.05
2.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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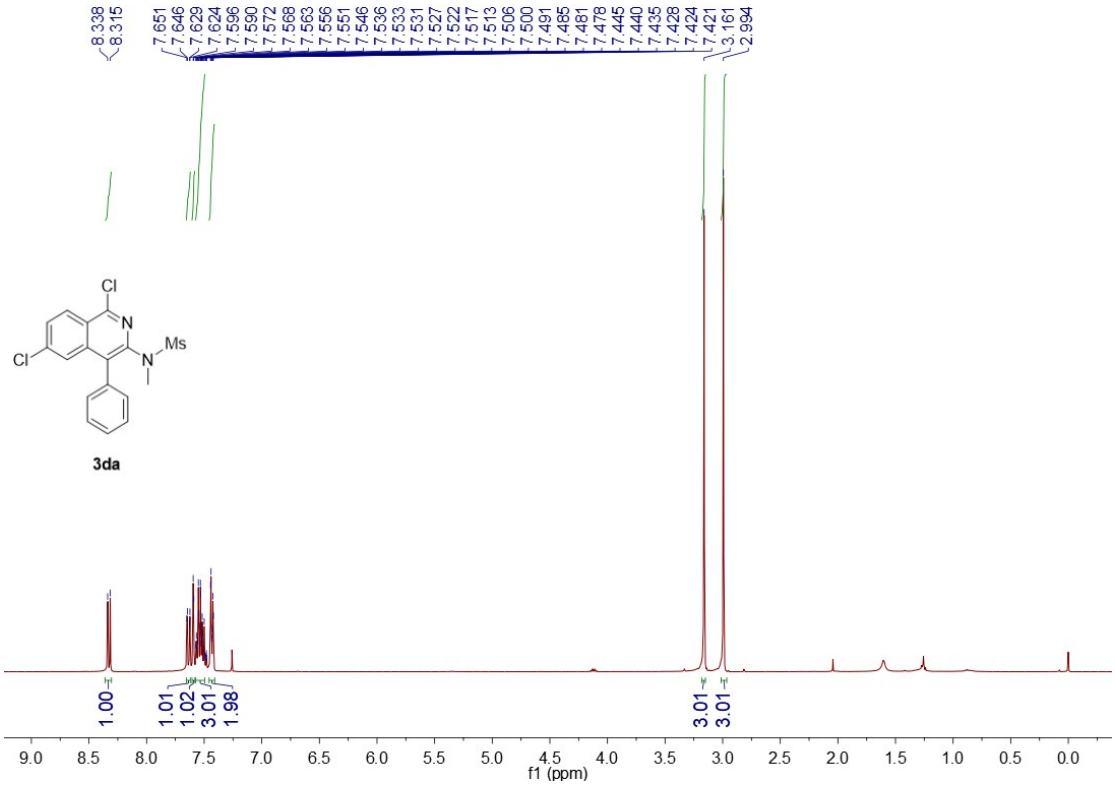
130.378
128.451
128.256
126.732
126.572
125.274
38.346
37.827
21.882
Cl
N
Ms
N
3ca
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.590
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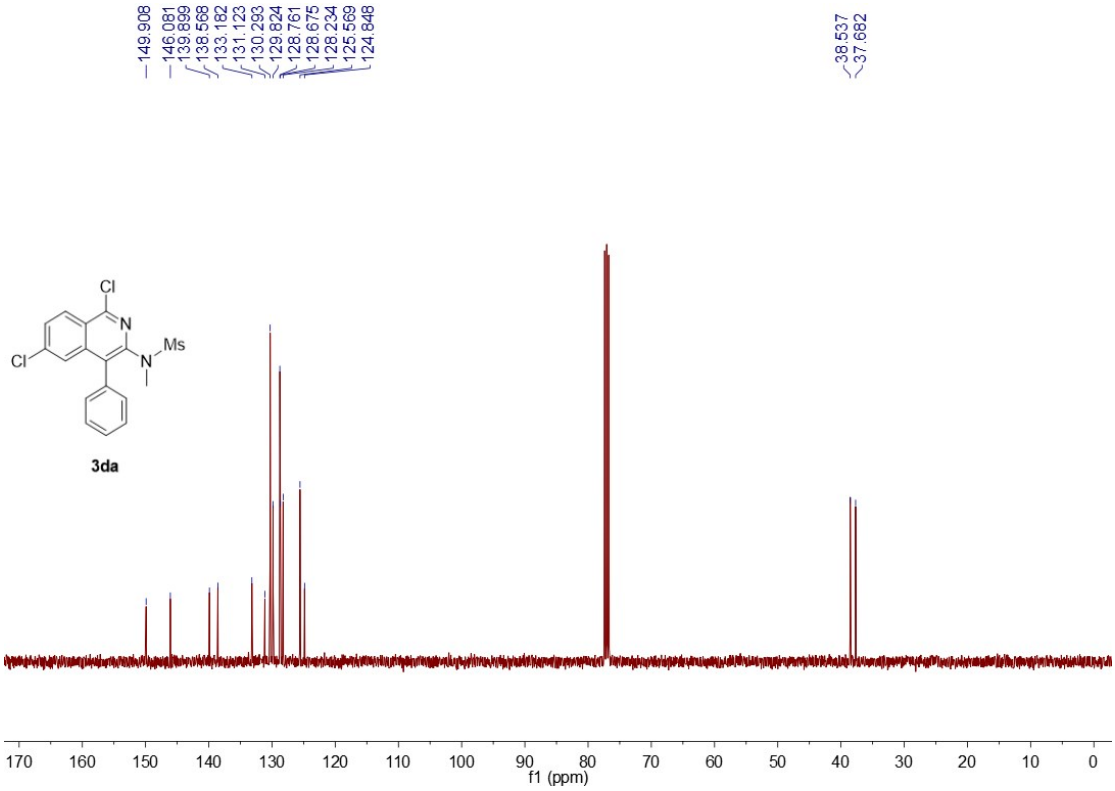
7.551
7.546
7.536
7.533
7.531
7.527
7.522
7.517
7.513
7.506
7.500
7.491
7.485
7.481
7.478
7.445
7.440
7.435
7.428
7.424
7.421
3.161
2.994
Cl
N
Ms
N
Cl
3da
1.00
1.01
1.02
3.01
1.98
3.01
3.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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130.293
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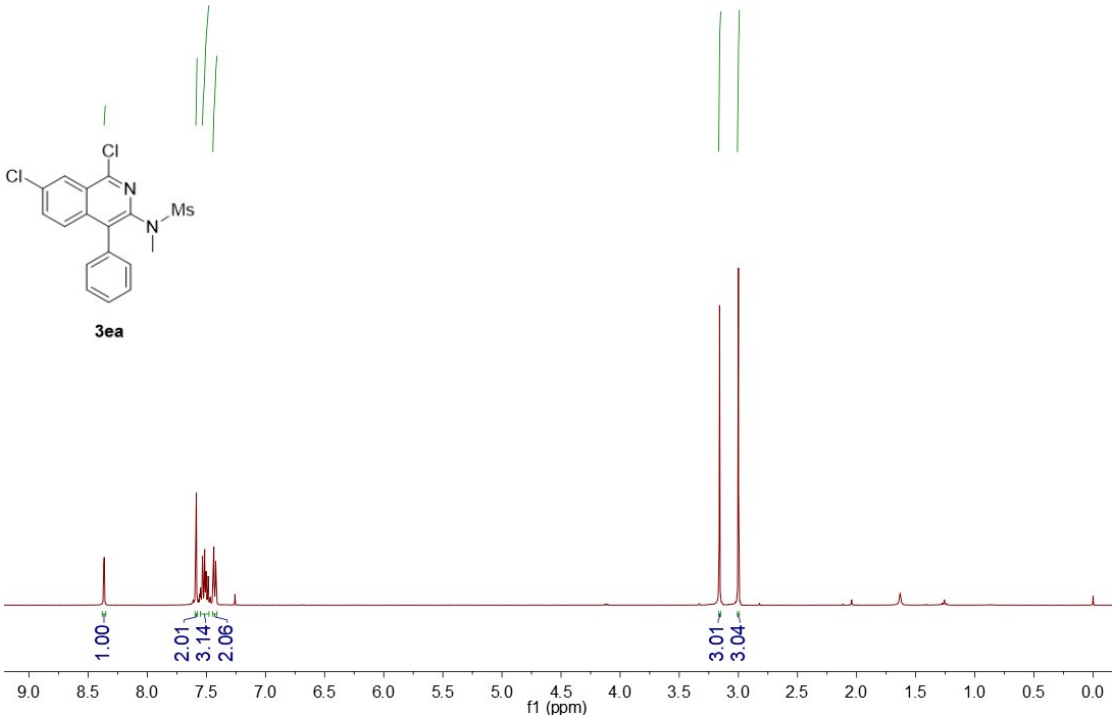
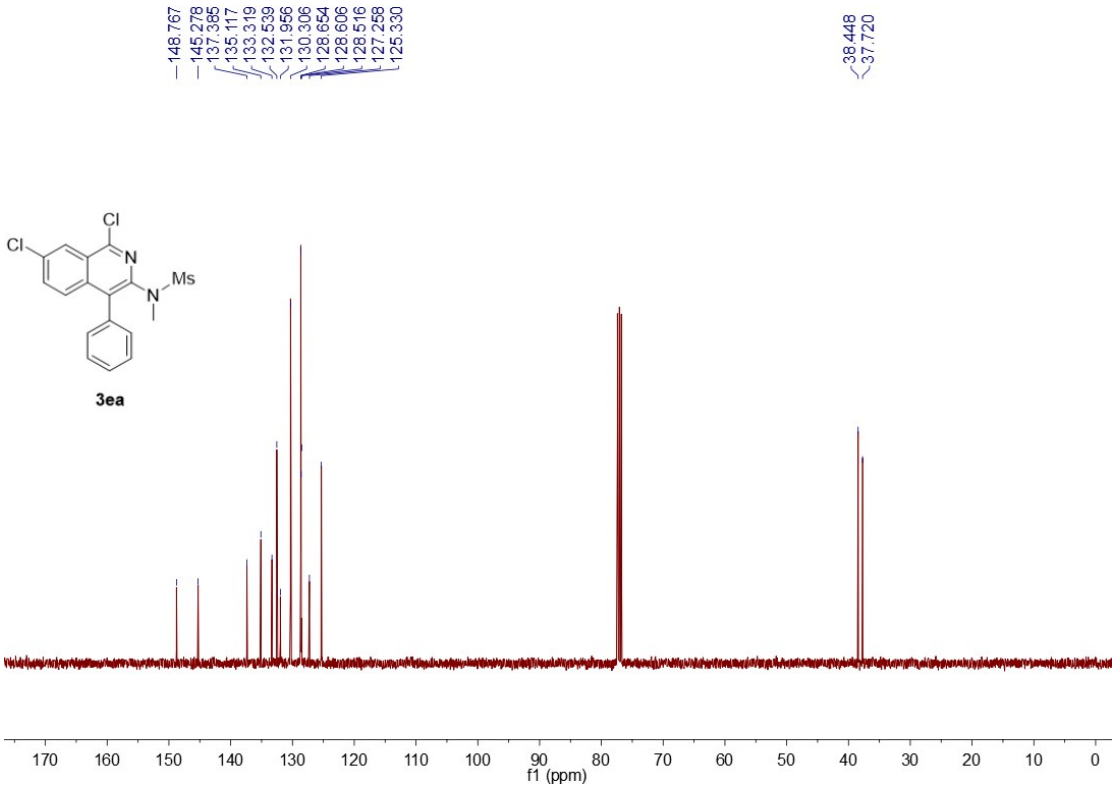
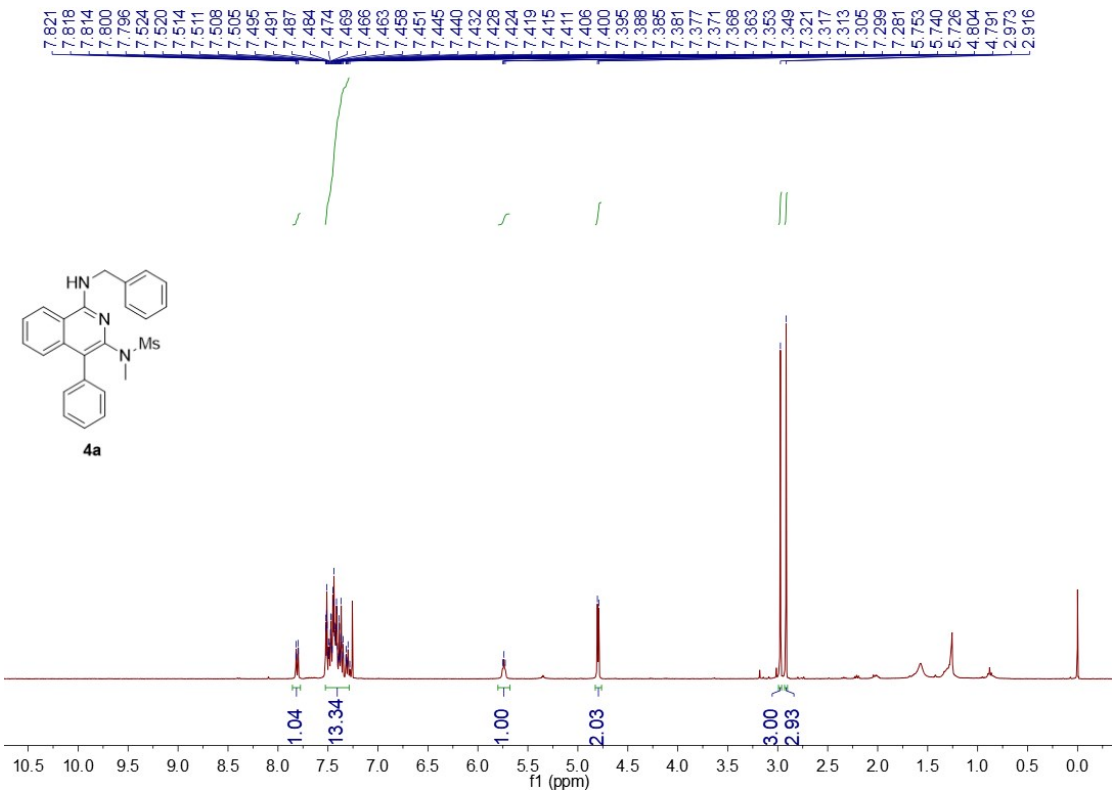
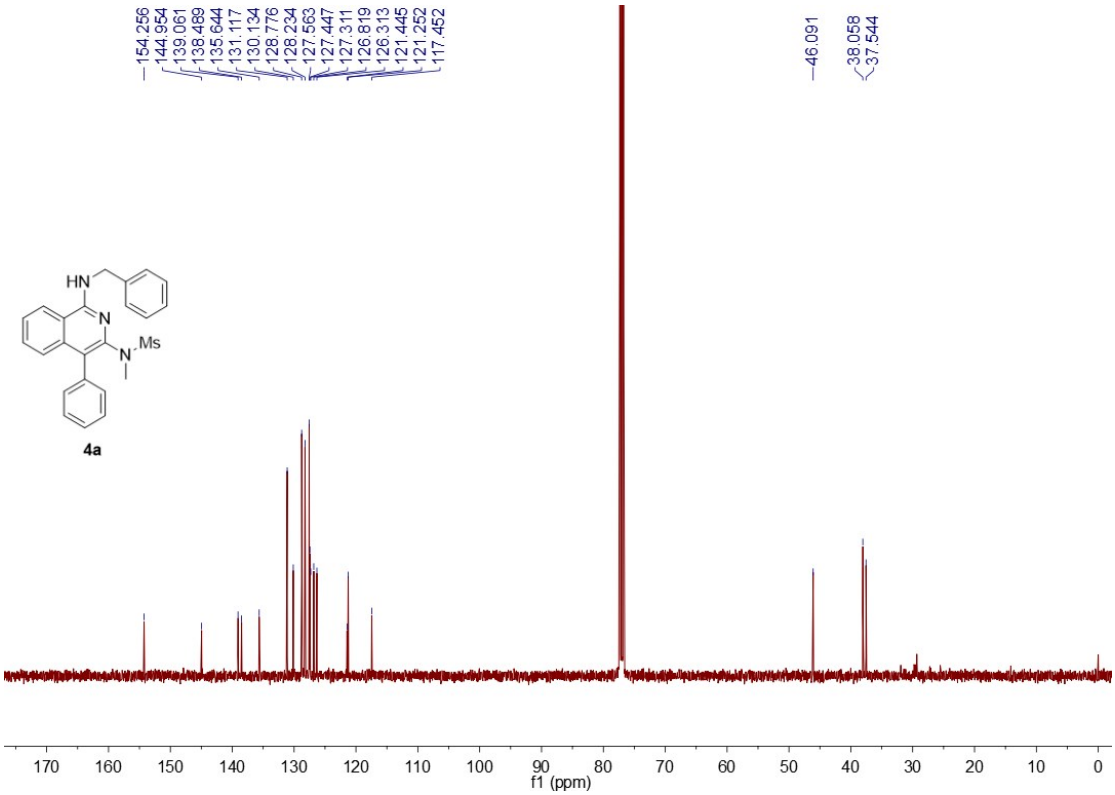
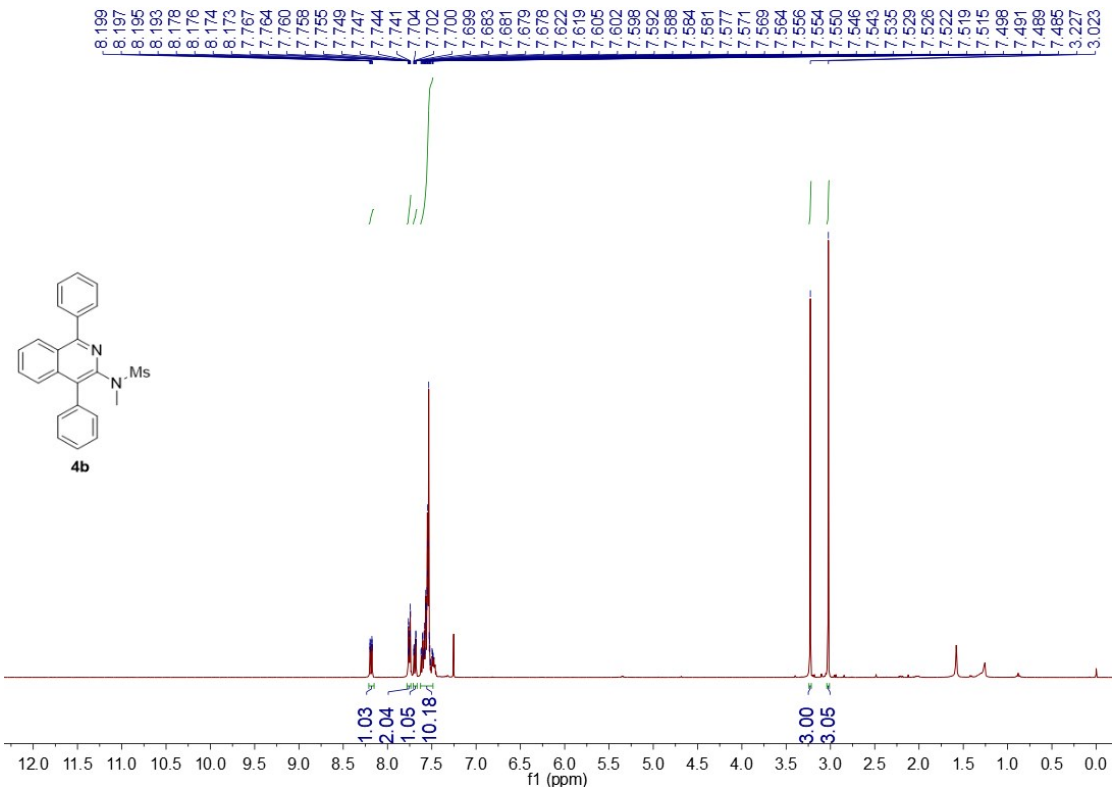
128.675
128.234
125.569
124.848
38.537
37.682
Cl
N
Cl
N
Ms
3da
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

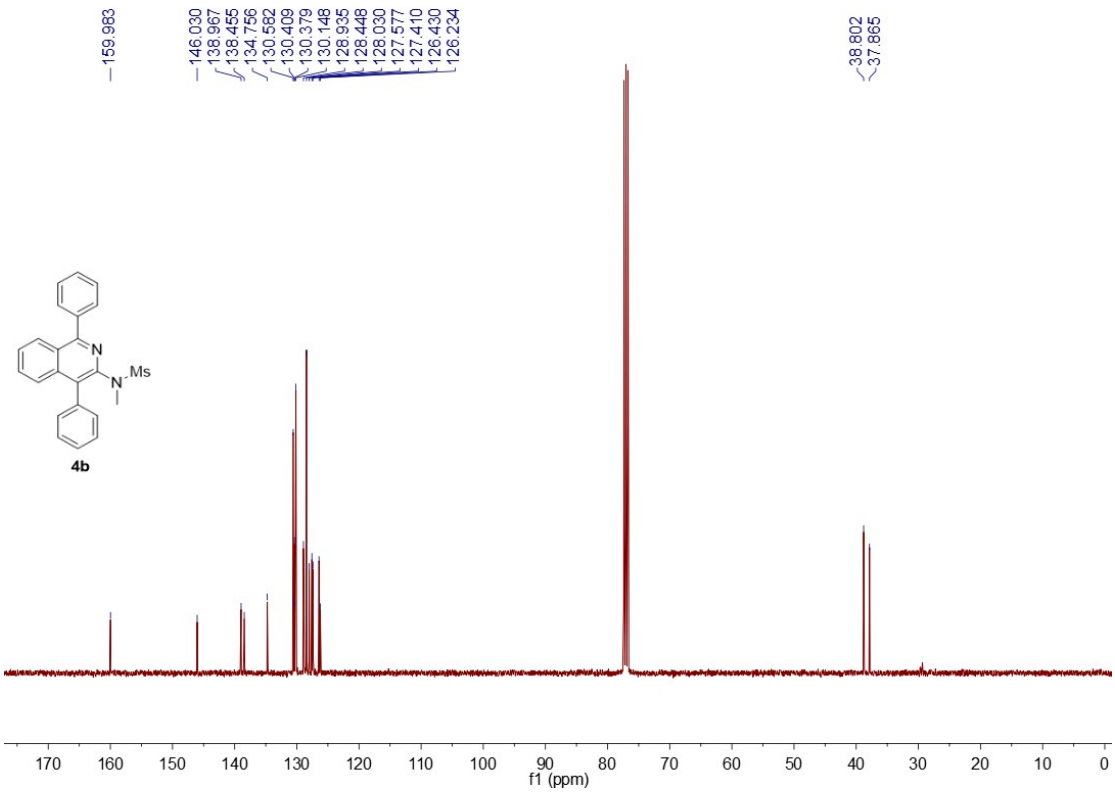

Cl
N
Cl
N
Ms
3ea
1.00
2.01
3.14
2.06
3.01
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


148.767
145.278
137.385
135.117
133.319
132.539
131.956
130.306
128.654
128.606
128.516
127.258
125.330
38.448
37.720
Cl
Cl
N
N
Ms
3ea
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.821
7.818
7.814
7.800
7.796
7.524
7.520
7.514
7.511
7.508
7.505
7.495
7.491
7.487
7.484
7.474
7.469
7.466
7.463
7.458
7.451
7.445
7.440
7.432
7.428
7.424
7.419
7.415
7.411
7.406
7.400
7.395
7.388
7.385
7.381
7.377
7.371
7.368
7.363
7.353
7.349
7.321
7.317
7.313
7.305
7.299
7.281
5.753
5.740
5.726
4.804
4.791
2.973
2.916
HN
N
N
Ms
4a
1.04
13.34
1.00
2.03
3.00
2.93
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


154.256
144.954
139.061
138.489
135.644
131.117
130.134
128.776
128.234
127.563
127.447
127.311
126.819
126.313
121.445
121.252
117.452
46.091
38.058
37.544
HN
N
N
Ms
4a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.199
8.197
8.195
8.193
8.178
8.176
8.174
8.173
7.767
7.764
7.760
7.758
7.755
7.749
7.747
7.744
7.741
7.704
7.702
7.700
7.699
7.683
7.681
7.679
7.678
7.622
7.619
7.605
7.602
7.598
7.592
7.588
7.584
7.581
7.577
7.571
7.569
7.564
7.556
7.554
7.550
7.546
7.543
7.535
7.529
7.526
7.522
7.519
7.515
7.498
7.491
7.489
7.485
3.227
3.023
N
N
Ms
4b
1.03
2.04
1.05
10.18
3.00
3.05
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


159.983
146.030
138.967
138.455
134.756
130.582
130.409
130.379
130.148
128.935
128.448
128.030
127.577
127.410
126.430
126.234
38.802
37.865
N
N
Ms
4b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

# 7. Cartesian Coordinates and Energies

**Cartesian Coordinates and Energies**
**1a**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.112516 | -0.414232 | -0.000356 |
| 2 | 6 | 0 | 0.933483 | 0.734074 | -0.000225 |
| 3 | 6 | 0 | 2.329826 | 0.624875 | -0.000044 |
| 4 | 6 | 0 | 2.883368 | -0.649094 | 0.000108 |
| 5 | 6 | 0 | 2.071170 | -1.801421 | 0.000181 |
| 6 | 6 | 0 | 0.689089 | -1.695203 | 0.000007 |
| 7 | 6 | 0 | -1.269599 | 0.003029 | -0.000031 |
| 8 | 1 | 0 | 2.962545 | 1.507303 | 0.000092 |
| 9 | 1 | 0 | 3.964183 | -0.759330 | 0.000034 |
| 10 | 1 | 0 | 2.536636 | -2.782458 | 0.000113 |
| 11 | 1 | 0 | 0.055112 | -2.576384 | 0.000052 |
| 12 | 17 | 0 | -2.578654 | -1.153085 | -0.000025 |
| 13 | 7 | 0 | -1.538373 | 1.270093 | 0.000381 |
| 14 | 16 | 0 | -0.088242 | 2.156906 | -0.000024 |

Zero-point correction= 0.093114 (Hartree/Particle)
Thermal correction to Energy= 0.100684
Thermal correction to Enthalpy= 0.101628
Thermal correction to Gibbs Free Energy= 0.060006
Sum of electronic and zero-point Energies= -1182.191468
Sum of electronic and thermal Energies= -1182.183898
Sum of electronic and thermal Enthalpies= -1182.182954
Sum of electronic and thermal Free Energies= -1182.224575
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -1182.121494

**2a**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.065456 | -1.243063 | -0.604216 |
| 2 | 6 | 0 | 2.698511 | -0.979143 | -0.628698 |
| 3 | 6 | 0 | 2.187121 | 0.184402 | -0.020021 |
| 4 | 6 | 0 | 3.082428 | 1.075092 | 0.604084 |
| 5 | 6 | 0 | 4.449682 | 0.810857 | 0.610143 |
| 6 | 6 | 0 | 4.945816 | -0.349194 | 0.010618 |
| 7 | 1 | 0 | 4.446127 | -2.146229 | -1.073565 |
| 8 | 1 | 0 | 2.011808 | -1.665112 | -1.115037 |
| 9 | 1 | 0 | 2.693048 | 1.971134 | 1.077913 |
| 10 | 1 | 0 | 5.129809 | 1.509403 | 1.090205 |
| 11 | 1 | 0 | 6.012586 | -0.555378 | 0.022052 |
| 12 | 6 | 0 | 0.784616 | 0.451839 | -0.036740 |
| 13 | 6 | 0 | -0.412282 | 0.656245 | -0.081981 |
| 14 | 7 | 0 | -1.739174 | 0.905275 | -0.076219 |
| 15 | 6 | 0 | -2.244819 | 2.096844 | -0.787671 |
| 16 | 1 | 0 | -3.311642 | 2.191982 | -0.587650 |
| 17 | 1 | 0 | -1.716018 | 2.967475 | -0.392648 |
| 18 | 1 | 0 | -2.074713 | 2.024239 | -1.867467 |
| 19 | 16 | 0 | -2.782601 | -0.482612 | 0.018080 |
| 20 | 8 | 0 | -4.140384 | 0.045760 | -0.123427 |
| 21 | 8 | 0 | -2.293772 | -1.551673 | -0.851507 |
| 22 | 6 | 0 | -2.500777 | -0.975978 | 1.727171 |
| 23 | 1 | 0 | -3.050355 | -1.907401 | 1.879611 |
| 24 | 1 | 0 | -1.430978 | -1.136233 | 1.871372 |
| 25 | 1 | 0 | -2.875115 | -0.189101 | 2.382815 |

Zero-point correction= 0.193727 (Hartree/Particle)
Thermal correction to Energy= 0.207980
Thermal correction to Enthalpy= 0.208924
Thermal correction to Gibbs Free Energy= 0.149893
Sum of electronic and zero-point Energies= -990.745514
Sum of electronic and thermal Energies= -990.731261
Sum of electronic and thermal Enthalpies= -990.730317
Sum of electronic and thermal Free Energies= -990.789348
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobeneze solvent = -990.705630

**INT1**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.415386 | 3.782663 | 0.162701 |
| 2 | 6 | 0 | -0.597520 | 2.682685 | 0.408252 |
| 3 | 6 | 0 | 0.793392 | 2.784624 | 0.214746 |
| 4 | 6 | 0 | 1.345804 | 4.008580 | -0.218717 |
| 5 | 6 | 0 | 0.519323 | 5.101881 | -0.457386 |
| 6 | 6 | 0 | -0.862323 | 4.990201 | -0.268456 |
| 7 | 1 | 0 | -2.487083 | 3.679891 | 0.301977 |
| 8 | 1 | 0 | -1.034221 | 1.749169 | 0.733524 |
| 9 | 1 | 0 | 2.419303 | 4.087326 | -0.362993 |
| 10 | 1 | 0 | 0.950826 | 6.041132 | -0.791786 |
| 11 | 1 | 0 | -1.505354 | 5.844635 | -0.461031 |
| 12 | 6 | 0 | 1.663969 | 1.672222 | 0.457467 |
| 13 | 6 | 0 | 2.540234 | 0.839401 | 0.646867 |
| 14 | 7 | 0 | 3.534953 | -0.024177 | 0.956604 |
| 15 | 6 | 0 | 3.694116 | -0.446405 | 2.371510 |
| 16 | 1 | 0 | 4.587603 | -1.064336 | 2.453119 |
| 17 | 1 | 0 | 3.815575 | 0.461000 | 2.965516 |
| 18 | 1 | 0 | 2.819686 | -1.003758 | 2.723560 |
| 19 | 16 | 0 | 3.935569 | -1.186920 | -0.263156 |
| 20 | 8 | 0 | 4.821864 | -2.163903 | 0.357678 |
| 21 | 8 | 0 | 2.693598 | -1.641692 | -0.932768 |
| 22 | 6 | 0 | 4.829372 | -0.177376 | -1.449893 |
| 23 | 1 | 0 | 5.034410 | -0.814532 | -2.313272 |
| 24 | 1 | 0 | 4.197308 | 0.664953 | -1.737312 |
| 25 | 1 | 0 | 5.755170 | 0.160522 | -0.982350 |
| 26 | 47 | 0 | 0.538602 | -0.812835 | -0.375120 |
| 27 | 51 | 0 | -2.658498 | -0.803611 | 0.062021 |
| 28 | 9 | 0 | -1.262465 | -0.410979 | 1.318585 |
| 29 | 9 | 0 | -3.561054 | -1.777298 | 1.341852 |
| 30 | 9 | 0 | -3.860618 | -1.194380 | -1.280031 |
| 31 | 9 | 0 | -1.552624 | 0.138075 | -1.185771 |
| 32 | 9 | 0 | -1.549584 | -2.279326 | -0.391080 |
| 33 | 9 | 0 | -3.456709 | 0.807825 | 0.513229 |

Zero-point correction= 0.209211 (Hartree/Particle)
Thermal correction to Energy= 0.235746
Thermal correction to Enthalpy= 0.236690
Thermal correction to Gibbs Free Energy= 0.147728
Sum of electronic and zero-point Energies= -1741.109166
Sum of electronic and thermal Energies= -1741.082630
Sum of electronic and thermal Enthalpies= -1741.081686
Sum of electronic and thermal Free Energies= -1741.170649
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -1742.336697

**TS1a**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.076362 | -3.879452 | -0.315508 |
| 2 | 6 | 0 | -3.103090 | -2.889382 | -0.447172 |
| 3 | 6 | 0 | -3.075412 | -1.786548 | 0.427034 |
| 4 | 6 | 0 | -4.030718 | -1.728689 | 1.459552 |
| 5 | 6 | 0 | -4.984081 | -2.735739 | 1.605720 |
| 6 | 6 | 0 | -5.018332 | -3.809986 | 0.713663 |
| 7 | 1 | 0 | -4.084059 | -4.717313 | -1.007304 |
| 8 | 1 | 0 | -2.352826 | -2.962824 | -1.230059 |
| 9 | 1 | 0 | -4.005470 | -0.902666 | 2.164415 |
| 10 | 1 | 0 | -5.700668 | -2.681581 | 2.421090 |
| 11 | 1 | 0 | -5.761832 | -4.593560 | 0.828731 |
| 12 | 6 | 0 | -2.048477 | -0.726236 | 0.244672 |
| 13 | 6 | 0 | -2.413645 | 0.522696 | 0.349962 |
| 14 | 7 | 0 | -3.407001 | 1.402628 | 0.338650 |
| 15 | 6 | 0 | -3.585011 | 2.385193 | 1.424240 |
| 16 | 1 | 0 | -4.569657 | 2.842201 | 1.334740 |
| 17 | 1 | 0 | -3.499710 | 1.854296 | 2.373991 |
| 18 | 1 | 0 | -2.814697 | 3.161113 | 1.367851 |
| 19 | 16 | 0 | -4.095921 | 1.826663 | -1.248991 |
| 20 | 8 | 0 | -4.915964 | 3.012479 | -1.010419 |
| 21 | 8 | 0 | -3.011913 | 1.821074 | -2.228797 |
| 22 | 6 | 0 | -5.160061 | 0.407898 | -1.555922 |
| 23 | 1 | 0 | -5.621628 | 0.580003 | -2.531572 |
| 24 | 1 | 0 | -4.554048 | -0.498932 | -1.569195 |
| 25 | 1 | 0 | -5.915711 | 0.363546 | -0.770612 |
| 26 | 6 | 0 | 1.386916 | 2.429204 | 0.933253 |
| 27 | 6 | 0 | 1.378271 | 2.781160 | -0.434203 |
| 28 | 6 | 0 | 2.492949 | 3.382333 | -1.032446 |
| 29 | 6 | 0 | 3.607076 | 3.610110 | -0.237761 |
| 30 | 6 | 0 | 3.625075 | 3.259489 | 1.129224 |

| | | | | | |
|---|---|---|---|---|---|
| 31 | 6 | 0 | 2.524412 | 2.672180 | 1.724835 |
| 32 | 6 | 0 | 0.137189 | 1.817212 | 1.269979 |
| 33 | 1 | 0 | 2.494232 | 3.642211 | -2.086025 |
| 34 | 1 | 0 | 4.491235 | 4.058036 | -0.681559 |
| 35 | 1 | 0 | 4.522012 | 3.439666 | 1.712879 |
| 36 | 1 | 0 | 2.533029 | 2.381345 | 2.769819 |
| 37 | 17 | 0 | -0.230475 | 1.255183 | 2.864860 |
| 38 | 7 | 0 | -0.742355 | 1.693672 | 0.307182 |
| 39 | 16 | 0 | -0.144752 | 2.340614 | -1.160662 |
| 40 | 47 | 0 | -0.025186 | -1.349196 | -0.132842 |
| 41 | 51 | 0 | 3.239479 | -1.190170 | -0.299519 |
| 42 | 9 | 0 | 1.913864 | -2.576071 | -0.479006 |
| 43 | 9 | 0 | 4.230117 | -2.266168 | 0.827868 |
| 44 | 9 | 0 | 4.346956 | 0.279084 | -0.096982 |
| 45 | 9 | 0 | 2.033756 | -0.181507 | -1.360917 |
| 46 | 9 | 0 | 2.166190 | -0.621471 | 1.160404 |
| 47 | 9 | 0 | 4.098815 | -1.798351 | -1.816718 |

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Zero-point correction= 0.302506 (Hartree/Particle)
Thermal correction to Energy= 0.337507
Thermal correction to Enthalpy= 0.338452
Thermal correction to Gibbs Free Energy= 0.229876
Sum of electronic and zero-point Energies= -2923.263615
Sum of electronic and thermal Energies= -2923.228614
Sum of electronic and thermal Enthalpies= -2923.227670
Sum of electronic and thermal Free Energies= -2923.336246
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.451937

**TS1a'**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.082351 | -3.359340 | 1.626552 |
| 2 | 6 | 0 | -0.214212 | -2.137228 | 0.970380 |
| 3 | 6 | 0 | 0.731352 | -1.110961 | 1.173046 |
| 4 | 6 | 0 | 1.778590 | -1.338165 | 2.089972 |
| 5 | 6 | 0 | 1.888732 | -2.553779 | 2.763527 |
| 6 | 6 | 0 | 0.965267 | -3.574131 | 2.525696 |
| 7 | 1 | 0 | -0.819085 | -4.137946 | 1.450361 |
| 8 | 1 | 0 | -1.054334 | -1.970724 | 0.303039 |
| 9 | 1 | 0 | 2.491220 | -0.544720 | 2.298932 |
| 10 | 1 | 0 | 2.693723 | -2.701348 | 3.479182 |
| 11 | 1 | 0 | 1.050170 | -4.521362 | 3.051221 |
| 12 | 6 | 0 | 0.584320 | 0.174238 | 0.480224 |
| 13 | 6 | 0 | 1.496901 | 0.933797 | -0.070321 |
| 14 | 7 | 0 | 1.668613 | 2.227689 | -0.500226 |
| 15 | 6 | 0 | 1.695595 | 2.485842 | -1.956922 |
| 16 | 1 | 0 | 1.971931 | 3.526520 | -2.127450 |
| 17 | 1 | 0 | 2.455726 | 1.836976 | -2.398760 |
| 18 | 1 | 0 | 0.722585 | 2.269956 | -2.412723 |
| 19 | 16 | 0 | 0.994724 | 3.534757 | 0.435282 |
| 20 | 8 | 0 | 1.662241 | 4.736072 | -0.064457 |
| 21 | 8 | 0 | -0.471314 | 3.471251 | 0.435214 |
| 22 | 6 | 0 | 1.579893 | 3.160586 | 2.095899 |
| 23 | 1 | 0 | 1.173372 | 3.956935 | 2.723966 |
| 24 | 1 | 0 | 1.191049 | 2.194065 | 2.415518 |
| 25 | 1 | 0 | 2.670375 | 3.187896 | 2.104848 |
| 26 | 6 | 0 | 4.848038 | -1.222837 | -0.867675 |
| 27 | 6 | 0 | 5.570964 | -0.269874 | -0.116052 |
| 28 | 6 | 0 | 6.951868 | -0.394998 | 0.078048 |
| 29 | 6 | 0 | 7.586980 | -1.491222 | -0.492740 |
| 30 | 6 | 0 | 6.875022 | -2.448386 | -1.245716 |
| 31 | 6 | 0 | 5.509773 | -2.324035 | -1.441172 |
| 32 | 6 | 0 | 3.459557 | -0.859771 | -0.921027 |
| 33 | 1 | 0 | 7.509603 | 0.336228 | 0.654124 |
| 34 | 1 | 0 | 8.657360 | -1.612612 | -0.355235 |
| 35 | 1 | 0 | 7.406334 | -3.291571 | -1.675218 |
| 36 | 1 | 0 | 4.950927 | -3.054168 | -2.017173 |
| 37 | 17 | 0 | 2.297746 | -1.759194 | -1.804048 |
| 38 | 7 | 0 | 3.131507 | 0.234366 | -0.273385 |
| 39 | 16 | 0 | 4.497022 | 0.984704 | 0.452746 |
| 40 | 47 | 0 | -1.468385 | 0.873957 | 0.146468 |
| 41 | 51 | 0 | -4.345036 | -0.633761 | -0.344188 |
| 42 | 9 | 0 | -5.172222 | -0.511805 | -1.992978 |
| 43 | 9 | 0 | -3.647069 | 1.150489 | -0.571813 |
| 44 | 9 | 0 | -5.804639 | 0.061768 | 0.551174 |
| 45 | 9 | 0 | -3.333270 | -0.621059 | 1.257649 |
| 46 | 9 | 0 | -4.845777 | -2.391862 | -0.066150 |
| 47 | 9 | 0 | -2.738760 | -1.192504 | -1.185187 |

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Zero-point correction= 0.302972 (Hartree/Particle)
Thermal correction to Energy= 0.337793
Thermal correction to Enthalpy= 0.338737
Thermal correction to Gibbs Free Energy= 0.229801
Sum of electronic and zero-point Energies= -2923.255693
Sum of electronic and thermal Energies= -2923.220872
Sum of electronic and thermal Enthalpies= -2923.219928
Sum of electronic and thermal Free Energies= -2923.328865
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.449833

**TS1b**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.771335 | -3.311004 | 0.089520 |
| 2 | 6 | 0 | -0.276577 | -2.054393 | -0.259467 |
| 3 | 6 | 0 | 0.792582 | -1.482635 | 0.453684 |
| 4 | 6 | 0 | 1.383953 | -2.225039 | 1.495839 |
| 5 | 6 | 0 | 0.912366 | -3.494202 | 1.815810 |
| 6 | 6 | 0 | -0.172657 | -4.037101 | 1.118571 |
| 7 | 1 | 0 | -1.643934 | -3.696693 | -0.428529 |
| 8 | 1 | 0 | -0.757314 | -1.496231 | -1.054223 |
| 9 | 1 | 0 | 2.201679 | -1.793550 | 2.065934 |
| 10 | 1 | 0 | 1.374052 | -4.052056 | 2.626062 |
| 11 | 1 | 0 | -0.556478 | -5.016943 | 1.388757 |
| 12 | 6 | 0 | 1.243927 | -0.123472 | 0.148772 |
| 13 | 6 | 0 | 0.779214 | 1.088744 | -0.009247 |
| 14 | 7 | 0 | 1.343947 | 2.263518 | -0.455210 |
| 15 | 6 | 0 | 2.520772 | 2.340456 | -1.337313 |
| 16 | 1 | 0 | 2.498748 | 3.288053 | -1.873158 |
| 17 | 1 | 0 | 3.457324 | 2.277616 | -0.773703 |
| 18 | 1 | 0 | 2.467947 | 1.520693 | -2.057723 |
| 19 | 16 | 0 | 0.482553 | 3.731828 | -0.164796 |
| 20 | 8 | 0 | 1.209825 | 4.780893 | -0.878864 |
| 21 | 8 | 0 | -0.951263 | 3.527249 | -0.408534 |
| 22 | 6 | 0 | 0.702127 | 3.972568 | 1.607691 |
| 23 | 1 | 0 | 0.136159 | 4.867301 | 1.877643 |
| 24 | 1 | 0 | 0.312682 | 3.100266 | 2.135449 |
| 25 | 1 | 0 | 1.765680 | 4.112225 | 1.808269 |
| 26 | 6 | 0 | 5.366958 | -0.627266 | 0.114893 |
| 27 | 6 | 0 | 5.197546 | -1.417602 | -1.044893 |
| 28 | 6 | 0 | 6.285541 | -2.065196 | -1.644245 |
| 29 | 6 | 0 | 7.535376 | -1.905924 | -1.059436 |
| 30 | 6 | 0 | 7.714198 | -1.120655 | 0.099291 |
| 31 | 6 | 0 | 6.640805 | -0.479072 | 0.693875 |
| 32 | 6 | 0 | 4.098412 | -0.088355 | 0.518023 |
| 33 | 1 | 0 | 6.158542 | -2.672894 | -2.534362 |
| 34 | 1 | 0 | 8.394626 | -2.398516 | -1.504872 |
| 35 | 1 | 0 | 8.706455 | -1.020641 | 0.527486 |
| 36 | 1 | 0 | 6.766939 | 0.126682 | 1.585333 |
| 37 | 17 | 0 | 3.905775 | 0.905375 | 1.915859 |
| 38 | 7 | 0 | 3.069044 | -0.398776 | -0.227868 |
| 39 | 16 | 0 | 3.518994 | -1.417127 | -1.527373 |
| 40 | 47 | 0 | -1.467836 | 1.018875 | 0.190724 |
| 41 | 51 | 0 | -4.192413 | -0.737810 | -0.195058 |
| 42 | 9 | 0 | -2.788556 | -0.549012 | -1.466928 |
| 43 | 9 | 0 | -4.215090 | -2.564144 | -0.520465 |
| 44 | 9 | 0 | -5.435996 | -0.340516 | -1.501426 |
| 45 | 9 | 0 | -5.475812 | -0.813141 | 1.132010 |
| 46 | 9 | 0 | -3.879275 | 1.120306 | 0.143690 |
| 47 | 9 | 0 | -2.825649 | -0.983288 | 1.099027 |

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Zero-point correction= 0.302749 (Hartree/Particle)
Thermal correction to Energy= 0.337674
Thermal correction to Enthalpy= 0.338619
Thermal correction to Gibbs Free Energy= 0.229543
Sum of electronic and zero-point Energies= -2923.254220
Sum of electronic and thermal Energies= -2923.219294
Sum of electronic and thermal Enthalpies= -2923.218350
Sum of electronic and thermal Free Energies= -2923.327426
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.443123

**TS1b'**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.643184 | 3.682165 | 0.356754 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | -3.751510 | 2.670256 | 0.692827 |
| 3 | 6 | 0 | -3.421355 | 1.669090 | -0.244703 |
| 4 | 6 | 0 | -3.999687 | 1.722313 | -1.530327 |
| 5 | 6 | 0 | -4.906095 | 2.730496 | -1.855744 |
| 6 | 6 | 0 | -5.226035 | 3.712076 | -0.916125 |
| 7 | 1 | 0 | -4.892310 | 4.447263 | 1.086518 |
| 8 | 1 | 0 | -3.300462 | 2.640303 | 1.679822 |
| 9 | 1 | 0 | -3.724761 | 0.969992 | -2.263117 |
| 10 | 1 | 0 | -5.350234 | 2.757027 | -2.846631 |
| 11 | 1 | 0 | -5.924322 | 4.503481 | -1.173873 |
| 12 | 6 | 0 | -2.581362 | 0.550970 | 0.095250 |
| 13 | 6 | 0 | -2.326975 | -0.716586 | 0.138730 |
| 14 | 7 | 0 | -3.269287 | -1.733217 | 0.133808 |
| 15 | 6 | 0 | -4.709272 | -1.433471 | 0.183404 |
| 16 | 1 | 0 | -5.275061 | -2.363522 | 0.182260 |
| 17 | 1 | 0 | -4.948329 | -0.842781 | 1.076823 |
| 18 | 1 | 0 | -4.979363 | -0.855091 | -0.704022 |
| 19 | 16 | 0 | -2.777139 | -3.334113 | 0.511753 |
| 20 | 8 | 0 | -3.922385 | -4.195331 | 0.225658 |
| 21 | 8 | 0 | -1.480143 | -3.571098 | -0.135605 |
| 22 | 6 | 0 | -2.492792 | -3.319556 | 2.294413 |
| 23 | 1 | 0 | -2.144919 | -4.317672 | 2.570681 |
| 24 | 1 | 0 | -1.729827 | -2.573563 | 2.524680 |
| 25 | 1 | 0 | -3.434441 | -3.091135 | 2.797761 |
| 26 | 6 | 0 | 1.207149 | 2.783554 | 0.348610 |
| 27 | 6 | 0 | 1.222921 | 2.390415 | 1.704598 |
| 28 | 6 | 0 | 2.291754 | 2.724460 | 2.543472 |
| 29 | 6 | 0 | 3.338325 | 3.454380 | 1.995476 |
| 30 | 6 | 0 | 3.332686 | 3.850289 | 0.642539 |
| 31 | 6 | 0 | 2.276467 | 3.519967 | -0.188617 |
| 32 | 6 | 0 | 0.012258 | 2.290486 | -0.278469 |
| 33 | 1 | 0 | 2.312423 | 2.411244 | 3.582302 |
| 34 | 1 | 0 | 4.185975 | 3.716046 | 2.622023 |
| 35 | 1 | 0 | 4.175704 | 4.407729 | 0.247013 |
| 36 | 1 | 0 | 2.269408 | 3.803150 | -1.235859 |
| 37 | 17 | 0 | -0.363427 | 2.576331 | -1.939054 |
| 38 | 7 | 0 | -0.802155 | 1.598346 | 0.471861 |
| 39 | 16 | 0 | -0.217731 | 1.471800 | 2.069507 |
| 40 | 47 | 0 | -0.190225 | -1.356571 | -0.232824 |
| 41 | 51 | 0 | 3.042309 | -0.918095 | -0.466577 |
| 42 | 9 | 0 | 1.674095 | 0.119170 | -1.293282 |
| 43 | 9 | 0 | 3.926173 | 0.636144 | 0.020299 |
| 44 | 9 | 0 | 3.929384 | -1.065179 | -2.079471 |
| 45 | 9 | 0 | 4.222797 | -2.024997 | 0.423136 |
| 46 | 9 | 0 | 1.912414 | -2.391820 | -0.899099 |
| 47 | 9 | 0 | 1.959585 | -0.789285 | 1.095403 |

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Zero-point correction= 0.302264 (Hartree/Particle)
Thermal correction to Energy= 0.337388
Thermal correction to Enthalpy= 0.338332
Thermal correction to Gibbs Free Energy= 0.228705
Sum of electronic and zero-point Energies= -2923.253343
Sum of electronic and thermal Energies= -2923.218219
Sum of electronic and thermal Enthalpies= -2923.217275
Sum of electronic and thermal Free Energies= -2923.326902
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.439698

**TS1c**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.234890 | 5.352976 | 0.326738 |
| 2 | 6 | 0 | 0.819813 | 4.102510 | -0.125505 |
| 3 | 6 | 0 | 1.427801 | 2.925922 | 0.353181 |
| 4 | 6 | 0 | 2.435991 | 3.040511 | 1.328870 |
| 5 | 6 | 0 | 2.830839 | 4.294054 | 1.796501 |
| 6 | 6 | 0 | 2.240747 | 5.454087 | 1.291953 |
| 7 | 1 | 0 | 0.759940 | 6.248999 | -0.063502 |
| 8 | 1 | 0 | 0.021660 | 4.027645 | -0.860021 |
| 9 | 1 | 0 | 2.885585 | 2.144973 | 1.744773 |
| 10 | 1 | 0 | 3.603898 | 4.359821 | 2.556988 |
| 11 | 1 | 0 | 2.550964 | 6.429015 | 1.657341 |
| 12 | 6 | 0 | 0.987311 | 1.602644 | -0.161601 |
| 13 | 6 | 0 | 1.921156 | 0.723233 | -0.494422 |
| 14 | 7 | 0 | 3.196347 | 0.728345 | -0.941877 |
| 15 | 6 | 0 | 3.593505 | 1.715713 | -1.969833 |
| 16 | 1 | 0 | 4.545061 | 1.422210 | -2.417524 |
| 17 | 1 | 0 | 2.826179 | 1.719695 | -2.745921 |
| 18 | 1 | 0 | 3.689008 | 2.712978 | -1.532635 |

| | | | | | |
|---|---|---|---|---|---|
| 19 | 16 | 0 | 4.470907 | 0.113627 | 0.091202 |
| 20 | 8 | 0 | 5.328868 | 1.235493 | 0.471313 |
| 21 | 8 | 0 | 3.788718 | -0.704345 | 1.092217 |
| 22 | 6 | 0 | 5.399966 | -0.950029 | -1.028464 |
| 23 | 1 | 0 | 6.134275 | -1.468840 | -0.407300 |
| 24 | 1 | 0 | 4.713475 | -1.654709 | -1.497610 |
| 25 | 1 | 0 | 5.912568 | -0.335363 | -1.769641 |
| 26 | 6 | 0 | 1.457131 | -3.125410 | 0.571784 |
| 27 | 6 | 0 | 0.596919 | -2.013619 | 0.500418 |
| 28 | 6 | 0 | -0.396827 | -1.796261 | 1.449203 |
| 29 | 6 | 0 | -0.472271 | -2.702530 | 2.510997 |
| 30 | 6 | 0 | 0.394426 | -3.801022 | 2.607575 |
| 31 | 6 | 0 | 1.361057 | -4.030274 | 1.633309 |
| 32 | 6 | 0 | 2.341926 | -3.124548 | -0.575756 |
| 33 | 1 | 0 | -1.115995 | -0.991476 | 1.372592 |
| 34 | 1 | 0 | -1.236534 | -2.553384 | 3.267546 |
| 35 | 1 | 0 | 0.298354 | -4.488713 | 3.441967 |
| 36 | 1 | 0 | 2.021904 | -4.889480 | 1.682106 |
| 37 | 17 | 0 | 3.543595 | -4.359287 | -0.793982 |
| 38 | 7 | 0 | 2.243989 | -2.179804 | -1.454456 |
| 39 | 16 | 0 | 0.962093 | -1.133625 | -1.008167 |
| 40 | 47 | 0 | -1.116419 | 1.326377 | -0.368197 |
| 41 | 51 | 0 | -3.980767 | -0.263057 | -0.139224 |
| 42 | 9 | 0 | -2.876048 | 0.302212 | 1.310811 |
| 43 | 9 | 0 | -5.404829 | 0.677921 | 0.560380 |
| 44 | 9 | 0 | -4.885789 | -0.724123 | -1.678817 |
| 45 | 9 | 0 | -2.383733 | -1.027714 | -0.823511 |
| 46 | 9 | 0 | -4.381085 | -1.827192 | 0.757571 |
| 47 | 9 | 0 | -3.330507 | 1.346003 | -0.979538 |

Zero-point correction= 0.302772 (Hartree/Particle)
Thermal correction to Energy= 0.337534
Thermal correction to Enthalpy= 0.338478
Thermal correction to Gibbs Free Energy= 0.231389
Sum of electronic and zero-point Energies= -2923.247970
Sum of electronic and thermal Energies= -2923.213209
Sum of electronic and thermal Enthalpies= -2923.212265
Sum of electronic and thermal Free Energies= -2923.319354
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.432162

**TS1d**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.723477 | 1.048354 | 2.025391 |
| 2 | 6 | 0 | 3.408599 | 0.954383 | 1.574936 |
| 3 | 6 | 0 | 3.063344 | 1.394971 | 0.278468 |
| 4 | 6 | 0 | 4.080557 | 1.892314 | -0.564919 |
| 5 | 6 | 0 | 5.392189 | 1.984572 | -0.108166 |
| 6 | 6 | 0 | 5.715199 | 1.564286 | 1.186145 |
| 7 | 1 | 0 | 4.975429 | 0.720089 | 3.029754 |
| 8 | 1 | 0 | 2.632147 | 0.554434 | 2.219865 |
| 9 | 1 | 0 | 3.822690 | 2.207297 | -1.570891 |
| 10 | 1 | 0 | 6.164566 | 2.380552 | -0.761019 |
| 11 | 1 | 0 | 6.740230 | 1.636478 | 1.539071 |
| 12 | 6 | 0 | 1.686977 | 1.368961 | -0.160258 |
| 13 | 6 | 0 | 0.514481 | 1.945609 | -0.239630 |
| 14 | 7 | 0 | 0.252336 | 3.209104 | 0.273369 |
| 15 | 6 | 0 | 1.273029 | 3.986721 | 0.994856 |
| 16 | 1 | 0 | 0.870968 | 4.965797 | 1.248894 |
| 17 | 1 | 0 | 1.586835 | 3.461127 | 1.903713 |
| 18 | 1 | 0 | 2.142018 | 4.122432 | 0.345054 |
| 19 | 16 | 0 | -1.343789 | 3.851320 | 0.234512 |
| 20 | 8 | 0 | -1.214201 | 5.291121 | 0.449372 |
| 21 | 8 | 0 | -2.013845 | 3.340834 | -0.971836 |
| 22 | 6 | 0 | -2.163895 | 3.125431 | 1.668343 |
| 23 | 1 | 0 | -3.183086 | 3.520012 | 1.676823 |
| 24 | 1 | 0 | -2.178542 | 2.036629 | 1.579503 |
| 25 | 1 | 0 | -1.628971 | 3.443431 | 2.565752 |
| 26 | 6 | 0 | 2.977813 | -2.415955 | 0.054464 |
| 27 | 6 | 0 | 1.689703 | -1.853960 | 0.125550 |
| 28 | 6 | 0 | 0.755985 | -2.262805 | 1.075415 |
| 29 | 6 | 0 | 1.157123 | -3.252538 | 1.973873 |
| 30 | 6 | 0 | 2.443279 | -3.815722 | 1.922868 |
| 31 | 6 | 0 | 3.364663 | -3.408142 | 0.962442 |
| 32 | 6 | 0 | 3.696390 | -1.820509 | -1.061098 |
| 33 | 1 | 0 | -0.246889 | -1.863035 | 1.101919 |
| 34 | 1 | 0 | 0.443966 | -3.601324 | 2.714444 |
| 35 | 1 | 0 | 2.716925 | -4.589593 | 2.633596 |

| | | | | | |
|---|---|---|---|---|---|
| 36 | 1 | 0 | 4.354609 | -3.849006 | 0.904269 |
| 37 | 17 | 0 | 5.325608 | -2.282561 | -1.439249 |
| 38 | 7 | 0 | 3.102272 | -0.932047 | -1.790649 |
| 39 | 16 | 0 | 1.531656 | -0.663183 | -1.180599 |
| 40 | 47 | 0 | -1.283305 | 0.905542 | -1.106539 |
| 41 | 51 | 0 | -3.114327 | -1.535991 | 0.156123 |
| 42 | 9 | 0 | -1.526167 | -1.678384 | -0.893521 |
| 43 | 9 | 0 | -2.466773 | -2.868181 | 1.275973 |
| 44 | 9 | 0 | -4.613786 | -1.194930 | 1.176308 |
| 45 | 9 | 0 | -3.498949 | -0.068181 | -1.000647 |
| 46 | 9 | 0 | -3.983703 | -2.715327 | -0.963429 |
| 47 | 9 | 0 | -2.126123 | -0.273633 | 1.190601 |

Zero-point correction= 0.302797 (Hartree/Particle)
Thermal correction to Energy= 0.337580
Thermal correction to Enthalpy= 0.338524
Thermal correction to Gibbs Free Energy= 0.231084
Sum of electronic and zero-point Energies= -2923.250858
Sum of electronic and thermal Energies= -2923.216075
Sum of electronic and thermal Enthalpies= -2923.215130
Sum of electronic and thermal Free Energies= -2923.322570
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.432635

**TS1d'**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.638278 | -2.597629 | -1.928378 |
| 2 | 6 | 0 | 1.648513 | -1.240729 | -1.609564 |
| 3 | 6 | 0 | 1.567575 | -0.822603 | -0.267633 |
| 4 | 6 | 0 | 1.503584 | -1.794272 | 0.745658 |
| 5 | 6 | 0 | 1.504014 | -3.151305 | 0.422055 |
| 6 | 6 | 0 | 1.568661 | -3.555136 | -0.912829 |
| 7 | 1 | 0 | 1.679188 | -2.907362 | -2.968893 |
| 8 | 1 | 0 | 1.694491 | -0.492737 | -2.395908 |
| 9 | 1 | 0 | 1.428399 | -1.479607 | 1.781569 |
| 10 | 1 | 0 | 1.433334 | -3.891777 | 1.213372 |
| 11 | 1 | 0 | 1.554728 | -4.612271 | -1.162584 |
| 12 | 6 | 0 | 1.528206 | 0.620209 | 0.058212 |
| 13 | 6 | 0 | 0.553786 | 1.523085 | 0.034455 |
| 14 | 7 | 0 | 0.447085 | 2.831092 | 0.389405 |
| 15 | 6 | 0 | 1.487103 | 3.602563 | 1.081582 |
| 16 | 1 | 0 | 1.085714 | 4.574381 | 1.364960 |
| 17 | 1 | 0 | 1.811030 | 3.063972 | 1.978933 |
| 18 | 1 | 0 | 2.349100 | 3.771527 | 0.426878 |
| 19 | 16 | 0 | -1.010251 | 3.704615 | -0.046348 |
| 20 | 8 | 0 | -0.632495 | 5.117038 | -0.011252 |
| 21 | 8 | 0 | -1.538357 | 3.094987 | -1.268329 |
| 22 | 6 | 0 | -2.147219 | 3.376497 | 1.311711 |
| 23 | 1 | 0 | -3.018874 | 4.010914 | 1.130708 |
| 24 | 1 | 0 | -2.448823 | 2.327296 | 1.305714 |
| 25 | 1 | 0 | -1.660389 | 3.661886 | 2.246339 |
| 26 | 6 | 0 | 5.272917 | -0.526804 | 0.093419 |
| 27 | 6 | 0 | 4.515046 | 0.482242 | -0.523399 |
| 28 | 6 | 0 | 4.705978 | 0.839126 | -1.855541 |
| 29 | 6 | 0 | 5.687026 | 0.149676 | -2.569416 |
| 30 | 6 | 0 | 6.454037 | -0.860279 | -1.964476 |
| 31 | 6 | 0 | 6.257378 | -1.207852 | -0.631141 |
| 32 | 6 | 0 | 4.843268 | -0.669493 | 1.477463 |
| 33 | 1 | 0 | 4.111901 | 1.616007 | -2.326239 |
| 34 | 1 | 0 | 5.858907 | 0.399445 | -3.612085 |
| 35 | 1 | 0 | 7.210849 | -1.376368 | -2.546867 |
| 36 | 1 | 0 | 6.847405 | -1.985728 | -0.157609 |
| 37 | 17 | 0 | 5.565020 | -1.840859 | 2.529797 |
| 38 | 7 | 0 | 3.903815 | 0.097913 | 1.927578 |
| 39 | 16 | 0 | 3.398374 | 1.159975 | 0.675192 |
| 40 | 47 | 0 | -1.248472 | 0.422805 | -0.686383 |
| 41 | 51 | 0 | -3.935700 | -1.213902 | 0.199537 |
| 42 | 9 | 0 | -2.197785 | -1.494782 | 0.893431 |
| 43 | 9 | 0 | -4.690227 | -1.433688 | 1.871271 |
| 44 | 9 | 0 | -5.535060 | -0.770438 | -0.610182 |
| 45 | 9 | 0 | -3.014278 | -0.861427 | -1.456807 |
| 46 | 9 | 0 | -4.070112 | -2.998827 | -0.256500 |
| 47 | 9 | 0 | -3.600509 | 0.627581 | 0.556780 |

Zero-point correction= 0.302332 (Hartree/Particle)
Thermal correction to Energy= 0.337218
Thermal correction to Enthalpy= 0.338162
Thermal correction to Gibbs Free Energy= 0.228277

Sum of electronic and zero-point Energies= -2923.246513
Sum of electronic and thermal Energies= -2923.211627
Sum of electronic and thermal Enthalpies= -2923.210683
Sum of electronic and thermal Free Energies= -2923.320568
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy chlorobenzene solvent = -2924.429210

**INT2**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.419439 | -3.487681 | -0.559705 |
| 2 | 6 | 0 | -3.315354 | -2.641231 | -0.655859 |
| 3 | 6 | 0 | -3.066810 | -1.660295 | 0.323591 |
| 4 | 6 | 0 | -3.941232 | -1.588460 | 1.425251 |
| 5 | 6 | 0 | -5.025406 | -2.458753 | 1.536824 |
| 6 | 6 | 0 | -5.277642 | -3.404153 | 0.540124 |
| 7 | 1 | 0 | -4.597521 | -4.227269 | -1.335828 |
| 8 | 1 | 0 | -2.633229 | -2.730156 | -1.497571 |
| 9 | 1 | 0 | -3.752179 | -0.859934 | 2.207911 |
| 10 | 1 | 0 | -5.676142 | -2.396722 | 2.405407 |
| 11 | 1 | 0 | -6.125012 | -4.078560 | 0.626467 |
| 12 | 6 | 0 | -1.890714 | -0.774813 | 0.198311 |
| 13 | 6 | 0 | -2.029474 | 0.560635 | 0.302876 |
| 14 | 7 | 0 | -3.222191 | 1.324389 | 0.397798 |
| 15 | 6 | 0 | -3.426615 | 2.198302 | 1.562943 |
| 16 | 1 | 0 | -4.422103 | 2.640206 | 1.517592 |
| 17 | 1 | 0 | -3.343020 | 1.591361 | 2.468336 |
| 18 | 1 | 0 | -2.695249 | 3.015812 | 1.606581 |
| 19 | 16 | 0 | -3.993152 | 1.777063 | -1.068198 |
| 20 | 8 | 0 | -4.578244 | 3.105223 | -0.864078 |
| 21 | 8 | 0 | -3.038569 | 1.524877 | -2.155434 |
| 22 | 6 | 0 | -5.340759 | 0.595612 | -1.233951 |
| 23 | 1 | 0 | -5.880630 | 0.866182 | -2.144727 |
| 24 | 1 | 0 | -4.924604 | -0.409444 | -1.308365 |
| 25 | 1 | 0 | -5.991169 | 0.683794 | -0.362289 |
| 26 | 6 | 0 | 1.229819 | 2.316742 | 0.862107 |
| 27 | 6 | 0 | 1.119937 | 2.764127 | -0.474615 |
| 28 | 6 | 0 | 2.128504 | 3.541169 | -1.057921 |
| 29 | 6 | 0 | 3.242048 | 3.837696 | -0.285649 |
| 30 | 6 | 0 | 3.365419 | 3.384874 | 1.046437 |
| 31 | 6 | 0 | 2.369178 | 2.629021 | 1.630457 |
| 32 | 6 | 0 | 0.091810 | 1.545664 | 1.217919 |
| 33 | 1 | 0 | 2.053524 | 3.880183 | -2.085805 |
| 34 | 1 | 0 | 4.046500 | 4.421828 | -0.722417 |
| 35 | 1 | 0 | 4.263434 | 3.620021 | 1.607660 |
| 36 | 1 | 0 | 2.459879 | 2.254326 | 2.643721 |
| 37 | 17 | 0 | -0.152316 | 0.881987 | 2.771846 |
| 38 | 7 | 0 | -0.806546 | 1.388368 | 0.247898 |
| 39 | 16 | 0 | -0.347011 | 2.211284 | -1.220004 |
| 40 | 47 | 0 | 0.024250 | -1.634622 | -0.158835 |
| 41 | 51 | 0 | 3.310804 | -1.045467 | -0.263111 |
| 42 | 9 | 0 | 2.079410 | -2.513195 | -0.502659 |
| 43 | 9 | 0 | 4.371283 | -2.118332 | 0.802353 |
| 44 | 9 | 0 | 4.343300 | 0.470760 | 0.003492 |
| 45 | 9 | 0 | 2.056823 | -0.048614 | -1.267565 |
| 46 | 9 | 0 | 2.239556 | -0.602898 | 1.233317 |
| 47 | 9 | 0 | 4.189049 | -1.533691 | -1.812442 |

Zero-point correction= 0.305176 (Hartree/Particle)
Thermal correction to Energy= 0.339819
Thermal correction to Enthalpy= 0.340763
Thermal correction to Gibbs Free Energy= 0.234596
Sum of electronic and zero-point Energies= -2923.281084
Sum of electronic and thermal Energies= -2923.246441
Sum of electronic and thermal Enthalpies= -2923.245497
Sum of electronic and thermal Free Energies= -2923.351665
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.476866

**TS2**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.058447 | -4.123908 | 1.431487 |
| 2 | 6 | 0 | 0.699687 | -2.938995 | 0.799417 |
| 3 | 6 | 0 | -0.607438 | -2.403583 | 0.956029 |
| 4 | 6 | 0 | -1.522013 | -3.093992 | 1.802170 |
| 5 | 6 | 0 | -1.147952 | -4.265099 | 2.442956 |
| 6 | 6 | 0 | 0.141687 | -4.786057 | 2.253648 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 1 | 0 | 2.059308 | -4.522404 | 1.297164 |
| 8 | 1 | 0 | 1.420582 | -2.411657 | 0.182009 |
| 9 | 1 | 0 | -2.513615 | -2.680659 | 1.955183 |
| 10 | 1 | 0 | -1.847911 | -4.774463 | 3.099398 |
| 11 | 1 | 0 | 0.431560 | -5.702927 | 2.759744 |
| 12 | 6 | 0 | -0.937820 | -1.156874 | 0.329337 |
| 13 | 6 | 0 | -2.222728 | -0.675011 | 0.108574 |
| 14 | 7 | 0 | -3.295174 | -1.455619 | -0.379087 |
| 15 | 6 | 0 | -4.655339 | -0.885538 | -0.331553 |
| 16 | 1 | 0 | -5.369749 | -1.645794 | -0.650054 |
| 17 | 1 | 0 | -4.876762 | -0.613640 | 0.701630 |
| 18 | 1 | 0 | -4.768948 | -0.013617 | -0.983692 |
| 19 | 16 | 0 | -2.988417 | -2.376709 | -1.859381 |
| 20 | 8 | 0 | -4.009706 | -1.992873 | -2.834590 |
| 21 | 8 | 0 | -1.562628 | -2.272514 | -2.156549 |
| 22 | 6 | 0 | -3.342692 | -4.051217 | -1.300360 |
| 23 | 1 | 0 | -3.202029 | -4.703893 | -2.165434 |
| 24 | 1 | 0 | -2.645502 | -4.306464 | -0.501379 |
| 25 | 1 | 0 | -4.377031 | -4.100801 | -0.954904 |
| 26 | 6 | 0 | -2.685349 | 2.975824 | 0.649111 |
| 27 | 6 | 0 | -1.911930 | 3.301298 | -0.502721 |
| 28 | 6 | 0 | -1.672906 | 4.660440 | -0.788437 |
| 29 | 6 | 0 | -2.216105 | 5.648601 | 0.018706 |
| 30 | 6 | 0 | -2.995262 | 5.322687 | 1.144709 |
| 31 | 6 | 0 | -3.222025 | 3.996715 | 1.462600 |
| 32 | 6 | 0 | -2.811418 | 1.568224 | 0.925692 |
| 33 | 1 | 0 | -1.065001 | 4.922479 | -1.648162 |
| 34 | 1 | 0 | -2.030116 | 6.691610 | -0.221932 |
| 35 | 1 | 0 | -3.407937 | 6.109240 | 1.768109 |
| 36 | 1 | 0 | -3.811152 | 3.734270 | 2.334238 |
| 37 | 17 | 0 | -3.501318 | 1.056956 | 2.462954 |
| 38 | 7 | 0 | -2.367310 | 0.692341 | 0.093444 |
| 39 | 16 | 0 | -1.287227 | 2.033404 | -1.512869 |
| 40 | 47 | 0 | 0.597860 | 0.272780 | -0.241844 |
| 41 | 51 | 0 | 3.868452 | 0.320917 | -0.091330 |
| 42 | 9 | 0 | 4.894943 | 0.494785 | -1.616207 |
| 43 | 9 | 0 | 5.002539 | -0.896971 | 0.712015 |
| 44 | 9 | 0 | 4.639011 | 1.788120 | 0.725235 |
| 45 | 9 | 0 | 2.628531 | 0.164212 | 1.340924 |
| 46 | 9 | 0 | 2.518180 | 1.457566 | -0.861417 |
| 47 | 9 | 0 | 2.880074 | -1.089832 | -0.894020 |

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Zero-point correction= 0.303639 (Hartree/Particle)
Thermal correction to Energy= 0.338114
Thermal correction to Enthalpy= 0.339058
Thermal correction to Gibbs Free Energy= 0.232058
Sum of electronic and zero-point Energies= -2923.244460
Sum of electronic and thermal Energies= -2923.209985
Sum of electronic and thermal Enthalpies= -2923.209041
Sum of electronic and thermal Free Energies= -2923.316040
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.425329

**INT3**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.651616 | -3.047378 | 2.002472 |
| 2 | 6 | 0 | 1.092176 | -2.287157 | 0.984356 |
| 3 | 6 | 0 | -0.284833 | -1.925111 | 1.022698 |
| 4 | 6 | 0 | -1.071007 | -2.355175 | 2.137852 |
| 5 | 6 | 0 | -0.502178 | -3.111549 | 3.146765 |
| 6 | 6 | 0 | 0.860277 | -3.457488 | 3.078734 |
| 7 | 1 | 0 | 2.708441 | -3.288766 | 1.962674 |
| 8 | 1 | 0 | 1.697953 | -1.960422 | 0.150429 |
| 9 | 1 | 0 | -2.111570 | -2.049308 | 2.199252 |
| 10 | 1 | 0 | -1.098322 | -3.423181 | 3.999487 |
| 11 | 1 | 0 | 1.302899 | -4.040437 | 3.882050 |
| 12 | 6 | 0 | -0.825806 | -1.128678 | -0.018658 |
| 13 | 6 | 0 | -2.177243 | -0.857662 | -0.273199 |
| 14 | 7 | 0 | -3.115869 | -1.745534 | -0.785953 |
| 15 | 6 | 0 | -4.431310 | -1.207744 | -1.193160 |
| 16 | 1 | 0 | -4.991181 | -2.001132 | -1.684726 |
| 17 | 1 | 0 | -4.973040 | -0.868541 | -0.307854 |
| 18 | 1 | 0 | -4.305527 | -0.377766 | -1.894949 |
| 19 | 16 | 0 | -2.600411 | -3.240481 | -1.551003 |
| 20 | 8 | 0 | -3.511847 | -3.462674 | -2.668523 |
| 21 | 8 | 0 | -1.155705 | -3.159994 | -1.730883 |
| 22 | 6 | 0 | -2.967321 | -4.455525 | -0.274872 |
| 23 | 1 | 0 | -2.699497 | -5.430022 | -0.691324 |

| | | | | | |
|---|---|---|---|---|---|
| 24 | 1 | 0 | -2.364745 | -4.237249 | 0.608170 |
| 25 | 1 | 0 | -4.034905 | -4.418869 | -0.050470 |
| 26 | 6 | 0 | -2.972344 | 2.677754 | 0.514513 |
| 27 | 6 | 0 | -2.022046 | 3.257344 | -0.399011 |
| 28 | 6 | 0 | -1.878701 | 4.666334 | -0.369205 |
| 29 | 6 | 0 | -2.666555 | 5.464485 | 0.441413 |
| 30 | 6 | 0 | -3.621790 | 4.890767 | 1.299287 |
| 31 | 6 | 0 | -3.757303 | 3.517965 | 1.340975 |
| 32 | 6 | 0 | -3.050420 | 1.240272 | 0.627106 |
| 33 | 1 | 0 | -1.137821 | 5.113400 | -1.023397 |
| 34 | 1 | 0 | -2.538042 | 6.543220 | 0.416584 |
| 35 | 1 | 0 | -4.236012 | 5.518068 | 1.937613 |
| 36 | 1 | 0 | -4.475670 | 3.069058 | 2.016519 |
| 37 | 17 | 0 | -3.889094 | 0.549709 | 2.078277 |
| 38 | 7 | 0 | -2.516381 | 0.445036 | -0.203754 |
| 39 | 16 | 0 | -1.090387 | 2.397992 | -1.603225 |
| 40 | 47 | 0 | 0.474083 | 0.699292 | -0.607140 |
| 41 | 51 | 0 | 3.720280 | 0.331050 | -0.093536 |
| 42 | 9 | 0 | 5.052812 | 0.282729 | -1.368096 |
| 43 | 9 | 0 | 4.206630 | -1.294622 | 0.670542 |
| 44 | 9 | 0 | 4.716615 | 1.333603 | 1.093070 |
| 45 | 9 | 0 | 2.232071 | 0.369221 | 1.112368 |
| 46 | 9 | 0 | 2.902145 | 1.851127 | -0.854066 |
| 47 | 9 | 0 | 2.547852 | -0.649554 | -1.249642 |

Zero-point correction= 0.303781 (Hartree/Particle)
Thermal correction to Energy= 0.339171
Thermal correction to Enthalpy= 0.340115
Thermal correction to Gibbs Free Energy= 0.231651
Sum of electronic and zero-point Energies= -2923.250393
Sum of electronic and thermal Energies= -2923.215003
Sum of electronic and thermal Enthalpies= -2923.214059
Sum of electronic and thermal Free Energies= -2923.322523
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.434022

**TS3**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.030178 | -2.060242 | 3.246776 |
| 2 | 6 | 0 | 0.005018 | -1.259501 | 2.115416 |
| 3 | 6 | 0 | 1.069987 | -0.346113 | 1.834270 |
| 4 | 6 | 0 | 2.139841 | -0.268160 | 2.786056 |
| 5 | 6 | 0 | 2.126699 | -1.037968 | 3.936525 |
| 6 | 6 | 0 | 1.083279 | -1.947956 | 4.162234 |
| 7 | 1 | 0 | -0.783749 | -2.754477 | 3.430524 |
| 8 | 1 | 0 | -0.839067 | -1.319949 | 1.439061 |
| 9 | 1 | 0 | 2.959606 | 0.420419 | 2.619667 |
| 10 | 1 | 0 | 2.933885 | -0.947216 | 4.657300 |
| 11 | 1 | 0 | 1.089256 | -2.562574 | 5.058403 |
| 12 | 6 | 0 | 0.945826 | 0.521323 | 0.711250 |
| 13 | 6 | 0 | 2.092693 | 1.323921 | 0.273799 |
| 14 | 7 | 0 | 1.940611 | 2.666967 | 0.090189 |
| 15 | 6 | 0 | 3.101264 | 3.453100 | -0.368849 |
| 16 | 1 | 0 | 2.860683 | 4.509903 | -0.282731 |
| 17 | 1 | 0 | 3.954495 | 3.202201 | 0.264814 |
| 18 | 1 | 0 | 3.337450 | 3.200367 | -1.407774 |
| 19 | 16 | 0 | 0.348823 | 3.452469 | -0.140199 |
| 20 | 8 | 0 | 0.694261 | 4.868730 | -0.206384 |
| 21 | 8 | 0 | -0.326006 | 2.804058 | -1.262524 |
| 22 | 6 | 0 | -0.555930 | 3.170838 | 1.392438 |
| 23 | 1 | 0 | -1.334686 | 3.939363 | 1.382454 |
| 24 | 1 | 0 | -0.999855 | 2.175419 | 1.394409 |
| 25 | 1 | 0 | 0.120418 | 3.334608 | 2.233083 |
| 26 | 6 | 0 | 3.685941 | -1.312014 | -0.844439 |
| 27 | 6 | 0 | 2.641993 | -1.248604 | -1.831529 |
| 28 | 6 | 0 | 2.421580 | -2.387851 | -2.640204 |
| 29 | 6 | 0 | 3.173415 | -3.541371 | -2.505249 |
| 30 | 6 | 0 | 4.192916 | -3.606321 | -1.541536 |
| 31 | 6 | 0 | 4.441414 | -2.512309 | -0.738155 |
| 32 | 6 | 0 | 3.978610 | -0.210430 | 0.053846 |
| 33 | 1 | 0 | 1.632248 | -2.333642 | -3.382707 |
| 34 | 1 | 0 | 2.969072 | -4.395437 | -3.144907 |
| 35 | 1 | 0 | 4.785079 | -4.508454 | -1.424045 |
| 36 | 1 | 0 | 5.222487 | -2.575239 | 0.007719 |
| 37 | 17 | 0 | 5.511728 | -0.306367 | 0.981160 |
| 38 | 7 | 0 | 3.354871 | 0.882381 | 0.291026 |
| 39 | 16 | 0 | 1.670003 | 0.164166 | -2.166687 |
| 40 | 47 | 0 | -0.605566 | 0.064472 | -0.890447 |

| | | | | | |
|---|---|---|---|---|---|
| 41 | 51 | 0 | -3.720079 | -0.595207 | -0.011083 |
| 42 | 9 | 0 | -2.907311 | 0.201565 | -1.547174 |
| 43 | 9 | 0 | -2.246411 | -1.810238 | -0.108045 |
| 44 | 9 | 0 | -4.275295 | -1.406298 | 1.555268 |
| 45 | 9 | 0 | -4.999542 | 0.733916 | 0.044537 |
| 46 | 9 | 0 | -4.726913 | -1.701339 | -1.092348 |
| 47 | 9 | 0 | -2.531754 | 0.501550 | 0.995353 |

Zero-point correction= 0.303392 (Hartree/Particle)
Thermal correction to Energy= 0.337886
Thermal correction to Enthalpy= 0.338830
Thermal correction to Gibbs Free Energy= 0.233450
Sum of electronic and zero-point Energies= -2923.247935
Sum of electronic and thermal Energies= -2923.213441
Sum of electronic and thermal Enthalpies= -2923.212497
Sum of electronic and thermal Free Energies= -2923.317877
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.430800

**INT4**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.109790 | -3.810286 | 0.068239 |
| 2 | 6 | 0 | 1.992319 | -2.512949 | -0.435407 |
| 3 | 6 | 0 | 1.515258 | -1.466162 | 0.369808 |
| 4 | 6 | 0 | 1.172247 | -1.767938 | 1.703294 |
| 5 | 6 | 0 | 1.299565 | -3.059629 | 2.205466 |
| 6 | 6 | 0 | 1.768668 | -4.093228 | 1.389729 |
| 7 | 1 | 0 | 2.475390 | -4.600425 | -0.582248 |
| 8 | 1 | 0 | 2.258562 | -2.322253 | -1.470313 |
| 9 | 1 | 0 | 0.785498 | -0.984646 | 2.351014 |
| 10 | 1 | 0 | 1.020887 | -3.260255 | 3.236316 |
| 11 | 1 | 0 | 1.861780 | -5.102536 | 1.779647 |
| 12 | 6 | 0 | 1.266413 | -0.071075 | -0.163107 |
| 13 | 6 | 0 | 1.808054 | 1.028143 | 0.711470 |
| 14 | 7 | 0 | 1.291435 | 2.259311 | 0.952497 |
| 15 | 6 | 0 | 2.124839 | 3.216612 | 1.714168 |
| 16 | 1 | 0 | 1.538849 | 4.107962 | 1.921895 |
| 17 | 1 | 0 | 2.446616 | 2.741487 | 2.643697 |
| 18 | 1 | 0 | 3.003899 | 3.500119 | 1.128489 |
| 19 | 16 | 0 | -0.237072 | 2.938525 | 0.279275 |
| 20 | 8 | 0 | -0.067591 | 4.377192 | 0.443233 |
| 21 | 8 | 0 | -0.432222 | 2.360528 | -1.043514 |
| 22 | 6 | 0 | -1.462653 | 2.373448 | 1.465065 |
| 23 | 1 | 0 | -2.422632 | 2.739617 | 1.094144 |
| 24 | 1 | 0 | -1.500536 | 1.284639 | 1.508707 |
| 25 | 1 | 0 | -1.207780 | 2.821614 | 2.427052 |
| 26 | 6 | 0 | 4.616917 | -0.014503 | -0.274683 |
| 27 | 6 | 0 | 3.871044 | 0.168804 | -1.477757 |
| 28 | 6 | 0 | 4.555225 | 0.139451 | -2.708467 |
| 29 | 6 | 0 | 5.921526 | -0.079706 | -2.773929 |
| 30 | 6 | 0 | 6.653986 | -0.303017 | -1.598649 |
| 31 | 6 | 0 | 6.008947 | -0.273827 | -0.377781 |
| 32 | 6 | 0 | 4.015091 | 0.146546 | 1.044719 |
| 33 | 1 | 0 | 3.985383 | 0.272600 | -3.624488 |
| 34 | 1 | 0 | 6.417848 | -0.093830 | -3.740025 |
| 35 | 1 | 0 | 7.721693 | -0.492492 | -1.642550 |
| 36 | 1 | 0 | 6.578296 | -0.434964 | 0.528500 |
| 37 | 17 | 0 | 4.913762 | -0.476867 | 2.432599 |
| 38 | 7 | 0 | 2.941854 | 0.766463 | 1.365084 |
| 39 | 16 | 0 | 2.111165 | 0.401899 | -1.685864 |
| 40 | 47 | 0 | -0.879879 | -0.312246 | -0.751262 |
| 41 | 51 | 0 | -4.134103 | -0.420382 | -0.065121 |
| 42 | 9 | 0 | -2.920980 | -1.146896 | -1.375090 |
| 43 | 9 | 0 | -2.649300 | -0.583709 | 1.131467 |
| 44 | 9 | 0 | -5.126317 | 0.387173 | 1.268881 |
| 45 | 9 | 0 | -5.431765 | -0.228621 | -1.362036 |
| 46 | 9 | 0 | -4.663827 | -2.131829 | 0.378635 |
| 47 | 9 | 0 | -3.357541 | 1.236330 | -0.527632 |

Zero-point correction= 0.305138 (Hartree/Particle)
Thermal correction to Energy= 0.339642
Thermal correction to Enthalpy= 0.340586
Thermal correction to Gibbs Free Energy= 0.234106
Sum of electronic and zero-point Energies= -2923.289108
Sum of electronic and thermal Energies= -2923.254604
Sum of electronic and thermal Enthalpies= -2923.253660
Sum of electronic and thermal Free Energies= -2923.360140
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.482597

**TS4**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.030773 | 4.668201 | -0.306458 |
| 2 | 6 | 0 | 2.140785 | 4.101180 | 0.569297 |
| 3 | 6 | 0 | 1.768492 | 2.728422 | 0.452227 |
| 4 | 6 | 0 | 2.238604 | 1.991440 | -0.701315 |
| 5 | 6 | 0 | 3.208346 | 2.601170 | -1.570638 |
| 6 | 6 | 0 | 3.593332 | 3.897364 | -1.364288 |
| 7 | 1 | 0 | 3.328275 | 5.704488 | -0.180997 |
| 8 | 1 | 0 | 1.744846 | 4.670584 | 1.402028 |
| 9 | 1 | 0 | 3.585847 | 2.027796 | -2.410177 |
| 10 | 1 | 0 | 4.314323 | 4.354626 | -2.035884 |
| 11 | 6 | 0 | 1.118975 | 2.016513 | 1.484493 |
| 12 | 6 | 0 | 2.060820 | -0.077977 | 1.033492 |
| 13 | 6 | 0 | 2.476212 | 0.123331 | -0.323511 |
| 14 | 7 | 0 | 1.278618 | 0.732053 | 1.739282 |
| 15 | 16 | 0 | 1.199320 | 0.696618 | -1.462744 |
| 16 | 17 | 0 | 0.182553 | 2.899808 | 2.682454 |
| 17 | 6 | 0 | 3.678231 | -0.540626 | -0.894335 |
| 18 | 6 | 0 | 4.907764 | -0.430278 | -0.220036 |
| 19 | 6 | 0 | 3.628946 | -1.258293 | -2.099495 |
| 20 | 6 | 0 | 6.052755 | -1.035578 | -0.731110 |
| 21 | 1 | 0 | 4.959744 | 0.137729 | 0.704278 |
| 22 | 6 | 0 | 4.777385 | -1.869072 | -2.607504 |
| 23 | 1 | 0 | 2.688545 | -1.346621 | -2.634539 |
| 24 | 6 | 0 | 5.991044 | -1.758948 | -1.926320 |
| 25 | 1 | 0 | 6.996135 | -0.936657 | -0.201602 |
| 26 | 1 | 0 | 4.721465 | -2.426517 | -3.538142 |
| 27 | 1 | 0 | 6.885735 | -2.227257 | -2.326658 |
| 28 | 7 | 0 | 2.465013 | -1.278424 | 1.674086 |
| 29 | 6 | 0 | 2.697292 | -1.216863 | 3.133655 |
| 30 | 1 | 0 | 1.784046 | -1.001957 | 3.692648 |
| 31 | 1 | 0 | 3.116434 | -2.167442 | 3.469139 |
| 32 | 1 | 0 | 3.430212 | -0.427069 | 3.312450 |
| 33 | 16 | 0 | 1.532815 | -2.664279 | 1.176426 |
| 34 | 8 | 0 | 0.715981 | -2.226113 | 0.026630 |
| 35 | 8 | 0 | 0.907956 | -3.260493 | 2.354491 |
| 36 | 6 | 0 | 2.782676 | -3.802622 | 0.561693 |
| 37 | 1 | 0 | 3.295419 | -3.345922 | -0.285039 |
| 38 | 1 | 0 | 3.477365 | -4.023099 | 1.374409 |
| 39 | 1 | 0 | 2.253219 | -4.709684 | 0.260109 |
| 40 | 47 | 0 | -0.984008 | -0.219471 | -0.247067 |
| 41 | 51 | 0 | -4.184672 | -0.140294 | -0.382894 |
| 42 | 9 | 0 | -2.973593 | 1.182314 | -1.025121 |
| 43 | 9 | 0 | -5.160273 | -0.048127 | -1.948432 |
| 44 | 9 | 0 | -2.963397 | -1.374081 | -1.182194 |
| 45 | 9 | 0 | -5.171090 | -1.539680 | 0.308049 |
| 46 | 9 | 0 | -2.978131 | -0.233152 | 1.105365 |
| 47 | 9 | 0 | -5.180628 | 1.153418 | 0.479606 |

Zero-point correction= 0.303975 (Hartree/Particle)
Thermal correction to Energy= 0.338153
Thermal correction to Enthalpy= 0.339098
Thermal correction to Gibbs Free Energy= 0.231424
Sum of electronic and zero-point Energies= -2923.287455
Sum of electronic and thermal Energies= -2923.253277
Sum of electronic and thermal Enthalpies= -2923.252333
Sum of electronic and thermal Free Energies= -2923.360007
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy chlorobenzene solvent = -2924.479830

**INT5**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.315128 | 4.515040 | -0.219907 |
| 2 | 6 | 0 | -0.153130 | 3.566080 | 0.664203 |
| 3 | 6 | 0 | 0.430830 | 2.276472 | 0.689623 |
| 4 | 6 | 0 | 1.463892 | 1.928714 | -0.213543 |
| 5 | 6 | 0 | 1.945684 | 2.925371 | -1.076113 |
| 6 | 6 | 0 | 1.381871 | 4.192487 | -1.079679 |
| 7 | 1 | 0 | -0.133304 | 5.502844 | -0.250445 |
| 8 | 1 | 0 | -0.972035 | 3.788960 | 1.337350 |
| 9 | 1 | 0 | 2.749320 | 2.689707 | -1.763261 |
| 10 | 1 | 0 | 1.764618 | 4.941595 | -1.767051 |
| 11 | 6 | 0 | 0.074696 | 1.269820 | 1.641145 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 6 | 0 | 1.408873 | -0.404110 | 0.744608 |
| 13 | 6 | 0 | 2.054230 | 0.520562 | -0.277979 |
| 14 | 7 | 0 | 0.514046 | 0.041610 | 1.648514 |
| 15 | 16 | 0 | 1.478216 | -0.136164 | -1.955639 |
| 16 | 17 | 0 | -0.967214 | 1.671617 | 2.966381 |
| 17 | 6 | 0 | 3.580920 | 0.637564 | -0.106229 |
| 18 | 6 | 0 | 4.086562 | 0.855346 | 1.184482 |
| 19 | 6 | 0 | 4.463783 | 0.642526 | -1.189486 |
| 20 | 6 | 0 | 5.453300 | 1.059009 | 1.389340 |
| 21 | 1 | 0 | 3.411040 | 0.886603 | 2.037467 |
| 22 | 6 | 0 | 5.827210 | 0.857283 | -0.985205 |
| 23 | 1 | 0 | 4.083110 | 0.449462 | -2.186504 |
| 24 | 6 | 0 | 6.328417 | 1.062512 | 0.301821 |
| 25 | 1 | 0 | 5.827475 | 1.228370 | 2.395489 |
| 26 | 1 | 0 | 6.501124 | 0.852845 | -1.837368 |
| 27 | 1 | 0 | 7.391310 | 1.225799 | 0.456160 |
| 28 | 7 | 0 | 1.624148 | -1.736367 | 0.865860 |
| 29 | 6 | 0 | 0.697805 | -2.500324 | 1.753723 |
| 30 | 1 | 0 | -0.329217 | -2.278530 | 1.461980 |
| 31 | 1 | 0 | 0.891400 | -3.560831 | 1.614376 |
| 32 | 1 | 0 | 0.848926 | -2.205522 | 2.794403 |
| 33 | 16 | 0 | 2.914688 | -2.786466 | 0.151621 |
| 34 | 8 | 0 | 3.632148 | -2.106266 | -0.906516 |
| 35 | 8 | 0 | 2.260260 | -4.068480 | -0.070073 |
| 36 | 6 | 0 | 3.986836 | -2.898125 | 1.596884 |
| 37 | 1 | 0 | 4.398021 | -1.906594 | 1.794386 |
| 38 | 1 | 0 | 3.420284 | -3.280948 | 2.447282 |
| 39 | 1 | 0 | 4.782103 | -3.597533 | 1.325865 |
| 40 | 47 | 0 | -0.937392 | -0.262302 | -1.722960 |
| 41 | 51 | 0 | -3.635563 | -0.344860 | 0.132938 |
| 42 | 9 | 0 | -2.328792 | 1.039621 | 0.105352 |
| 43 | 9 | 0 | -4.961313 | 0.893680 | -0.206573 |
| 44 | 9 | 0 | -3.250841 | -0.464405 | -1.748044 |
| 45 | 9 | 0 | -4.781807 | -1.784906 | 0.013396 |
| 46 | 9 | 0 | -2.149728 | -1.516673 | 0.318954 |
| 47 | 9 | 0 | -3.771395 | -0.195282 | 1.970353 |

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Zero-point correction= 0.307028 (Hartree/Particle)
Thermal correction to Energy= 0.341200
Thermal correction to Enthalpy= 0.342144
Thermal correction to Gibbs Free Energy= 0.237719
Sum of electronic and zero-point Energies= -2923.319383
Sum of electronic and thermal Energies= -2923.285211
Sum of electronic and thermal Enthalpies= -2923.284267
Sum of electronic and thermal Free Energies= -2923.388692
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.517281

**TS5**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.189577 | 4.671989 | -0.477080 |
| 2 | 6 | 0 | 2.045594 | 4.159213 | 0.106344 |
| 3 | 6 | 0 | 1.940257 | 2.777894 | 0.369165 |
| 4 | 6 | 0 | 3.012308 | 1.895624 | 0.027454 |
| 5 | 6 | 0 | 4.180149 | 2.459631 | -0.542755 |
| 6 | 6 | 0 | 4.261545 | 3.816948 | -0.794356 |
| 7 | 1 | 0 | 3.263430 | 5.735726 | -0.681382 |
| 8 | 1 | 0 | 1.220465 | 4.811268 | 0.367101 |
| 9 | 1 | 0 | 5.016750 | 1.816366 | -0.785239 |
| 10 | 1 | 0 | 5.164556 | 4.225865 | -1.238154 |
| 11 | 6 | 0 | 0.814739 | 2.177376 | 1.026612 |
| 12 | 6 | 0 | 1.685401 | 0.052689 | 0.913773 |
| 13 | 6 | 0 | 2.887249 | 0.484115 | 0.291285 |
| 14 | 7 | 0 | 0.705289 | 0.910364 | 1.284689 |
| 15 | 16 | 0 | 1.088709 | 0.192779 | -2.027139 |
| 16 | 17 | 0 | -0.507011 | 3.179812 | 1.563151 |
| 17 | 6 | 0 | 4.088944 | -0.390826 | 0.179258 |
| 18 | 6 | 0 | 4.702787 | -0.851707 | 1.355855 |
| 19 | 6 | 0 | 4.673601 | -0.701030 | -1.058867 |
| 20 | 6 | 0 | 5.878865 | -1.603190 | 1.294389 |
| 21 | 1 | 0 | 4.266423 | -0.608239 | 2.320320 |
| 22 | 6 | 0 | 5.842875 | -1.457188 | -1.117064 |
| 23 | 1 | 0 | 4.184858 | -0.375767 | -1.971915 |
| 24 | 6 | 0 | 6.450688 | -1.908982 | 0.057870 |
| 25 | 1 | 0 | 6.349019 | -1.941496 | 2.213732 |
| 26 | 1 | 0 | 6.275348 | -1.701108 | -2.083194 |
| 27 | 1 | 0 | 7.363512 | -2.496004 | 0.009040 |
| 28 | 7 | 0 | 1.475211 | -1.274910 | 1.351029 |

| | | | | | |
|---|---|---|---|---|---|
| 29 | 6 | 0 | 0.450532 | -1.464201 | 2.414851 |
| 30 | 1 | 0 | 0.679192 | -0.766780 | 3.220708 |
| 31 | 1 | 0 | -0.564129 | -1.291755 | 2.052166 |
| 32 | 1 | 0 | 0.539989 | -2.484320 | 2.794081 |
| 33 | 16 | 0 | 1.435102 | -2.571465 | 0.181171 |
| 34 | 8 | 0 | 2.056329 | -2.067147 | -1.053239 |
| 35 | 8 | 0 | 0.087056 | -3.134731 | 0.153867 |
| 36 | 6 | 0 | 2.548192 | -3.782331 | 0.908940 |
| 37 | 1 | 0 | 3.545020 | -3.345765 | 0.975437 |
| 38 | 1 | 0 | 2.165994 | -4.063120 | 1.892044 |
| 39 | 1 | 0 | 2.536321 | -4.646154 | 0.239961 |
| 40 | 47 | 0 | -1.119085 | -0.321662 | -1.275670 |
| 41 | 51 | 0 | -4.011616 | -0.102114 | 0.144898 |
| 42 | 9 | 0 | -3.462343 | -0.644538 | -1.611530 |
| 43 | 9 | 0 | -4.964509 | -1.670959 | 0.341789 |
| 44 | 9 | 0 | -2.407008 | -1.019607 | 0.670126 |
| 45 | 9 | 0 | -4.297345 | 0.434241 | 1.888974 |
| 46 | 9 | 0 | -2.854892 | 1.363011 | -0.164825 |
| 47 | 9 | 0 | -5.448297 | 0.827860 | -0.545105 |

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Zero-point correction= 0.305949 (Hartree/Particle)
Thermal correction to Energy= 0.339940
Thermal correction to Enthalpy= 0.340884
Thermal correction to Gibbs Free Energy= 0.235593
Sum of electronic and zero-point Energies= -2923.270405
Sum of electronic and thermal Energies= -2923.236414
Sum of electronic and thermal Enthalpies= -2923.235469
Sum of electronic and thermal Free Energies= -2923.340761
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.464803

**INT6**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.908154 | -3.667726 | 3.454091 |
| 2 | 6 | 0 | 0.422349 | -2.379534 | 3.460178 |
| 3 | 6 | 0 | 0.793563 | -1.473913 | 2.435423 |
| 4 | 6 | 0 | 1.669567 | -1.901731 | 1.385786 |
| 5 | 6 | 0 | 2.157718 | -3.234442 | 1.419282 |
| 6 | 6 | 0 | 1.783392 | -4.093954 | 2.428933 |
| 7 | 1 | 0 | 0.616447 | -4.360524 | 4.237540 |
| 8 | 1 | 0 | -0.252367 | -2.046914 | 4.240001 |
| 9 | 1 | 0 | 2.824624 | -3.570288 | 0.633849 |
| 10 | 1 | 0 | 2.161076 | -5.112390 | 2.435569 |
| 11 | 6 | 0 | 0.343516 | -0.124487 | 2.363261 |
| 12 | 6 | 0 | 1.493821 | 0.289536 | 0.422977 |
| 13 | 6 | 0 | 2.043293 | -0.976374 | 0.355198 |
| 14 | 7 | 0 | 0.661381 | 0.705900 | 1.409171 |
| 15 | 16 | 0 | -0.351727 | 4.059376 | -0.109529 |
| 16 | 17 | 0 | -0.707904 | 0.515225 | 3.613410 |
| 17 | 6 | 0 | 2.931308 | -1.407368 | -0.764722 |
| 18 | 6 | 0 | 2.394034 | -2.161996 | -1.820565 |
| 19 | 6 | 0 | 4.296927 | -1.091656 | -0.773821 |
| 20 | 6 | 0 | 3.213537 | -2.582306 | -2.869195 |
| 21 | 1 | 0 | 1.332844 | -2.393990 | -1.817067 |
| 22 | 6 | 0 | 5.113266 | -1.512554 | -1.825488 |
| 23 | 1 | 0 | 4.726069 | -0.531917 | 0.053923 |
| 24 | 6 | 0 | 4.572406 | -2.257786 | -2.875035 |
| 25 | 1 | 0 | 2.787098 | -3.161220 | -3.683568 |
| 26 | 1 | 0 | 6.170676 | -1.262648 | -1.821604 |
| 27 | 1 | 0 | 5.207518 | -2.585520 | -3.693250 |
| 28 | 7 | 0 | 1.747822 | 1.260390 | -0.612164 |
| 29 | 6 | 0 | 1.240576 | 1.046334 | -2.004377 |
| 30 | 1 | 0 | 2.011363 | 0.563251 | -2.606000 |
| 31 | 1 | 0 | 0.351981 | 0.420069 | -1.933137 |
| 32 | 1 | 0 | 0.971111 | 2.004544 | -2.446195 |
| 33 | 16 | 0 | 2.259047 | 2.770284 | -0.207630 |
| 34 | 8 | 0 | 1.229111 | 3.574094 | 0.670070 |
| 35 | 8 | 0 | 2.727984 | 3.453592 | -1.402888 |
| 36 | 6 | 0 | 3.535328 | 2.552483 | 1.034584 |
| 37 | 1 | 0 | 3.121539 | 2.021716 | 1.891929 |
| 38 | 1 | 0 | 4.349305 | 1.998649 | 0.564345 |
| 39 | 1 | 0 | 3.852945 | 3.557450 | 1.319099 |
| 40 | 47 | 0 | -1.532785 | 1.934384 | 0.222827 |
| 41 | 51 | 0 | -2.587180 | -1.130351 | -0.961745 |
| 42 | 9 | 0 | -2.207934 | 0.533025 | -1.802016 |
| 43 | 9 | 0 | -2.508537 | -2.012130 | -2.582733 |
| 44 | 9 | 0 | -0.715605 | -1.289624 | -0.766982 |
| 45 | 9 | 0 | -2.830053 | -2.669449 | 0.031395 |

| | | | | | |
|---|---|---|---|---|---|
| 46 | 9 | 0 | -2.533116 | -0.106033 | 0.670208 |
| 47 | 9 | 0 | -4.396491 | -0.784952 | -1.086351 |

Zero-point correction= 0.306843 (Hartree/Particle)
Thermal correction to Energy= 0.340567
Thermal correction to Enthalpy= 0.341511
Thermal correction to Gibbs Free Energy= 0.237909
Sum of electronic and zero-point Energies= -2923.317876
Sum of electronic and thermal Energies= -2923.284152
Sum of electronic and thermal Enthalpies= -2923.283208
Sum of electronic and thermal Free Energies= -2923.386811
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2924.511515

**3aa**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.081268 | 2.186593 | -0.513114 |
| 2 | 6 | 0 | -3.935053 | 0.835930 | -0.292714 |
| 3 | 6 | 0 | -2.652242 | 0.284701 | -0.050236 |
| 4 | 6 | 0 | -1.497228 | 1.133552 | -0.044001 |
| 5 | 6 | 0 | -1.692413 | 2.525630 | -0.260824 |
| 6 | 6 | 0 | -2.950617 | 3.035228 | -0.490727 |
| 7 | 1 | 0 | -5.066795 | 2.603133 | -0.699701 |
| 8 | 1 | 0 | -4.796178 | 0.177955 | -0.300184 |
| 9 | 1 | 0 | -0.832612 | 3.185397 | -0.243466 |
| 10 | 1 | 0 | -3.076678 | 4.101734 | -0.656099 |
| 11 | 6 | 0 | -2.407265 | -1.093761 | 0.217841 |
| 12 | 6 | 0 | -0.142613 | -0.807942 | 0.406181 |
| 13 | 6 | 0 | -0.206346 | 0.563281 | 0.209351 |
| 14 | 7 | 0 | -1.236966 | -1.610918 | 0.421638 |
| 15 | 17 | 0 | -3.772546 | -2.218188 | 0.288849 |
| 16 | 6 | 0 | 1.007803 | 1.428390 | 0.285334 |
| 17 | 6 | 0 | 1.615684 | 1.682862 | 1.523990 |
| 18 | 6 | 0 | 1.549032 | 2.017884 | -0.867419 |
| 19 | 6 | 0 | 2.740034 | 2.504480 | 1.609332 |
| 20 | 1 | 0 | 1.201888 | 1.232630 | 2.421932 |
| 21 | 6 | 0 | 2.673189 | 2.841544 | -0.781053 |
| 22 | 1 | 0 | 1.099859 | 1.806619 | -1.832456 |
| 23 | 6 | 0 | 3.271954 | 3.087026 | 0.456467 |
| 24 | 1 | 0 | 3.197997 | 2.692484 | 2.576838 |
| 25 | 1 | 0 | 3.083170 | 3.286914 | -1.683587 |
| 26 | 1 | 0 | 4.146791 | 3.728331 | 0.522473 |
| 27 | 7 | 0 | 1.103449 | -1.467450 | 0.644202 |
| 28 | 6 | 0 | 1.067328 | -2.572088 | 1.622848 |
| 29 | 1 | 0 | 0.504564 | -3.436854 | 1.263942 |
| 30 | 1 | 0 | 2.090433 | -2.876387 | 1.855211 |
| 31 | 1 | 0 | 0.602573 | -2.189329 | 2.534635 |
| 32 | 16 | 0 | 2.059945 | -1.813037 | -0.756248 |
| 33 | 8 | 0 | 1.511553 | -1.038963 | -1.871353 |
| 34 | 8 | 0 | 2.243316 | -3.263898 | -0.861849 |
| 35 | 6 | 0 | 3.648786 | -1.102372 | -0.287979 |
| 36 | 1 | 0 | 3.528613 | -0.028184 | -0.148014 |
| 37 | 1 | 0 | 3.993267 | -1.583608 | 0.629204 |
| 38 | 1 | 0 | 4.340343 | -1.317224 | -1.106096 |

Zero-point correction= 0.290067 (Hartree/Particle)
Thermal correction to Energy= 0.310423
Thermal correction to Enthalpy= 0.311368
Thermal correction to Gibbs Free Energy= 0.240379
Sum of electronic and zero-point Energies= -1774.834685
Sum of electronic and thermal Energies= -1774.814329
Sum of electronic and thermal Enthalpies= -1774.813385
Sum of electronic and thermal Free Energies= -1774.884373
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -1774.734357

**TS1f**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.041338 | -3.907467 | -0.369112 |
| 2 | 6 | 0 | -3.092255 | -2.893916 | -0.498180 |
| 3 | 6 | 0 | -3.037499 | -1.836197 | 0.428949 |
| 4 | 6 | 0 | -3.941251 | -1.848714 | 1.509129 |
| 5 | 6 | 0 | -4.869788 | -2.879110 | 1.650700 |
| 6 | 6 | 0 | -4.930931 | -3.907915 | 0.707806 |
| 7 | 1 | 0 | -4.070620 | -4.709163 | -1.101900 |
| 8 | 1 | 0 | -2.382447 | -2.912642 | -1.320849 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 1 | 0 | -3.895158 | -1.057956 | 2.252682 |
| 10 | 1 | 0 | -5.545515 | -2.879175 | 2.501953 |
| 11 | 1 | 0 | -5.654685 | -4.710194 | 0.819513 |
| 12 | 6 | 0 | -2.040716 | -0.748762 | 0.249013 |
| 13 | 6 | 0 | -2.391900 | 0.484735 | 0.476099 |
| 14 | 7 | 0 | -3.348052 | 1.393527 | 0.556365 |
| 15 | 6 | 0 | -3.444320 | 2.328832 | 1.691979 |
| 16 | 1 | 0 | -4.400417 | 2.848398 | 1.646189 |
| 17 | 1 | 0 | -3.376100 | 1.749924 | 2.615611 |
| 18 | 1 | 0 | -2.627536 | 3.055715 | 1.650643 |
| 19 | 16 | 0 | -4.165711 | 1.866449 | -0.963560 |
| 20 | 8 | 0 | -4.929185 | 3.066783 | -0.629175 |
| 21 | 8 | 0 | -3.174938 | 1.848507 | -2.034797 |
| 22 | 6 | 0 | -5.291802 | 0.481008 | -1.195375 |
| 23 | 1 | 0 | -5.838177 | 0.687119 | -2.119329 |
| 24 | 1 | 0 | -4.713234 | -0.439233 | -1.285444 |
| 25 | 1 | 0 | -5.972346 | 0.437165 | -0.344123 |
| 26 | 6 | 0 | 1.438616 | 2.582950 | 0.968013 |
| 27 | 6 | 0 | 1.217848 | 3.190352 | -0.286576 |
| 28 | 6 | 0 | 2.167077 | 4.044753 | -0.861133 |
| 29 | 6 | 0 | 3.343259 | 4.272762 | -0.158403 |
| 30 | 6 | 0 | 3.582582 | 3.664580 | 1.090652 |
| 31 | 6 | 0 | 2.641089 | 2.822229 | 1.658884 |
| 32 | 6 | 0 | 0.323020 | 1.748001 | 1.340169 |
| 33 | 1 | 0 | 1.997235 | 4.506136 | -1.828871 |
| 34 | 1 | 0 | 4.098863 | 4.925904 | -0.585701 |
| 35 | 1 | 0 | 4.520889 | 3.849703 | 1.604019 |
| 36 | 1 | 0 | 2.833698 | 2.337989 | 2.611019 |
| 37 | 7 | 0 | -0.649630 | 1.708380 | 0.453706 |
| 38 | 16 | 0 | -0.321240 | 2.677294 | -0.922254 |
| 39 | 47 | 0 | -0.038085 | -1.281552 | -0.335254 |
| 40 | 51 | 0 | 3.231608 | -1.284643 | -0.208429 |
| 41 | 9 | 0 | 1.893820 | -2.397925 | -1.029411 |
| 42 | 9 | 0 | 4.135825 | -2.778099 | 0.390920 |
| 43 | 9 | 0 | 4.325031 | -0.080968 | 0.673706 |
| 44 | 9 | 0 | 2.105305 | 0.124879 | -0.799408 |
| 45 | 9 | 0 | 2.081438 | -1.358692 | 1.304713 |
| 46 | 9 | 0 | 4.180101 | -1.213400 | -1.790503 |
| 47 | 6 | 0 | 0.259937 | 0.964234 | 2.617036 |
| 48 | 1 | 0 | 1.023498 | 0.178727 | 2.596898 |
| 49 | 1 | 0 | 0.460430 | 1.615685 | 3.475394 |
| 50 | 1 | 0 | -0.715867 | 0.493832 | 2.745363 |

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Zero-point correction= 0.340123 (Hartree/Particle)
Thermal correction to Energy= 0.375549
Thermal correction to Enthalpy= 0.376493
Thermal correction to Gibbs Free Energy= 0.266549
Sum of electronic and zero-point Energies= -2502.960937
Sum of electronic and thermal Energies= -2502.925512
Sum of electronic and thermal Enthalpies= -2502.924567
Sum of electronic and thermal Free Energies= -2503.034512
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2504.15863

**INT2f**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.985323 | -3.767193 | -0.706542 |
| 2 | 6 | 0 | -3.028525 | -2.760611 | -0.834483 |
| 3 | 6 | 0 | -2.740339 | -1.894772 | 0.238142 |
| 4 | 6 | 0 | -3.417207 | -2.101911 | 1.455391 |
| 5 | 6 | 0 | -4.349825 | -3.130258 | 1.591543 |
| 6 | 6 | 0 | -4.647490 | -3.960960 | 0.509063 |
| 7 | 1 | 0 | -4.199458 | -4.413941 | -1.553299 |
| 8 | 1 | 0 | -2.496037 | -2.631741 | -1.773283 |
| 9 | 1 | 0 | -3.192583 | -1.463718 | 2.305183 |
| 10 | 1 | 0 | -4.846202 | -3.281665 | 2.546741 |
| 11 | 1 | 0 | -5.376284 | -4.759636 | 0.614978 |
| 12 | 6 | 0 | -1.717709 | -0.837731 | 0.080971 |
| 13 | 6 | 0 | -2.021208 | 0.443938 | 0.364123 |
| 14 | 7 | 0 | -3.294990 | 0.985285 | 0.698344 |
| 15 | 6 | 0 | -3.451069 | 1.699593 | 1.972658 |
| 16 | 1 | 0 | -4.485092 | 2.025891 | 2.084660 |
| 17 | 1 | 0 | -3.200820 | 1.018051 | 2.791473 |
| 18 | 1 | 0 | -2.810096 | 2.588926 | 2.031666 |
| 19 | 16 | 0 | -4.362103 | 1.402713 | -0.578703 |
| 20 | 8 | 0 | -5.064877 | 2.626728 | -0.181885 |
| 21 | 8 | 0 | -3.586123 | 1.339039 | -1.822642 |
| 22 | 6 | 0 | -5.567146 | 0.065984 | -0.607016 |

| | | | | | |
|---|---|---|---|---|---|
| 23 | 1 | 0 | -6.293402 | 0.322174 | -1.382377 |
| 24 | 1 | 0 | -5.057343 | -0.868878 | -0.840228 |
| 25 | 1 | 0 | -6.054000 | 0.012587 | 0.368113 |
| 26 | 6 | 0 | 0.905524 | 2.724623 | 0.709585 |
| 27 | 6 | 0 | 0.431574 | 3.371335 | -0.452614 |
| 28 | 6 | 0 | 1.110692 | 4.464983 | -1.004766 |
| 29 | 6 | 0 | 2.277559 | 4.884039 | -0.379479 |
| 30 | 6 | 0 | 2.774336 | 4.234065 | 0.769914 |
| 31 | 6 | 0 | 2.100055 | 3.158327 | 1.318699 |
| 32 | 6 | 0 | 0.057899 | 1.641646 | 1.101437 |
| 33 | 1 | 0 | 0.746064 | 4.962291 | -1.897668 |
| 34 | 1 | 0 | 2.826243 | 5.725116 | -0.793193 |
| 35 | 1 | 0 | 3.702509 | 4.574365 | 1.217281 |
| 36 | 1 | 0 | 2.497479 | 2.635007 | 2.181822 |
| 37 | 7 | 0 | -0.972210 | 1.470905 | 0.273490 |
| 38 | 16 | 0 | -1.009255 | 2.610438 | -1.054834 |
| 39 | 47 | 0 | 0.225108 | -1.442820 | -0.541667 |
| 40 | 51 | 0 | 3.495598 | -1.022590 | -0.047749 |
| 41 | 9 | 0 | 2.327383 | -2.089878 | -1.150321 |
| 42 | 9 | 0 | 4.544666 | -2.499290 | 0.302456 |
| 43 | 9 | 0 | 4.414594 | 0.102980 | 1.100719 |
| 44 | 9 | 0 | 2.264474 | 0.373131 | -0.410233 |
| 45 | 9 | 0 | 2.318219 | -1.502099 | 1.359131 |
| 46 | 9 | 0 | 4.480031 | -0.547155 | -1.535522 |
| 47 | 6 | 0 | 0.292673 | 0.788052 | 2.301130 |
| 48 | 1 | 0 | 1.121113 | 0.099779 | 2.091046 |
| 49 | 1 | 0 | 0.575611 | 1.417643 | 3.150979 |
| 50 | 1 | 0 | -0.584272 | 0.194399 | 2.557058 |

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Zero-point correction= 0.343125 (Hartree/Particle)
Thermal correction to Energy= 0.378031
Thermal correction to Enthalpy= 0.378975
Thermal correction to Gibbs Free Energy= 0.271958
Sum of electronic and zero-point Energies= -2502.985661
Sum of electronic and thermal Energies= -2502.950755
Sum of electronic and thermal Enthalpies= -2502.949811
Sum of electronic and thermal Free Energies= -2503.056828
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2504.191171

**TS2f**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.693853 | -3.593431 | 1.435337 |
| 2 | 6 | 0 | 1.082204 | -2.578623 | 0.708660 |
| 3 | 6 | 0 | -0.277641 | -2.235295 | 0.944736 |
| 4 | 6 | 0 | -0.986697 | -2.952003 | 1.954956 |
| 5 | 6 | 0 | -0.368665 | -3.960974 | 2.674557 |
| 6 | 6 | 0 | 0.974774 | -4.282896 | 2.414779 |
| 7 | 1 | 0 | 2.737608 | -3.826020 | 1.249711 |
| 8 | 1 | 0 | 1.642948 | -2.030954 | -0.037957 |
| 9 | 1 | 0 | -2.020102 | -2.689378 | 2.161808 |
| 10 | 1 | 0 | -0.913832 | -4.493868 | 3.448601 |
| 11 | 1 | 0 | 1.459005 | -5.067045 | 2.990650 |
| 12 | 6 | 0 | -0.860189 | -1.154075 | 0.218285 |
| 13 | 6 | 0 | -2.214516 | -0.814162 | 0.168482 |
| 14 | 7 | 0 | -3.246925 | -1.698495 | -0.212403 |
| 15 | 6 | 0 | -4.631605 | -1.189310 | -0.173041 |
| 16 | 1 | 0 | -5.309815 | -1.985485 | -0.478352 |
| 17 | 1 | 0 | -4.869702 | -0.903442 | 0.853783 |
| 18 | 1 | 0 | -4.776427 | -0.334276 | -0.840730 |
| 19 | 16 | 0 | -2.937064 | -2.796818 | -1.562525 |
| 20 | 8 | 0 | -4.056863 | -2.660064 | -2.492865 |
| 21 | 8 | 0 | -1.553826 | -2.604457 | -1.984572 |
| 22 | 6 | 0 | -3.076269 | -4.396330 | -0.747636 |
| 23 | 1 | 0 | -2.923460 | -5.152660 | -1.521555 |
| 24 | 1 | 0 | -2.304722 | -4.466732 | 0.020364 |
| 25 | 1 | 0 | -4.075378 | -4.491711 | -0.318321 |
| 26 | 6 | 0 | -2.927652 | 2.746778 | 0.844477 |
| 27 | 6 | 0 | -2.222376 | 3.210765 | -0.306133 |
| 28 | 6 | 0 | -2.139926 | 4.603518 | -0.517499 |
| 29 | 6 | 0 | -2.769314 | 5.495625 | 0.338399 |
| 30 | 6 | 0 | -3.482873 | 5.036031 | 1.457221 |
| 31 | 6 | 0 | -3.546431 | 3.676663 | 1.709177 |
| 32 | 6 | 0 | -2.924341 | 1.324339 | 1.151821 |
| 33 | 1 | 0 | -1.581903 | 4.968234 | -1.373662 |
| 34 | 1 | 0 | -2.701127 | 6.561948 | 0.140742 |
| 35 | 1 | 0 | -3.969278 | 5.739265 | 2.125926 |
| 36 | 1 | 0 | -4.089295 | 3.322142 | 2.579771 |

| | | | | | |
|---|---|---|---|---|---|
| 37 | 7 | 0 | -2.505684 | 0.510166 | 0.241612 |
| 38 | 16 | 0 | -1.489235 | 2.130749 | -1.470164 |
| 39 | 47 | 0 | 0.355855 | 0.625022 | -0.468241 |
| 40 | 51 | 0 | 3.628425 | 0.442847 | -0.133331 |
| 41 | 9 | 0 | 4.852656 | 0.720445 | -1.486877 |
| 42 | 9 | 0 | 4.399016 | -1.146397 | 0.434085 |
| 43 | 9 | 0 | 4.558268 | 1.488086 | 1.072485 |
| 44 | 9 | 0 | 2.244516 | 0.182989 | 1.156671 |
| 45 | 9 | 0 | 2.560497 | 1.909123 | -0.695888 |
| 46 | 9 | 0 | 2.523580 | -0.575525 | -1.312924 |
| 47 | 6 | 0 | -3.329824 | 0.834284 | 2.525365 |
| 48 | 1 | 0 | -2.823326 | 1.415028 | 3.302224 |
| 49 | 1 | 0 | -4.409974 | 0.951378 | 2.674800 |
| 50 | 1 | 0 | -3.073384 | -0.219988 | 2.647869 |

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Zero-point correction= 0.341054 (Hartree/Particle)
Thermal correction to Energy= 0.375910
Thermal correction to Enthalpy= 0.376854
Thermal correction to Gibbs Free Energy= 0.270585
Sum of electronic and zero-point Energies= -2502.936447
Sum of electronic and thermal Energies= -2502.901592
Sum of electronic and thermal Enthalpies= -2502.900648
Sum of electronic and thermal Free Energies= -2503.006917
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2504.191173

**INT3f**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.733299 | -3.486686 | 1.480037 |
| 2 | 6 | 0 | 1.097300 | -2.521136 | 0.708970 |
| 3 | 6 | 0 | -0.266564 | -2.188994 | 0.938864 |
| 4 | 6 | 0 | -0.957586 | -2.871235 | 1.985831 |
| 5 | 6 | 0 | -0.317851 | -3.835767 | 2.745482 |
| 6 | 6 | 0 | 1.031175 | -4.143046 | 2.493634 |
| 7 | 1 | 0 | 2.781803 | -3.701608 | 1.301355 |
| 8 | 1 | 0 | 1.642228 | -2.001556 | -0.067801 |
| 9 | 1 | 0 | -1.993978 | -2.616428 | 2.188410 |
| 10 | 1 | 0 | -0.848787 | -4.343372 | 3.545928 |
| 11 | 1 | 0 | 1.532764 | -4.889668 | 3.103550 |
| 12 | 6 | 0 | -0.868749 | -1.152660 | 0.168041 |
| 13 | 6 | 0 | -2.225978 | -0.813007 | 0.133786 |
| 14 | 7 | 0 | -3.264038 | -1.690880 | -0.236188 |
| 15 | 6 | 0 | -4.640337 | -1.156787 | -0.234313 |
| 16 | 1 | 0 | -5.324583 | -1.943958 | -0.548210 |
| 17 | 1 | 0 | -4.897565 | -0.852526 | 0.782657 |
| 18 | 1 | 0 | -4.749830 | -0.306923 | -0.915086 |
| 19 | 16 | 0 | -2.951816 | -2.866220 | -1.516879 |
| 20 | 8 | 0 | -4.068023 | -2.778537 | -2.456568 |
| 21 | 8 | 0 | -1.566595 | -2.701549 | -1.943476 |
| 22 | 6 | 0 | -3.099495 | -4.416701 | -0.613726 |
| 23 | 1 | 0 | -2.947533 | -5.215678 | -1.343768 |
| 24 | 1 | 0 | -2.330005 | -4.447971 | 0.158972 |
| 25 | 1 | 0 | -4.100287 | -4.483580 | -0.182979 |
| 26 | 6 | 0 | -2.890142 | 2.748371 | 0.848220 |
| 27 | 6 | 0 | -2.187502 | 3.228165 | -0.299282 |
| 28 | 6 | 0 | -2.097891 | 4.625110 | -0.482890 |
| 29 | 6 | 0 | -2.716952 | 5.506951 | 0.390549 |
| 30 | 6 | 0 | -3.428091 | 5.032212 | 1.504325 |
| 31 | 6 | 0 | -3.497647 | 3.669081 | 1.731653 |
| 32 | 6 | 0 | -2.898919 | 1.322724 | 1.144527 |
| 33 | 1 | 0 | -1.541057 | 5.000960 | -1.334972 |
| 34 | 1 | 0 | -2.642207 | 6.576065 | 0.210994 |
| 35 | 1 | 0 | -3.907214 | 5.725887 | 2.188154 |
| 36 | 1 | 0 | -4.038199 | 3.303263 | 2.598943 |
| 37 | 7 | 0 | -2.514252 | 0.507262 | 0.221423 |
| 38 | 16 | 0 | -1.467593 | 2.180808 | -1.503887 |
| 39 | 47 | 0 | 0.335507 | 0.655792 | -0.536093 |
| 40 | 51 | 0 | 3.607324 | 0.408855 | -0.134903 |
| 41 | 9 | 0 | 4.892207 | 0.596672 | -1.446765 |
| 42 | 9 | 0 | 4.243900 | -1.237805 | 0.446232 |
| 43 | 9 | 0 | 4.573105 | 1.372887 | 1.109434 |
| 44 | 9 | 0 | 2.172651 | 0.229465 | 1.116316 |
| 45 | 9 | 0 | 2.655942 | 1.935829 | -0.717761 |
| 46 | 9 | 0 | 2.473923 | -0.536984 | -1.351729 |
| 47 | 6 | 0 | -3.283616 | 0.828685 | 2.523340 |
| 48 | 1 | 0 | -2.757502 | 1.397830 | 3.295616 |
| 49 | 1 | 0 | -4.359758 | 0.955231 | 2.693254 |
| 50 | 1 | 0 | -3.037404 | -0.229465 | 2.633552 |

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Zero-point correction= 0.341139 (Hartree/Particle)
Thermal correction to Energy= 0.376885
Thermal correction to Enthalpy= 0.377829
Thermal correction to Gibbs Free Energy= 0.268498
Sum of electronic and zero-point Energies= -2502.936386
Sum of electronic and thermal Energies= -2502.900641
Sum of electronic and thermal Enthalpies= -2502.899697
Sum of electronic and thermal Free Energies= -2503.009028
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2504.135695

**TS1g**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.875545 | -4.059774 | -0.322701 |
| 2 | 6 | 0 | -2.977033 | -3.003636 | -0.471382 |
| 3 | 6 | 0 | -3.029504 | -1.886036 | 0.382159 |
| 4 | 6 | 0 | -3.991281 | -1.878286 | 1.411066 |
| 5 | 6 | 0 | -4.870660 | -2.947724 | 1.573669 |
| 6 | 6 | 0 | -4.823445 | -4.039051 | 0.702667 |
| 7 | 1 | 0 | -3.820467 | -4.908594 | -0.998794 |
| 8 | 1 | 0 | -2.221993 | -3.036133 | -1.252430 |
| 9 | 1 | 0 | -4.031024 | -1.038403 | 2.098649 |
| 10 | 1 | 0 | -5.593428 | -2.929444 | 2.385230 |
| 11 | 1 | 0 | -5.509314 | -4.871651 | 0.831023 |
| 12 | 6 | 0 | -2.081070 | -0.759118 | 0.179463 |
| 13 | 6 | 0 | -2.487457 | 0.463593 | 0.354746 |
| 14 | 7 | 0 | -3.474955 | 1.335502 | 0.455431 |
| 15 | 6 | 0 | -3.552925 | 2.287163 | 1.581040 |
| 16 | 1 | 0 | -4.572450 | 2.662347 | 1.661667 |
| 17 | 1 | 0 | -3.267444 | 1.748309 | 2.485320 |
| 18 | 1 | 0 | -2.858888 | 3.118206 | 1.422604 |
| 19 | 16 | 0 | -4.263801 | 1.847382 | -1.062037 |
| 20 | 8 | 0 | -5.177333 | 2.918108 | -0.669363 |
| 21 | 8 | 0 | -3.235308 | 2.047384 | -2.080087 |
| 22 | 6 | 0 | -5.200228 | 0.365177 | -1.469671 |
| 23 | 1 | 0 | -5.717612 | 0.584341 | -2.407055 |
| 24 | 1 | 0 | -4.512402 | -0.471603 | -1.596922 |
| 25 | 1 | 0 | -5.912534 | 0.169930 | -0.667278 |
| 26 | 6 | 0 | 1.343223 | 2.471753 | 0.873980 |
| 27 | 6 | 0 | 1.296074 | 2.861224 | -0.484575 |
| 28 | 6 | 0 | 2.374458 | 3.501117 | -1.107820 |
| 29 | 6 | 0 | 3.512931 | 3.744410 | -0.355137 |
| 30 | 6 | 0 | 3.578517 | 3.369591 | 1.000516 |
| 31 | 6 | 0 | 2.510511 | 2.743097 | 1.619348 |
| 32 | 6 | 0 | 0.086495 | 1.838036 | 1.231173 |
| 33 | 1 | 0 | 2.324353 | 3.784003 | -2.154670 |
| 34 | 1 | 0 | 4.369150 | 4.224600 | -0.819706 |
| 35 | 1 | 0 | 4.484272 | 3.563777 | 1.566047 |
| 36 | 1 | 0 | 2.591993 | 2.456603 | 2.659091 |
| 37 | 7 | 0 | -0.801044 | 1.752280 | 0.261121 |
| 38 | 16 | 0 | -0.244265 | 2.453137 | -1.189425 |
| 39 | 47 | 0 | -0.035002 | -1.227848 | -0.303546 |
| 40 | 51 | 0 | 3.243947 | -1.210256 | -0.280741 |
| 41 | 9 | 0 | 1.901660 | -2.545271 | -0.594718 |
| 42 | 9 | 0 | 4.180813 | -2.378963 | 0.799347 |
| 43 | 9 | 0 | 4.360777 | 0.221549 | 0.069950 |
| 44 | 9 | 0 | 2.076455 | -0.106600 | -1.292355 |
| 45 | 9 | 0 | 2.139944 | -0.725762 | 1.195085 |
| 46 | 9 | 0 | 4.141814 | -1.714843 | -1.812329 |
| 47 | 8 | 0 | -0.318128 | 1.368623 | 2.420941 |
| 48 | 6 | 0 | 0.627439 | 0.939245 | 3.416678 |
| 49 | 1 | 0 | 0.059222 | 0.288973 | 4.083643 |
| 50 | 1 | 0 | 1.444236 | 0.377812 | 2.961673 |
| 51 | 1 | 0 | 0.999161 | 1.797480 | 3.985846 |

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Zero-point correction= 0.345130 (Hartree/Particle)
Thermal correction to Energy= 0.381704
Thermal correction to Enthalpy= 0.382648
Thermal correction to Gibbs Free Energy= 0.269682
Sum of electronic and zero-point Energies= -2578.156789
Sum of electronic and thermal Energies= -2578.120215
Sum of electronic and thermal Enthalpies= -2578.119270
Sum of electronic and thermal Free Energies= -2578.232237
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2579.353372

**INT2g**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.414067 | -3.522182 | -0.599089 |
| 2 | 6 | 0 | -3.338007 | -2.644255 | -0.728019 |
| 3 | 6 | 0 | -3.041544 | -1.707693 | 0.280952 |
| 4 | 6 | 0 | -3.839008 | -1.711890 | 1.441616 |
| 5 | 6 | 0 | -4.894838 | -2.612317 | 1.582722 |
| 6 | 6 | 0 | -5.195497 | -3.514348 | 0.559531 |
| 7 | 1 | 0 | -4.630234 | -4.226759 | -1.397941 |
| 8 | 1 | 0 | -2.714669 | -2.674113 | -1.618149 |
| 9 | 1 | 0 | -3.612350 | -1.015550 | 2.243432 |
| 10 | 1 | 0 | -5.486216 | -2.607530 | 2.495006 |
| 11 | 1 | 0 | -6.020566 | -4.212731 | 0.669006 |
| 12 | 6 | 0 | -1.893893 | -0.789478 | 0.125482 |
| 13 | 6 | 0 | -2.050787 | 0.538156 | 0.279738 |
| 14 | 7 | 0 | -3.266440 | 1.251268 | 0.485959 |
| 15 | 6 | 0 | -3.398689 | 2.088718 | 1.687814 |
| 16 | 1 | 0 | -4.428620 | 2.433911 | 1.783671 |
| 17 | 1 | 0 | -3.141841 | 1.474556 | 2.554390 |
| 18 | 1 | 0 | -2.744609 | 2.969907 | 1.662984 |
| 19 | 16 | 0 | -4.124456 | 1.762793 | -0.908097 |
| 20 | 8 | 0 | -4.725203 | 3.065045 | -0.602826 |
| 21 | 8 | 0 | -3.234503 | 1.589157 | -2.063834 |
| 22 | 6 | 0 | -5.454948 | 0.559572 | -1.056485 |
| 23 | 1 | 0 | -6.048553 | 0.856667 | -1.924562 |
| 24 | 1 | 0 | -5.023101 | -0.431705 | -1.197356 |
| 25 | 1 | 0 | -6.059667 | 0.593968 | -0.148877 |
| 26 | 6 | 0 | 1.181172 | 2.343630 | 0.777025 |
| 27 | 6 | 0 | 1.006137 | 2.812232 | -0.546823 |
| 28 | 6 | 0 | 1.958841 | 3.627759 | -1.168839 |
| 29 | 6 | 0 | 3.102756 | 3.955840 | -0.458047 |
| 30 | 6 | 0 | 3.302246 | 3.487615 | 0.854716 |
| 31 | 6 | 0 | 2.358464 | 2.691417 | 1.476434 |
| 32 | 6 | 0 | 0.052596 | 1.537602 | 1.165829 |
| 33 | 1 | 0 | 1.813199 | 3.975976 | -2.186374 |
| 34 | 1 | 0 | 3.863124 | 4.573084 | -0.927052 |
| 35 | 1 | 0 | 4.217034 | 3.739466 | 1.380539 |
| 36 | 1 | 0 | 2.547916 | 2.326664 | 2.475431 |
| 37 | 7 | 0 | -0.865155 | 1.401132 | 0.197230 |
| 38 | 16 | 0 | -0.475374 | 2.261851 | -1.264332 |
| 39 | 47 | 0 | 0.025242 | -1.599279 | -0.292839 |
| 40 | 51 | 0 | 3.335324 | -1.048758 | -0.242186 |
| 41 | 9 | 0 | 2.097361 | -2.482974 | -0.592059 |
| 42 | 9 | 0 | 4.338258 | -2.187757 | 0.811043 |
| 43 | 9 | 0 | 4.370013 | 0.434542 | 0.161752 |
| 44 | 9 | 0 | 2.126938 | 0.013769 | -1.226312 |
| 45 | 9 | 0 | 2.221688 | -0.667951 | 1.251679 |
| 46 | 9 | 0 | 4.271604 | -1.462709 | -1.777706 |
| 47 | 8 | 0 | -0.247714 | 0.963232 | 2.311967 |
| 48 | 6 | 0 | 0.698052 | 0.828625 | 3.394484 |
| 49 | 1 | 0 | 0.190476 | 0.189669 | 4.116455 |
| 50 | 1 | 0 | 1.605057 | 0.344785 | 3.034813 |
| 51 | 1 | 0 | 0.896798 | 1.805576 | 3.843800 |

Zero-point correction= 0.348389 (Hartree/Particle)
Thermal correction to Energy= 0.384372
Thermal correction to Enthalpy= 0.385316
Thermal correction to Gibbs Free Energy= 0.276346
Sum of electronic and zero-point Energies= -2578.181678
Sum of electronic and thermal Energies= -2578.145695
Sum of electronic and thermal Enthalpies= -2578.144751
Sum of electronic and thermal Free Energies= -2578.253721
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2579.387327

**TS2g**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.320763 | -3.948036 | 1.384868 |
| 2 | 6 | 0 | 0.868225 | -2.824726 | 0.701491 |
| 3 | 6 | 0 | -0.458310 | -2.350647 | 0.888123 |
| 4 | 6 | 0 | -1.294849 | -3.037190 | 1.815634 |
| 5 | 6 | 0 | -0.829445 | -4.147401 | 2.502598 |
| 6 | 6 | 0 | 0.478828 | -4.608477 | 2.283775 |
| 7 | 1 | 0 | 2.336408 | -4.298119 | 1.228702 |
| 8 | 1 | 0 | 1.529689 | -2.296410 | 0.022911 |
| 9 | 1 | 0 | -2.301969 | -2.671045 | 1.988572 |
| 10 | 1 | 0 | -1.471097 | -4.655594 | 3.217135 |

| | | | | | |
|---|---|---|---|---|---|
| 11 | 1 | 0 | 0.840786 | -5.477425 | 2.826749 |
| 12 | 6 | 0 | -0.881615 | -1.165319 | 0.202649 |
| 13 | 6 | 0 | -2.198987 | -0.730891 | 0.065574 |
| 14 | 7 | 0 | -3.282031 | -1.562220 | -0.294659 |
| 15 | 6 | 0 | -4.647820 | -1.015126 | -0.171815 |
| 16 | 1 | 0 | -5.366765 | -1.819912 | -0.334021 |
| 17 | 1 | 0 | -4.768205 | -0.634066 | 0.843329 |
| 18 | 1 | 0 | -4.847359 | -0.221901 | -0.899050 |
| 19 | 16 | 0 | -3.069714 | -2.580759 | -1.719936 |
| 20 | 8 | 0 | -4.153113 | -2.264975 | -2.651006 |
| 21 | 8 | 0 | -1.666451 | -2.499736 | -2.114060 |
| 22 | 6 | 0 | -3.381018 | -4.213322 | -1.026383 |
| 23 | 1 | 0 | -3.298563 | -4.922539 | -1.853629 |
| 24 | 1 | 0 | -2.628889 | -4.416679 | -0.262976 |
| 25 | 1 | 0 | -4.388982 | -4.239308 | -0.607990 |
| 26 | 6 | 0 | -2.803117 | 2.882661 | 0.599728 |
| 27 | 6 | 0 | -2.008473 | 3.278221 | -0.510906 |
| 28 | 6 | 0 | -1.839690 | 4.656902 | -0.748769 |
| 29 | 6 | 0 | -2.481524 | 5.590846 | 0.053918 |
| 30 | 6 | 0 | -3.297065 | 5.191710 | 1.127763 |
| 31 | 6 | 0 | -3.450173 | 3.843482 | 1.402406 |
| 32 | 6 | 0 | -2.868632 | 1.469418 | 0.893776 |
| 33 | 1 | 0 | -1.215137 | 4.979555 | -1.575439 |
| 34 | 1 | 0 | -2.350297 | 6.648788 | -0.156348 |
| 35 | 1 | 0 | -3.798317 | 5.935289 | 1.739242 |
| 36 | 1 | 0 | -4.079346 | 3.509826 | 2.221696 |
| 37 | 7 | 0 | -2.390619 | 0.622144 | 0.044794 |
| 38 | 16 | 0 | -1.295443 | 2.082167 | -1.562747 |
| 39 | 47 | 0 | 0.538848 | 0.387790 | -0.414084 |
| 40 | 51 | 0 | 3.815227 | 0.354504 | -0.107324 |
| 41 | 9 | 0 | 4.935143 | 0.648806 | -1.545562 |
| 42 | 9 | 0 | 4.870503 | -0.975598 | 0.625422 |
| 43 | 9 | 0 | 4.575444 | 1.702636 | 0.902140 |
| 44 | 9 | 0 | 2.502257 | 0.080218 | 1.242834 |
| 45 | 9 | 0 | 2.539146 | 1.596891 | -0.823897 |
| 46 | 9 | 0 | 2.842395 | -0.941581 | -1.100503 |
| 47 | 8 | 0 | -3.413050 | 1.034783 | 2.065246 |
| 48 | 6 | 0 | -2.557388 | 1.153146 | 3.226123 |
| 49 | 1 | 0 | -1.687593 | 0.496000 | 3.122230 |
| 50 | 1 | 0 | -2.230040 | 2.187183 | 3.365897 |
| 51 | 1 | 0 | -3.167000 | 0.834106 | 4.071850 |

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Zero-point correction= 0.345899 (Hartree/Particle)
Thermal correction to Energy= 0.382013
Thermal correction to Enthalpy= 0.382957
Thermal correction to Gibbs Free Energy= 0.272344
Sum of electronic and zero-point Energies= -2578.138164
Sum of electronic and thermal Energies= -2578.102050
Sum of electronic and thermal Enthalpies= -2578.101106
Sum of electronic and thermal Free Energies= -2578.211720
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2579.330462

**INT3g**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.323551 | -3.914559 | 1.426386 |
| 2 | 6 | 0 | 0.872824 | -2.810423 | 0.708322 |
| 3 | 6 | 0 | -0.455902 | -2.327929 | 0.891467 |
| 4 | 6 | 0 | -1.290970 | -2.980895 | 1.844612 |
| 5 | 6 | 0 | -0.827239 | -4.072077 | 2.560216 |
| 6 | 6 | 0 | 0.477490 | -4.541588 | 2.344674 |
| 7 | 1 | 0 | 2.336431 | -4.269656 | 1.283352 |
| 8 | 1 | 0 | 1.524280 | -2.305947 | 0.004507 |
| 9 | 1 | 0 | -2.295207 | -2.603640 | 2.010281 |
| 10 | 1 | 0 | -1.470849 | -4.562317 | 3.287909 |
| 11 | 1 | 0 | 0.834654 | -5.403649 | 2.908015 |
| 12 | 6 | 0 | -0.888923 | -1.192247 | 0.135130 |
| 13 | 6 | 0 | -2.213577 | -0.739613 | 0.042810 |
| 14 | 7 | 0 | -3.303140 | -1.563171 | -0.309580 |
| 15 | 6 | 0 | -4.657714 | -0.978148 | -0.221149 |
| 16 | 1 | 0 | -5.395618 | -1.765111 | -0.386291 |
| 17 | 1 | 0 | -4.784662 | -0.581863 | 0.790360 |
| 18 | 1 | 0 | -4.816355 | -0.183092 | -0.955379 |
| 19 | 16 | 0 | -3.094945 | -2.618866 | -1.713675 |
| 20 | 8 | 0 | -4.165204 | -2.300065 | -2.657878 |
| 21 | 8 | 0 | -1.689573 | -2.578484 | -2.090127 |
| 22 | 6 | 0 | -3.449016 | -4.224374 | -0.984908 |
| 23 | 1 | 0 | -3.376186 | -4.958676 | -1.788068 |

| | | | | | |
|---|---|---|---|---|---|
| 24 | 1 | 0 | -2.708222 | -4.428821 | -0.204687 |
| 25 | 1 | 0 | -4.464788 | -4.219213 | -0.570880 |
| 26 | 6 | 0 | -2.742880 | 2.883524 | 0.570068 |
| 27 | 6 | 0 | -1.879659 | 3.286355 | -0.492106 |
| 28 | 6 | 0 | -1.708541 | 4.667810 | -0.704172 |
| 29 | 6 | 0 | -2.410636 | 5.602613 | 0.052152 |
| 30 | 6 | 0 | -3.288606 | 5.196012 | 1.071502 |
| 31 | 6 | 0 | -3.443961 | 3.845241 | 1.332175 |
| 32 | 6 | 0 | -2.847541 | 1.467728 | 0.892879 |
| 33 | 1 | 0 | -1.029356 | 4.995706 | -1.488564 |
| 34 | 1 | 0 | -2.268295 | 6.657678 | -0.147858 |
| 35 | 1 | 0 | -3.833299 | 5.931556 | 1.656860 |
| 36 | 1 | 0 | -4.121842 | 3.506272 | 2.109280 |
| 37 | 7 | 0 | -2.398368 | 0.597545 | 0.070666 |
| 38 | 16 | 0 | -1.088826 | 2.158005 | -1.573687 |
| 39 | 47 | 0 | 0.507798 | 0.420816 | -0.446415 |
| 40 | 51 | 0 | 3.793786 | 0.310249 | -0.100724 |
| 41 | 9 | 0 | 4.970286 | 0.558061 | -1.505951 |
| 42 | 9 | 0 | 4.784529 | -1.053534 | 0.671073 |
| 43 | 9 | 0 | 4.568325 | 1.629113 | 0.937661 |
| 44 | 9 | 0 | 2.424723 | 0.071581 | 1.209524 |
| 45 | 9 | 0 | 2.581243 | 1.582642 | -0.850572 |
| 46 | 9 | 0 | 2.806888 | -0.966237 | -1.106066 |
| 47 | 8 | 0 | -3.418957 | 1.071894 | 2.071086 |
| 48 | 6 | 0 | -2.626284 | 1.293939 | 3.263642 |
| 49 | 1 | 0 | -1.726510 | 0.657802 | 3.240625 |
| 50 | 1 | 0 | -2.331128 | 2.343899 | 3.354377 |
| 51 | 1 | 0 | -3.260296 | 1.011605 | 4.096926 |

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Zero-point correction= 0.346090 (Hartree/Particle)
Thermal correction to Energy= 0.383115
Thermal correction to Enthalpy= 0.384059
Thermal correction to Gibbs Free Energy= 0.272226
Sum of electronic and zero-point Energies= -2578.147060
Sum of electronic and thermal Energies= -2578.110035
Sum of electronic and thermal Enthalpies= -2578.109091
Sum of electronic and thermal Free Energies= -2578.220925
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -2579.349826