Supporting Information

Ruthenium(II) Catalyzed Regioselective 1,2-Hydrosilylation of *N*-Heteroarenes and Tetrel Bonding Mechanism

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General Experimental: All catalytic reactions were performed under nitrogen atmosphere. All stoichiometric reactions were performed in nitrogen atmosphere MBraun glove box. Catalyst **1** was prepared from previous reported procedure.[1] Deuterated solvents are stored under molecular sieves (heated at 400°C and cooled under nitrogen atmosphere) inside the glove box. Chemicals were purchased from Sigma-Aldrich, Alfa-aesar, Acros, and TCI chemicals used without further purification. ^{1}H and ^{13}C spectra were recorded at Bruker AV-400 (^{1}H: 400 MHz, ^{13}C: 100.6 MHz, ^{31}P: 162 MHz). ^{29}Si NMR spectrum was recorded at Jeol-400 MHz spectrometer. ^{1}H and $^{13}C\{^{1}H\}$ NMR chemical shifts were reported in ppm downfield from tetramethylsilane. Multiplicity is abbreviated as: s, singlet; d, doublet; t, triplet; q, quartet; quint, quintet; sept, septet; m, multiplet.

General Optimization Procedure for 1,2-Hydrosilylation of Quinoline: To a PTFE screw cap scintillation vial charged with a stir bar, quinoline (0.5 mmol), silane (0.5-0.75 mmol), and catalyst **1** (0.01-0.02 mmol) were added inside the glove box. The reaction vial was taken out from box and stirred at indicated temperature. After completion of the reaction, the reaction mixture cooled to room temperature and taken inside the glove box, internal standard cyclohexane (0.25 mmol) was added. Then 200 µl $CDCl_3$ was added into the reaction mixture and stirred for 10 minutes. From the resulting mixture 100 µl solution was transferred to NMR tube and used for the NMR analyses. The products are highly air and moisture sensitive. All experimental procedures were carried out under nitrogen atmosphere and reaction mixture NMR samples were prepared under the nitrogen atmosphere glove-box.

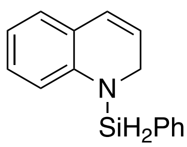
General Procedure for 1,2-Hydrosilylation of Quinoline Derivatives: To a PTFE screw cap scintillation vial charged with a stir bar, quinoline derivative (0.5 mmol), phenylsilane (0.6 mmol) or diethyl silane (0.75 mmol) and catalyst **1** (0.02 mmol, 2 mol%) [C_6D_6 or $CDCl_3$ (0.3 mL) for solid substrates] were added inside the glove box. The reaction mixture was allowed to stir at 60 °C for 18 h. After completion of the reaction, the reaction mixture was cooled to room temperature, taken inside the glove box and internal standard cyclohexane (0.25 mmol) was added. Then 200 µl of $CDCl_3$ or C_6D_6 was added into the reaction mixture and stirred for 10 minutes. From the resulting mixture 100 µl solution was transferred to NMR tube and used for the NMR analyses. The products are highly air and moisture sensitive. All experimental procedures were carried out under nitrogen atmosphere and reaction mixture NMR samples were prepared under the nitrogen atmosphere glove-box.

General Procedure for 1,2-Hydrosilylation of *N*-Heteroarenes:

To a PTFE screw cap scintillation vial charged with a stir bar, *N*-heterocycle derivative (0.5 mmol), phenylsilane (0.6 mmol) or diethyl silane (0.75 mmol or 1.25 mmol) and catalyst **1** (0.02 mmol, 2 mol%) [C_6D_6 or $CDCl_3$ (0.3 mL) for solid substrates] were added inside the glove box. The reaction mixture was allowed to stir at 60 °C for 18 h. After completion of the reaction, the reaction mixture was cooled to room temperature taken inside the glove box, and internal standard cyclohexane (0.25 mmol) was added. Then 200 µl $CDCl_3$ or C_6D_6 was added into the reaction mixture and stirred for 10 minutes. From the resulting mixture 100 µl solution was transferred to NMR tube and used for the NMR analyses. The products are highly air and moisture sensitive. Thus, the NMR samples were prepared under the nitrogen atmosphere glove-box.

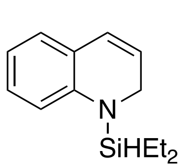
Spectral Data of *N*-Silyl-1,2-Dihydroheteroarenes:

1-(Phenylsilyl)-1,2-dihydroquinoline (2a).[2] Yield: >99%. ^{1}H NMR (400 MHz, $CDCl_3$):



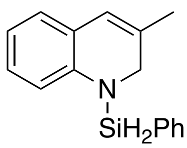
δ 7.72-7.70 (d, 2H, *J* = 8Hz, ArC*H*), 7.49-7.42 (m, 3H, ArC*H*), 7.06-6.98 (m, 2H, ArC*H*), 6.86-6.81 (m, 2H, ArC*H*), 6.49-6.46 (d, 1H, *J* = 12Hz, olefinic-C*H*), 5.79-5.77 (m, 1H, olefinic-C*H*), 5.21 (s, 2H, Si-*H*), 4.15-4.12 (m, 2H, C*H*$_2$). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 145.17, 135.82, 134.67, 132.43, 130.51, 128.41, 128.26, 127.09, 126.72, 122.77, 119.95, 117.13, 46.71.

1-(Diethylsilyl)-1,2-dihydroquinoline (2b).[3] Yield: >99%. ^{1}H NMR (400 MHz, $CDCl_3$): δ



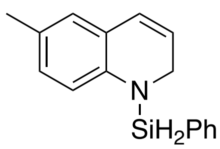
7.06 (t, J = 7.7 Hz, 1H, ArCH), 6.96 (d, J = 7.3 Hz, 1H, ArCH), 6.83 (d, J = 8.0 Hz, 1H, ArCH), 6.78 (t, J = 7.4 Hz, 1H, ArCH), 6.43 (d, J = 9.5 Hz, 1H, olefinic-CH), 5.79-5.75 (m, 1H, olefinic-CH), 4.56-4.52 (m, 1H, Si-H), 4.00-3.99 (m, 2H, CH_2), 1.06 (t, J = 7.9 Hz, 6H, CH_3), 0.92-0.81 (m, 4H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 146.08, 127.88, 127.04, 126.82, 126.18, 122.77, 119.27, 117.27, 45.35, 7.63, 5.35.

3-Methyl-1-(phenylsilyl)-1,2-dihydroquinoline (2c). Yield: >99%. ^{1}H NMR (400 MHz,



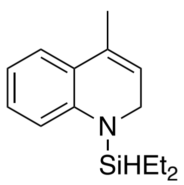
$CDCl_3$): δ 7.74-7.72 (d, 2H, J = 8Hz, ArCH), 7.52-7.45 (m, 3H, ArCH), 7.05-6.96 (m, 2H, ArCH), 6.88-6.82 (m, 2H, ArCH), 6.24 (s, 1H, olefinic-CH), 5.24 (s, 2H, Si-H), 4.05 (s, 2H, CH_2), 1.85 (s, 3H, CH_3). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 143.52, 135.81, 134.62, 132.45, 130.49, 128.40, 128.25, 127.30, 126.16, 121.63, 119.89, 116.58, 51.29, 20.81.

6-Methyl-1-(phenylsilyl)-1,2-dihydroquinoline (2d). Yield: >99%. ^{1}H NMR (400 MHz,



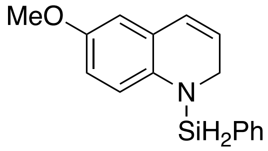
$CDCl_3$): δ 7.75-7.73 (d, 2H, J = 8Hz, ArCH), 7.52-7.46 (m, 3H, ArCH), 6.91-6.79 (m, 3H, ArCH), 6.49-6.46 (d, 1H, J = 12Hz, olefinic-CH), 5.83-5.80 (m, 1H, olefinic-CH), 5.24 (s, 2H, Si-H), 4.15-4.11 (m, 2H, CH_2), 2.31 (s, 3H, CH_3). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 142.56, 135.75, 134.59, 132.63, 130.37, 129.06, 128.63, 128.31, 127.62, 126.69, 122.90, 116.98, 46.64, 20.52.

1-(Diethylsilyl)-4-methyl-1,2-dihydroquinoline (2e).[3] Yield: >99%. ^{1}H NMR (400 MHz,



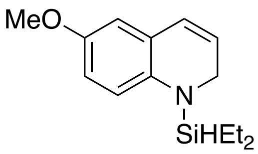
$CDCl_3$): δ 7.19 (d, J = 7.6 Hz, 1H, ArCH), 7.09 (t, J = 7.7 Hz, 1H, ArCH), 6.84 (dd, J_1 = 14.6 Hz, J_2= 7.7 Hz, 2H, ArCH), 5.61 (s, 1H, olefinic-CH), 4.78-4.32 (m, 1H, Si-H), 3.92 (dd, J = 2.5, 1.1 Hz, 2H, CH_2), 2.05 (s, 3H), 1.07 (t, J = 8.0 Hz, 6H, CH_3), 0.90-0.84 (m, 4H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 146.23, 131.59, 127.78, 127.67, 123.85, 119.71, 118.96, 117.30, 45.16, 18.79, 7.66, 5.34.

6-Methoxy-1-(phenylsilyl)-1,2-dihydroquinoline (2f). Yield: 86%. ^{1}H NMR (400 MHz,



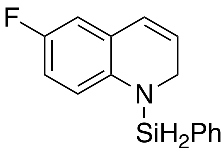
CDCl$_3$): δ 7.70-7.66 (d, 2H, J = 8Hz, ArCH), 7.47-7.42 (m, 3H, ArCH), 6.85-6.78 (m, 1H, ArCH), 6.65-6.62 (m, 2H, ArCH), 6.46-6.43 (d, 1H, J = 12Hz, olefinic-CH), 5.86-5.82 (m, 1H, olefinic-CH), 5.19 (s, 2H, Si-H), 4.08-4.07 (m, 2H, CH_2), 3.77 (s, 3H, OCH_3). ^{13}C {^{1}H} NMR (100.6 MHz, CDCl$_3$): δ 153.61, 138.56, 135.78, 134.62, 130.41, 128.34, 123.23, 126.65, 124.11, 117.99, 113.41, 112.59, 55.67, 46.66.

6-Methoxy-1-(diethylsilyl)-1,2-dihydroquinoline (2g).[3] Yield: >99%. ^{1}H NMR (400 MHz,



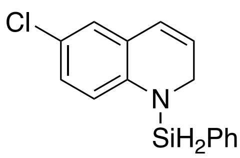
CDCl$_3$): δ 6.76 (d, J = 8.6 Hz, 1H, ArCH), 6.65 (dd, J_1 = 8.6 Hz, J_2= 2.9 Hz, 1H, ArCH), 6.57 (d, J = 2.8 Hz, 1H, ArCH), 6.39 (d, J = 9.5 Hz, 1H, olefinic-CH), 5.84-5.80 (m, 1H, olefinic-CH), 4.49-4.45 (m, 1H, Si-H), 3.91 (dd, J_1 = 4.1 Hz, J_2 = 1.4 Hz, 2H, CH_2), 3.77 (s, 3H, OCH_3), 1.03 (t, J = 7.2 Hz, 6H, CH_3), 0.85-0.78 (m, 4H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, CDCl$_3$): δ 153.21, 139.47, 127.34, 126.73, 124.21, 118.26, 113.28, 112.34, 55.68, 45.36, 7.60, 5.47.

6-Fluoro-1-(phenylsilyl)-1,2-dihydroquinoline (2h). Yield: 87%. ^{1}H NMR (400 MHz,



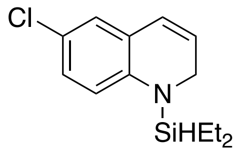
CDCl$_3$): δ 7.70-7.67 (m, 2H, ArCH), 7.50-7.43 (m, 3H, ArCH), 6.76-6.72 (m, 3H, ArCH & olefinic-CH), 6.42 (d, J = 9.6 Hz, 1H, ArCH), 5.88-5.84 (m, 1H, olefinic-CH), 5.19 (d, J = 1.6 Hz, 2H, Si-H), 4.11-4.04 (m, 2H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, CDCl$_3$): δ 157.18 (d, J = 237.4 Hz), 140.99, 135.81, 134.64, 130.60, 128.44, 128.25, 126.13, 124.55, 117.96 (d, J = 7.7 Hz), 114.20 (d, J = 22.4 Hz), 113.29 (d, J = 22.8 Hz), 46.65.

6-Chloro-1-(phenylsilyl)-1,2-dihydroquinoline (2i). Yield: >99%. ^{1}H NMR (400 MHz,



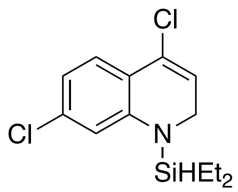
CDCl$_3$): δ 7.68 (d, J = 6.4 Hz, 2H, ArCH), 7.50-7.43 (m, 3H, ArCH), 6.98-6.95 (m, 2H, ArCH), 6.74 (d, J = 8.5 Hz, 1H, ArCH), 6.38 (d, J = 9.7 Hz, 1H, olefinic-CH), 5.83-5.79 (m, 1H, olefinic-CH), 5.17 (s, 2H, Si-*H*), 4.13 (dd, J_1 = 4.0 Hz, J_2 = 1.5 Hz, 2H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 143.66, 135.80, 134.65, 130.69, 128.49, 128.25, 127.73, 126.60, 125.85, 124.67, 124.10, 118.14, 46.74.

6-Chloro-1-(diethylsilyl)-1,2-dihydroquinoline (2j).[3] Yield: >99%. ^{1}H NMR (400 MHz,



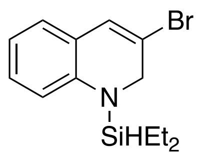
$CDCl_3$): δ 6.96 (dd, J_1 = 8.5 Hz, J_2= 2.5 Hz, 1H, ArC*H*), 6.88 (d, *J* = 2.5 Hz, 1H, ArC*H*), 6.70 (d, *J* = 8.5 Hz, 1H, ArC*H*), 6.32 (d, *J* = 9.5 Hz, 1H, olefinic-C*H*), 5.81-5.74 (m, 1H, olefinic-C*H*), 4.47-4.44 (m, 1H, Si-*H*), 3.93 (dd, J_1= 4.2 Hz, J_2= 1.6 Hz, 2H, CH_2), 1.03-0.99 (m, 6H, CH_3), 0.87-0.77 (m, 4H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 144.59, 127.54, 127.40, 126.52, 125.95, 124.10, 123.96, 118.31, 45.31, 7.57, 5.22.

4,7-Dichloro-1-(diethylsilyl)-1,2-dihydroquinoline (2k). Yield: >99%. ^{1}H NMR (400 MHz,



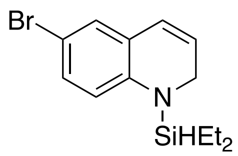
$CDCl_3$): δ 7.36 (d, *J* = 8.8 Hz, 1H, ArC*H*), 6.81-6.78 (m, 2H, ArC*H*), 5.84 (t, *J* = 4.6 Hz, 1H, olefinic-C*H*), 4.50-4.47 (m, 1H, Si-*H*), 3.99 (d, *J* = 4.6 Hz, 2H, CH_2), 1.09-1.02 (m, 6H, CH_3), 0.90-0.80 (m, 4H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 147.79, 134.72, 129.16, 126.16, 122.91, 119.70, 119.35, 117.25, 46.13, 7.51, 5.04.

3-Bromo-1-(diethylsilyl)-1,2-dihydroquinoline (2l).[3] Yield: >99%. ^{1}H NMR (400 MHz,



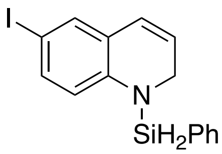
$CDCl_3$): δ 7.08 (td, J_1 = 8.0 Hz, J_2= 1.6 Hz, 1H, ArC*H*), 6.92 (dd, J_1 = 7.4 Hz, J_2= 1.4 Hz, 1H, ArC*H*), 6.84-6.79 (m, 2H, ArC*H*), 6.74 (s, 1H, olefinic-C*H*), 4.49 (quint, *J*= 3.6 Hz 1H, Si-*H*), 4.15 (d, *J* = 1.1 Hz, 2H, CH_2), 1.04 (t, *J* = 7.7 Hz, 6H, CH_3), 0.91-0.80 (m, 4H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 143.88, 128.25, 128.12, 126.56, 126.33, 120.06, 117.80, 115.55, 52.99, 7.50, 5.31.

6-Bromo-1-(diethylsilyl)-1,2-dihydroquinoline (2m).[3] Yield: >99%. ^{1}H NMR (400 MHz,

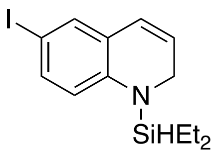


$CDCl_3$): δ 7.09 (dd, *J* = 8.5, 2.4 Hz, 1H, ArC*H*), 7.02 (d, *J* = 2.3 Hz, 1H, ArC*H*), 6.65 (d, *J* = 8.5 Hz, 1H, ArC*H*), 6.31 (d, *J* = 9.5 Hz, 1H, olefinic-CH), 5.79-5.74 (m, 1H, olefinic-CH), 4.45 (quint, J = 3.2 Hz 1H, Si-H), 3.94 (dd, J_1 = 4.2 Hz, J_2= 1.6 Hz, 2H, CH_2), 1.04-0.99 (m, 6H, CH_3), 0.887-0.78 (m, 4H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 145.11, 130.32, 129.38, 128.02, 125.85, 124.03, 118.76, 111.21, 45.30, 7.58, 5.19.

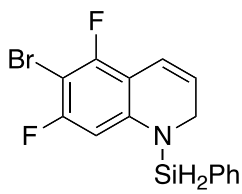
6-Iodo-1-(phenylsilyl)-1,2-dihydroquinoline (2n). Yield: >99%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, J = 7.4 Hz, 2H, ArCH), 7.52-7.45 (m, 3H, ArCH), 7.33-7.27 (m, 2H, ArCH), 6.60 (d, J = 8.1 Hz, 1H, olefinic-CH), 6.38 (d, J = 9.6 Hz, 1H, ArCH), 5.84-5.78 (m, 1H, olefinic-CH), 5.17 (s, 2H, Si-H), 4.16-4.08 (m, 2H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 144.92, 136.64, 135.81, 135.28, 134.65, 128.51, 128.25, 128.03, 125.58, 123.80, 119.09, 81.57, 46.71.



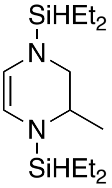
1-(Diethylsilyl)-6-iodo-1,2-dihydroquinoline (2o). Yield: 80%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30-7.27 (m, 1H, ArCH), 7.21 (d, J = 2.1 Hz, 1H, ArCH), 6.56 (d, J = 8.5 Hz, 1H, ArCH), 6.31 (d, J = 9.6 Hz, 1H, olefinic-CH), 5.78-5.74 (m, 1H, olefinic-CH), 4.47-4.44 (m, 1H, Si-H), 3.96 (dd, J_1 = 4.2 Hz, J_2 = 1.6 Hz, 2H, CH_2), 1.05-1.01 (m, 6H, CH_3), 0.90-0.78 (m, 4H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 145.84, 136.31, 135.23, 128.50, 125.67, 123.78, 119.26, 80.69, 45.26, 7.59, 5.14.



6-Bromo-5,7-difluoro-1-(phenylsilyl)-1,2-dihydroquinoline (2p). Yield: >99%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67-7.65 (m, 2H, ArCH), 7.51-7.41 (m, 3H, ArCH), 6.63 (d, J = 9.8 Hz, 1H, olefinic-CH), 6.48-6.46 (m, 1H, ArCH), 5.78-5.74 (m, 1H, olefinic-CH), 5.15 (s, 2H, Si-H), 4.11 (dd, J_1 = 4.0 Hz, J_2= 1.5 Hz, 2H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 158.99 (dd, J_1 = 245.3 Hz, J_2= 7.0 Hz), 155.78 (dd, J_1 = 247.3 Hz, J_2 = 6.7 Hz), 146.28 (dd, J_1 = 12.2 Hz, J_2 = 8.5 Hz), 135.79, 134.67, 131.06, 128.66, 128.24, 122.06, 118.40 (d, J = 3.2 Hz), 101.01 (dd, J_1 = 26.1 Hz, J_2= 3.0 Hz), 86.78 (t, J = 25.2 Hz), 46.40.

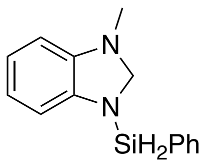


1,4-Bis(diethylsilyl)-2-methyl-1,2,3,4-tetrahydropyrazine (3e).[3] Yield: >99%. ^{1}H NMR



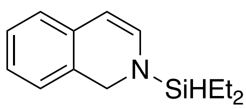
(400 MHz, $CDCl_3$): δ 5.29 (d, J = 6.0 Hz, 1H, olefinic-C*H*), 5.25 (d, J = 6.0 Hz, 1H, olefinic-C*H*), 4.24-4.19 (m, 1H, Si-*H*), 4.19-4.13 (m, 1H, Si-*H*), 3.47-3.38 (m, 1H, C*H*), 3.00 (qd, J_1 = 11.3 Hz, J_2= 1.6 Hz, 2H, CH_2), 1.08 (d, J = 6.4 Hz, 3H, CH_3), 1.01-0.96 (m, 12H, CH_3), 0.71-0.63 (m, 8H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 110.17, 109.55, 49.04, 47.94, 18.87, 7.47, 7.45, 4.94, 4.84.

1-Methyl-3-(phenylsilyl)-2,3-dihydro-1*H*-benzo[*d*]imidazole (3g). Yield: >99%. ^{1}H NMR



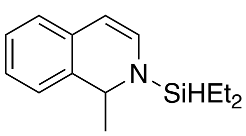
(400 MHz, $CDCl_3$): δ 7.79-7.77 (m, 2H, ArC*H*), 7.53-7.47 (m, 3H, ArC*H*), 6.79 (dd, J_1 = 10.7 Hz, J_2 = 4.3 Hz, 1H, ArC*H*), 6.70 (t, J = 7.5 Hz, 1H, ArC*H*), 6.63 (d, J = 7.4 Hz, 1H, ArC*H*), 6.51 (d, J = 7.4 Hz, 1H, ArC*H*), 5.25 (s, 2H, Si-*H*), 4.88 (s, 2H, CH_2), 2.80 (s, 3H, CH_3). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 144.22, 141.52, 135.77, 134.95, 130.76, 128.42, 119.56, 118.92, 107.74, 106.08, 77.48, 77.16, 76.84, 75.58, 34.29.

2-(Diethylsilyl)-1,2-dihydroisoquinoline (3h).[3] Yield: >99%. ^{1}H NMR (400 MHz, $CDCl_3$):



δ 7.14 (t, J = 7.2 Hz, 1H, ArC*H*), 7.05 (t, J = 7.0 Hz, 1H, ArC*H*), 6.94 (d, J = 7.3 Hz, 1H, ArC*H*), 6.90 (d, J = 7.4 Hz, 1H, ArC*H*), 6.37 (d, J = 7.2 Hz, 1H, olefinic-C*H*), 5.56 (d, J = 7.2 Hz, 1H, olefinic-C*H*), 4.35 (s, 3H, CH_2& Si-*H*), 1.05 (t, J = 7.8 Hz, 6H, CH_3), 0.83-0.78 (m, 4H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 137.02, 134.22, 127.43, 126.78, 125.12, 124.89, 122.30, 102.12, 48.11, 7.31, 4.30.

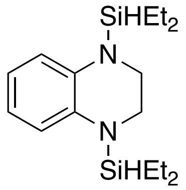
2-(Diethylsilyl)-1-methyl-1,2-dihydroisoquinoline (3i). Yield: >99%. ^{1}H NMR (400 MHz,



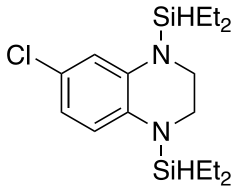
$CDCl_3$): δ 7.16 (t, J = 7.4 Hz, 1H, ArC*H*), 7.08 (t, J = 7.4 Hz, 1H, ArC*H*), 6.97-6.94 (m, 2H, ArC*H*), 6.27 (d, J = 7.2 Hz, 1H, olefinic-C*H*), 5.57 (d, J = 7.2 Hz, 1H, olefinic-C*H*), 4.49 (q, J = 6.5 Hz, 1H, C*H*), 4.41 (s, 1H, Si-*H*), 1.26 (d, J = 6.6 Hz, 3H, CH_3), 1.08-1.04 (m, 6H, CH_3), 0.87-0.70 (m, 4H, CH_2). ^{13}C {^{1}H}

NMR (100.6 MHz, $CDCl_3$): δ 133.53, 132.32, 132.22, 127.06, 125.14, 125.01, 122.81, 101.40, 53.37, 22.50, 7.31, 7.29, 5.29, 4.47.

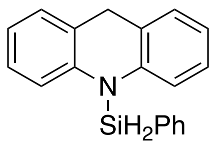
1,4-Bis(diethylsilyl)-1,2,3,4-tetrahydroquinoxaline (3j). Yield: >99%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.84-6.82 (m, 2H, ArC*H*), 6.69-6.67 (m, 2H, ArC*H*), 4.54 (s, 2H, Si-*H*), 3.38 (s, 4H, CH_2), 1.05 (t, J = 7.7 Hz, 12H, CH_3), 0.93-0.82 (m, 8H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 136.06, 118.55, 117.00, 45.62, 7.69, 5.08.



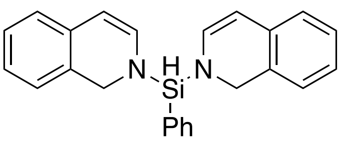
6-Chloro-1,4-bis(diethylsilyl)-1,2,3,4-tetrahydroquinoxaline (3k). Yield: >99%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.79-6.78 (m, 1H, ArC*H*), 6.70 (dd, J_1= 8.5 Hz, J_2= 1.7 Hz, 1H, ArC*H*), 6.61 (dd, J = 8.5, 2.2 Hz, 1H, ArC*H*), 4.54-4.50 (m, 2H, Si-*H*), 3.33 (d, J = 1.4 Hz, 4H, CH_2), 1.05-1.01 (m, 12H, CH_3), 0.88-0.83 (m, 8H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 137.36, 134.72, 123.30, 118.04, 117.56, 116.57, 45.37, 45.21, 7.61, 4.97, 4.83.



10-(Phenylsilyl)-9,10-dihydroacridine (3l).[2] Yield: 85%. ^{1}H NMR (400 MHz, C_6D_6): δ 7.53-7.51 (m, 2H, ArC*H*), 7.13-7.05 (m, 6H, ArC*H*), 6.96-6.86 (m, 5H, ArC*H*), 5.31 (s, 2H, Si-*H*), 3.64 (s, 2H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, C_6D_6): δ 144.61, 134.57, 132.66, 130.67, 128.76, 128.15, 127.94, 126.97, 122.69, 118.71, 33.27.

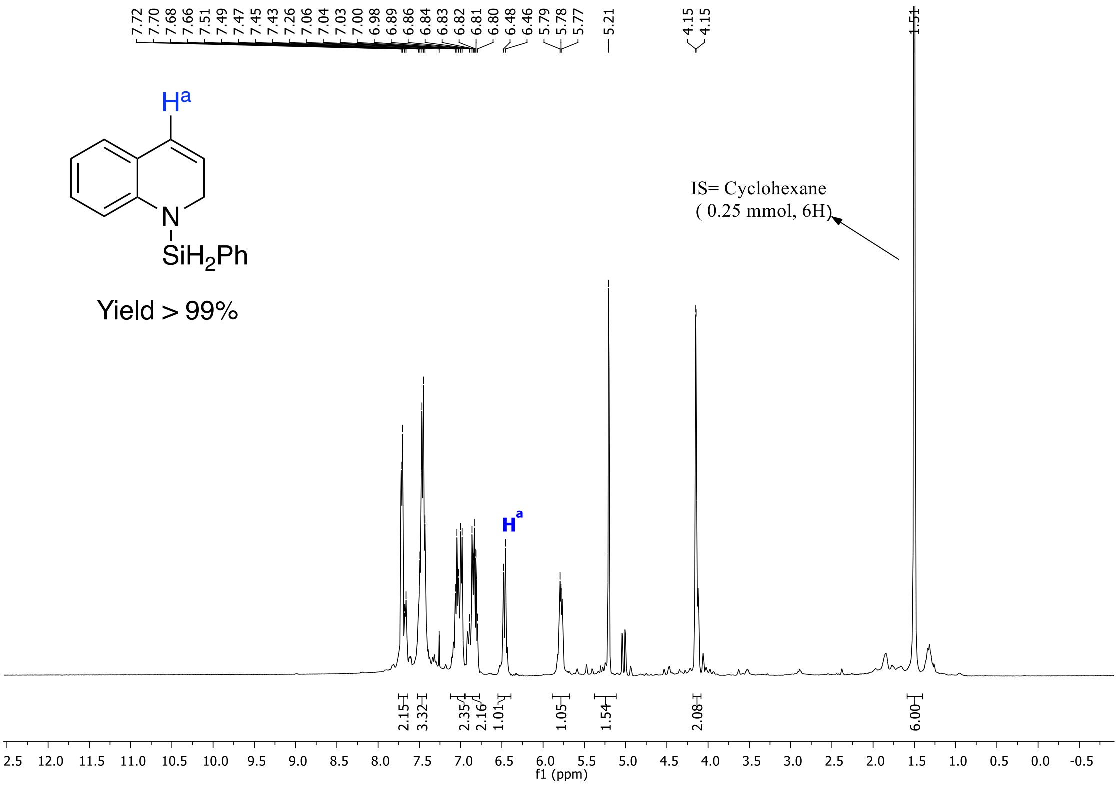


2,2'-(Phenylsilanediyl)bis(1,2-dihydroisoquinoline) (3m).[2] Yield: >99%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70-7.68 (m, 2H, ArC*H*), 7.50-7.43 (m, 3H, ArC*H*), 7.19 (d, J = 7.5 Hz, 2H, ArC*H*), 7.11 (t, J = 7.4 Hz, 2H, ArC*H*), 6.97 (d, J = 7.5 Hz, 2H, ArC*H*), 6.93 (d, J = 7.2 Hz, 2H, ArC*H*), 6.45 (d, J = 7.3 Hz, 2H, olefinic-C*H*), 5.71 (d, J = 7.3 Hz, 2H, olefinic-C*H*), 5.22 (s, 1H, Si-*H*), 4.44 (s, 4H, CH_2). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 135.14, 134.89, 133.64, 131.38, 128.66, 128.25, 127.62, 127.12, 125.80, 125.12, 122.84, 104.89, 77.48, 77.16, 76.84, 47.12.

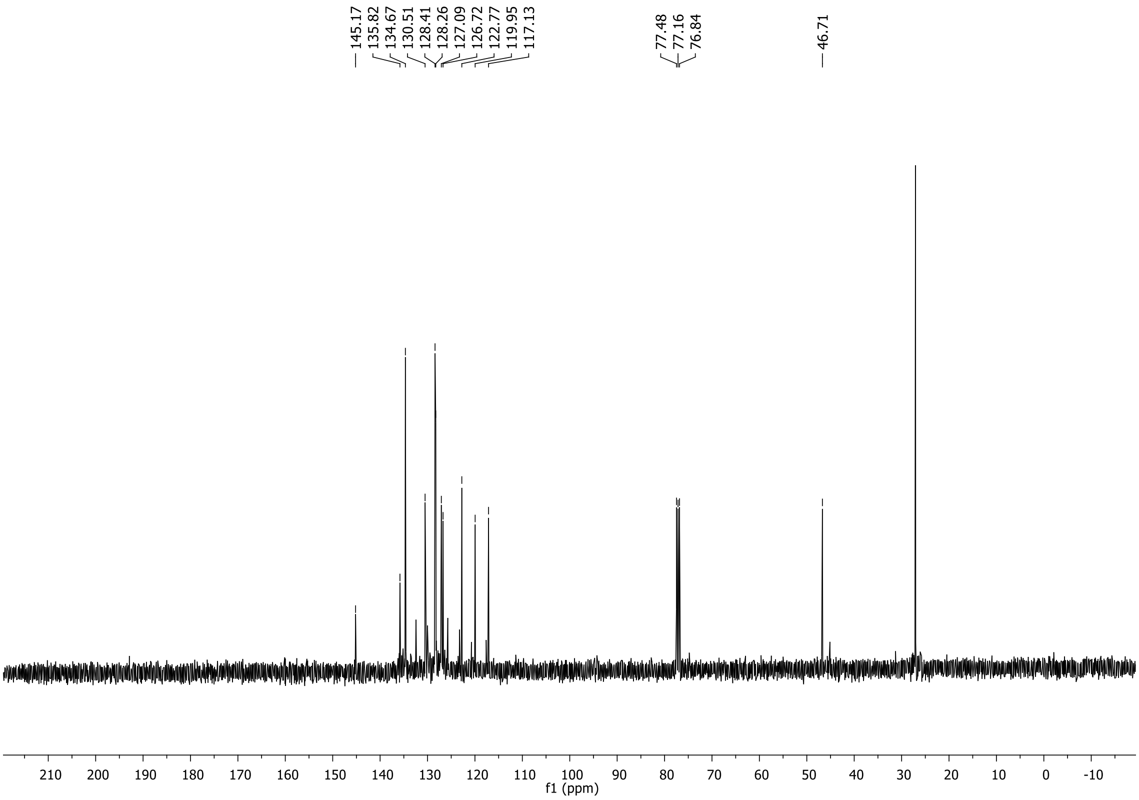


NMR Spectra of *N*-Silyl-1,2-Dihydroheteroarenes:

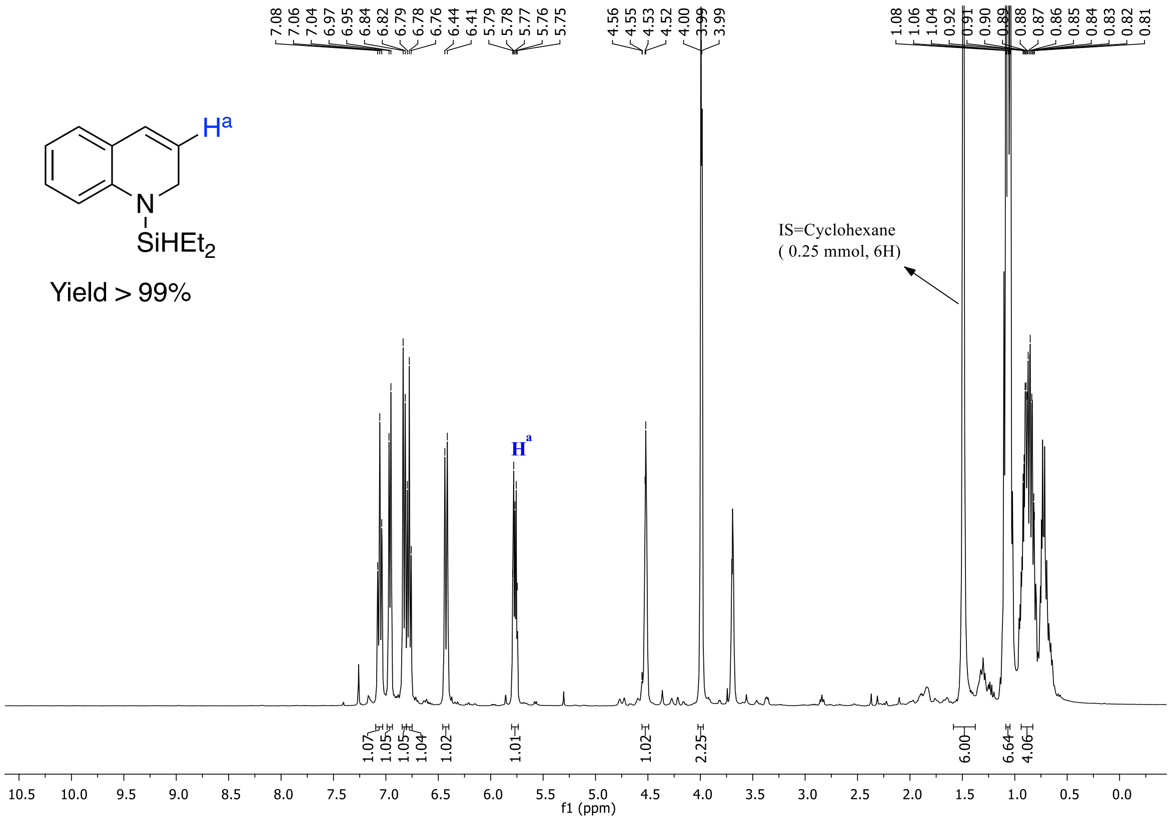
^{1}H NMR reaction mixture spectrum of 1-(phenylsilyl)-1,2-dihydroquinoline **(2a):**



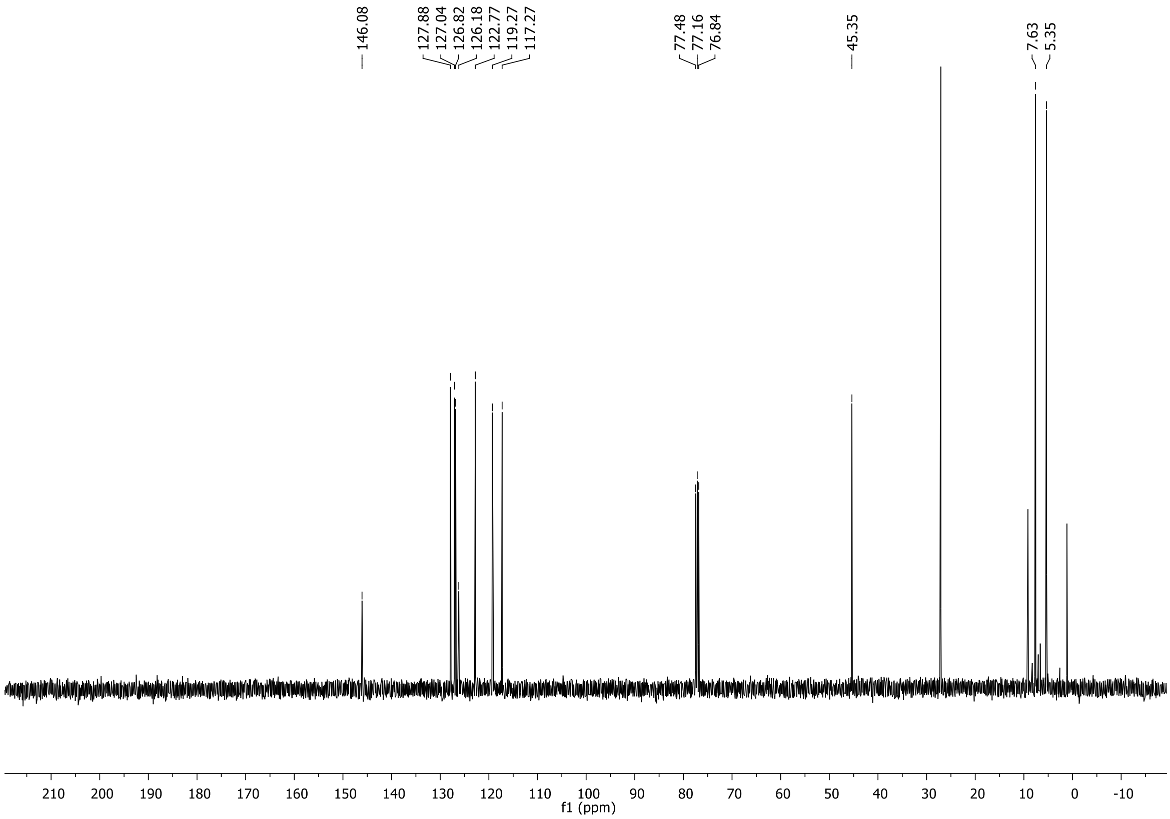
^{13}C NMR reaction mixture spectrum of 1-(phenylsilyl)-1,2-dihydroquinoline **(2a):**



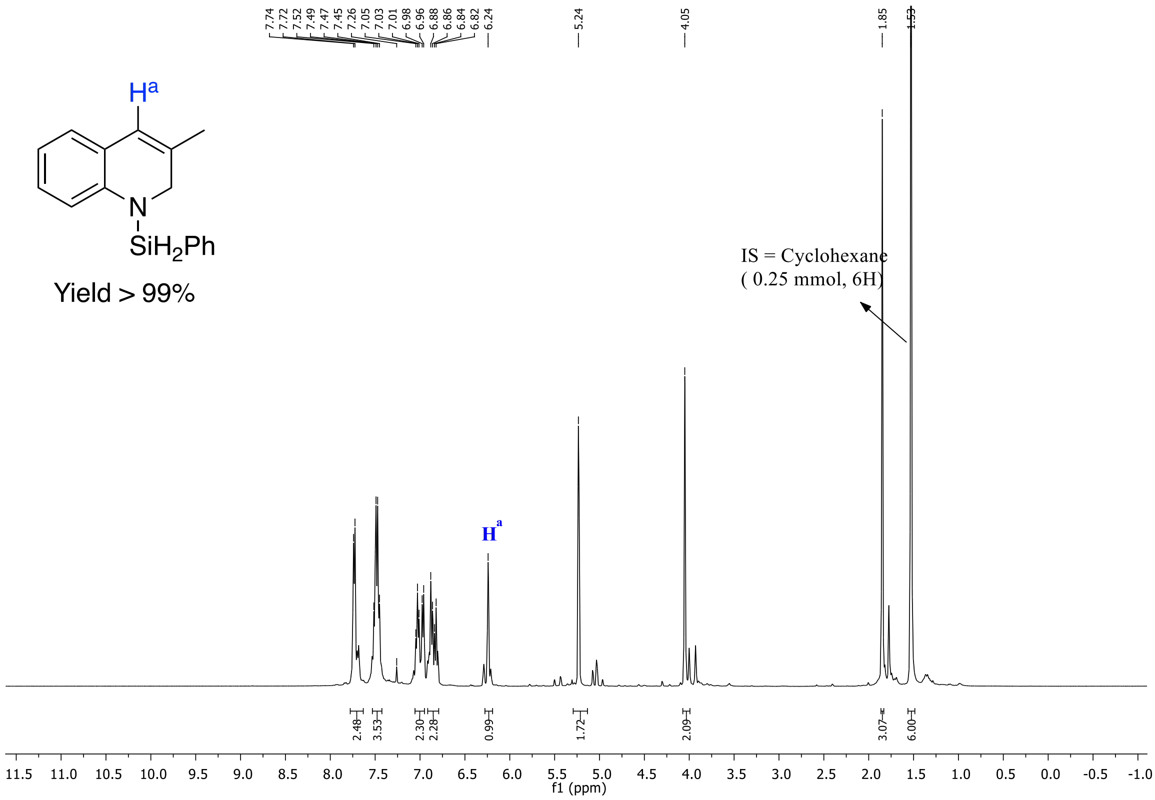
[1]H NMR reaction mixture spectrum of 1-(diethylsilyl)-1,2-dihydroquinoline **(2b):**



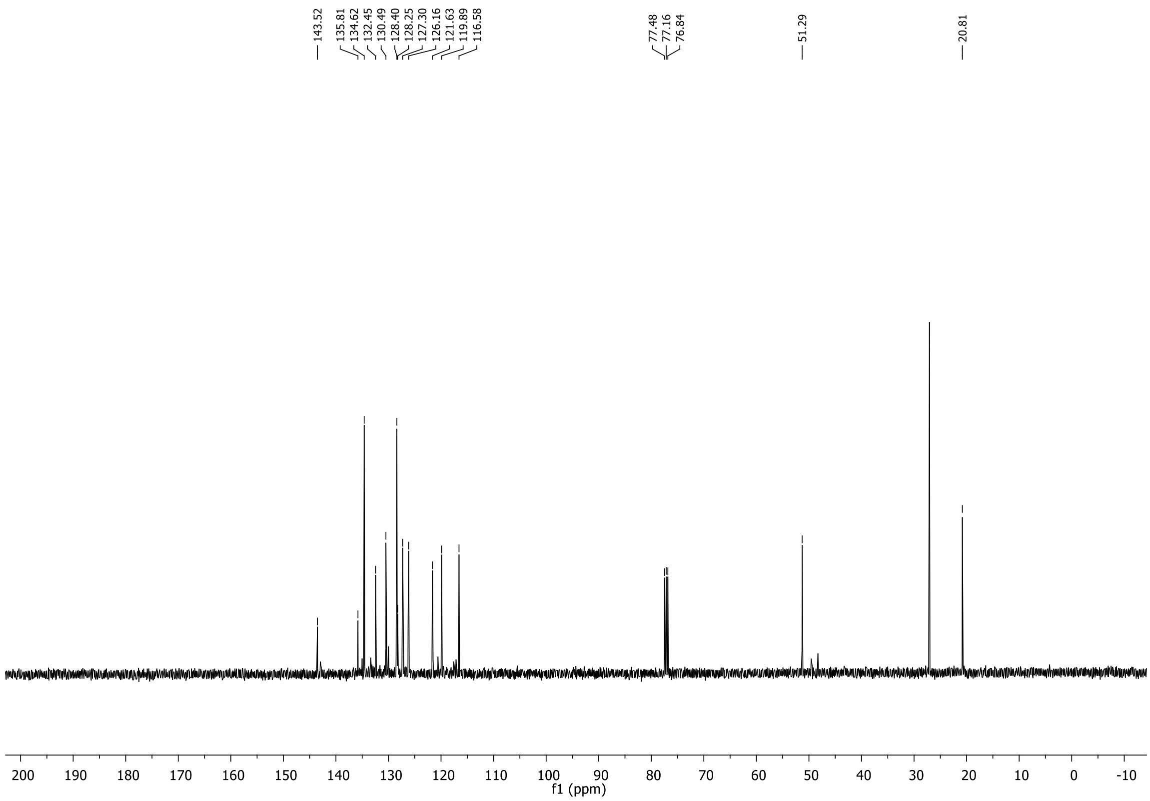
[13]C NMR reaction mixture spectrum of 1-(diethylsilyl)-1,2-dihydroquinoline **(2b):**



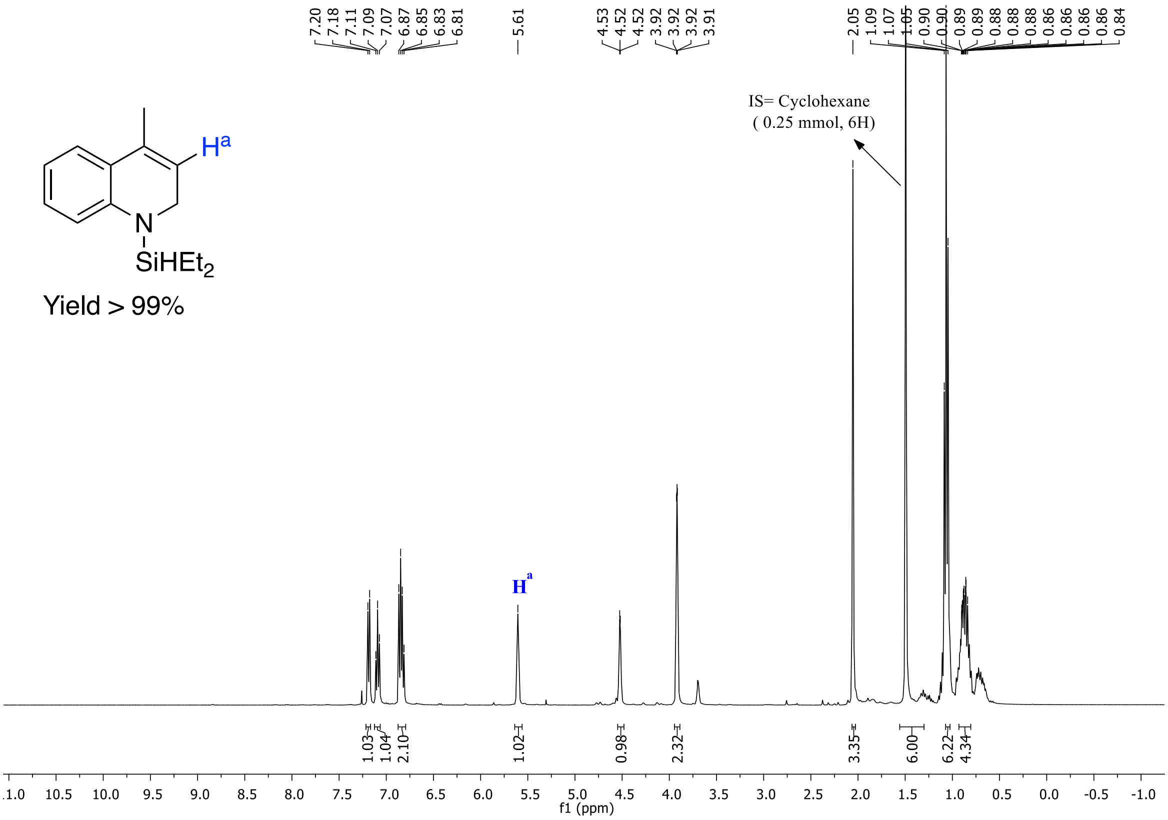
[1]H NMR reaction mixture spectrum of 3-methyl-1-(phenylsilyl)-1,2-dihydroquinoline **(2c):**



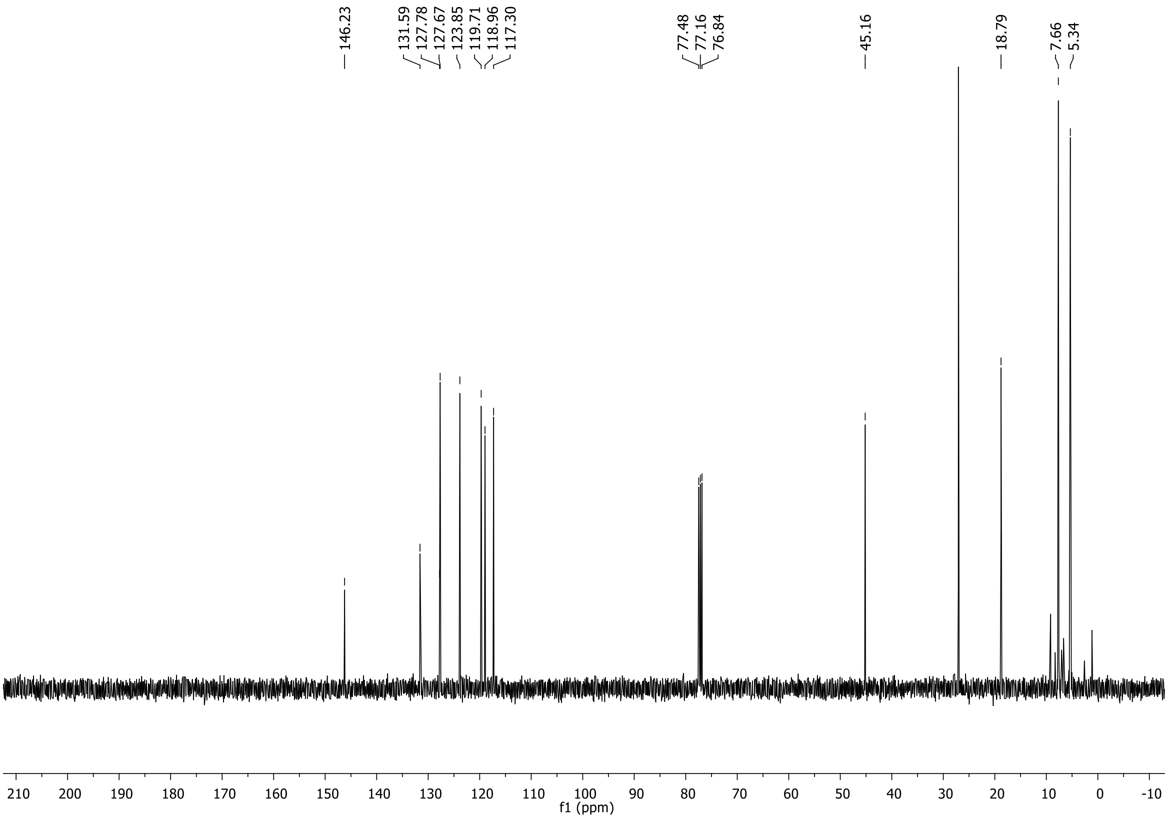
[13]C NMR reaction mixture spectrum of 3-methyl-1-(phenylsilyl)-1,2-dihydroquinoline **(2c):**



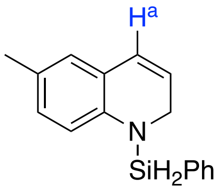
[1]H NMR reaction mixture spectrum of 1-(diethylsilyl)-4-methyl-1,2-dihydroquinoline **(2d):**



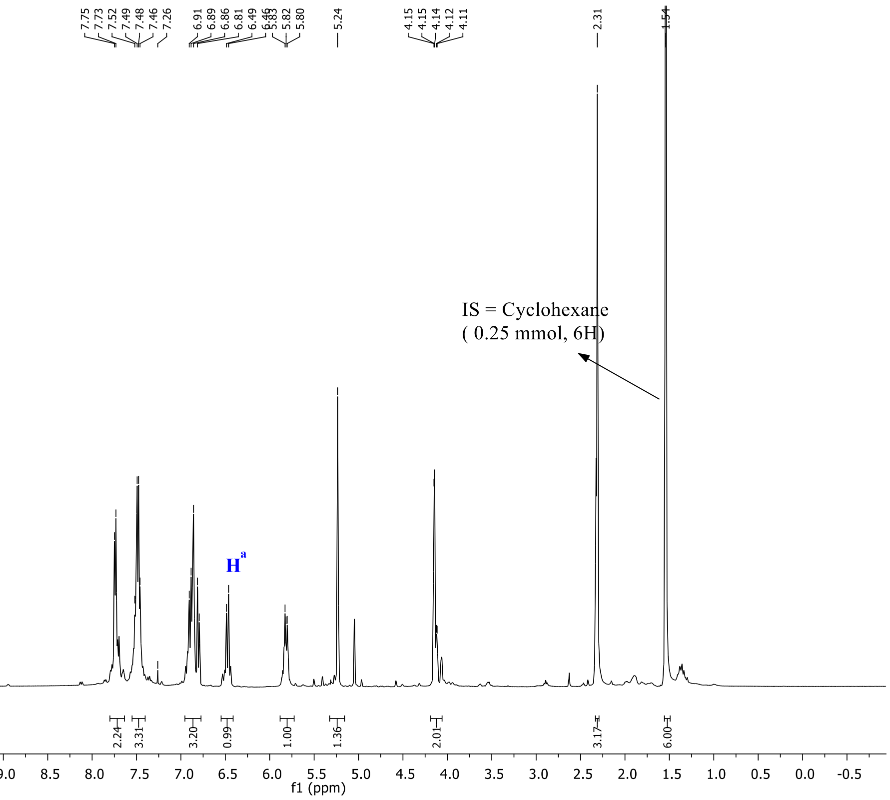
[13]C NMR reaction mixture spectrum of 1-(diethylsilyl)-4-methyl-1,2-dihydroquinoline **(2d):**



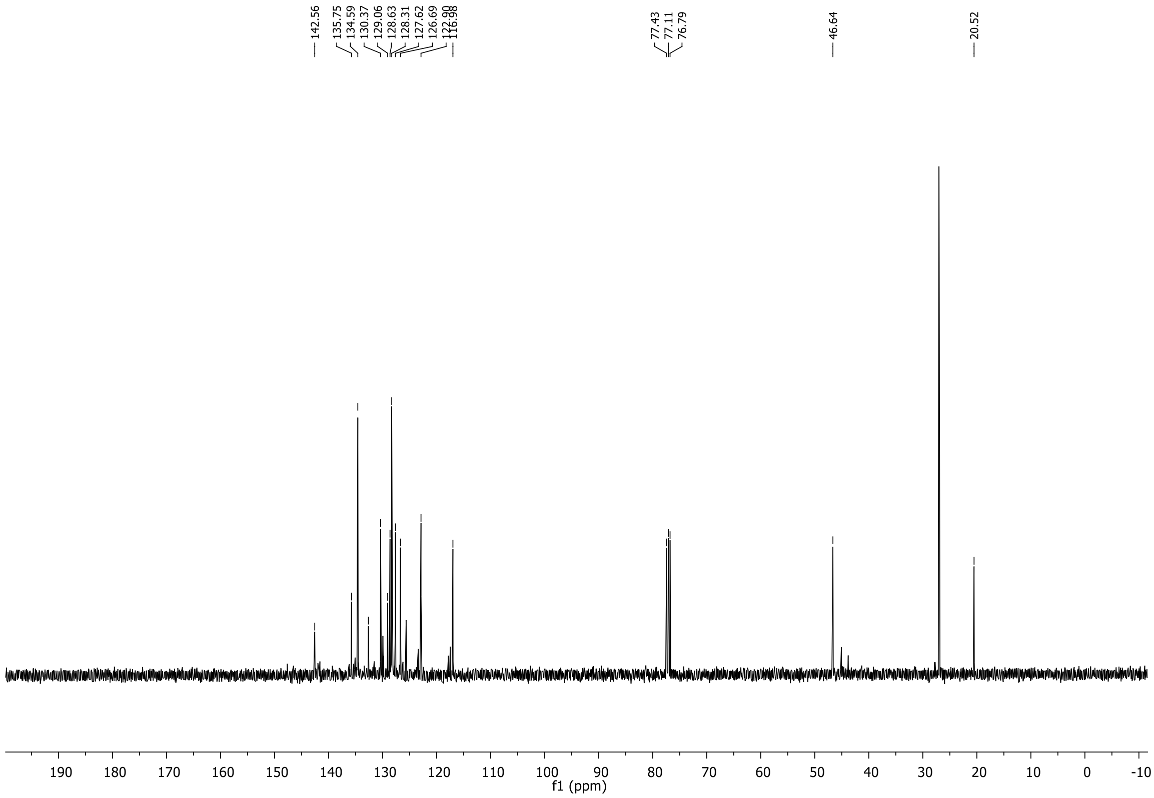
[1]H NMR reaction mixture spectrum of 6-methyl-1-(phenylsilyl)-1,2-dihydroquinoline **(2e):**



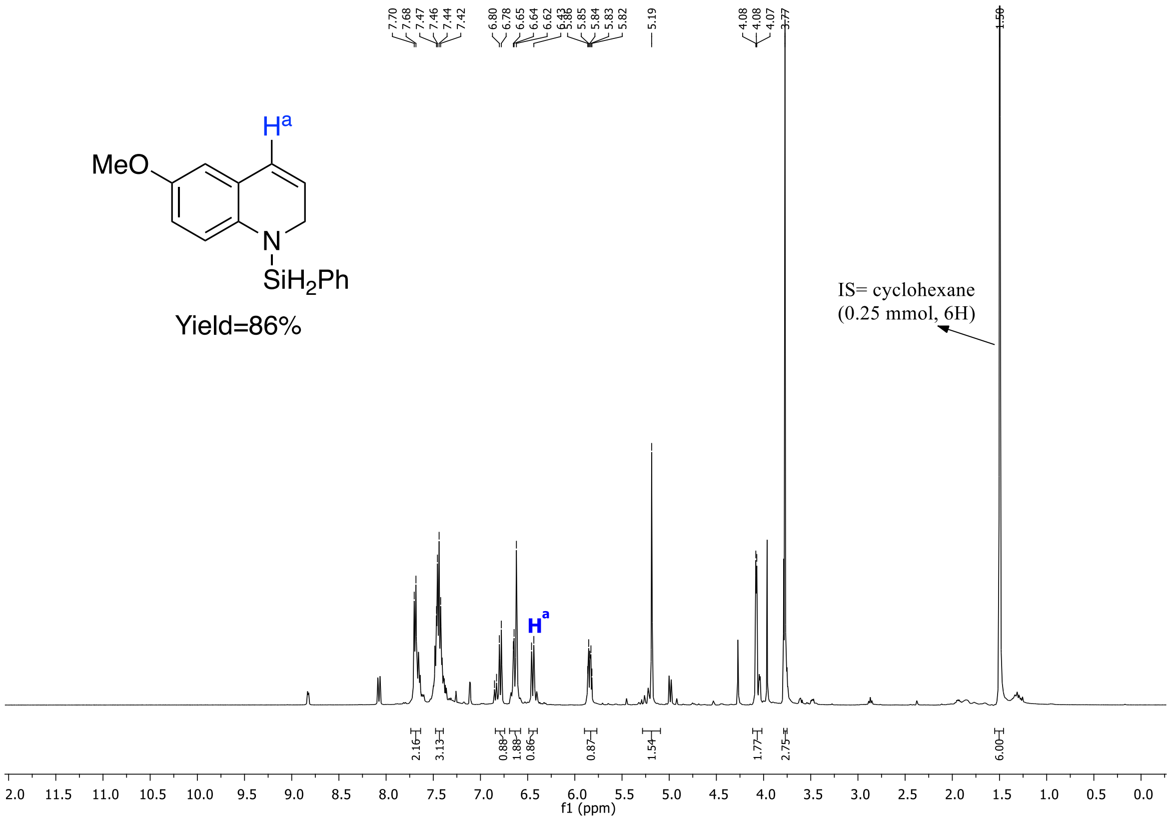
Yield > 99%



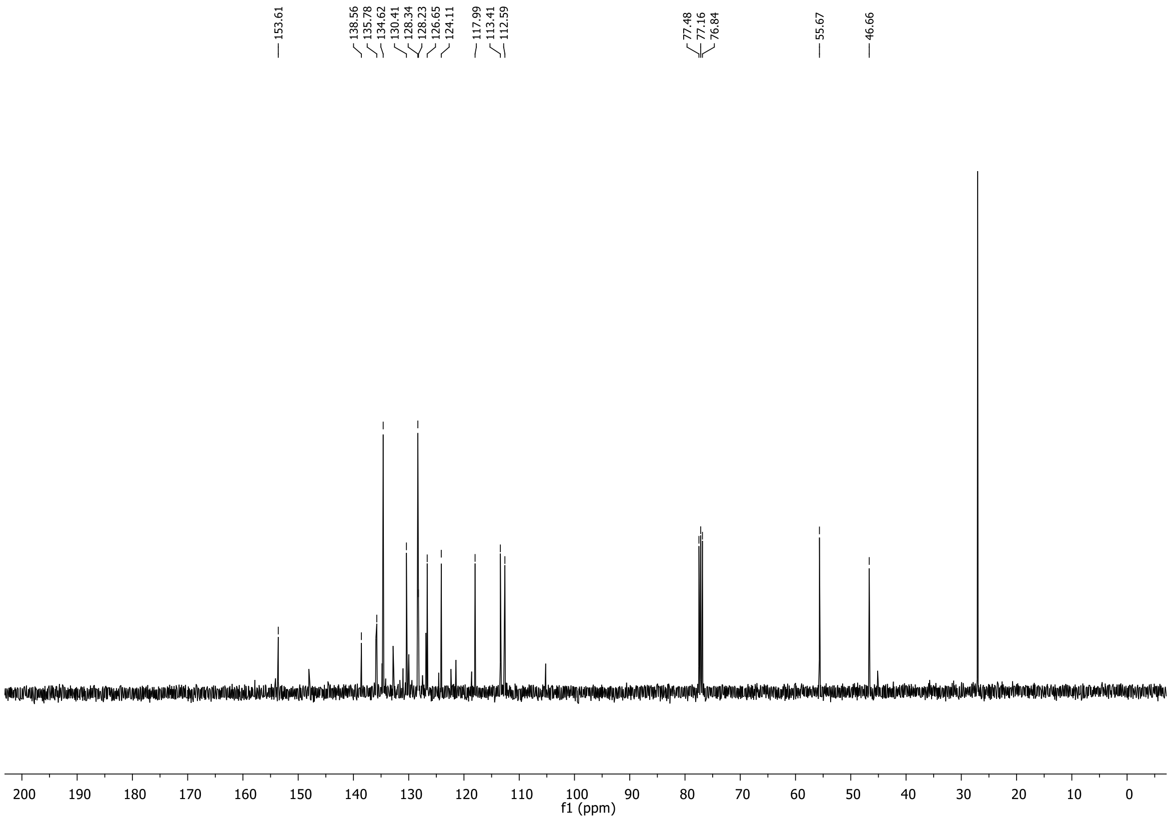
[13]C NMR reaction mixture spectrum of 6-methyl-1-(phenylsilyl)-1,2-dihydroquinoline **(2e):**



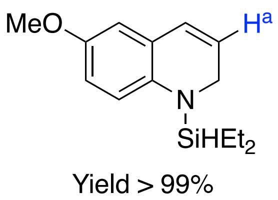
^{1}H NMR reaction mixture spectrum of 6-methoxy-1-(phenylsilyl)-1,2-dihydroquinoline **(2f):**

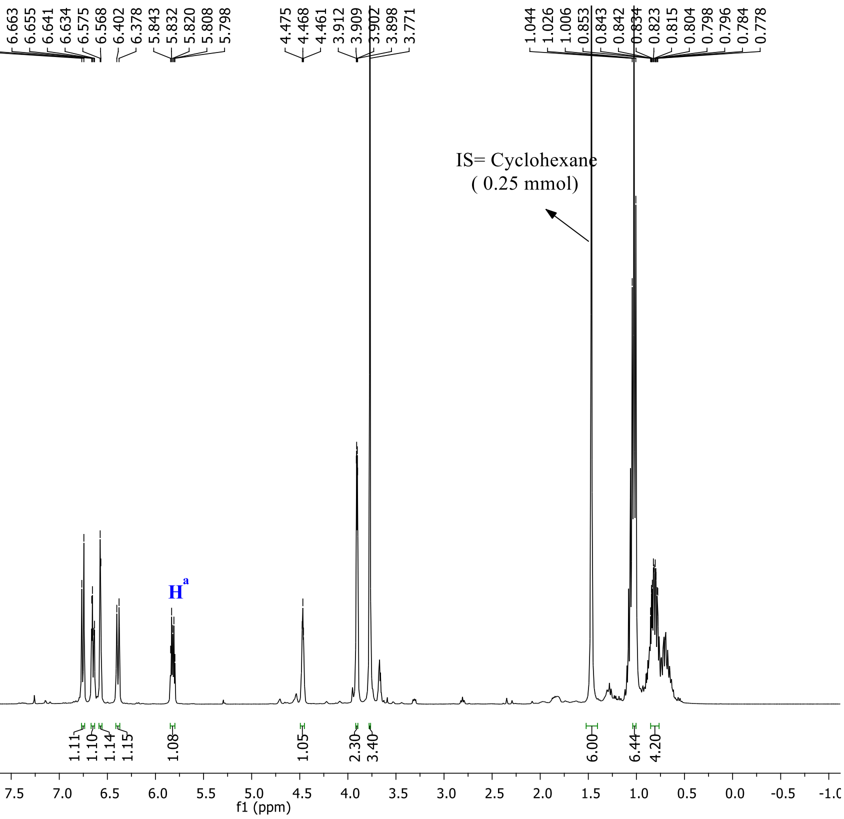


^{13}C NMR reaction mixture spectrum of 6-methoxy-1-(phenylsilyl)-1,2-dihydroquinoline **(2f):**

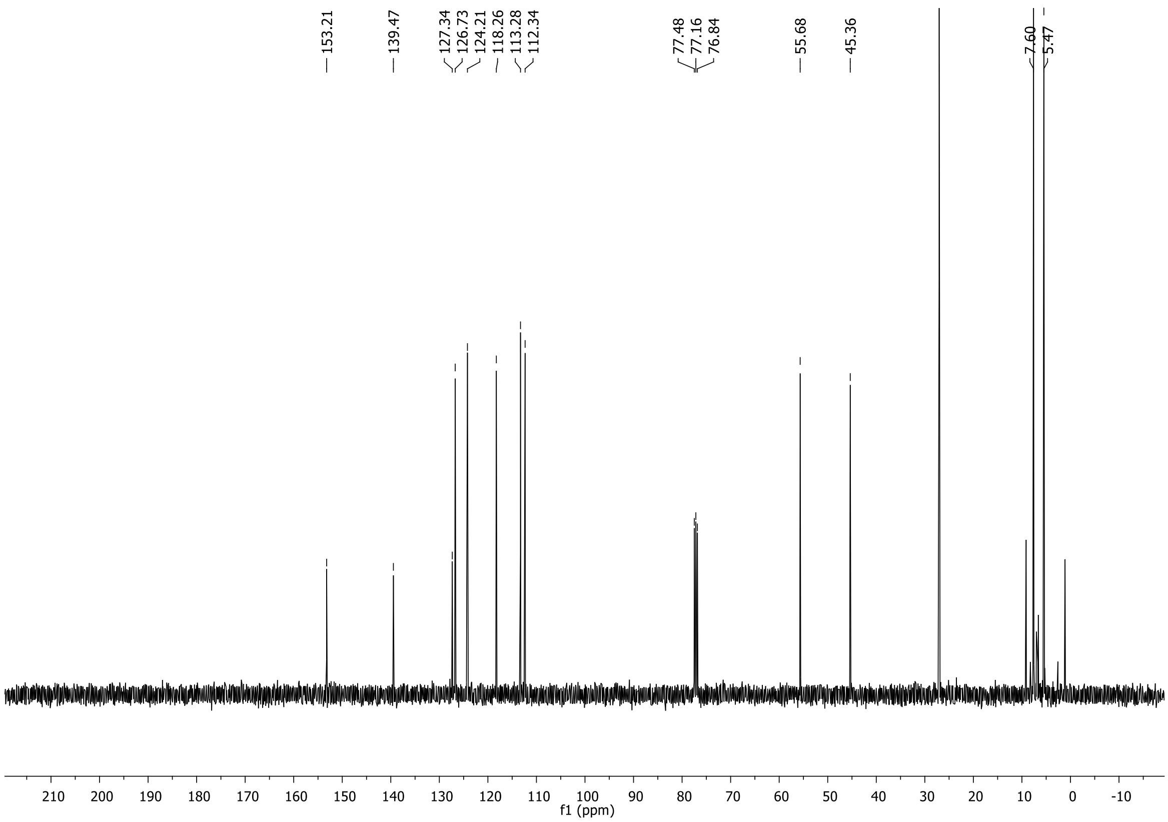


^{1}H NMR reaction mixture spectrum of 6-methoxy-1-(diethylsilyl)-1,2-dihydroquinoline **(2g):**

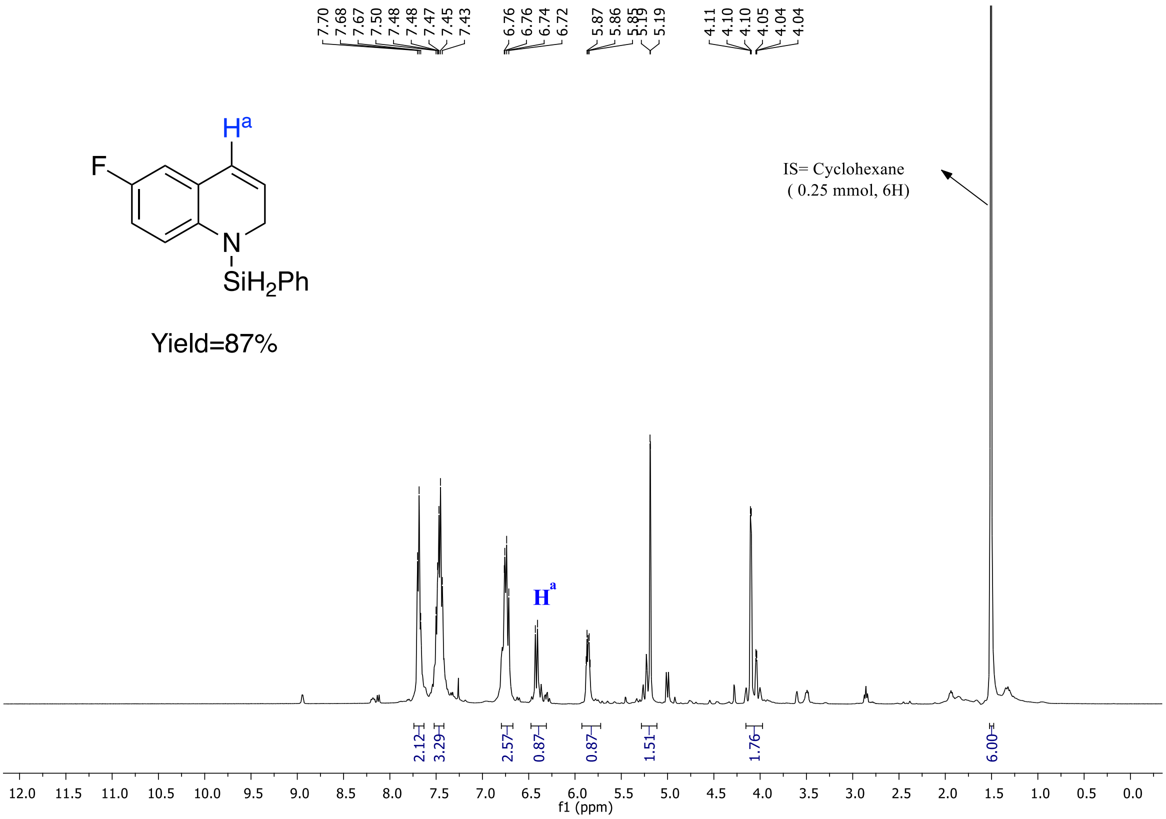




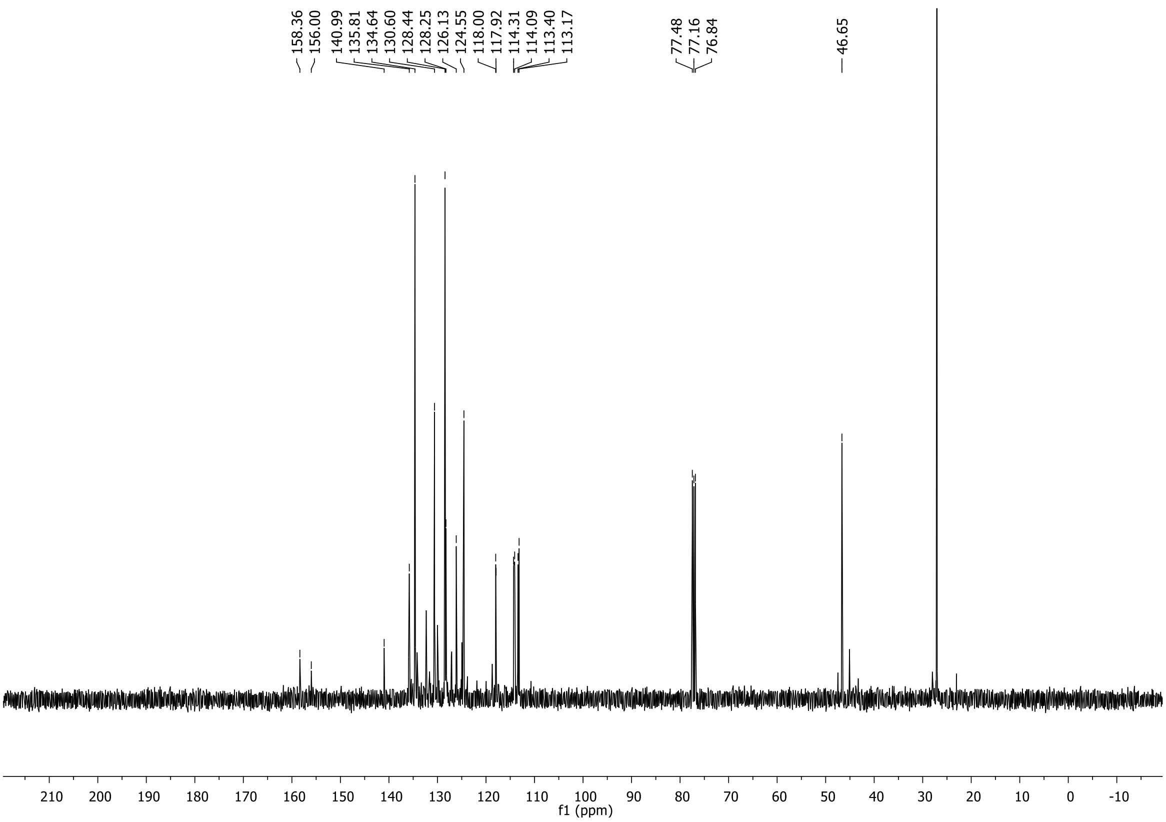
^{13}C NMR reaction mixture spectrum of 6-methoxy-1-(diethylsilyl)-1,2-dihydroquinoline **(2g):**



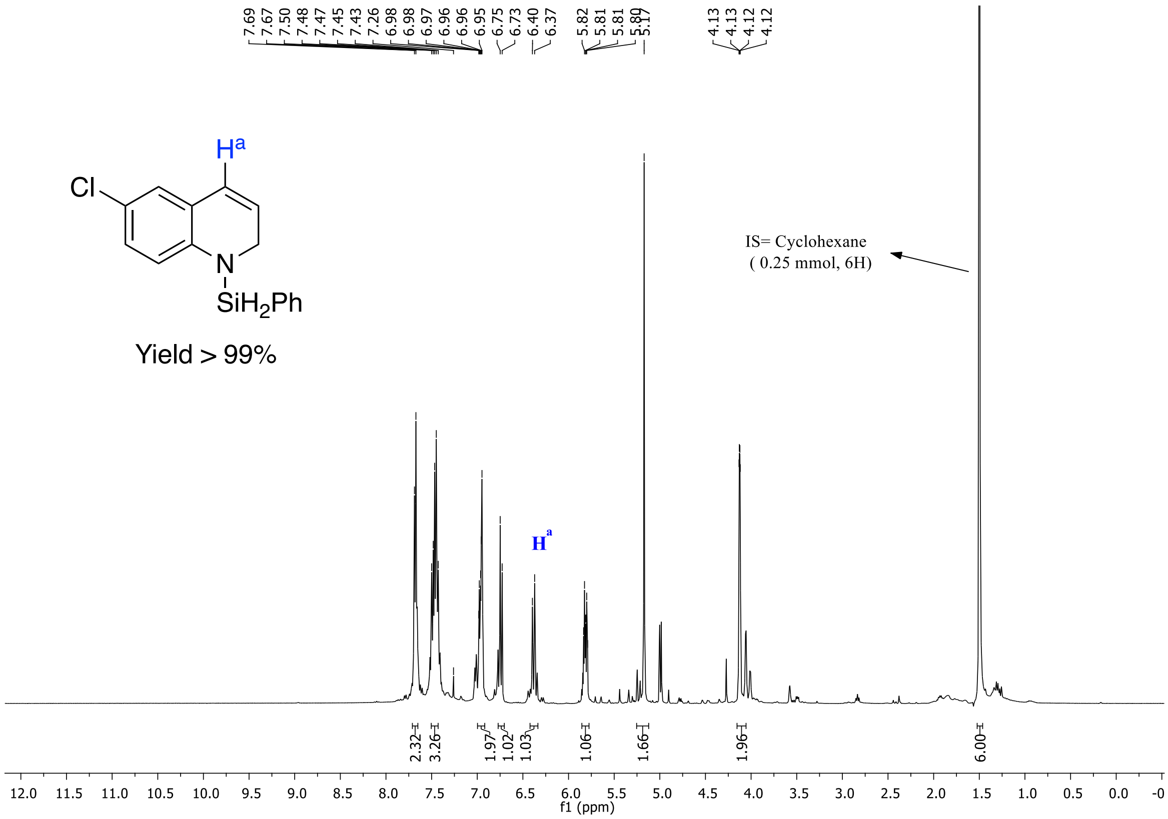
^{1}H NMR reaction mixture spectrum of 6-fluoro-1-(phenylsilyl)-1,2-dihydroquinoline **(2h):**



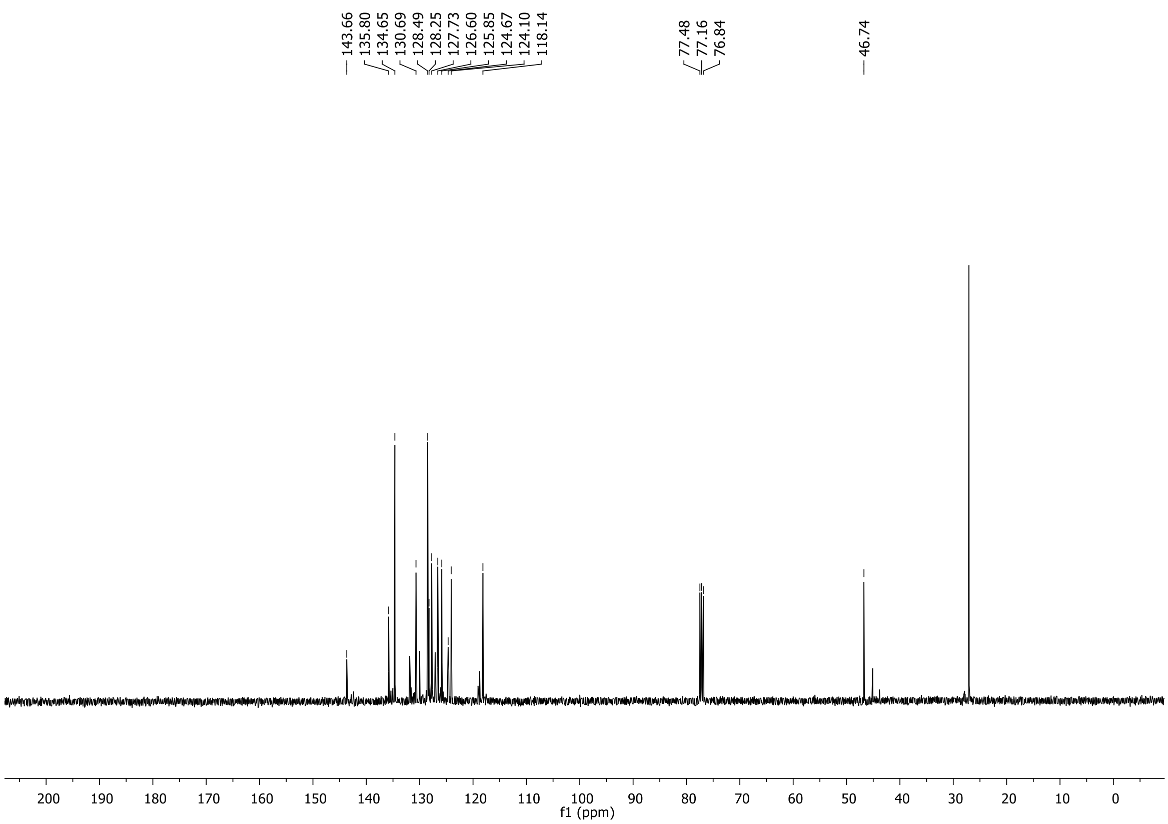
^{13}C NMR reaction mixture spectrum of 6-fluoro-1-(phenylsilyl)-1,2-dihydroquinoline **(2h):**



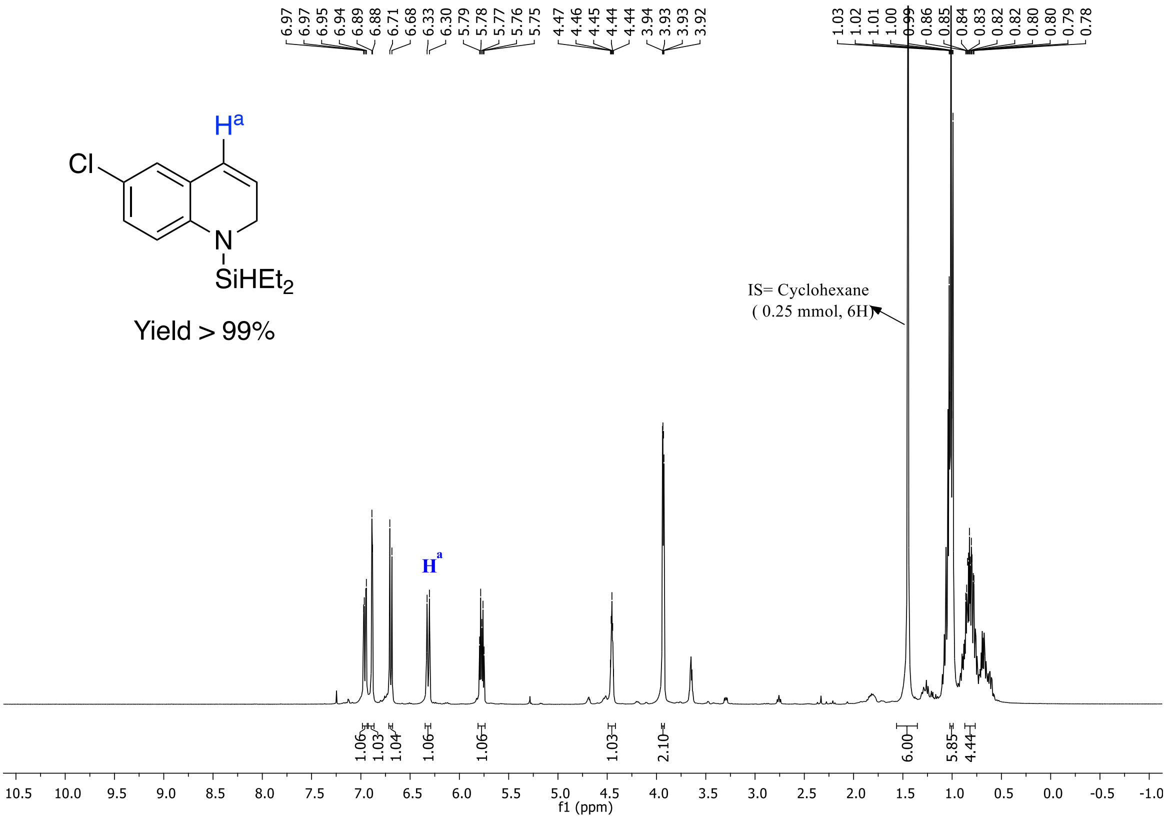
^{1}H NMR reaction mixture spectrum of 6-chloro-1-(phenylsilyl)-1,2-dihydroquinoline **(2i):**



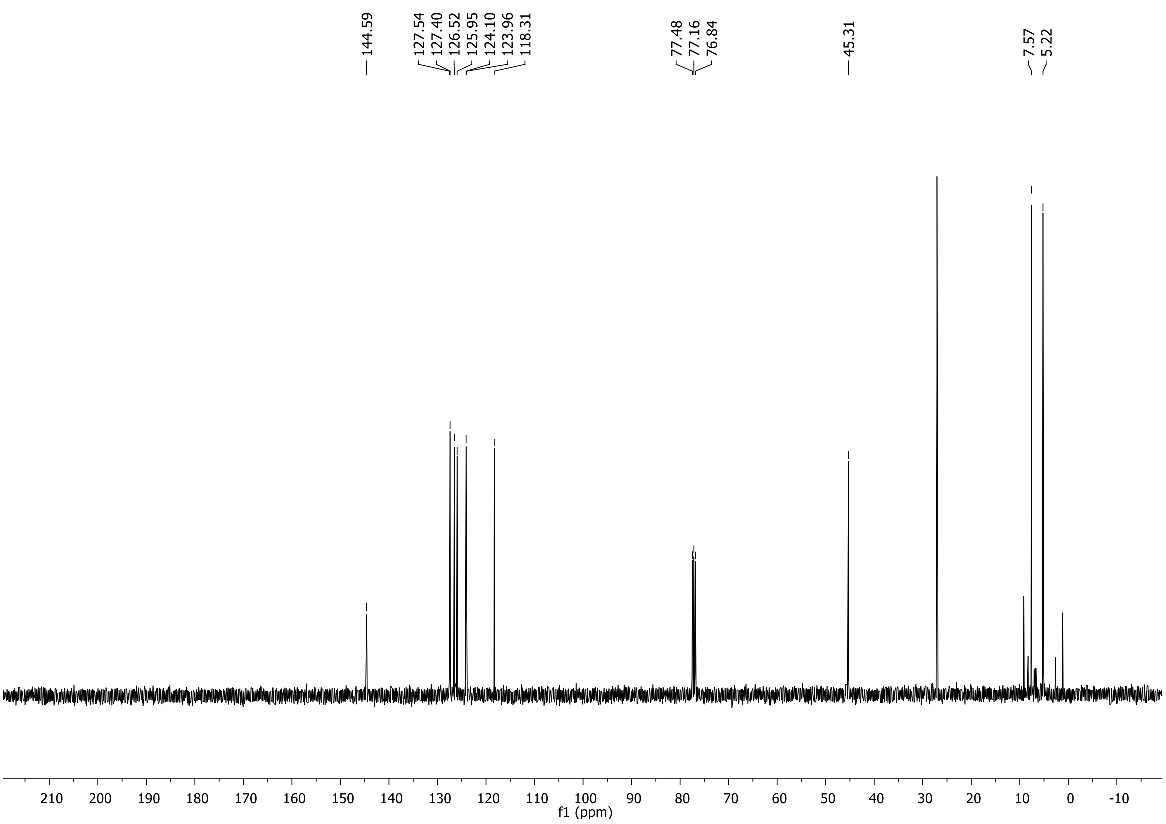
^{13}C NMR reaction mixture spectrum of 6-chloro-1-(phenylsilyl)-1,2-dihydroquinoline **(2i):**



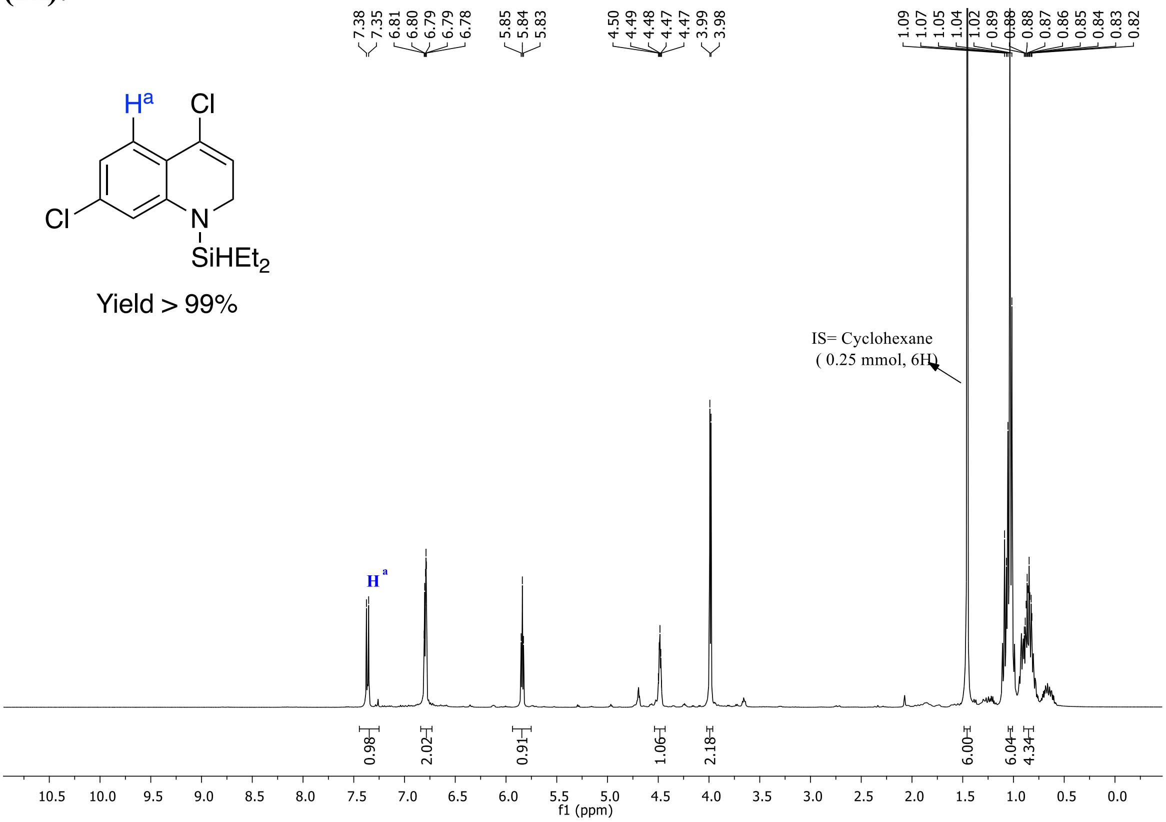
^{1}H NMR reaction mixture spectrum of 6-chloro-1-(diethylsilyl)-1,2-dihydroquinoline **(2j):**



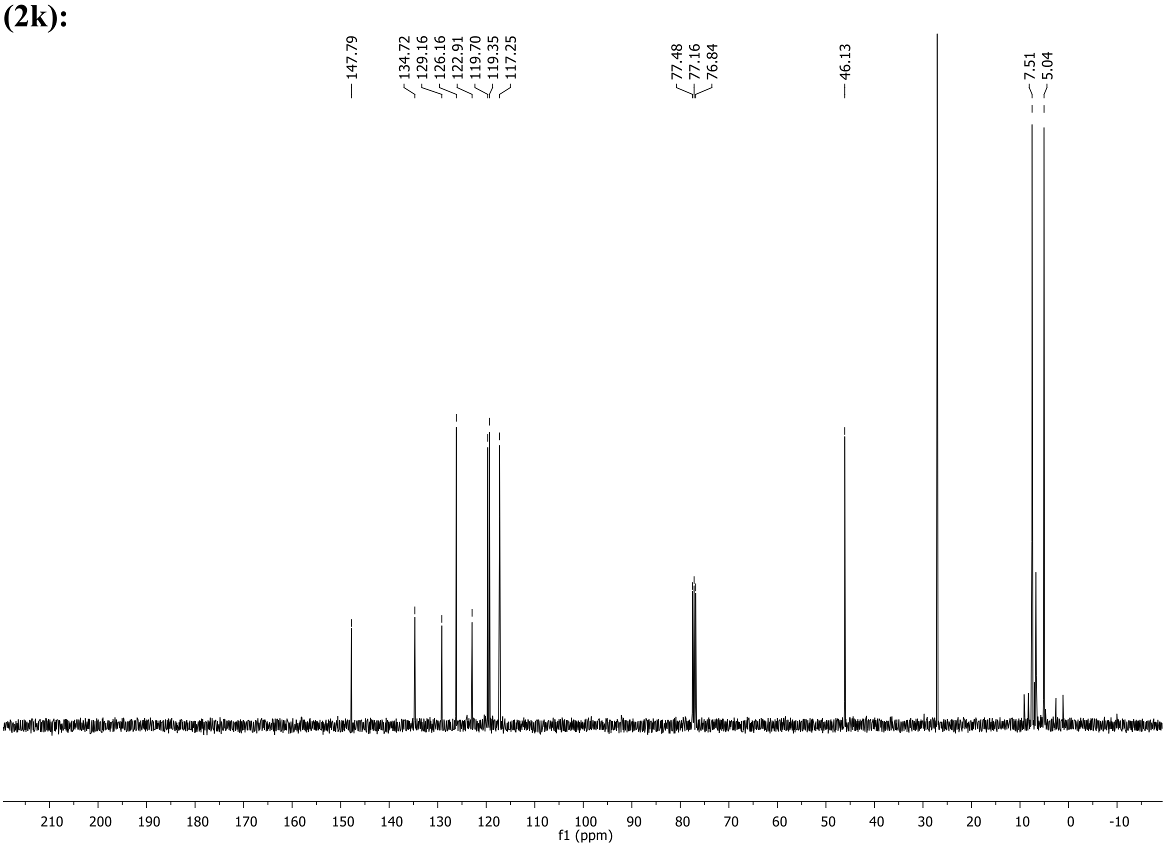
^{13}C NMR reaction mixture spectrum of 6-chloro-1-(diethylsilyl)-1,2-dihydroquinoline **(2j):**



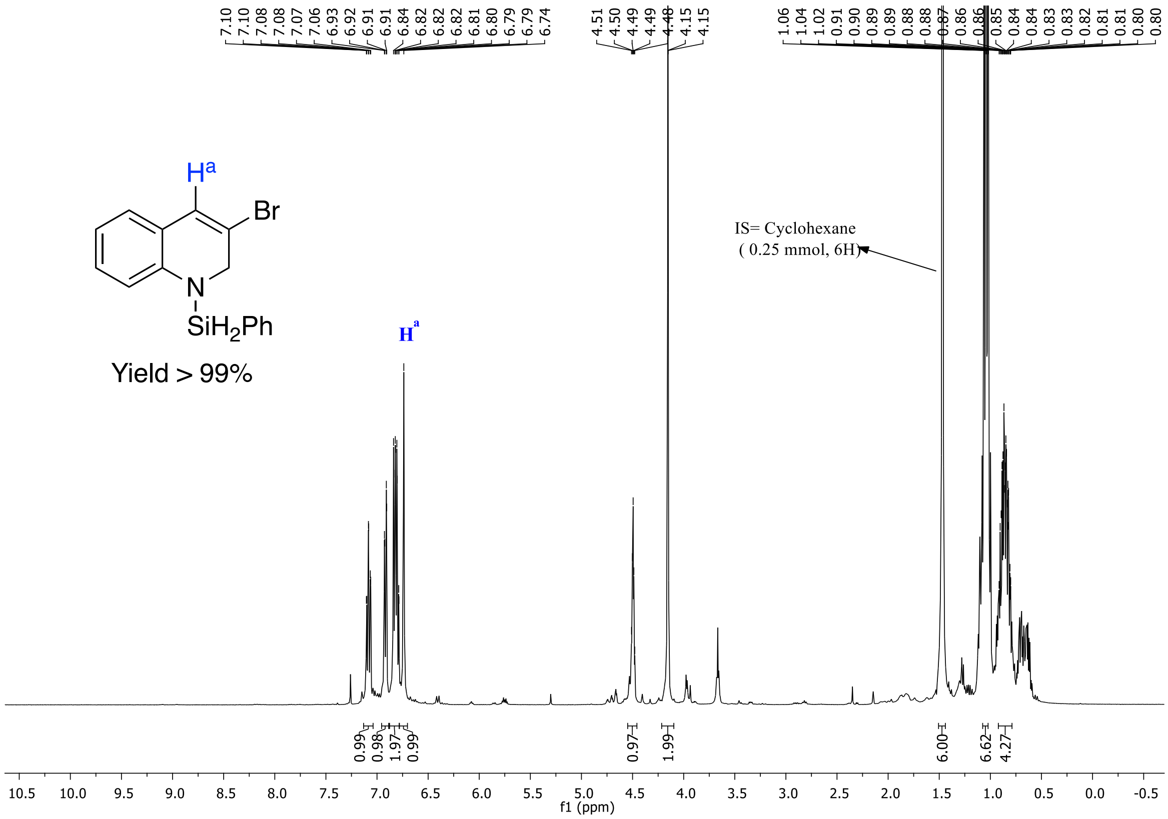
[1]H NMR reaction mixture spectrum of 4,7-dichloro-1-(diethylsilyl)-1,2-dihydroquinoline **(2k):**



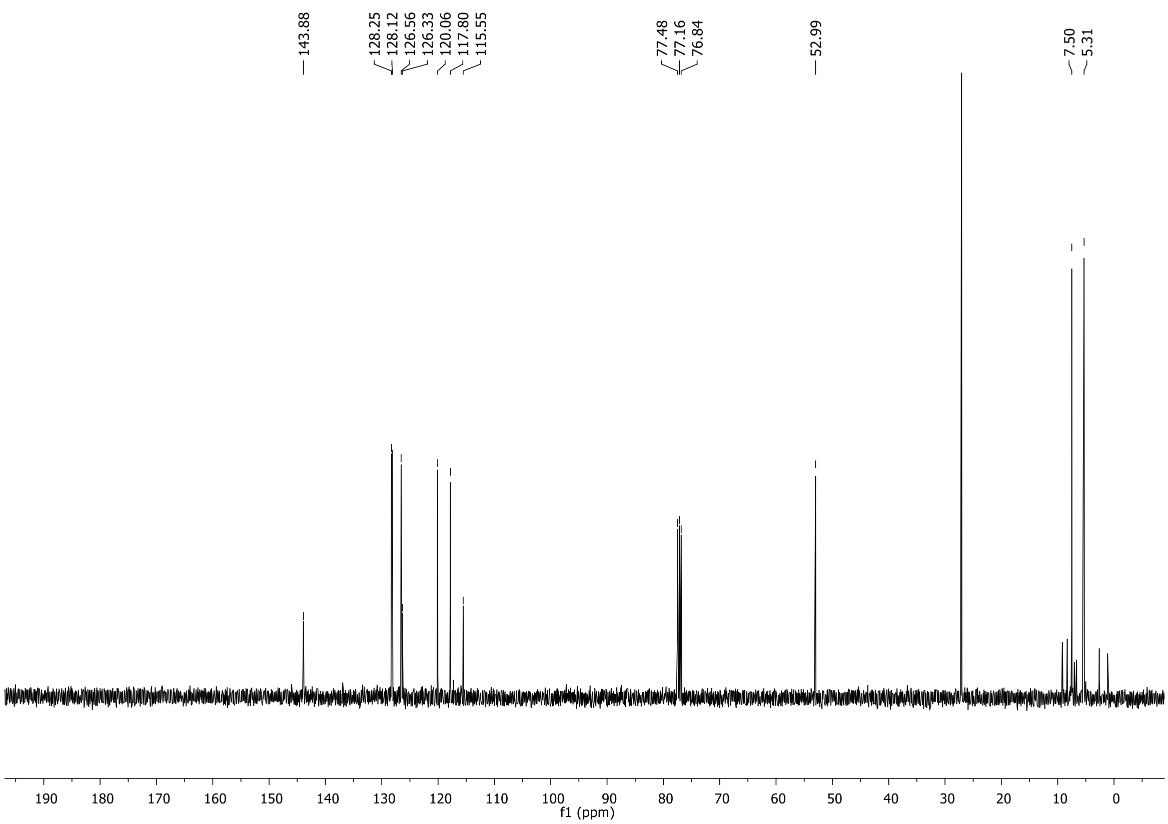
[13]C NMR reaction mixture spectrum of 4,7-dichloro-1-(diethylsilyl)-1,2-dihydroquinoline **(2k):**



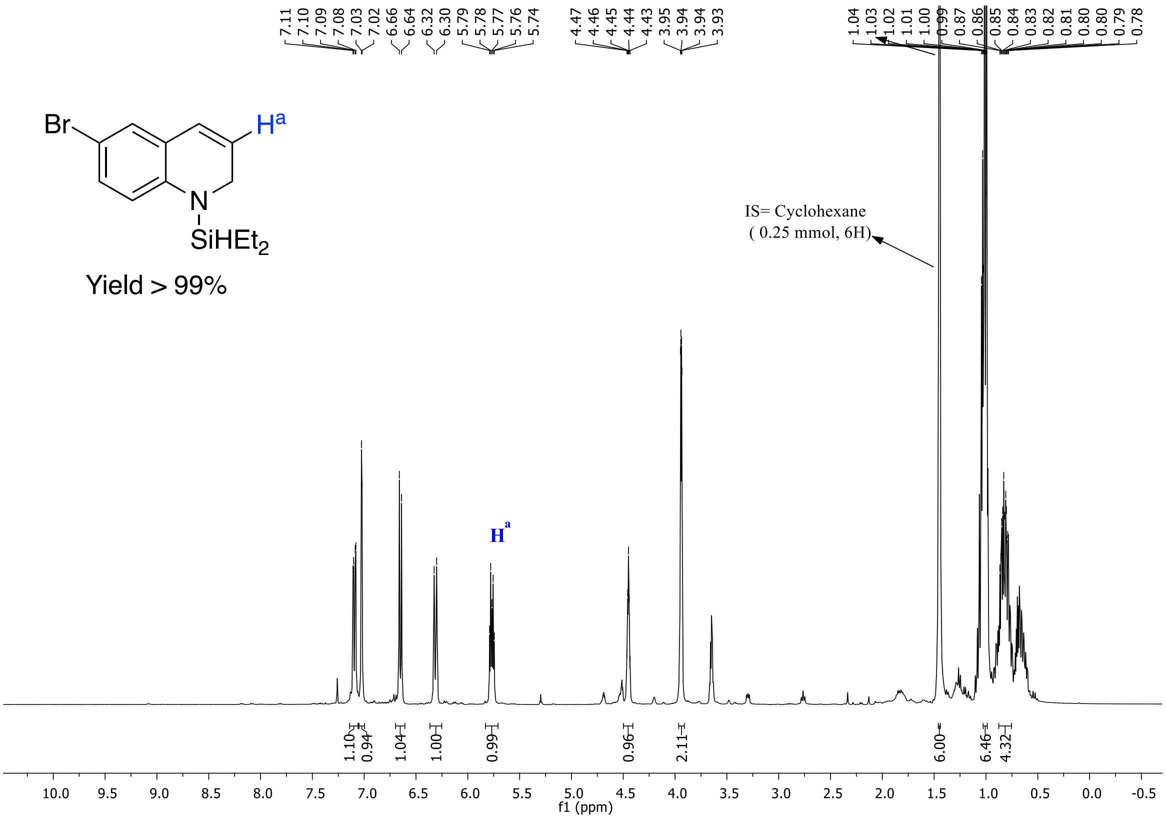
[1]H NMR reaction mixture spectrum of 3-bromo-1-(diethylsilyl)-1,2-dihydroquinoline **(2l):**



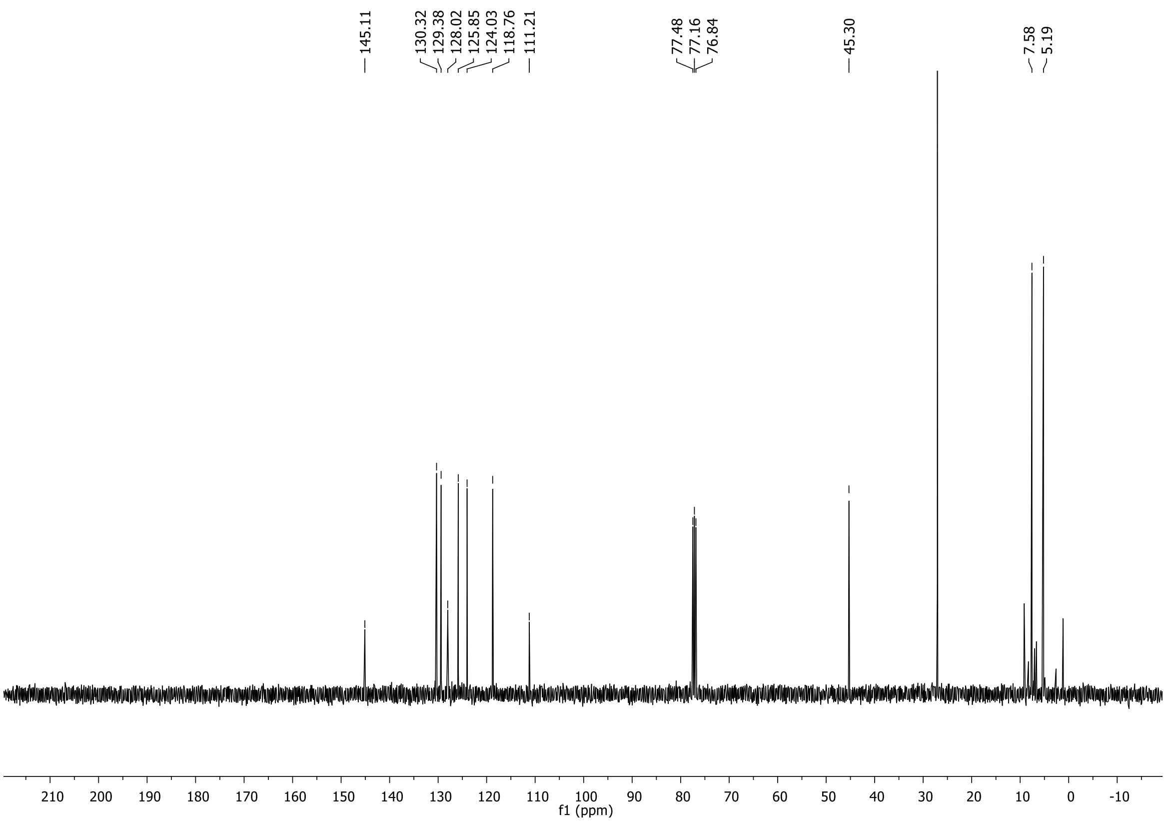
[13]C NMR reaction mixture spectrum of 3-bromo-1-(diethylsilyl)-1,2-dihydroquinoline **(2l):**



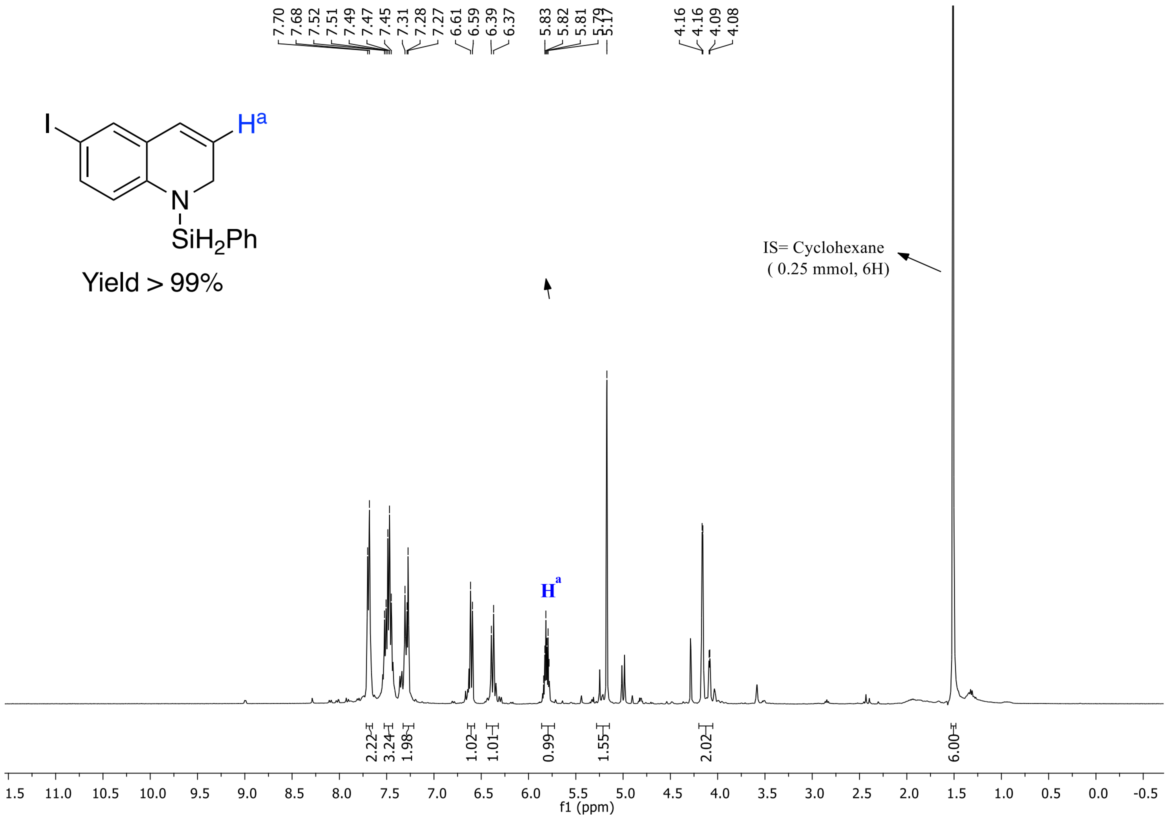
[1]H NMR reaction mixture spectrum of 6-bromo-1-(diethylsilyl)-1,2-dihydroquinoline **(2m):**



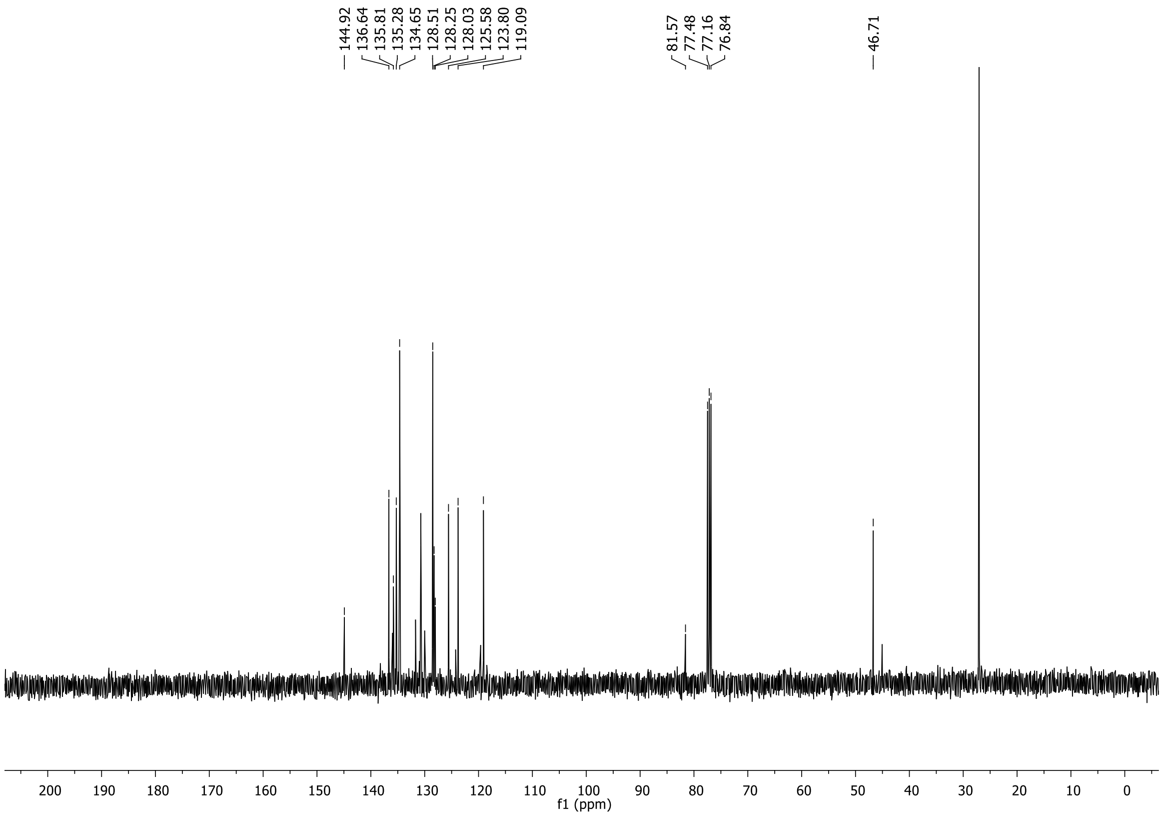
[13]C NMR reaction mixture spectrum of 6-bromo-1-(diethylsilyl)-1,2-dihydroquinoline **(2m):**



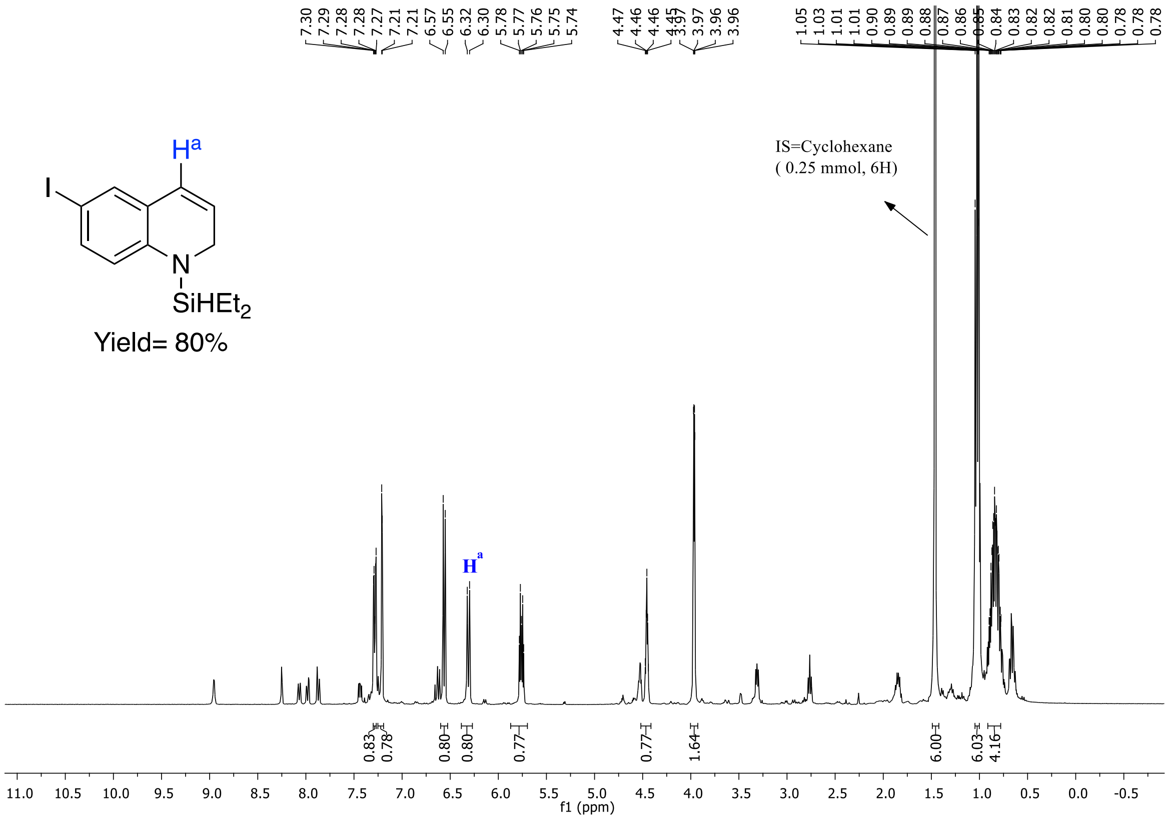
[1]H NMR reaction mixture spectrum of 6-iodo-1-(phenylsilyl)-1,2-dihydroquinoline **(2n):**



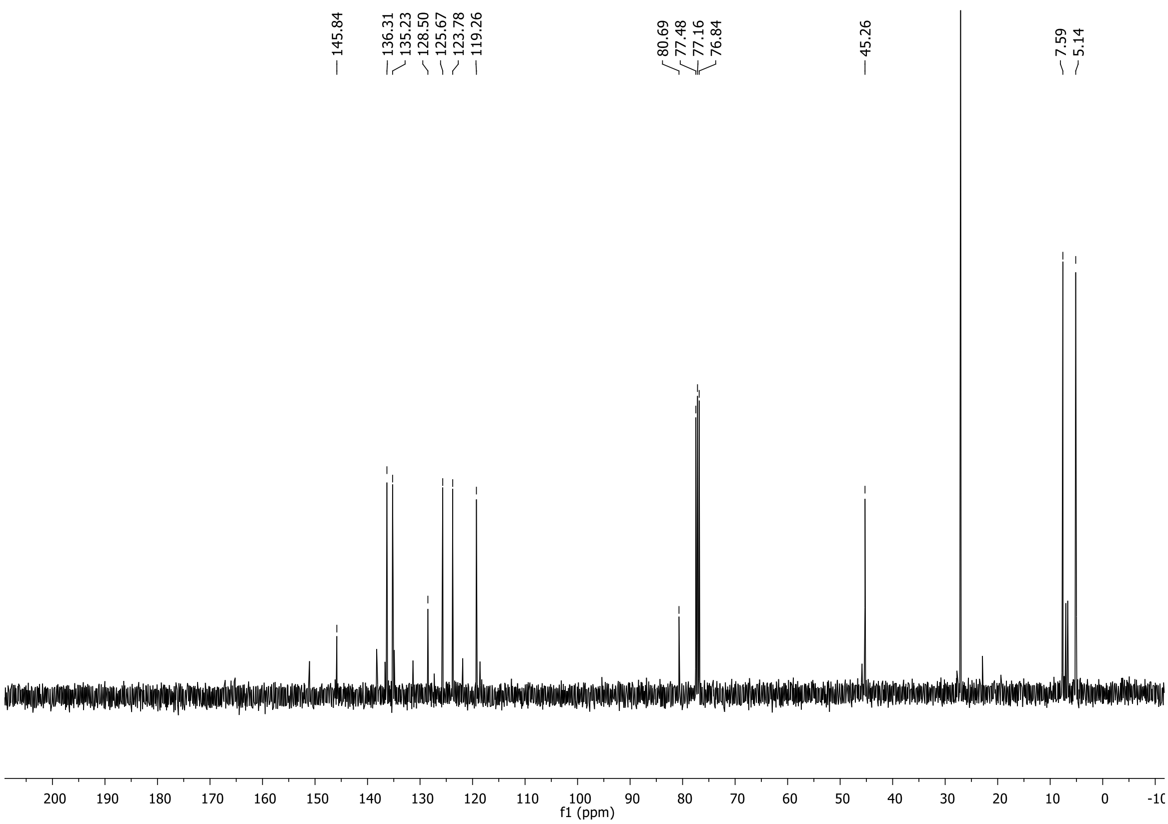
[13]C NMR reaction mixture spectrum of 6-iodo-1-(phenylsilyl)-1,2-dihydroquinoline **(2n):**



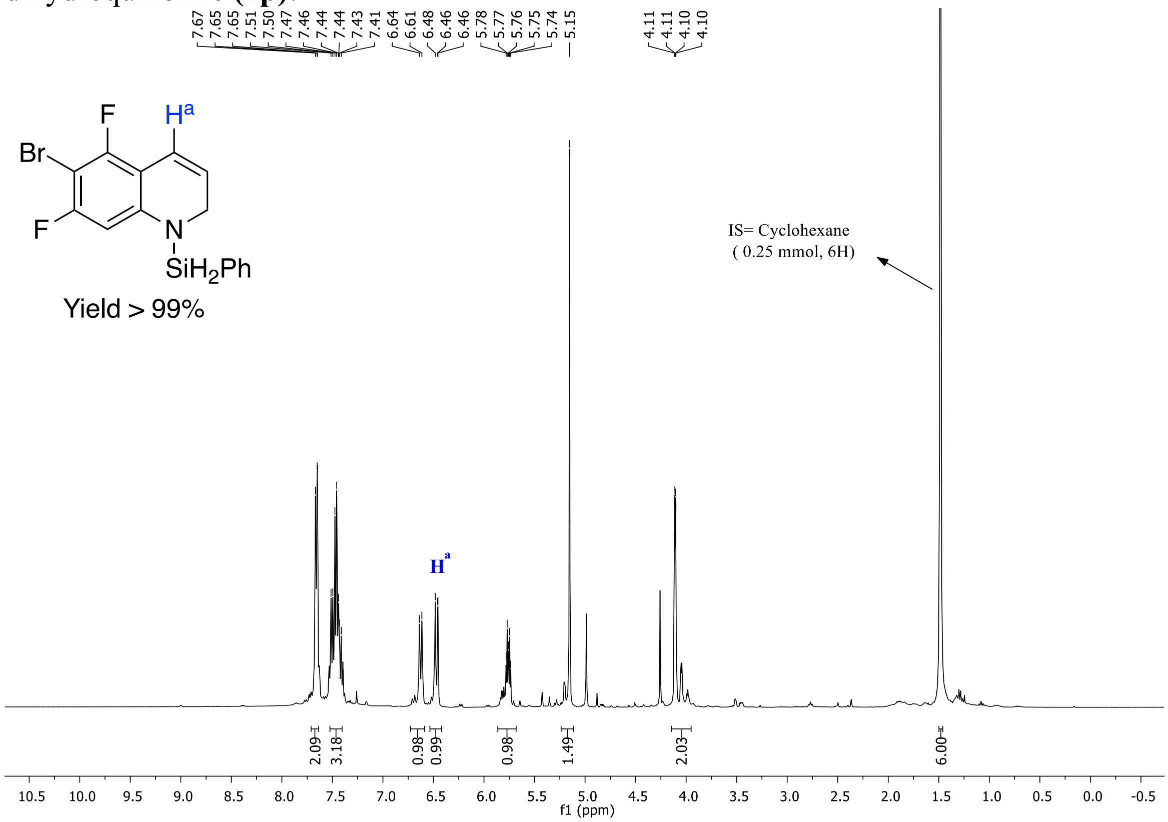
[1]H NMR reaction mixture spectrum of 1-(diethylsilyl)-6-iodo-1,2-dihydroquinoline **(2o):**



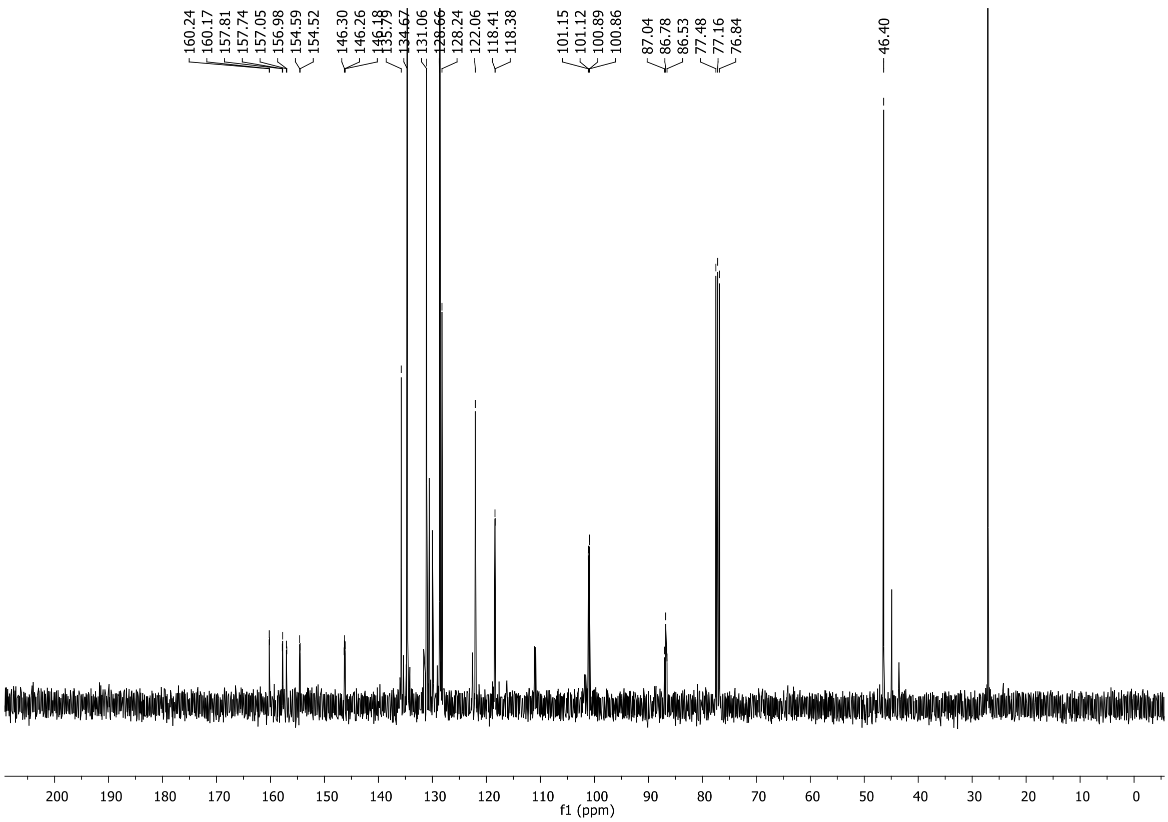
[13]C NMR reaction mixture spectrum of 1-(diethylsilyl)-6-iodo-1,2-dihydroquinoline **(2o):**



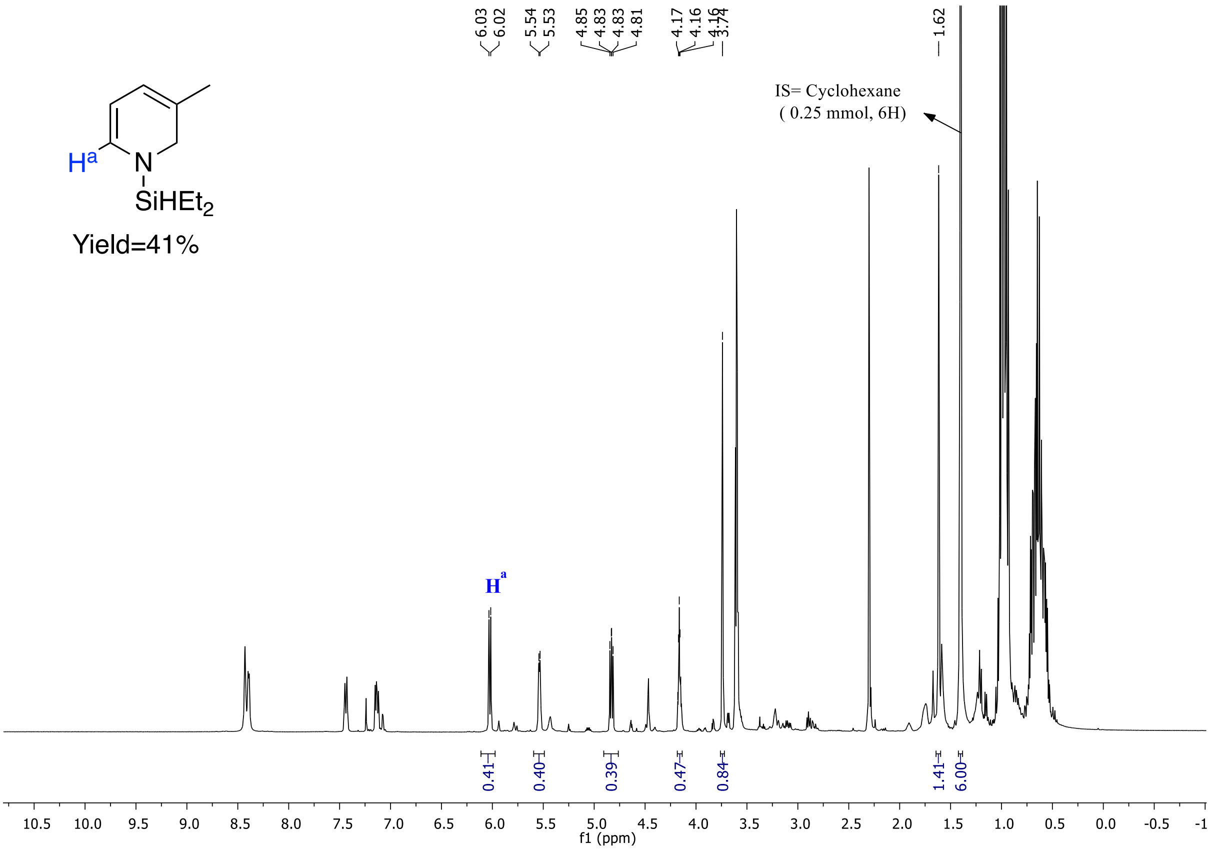
^{1}H NMR reaction mixture spectrum of 6-bromo-5,7-difluoro-1-(phenylsilyl)-1,2-dihydroquinoline **(2p):**



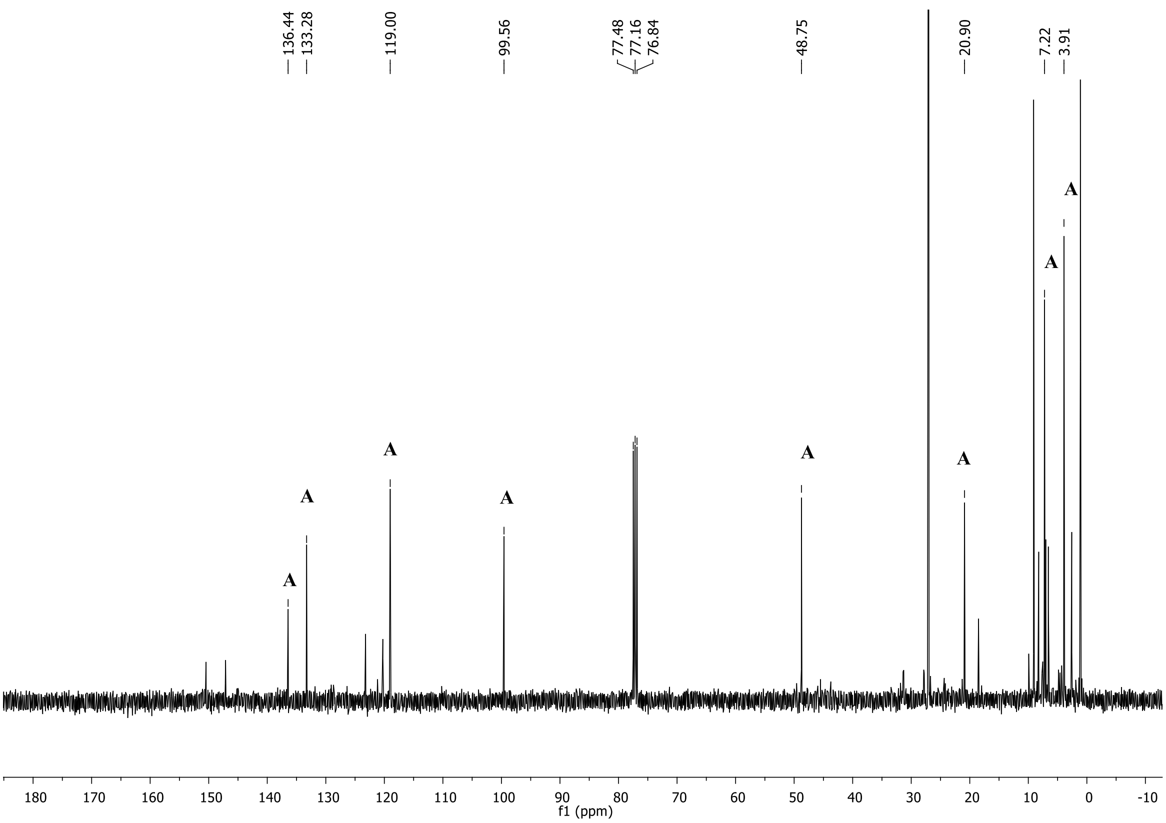
^{13}C NMR reaction mixture spectrum of 6-bromo-5,7-difluoro-1-(phenylsilyl)-1,2-dihydroquinoline **(2p):**



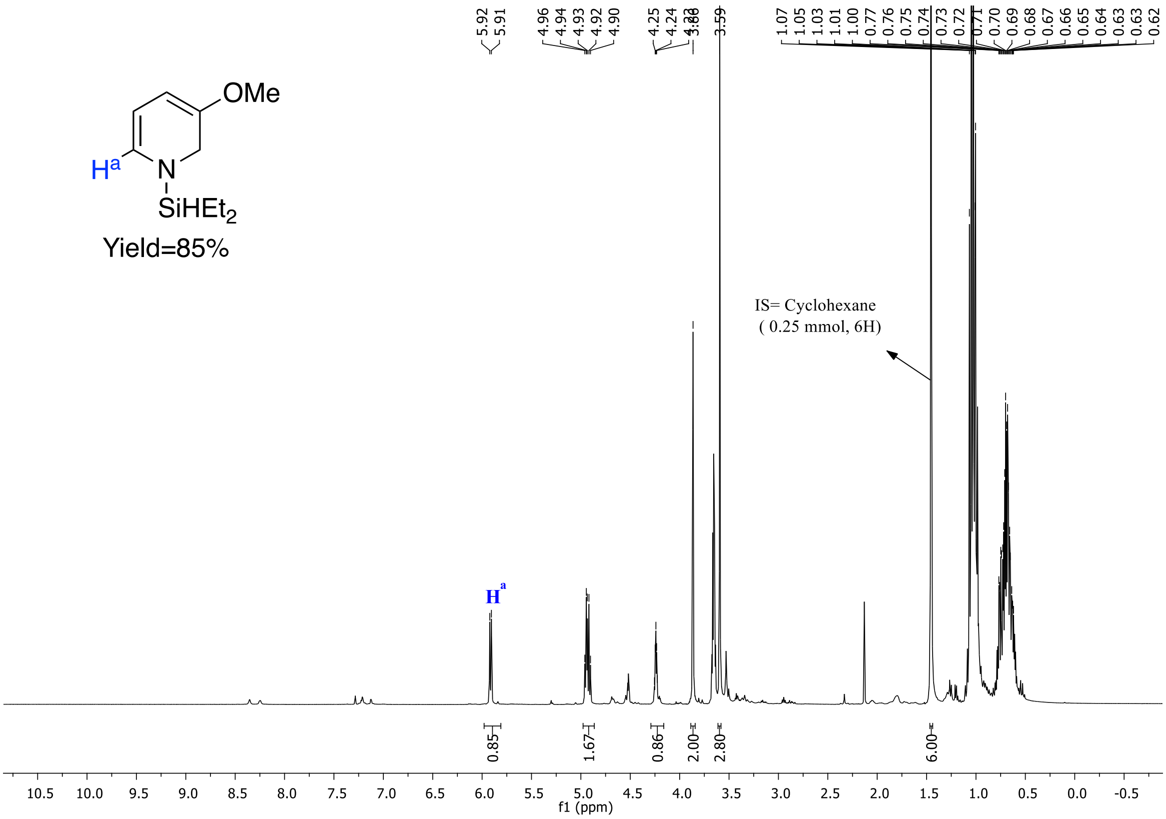
[1]H NMR reaction mixture spectrum of 1-(diethylsilyl)-3-methyl-1,2-dihydropyridine **(3a):**



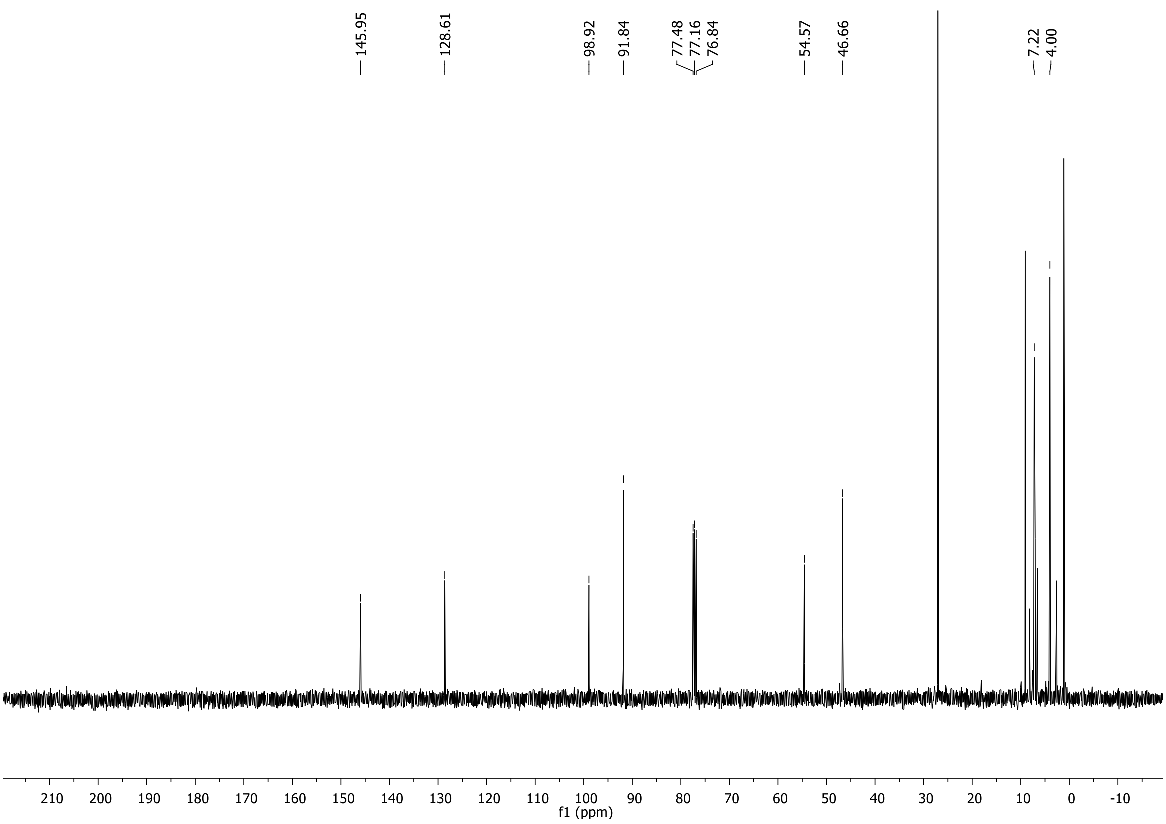
[13]C NMR reaction mixture spectrum of 1-(diethylsilyl)-3-methyl-1,2-dihydropyridine **(3a):**



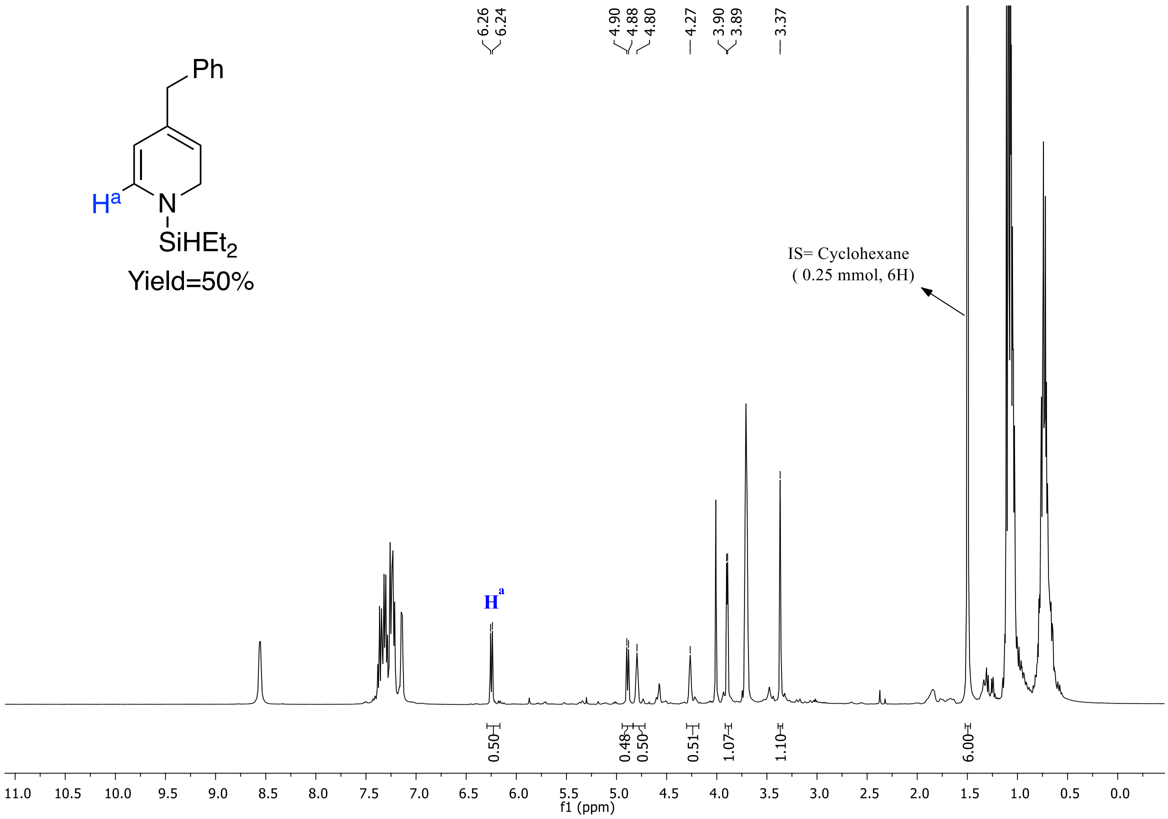
[1]H NMR reaction mixture spectrum of 1-(diethylsilyl)-3-methoxy-1,2-dihydropyridine **(3b):**



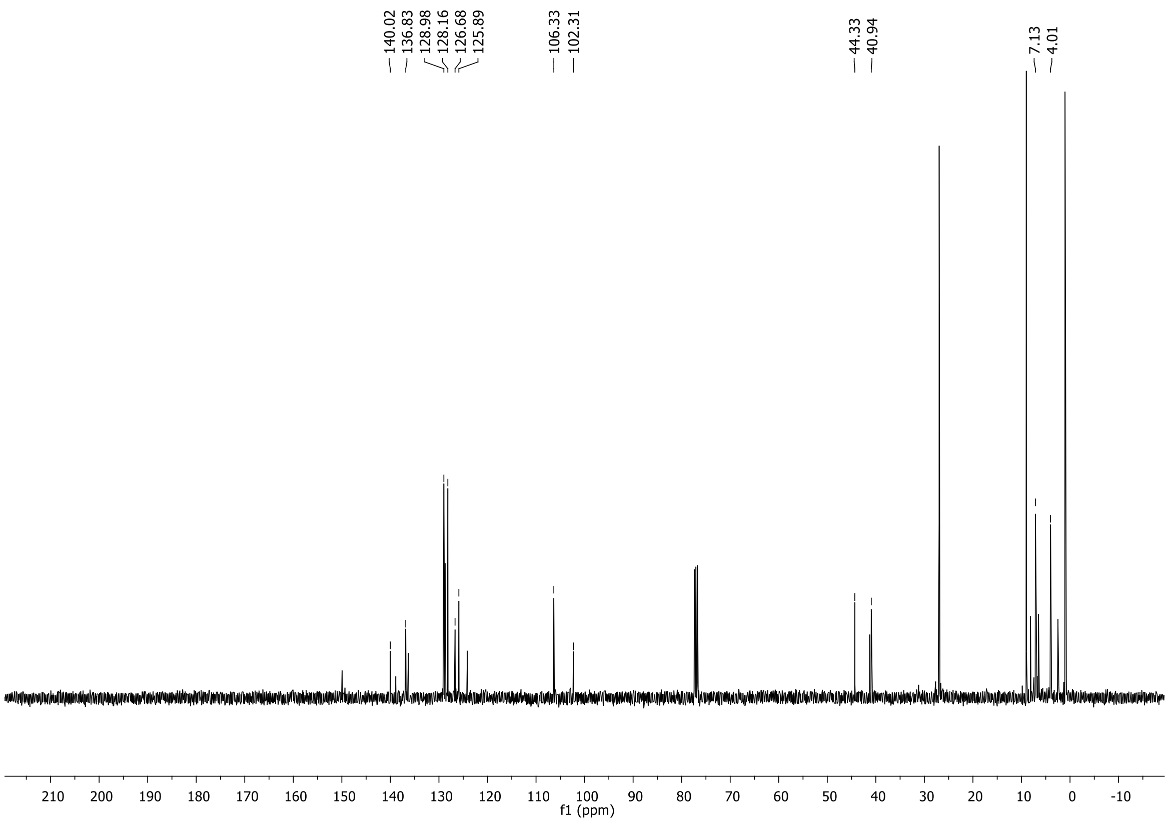
[13]C NMR reaction mixture spectrum of 1-(diethylsilyl)-3-methoxy-1,2-dihydropyridine **(3b):**



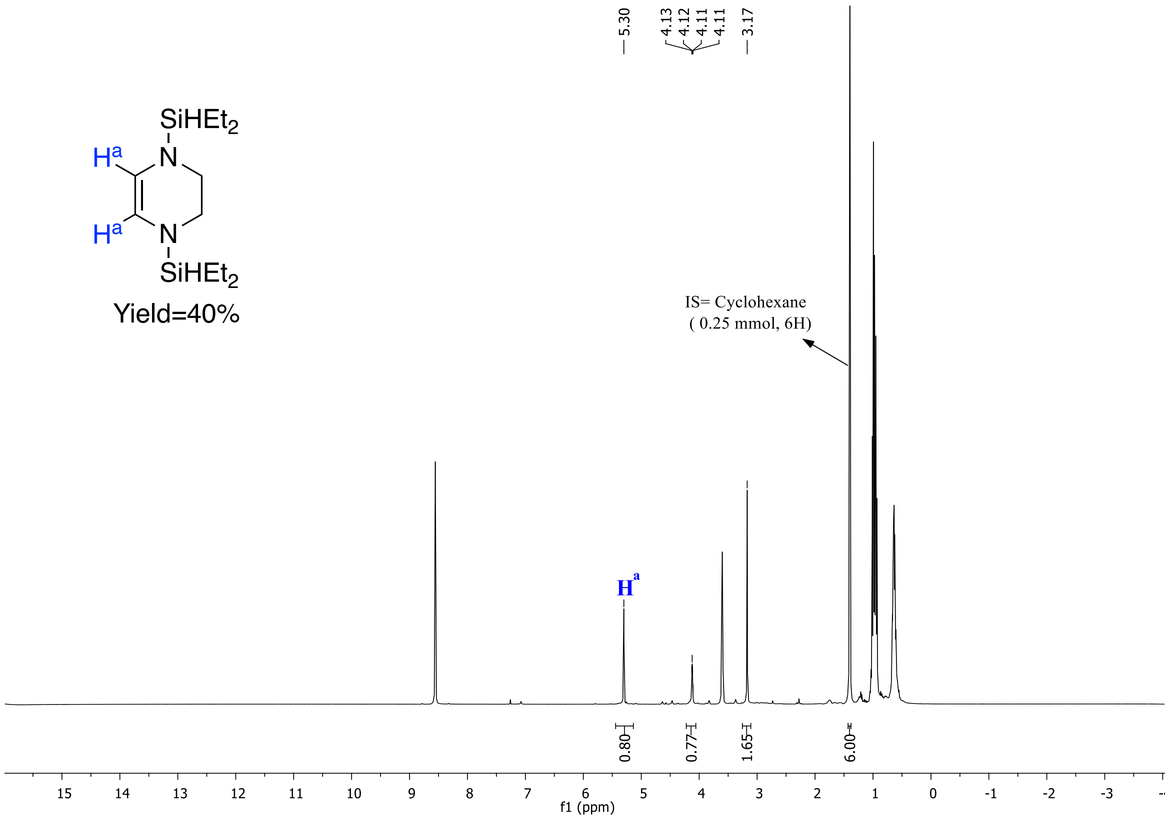
[1]H NMR reaction mixture spectrum of 4-benzyl-1-(diethylsilyl)-1,2-dihydropyridine **(3c):**



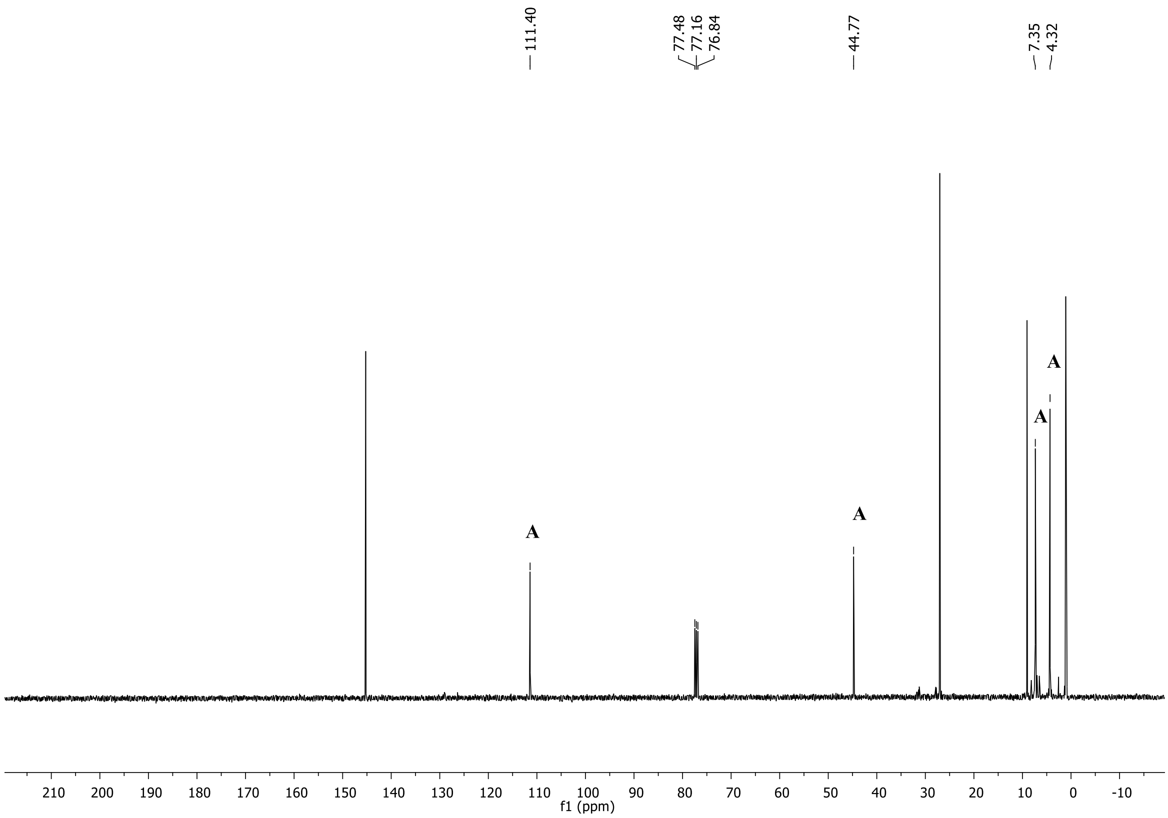
[13]C NMR reaction mixture spectrum of 4-benzyl-1-(diethylsilyl)-1,2-dihydropyridine **(3c):**



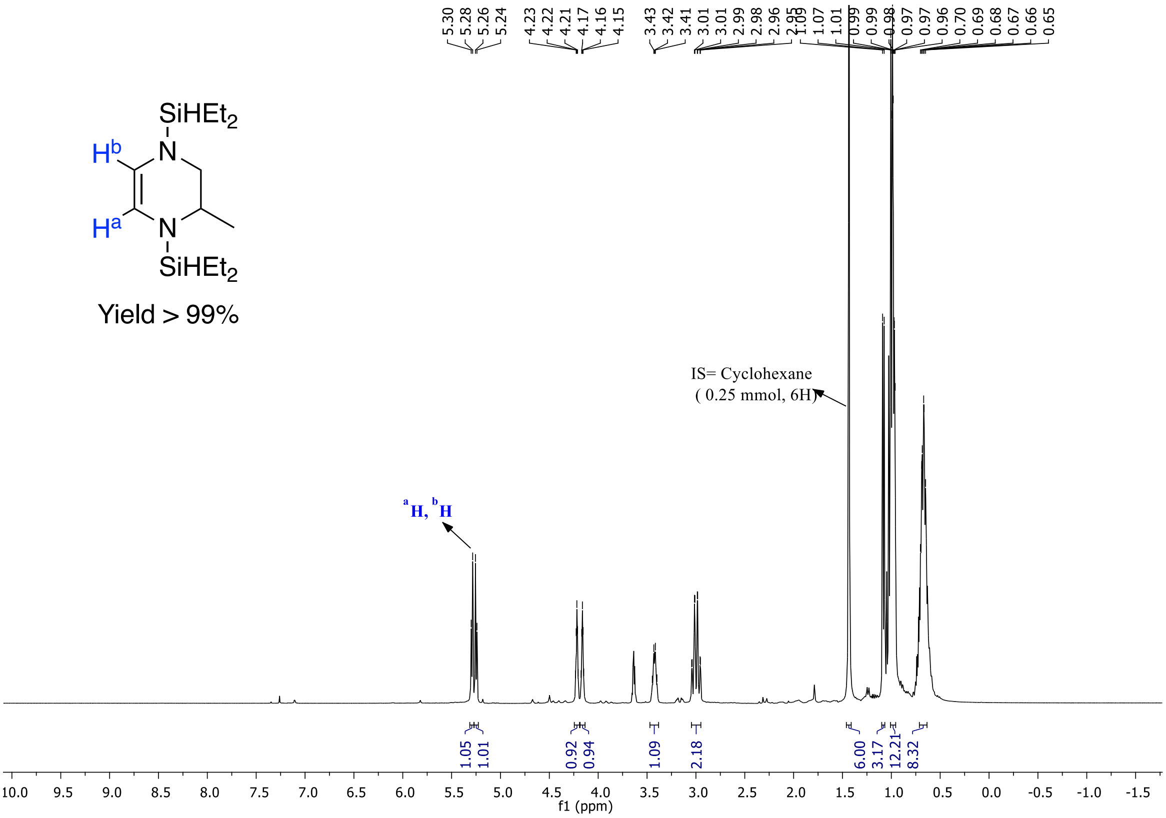
[1]H NMR reaction mixture spectrum of 1,4-bis(diethylsilyl)-1,2,3,4-tetrahydropyrazine **(3d):**



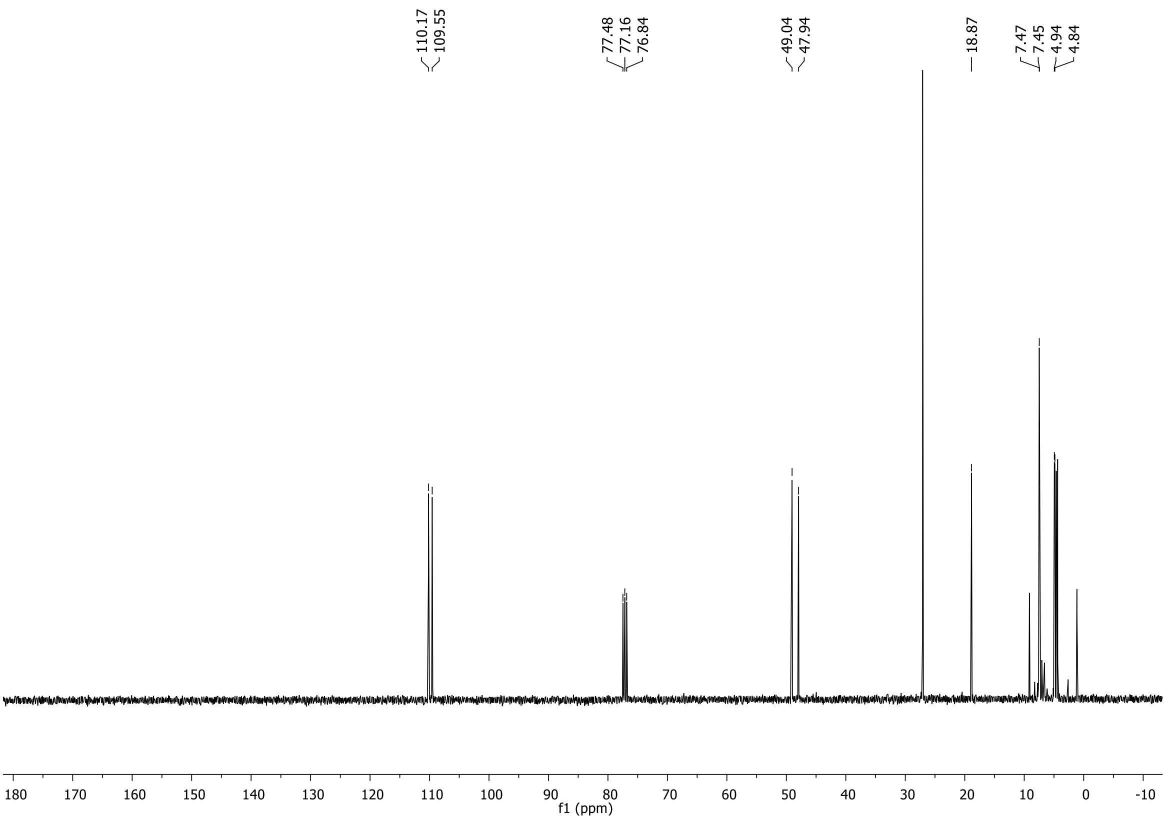
[13]C NMR reaction mixture spectrum of 1,4-bis(diethylsilyl)-1,2,3,4-tetrahydropyrazine **(3d):**



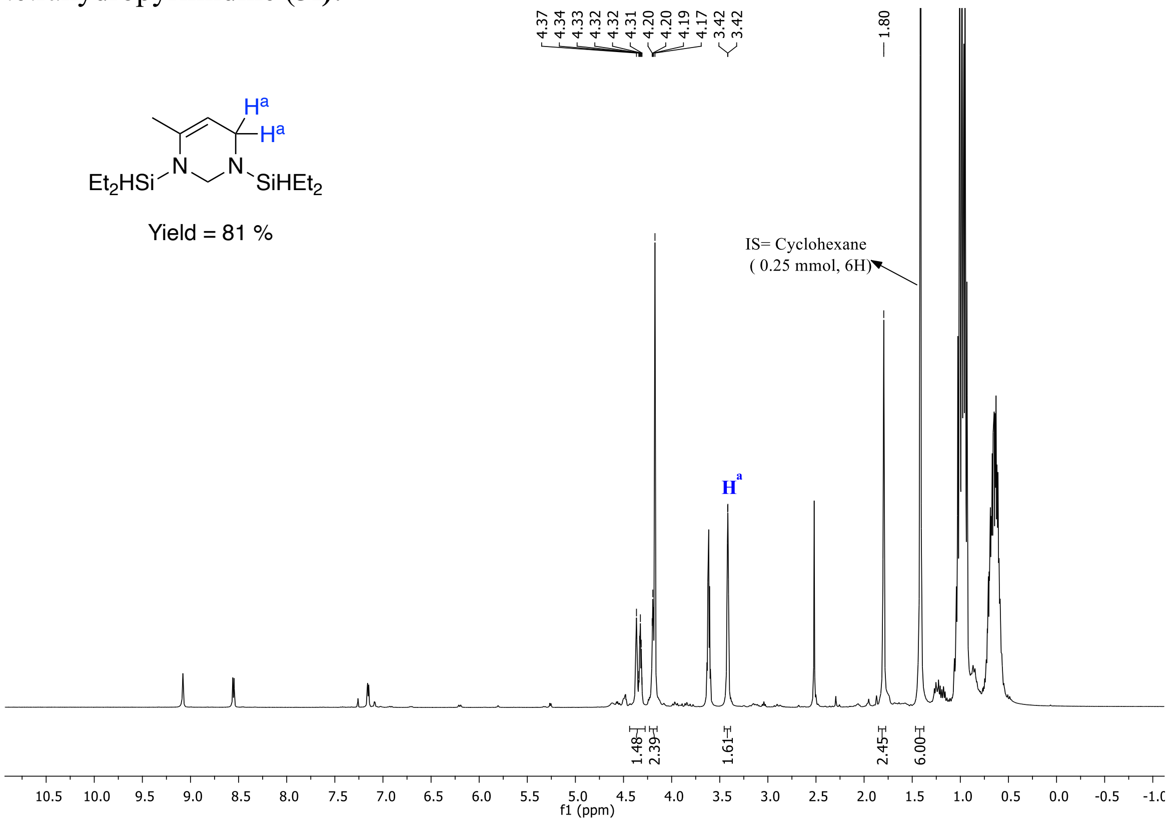
^{1}H NMR reaction mixture spectrum of 1,4-bis(diethylsilyl)-2-methyl-1,2,3,4-tetrahydropyrazine **(3e):**



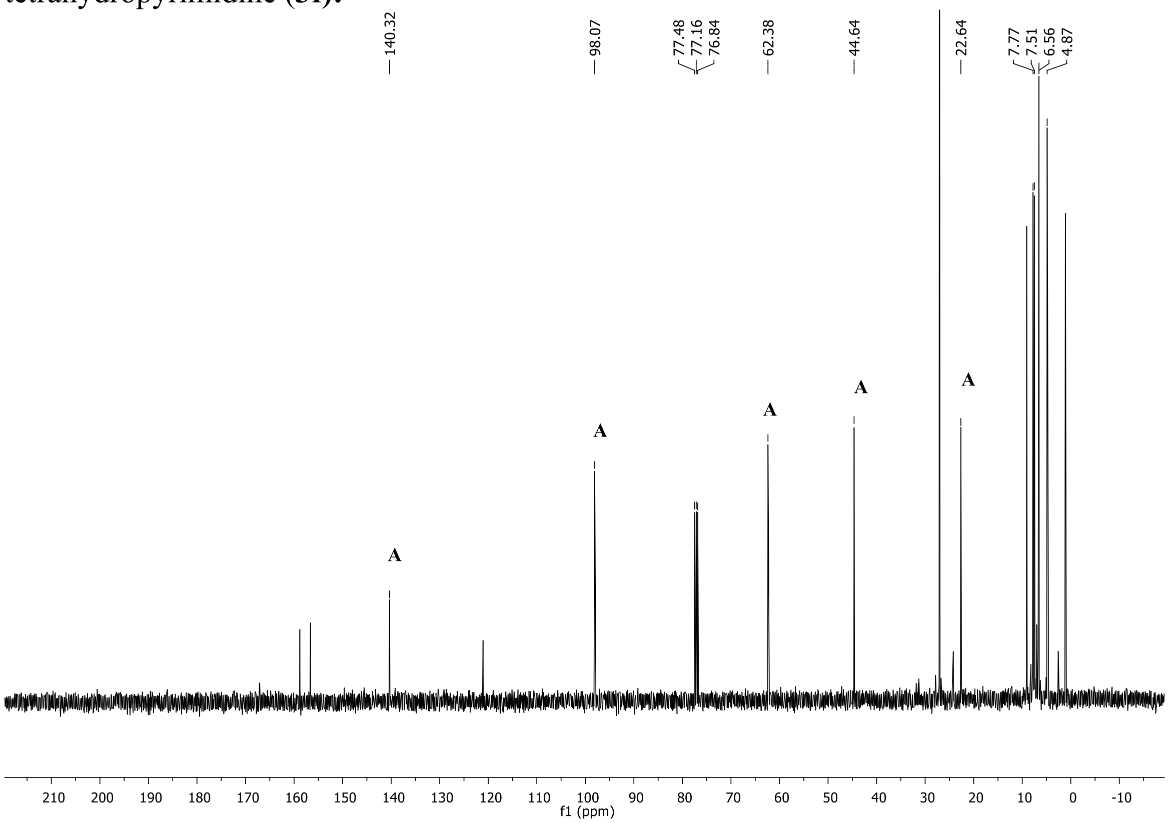
^{13}C NMR reaction mixture spectrum of 1,4-bis(diethylsilyl)-2-methyl-1,2,3,4-tetrahydropyrazine **(3e):**



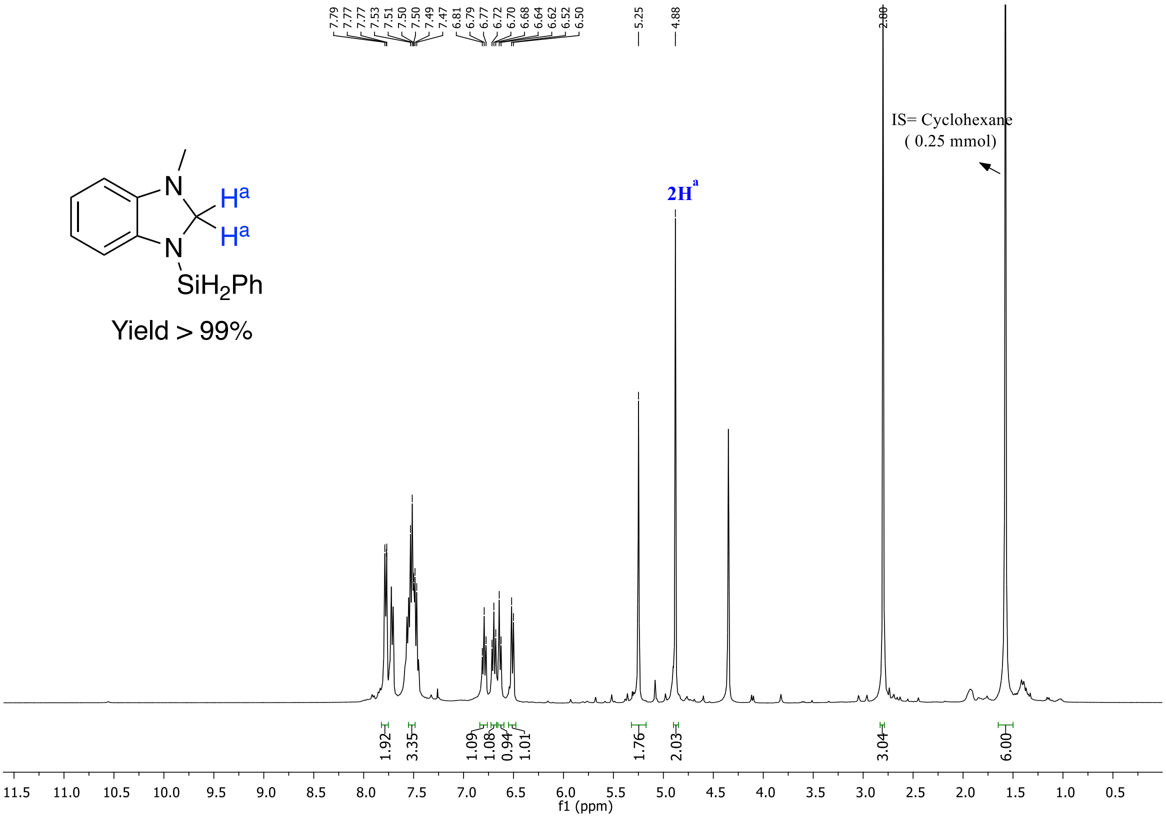
^{1}H NMR reaction mixture spectrum of 1,3-bis(diethylsilyl)-6-methyl-1,2,3,4-tetrahydropyrimidine (**3f**):



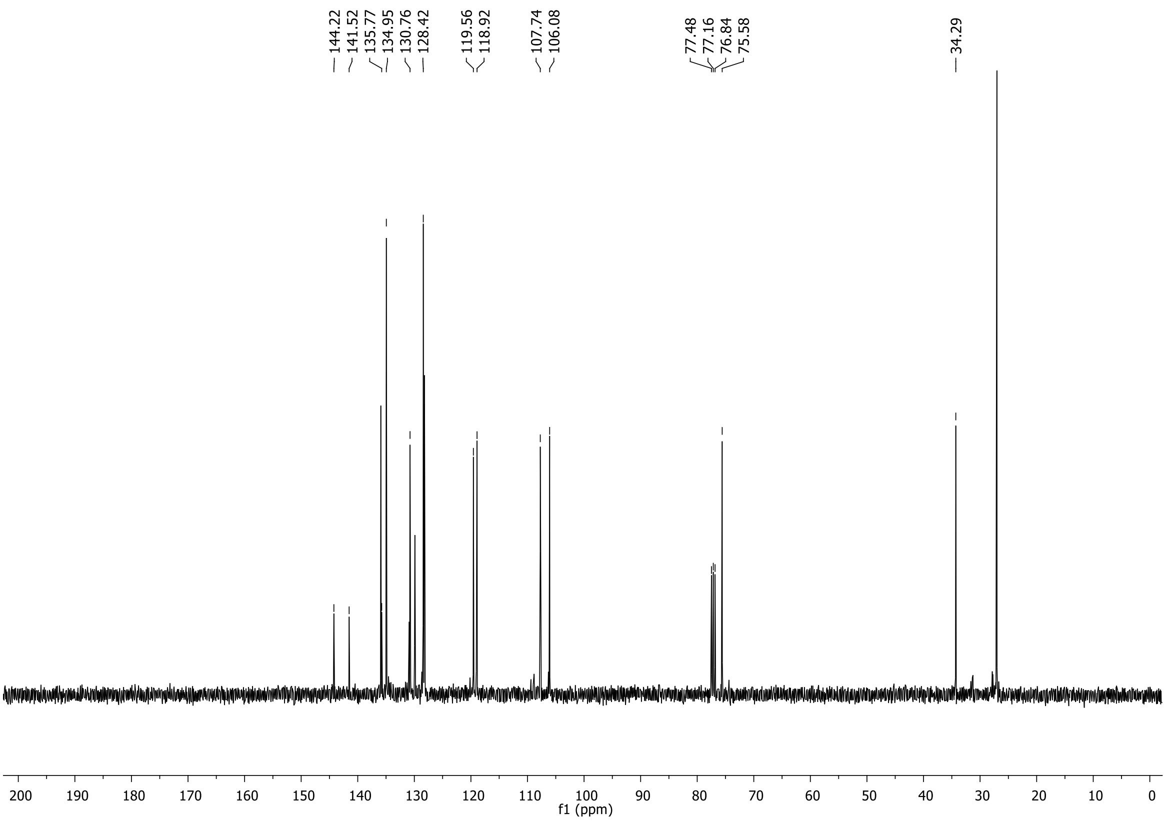
^{13}C NMR reaction mixture spectrum of 1,3-bis(diethylsilyl)-6-methyl-1,2,3,4-tetrahydropyrimidine (**3f**):



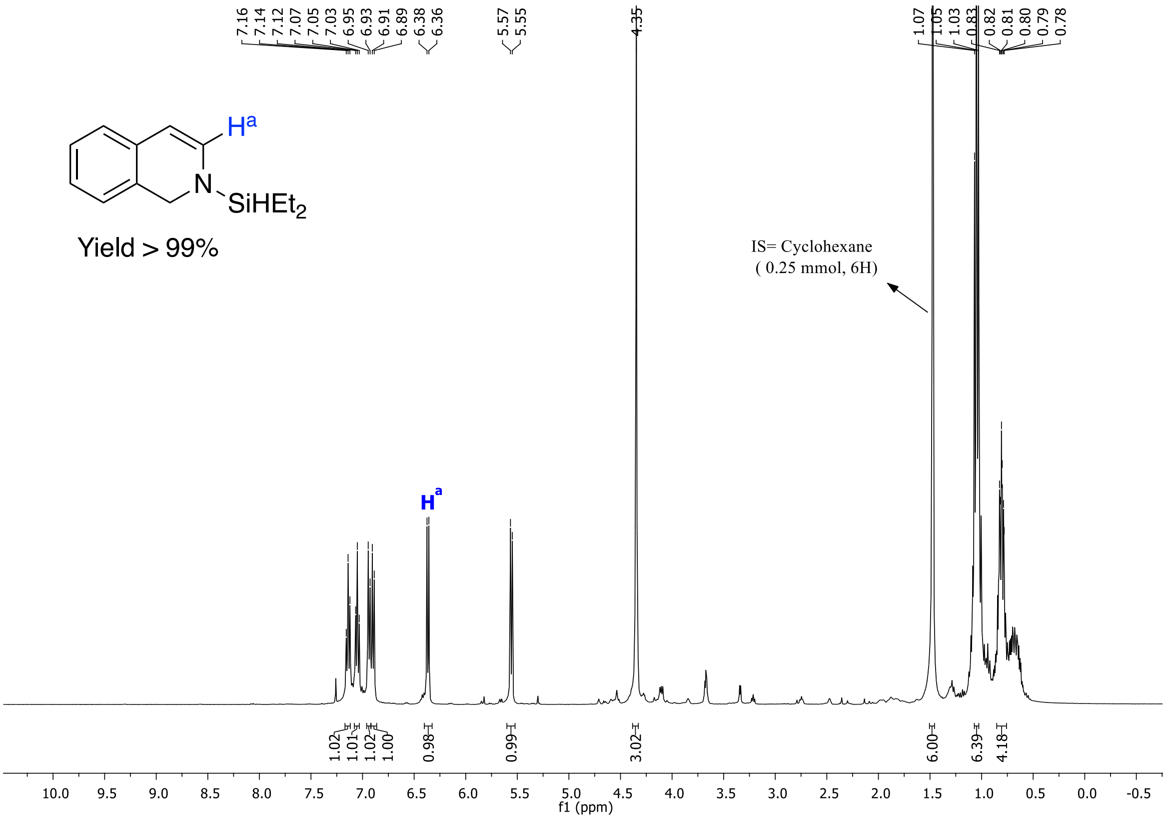
[1]H NMR reaction mixture spectrum of 1-methyl-3-(phenylsilyl)-2,3-dihydro-1*H*-benzo[*d*]imidazole **(3g):**



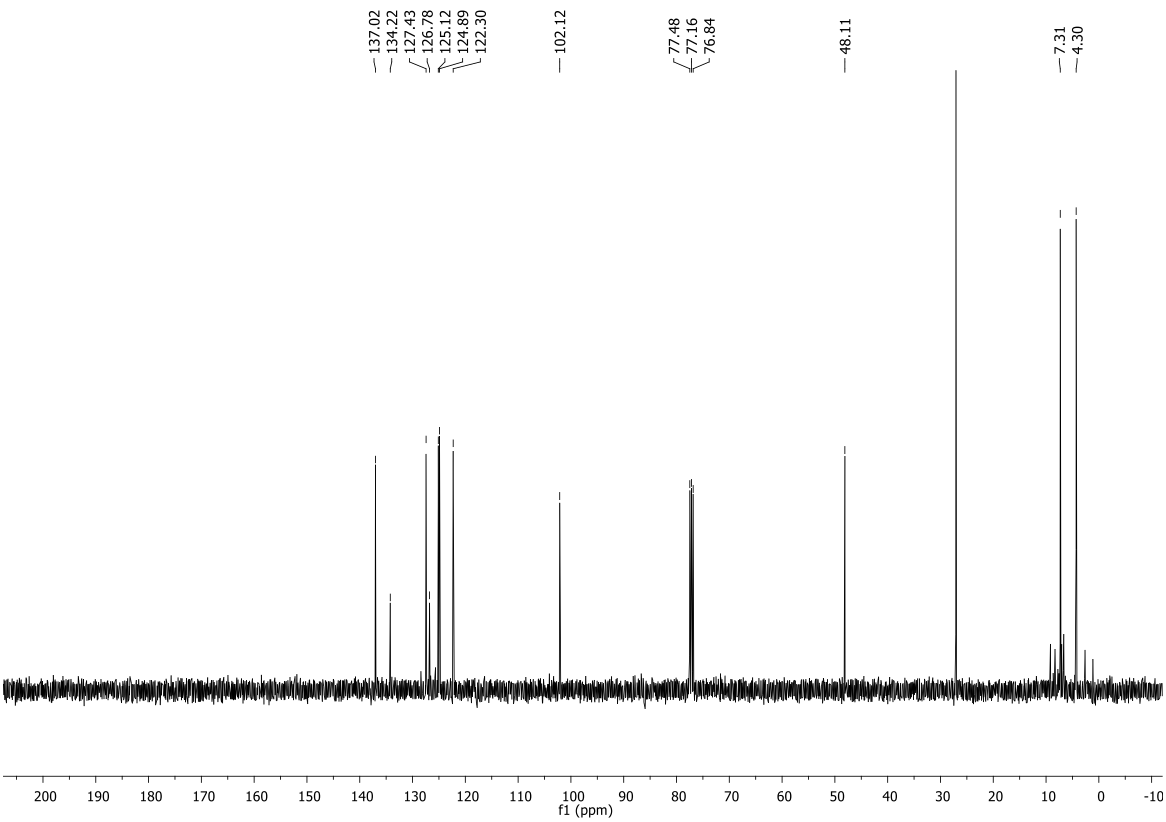
[13]C NMR reaction mixture spectrum of 1-methyl-3-(phenylsilyl)-2,3-dihydro-1*H*-benzo[*d*]imidazole **(3g):**



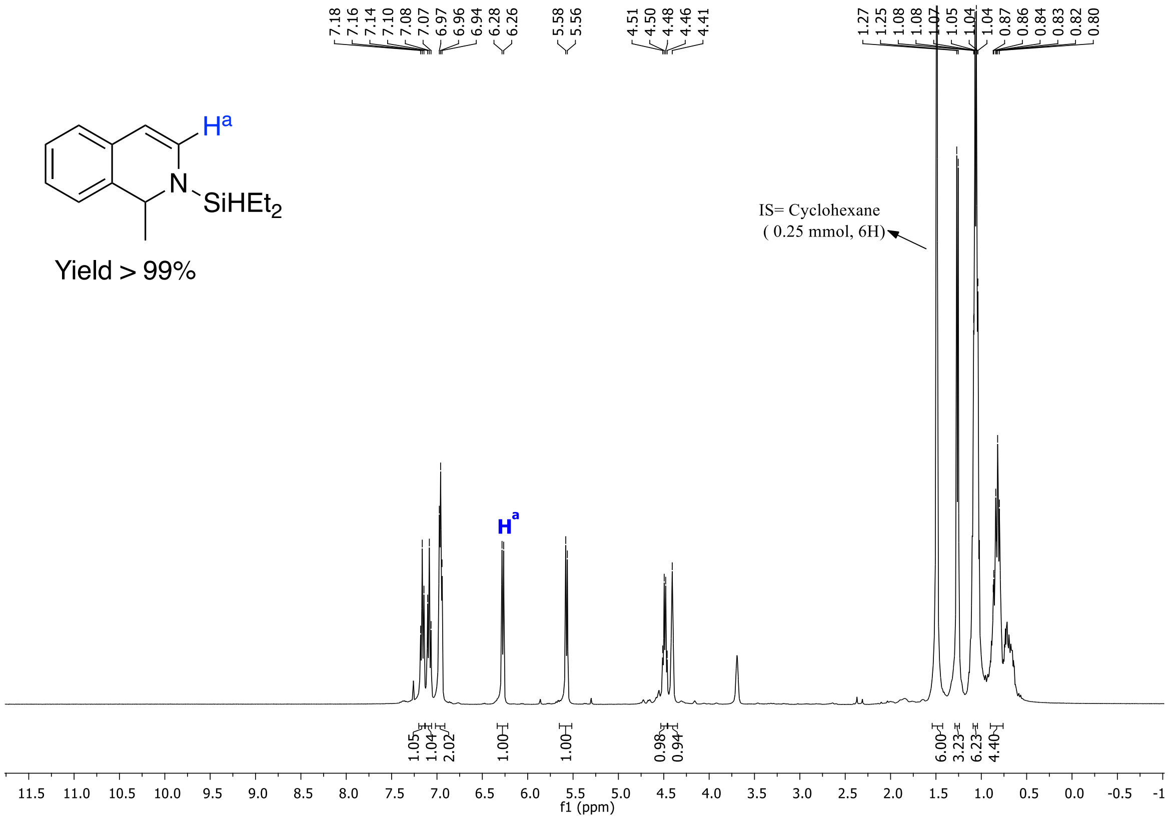
[1]H NMR reaction mixture spectrum of 2-(diethylsilyl)-1,2-dihydroisoquinoline **(3h):**



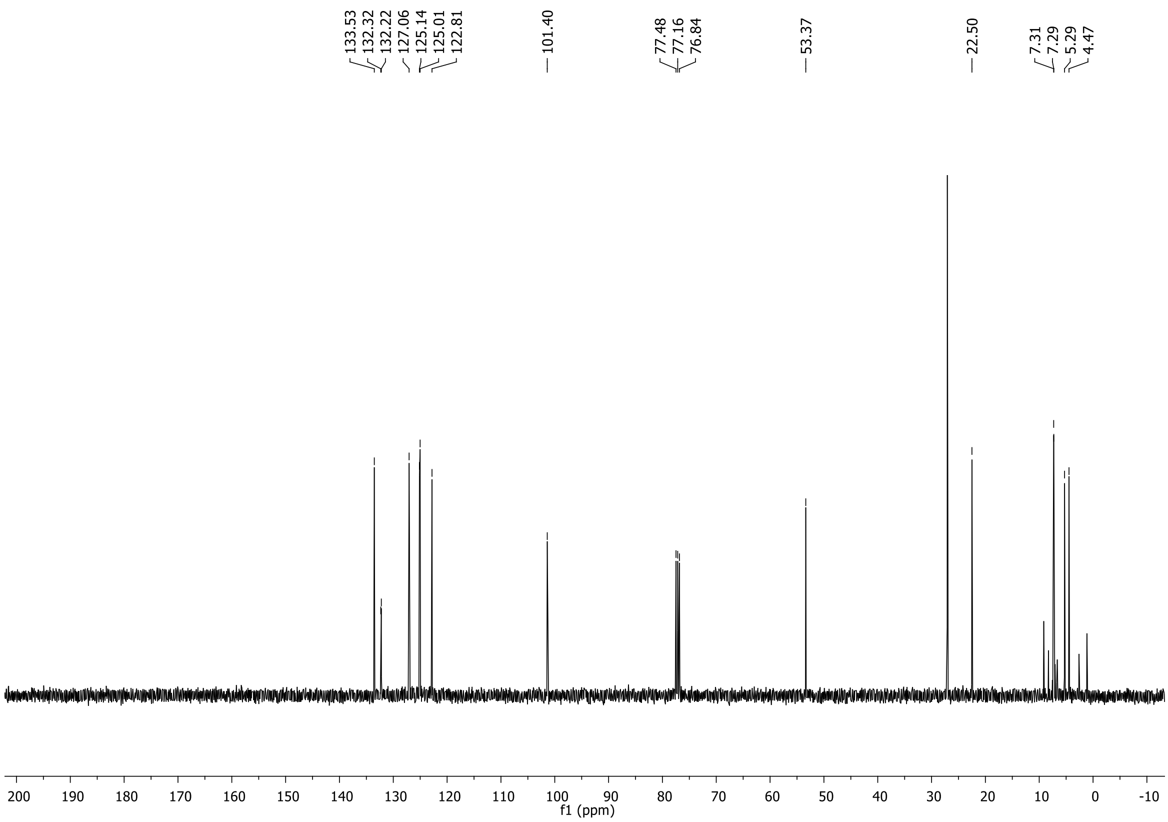
[13]C NMR reaction mixture spectrum of 2-(diethylsilyl)-1,2-dihydroisoquinoline **(3h):**



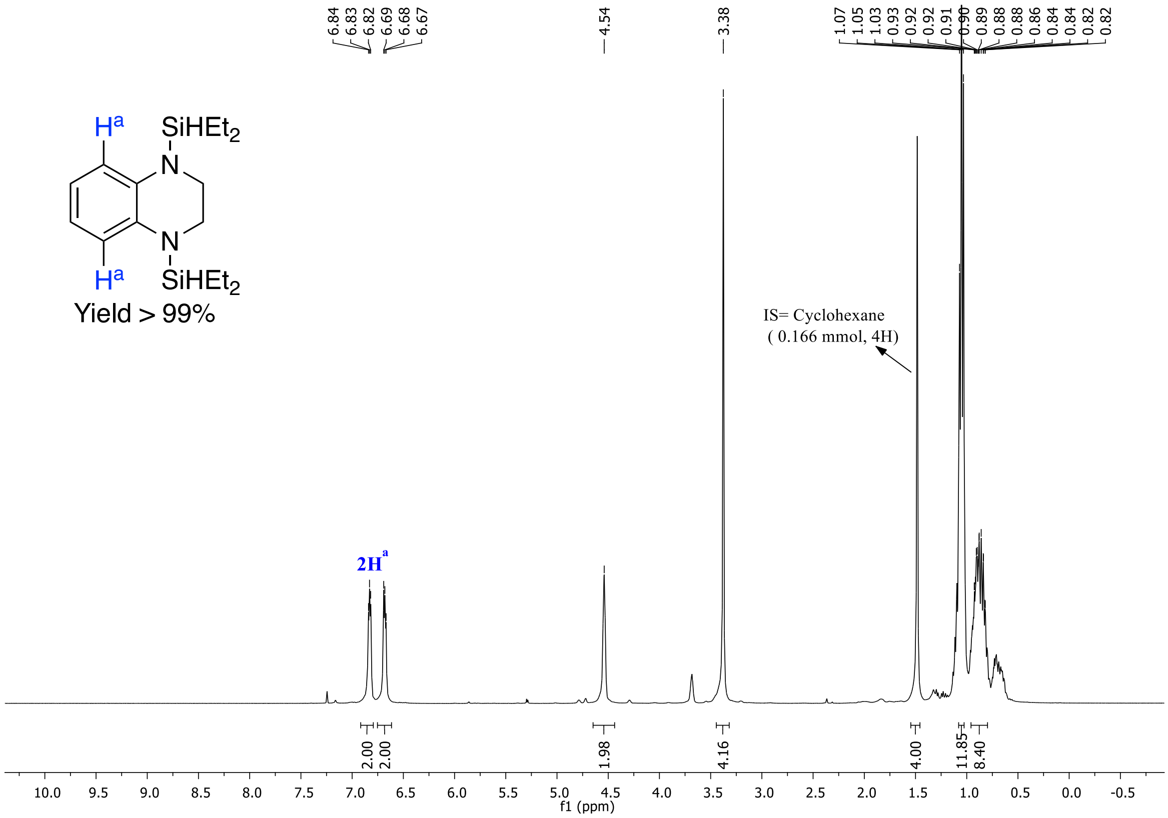
[1]H NMR reaction mixture spectrum of 2-(diethylsilyl)-1-methyl-1,2-dihydroisoquinoline **(3i):**



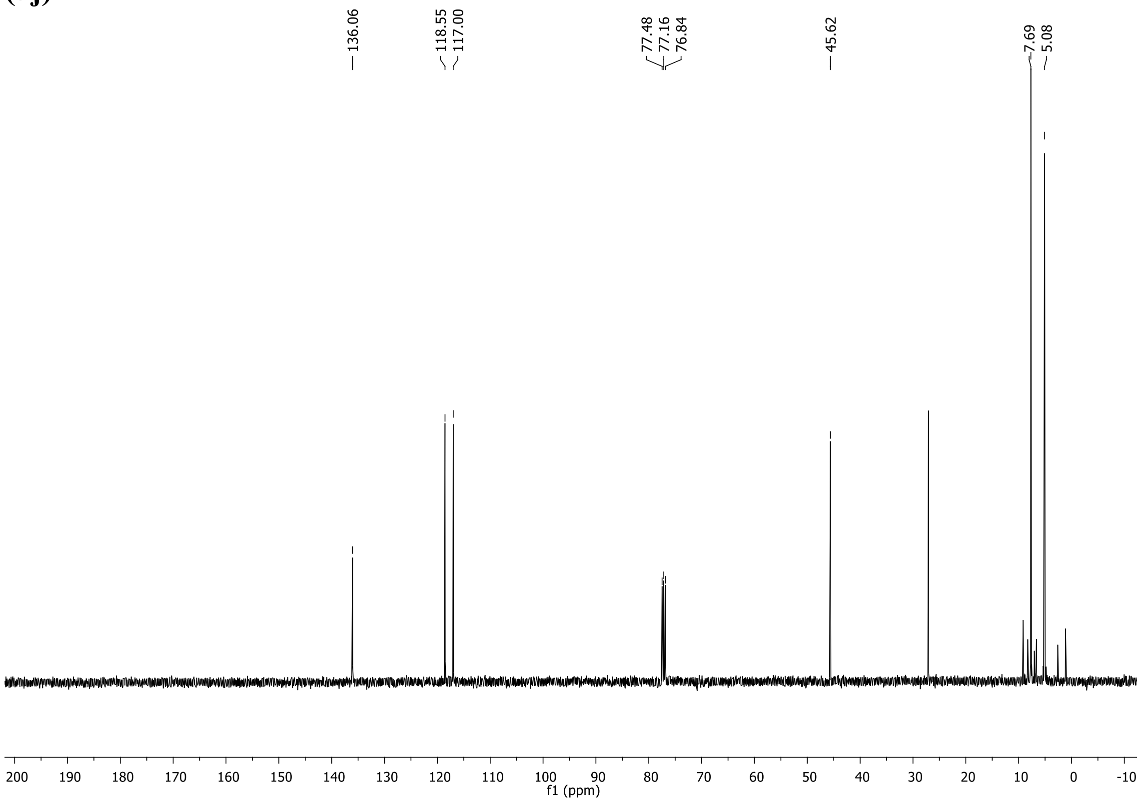
[13]C NMR reaction mixture spectrum of 2-(diethylsilyl)-1-methyl-1,2-dihydroisoquinoline **(3i):**



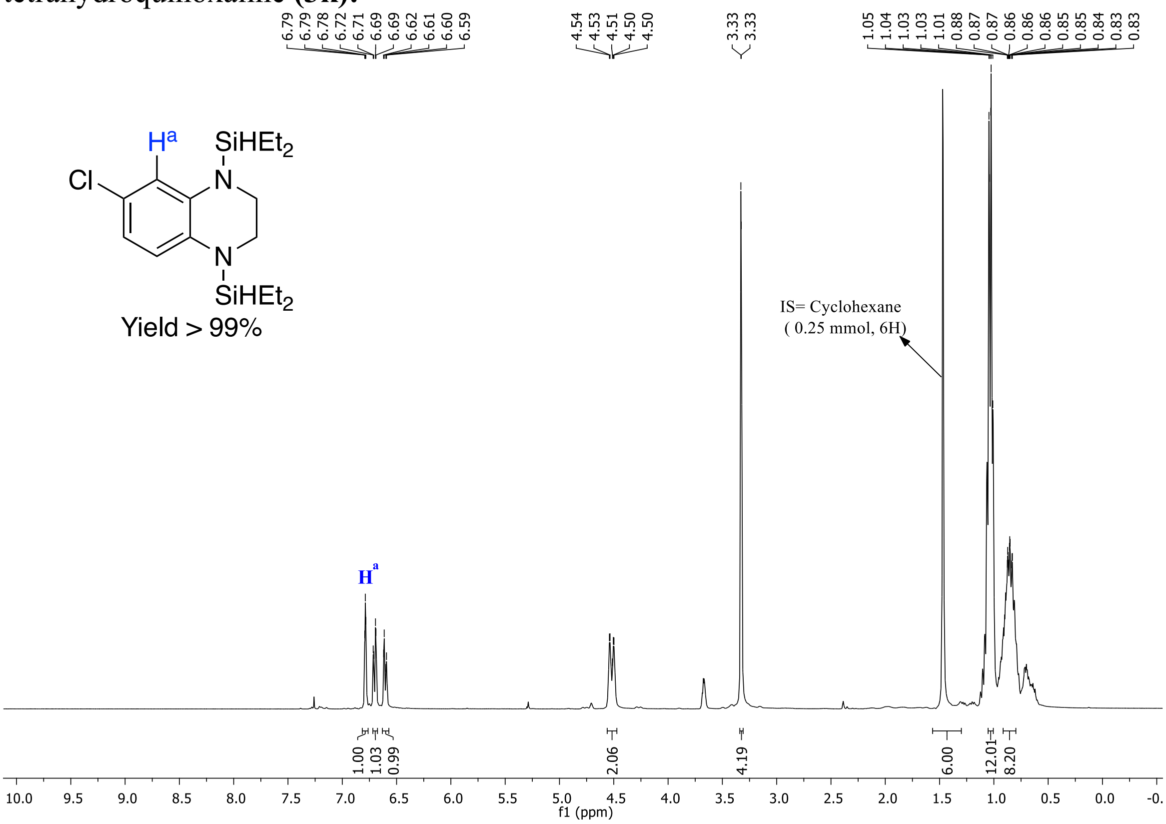
^{1}H NMR reaction mixture spectrum of 1,4-bis(diethylsilyl)-1,2,3,4-tetrahydroquinoxaline **(3j):**



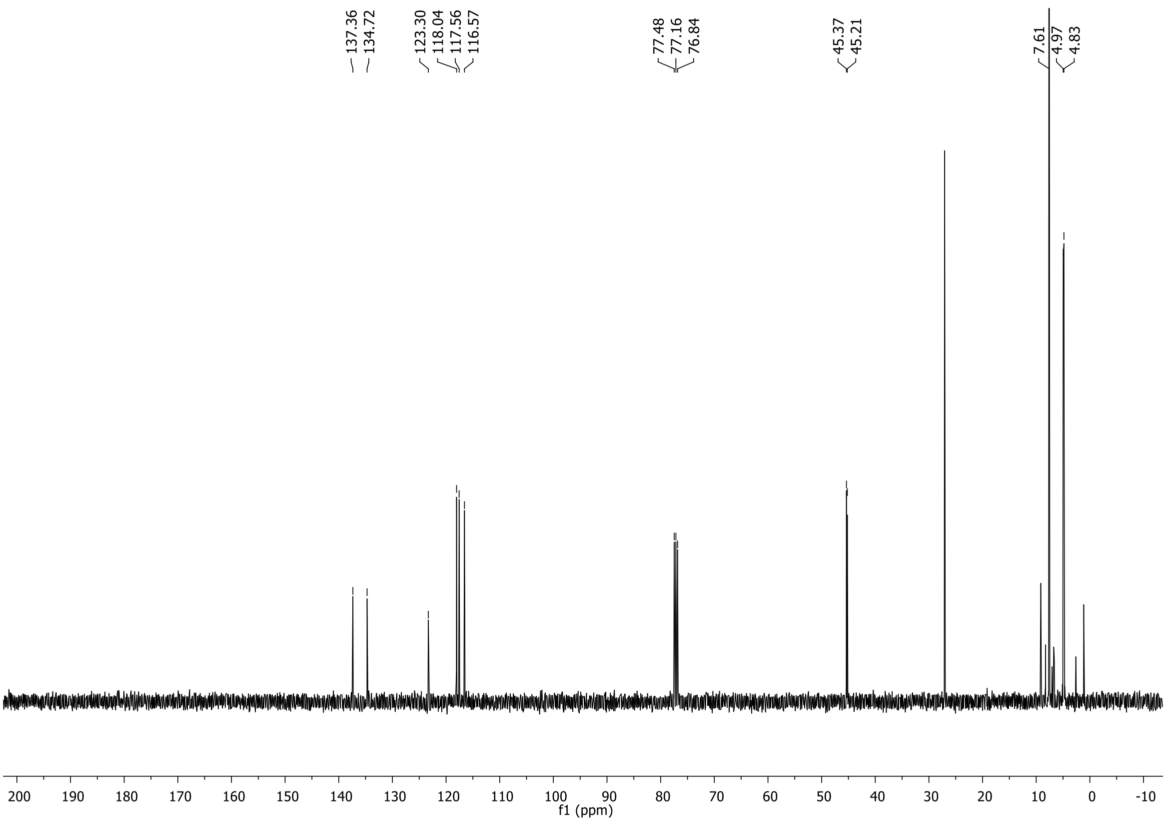
^{13}C NMR reaction mixture spectrum of 1,4-bis(diethylsilyl)-1,2,3,4-tetrahydroquinoxaline **(3j):**



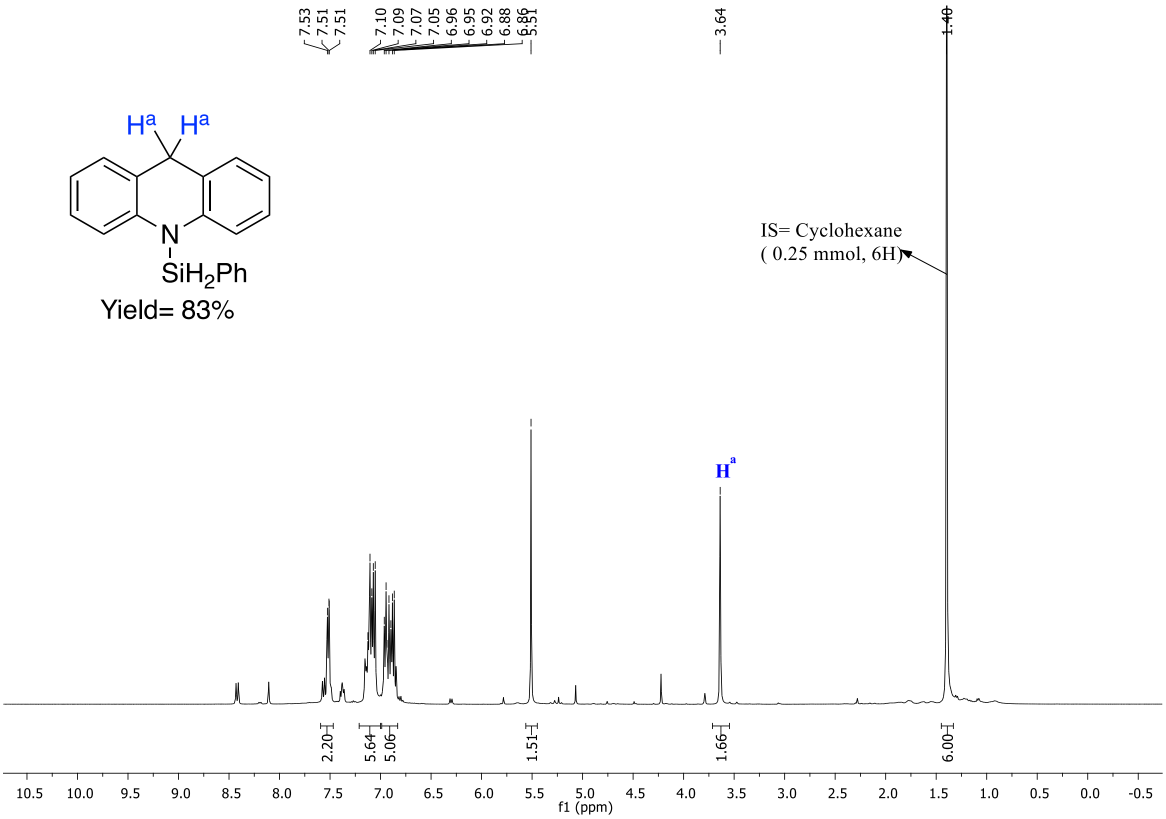
^{1}H NMR reaction mixture spectrum of 6-chloro-1,4-bis(diethylsilyl)-1,2,3,4-tetrahydroquinoxaline **(3k):**



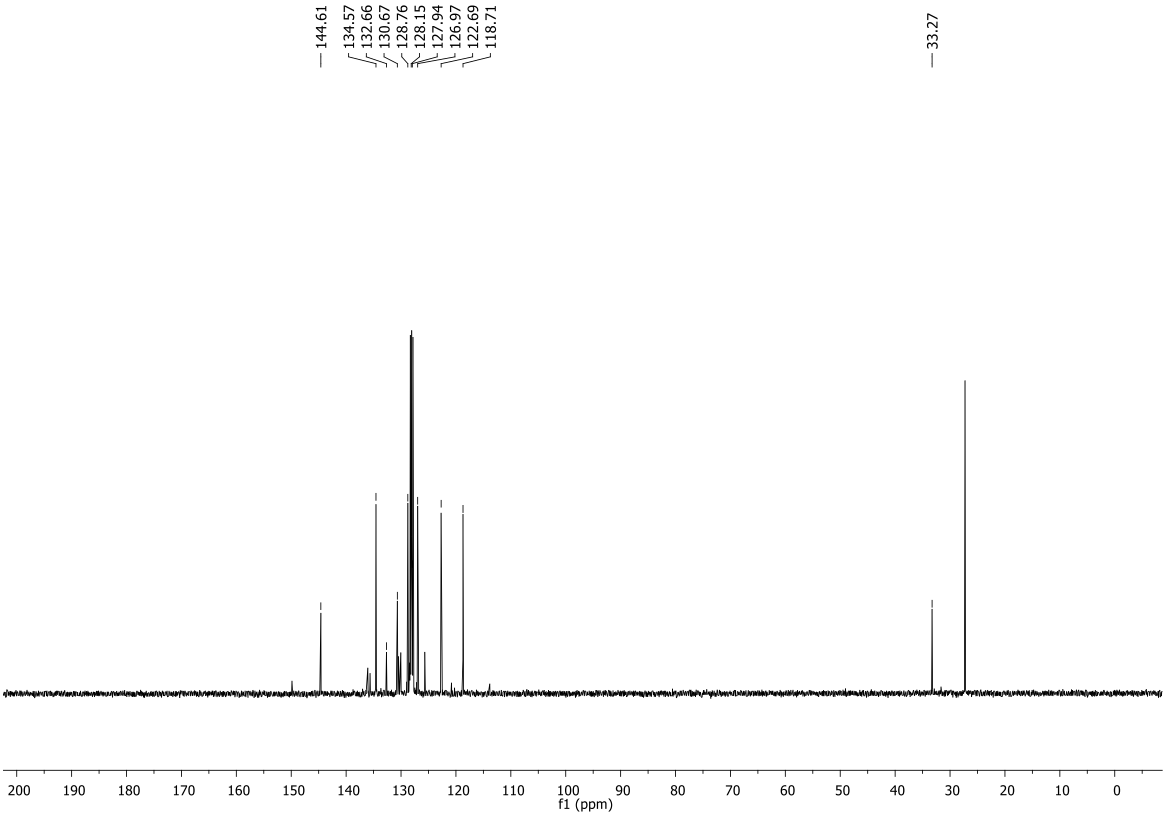
^{13}C NMR reaction mixture spectrum of 6-chloro-1,4-bis(diethylsilyl)-1,2,3,4-tetrahydroquinoxaline **(3k):**



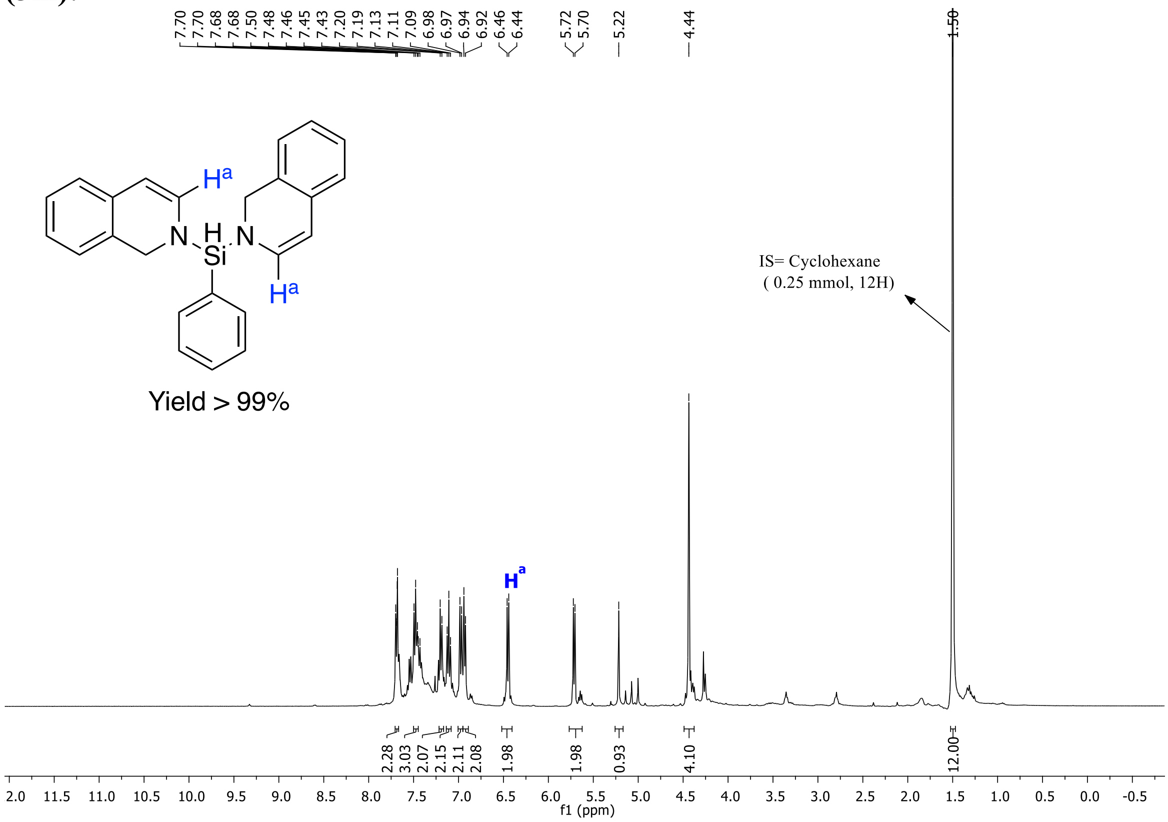
[1]H NMR reaction mixture spectrum of 10-(phenylsilyl)-9,10-dihydroacridine **(3l):**



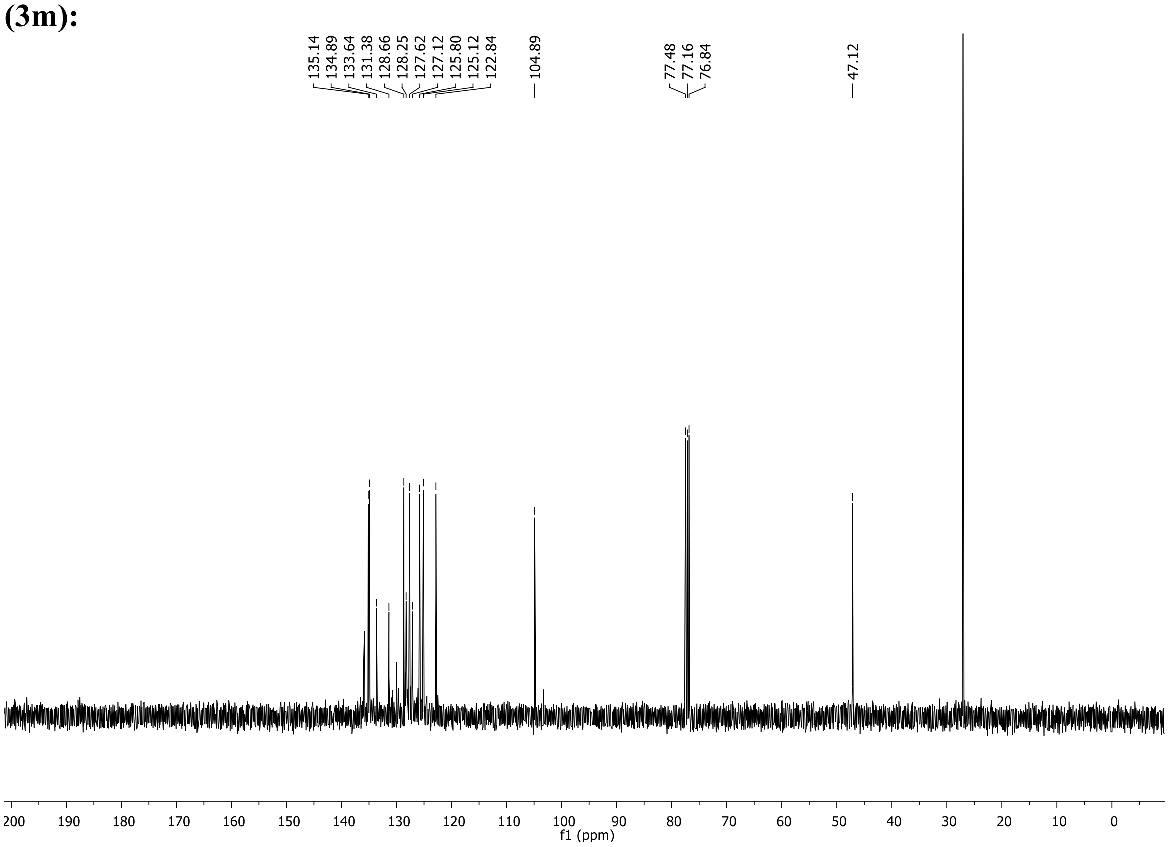
[13]C NMR reaction mixture spectrum of 10-(phenylsilyl)-9,10-dihydroacridine **(3l):**



[1]H NMR reaction mixture spectrum of 2,2'-(phenylsilanediyl)bis(1,2-dihydroisoquinoline) **(3m):**



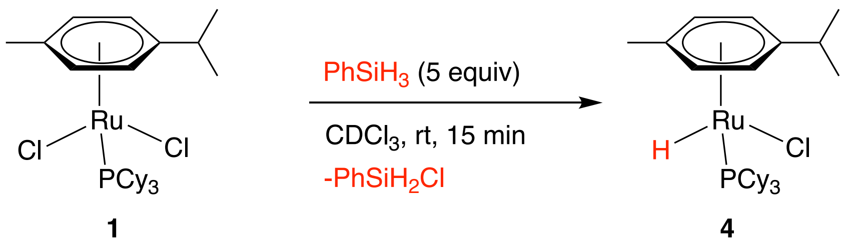
[13]C NMR reaction mixture spectrum of 2,2'-(phenylsilanediyl)bis(1,2-dihydroisoquinoline) **(3m):**



Stoichiometric Experiments:

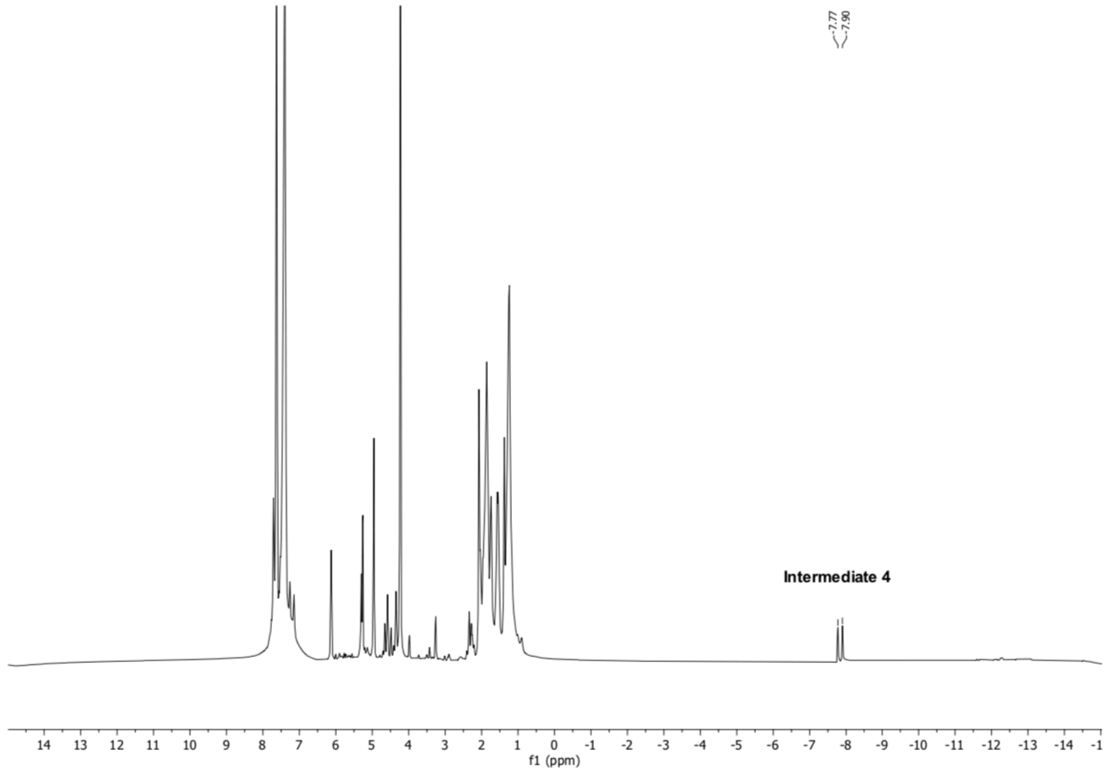
A screw cap NMR tube was charged with [Ru(*p*-cymene)(PCy_3)Cl_2] (**1**) (0.050 mmol, 30 mg), phenylsilane (5 equiv. 0.250 mmol, 27 mg), solvent $CDCl_3$ (0.5 mL) and the reaction was analysed by ^{1}H, and ^{31}P NMR spectroscopy.

Scheme S1: Stoichiometric Reaction of Catalyst **1** and Phenylsilane

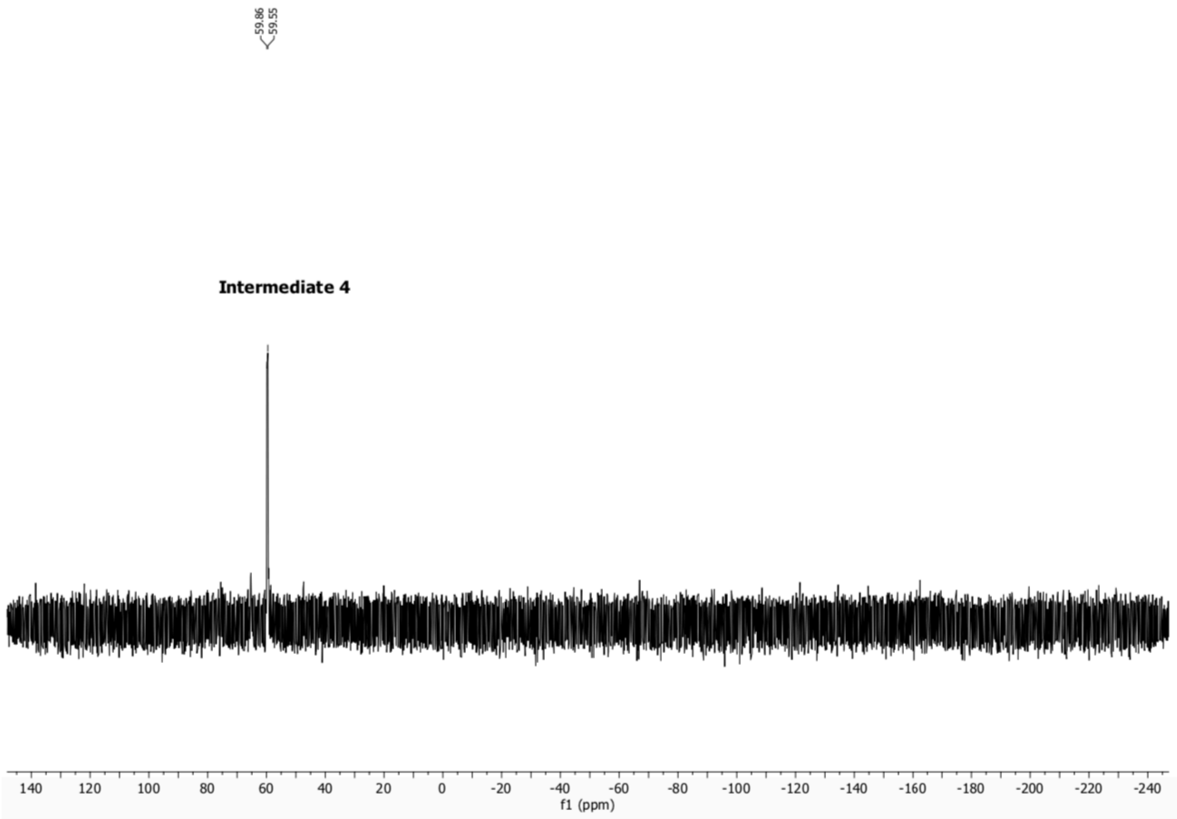


^{1}H NMR: δ = -7.84 ppm (d, J_{PH}= 49.2 Hz)
^{31}P NMR: δ = 59.70 ppm (d, J_{PH}= 50.6 Hz)

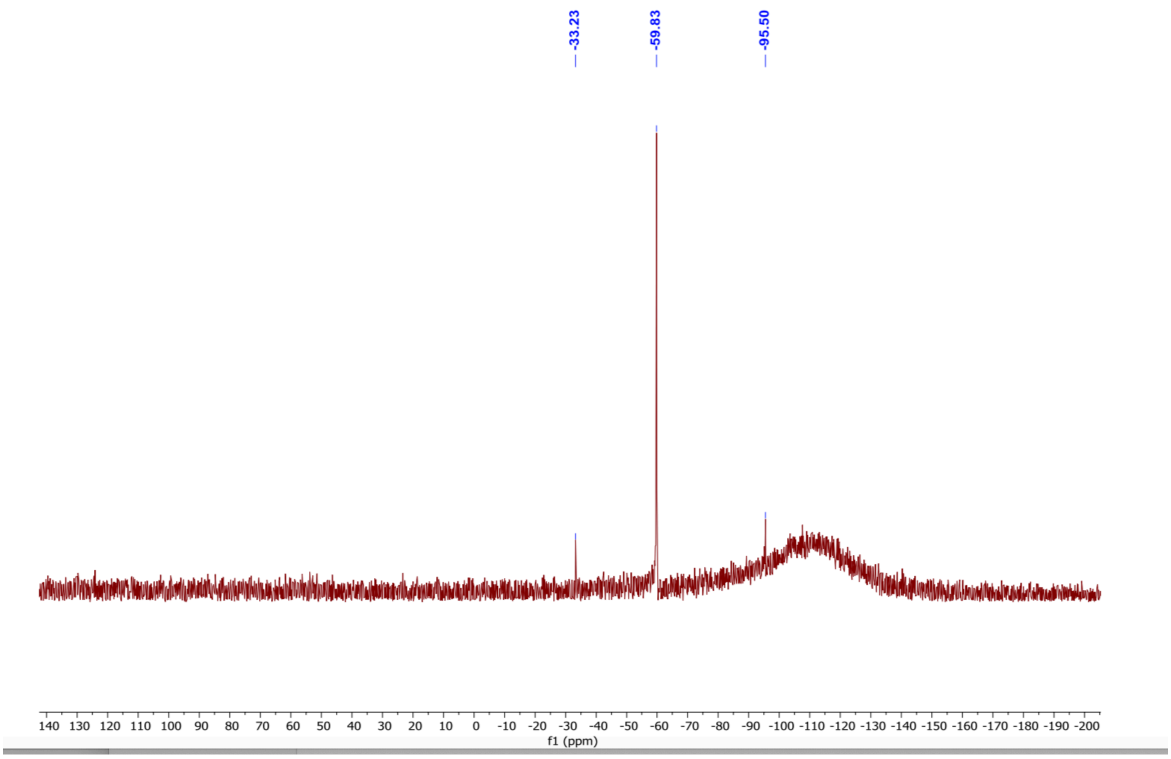
^{1}H NMR spectrum of the stoichiometric reaction of **1** and phenylsilane:



^{31}P NMR spectrum of the stoichiometric reaction of **1** and phenylsilane:

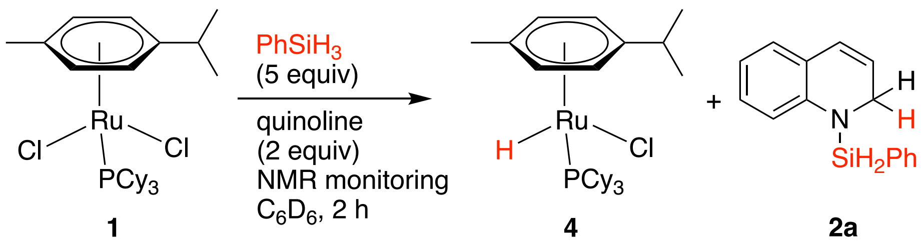


^{29}Si NMR spectrum of the stoichiometric reaction of **1** and phenylsilane:

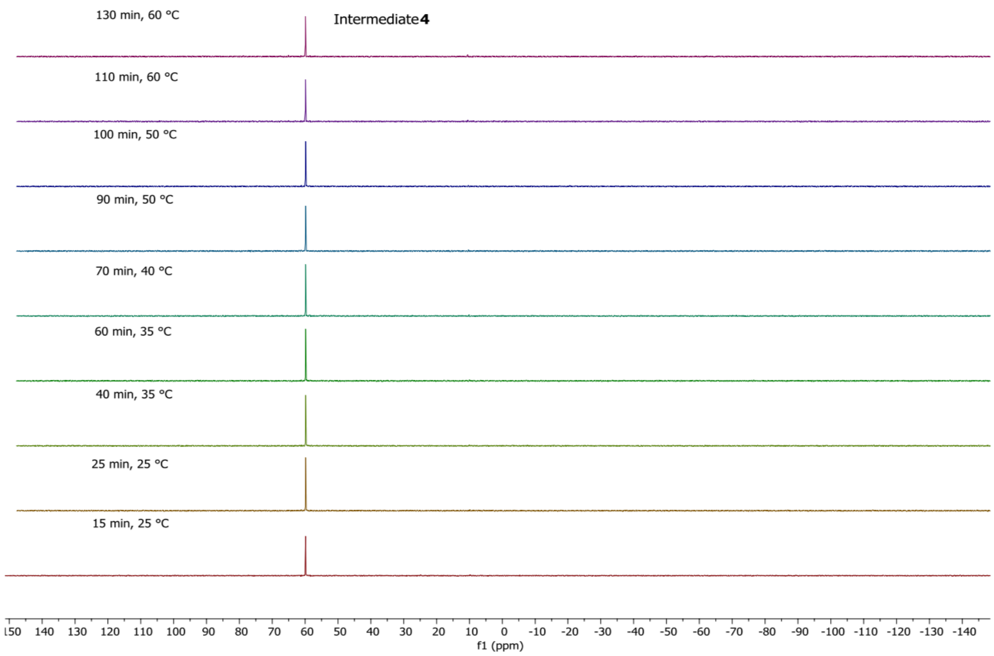


A screw cap NMR tube was charged with [Ru(p-cymene)(PCy_3)Cl_2] (**1**) (0.050 mmol, 30 mg), quinoline (2 equiv. 0.10 mmol, 13 mg), phenylsilane (5 equiv. 0.250 mmol, 27 mg), solvent C_6D_6 (0.5 ml) and the reaction was monitored by ^{1}H, and ^{31}P NMR spectroscopy at regular interval varying the temperature.

Scheme S2: NMR Monitoring of the Stoichiometric Reaction of Catalyst **1**, Phenylsilane and Quinoline

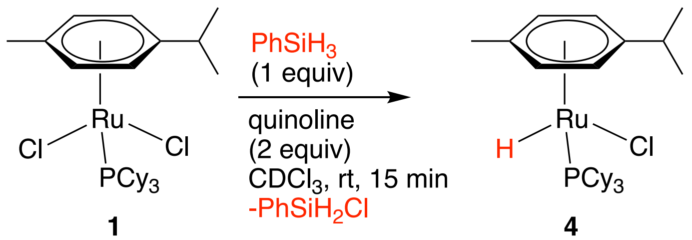


Stacked ^{31}P NMR spectra of the stoichiometric reaction of **1**, quinoline, and phenylsilane:



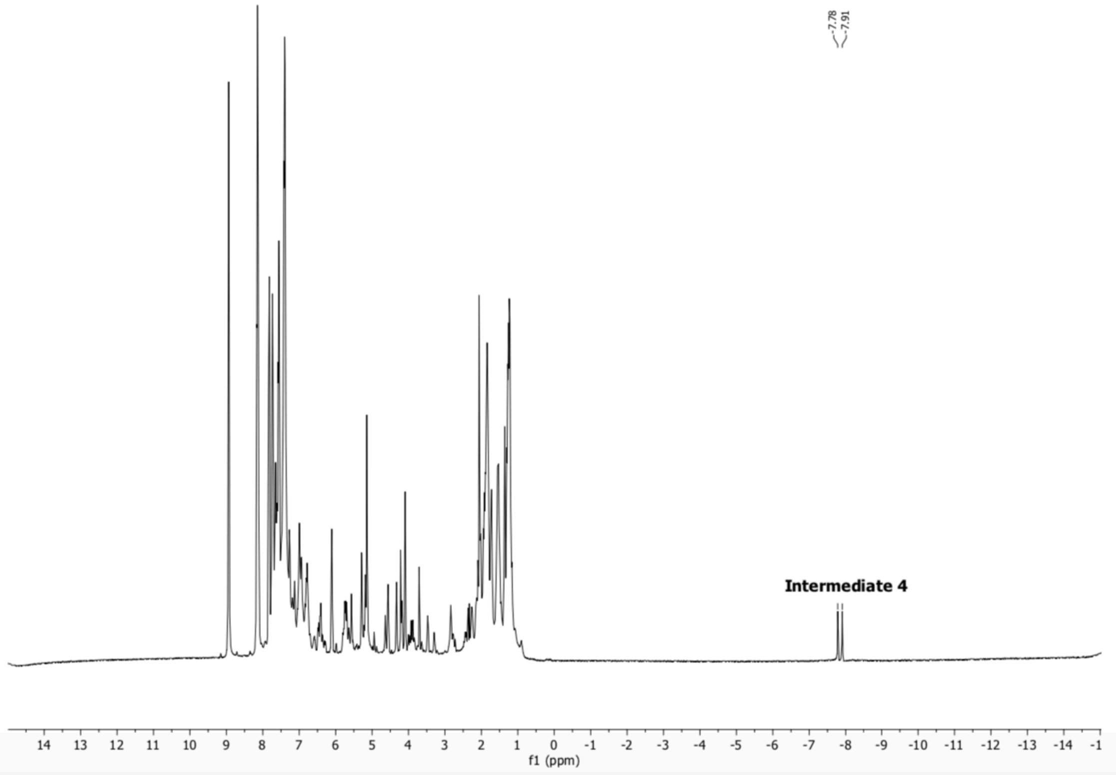
In a screw cap NMR tube was charged with [Ru(p-cymene)(PCy_3)Cl_2] (**1**, 0.050 mmol, 30 mg), quinoline (2 equiv. 0.050 mmol, 13 mg), phenylsilane (1 equiv. 0.050 mmol, 5.4 mg), solvent $CDCl_3$ (0.5 mL) and the reaction progress was analysed by ^1H, and ^{31}P NMR spectroscopy.

Scheme S3: Stoichiometric Reaction of Catalyst **1**, Phenylsilane and Quinoline

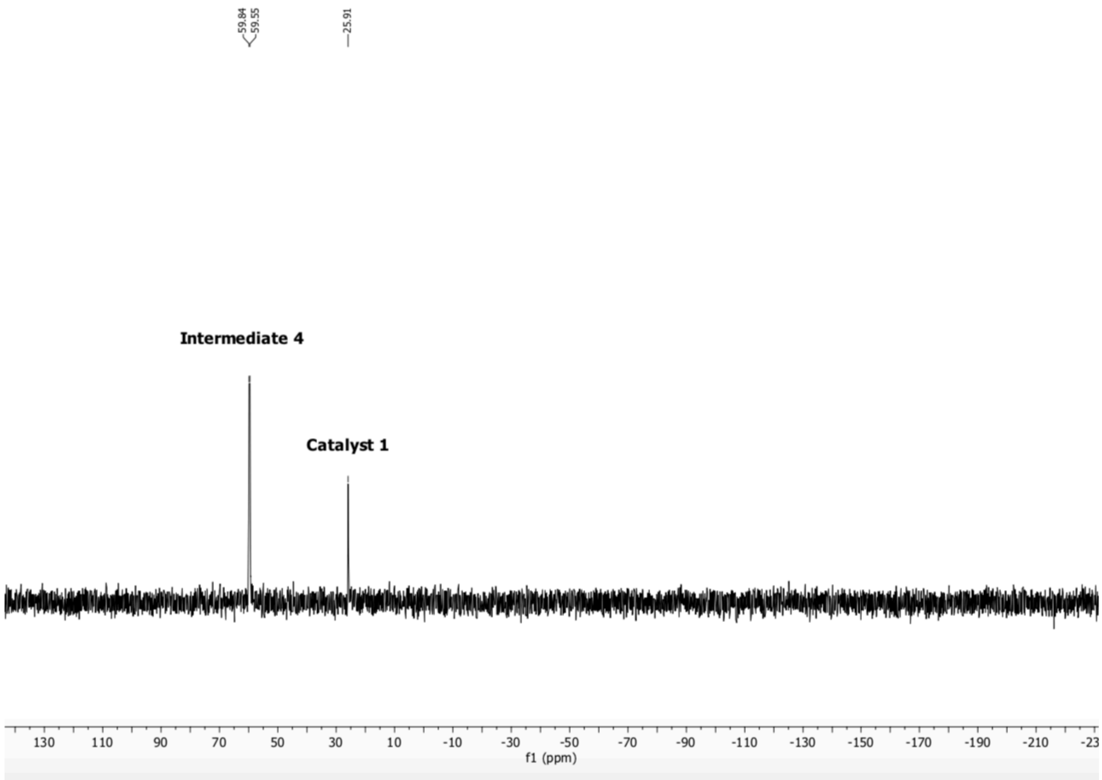


^{1}H NMR: δ = -7.84 ppm (d, J_{PH}= 49.5 Hz)
^{31}P NMR: δ = 59.70 ppm (d, J_{PH}= 46.8 Hz)

[1]H NMR spectra of the stoichiometric reaction of **1**, quinoline, and phenylsilane:

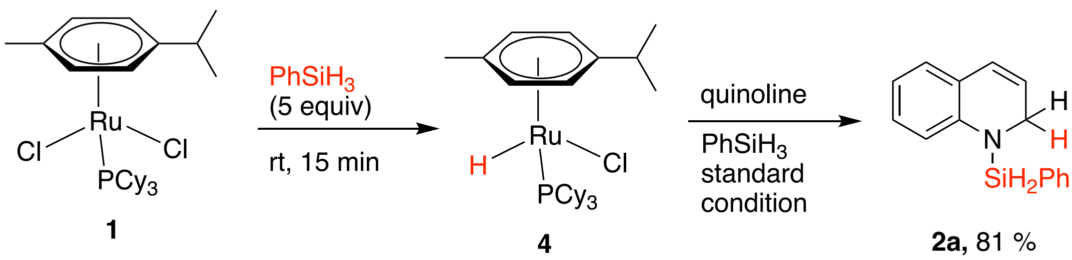


[31]P NMR spectra of the stoichiometric reaction of catalyst **1**, quinoline, and phenylsilane:



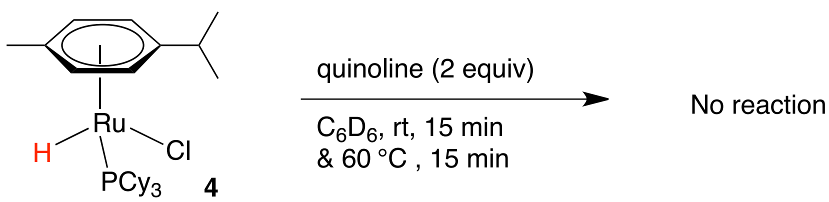
To a PTFE screw cap scintillation vial charged with a stir bar, catalyst **1** (0.02 mmol, 2 mol%), phenylsilane (0.1 mmol, 5 equiv) and $CDCl_3$ (0.1 mL) were stirred inside the glove box for 15 minutes. After complete formation of hydride intermediate **4** the reaction mixture was filtered out and subjected to high vacuum for 30 minutes. To the same vial, quinoline (0.5 mmol), phenylsilane (0.6 mmol) were added and the reaction performed at 60 °C for 18 h (standard reaction condition), which resulted 81 % of our desired 1,2-hydrosilylated product **2a**.

Scheme S4: Catalytic Reaction of Intermediate **4**, Phenylsilane and Quinoline Under Standard Reaction Condition

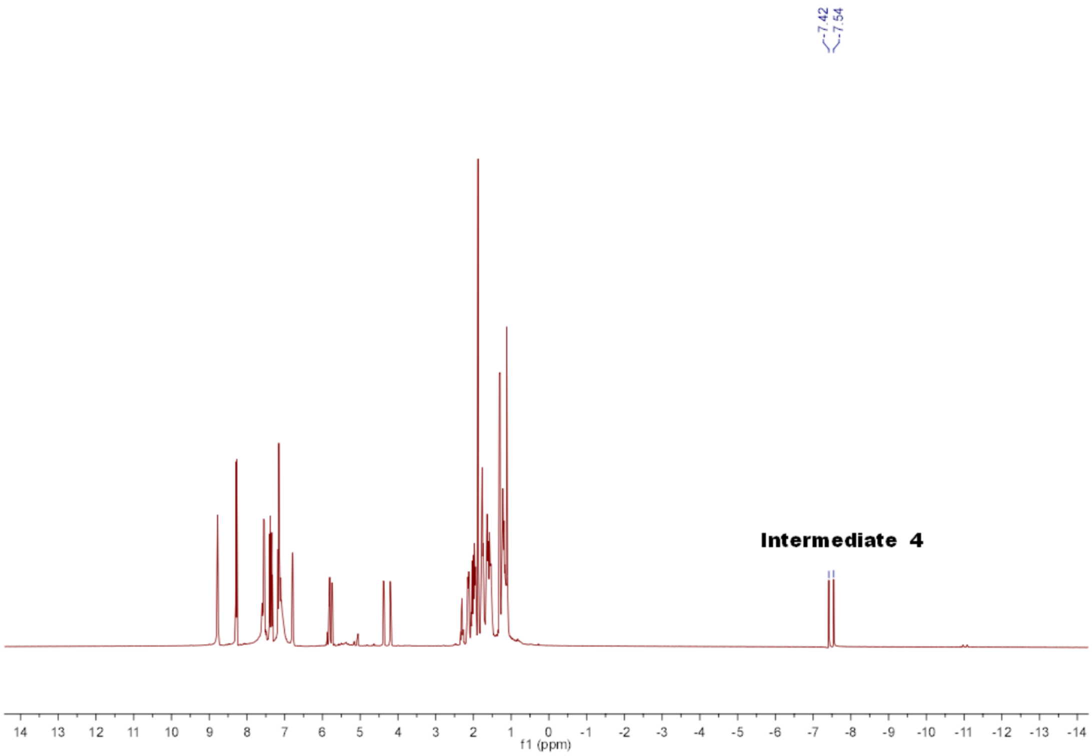


To a PTFE screw cap scintillation vial charged with a stir bar, catalyst **4** (0.03 mmol, 3 mol%), quinoline (0.06 mmol, 2 equiv) and C_6D_6 (0.4 mL) were stirred inside the glove box for 15 minutes. After that the reaction mixture was subjected to ^1H, and ^{31}P NMR analyses. Further, the reaction mixture also heated to 60 °C for another 15 minutes and again subjected to ^1H, and ^{31}P NMR analyses. Reaction performed both at room temperature and at 60 °C provided same results.

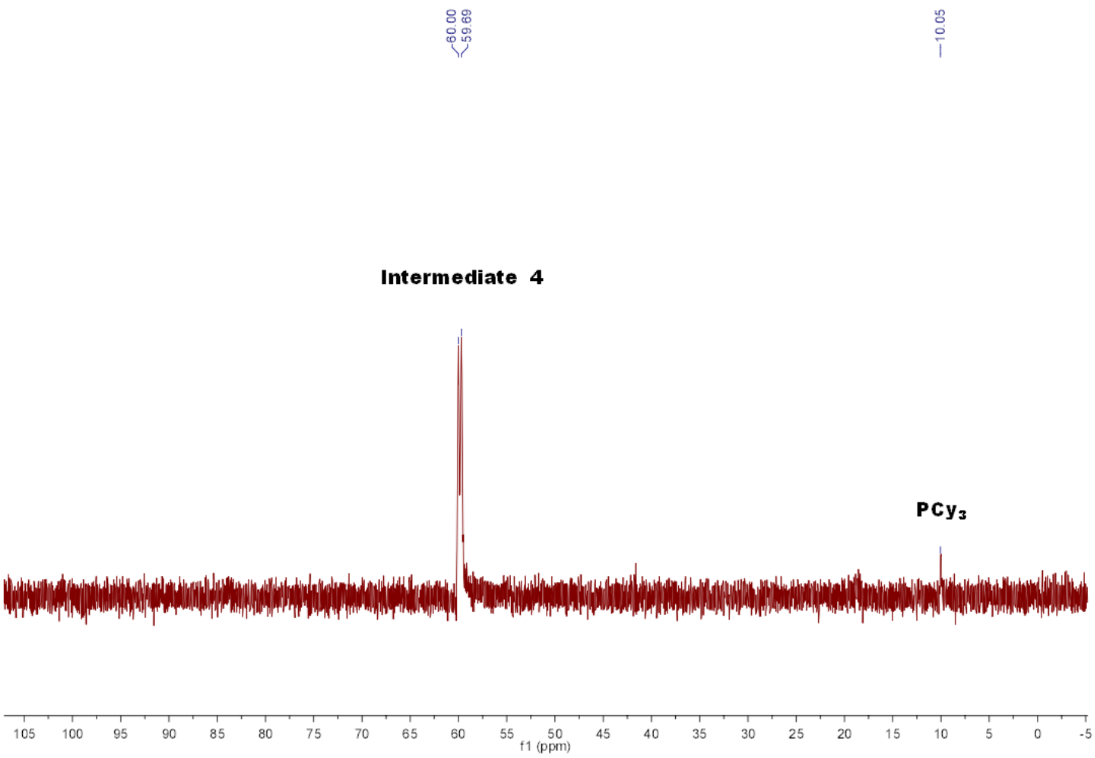
Scheme S5: Stoichiometric Reaction of Intermediate **4** and Quinoline



[1]H NMR spectra of the stoichiometric reaction of intermediate **4** and quinoline:



[13]P NMR spectra of the stoichiometric reaction of intermediate **4** and quinoline:



DFT Calculations

Methodology:

For optimization of all the geometries, the density functional theory (DFT) calculation[4] at M06L/BS1/SMD method is used where BS1 stands for a mixed basis set (basis set LANL2DZ for ruthenium and 6-31g** for other atoms).[5] M06L stands for Minnesota 2006 local functional while SMD describes the self-consistent reaction field method to simulate the implicit solvation effect. The selected solvent is $CHCl_3$. All the transition states were characterized by a single imaginary frequency along the reaction coordinate, whereas all the intermediates were confirmed to be a minima by locating zero imaginary frequency in the vibrational frequency analysis. All the calculations were done with the Gaussian 16 suite of programmes.[6]The energy data of all the structures are given in Table S1. Further, the reliability of the M06L/BS1/SMD method is assessed by evaluating the free energy of all the structures using various basis sets, viz. M06L/BS2/SMD (BS2 stands for 6-311++G(d,p)/lanl2dz), M06L/BS4/SMD (BS3 stands for 6-311G*/lanl2dz),[7] M06L/BS6/SMD (BS4 stands for 6-31g**/def2tzvp).[8]

Molecular electrostatic potential analysis (MESP)[9] is used to characterize the electron rich and electron deficient regions of the molecules. MESP is calculated rigorously by using Eq. 1 as implemented in Gaussian 16,

$$V(\boldsymbol{r}) = \sum_{A}^{N} \frac{Z_A}{|\boldsymbol{r} - \boldsymbol{R_A}|} - \int \frac{\rho(\boldsymbol{r'}) d^3\boldsymbol{r'}}{|\boldsymbol{r} - \boldsymbol{r'}|} \qquad \text{-------------------(1)}$$

where Z_A is the nuclear charge of the atom A positioned at $\mathbf{R}_A$, $\rho(\mathbf{r})$ being the molecular electron density and **r'** is a dummy integration variable. MESP analysis has been widely used for understanding electrostatic distribution of molecules and their chemical reactivity.

Table S1. Energy data of optimized geometries at M06L/BS1/SMD level (solvent = $CHCl_3$).

Molecule	SCF energy (hartree)	Gibb's energy (hartree)	Lowest frequency (cm-1)	No. of imaginary frequency
5	-1926.768884	-1926.490463	19.2	0
TS1	-1926.725816	-1926.446213	-209.6	1
6	-1926.760559	-1926.483139	19.1	0
7	-944.210256	-944.028127	44.6	0

8	-982.5387109	-982.463788	15.2	0
9	-1346.148342	-1345.838849	22.7	0
TS2	-1346.112370	-1345.805290	-705.5	1
10	-1346.130795	-1345.818906	24.4	0
11	-1869.041306	-1868.620555	15.4	0
TS3	-1869.041187	-1868.616848	-45.4	1
12	-1869.052503	-1868.630864	20.4	0
2a	-924.816911	-924.603933	15.4	0
[Ru(*p*-cymene)Cl_2(PCy_3)]	-2451.018277	-2450.378275	27.5	0
20 [Ru-(*p*-cymene)Cl_2]	-1403.857276	-1403.683159	55.5	0
PCy_3	-1047.108994	-1046.671871	38.4	0
$PhSiH_3$	-522.9037868	-522.820485	29.5	0
Quinoline	-401.9003236	-401.795585	172.5	0
13	-1815.701309	-1815.349065	28.1	0
TS4	-1815.689528	-1815.335771	-116.1	2
14	-1815.686436	-1815.337651	16.5	0
15 (ClBpin)	-871.4660151	-871.318610	96.6	0
16	-660.1162167	-659.875799	37.9	0
17	-1119.761311	-1119.530226	31.6	0
18	-2063.983832	-2063.546942	22.9	0
TS5	-2063.97421	-2063.541769	-472.0	1
19	-2063.995242	-2063.557816	22.2	0
21	-660.1248904	-659.883324	40.4	0
HBpin	-411.8346587	-411.677119	101.9	0
pyridine	-248.2643142	-248.202240	375.2	0

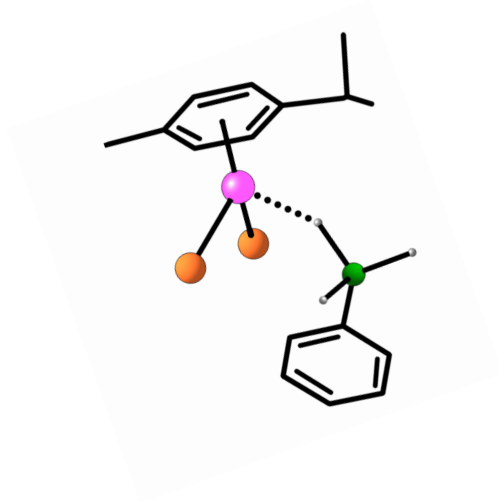
Table S2. Relative free energy data in kcal/mol for all the structures using various basis sets at M06L and SMD method (solvent = $CHCl_3$).

Molecule	BS1	BS2	BS3	BS4
Stage 1				
5	0.0	0.0	0.0	0.0
TS1	27.8	28.6	29.1	27.8
5	4.6	5.3	6.0	6.7
7+8	-4.1	0.7	1.6	-3.0
Stage 2				
9	0.0	0.0	0.0	0.0
TS2	21.1	19.8	20.2	20.7
10	12.5	11.2	11.1	11.2
Stage 3				
11	0.0	0.0	0.0	0.0
TS3	2.3	2.4	2.3	2.5
12	-6.5	-6.1	-6.8	-5.1
2a+7	-10.2	-8.5	-8.4	-10.3

Table S3. Cartesian coordinates of optimized structures using M06L/BS1/SMD method. Atomic number followed by X, Y and Z coordinates in Ǎ.

5

44	0.862103000	0.305141000	-0.029398000
17	-0.398267000	-0.929242000	-1.716123000
6	2.127251000	1.735810000	1.070875000
6	2.880644000	-0.406895000	0.074559000
6	2.151730000	1.477281000	-1.371855000
1	1.868663000	1.834166000	-2.356821000
6	2.637400000	0.429812000	1.213692000
1	2.701980000	-0.009973000	2.205106000
6	1.855508000	2.271311000	-0.227936000
6	2.645901000	0.158281000	-1.218911000
1	1.824685000	2.295095000	1.951086000
1	2.709167000	-0.478656000	-2.095860000
17	-0.230505000	-1.047868000	1.697081000
6	1.195558000	3.598259000	-0.372892000
1	0.591183000	3.844497000	0.503535000
1	1.959401000	4.377812000	-0.474964000
1	0.562733000	3.636681000	-1.262590000
6	3.350674000	-1.824418000	0.269807000
1	2.948741000	-2.150995000	1.237730000
6	4.878048000	-1.824175000	0.359029000
6	2.855364000	-2.783275000	-0.801652000
1	1.767942000	-2.730132000	-0.918499000
1	3.312833000	-2.577889000	-1.775888000
1	3.120729000	-3.809640000	-0.534004000
1	5.324300000	-1.486299000	-0.583252000
1	5.245104000	-2.835326000	0.557747000
1	5.242663000	-1.170334000	1.157446000
14	-2.241050000	1.615771000	0.736071000
6	-3.558942000	0.376250000	0.304050000
6	-3.763775000	-0.788101000	1.060732000
6	-4.755421000	-1.699997000	0.711499000
6	-5.559627000	-1.465520000	-0.401938000
6	-5.372717000	-0.314551000	-1.164384000
6	-4.382576000	0.597887000	-0.811842000
1	-1.911542000	1.648929000	2.175472000
1	-0.963373000	1.377246000	-0.023772000
1	-2.669460000	2.965000000	0.282951000
1	-3.132950000	-0.986492000	1.923800000
1	-4.899356000	-2.596762000	1.308174000
1	-6.332833000	-2.178927000	-0.674905000
1	-5.998838000	-0.126852000	-2.032580000
1	-4.250621000	1.494967000	-1.414700000



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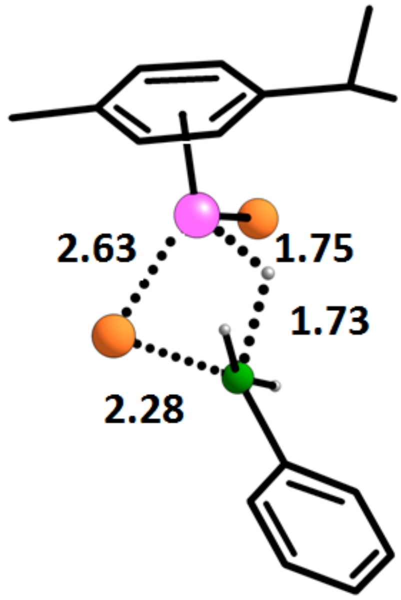

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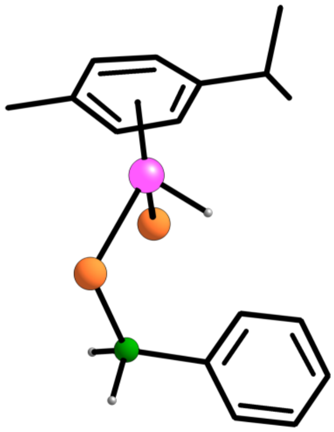

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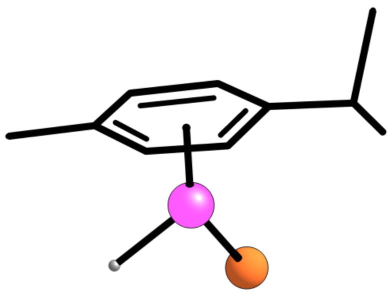

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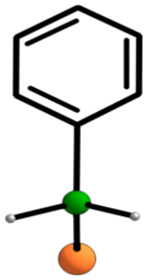

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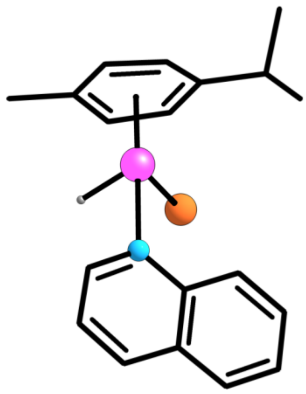

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TS2

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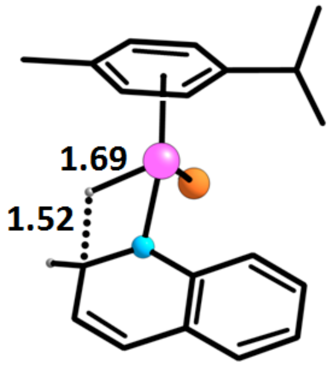
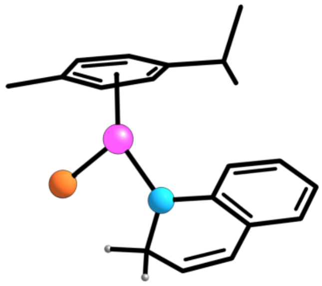


10				
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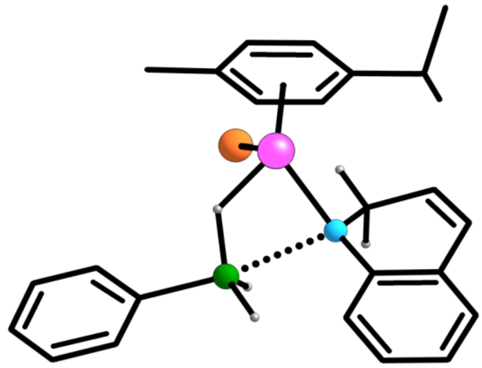
17	1.383730000	-1.244333000	1.991927000	
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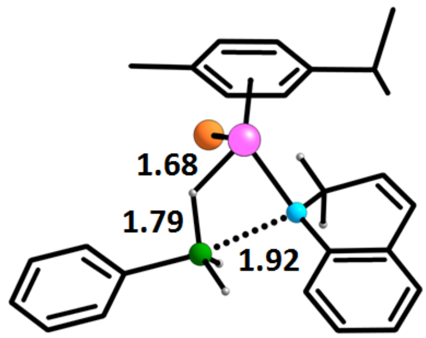
TS3				
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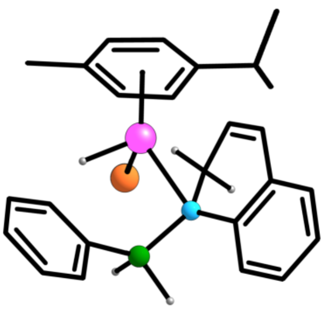

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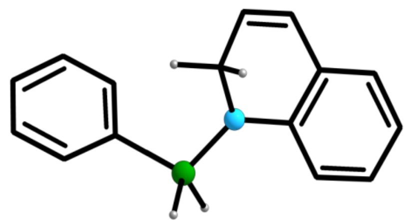

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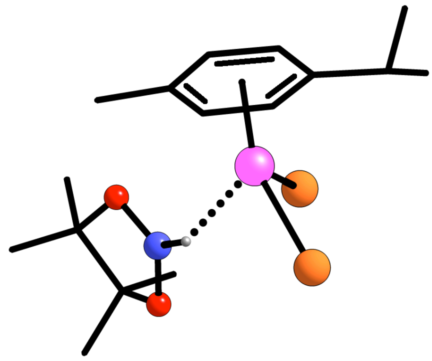
6	1.759496000	1.951398000	1.203325000	
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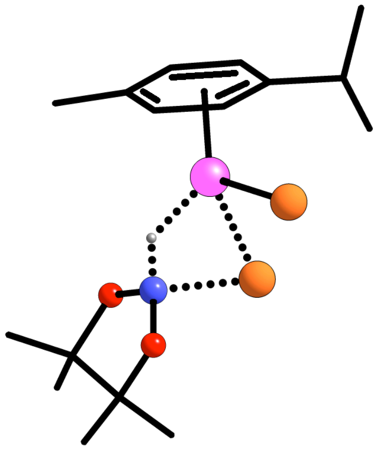

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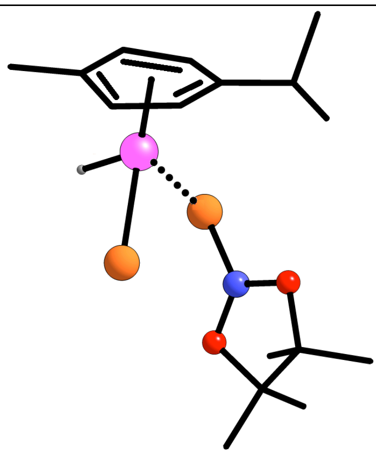
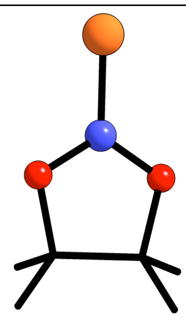


15				
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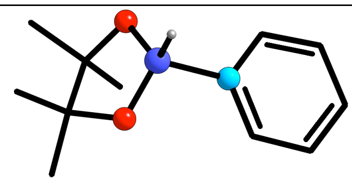
16				
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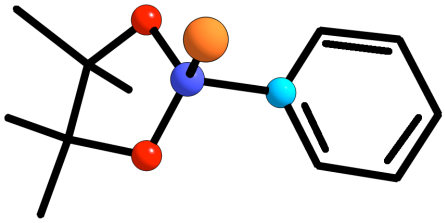
17				
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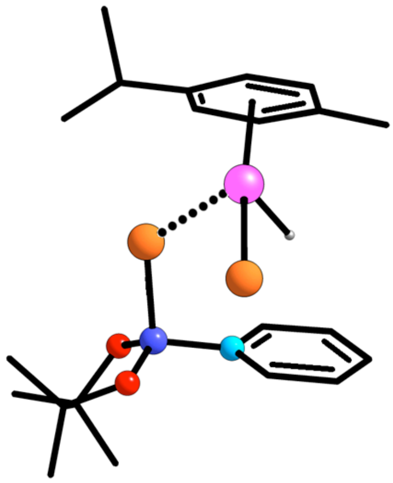
18				
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TS5

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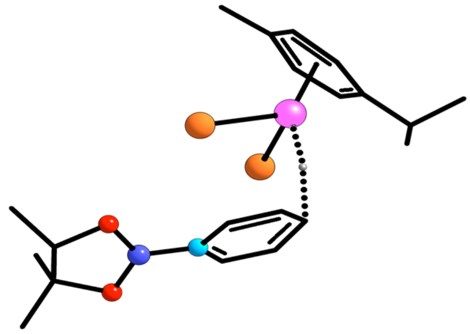

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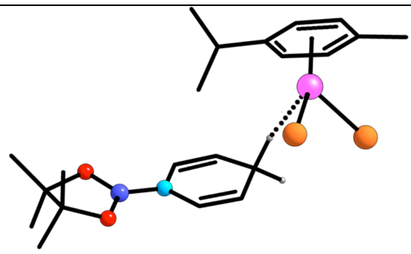
19				
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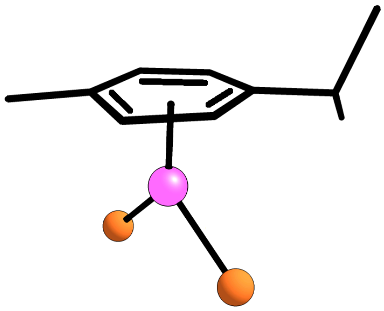
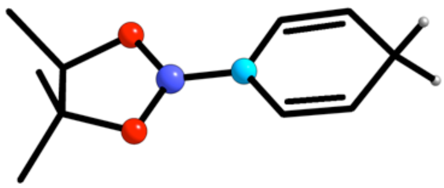
20 44 -0.817670000 0.301610000 -0.433959000 17 -1.199687000 2.640799000 0.040524000 6 3.204515000 1.126759000 0.756950000 1 2.495231000 1.957827000 0.825420000 1 4.168280000 1.533370000 0.438347000 1 3.343131000 0.716246000 1.763548000 6 1.365594000 -0.485777000 0.092186000 6 -0.674282000 -0.690434000 1.423130000 1 -1.238957000 -0.391464000 2.302230000 6 -0.587817000 -1.841600000 -0.723945000 1 -1.060095000 -2.408736000 -1.519120000 6 -2.655281000 -2.136926000 0.733635000 1 -3.258133000 -1.450326000 1.332709000 1 -2.578549000 -3.079849000 1.287703000 1 -3.184277000 -2.338430000 -0.200380000 6 0.689761000 -0.260745000 1.284846000 1 1.120479000 0.374027000 2.052081000 6 0.648265000 -1.182873000 -0.952033000 1 1.109068000 -1.259522000 -1.934534000 6 -1.295299000 -1.582624000 0.482936000 6 3.739125000 -1.092033000 -0.303426000 1 4.722798000 -0.721365000 -0.606818000 1 3.430213000 -1.852062000 -1.028023000 1 3.851112000 -1.583710000 0.669186000 6 2.735919000 0.060234000 -0.218136000 1 2.667055000 0.512100000 -1.218826000 1 -2.238171000 0.343567000 -1.215095000	
21 6 -2.262409000 -1.179681000 0.173329000 6 -3.599952000 -1.217409000 0.179437000 6 -4.457274000 0.000000000 0.000003000 6 -3.599952000 1.217409000 -0.179437000 6 -2.262409000 1.179681000 -0.173332000 7 -1.523538000 0.000000000 -0.000002000 1 -1.655843000 -2.069708000 0.303297000 1 -4.082598000 -2.179941000 0.320599000 1 -4.082598000 2.179941000 -0.320600000 1 -1.655843000 2.069707000 -0.303304000 1 -5.139458000 0.126739000 0.858347000	

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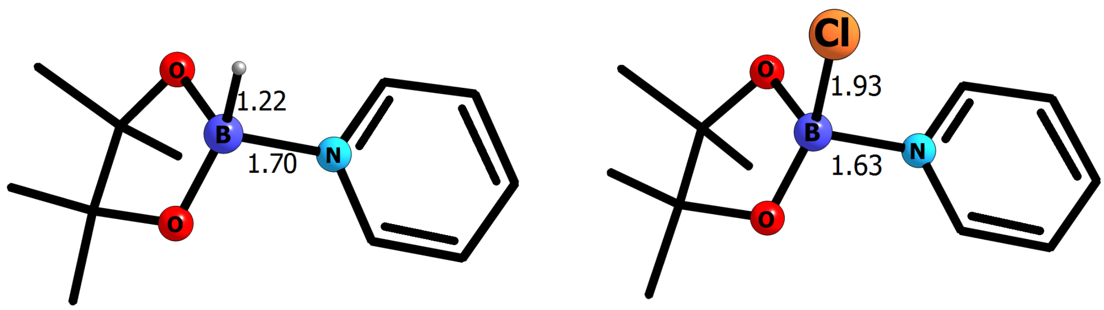
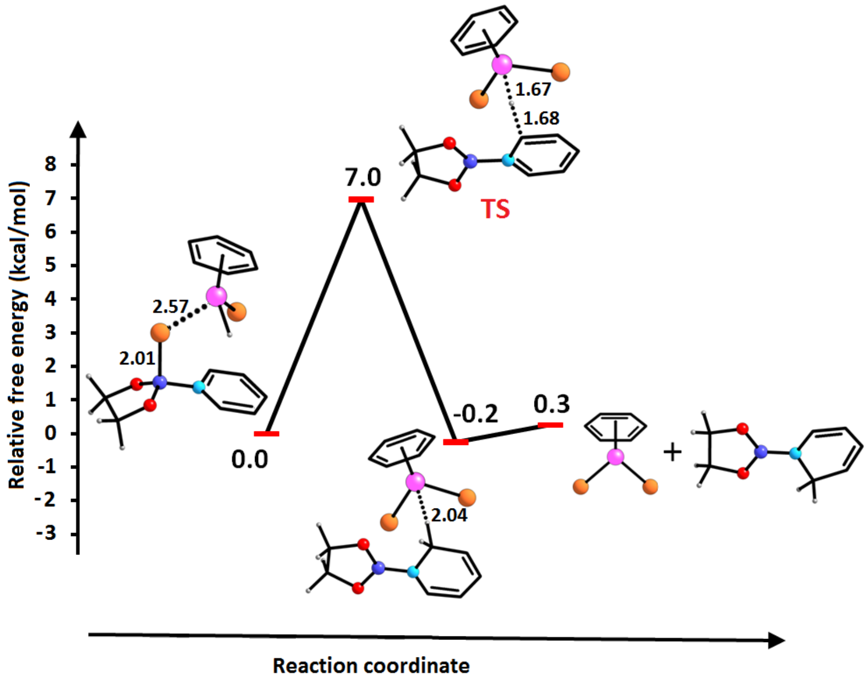
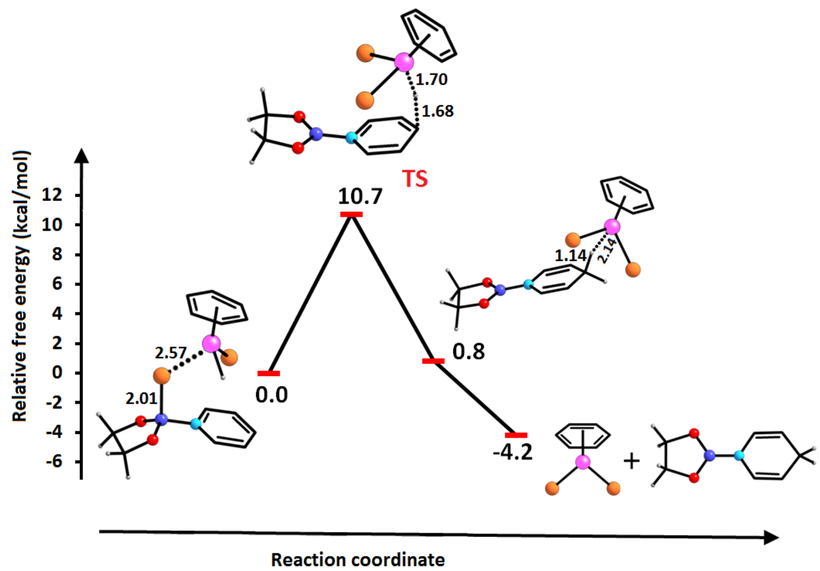


(16) (17)

Figure S1. Complex of HBpin (16) and ClBpin (17) with pyridine.



(a)



(b)

Figure S2. Mechanism for (a) 1,2-hydroboration and (b) 1,4-hydroboration using the 'reduced' model.

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