

Supplementary Materials: DFT Studies on the Stereoselectivity of α -Silyloxy Diazoalkane Cycloadditions

Matthew J. O'Connor, Huaqing Liu, Daesung Lee, Tao Zhou and Yuanzhi Xia

Table of Contents

1. General Information	S2
2. General Procedure for Preparation of Pyrazolines	S2
3. Characterization Data	S3
4. Computational Data	S6
5. ^1H -NMR and ^{13}C -NMR Spectra	S14
6. ORTEP Diagrams of Compounds 1a , 1b , 1e , PNB-2a	S28
7. Geometric TSs with Bond Lengths	S29

1. General Information

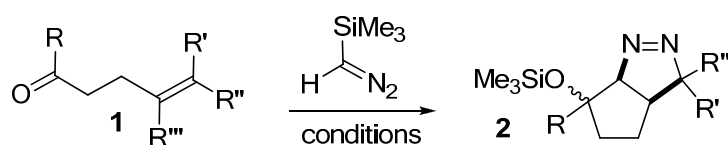
1.1. Calculation Details

All calculations were carried out with the Gaussian 09 suite of computational programs. The geometry optimizations were done at the B3LYP/6-31+G(d) level of theory. Frequencies were analytically computed at the same level of theory to obtain the enthalpies and free energies and to confirm whether the structures are minima (no imaginary frequency) or transition states (only one imaginary frequency). The effect of THF solvent was included in all optimizations by using the PCM model with the default UFF atomic radii. Unless stated otherwise, all the energy values discussed in the main text are relative enthalpies (ΔH_{sol}) in kcal/mol, and the relative free energies (ΔG_{sol}) are given in related figures for reference. Only the intermediate or transition state that has the lowest energy value among all possible conformers is used for discussion.

1.2. Experimental Details

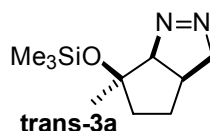
All reactions were carried out under an inert nitrogen atmosphere, unless otherwise indicated. Flasks were oven-dried overnight and cooled under a stream of nitrogen. Compounds were purchased from Aldrich unless otherwise noted. CH_2Cl_2 , THF, Et₂O were purified based on standard procedures. Flash chromatography was performed using silica gel 60 Å (32–63 mesh) purchased from Sorbent Technologies. Analytical thin layer chromatography (TLC) was performed on 0.25 mm E. Merck precoated silica gel 60 (particle size 0.040–0.063 mm). ¹H NMR and ¹³C NMR spectra were recorded on a Bruker DRX-500 spectrometer. ¹H and ¹³C chemical shifts were referenced to internal solvent resonances and reported relative to SiMe₄; multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), qn (quintet), m (multiplet) and br (broad). Coupling constants, *J*, are reported in Hz (Hertz). Electrospray ionization (ESI) mass spectra were recorded on a Micromass LCT equipped with a time-of-flight analyzer on a Waters Micromass Q-ToF Ultima in the University of Illinois at Urbana-Champaign. Electron impact (EI) mass spectra were obtained using a Micromass AutoSpecTM. Fast atom bombardment (FAB) mass spectra were taken at the Mass Spectrometry Laboratory in the University of Illinois at Urbana-Champaign, using a Micromass 70-VS-4F and 70-VSE for HRFAB and LRFAB, respectively. IR spectra were recorded using ATI Mattson, Genesis series FTIR. Optical rotations were measured on a JASCO DIP-370 digital polarimeter.

2. General Procedure for the Preparation of Δ^1 -Pyrazolines

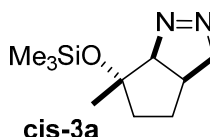


To a stirred solution of carbonyl compound (1 mmol) in anhydrous THF (5 mL) under an atmosphere of nitrogen was added trimethylsilyldiazomethane (0.55 mL, 2.0 M in ether, 1.1 mmol). The appropriate catalyst was added, and the reaction was monitored by TLC. The reaction mixture was quenched with several drops of saturated aqueous solution of NH_4Cl , and then dried over MgSO_4 . The drying reagent was filtered and solvent was removed under reduced pressure to give the crude product. Subsequent purification using flash chromatography (gradient elution, hexane:ethyl acetate, 1:0→6:1) to afford the pure pyrazoline **2**.

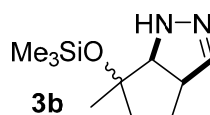
3. Characterization Data



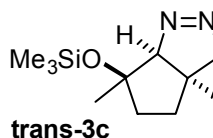
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 4.75–4.60 (m, 1H), 4.47 (ddd, J = 18.3, 9.2, 2.2 Hz, 1H), 4.33 (dt, J = 18.3, 3.0 Hz, 1H), 2.51 (q, J = 8.9 Hz, 1H), 2.13–1.92 (m, 1H), 1.66 (s, 3H), 1.62–1.49 (m, 1H), 1.27–1.12 (m, 1H), 0.83 (td, J = 12.9, 7.4 Hz, 1H), 0.23–0.11 (m, 9H). $^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 103.85, 85.51, 83.07, 37.97, 32.48, 31.13, 24.54, 2.24. HRMS (ESI) calc. for $\text{C}_{10}\text{H}_{21}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 213.1423, found 213.1421.



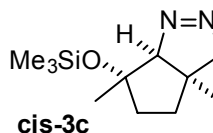
$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 4.71 (dd, J = 7.5, 1.1 Hz, 1H), 4.51 (ddd, J = 17.9, 9.7, 1.4 Hz, 1H), 4.22–4.12 (m, 1H), 2.39–2.26 (m, 1H), 1.79 (tdt, J = 11.5, 7.2, 5.7 Hz, 1H), 1.56 (s, 3H), 1.51 (dd, J = 13.0, 6.3 Hz, 1H), 1.48–1.40 (m, 1H), 1.36–1.27 (m, 1H), 0.11 (s, 9H). $^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 101.18, 84.99, 82.03, 40.07, 32.74, 29.89, 27.17, 2.19. HRMS (ESI) calc. for $\text{C}_{10}\text{H}_{21}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 213.1418, found 213.1421.



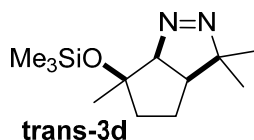
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 6.58 (d, J = 1.43 Hz, 1H, major), 6.48 (s, 1H, minor), 3.74 (d, J = 1.43 Hz), 3.54 (t, J = 9.68, 9.68 Hz), 3.47–3.41 (m), 2.09–2.00 (m), 1.76–1.63 (m), 1.57–1.52 (m), 1.49–1.43 (m), 1.41–1.34 (m), 1.37 (s, 3H minor), 1.25 (s, 3H, major), 0.12 (s, 9H, minor), 0.10 (s, 9H, major). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) δ 147.80, 146.56, 85.22, 82.76, 77.28, 72.79, 68.12, 51.01, 50.13, 37.92, 28.59, 28.26, 27.85, 22.86, 2.38, 2.19. HRMS (ESI) calc. for $\text{C}_{10}\text{H}_{21}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 213.1423, found 213.1423.



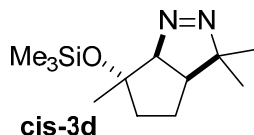
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 4.37 (dt, J = 10.9, 5.4 Hz, 1H), 4.29–4.18 (m, 2H), 1.87–1.73 (m, 1H), 1.65–1.60 (m, 1H), 1.59 (d, J = 4.5 Hz, 3H), 1.45 (dd, J = 12.4, 7.1 Hz, 1H), 1.19 (s, 3H), 0.89 (ddd, J = 21.0, 13.5, 6.8 Hz, 1H), 0.20–0.09 (m, 9H). $^{13}\text{C-NMR}$ (126 MHz, CDCl_3) δ 108.21, 92.05, 83.33, 41.37, 38.99, 38.70, 26.50, 24.55, 2.25. HRMS (ESI) calc. for $\text{C}_{11}\text{H}_{23}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 227.1580, found 227.1590.



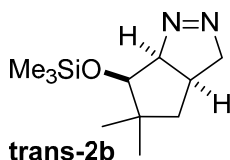
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 4.34 (t, J = 3.9 Hz, 1H), 4.31 (d, J = 17.9 Hz, 1H), 4.12 (dd, J = 17.9, 2.9 Hz, 1H), 1.72–1.62 (m, 1H), 1.60–1.57 (m, 1H), 1.55 (dd, J = 11.7, 5.7 Hz, 1H), 1.50–1.43 (m, 1H), 1.03 (s, 1H), 0.10–0.05 (m, 1H). $^{13}\text{C-NMR}$ (126 MHz, CDCl_3) δ 107.10, 91.54, 82.56, 41.50, 40.96, 37.04, 27.01, 26.87, 2.12. HRMS (ESI) calc. for $\text{C}_{11}\text{H}_{23}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 227.1580, found 227.1587.



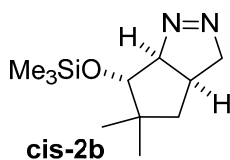
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 4.71 (d, $J = 7.09$ Hz, 1H), 2.20 (t, $J = 8.27$, 1H), 1.82–1.74 (m, 1H), 1.70 (s, 3H), 1.54 (dd, $J = 12.88, 6.66$ Hz, 1H), 1.45 (s, 3H), 1.45–1.40 (m, 1H), 1.15 (s, 3H), 0.85 (dt, $J = 12.71, 12.69, 7.24$ Hz, 1H), 0.16 (s, 9H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) δ 104.19, 90.39, 83.39, 43.94, 39.01, 27.61, 25.08, 24.60, 21.69, 2.39. HRMS (ESI) calc. for $\text{C}_{12}\text{H}_{25}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 241.1736, found 241.1736.



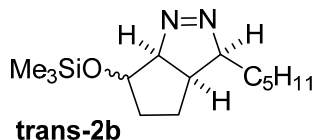
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 4.72 (d, $J = 8.47$ Hz, 1H), 2.00 (q, $J = 13.24, 8.41$ Hz, 1H), 1.56 (s, 3H), 1.54–1.45 (m, 4H), 1.40 (s, 3H), 1.19 (s, 3H), 0.14 (s, 9H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) δ 101.96, 89.74, 81.82, 43.57, 40.72, 28.21, 27.44, 24.14, 21.42, 2.42. HRMS (ESI) calc. for $\text{C}_{12}\text{H}_{25}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 241.1736, found 241.1736.



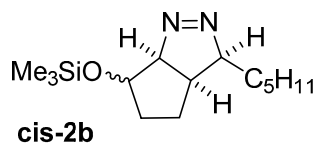
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 4.84–4.72 (m, 1H), 4.38–4.20 (m, 2H), 3.49 (t, $J = 13.2$ Hz, 1H), 2.46 (pd, $J = 9.2, 3.1$ Hz, 1H), 1.83–1.70 (m, 1H), 0.92 (d, $J = 7.7$ Hz, 3H), 0.89–0.83 (m, 4H), 0.74 (dd, $J = 12.8, 10.1$ Hz, 2H), 0.17 (s, 9H). $^{13}\text{C-NMR}$ (126 MHz, CDCl_3) δ 102.54, 82.95, 82.32, 44.51, 42.71, 30.67, 25.93, 20.74, 0.22. HRMS (ESI) calc. for $\text{C}_{11}\text{H}_{23}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 227.1580, found 227.1587.



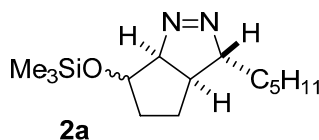
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 5.32 (dt, $J = 8.5, 3.9$ Hz, 1H), 4.54 (ddd, $J = 15.5, 7.8, 2.7$ Hz, 1H), 4.05 (t, $J = 5.4$ Hz, 1H), 4.01–3.92 (m, 1H), 2.53–2.23 (m, 1H), 1.70–1.49 (m, 1H), 1.39–1.16 (m, 2H), 0.92 (d, $J = 6.6$ Hz, 4H), 0.85 (d, $J = 6.4$ Hz, 4H), 0.08 (d, $J = 3.2$ Hz, 9H). $^{13}\text{C-NMR}$ (126 MHz, CDCl_3) δ 97.84, 83.42, 80.00, 77.25, 76.99, 76.74, 46.18, 43.55, 32.52, 25.46, 22.35. HRMS (ESI) calc. for $\text{C}_{11}\text{H}_{23}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 227.1580, found 227.1587.



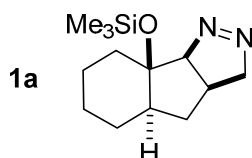
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 6.69–4.65 (m, 2H), 4.01 (dq, $J = 7.87, 7.77, 7.77, 2.55$ Hz, 1H), 2.58–2.52 (m, 1H), 2.10–2.02 (m, 1H), 1.80–1.73 (m, 1H), 1.69–1.54 (m, 3H), 1.52–1.46 (m, 1H), 1.41–1.34 (m, 5H), 1.32–1.26 (m, 3H), 1.25–1.18 (m, 1H), 0.91 (t, $J = 7.05, 7.05$ Hz, 3H), 0.19 (s, 9H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) δ 102.73, 90.98, 74.87, 36.82, 34.04, 31.95, 28.64, 27.84, 23.42, 22.58, 14.08, 0.16. HRMS (ESI) calc. for $\text{C}_{14}\text{H}_{29}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 269.2049, found 269.2059.



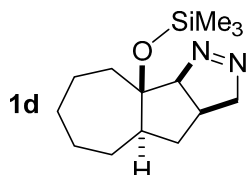
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 4.05 (td, $J = 10.23, 6.42, 6.42$ Hz, 1H), 3.85 (dd, $J = 8.88, 7.05$ Hz, 1H), 3.37 (t, $J = 8.45, 8.45$ Hz, 1H), 2.33–2.22 (m, 1H), 2.16–2.10 (m, 1H), 1.83–1.74 (m, 2H), 1.66–1.57 (m, 3H), 1.54–1.48 (m, 1H), 1.32–1.22 (m, 7H), 0.89 (t, $J = 6.34, 6.34$ Hz, 3H), 0.12 (s, 9H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) δ 75.96, 62.10, 51.91, 31.95, 31.73, 27.61, 26.36, 25.65, 22.49, 14.02, 0.01. HRMS (ESI) calc. for $\text{C}_{14}\text{H}_{29}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 269.2049, found 269.2062.



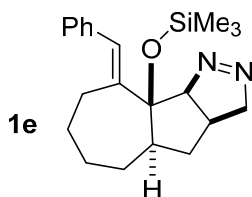
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 4.90 (d, $J = 7.44$ Hz, 1H), 4.58 (bs, 1H), 4.30 (bs, 1H), 2.18 (t, $J = 7.94, 7.94$ Hz, 1H), 2.09–2.01 (m, 1H), 1.87–1.80 (m, 1H), 1.53–1.50 (m, 1H), 1.43–1.39 (m, 2H), 1.33–1.26 (m, 6H), 1.18–1.12 (m, 1H), 0.90 (bt, $J = 6.45, 6.45$ Hz, 3H), 0.20 (s, 9H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) δ 102.14, 97.46, 74.12, 38.80, 33.37, 32.62, 31.77, 30.43, 26.09, 22.53, 14.04, 0.16. HRMS (ESI) calc. for $\text{C}_{14}\text{H}_{29}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 269.2049, found 269.2062.



$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 4.99 (dd, $J = 10.1, 3.1$ Hz, 1H), 4.55 (dd, $J = 17.9, 10.5$ Hz, 1H), 3.86 (ddd, $J = 18.0, 6.4, 3.2$ Hz, 1H), 2.57 (d, $J = 13.1$ Hz, 1H), 2.33–2.16 (m, 1H), 1.85 (ddd, $J = 14.1, 8.6, 5.3$ Hz, 1H), 1.73–1.51 (m, 4H), 1.47–1.37 (m, 3H), 1.28–1.05 (m, 3H), 0.08 (d, $J = 3.0$ Hz, 9H). $^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 102.88, 83.26, 81.95, 77.31, 76.99, 76.67, 51.58, 36.05, 35.56, 32.94, 25.41, 24.55, 21.46, 2.64. HRMS (ESI) calc. for $\text{C}_{13}\text{H}_{25}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 253.1736, found 253.1734.

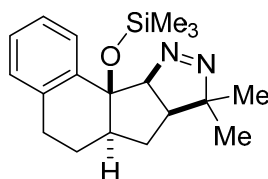


$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 4.96 (dd, $J = 10.1, 2.9$ Hz, 1H), 4.57–4.42 (m, 1H), 3.97 (ddd, $J = 17.9, 5.6, 3.2$ Hz, 1H), 2.66 (ddd, $J = 14.8, 5.8, 2.4$ Hz, 1H), 2.32–2.19 (m, 1H), 1.94–1.79 (m, 3H), 1.76–1.44 (m, 10H), 1.39–1.30 (m, 1H), 1.14–1.04 (m, 1H), 0.13–0.06 (m, 9H). $^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 104.68, 86.44, 82.77, 77.31, 76.99, 76.67, 51.19, 41.35, 38.51, 32.88, 27.60, 25.60, 24.19, 23.61, 2.67. HRMS (ESI) calc. for $\text{C}_{14}\text{H}_{27}\text{N}_2\text{OSi}$ $[\text{M} + \text{H}]^+$ 267.1893, found 267.1890.



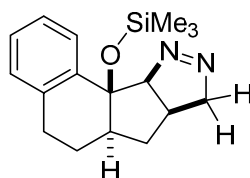
$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 7.62 (s, 1H), 7.37 (t, $J = 7.6$ Hz, 2H), 7.31–7.0 (m, 2H), 7.26–7.24 (m, 1H), 5.48 (dd, $J = 10.3, 3.0$ Hz, 1H), 4.64 (dd, $J = 17.8, 10.3$ Hz, 1H), 3.94 (ddd, $J = 17.8, 6.6, 3.1$ Hz, 1H), 2.65 (dd, $J = 14.9, 7.8$ Hz, 1H), 2.33–2.27 (m, 2H), 2.09–2.05 (m, 1H), 1.94 (ddd, $J = 11.9, 8.7, 6.6$ Hz, 1H), 1.81–1.72 (m, 4H), 1.51–1.42 (m, 2H), 1.26 (td, $J = 12.2, 7.6$ Hz, 1H), 0.05 (s, 9H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) δ

145.37, 138.17, 130.58, 128.91, 128.20, 126.50, 103.13, 88.19, 83.30, 51.84, 37.35, 32.28, 27.83, 27.67, 27.29, 25.45, 2.84. HRMS (ESI) calc. for C₁₄H₃₁N₂OSi [M + H]⁺ 355.2206, found 355.2206.



1c

¹H-NMR (400 MHz, CDCl₃) δ 8.50–8.01 (m, 1H), 7.33–7.22 (m, 2H), 7.21–7.12 (m, 1H), 5.48 (d, *J* = 10.2 Hz, 1H), 3.02–2.80 (m, 2H), 2.15 (dd, *J* = 18.7, 8.8 Hz, 1H), 1.93 (pd, *J* = 12.6, 6.5 Hz, 2H), 1.82–1.60 (m, 2H), 1.55–1.44 (m, 1H), 1.38 (d, *J* = 5.6 Hz, 6H), –0.29 (s, 9H). ¹³C-NMR (101 MHz, CDCl₃) δ 138.78, 137.83, 129.27, 128.87, 128.26, 125.48, 102.74, 87.42, 80.54, 77.31, 76.99, 76.67, 49.02, 43.94, 29.54, 29.25, 29.03, 21.43, 20.62, 1.42. HRMS (ESI) calc. for C₁₉H₂₉N₂OSi [M + H]⁺ 329.2049, found 329.2049.



1b

¹H-NMR (400 MHz, CDCl₃) δ 8.38–8.22 (m, 1H), 7.34–7.23 (m, 2H), 7.15 (dd, *J* = 5.0, 3.8 Hz, 1H), 5.47 (dd, *J* = 10.0, 2.9 Hz, 1H), 4.70 (dd, *J* = 17.7, 10.5 Hz, 1H), 3.91 (ddd, *J* = 17.7, 7.1, 3.0 Hz, 1H), 3.00–2.79 (m, 2H), 2.52–2.29 (m, 1H), 2.14–1.82 (m, 3H), 1.79–1.65 (m, 1H), 1.43–1.17 (m, 2H), 0.32 (s, 9H). ¹³C-NMR (101 MHz, CDCl₃) δ 138.21, 137.78, 129.48, 128.88, 128.38, 125.55, 101.29, 83.00, 81.48, 77.31, 76.99, 76.67, 49.15, 34.59, 34.15, 29.07, 20.98, 1.35. HRMS (ESI) calc. for C₁₇H₂₅N₂OSi [M + H]⁺ 301.1736, found 301.1737.

4. Computational Data

4.1. Table of Energy Values (in a.u.)

Species	Enthalpy	Free Energy
IN-1b	–983.704537	–983.777262
<i>syn</i> -TS-1b	–983.679348	–983.746287
<i>anti</i> -TS-1b	–983.67826	–983.745288
<i>syn</i> -1b	–983.74574	–983.810444
<i>anti</i> -1b	–983.749865	–983.815234
IN-1b'	–983.705843	–983.779457
<i>syn</i> -TS-1b'	–983.679466	–983.745844
<i>anti</i> -TS-1b'	–983.673821	–983.740303
<i>syn</i> -1b'	–983.747524	–983.812473
<i>anti</i> -1b'	–983.747361	–983.813072
IN-2a	–867.043546	–867.114206
<i>syn</i> -TS-2a	–867.012163	–867.077092
<i>anti</i> -TS-2a	–867.014639	–867.079784
<i>syn</i> -2a	–867.081985	–867.144665
<i>anti</i> -2a	–867.085089	–867.148929
IN-2b	–827.7535	–827.820651
<i>syn</i> -TS-2b	–827.725581	–827.786484
<i>anti</i> -TS-2b	–827.727787	–827.789079

<i>syn-2b</i>	-827.793632	-827.852806
<i>anti-2b</i>	-827.797055	-827.856769
<i>IN-2c</i>	-867.040993	-867.111917
<i>syn-TS-2c</i>	-867.009754	-867.073989
<i>anti-TS-2c</i>	-867.011746	-867.076989
<i>syn-2c</i>	-867.079217	-867.142494
<i>anti-2c</i>	-867.083341	-867.145937
<i>IN-3a</i>	-867.03829	-867.106675
<i>syn-TS-3a</i>	-867.010656	-867.073362
<i>anti-TS-3a</i>	-867.01093	-867.072946
<i>syn-3a</i>	-867.079024	-867.140659
<i>anti-3a</i>	-867.078842	-867.140627

4.2. Cartesian Coordinates for All Species

IN-1b				O	2.28178100	6.92501300	0.66833500
C	1.43846400	3.44680200	-0.58971600	C	1.31655900	7.40133800	-1.50596600
C	2.65870900	4.34459500	-0.78524000	H	1.09614600	7.03668600	-2.50843700
C	2.21124700	5.75903800	-1.13882600	N	1.84314290	8.61866745	-1.72418237
C	1.27944200	6.37116600	-0.07573200	N	1.61218461	9.75158240	-1.56414267
C	0.06715600	5.45373500	0.19087200	C	-0.57095100	7.14824400	0.44463100
C	0.53371300	4.02450700	0.49545000	H	-1.60876800	6.87147100	0.67916600
H	0.88402300	3.37121100	-1.53363300	H	-0.13397000	7.56750000	1.35864800
H	3.24402700	4.37349900	0.13895700	C	-0.55258400	8.18881700	-0.66398500
H	1.67450100	5.74903400	-2.09430300	H	-1.12670000	7.92303900	-1.55317000
H	-0.34669600	3.39445000	0.64724400	C	-0.31061300	9.53307100	-0.44678300
H	3.07057000	6.42781700	-1.25304700	H	-0.61963200	10.28616600	-1.16555000
H	3.30802600	3.95576100	-1.57406400	H	-0.01389000	9.89792700	0.53354200
H	1.74548800	2.43318400	-0.31918300	Si	3.81657000	7.38866900	1.18843300
H	1.08458500	4.04728500	1.44262900	C	5.10657000	7.44796200	-0.19103000
H	-0.53344400	5.43163300	-0.72983900	H	6.03266300	7.88193000	0.21028400
C	0.86638400	7.74197200	-0.58249700	H	5.35489600	6.45196800	-0.57666200
H	1.59397400	8.45378500	-0.94727000	H	4.78673000	8.07135200	-1.03383800
N	-0.36814600	8.04080300	-0.82005400	C	3.59570400	9.09752600	1.95282800
N	-1.45930100	8.28234900	-1.00250600	H	4.53466900	9.43977700	2.40768500
O	2.02248200	6.45981000	1.13495300	H	3.29108300	9.83925200	1.20564800
C	-0.80903600	5.96176400	1.35484400	H	2.83149300	9.07781100	2.74002200
H	-0.31557900	5.70699000	2.29747100	C	4.38814600	6.19636200	2.53787300
H	-0.89640700	7.05193400	1.33570000	H	5.28223900	6.59705200	3.03444400
C	-2.18757200	5.37026300	1.31640000	H	3.61363600	6.06602100	3.30412900
H	-2.79946700	5.65253100	0.46009300	H	4.64537200	5.20590300	2.14463000
C	-2.68873500	4.54205300	2.22589200	anti-TS-1b			
H	-2.10642900	4.23921900	3.09108500	C	0.78452600	3.41984400	-0.07913800
H	-3.69284500	4.14381300	2.13986700	C	2.29946000	3.63037000	-0.15123000
Si	2.44166200	7.75217800	2.10692900	C	2.64160700	4.94453400	-0.85712400
C	0.95343100	8.65337500	2.80234000	C	1.95871700	6.12488700	-0.15483200
H	1.29226700	9.47088800	3.44654100	C	0.43500600	5.91495100	-0.10529700
H	0.33549500	9.08830400	2.01252100	C	0.09121700	4.60529500	0.59911000
H	0.32361100	7.99499500	3.40524000	H	0.38882700	3.30426700	-1.09585400
C	3.41465700	6.95148400	3.48465600	H	2.71027800	3.65470600	0.86355200
H	3.75256200	7.69207300	4.21437600	H	2.29426100	4.91440900	-1.89591500
H	2.80360000	6.21308300	4.00925000	H	-0.99348000	4.46336800	0.60346600
H	4.29466300	6.43831800	3.08983700	H	3.72201400	5.11229700	-0.88050800
C	3.52619900	8.97659900	1.18139300	H	2.77668100	2.79712700	-0.67365000
H	4.09261300	9.58415500	1.89346900	H	0.55875900	2.49339800	0.45525300
H	4.24863200	8.46151700	0.54238900	H	0.41662200	4.67580300	1.64252500
H	2.94403300	9.66209900	0.56152600	H	0.08811100	5.84993100	-1.14694200
syn-TS-1b				O	2.40200100	6.20683300	1.18539700
C	1.03811700	3.55244900	0.49685600	C	2.19060300	7.47628600	-0.82620600
C	2.43539700	3.94608600	-0.00812000	H	3.07646800	8.04141000	-0.55035000
C	2.38417100	5.11586600	-1.00688600	N	1.12185000	7.94844500	-2.88268300
C	1.62600300	6.33818300	-0.44463800	N	1.90820500	7.57294900	-2.13340900
C	0.20543900	5.89268200	0.02284900	C	-0.17919800	7.16495600	0.52959200
C	0.27705500	4.76556500	1.05910300	H	-1.27012700	7.10011600	0.48280000
H	0.45959800	3.11888400	-0.33309200	H	0.10375600	7.19001800	1.58494800
H	3.06203700	4.22083700	0.84840300	C	0.29974500	8.42590800	-0.17681700
H	1.86534700	4.78985200	-1.91893300	H	0.81951600	9.16515100	0.42465200
H	-0.74057900	4.47175100	1.34960600	C	-0.28214700	8.83305100	-1.35586700
H	3.39386400	5.41249700	-1.31269600	H	-1.09960300	8.26511500	-1.78757200
H	2.92184200	3.08642000	-0.48717900	H	-0.15607000	9.84231700	-1.72704200
H	1.12385100	2.76962700	1.26166700	Si	3.74080700	6.83665800	1.95315000
H	0.77435800	5.13423500	1.96616300	C	3.81725600	5.92332600	3.57745000
H	-0.29140100	5.48672400	-0.87377800	H	3.94736200	4.85115700	3.41136900
				H	4.64865600	6.27424500	4.19416000
				H	2.89289100	6.06566700	4.14230100

C	5.30528200	6.54570200	0.96043000
H	6.16271800	6.98715000	1.47686200
H	5.50107200	5.47637200	0.84485000
H	5.25880600	6.98852400	-0.03806000
C	3.48254400	8.66866000	2.25843500
H	2.50640400	8.83242000	2.72395300
H	4.24545100	9.05654200	2.93949000
H	3.51986400	9.26769100	1.34535200

syn-1b

C	1.63031100	3.69600200	0.01311800
C	2.86338900	4.48116800	-0.45503900
C	2.47826800	5.73867000	-1.24414500
C	1.51699000	6.59273200	-0.42827900
C	0.26887600	5.78501800	-0.03206600
C	0.64981800	4.57349600	0.80467100
H	1.11281200	3.28971100	-0.86506400
H	3.45455700	4.77058000	0.41863000
H	1.96720100	5.44882800	-2.16948200
H	-0.23958500	3.99868700	1.07915700
H	3.35820900	6.31851400	-1.53228800
H	3.50255300	3.84192400	-1.06969900
H	1.94404100	2.84026500	0.61648800
H	1.11921800	4.91889800	1.73180600
H	-0.18875000	5.43449800	-0.96873100
O	2.08357100	7.05060300	0.78615500
C	0.86148200	7.78940000	-1.15169800
H	0.68690800	7.54472300	-2.20125800
N	1.69802000	8.99812400	-1.08809600
N	1.25394000	9.83631600	-0.30591400
C	-0.64142400	6.85674800	0.57761700
H	-1.68756900	6.54803200	0.60926000
H	-0.31647000	7.06825900	1.59927800
C	-0.41666200	8.09119800	-0.33144400
H	-1.27000700	8.24925000	-0.99176400
C	-0.01509800	9.40473800	0.34286800
H	-0.73287300	10.21866700	0.23320700
H	0.21252600	9.29132700	1.40730300
Si	3.53411300	7.64369400	1.37009400
C	4.18780700	6.40703200	2.62331200
H	4.60527400	5.50831500	2.16495500
H	4.97867000	6.86772100	3.22278500
H	3.39113700	6.09997800	3.30651500
C	3.15285200	9.22928500	2.28561100
H	4.04057600	9.56973100	2.82699400
H	2.83794900	10.02550600	1.60825700
H	2.36125600	9.06606300	3.02280000
C	4.80256500	7.93967600	0.02515000
H	5.63703800	8.51263900	0.44079700
H	5.20885000	7.00547900	-0.37045700
H	4.37120400	8.51746800	-0.79613800

anti-1b

C	0.89095100	3.35715000	-0.62757700
C	2.39560700	3.63240200	-0.75478600
C	2.68067000	5.09657000	-1.11509200
C	2.01755900	6.00164600	-0.08392500
C	0.50373100	5.74552500	-0.02305900
C	0.21081200	4.30508100	0.37095200
H	0.42184800	3.48266200	-1.61141300
H	2.88524800	3.39740800	0.19584900
H	2.27226600	5.33350600	-2.10174700
H	-0.86774000	4.12456400	0.39535800
H	3.75615900	5.28945500	-1.15832700
H	2.83042500	2.97560800	-1.51254200
H	0.72801400	2.31767200	-0.33104600
H	0.60074300	4.12951500	1.37836800
H	0.11634100	5.91324100	-1.03860300
O	2.52432400	5.71586600	1.21464100
C	2.07123300	7.52316200	-0.31756500
H	3.03750600	7.94511500	-0.02957200
N	0.90790300	8.56544200	-1.96044900
N	1.88772300	7.85482700	-1.75290900
C	0.01370300	6.87796700	0.88053800
H	-1.06255100	7.04944900	0.80687900
H	0.25046800	6.63677600	1.91924500
C	0.83437600	8.10579500	0.41468400
H	1.10977300	8.75139500	1.24723300
C	0.17580400	8.90655300	-0.71487000
H	-0.87778200	8.66595100	-0.87695800
H	0.25118100	9.99029400	-0.59471400
Si	3.92349300	6.14177800	2.01158800
C	3.71213700	7.82770700	2.81142200
H	4.51265700	8.00946800	3.53442300
H	3.73010900	8.64768400	2.08928100
H	2.76201500	7.87334700	3.35118400
C	4.12948300	4.83932000	3.33283900

H	4.24756400	3.84957500	2.88496200
H	5.00791600	5.03910800	3.95224000
H	3.25407200	4.81020200	3.98610200
C	5.40948700	6.15456200	0.86699300
H	6.30538500	6.43501100	1.42890200
H	5.58240100	5.16463200	0.43652200
H	5.29988400	6.86575300	0.04396900

IN-1b'

C	1.56744100	3.27029600	-0.20477000
C	2.83555000	4.11900600	-0.09750900
C	2.55227600	5.56837400	-0.49611200
C	1.42042400	6.20061800	0.32987500
C	0.14495100	5.33139400	0.19289900
C	0.42369000	3.88241500	0.60432300
H	1.26679200	3.20889300	-1.25793000
H	3.22122800	4.08077600	0.92730000
H	2.24130100	5.58291300	-1.54918900
H	-0.48999700	3.29479400	0.48276400
H	3.44399600	6.19426100	-0.40380500
H	3.62361700	3.71283700	-0.73657700
H	1.76456900	2.24798400	0.12813900
H	0.66789600	3.85750300	1.67434000
H	-0.10440300	5.33252500	-0.87753600
C	-1.04149800	5.92799800	0.96247300
H	-0.89087700	5.78475200	2.03762600
H	-1.06732800	7.00741900	0.77779400
C	-2.34663500	5.31886600	0.54366200
H	-2.63287000	5.47538600	-0.49624800
C	-3.14770400	4.60830600	1.32995600
H	-2.89724500	4.42723000	2.37086700
H	-4.07891900	4.19145100	0.96443500
C	1.85228000	6.32924800	1.78359600
H	2.30513000	5.54325700	2.36507400
N	1.63272700	7.44147200	2.40303800
N	1.43786600	8.42916000	2.91813100
O	1.14751500	7.51755200	-0.10026300
Si	1.02260200	8.25378600	-1.59338900
C	-0.09690500	7.28677000	-2.74929600
H	-0.24991800	7.85368800	-3.67252900
H	0.32142100	6.31575800	-3.02697700
H	-1.07810400	7.11872100	-2.29640800
C	2.70971400	8.47334400	-2.38017200
H	3.12936100	7.53107100	-2.73929000
H	2.64027200	9.15355500	-3.23416900
H	3.41323500	8.90721600	-1.66489700
C	0.26461100	9.91241300	-1.20576400
H	0.89434400	10.47268000	-0.51085700
H	0.14026200	10.51184700	-2.11144000
H	-0.71723900	9.78956400	-0.74199300

syn-TS-1b'

C	1.10632300	3.27869900	-0.35129000
C	2.31957500	3.59488700	0.52380600
C	2.80719800	5.02500600	0.28418800
C	1.70567100	6.07708800	0.47433400
C	0.46261900	5.73060600	-0.37544800
C	-0.01110500	4.29589400	-0.11786500
H	1.40688300	3.31024000	-1.40544500
H	2.05775700	3.45444800	1.57868700
H	3.15447900	5.11176100	-0.75201600
H	-0.86358100	4.08458300	-0.76991600
H	3.65464200	5.26046100	0.93594100
H	3.13406600	2.89652900	0.31594400
H	0.74804900	2.26540200	-0.15238000
H	-0.38027500	4.20248800	0.91089800
H	0.76785100	5.81285200	-1.42609800
C	-0.60701400	6.77658000	-0.04887100
H	-0.30433600	7.73819300	-0.46840200
H	-1.55357400	6.49335400	-0.52221800
C	-0.80581100	6.93821400	1.44738200
C	-0.84249100	8.17762800	2.04605900
O	2.12805300	7.35726300	0.06726300
C	1.18125400	6.17038100	1.91043000
H	1.10114000	5.26216300	2.49857500
N	1.55914100	7.23514100	2.62464800
N	1.22533800	8.28087000	2.96232800
H	-1.32248400	6.12503800	1.95191600
H	-1.31977200	8.32441600	3.00662000
H	-0.64492200	9.07158600	1.46451700
Si	3.59859300	8.15951000	0.05931500
C	4.71958300	7.45420700	-1.27050600
H	4.17382800	7.30268500	-2.20533700
H	5.53931700	8.15016400	-1.47219800
H	5.16256200	6.50021500	-0.97461800
C	3.12479500	9.91740700	-0.34336300
H	4.00226300	10.56924900	-0.35914200

H	2.63538600	9.98103600	-1.31789200
H	2.43087400	10.29977700	0.40956100
C	4.48789600	8.09373400	1.70841200
H	3.94710800	8.64831100	2.47806500
H	4.63606100	7.07397700	2.07190500
H	5.47697900	8.54875000	1.59423700

anti-TS-1b'

C	1.14585800	2.91043800	-0.49137100
C	2.54167500	3.30302500	-0.00790500
C	2.89241500	4.71698400	-0.47241400
C	1.85925700	5.77588300	-0.06069500
C	0.42669900	5.34696500	-0.42976000
C	0.10055900	3.91039900	0.00213600
H	1.13832300	2.88917300	-1.58803300
H	2.58858200	3.23760000	1.08331900
H	2.92929300	4.73060000	-1.56812200
H	-0.88639800	3.65391500	-0.39443400
H	3.88148600	5.01316500	-0.10655200
H	3.29044900	2.60585500	-0.39271900
H	0.89586700	1.90266200	-0.15057800
H	0.01665300	3.84508500	1.09057000
H	0.37401900	5.38774900	-1.52480200
O	2.08321400	6.99581500	-0.75068000
C	1.87975800	6.15609900	1.42242900
H	2.52817800	6.98480200	1.68814400
N	1.82849600	5.22839000	2.38603100
N	1.15789100	4.75285900	3.18827200
C	-0.54389100	6.37849000	0.16927900
H	-0.51243100	7.28117300	-0.44276900
H	-1.56253200	5.98305900	0.11470900
C	-0.20934600	6.75068800	1.61056800
H	0.06937400	7.78696700	1.77600600
C	-0.68649400	6.04499500	2.69077500
H	-1.29795400	5.16018600	2.55217000
H	-0.70075200	6.48202800	3.68118800
Si	3.47063800	7.83046800	-1.16664600
C	4.59238900	8.08912600	0.31619100
H	4.11016600	8.69193000	1.09031500
H	4.91274300	7.14632200	0.76803400
H	5.49381700	8.62310900	0.00078200
C	2.83347800	9.46611600	-1.79834200
H	3.65619500	10.12007000	-2.09895100
H	2.18454000	9.31813000	-2.66472600
H	2.25323000	9.98032500	-1.02882100
C	4.43283700	6.95603000	-2.51905100
H	4.96919000	6.07748100	-2.15419000
H	3.76987900	6.63900300	-3.32824700
H	5.17088600	7.64238100	-2.94513900

syn-1b'

C	0.95494800	3.02980900	0.06375400
C	2.31013300	3.71295700	0.25078500
C	2.31940800	5.09620100	-0.40564100
C	1.14585800	5.97238200	0.02813200
C	-0.22641500	5.27095900	0.00495600
C	-0.16437100	3.88477200	0.65614300
H	0.76909800	2.88160300	-1.00753400
H	2.52785000	3.79604200	1.32122200
H	2.25965100	4.96696400	-1.49036900
H	-1.13513500	3.39456600	0.53747800
H	3.24688700	5.63595200	-0.19366100
H	3.10888500	3.10376300	-0.17931700
H	0.95988500	2.03906900	0.52545400
H	-0.00358600	3.99468900	1.73645900
H	-0.55612700	5.14913400	-1.03445000
C	-1.12893200	6.24057800	0.79104300
H	-1.52766800	7.01447500	0.13388500
H	-1.97973200	5.71820500	1.23425600
C	-0.20888100	6.87032200	1.86610900
C	-0.06032200	8.39593000	1.85121100
O	1.09519100	7.15519500	-0.75015800
C	1.22652600	6.44920300	1.50067800
H	1.65111400	5.67282200	2.13765900
N	2.06844200	7.65454300	1.63183000
N	1.40165400	8.67085200	1.80667800
H	-0.47676800	6.52772200	2.86608400
H	-0.46863400	8.90603900	2.72445600
H	-0.48488700	8.85727900	0.95425000
Si	0.64824900	7.52651700	-2.31165900
C	1.54599100	9.11638100	-2.68718800
H	2.62699500	8.96043300	-2.67810100
H	1.26366600	9.51404400	-3.66553000
H	1.31559800	9.87085200	-1.93089500
C	1.12281900	6.18915600	-3.54038100
H	0.78834300	6.48740200	-4.53867200
H	2.20462900	6.04292900	-3.58425800

H	0.65635800	5.22634300	-3.31354200
C	-1.20528900	7.80526000	-2.43186200
H	-1.53837300	8.57695600	-1.73259900
H	-1.45872500	8.14551600	-3.44050100
H	-1.78036800	6.89665700	-2.23609700

anti-1b'

C	1.09840400	2.93253200	-0.61796800
C	2.46884500	3.28604500	-0.04048900
C	2.86134500	4.72029900	-0.40537000
C	1.79876700	5.77737000	-0.09438100
C	0.36802300	5.35321300	-0.47566300
C	0.03996800	3.90281800	-0.09615400
H	1.13365000	2.98698300	-1.71332200
H	2.45117000	3.16535100	1.04476500
H	3.02718300	4.76682000	-1.48755800
H	-0.94635200	3.65767800	-0.50174500
H	3.80408500	4.99526700	0.08207100
H	3.23158900	2.60465000	-0.42679100
H	0.83200800	1.90511000	-0.35694600
H	-0.03621900	3.78883700	0.99048700
H	0.27622700	5.45556800	-1.56140000
O	2.04366300	6.97232600	-0.83499900
C	1.67304800	6.21834600	1.38652200
H	2.43891400	6.96402100	1.60446400
N	1.88617700	5.12752200	2.36830000
N	0.92136700	4.94939500	3.10783700
C	-0.50947000	6.38141200	0.25540600
H	-0.57720000	7.29149900	-0.34156200
H	-1.52473400	6.01010100	0.41999900
C	0.21856600	6.69449400	1.58334900
H	0.16720300	7.75736600	1.81289900
C	-0.20852100	5.86225800	2.79925800
H	-1.09178300	5.24063300	2.62751100
H	-0.39370500	6.45186400	3.70010800
Si	3.44159600	7.82072300	-1.17295200
C	4.44463800	8.16924100	0.37635700
H	3.89035400	8.78412500	1.09024100
H	4.75864100	7.25374000	0.88527500
H	5.35087900	8.71838100	0.10350200
C	2.82745900	9.41786800	-1.91888100
H	3.66019100	10.07566700	-2.18154400
H	2.25135700	9.22303900	-2.82646600
H	2.18071200	9.95117600	-1.21837600
C	4.53152100	6.92220600	-2.40693200
H	5.04880300	6.06951300	-1.96213800
H	3.94830200	6.56159600	-3.25826200
H	5.29156600	7.60848800	-2.79247700

IN-2a

C	0.98292900	4.03619300	0.43968400
C	1.10347600	2.76188500	0.08016600
H	1.66611600	2.52099400	-0.82222200
C	0.53286200	1.59500700	0.83180400
H	-0.03165500	1.95734100	1.69794000
H	-0.17589700	1.05776100	0.19090900
C	1.62226800	0.62289700	1.28828000
H	2.19398200	0.26007900	0.42605400
H	2.33254200	1.13323000	1.94367000
C	1.07833800	-0.58754600	2.04324600
H	0.48249200	-0.23998100	2.89831000
C	0.13685100	-1.43393400	1.21500500
H	-0.89279100	-1.64489400	1.45618500
N	0.59246300	-1.96627900	0.12427600
N	1.04257100	-2.42625800	-0.80443300
O	2.20024000	-1.31727600	2.50848000
Si	2.12655100	-2.76801200	3.34696800
C	3.77842200	-2.90595300	4.20209800
H	3.85848600	-3.84551200	4.75508400
H	4.59082700	-2.87424400	3.47220900
H	3.92645500	-2.08279800	4.90433200
C	0.72028400	-2.68701700	4.58565700
H	0.83059200	-1.82724500	5.25193200
H	-0.25163500	-2.61152100	4.09022600
H	0.70270900	-3.58740200	5.20597600
C	1.88329800	-4.21118600	2.17794100
H	0.86842800	-4.24610300	1.77485000
H	2.57803600	-4.14863100	1.33623500
H	2.07098100	-5.15676000	2.69474100
H	0.42194200	4.27204200	1.34325600
C	1.56110600	5.19743700	-0.31222600
H	2.11423400	4.86096600	-1.19078200
H	0.77392700	5.88036200	-0.64392000
H	2.24021900	5.77577500	0.32029900

syn-TS-2a

C	0.62583700	0.35825200	-1.80742300
C	0.92844700	0.89957800	-0.57709500
H	0.32737000	1.74548000	-0.24229600
C	2.29566400	0.77976100	0.06599300
H	2.88029400	0.02547700	-0.46642400
H	2.83547400	1.72809400	-0.01810700
C	2.17378100	0.37984400	1.53680600
H	3.14052200	0.16426200	1.99918900
H	1.69937000	1.18442900	2.10995400
C	1.28205100	-0.86047400	1.59761500
H	1.06845300	-1.12722200	2.64171900
C	0.00254100	-0.46424100	0.87201000
H	-0.76327100	0.06651400	1.42879300
N	-0.46710800	-1.31156000	-0.04482800
N	-0.46071600	-1.53117700	-1.17462900
O	1.92006100	-1.91832900	0.92185100
Si	1.84451900	-3.52039100	1.43453700
C	2.67740900	-4.48890100	0.07964400
H	2.68131100	-5.55858300	0.30556700
H	2.16035400	-4.34978300	-0.87306000
H	3.71469500	-4.17090200	-0.05091300
C	2.76146300	-3.67148600	3.05967800
H	3.79155400	-3.31828100	2.96502500
H	2.28113000	-3.09495400	3.85531900
H	2.79558100	-4.71373800	3.38993100
C	0.05806000	-4.02681600	1.66367900
H	-0.46266600	-3.35611700	2.35377200
H	-0.48772400	-4.01849300	0.71726100
H	-0.00285300	-5.03662600	2.07983300
H	1.38600600	-0.24135500	-2.30308300
C	-0.49748000	0.87609500	-2.66695400
H	-0.15791300	1.67532800	-3.33490400
H	-0.92590700	0.08960600	-3.29230500
H	-1.30199200	1.28644600	-2.04979500

anti-TS-2a

C	1.36095000	0.22130200	-1.81572200
C	0.81641200	0.57802600	-0.60243700
H	-0.27046000	0.62069600	-0.53190100
C	1.56266500	1.39968400	0.43118100
H	2.63194100	1.39553000	0.19196100
H	1.23492700	2.44311300	0.39354600
C	1.34468100	0.82868100	1.82961300
H	1.94644000	1.32785300	2.59263200
H	0.29274600	0.92220100	2.12177900
C	1.69847300	-0.65593200	1.77488300
C	0.90497700	-1.23220900	0.61911000
H	-0.09895100	-1.59196600	0.82741900
N	1.56700500	-1.95906600	-0.29151100
N	2.04463000	-1.89966400	-1.33625400
H	2.76637500	-0.75156500	1.53473600
O	1.42436000	-1.26466700	3.01761900
Si	1.83518200	-2.85751200	3.38556800
C	0.57264500	-4.04199400	2.66969300
H	-0.44454400	-3.74434000	2.93860600
H	0.63199600	-4.09850900	1.57991200
H	0.73580300	-5.05028700	3.06238200
C	3.53194000	-3.22277500	2.68424200
H	4.27433600	-2.49930700	3.03251100
H	3.86569000	-4.21563200	2.99894000
H	3.53565100	-3.21174900	1.59041100
C	1.82080300	-2.93332800	5.24821900
H	2.07197300	-3.93734500	5.60064300
H	2.54385100	-2.23570000	5.67772700
H	0.83399900	-2.67998800	5.64396400
H	2.39383000	0.49605500	-2.01740600
C	0.51574900	-0.15956400	-3.00238200
H	0.26704700	0.71328800	-3.61559600
H	1.02525700	-0.87749900	-3.64878400
H	-0.42650100	-0.61109600	-2.67892700

syn-2a

C	0.62903100	-1.37876300	-1.28975000
C	0.79846900	-0.04567900	-0.54844100
H	0.08370800	0.68390500	-0.93590300
C	2.22780000	0.54446900	-0.47731000
H	2.93957400	-0.13026700	-0.95646900
H	2.30132900	1.51293800	-0.97256300
C	2.53964700	0.63567100	1.02889600
H	3.60580600	0.60278000	1.25795900
H	2.11822900	1.55174100	1.45497600
C	1.80710700	-0.57457800	1.60112400
C	0.43869900	-0.46733400	0.88792800
H	-0.21689100	0.21768200	1.42818400
N	-0.21992300	-1.78144300	0.78389600
N	-0.09839000	-2.27093600	-0.33706700
H	1.71429800	-0.55843100	2.69277200
O	2.46902800	-1.73502500	1.14956300

Si	2.74478600	-3.13424600	2.03460600
C	1.23051700	-3.63139300	3.01229900
H	1.46629700	-4.49365600	3.64339000
H	0.88631900	-2.82703300	3.66824600
H	0.40134500	-3.89351200	2.35303600
C	4.17022900	-2.80585900	3.20727900
H	3.92344200	-2.00965400	3.91573400
H	4.41831900	-3.69791800	3.78883900
H	5.06434500	-2.50123700	2.65777500
C	3.18310100	-4.40980600	0.74946300
H	3.39093600	-5.38149000	1.20468200
H	2.34932200	-4.53264800	0.05326200
H	4.06395500	-4.10676100	0.17862600
H	1.59806100	-1.86828900	-1.43886700
C	-0.13513000	-1.31437800	-2.60171300
H	0.40469500	-0.69693000	-3.32287500
H	-0.26402200	-2.31220600	-3.02329400
H	-1.12434200	-0.87687300	-2.44476200

anti-2a

C	0.43760800	0.12081600	-1.91131900
H	1.22501900	0.47985800	-2.57970500
C	0.76489700	0.32800200	-0.43472000
H	0.18965200	1.14722800	-0.00005400
C	2.25994900	0.46851400	-0.09633100
H	2.85294800	-0.08833700	-0.83114900
H	2.60509000	1.50323000	-0.10918500
C	2.37830500	-0.19622200	1.27633400
H	3.40672800	-0.43408000	1.55920700
H	1.95003700	0.44913000	2.05077200
C	1.49256000	-1.44558900	1.15339800
C	0.38105200	-1.02917900	0.17242800
H	-0.58509800	-1.07584400	0.67880800
N	0.31769100	-1.95500300	-0.99338100
N	0.37838900	-1.36644100	-2.06938300
H	2.06328800	-2.26344700	0.69180700
O	0.93893300	-1.87825200	2.37354000
Si	1.80949800	-2.57571200	3.62103400
C	0.55464600	-3.49485200	4.64741300
H	-0.22043100	-2.81350700	5.00602100
H	0.06918900	-4.27700700	4.05979600
H	1.02218900	-3.96176600	5.51809800
C	3.10226000	-3.72830100	2.90426200
H	3.86849500	-3.18413000	2.34499000
H	3.60946600	-4.27306200	3.70536200
H	2.65113200	-4.46308700	2.23259200
C	2.64684200	-1.24877500	4.64763300
H	3.13879400	-1.69161800	5.51841200
H	3.40608700	-0.71027800	4.07558800
H	1.91739900	-0.52027200	5.01094900
C	-0.91134400	0.68258400	-2.34772800
H	-0.89397600	1.77349200	-2.32474900
H	-1.15308500	0.35594100	-3.35995400
H	-1.70111500	0.33369700	-1.67693100

IN-2b

C	0.93953600	4.04175200	0.48804100
H	0.37505600	4.30201100	1.37826100
H	1.38228000	4.85643900	-0.07241300
C	1.07744400	2.77775500	0.10510300
H	1.65287500	2.55413100	-0.79194400
C	0.50939300	1.59347100	0.83015900
H	-0.07865900	1.93621700	1.68834200
H	-0.17515400	1.05376500	0.16557000
C	1.60723300	0.63539600	1.29630600
H	2.20033100	0.29002400	0.44151500
H	2.29644600	1.15111300	1.96969000
C	1.06841300	-0.59008800	2.03067600
H	0.44734700	-0.25865800	2.87410200
C	0.16166000	-1.44801800	1.17596300
H	-0.87161000	-1.67230600	1.38774400
N	0.65661100	-1.97670200	0.10050100
N	1.14043100	-2.43259900	-0.81304000
O	2.19277800	-1.30183500	2.51534600
Si	2.12495100	-2.75217600	3.35600400
C	3.75688800	-2.85739100	4.25236000
H	3.83928100	-3.79297000	4.81168900
H	4.58661600	-2.81484000	3.54283200
H	3.87291700	-2.02860300	4.95401500
C	0.68481700	-2.69494500	4.55691100
H	0.75243500	-1.82547500	5.21626300
H	-0.27471000	-2.65254800	4.03409900
H	0.67500400	-3.58885900	5.18669700
C	1.93706600	-4.20106200	2.18414000
H	0.93322900	-4.25602600	1.75626200
H	2.65114500	-4.12700300	1.35970700
H	2.12947100	-5.14214100	2.70738000

syn-TS-2b

C	0.69087100	0.27725900	-1.78909700
H	-0.11517200	0.61850200	-2.42569500
H	1.43672100	-0.35816300	-2.25375500
C	0.95457400	0.88453100	-0.58139300
H	0.35525500	1.75099700	-0.30871200
C	2.31119900	0.79235700	0.09200100
H	2.90764000	0.02906700	-0.41245300
H	2.84103800	1.74426400	-0.00465300
C	2.16726600	0.41715700	1.56803500
H	3.12674800	0.20209000	2.04468500
H	1.68547100	1.23042300	2.12307100
C	1.27019800	-0.82005000	1.62432500
H	1.05176300	-1.09241700	2.66712700
C	0.00008700	-0.41388200	0.88745400
H	-0.75809000	0.13598900	1.43629100
N	-0.48859000	-1.28240300	-0.00476400
N	-0.49459500	-1.53531500	-1.12530100
O	1.90803100	-1.87220000	0.94611000
Si	1.83187200	-3.48548600	1.40669200
C	2.63982300	-4.41319000	0.01000600
H	2.64539500	-5.48964700	0.19839500
H	2.10261000	-4.23355300	-0.92424100
H	3.67318300	-4.08617800	-0.12552900
C	2.77119300	-3.68964200	3.01543500
H	3.80084400	-3.33845500	2.91349400
H	2.30253100	-3.12968200	3.82961800
H	2.80169200	-4.74018800	3.31766200
C	0.04847300	-3.99708800	1.65380500
H	-0.46252400	-3.32952400	2.35407900
H	-0.50629600	-3.98039200	0.71307700
H	-0.00474800	-5.00928000	2.06458100

anti-TS-2b

C	1.40937100	0.23122600	-1.79581600
H	0.81569200	-0.05509000	-2.65448900
H	2.44561200	0.48379800	-1.99238900
C	0.81752700	0.58929300	-0.60554500
H	-0.26830700	0.64363600	-0.57315500
H	1.53742200	1.42118000	0.44158200
C	2.60766200	1.43629800	0.20769700
H	1.18933700	2.45712600	0.40019000
C	1.32299600	0.83989600	1.83658800
H	1.92112200	1.33383300	2.60518500
H	0.27109300	0.92002300	2.13204500
C	1.68451200	-0.64219600	1.76618900
C	0.87989500	-1.20467900	0.61163700
H	-0.12487600	-1.55337000	0.83495400
N	1.52649000	-1.95495000	-0.29569400
N	1.99585300	-1.92485600	-1.34307800
H	2.74996600	-0.73083100	1.50888200
O	1.42639500	-1.26154300	3.00347400
Si	1.83727000	-2.84863300	3.37115200
C	0.56650300	-4.03557900	2.67107100
H	-0.44482800	-3.74070400	2.96299800
H	0.61005200	-4.08074900	1.58019300
H	0.74124400	-5.04576000	3.05290700
C	3.52419700	-3.22447000	2.64840400
H	4.27534100	-2.51017700	2.99611100
H	3.85126100	-4.22329300	2.95008900
H	3.51043800	-3.20296500	1.55488300
C	1.84508600	-2.92463900	5.23360700
H	2.09232400	-3.92953000	5.58543200
H	2.57649200	-2.22793700	5.64896000
H	0.86361300	-2.65920300	5.63335600

syn-2b

C	0.60645500	-1.40988600	-1.29821000
H	0.00272200	-1.35796100	-2.20510500
H	1.54674000	-1.91488200	-1.53789400
C	0.81172100	-0.07323900	-0.57765100
H	0.11184300	0.67277800	-0.95544500
C	2.25471400	0.48473800	-0.52191300
H	2.94952200	-0.21842200	-0.98419300
H	2.34977800	1.43889200	-1.04058800
C	2.57104500	0.60231100	0.98062800
H	3.63751400	0.56416700	1.20740400
H	2.15830800	1.52929400	1.39150100
C	1.82973300	-0.59232500	1.57401000
C	0.45854100	-0.48258300	0.86717900
H	-0.19159900	0.21106000	1.40265900
N	-0.20369300	-1.79537200	0.78317900
N	-0.10511100	-2.29506100	-0.33555900
H	1.74327800	-0.55999900	2.66596100
O	2.47812500	-1.76522700	1.13388900
Si	2.75664000	-3.14492900	2.04874200
C	1.21635800	-3.68011700	2.96174500

H	1.45151300	-4.51663900	3.62669100
H	0.80481600	-2.87360400	3.57453100
H	0.43367900	-3.99083800	2.26751400
C	4.11862100	-2.76077600	3.27892100
H	3.81547400	-1.97572600	3.97772700
H	4.37462100	-3.64412000	3.87046900
H	5.02328600	-2.42403700	2.76672600
C	3.29447900	-4.42054700	0.80194900
H	3.51394600	-5.37793400	1.28131700
H	2.49917500	-4.58301700	0.06997200
H	4.18996600	-4.09502700	0.26751100

anti-2b

C	0.44910100	0.10719600	-1.91005400
H	-0.51860800	0.51184800	-2.21891700
H	1.20577400	0.47860200	-2.60372000
C	0.76519200	0.33087300	-0.43651200
H	0.19227100	1.15163000	-0.00517700
C	2.26092200	0.46890500	-0.09750400
H	2.85342600	-0.08974400	-0.83148100
H	2.60784600	1.50292900	-0.11112900
C	2.37696600	-0.19480600	1.27579200
H	3.40486900	-0.43442400	1.55876800
H	1.95005100	0.45226400	2.04950400
C	1.48889200	-1.44288100	1.15449800
C	0.37735900	-1.02438200	0.17527400
H	-0.58900200	-1.06095700	0.68208700
N	0.30330600	-1.95429000	-0.98584100
N	0.35589300	-1.37296800	-2.06611100
H	2.05782600	-2.26131100	0.69164900
O	0.93682800	-1.87461500	2.37529000
Si	1.80897100	-2.57357600	3.62115800
C	0.55519900	-3.49160400	4.64959400
H	-0.21870900	-2.80968500	5.00960800
H	0.06812200	-4.27336800	4.06281500
H	1.02394100	-3.95890900	5.51942100
C	3.09903700	-3.72710000	2.90107400
H	3.86456400	-3.18362400	2.34016000
H	3.60757800	-4.27237300	3.70097000
H	2.64574400	-4.46150000	2.23044400
C	2.64982000	-1.24758700	4.64609100
H	3.14286900	-1.69117000	5.51587900
H	3.40873400	-0.70994000	4.07283100
H	1.92197500	-0.51827400	5.01095600

IN-2c

C	0.74070849	4.03478348	0.36627966
H	1.23543550	4.79477368	-0.23117424
C	1.02050200	2.75863300	0.10897200
H	1.73119861	2.53297529	-0.68327963
C	0.46157500	1.57252500	0.84040500
H	-0.12559300	1.89804600	1.70454700
H	-0.22059200	1.02500000	0.17960600
C	1.57208400	0.62577300	1.30237800
H	2.17056100	0.29377700	0.44617500
H	2.25445600	1.14768400	1.97835000
C	1.04921300	-0.60989400	2.03087500
H	0.41746500	-0.29026100	2.87098700
C	0.16212300	-1.48069100	1.16853400
H	-0.87045100	-1.71736700	1.36990900
N	0.67329400	-2.00114500	0.09669900
N	1.17100300	-2.45019300	-0.81281800
O	2.18124700	-1.30566100	2.52175600
Si	2.12937300	-2.76022500	3.35570500
C	3.75356600	-2.84151400	4.26879800
H	3.84545900	-3.77727500	4.82634600
H	4.58959400	-2.78347400	3.56780600
H	3.84887000	-2.01283400	4.97373400
C	0.67569200	-2.73323500	4.54169900
H	0.71923000	-1.86394000	5.20330900
H	-0.27839800	-2.70820200	4.00795900
H	0.67586400	-3.62855200	5.16953900
C	1.97864800	-4.20881400	2.17800100
H	0.98073700	-4.27979700	1.73877200
H	2.70059200	-4.12127900	1.36177600
H	2.18085100	-5.14761800	2.70169800
C	-0.21002050	4.52113546	1.43219302
H	-1.19776630	4.06547885	1.33034644
H	0.15897311	4.28351694	2.43410323
H	-0.33747313	5.60191547	1.37731676

syn-TS-2c

C	0.79142100	0.12936400	-1.78555600
H	0.00632200	0.47415200	-2.45005300
C	0.98960200	0.82917400	-0.61025500
H	0.36079200	1.70164100	-0.44786100
C	2.30186700	0.83448000	0.15538300

H	2.99141500	0.11076300	-0.27964400
H	2.76989300	1.81959800	0.06978600
C	2.09046200	0.48178000	1.63063000
H	3.03062700	0.29454200	2.15538800
H	1.56653300	1.29251600	2.14950900
C	1.21502600	-0.77137200	1.66341600
H	0.98892200	-1.05971500	2.70018900
C	-0.04511500	-0.37821300	0.90842200
H	-0.79284500	0.21238300	1.42830300
N	-0.54133200	-1.26873700	0.04442500
N	-0.52603600	-1.55959000	-1.06838700
O	1.87868900	-1.80388800	0.98007100
Si	1.82576600	-3.43460600	1.37887000
C	2.54314300	-4.29937900	-0.10553500
H	2.59280100	-5.38022800	0.04894600
H	1.92707600	-4.10911100	-0.98807900
H	3.55344800	-3.93933700	-0.31401800
C	2.86589900	-3.70452500	2.91292500
H	3.88938700	-3.35666600	2.75335300
H	2.45853300	-3.16834300	3.77455300
H	2.90716900	-4.76495800	3.17665200
C	0.06032000	-3.96146800	1.70922900
H	-0.42011800	-3.31409900	2.44874600
H	-0.54035100	-3.93105900	0.79753100
H	0.03665000	-4.98247100	2.10056600
C	1.80824900	-0.80855700	-2.38760700
H	1.33468900	-1.46295000	-3.12153400
H	2.61064600	-0.26260000	-2.89608700
H	2.26439000	-1.44189100	-1.62251400

anti-TS-2c

C	1.49422800	0.23675900	-1.77532500
H	0.87498600	-0.03021200	-2.62502000
C	0.85408800	0.60452000	-0.60757900
H	-0.23164300	0.65402100	-0.63724800
C	1.49659900	1.45016500	0.48031400
H	2.57280900	1.53069000	0.30610900
H	1.09810100	2.46808500	0.43609900
C	1.25325100	0.84076000	1.85933500
H	1.81722200	1.33529600	2.65305500
H	0.19175000	0.89086000	2.12609200
C	1.65038100	-0.63206400	1.77680600
C	0.85078500	-1.19690300	0.62374200
H	-0.16498600	-1.51694500	0.84187400
N	1.48097200	-1.96606000	-0.27724700
N	1.93613100	-1.94551600	-1.33271700
H	2.71658900	-0.69627500	1.51339600
O	1.41269500	-1.26358100	3.01253800
Si	1.83912300	-2.85042900	3.36234600
C	0.55139200	-4.03789500	2.69577200
H	-0.45057400	-3.74765500	3.02248600
H	0.55940500	-4.07427200	1.60384000
H	0.74126500	-5.05023600	3.06437100
C	3.50720700	-3.21769200	2.59211600
H	4.26610200	-2.50465500	2.92535100
H	3.84385500	-4.21808800	2.87773800
H	3.46421500	-3.18784100	1.49953500
C	1.90023600	-2.93473300	5.22364000
H	2.16158000	-3.94033700	5.56312700
H	2.64010400	-2.23705100	5.62198900
H	0.92932600	-2.67568800	5.65240800
C	2.93863500	0.54558100	-2.08595300
H	3.28146500	-0.05576700	-2.92898300
H	3.08153500	1.60010600	-2.34548200
H	3.59781000	0.32306200	-1.24241700

syn-2c

C	0.56990500	-1.38744000	-1.36600400
H	-0.19028500	-1.21949500	-2.13374000
C	0.85413300	-0.09132400	-0.57363100
H	0.17486100	0.69141700	-0.91195100
C	2.30093200	0.45286300	-0.49581600
H	3.01099800	-0.25491900	-0.92226400
H	2.41070200	1.39708600	-1.02986200
C	2.58020000	0.59703300	1.01105600
H	3.64186400	0.58207800	1.26249500
H	2.14041700	1.52069200	1.40093100
C	1.84855400	-0.60384700	1.60343600
C	0.49520500	-0.53192800	0.86133400
H	-0.18971800	0.13509200	1.38836200
N	-0.13016900	-1.85998300	0.75541300
N	-0.07328800	-2.31555400	-0.38354400
H	1.73317800	-0.55546600	2.69212500
O	2.53240200	-1.77108200	1.20264100
Si	2.80096400	-3.13264400	2.14669500
C	1.24796300	-3.66670900	3.03799600
H	1.47700200	-4.48923900	3.72223600
H	0.81675000	-2.85355500	3.62811200

H	0.48277500	-3.99602500	2.33306400
C	4.13493400	-2.71717100	3.39693400
H	3.81092200	-1.92210200	4.07468200
H	4.38565800	-3.58742800	4.00978500
H	5.04728500	-2.38184800	2.89763500
C	3.37410300	-4.42430800	0.93137000
H	3.61518900	-5.36389800	1.43495300
H	2.58665600	-4.62397300	0.19983700
H	4.26434700	-4.09033100	0.39276300
C	1.74628500	-2.12183300	-1.99718100
H	1.39221500	-3.04931600	-2.44980800
H	2.20916800	-1.51102500	-2.77488500
H	2.49391300	-2.36523600	-1.24061900

anti-2c

C	0.50083800	0.14117300	-1.89597300
C	0.86515500	0.30202400	-0.42059000
H	0.30241400	1.10676500	0.05441400
C	2.36303500	0.42114000	-0.08289200
H	2.95590000	-0.15545200	-0.80088200
H	2.72928500	1.44853300	-0.10051500
C	2.45625400	-0.23966100	1.29422200
H	3.47941600	-0.48288900	1.59098600
H	2.02208200	0.41100200	2.06077300
C	1.56304000	-1.48481100	1.16380200
C	0.49093500	-1.07487200	0.14065100
H	-0.50146700	-1.15624500	0.58982800
N	0.50881700	-1.96866200	-1.05559000
N	0.52800200	-1.34059300	-2.11035300
H	2.13907300	-2.31751000	0.73683600
O	0.96556300	-1.88706200	2.37459200
Si	1.78774000	-2.58361000	3.65504100
C	0.48501200	-3.44661100	4.67049300
H	-0.27910600	-2.73734000	4.99722700
H	-0.00824800	-4.22827800	4.08882600
H	0.92054300	-3.90656100	5.56122700
C	3.06338200	-3.78432800	2.98737000
H	3.85465600	-3.26886800	2.43571700
H	3.53969600	-4.32875100	3.80737800
H	2.60710600	-4.51779000	2.31773900
C	2.64114500	-1.26212600	4.67568700
H	3.10240600	-1.70287900	5.56413500
H	3.42731300	-0.75570100	4.11059700
H	1.92567900	-0.50686400	5.01093000
H	-0.54765100	0.42184700	-2.05364600
C	1.36572400	0.84210600	-2.92917900
H	0.99878700	0.62524600	-3.93306200
H	1.34318900	1.92305600	-2.77620800
H	2.40211000	0.50615600	-2.86940700

IN-3a

C	1.25616600	3.84611100	-0.02967900
H	0.76023800	4.35485800	0.79150000
H	1.78675400	4.46282300	-0.74508000
C	1.20958700	2.52440700	-0.14875000
H	1.72054300	2.04656200	-0.98324700
C	0.50996900	1.60208200	0.80679400
H	-0.01685100	2.19562300	1.55895300
H	-0.24624200	1.02228800	0.26371400
C	1.49811000	0.64386600	1.47760200
H	2.12488900	0.16078200	0.71925300
H	2.18072900	1.20263700	2.12326000
C	0.86521800	-0.45821300	2.33811900
C	-0.01541700	-1.37458300	1.51121300
H	-0.95436900	-1.78766300	1.84811300
N	0.36260100	-1.71542000	0.32035500
N	0.73430700	-1.98524600	-0.71254700
O	1.97308300	-1.14389200	2.92008600
Si	2.11555300	-2.74270300	3.38855900
C	3.71632200	-2.78929900	4.34696800
H	3.92232900	-3.79655800	4.71871800
H	4.55388000	-2.48383400	3.71562100
H	3.67679800	-2.11153500	5.20261300
C	0.68377900	-3.26648400	4.48548800
H	0.61516900	-2.63938300	5.37818100
H	-0.27358500	-3.22199600	3.95970500
H	0.82798800	-4.29950000	4.81564300
C	2.22088400	-3.88810200	1.90729400
H	1.24753300	-4.06016400	1.44190100
H	2.89221900	-3.48178800	1.14597400
H	2.61802800	-4.86040400	2.21366100
C	0.00931100	0.12135800	3.46386800
H	-0.84651200	0.67208100	3.06974700
H	-0.36095600	-0.68225600	4.10407900
H	0.62249500	0.79084000	4.06984700

syn-TS-3a

C	0.63913700	0.06806000	-1.77771800
H	-0.17476800	0.36956800	-2.42440300
H	1.35534400	-0.63043800	-2.19668800
C	0.94719500	0.77534900	-0.63762600
H	0.38050400	1.68210800	-0.43510200
C	2.31468000	0.70353300	0.01443400
H	2.87165500	-0.13214600	-0.41490200
H	2.87610400	1.61873900	-0.19561300
C	2.18726000	0.49685900	1.52167300
H	3.15005300	0.30833700	2.00485600
H	1.74016000	1.38221800	1.98903600
C	1.25826400	-0.70476000	1.75288300
C	-0.00648900	-0.34140500	0.97012000
H	-0.74617600	0.28076800	1.46601800
N	-0.53052000	-1.28161500	0.17810800
N	-0.57103400	-1.64592700	-0.91058100
O	1.87367000	-1.81717500	1.14760800
Si	1.81311000	-3.46888700	1.42611300
C	2.73788600	-4.18274400	-0.02604200
H	2.78149300	-5.27361000	0.02882600
H	2.23970000	-3.90939200	-0.95961000
H	3.76098400	-3.80206800	-0.06446000
C	2.68023500	-3.88516500	3.03689400
H	3.63633100	-3.36074100	3.11298200
H	2.07806200	-3.62607400	3.91073400
H	2.88437400	-4.95882900	3.08349000
C	0.06123800	-4.13417100	1.47315300
H	-0.56715800	-3.62102600	2.20525800
H	-0.42424400	-4.04820200	0.49870200
H	0.08751900	-5.19370100	1.74684700
C	0.98765500	-0.92663000	3.23908500
H	0.30877700	-1.76877700	3.39402300
H	1.92592800	-1.12798500	3.76160400
H	0.53045300	-0.03663900	3.67676000

anti-TS-3a

C	1.37209000	0.24037500	-1.82254400
H	0.85350700	-0.14953700	-2.68842100
H	2.32990300	0.71399000	-2.01221800
C	0.71951800	0.43880800	-0.62559100
H	-0.34892300	0.23639600	-0.59861900
C	1.21038800	1.41694900	0.42937200
H	2.20839500	1.77207300	0.15790000
H	0.56257400	2.29806000	0.44241000
C	1.23151700	0.76061400	1.80831600
H	1.72867000	1.36871600	2.56837000
H	0.20953500	0.57370800	2.15504300
C	1.93493100	-0.60251600	1.69985800
C	1.19513100	-1.29474700	0.56316000
H	0.26604600	-1.79667500	0.81571800
N	1.91229700	-1.92487900	-0.38111800
N	2.33209700	-1.80204500	-1.44279800
O	1.77445600	-1.25464500	2.94734600
Si	1.87952200	-2.87096800	3.36769600
C	0.36682000	-3.81656400	2.78235900
H	-0.55188600	-3.26234100	2.99215100
H	0.40380000	-4.03476700	1.71244200
H	0.30252500	-4.77353000	3.30887100
C	3.40826800	-3.69196400	2.65868700
H	4.32620900	-3.19231700	2.97762700
H	3.45578400	-4.72859500	3.00616000
H	3.38809600	-3.71396000	1.56550500
C	1.93729300	-2.84543200	5.23180100
H	1.99361500	-3.85820300	5.63909900
H	2.80800700	-2.28768000	5.58386100
H	1.04436300	-2.36512700	5.63837500
C	3.42069200	-0.43202700	1.39143100
H	3.91952300	-1.40042700	1.33912800
H	3.57836500	0.07884500	0.43983300
H	3.87680500	0.15486100	2.19035500

syn-3a

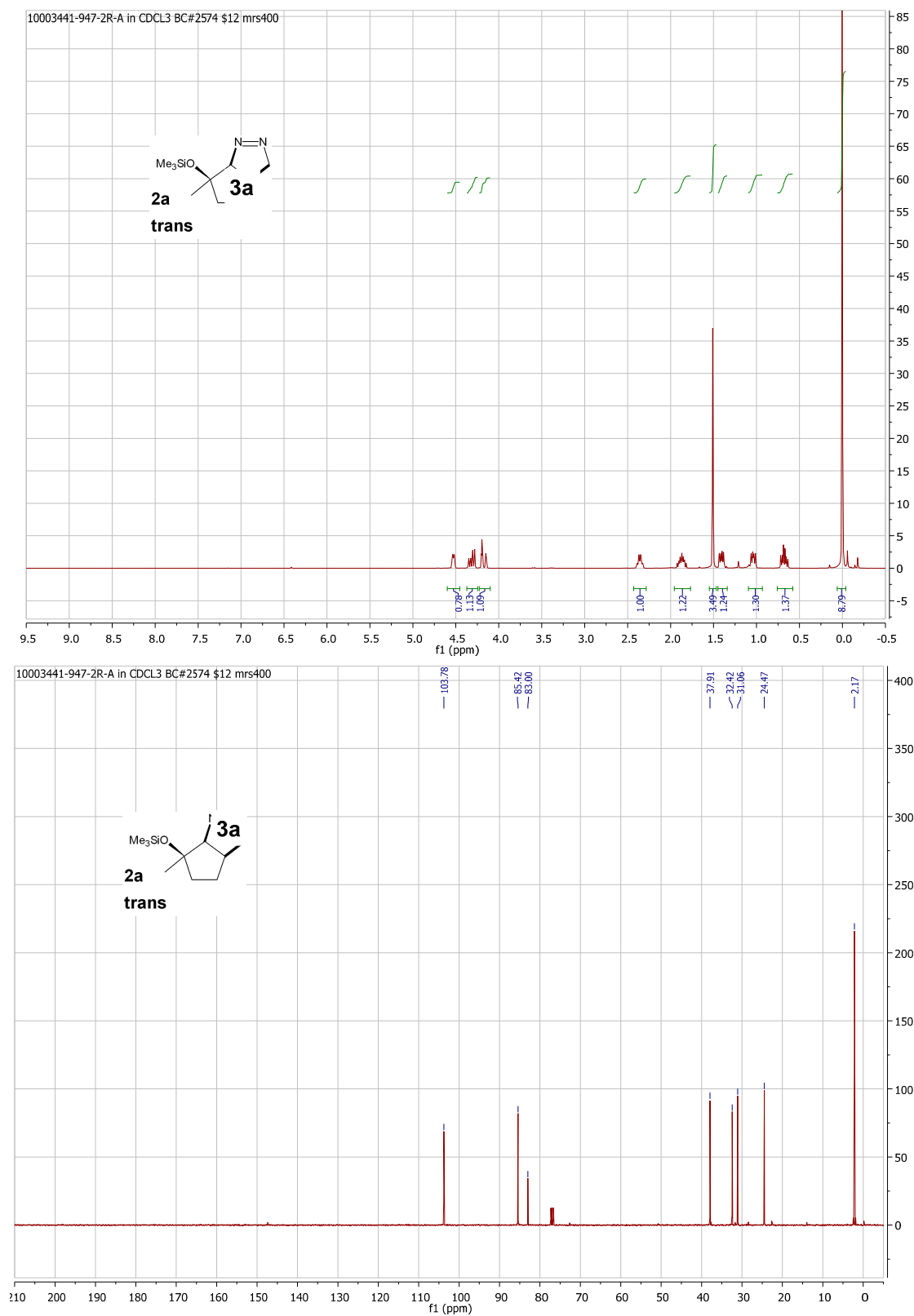
C	0.47721800	-1.54827500	-1.12343900
H	-0.18345500	-1.56381300	-1.99130500
H	1.38448700	-2.10576400	-1.37338000
C	0.76720500	-0.15616100	-0.55507300
H	0.08503200	0.57925200	-0.98278700
C	2.23353000	0.33831400	-0.61187300
H	2.88305300	-0.45014300	-0.99602100
H	2.34999300	1.21225700	-1.25340600
C	2.59901100	0.63094700	0.85133600
H	3.67075400	0.58619700	1.05452800
H	2.22562300	1.61505900	1.15410000
C	1.84814800	-0.45469900	1.62808000
C	0.45834900	-0.39298200	0.93626900
H	-0.16318200	0.36995500	1.40875100
N	-0.22770300	-1.69075900	1.02632000
N	-0.19512700	-2.31024100	-0.03510400

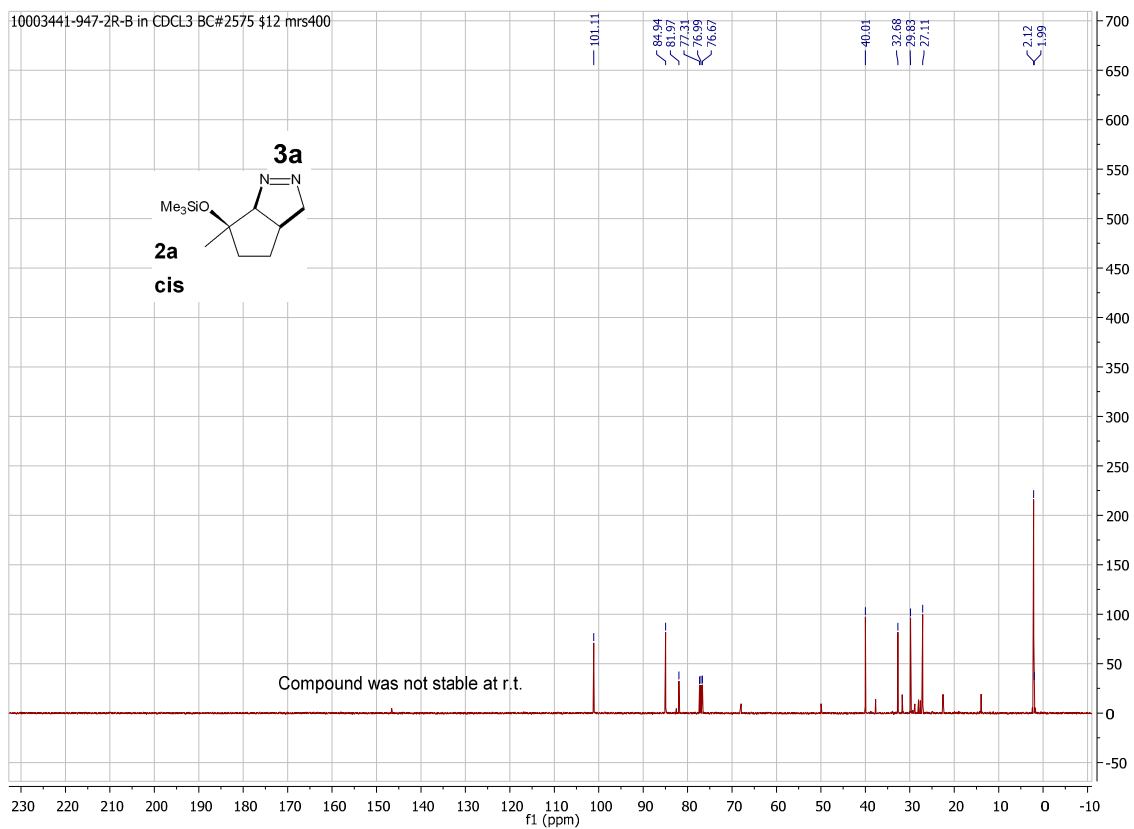
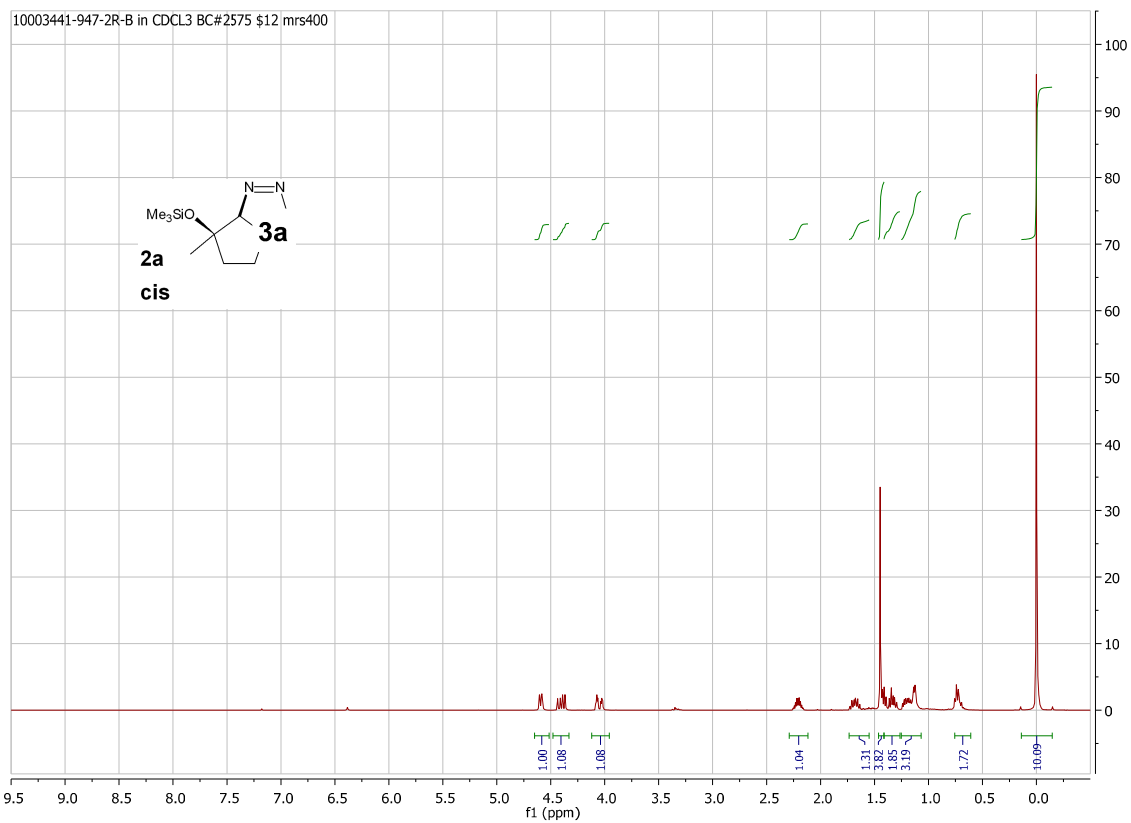
O	2.45713400	-1.68149200	1.26785700
Si	2.74042200	-3.13188100	2.05760100
C	1.19884800	-3.94561700	2.73429600
H	1.48150000	-4.87899500	3.23200900
H	0.67704900	-3.32212500	3.46331300
H	0.49098000	-4.17520600	1.93577600
C	3.97115500	-2.87459300	3.45357700
H	3.50971400	-2.41395200	4.33020700
H	4.38283300	-3.83801700	3.76858200
H	4.80512400	-2.24417400	3.13400500
C	3.48840900	-4.19239500	0.71510000
H	3.77340900	-5.17568800	1.09819600
H	2.76574000	-4.34373800	-0.09105100
H	4.37805700	-3.72087100	0.29148300
C	1.80281900	-0.23572300	3.13017100
H	1.21795000	-1.01858200	3.61984500
H	2.81399800	-0.23789500	3.54313300
H	1.33939000	0.72674600	3.35695700

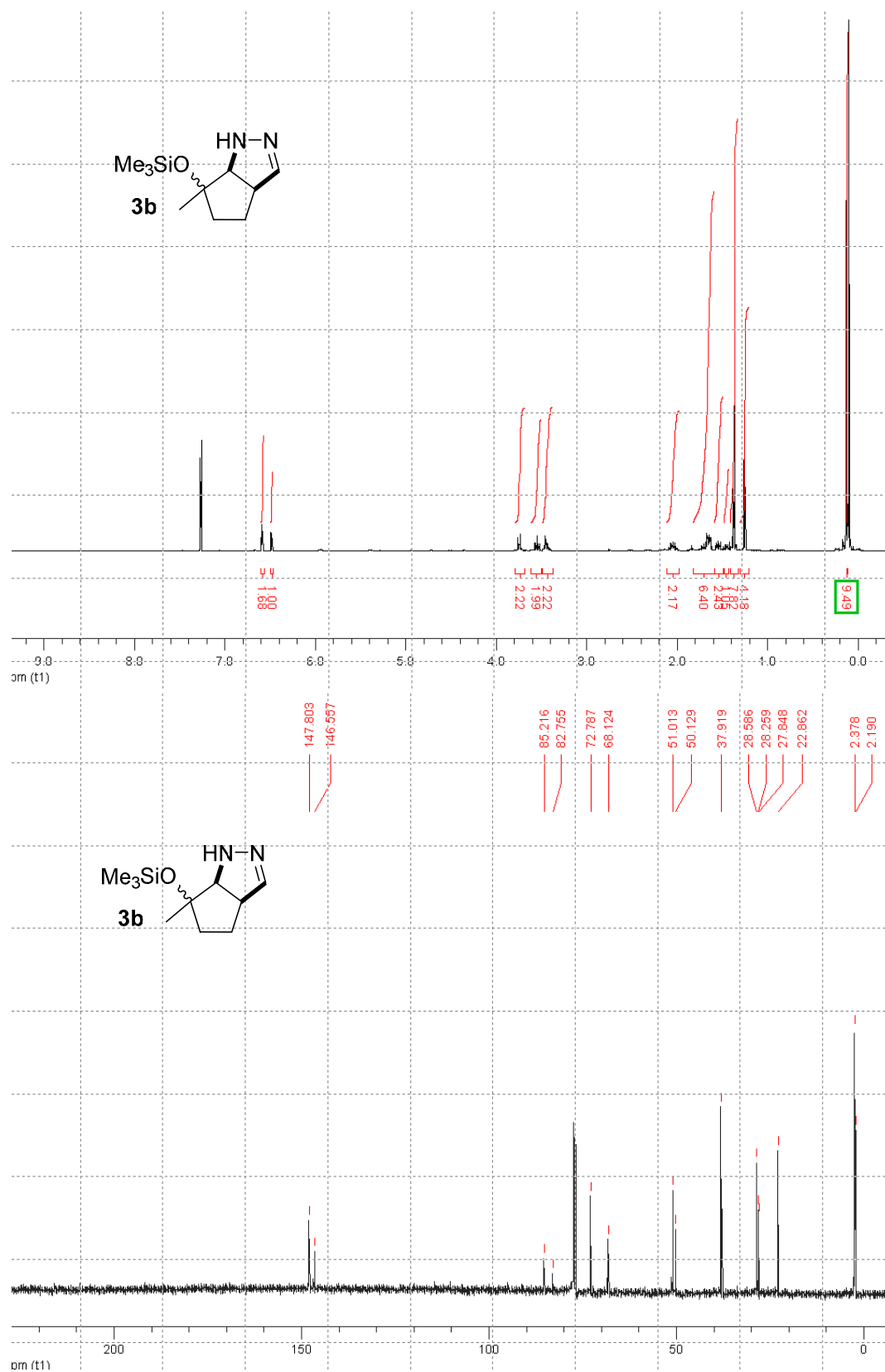
anti-3a

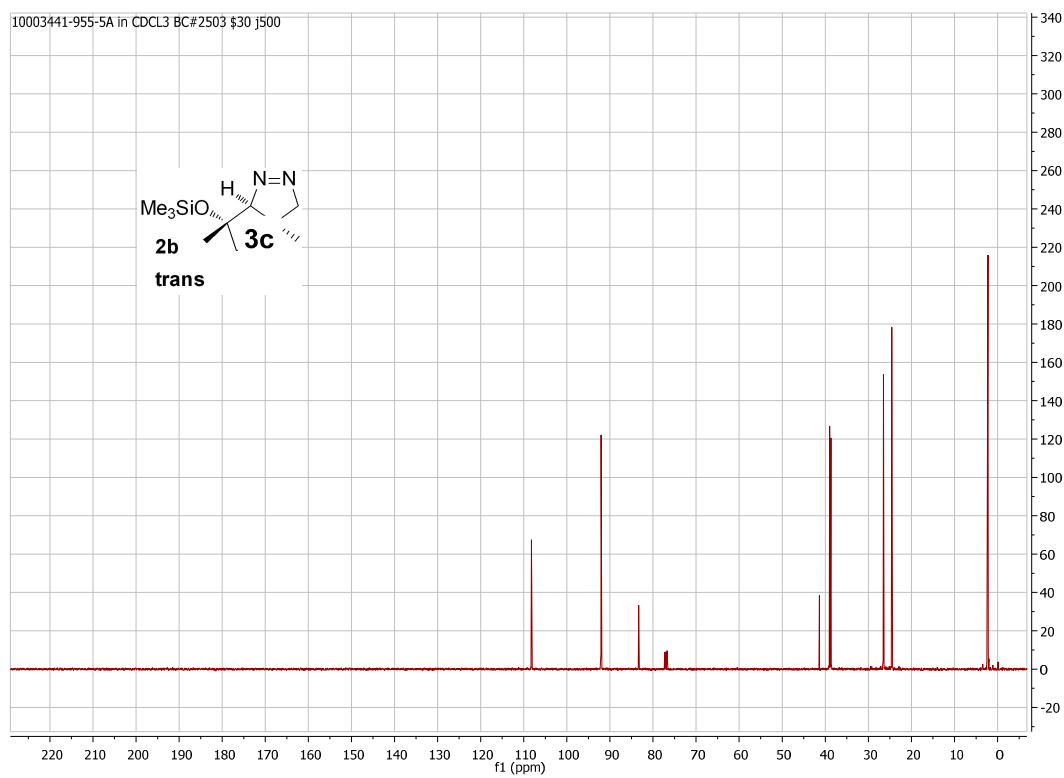
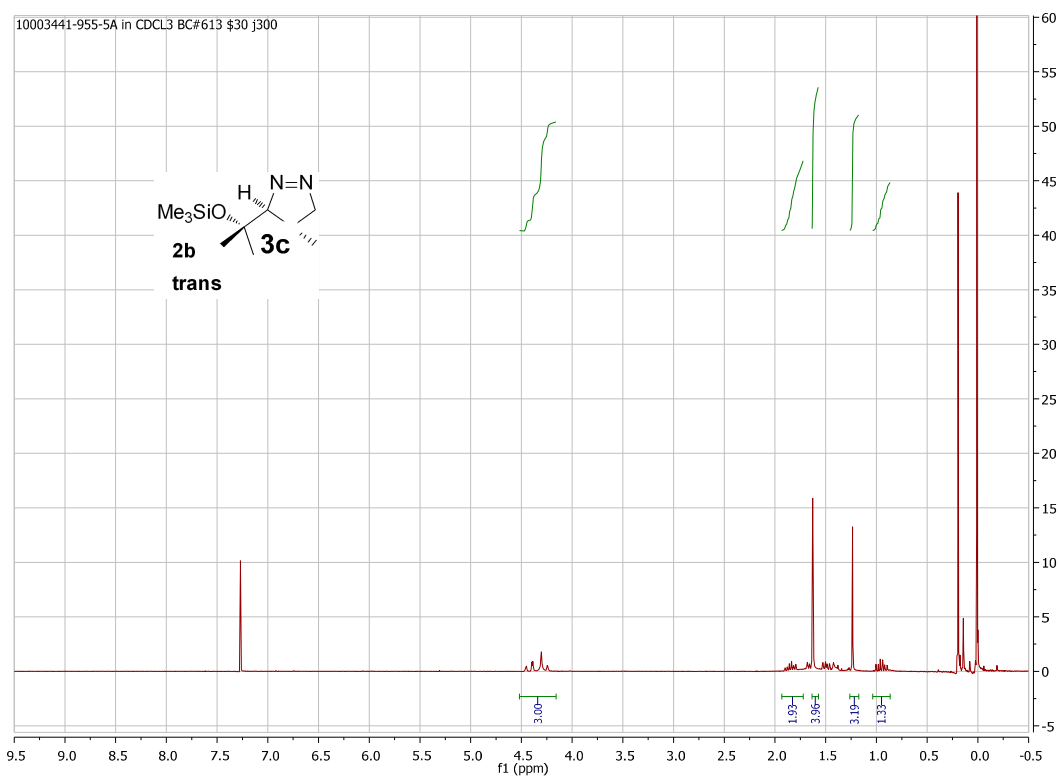
C	0.24425900	0.33507400	-1.74362100
H	-0.72722500	0.81558000	-1.88615600
H	0.94221100	0.76952200	-2.46234400
C	0.72684500	0.34258300	-0.29896500
H	0.20849100	1.08628400	0.30642000
C	2.24725100	0.45012100	-0.09761000
H	2.76751100	0.00833300	-0.95467300
H	2.59201200	1.48047400	0.00074600
C	2.48330900	-0.38819800	1.15870600
H	3.53339100	-0.63841100	1.33538500
H	2.10681100	0.15418100	2.03146700
C	1.60998900	-1.64441500	0.95557200
C	0.39430400	-1.09021300	0.15496600
H	-0.50006700	-1.18785900	0.77290700
N	0.12530300	-1.83444600	-1.10391100
N	0.05676200	-1.10292100	-2.08794000
O	1.12213300	-2.17297600	2.17532300
Si	1.87621300	-2.60357900	3.59975400
C	0.52307500	-3.41257000	4.59619800
H	-0.30377700	-2.71733100	4.75833300
H	0.12842500	-4.28578000	4.07193800
H	0.88958800	-3.73822300	5.57310500
C	3.29633700	-3.80060500	3.33114500
H	4.15776200	-3.32265700	2.85752500
H	3.63103800	-4.18646200	4.29890700
H	2.99632900	-4.65254900	2.71632000
C	2.53612800	-1.09897700	4.50800200
H	2.87018900	-1.39254300	5.50773700
H	3.38807700	-0.64487800	3.99663800
H	1.76321000	-0.33529300	4.62740900
C	2.36257300	-2.72676200	0.18402300
H	3.24284300	-3.03654300	0.74907500
H	1.71588700	-3.58795100	0.01751900
H	2.69025400	-2.35940200	-0.79116300

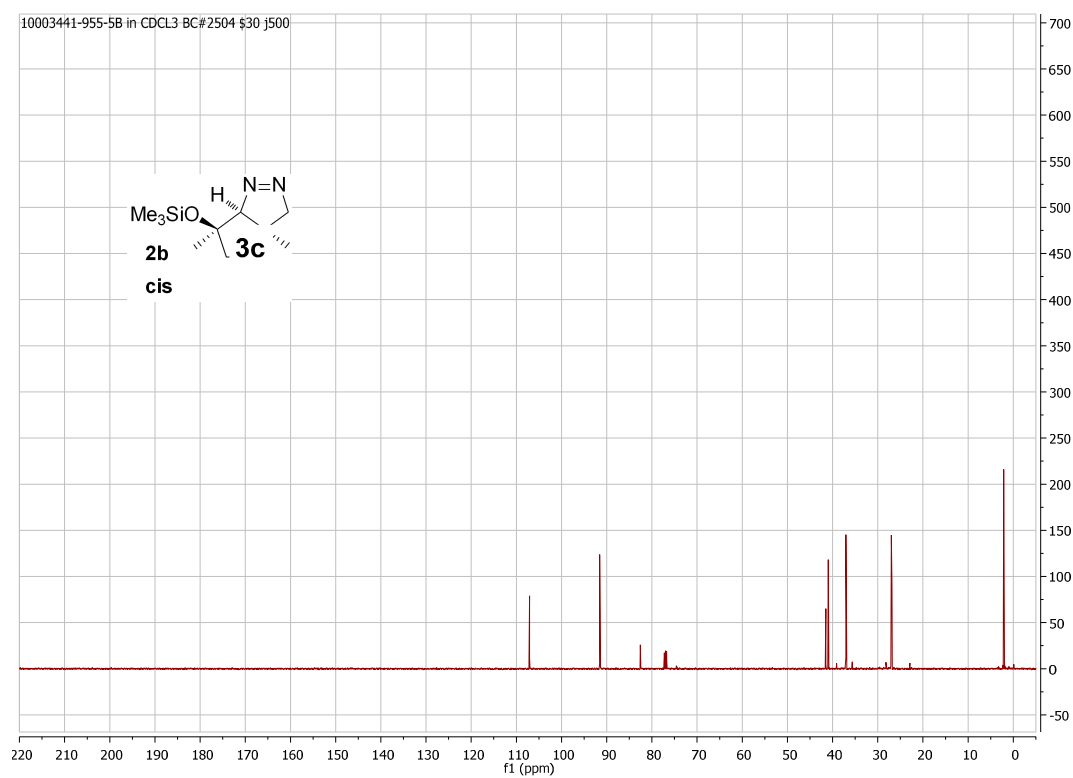
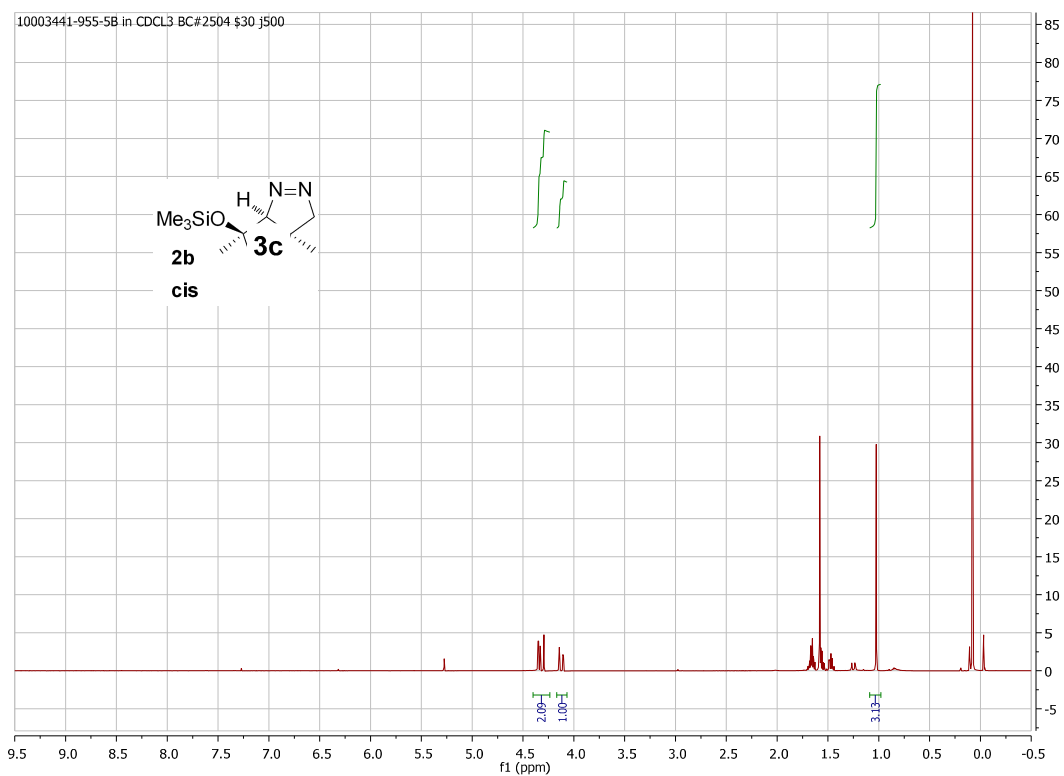
5. Select ^1H -NMR and ^{13}C -NMR-Spectra

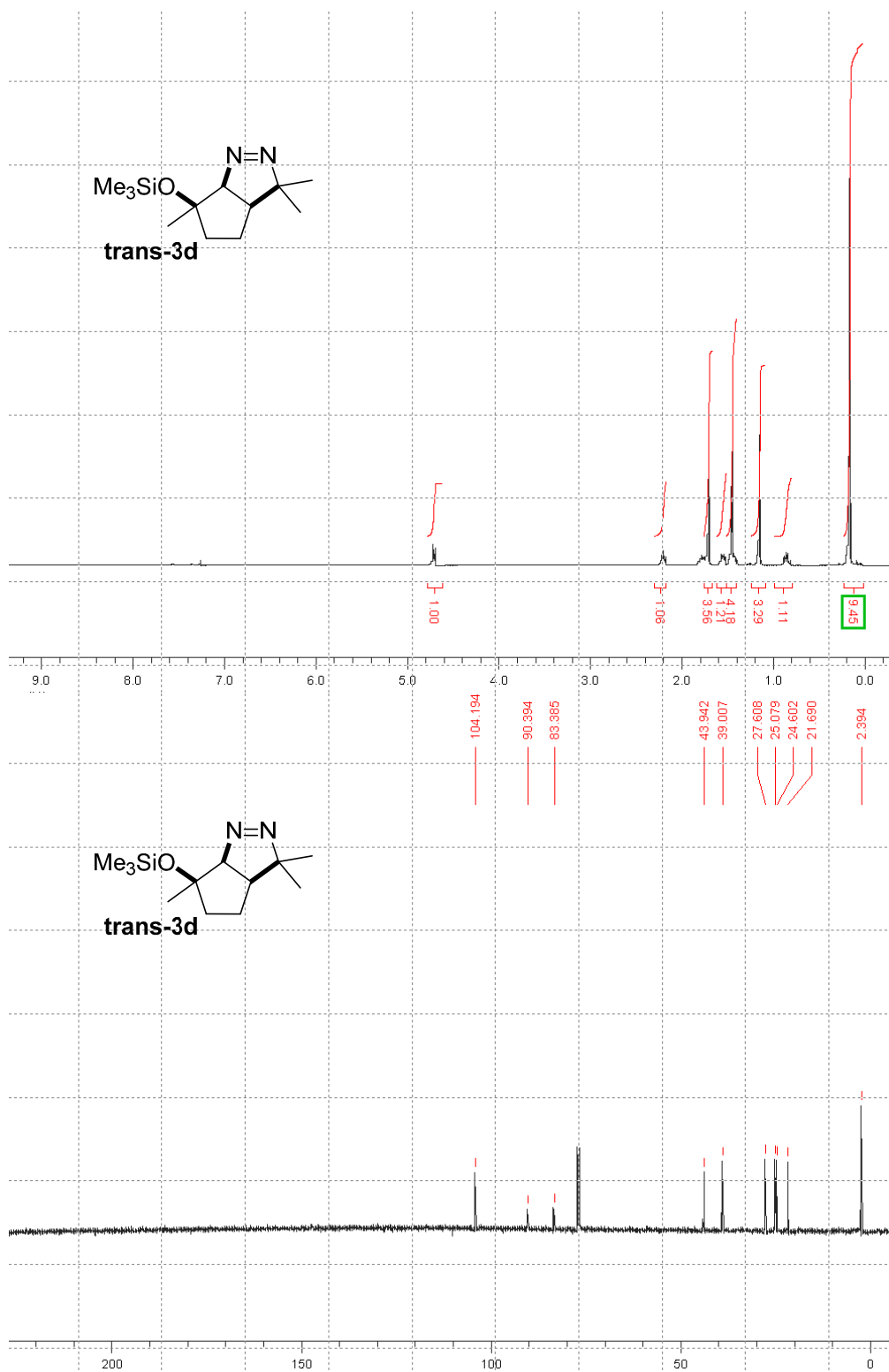


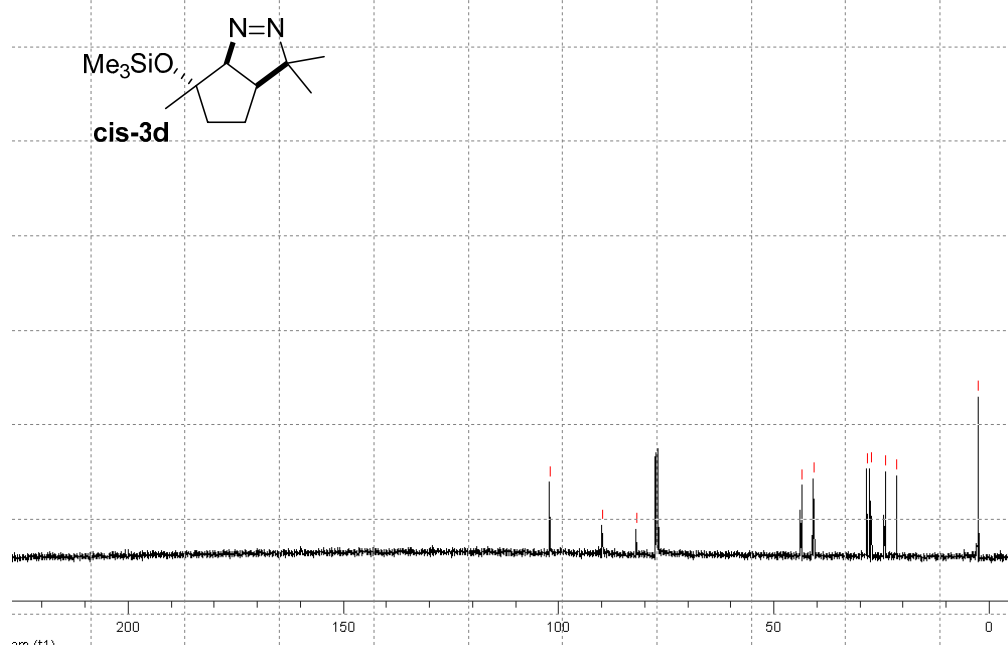
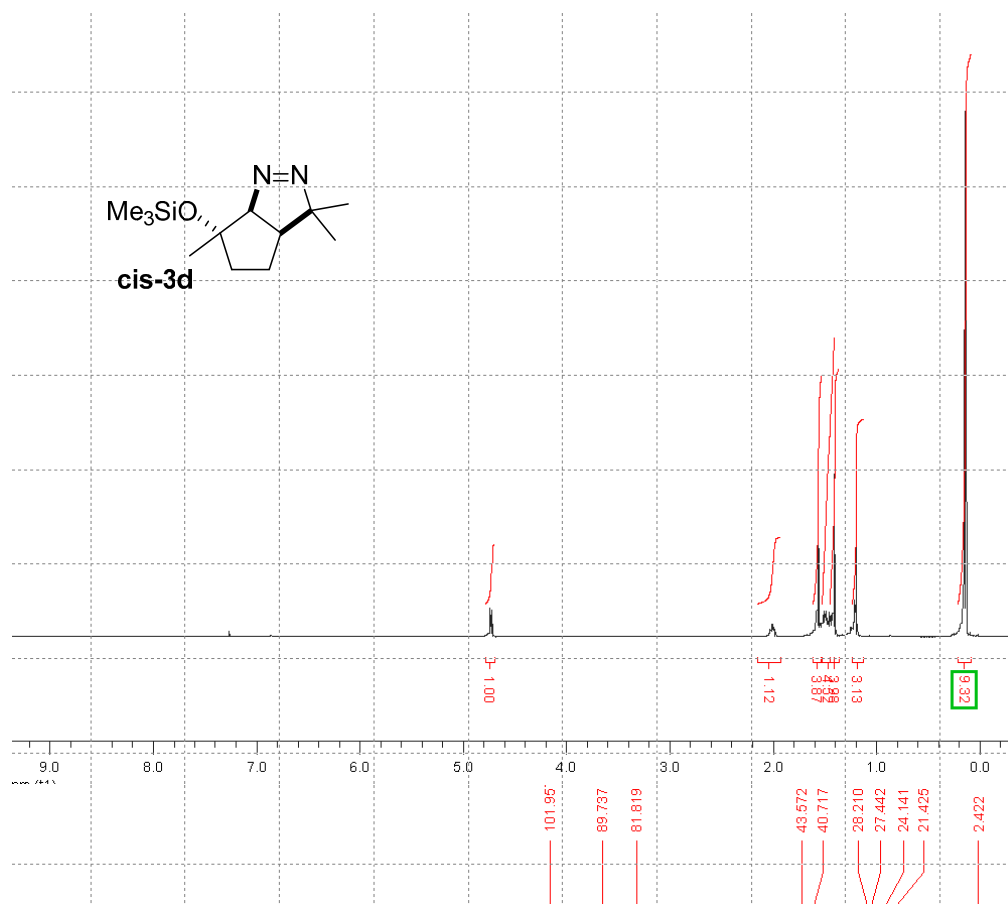


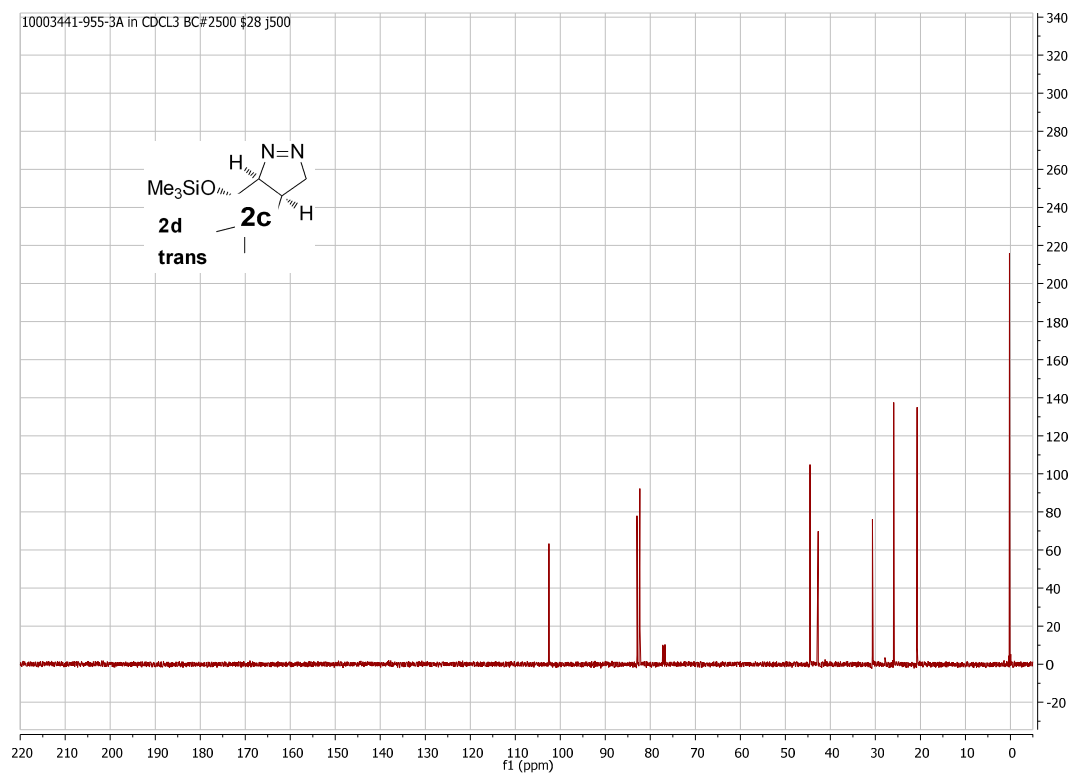
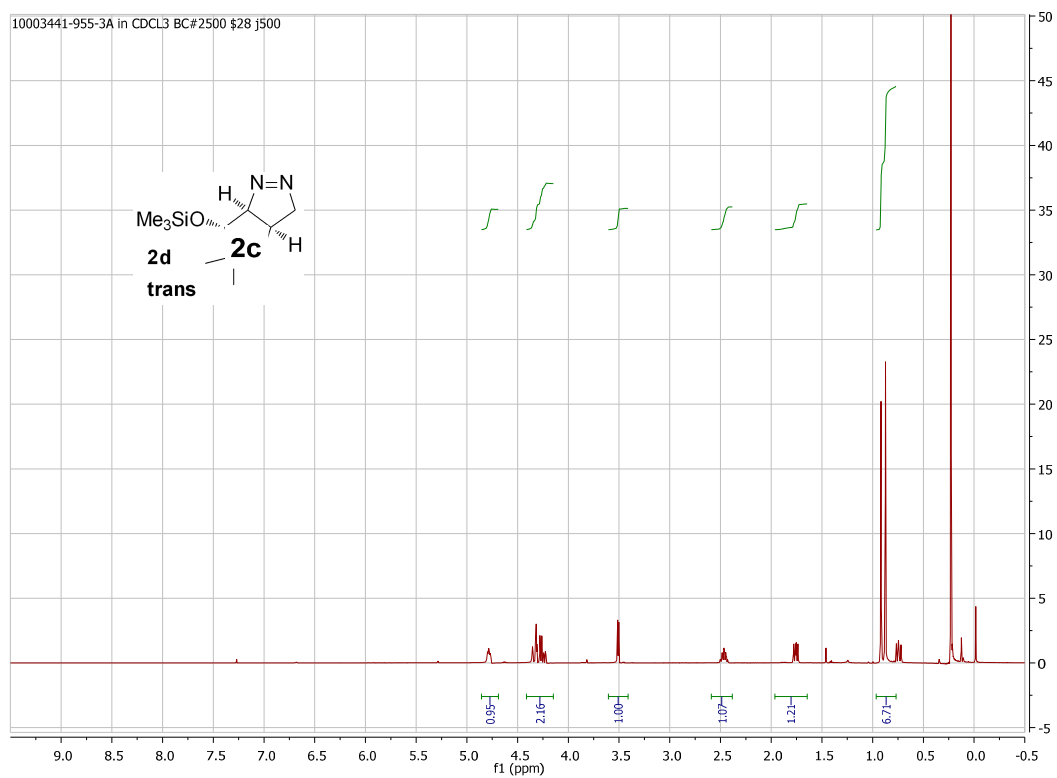


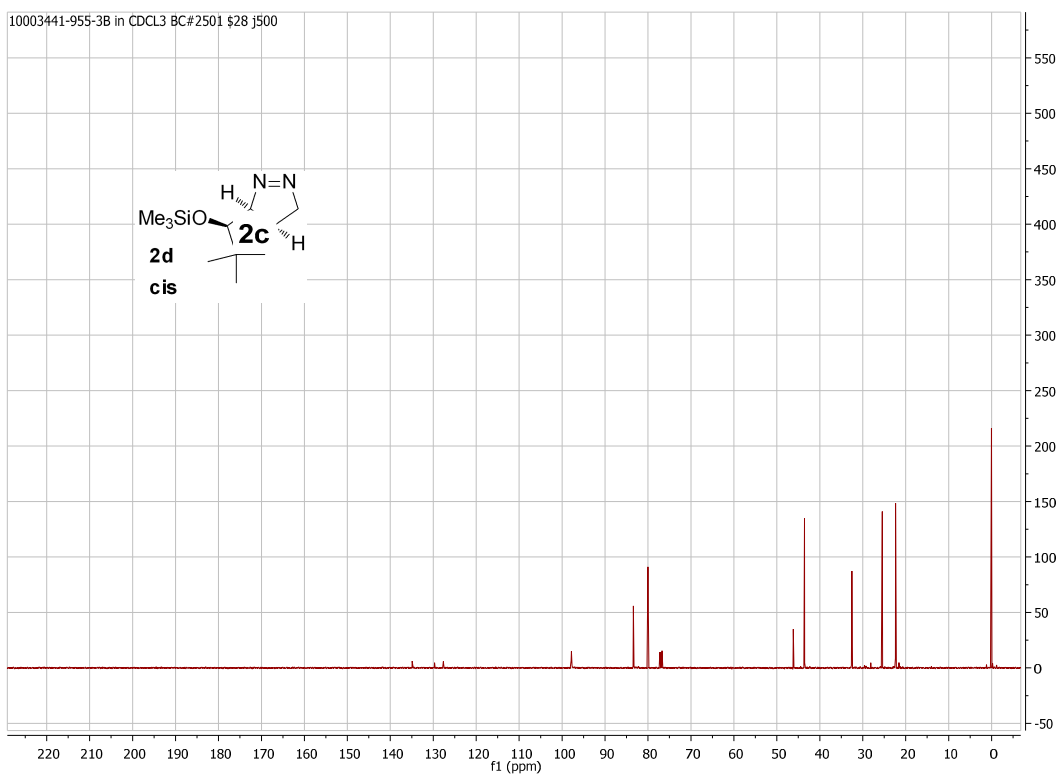
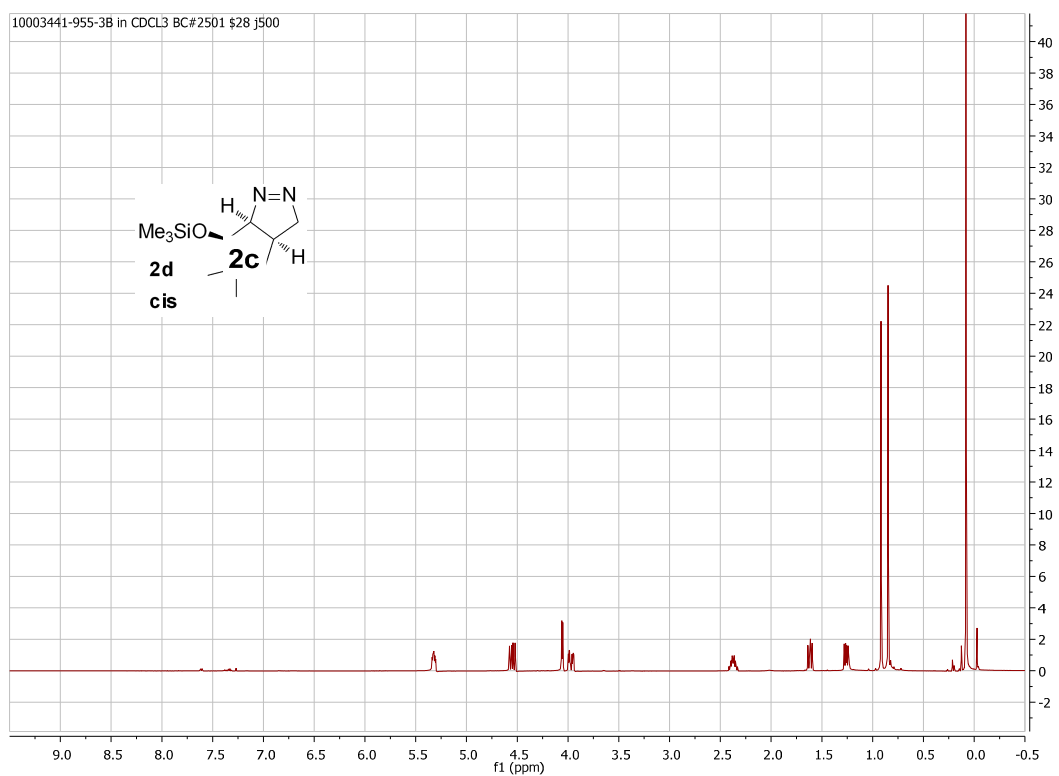


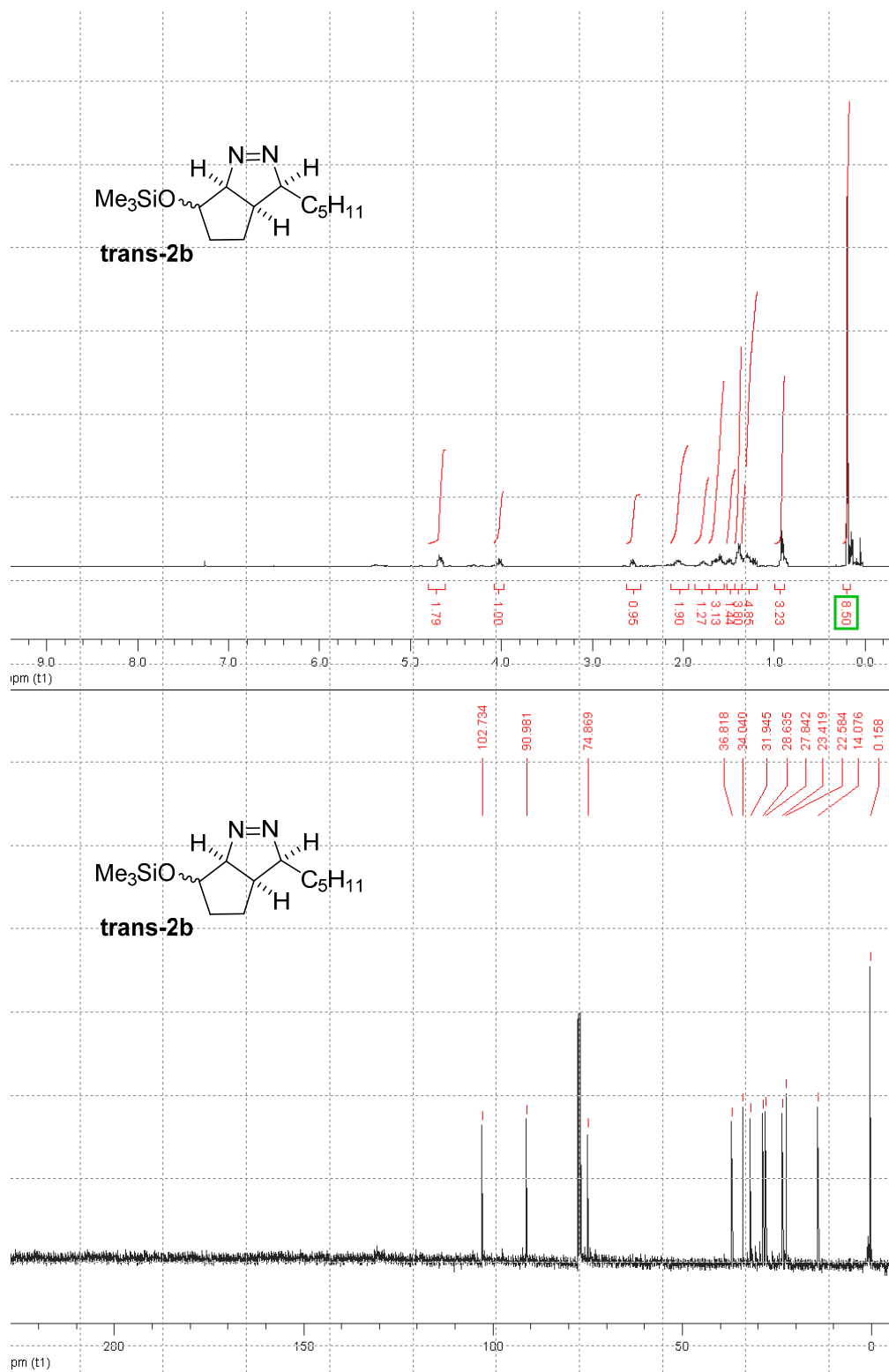




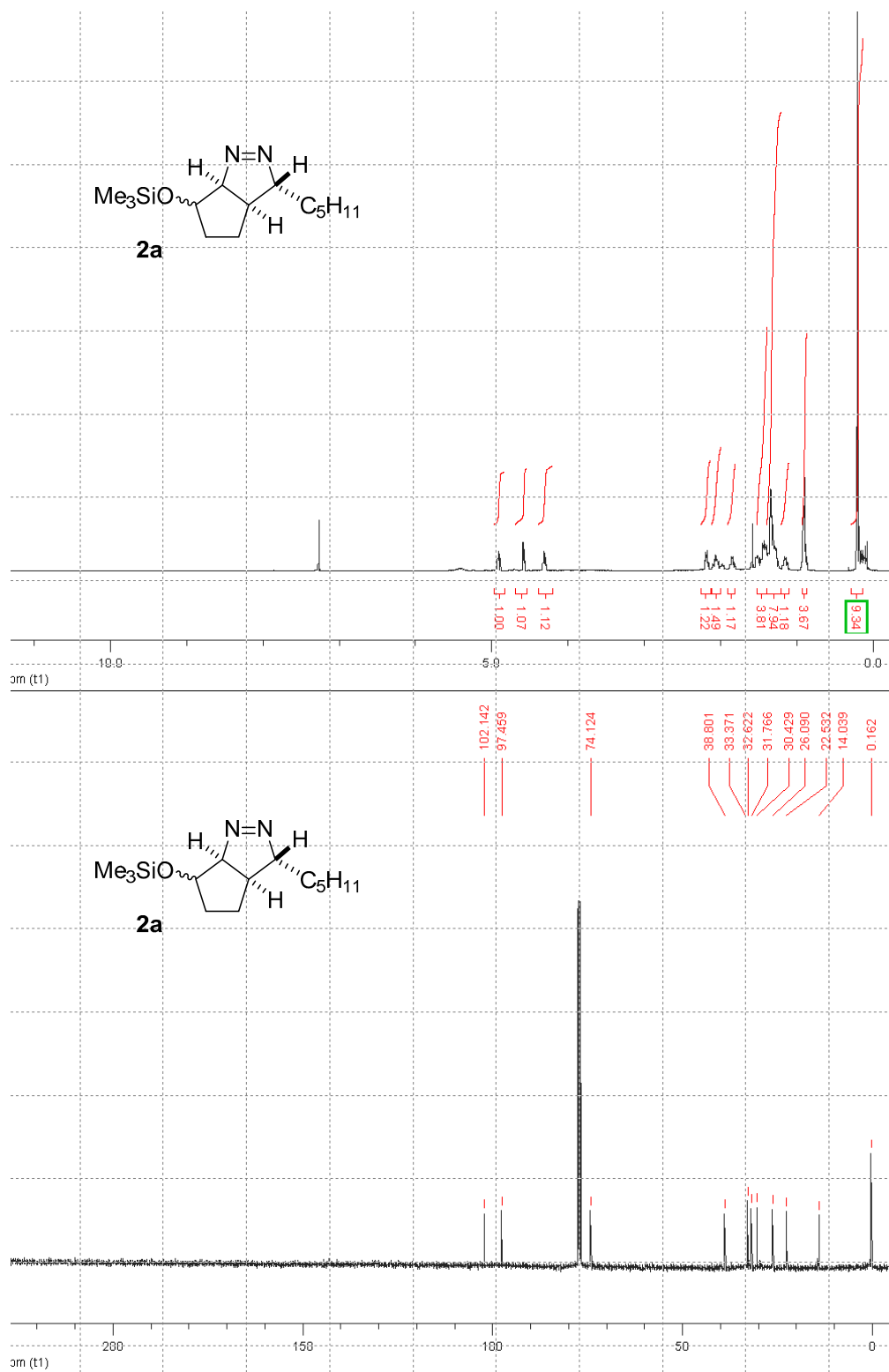


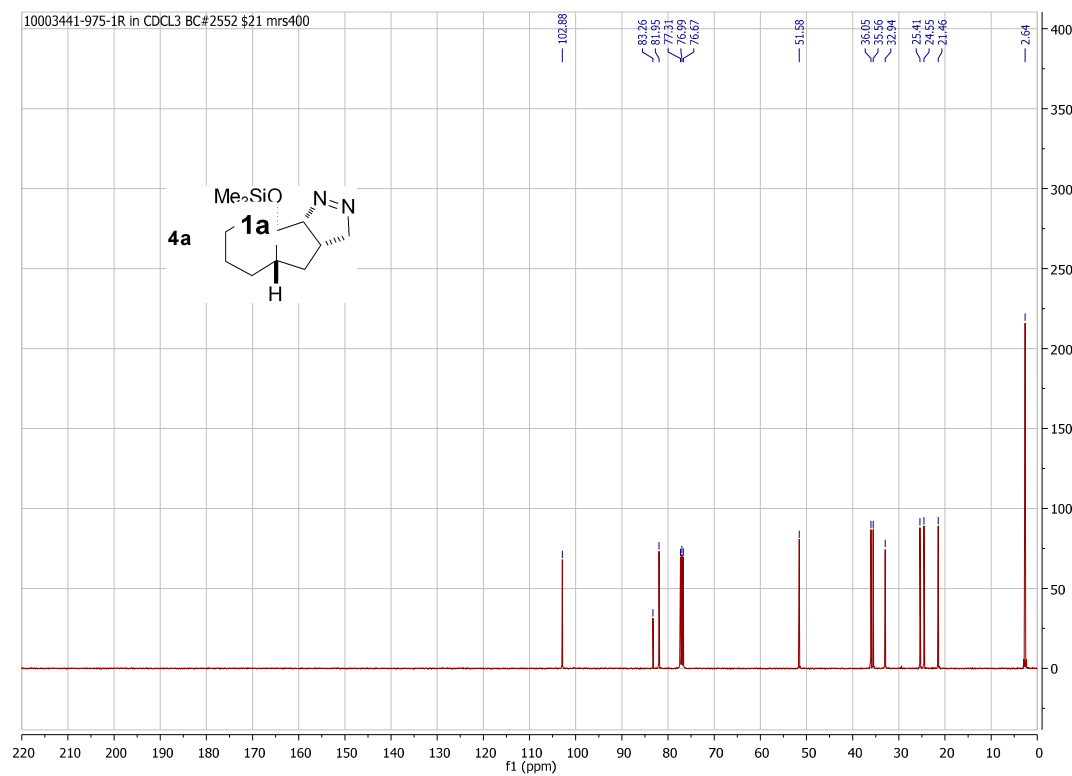
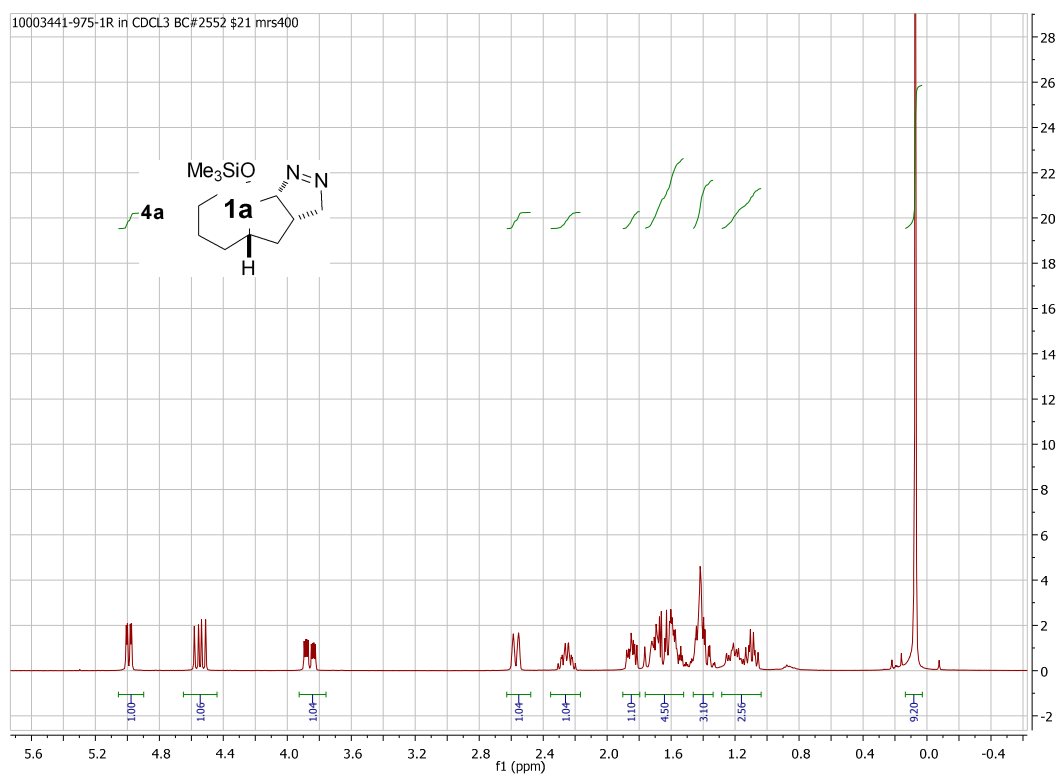


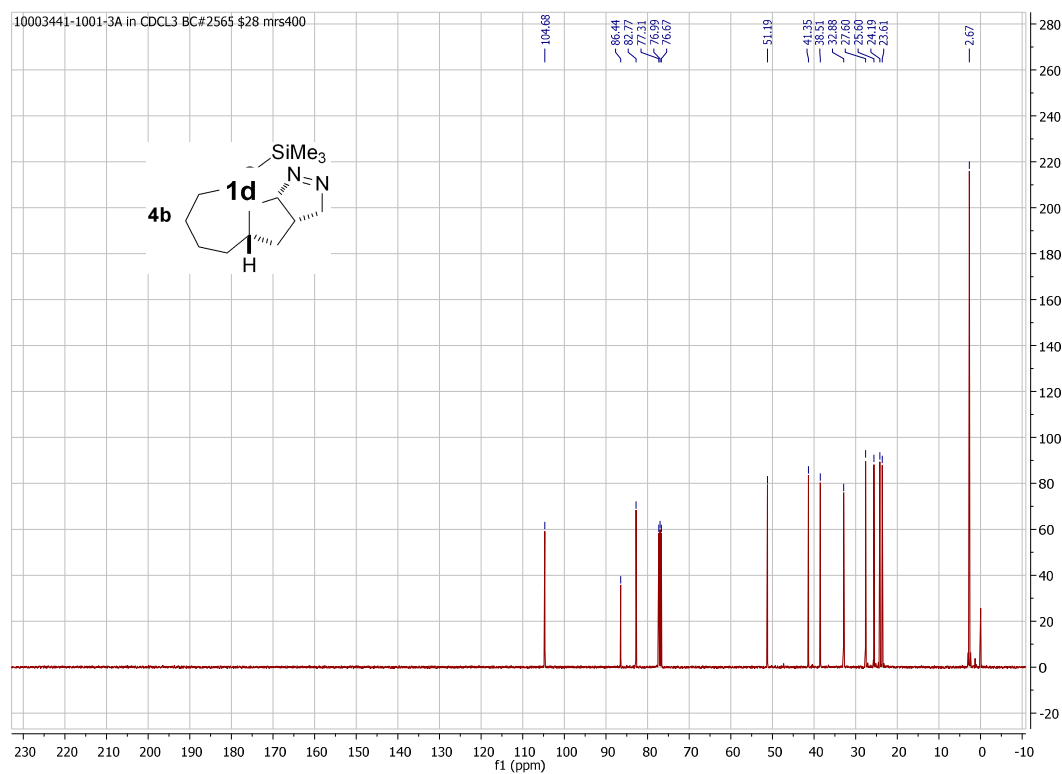
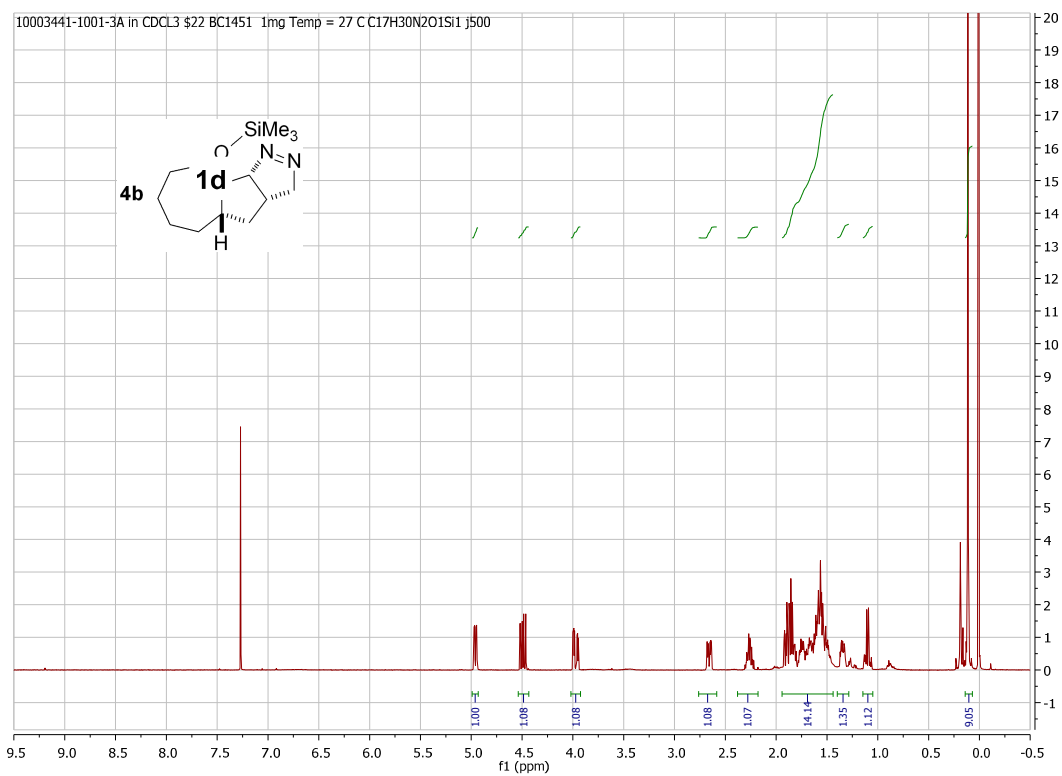




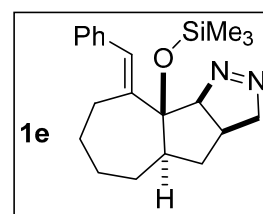
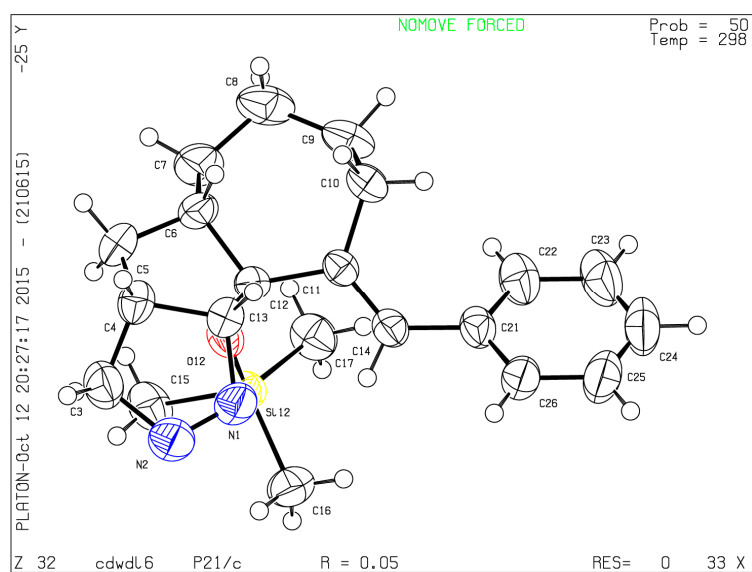
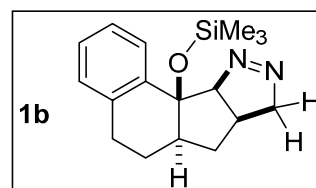
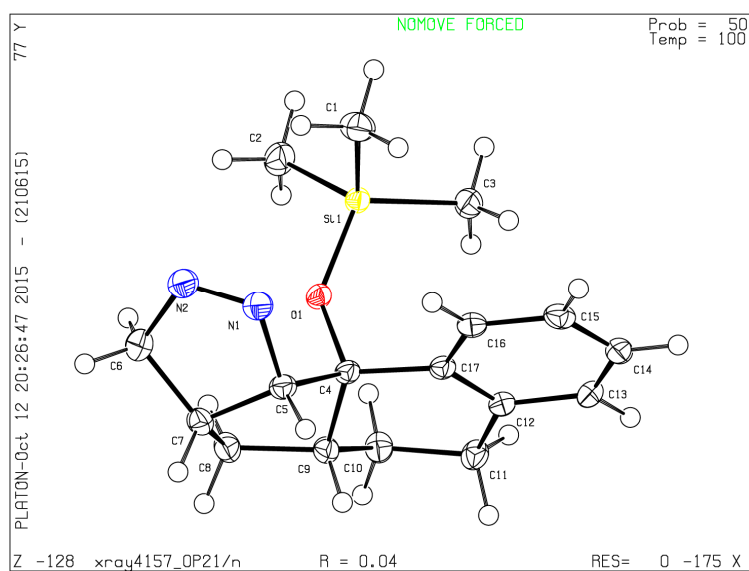
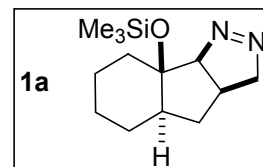
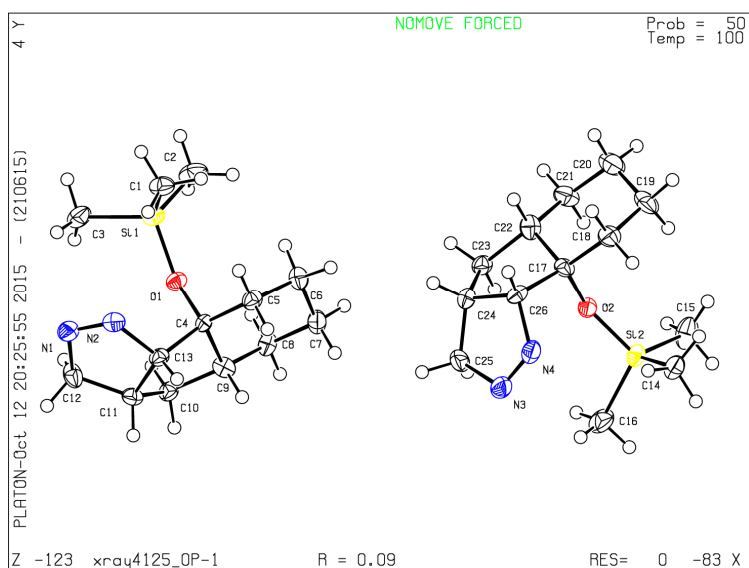


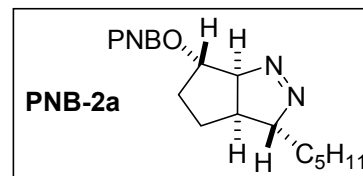
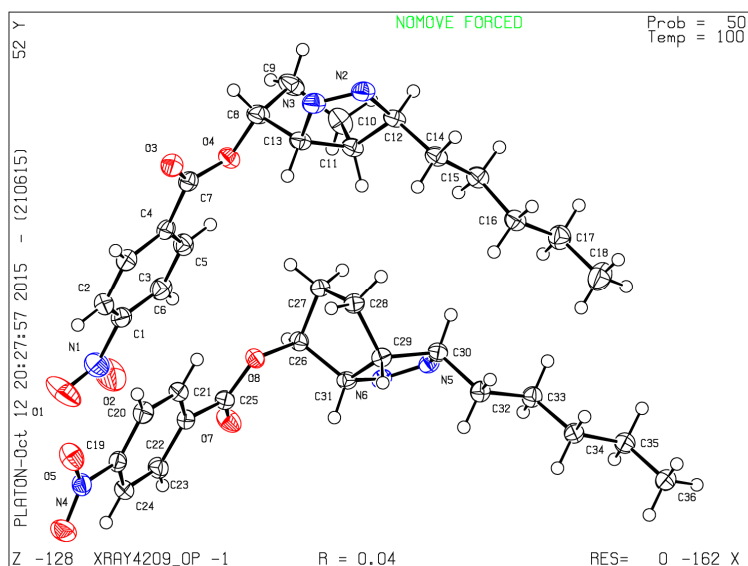






6. ORTEP Diagrams





7. Geometric TSs with Bond Lengths

