

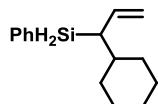
Supporting Information

**Highly efficient regioselective hydrosilylation of allenes by a [(3IP)Pd(allyl)]OTf catalyst; first example of
allene hydrosilylation with phenyl- and diphenylsilane**

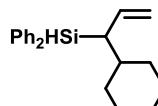
Hosein Tafazolian and Joseph A. R. Schmidt*

General methods and instrumentation: [(3IP)Pd(allyl)]OTf catalyst was synthesized via the reported procedure.¹ All NMR-scale reactions were set up in a nitrogen-filled glovebox. CDCl₃ was purchased from Cambridge Isotope Laboratories, dried over calcium hydride, freeze-pumped-thawed three times, vacuum transferred, and stored over molecular sieves in the glovebox. Cyclohexylallene and dimethylallene were supplied by Alfa Aesar and Sigma-Aldrich, respectively. All of the hydrosilanes (phenylsilane, diphenylsilane, triphenylsilane, triethylsilane, tri-n-propylsilane, tri-isopropylsilane, di-isopropylsilane, methyldiphenylsilane, dimethylphenylsilane, methylphenylsilane, 1,4-bis(dimethylsilyl)benzene, tert-butyldimethylsilane, triethoxysilane and trichlorosilane) were purchased from either Acros or Gelest and freeze-pump-thawed three times before transferring into the glovebox. ¹H and ¹³C NMR data were obtained on a 400 MHz Varian VXRS NMR spectrometer at 399.95 MHz for ¹H NMR and 100.56 MHz for ¹³C NMR. HMQC and gCOSY experiments to analyze the ¹H NMR and ¹³C NMR spectra of **3c** (to characterize diastereomers) were performed on a 600 MHz Bruker Avance III at 599.9 MHz for ¹H NMR and 150.8 MHz for ¹³C NMR. High resolution mass spectrometry data were determined by the University of Illinois Mass Spectrometry Laboratory, Urbana, IL, USA.

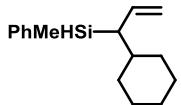
Catalytic reactions and isolation: All catalytic reactions were set up inside a nitrogen-filled glovebox in an NMR tube. Allene (0.50 mmol) was added to a mixture of Pd catalyst (1 mol%, 3.2 mg) and hydrosilane (0.50 mmol) in 800 μ l CDCl₃. Formation of the product and reaction completion time were monitored by ¹H NMR spectroscopy. After reaction completion, the reaction mixture was concentrated under vacuum and the product was extracted with hexane and passed through a small silica gel-packed column to remove the catalyst residue. All volatiles were removed under vacuum to give the product as a colorless liquid. Catalytic products **3e**,² **3g**³ and **4b**⁴ were reported previously and the reported ¹H NMR data were used as a reference. **3e**, **3g** and **4b** were isolated as colorless liquids with isolated yields of 82%, 91% and 98%, respectively.



(1-Cyclohexylallyl)(phenyl)silane (3a): Colorless liquid (106 mg, 92%). ¹H NMR (CDCl₃) δ 7.62 (dm, ³J_{H-H}= 7.8 Hz, 2H), 7.44-7.37 (m, 3H), 5.80 (dt, ³J_{H-H}= 16.8 Hz, ³J_{H-H}= 10.2 Hz, 1H), 4.98 (dd, ³J_{H-H}= 10.2 Hz, ²J_{H-H}= 1.8 Hz, 1H), 4.90 (dd, ³J_{H-H}= 16.8 Hz, ²J_{H-H}= 1.8 Hz, 1H), 4.41 (dd, ²J_{H-H}= 6.6 Hz, ³J_{H-H}= 2.4 Hz, 1H), 4.35 (dd, ²J_{H-H}= 6.6 Hz, ³J_{H-H}= 3.6 Hz, 1H), 2.02-1.96 (m, 1H), 1.89-1.54 (m, 6H), 1.31-1.06 (m, 5H); ¹³C{¹H} NMR (CDCl₃) δ 138.1, 135.9, 132.0, 129.7, 127.9, 114.5, 39.2, 38.2, 33.5, 32.2, 26.73, 26.68, 26.5; HRMS (EI) (m/z): [M]⁺ calc for C₁₅H₂₂Si, 230.1491; found, 230.1490.



(1-Cyclohexylallyl)diphenylsilane (3b): Colorless liquid (133 mg, 87%). ¹H NMR (CDCl₃) δ 7.72-7.68 (m, 4H), 7.47-7.41 (m, 6H), 5.87 (dt, ³J_{H-H}= 16.8 Hz, ³J_{H-H}= 10.8 Hz, 1H), 5.06 (d, ³J_{H-H}= 3.0 Hz, 1H), 5.02 (dd, ³J_{H-H}= 10.8 Hz, ²J_{H-H}= 1.8 Hz, 1H), 4.94 (dd, ³J_{H-H}= 16.8 Hz, ²J_{H-H}= 1.8 Hz, 1H), 2.30-2.25 (m, 1H), 1.93-1.67 (m, 6H), 1.29-1.12 (m, 5H); ¹³C{¹H} NMR (CDCl₃) δ 137.3, 136.0, 135.6, 134.2, 133.8, 129.6, 128.0, 127.9, 115.2, 39.7, 38.9, 33.9, 31.9, 26.8, 26.7, 26.4; HRMS (EI) (m/z): [M]⁺ calc for C₂₁H₂₆Si, 306.1804; found, 306.1809.

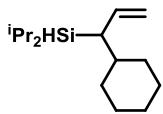


(1-Cyclohexylallyl)(methyl)(phenyl)silane (3c) as 50/50 mixture of diastereomers: Colorless liquid (100 mg, 82%).

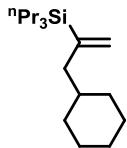
Diastereomer A: ^1H NMR (CDCl_3) δ 7.58-7.56 (m, 2H), 7.41-7.36 (m, 3H), 5.77 (dt, $^3\text{J}_{\text{H-H}}=17.2$ Hz, $^3\text{J}_{\text{H-H}}=10.2$ Hz, 1H), 4.95 (dd, $^3\text{J}_{\text{H-H}}=10.2$ Hz, $^2\text{J}_{\text{H-H}}=2.2$ Hz, 1H), 4.82 (dd, 17.2 Hz, $^2\text{J}_{\text{H-H}}=2.2$ Hz, 1H), 4.48-4.46 (m, 1H), 1.87-1.63 (m, 6H), 1.52-1.48 (m, 1H), 1.28-0.99 (m, 5H), 0.37 (d, $^3\text{J}_{\text{H-H}}=3.6$ Hz, 3H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 137.60, 135.61, 134.89, 129.31, 127.80, 114.21, 40.50, 38.59, 33.71, 31.92, 26.79, 26.68, 26.51, -6.65

Diastereomer B: ^1H NMR (CDCl_3) δ 7.58-7.56 (m, 2H), 7.41-7.36 (m, 3H), 5.69 (dt, $^3\text{J}_{\text{H-H}}=17.2$ Hz, $^3\text{J}_{\text{H-H}}=10.2$ Hz, 1H), 4.97 (dd, $^3\text{J}_{\text{H-H}}=10.2$ Hz, $^2\text{J}_{\text{H-H}}=2.2$ Hz, 1H), 4.84 (dd, 17.2 Hz, $^2\text{J}_{\text{H-H}}=2.2$ Hz, 1H), 4.50-4.48 (m, 1H), 1.87-1.63 (m, 6H), 1.55-1.53 (m, 1H), 1.28-0.99 (m, 5H), 0.39 (d, $^3\text{J}_{\text{H-H}}=3.6$ Hz, 3H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 138.00, 136.15, 135.10, 129.33, 127.84, 113.97, 40.95, 38.91, 33.77, 32.38, 26.81, 26.75, 26.53, -6.16

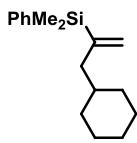
HRMS (EI) (m/z): [M]⁺ calc for $\text{C}_{16}\text{H}_{24}\text{Si}$, 244.1647; found, 244.1645.



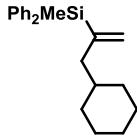
(1-Cyclohexylallyl)diisopropylsilane (3d): Colorless liquid (89 mg, 75%). ^1H NMR (CDCl_3) δ 5.76 (dt, $^3\text{J}_{\text{H-H}}=16.2$ Hz, $^3\text{J}_{\text{H-H}}=11.0$ Hz, 1H), 4.89 (dd, $^3\text{J}_{\text{H-H}}=11.0$ Hz, $^2\text{J}_{\text{H-H}}=2.2$ Hz, 1H), 4.87 (dd, $^3\text{J}_{\text{H-H}}=16.2$ Hz, $^2\text{J}_{\text{H-H}}=2.2$ Hz, 1H), 3.53 (s, 1H), 1.84-1.46 (m, 7H), 1.29-0.89 (m, 7H), 1.07 (d, $^3\text{J}_{\text{H-H}}=5.5$ Hz, 12H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 139.2, 113.5, 39.0, 38.3, 33.9, 32.3, 26.9, 26.6, 20.1, 19.3, 10.8, 10.5; HRMS (EI) (m/z): [M]⁺ calc for $\text{C}_{15}\text{H}_{30}\text{Si}$, 238.2117; found, 238.2122.



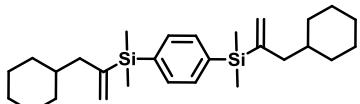
(3-Cyclohexylprop-1-en-2-yl)tripropylsilane (3f): Colorless liquid (111 mg, 79%). ^1H NMR (CDCl_3) δ 5.56 (dt, $^2\text{J}_{\text{H-H}}=3.3$ Hz, $^4\text{J}_{\text{H-H}}=1.5$ Hz, 1H), 5.32 (d, $^2\text{J}_{\text{H-H}}=3.3$ Hz, 1H), 1.98 (d, $^3\text{J}_{\text{H-H}}=7.0$ Hz, 2H), 1.72-1.64 (m, 5H), 1.39-1.27 (m, 7H), 1.24-1.16 (m, 3H), 0.96 (t, $^3\text{J}_{\text{H-H}}=7.3$ Hz, 9H), 0.89-0.81 (m, 2H), 0.61-0.53 (m, 6H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 148.1, 126.4, 45.3, 36.6, 33.7, 26.9, 26.6, 18.8, 17.6, 15.2; HRMS (EI) (m/z): [M]⁺ calc for $\text{C}_{18}\text{H}_{36}\text{Si}$, 280.2586; found, 280.2578.



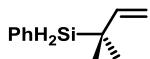
(3-Cyclohexylprop-1-en-2-yl)dimethyl(phenyl)silane (3g): Colorless liquid (118 mg, 91%). ^1H NMR (CDCl_3) δ 7.59-7.57 (m, 2H), 7.41-7.39 (m, 3H), 5.69 (dt, $^2\text{J}_{\text{H-H}}=3.0$ Hz, $^4\text{J}_{\text{H-H}}=1.8$ Hz, 1H), 4.50 (d, $^2\text{J}_{\text{H-H}}=3.0$ Hz, 1H), 2.08 (d, $^3\text{J}_{\text{H-H}}=7.2$ Hz, 2H), 1.69-1.66 (m, 5H), 1.36-1.29 (m, 1H), 1.15-1.11 (m, 3H), 0.86-0.78 (m, 2H), 0.44 (s, 6H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 149.1, 138.8, 134.2, 129.1, 127.9, 127.5, 45.2, 36.7, 33.6, 26.9, 26.6, -2.5; HRMS (EI) (m/z): [M]⁺ calc for $\text{C}_{17}\text{H}_{26}\text{Si}$, 258.1804; found, 258.1814.³



(3-Cyclohexylprop-1-en-2-yl)(methyl)diphenylsilane (3h): Colorless liquid (151 mg, 94%). ^1H NMR (CDCl_3) δ 7.63 (dd, $^3J_{\text{H-H}}=8.4$ Hz, 4H), 7.47-7.42 (m, 6H), 5.89 (dt, $^2J_{\text{H-H}}=3.3$ Hz, $^4J_{\text{H-H}}=1.1$ Hz, 1H), 5.54 (d, $^2J_{\text{H-H}}=3.3$ Hz, 1H), 2.19 (d, $^3J_{\text{H-H}}=7.2$ Hz, 2H), 1.74-1.66 (m, 5H), 1.38-1.29 (m, 1H), 1.17-1.11 (m, 3H), 0.90-0.84 (m, 2H), 0.76 (s, 3H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 146.8, 136.4, 135.2, 129.9, 129.3, 127.9, 44.9, 36.4, 33.4, 26.7, 26.5, -3.7; HRMS (EI) (m/z): $[\text{M}]^+$ calc for $\text{C}_{22}\text{H}_{28}\text{Si}$, 320.1960; found, 320.1965.



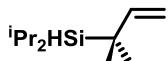
1,4-bis((3-Cyclohexylprop-1-en-2-yl)dimethylsilyl)benzene (3i): Colorless liquid (195 mg, 89%). ^1H NMR (CDCl_3) δ 7.55 (s, 4H), 5.68 (dt, $^2J_{\text{H-H}}=3.3$ Hz, $^4J_{\text{H-H}}=1.1$ Hz, 2H), 5.49 (d, $^2J_{\text{H-H}}=3.3$ Hz, 2H), 2.07 (d, $^3J_{\text{H-H}}=7.0$ Hz, 4H), 1.67-1.63 (m, 10H), 1.36-1.10 (m, 8H), 0.85-0.80 (m, 4H), 0.42 (s, 12H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 148.9, 139.3, 133.2, 127.3, 45.1, 36.6, 33.5, 26.8, 26.5, -2.7; HRMS (EI) (m/z): $[\text{M}]^+$ calc for $\text{C}_{28}\text{H}_{46}\text{Si}_2$, 438.3138; found, 438.3156.



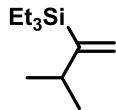
(2-Methylbut-3-en-2-yl)(phenyl)silane (4a): Colorless liquid (77 mg, 87%). ^1H NMR (CDCl_3) δ 7.60 (dd, $^3J_{\text{H-H}}=7.8$ Hz, $^4J_{\text{H-H}}=1.2$ Hz, 2H), 7.45-7.37 (m, 3H), 5.96 (dd, $^3J_{\text{H-H}}=17.4$ Hz, $^3J_{\text{H-H}}=10.8$ Hz, 1H), 4.98 (dd, $^3J_{\text{H-H}}=10.8$ Hz, $^2J_{\text{H-H}}=1.2$ Hz, 1H), 4.85 (dd, $^3J_{\text{H-H}}=17.4$ Hz, $^2J_{\text{H-H}}=1.2$ Hz, 1H), 4.21 (s, 2H), 1.19 (s, 6H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 145.9, 136.2, 131.5, 129.9, 127.9, 110.6, 26.1, 23.7; HRMS (EI) (m/z): $[\text{M}]^+$ calc for $\text{C}_{11}\text{H}_{16}\text{Si}$, 176.1021; found, 176.1023.



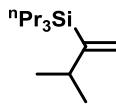
Methyl(2-methylbut-3-en-2-yl)(phenyl)silane (4c): Colorless liquid (71 mg, 75%). ^1H NMR (CDCl_3) δ 7.56 (dd, $^3J_{\text{H-H}}=7.8$ Hz, $^4J_{\text{H-H}}=1.2$ Hz, 2H), 7.43-7.37 (m, 3H), 5.90 (dd, $^3J_{\text{H-H}}=17.2$ Hz, $^3J_{\text{H-H}}=10.6$ Hz, 1H), 4.97 (dd, $^3J_{\text{H-H}}=10.6$ Hz, $^2J_{\text{H-H}}=1.5$ Hz, 1H), 4.80 (dd, $^3J_{\text{H-H}}=17.2$ Hz, $^2J_{\text{H-H}}=1.5$ Hz, 1H), 4.19 (t, $^3J_{\text{H-H}}=3.7$ Hz, 1H), 1.12 (s, 3H), 1.10 (s, 3H), 0.38 (d, $^3J_{\text{H-H}}=3.7$ Hz, 3H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 146.1, 135.4, 134.7, 129.6, 127.7, 110.1, 26.7, 23.2, 23.0, -8.3.



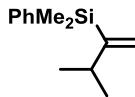
Diisopropyl(2-methylbut-3-en-2-yl)silane (4d): Colorless liquid (73 mg, 79%). ^1H NMR (CDCl_3) δ 5.99 (dd, $^3J_{\text{H-H}}=17.2$ Hz, $^3J_{\text{H-H}}=10.6$ Hz, 1H), 4.87 (dd, $^3J_{\text{H-H}}=10.6$ Hz, $^2J_{\text{H-H}}=1.5$ Hz, 1H), 4.80 (dd, $^3J_{\text{H-H}}=17.2$ Hz, $^2J_{\text{H-H}}=1.5$ Hz, 1H), 3.33 (s, 1H), 1.15 (s, 6H), 1.13-1.08 (m, 14H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 147.7, 109.1, 24.8, 20.6, 19.8, 11.3; HRMS (EI) (m/z): $[\text{M}]^+$ calc for $\text{C}_{11}\text{H}_{24}\text{Si}$, 184.1647; found, 184.1644.



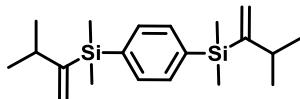
Triethyl(3-methylbut-1-en-2-yl)silane (4e): Colorless liquid, (79 mg, 86%). ^1H NMR (CDCl_3) δ 5.71 (dd, $^2J_{\text{H-H}}=2.4$ Hz, 1H), 5.30 (d, $^2J_{\text{H-H}}=2.4$ Hz, 1H), 2.40 (septd, $^3J_{\text{H-H}}=6.6$ Hz, $^4J_{\text{H-H}}=1.2$ Hz, 1H), 1.02 (d, $^3J_{\text{H-H}}=6.6$ Hz, 6H), 0.93 (t, $^3J_{\text{H-H}}=7.8$ Hz, 9H), 0.062 (q, $^3J_{\text{H-H}}=7.8$ Hz, 6H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 155.7, 122.9, 32.5, 23.2, 7.6, 3.3; HRMS (EI) (m/z): [M] $^+$ calc for $\text{C}_{11}\text{H}_{24}\text{Si}$, 184.1647; found, 184.1646.⁵



(3-Methylbut-1-en-2-yl)tripropylsilane (4f): Colorless liquid (86 mg, 76%). ^1H NMR (CDCl_3) δ 5.68 (dd, $^2J_{\text{H-H}}=2.6$ Hz, 1H), 5.28 (d, $^2J_{\text{H-H}}=2.6$ Hz, 1H), 2.40 (septd, $^3J_{\text{H-H}}=6.6$ Hz, $^4J_{\text{H-H}}=1.1$ Hz, 1H), 1.36-1.26 (m, 6H), 1.01 (d, $^3J_{\text{H-H}}=6.6$ Hz, 6H), 0.95 (t, $^3J_{\text{H-H}}=6.9$ Hz, 9H), 0.62-0.58 (m, 6H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 156.5, 122.6, 32.4, 23.2, 18.8, 17.6, 15.3; HRMS (EI) (m/z): [M] $^+$ calc for $\text{C}_{14}\text{H}_{30}\text{Si}$, 226.2117; found, 226.2117.



Dimethyl(3-methylbut-1-en-2-yl)(phenyl)silane (4g): Colorless liquid (87 mg, 85%). ^1H NMR (CDCl_3) δ 7.62-7.58 (m, 2H), 7.42-7.39 (m, 3H), 5.82 (dd, $^2J_{\text{H-H}}=2.4$ Hz, $^4J_{\text{H-H}}=1.2$ Hz, 1H), 5.48 (d, $^2J_{\text{H-H}}=2.4$ Hz, 1H), 4.59 (sept, $^3J_{\text{H-H}}=6.1$ Hz, 1H), 1.03 (d, $^3J_{\text{H-H}}=6.1$ Hz, 6H), 0.45 (s, 6H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 157.0, 139.0, 134.1, 129.0, 127.8, 123.8, 33.0, 23.2, -2.2; HRMS (EI) (m/z): [M] $^+$ calc for $\text{C}_{13}\text{H}_{20}\text{Si}$, 204.1334; found, 204.1334.

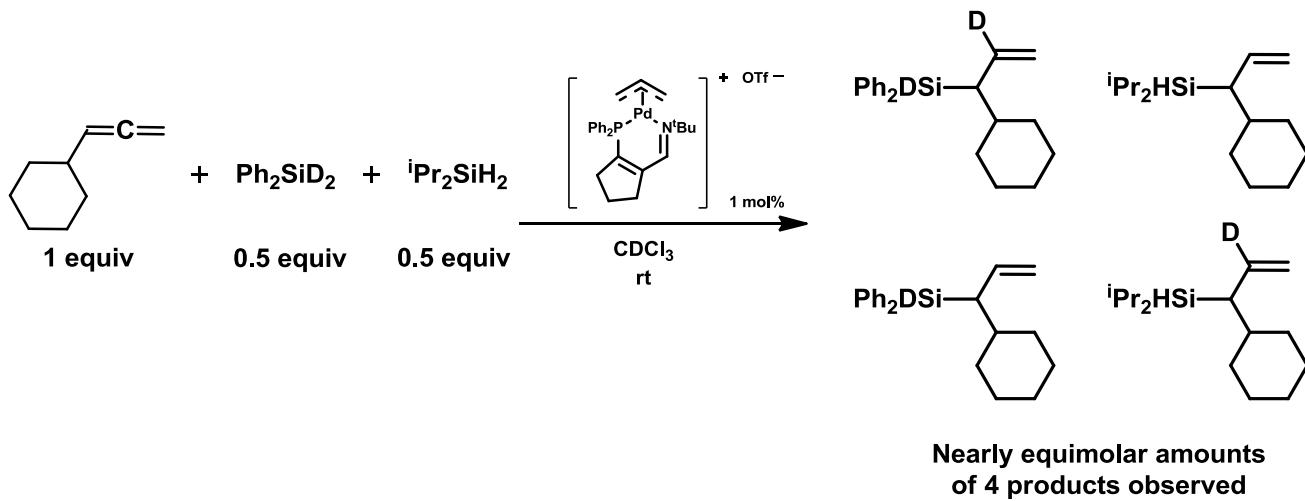


1,4-Bis(dimethyl(3-methylbut-1-en-2-yl)silyl)benzene (4i): Colorless liquid (155 mg, 94%). ^1H NMR (CDCl_3) δ 7.54 (s, 4H), 5.79 (dd, $^2J_{\text{H-H}}=2.5$ Hz, $^4J_{\text{H-H}}=1.1$ Hz, 2H), 5.45 (d, $^2J_{\text{H-H}}=2.5$ Hz, 2H), 2.49 (septd, $^3J_{\text{H-H}}=6.9$ Hz, $^4J_{\text{H-H}}=1.1$ Hz, 2H), 1.01 (d, $^3J_{\text{H-H}}=6.9$ Hz, 12H), 0.43 (s, 12H); $^{13}\text{C}\{\text{H}\}$ NMR (CDCl_3) δ 157.0, 133.3, 125.4, 123.7, 32.9, 23.2, -2.25; HRMS (EI) (m/z): [M] $^+$ calc for $\text{C}_{20}\text{H}_{34}\text{Si}_2$, 330.2199; found, 330.2203.

Crossover experiments related to operable mechanism: Diphenylsilane-d₂ (Ph_2SiD_2) was supplied by Santa Cruz Biotechnology and transferred to the glovebox as received.

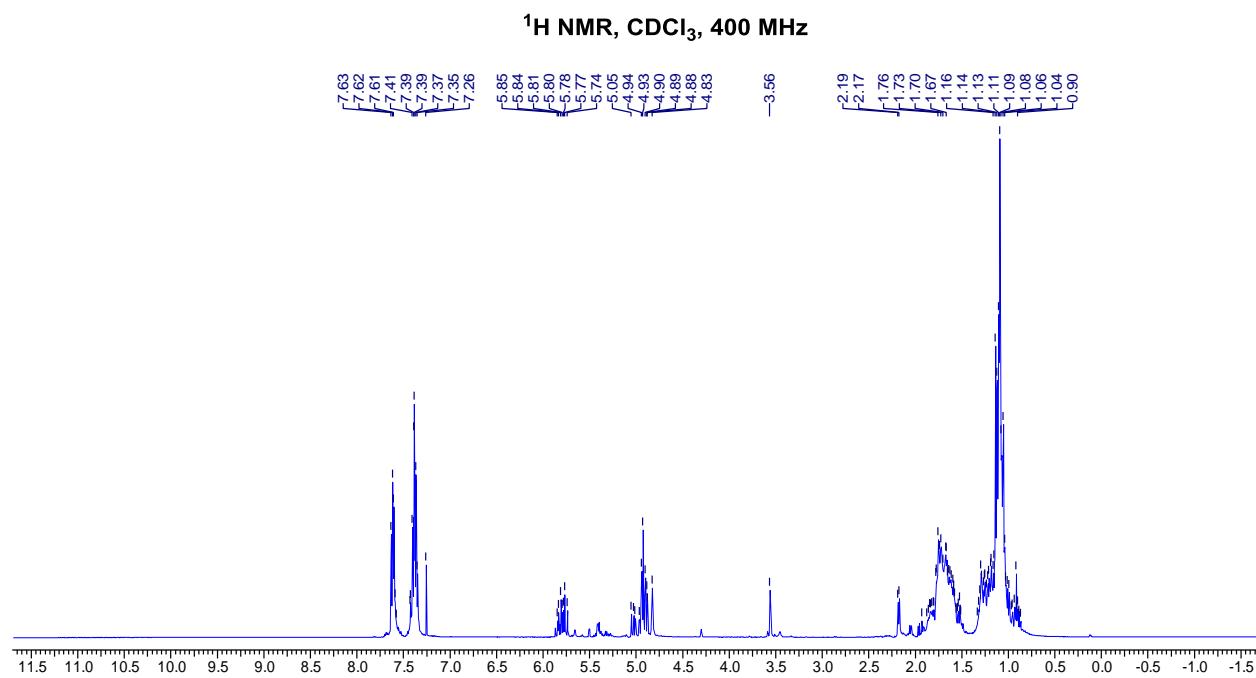
Control experiment: Into two separate vials in the glovebox, Pd catalyst (0.5 mol%, 1.6 mg) and 400 μl CDCl_3 were added, followed by addition of diphenylsilane-d₂ (0.25 mmol) to the first vial and diisopropylsilane (0.25 mmol) to the second vial. No cyclohexylallene was added and the contents of the two vials were immediately mixed. After 7 hours, the mixture was observed by ¹H and ²H NMR spectroscopy. No H/D exchange was observed.

Crossover experiment: Into two separate vials in the glovebox, Pd catalyst (0.5 mol%, 1.6 mg) and 400 μl CDCl_3 were added, followed by addition of diphenylsilane-d₂ (0.25 mmol) to the first vial and diisopropylsilane (0.25 mmol) to the second vial. To each of these, cyclohexylallene (0.25 mmol) was added and the contents of the two vials were immediately mixed. After 7 hours, reaction completion was observed by ¹H NMR spectroscopy. The resultant ¹H NMR confirmed formation of four products in an approximately equimolar ratio (see Scheme S1 and spectra below):

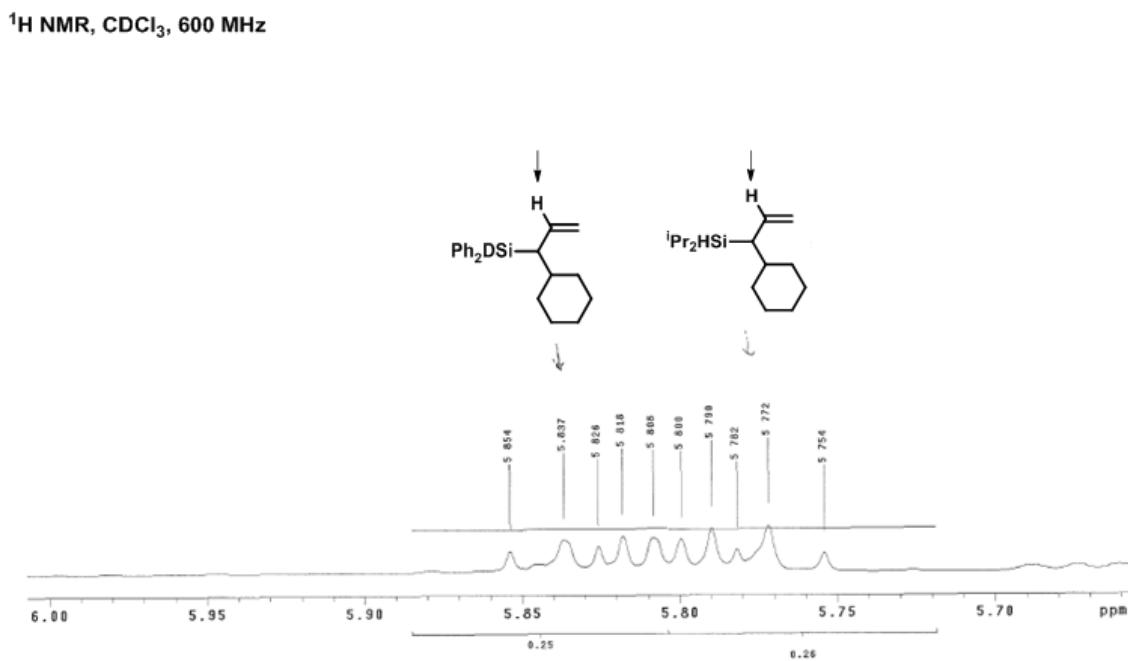


Scheme S1. Products formed in crossover experiment. No Si-H/Si-D crossover was observed. That is, for all Ph_2Si fragments, the silane retains one deuterium atom, and for all $^i\text{Pr}_2\text{Si}$ fragments, the silane retains one hydrogen atom. At the same time, complete H/D scrambling at the vinylic position was observed.

¹NMR spectrum of crude reaction mixture from crossover experiment:

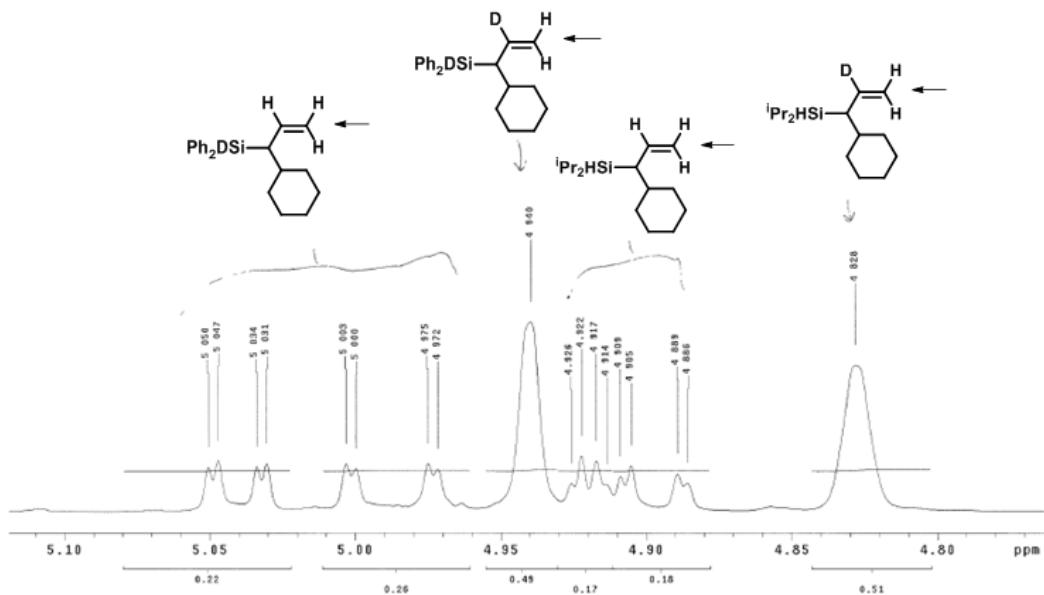


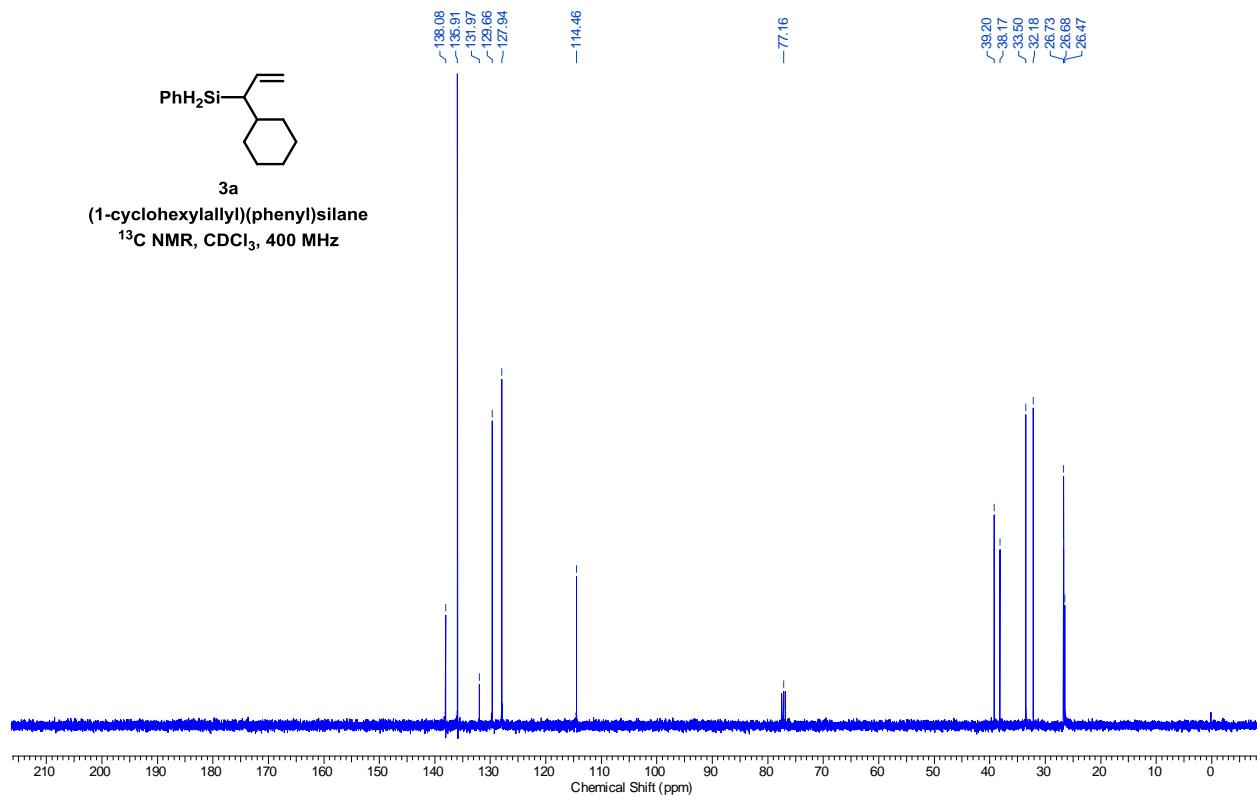
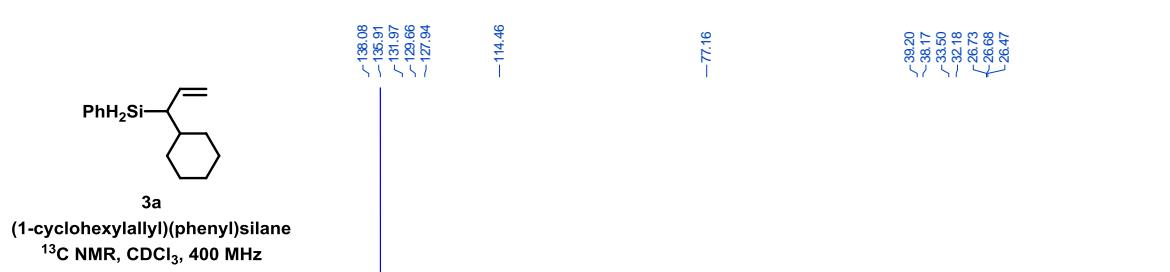
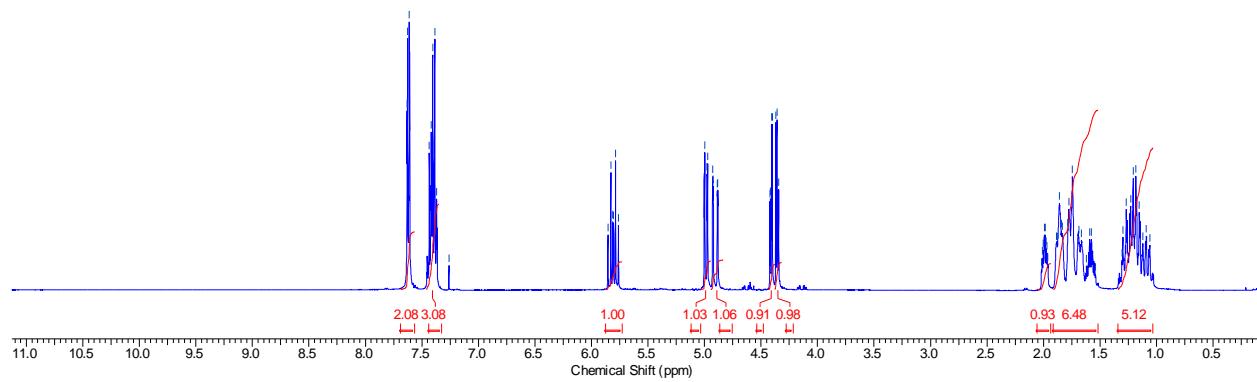
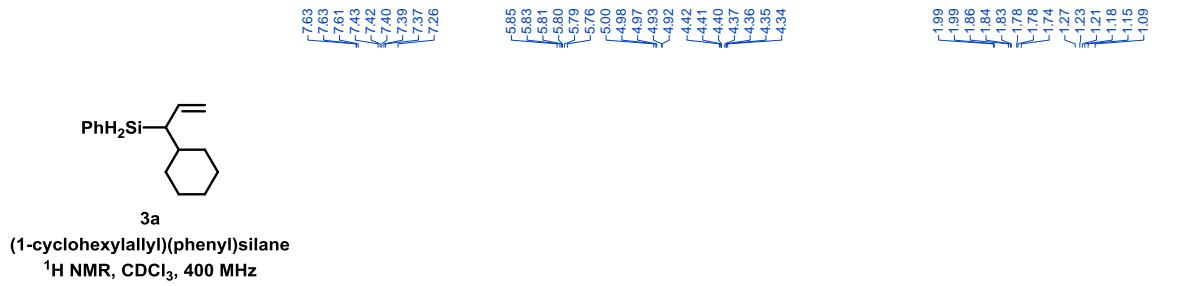
Internal vinylic hydrogen region from ¹NMR spectrum of crossover experiment:

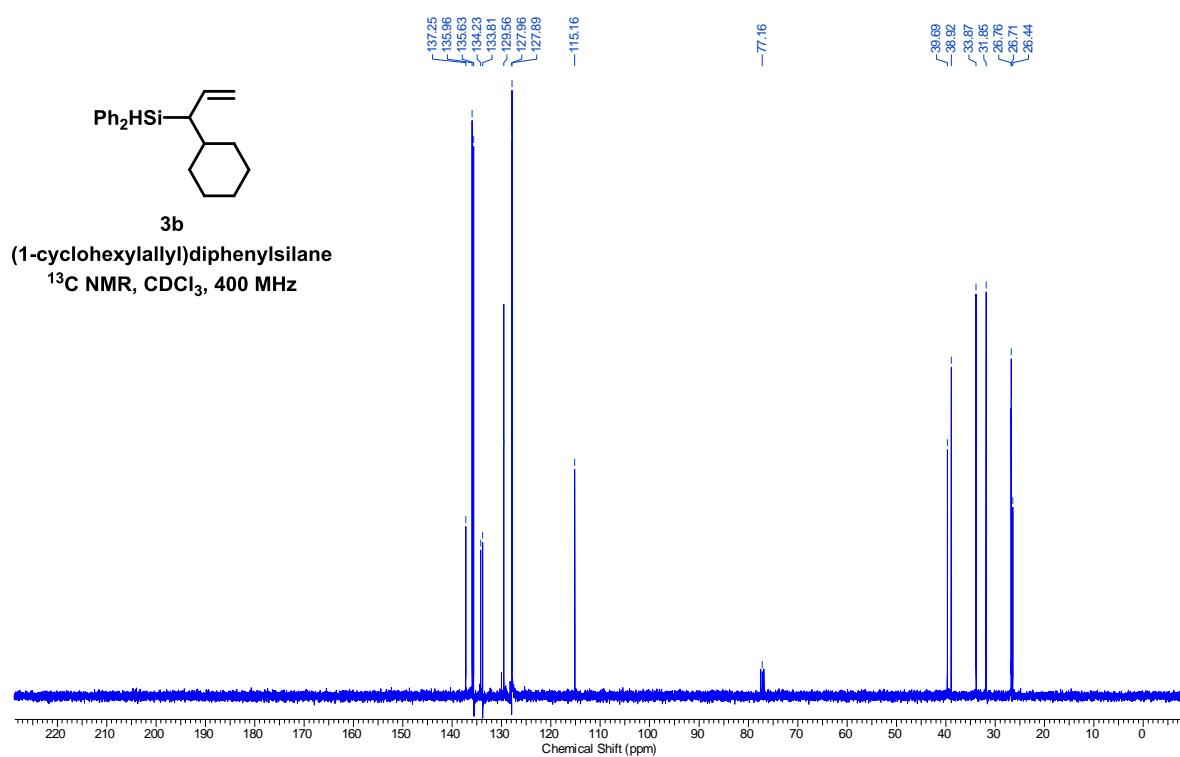
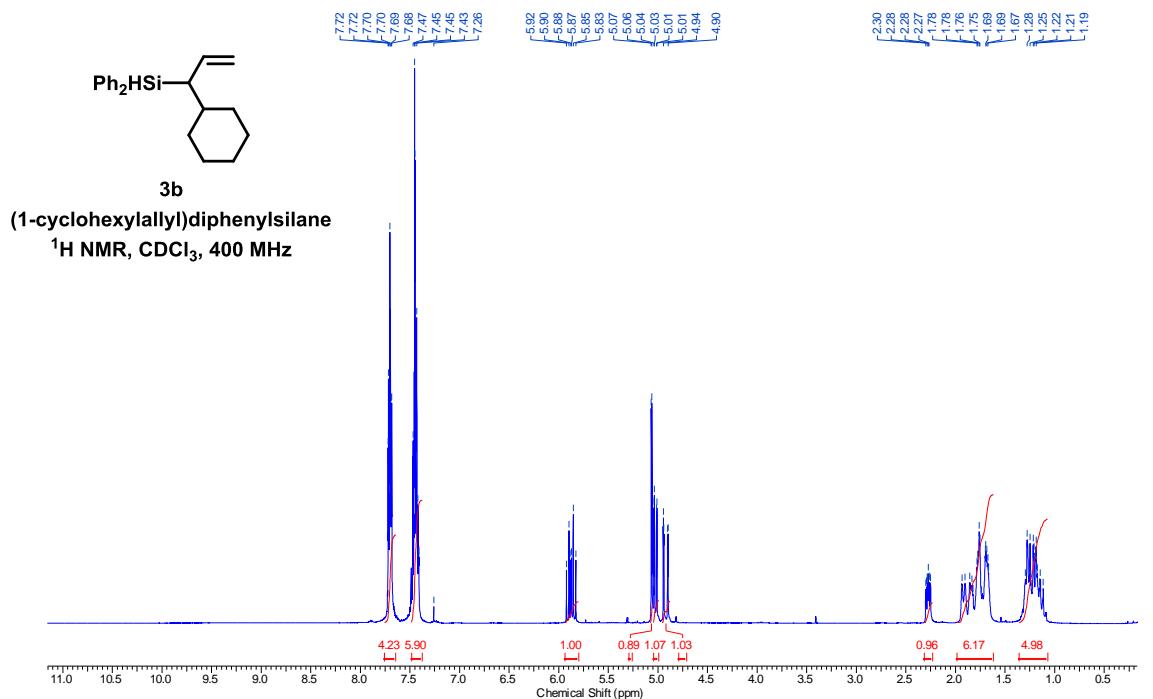


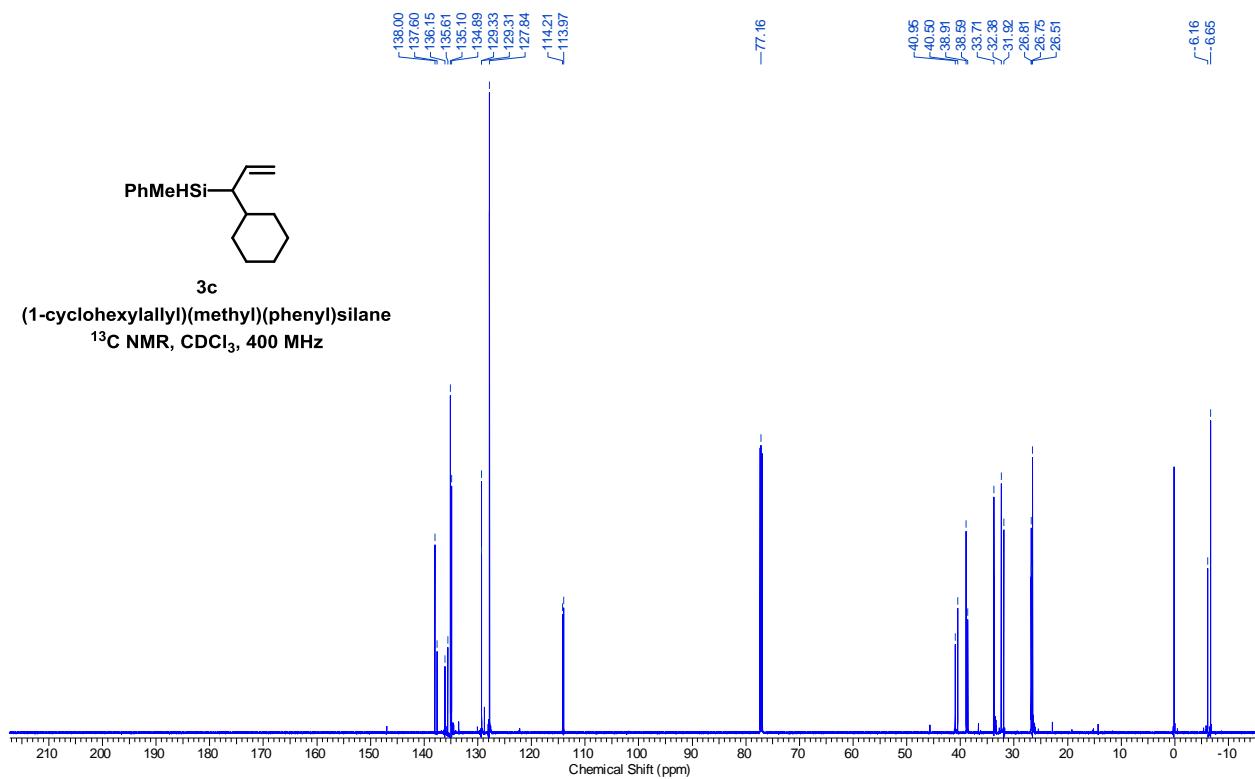
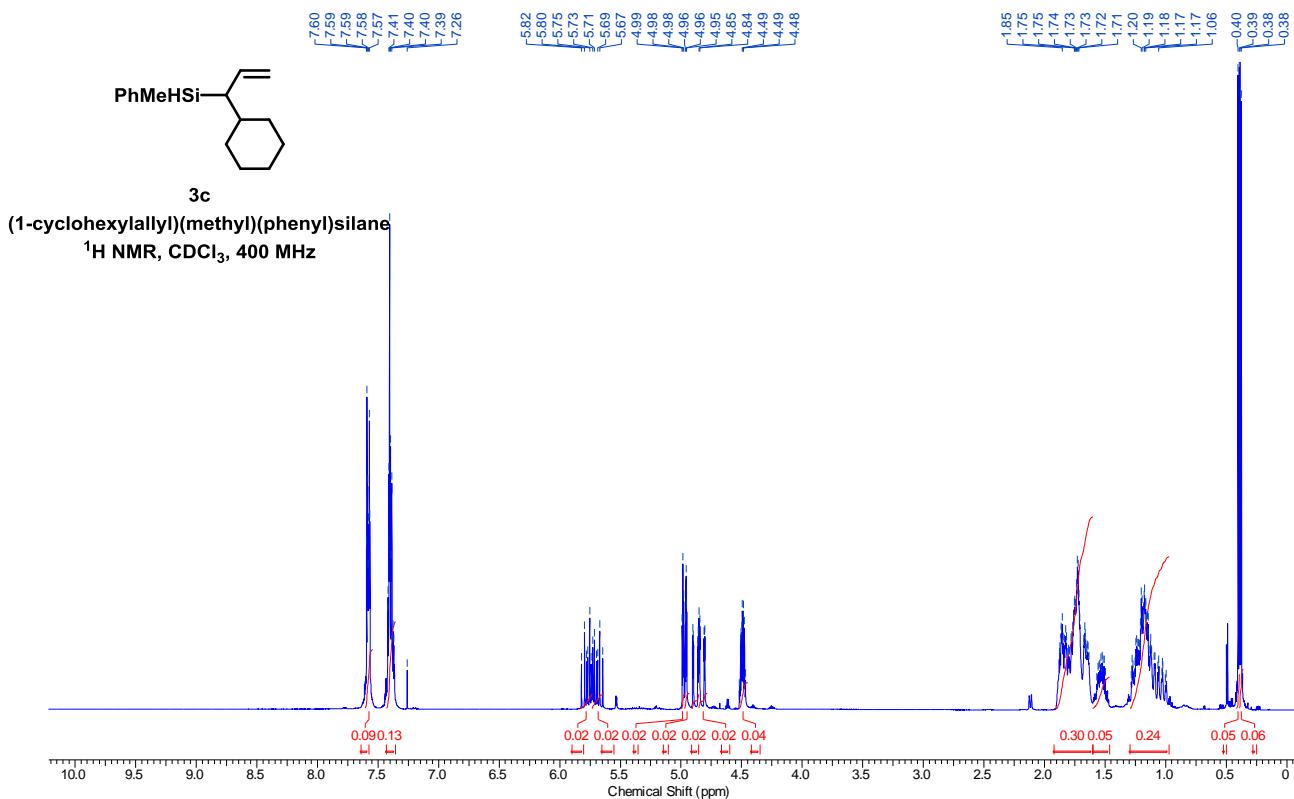
External vinylic hydrogen region from ^1H NMR spectrum of crossover experiment:

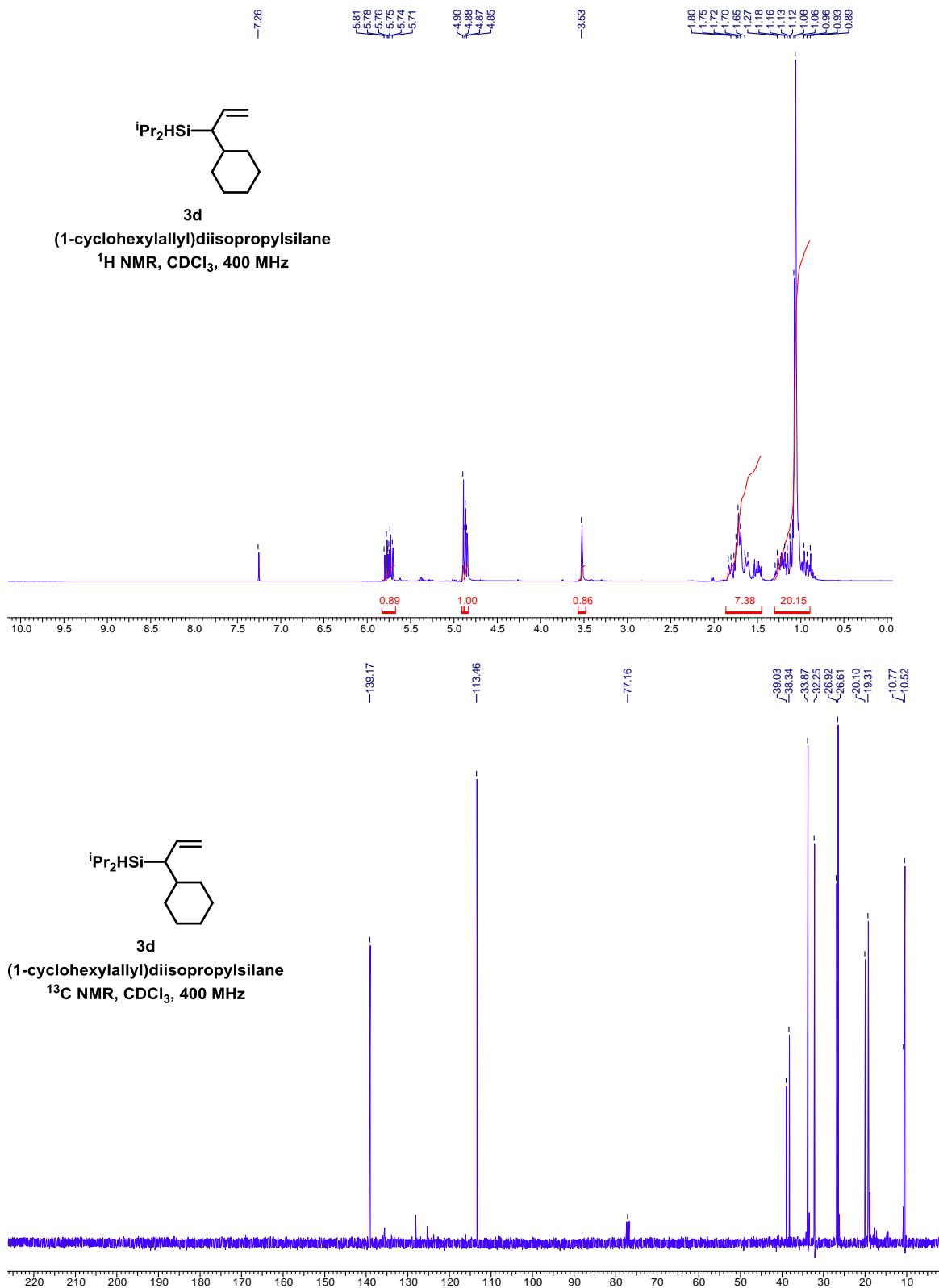
^1H NMR, CDCl_3 , 600 MHz

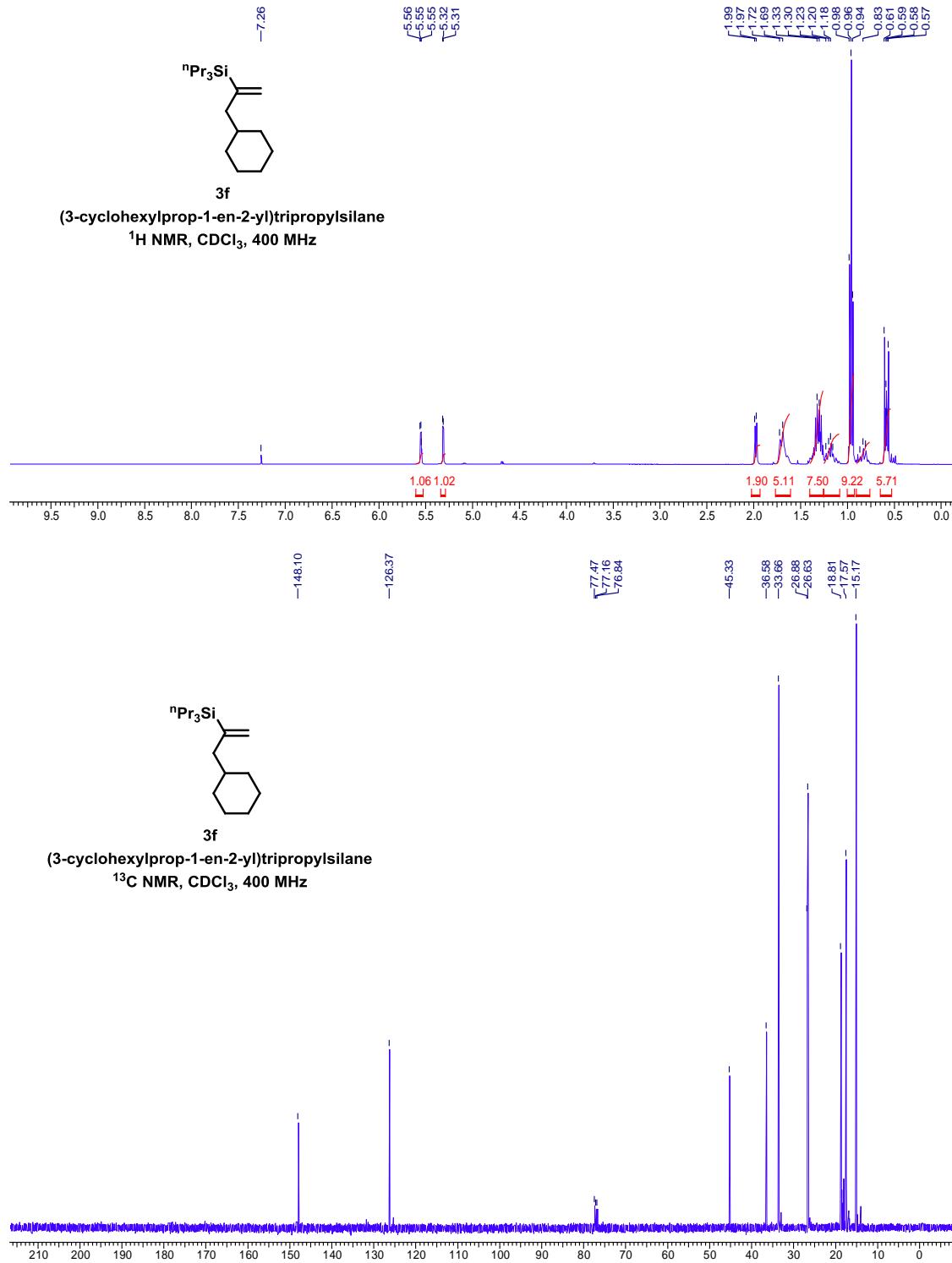


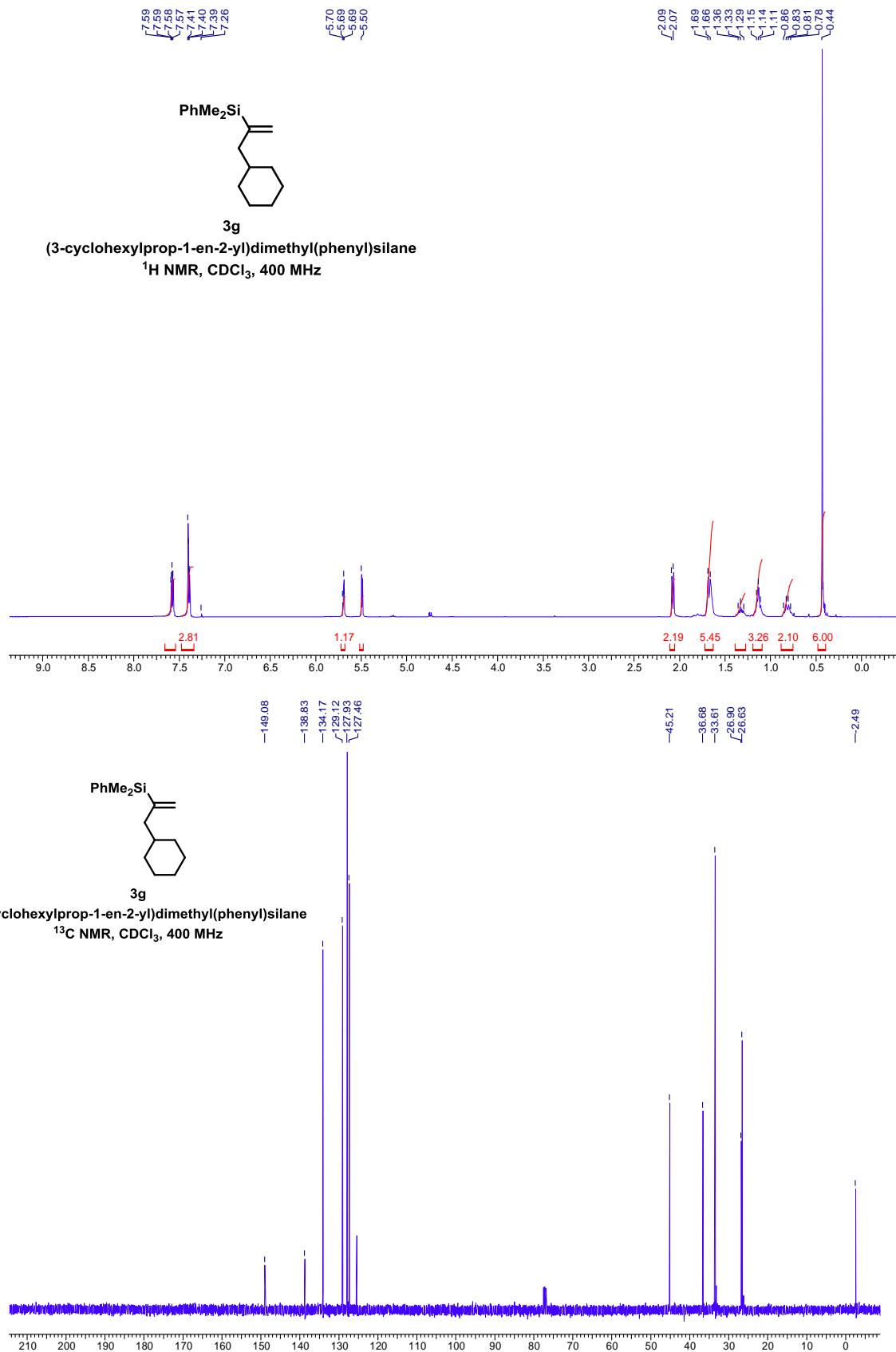


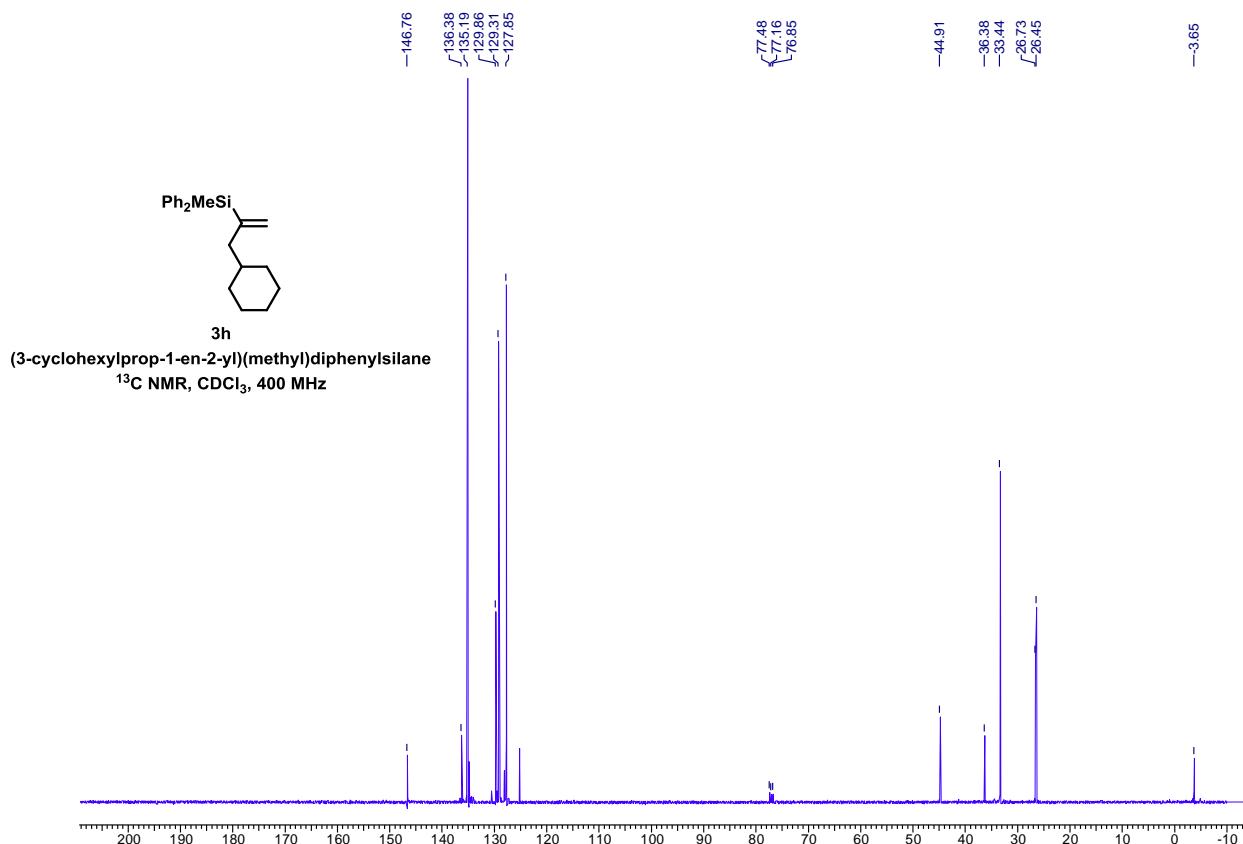
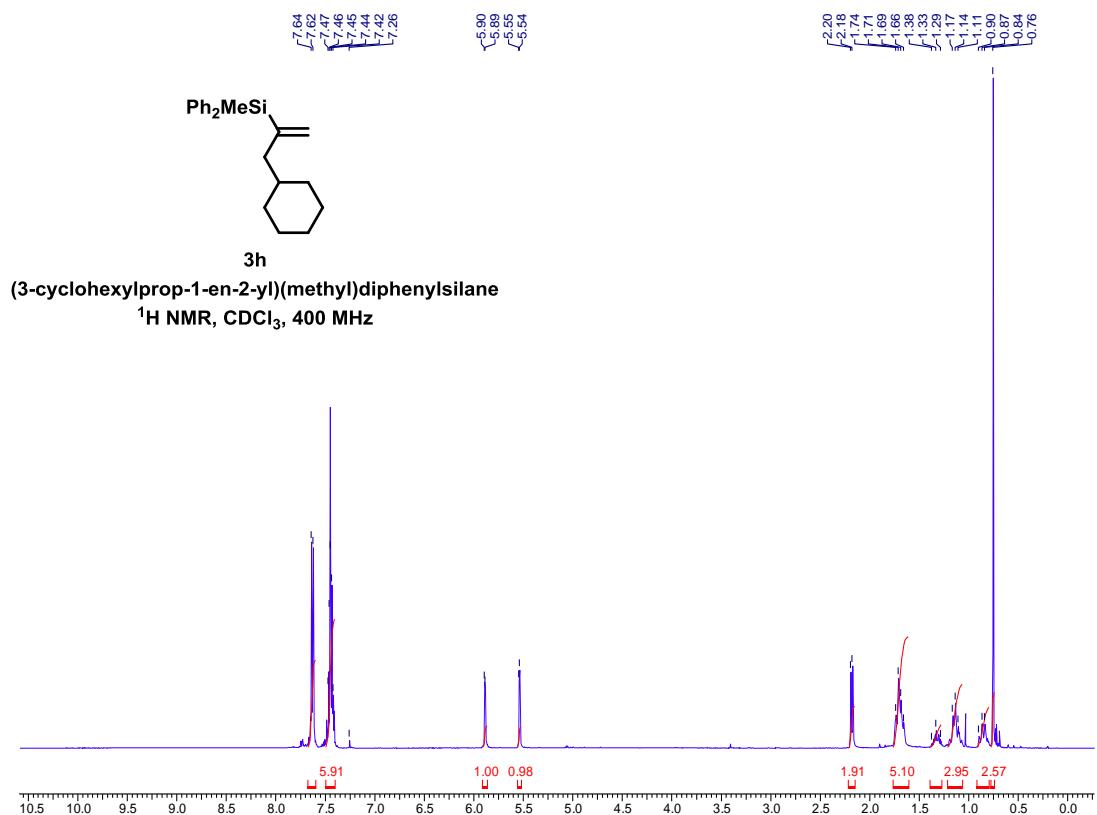


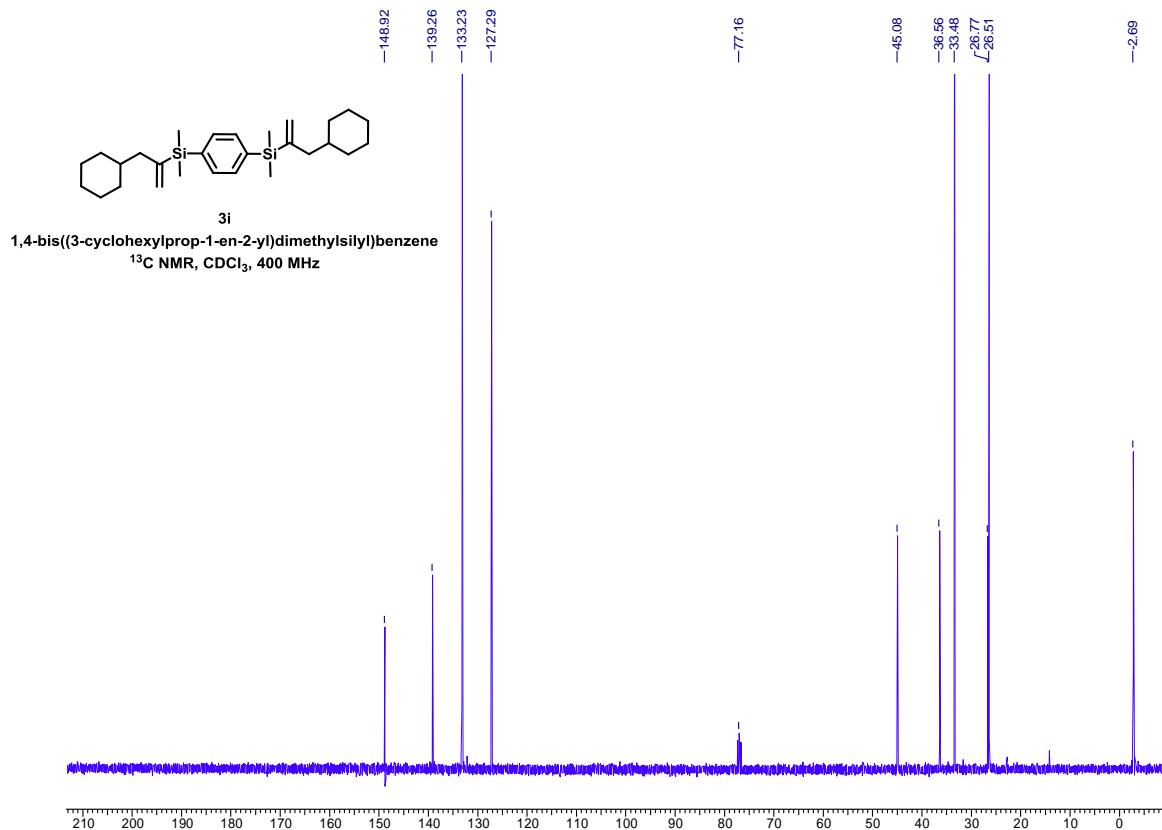
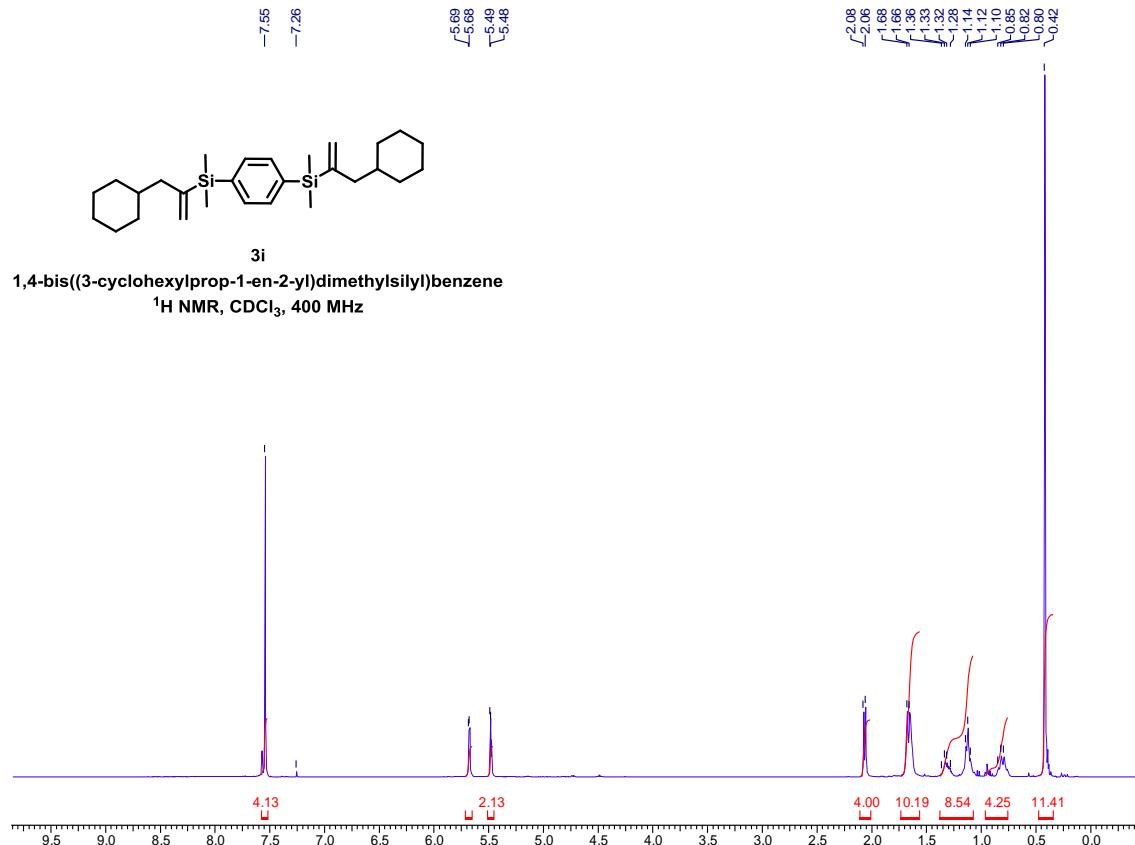


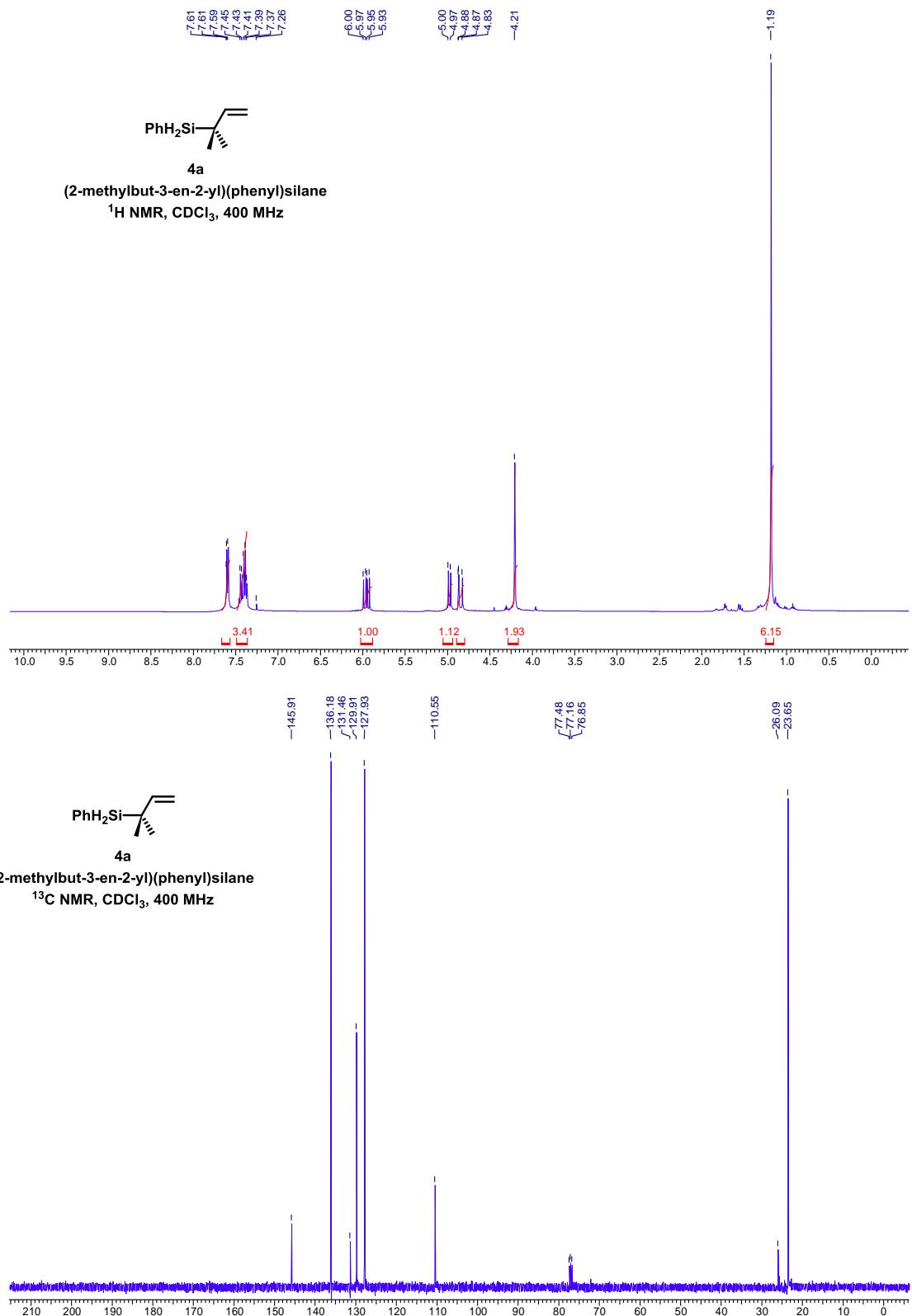


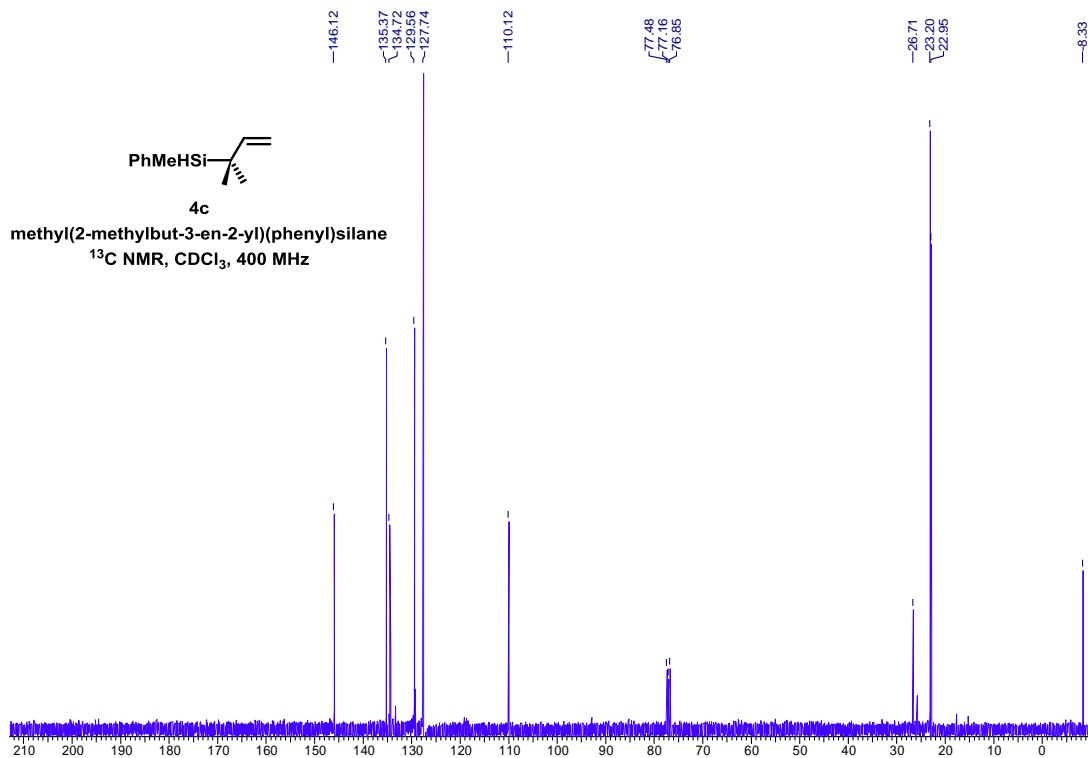
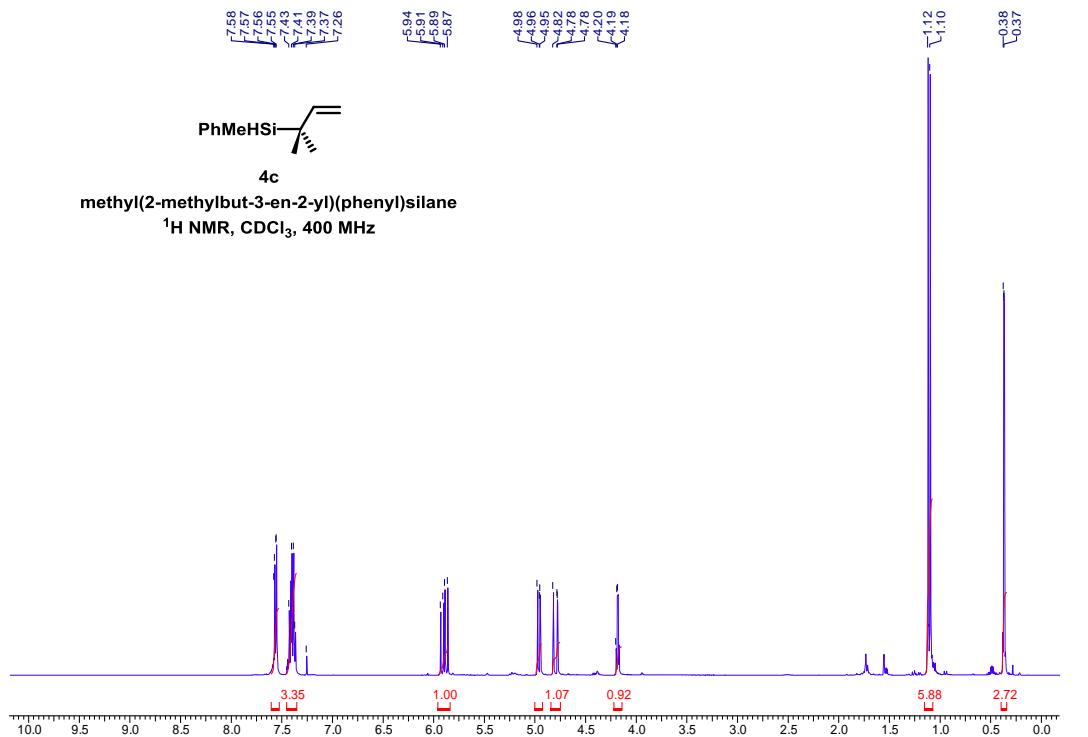


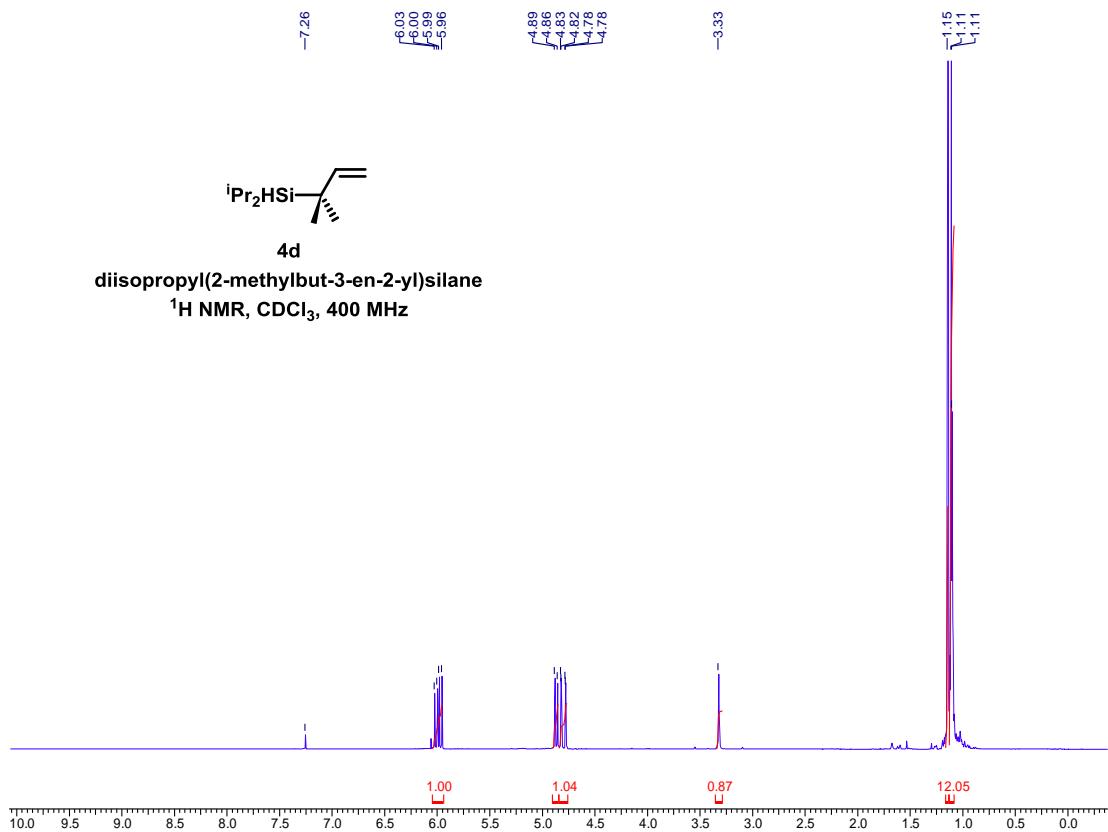


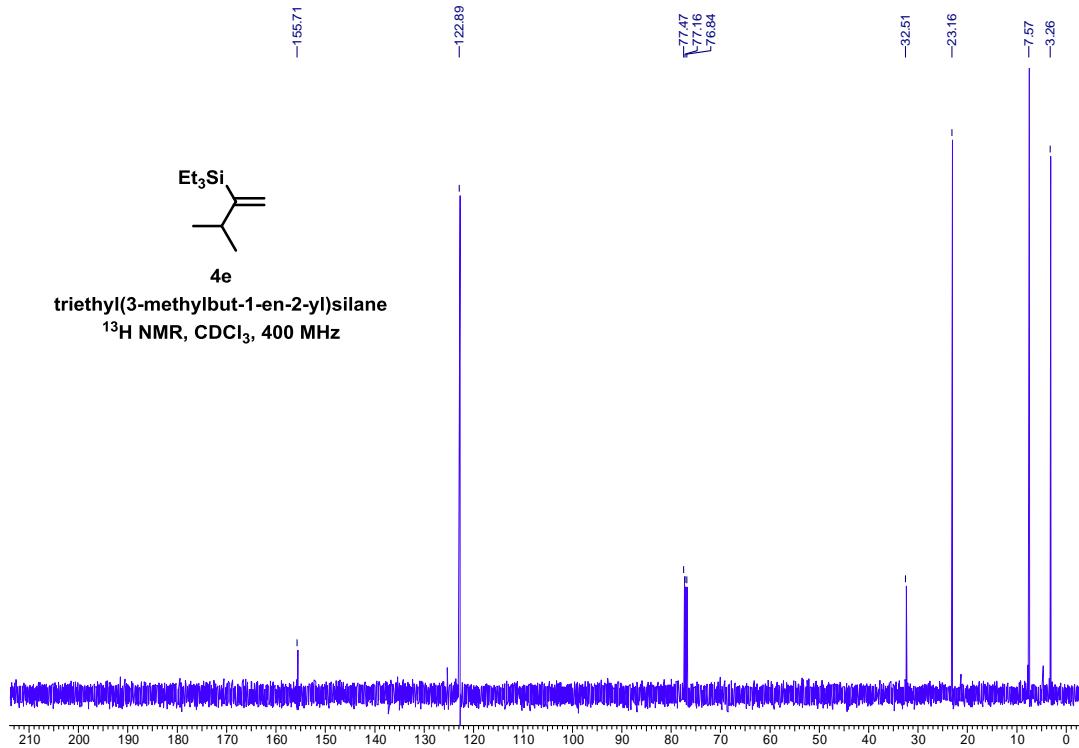
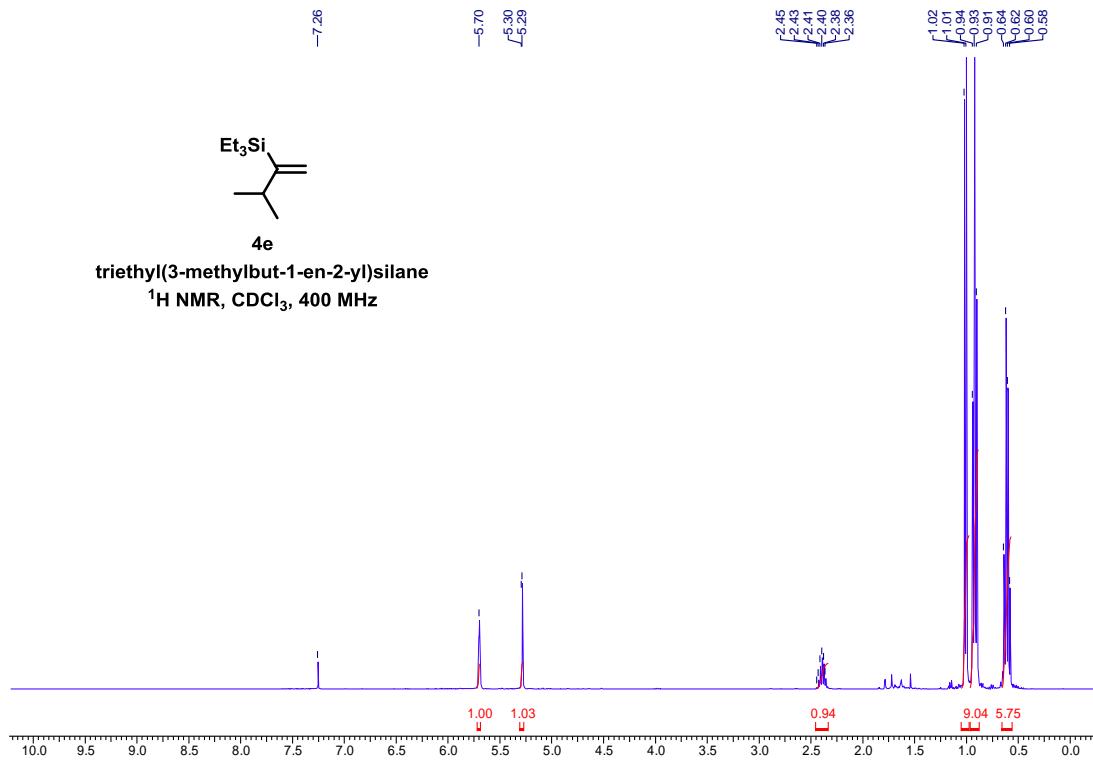


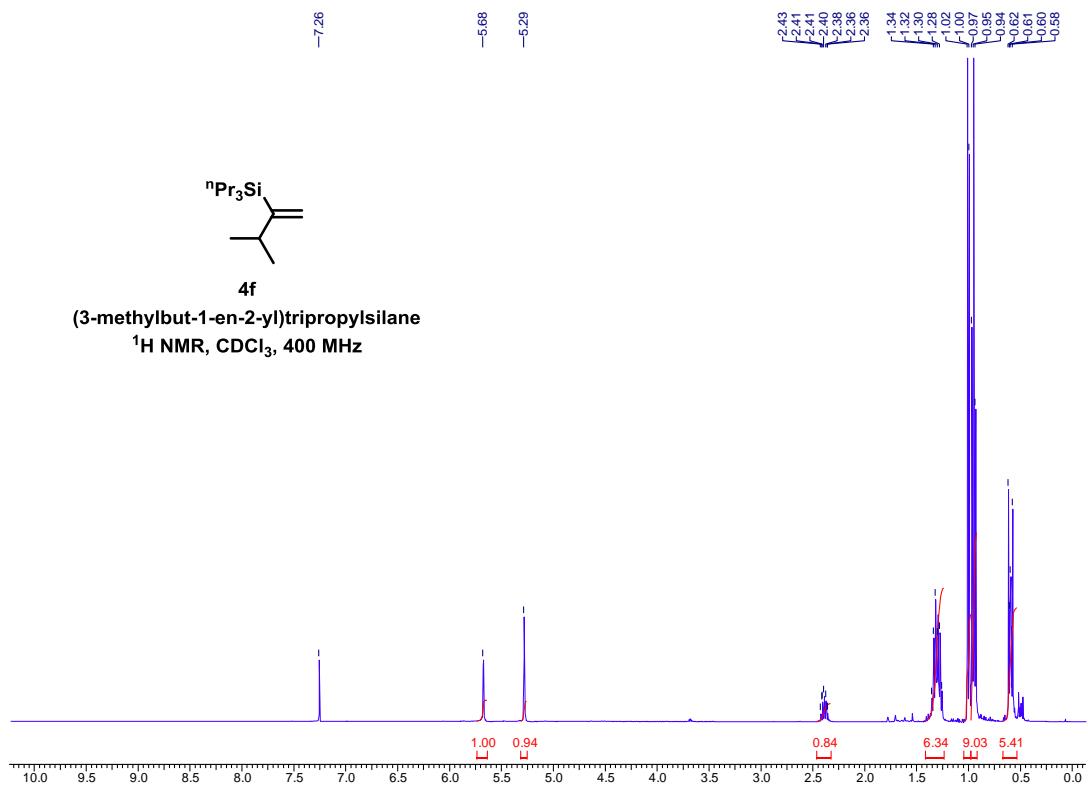


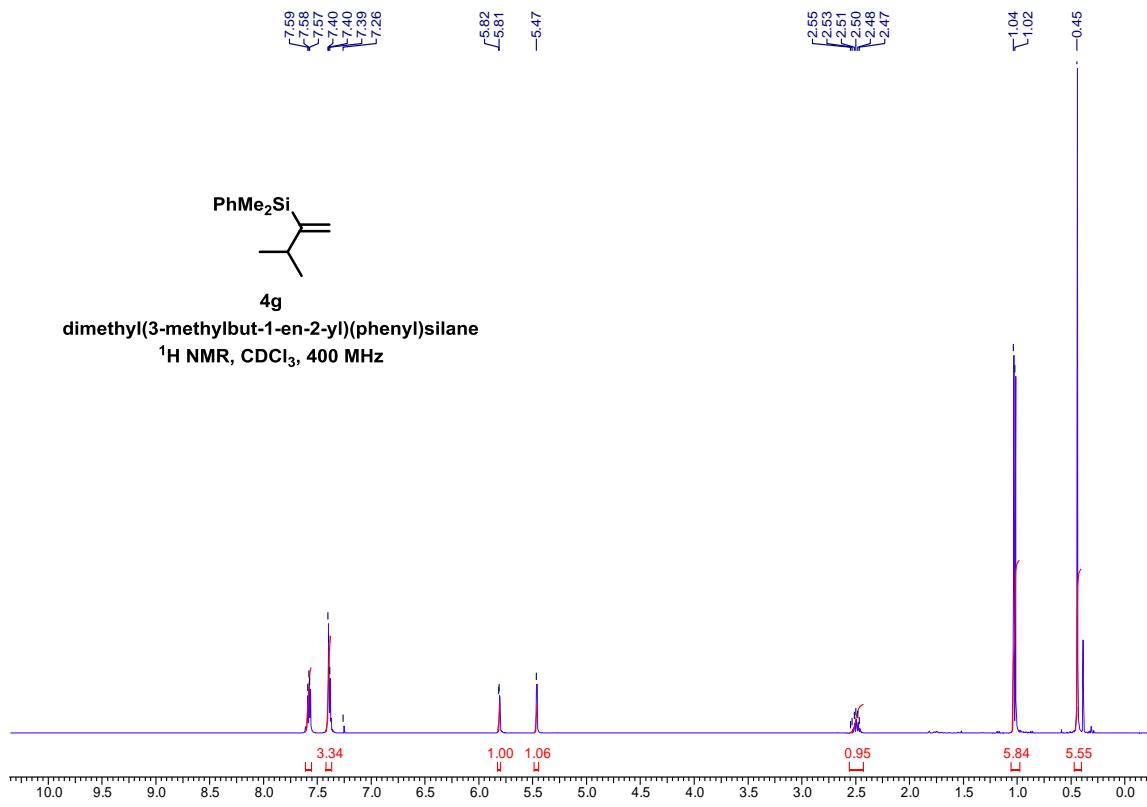






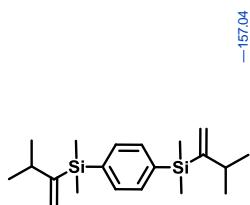
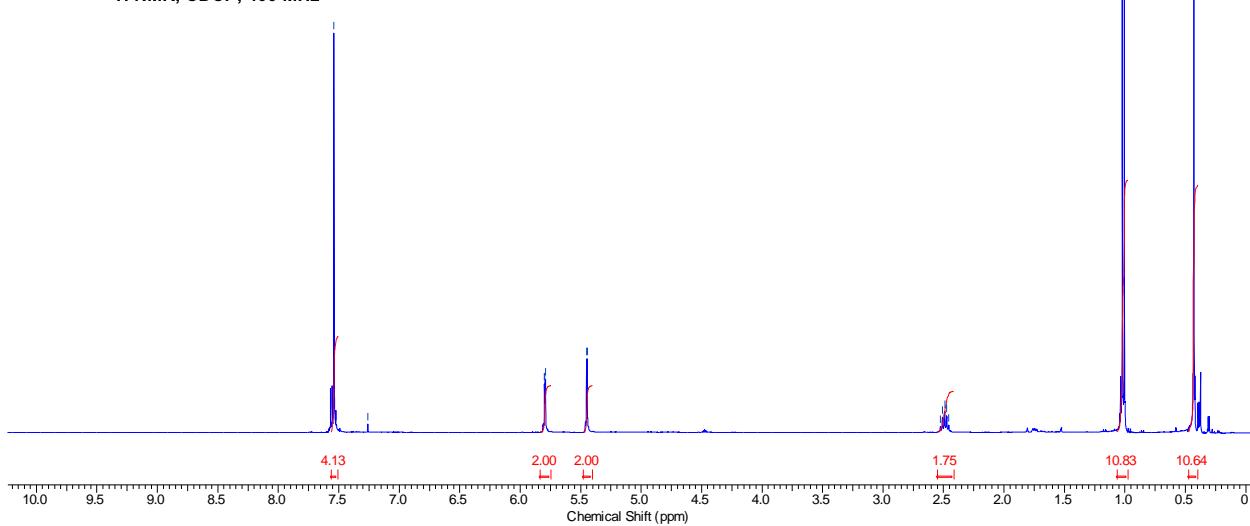




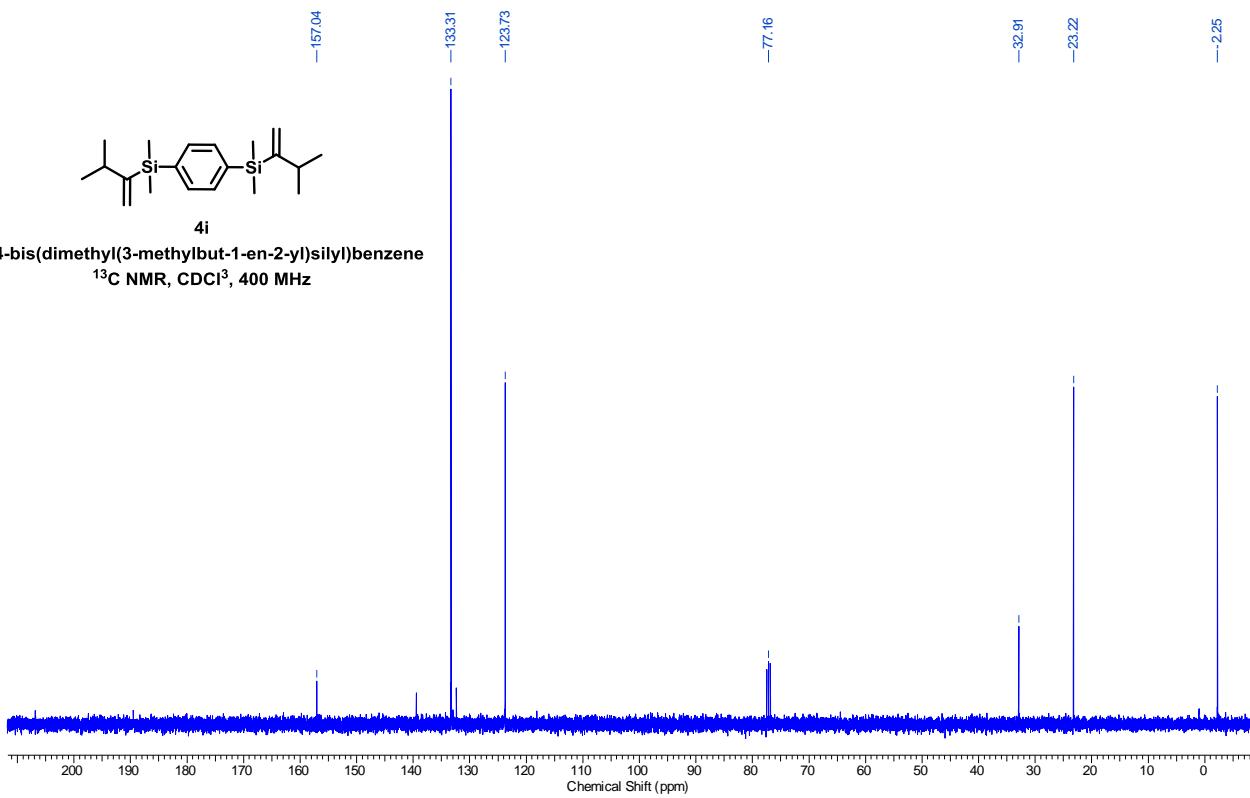




1,4-bis(dimethyl(3-methylbut-1-en-2-yl)silyl)benzene
 ^1H NMR, CDCl_3 , 400 MHz



1,4-bis(dimethyl(3-methylbut-1-en-2-yl)silyl)benzene
 ^{13}C NMR, CDCl_3 , 400 MHz



1. A. R. Shaffer and J. A. R. Schmidt, *Organometallics*, 2009, **28**, 2494-2504.
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