

## SUPPORTING INFORMATION

# Hydrosilylation-Promoted Furan Diels–Alder Cycloadditions with Stereoselectivity Controlled by the Silyl Group

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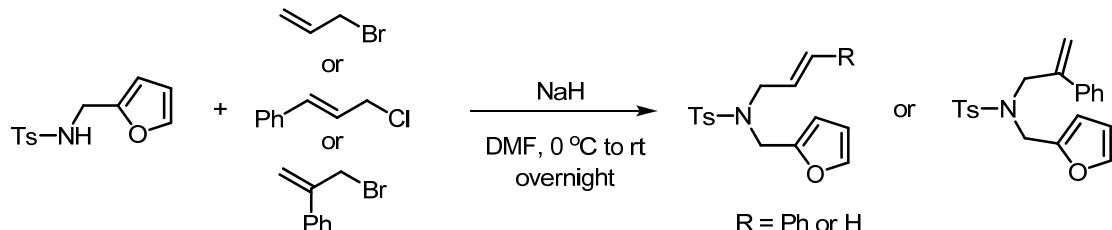
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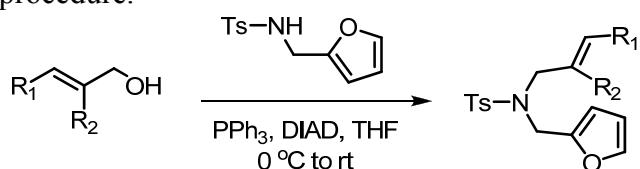
## 1. General Information

Unless otherwise noted, all materials were used as received from commercial sources without further purification. Dry solvents were obtained by distillation from drying reagents according to procedures described in Purification of Laboratory Chemicals (5th Edition) written by Wilfred L.F. Armarego and Christina L.L. Chai (Elsevier, 2003). Analytical thin layer chromatography (TLC) was performed on Huanghai precoated (0.25 mm thickness) silica gel plates with F254 indicator. Visualization was accomplished with UV light (254 nm) or the potassium permanganate stain solution. Flash chromatography was performed with silica gel (32-63  $\mu\text{m}$ ) supplied by Sanpont Group.  $^1\text{H}$  NMR spectra were recorded on a Bruker DRX-400 (400 MHz) spectrometer and chemical shifts were reported in ppm. The peak information was described as: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet; coupling constants in Hz.  $^{13}\text{C}$  NMR spectra were recorded on a Bruker DRX-400 (101 MHz) spectrometer with complete proton decoupling. Chemical shifts of the NMR spectra were calibrated by the literature values of the solvent residual peaks. High-resolution mass spectra (HRMS) were obtained on a Varian 7.0T FTMS (ESI or MALDI).  $\text{B}(\text{C}_6\text{F}_5)_3$  was prepared according to the previous literature.<sup>[1]</sup>

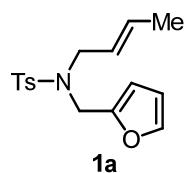
## 2. Preparation of Starting Materials



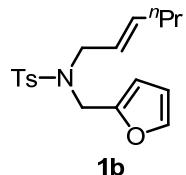
**General procedure A:** The tosylated furfurylamine<sup>[2]</sup> (10 mmol, 1 equiv) was added to a solution of NaH (60 % in mineral oil, 15 mmol, 1.5 equiv) in dry DMF (30 mL). The solution was stirred under argon at room temperature for 1 h, followed by the addition of the corresponding allylic halide (12 mmol, 1.2 equiv). The resulting mixture was stirred at room temperature for 20 h, and then was poured into a mixture of ice and water (60 mL). The mixture was extracted with dichloromethane (3 x 30 mL). The combined organic layers were dried over  $\text{MgSO}_4$ , filtered and concentrated in vacuo. The residue was subjected to column chromatography on silica gel (PE/EA = 20:1 as eluent) to give the corresponding product. Substrates **1g**, **1h** and **1k** were prepared using this procedure.



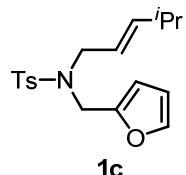
**General procedure B:** The corresponding allylic alcohol (7.2 mmol, 1.2 equiv) and PPh<sub>3</sub> (8.4 mmol, 1.4 equiv) were added to a solution of the tosylated furfurylamine (6 mmol, 1 equiv) in dry THF (20 mL) under argon. Diisopropyl azodicarboxylate (8.4 mmol, 1.4 equiv) was then added dropwise at 0 °C, and the resulting mixture was stirred at room temperature for 5 h. The mixture was concentrated in vacuo. The residue was subjected to column chromatography on silica gel (PE/EA = 20:1 as eluent) to give the corresponding product. Substrates **1a**, **1b**, **1c**, **1d**, **1e**, **1f**, **1i**, **1j**, **1l**, **1m**, **1n**, **1o**, **1p**, **1q**, **1r** were prepared using this procedure. The allylic alcohol precursors for preparation of **1a**<sup>[3]</sup>, **1c**<sup>[4]</sup>, **1d**<sup>[5]</sup>, **1e**<sup>[6]</sup>, **1j**<sup>[7]</sup>, **1m**<sup>[8]</sup>, **1n**<sup>[8]</sup> and **1p**<sup>[8]</sup> had been synthesized and characterized in the previous literatures. The allylic alcohol precursors for preparation of **1l** was prepared according to the previous literature<sup>[9]</sup>, The allylic alcohol precursors for preparation of **1b**, **1f**, **1i**, **1o**, **1q** and **1r** were purchased from commercial sources.



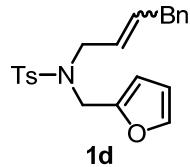
**(E)-N-(But-2-en-1-yl)-N-(furan-2-ylmethyl)-4-methylbenzenesulfonamide (1a).** Colorless oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.62 (d, *J* = 8.3 Hz, 2H), 7.25-7.20 (m, 3H), 6.23 (dd, *J* = 3.1, 1.9 Hz, 1H), 6.11 (d, *J* = 3.1 Hz, 1H), 5.62-5.51 (m, 1H), 5.29-5.20 (m, 1H), 4.36 (s, 2H), 3.69 (d, *J* = 6.7 Hz, 2H), 2.38 (s, 3H), 1.62 (dd, *J* = 6.5, 1.1 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 149.9, 143.1, 142.3, 137.3, 131.0, 129.5, 127.2, 125.1, 110.3, 109.3, 49.0, 42.4, 21.5, 17.7. HRMS (ESI) calcd. for C<sub>16</sub>H<sub>20</sub>NO<sub>3</sub>S<sup>+</sup> (M+H)<sup>+</sup>: 306.1158, Found: 306.1158.



**(E)-N-(Furan-2-ylmethyl)-N-(hex-2-en-1-yl)-4-methylbenzenesulfonamide (1b).** Colorless oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.27-7.22 (m, 3H), 6.25 (dd, *J* = 3.0, 1.9 Hz, 1H), 6.13 (d, *J* = 3.0 Hz, 1H), 5.56 (dt, *J* = 13.8, 6.7 Hz, 1H), 5.32-5.19 (m, 1H), 4.38 (s, 2H), 3.72 (d, *J* = 6.7 Hz, 2H), 2.41 (s, 3H), 1.95 (q, *J* = 7.0 Hz, 2H), 1.43-1.25 (m, 2H), 0.86 (t, *J* = 7.4 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 150.1, 143.1, 142.4, 137.5, 136.4, 129.6, 127.4, 124.0, 110.4, 109.4, 49.1, 42.4, 34.3, 22.3, 21.6, 13.7. HRMS (ESI) calcd. for C<sub>18</sub>H<sub>24</sub>NO<sub>3</sub>S<sup>+</sup> (M+H)<sup>+</sup>: 334.1471, Found: 334.1472.

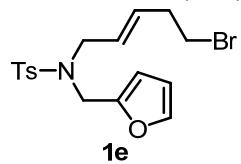


**(E)-N-(Furan-2-ylmethyl)-4-methyl-N-(4-methylpent-2-en-1-yl)benzenesulfonamide (1c).** Colorless oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 (d,  $J = 8.2$  Hz, 2H), 7.28-7.21 (m, 3H), 6.25 (dd,  $J = 3.1, 1.9$  Hz, 1H), 6.13 (d,  $J = 3.1$  Hz, 1H), 5.56-5.46 (m, 1H), 5.23-5.12 (m, 1H), 4.37 (s, 2H), 3.72 (d,  $J = 6.7$  Hz, 2H), 2.41 (s, 3H), 2.32-2.13 (m, 1H), 0.94-0.88 (m, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.0, 143.4, 143.1, 142.4, 137.5, 129.6, 127.3, 120.9, 110.4, 109.4, 49.2, 42.5, 30.8, 22.2, 21.6. HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{24}\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 334.1471, Found: 334.1469.



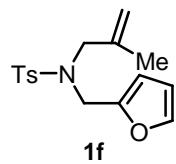
**N-(Furan-2-ylmethyl)-4-methyl-N-(4-phenylbut-2-en-1-yl)benzenesulfonamide (1d).**

Colorless oil.  $E/Z = 8.5:1$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  ( $E$ ): 7.63 (d,  $J = 8.2$  Hz, 2H), 7.31-7.16 (m, 6H), 7.10 (d,  $J = 7.2$  Hz, 2H), 6.24-6.20 (m, 0.89H), 6.11-6.09 (m, 0.89H), 5.78-5.64 (m, 1H), 5.39-5.28 (m, 1H), 4.37 (s, 1.79H), 3.75 (d,  $J = 6.7$  Hz, 1.79H), 3.30 (d,  $J = 6.7$  Hz, 2H), 2.39 (s, 3H). ( $Z$ ) (distinguishable peaks): 6.26-6.24 (m, 0.11H), 6.15-6.12 (m, 0.11H), 4.41 (s, 0.21H), 3.94 (d,  $J = 7.0$  Hz, 0.21H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , signals of the dominant  $E$  isomer)  $\delta$  149.8, 143.1, 142.4, 139.7, 137.3, 134.7, 129.5, 128.6, 128.5, 127.3, 126.2, 125.4, 110.3, 109.4, 48.9, 42.7, 38.7, 21.6. HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{24}\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 382.1471, Found: 382.1470.



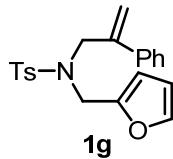
**(E)-N-(5-Bromopent-2-en-1-yl)-N-(furan-2-ylmethyl)-4-methylbenzenesulfonamide (1e).**

White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 (d,  $J = 8.3$  Hz, 2H), 7.30-7.23 (m, 3H), 6.29-6.24 (m, 1H), 6.17 (d,  $J = 2.9$  Hz, 1H), 5.61-5.48 (m, 1H), 5.42-5.34 (m, 1H), 4.40 (s, 2H), 3.74 (d,  $J = 6.5$  Hz, 2H), 3.34 (t,  $J = 6.8$  Hz, 2H), 2.54 (q,  $J = 6.5$  Hz, 2H), 2.42 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.8, 143.3, 142.5, 137.3, 132.2, 129.6, 127.4, 127.3, 110.4, 109.6, 48.8, 42.7, 35.3, 32.2, 21.6. HRMS (ESI) calcd. for  $\text{C}_{17}\text{H}_{21}\text{BrNO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 398.0420, Found: 398.0422.

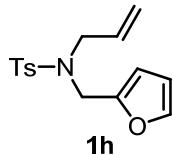


**N-(Furan-2-ylmethyl)-4-methyl-N-(2-methylallyl)benzenesulfonamide (1f).**

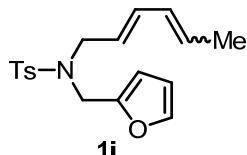
Colorless oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 (d,  $J = 8.2$  Hz, 2H), 7.26-7.16 (m, 3H), 6.24-6.17 (m, 1H), 6.08 (d,  $J = 3.2$  Hz, 1H), 4.91 (d,  $J = 17.3$  Hz, 2H), 4.36 (s, 2H), 3.70 (s, 2H), 2.39 (s, 3H), 1.69 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.7, 143.0, 142.3, 139.9, 137.2, 129.4, 127.3, 114.8, 110.2, 109.7, 53.2, 42.4, 21.5, 19.7. HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{20}\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 306.1158, Found: 306.1157.



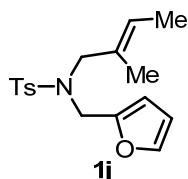
**N-(Furan-2-ylmethyl)-4-methyl-N-(2-phenylallyl)benzenesulfonamide (1g).** White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 (d,  $J = 8.3$  Hz, 2H), 7.42-7.35 (m, 2H), 7.34-7.28 (m, 3H), 7.22 (d,  $J = 8.1$  Hz, 2H), 7.18 (d,  $J = 1.0$  Hz, 1H), 6.21 (dd,  $J = 3.1, 1.9$  Hz, 1H), 6.05 (d,  $J = 3.1$  Hz, 1H), 5.48 (s, 1H), 5.28 (d,  $J = 0.7$  Hz, 1H), 4.35 (s, 2H), 4.25 (s, 2H), 2.41 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.7, 143.2, 142.5, 142.4, 138.6, 136.9, 129.5, 128.5, 128.1, 127.5, 126.6, 116.5, 110.4, 109.8, 50.8, 42.7, 21.6. HRMS (ESI) calcd. for  $\text{C}_{21}\text{H}_{22}\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 368.1315, Found: 368.1313.



**N-Allyl-N-(furan-2-ylmethyl)-4-methylbenzenesulfonamide (1h).** Colorless oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 (d,  $J = 8.3$  Hz, 2H), 7.28-7.23 (m, 3H), 6.25 (dd,  $J = 3.1, 1.9$  Hz, 1H), 6.14 (d,  $J = 3.1$  Hz, 1H), 5.70-5.54 (m, 1H), 5.21-5.16 (m, 1H), 5.16-5.12 (m, 1H), 4.39 (s, 2H), 3.77 (d,  $J = 6.3$  Hz, 2H), 2.40 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.7, 143.2, 142.4, 137.2, 132.5, 129.6, 127.2, 119.2, 110.3, 109.5, 49.6, 42.7, 21.5. HRMS (ESI) calcd. for  $\text{C}_{15}\text{H}_{18}\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 292.1002, Found: 292.1000. This compound was characterized by previous literature<sup>[10]</sup>.

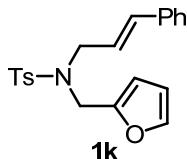


**N-(Furan-2-ylmethyl)-N-((2E)-hexa-2,4-dien-1-yl)-4-methylbenzenesulfonamide (1i).** Colorless oil.  $E/Z = 5.1:1$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  ( $E$ ): 7.65 (d,  $J = 7.1$  Hz, 2H), 7.28-7.21 (m, 3H), 6.31-6.21 (m, 1H), 6.17-6.12 (m, 1H), 6.10-5.90 (m, 1.85H), 5.72-5.61 (m, 0.84H), 5.35-5.26 (m, 0.84H), 4.38 (s, 2H), 3.78 (d,  $J = 6.8$  Hz, 1.67H), 2.41 (s, 3H), 1.74 (d,  $J = 6.7$  Hz, 3H). ( $Z$ ) (distinguishable peaks): 5.54-5.37 (m, 0.33H), 5.18-5.02 (m, 0.14H), 3.83 (d,  $J = 6.9$  Hz, 0.33H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , signals of the dominant  $E$  isomer)  $\delta$  149.9, 143.2, 142.5, 137.4, 135.1, 130.6, 130.5, 129.6, 127.4, 124.1, 110.4, 109.5, 48.9, 42.5, 21.6, 18.2. HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{22}\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 332.1315, Found: 332.1314.

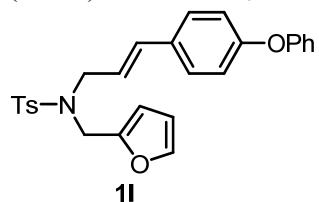


**(E)-N-(Furan-2-ylmethyl)-4-methyl-N-(2-methylbut-2-en-1-yl)benzenesulfonamide (1j).** Colorless oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 (d,  $J = 8.2$  Hz, 2H), 7.21 (d,  $J = 8.2$  Hz, 2H), 7.18-7.13 (m, 1H), 6.20 (dd,  $J = 3.0, 1.8$  Hz, 1H), 6.04 (d,  $J = 3.0$  Hz, 1H), 5.39 (q,  $J = 6.6$  Hz, 1H), 4.31 (s, 2H), 3.66 (s, 2H), 2.38 (s, 3H), 1.59 (d,  $J = 6.6$

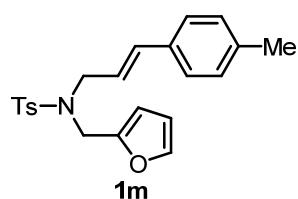
Hz, 3H), 1.55 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.1, 142.9, 142.2, 137.3, 130.4, 129.4, 127.3, 124.7, 110.2, 109.4, 55.3, 42.1, 21.6, 13.6. HRMS (ESI) calcd. for  $\text{C}_{17}\text{H}_{22}\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 320.1315, Found: 320.1312.



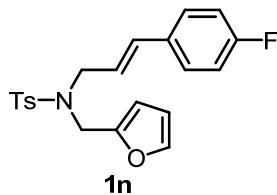
**N-Cinnamyl-N-(furan-2-ylmethyl)-4-methylbenzenesulfonamide (1k).** White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (d,  $J = 8.3$  Hz, 2H), 7.35-7.18 (m, 8H), 6.43 (d,  $J = 15.9$  Hz, 1H), 6.26 (dd,  $J = 3.1, 1.9$  Hz, 1H), 6.17 (d,  $J = 3.1$  Hz, 1H), 5.96 (dt,  $J = 15.9, 6.7$  Hz, 1H), 4.43 (s, 2H), 3.93 (d,  $J = 6.7$  Hz, 2H), 2.41 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.9, 143.3, 142.6, 137.3, 136.3, 134.3, 129.7, 128.7, 128.0, 127.4, 126.6, 123.7, 110.5, 109.6, 49.3, 42.9, 21.6. HRMS (ESI) calcd. for  $\text{C}_{21}\text{H}_{22}\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 368.1315, Found: 368.1316.



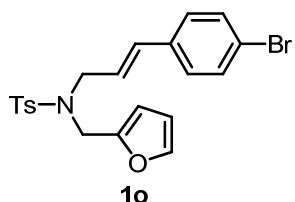
**(E)-N-(Furan-2-ylmethyl)-4-methyl-N-(3-(4-phenoxyphenyl)allyl)benzenesulfonamide (1l).** Colorless oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (d,  $J = 8.2$  Hz, 2H), 7.33 (t,  $J = 8.0$  Hz, 2H), 7.28-7.21 (m, 5H), 7.11 (t,  $J = 7.4$  Hz, 1H), 7.00 (d,  $J = 7.7$  Hz, 2H), 6.93 (d,  $J = 8.6$  Hz, 2H), 6.40 (d,  $J = 15.8$  Hz, 1H), 6.26 (dd,  $J = 3.0, 1.9$  Hz, 1H), 6.16 (d,  $J = 3.0$  Hz, 1H), 5.87 (dt,  $J = 15.8, 6.8$  Hz, 1H), 4.43 (s, 2H), 3.92 (d,  $J = 6.8$  Hz, 2H), 2.40 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  157.2, 157.0, 149.9, 143.3, 142.6, 137.3, 133.5, 131.5, 129.9, 129.6, 127.9, 127.4, 123.6, 122.7, 119.1, 118.9, 110.4, 109.6, 49.4, 42.9, 21.6. HRMS (ESI) calcd. for  $\text{C}_{27}\text{H}_{25}\text{NO}_4\text{SNa}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 482.1397, Found: 482.1394.



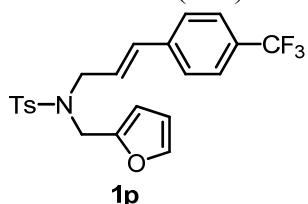
**(E)-N-(Furan-2-ylmethyl)-4-methyl-N-(3-(p-tolyl)allyl)benzenesulfonamide (1m).** White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (d,  $J = 8.2$  Hz, 2H), 7.29-7.23 (m, 3H), 7.17 (d,  $J = 8.1$  Hz, 2H), 7.11 (d,  $J = 8.1$  Hz, 2H), 6.40 (d,  $J = 15.8$  Hz, 1H), 6.26 (dd,  $J = 3.1, 1.9$  Hz, 1H), 6.16 (d,  $J = 3.1$  Hz, 1H), 5.90 (dt,  $J = 15.8, 6.8$  Hz, 1H), 4.43 (s, 2H), 3.92 (d,  $J = 6.8$  Hz, 2H), 2.42 (s, 3H), 2.33 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.9, 143.3, 142.6, 137.9, 137.4, 134.3, 133.5, 129.6, 129.4, 127.4, 126.5, 122.6, 110.4, 109.6, 49.4, 42.8, 21.6, 21.3. HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{24}\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 382.1471, Found: 382.1473.



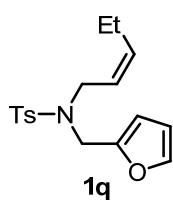
**(E)-N-(3-(4-Fluorophenyl)allyl)-N-(furan-2-ylmethyl)-4-methylbenzenesulfonamide (1n).** White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (d,  $J = 8.3$  Hz, 2H), 7.30-7.18 (m, 5H), 7.03-6.93 (m, 2H), 6.39 (d,  $J = 15.8$  Hz, 1H), 6.28-6.24 (m, 1H), 6.16 (d,  $J = 3.0$  Hz, 1H), 5.88 (dt,  $J = 15.8, 6.7$  Hz, 1H), 4.42 (s, 2H), 3.92 (d,  $J = 6.7$  Hz, 2H), 2.41 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  162.5 (d,  $J = 247.3$  Hz), 149.8, 143.3, 142.6, 137.2, 132.9, 132.5 (d,  $J = 3.1$  Hz), 129.6, 128.1 (d,  $J = 8.0$  Hz), 127.4, 123.6 (d,  $J = 1.9$  Hz), 115.5 (d,  $J = 21.6$  Hz), 110.4, 109.6, 49.3, 43.0, 21.6. HRMS (ESI) calcd. for  $\text{C}_{21}\text{H}_{21}\text{FNO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 386.1221, Found: 386.1222.



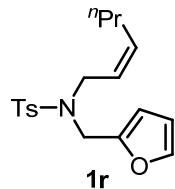
**(E)-N-(3-(4-Bromophenyl)allyl)-N-(furan-2-ylmethyl)-4-methylbenzenesulfonamide (1o).** White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 (d,  $J = 8.1$  Hz, 2H), 7.39 (d,  $J = 8.3$  Hz, 2H), 7.33-7.19 (m, 3H), 7.11 (d,  $J = 8.3$  Hz, 2H), 6.35 (d,  $J = 15.9$  Hz, 1H), 6.29-6.20 (m, 1H), 6.18-6.12 (m, 1H), 5.95 (dt,  $J = 15.7, 6.6$  Hz, 1H), 4.41 (s, 2H), 3.91 (d,  $J = 6.6$  Hz, 2H), 2.39 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.7, 143.3, 142.6, 137.1, 135.2, 132.7, 131.6, 129.6, 128.0, 127.3, 124.7, 121.6, 110.4, 109.6, 49.2, 43.1, 21.5. HRMS (ESI) calcd. for  $\text{C}_{21}\text{H}_{21}\text{BrNO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 446.0420, Found: 446.0418.



**(E)-N-(Furan-2-ylmethyl)-4-methyl-N-(3-(4-(trifluoromethyl)phenyl)allyl)benzenesulfonamide (1p).** White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J = 8.0$  Hz, 2H), 7.55 (d,  $J = 8.0$  Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 7.29-7.25 (m, 3H), 6.46 (d,  $J = 15.9$  Hz, 1H), 6.28-6.24 (m, 1H), 6.20-6.15 (m, 1H), 6.13-6.01 (m, 1H), 4.43 (s, 2H), 3.95 (d,  $J = 6.4$  Hz, 2H), 2.41 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.7, 143.5, 142.7, 139.9, 137.2, 132.5, 129.7 (q,  $J = 32.5$  Hz), 129.7, 127.5, 126.9, 126.7, 125.6 (q,  $J = 3.8$  Hz), 124.2 (q,  $J = 271.9$  Hz), 110.6, 109.8, 49.3, 43.4, 21.6. HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{21}\text{F}_3\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 436.1189, Found: 436.1190.



**(Z)-N-(Furan-2-ylmethyl)-4-methyl-N-(pent-2-en-1-yl)benzenesulfonamide (1q).** Colorless oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 (d,  $J = 8.3$  Hz, 2H), 7.29-7.21 (m, 3H), 6.26 (dd,  $J = 3.2, 1.9$  Hz, 1H), 6.14 (d,  $J = 3.2$  Hz, 1H), 5.59-5.48 (m, 1H), 5.23-5.12 (m, 1H), 4.38 (s, 2H), 3.83 (d,  $J = 7.0$  Hz, 2H), 2.40 (s, 3H), 1.96 (pd,  $J = 7.5, 1.3$  Hz, 2H), 0.92 (t,  $J = 7.5$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.0, 143.1, 142.4, 137.3, 136.6, 129.5, 127.3, 122.9, 110.4, 109.2, 43.7, 42.7, 21.5, 20.5, 14.1. HRMS (ESI) calcd. for  $\text{C}_{17}\text{H}_{22}\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 320.1315, Found: 320.1313.



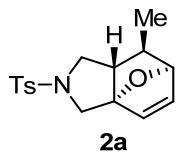
**(Z)-N-(Furan-2-ylmethyl)-N-(hex-2-en-1-yl)-4-methylbenzenesulfonamide (1r).** Colorless oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 (d,  $J = 8.3$  Hz, 2H), 7.30-7.19 (m, 3H), 6.26 (dd,  $J = 3.1, 1.9$  Hz, 1H), 6.14 (d,  $J = 3.1$  Hz, 1H), 5.61-5.45 (m, 1H), 5.27-5.16 (m, 1H), 4.38 (s, 2H), 3.84 (d,  $J = 7.0$  Hz, 2H), 2.40 (s, 3H), 1.93 (q,  $J = 7.0$  Hz, 2H), 1.39-1.23 (m, 2H), 0.85 (t,  $J = 7.4$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.9, 143.1, 142.3, 137.3, 134.8, 129.5, 127.2, 123.7, 110.3, 109.2, 43.7, 42.6, 29.1, 22.6, 21.5, 13.7. HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{24}\text{NO}_3\text{S}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 334.1471, Found: 334.1473.

### 3. Optimization of the Reaction Conditions

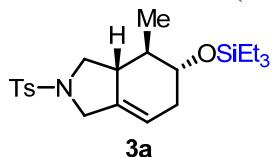
**General procedure:** In a glovebox, hydrosilane (0.15 mmol, 1.5 equiv) and **1a** (0.1 mmol, 1 equiv) were dissolved in dry toluene (0.25 mL) in an 8 mL vial.  $\text{B}(\text{C}_6\text{F}_5)_3$  (0.005 mmol, 5 mol %) was then added before the vial was capped and closed tightly. The reaction mixture was then stirred at 120 °C for 24 h. After being allowed to cool to room temperature, one drop of  $\text{Et}_3\text{N}$  was added to the solution. After evaporation of the solvent in vacuo, the residue was analyzed with  $^1\text{H}$  NMR spectroscopy to determine the yields of products using  $\text{CH}_2\text{Br}_2$  (5  $\mu\text{L}$ , 0.071 mmol) as the internal standard.

### 4. Substrate Scope

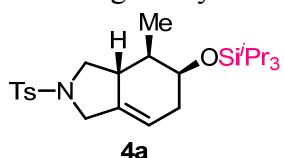
**General procedure:** In a glovebox,  $i\text{Pr}_3\text{SiH}$  (61  $\mu\text{L}$ , 0.3 mmol, 1.5 equiv) or  $\text{Et}_3\text{SiH}$  (48  $\mu\text{L}$ , 0.3 mmol, 1.5 equiv) and a furan substrate (0.2 mmol, 1 equiv) were dissolved in a dry solvent (0.5 mL of toluene or DCE) in an 8 mL vial.  $\text{B}(\text{C}_6\text{F}_5)_3$  (5.1 mg, 0.01 mmol, 5 mol %) was then added before the vial was capped and closed tightly. The reaction mixture was stirred at the corresponding temperature for 24 h. After being allowed to cool to room temperature, one drop of  $\text{Et}_3\text{N}$  was added to the solution. After evaporation of the solvent in vacuo, the residue was subjected to column chromatography on silica gel to give the corresponding product. The relative stereochemistry was determined by NOE experiment, X-ray crystallography or analogy to that of similar products.



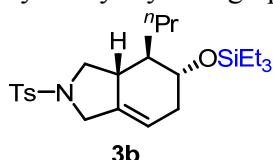
**(±)-7-Methyl-2-tosyl-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole (2a).** Reaction conditions: no  $B(C_6F_5)_3$ , no hydrosilane, toluene, 120 °C. White solid (4 mg, 7% yield).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.70 (d,  $J = 7.9$  Hz, 2H), 7.31 (d,  $J = 7.9$  Hz, 2H), 6.41 (d,  $J = 5.7$  Hz, 1H), 6.35-6.28 (m, 1H), 4.78-4.71 (m, 1H), 3.97-3.84 (m, 2H), 3.42 (d,  $J = 12.1$  Hz, 1H), 2.72 (t,  $J = 9.3$  Hz, 1H), 2.41 (s, 3H), 2.10-2.01 (m, 1H), 1.67-1.58 (m, 1H), 0.81 (d,  $J = 7.0$  Hz, 3H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  143.6, 135.3, 135.3, 133.6, 129.8, 127.5, 96.0, 83.8, 53.0, 51.0, 49.7, 38.8, 21.6, 16.5. HRMS (ESI) calcd. for  $C_{16}H_{20}NO_3S^+$  ( $M+H$ ) $^+$ : 306.1158, Found: 306.1158.



**(±)-4-Methyl-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3a).** Reaction conditions:  $Et_3SiH$  (1.5 equiv),  $B(C_6F_5)_3$  (5 mol %), toluene, 120 °C. White solid (38 mg, 45% yield).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.69 (d,  $J = 8.0$  Hz, 2H), 7.32 (d,  $J = 8.0$  Hz, 2H), 5.37 (s, 1H), 3.99-3.91 (m, 1H), 3.82-3.76 (m, 1H), 3.67-3.59 (m, 1H), 3.52-3.44 (m, 1H), 2.59 (t,  $J = 9.8$  Hz, 1H), 2.42 (s, 3H), 2.38-2.18 (m, 2H), 2.01-1.90 (m, 1H), 1.30-1.22 (m, 1H), 0.99-0.90 (m, 12H), 0.63-0.52 (m, 6H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  143.6, 136.1, 133.8, 129.9, 127.7, 118.1, 72.6, 53.5, 51.1, 46.3, 40.3, 35.9, 21.7, 16.3, 7.0, 5.1. HRMS (MALDI) calcd. for  $C_{22}H_{35}NNaO_3SSi^+$  ( $M+Na$ ) $^+$ : 444.1999, Found: 444.2002. The relative stereochemistry of this compound was assigned by NOE experiment.

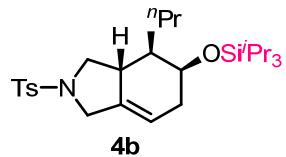


**(±)-4-Methyl-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4a).** Reaction conditions:  $iPr_3SiH$  (1.5 equiv),  $B(C_6F_5)_3$  (5 mol %), toluene, 110 °C. White solid (79 mg, 85% yield).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.70(d,  $J = 8.0$  Hz, 2H), 7.30(d,  $J = 8.0$  Hz, 2H), 5.31 (s, 1H), 4.09-3.95 (m, 2H), 3.86-3.79 (m, 1H), 3.67 (d,  $J = 13.5$  Hz, 1H), 2.66-2.54 (m, 1H), 2.55-2.38 (m, 4H), 2.27-2.07 (m, 2H), 1.27-1.17 (m, 1H), 1.12-0.84 (m, 24H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  143.4, 136.6, 133.9, 129.8, 127.6, 115.8, 70.2, 53.4, 51.4, 40.2, 38.5, 35.2, 21.6, 18.3, 18.2, 17.2, 12.9. HRMS (MALDI) calcd. for  $C_{25}H_{41}NNaO_3SSi^+$  ( $M+Na$ ) $^+$ : 486.2469, Found: 486.2473. The structure and relative stereochemistry of this compound was determined by X-ray crystallography and NOE experiment.



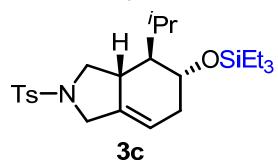
**(±)-4-Propyl-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole**

**(3b).** Reaction conditions: Et<sub>3</sub>SiH (2.0 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol%), DCE, 120 °C. White solid (49 mg, 54% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.69 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.32- 5.38 (m, 1H), 3.92 (d, *J* = 13.3 Hz, 1H), 3.85-3.79 (m, 1H), 3.66- 3.55 (m, 2H), 2.60 (dd, *J* = 10.5, 9.3 Hz, 1H), 2.43 (s, 3H), 2.39-2.25 (m, 2H), 2.00-1.90 (m, 1H), 1.55-1.47 (m, 1H), 1.40-1.19 (m, 4H), 0.96-0.86 (m, 12H), 0.57 (q, *J* = 7.9 Hz, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.6, 136.4, 133.8, 129.8, 127.7, 117.9, 70.8, 53.7, 50.8, 44.7, 44.1, 36.1, 32.5, 21.7, 19.7, 14.8, 7.0, 5.2. HRMS (MALDI) calcd. for C<sub>24</sub>H<sub>39</sub>NNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 472.2312, Found: 472.2316. The structure and relative stereochemistry of this compound was determined by X-ray crystallography.



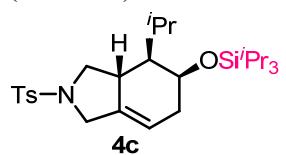
**(±)-4-Propyl-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole**

**e (4b).** Reaction conditions: iPr<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), toluene, 110 °C. White solid (91 mg, 93% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 5.31 (s, 1H), 4.18-4.13 (m, 1H), 4.00 (d, *J* = 13.5 Hz, 1H), 3.86-3.80 (m, 1H), 3.67 (d, *J* = 13.5 Hz, 1H), 2.68-2.56 (m, 1H), 2.55-2.45 (m, 1H), 2.41 (s, 3H), 2.17-2.10 (m, 2H), 1.56-1.44 (m, 1H), 1.44-1.29 (m, 1H), 1.20-1.10 (m, 2H), 1.07-0.90 (m, 22H), 0.86 (t, *J* = 7.0 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.4, 136.9, 133.9, 129.8, 127.6, 115.8, 66.6, 53.6, 51.3, 43.5, 39.7, 35.2, 32.9, 21.6, 20.4, 18.3, 18.2, 14.4, 13.0. HRMS (MALDI) calcd. for C<sub>27</sub>H<sub>45</sub>NNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 514.2782, Found: 514.2783.



**(±)-4-Isopropyl-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole**

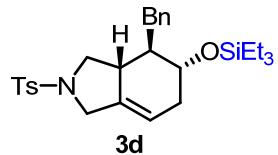
**(3c).** Reaction conditions: Et<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), toluene, 120 °C. White solid (48 mg, 53% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 5.38-5.33 (m, 1H), 3.93-3.81 (m, 2H), 3.67 (td, *J* = 9.7, 5.8 Hz, 1H), 3.58 (d, *J* = 13.4 Hz, 1H), 2.67-2.56 (m, 1H), 2.43 (s, 3H), 2.40-2.20 (m, 3H), 2.02-1.91 (m, 1H), 1.27-1.17 (m, 1H), 0.95-0.89 (m, 12H), 0.81 (d, *J* = 7.0 Hz, 3H), 0.57 (q, *J* = 7.8 Hz, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.6, 136.8, 133.9, 129.9, 127.7, 117.5, 69.3, 54.0, 50.3, 50.2, 40.2, 36.2, 25.3, 21.9, 21.7, 17.0, 7.0, 5.3. HRMS (MALDI) calcd. for C<sub>24</sub>H<sub>39</sub>NNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 472.2312, Found: 472.2316.



**(±)-4-Isopropyl-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoin-**

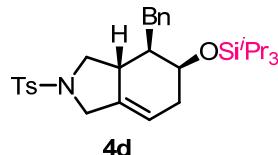
**dole (4c).** Reaction conditions: iPr<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), toluene,

120 °C. Colorless oil. (42 mg, 43% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 7.7$  Hz, 2H), 7.31 (d,  $J = 7.7$  Hz, 2H), 5.33 (s, 1H), 4.31-4.18 (m, 1H), 4.02-3.88 (m, 2H), 3.67 (d,  $J = 13.5$  Hz, 1H), 2.73-2.62 (m, 1H), 2.58-2.49 (m, 1H), 2.41 (s, 3H), 2.18-2.09 (m, 2H), 1.82-1.68 (m, 1H), 1.36-1.25 (m, 1H), 1.00-0.88 (m, 27H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.5, 137.4, 134.0, 129.8, 127.6, 115.9, 67.9, 54.4, 50.8, 49.7, 38.2, 35.7, 29.8, 21.7, 21.6, 21.5, 18.4, 18.2, 13.3. HRMS (MALDI) calcd. for  $\text{C}_{27}\text{H}_{45}\text{NNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 514.2782, Found: 514.2785.



**(±)-4-Benzyl-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole**

**(3d).** Reaction conditions:  $\text{Et}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), toluene, 120 °C. White solid (41 mg, 41% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.50 (d,  $J = 7.9$  Hz, 2H), 7.34-7.22 (m, 5H), 7.15 (d,  $J = 7.0$  Hz, 2H), 5.38 (s, 1H), 3.78 (d,  $J = 13.2$  Hz, 1H), 3.67-3.59 (m, 1H), 3.53 (d,  $J = 13.4$  Hz, 1H), 3.31 (dd,  $J = 13.6, 2.5$  Hz, 1H), 2.95-2.88 (m, 1H), 2.43 (s, 3H), 2.41-2.32 (m, 1H), 2.25 (dd,  $J = 13.4, 9.7$  Hz, 1H), 2.16-2.01 (m, 3H), 1.66-1.57 (m, 1H), 0.97 (t,  $J = 7.9$  Hz, 9H), 0.62 (q,  $J = 7.9$  Hz, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.4, 140.6, 136.4, 133.9, 129.7, 129.4, 128.5, 127.7, 126.5, 117.9, 71.3, 53.4, 50.3, 47.3, 44.6, 37.6, 35.6, 21.7, 7.1, 5.4. HRMS (MALDI) calcd. for  $\text{C}_{28}\text{H}_{39}\text{NNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 520.2312, Found: 520.2315.

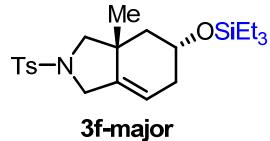


**(±)-4-Benzyl-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4d).** Reaction conditions:  $\text{iPr}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), toluene, 110 °C. White solid (90 mg, 84% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64 (d,  $J = 8.0$  Hz, 2H), 7.34-7.22 (m, 5H), 7.12 (d,  $J = 7.2$  Hz, 2H), 5.34 (s, 1H), 4.04-3.92 (m, 2H), 3.66 (d,  $J = 13.7$  Hz, 1H), 3.51-3.44 (m, 1H), 2.79 (dd,  $J = 13.8, 8.4$  Hz, 1H), 2.63 (dd,  $J = 13.8, 6.4$  Hz, 1H), 2.56-2.48 (m, 1H), 2.44-2.38 (m, 4H), 2.18-2.08 (m, 2H), 1.51-1.43 (m, 1H), 1.10-0.94 (m, 21H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.4, 140.2, 136.9, 133.8, 129.7, 129.1, 128.5, 127.6, 126.4, 116.0, 67.4, 53.4, 51.1, 45.7, 39.5, 37.7, 35.1, 21.7, 18.4, 18.3, 13.1. HRMS (MALDI) calcd. for  $\text{C}_{31}\text{H}_{45}\text{NNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 562.2782, Found: 562.2785.



**(±)-4-(2-Bromoethyl)-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4e).** Reaction conditions:  $\text{iPr}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), toluene, 110 °C. Colorless oil (69 mg, 62% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71

(d,  $J = 8.1$  Hz, 2H), 7.32 (d,  $J = 8.1$  Hz, 2H), 5.38-5.33 (m, 1H), 4.17-4.13 (m, 1H), 4.03 (d,  $J = 13.5$  Hz, 1H), 3.86-3.79 (m, 1H), 3.67 (d,  $J = 13.5$  Hz, 1H), 3.50-3.42 (m, 1H), 3.42-3.34 (m, 1H), 2.66 (dd,  $J = 11.1, 8.9$  Hz, 1H), 2.60-2.50 (m, 1H), 2.42 (s, 3H), 2.24-2.17 (m, 2H), 2.16-2.07 (m, 1H), 1.84-1.73 (m, 1H), 1.38 (td,  $J = 9.5, 3.7$  Hz, 1H), 1.03-0.94 (m, 21H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.6, 136.5, 133.7, 129.8, 127.6, 115.9, 66.3, 53.1, 51.2, 41.9, 39.1, 34.9, 33.7, 31.5, 21.7, 18.3, 18.2, 13.0. HRMS (MALDI) calcd. for  $\text{C}_{26}\text{H}_{43}\text{BrNO}_3\text{SSi}^+$  ( $\text{M}+\text{H}$ ) $^+$ : 556.1911, Found: 556.1915.



**( $\pm$ )-3a-Methyl-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3f).**

Reaction conditions:  $\text{Et}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol%), DCE, 110 °C. Colorless oil (77 mg, 91% yield), dr = 8.2:1.0. Major:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J = 8.2$  Hz, 2H), 7.30 (d,  $J = 8.2$  Hz, 2H), 5.32-5.28 (m, 1H), 4.03-3.93 (m, 2H), 3.64 (dd,  $J = 12.9, 1.1$  Hz, 1H), 3.39 (d,  $J = 8.9$  Hz, 1H), 2.70 (d,  $J = 8.9$  Hz, 1H), 2.41 (s, 3H), 2.35-2.25 (m, 1H), 1.94-1.84 (m, 1H), 1.78 (dd,  $J = 11.9, 3.6$  Hz, 1H), 1.27 (t,  $J = 11.9$  Hz, 1H), 0.99 (s, 3H), 0.92 (t,  $J = 7.9$  Hz, 9H), 0.56 (q,  $J = 7.9$  Hz, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.5, 139.2, 134.1, 129.7, 127.5, 118.0, 65.4, 61.5, 49.9, 42.7, 42.5, 35.4, 24.5, 21.6, 6.9, 4.9. Minor (distinguishable peaks):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  5.35 (s, 1H), 3.32 (d,  $J = 8.8$  Hz, 1H), 1.46-1.38 (m, 1H), 1.03 (s, 3H). HRMS (MALDI) calcd. for  $\text{C}_{22}\text{H}_{35}\text{NNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 444.1999, Found: 444.2002. The relative stereochemistry of this major compound was assigned by NOE experiment.



**( $\pm$ )-3a-Methyl-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4f).**

Reaction conditions:  $^i\text{Pr}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), toluene, 110 °C. Colorless oil (85 mg, 92% yield), dr = 3.3:1.0. Major:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 (d,  $J = 8.1$  Hz, 2H), 7.30 (d,  $J = 8.1$  Hz, 2H), 5.38-5.32 (m, 1H), 4.13-4.05 (m, 1H), 4.02-3.95 (m, 1H), 3.72 (d,  $J = 12.5$  Hz, 1H), 3.33 (d,  $J = 8.9$  Hz, 1H), 2.76 (d,  $J = 8.9$  Hz, 1H), 2.41 (s, 3H), 2.30-2.20 (m, 1H), 2.12-2.02 (m, 1H), 1.81 (dd,  $J = 13.6, 5.2$  Hz, 1H), 1.45 (dd,  $J = 13.6, 3.5$  Hz, 1H), 1.07-0.96 (m, 24H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.4, 139.4, 134.5, 129.7, 127.5, 117.0, 65.9, 62.0, 50.5, 40.0, 39.9, 34.3, 25.3, 21.6, 18.2, 18.1, 12.3. HRMS (MALDI) calcd. for  $\text{C}_{25}\text{H}_{41}\text{NNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 486.2469, Found: 486.2470. The relative stereochemistry of this compound was assigned by NOE experiment.



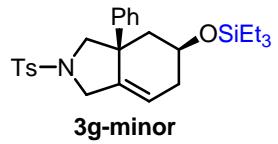
Minor:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 (d,  $J = 8.1$  Hz, 2H), 7.31 (d,  $J = 8.1$  Hz, 2H), 5.34-5.30 (m, 1H), 4.16-4.06 (m, 1H), 3.99 (dd,  $J = 13.0, 2.6$  Hz 1H), 3.65 (d,  $J = 13.0$

Hz, 1H), 3.41 (d,  $J$  = 8.9 Hz, 1H), 2.72 (d,  $J$  = 8.9 Hz, 1H), 2.45-2.34 (m, 4H), 1.97-1.85 (m, 2H), 1.32-1.25 (m, 1H), 1.06-1.02 (m, 2H), 1.00 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.5, 139.4, 134.6, 129.8, 127.6, 118.1, 65.7, 61.6, 50.1, 42.8, 42.7, 35.8, 24.6, 21.6, 18.2, 12.5. HRMS (MALDI) calcd. for  $\text{C}_{25}\text{H}_{41}\text{NNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 486.2469, Found: 486.2472.



**( $\pm$ )-3a-Phenyl-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3g).**

Reaction conditions:  $\text{Et}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), toluene, 120 °C. White solid (62 mg, 64% yield), dr = 6.8:1.0. Major:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.39 (d,  $J$  = 8.1 Hz, 2H), 7.19-7.12 (m, 3H), 7.08-7.01 (m, 4H), 5.76 (s, 1H), 4.04 (d,  $J$  = 9.7 Hz, 1H), 3.93 (dd,  $J$  = 12.9, 2.4 Hz, 1H), 3.83 (d,  $J$  = 12.9 Hz, 1H), 3.49-3.39 (m, 1H), 3.19 (d,  $J$  = 9.7 Hz, 1H), 2.37-2.28 (m, 4H), 2.09 (dd,  $J$  = 11.7, 3.0 Hz, 1H), 2.06-1.95 (m, 1H), 1.58 (t,  $J$  = 11.7 Hz, 1H), 0.71 (t,  $J$  = 7.9 Hz, 9H), 0.30 (q,  $J$  = 7.9 Hz, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.9, 143.0, 136.9, 133.9, 129.4, 128.4, 127.1, 126.8, 126.6, 122.4, 64.7, 62.2, 52.0, 50.8, 44.4, 35.3, 21.5, 6.6, 4.6. HRMS (MALDI) calcd. for  $\text{C}_{27}\text{H}_{37}\text{NNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 506.2156, Found: 506.2158. The relative stereochemistry of this compound was assigned by NOE experiment.



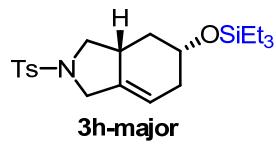
Minor:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.35 (d,  $J$  = 8.2 Hz, 2H), 7.10-7.01 (m, 7H), 5.82-5.77 (m, 1H), 4.02 (d,  $J$  = 9.5 Hz, 1H), 3.97-3.85 (m, 3H), 3.19 (d,  $J$  = 9.5 Hz, 1H), 2.37-2.24 (m, 4H), 2.15-2.01 (m, 2H), 1.78 (dd,  $J$  = 13.5, 3.1 Hz, 1H), 0.73 (t,  $J$  = 7.9 Hz, 9H), 0.26 (q,  $J$  = 7.9 Hz, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  145.4, 142.9, 137.1, 134.5, 129.4, 128.1, 127.1, 126.6, 125.8, 121.6, 65.5, 62.7, 51.4, 48.6, 42.0, 34.5, 21.5, 6.8, 4.5. HRMS (ESI) calcd. for  $\text{C}_{27}\text{H}_{37}\text{NNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 506.2156, Found: 506.2160.



**( $\pm$ )-3a-Phenyl-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4g).**

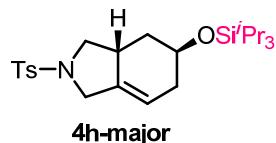
Reaction conditions:  $^i\text{Pr}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), toluene, 110 °C. White solid (95 mg, 90% yield), dr = 8.4:1.0. Major:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.37 (d,  $J$  = 7.9 Hz, 2H), 7.10-7.02 (m, 7H), 5.84-5.78 (m, 1H), 4.07-3.97 (m, 2H), 3.90-3.85 (m, 2H), 3.19 (d,  $J$  = 9.5 Hz, 1H), 2.39-2.29 (m, 4H), 2.15-2.03 (m, 2H), 1.89 (dd,  $J$  = 13.7, 3.5 Hz, 1H), 0.91-0.78 (m, 21H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  145.1, 142.9, 137.3, 134.5, 129.4, 128.4, 127.1, 126.4, 126.0, 121.6, 66.2, 62.0, 51.3, 49.0, 42.4, 34.5, 21.5, 18.1, 18.0, 12.1. Minor (distinguishable peaks):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 (d,  $J$  = 8.2 Hz, 2H), 5.78-5.75 (m, 1H), 4.07 (d,  $J$  = 10.1 Hz, 1H),

1.82 (dd,  $J$  = 13.6, 3.1 Hz, 1H), 1.62-1.54 (m, 1H). HRMS (MALDI) calcd. for  $C_{30}H_{43}NNaO_3SSi^+$  ( $M+Na$ ) $^+$ : 548.2625, Found: 548.2630. The relative stereochemistry of this major compound was assigned by NOE experiment.



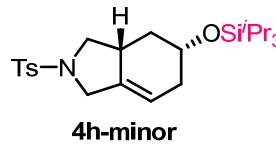
**( $\pm$ )-2-Tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3h).**

Reaction conditions: Et<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), DCE, 80 °C. White solid (50 mg, 61% yield), dr = 12.0:1.0. Major: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.69 (d,  $J$  = 8.2 Hz, 2H), 7.31 (d,  $J$  = 8.2 Hz, 2H), 5.43-5.38 (m, 1H), 3.96-3.89 (m, 1H), 3.88-3.79 (m, 1H), 3.78-3.68 (m, 1H), 3.62 (d,  $J$  = 13.4 Hz, 1H), 2.62-2.52 (m, 2H), 2.42 (s, 3H), 2.33-2.23 (m, 1H), 2.01-1.87 (m, 2H), 1.18-1.08 (m, 1H), 0.92 (t,  $J$  = 7.9 Hz, 9H), 0.56 (q,  $J$  = 7.9 Hz, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.6, 136.3, 133.8, 129.8, 127.7, 118.4, 67.7, 53.9, 50.6, 39.4, 35.8, 35.2, 21.7, 6.9, 4.9. Minor (distinguishable peaks): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 5.37 (s, 1H), 4.01 (d,  $J$  = 13.5 Hz, 1H), 2.23-2.14 (m, 1H). HRMS (MALDI) calcd. for  $C_{21}H_{33}NNaO_3SSi^+$  ( $M+Na$ ) $^+$ : 430.1843, Found: 430.1846. The relative stereochemistry of this compound was assigned by NOE experiment.

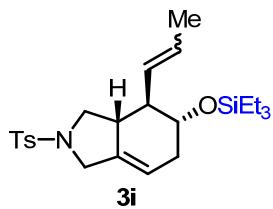


**( $\pm$ )-2-Tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4h).**

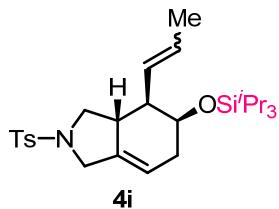
Reaction conditions: iPr<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), toluene, 80 °C. White solid (79 mg, 88% yield), dr = 2.4:1.0. Major: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.71 (d,  $J$  = 8.0 Hz, 2H), 7.30 (d,  $J$  = 8.0 Hz, 2H), 5.36 (s, 1H), 4.23 (s, 1H), 4.03 (d,  $J$  = 13.5 Hz, 1H), 3.78 (t,  $J$  = 8.3 Hz, 1H), 3.68 (d,  $J$  = 13.5 Hz, 1H), 2.78-2.66 (m, 1H), 2.65-2.56 (m, 1H), 2.41 (s, 3H), 2.18 (d,  $J$  = 18.5 Hz, 1H), 2.06 (d,  $J$  = 18.5 Hz, 1H), 2.01-1.93 (m, 1H), 1.05-0.94 (m, 22H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.5, 136.6, 133.9, 129.8, 127.7, 116.3, 64.7, 54.1, 51.2, 34.2, 33.4, 33.2, 21.7, 18.2, 12.3. HRMS (MALDI) calcd. for  $C_{24}H_{39}NNaO_3SSi^+$  ( $M+Na$ ) $^+$ : 472.2312, Found: 472.2315.



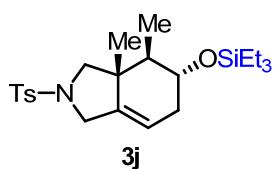
Minor: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.69 (d,  $J$  = 8.1 Hz, 2H), 7.32 (d,  $J$  = 8.1 Hz, 2H), 5.44-5.39 (m, 1H), 3.99-3.89 (m, 2H), 3.79-3.69 (m, 1H), 3.62 (d,  $J$  = 13.4 Hz, 1H), 2.63-2.51 (m, 2H), 2.43 (s, 3H), 2.40-2.30 (m, 1H), 2.04 (dt,  $J$  = 11.9, 3.5 Hz, 1H), 1.99-1.89 (m, 1H), 1.19-1.10 (m, 1H), 1.07-0.96 (m, 21H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.6, 136.3, 133.7, 129.8, 127.7, 118.5, 67.9, 53.9, 50.7, 39.4, 35.9, 35.4, 21.7, 18.2, 12.4. HRMS (ESI) calcd. for  $C_{24}H_{39}NNaO_3SSi^+$  ( $M+Na$ ) $^+$ : 472.2312, Found: 472.2318.



**( $\pm$ )-4-(Prop-1-en-1-yl)-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3i).** Reaction conditions: Et<sub>3</sub>SiH (2.0 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), DCE, 120 °C. White solid (41 mg, 46% yield), *E/Z* = 4.5:1.0. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ (*E*): 7.70 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.49-5.34 (m, 1.85H), 5.26-5.18 (m, 0.81H), 3.95 (d, *J* = 13.4 Hz, 1H), 3.75-3.56 (m, 3H), 2.60-2.51 (m, 1H), 2.47-2.29 (m, 5H), 2.05-1.94 (m, 1H), 1.79 (dd, *J* = 18.9, 9.9 Hz, 1H), 1.67-1.64 (m, 2.48H), 0.95-0.87 (m, 9H), 0.57-0.48 (m, 6H). (*Z*) (distinguishable peaks): 5.64-5.53 (m, 0.18H), 5.14-5.03 (m, 0.18H), 1.60-1.56 (m, 0.54H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.6, 135.6, 133.7, 131.5, 129.8, 127.7, 127.2, 118.0, 70.9, 53.5, 51.1, 49.5, 44.2, 35.9, 21.7, 18.2, 6.9, 5.0. HRMS (MALDI) calcd. for C<sub>24</sub>H<sub>37</sub>NNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 470.2156, Found: 470.2158.

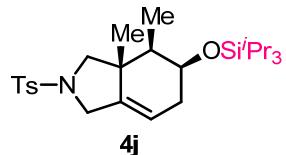


**( $\pm$ )-4-(Prop-1-en-1-yl)-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4i).** Reaction conditions: iPr<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), toluene, 110 °C. White solid (66 mg, 67% yield), *E/Z* = 5.5:1.0. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ (*E*): 7.70 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 5.56-5.47 (m, 1H), 5.45-5.36 (m, 1H), 5.32 (s, 1H), 4.08-4.00 (m, 2H), 3.76-3.65 (m, 2H), 2.74-2.63 (m, 1H), 2.62-2.51 (m, 1H), 2.41 (s, 3H), 2.26-2.08 (m, 2H), 1.72-1.66 (m, 1H), 1.66-1.61 (m, 2.54H), 1.03-0.90 (m, 21H). (*Z*) (distinguishable peaks): 1.59-1.51 (m, 0.43H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.4, 136.3, 133.9, 132.4, 129.8, 127.7, 126.1, 115.8, 70.0, 53.5, 51.5, 47.8, 38.1, 35.1, 21.6, 18.3, 18.2, 18.1, 12.8. HRMS (MALDI) calcd. for C<sub>27</sub>H<sub>43</sub>NNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 512.2625, Found: 512.2630.

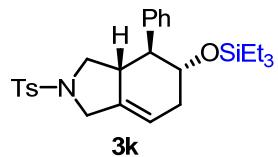


**( $\pm$ )-3a,4-Dimethyl-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3j).** Reaction conditions: Et<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), toluene, 120 °C. Colorless oil (47 mg, 54% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.69 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 5.27 (s, 1H), 4.07-3.98 (m, 1H), 3.71-3.60 (m, 2H), 3.42 (d, *J* = 8.9 Hz, 1H), 2.71 (d, *J* = 8.9 Hz, 1H), 2.42 (s, 3H), 2.40-2.30 (m, 1H), 1.99-1.88 (m, 1H), 1.43-1.33 (m, 1H), 0.93 (t, *J* = 7.9 Hz, 12H), 0.84 (s, 3H), 0.57 (q, *J* = 7.9 Hz,

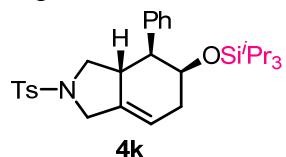
6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.5, 140.4, 134.1, 129.8, 127.5, 117.4, 69.5, 61.4, 50.5, 45.7, 43.6, 36.2, 21.7, 18.9, 12.7, 7.0, 5.1. HRMS (MALDI) calcd. for  $\text{C}_{23}\text{H}_{37}\text{NNaO}_3\text{SSI}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 458.2156, Found: 458.2158. The relative stereochemistry of this compound was assigned by NOE experiment.



**( $\pm$ )-3a,4-Dimethyl-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4j).** Reaction conditions:  $i\text{Pr}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (10 mol %), toluene, 130 °C. White solid (34 mg, 36% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 7.9$  Hz, 2H), 7.31 (d,  $J = 7.9$  Hz, 2H), 5.31 (s, 1H), 4.10-3.91 (m, 2H), 3.75 (d,  $J = 12.5$  Hz, 1H), 3.37 (d,  $J = 8.8$  Hz, 1H), 2.74 (d,  $J = 8.8$  Hz, 1H), 2.42 (s, 3H), 2.34-2.25 (m, 1H), 2.18 (d,  $J = 19.1$  Hz, 1H), 1.40-1.33 (m, 1H), 1.07-0.95 (m, 27H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.3, 140.3, 134.7, 129.7, 127.5, 116.0, 70.6, 62.6, 51.0, 42.9, 41.3, 35.3, 21.7, 19.1, 18.4, 18.4, 14.4, 12.9. HRMS (MALDI) calcd. for  $\text{C}_{26}\text{H}_{43}\text{NNaO}_3\text{SSI}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 500.2625, Found: 500.2628. The relative stereochemistry of this compound was assigned by NOE experiment.

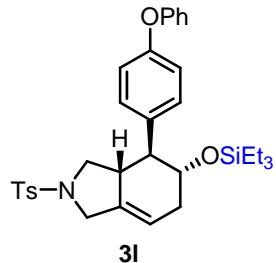


**( $\pm$ )-4-Phenyl-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3k).** Reaction conditions:  $\text{Et}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), DCE, 90 °C. White solid (60 mg, 62% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64 (d,  $J = 8.2$  Hz, 2H), 7.31 (d,  $J = 8.2$  Hz, 2H), 7.27 (d,  $J = 6.5$  Hz, 2H), 7.24-7.18 (m, 1H), 7.13-7.09 (m, 2H), 5.49-5.45 (m, 1H), 4.08-4.01 (m, 1H), 3.98-3.90 (m, 1H), 3.73-3.66 (m, 1H), 3.46 (dd,  $J = 9.0, 8.0$  Hz, 1H), 2.95-2.84 (m, 1H), 2.56-2.46 (m, 2H), 2.44 (s, 3H), 2.33 (t,  $J = 10.6$  Hz, 1H), 2.19-2.07 (m, 1H), 0.67 (t,  $J = 7.9$  Hz, 9H), 0.34-0.12 (m, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.6, 141.0, 136.2, 133.6, 129.8, 128.4, 128.3, 127.7, 126.9, 118.0, 71.7, 53.3, 52.4, 51.1, 45.3, 36.9, 21.7, 6.7, 4.7. HRMS (MALDI) calcd. for  $\text{C}_{27}\text{H}_{37}\text{NNaO}_3\text{SSI}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 506.2156, Found: 506.2160. The structure and relative stereochemistry of this compound was determined by X-ray crystallography and NOE experiment.

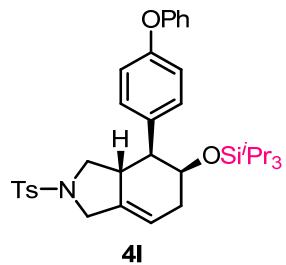


**( $\pm$ )-4-Phenyl-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4k).** Reaction conditions:  $i\text{Pr}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), toluene, 95 °C. Colorless oil (58 mg, 55% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (d,  $J = 8.2$  Hz, 2H), 7.31 (d,  $J = 8.2$  Hz, 2H), 7.29-7.25 (m, 2H), 7.24-7.16 (m, 3H), 5.43 (s, 1H), 4.21-4.06 (m, 2H), 3.78-3.70 (m, 2H), 3.34-3.23 (m, 1H), 2.50 (dd,  $J = 10.9, 9.7$  Hz, 1H), 2.45-2.33 (m, 5H), 2.31-2.22 (m, 1H), 0.87-0.72 (m, 21H).  $^{13}\text{C}$  NMR (101 MHz,

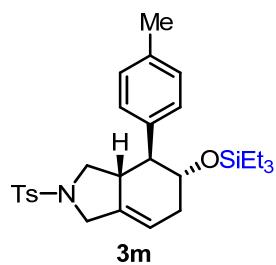
$\text{CDCl}_3$ )  $\delta$  143.5, 141.5, 136.8, 133.8, 129.8, 128.4, 128.3, 127.8, 126.9, 115.9, 71.3, 53.3, 51.5, 49.9, 37.0, 35.9, 21.7, 18.1, 17.9, 13.0. HRMS (MALDI) calcd. for  $\text{C}_{30}\text{H}_{43}\text{NNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 548.2625, Found: 548.2630. The relative stereochemistry of this compound was assigned by NOE experiment.



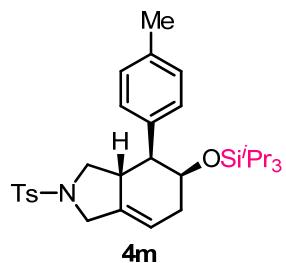
**(±)-4-(4-Phenoxyphenyl)-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3l).** Reaction conditions:  $\text{Et}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), DCE, 95 °C. White solid (59 mg, 51% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71-7.63 (m, 2H), 7.36-7.30 (m, 4H), 7.12-7.06 (m, 3H), 7.01-6.93 (m, 4H), 5.47 (s, 1H), 4.05 (d,  $J = 13.5$  Hz, 1H), 3.95-3.86 (m, 1H), 3.69 (d,  $J = 13.5$  Hz, 1H), 3.50 (t,  $J = 8.4$  Hz, 1H), 2.95-2.83 (m, 1H), 2.58-2.40 (m, 5H), 2.33 (t,  $J = 10.5$  Hz, 1H), 2.20-2.08 (m, 1H), 0.73 (t,  $J = 7.9$  Hz, 9H), 0.38-0.20 (m, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  157.8, 156.0, 143.7, 136.2, 136.1, 133.5, 129.8, 129.8, 129.5, 127.7, 123.0, 119.3, 118.5, 118.0, 71.8, 53.3, 51.6, 51.1, 45.3, 36.8, 21.7, 6.8, 4.8. HRMS (ESI) calcd. for  $\text{C}_{33}\text{H}_{41}\text{NNaO}_4\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 598.2418, Found: 598.2422.



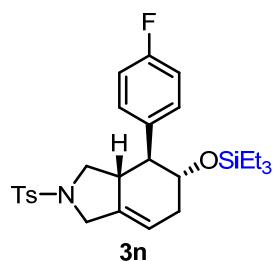
**(±)-4-(4-Phenoxyphenyl)-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4l).** Reaction conditions:  $\text{iPr}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), toluene, 95 °C. Colorless oil (68 mg, 55% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75-7.64 (m, 2H), 7.37-7.28 (m, 4H), 7.20-7.12 (m, 2H), 7.12-7.05 (m, 1H), 7.00-6.93 (m, 4H), 5.44 (s, 1H), 4.24-4.08 (m, 2H), 3.80-3.70 (m, 2H), 3.31-3.17 (m, 1H), 2.54 (t,  $J = 10.3$  Hz, 1H), 2.46-2.33 (m, 5H), 2.32-2.23 (m, 1H), 0.91-0.82 (m, 21H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  157.9, 155.8, 143.6, 136.7, 133.6, 129.8, 129.8, 129.6, 127.7, 123.0, 119.3, 118.4, 115.9, 71.3, 53.3, 51.4, 49.2, 37.2, 35.8, 21.7, 18.2, 18.0, 13.0. HRMS (ESI) calcd. for  $\text{C}_{36}\text{H}_{47}\text{NNaO}_4\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 640.2887, Found: 640.2892.



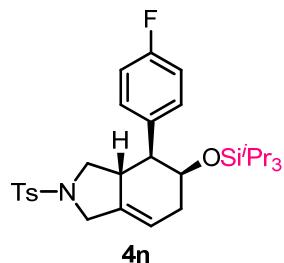
**( $\pm$ )-4-(*p*-Tolyl)-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3m).** Reaction conditions: Et<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), DCE, 95 °C. White solid (56 mg, 56% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.10-7.05 (m, 2H), 7.02-6.96 (m, 2H), 5.45 (s, 1H), 4.03 (d, *J* = 13.5 Hz, 1H), 3.96-3.86 (m, 1H), 3.69 (d, *J* = 13.5 Hz, 1H), 3.46 (t, *J* = 8.5 Hz, 1H), 2.92-2.80 (m, 1H), 2.55-2.49 (m, 1H), 2.48-2.38 (m, 4H), 2.35-2.24 (m, 4H), 2.19-2.06 (m, 1H), 0.67 (t, *J* = 7.9 Hz, 9H), 0.35-0.15 (m, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.6, 137.9, 136.3, 136.2, 133.6, 129.8, 129.0, 128.1, 127.7, 117.9, 71.7, 53.3, 51.9, 51.1, 45.3, 36.8, 21.7, 21.1, 6.7, 4.7. HRMS (MALDI) calcd. for C<sub>28</sub>H<sub>39</sub>NNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 520.2312, Found: 520.2316.



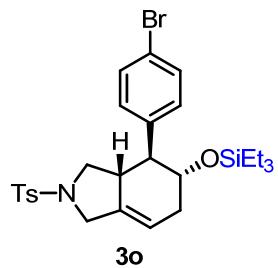
**( $\pm$ )-4-(*p*-Tolyl)-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4m).** Reaction conditions: iPr<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), toluene, 95 °C. White solid (65 mg, 60% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.68 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.10-7.05 (m, 4H), 5.42 (s, 1H), 4.20-4.10 (m, 2H), 3.78-3.68 (m, 2H), 3.31-3.20 (m, 1H), 2.49 (dd, *J* = 10.9, 9.8 Hz, 1H), 2.42 (s, 3H), 2.38-2.21 (m, 6H), 0.88-0.79 (m, 21H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.5, 138.4, 136.8, 136.3, 133.6, 129.8, 128.9, 128.2, 127.7, 115.8, 71.3, 53.3, 51.5, 49.5, 37.1, 35.9, 21.7, 21.1, 18.1, 17.9, 13.0. HRMS (MALDI) calcd. for C<sub>31</sub>H<sub>45</sub>NNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 562.2782, Found: 562.2785.



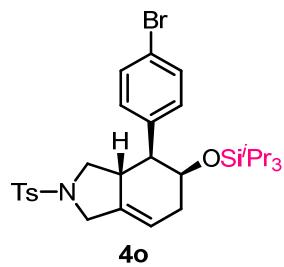
**( $\pm$ )-4-(4-Fluorophenyl)-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoinole (3n).** Reaction conditions: Et<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), DCE, 90 °C. White solid (67 mg, 67% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.11-7.04 (m, 2H), 7.01-6.95 (m, 2H), 5.46 (s, 1H), 4.03 (d, *J* = 13.5 Hz, 1H), 3.88 (ddd, *J* = 10.0, 8.9, 6.2 Hz, 1H), 3.68 (d, *J* = 13.5 Hz, 1H), 3.44 (dd, *J* = 9.0, 7.9 Hz, 1H), 2.90-2.79 (m, 1H), 2.54-2.40 (m, 5H), 2.32 (t, *J* = 10.6 Hz, 1H), 2.19-2.06 (m, 1H), 0.68 (t, *J* = 7.9 Hz, 9H), 0.34-0.15 (m, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 162.0 (d, *J* = 244.4 Hz), 143.7, 136.8 (d, *J* = 3.1 Hz), 136.0, 133.5, 129.8, 129.6 (d, *J* = 7.9 Hz), 127.7, 118.0, 115.2 (d, *J* = 21.1 Hz), 71.7, 53.2, 51.6, 51.0, 45.3, 36.8, 21.7, 6.7, 4.7. HRMS (MALDI) calcd. for C<sub>27</sub>H<sub>36</sub>FNNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 524.2061, Found: 524.2065.



**(±)-4-(4-Fluorophenyl)-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4n).** Reaction conditions: *i*Pr<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), toluene, 95 °C. White solid (75 mg, 69% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.67 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.18-7.12 (m, 2H), 7.00-6.93 (m, 2H), 5.43 (s, 1H), 4.18-4.02 (m, 2H), 3.73 (d, *J* = 13.7 Hz, 1H), 3.70-3.64 (m, 1H), 3.27-3.15 (m, 1H), 2.51-2.45 (m, 1H), 2.42 (s, 3H), 2.39-2.21 (m, 3H), 0.90-0.72 (m, 21H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 161.9 (d, *J* = 244.7 Hz), 143.6, 137.2 (d, *J* = 3.1 Hz), 136.5, 133.6, 129.8, 129.7 (d, *J* = 7.9 Hz), 127.7, 115.9, 115.0 (d, *J* = 21.0 Hz), 71.1, 53.1, 51.4, 49.2, 37.3, 35.8, 21.6, 18.1, 17.9, 12.9. HRMS (MALDI) calcd. for C<sub>30</sub>H<sub>42</sub>FNNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 566.2531, Found: 566.2536. The structure and relative stereochemistry of this compound was determined by X-ray crystallography.

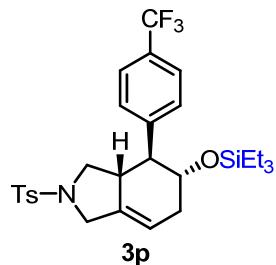


**(±)-4-(4-Bromophenyl)-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isooindole (3o).** Reaction conditions: Et<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), DCE, 90 °C. White solid (74 mg, 66% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 (d, *J* = 8.1 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.00 (d, *J* = 8.4 Hz, 2H), 5.49-5.44 (m, 1H), 4.03 (d, *J* = 13.6 Hz, 1H), 3.93-3.85 (m, 1H), 3.69 (d, *J* = 13.6 Hz, 1H), 3.42 (dd, *J* = 9.1, 7.9 Hz, 1H), 2.88-2.78 (m, 1H), 2.53-2.42 (m, 5H), 2.30 (t, *J* = 10.6 Hz, 1H), 2.18-2.06 (m, 1H), 0.68 (t, *J* = 7.9 Hz, 9H), 0.35-0.18 (m, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.7, 140.2, 136.0, 133.6, 131.5, 130.0, 129.9, 127.7, 120.6, 118.1, 71.6, 53.1, 51.9, 51.0, 45.1, 36.8, 21.7, 6.7, 4.8. HRMS (MALDI) calcd. for C<sub>27</sub>H<sub>36</sub>BrNNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 584.1261, Found: 584.1265.

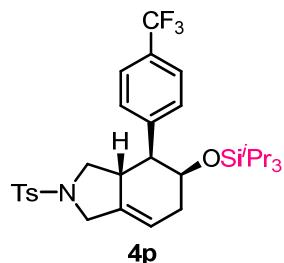


**(±)-4-(4-Bromophenyl)-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4o).** Reaction conditions: *i*Pr<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %),

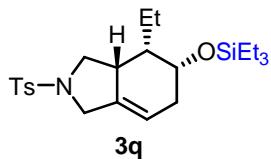
toluene, 95 °C. White solid (83 mg, 69% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 (d,  $J$  = 8.2 Hz, 2H), 7.43-7.37 (m, 2H), 7.31 (d,  $J$  = 8.0 Hz, 2H), 7.09-7.03 (m, 2H), 5.43 (s, 1H), 4.19-4.02 (m, 2H), 3.77-3.70 (m, 1H), 3.66 (dd,  $J$  = 9.3, 7.9 Hz, 1H), 3.26-3.13 (m, 1H), 2.51-2.43 (m, 1H), 2.42 (s, 3H), 2.38-2.21 (m, 3H), 0.89-0.73 (m, 21H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.6, 140.6, 136.5, 133.6, 131.3, 130.1, 129.8, 127.7, 120.7, 115.9, 71.0, 53.0, 51.4, 49.4, 37.1, 35.8, 21.7, 18.1, 17.9, 13.0. HRMS (MALDI) calcd. for  $\text{C}_{30}\text{H}_{42}\text{BrNNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 626.1730, Found: 626.1735.



**( $\pm$ )-2-Tosyl-5-((triethylsilyl)oxy)-4-(4-(trifluoromethyl)phenyl)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3p).** Reaction conditions:  $\text{Et}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), DCE, 75 °C. White solid (68 mg, 62% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 (d,  $J$  = 8.2 Hz, 2H), 7.56 (d,  $J$  = 8.1 Hz, 2H), 7.32 (d,  $J$  = 8.0 Hz, 2H), 7.25 (d,  $J$  = 7.5 Hz, 2H), 5.52-5.47 (m, 1H), 4.04 (d,  $J$  = 13.6 Hz, 1H), 3.96 (td,  $J$  = 9.0, 6.2 Hz, 1H), 3.70 (d,  $J$  = 13.6 Hz, 1H), 3.42 (dd,  $J$  = 9.0, 8.0 Hz, 1H), 2.97-2.85 (m, 1H), 2.55-2.48 (m, 2H), 2.45-2.39 (m, 4H), 2.22-2.09 (m, 1H), 0.65 (t,  $J$  = 7.9 Hz, 9H), 0.35-0.13 (m, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  145.4 (q,  $J$  = 1.2 Hz), 143.7, 135.9, 133.5, 129.9, 129.4 (q,  $J$  = 32.3), 128.6, 127.7, 125.3 (q,  $J$  = 3.8), 124.3 (q,  $J$  = 271.9 Hz), 118.1, 71.6, 53.0, 52.3, 51.0, 45.1, 36.7, 21.7, 6.6, 4.7. HRMS (MALDI) calcd. for  $\text{C}_{28}\text{H}_{36}\text{F}_3\text{NNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 574.2029, Found: 574.2033.

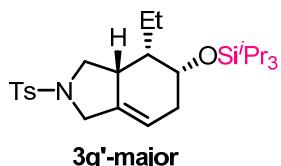


**( $\pm$ )-2-Tosyl-4-(4-(trifluoromethyl)phenyl)-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (4p).** Reaction conditions:  $i\text{Pr}_3\text{SiH}$  (1.5 equiv),  $\text{B}(\text{C}_6\text{F}_5)_3$  (5 mol %), toluene, 95 °C. White solid (70 mg, 59% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (d,  $J$  = 8.0 Hz, 2H), 7.55 (d,  $J$  = 7.9 Hz, 2H), 7.32 (d,  $J$  = 7.9 Hz, 4H), 5.50-5.43 (m, 1H), 4.23-4.06 (m, 2H), 3.76 (d,  $J$  = 13.7 Hz, 1H), 3.69 (dd,  $J$  = 9.3, 8.0 Hz, 1H), 3.34-3.22 (m, 1H), 2.54-2.47 (m, 1H), 2.45-2.39 (m, 5H), 2.33-2.24 (m, 1H), 0.88-0.74 (m, 21H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  145.7, 143.7, 136.4, 133.5, 129.8, 129.3 (q,  $J$  = 32.4 Hz), 128.7, 127.7, 125.2 (q,  $J$  = 3.6 Hz), 124.3 (q,  $J$  = 271.9 Hz), 116.0, 71.0, 53.0, 51.3, 49.8, 36.9, 35.8, 21.7, 18.0, 17.8, 12.9. HRMS (MALDI) calcd. for  $\text{C}_{31}\text{H}_{42}\text{F}_3\text{NNaO}_3\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 616.2499, Found: 616.2502.



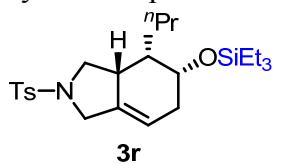
**( $\pm$ )-4-Ethyl-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3q).**

Reaction conditions: Et<sub>3</sub>SiH (2.0 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), DCE, 120 °C. White solid (33 mg, 38% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 5.37 (s, 1H), 3.92 (d, *J* = 13.5 Hz, 1H), 3.87-3.80 (m, 1H), 3.64-3.58 (m, 1H), 3.55 (d, *J* = 13.5 Hz, 1H), 2.82 (dd, *J* = 11.2, 8.9 Hz, 1H), 2.74-2.65 (m, 1H), 2.43 (s, 3H), 2.12-2.01 (m, 1H), 1.99-1.87 (m, 1H), 1.71-1.64 (m, 1H), 1.54-1.47 (m, 1H), 0.93-0.82 (m, 13H), 0.52 (q, *J* = 7.9 Hz, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.6, 135.1, 133.6, 129.8, 127.7, 117.6, 70.2, 50.6, 50.5, 43.1, 42.5, 31.4, 21.7, 16.0, 14.8, 7.0, 5.0. HRMS (MALDI) calcd. for C<sub>23</sub>H<sub>37</sub>NNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 458.2156, Found: 458.2160. The relative stereochemistry of this compound was assigned by NOE experiment.



**( $\pm$ )-4-Ethyl-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3q').**

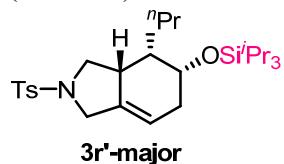
Reaction conditions: iPr<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), toluene, 115 °C. White solid (44 mg, 46% yield), dr = 4.1:1.0. Major: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 5.37 (s, 1H), 3.97-3.87 (m, 2H), 3.67-3.60 (m, 1H), 3.55 (d, *J* = 13.6 Hz, 1H), 2.86-2.77 (m, 1H), 2.75-2.66 (m, 1H), 2.43 (s, 3H), 2.18-2.08 (m, 1H), 1.98-1.87 (m, 1H), 1.79-1.73 (m, 1H), 1.60-1.51 (m, 1H), 1.05-0.97 (m, 21H), 0.88-0.83 (m, 4H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.6, 134.9, 133.6, 129.8, 127.7, 117.7, 70.6, 50.6, 50.5, 43.3, 42.6, 31.4, 21.7, 18.2, 15.4, 15.0, 12.4. Minor (distinguishable peaks): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 5.32 (s, 1H), 4.07-3.97 (m, 1H). HRMS (MALDI) calcd. for C<sub>26</sub>H<sub>43</sub>NNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 500.2625, Found: 500.2630. The relative stereochemistry of this major compound was assigned by NOE experiment.



**( $\pm$ )-4-Propyl-2-tosyl-5-((triethylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (3r).**

Reaction conditions: Et<sub>3</sub>SiH (2.0 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), DCE, 120 °C. White solid (33 mg, 37% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 5.39-5.34 (m, 1H), 3.92 (d, *J* = 13.5 Hz, 1H), 3.85-3.78 (m, 1H), 3.60 (t, *J* = 7.9 Hz, 1H), 3.55 (d, *J* = 13.5 Hz, 1H), 2.78 (dd, *J* = 11.2, 8.6 Hz, 1H), 2.74-2.64 (m, 1H), 2.43 (s, 3H), 2.12-2.01 (m, 1H), 1.98-1.87 (m, 1H), 1.78-1.71 (m, 1H), 1.47-1.34 (m, 1H), 1.23-1.14 (m, 2H), 0.90 (t, *J* = 7.9 Hz, 9H), 0.82 (t, *J* = 7.3 Hz, 4H), 0.57-0.49 (m, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.6, 135.0, 133.5, 129.8,

127.8, 117.7, 70.1, 50.7, 50.5, 43.1, 40.3, 31.4, 25.1, 23.4, 21.7, 14.5, 7.0, 5.0. HRMS (MALDI) calcd. for C<sub>24</sub>H<sub>39</sub>NNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 472.2312, Found: 472.2318.

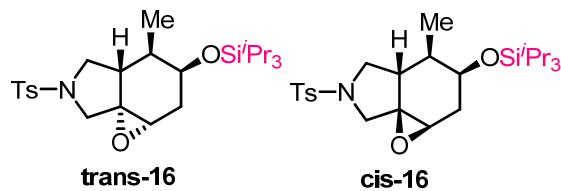


**(±)-4-Propyl-2-tosyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole e (3r').** Reaction conditions: *i*Pr<sub>3</sub>SiH (1.5 equiv), B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5 mol %), toluene, 115 °C. White solid (43 mg, 44% yield), dr = 7.0:1.0. Major: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.70 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.40-5.34 (m, 1H), 3.97-3.88 (m, 2H), 3.62 (t, *J* = 7.6 Hz, 1H), 3.55 (t, *J* = 13.7 Hz, 1H), 2.80-2.65 (m, 2H), 2.43 (s, 3H), 2.18-2.09 (m, 1H), 1.97-1.88 (m, 1H), 1.86-1.79 (m, 1H), 1.51-1.42 (m, 1H), 1.23-1.15 (m, 2H), 1.05-0.94 (m, 22H), 0.82 (t, *J* = 7.3 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.6, 134.9, 133.5, 129.8, 127.8, 117.8, 70.5, 50.6, 50.6, 43.3, 40.6, 31.4, 23.7, 21.7, 18.2, 18.2, 14.7, 12.4. Minor (distinguishable peaks): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 5.32 (s, 1H), 4.01-4.98 (m, 1H), 2.94-2.86 (m, 2H). HRMS (MALDI) calcd. for C<sub>27</sub>H<sub>45</sub>NNaO<sub>3</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 514.2782, Found: 514.2786.

## 5. Transformations of Product 4a



**(±)-4-Methyl-5-((triisopropylsilyl)oxy)-2,3,3a,4,5,6-hexahydro-1H-isoindole (15).** Magnesium turnings (84 mg, 3.84 mmol, 20 equiv) were added to a solution of **4a** (80 mg, 0.19 mmol, 1 equiv) in dry MeOH (4 mL), and the mixture was refluxed for 1 hours under argon. After being allowed to cool to room temperature, the suspension was filtered through a short plug of Celite. The filtrate was concentrated in vacuo, and the residue was purified by flash column chromatography (from MeOH/DCM = 10:1 to MeOH/DCM/NH<sub>4</sub>OH = 8:1:0.08) to afford the title compound as a colorless oil (41 mg, 70 % yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 5.35 (s, 1H), 4.07-3.93(m, 1H), 3.69 (d, *J* = 14.4 Hz, 1H), 3.55-3.42 (m, 2H), 3.40-3.31 (m, 1H), 2.46-2.33 (m, 2H), 2.33-2.14 (m, 2H), 1.33-1.25 (m, 1H), 1.08-0.98 (m, 24H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 141.0, 114.1, 70.9, 52.2, 49.9, 41.8, 39.1, 35.8, 18.4, 18.3, 17.5, 13.1. HRMS (ESI) calcd. for C<sub>15</sub>H<sub>36</sub>NOSi<sup>+</sup> (M+H)<sup>+</sup>: 310.2561, Found: 310.2565.

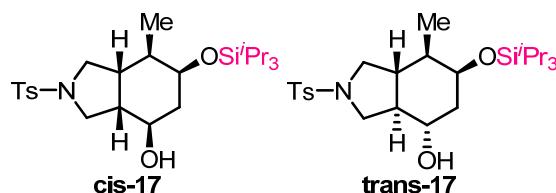


**(±)-4-Methyl-6-tosyl-3-((triisopropylsilyl)oxy)octahydrooxireno[2,3-d]isoindole (16).** *m*-CPBA (34.5 mg, 0.2 mmol, 2 equiv) was added in portions to a solution of **4a** (46.4 mg, 0.1 mmol, 1 equiv) in dry DCM (8 mL) at 0 °C. The reaction mixture was

allowed to warm to room temperature and stirred for 16 h. The mixture was washed with aqueous Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>. The organic layer was dried, filtered and concentrated in vacuo. The residue was purified by column chromatography (PE/EA = 10 :1) to afford ( $\pm$ ) **trans-16** (32 mg, 67% yield) and ( $\pm$ ) **cis-16** (12 mg, 25% yield).

( $\pm$ ) **trans-16**: White solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.71 (d,  $J$  = 8.2 Hz, 2H), 7.31 (d,  $J$  = 8.2 Hz, 2H), 3.82-3.71 (m, 3H), 3.40 (d,  $J$  = 3.5 Hz, 1H), 3.14 (d,  $J$  = 11.4 Hz, 1H), 2.90 (dd,  $J$  = 12.3, 8.8 Hz, 1H), 2.41 (s, 3H), 2.35 (td,  $J$  = 11.8, 7.3 Hz, 1H), 2.06-1.91 (m, 2H), 1.55 (dq,  $J$  = 13.7, 6.9 Hz, 1H), 1.02-0.95 (m, 21H), 0.90 (d,  $J$  = 6.9 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  143.6, 134.3, 129.9, 127.5, 70.1, 67.1, 53.4, 52.4, 50.2, 39.1, 34.5, 32.7, 21.7, 18.3, 18.2, 16.3, 12.9. HRMS (MALDI) calcd. for C<sub>25</sub>H<sub>41</sub>NNaO<sub>4</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 502.2418, Found: 502.2423. The relative stereochemistry of this compound was assigned by NOE experiment.

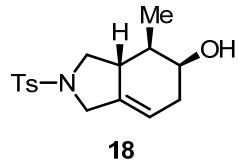
( $\pm$ ) **cis-16**: White solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.71 (d,  $J$  = 8.1 Hz, 2H), 7.35 (d,  $J$  = 8.1 Hz, 2H), 3.89-3.77 (m, 1H), 3.61 (t,  $J$  = 9.5 Hz, 1H), 3.33-3.25 (m, 2H), 3.14-3.09 (m, 1H), 2.94 (dd,  $J$  = 10.0, 8.0 Hz, 1H), 2.44 (s, 3H), 2.34-2.19 (m, 2H), 1.87-1.77 (m, 1H), 1.29-1.24 (m, 1H), 1.06-0.91 (m, 24H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  144.1, 132.1, 129.9, 128.2, 69.3, 63.8, 56.1, 52.4, 52.0, 39.0, 37.9, 33.1, 21.7, 18.3, 18.2, 17.0, 12.8. HRMS (MALDI) calcd. for C<sub>25</sub>H<sub>41</sub>NNaO<sub>4</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 502.2418, Found: 502.2422.



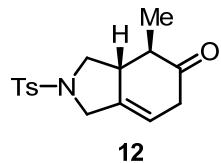
( $\pm$ )-**7-Methyl-2-tosyl-6-((triisopropylsilyl)oxy)octahydro-1H-isoindol-4-ol (17). 4a** (120 mg, 0.26 mmol, 1 equiv) was dissolved in dry THF (8 mL). The solution was cooled to 0 °C, and then BH<sub>3</sub>•THF (1.29 mL, 1.29 mmol, 5 equiv) was added dropwise. The mixture was stirred overnight at room temperature under argon. The mixture was then cooled to 0 °C, and treated dropwise with aqueous NaOH (10%, 2 mL) and subsequently aqueous H<sub>2</sub>O<sub>2</sub> (30%, 2 mL). This mixture was heated to 60 °C for 1 h. The volatiles were removed in vacuo, followed by the addition of H<sub>2</sub>O (30 mL). The mixture was extracted with ethyl acetate (3 x 5 mL). The combined organic layers were dried, filtered, and concentrated to give a viscous liquid which was chromatographed (PE/EA = 5:1) on silica gel to afford ( $\pm$ ) **cis-17** (43.9 mg, 35% yield) and ( $\pm$ ) **trans-17** (43.8 mg, 35% yield).

( $\pm$ ) **cis-17**: Colorless oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.71 (d,  $J$  = 8.1 Hz, 2H), 7.32 (d,  $J$  = 8.1 Hz, 2H), 4.01-3.94 (m, 1H), 3.49-3.41 (m, 1H), 3.31-3.19 (m, 4H), 3.16-3.04 (m, 1H), 2.42 (s, 3H), 2.23-2.05 (m, 2H), 1.92-1.79 (m, 1H), 1.66 (dt,  $J$  = 13.7, 3.3 Hz, 1H), 1.57-1.46 (m, 1H), 1.11-0.99 (m, 21H), 0.96 (d,  $J$  = 6.9 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  143.6, 133.9, 129.8, 127.5, 70.8, 67.1, 51.0, 49.5, 44.4, 40.2, 35.6, 34.4, 21.7, 18.3, 18.2, 15.5, 12.6. HRMS (ESI) calcd. for C<sub>25</sub>H<sub>43</sub>NNaO<sub>4</sub>SSi<sup>+</sup> (M+Na)<sup>+</sup>: 504.2574, Found: 504.2578. The relative stereochemistry of this compound was assigned by NOE experiment.

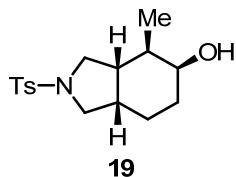
**(±) trans-17:** White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 (d,  $J = 8.1$  Hz, 2H), 7.30 (d,  $J = 8.1$  Hz, 2H), 4.07-4.03 (m, 1H), 3.79-3.66 (m, 2H), 3.58 (dd,  $J = 9.1, 7.1$  Hz, 1H), 3.03 (t,  $J = 10.2$  Hz, 1H), 2.79 (dd,  $J = 11.4, 9.1$  Hz, 1H), 2.41 (s, 3H), 2.11 (dt,  $J = 13.2, 3.8$  Hz, 1H), 1.79 (s, 1H), 1.77-1.63 (m, 1H), 1.47-1.37 (m, 1H), 1.37-1.25 (m, 2H), 1.07-0.94 (m, 21H), 0.89 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.4, 134.6, 129.8, 127.4, 73.3, 69.3, 52.2, 52.1, 51.6, 43.8, 42.0, 40.3, 21.7, 18.3, 18.3, 16.2, 12.9. HRMS (ESI) calcd. for  $\text{C}_{25}\text{H}_{43}\text{NNaO}_4\text{SSi}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 504.2574, Found: 504.2578.



**(±)-4-Methyl-2-tosyl-2,3,3a,4,5,6-hexahydro-1H-isoindol-5-ol (18).** **4a** (50 mg, 0.11 mmol, 1 equiv) was dissolved in dry THF (5 mL). The solution was cooled to 0 °C, and then TBAF in THF (0.22 mL, 1 M, 0.216 mmol, 2 equiv) was added dropwise. The resulting mixture was stirred overnight at room temperature. After the addition of  $\text{H}_2\text{O}$  (5 mL), the mixture was extracted with ethyl acetate (3 x 5 mL). The combined organic layers were dried, filtered, and concentrated in vacuo. The residue was purified by column chromatography (PE/EA = 3:2) to afford the title compound as a colorless oil (28 mg, 84%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 (d,  $J = 8.1$  Hz, 2H), 7.31 (d,  $J = 8.1$  Hz, 2H), 5.38 (s, 1H), 3.99 (d,  $J = 13.3$  Hz, 1H), 3.85-3.78 (m, 2H), 3.70 (d,  $J = 13.3$  Hz, 1H), 2.63 (dd,  $J = 10.6, 9.1$  Hz, 1H), 2.48-2.38 (m, 4H), 2.37-2.27 (m, 1H), 2.16 (d,  $J = 18.8$  Hz, 1H), 1.69 (br, 1H), 1.34-1.26 (m, 1H), 1.01 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  143.6, 136.2, 133.8, 129.8, 127.6, 116.0, 69.1, 53.3, 51.4, 39.8, 37.2, 34.7, 21.6, 16.7. HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{21}\text{NNaO}_3\text{S}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 330.1134, Found: 330.1138.



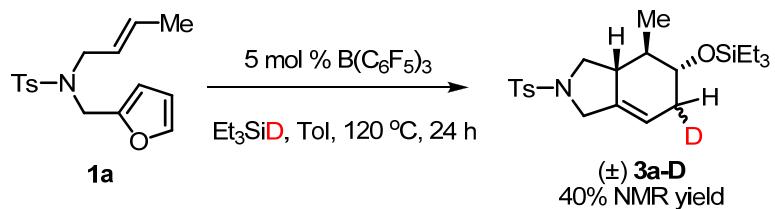
**(±)-4-Methyl-2-tosyl-1,2,3,3a,4,6-hexahydro-5H-isoindol-5-one. (12).** PCC (86.2 mg, 0.4 mmol, 4 equiv) was added in portions to a solution of **18** (30.7 mg, 0.1 mmol, 1 equiv) in dry DCM (5 mL). The resulting mixture was stirred at room temperature for 16 h. The reaction mixture was then filtered through a plug of Celite. The filtrate was concentrated in vacuo, and the residue was purified by column chromatography (PE/EA = 4 : 1) to afford the title compound as a white solid (30 mg, 98% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J = 8.1$  Hz, 2H), 7.34 (d,  $J = 8.1$  Hz, 2H), 5.65-5.59 (m, 1H), 4.06 (d,  $J = 14.0$  Hz, 1H), 3.89 (t,  $J = 8.6$  Hz, 1H), 3.77 (d,  $J = 14.0$  Hz, 1H), 2.96-2.84 (m, 1H), 2.84-2.72 (m, 2H), 2.65-2.43 (m, 1H), 2.45 (s, 3H), 2.23-2.14 (m, 1H), 1.05 (d,  $J = 6.5$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  208.9, 144.0, 137.9, 133.4, 130.0, 127.8, 116.5, 54.1, 51.0, 46.6, 45.9, 39.0, 21.7, 12.1. HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{19}\text{NNaO}_3\text{S}^+$  ( $\text{M}+\text{Na}$ ) $^+$ : 328.0978, Found: 328.0984.



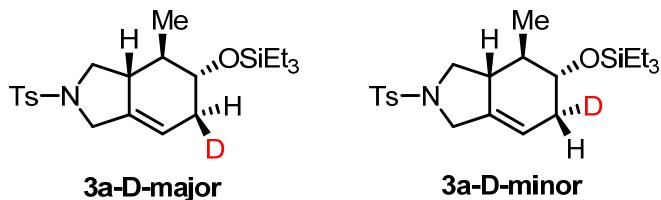
**( $\pm$ )-4-Methyl-2-tosyloctahydro-1H-isoindol-5-ol (19).** **18** (38 mg, 0.12 mmol, 1 equiv) and Pd/C (3.8 mg, 10%) were dissolved in DCM (3 mL) in a 10 mL glass test tube. The tube was then placed in a stainless-steel autoclave. After being sealed, the autoclave was purged three times with H<sub>2</sub> and the final pressure of hydrogen was adjusted to 5 bar. After being stirred at room temperature for 4 h, the reaction mixture was filtered through a short plug of Celite. The filtrate was then concentrated, and purified by column chromatography (PE/EA = 1.5:1) to afford the title compound as a colorless oil (37 mg, 99% yield), dr = 13.0:1.0. Major (( $\pm$ ) **cis-19**): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.70 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 3.74-3.68 (m, 1H), 3.32 (dd, *J* = 10.0, 2.7 Hz, 1H), 3.26-3.16 (m, 2H), 3.12 (t, *J* = 9.5 Hz, 1H), 2.42 (s, 3H), 2.21-2.12 (m, 1H), 1.98-1.91 (m, 1H), 1.96-1.74 (m, 1H), 1.62-1.54 (m, 1H), 1.52-1.41 (m, 2H), 1.33-1.24 (m, 1H), 1.24-1.17 (m, 1H), 0.88 (d, *J* = 6.8 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  143.4, 134.2, 129.7, 127.4, 69.6, 51.7, 49.6, 41.0, 36.1, 33.6, 27.7, 21.6, 19.3, 16.1. Minor (( $\pm$ ) **trans-19**, distinguishable peaks): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  3.76 (s, 1H), 3.53-3.46 (m, 2H), 2.83-2.74 (m, 2H), 0.97 (d, *J* = 7.3 Hz, 3H). HRMS (ESI) calcd. for C<sub>16</sub>H<sub>22</sub>NO<sub>3</sub>S<sup>+</sup> (M+H)<sup>+</sup>: 310.1471, Found: 310.1478. The relative stereochemistry of this major compound was assigned by NOE experiment.

## 6. Mechanistic Studies

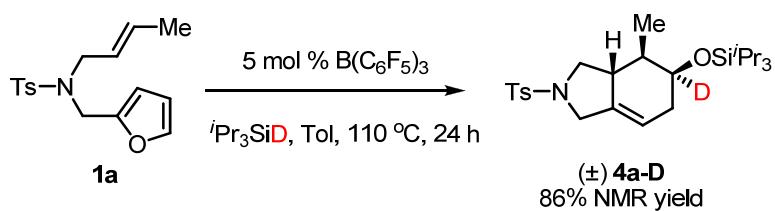
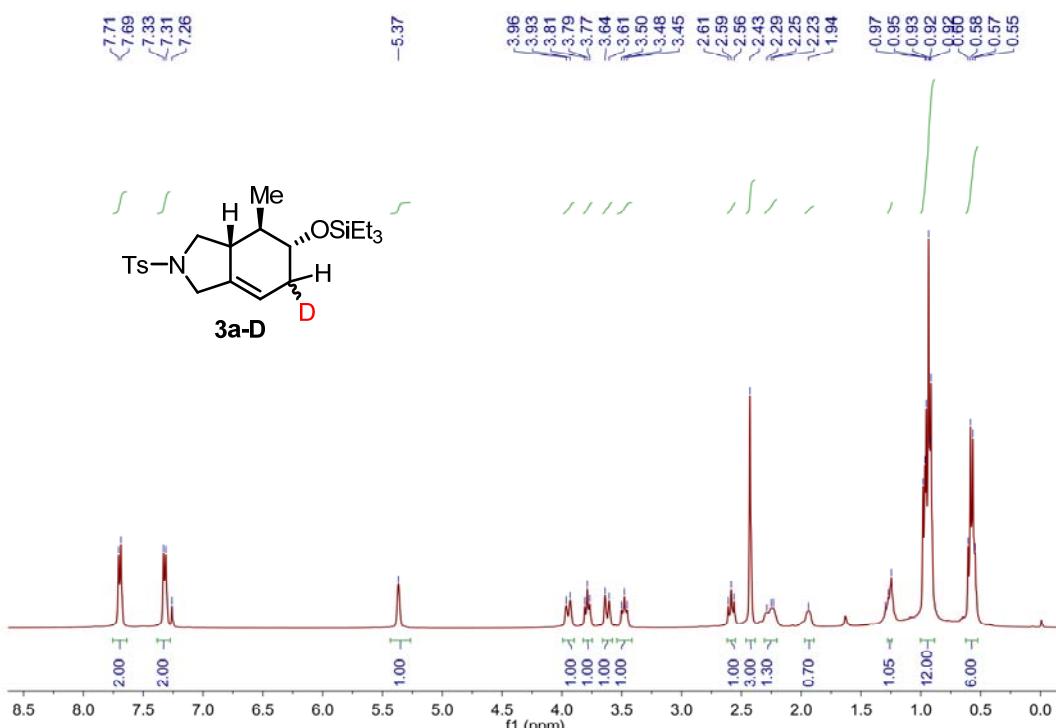
### 6.1 Deuterium-Labelling Experiments



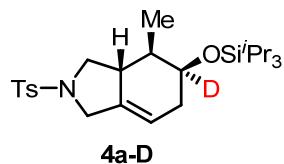
In a glovebox, Et<sub>3</sub>SiD (48  $\mu$ L, 0.3 mmol, 1.5 equiv) was added to a solution of **1a** (61 mg, 0.2 mmol, 1 equiv) in dry toluene (0.5 mL) in an 8 mL vial. B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (5.1 mg, 0.01 mmol, 5 mol %) was then added before the vial was capped and closed tightly. The reaction mixture was stirred at 120 °C for 24 h. After being allowed to cool to room temperature, one drop Et<sub>3</sub>N was added to the solution. After evaporation of the solvent in vacuo, the residue was subjected to column chromatography on silica gel (PE/EA = 30:1 to 20:1 as eluent) to give the product.



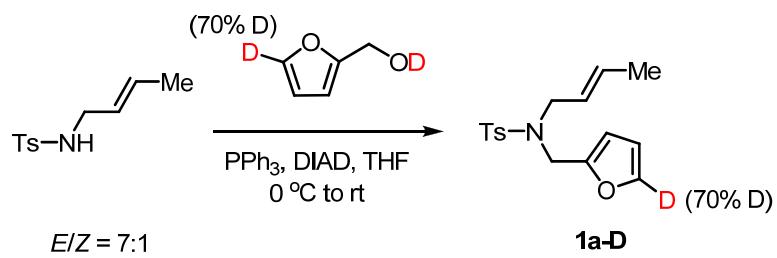
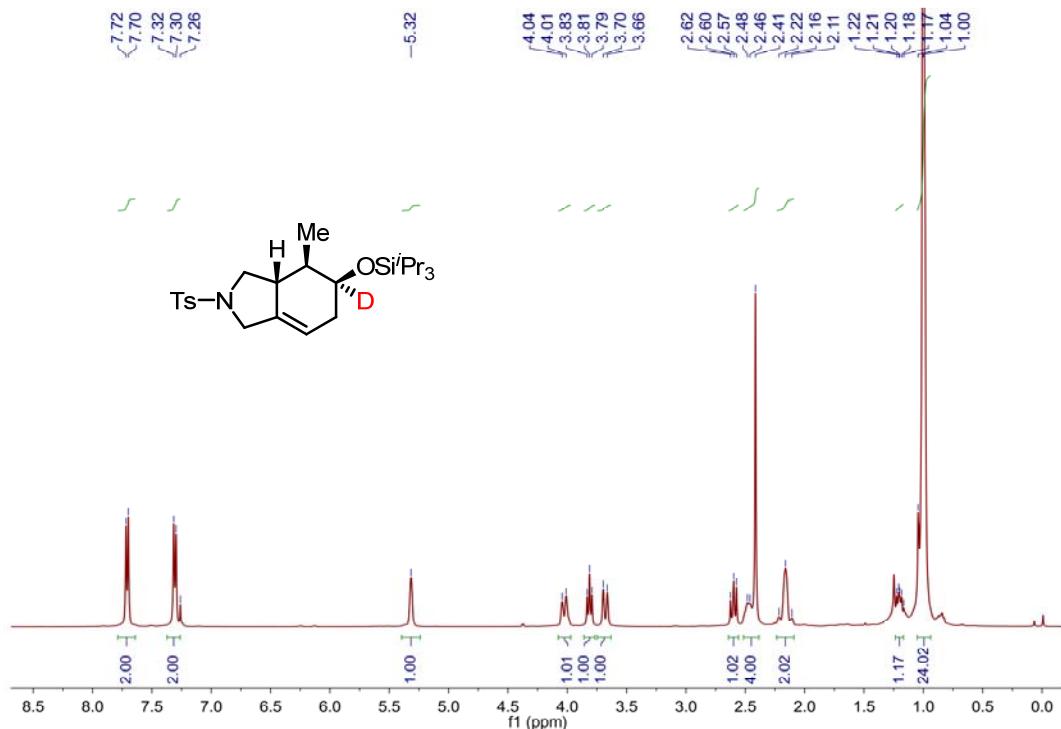
**3a-D:** dr = 7:3. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) (mixture of two diastereomers)  $\delta$  7.69 (d,  $J$  = 7.9 Hz, 2H), 7.32 (d,  $J$  = 7.9 Hz, 2H), 5.37 (s, 1H), 3.99-3.91 (m, 1H), 3.82-3.76 (m, 1H), 3.67-3.59 (m, 1H), 3.52-3.44 (m, 1H), 2.59 (t,  $J$  = 9.8 Hz, 1H), 2.43 (s, 3H), 2.32-2.18 (m, 1.3H), 2.00-1.90 (m, 0.7H), 1.30-1.22 (m, 1H), 0.99-0.87 (m, 12H), 0.63-0.52 (m, 6H).



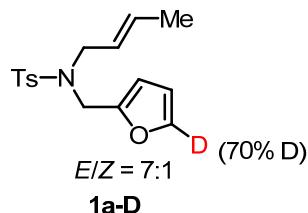
In a glovebox,  $i\text{Pr}_3\text{SiD}$  (61  $\mu\text{L}$ , 0.3 mmol, 1.5 equiv) was added to a solution of **1a** (61 mg, 0.2 mmol, 1 equiv) in dry toluene (0.5 mL) in an 8 mL vial.  $\text{B}(\text{C}_6\text{F}_5)_3$  (5.1 mg, 0.01 mmol, 5 mol %) was then added before the vial was capped and closed tightly. The reaction mixture was stirred at 110 °C for 24 h. After being allowed to cool to room temperature, one drop of  $\text{Et}_3\text{N}$  was added to the solution. After evaporation of the solvent in vacuo, the residue was subjected to column chromatography on silica gel (PE/EA = 30:1 to 20:1 as eluent) to give the product.



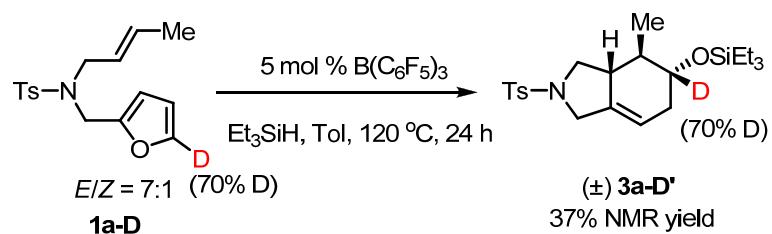
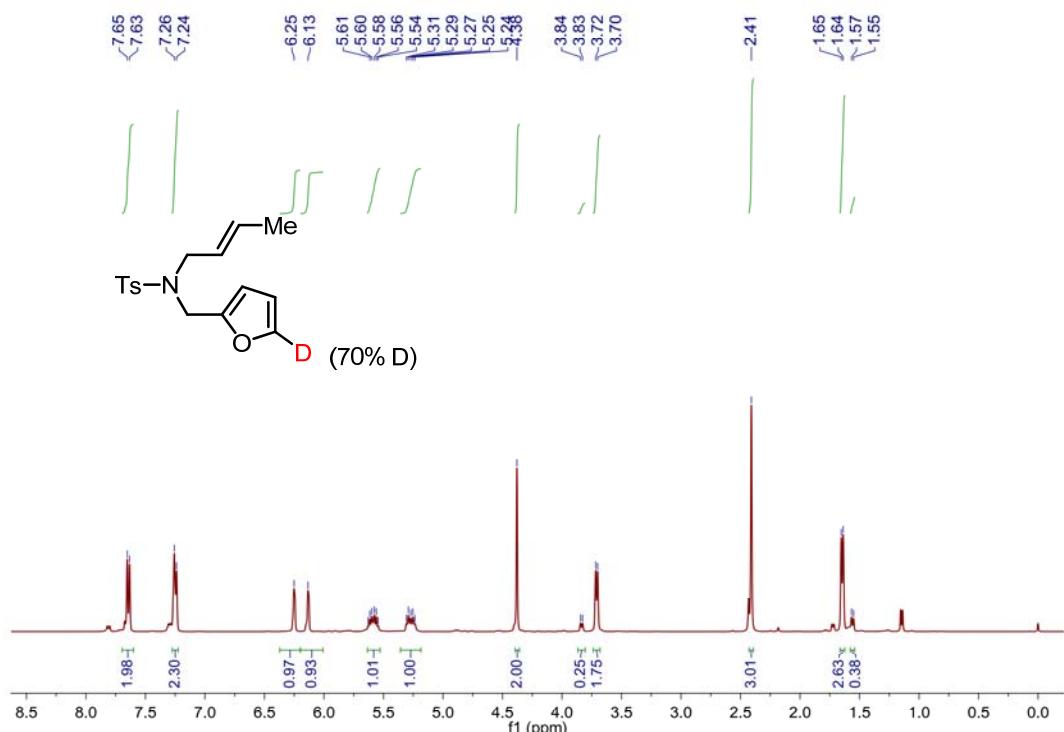
**4a-D:** White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J = 8.0$  Hz, 2H), 7.31 (d,  $J = 8.0$  Hz, 2H), 5.31 (s, 1H), 4.09-3.95 (m, 1H), 3.86-3.79 (m, 1H), 3.67 (d,  $J = 13.5$  Hz, 1H), 2.66-2.54 (m, 1H), 2.55-2.38 (m, 4H), 2.27-2.07 (m, 2H), 1.27-1.17 (m, 1H), 1.12-0.84 (m, 24H).



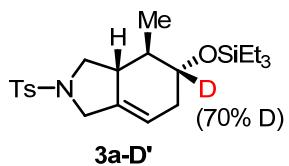
The deuterated furfuryl alcohol<sup>[11]</sup> (0.72 g, 7.2 mmol, 1.2 equiv) and  $\text{PPh}_3$  (2.20 g, 8.4 mmol, 1.4 equiv) were added to a solution of the tosylated but-2-en-1-amine<sup>[12]</sup> (1.35 g, 6 mmol, 1 equiv) in dry THF (20 mL) under argon. Diisopropyl azodicarboxylate (1.70 g, 8.4 mmol, 1.4 equiv) was then added dropwise at 0 °C, and the resulting mixture was stirred for 5 h at room temperature. The mixture was concentrated in vacuo. The residue was then subjected to column chromatography on silica gel (PE/EA = 20:1 as eluent) to give the product.



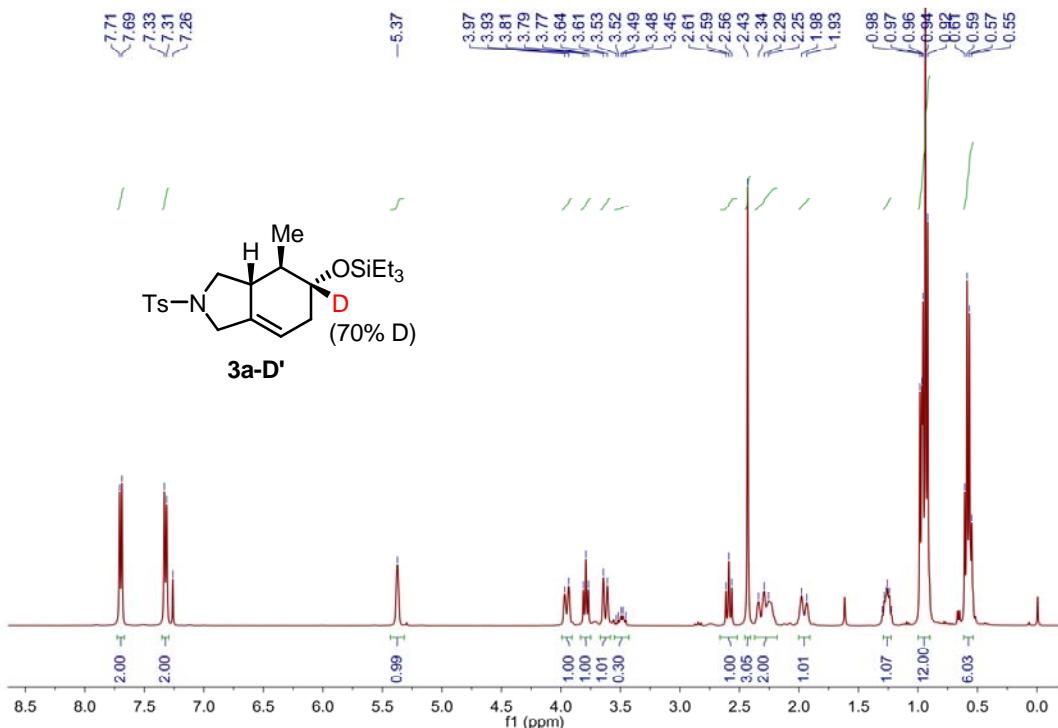
**1a-D:** Colorless oil,  $E/Z = 7:1$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.62 (d,  $J = 8.3$  Hz, 2H), 7.25-7.20 (m, 2.3H), 6.26-6.20 (m, 1H), 6.19-6.01 (m, 1H), 5.62-5.53 (m, 1H), 5.35-5.19 (m, 1H), 4.38 (s, 2H), 3.71 (d,  $J = 6.6$  Hz, 1.75H), 2.41 (s, 3H), 1.65 (d,  $J = 6.5, 2.63$  Hz); (Z) (distinguishable peaks): 3.84 (d,  $J = 7.0$  Hz, 0.25H), 1.56 (d,  $J = 6.9, 0.38$  Hz).



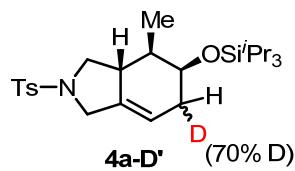
In a glovebox,  $\text{Et}_3\text{SiH}$  (48  $\mu\text{L}$ , 0.3 mmol, 1.5 equiv) was added to a solution of **1a-D** (61 mg, 0.2 mmol, 1 equiv) in dry toluene (0.5 mL) in an 8 mL vial.  $\text{B}(\text{C}_6\text{F}_5)_3$  (5.1 mg, 0.01 mmol, 5 mol %) was then added before the vial was capped and closed tightly. The reaction mixture was stirred at 120 °C for 24 h. After being allowed to cool to room temperature, one drop of  $\text{Et}_3\text{N}$  was added to the solution. After evaporation of the solvent in vacuo, the residue was subjected to column chromatography on silica gel (PE/EA = 30:1 to 20:1 as eluent) to give the product. We did not observe the product from the reaction of the *Z* isomer of **1a-D**.



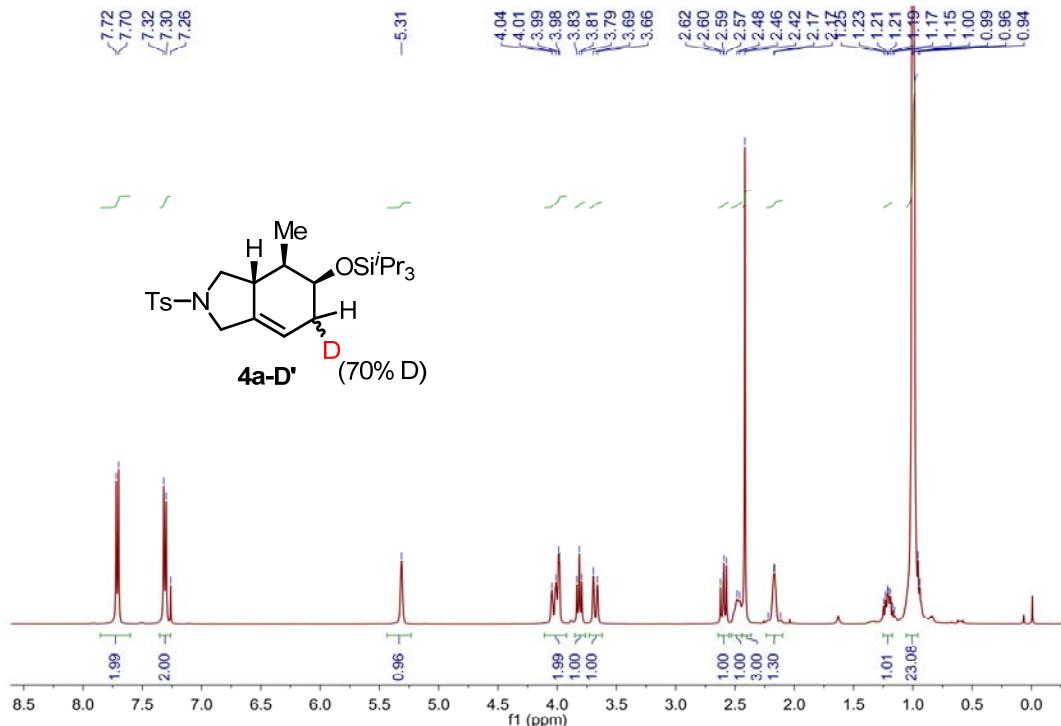
**3a-D':** White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J = 7.9$  Hz, 2H), 7.32 (d,  $J = 7.9$  Hz, 2H), 5.37 (s, 1H), 3.95 (d,  $J = 13.5$  Hz, 1H), 3.79 (t,  $J = 8.4$  Hz, 1H), 3.63 (d,  $J = 13.5$  Hz, 1H), 3.52-3.44 (m, 0.3H), 2.59 (t,  $J = 9.8$  Hz, 1H), 2.43 (s, 3H), 2.38-2.18 (m, 2H), 1.96 (d,  $J = 17.6$  Hz, 1H), 1.30-1.22 (m, 1H), 0.99-0.90 (m, 12H), 0.58 (q,  $J = 7.9$  Hz, 6H).



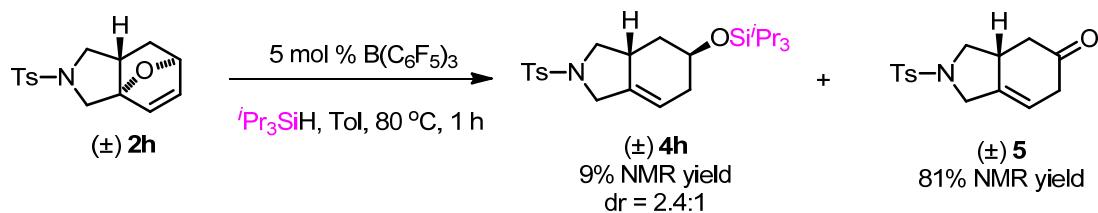
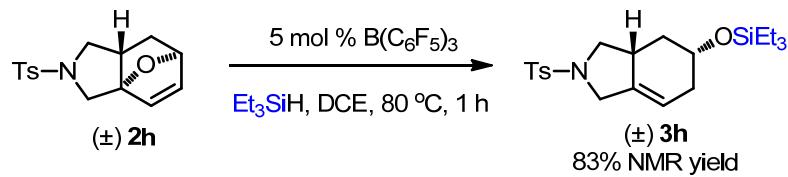
In a glovebox,  $i\text{Pr}_3\text{SiH}$  (61  $\mu\text{L}$ , 0.3 mmol, 1.5 equiv) was added to a solution of **1a-D** (61 mg, 0.2 mmol, 1 equiv) in dry toluene (0.5 mL) in an 8 mL vial.  $\text{B}(\text{C}_6\text{F}_5)_3$  (5.1 mg, 0.01 mmol, 5 mol %) was then added before the vial was capped and closed tightly. The reaction mixture was stirred at 110 °C for 24 h. After being allowed to cool to room temperature, one drop of  $\text{Et}_3\text{N}$  was added to the solution. After evaporation of the solvent in vacuo, the residue was subjected to column chromatography on silica gel (PE/EA = 30:1 to 20:1 as eluent) to give the product. We did not observe the product from the reaction of the Z isomer of **1a-D**.



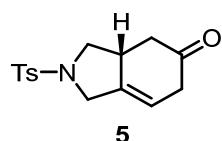
**4a-D':** White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J = 8.0$  Hz, 2H), 7.31 (d,  $J = 8.0$  Hz, 2H), 5.31 (s, 1H), 4.09-3.95 (m, 2H), 3.81 (t,  $J = 8.3$  Hz, 1H), 3.68 (d,  $J = 13.6$  Hz, 1H), 2.64-2.55 (dd,  $J = 10.9, 9.1$  Hz, 1H), 2.54-2.35 (m, 4H), 2.24-2.09 (m, 1.3H), 1.25-1.17 (m, 1H), 1.07-0.95 (m, 24H).



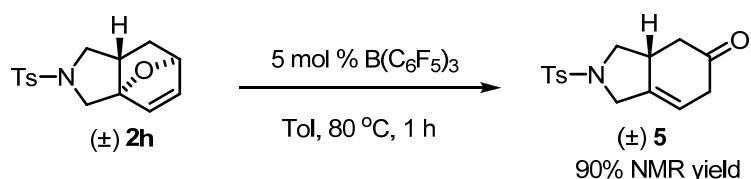
## 6.2 Control Experiments



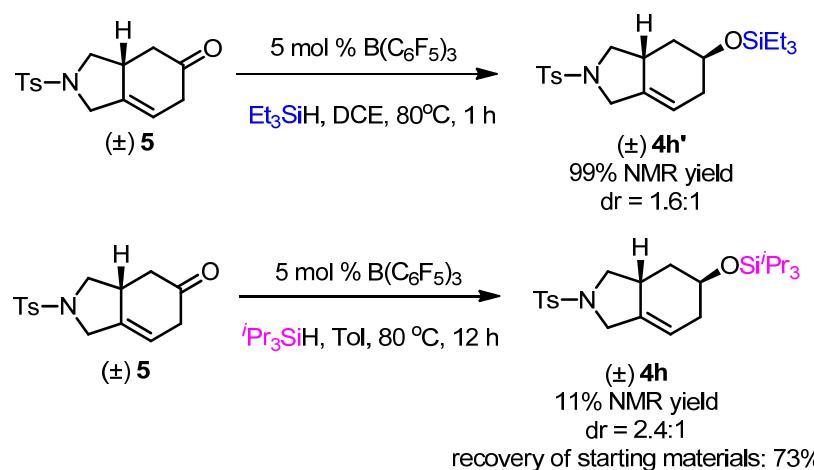
In a glovebox, *t*Pr<sub>3</sub>SiH (61  $\mu$ L, 0.15 mmol, 1.5 equiv) or Et<sub>3</sub>SiH (48  $\mu$ L, 0.15 mmol, 1.5 equiv) and **2h**<sup>[13]</sup> (29.1 mg, 0.1 mmol, 1 equiv) were dissolved in a dry solvent (0.25 mL of toluene or DCE) in an 8 mL vial. B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (2.6 mg, 0.005 mmol, 5 mol %) was then added before the vial was capped and closed tightly. The reaction mixture was then stirred at 80 °C for 1 h. After being allowed to cool to room temperature, one drop of Et<sub>3</sub>N was added to the solution. After removing all the volatiles, the resulting reaction mixture was analyzed by <sup>1</sup>H NMR spectroscopy using CH<sub>2</sub>Br<sub>2</sub> as the internal standard.



**(±)-2-Tosyl-1,2,3,3a,4,6-hexahydro-5H-isoindol-5-one (5).** White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 7.9$  Hz, 2H), 7.34 (d,  $J = 7.9$  Hz, 2H), 5.65 (s, 1H), 4.08 (d,  $J = 14.0$  Hz, 1H), 3.88 (t,  $J = 8.6$  Hz, 1H), 3.75 (d,  $J = 14.0$  Hz, 1H), 2.99-2.75 (m, 3H), 2.74-2.67 (m, 1H), 2.61 (dd,  $J = 14.5, 5.1$  Hz, 1H) 2.44 (s, 3H), 2.14-2.02 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  208.0, 144.0, 138.3, 132.9, 130.0, 127.8, 116.4, 54.3, 50.6, 42.4, 38.8, 38.6, 21.7. HRMS (ESI) calcd. for  $\text{C}_{15}\text{H}_{18}\text{NO}_3\text{S}^+ (\text{M}+\text{H})^+$ : 292.1002. Found: 292.1004.

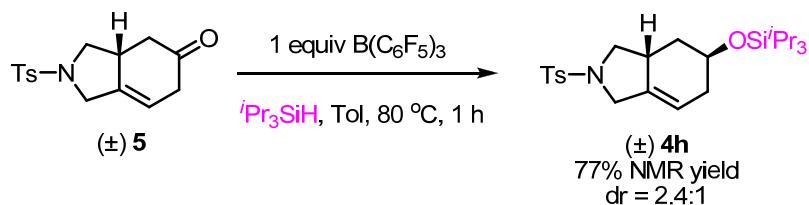


In a glovebox,  $B(C_6F_5)_3$  (2.6 mg, 0.005 mmol, 5 mol %) was added to a solution of **2h** (29.1 mg, 0.1 mmol, 1 equiv) in dry toluene (0.25 mL) before the vial was capped and closed tightly. The reaction mixture was then stirred at 80 °C for 1 h. After being allowed to cool to room temperature, one drop of  $Et_3N$  was added to the solution. After evaporation of all the volatiles in vacuo, the resulting mixture was analyzed by  $^1H$  NMR spectroscopy using  $CH_2Br_2$  as the internal standard.



In a glovebox,  $^t\text{Pr}_3\text{SiH}$  (31  $\mu\text{L}$ , 0.15 mmol, 1.5 equiv) or  $\text{Et}_3\text{SiH}$  (24  $\mu\text{L}$ , 0.15 mmol, 1.5 equiv) was added to a solution of **5** (29.1 mg, 0.1 mmol, 1 equiv) in a dry solvent

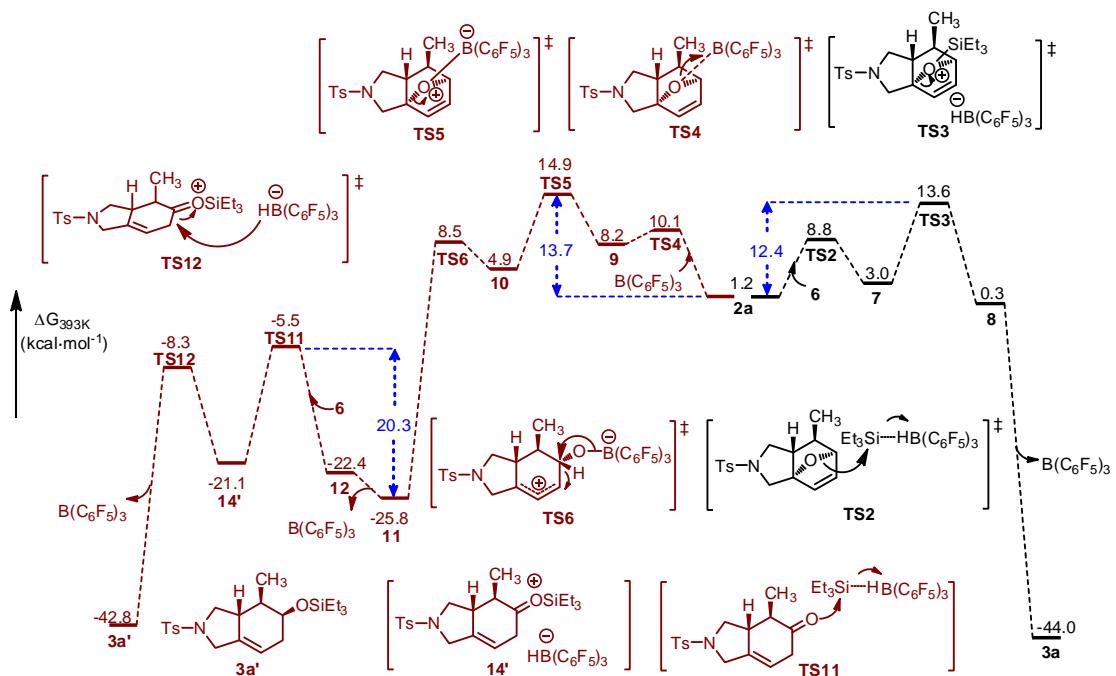
(0.25 mL of toluene or DCE) in an 8 mL vial.  $B(C_6F_5)_3$  (2.6 mg, 0.005 mmol, 5 mol %) was then added before the vial was capped and closed tightly. The reaction mixture was stirred at 80 °C. After being allowed to cool to room temperature, one drop of  $Et_3N$  was added to the solution. After evaporation of all the volatiles in vacuo, the resulting mixture was analyzed by  $^1H$  NMR spectroscopy using  $CH_2Br_2$  as the internal standard.



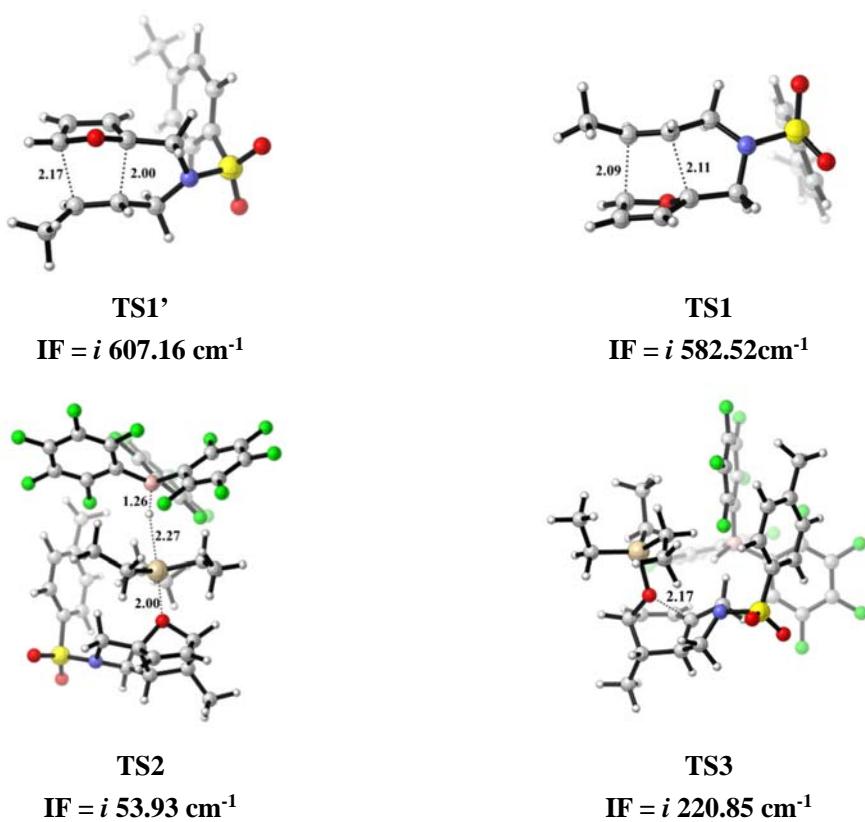
In a glovebox,  $iPr_3SiH$  (31  $\mu L$ , 0.15 mmol, 1.5 equiv) was added to a solution of **5** (29.1 mg, 0.1 mmol, 1 equiv) in dry toluene (0.25 mL) in an 8 mL vial.  $B(C_6F_5)_3$  (51.2 mg, 0.1 mmol, 1 equiv) was then added before the vial was capped and closed tightly. The reaction mixture was stirred at 80 °C for 1 h. After being allowed to cool to room temperature, one drop of  $Et_3N$  was added to the solution. After evaporation of all the volatiles in vacuo, the resulting mixture was analyzed by  $^1H$  NMR spectroscopy using  $CH_2Br_2$  as the internal standard.

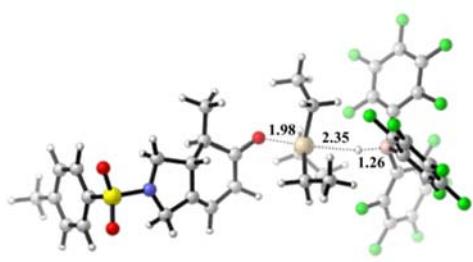
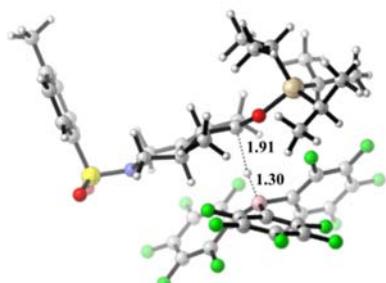
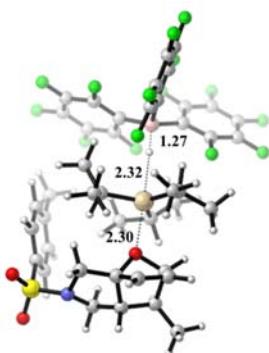
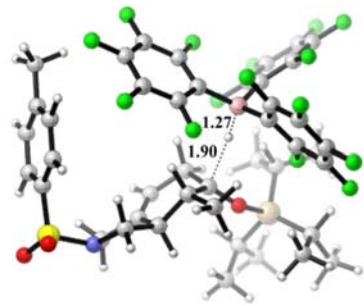
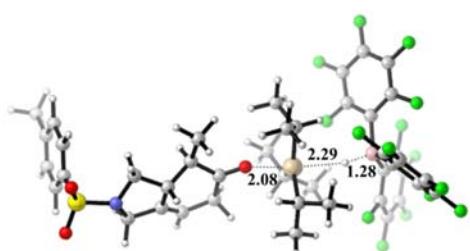
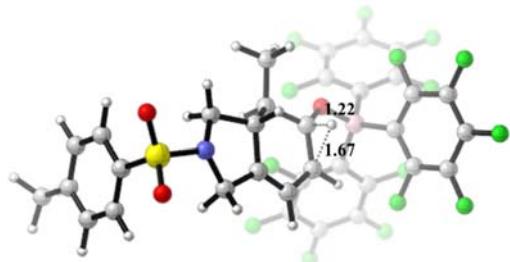
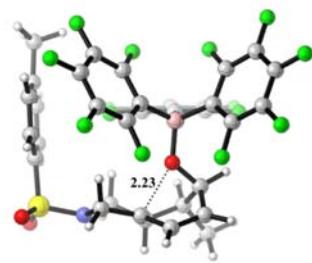
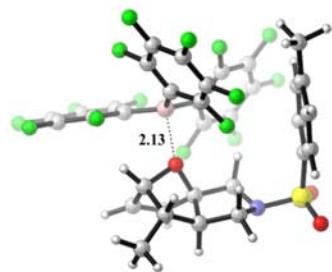
### 6.3 DFT studies

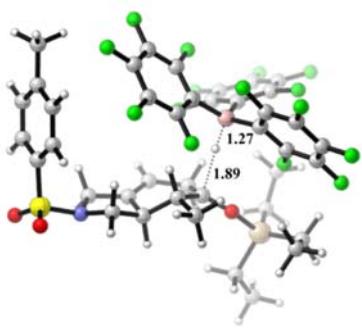
**Computational Methods:** All quantum chemical calculations were performed with Gaussian 09.<sup>[14]</sup> Geometrical optimizations and vibrational frequency analysis were calculated with the M06-2X<sup>[15]</sup> density functional and the 6-31G(d) basis set. Intrinsic Reaction Coordinate (IRC)<sup>[16,17]</sup> calculations were conducted to determine the connectivity of minima and transition states. Single point energy calculations were carried out with the M06-2X density functional, 6-311++G(d,p) basis set, and the SMD solvation model<sup>[18]</sup> with toluene as the solvent. Grimme's D3 empirical dispersion was used with M06-2X functional.<sup>[19]</sup> Gibbs free energies were evaluated at the reaction temperature (383 K or 393 K) using vibrational frequencies: rigid rotor harmonic oscillator (RRHO) vibrational entropies were used above 100  $cm^{-1}$ , while a free rotor description was used below this value, as described by Grimme.<sup>[20]</sup> Concentration was corrected from 1 atm to 1 mol/L. This was implemented using Goodvibes.<sup>[21]</sup> The calculated structures were displayed with the CYLview software.<sup>[22]</sup>



**Figure S1.** Energy profile (kcal/mol) for two possible pathways of the reaction of **2a** with Et<sub>3</sub>SiH (The sum of the energy values of **1a**, Et<sub>3</sub>SiH and B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> is the energy zero point).



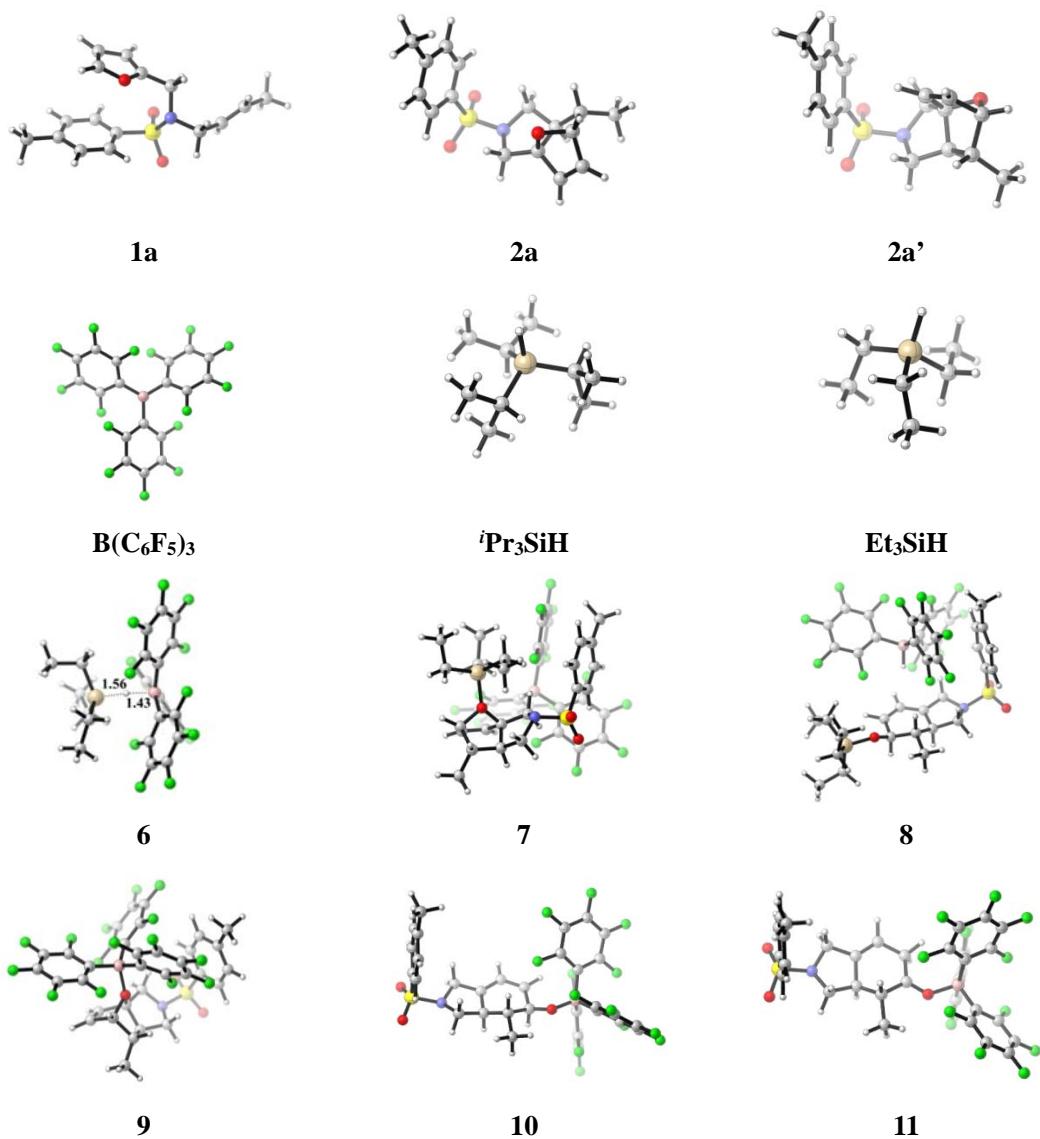


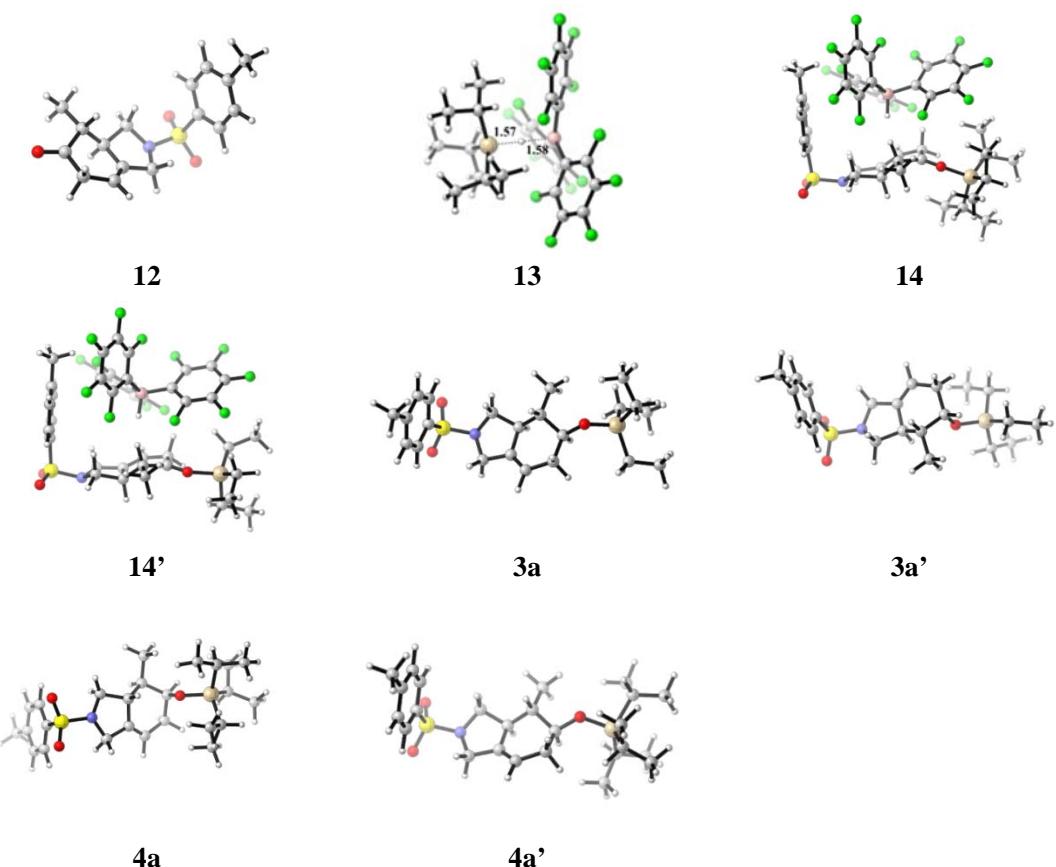


**TS12**

$\text{IF} = i \ 158.12 \text{ cm}^{-1}$

**Figure S2.** Optimized transition states and their corresponding imaginary frequencies (IF,  $\text{cm}^{-1}$ ). Bond distances are given in Å.





**Figure S3.** Optimized structures of starting materials and intermediates.

**Optimized Cartesian coordinates calculated at the M06-2X/6-31G(d) level**

<b>B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub></b>				<b>Et<sub>3</sub>SiH</b>			
B	-0.00049200	-0.00206900	-0.00018300	Si	0.02983400	-0.17970400	0.80563700
C	-1.47156100	-0.54385300	0.00102700	H	0.45450300	-0.54729100	2.18833400
C	-2.51595700	0.13476500	0.63751900	C	1.05240100	-1.19294700	-0.42038200
C	-1.82954300	-1.73673400	-0.63540100	H	0.68393700	-1.00187000	-1.43695900
C	-3.82129900	-0.33059800	0.65491800	H	0.87391000	-2.25955500	-0.23232900
C	-3.12655800	-2.22492800	-0.65356600	C	2.55296600	-0.88671800	-0.34264100
C	-4.12675300	-1.51681200	0.00020100	H	3.13386200	-1.51630000	-1.02424600
C	0.26461600	1.54321100	0.00015400	H	2.75727900	0.15676200	0.60585200
C	1.37600200	2.10979500	0.63252200	H	2.94092800	-1.05013400	0.66867000
C	-0.59324700	2.44858900	-0.63282500	C	0.37373800	1.66222200	0.55202600
C	1.62402900	3.47336900	0.64907800	H	1.44376200	1.84644000	0.71137700
C	-0.36940500	3.81649700	-0.65151800	H	-0.14792200	2.22788200	1.33426500
C	0.74544300	4.32987500	-0.00163700	C	-0.04813500	2.17429900	-0.83117300
C	1.20542600	-1.00360100	-0.00045800	H	-1.12876000	2.07033300	-0.97824200
C	2.41955300	-0.71077900	-0.63049100	H	0.19904200	3.23212400	0.96734800
C	1.14114800	-2.25049700	0.62994200	H	0.44726200	1.61623300	1.63416100
C	3.49386200	-1.58620500	-0.64798800	C	-1.81720800	-0.55528600	0.59009200
C	2.19986500	-3.14485700	0.64785000	H	-2.39218400	0.31155200	0.94158100
C	3.38191100	-2.80951700	0.00013200	H	-2.09019300	-1.38448200	1.25355900
F	-1.67869700	2.01439100	-1.27521700	C	-2.21885700	-0.90179100	-0.85064700
F	-1.20795300	4.63559400	-1.27708700	H	-1.71508000	-1.81240200	-1.19045700
F	0.97074900	5.63406800	-0.00279800	H	-3.29728400	-1.06828800	-0.93962400
F	2.68874800	3.96467400	1.27388400	H	-1.95016100	-0.10381800	-1.55113900
F	2.25369700	1.33711800	1.27432700				
F	-0.91269200	-2.45960100	-1.28061300				
F	-3.41971100	-3.35764700	-1.28338400	<b><i>i</i>Pr<sub>3</sub>SiH</b>			
F	-5.36920500	-1.97274100	0.00046000	Si	0.04670300	-0.04282500	-0.53058400
F	-4.77718300	0.34422600	1.28466600	H	-0.16943300	-0.07035100	-2.01086100
F	-2.28269400	1.27733500	1.28540300	C	1.86168200	-0.48964700	-0.20089800
F	0.03383700	-2.62755800	1.27100100	H	2.00838200	-1.49941200	-0.61098400
F	2.09474600	-4.31286600	1.27258800	C	2.82255200	0.45660700	-0.93025700
F	4.62280200	-1.26655600	-1.27161000	H	2.73199100	1.48163200	-0.55120300
F	2.58539000	0.44729000	-1.27149100	H	3.86513900	0.14956500	-0.78172200
F	4.40008400	-3.65505600	0.00033400	H	2.63119400	0.48234000	-2.00816900
				C	2.17604500	-0.52892100	1.29981700
				H	1.51330700	-1.21136000	1.84521800
				H	3.20840100	-0.85300700	1.48005500
<b>TS1'</b>				H	2.06839600	0.46723300	1.74694900
N	0.57267700	-1.62123300	-0.16117100	C	-1.10849400	-1.34004500	0.23786900
C	0.96874200	-0.96036200	-1.43079900	H	-1.07887400	-1.20539500	1.32947200
C	2.51450300	-0.466667300	0.56496500	C	-2.55582900	-1.14108200	-0.23054600
C	1.24270700	-1.09302900	1.05912200	H	-2.62977100	-1.23279600	-1.32079200
C	3.24820400	0.61570300	1.07337200	H	-3.21940400	-1.89634900	0.20856900

C	-2.46617600	-0.07997400	-1.06338400	H	-2.94899600	-0.15633500	0.04493400
C	-3.11315000	1.14758000	-0.98980500	C	-0.63094100	-2.76183600	-0.08255500
C	-3.27494700	1.80559000	0.23416900	H	0.35716000	-2.96760200	0.34270200
C	-2.78499300	1.19615900	1.39301300	H	-1.32764000	-3.50900000	0.31706800
C	-2.13560400	-0.03332400	1.33885600	H	-0.56678200	-2.92249400	-1.16613400
C	-4.00031200	3.12445100	0.30139800	C	-0.34916200	1.70733700	0.11338100
S	-0.99148000	-2.14171000	-0.00668100	H	0.60108700	2.26180400	0.10900300
O	-1.06307400	-2.81119500	1.28083700	C	-0.87124600	1.68799100	1.55699800
O	-1.34631800	-2.79423800	-1.25551600	H	-1.01912400	2.70790200	1.93244600
H	3.12567500	-1.18450100	0.01188700	H	-1.83833900	1.17533200	1.61922400
H	2.77855000	1.23206100	1.83837400	H	-0.18607200	1.17701200	2.24253300
H	-2.35870300	-0.60335400	-2.00847900	C	-1.32758800	2.45508700	-0.80232500
H	-3.50411000	1.60286000	-1.89599000	H	-1.53592400	3.46049300	-0.41562500
H	-2.92034800	1.68841600	2.35243500	H	-0.93368100	2.55851600	-1.81797100
H	-1.77547700	-0.52063300	2.23974100	H	-2.28697500	1.92887800	-0.87543900
H	-3.77220300	3.74518300	-0.56936100				
H	-5.08437300	2.96764400	0.31957900	<b>1a</b>			
H	-3.73040200	3.68200900	1.20171400	C	-0.09212100	1.88710200	-0.17213900
C	4.75655800	0.54165600	1.13765800	C	0.42332000	2.56199500	0.88867300
H	5.15276100	0.06551600	0.23403700	C	1.76646600	2.90501000	0.52985300
H	5.20973800	1.53412400	1.22606600	C	1.95562500	2.40226900	-0.71703500
H	5.09096800	-0.05077300	1.99792300	O	0.83312000	1.79170600	-1.16113700
C	1.57742100	0.34023500	-1.00893400	H	-0.08799400	2.75701800	1.82020200
C	0.85648800	1.45089600	-0.48634000	H	2.49218800	3.43975400	1.12440700
O	2.77267200	0.80287000	-1.49987300	H	2.79531400	2.39093200	-1.39467700
C	1.79491900	2.42893900	-0.27291600	C	-1.41800000	1.25874800	-0.41765500
C	3.02861900	1.86849700	-0.68231800	H	-2.07373900	1.48293900	0.43174400
H	0.09107700	-0.83659200	-2.07073900	H	-1.87324300	1.68174800	-1.32063600
H	1.69585400	-1.57690200	-1.96689500	N	-1.32204900	-0.18993500	-0.66468200
H	0.62281500	-0.34405200	1.57465000	C	-2.56105600	-0.77686800	-1.22078100
H	1.40652500	-1.93561000	1.73462100	H	-2.73858100	-0.25834300	-2.16956400
H	3.96649200	2.37605700	-0.87139800	H	-2.34846400	-1.82467600	-1.43928700
H	1.67379800	3.37659300	0.23401700	C	-3.75410700	-0.64498000	-0.31613500
H	-0.18367500	1.43964900	-0.18391200	C	-4.80675300	0.12443900	-0.58740300
				H	-3.71568900	-1.21464800	0.61348600
<b>6</b>				H	-4.81680200	0.68488800	-1.52470200
Si	0.02273700	-0.21319100	2.49838000	C	-6.00835100	0.27880300	0.29535100
C	1.86453400	-0.38457500	2.85886300	H	-6.16128400	1.32825600	0.57050400
H	2.40866500	-0.05740800	1.96434900	H	-6.91791100	-0.05164200	-0.21866800
H	2.10513100	0.35881600	3.63029200	H	-5.90101700	-0.30484800	1.21333800
C	2.34442600	-1.77402300	3.29897900	S	-0.64888500	-1.06343600	0.61098000
H	3.42346200	-1.77185800	3.47948200	O	-0.92871700	-0.40542700	1.88273000
H	1.85794100	-2.09115700	4.22698600	O	-1.05477900	-2.44721100	0.40020100
H	2.13681500	-2.53241800	2.53966200	C	1.09509500	-0.93612400	0.29369800

C	-1.02472900	-1.74905700	2.80133600	C	1.59542700	-1.39710400	-0.92293900
H	-1.00978300	-2.34723200	1.88207400	C	1.93237700	-0.44028200	1.28124100
H	-0.50385300	-2.35732900	3.55267000	C	2.96279200	-1.35312800	-1.14358900
C	-2.47166000	-1.48985400	3.24440100	H	0.91465200	-1.77520500	-1.67929600
H	-2.99957200	-2.43424900	3.40671400	C	3.30564900	-0.41115700	1.04407500
H	-2.51212300	-0.92643600	4.18189600	H	1.50732000	-0.07829300	2.21169300
H	-3.03267100	-0.92157300	2.49854500	C	3.83651500	-0.86274300	-0.16283300
C	-0.71359400	1.36878900	3.18687400	H	3.36636900	-1.70840000	-2.08835000
H	-0.19479000	2.22525300	2.74084400	H	3.97244300	-0.02462800	1.81003500
H	-1.76336100	1.43593000	2.87966300	C	5.31884200	-0.81235300	-0.42935000
C	-0.59151000	1.42641300	4.71910600	H	5.68773700	-1.77840100	-0.78717200
H	-1.04370500	2.34047600	5.11408500	H	5.55119000	-0.06924400	-1.20025200
H	-1.09112600	0.57959300	5.20153200	H	5.87672600	-0.54699500	0.47176000
H	0.45559400	1.41584100	5.03780100				
H	-0.03750800	-0.00512500	0.95221200				
B	0.00538200	0.07599600	-0.47932900	<b>TS1</b>			
C	-0.26626600	1.64581000	-0.61904500	C	2.09865200	-0.08451300	-1.10349500
C	0.53253600	2.55504200	0.06845400	C	3.41668100	0.10984000	-1.58097200
C	-1.28771400	2.20627200	-1.37857400	C	4.11164200	-1.02730100	-1.23867500
C	0.34830400	3.92653600	0.02941400	C	3.18489300	-1.85057300	-0.55223100
C	-1.50260800	3.57795500	-1.45766800	O	1.92437200	-1.41945900	-0.86354300
C	-0.67932200	4.44169000	-0.75144900	H	3.79984300	1.03528300	-1.98917300
C	1.49945400	-0.44401100	-0.72165000	H	5.17425800	-1.20782500	-1.32179300
C	1.90039800	-1.66733000	-0.19158800	H	3.27135000	-2.91126000	-0.35093700
C	2.49650400	0.26838600	-1.38140200	C	0.84000100	0.69796100	-1.30622300
C	3.18981300	-2.16315800	-0.27007300	N	0.46475200	1.27388300	-0.00041300
C	3.80200900	-0.19793000	-1.50242500	C	0.94812000	0.48008300	1.14037900
C	4.15134800	-1.41690600	-0.94100300	S	-1.05399900	1.93992500	0.09543900
C	-1.20210100	-0.92464600	-0.79229900	O	-1.15018200	2.56523400	1.40314100
C	-2.43874600	-0.71378100	-0.18850400	O	-1.24063100	2.68394500	-1.13986300
C	-1.11704700	-2.06239700	-1.58807900	C	-2.18973400	0.56913900	0.07235800
C	-3.52016800	-1.56709800	-0.32291000	C	-2.49749300	-0.07863800	1.26771400
C	-2.18288900	-2.93802400	-1.76824900	C	-2.71323800	0.12871200	-1.13973500
C	-3.38897200	-2.69169800	-1.12875000	C	-3.33614000	-1.18522600	1.23822500
F	0.01714100	-2.36891100	-2.22516700	H	-2.10026100	0.30230100	2.20373500
F	-2.05193500	-4.01173400	-2.54202600	C	-3.55201400	-0.98168100	-1.14918700
F	-4.41028400	-3.52511600	-1.28280300	H	-2.48070600	0.66927800	-2.05208200
F	-4.66423300	-1.32415900	0.31320500	C	-3.87238000	-1.65243100	0.03309800
F	-2.60222700	0.35736500	0.60855100	H	-3.58636900	-1.69422600	2.16546400
F	-2.12238100	1.43311200	-2.08024200	H	-3.96891000	-1.33058600	-2.09009100
F	-2.48968000	4.06541000	-2.20419400	C	-4.80304200	-2.83743800	0.02334300
F	1.52984800	2.09502500	0.84777500	H	-5.80942100	-2.54070300	0.33847800
F	1.13637000	4.74530100	0.72226000	H	-4.88190200	-3.27347100	-0.97550800
F	-0.87437100	5.75307400	-0.81483100	H	-4.45942700	-3.61480300	0.71159400
				C	2.42675500	0.27773700	0.95004400

F	1.00568600	-2.40818400	0.48845000	H	3.00086100	1.20248100	0.92438600
F	3.51080100	-3.32678600	0.29086300	C	3.09291500	-0.90112100	1.30891100
F	5.39533300	-1.86764800	-1.04157000	H	2.47677000	-1.69745300	1.72692000
F	4.71663500	0.51871000	-2.14937900	C	4.51652800	-0.85039000	1.80895200
F	2.23703500	1.45333400	-1.94111700	H	4.55725300	-0.58502600	2.87166200
<b>7</b>				H	5.02613600	-1.81228600	1.68652800
				H	5.08468100	-0.09443200	1.25692700
N	3.20226000	-0.51024600	1.36802300	H	0.44025500	-0.49658400	1.19789900
C	1.92160900	0.14344800	1.05762200	H	0.72414500	1.05093500	2.04567700
C	2.31204400	1.58099300	0.98565000	H	0.06687700	0.01164300	-1.68267000
C	3.35206600	1.78404900	2.11478000	H	0.97394300	1.50804900	-2.02407000
C	4.03490400	0.40244000	2.20773100	<b>2a</b>			
C	1.36922700	2.74946900	0.89515400	C	2.40603500	0.34206700	0.61546300
C	2.08879900	3.78743100	0.46406600	C	2.08090800	-0.01341000	-0.87799100
C	3.50408100	3.29241900	0.25561000	C	3.38926600	-0.08568800	-1.63824900
C	4.19651200	2.98225400	1.61227100	C	3.96995400	-1.20869700	-1.21356300
O	3.24635600	1.89594900	-0.17120500	C	2.99454200	-1.81417100	-0.21242200
C	4.24962400	4.17637700	2.55539800	C	3.04978400	-0.97066500	1.11147200
C	2.02471800	-2.86869600	0.87874600	C	0.65945600	1.11377000	0.44628300
C	-0.12635500	-3.63706500	0.16373000	C	0.88733900	0.82801100	-1.28684000
C	0.43618500	-4.14177500	-1.01120700	C	1.81230800	-3.98839700	-1.73715600
C	2.61827900	-3.36804500	-0.27924200	C	-2.15427300	0.55916500	0.06892500
C	-0.42140100	-4.86548000	-2.01616100	C	-2.43465300	-0.09719900	1.26690800
S	3.02216600	-2.03827400	2.08203900	C	-3.20610200	-1.25126000	1.23874600
O	2.24294400	-1.89549700	3.30754800	C	-3.70203700	-1.75885000	0.03226000
O	4.36223300	-2.60008800	2.12454300	C	-3.41737700	-1.07492300	-1.15099800
H	1.19262900	0.06277100	1.87524700	C	-2.64530800	0.08311500	-1.14296600
H	1.46788100	-0.25298600	0.15137100	C	-4.52520800	-3.02093600	0.02189900
H	2.82385100	2.01983900	3.04257400	S	-1.10425300	1.99508800	0.08880500
H	4.07347200	0.06054000	3.24696200	O	-1.34147500	2.72702600	-1.14451000
H	5.05300100	0.41138100	1.80962100	O	-1.22708100	2.60840700	1.40031200
H	0.33192000	2.70197300	1.20015100	C	4.43346200	-0.82255100	1.72921600
H	1.76874800	4.81274800	0.33153400	H	3.07395400	1.20554600	0.68953300
H	4.12287800	3.79955800	-0.48224900	H	2.37723700	-1.46060100	1.82447300
H	5.21140100	2.63944500	1.38363700	H	1.01339400	1.34999300	2.01215300
H	4.77070000	3.90597800	3.47746400	H	0.44863100	-0.21811800	1.35513000
H	4.78373300	5.01787300	2.10275000	H	-2.07234000	0.31612300	2.20327100
H	3.24221900	4.50899200	2.82257300	H	-3.43799400	-1.76507800	2.16821000
H	0.23138200	-2.59933800	2.03140100	H	-3.81169000	-1.44912200	-2.09174500
H	-1.19455900	-3.74320600	0.32913200	H	-2.44431000	0.63396500	-2.05659700
H	2.25398700	-4.37389200	-2.14002200	H	-3.90252900	-3.89220100	0.25151500
H	3.69136400	-3.27284200	-0.42103100	H	-5.31899000	-2.97840700	0.77375900

H	-1.47952500	-4.63714600	-1.86243900	H	-4.98753500	-3.18613900	-0.95409000
H	-0.15077300	-4.58732100	-3.03810300	H	4.38444000	-0.26171500	2.66732200
H	-0.29322100	-5.94921000	-1.91851600	H	4.87621700	-1.80061200	1.94709700
Si	3.03482200	1.39485600	-1.92524300	H	5.10737000	-0.28606200	1.05367300
C	3.58705500	-0.38410100	-1.93803600	H	0.12569700	0.17548900	-1.73376200
H	2.90555900	-0.99860100	-1.34310700	H	1.13916500	1.62100300	-1.99390900
C	4.32073400	2.49238100	-2.74163000	H	3.78667500	0.68761300	-2.28432400
H	5.23671300	2.49322400	-2.13557200	H	4.96243400	-1.58020400	-1.43667500
C	1.27849800	1.75432100	-2.41425700	H	3.02167300	-2.89551600	-0.07568200
H	1.11807600	2.83866100	-2.44358500				
C	0.92476500	1.11932000	-3.77142900	<b>2a'</b>			
H	-0.14256800	1.24323500	-3.97585200	C	2.41937800	-0.35134600	0.37386100
H	1.47505500	1.58298100	-4.59653500	C	1.71468900	0.26151300	-0.86246000
H	1.13838400	0.04588900	-3.78413600	C	0.86675600	1.45135900	-0.42471800
C	5.03442300	-0.56883200	-1.46509400	C	1.74140600	2.42076000	-0.16577400
H	5.15144500	-0.22539600	-0.43308100	C	3.09783300	1.78133600	-0.39398000
H	5.32398400	-1.62335800	-1.48932600	C	3.31036500	0.81001200	0.84479000
H	5.74307200	-0.01929500	-2.09473500	C	1.25887400	-1.04820300	1.05758300
C	4.65130400	2.00543600	-4.16405700	N	0.56718200	-1.60099300	-0.14712500
H	5.40935400	2.64205400	-4.62794000	C	0.96636900	-0.93028600	-1.41958200
H	5.03818900	0.98153500	-4.15674900	O	2.82755600	0.88438800	-1.48793700
H	3.76928200	2.02176800	-4.81099900	C	-1.98118000	-0.66721500	0.10702200
H	3.46841100	-0.73963600	-2.97232500	C	-2.49300200	-0.12391100	-1.07018000
H	0.60054000	1.37716600	-1.64039600	C	-3.15586100	1.09657000	-1.02020700
H	3.96237300	3.52847100	-2.78380000	C	-3.31917800	1.77967500	0.18959900
B	-1.62197500	0.34725300	0.00576300	C	-2.81378500	1.20317900	1.35877700
C	-1.78718600	-0.54220700	1.36758500	C	-2.14859600	-0.01836300	1.32837100
C	-1.23235100	-0.09342500	2.56099300	C	-4.06272500	3.08937300	0.23157300
C	-2.44971900	-1.75985800	1.47789400	S	-0.98529700	-2.14098100	0.02154700
C	-1.25200400	-0.79844400	3.75773400	O	-1.04220300	-2.78737700	1.32178300
C	-2.49966600	-2.50943200	2.64732600	O	-1.33179100	-2.81970000	-1.21504300
C	-1.89782200	-2.02624500	3.80130800	C	4.77031500	0.40787000	1.01670300
C	-1.76853200	-0.53792600	-1.36536300	H	3.07740500	-1.13173000	-0.02891600
C	-2.98138500	-0.78451000	-2.00920600	H	2.93711500	1.28938500	1.75494600
C	-0.67669300	-1.12382500	-1.99097000	H	1.52661800	-1.86884900	1.72319600
C	-3.10391600	-1.52298400	-3.18003700	H	0.62134700	-0.33466900	1.59938500
C	-0.74188800	-1.85689000	-3.16789400	H	0.08889400	-0.66568700	-2.01513200
C	-1.96955100	-2.06568100	-3.77046800	H	1.61128400	-1.58855200	-2.00805700
C	-2.61607700	1.64333100	0.04053500	H	-2.38349800	-0.66775600	-2.00342400
C	-3.90345800	1.62545700	0.57341000	H	-3.55853800	1.52569100	-1.93400000
C	-2.20719100	2.88475500	-0.43231600	H	-2.94980200	1.71531500	2.30761300
C	-4.71992700	2.74719000	0.64898900	H	-1.77710800	-0.48016200	2.23802800
C	-2.98594000	4.03419800	-0.37991000	H	-3.84754000	3.69391700	-0.65375700
C	-4.25667000	3.96371900	0.16739100	H	-5.14435700	2.91773100	0.25859800

H	-0.48844700	0.78495400	0.02208200	H	-3.79634900	3.67016000	1.11811200
F	-4.12105800	-0.32052400	-1.48776200	H	5.38461200	1.26744300	1.30287400
F	-4.29630800	-1.72499600	-3.74036200	H	4.88490100	-0.36176800	1.78627000
F	-2.05902700	-2.78474700	-4.88824600	H	5.16098000	0.00806800	0.07481600
F	0.37619100	-2.36057900	-3.71341500	H	3.94421500	2.42579700	-0.63279200
F	0.57322400	-1.00861200	-1.47906100	H	-0.21169800	1.44649700	-0.30236500
F	-0.59053600	1.10022900	2.59965100	H	1.56755400	3.40938100	0.24104800
F	-0.68045600	-0.30105200	4.85352100				
F	-1.94954000	-2.72291300	4.93308300				
F	-3.11222900	-3.69404500	2.66246700	<b>TS2</b>			
F	-3.05747300	-2.31143100	0.41394700	C	-5.03739300	2.29788900	0.13895500
F	-0.97893300	3.03919700	-0.97473800	C	-3.91481800	2.07495500	-0.92358900
F	-2.52127400	5.19842900	-0.84608100	C	-3.79257600	3.33302700	-1.74890000
F	-5.02392400	5.05099800	0.23054400	C	-3.28748400	4.26250900	-0.93696100
F	-5.94123200	2.67115400	1.17876100	C	-3.04800500	3.58614200	0.39960500
F	-4.42232000	0.48704100	1.04882600	C	-4.40571700	3.31545100	1.10988400
				C	-5.30808100	0.86676600	0.59868100
				N	-5.24829200	0.17165300	-0.68905500
<b>8</b>				C	-4.12587700	0.67703300	-1.49007300
N	0.99347400	-3.42217400	-1.61687600	O	-2.73498300	2.22095300	-0.03285300
C	0.65190500	-2.07195300	-2.05532600	C	-4.24871900	-2.30119300	-0.10415700
C	-0.79035300	-1.97378300	-1.76849600	C	-4.13979400	-2.41598700	1.28184100
C	-1.27687800	-3.22379400	-1.12787700	C	-2.98842600	-2.98011800	1.81552400
C	0.00305300	-3.93345900	-0.65835600	C	-1.94652300	-3.42317000	0.98996100
C	-1.62078200	-0.87591900	-2.00573600	C	-2.10444300	-3.33954100	-0.39709900
C	-2.86829700	-0.91115200	-1.44655100	C	-3.24802600	-2.77217000	-0.95100400
C	-3.45560400	-2.08317200	-0.72025300	S	-5.63905400	-1.44758000	-0.79552200
C	-2.37748700	-2.97596800	-0.08725300	O	-5.68134300	-1.73641400	-2.21733800
C	-2.96474300	-4.27310800	0.45123500	O	-6.78078400	-1.62272000	0.08317900
C	3.13434300	-2.81874000	0.04544100	C	-5.23534100	4.56761000	1.35946000
C	3.70572500	-1.56183000	-0.14850600	H	-5.93071700	2.69039000	-0.35553500
C	4.16436200	-0.85379900	0.95818000	H	-4.17820300	2.82295900	2.06181900
C	4.04612400	-1.37659300	2.24858400	H	-6.29017400	0.71967900	1.04872600
C	3.45886600	-2.63654100	2.41456000	H	-4.52591600	0.52084200	1.29530800
C	3.00545200	-3.36610200	1.32231900	H	-4.95611600	-2.08807400	1.91895100
C	4.56238200	-0.60289900	3.43368900	H	-2.88847800	-3.07643000	2.89406200
S	2.61326800	-3.76393400	-1.36461000	H	-1.31567100	-3.70086800	-1.04916400
O	3.28444600	-3.22755700	-2.53439500	H	-3.37911400	-2.70406700	-2.02701500
O	2.63934500	-5.16858300	-1.00202200	H	-6.16692600	4.31075500	1.87059800
O	-4.34656500	-1.68406900	0.27156000	H	-4.69534700	5.28331300	1.98711900
Si	-5.84665200	-0.91185900	0.06306800	H	-5.49438700	5.05971100	0.41678600
C	-5.61245900	0.95636900	-0.11072900	H	-3.22249600	0.05933600	-1.38884900
C	-5.75367900	1.54656000	-1.52192700	H	-4.40063500	0.70344200	-2.54767000
C	-6.75695200	-1.32159800	1.64539200	H	-4.16458000	3.44017500	-2.76041300
C	-5.97428800	-0.89378100	2.89571400	H	-3.13731400	5.31698800	-1.13087300

C	-6.68279800	-1.64860200	-1.45551200	H	-2.25237400	3.97780500	1.02908300
C	-8.18901800	-1.33969400	-1.47023500	Si	-0.90356700	1.43022200	-0.22264900
H	0.89981100	-1.89250600	-3.10894400	B	2.23175300	-0.12312600	-0.04840600
H	1.14086500	-1.26517900	-1.47179700	C	3.17648300	1.19760500	-0.05049100
H	-1.70973100	-3.80251100	-1.96912200	C	4.12253100	1.53757800	0.90895400
H	-0.05604100	-5.01867500	-0.74112900	C	2.99192700	2.15369100	-1.04415800
H	0.23040500	-3.65483600	0.38003400	C	4.81632900	2.74539800	0.90283100
H	-1.24245300	0.01022100	-2.49976700	C	3.64552200	3.37344600	-1.08787200
H	-3.97569000	-2.67646200	-1.50645500	C	4.57260100	3.67279800	-0.09762600
H	-1.93410400	-2.40236600	0.73484400	C	2.17109500	-0.86622500	1.40538800
H	-3.75059700	-4.05297100	1.17692800	C	1.62331300	-0.19370100	2.49124500
H	-2.19565900	-4.86897300	0.95140700	C	2.60209700	-2.15617700	1.70126900
H	-3.39499200	-4.87592800	-0.35739700	C	1.45376300	-0.73318800	3.75671900
H	3.81969600	-1.16477700	-1.15416500	C	2.46926700	-2.74223700	2.95769900
H	4.62708600	0.11857500	0.82241600	C	1.88626000	-2.03001500	3.99468000
H	3.34648400	-3.04610800	3.41547800	C	2.49071300	-1.15702000	-1.27437000
H	2.58383100	-4.35866900	1.44707300	C	1.60861200	-2.22105500	-1.42670400
H	3.98137300	-0.81935100	4.33472900	C	3.47098100	-1.07897000	-2.25504300
H	5.60625500	-0.86562600	3.63888700	C	1.66313600	-3.14868200	-2.44937800
H	4.52010700	0.47383200	3.24606100	C	3.57013600	-1.98805700	-3.30755700
H	-4.63436100	1.22985900	0.30501800	C	2.66254200	-3.02973800	-3.40754900
H	-5.04748500	1.10810400	-2.23746900	F	4.39185400	-0.10678200	-2.23887400
H	-5.56735400	2.62301100	-1.51300800	F	4.53210400	-1.86133600	-4.22143100
H	-6.75474700	1.37827900	-1.93143200	F	2.74211400	-3.90358500	-4.40821800
H	-6.95424400	-2.40100900	1.67314300	F	0.76392900	-4.13719700	-2.52832600
H	-5.00166300	-1.39273800	2.93797800	F	0.60252900	-2.36435200	-0.53691400
H	-6.51859100	-1.13834700	3.81245400	F	2.09094800	1.91845900	-2.02178400
H	-5.79062200	0.18595700	2.89984100	F	3.37761400	4.26074600	-2.04988100
H	-6.53033900	-2.73625000	-1.46341100	F	4.41425200	0.70203600	1.91498900
H	-8.69416600	-1.81771600	-0.62520200	F	5.70742900	3.02050600	1.85492300
H	-8.66590400	-1.69732800	-2.38718700	F	5.21329200	4.83976700	-0.10939900
H	-8.38143600	-0.26320900	-1.39856200	F	1.21243900	1.08303500	2.33440300
H	-3.49502000	-0.02385600	-1.51753300	F	0.88756800	-0.01842800	4.73274500
B	0.62226100	1.35077700	-0.20482900	F	1.74284700	-2.58032500	5.19836700
C	1.98304900	1.40555600	-1.11384800	F	2.88283900	-3.99219200	3.16605800
C	1.95296300	1.02050500	-2.45123800	C	-1.36114200	-0.00085500	0.90155600
C	3.25313400	1.75116700	-0.66064900	H	-2.18683200	-0.54533000	0.42082800
C	3.06864000	0.92926200	-3.27511800	H	-0.52697600	-0.70917200	0.93703500
C	4.40131600	1.67567700	-1.43918400	C	-0.92185600	1.24039400	-2.09355900
C	4.31339300	1.26142600	-2.76142300	H	-1.87957100	1.62107400	-2.46743000
C	0.87780100	0.75602800	1.29774700	H	-0.16504400	1.92549500	-2.48740900
C	1.34124600	1.47783800	2.39636700	C	0.05880000	2.89641000	0.43702600
C	0.60342900	-0.57363600	1.57727800	C	-0.65241600	-0.17545600	-2.62140800
C	1.56185000	0.90989200	3.64719500	H	-1.00889900	-0.28327700	-3.64994200

C	0.77057700	-1.18319500	2.80982500	H	0.42123700	-0.36799800	-2.61636600
C	1.27761600	-0.43307000	3.855579700	H	-1.12793900	-0.95627000	-2.01404400
C	-0.21175900	2.74731100	-0.17135000	C	0.17915200	4.08898700	-0.52216600
C	-1.60055700	2.73783700	-0.20444200	H	0.66827600	4.93268900	-0.02614000
C	0.35806000	4.01470900	-0.10444700	H	0.79057200	3.82457400	-1.38924500
C	-2.38778000	3.87968200	-0.17674600	H	-0.78633600	4.43840700	-0.90296200
C	-0.38638300	5.18914200	-0.08069000	C	-1.77898700	0.41287300	2.31907900
C	-1.77246300	5.12071500	-0.11636200	H	-2.14248300	-0.45819100	2.87402000
H	-0.09037100	0.54994900	-0.74834000	H	-0.94584800	0.84140900	2.87967600
F	1.59533300	2.78443200	2.28590500	H	-2.58861200	1.15195900	2.30295300
F	2.06655100	1.63240800	4.64737800	F	3.17470400	-2.92877700	0.76858600
F	1.53892300	-1.00484100	5.03297400	H	1.07641200	0.32189400	-0.25468100
F	0.49636500	-2.48442300	2.96785900	H	-0.34453700	3.18879600	1.41512100
F	0.12457200	-1.39815700	0.60656000	H	1.06071500	2.51935900	0.65909200
F	0.78297700	0.66721000	-3.04038100	C	-0.67239800	-3.93764900	1.60300700
F	2.94644900	0.53963800	-4.54413000	H	-0.10352700	-3.09870500	2.02363800
F	5.40030300	1.19234900	-3.52311900	H	-0.87757200	-4.63906800	2.41696300
F	5.59065200	1.96824900	-0.91013500	H	-0.03526100	-4.42625500	0.86355000
F	3.44369600	2.13657400	0.60782700				
F	1.68791100	4.14998300	-0.06186400				
F	0.21217600	6.37849200	-0.02493600	<b>TS3</b>			
F	-2.50475800	6.23292200	-0.09279000	N	-3.10496600	-0.50359400	-1.49237900
F	-3.72421200	3.79254200	-0.20966200	C	-1.73046800	-0.01941300	-1.57356400
F	-2.27759700	1.56377500	-0.26787900	C	-1.90160200	1.41018000	-1.82467300
H	-7.73818500	-0.82908900	1.62751400	C	-3.16349900	1.62824900	-2.60786900
H	-6.34935000	1.43692100	0.54705000	C	-3.98623800	0.34789000	-2.33904400
H	-6.21749700	-1.26236600	-2.37289600	C	-0.96030500	2.49339300	-1.66682200
				C	-1.56236700	3.60080700	-1.20047800
				C	-3.03610100	3.37323200	-0.91152200
<b>TS4</b>				C	-3.77382800	3.00099700	-2.21313500
C	0.64339900	-1.14060700	3.36592200	O	-3.10319300	2.14831600	-0.17714100
C	0.12416100	-1.64269300	1.97560600	C	-3.68863000	4.05959400	-3.30566500
C	-1.09144200	-2.50039100	2.25979500	C	-2.33329500	-2.84344600	-0.46604900
C	-2.04282600	-1.65306400	2.65391000	C	-1.01054100	-3.22356800	-0.67236700
C	-1.42417200	-0.26693900	2.57777800	C	-0.28636500	-3.72510200	0.40374100
C	-0.39909400	-0.07319900	3.73553600	C	-0.86253400	-3.82845900	1.67293300
C	2.08332300	-0.73750900	3.06736900	C	-2.19586100	-3.43759500	1.84628800
N	2.46732500	-1.80454900	2.13031900	C	-2.94343600	-2.95316600	0.78143500
C	1.36056600	-2.05970100	1.19224400	C	-0.05639600	-4.36092600	2.82825400
O	-0.51102900	-0.42671500	1.46342400	S	-3.25837300	-2.16160100	-1.80883300
C	4.08066800	-0.35681300	0.46220500	O	-2.56936600	-2.46515700	-3.05866400
C	4.46482800	0.85893500	1.02356600	O	-4.67828600	-2.43204700	-1.66009000
C	4.38250900	2.01122700	0.25305700	H	-1.19450800	-0.39429100	-2.47266800
C	3.91155100	1.96658500	-1.06274200	H	-1.12755300	-0.25771900	-0.69489000
C	3.57395900	0.72883400	-1.61573300	H	-2.83780800	1.65950700	-3.65868200

C	3.65370800	-0.43722000	-0.86119500	H	-4.24769700	-0.15298300	-3.27706500
C	3.78277100	3.22849700	-1.87524900	H	-4.90350600	0.56159900	-1.78689700
S	4.00753500	-1.80053000	1.49394700	H	0.10697000	2.34143100	-1.77718300
O	4.07737200	-2.96991800	0.63450000	H	-1.02555400	4.51043100	-0.95126900
O	4.90239800	-1.59543800	2.61932300	H	-3.51459800	4.20032800	-0.37941400
C	-0.99657700	-0.20012400	5.12954100	H	-4.81884800	2.82873000	-1.93558100
H	0.64663400	-1.97815300	4.07000000	H	-4.28496400	3.76482800	-4.17334900
H	0.03548200	0.92407500	3.60103000	H	-4.07081300	5.02071000	-2.94792100
H	2.74230600	-0.76333100	3.93617400	H	-2.65665800	4.20543400	-3.64001900
H	2.12532900	0.25618100	2.59821400	H	-0.56322000	-3.13070300	-1.65860600
H	4.82617500	0.88705300	2.04694900	H	0.74558500	-4.03346500	0.26186800
H	4.66738800	2.96666000	0.68443100	H	-2.64792900	-3.51002600	2.83136200
H	3.24035000	0.68390600	-2.64865700	H	-3.98295100	-2.66163400	0.90307000
H	3.40205000	-1.40558200	-1.28615300	H	1.00640200	-4.14081000	2.69161400
H	4.72091700	3.46257100	-2.39036000	H	-0.38446900	-3.91967500	3.77328300
H	3.00233400	3.12408000	-2.63433900	H	-0.16648800	-5.44814500	2.90850300
H	3.53227800	4.07854900	-1.23473100	Si	-2.92639900	2.04833300	1.54725900
H	-0.22901000	-0.05214000	5.89439700	C	-3.56546400	0.35859800	2.02010400
H	-1.78152500	0.54522600	5.29332000	H	-2.85664000	-0.40955500	1.69577900
H	-1.43050600	-1.19430000	5.27709800	C	-4.06397100	3.39919200	2.21621700
H	1.44921300	-1.42846000	0.30178800	H	-4.94793200	3.47066500	1.56755200
H	1.35431400	-3.11000400	0.89337200	C	-1.12586300	2.33427600	1.97011900
H	-1.10308400	-3.58299200	2.23580500	H	-0.83131500	3.35961200	1.70957500
H	-3.03441800	-1.87800200	3.02636900	C	-0.81571700	2.05949200	3.45106300
H	-2.08116200	0.58130700	2.42364100	H	0.26382400	2.06689100	3.63201400
B	-1.19483100	0.15894900	-0.46487400	H	-1.26643800	2.81552100	4.10282700
C	-0.28000500	-0.71974400	-1.43446800	H	-1.19374600	1.08087900	3.76704100
C	0.48521200	-0.15444600	-2.45524600	C	-4.97277600	0.05557300	1.49056000
C	-0.21750700	-2.11260700	-1.36906200	H	-4.95231900	-0.09557200	0.40694300
C	1.23016500	-0.91254900	-3.35392700	H	-5.37995000	-0.85583800	1.94029100
C	0.54106400	-2.90046300	-2.21545800	H	-5.67934800	0.86540700	1.70884800
C	1.27411400	-2.29055700	-3.22792300	C	-4.51398900	3.13766700	3.66257700
C	-0.74104200	1.67884900	-0.29282500	H	-5.14153500	3.95130600	4.03776700
C	-1.52640700	2.73587200	-0.74933700	H	-5.09420200	2.21209800	3.73291600
C	0.51347100	2.03841100	0.19967600	H	-3.66066100	3.04144700	4.34147800
C	-1.13844700	4.06615700	-0.67038200	H	-3.55567100	0.31892000	3.11901500
C	0.92216600	3.35885700	0.32771900	H	-0.51558700	1.68423100	1.33118100
C	0.09516900	4.37855400	-0.12099500	H	-3.55648500	4.37122700	2.15671400
C	-2.75643800	-0.18172900	-0.35173200	B	1.68660500	0.24426500	-0.05529700
C	-3.62914100	0.57497300	0.44331100	C	1.79186700	-0.95995600	-1.15642300
C	-3.39420900	-1.20942500	-1.05755500	C	1.35731700	-0.75375500	-2.45960400
C	-4.97519500	0.29663700	0.61302900	C	2.28262100	-2.23991500	-0.92338500
C	-4.74421100	-1.51687900	-0.92291200	C	1.34379500	-1.72122600	-3.45548500
C	-5.54106500	-0.76774800	-0.07450400	C	2.29353200	-3.24708700	-1.88159400

F	1.39608200	1.10181300	0.56596000	C	1.82246600	-2.99096400	-3.16214400
F	2.10664600	3.66695900	0.85739000	C	1.61816900	-0.31025600	1.47936600
F	0.48575400	5.64289500	-0.02042200	C	2.68874100	-0.40288700	2.36559800
F	-1.93232900	5.03473100	-1.11796200	C	0.40543500	-0.72852600	2.00964200
F	-2.71560700	2.50071700	-1.31484000	C	2.56408200	-0.84291600	3.67942800
F	-0.89873200	-2.75703300	-0.41325100	C	0.22340600	-1.15110900	3.31764500
F	0.57584600	-4.22024000	-2.06575200	C	1.31824000	-1.21787800	4.16307100
F	1.99686300	-3.01878600	-4.06472900	C	2.84493900	1.36351000	-0.29495800
F	1.93657400	-0.30877500	-4.31014100	C	4.16380000	1.04055800	-0.60330400
F	0.53030100	1.16706100	-2.65285900	C	2.58190400	2.72568300	-0.22860900
F	-2.74974200	-1.95681400	-1.95541100	C	5.15100400	1.98702900	-0.84255900
F	-5.27306100	-2.51692700	-1.62060100	C	3.53407700	3.71127500	-0.45990700
F	-5.72678700	1.05104100	1.41006000	C	4.83183100	3.33663700	-0.76985900
F	-3.19300400	1.65526600	1.11150600	H	0.62449100	0.79685500	-0.25912800
F	-6.82800800	-1.04883900	0.06533900	F	3.92440200	-0.07203200	1.97509000
				F	3.62783500	-0.91036100	4.47940600
				F	1.17154500	-1.63637700	5.41953000
<b>TS5</b>				F	-0.99671900	-1.47049600	3.77388100
C	1.13061900	1.92941100	2.66327500	F	-0.70996400	-0.71813500	1.24137100
C	0.86286400	0.51675700	3.08528100	F	0.86756200	0.45954800	-2.82207900
C	-0.22019000	0.28322000	3.99177700	F	0.88085100	-1.43783800	-4.67328100
C	-1.35276900	0.91501900	3.61321400	F	1.83432400	-3.94187300	-4.09114400
C	-1.23882900	1.51580700	2.22170200	F	2.72943300	-4.46780900	-1.56474400
C	-0.17440400	2.63230100	2.22866900	F	2.74880200	-2.58753300	0.28493300
C	2.31378500	1.78628800	1.70054400	F	1.33834500	3.17281600	0.06469000
N	3.01807000	0.65987900	2.32505800	F	3.21002700	5.00600600	-0.38431100
C	2.02654100	-0.33580700	2.73335900	F	5.76365300	4.26161500	-0.99446200
O	-0.67202100	0.46268100	1.46884900	F	6.39846800	1.61862300	-1.13402000
C	4.15535500	-0.32140600	0.01377000	F	4.53546600	-0.24369300	-0.67165000
C	4.29894400	0.64255500	-0.98235400				
C	3.99278000	0.30194400	-2.29321200	<b>3a</b>			
C	3.54559700	-0.98155500	-2.61783100	N	-2.29866900	-1.65869800	-0.03000900
C	3.45725700	-1.94248700	-1.60428400	C	-1.90374100	-1.42087200	1.37114700
C	3.74438800	-1.62028900	-0.28296500	C	-0.49284500	-0.89605000	1.22377500
C	3.11098300	-1.30935200	-4.02017200	C	-0.07802600	-1.00889700	-0.22654100
S	4.47892400	0.13136300	1.69436300	C	-1.42633900	-0.91069400	-0.94625300
O	4.78307800	-1.06698200	2.45710900	C	0.24350600	-0.29091900	2.15085900
O	5.33355900	1.30261100	1.68666400	C	1.59395700	0.29957800	1.84268600
C	-0.54100400	3.84070800	3.08296000	C	2.09854300	-0.04869600	0.43951600
H	1.52000700	2.38589300	3.58955900	C	0.97546800	0.02896900	-0.60241100
H	-0.04819900	2.93294900	1.18153400	C	1.50230000	-0.17253400	-2.01937700
H	2.96328700	2.66252000	1.67593900	C	-4.58318000	-0.15103500	-0.18114400
H	1.96841200	1.53948900	0.68751400	C	-5.10265300	0.23293500	1.05153000
H	4.65495700	1.63581200	-0.72670500	C	-5.57272500	1.53317600	1.21134000

H	3.16450000	-2.95822800	-1.85734000	C	-5.53150300	2.44851400	0.15783500
H	3.69462000	-2.36840500	0.50355400	C	-5.01133200	2.03396100	-1.07360100
H	2.03539900	-1.12492700	-4.11956600	C	-4.53822900	0.74056200	-1.25222200
H	3.63129400	-0.68943200	-4.75444600	C	-6.06115600	3.84923500	0.32527300
H	3.28466500	-2.36150600	-4.25873800	S	-3.91006700	-1.78726100	-0.37906300
H	0.23439600	4.60955600	3.02275200	O	-4.48199500	-2.62153900	0.66461400
H	-1.48062600	4.28427300	2.74053000	O	-3.99542600	-2.12457400	-1.78963700
H	-0.65732800	3.56316500	4.13650100	O	3.13599400	0.84544200	0.08795400
H	1.70019900	-0.99842300	1.91013900	Si	4.75422800	0.41817700	0.03794100
H	2.38408600	-0.96212600	3.55518300	C	4.98733500	-1.00695500	-1.17790100
H	-0.13965600	-0.41990100	4.81361700	C	6.39405200	-1.61958000	-1.14602900
H	-2.28331400	0.86182200	4.16692100	C	5.34757900	-0.05852600	1.76694200
H	-2.19811800	1.85526300	1.81707300	C	6.85661900	0.12939200	1.98502200
B	-1.19553200	0.06811500	0.11297800	C	5.62586100	1.96725500	-0.56222500
C	-0.41213900	-1.31747800	-0.27603000	C	4.98126900	2.55937100	-1.82290600
C	-0.09958300	-2.27713200	0.68407500	H	-1.97432000	-2.35808700	1.92926100
C	-0.11484600	-1.69006700	-1.58568800	H	-2.54834200	-0.67581200	1.86102600
C	0.51989200	-3.48960700	0.39510200	H	0.32233600	-2.01794600	-0.41277800
C	0.47835600	-2.89802900	-1.91882000	H	-1.44827800	-1.37667400	-1.93241000
C	0.80746300	-3.80288400	-0.92148000	H	-1.73196900	0.14622500	-1.03217000
C	-0.87864800	1.35331300	-0.86457900	H	-0.13643200	-0.17719500	3.16506500
C	-1.75254300	2.41955200	-1.05047300	H	2.33555300	-0.01984800	2.58619300
C	0.38956300	1.55733700	-1.39529300	H	1.54362100	1.39482800	1.91356800
C	-1.41314700	3.58913400	-1.72309400	H	2.46924700	-1.08984500	0.44343100
C	0.78266100	2.70574800	-2.06724400	H	0.52473200	1.02952600	-0.51879400
C	-0.13332000	3.73420700	-2.23849900	H	2.25738500	0.57963900	-2.26252600
C	-2.78856100	-0.33799300	0.14570800	H	0.69443600	-0.09939700	-2.75494700
C	-3.46443900	-0.80719400	1.26452800	H	1.96065000	-1.16426400	-2.12249000
C	-3.53251800	-0.37165700	-1.03277100	H	-5.15922700	-0.49148400	1.85821000
C	-4.78541600	-1.24278200	1.24582600	H	-5.98573400	1.84026600	2.16842200
C	-4.84894400	-0.80261600	-1.10371600	H	-4.98552200	2.73441700	-1.90448600
C	-5.48410500	-1.24225400	0.05015700	H	-4.16056500	0.40527600	-2.21336700
F	1.34368200	0.62297500	-1.23054600	H	-7.01379400	3.96892600	-0.20183100
F	2.02824900	2.83133700	-2.53212700	H	-6.22957500	4.08738500	1.37822800
F	0.21451100	4.84971300	-2.87298200	H	-5.36435100	4.58558900	-0.08576200
F	-2.29844500	4.57489500	-1.86083100	H	4.24397100	-1.78817800	-0.97024300
F	-2.99533300	2.38424400	-0.53791400	H	6.59532600	-2.09039900	-0.17805000
F	-0.36484900	-0.85894200	-2.60644100	H	6.51997000	-2.38716500	-1.91584300
F	0.81098300	-3.17381300	-3.18182600	H	7.16923700	-0.86223200	-1.31020800
F	1.45060500	-4.92746800	-1.23126000	H	4.79797700	0.56756600	2.48241400
F	0.83747700	-4.33871500	1.37282900	H	7.14826100	1.17251500	1.82340600
F	-0.36810400	-2.07542000	1.99039500	H	7.15362000	-0.14108800	3.00321300
F	-2.97361600	0.02396200	-2.18476300	H	7.44803700	-0.48362800	1.29761300
F	-5.50474800	-0.80504800	-2.26270700	H	5.61379600	2.70917200	0.24717100

F	-5.37518200	-1.66548300	2.36508700	H	3.93113600	2.80560000	-1.63979300
F	-2.85603000	-0.86374900	2.46662500	H	5.49185800	3.47088200	-2.14920000
F	-6.74557900	-1.66108100	0.00542100	H	5.01326600	1.84969500	-2.65723900
				H	6.68422600	1.73935500	-0.74703300
				H	5.05899000	-1.09574500	1.98687200
<b>TS6</b>				H	4.75588000	-0.63906100	-2.18636300
N	-4.85995800	1.90345800	-0.38583400				
C	-4.28809200	1.64568700	0.93896400	<b>9</b>			
C	-2.83536000	1.45558900	0.63177400	C	0.77174200	-1.18356300	3.27851400
C	-2.62117100	1.49995000	-0.84909300	C	0.23341200	-1.70406900	1.90536700
C	-4.02583700	1.27236000	-1.41582200	C	-0.95399200	-2.58221400	2.23872400
C	-1.80384500	1.28181900	1.49357600	C	-1.90709400	-1.76293000	2.68336100
C	-0.51548200	0.98824200	0.96396500	C	-1.34679300	-0.35553600	2.58512500
C	-1.50944800	0.56244900	-1.31367500	C	-0.26163300	-0.11598800	3.66701200
C	-1.20141800	0.71037900	-2.79838300	C	2.22372900	-0.80669700	3.00370100
C	-6.91718700	0.09541400	-0.35830600	N	2.58632300	-1.84179600	2.02270000
C	-6.90797500	-0.72375600	-1.48724200	C	1.46463800	-2.08512400	1.09957600
C	-7.15540100	-2.08160400	-1.33384300	O	-0.48197300	-0.48858300	1.40714100
C	-7.41097300	-2.63167000	-0.07225300	C	4.08906600	-0.30621400	0.33711500
C	-7.42842800	-1.78476300	1.03906200	C	4.49654300	0.89863200	0.90471200
C	-7.18376500	-0.42148700	0.90716900	C	4.32618800	2.07428800	0.18425900
C	-7.65631200	-4.11008000	0.07645600	S	3.74197000	2.06324500	-1.08558300
S	-6.52414300	1.81814000	-0.53412700	C	3.38544300	0.83581300	-1.65171100
O	-7.03974900	2.52088400	0.62644600	C	3.55441600	-0.35225900	-0.94962100
H	-4.49712400	2.47317100	1.62234900	C	3.51146900	3.34404400	-1.84468400
H	-4.67259700	0.71555000	1.39623800	S	4.10628900	-1.77787900	1.32906100
H	-2.31462200	2.53989100	-1.07802400	O	4.17338600	-2.92414300	0.43955700
H	-4.19893400	1.75425900	-2.37820100	O	5.03288700	-1.57555800	2.42828100
H	-4.22247200	0.19017000	-1.50605200	C	-0.78568100	-0.20755200	5.09297200
H	-1.92197700	1.35665400	2.56939900	H	0.75900600	-2.02578600	3.97701300
H	-1.79604700	-0.47837700	-1.10038600	H	0.15363200	0.88025600	3.47589900
H	-2.08176900	0.45998400	-3.39761300	H	2.86759400	-0.90113100	3.87921400
H	-0.90343100	1.73833800	-3.03263100	H	2.31032900	0.20710100	2.59362500
H	-0.38540900	0.04237300	-3.07708700	H	4.94049600	0.90129100	1.89557700
H	-6.74145700	-0.28776300	-2.46773000	H	4.62732700	3.02084400	0.62353800
H	-7.16213600	-2.72672500	-2.20819200	H	2.96778700	0.81655500	-2.65485000
H	-7.64816400	-2.19666200	2.02007000	H	3.28721100	-1.30971400	-1.39032900
H	-7.23223300	0.24486400	1.76322200	H	2.60626300	3.27148800	-2.45522800
H	-8.31300400	-4.48132700	-0.71518900	H	3.40112100	4.19052200	-1.16186600
H	-6.71439800	-4.66528900	0.01011200	H	4.34972600	3.55909100	-2.51643400
H	-8.11470500	-4.34231700	1.04044400	H	0.02268000	-0.04253400	5.81055400
O	0.80791900	0.20302700	-0.92279600	H	-1.55963500	0.54322200	5.28041500
C	2.58746700	1.51364500	0.28730800	H	-1.21062700	-1.19782200	5.28733400
C	2.95755700	2.39783000	-0.72646600	H	1.53179100	-1.43648400	0.22144400

C	3.38129100	3.69895500	-0.49840100	H	1.46236900	-3.12793300	0.77844200
C	3.43289900	4.17902300	0.80408800	H	-0.94277400	-3.66407700	2.19812900
C	3.05260100	3.35044800	1.84716700	H	-2.87980700	-2.01586400	3.08535500
C	2.64059000	2.05206400	1.56626800	H	-2.03668600	0.46947200	2.46067000
C	3.08135300	-0.78175900	-1.15116800	B	-1.10438500	0.01102600	-0.13220600
C	2.59944500	-1.90604200	-1.81744000	C	-0.29237400	-0.77389800	-1.30657100
C	3.37139400	-2.68155800	-2.67118700	C	0.32286800	-0.12665500	-2.37944600
C	4.70327300	-2.34707000	-2.86990400	C	-0.18236400	-2.16456500	-1.35843800
C	5.23416500	-1.24824500	-2.21220400	C	0.99124500	-0.79912200	-3.40124900
C	4.42424300	-0.49673100	-1.36775800	C	0.49146200	-2.87324500	-2.33632200
C	0.75292900	-1.82587500	1.35992700	C	1.09045000	-2.17829000	-3.38081800
C	1.86387300	-1.03012700	1.12350700	C	-0.70423800	1.58654700	-0.09281100
C	2.95664900	-1.29367400	1.94688700	C	-1.48582900	2.59102100	-0.66143300
C	2.95606500	-2.25339400	2.94619100	C	0.52917300	2.01867400	0.38583600
C	1.81225400	-3.01748800	3.14844200	C	-1.11243700	3.92694200	-0.70337200
C	0.70051700	-2.80011500	2.35173200	C	0.92669300	3.34992700	0.40167000
B	2.07722400	0.00683500	-0.13703300	C	0.10530400	4.31179400	-0.16256000
F	-0.38311100	-1.66594900	0.64278800	C	-2.72309900	-0.26570500	-0.10538600
F	-0.40882600	-3.51697000	2.54092900	C	-3.60241600	0.56367900	0.60460500
F	1.78350900	-3.94235300	4.10363100	C	-3.38698100	-1.27171200	-0.81601300
F	4.02945900	-2.45564900	3.70667900	C	-4.97471600	0.39142500	0.68146300
F	4.08187900	-0.58782500	1.77366400	C	-4.76370400	-1.48114100	-0.77232300
F	1.32867000	-2.30274900	-1.63402500	C	-5.56840700	-0.65126500	-0.01379100
F	2.85280400	-3.74562400	-3.28681300	F	1.42681900	1.13381400	0.85067500
F	5.46351600	-3.07537200	-3.68428100	F	2.09475400	3.71366900	0.93547100
F	6.51410200	-0.92260700	-2.39173500	F	0.48350100	5.58487600	-0.18480200
F	5.01247800	0.54504300	-0.76470300	F	-1.90618700	4.83557800	-1.26424200
F	2.92728800	1.99600000	-2.00243100	F	-2.65900800	2.29865700	-1.23579200
F	3.73316400	4.49135600	-1.50906400	F	-0.72531700	-2.90385200	-0.37804700
F	3.82426900	5.42636100	1.04418500	F	0.56905400	-4.19919200	-2.28065900
F	3.06315400	3.80554400	3.09963800	F	1.73809600	-2.82656800	-4.33784000
F	2.22541100	1.33353600	2.63163700	F	1.57391000	-0.10190500	-4.37757300
C	-0.27627700	0.79054400	-0.44332900	F	0.31861400	1.20520500	-2.51480500
H	0.33998300	0.95062600	1.63645000	F	-2.74760500	-2.11235500	-1.63380000
H	-0.10880500	1.98645400	-0.30594900	F	-5.30554900	-2.47394400	-1.47229200
				F	-5.72113800	1.22892000	1.39763500
<b>12</b>				F	-3.14426500	1.63395800	1.28346200
N	0.20954900	-1.45912200	-0.09993300	F	-6.88006800	-0.83891000	0.04122500
C	0.58194000	-0.95548900	-1.43279800				
C	1.89873400	-0.26306200	-1.16052200	<b>10</b>			
C	2.25379700	-0.42967500	0.30079000	N	4.87053100	-1.91916000	-0.47385900
C	0.88507200	-0.67839700	0.94339700	C	4.27778400	-1.70898300	0.84559400
C	2.60988200	0.48113800	-2.00174000	C	2.83019800	-1.53880800	0.53745000
C	3.88449800	1.16374200	-1.58253400	C	2.62218600	-1.54536500	-0.93670700

C	3.02032300	0.78359700	0.83578600	C	4.02669400	-1.28274000	-1.49341700
C	3.46396600	0.63320800	2.28322500	C	1.80754700	-1.33967900	1.43331600
C	-2.32695500	-0.44410000	0.10224100	C	0.55131300	-1.00949800	0.92477900
C	-2.48678700	0.29651200	1.27150600	C	1.48766200	-0.61101600	-1.36615500
C	-3.18974900	1.49441200	1.22113500	C	1.19678000	-0.68855100	-2.85729700
C	-3.73848800	1.95850900	0.02152400	C	6.85939900	-0.04138400	-0.36741700
C	-3.57033700	1.19213600	-1.13489000	C	6.82627800	0.80838200	-1.47232200
C	-2.86978500	-0.00882700	-1.10444400	C	7.01551800	2.17091500	-1.27763500
S	-1.35911100	-1.93677500	0.14323400	C	7.23552700	2.69424100	0.00136400
O	-1.72132700	-2.72424700	-1.02193000	C	7.28087500	1.81629400	1.08855400
O	-1.41664000	-2.45996600	1.49692000	C	7.09417000	0.44914000	0.91587600
H	0.65712100	-1.79286200	-2.13055400	C	7.40703200	4.17655300	0.20252100
H	-0.15770000	-0.24013100	-1.82450600	S	6.53682100	-1.77120400	-0.59486300
H	2.86240800	-1.33662900	0.43252100	O	7.05436200	-2.48584700	0.55736900
H	0.91887000	-1.25375700	1.86929700	O	6.85442100	-2.12002100	-1.96439000
H	0.37804600	0.28510900	1.12833900	H	4.49325800	-2.54218200	1.52229300
H	2.28775600	0.61138900	-3.03329800	H	4.62608400	-0.77831600	1.33557100
H	2.35081000	1.65268700	0.72723900	H	2.33133100	-2.58438700	-1.18863500
H	2.60057300	0.49535600	2.94122400	H	4.20782000	-1.74225400	-2.46499800
H	4.12638500	-0.23086600	2.39065000	H	4.20338300	-0.19590100	-1.56187700
H	4.01882400	1.51398700	2.61316400	H	1.97676300	-1.37089700	2.50487700
H	-2.08412300	-0.08180700	2.20624400	H	1.74947100	0.42091900	-1.09639400
H	-3.32413800	2.07588700	2.12947800	H	2.07468600	-0.39368300	-3.44086300
H	-4.00136000	1.53762500	-2.07085600	H	0.91368700	-1.70689200	-3.14746700
H	-2.76138000	-0.62224300	-1.99378600	H	0.37171800	-0.01749400	-3.10057000
O	5.33038400	1.16282500	0.31537500	H	6.68655600	0.39517000	-2.46676400
C	4.19989400	1.04157100	-0.09481300	H	7.00314600	2.84036900	-2.13317400
H	4.75210400	0.78341400	-2.13374600	H	7.47676900	2.20876500	2.08256800
H	3.83305300	2.23744500	-1.81460800	H	7.16601700	-0.23996400	1.75217500
C	-4.53059300	3.23959000	-0.01502900	H	7.89588600	4.63943400	-0.65835000
H	-4.47430500	3.71284300	-0.99870300	H	6.43236700	4.66051600	0.32927300
H	-5.58725200	3.04491600	0.19883100	H	8.00181200	4.39078300	1.09371000
H	-4.16855300	3.95181000	0.73093400	O	-0.79482800	-0.18649600	-0.92927500
<b>13</b>				C	-2.54339900	-1.49624700	0.36042200
Si	0.00994100	0.01229800	2.30440200	C	-2.90347700	-2.44179400	-0.59960200
C	1.84434700	0.15307900	2.76090200	C	-3.30781100	-3.73351300	-0.29758900
H	2.36238100	-0.62073800	2.18061300	C	-3.35134000	-4.13949400	1.03092100
C	2.10256300	-0.15467900	4.24613600	C	-2.98130600	-3.24808600	2.02361500
H	3.16675300	-0.02137700	4.47376700	C	-2.58666800	-1.96139000	1.66814000
H	1.54203400	0.50922400	4.91294600	C	-3.08485000	0.73082900	-1.17173100
H	1.84018200	-1.18583600	4.50156900	C	-2.63496000	1.83939200	-1.88556700
C	-0.78429500	-1.64257000	2.77626900	C	-3.43179200	2.56505500	-2.76054900
H	-1.71399300	-1.70719700	2.19724300	C	-4.75612200	2.19253400	-2.93773100
				C	-5.25492600	1.10575100	-2.23685800

C	-1.17908100	-1.70416500	4.26194000	C	-4.42137500	0.40612600	-1.37143400
H	-1.60211500	-2.68885800	4.49319000	C	-0.69432900	1.77688300	1.38742700
H	-0.32245500	-1.55432600	4.92765300	C	-1.84860600	1.07059500	1.09273100
H	-1.93544900	-0.95534800	4.51566100	C	-2.96110500	1.43796200	1.84652700
C	-1.02593000	1.53123100	2.76535500	C	-2.94417700	2.42898300	2.81502700
H	-0.61983100	2.36430400	2.17822800	C	-1.75820500	3.11056100	3.06591800
C	-0.87946700	1.91707300	4.24748400	C	-0.61943900	2.77606300	2.35199800
H	-1.52456700	2.77429400	4.47352500	B	-2.04627700	-0.00718600	-0.14586600
H	-1.17160200	1.10417000	4.92090700	F	0.47895500	1.47791100	0.77025200
H	0.14659900	2.20528800	4.49545100	F	0.53436900	3.40177200	2.59824500
H	0.00057900	0.00729900	0.73818700	F	-1.71341200	4.06189400	3.99499300
B	-0.00205200	-0.00309200	-0.83979900	F	-4.04039000	2.73495600	3.50607000
C	-1.00832700	1.22017200	-1.03602200	F	-4.11986800	0.79761400	1.64394400
C	-0.73335300	2.46253000	-0.46665900	F	-1.37292200	2.27457100	-1.73392500
C	-2.23541900	1.13172000	-1.69078500	F	-2.94187300	3.61772200	-3.41910600
C	-1.61288600	3.53127400	-0.48120300	F	-5.54021700	2.87278900	-3.77176600
C	-3.14135800	2.18493400	-1.74712800	F	-6.52823300	0.74291800	-2.39669400
C	-2.83149400	3.38935200	-1.13286500	F	-4.98359200	-0.62572700	-0.72666000
C	1.56093400	0.25367100	-1.03566100	F	-2.87503500	-2.11359700	-1.89706200
C	2.49820400	-0.60245100	-0.45997700	F	-3.64730300	-4.58865900	-1.26081100
C	2.09930500	1.35417600	-1.69994100	F	-3.72564100	-5.37697200	1.34235400
C	3.86414700	-0.37885300	-0.47927200	F	-2.98606600	-3.62970800	3.30089400
C	3.46491300	1.60814300	-1.76126700	F	-2.18403200	-1.17881700	2.69285800
C	4.35209600	0.74049000	-1.14153900	C	0.24275100	-0.96555200	-0.52947400
C	-0.56072300	-1.48701700	-1.02276800	H	-0.26080900	-0.81913300	1.62583200
C	-1.77117400	-1.86663900	-0.44523700	H	0.02735300	-2.05959300	-0.70912500
C	0.12333800	-2.50795500	-1.68021900				
C	-2.26090300	-3.16141700	-0.45712200	<b>11</b>			
C	-0.34006000	-3.81765500	-1.73424200	N	-4.87011300	1.91058000	-0.52406100
C	-1.53562100	-4.14776500	-1.11350700	C	-4.34268900	1.78931200	0.84347700
F	1.28249000	-2.26846600	-2.29868200	C	-2.86552300	1.59213900	0.59645600
F	0.35302900	-4.75316600	-2.37661100	C	-2.61121100	1.50503600	-0.89338900
F	-1.98660600	-5.39448800	-1.15121300	C	-4.00140900	1.18790000	-1.45618500
F	-3.40547400	-3.46264300	0.15057600	C	-1.89387200	1.41642900	1.48465300
F	-2.51109500	-0.95469200	0.20587200	C	-0.46925100	1.22001500	1.03663300
F	-2.60612000	0.00431200	-2.30312400	C	-1.55483100	0.44411400	-1.20224100
F	-4.30087100	2.04552200	-2.38311600	C	-1.21025700	0.28818700	-2.68013300
F	0.42689100	2.65342700	0.18185100	C	-6.93704800	0.12062000	-0.34801000
F	-1.30398400	4.67602100	0.12249400	C	-6.86070500	-0.84950500	-1.34644700
F	-3.69032600	4.39928400	-1.16991100	C	-7.13387000	-2.17264700	-1.02249800
F	2.08218100	-1.69667800	0.19777600	C	-7.48250400	-2.53937600	0.28195400
F	4.69975800	-1.21631200	0.12952600	C	-7.56655600	-1.54420800	1.25946500
F	5.65684600	0.97464000	-1.18515500	C	-7.29580300	-0.21423400	0.95533800
F	3.92507000	2.67509700	-2.40795100	C	-7.75027800	-3.98162600	0.62436000

F	1.30927800	2.23515000	-2.31888600	S	-6.51889000	1.80427500	-0.73518300
C	0.10494500	-2.83415600	2.39374300	O	-7.09987300	2.65218600	0.28988300
H	1.06190600	-2.80995000	2.92868600	O	-6.74727000	2.00414200	-2.15464100
H	-0.39221000	-3.77631600	2.65412300	H	-4.58004800	2.69104400	1.41189100
H	0.32921000	-2.85569300	1.32297800	H	-4.76306000	0.91885300	1.37265800
C	2.42766400	1.51895300	2.37263900	H	-2.28712300	2.48274400	-1.27806900
H	1.93198300	2.33512100	2.91173500	H	-4.16969300	1.54847300	-2.47150000
H	3.49434300	1.56059100	2.62368500	H	-4.17719700	0.09747600	-1.42194500
H	2.32487200	1.72390300	1.30263500	H	-2.08068800	1.44504400	2.55417800
C	-2.50282400	1.35109200	2.38686700	H	-1.94839100	-0.51524500	-0.81683500
H	-2.95750500	0.51369300	2.92952600	H	-2.11657200	0.06845200	-3.25038700
H	-3.07146600	2.25371600	2.64075500	H	-0.76885500	1.20894700	-3.07339200
H	-2.63537800	1.15882900	1.31774800	H	-0.49876700	-0.52621600	-2.82583700
				H	-6.62253300	-0.55660900	-2.36459300
<b>14</b>				H	-7.08745200	-2.93457300	-1.79617300
N	1.24664700	-4.20304300	0.09754800	H	-7.85852300	-1.81338100	2.27083000
C	0.91154800	-3.49151400	1.34411300	H	-7.39093400	0.56637000	1.70394500
C	-0.33866900	-2.73440900	0.96588100	H	-8.26121800	-4.49434200	-0.19485000
C	-0.70168700	-3.05880200	-0.46737300	H	-6.81117900	-4.51383000	0.81211500
C	0.63861200	-3.51685000	-1.04971300	H	-8.36669800	-4.06826600	1.52243700
C	-0.94267300	-1.78503400	1.67155900	O	0.73789300	0.22804800	-0.79569200
C	-2.05572700	-0.95247500	1.08815800	C	2.59728200	1.48129900	0.43091400
C	-2.37196400	-1.31782200	-0.31657400	C	2.87328400	2.46382000	-0.51796500
C	-1.28807000	-1.82678700	-1.19072300	C	3.29194300	3.74660900	-0.19773800
C	-1.70441500	-2.07874900	-2.62994100	C	3.44025900	4.09376200	1.13859200
C	3.74011900	-3.19829900	-0.39304400	C	3.15816600	3.15831700	2.12268000
C	3.84427000	-2.73429500	-1.70396700	C	2.74026800	1.88447700	1.75445300
C	4.46155900	-1.51345900	-1.94064000	C	3.04452800	-0.65547400	-1.23162600
C	4.97599400	-0.74999600	-0.88687600	C	4.36952000	-0.32991900	-1.50038100
C	4.86764400	-1.24170200	0.41808400	C	5.13250600	-0.99205300	-2.45588600
C	4.25107900	-2.46221600	0.67440900	C	4.57150400	-2.03278200	-3.18032300
C	5.62027400	0.58059400	-1.16496900	C	3.25494600	-2.40054500	-2.93922300
S	2.83653800	-4.69449600	-0.08623100	C	2.53220000	-1.71777200	-1.97213700
O	3.22740800	-5.22210700	1.20955000	C	3.08300000	-1.45565500	1.81495400
O	2.86213700	-5.49141400	-1.29970600	C	1.94385100	-1.12906100	1.08070600
O	-3.53549800	-1.22314200	-0.79065700	C	0.84036400	-1.93304900	1.32855800
Si	-5.22019100	-1.17393700	-0.18144100	C	0.83975400	-2.97076300	2.25526200
C	-5.43175000	-2.95430600	0.39633100	C	1.99570700	-3.24879300	2.96569900
C	-4.44686300	-3.38481400	1.49067200	C	3.13324700	-2.48043600	2.74484900
C	-6.88162600	-3.18565300	0.85415400	B	2.12768500	0.01126500	-0.06999000
C	-5.48962100	0.11086200	1.17263900	F	4.19950600	-0.74233600	1.62078500
C	-6.99238800	0.46263400	1.17239000	F	4.25046200	-2.74109300	3.41735500
C	-4.66483600	1.40188800	1.06984800	F	2.01661600	-4.23656300	3.85350900
C	-6.10362600	-0.79946200	-1.79206600	F	-0.26102000	-3.69299700	2.45778300

C	-5.63255700	0.54018200	-2.38011100	F	-0.33310100	-1.72950700	0.68713900
C	-5.91739500	-1.93691500	-2.80677700	F	4.98265700	0.65628400	-0.83610700
H	0.77320000	-4.21316100	2.15225300	F	6.39628000	-0.63695600	-2.67627100
H	1.69385700	-2.77686900	1.64182200	F	5.28981100	-2.67757900	-4.09388500
H	-1.41129800	-3.89931700	-0.50244900	F	2.70772200	-3.40618500	-3.62056000
H	0.54707100	-4.21177800	-1.88609300	F	1.27198300	-2.13961400	-1.75446100
H	1.22010100	-2.63519300	-1.35958800	F	2.73992400	2.17781200	-1.81993500
H	-0.62019400	-1.51188900	2.67167200	F	3.54561600	4.64117700	-1.14946600
H	-1.69659100	0.09260200	1.03471100	F	3.83402200	5.31694800	1.47225600
H	-2.96207200	-0.94890800	1.70373400	F	3.27349000	3.48977600	3.40657600
H	-0.50623800	-1.05341800	-1.14344200	F	2.43085300	1.05443000	2.76291200
H	-2.13793900	-1.17748200	-3.07158400	C	-0.34429000	0.62295800	-0.33457700
H	-0.82377800	-2.35212700	-3.21639700	H	0.05699500	2.18803500	0.97698500
H	-2.43517100	-2.89155200	-2.70014400	H	0.12376500	0.62832300	1.74331400
H	3.46226700	-3.33807400	-2.52163600				
H	4.54423800	-1.14481000	-2.95976500	<b>TS7</b>			
H	5.26914800	-0.65822900	1.24237600	N	7.41600900	-1.72988600	0.19084400
H	4.19017000	-2.86075300	1.68286100	C	6.96401000	-1.32298200	1.53000200
H	6.22226800	0.91634600	-0.31771500	C	5.49560000	-1.04887700	1.29872200
H	6.25543200	0.53211500	-2.05424600	C	5.16548800	-1.30221500	-0.15425900
H	4.85111100	1.33936400	-1.34157600	C	6.53477600	-1.16111100	-0.83043300
H	-5.24902700	-3.57708400	-0.49122300	C	4.60945500	-0.55297700	2.15417100
H	-4.64466900	-4.41940400	1.79170100	C	3.17891600	-0.29939100	1.75906300
H	-3.39989000	-3.34386500	1.16616400	C	4.09503900	-0.32976200	-0.66505800
H	-4.54421800	-2.76287800	2.38898700	C	3.72938300	-0.55079300	-2.12563100
H	-7.04874900	-4.24603700	1.07070300	C	9.58494500	-0.07825700	-0.09332000
H	-7.61427700	-2.88386800	0.09642000	C	9.51948100	0.66374600	-1.27130700
H	-7.09667600	-2.62930500	1.77398700	C	9.88411600	2.00466800	-1.24379900
H	-5.26016800	-0.37886200	2.13105500	C	10.31693100	2.61066900	-0.05967600
H	-7.22363600	1.10415900	2.02895700	C	10.38023600	1.84046100	1.10552100
H	-7.64394800	-0.41582600	1.23244200	C	10.01933700	0.49760800	1.09867800
H	-7.25918600	1.01747100	0.26589900	S	9.05474100	-1.77477600	-0.10324900
H	-4.97602100	2.10276900	1.85274700	O	9.63793400	-2.42916400	1.05338600
H	-3.59082800	1.23947500	1.19464200	O	9.19640400	-2.27663800	-1.45743100
H	-4.81393300	1.90012000	0.10760200	H	7.15600100	-2.12739900	2.24341200
H	-7.17492800	-0.71859900	-1.55638100	H	7.47435700	-0.41254900	1.88153200
H	-6.09033300	0.70288500	-3.36200700	H	4.82171100	-2.33809100	-0.28694000
H	-5.90226400	1.39023500	-1.74667700	H	6.63829300	-1.72165000	-1.76006600
H	-4.54528900	0.56314600	-2.51491900	H	6.75270600	-0.09428400	-1.01861300
H	-6.42459100	-1.69147100	-3.74591600	H	4.87715600	-0.33361700	3.18439700
H	-6.32712200	-2.88631100	-2.44699700	H	4.50643900	0.68560600	-0.52373400
H	-4.85653400	-2.08805600	-3.03775900	H	4.62091500	-0.44861300	-2.75009300
B	0.78251400	1.26308200	0.19006600	H	3.32162100	-1.55558600	-2.27321600
C	-0.47653500	2.31358800	0.18189900	H	2.98601400	0.17045600	-2.47030000

C	-0.56840700	3.45872600	0.97091500	H	9.21537000	0.18120600	-2.19525000
C	-1.53643700	2.13977500	-0.70156900	H	9.84414000	2.59010800	-2.15832500
C	-1.62233500	4.36318600	0.89164400	H	10.72757600	2.29717100	2.02821600
C	-2.59407500	3.02715900	-0.83568600	H	10.09783100	-0.11289000	1.99302400
C	-2.64596900	4.14515200	-0.01899700	H	2.50199100	-1.00514600	2.25577400
C	1.72129900	1.61621300	-1.09358700	H	2.85453400	0.69873800	2.08874400
C	2.31522500	2.86852100	-1.23140800	C	2.91053400	-0.36947900	0.27297900
C	1.93155200	0.75221500	-2.15715400	Si	-0.28093900	-0.30429000	0.14162700
C	3.05996800	3.25325400	-2.33713800	C	-0.01755000	0.79664900	1.66251900
C	2.67850100	1.08525500	-3.28335200	B	-3.80716300	0.08307900	0.01875600
C	3.24468100	2.34627800	-3.37540500	C	-3.84325000	1.30592300	-1.06104400
C	1.56046700	1.18316000	1.62104900	C	-2.92612700	2.34310400	-0.96685600
C	0.84148400	0.91859900	2.78248900	C	-4.74410600	1.44161100	-2.11391200
C	2.93629700	1.21694600	1.81264600	C	-2.84004100	3.41128100	-1.84468800
C	1.40610200	0.64220100	4.01716800	C	-4.71034500	2.49862700	-3.01864900
C	3.55544900	0.94586400	3.02933200	C	-3.74948100	3.49039900	-2.88864600
C	2.78869100	0.64881100	4.14381300	C	-4.36726700	0.52132200	1.48107800
H	0.33518000	0.14764700	0.02597700	C	-5.06252200	1.68704000	1.78027800
F	2.17169900	3.76654200	-0.24759500	C	-4.12472400	-0.30206100	2.57562400
F	3.60098800	4.46880200	-2.41732400	C	-5.46217800	2.02763200	3.07156300
F	3.95972300	2.68658400	-4.44620500	C	-4.49296100	-0.00695600	3.87561300
F	2.86066000	0.19828000	-4.26818400	C	-5.17452500	1.17786500	4.12605400
F	1.39785100	-0.48906700	-2.16201200	C	-4.50985700	-1.26596600	-0.57111300
F	0.37662300	3.73923500	1.87178400	C	-4.05700600	-1.79792200	-1.77472300
F	-1.66474000	5.43265200	1.68413700	C	-5.55493400	-1.98141600	0.00575300
F	-3.67488000	4.98714400	-0.10145900	C	-4.54772200	-2.94981300	-2.36430900
F	-3.59389900	2.78585700	-1.69584700	C	-6.08945300	-3.14206900	-0.54997600
F	-1.59414000	1.03373300	-1.48946400	C	-5.58422000	-3.63220400	-1.74186200
F	3.77159600	1.50040800	0.80047300	F	-5.59642300	2.56842400	-4.01128700
F	4.88935300	0.95241700	3.12010400	F	-5.71539800	0.54184200	-2.31008700
F	3.36332900	0.37640200	5.31357600	F	-3.70060100	4.50268900	-3.75166000
F	0.63567300	0.35529600	5.07026100	F	-1.89405900	4.34386700	-1.69431600
F	-0.51284200	0.89771700	2.74334200	F	-2.01441400	2.32637000	0.03278400
				F	-3.45005400	-1.45688600	2.39140200
<b>TS9</b>				F	-4.19363800	-0.83209000	4.88121100
C	-5.29330400	-2.24534600	-0.85241900	F	-5.54316800	1.49104800	5.36664200
C	-4.34373200	-2.23412200	0.39580700	F	-6.12078100	3.16461900	3.29834400
C	-4.20947700	-3.66098100	0.87398600	F	-5.39142700	2.56714600	0.82353300
C	-3.50011100	-4.29248100	-0.06332500	F	-6.12671400	-1.58771500	1.15207300
C	-3.15954800	-3.24657900	-1.10789400	F	-7.08821000	-3.78252800	0.05806400
C	-4.42664300	-2.90045600	-1.93927700	F	-6.07947800	-4.74352400	-2.28221500
C	-5.65224000	-0.77188600	-0.98787000	F	-4.03196900	-3.40984400	-3.50626300
N	-5.81368700	-0.39722400	0.41823400	F	-3.03732500	-1.19269500	-2.42164700
C	-4.82464000	-1.08441400	1.26697300	H	-2.57036000	-0.19584100	0.20041400

O	-3.04742300	-2.04887200	-0.28718300	H	0.70177300	0.17641400	2.21394100
C	-4.91387200	2.18990400	0.17839900	C	-0.36438300	-2.16675900	0.49846500
C	-4.97289800	2.63253800	-1.14349500	H	0.50779500	-2.55365200	-0.05122100
C	-3.94032200	3.41740900	-1.63846800	C	-0.47006800	0.27372400	-1.64354800
C	-2.85259200	3.77317300	-0.83197800	H	-1.54164300	0.42773300	-1.79483400
C	-2.82706800	3.33039500	0.49344400	C	-0.19147600	-2.50180100	1.98800200
C	-3.84905000	2.53666700	1.00756200	H	-0.11198500	-3.58694000	2.11535400
S	-6.23014600	1.16815600	0.79941700	H	0.69986000	-2.05500000	2.44108700
O	-6.20355400	1.22509400	2.25073600	H	-1.06429600	-2.17030900	2.55838900
O	-7.41458700	1.46255000	0.01509700	C	0.24973200	1.59443100	-1.95223100
C	-5.05765600	-4.08937500	-2.65075300	H	1.32657000	1.52633000	-1.75734400
H	-6.19255500	-2.82407200	-0.62157300	H	0.12510800	1.83540300	-3.01435800
H	-4.12587900	-2.14174600	-2.67187500	H	-0.14752700	2.43231000	-1.37559700
H	-6.58290300	-0.58566600	-1.52709000	C	0.65435300	2.14813200	1.37836600
H	-4.82970000	-0.21878900	-1.47221300	H	1.50105800	2.07554300	0.68533100
H	-5.83660500	2.38818900	-1.75439300	H	-0.05835400	2.85367300	0.94762200
H	-3.98108100	3.77392700	-2.66437100	H	1.02105300	2.58268300	2.31659500
H	-1.99916500	3.62287800	1.13368500	O	1.76971500	-0.41799900	-0.18908600
H	-3.84909400	2.22173600	2.04811100	C	-1.21294800	0.96775200	2.60422500
H	-5.93013400	-3.77216100	-3.22840400	H	-1.99710700	1.57554100	2.15195000
H	-4.35088600	-4.55826400	-3.34272800	H	-1.64745400	0.00462100	2.88034700
H	-5.38895300	-4.84467600	-1.93116200	H	-0.88244400	1.46394500	3.52443600
H	-4.01284600	-0.42367900	1.57149100	C	-1.60386500	-2.89570400	-0.03126900
H	-5.31104100	-1.45501900	2.17302200	H	-2.49294600	-2.60741700	0.53408100
H	-4.70578700	-4.07045200	1.74555300	H	-1.79443000	-2.68737300	-1.08532800
H	-3.26567300	-5.34739200	-0.13491500	H	-1.46522900	-3.97719900	0.07972600
H	-2.25773300	-3.39908100	-1.69583100	C	-0.02918100	-0.82487600	-2.62440500
Si	-0.87358300	-1.35382900	-0.01742500	H	-0.59360600	-1.75064500	-2.49649500
B	2.38934900	0.14464900	0.04764100	H	-0.20175400	-0.48230000	-3.65074200
C	2.15900300	1.75328900	0.21761400	H	1.03530100	-1.05254000	-2.52290700
C	2.19914500	2.42865600	1.43508000	C	10.74700600	4.05428100	-0.05008000
C	1.80162600	2.55781100	-0.86234500	H	11.81394600	4.13760700	-0.28388400
C	1.88844200	3.77684200	1.58822400	H	10.19956200	4.63689400	-0.79531500
C	1.52189200	3.91256400	-0.76742900	H	10.58711200	4.51004900	0.93024700
C	1.54407200	4.52674500	0.47556300				
C	3.12058500	-0.54174300	1.33658600	<b>TS8</b>			
C	2.46485000	-1.23974500	2.33774300	N	4.48408500	2.65191700	0.59444100
C	4.49949100	-0.45173500	1.51916200	C	3.94325800	3.02480500	-0.73114500
C	3.09018100	-1.85778700	3.41097400	C	2.54655900	2.46762400	-0.69396300
C	5.17714200	-1.04194700	2.57905500	C	2.14758600	2.32903300	0.75211600
C	4.46701000	-1.76003600	3.53175900	C	3.47693300	1.96888600	1.42855700
C	3.24557400	-0.26142600	-1.28785000	C	1.81989600	2.01720700	-1.71159600
C	3.16407400	-1.54139600	-1.81874700	C	0.49738700	1.30377300	-1.51010900
C	4.15067400	0.56752700	-1.94751500	C	0.03295400	1.54000300	-0.09906100

C	3.85525900	-1.97795100	-2.93977800	C	1.03403100	1.27972400	0.98783400
C	4.87273200	0.17949200	-3.06968300	C	0.47699900	1.37936500	2.40101700
C	4.72477400	-1.10474600	-3.57306200	C	5.90498700	0.44379800	-0.17703900
F	4.37456800	1.81425100	-1.51723200	C	5.55649800	-0.68960000	0.55843500
F	5.71353800	1.02681200	-3.66238000	C	5.37791000	-1.89857400	-0.10381600
F	5.40545400	-1.49216400	-4.64932600	C	5.53958300	-1.99331100	-1.49136800
F	3.68894300	-3.22009500	-3.40202600	C	5.91397400	-0.84785400	-2.20003300
F	2.33451400	-2.44753300	-1.25664500	C	6.10136600	0.36973400	-1.55449600
F	1.70166600	2.03353500	-2.09743300	C	5.31917300	-3.30199500	-2.20501500
F	1.21405100	4.62536000	-1.85476200	S	6.02829200	2.02101300	0.63752700
F	2.47839500	1.77913900	2.57694300	O	6.83493700	2.89143200	-0.19839500
F	1.90720200	4.34496900	2.79364500	O	6.31093700	1.78179300	2.04079300
F	1.21714800	5.81351300	0.59177900	O	-0.91587000	2.33021500	0.19307900
F	1.11238600	-1.32724500	2.33302600	Si	-2.20575000	3.17050200	-0.71734100
F	2.37501200	-2.52714200	4.31834800	C	-2.94117700	1.88612800	-1.89292800
F	5.09700800	-2.33300500	4.55422100	C	-4.44685900	1.65991100	-1.68724600
F	6.49812300	-0.91972400	2.69543800	C	-2.64832600	2.09215300	-3.38717600
C	-1.07121500	-0.70769300	-1.79391600	C	-3.34213100	3.72884700	0.67806500
H	-1.84068900	-1.36088000	-2.22784200	C	-4.08004000	5.02866000	0.32116600
C	-1.48402500	-0.21174600	1.35470500	C	-2.61965000	3.85622100	2.02656500
H	-2.39465900	0.17197100	0.87318000	C	-1.18821700	4.52192500	-1.56069700
C	-0.03594700	-3.02198800	0.31121000	C	-2.02138100	5.44395600	-2.46496600
C	-1.87127500	-0.95071100	2.64458600	C	-0.36168000	5.34528300	-0.56279700
H	-0.97896000	-1.18996900	3.22599300	H	3.96143500	4.11505100	-0.83489600
H	-2.50473000	-0.30587200	3.26647600	H	4.53056300	2.59742700	-1.54992100
H	-2.41514200	-1.88612000	2.46513200	H	1.80377900	3.30250100	1.13212500
C	-0.41618600	-3.75637100	1.60698800	H	3.55446100	2.31200400	2.46113900
C	0.15312100	-0.77106700	-2.71308900	H	3.60727600	0.87658100	1.40820600
H	-0.15729700	-0.53275100	-3.73686700	H	2.18090600	2.08106100	-2.73538900
H	0.90160600	-0.03606900	-2.41576500	H	0.64413500	0.22961600	-1.66224000
H	0.63184100	-1.75266100	-2.72423600	H	-0.25873200	1.62133000	-2.23097900
F	5.24429600	0.25418200	0.65835800	H	1.46904700	0.29421800	0.79404500
H	1.22626300	-0.36255100	-0.06520100	H	-0.36241000	0.69809600	2.54631400
H	0.99478400	-2.67099600	0.43640300	H	1.25614500	1.10944800	3.11901300
C	-0.00851600	-4.02121200	-0.86149200	H	0.14485000	2.40068100	2.60966200
H	-0.86539500	-4.70091600	-0.81464400	H	5.46065200	-0.62785700	1.63843100
H	0.01012000	-3.55137600	-1.84909200	H	5.12437100	-2.78509700	0.46883700
H	0.89366000	-4.63545900	-0.78606000	H	6.07620200	-0.91459900	-3.27245400
C	-1.64264000	0.71917500	-1.77827400	H	6.43264700	1.24898900	-2.09886000
H	-1.85942700	1.04475600	-2.80274100	H	5.79570800	-3.29747400	-3.18845600
H	-2.57111100	0.80562400	-1.20088700	H	5.72069500	-4.13851300	-1.62768000
H	-0.91370100	1.42496000	-1.36242700	H	4.25104300	-3.49846900	-2.35260000
C	-0.64259000	1.02310600	1.68366500	H	-2.43645400	0.96704800	-1.56936400
H	-0.44318900	1.63474800	0.79951900	H	-4.80332600	0.89917900	-2.39219500

H	-1.19204000	1.64280200	2.40426000	H	-4.67230300	1.30818000	-0.67882600
H	0.31076900	0.75149100	2.13736500	H	-5.02301200	2.57419100	-1.87452300
H	0.16979200	-4.68128600	1.66397400	H	-2.82397000	1.15917200	-3.93282200
H	-1.47304500	-4.03573100	1.62689700	H	-1.62063300	2.40736800	-3.60184600
H	-0.18824400	-3.17215500	2.49774100	H	-3.31526100	2.85016200	-3.81174400
C	-1.72392900	4.59008600	-1.39676300	H	-4.09100600	2.93610400	0.79042700
H	-1.05549000	3.96029500	-1.99393300	H	-4.83779700	5.25097200	1.08018500
H	-2.09732300	5.37978700	-2.05507900	H	-4.59141700	4.97308400	-0.64745600
H	-1.12400700	5.05657300	-0.61080700	H	-3.39226400	5.88117800	0.28845400
				H	-3.32329800	4.19225500	2.79628000
<b>14'</b>				H	-2.20656000	2.89662100	2.34809100
N	-2.02043000	4.03695100	0.30607400	H	-1.79986300	4.58342000	1.98353500
C	-1.53364900	3.34117500	1.50998300	H	-0.47852900	3.97791700	-2.20483000
C	-0.13247300	2.94212100	1.11638100	H	-1.36281600	6.09833400	-3.04684100
C	0.15563200	3.44378900	-0.28091400	H	-2.64399100	4.88984300	-3.17403900
C	-1.25079700	3.60448400	-0.86776600	H	-2.67901300	6.08817400	-1.87384600
C	0.68352600	2.13376800	1.78099600	H	0.30147400	6.03793700	-1.09344400
C	1.98353600	1.65952300	1.19092600	H	0.26031500	4.71140700	0.07854300
C	2.19307300	2.07832700	-0.22211600	H	-1.00798700	5.94506100	0.08762500
C	1.03088000	2.44880800	-1.06449100	B	-1.24545500	-1.31756800	0.19507800
C	1.39392700	2.88534700	-2.47505100	C	-2.39763800	-1.68777700	-0.90357000
C	-4.19450600	2.48669700	-0.27331200	C	-2.29392700	-1.32469300	-2.24283400
C	-4.17695100	2.07100400	-1.60406600	C	-3.57083000	-2.37085200	-0.59068400
C	-4.48322900	0.74973400	-1.90184400	C	-3.26112300	-1.57302000	-3.20184600
C	-4.80370300	-0.16174600	-0.88977500	C	-4.57623300	-2.64057100	-1.51672700
C	-4.82224400	0.28204700	0.43642100	C	-4.42476800	-2.23461000	-2.83194300
C	-4.52035000	1.60224000	0.75354900	C	-1.92119300	-1.15585900	1.66657300
C	-5.10845100	-1.59410800	-1.23380700	C	-1.77866100	-2.00231700	2.75966900
S	-3.68058200	4.13984800	0.11575200	C	-2.76849100	-0.07765500	1.88284300
O	-4.19859000	4.49045400	1.42675000	C	-2.38136600	-1.76511500	3.99057500
O	-3.88760900	4.96682100	-1.06012000	C	-3.39448000	0.20558100	3.08588800
O	3.34357700	2.09857400	-0.73664300	C	-3.19229000	-0.65094300	4.15881800
Si	4.99704000	1.71523700	-0.14363600	C	0.10892600	-2.22993000	0.11569400
C	5.50687700	3.30098900	0.70592800	C	1.07388700	-2.19568600	1.12574200
C	6.97515800	3.21033600	1.15706900	C	0.44897900	-3.05805200	-0.95626200
C	4.95615800	0.24678700	1.02132500	C	2.25618800	-2.92021700	1.11062600
C	6.14957300	-0.70254000	0.81518600	C	1.61979300	-3.81013300	-1.01082900
C	5.87015600	1.44307500	-1.76514500	C	2.52084400	-3.75619900	0.03732600
C	5.93914800	2.71203600	-2.626662700	H	-0.85108800	-0.13991600	-0.07035500
H	-1.58345100	4.01419200	2.36898800	F	-1.03941500	-3.11365900	2.66543600
H	-2.11898100	2.43732500	1.73764800	F	-2.19666600	-2.60355300	5.00852300
H	0.63891000	4.43075400	-0.23899300	F	-3.77602500	-0.41118900	5.32958800
H	-1.32467400	4.35967800	-1.65192800	F	-4.17596300	1.28223500	3.21178900
H	-1.59761300	2.63318700	-1.25409100	F	-3.01895600	0.78143700	0.86593400

H	0.42789500	1.73052000	2.75619900	F	-1.19099700	-0.67833100	-2.67197900
H	1.96575200	0.55408200	1.16319600	F	-3.09180500	-1.17581600	-4.46717900
H	2.85610800	1.93772800	1.79656900	F	-5.37131500	-2.48265500	-3.73218400
H	0.45191200	1.50735400	-1.09861000	F	-5.67890200	-3.28953000	-1.14653500
H	1.98741700	2.11810200	-2.97795700	F	-3.79596000	-2.82715400	0.64806900
H	0.47838400	3.03786700	-3.05188000	F	-0.35348600	-3.19261400	-2.01936600
H	1.96197800	3.82133400	-2.46996200	F	1.88700800	-4.57503000	-2.07067100
H	-3.94780200	2.78512300	-2.38928900	F	3.63559700	-4.48847700	0.00967300
H	-4.47056000	0.41804800	-2.93679800	F	3.13729400	-2.81893800	2.10817600
H	-5.07181300	-0.41792200	1.22934500	F	0.89503500	-1.41616300	2.20745600
H	-4.56405200	1.95873100	1.77840000				
H	-5.63068500	-2.09810500	-0.41755500				
H	-5.71986000	-1.65902300	-2.13859400	N	-3.94681400	-0.57559400	0.00692400
H	-4.17867600	-2.14220300	-1.41646400	C	-3.53397800	-0.24964100	-1.36741600
H	4.86028700	3.49108700	1.57212400	C	-2.13704200	0.28992200	-1.15366800
H	7.29356700	4.12985500	1.65490500	C	-1.82934700	0.28275700	0.32612600
H	7.12771100	2.38639300	1.86285700	C	-3.22493700	0.27842600	0.95576900
H	7.64597200	3.04827200	0.30607900	C	-1.31342500	0.78640300	-2.07031400
H	4.95091700	0.62773700	2.05133100	C	0.03655800	1.35970000	-1.72557900
H	6.11380800	-1.52430000	1.53562600	C	0.24406300	1.54797700	-0.24636900
H	7.10741700	-0.18774800	0.94806800	C	-0.93421600	1.46157700	0.68886300
H	6.13618100	-1.14041800	-0.18603400	C	-0.54841800	1.62960600	2.15961100
H	6.87951500	1.06428500	-1.55703800	C	-6.40537400	0.63156000	0.06130300
H	6.42029300	2.50853100	-3.58676000	C	-6.54071300	1.49905900	1.14140900
H	6.51174400	3.50309800	-2.13112300	C	-7.16656400	2.72670500	0.94750100
H	4.93865100	3.10512600	-2.83577700	C	-7.65717500	3.09462100	-0.30738200
B	-0.22676600	-1.17461800	0.14641900	C	-7.51797800	2.19878200	-1.37336700
C	1.24137300	-1.90261900	0.08669600	C	-6.89577600	0.96884000	-1.19957300
C	1.62354900	-3.03471700	0.80452700	C	-8.33183500	4.42546000	-0.51847500
C	2.21596800	-1.41758500	-0.77607700	S	-5.54871500	-0.91278200	0.28630800
C	2.87547500	-3.63184600	0.68623600	O	-5.95721500	-1.80316900	-0.78469800
C	3.47099900	-1.98570500	-0.93896000	O	-5.64601700	-1.26466700	1.69105600
C	3.81199800	-3.10087900	-0.19074000	O	1.23038100	2.22907000	0.17848200
C	-1.06640100	-1.67191000	-1.15688800	Si	2.50587800	3.36522800	-0.27791800
C	-1.34438900	-3.02089700	-1.36159600	C	3.18852900	3.10655000	-2.03005200
C	-1.48213600	-0.82934400	-2.17664200	C	2.44448300	3.78505600	-3.18826200
C	-1.98121000	-3.51599600	-2.49012600	C	4.65002000	3.59973800	-2.05221400
C	-2.13254600	-1.27402400	-3.32363500	C	1.55177200	4.99001500	-0.07303300
C	-2.38241800	-2.62776900	-3.48229300	C	1.18875500	5.28362800	1.39073400
C	-0.98443000	-1.35112300	1.57856400	C	0.26285100	5.04876100	-0.90881200
C	-0.32844100	-1.00218500	2.75443300	C	3.81824500	3.06455500	1.04854700
C	-2.31440300	-1.70832400	1.76507500	C	4.63477200	4.32810200	1.36827500
C	-0.92186500	-0.94816400	4.00540400	C	3.24384000	2.42526900	2.32247100
C	-2.96072200	-1.66770200	2.99674400	H	-3.57365800	-1.14269700	-1.99386800

C	-2.26398800	-1.28123800	4.12986600	H	-4.17750800	0.52449200	-1.81611800
H	-0.03988900	0.01918100	0.03617200	H	-1.33984700	-0.65698400	0.59423500
F	-0.97962500	-3.90707900	-0.42540100	H	-3.26116800	-0.16622400	1.95128800
F	-2.21383000	-4.82034800	-2.63648900	H	-3.64434400	1.30053100	0.99026800
F	-2.99971200	-3.07404100	-4.57446400	H	-1.57782100	0.77928300	-3.12456000
F	-2.52499700	-0.41031000	-4.26681800	H	0.14621900	2.36217300	-2.16644100
F	-1.25775300	0.50156700	-2.11327500	H	0.85684700	0.75231500	-2.13245400
F	0.78407700	-3.60238600	1.67294800	H	-1.49703100	2.36359700	0.37006500
F	3.19104600	-4.70330800	1.41063800	H	-0.42764100	2.68575800	2.40964800
F	5.02701200	-3.63796200	-0.29834000	H	-1.31822500	1.20810300	2.80922300
F	4.37777300	-1.41826000	-1.75190500	H	0.39552700	1.12939900	2.38014200
F	1.98481600	-0.29447700	-1.50232500	H	-6.18830800	1.19493900	2.12244600
F	-3.07539600	-2.11019600	0.73499900	H	-7.28786200	3.40539200	1.78738800
F	-4.25532000	-1.98676300	3.08786300	H	-7.91479500	2.46638700	-2.34944900
F	-2.86597600	-1.23242800	5.31612900	H	-6.81398800	0.25531500	-2.01406500
F	-0.22224200	-0.56377200	5.07626800	H	-7.73077100	5.06823100	-1.17028900
F	0.98239900	-0.66036700	2.71450600	H	-9.30853000	4.29836900	-0.99495500
H	5.36968800	4.14624900	0.02130000	H	-8.48088200	4.94999200	0.42821700
H	5.35282600	0.63809000	-2.29830600	H	3.20128600	2.02414200	-2.21114500
H	4.02304600	-0.31550200	0.90309700	H	2.97330000	3.58962900	-4.12780700
				H	1.41821700	3.43178800	-3.31907600
<b>3a'</b>				H	2.41350900	4.87257300	-3.05533200
N	1.79786200	-1.37424100	-0.21211000	H	5.09650800	3.38452800	-3.02868300
C	1.32778300	-0.98954200	1.13286900	H	5.27471400	3.11972600	-1.29668900
C	0.14025500	-0.10740200	0.82003300	H	4.69768000	4.68614900	-1.90406600
C	-0.14614500	-0.18219300	-0.66127000	H	2.23266900	5.77907900	-0.43053100
C	1.24232100	-0.47664800	-1.23569100	H	0.66915600	6.24562800	1.46712700
C	-0.48705500	0.72088800	1.64982300	H	2.05562600	5.32039500	2.05308400
C	-1.58505000	1.64272200	1.18455800	H	0.51002900	4.51524900	1.77732100
C	-2.03843600	1.35900200	-0.25194700	H	-0.23349800	6.01572800	-0.76847100
C	-0.83934600	1.07915700	-1.16895300	H	0.42833800	4.91784000	-1.98008400
C	-1.26574900	0.95644000	-2.62797600	H	-0.44926900	4.28138600	-0.57731600
C	4.39312400	-0.49854500	-0.08858700	H	4.50916000	2.33711100	0.60746300
C	4.70054500	0.35212700	-1.14898700	H	5.46984300	4.07067900	2.02898200
C	5.46923800	1.48379000	-0.90546600	H	5.06003900	4.79131000	0.47189100
C	5.93777500	1.77514600	0.37970100	H	4.04044600	5.08761300	1.88420300
C	5.62053200	0.90239100	1.42357000	H	4.04126300	2.27865700	3.06000500
C	4.85261500	-0.23516800	1.19903400	H	2.79841500	1.44726800	2.11108500
C	6.80119700	2.98569500	0.62265600	H	2.47502800	3.05317300	2.78785500
S	3.35057100	-1.91525400	-0.37344800	B	1.36500600	-1.44099300	0.06938000
O	3.57261800	-2.84097700	0.72475400	C	2.52348700	-1.45005300	-1.07258300
O	3.50840900	-2.29670800	-1.76675800	C	3.43813400	-0.40895900	-1.11993600
O	-2.88291300	0.22354000	-0.30812100	C	2.73615500	-2.43681600	-2.03235200
Si	-4.51953800	0.19938700	0.04761500	C	4.48643700	-0.31257000	-2.01787300

C	-5.31625800	1.78617600	-0.58725000	C	3.76618600	-2.38291000	-2.96811200
C	-6.85016500	1.71900500	-0.59807100	C	4.64794100	-1.31328600	-2.96525200
C	-5.16957800	-1.32187400	-0.84719500	C	0.13486700	-2.45053900	-0.25429500
C	-6.42545800	-1.95198600	-0.22905000	C	-0.46446300	-3.34533400	0.62758500
C	-4.78525700	0.01257600	1.90484500	C	-0.50523400	-2.34555700	-1.48848300
H	1.07400100	-1.89063900	1.69728600	C	-1.66011300	-4.00647700	0.35391400
H	2.09229400	-0.43255300	1.69430500	C	-1.69010500	-2.98451800	-1.80567300
H	-0.79236700	-1.04831200	-0.85893800	C	-2.29328700	-3.80618700	-0.86202800
H	1.23322800	-0.98642700	-2.20010000	C	1.94312800	-1.45374000	1.59497600
H	1.82552200	0.45664700	-1.31994000	C	1.07877800	-1.23386600	2.66652900
H	-0.19260800	0.77842200	2.69688000	C	3.28234700	-1.55914100	1.96649700
H	-1.23352800	2.68232500	1.25181300	C	1.47733700	-1.07047100	3.98260600
H	-2.45198200	1.57500000	1.85437300	C	3.73264200	-1.41581300	3.27695300
H	-2.57704400	2.24074200	-0.63438100	C	2.82738200	-1.16160300	4.29335900
H	-0.14212100	1.92341400	-1.05744800	H	0.82436100	-0.26054500	-0.01181900
H	-1.75783100	1.87292500	-2.97148300	F	0.08984800	-3.62413700	1.81413300
H	-0.40584100	0.77289300	-3.28049000	F	-2.19710800	-4.82647300	1.25436000
H	-1.96951700	0.12654100	-2.74448500	F	-3.44444200	-4.40615100	-1.13595700
H	4.35919000	0.10722400	-2.15022100	F	-2.27876800	-2.78493900	-2.99081900
H	5.71913500	2.14943200	-1.72761500	F	0.03158500	-1.56960500	-2.45024500
H	5.98826100	1.11183900	2.42463400	F	3.34095700	0.57824200	-0.19951200
H	4.62916100	-0.93263800	2.00042200	F	5.32859200	0.72735600	-1.98379300
H	6.49535900	3.82443300	-0.00864900	F	5.63568300	-1.24634200	-3.85337200
H	6.75262400	3.30537900	1.66670000	F	3.91168200	-3.35314600	-3.86843400
H	7.84909200	2.76450300	0.39172400	F	1.95082400	-3.51587400	-2.09993100
H	-4.98646000	2.63497000	0.02695400	F	4.24209300	-1.80824200	1.06397500
H	-7.29588000	2.65994400	-0.93550700	F	5.03133500	-1.52100300	3.55826200
H	-7.24992400	1.50697800	0.40007400	F	3.24169300	-1.00986100	5.54813500
H	-7.20470100	0.92938000	-1.26905600	F	0.58353300	-0.82228200	4.94032400
H	-5.35658300	-1.05448200	-1.89579000	F	-0.24670400	-1.13814700	2.44571700
H	-6.77555300	-2.80786900	-0.81444100				
H	-7.25303300	-1.23681600	-0.16608800	<b>TS11</b>			
H	-6.22832500	-2.30848000	0.78761700	N	6.85729700	1.37214600	-0.63125000
H	-5.84418200	-0.21384200	2.08999600	C	6.31545700	0.40387700	-1.59796000
H	-4.35578700	-2.05789000	-0.86916200	C	5.03098100	-0.02993700	-0.92860400
H	-4.94498500	1.98102300	-1.60283900	C	4.85377100	0.76506600	0.34670500
H	-4.59469400	0.96737000	2.41223700	C	6.30018700	1.13007500	0.70039400
C	-3.89672500	-1.09075400	2.49673700	C	4.22672100	-1.02751400	-1.28141000
H	-2.83632600	-0.87610500	2.32313100	C	3.00554400	-1.39892200	-0.47225400
H	-4.04941600	-1.20641200	3.57437800	C	4.10444600	-0.04641600	1.41928600
H	-4.10570600	-2.05945000	2.02812900	C	3.84332300	0.72877400	2.70253300
			C	9.37990900	0.35299400	-0.30133600	
<b>4a'</b>			C	9.67281300	0.12998400	1.04297900	
N	2.93879500	-1.66113000	-0.18054900	C	10.34529000	-1.03228000	1.40160800

C	2.44734400	-1.19329800	-1.49106600	C	10.73246400	-1.96892700	0.43733900
C	1.03024700	-0.77296400	-1.17207400	C	10.43243700	-1.71565600	-0.90457300
C	0.70198300	-1.19813800	0.24140900	C	9.76001600	-0.55902100	-1.28368700
C	2.08270400	-1.15842200	0.90344700	S	8.46115500	1.80282900	-0.76257200
C	0.22610500	-0.01866300	-1.91520300	O	8.68329400	2.03813000	-2.17690100
C	-1.12974400	0.42342000	-1.43071300	O	8.67855600	2.81087900	0.25823900
C	-1.55060900	-0.26638000	-0.12842000	H	6.16476700	0.89364000	-2.56278500
C	-0.38096100	-0.32172400	0.86385300	H	6.98361400	-0.45872600	-1.74299000
C	-0.82014700	-0.82822700	2.23264700	H	4.30769900	1.69613300	0.13691500
C	5.14653200	-0.06239700	0.11221400	H	6.40076800	2.02785300	1.31105200
C	5.57287000	0.55618700	-1.06029200	H	6.78906200	0.28024200	1.20926800
C	5.96547100	1.88972500	-1.01577700	H	4.41362900	-1.61810800	-2.17418600
C	5.94046000	2.60869200	0.18208300	H	4.71269500	-0.94337600	1.61346700
C	5.51476600	1.96127100	1.34631200	H	4.79112800	1.03475400	3.15262800
C	5.11954600	0.62923700	1.32167600	H	3.24960800	1.62472500	2.50089600
C	6.40128600	4.04250100	0.22895800	H	3.29906800	0.12142900	3.42951300
S	4.57300500	-1.74686200	0.05861800	H	9.40156100	0.87563800	1.78424700
O	5.12361800	-2.35500500	-1.14095900	H	10.58622000	-1.21190400	2.44583100
O	4.76141300	-2.31227800	1.38333200	H	10.74037900	-2.42948300	-1.66366300
O	-2.63544500	0.41105300	0.46484600	H	9.55443400	-0.34156100	-2.32733800
Si	-4.26807500	0.30201800	0.07974600	H	2.09372000	-1.37857400	-1.07629600
C	-4.66534300	-1.45369300	-0.52707200	H	3.10287300	-2.43238600	-0.10197500
C	-4.20969100	-1.70549000	-1.97270600	C	2.84799900	-0.52602700	0.74517200
C	-6.15429800	-1.80985800	-0.38527500	O	1.75445500	-0.16691000	1.19301000
C	-4.64166000	1.60870500	-1.24292100	C	11.49628700	-3.20538000	0.83331400
C	-4.35203000	3.01020600	-0.68733100	H	11.31151900	-4.02692700	0.13674400
C	-6.04997700	1.53599600	-1.84737700	H	12.57352400	-3.00656900	0.83237100
C	-5.06947700	0.70958100	1.74324000	H	11.22301000	-3.53640400	1.83843900
C	-4.82112100	-0.42346700	2.74969200	Si	-0.12615500	-0.32189800	0.58333700
C	-6.55330300	1.09648000	1.70938300	B	-3.63755700	-0.03708100	-0.12166000
H	2.51650100	-2.01015600	-2.21446800	C	-4.20028000	-0.05851500	1.40979200
H	3.03090700	-0.34255900	-1.87270500	C	-5.28985100	0.67538400	1.87417400
H	0.36706300	-2.24724200	0.23966200	C	-3.58521600	-0.83478300	2.38157200
H	2.18375500	-1.80384500	1.77689800	C	-5.70405400	0.67506100	3.20149900
H	2.33823300	-0.12134700	1.18024500	C	-3.94906000	-0.86229900	3.72005400
H	0.54705000	0.32356100	-2.89784200	C	-5.02584000	-0.09523800	4.13585200
H	-1.88560200	0.24829100	-2.20730100	C	-4.00854100	1.36791300	-0.86612900
H	-1.12802600	1.50815500	-1.24982400	C	-3.51662100	2.56732600	-0.36011600
H	-1.83525500	-1.31064500	-0.34728600	C	-4.81139700	1.51058500	-1.99376900
H	0.01621000	0.69992900	0.96421200	C	-3.75438100	3.81247400	-0.91814100
H	-1.53679500	-0.13904800	2.68361000	C	-5.08556200	2.73989100	-2.58872500
H	0.03494700	-0.92955200	2.90907800	C	-4.55453600	3.89951500	-2.04928600
H	-1.29923300	-1.81179900	2.14389600	C	-4.07622700	-1.33690700	-0.99083000
H	5.61707700	-0.01647000	-1.98161300	C	-3.30847300	-1.73067100	-2.07980500

H	6.30521600	2.37944200	-1.92461800	C	-5.19938200	-2.12104300	-0.75699600
H	5.50200800	2.50789700	2.28562600	C	-3.57983300	-2.84030000	-2.86329500
H	4.81699000	0.11420200	2.22848300	C	-5.52231000	-3.23848500	-1.52149000
H	6.27573600	4.53177300	-0.74032900	C	-4.70537700	-3.60247400	-2.58093000
H	5.84544100	4.61325700	0.97767300	F	-6.04527400	-1.82191700	0.23807700
H	7.46314900	4.09749500	0.49350600	F	-6.60937700	-3.96031700	-1.24753400
H	-4.09906200	-2.13093300	0.13227700	F	-4.99314000	-4.67436500	-3.31767800
H	-3.13024400	-1.58203800	-2.10421100	F	-2.76991100	-3.18620300	-3.86793900
H	-4.46172900	-2.72638400	-2.28510500	F	-2.19455600	-1.03506000	-2.39724600
H	-4.70595100	-1.02114300	-2.67099800	F	-2.53687300	-1.61951700	2.04329300
H	-6.49170600	-1.77698600	0.65457000	F	-3.27191100	-1.61232200	4.59563300
H	-6.34221900	-2.82292100	-0.76181200	F	-6.01122300	1.43053000	1.03741100
H	-6.79173700	-1.12856100	-0.96083900	F	-6.75005600	1.40527600	3.58725200
H	-3.92306200	1.41920200	-2.05519700	F	-5.40659600	-0.10049900	5.41174900
H	-3.33919300	3.08022600	-0.27650900	F	-2.72100800	2.54972600	0.72936900
H	-4.45613000	3.77321300	-1.46814300	F	-3.22399400	4.91663600	-0.38718200
H	-5.05330500	3.26838600	0.11552900	F	-4.80279700	5.08204400	-2.60920000
H	-6.22976400	0.58406400	-2.35697400	F	-5.85884400	2.80901600	-3.67283700
H	-6.19649600	2.33582200	-2.58378400	C	0.20482100	0.42947900	-1.11660000
H	-6.82729600	1.65242400	-1.08451400	H	1.26195500	0.72933500	-1.12209500
H	-4.50103400	1.58662300	2.08986300	H	0.09994200	-0.36317200	-1.86780300
H	-3.76328000	-0.70168600	2.79420300	C	-0.13815600	-2.19959500	0.73999000
H	-5.13414300	-0.12604700	3.75783900	H	0.89668500	-2.53445700	0.59800700
H	-5.39017500	-1.32286200	2.48692400	H	-0.38529600	-2.43348200	1.78102700
H	-6.72777200	2.00724100	1.12824000	C	-0.66284300	0.74732100	2.01682600
H	-6.92540000	1.28036300	2.72498100	C	-1.05386000	-2.98512600	-0.20410800
H	-7.17468400	0.30426600	1.27639600	H	-0.88732900	-4.05984600	-0.08578500
				H	-2.10148800	-2.78004400	0.01708100
<b>TS12</b>				H	-0.87658800	-2.73042000	-1.25376300
N	-3.83028100	3.00599400	-0.16110200	C	-0.35509700	0.13921500	3.39236500
C	-3.34556300	2.75723100	1.20723600	H	-0.59481800	0.85424800	4.18454500
C	-1.86079500	2.57752100	1.00096000	H	-0.95322900	-0.75822800	3.57023700
C	-1.53108100	2.76641700	-0.46447000	H	0.70212600	-0.12687700	3.49788200
C	-2.87754400	2.47394200	-1.13927900	C	-0.65481200	1.63061900	-1.52769600
C	-0.95317600	2.18273200	1.88784100	H	-0.20541900	2.13755600	-2.38643200
C	0.50090500	2.10967400	1.50746600	H	-1.65244500	1.30020600	-1.81355900
C	0.72775200	1.92856800	0.02850300	H	-0.75872100	2.36011900	-0.71894800
C	-0.44238100	1.77332800	-0.90624300	F	-5.38317000	0.45034400	-2.58187900
C	-0.03569600	1.89471500	-2.36685200	H	-2.38495100	-0.09906300	-0.03602200
C	-5.74487900	1.05532200	-0.09770000	H	-0.14417800	1.70870400	1.89750200
C	-5.47046900	0.09106300	-1.06635800	H	-1.72753800	0.96935800	1.92881900
C	-5.62596400	-1.25277500	-0.74448000				
C	-6.05114700	-1.64489500	0.53071600	<b>4a</b>			
C	-6.33447500	-0.65463600	1.47637600	N	2.23782300	-1.33685700	0.07894200

C	-6.18272500	0.69311300	1.17437000	C	1.79407800	-0.70041500	1.33438000
C	-6.19783300	-3.10001000	0.89322700	C	0.60583600	0.11706700	0.87947000
S	-5.45632800	2.77169700	-0.45123300	C	0.29188700	-0.24106400	-0.55561600
O	-6.15275900	3.55210400	0.55585400	C	1.67076600	-0.64171300	-1.08580800
O	-5.63201500	2.98657100	-1.87660200	C	-0.00063400	1.09679900	1.54389000
O	1.83468400	2.29733900	-0.47977700	C	-1.10188400	1.92042200	0.92649200
Si	3.23746500	3.23947700	0.05668900	C	-1.59809200	1.33868500	-0.39885100
C	2.53590000	4.97801700	-0.06148900	C	-0.41864000	0.89908000	-1.27995200
C	3.51804000	6.03685500	0.46368200	C	-0.87928200	0.50981900	-2.68030600
C	3.80344900	2.88144900	1.80847800	C	4.84283400	-0.48863100	-0.01539100
C	4.08024500	1.42688600	2.20677900	C	5.13211700	0.13880800	-1.22353400
C	4.51483300	2.90486400	-1.25694800	C	5.91490200	1.28946800	-1.21795000
C	3.91559700	2.76489600	-2.66362900	C	6.41240600	1.81618000	-0.02401700
H	-3.59610700	3.60940200	1.84413700	C	6.11587500	1.15967500	1.17553500
H	-3.78577700	1.84995800	1.64780900	C	5.33540000	0.01073600	1.18984200
H	-1.23527300	3.80488500	-0.67341600	C	7.26628700	3.05784000	-0.01610400
H	-3.01895600	2.96906400	-2.09998500	S	3.78204700	-1.91857900	-0.00532200
H	-2.98543500	1.38270400	-1.27441300	O	4.01846500	-2.62267400	1.24392600
H	-1.20907800	1.96283100	2.91996700	O	3.90525800	-2.55942200	-1.30343300
H	1.03781700	1.32521900	2.04982800	O	-2.40608600	0.19634800	-0.17898900
H	0.99745700	3.05254900	1.78227300	Si	-4.05988500	0.09999700	0.07545700
H	-0.87092200	0.78786300	-0.70498100	C	-4.80918400	1.85064800	0.06795000
H	0.74632100	1.16995600	-2.60750500	C	-5.06661700	2.36172700	-1.35706000
H	-0.89541200	1.68626900	-3.00803200	C	-6.09375600	1.95075900	0.90371000
H	0.33812000	2.90022600	-2.58649400	C	-4.74600500	-0.92239200	-1.36100900
H	-5.16944900	0.39288500	-2.06537600	C	-6.22878300	-1.27196200	-1.17813400
H	-5.42005500	-2.00709600	-1.49720000	C	-3.92221900	-2.18215400	-1.66520700
H	-6.68662900	-0.94602700	2.46224600	C	-4.32390900	-0.70235200	1.76964100
H	-6.42197700	1.46598200	1.89846500	C	-3.90241600	-2.17644100	1.80828300
H	-6.96006400	-3.23330700	1.66519600	C	-3.56121000	0.08374300	2.84519300
H	-6.47383400	-3.70057400	0.02368700	H	1.54480000	-1.47602500	2.06354000
H	-5.25504400	-3.50183600	1.28020300	H	2.57222500	-0.05459400	1.76734900
H	2.28430500	5.18096600	-1.11025200	H	-0.35384800	-1.13015200	-0.56919200
H	3.11306800	7.04558400	0.34647100	H	1.64761500	-1.32093900	-1.93893800
H	4.47121000	6.00377900	-0.07493600	H	2.25470100	0.25731700	-1.34863800
H	3.73263500	5.88897600	1.52697000	H	0.31461300	1.35389500	2.55428600
H	3.10861900	3.34874400	2.51812600	H	-0.73616600	2.94309500	0.75464800
H	4.45199500	1.37224600	3.23409100	H	-1.94804800	2.01205200	1.61808400
H	3.17642300	0.81454800	2.14259900	H	-2.17334400	2.11117600	-0.93178500
H	4.82384900	0.96518200	1.55237500	H	0.27523000	1.75068200	-1.34508500
H	5.22512700	3.74320500	-1.23159700	H	-1.35765500	1.35683900	-3.18425700
H	4.69833700	2.58214000	-3.40372100	H	-0.03989300	0.18111900	-3.30164700
H	3.37249500	3.66796400	-2.96350200	H	-1.60611300	-0.30689100	-2.62557500
H	3.21233100	1.92766500	-2.70778300	H	4.76851700	-0.29025700	-2.15231000

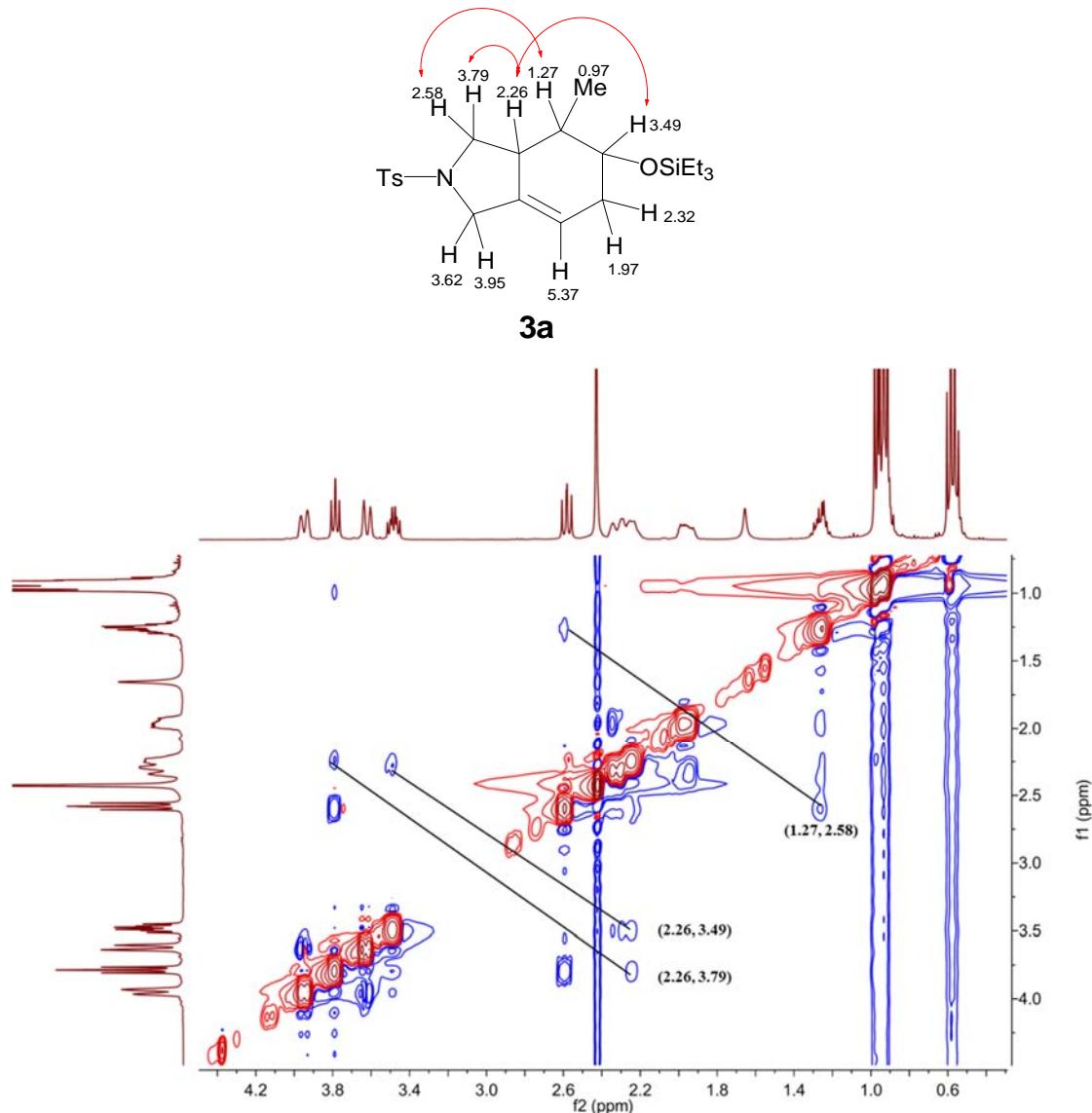
B	1.12493600	-1.20778500	0.02233500	H	6.15170800	1.78116900	-2.15754600
C	1.83346500	-1.45896800	1.46582800	H	6.51163700	1.55131800	2.10926800
C	1.16626300	-1.04970400	2.61979500	H	5.12677800	-0.52004900	2.11362400
C	3.12246700	-1.93272200	1.68871100	H	8.25981500	2.84553100	0.39184700
C	1.71509300	-1.06303700	3.89175300	H	7.39324600	3.46079800	-1.02354800
C	3.71639400	-1.97233500	2.94790000	H	6.81734400	3.83739800	0.60780800
C	3.01342600	-1.52854100	4.05633500	H	-4.06137700	2.51164000	0.53385800
C	2.10920900	-1.41521500	-1.25846700	H	-5.38894800	3.40981200	-1.34681500
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C	2.80929800	-2.40609000	-3.39025100	H	-6.51137200	2.96381900	0.85325000
C	4.15357300	-0.68969100	-2.41468000	H	-5.91964900	1.71528800	1.95824400
C	3.92375400	-1.58594700	-3.44916000	H	-6.86623500	1.26460700	0.53680400
C	-0.34320700	-1.89893300	-0.15808100	H	-4.65811300	-0.26010100	-2.23670500
C	-1.10461100	-1.65399900	-1.30126600	H	-6.60383400	-1.85349100	-2.02920600
C	-0.92916400	-2.80437500	0.72623000	H	-6.85772600	-0.37898900	-1.08852600
C	-2.33680800	-2.23012500	-1.56743500	H	-6.38370400	-1.87825700	-0.27659000
C	-2.15572600	-3.42107400	0.49557600	H	-4.22324100	-2.61581200	-2.62650000
C	-2.85300300	-3.14967100	-0.66822000	H	-2.84959500	-1.96764000	-1.70864300
H	0.93403200	0.04732500	0.05685100	H	-4.07147000	-2.95236700	-0.90248800
F	0.90181700	-3.16194400	-2.33398600	H	-5.40000700	-0.64492700	1.99377300
F	2.58096300	-3.28233100	-4.36675500	H	-3.94913300	-2.56727400	2.83234600
F	4.76970500	-1.66221500	-4.47254300	H	-4.55042800	-2.80174400	1.18732200
F	5.23459100	0.09811400	-2.44157400	H	-2.87177800	-2.30201700	1.45468700
F	3.54853700	0.23537900	-0.36959300	H	-3.76275100	-0.32178800	3.84398400
F	-0.09753700	-0.58867800	2.51861600	H	-3.83027200	1.14757800	2.85859900
F	1.01854300	-0.63111300	4.94430800	H	-2.48088300	0.01148500	2.66931700
F	3.57320900	-1.54688200	5.26295000				
F	4.96073400	-2.42607600	3.09291600				
F	3.88357100	-2.37912500	0.68115800				
F	-0.31769900	-3.17055200	1.85939200				
F	-2.66111300	-4.28499300	1.37837100				
F	-4.00474100	-3.77179300	-0.92588000				
F	-3.01284700	-1.93454400	-2.68098200				
F	-0.62258400	-0.84081000	-2.26151900				
H	1.59059700	5.03992400	0.49469400				
H	4.73322800	3.46564600	1.89488500				
H	5.08394500	2.00643300	-1.00365300				

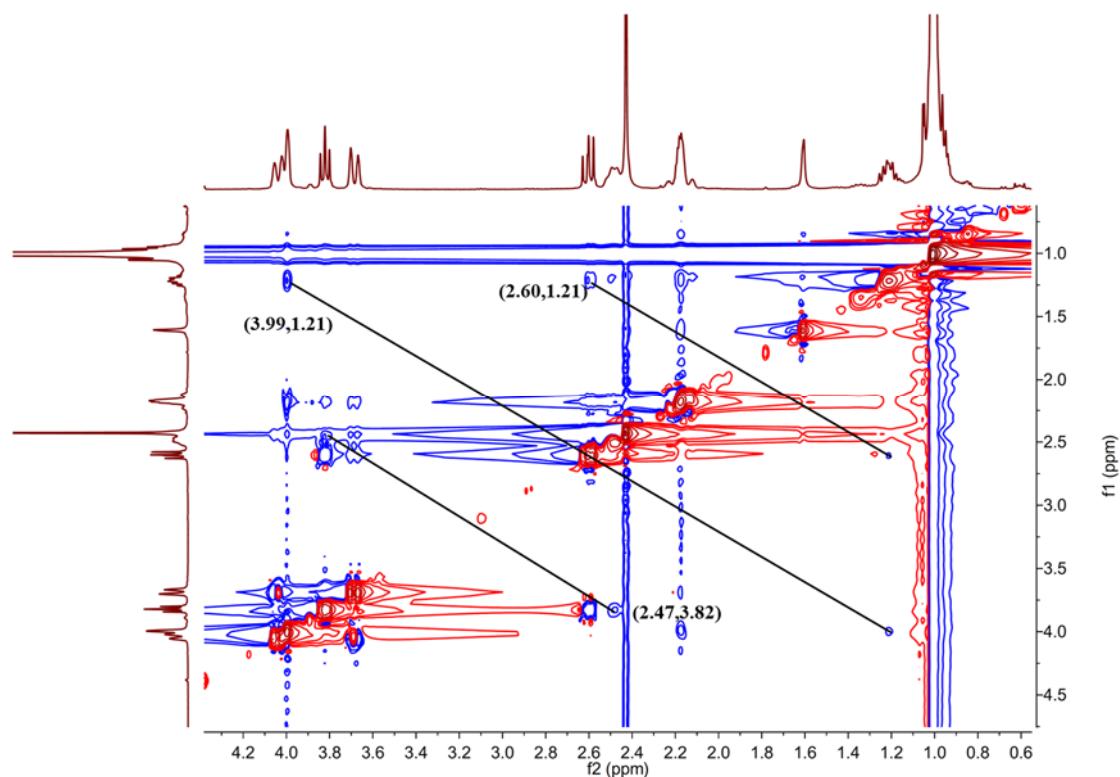
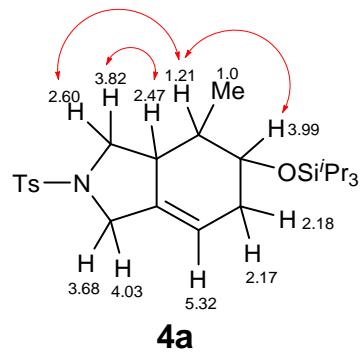
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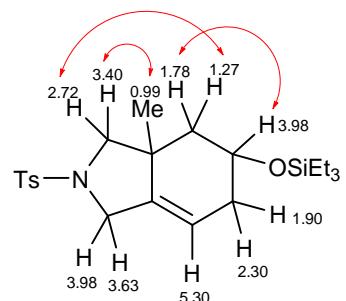
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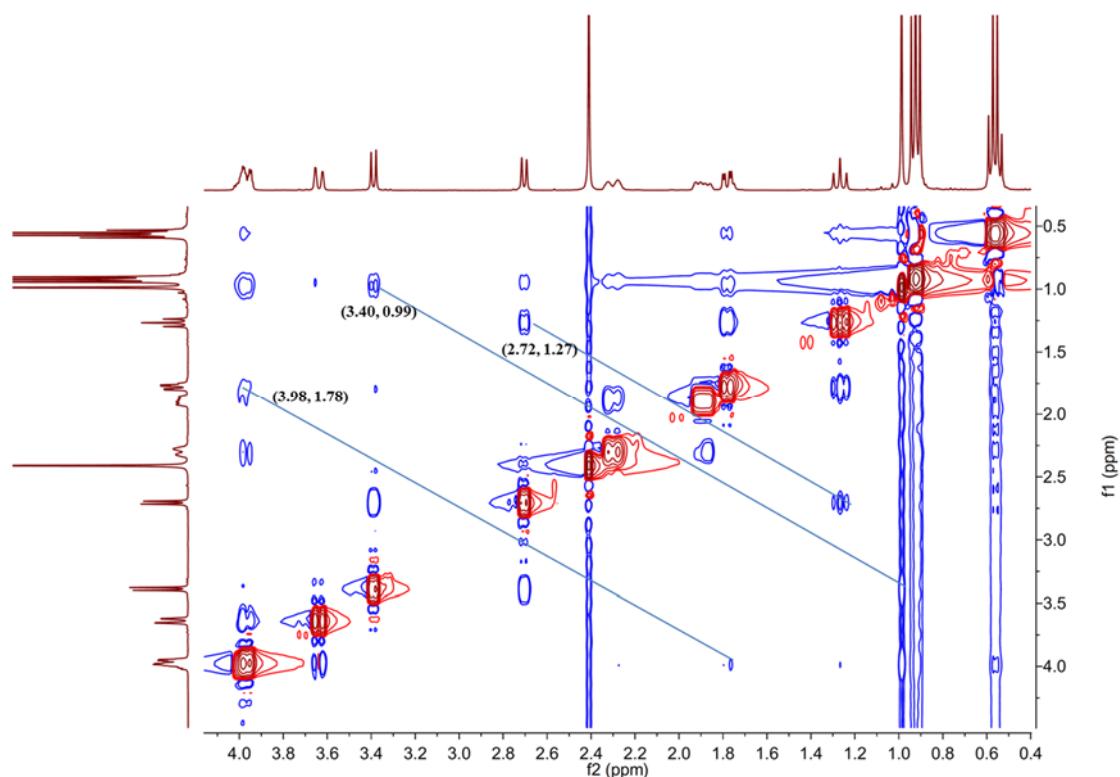
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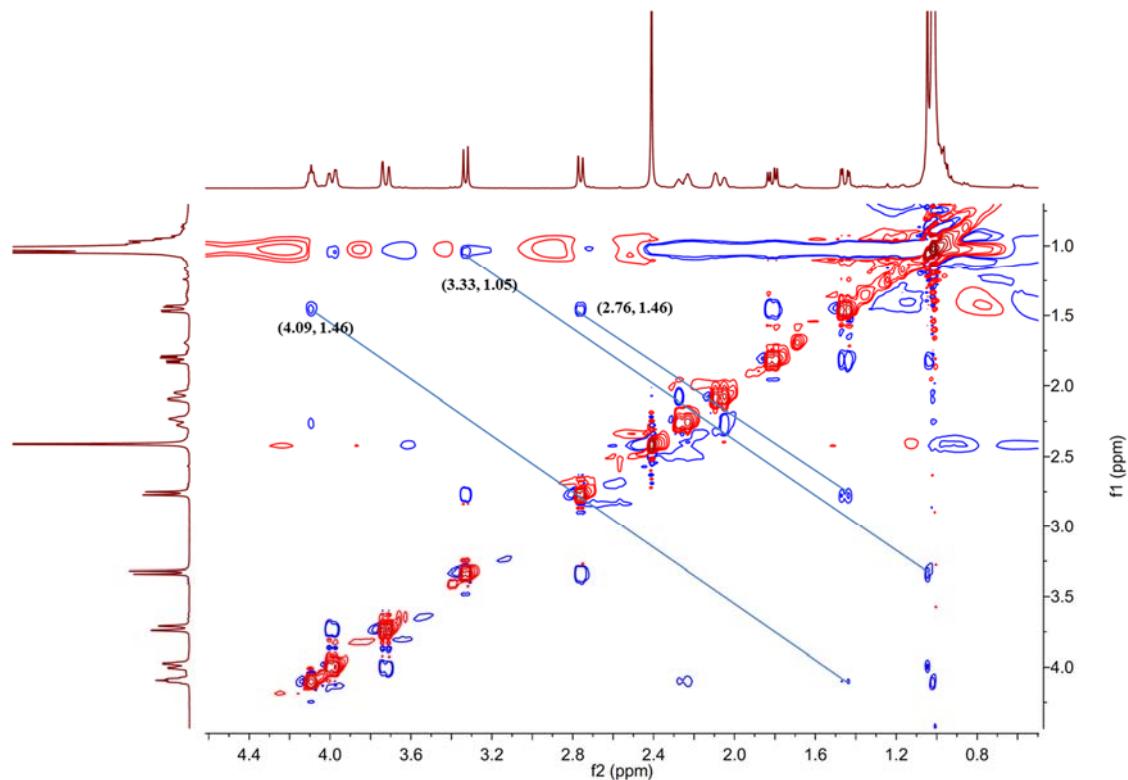
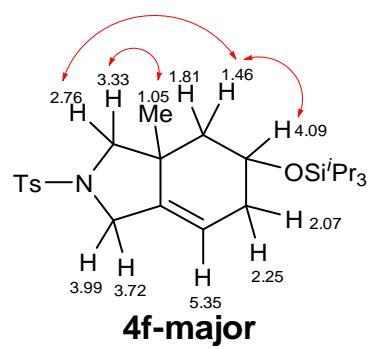


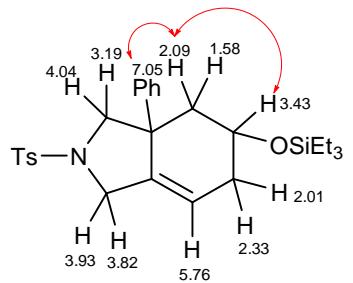




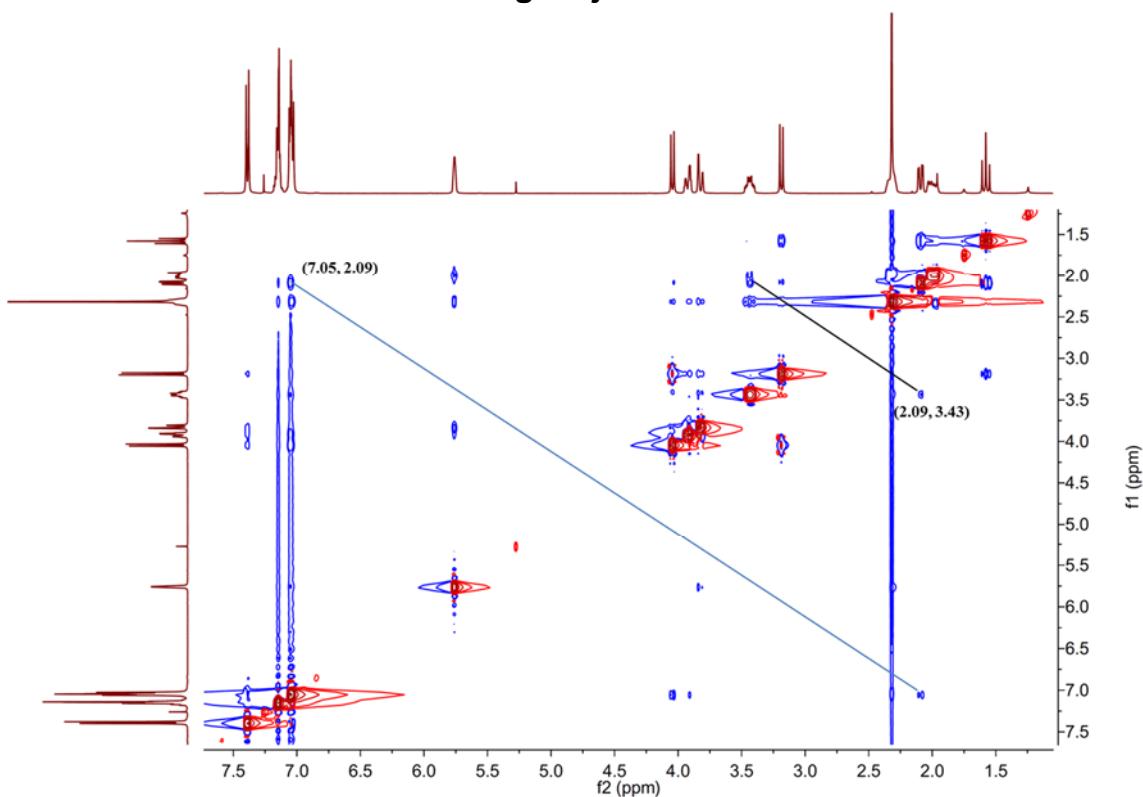
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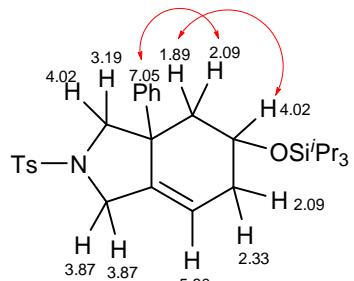




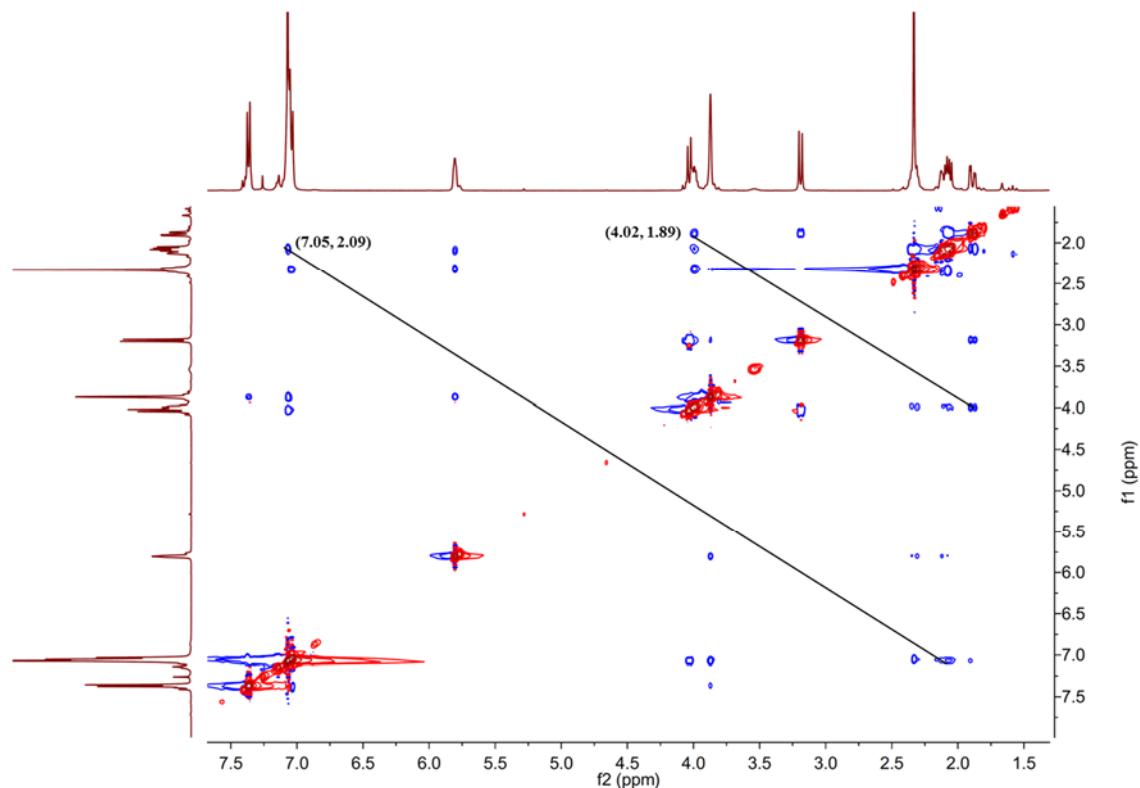


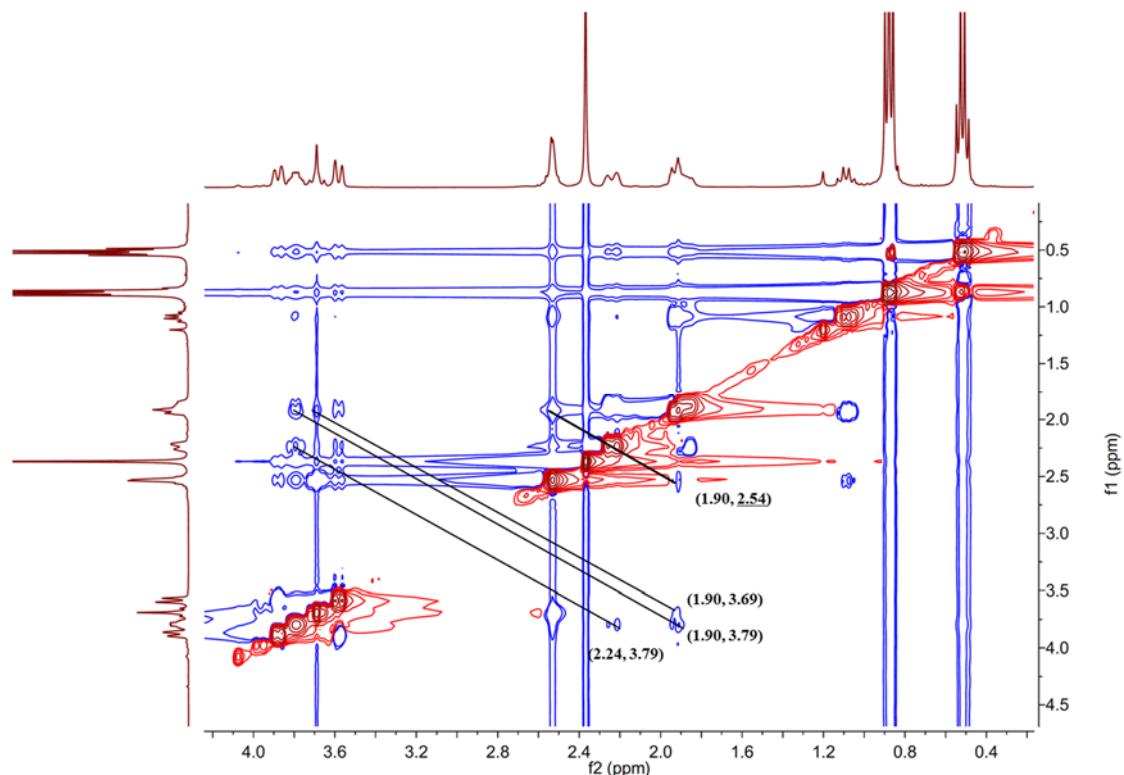
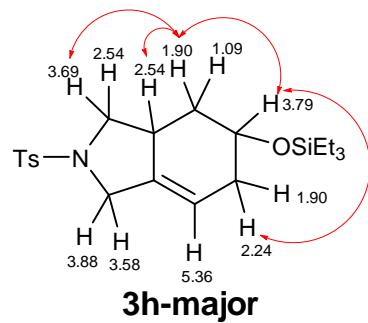
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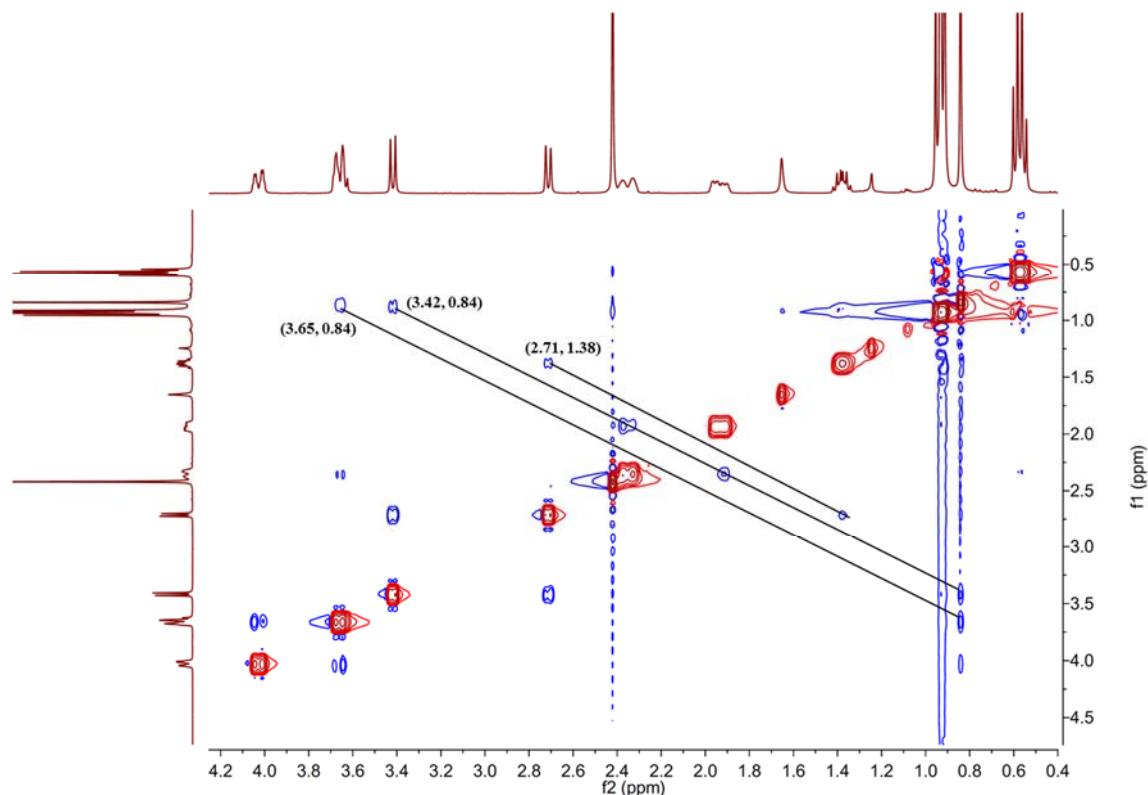
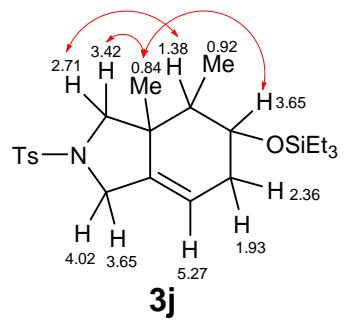


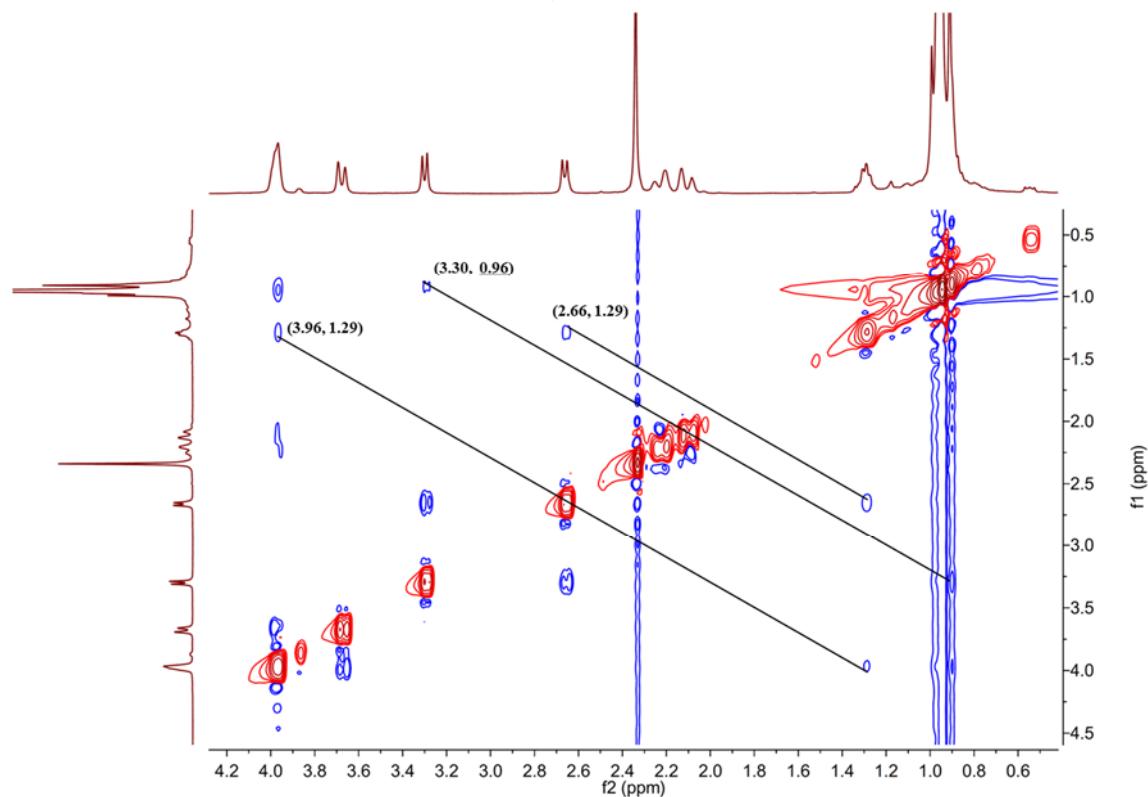
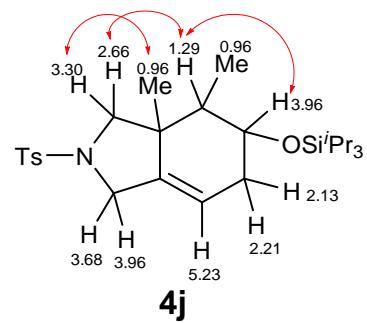


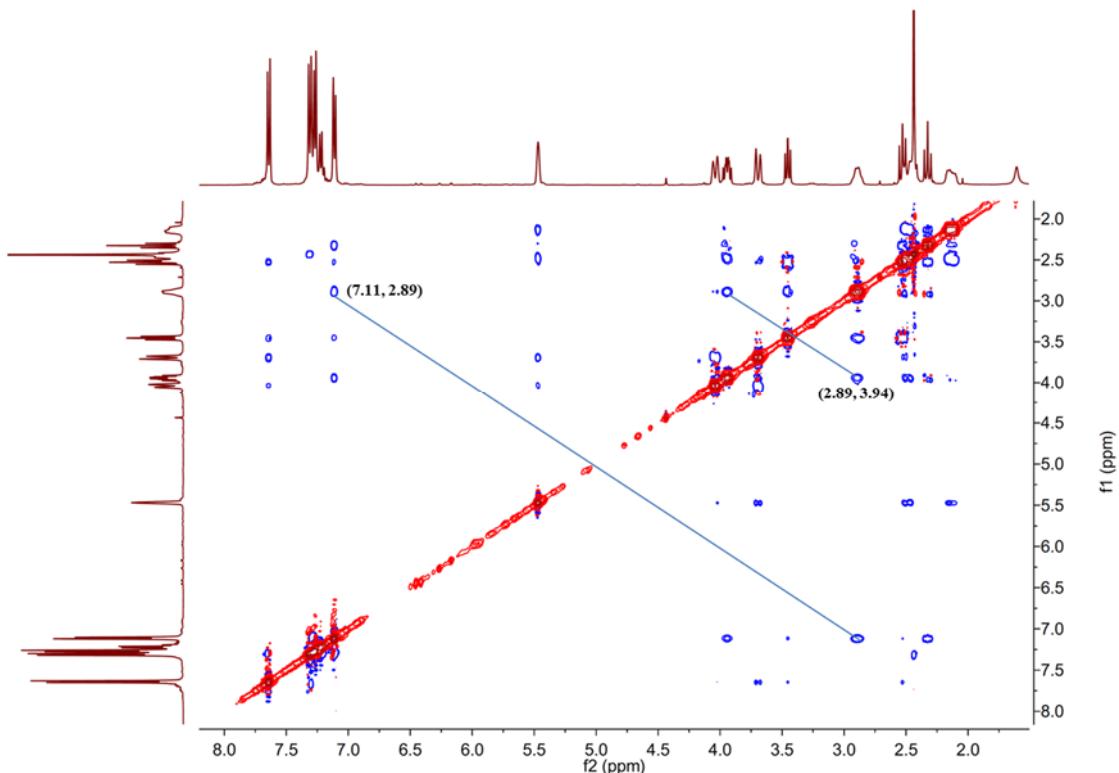
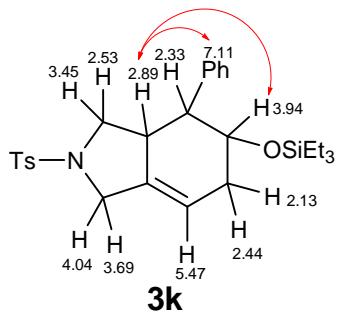
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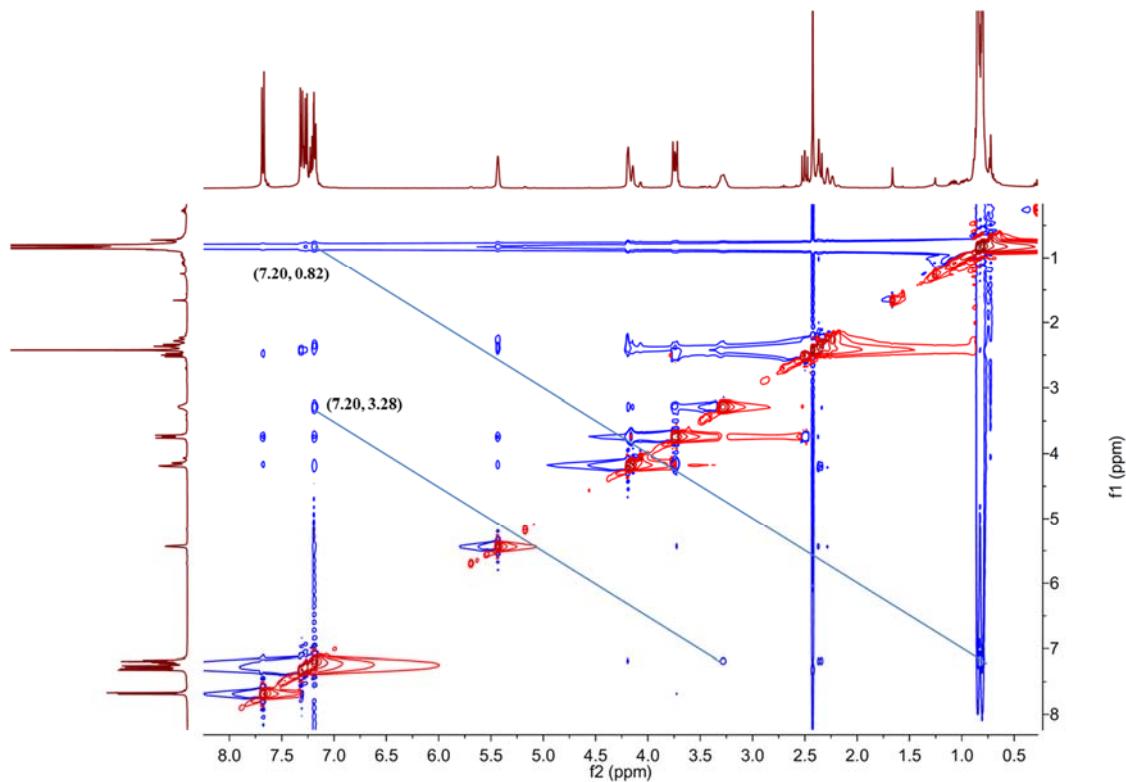
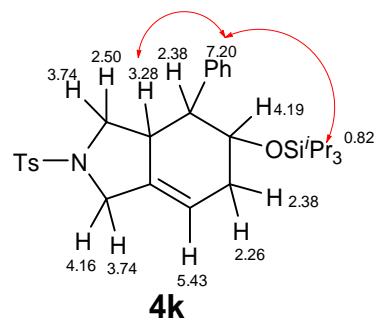


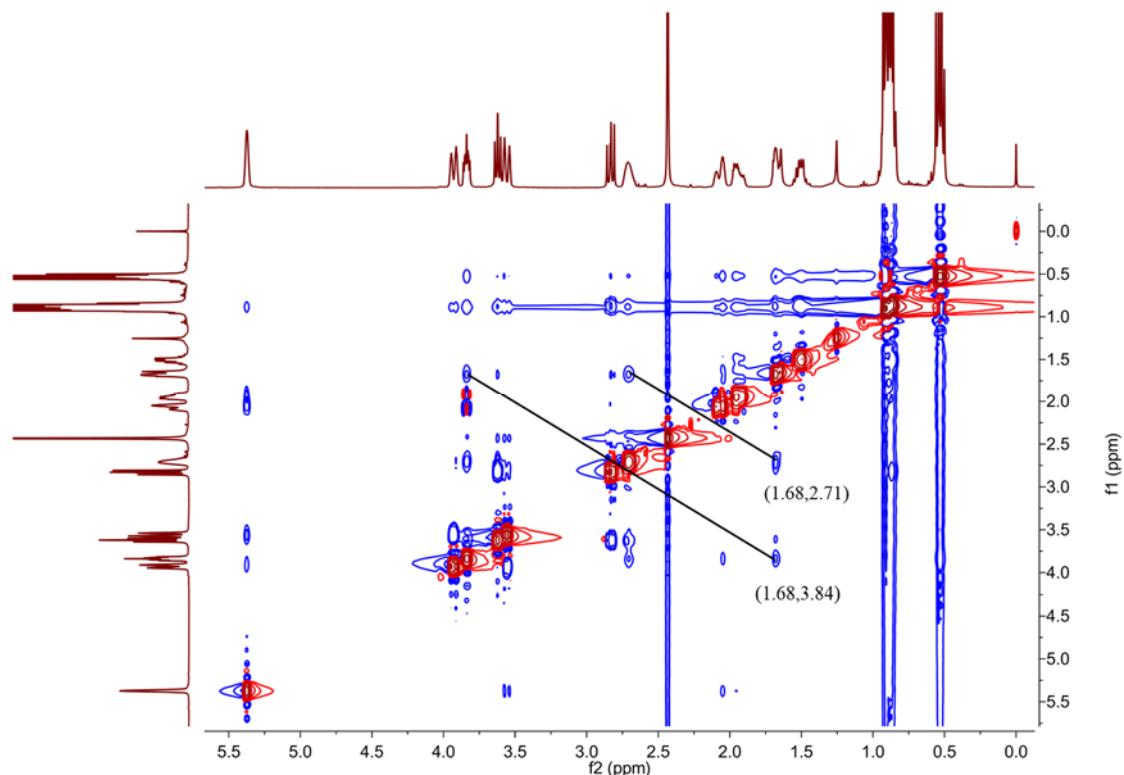
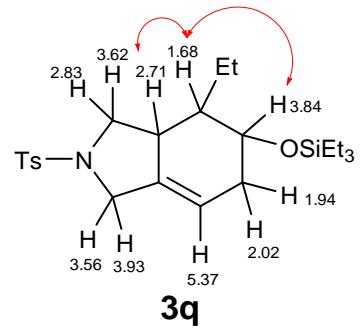


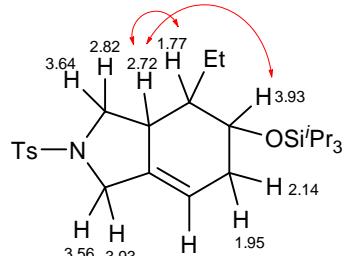




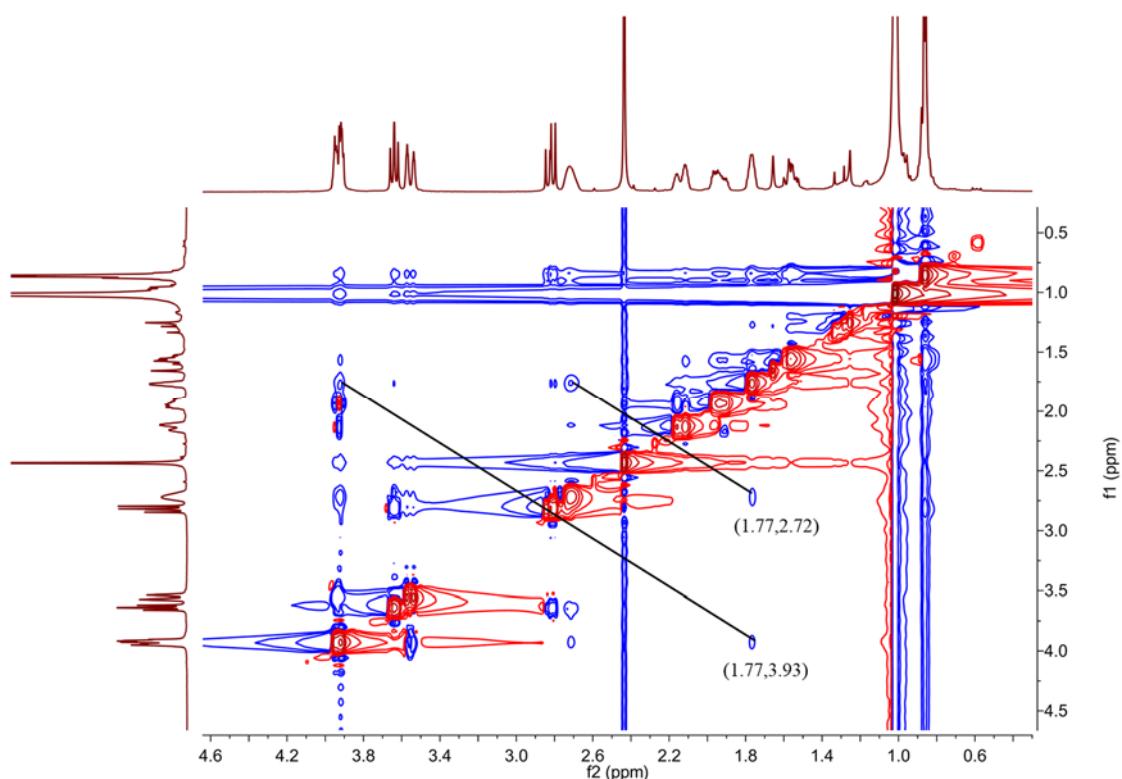


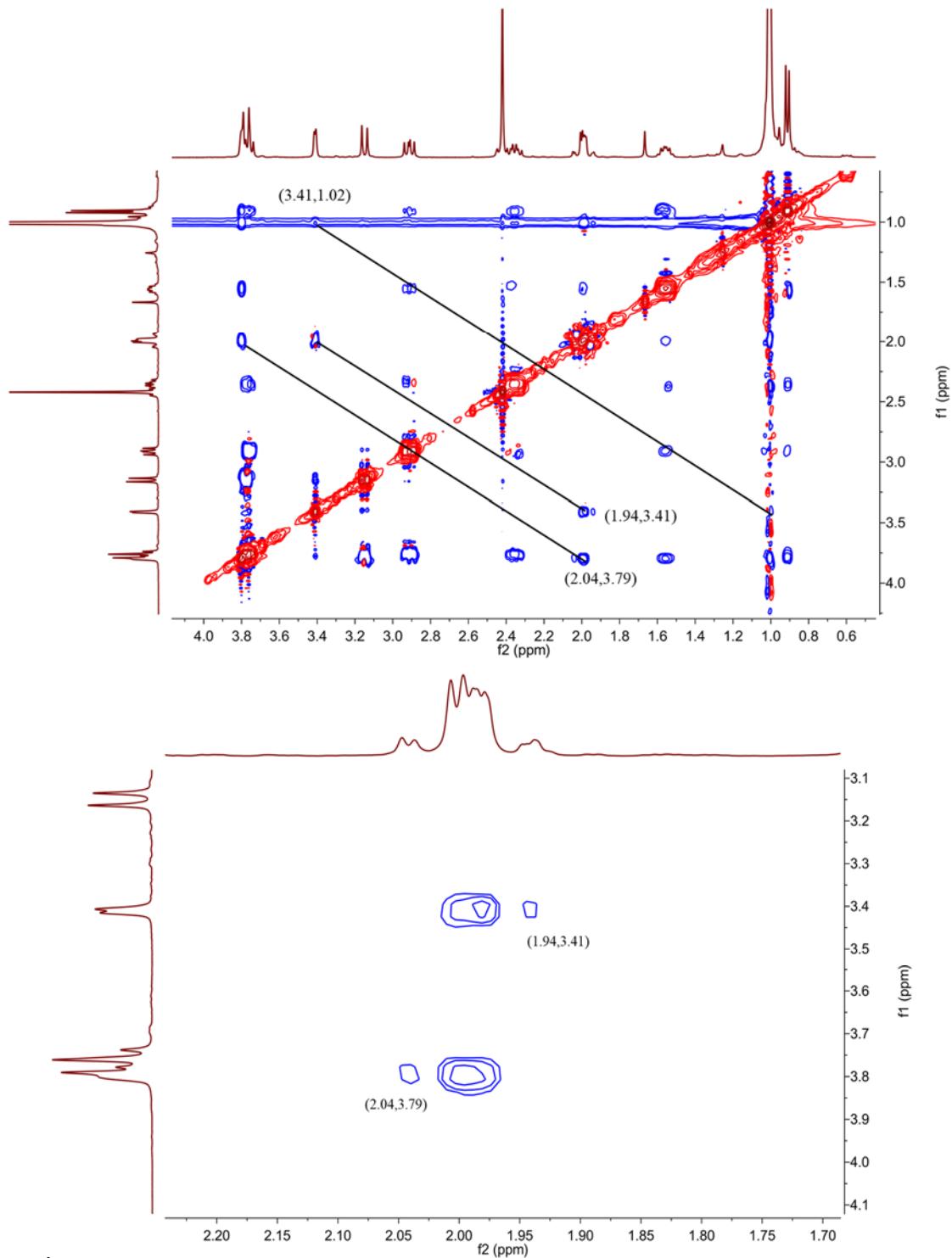
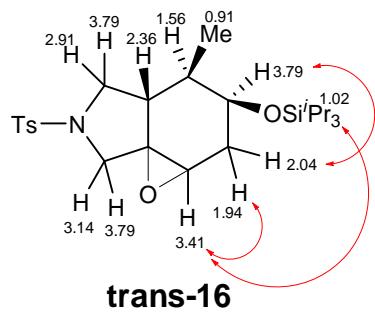


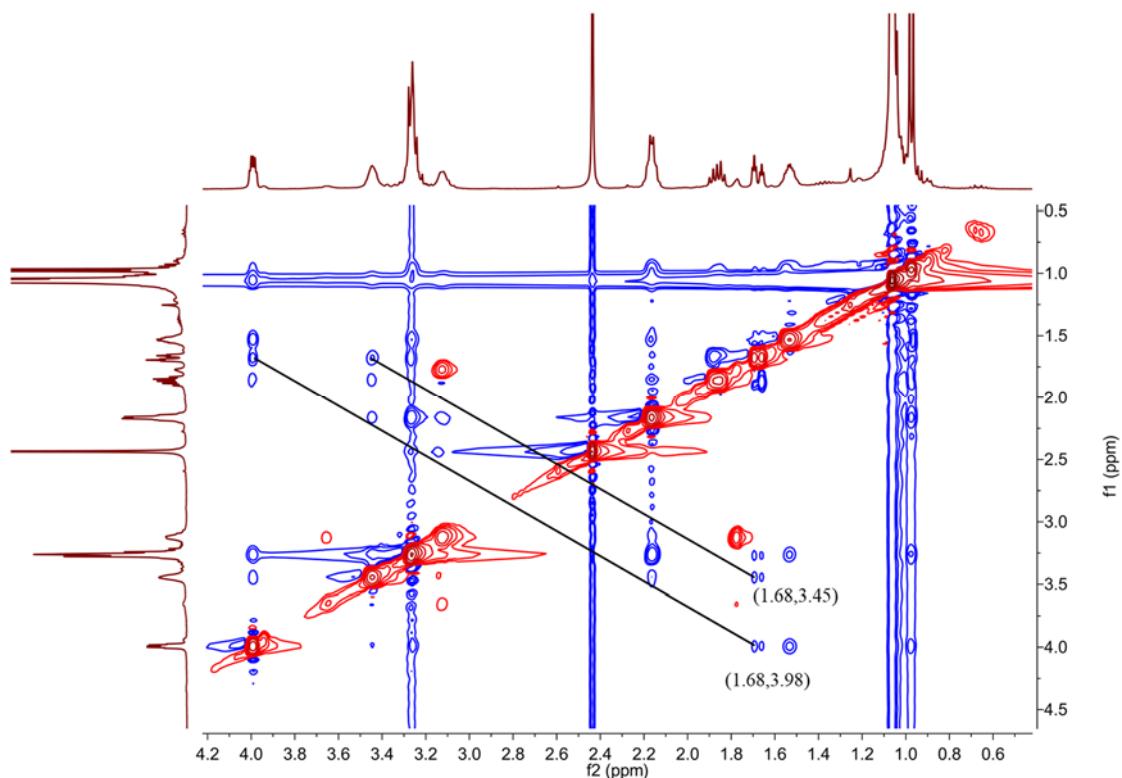
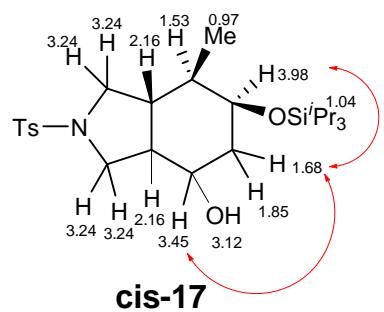


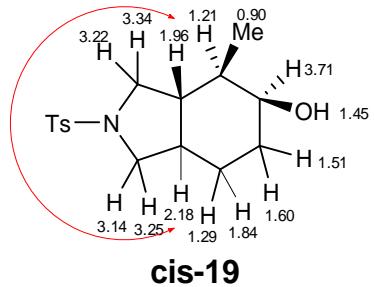


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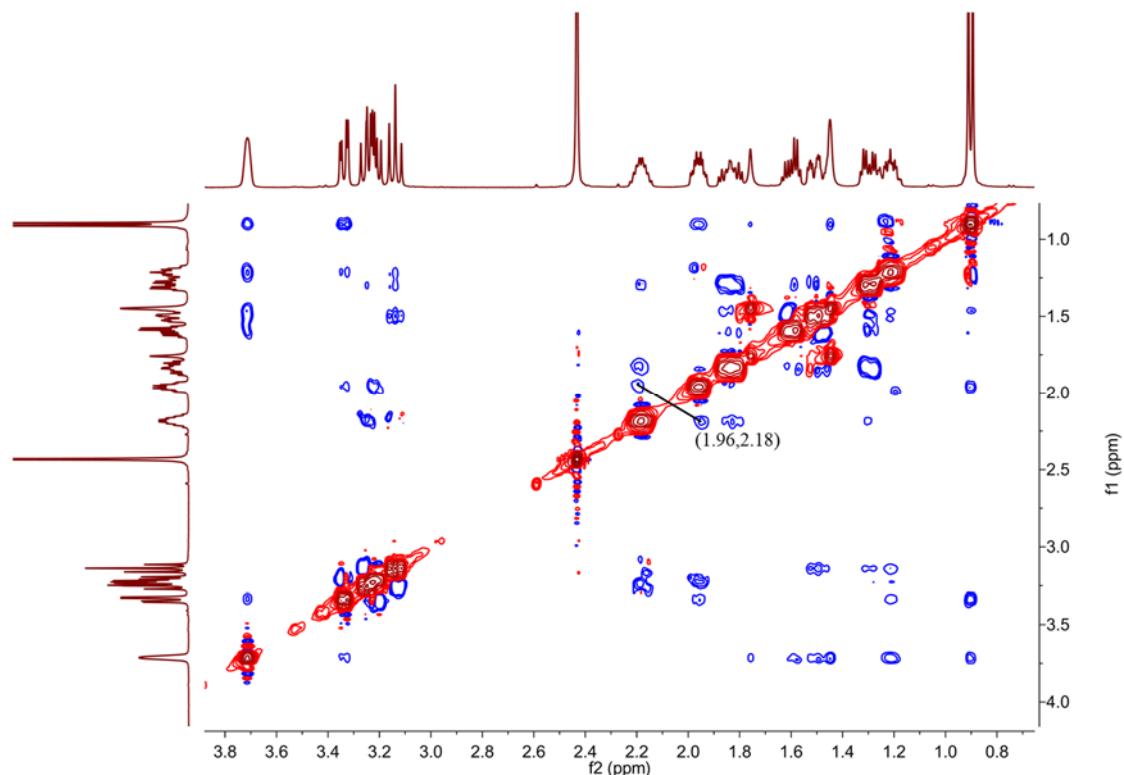




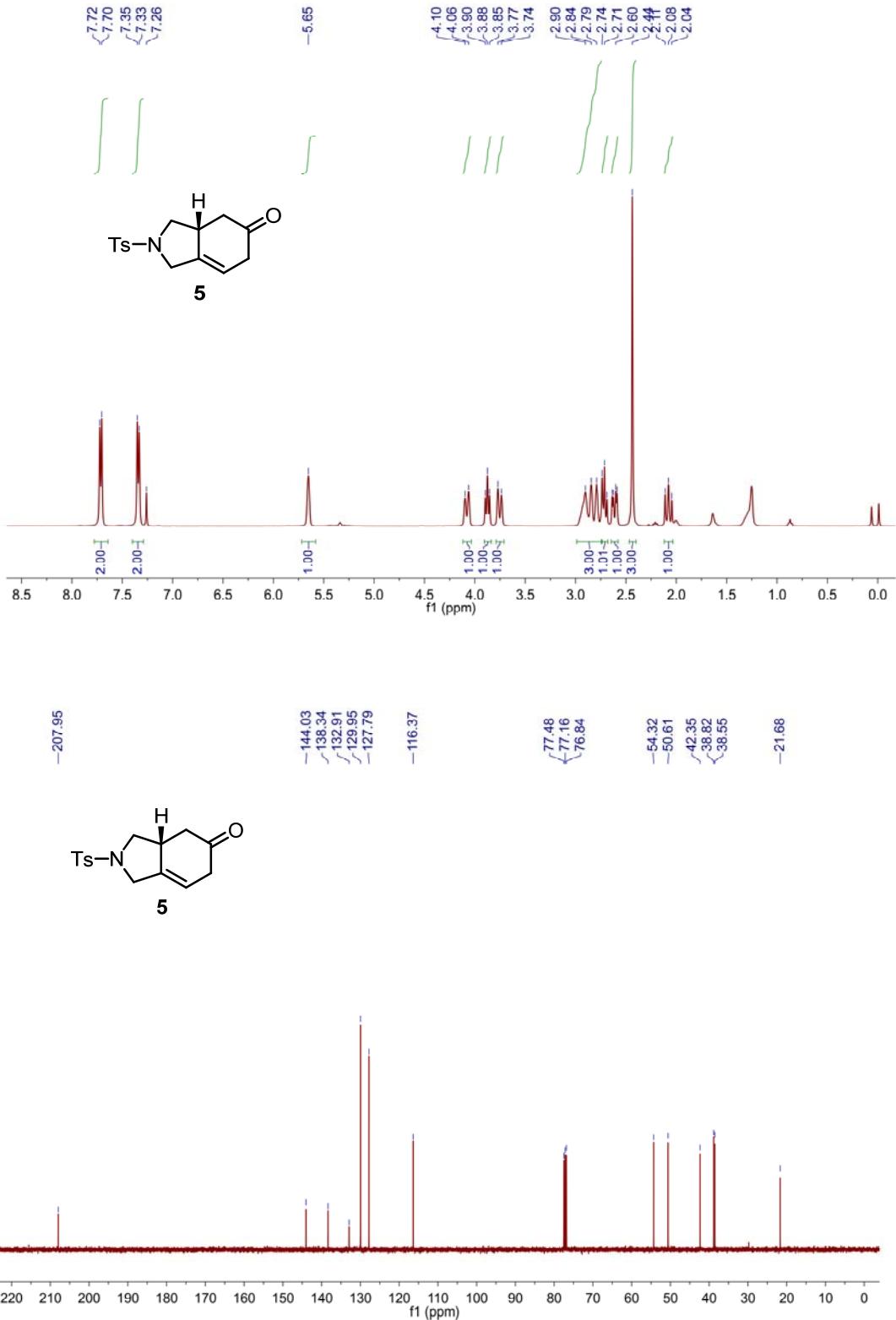


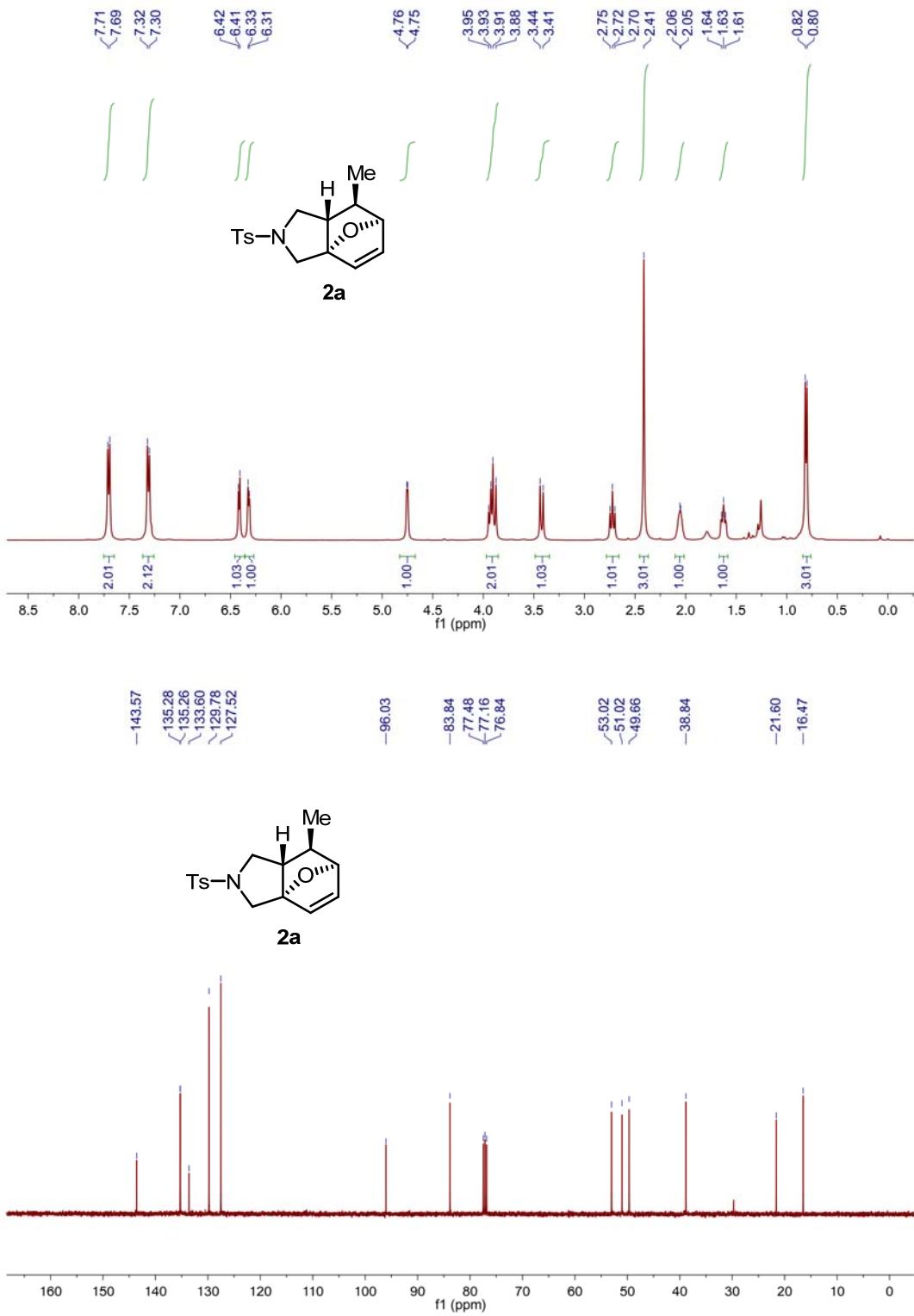


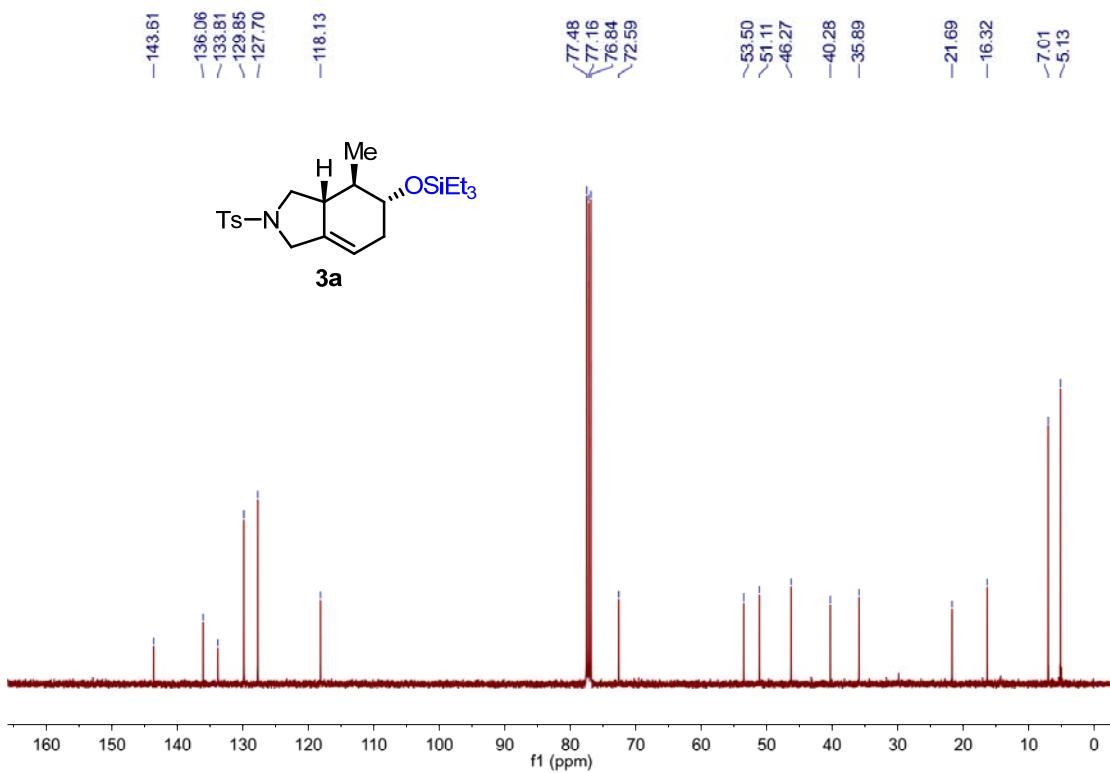
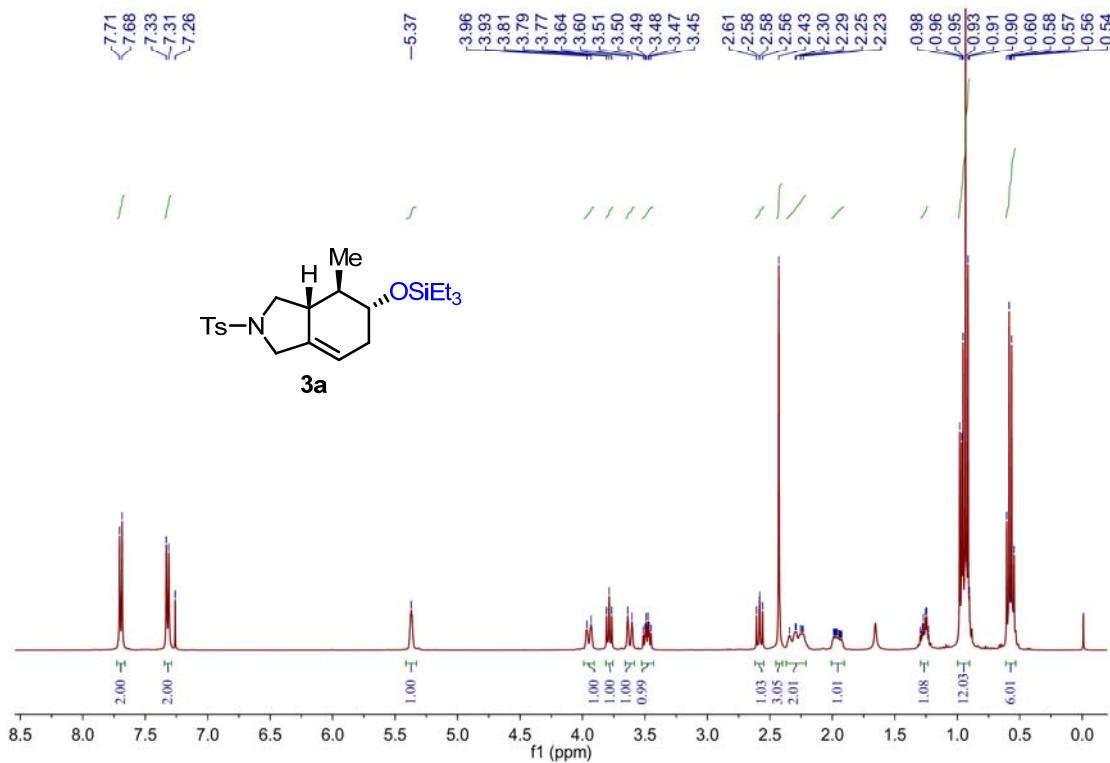
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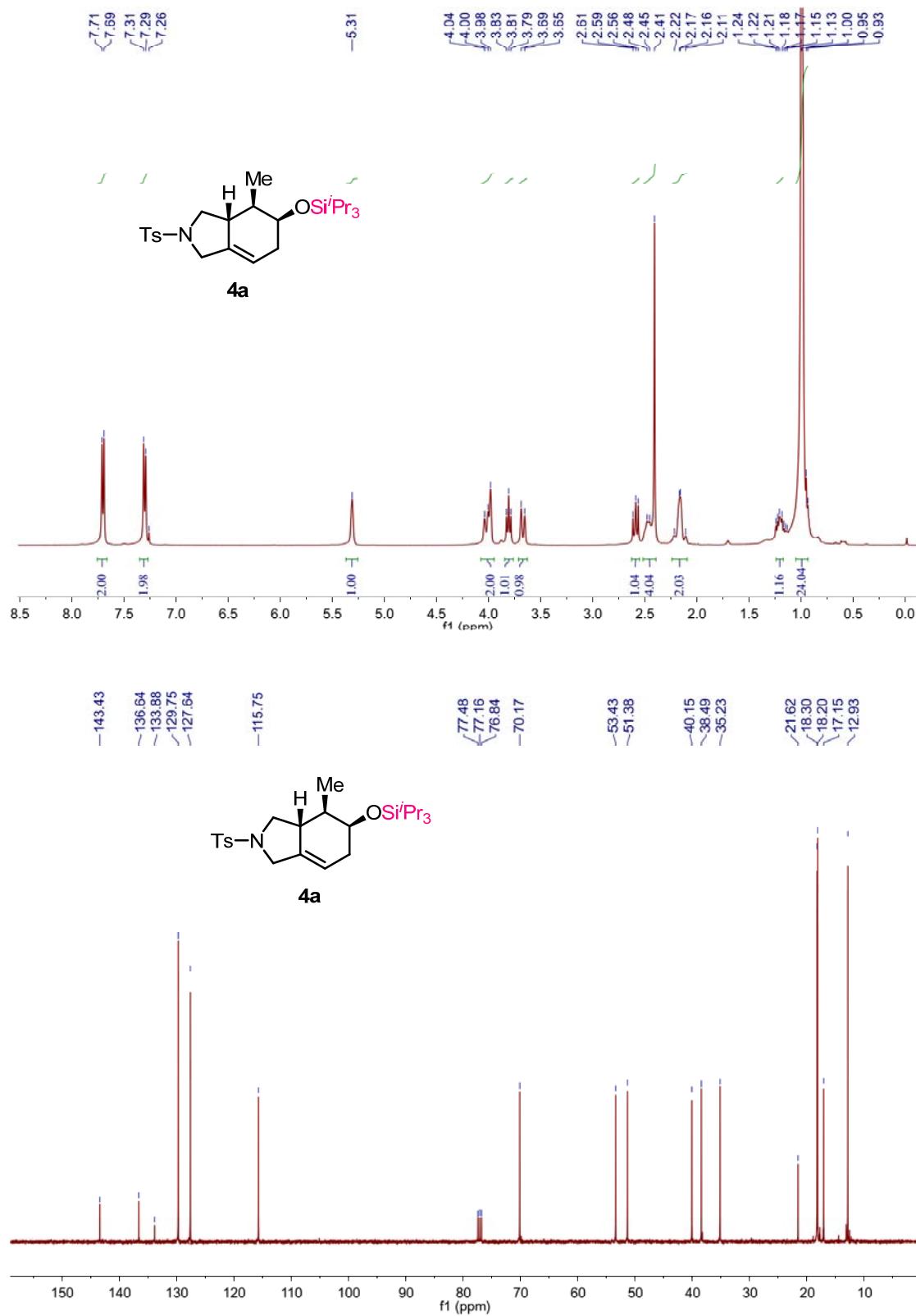


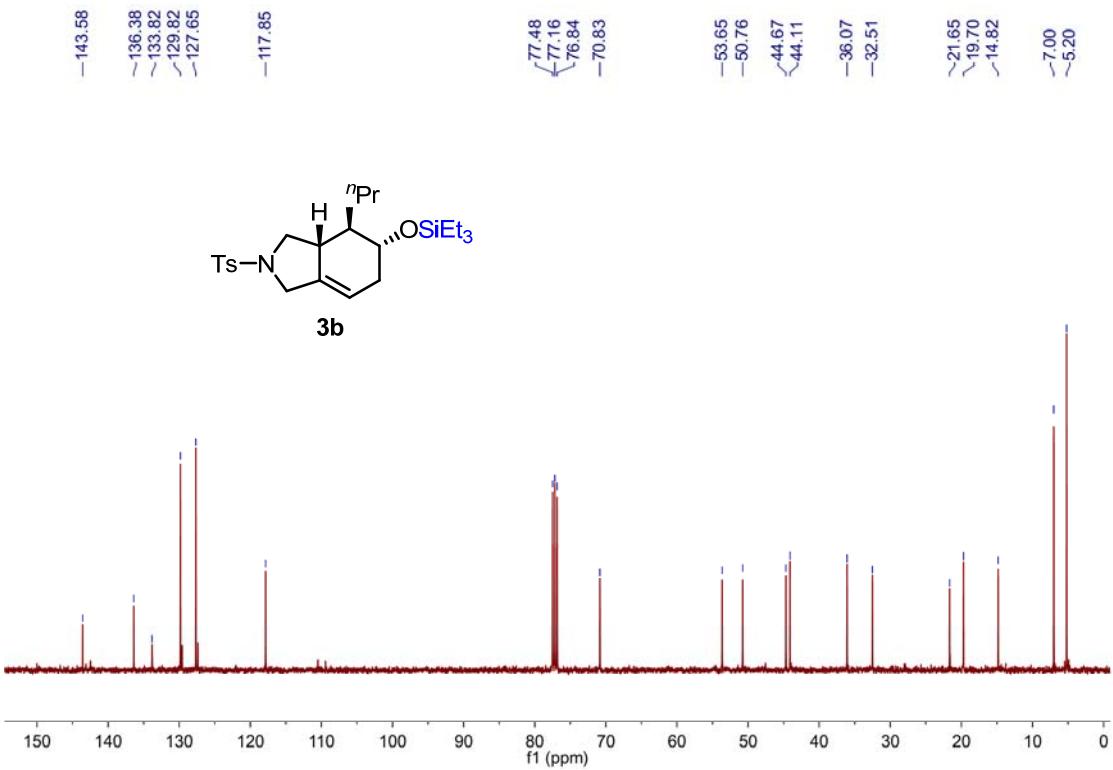
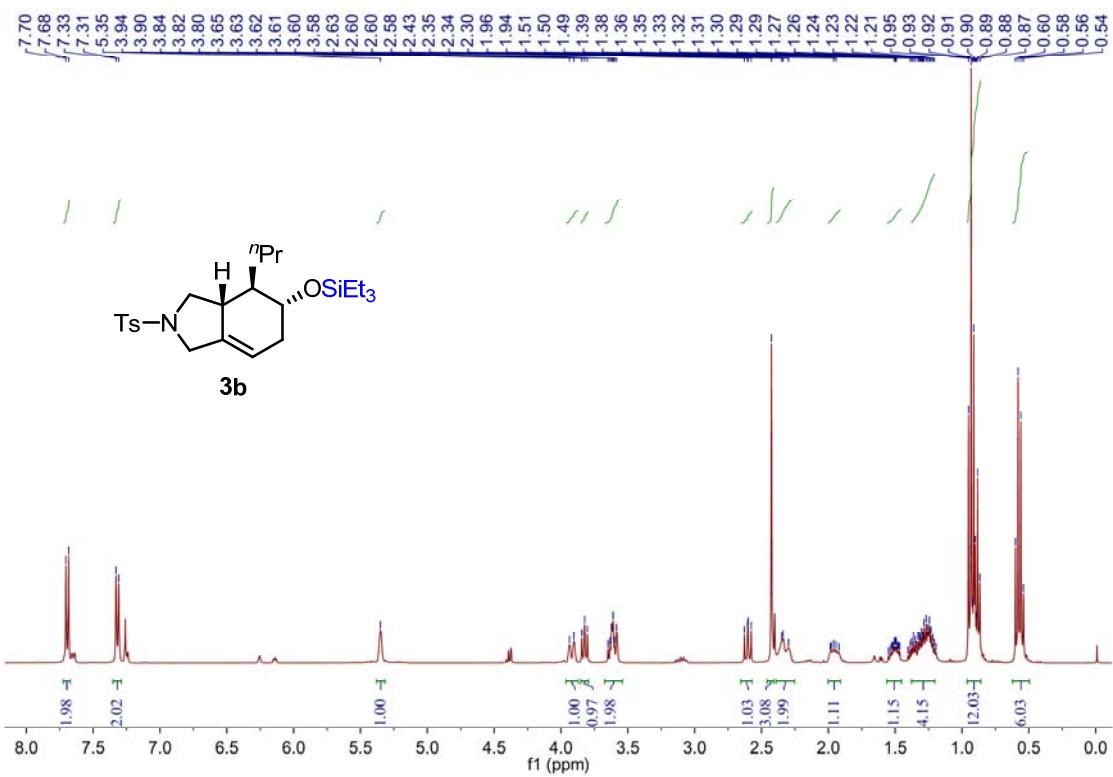
## 9. NMR Spectra





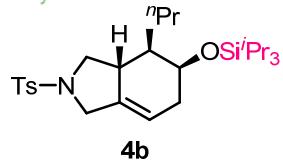




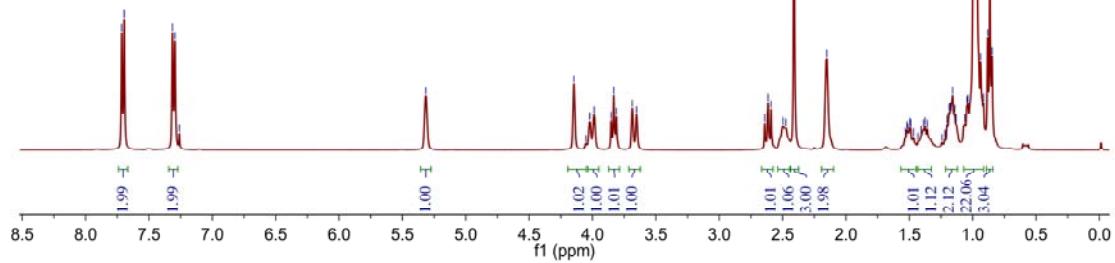




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4b



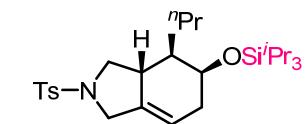
-115.80



-53.63



✓21.64 ✓20.41 ✓18.29 ✓18.20 ✓14.36 ✓12.99



4b

