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Supporting Information

Transfer Hydrogenation of *N*-Heteroarenes with 2-Propanol and Ethanol Enabled by Manganese Catalysis

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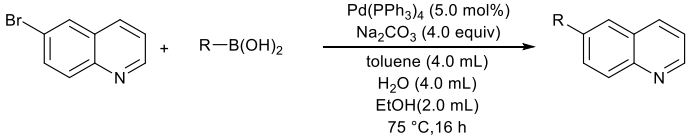
General remarks

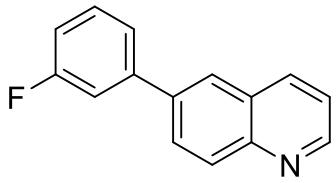
All catalytic reactions were performed under argon atmosphere using standard Schlenk techniques. Extra dry solvents were was purchased from Adamas and degassed before using. Other chemicals were obtained from commercial sources and were used without further purification. Substrate and catalysts **1g**,[1] **1k**,[2] **1n**,[3] **1o–1q**,[4] **1s–1u**,[4] **1w,**[5] **Mn-1–Mn-4**,[6] and **Mn-5**[7] were synthesized according to literatures methods. ^{1}H NMR, ^{13}C NMR , ^{31}P NMR and ^{19}F NMR spectra were recorded on a Bruker AV 400 or Bruker AV 600 spectrometer. Multiplicity is abbreviated as: s, singlet; d, doublet; dd, doublet of doublets; t, triplet; q, quartet; m, multiplet; br, broad. GC yields were determined by GC-FID, Agilent 8860 Network with FID detector, using *n*-hexadecane as an internal standard.

Synthesis of Substrates

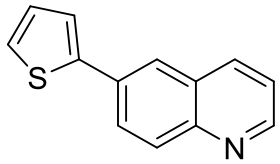
Synthesis of 6-arylquinoline:



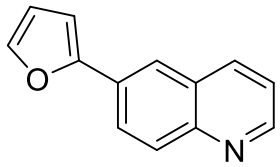
A Schlenk flask (50.0 mL) containing a stirring bar was sequentially charged with 6-bromo-quinoline (0.7 mL, 5.0 mmol, 1.0 equiv.), sodium carbonate (2.12 g, 20.0 mmol, 4.0 equiv.), boronic acid (6.0 mmol, 1.2 equiv.), water (4.0 mL), toluene (4.0 mL), ethanol (2.0 mL) and $Pd(PPh_3)_4$ (0.29 g, 0.25 mmol, 5.0 mol%) under argon, then the mixture was heated to 75–90 ℃ for 12–16 hours. Thereafter the mixture was filtered through a plug of celite, the filtrate was diluted with water (20.0 mL) and extracted with CH_2Cl_2 (3 x 20.0 mL). The combined organic phase were washed with brine (20.0 mL) and dried over $MgSO_4$. The drying agent was filtered off and the solvent was evaporated. The crude material was purified by chromatography on silica gel.



6-(3-Fluorophenyl)quinoline (1r): The procedure was followed using (3-fluorophenyl)boronic acid (839.5 mg, 6.0 mmol), 80 ^{o}C for 12 h. Purification by silica gel column chromatography (Petroleum ether/ Ethyl acetate: 50:1→10:1) yielded **1r** (0.92 g, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.93 (dd, J = 4.2, 1.7 Hz, 1H), 8.24–8.17 (m, 2H), 8.01–7.89 (m, 2H), 7.51–7.36 (m, 4H), 7.15–7.02 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ = 163.3 (d, $^{1}J_{C\text{-}F}$ = 245 Hz), 150.5, 147.6, 142.4 (d, $^{3}J_{C\text{-}F}$ = 8 Hz), 138.0 (d, $^{4}J_{C\text{-}F}$ = 2 Hz), 136.6, 130.5 (d, $^{3}J_{C\text{-}F}$ = 8 Hz), 129.9, 129.0, 128.4, 125.7, 123.1 (d, $^{4}J_{C\text{-}F}$ = 3 Hz), 121.6, 114.5 (d, $^{2}J_{C\text{-}F}$ = 21 Hz), 114.3 (d, $^{2}J_{C\text{-}F}$ = 23 Hz). ^{19}F NMR (565 MHz, $CDCl_3$) δ = -112.53. HR-MS (ESI): *m/z* calculated for $C_{15}H_{11}F_1N_1$ [M+H^{+}]: 224.0870, found: 224.0867.

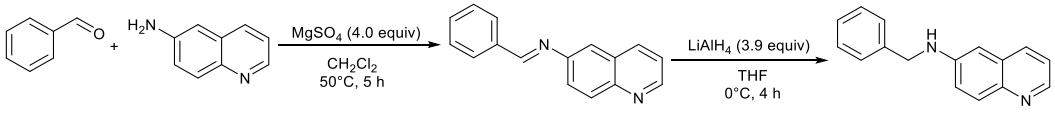


6-(Thiophen-2-yl)quinoline (1t): The procedure was followed using thiophen-2-ylboronic acid (767.8 mg, 6.0 mmol), 90 ℃ for 16 h. Purification by silica gel column chromatography (Petroleum ether/ Ethyl acetate: 40:1→5:1) yielded **1t** (1.05 g, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.88 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.17 (dd, *J* = 8.3, 1.6 Hz, 1H), 8.11 (d, *J* = 8.7 Hz, 1H), 8.03–7.97 (m, 2H), 7.47 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.41 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.36 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.14 (dd, *J* = 5.1, 3.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ = 150.3, 147.7, 143.5, 136.0, 132.6, 130.0, 128.6, 128.3, 128.0, 125.7, 124.1, 123.7, 121.7. HR-MS (ESI): *m/z* calculated for $C_{13}H_{10}S_1N_1$ [M+H$^+$]: 212.0528, found: 212.0526.



6-(Furan-2-yl)quinoline (1u): The procedure was followed using furan-2-ylboronic acid (685.0 mg, 6.0 mmol), 90 ℃ for 16 h. Purification by silica gel column chromatography (Petroleum ether/ Ethyl acetate: 40:1→5:1) yielded **1u** (0.95 g, 98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.87 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.16 (dd, *J* = 8.4, 1.7 Hz, 1H), 8.12–8.07 (m, 2H), 8.00 (dd, *J* = 8.9, 1.9 Hz, 1H), 7.54 (d, *J* = 1.7 Hz, 1H), 7.40 (dd, *J* = 8.3, 4.2 Hz, 1H), 6.81 (dd, *J* = 3.4, 0.7 Hz, 1H), 6.53 (dd, *J* = 3.4, 1.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ = 153.2, 150.1, 147.6, 142.8, 136.1, 129.8, 128.8, 128.5, 125.9, 121.6, 121.6, 112.0, 106.5. HR-MS (ESI): *m/z* calculated for $C_{13}H_{10}O_1N_1$ [M+H$^+$]: 196.0757, found: 196.0755.

Synthesis of *N*-benzylquinolin-6-amine:



Benzaldehyde (0.51 mL, 5.0 mmol) and quinolin-6-amine (0.720 mg, 5.0 mmol) were

dissolved in CH_2Cl_2 (20.0 mL), then $MgSO_4$ (2.407 g, 20.0 mmol) were added and the mixture was stirred at 50 ℃ for 5 hours. Afterwards, the mixture was filtered over Celite®. The filtrate was concentrated in *vacuum* to obtain a clear yellow liquid. Then dissolved in THF (8.0 mL) and cooled to 0 ℃. Lithium aluminium hydride (0.759 mg, 20 mmol) was added slowly to the solution and the mixture was stirred for 4 h. CH_2Cl_2 and small amount of MeOH and water was added, and then the mixture was extracted twice with CH_2Cl_2. The combined organic layer was washed with brine, dried over $MgSO_4$, filtered and concentrated in *vacuum*. The crude product was purified by silica gel column chromatography (Ethyl acetate/ Petroleum ether/ NEt_3= 50:50:1) to afford *N*-benzylquinolin-6-amine as a brown solid (0.714 g, 61%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.63–8.57 (m, 1H), 7.91–7.82 (m, 2H), 7.43–7.32 (m, 4H), 7.31–7.26 (m, 1H), 7.28–7.19 (m, 1H), 7.13–7.07 (m, 1H), 6.72–6.66 (m, 1H), 4.42 (s, 3H).

The analytical data are consistent with those previously reported literature. [8]

General procedure of catalytic experiments

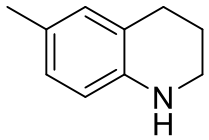
General procedure for the transfer hydrogenation of *N*-heteroarenes with *i*-Propanol:

In glovebox, a Schlenk sealed pressure tube (10.0 mL) containing a stirring bar was sequentially charged with **Mn-1** (2.0-3.0 mol%) and KO*t*-Bu (0.6 mmol, 1.2 equiv.). Afterwards, the reaction tube was capped and brought out of the glovebox. Then dry THF (1.0 mL), substrate (0.5 mmol, 1.0 equiv.) and *i*-Propanol (0.1 mL) were added under argon flow. Then the pressure tube was placed into a preheated aluminum block for 16−24 h. After the tube was cooled to ambient temperature, the reaction mixture was diluted with DCM (3.0 mL) and analyzed by GC using hexadecane as internal standard. The reaction mixture was purified by silica gel column chromatography to give the corresponding products.

General procedure for the transfer hydrogenation of *N*-heteroarenes with EtOH:

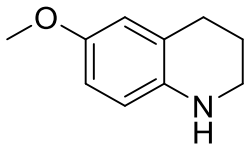
In glovebox, a Schlenk sealed pressure tube (10.0 mL) containing a stirring bar was sequentially charged with **Mn-2** (2.0 mol%) and KO*t*-Bu (0.6 mmol, 1.2 equiv.). Afterwards, the reaction tube was capped and brought out of the glovebox. Then dry 1,4-dioxane (1.0 mL), substrate (0.5 mmol, 1.0 equiv.) and EtOH (0.1 mL) were added under argon flow. Then the pressure tube was placed into a preheated aluminum block for 16 h. After the tube was cooled to ambient temperature, the reaction mixture was diluted with DCM (3.0 mL) and purified by silica gel column chromatography to give the corresponding products.

Characterization data of isolated products



6-Methyl-1,2,3,4-tetrahydroquinoline (2b): The procedure was followed using 6-methylquinoline (68 μL, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (8.3 mg, 0.015 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2b** (58.7 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.83–6.78 (m, 2H), 6.43 (d, J = 8.6 Hz, 1H), 3.50–3.06 (m, 3H), 2.76 (t, J = 6.5 Hz, 2H), 2.23 (s, 3H), 2.00–1.91 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 142.5, 130.1, 127.3, 126.3, 121.6, 114.5, 42.2, 27.0, 22.5, 20.4. HR-MS (ESI): *m/z* calculated for $C_{10}H_{14}N_1$ [M+H$^+$]: 148.1121, found: 148.1118.

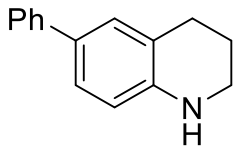
The analytical data are consistent with those previously reported literature. [9]



6-Methoxy-1,2,3,4-tetrahydroquinoline (2c): The procedure was followed using 6-methoxyquinoline (70 μL, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 100 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2c** (71.0 mg, 87%). ^{1}H NMR (600 MHz, $CDCl_3$) δ = 6.62–6.58 (m, 1H), 6.58–6.55 (m, 1H), 6.46 (d, J = 8.6 Hz, 1H), 3.73 (s, 3H), 3.28–3.23 (m, 2H), 3.20 (s, 1H), 2.76 (t, J = 6.5 Hz, 2H), 1.96–1.90 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 151.9, 138.9, 122.9, 115.7, 114.9, 112.9, 55.8, 42.4, 27.2, 22.5. HR-MS (ESI): *m/z* calculated for $C_{10}H_{14}N_1O_1$ [M+H$^+$]: 164.1070, found: 164.1068.

Ethanol as hydrogen source: The procedure was followed using 6-methoxyquinoline (70 μL, 0.5 mmol), EtOH (0.1 mL) and **Mn-2** (6.2 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2c** (49.0 mg, 60%).

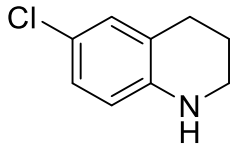
The analytical data are consistent with those previously reported literature. [9]



6-Phenyl-1,2,3,4-tetrahydroquinoline (2d): The procedure was followed using 6-phenylquinoline (102.7 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2d** (103.6 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.55–7.46 (m, 2H), 7.40–7.30 (m, 2H), 7.25–7.15 (m, 3H), 6.50–6.43 (m, 1H), 3.52 (s, 1H), 3.29–3.20 (m, 2H), 2.78 (t, J = 6.4 Hz, 2H), 1.96–1.87 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 144.4, 141.6, 129.9, 128.7, 128.3, 126.4, 126.0, 125.6, 121.7, 114.6, 42.1, 27.3, 22.3. HR-MS (ESI): *m/z* calculated for $C_{15}H_{16}N_1$ [M+H$^+$]: 210.1277, found: 210.1271.

Ethanol as hydrogen source: The procedure was followed using 6-phenylquinoline (102.7 mg, 0.5 mmol), EtOH (0.1 mL) and **Mn-2** (6.2 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2d** (86.5 mg, 83%).

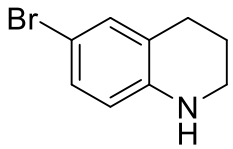
The analytical data are consistent with those previously reported literature. [10]



6-Chloro-1,2,3,4-tetrahydroquinoline (2e): The procedure was followed using 6-chloroquinoline (81.8 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2e** (79.6 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.93–6.87 (m, 2H), 6.41–6.35 (m, 1H), 3.66 (s, 1H), 3.33–3.23 (m, 2H), 2.72 (t, J = 6.4 Hz, 2H), 1.96–1.86 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 143.3, 129.0, 126.5, 122.9, 121.2, 115.1, 41.9, 26.9, 21.8. HR-MS (ESI):

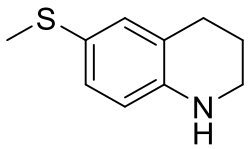
m/z calculated for $C_9H_{11}Cl_1N_1$ [M+H$^+$]: 168.0575, found: 168.0572.

The analytical data are consistent with those previously reported literature. [9]



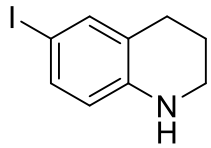
6-Bromo-1,2,3,4-tetrahydroquinoline (2f): The procedure was followed using 6-bromoquinoline (68 μL, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 100 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2f** (84.8 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.09–6.98 (m, 2H), 6.34 (d, J = 8.3 Hz, 1H), 3.77 (s, 1H), 3.32–3.24 (m, 2H), 2.73 (t, J = 6.4 Hz, 2H), 1.95–1.87 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 143.7, 131.9, 129.4, 123.4, 115.5, 108.2, 41.8, 26.8, 21.7. HR-MS (ESI): *m/z* calculated for $C_9H_{11}Br_1N_1$ [M+H$^+$]: 212.0069, found: 212.0068.

The analytical data are consistent with those previously reported literature. [11]

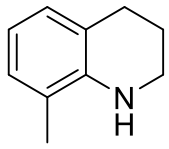


6-(Methylthio)-1,2,3,4-tetrahydroquinoline (2g): The procedure was followed using 6-(methylthio)quinoline (87.7 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 40:1→10:1) yielded **2g** (56.1 mg, 63%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.05–6.99 (m, 2H), 6.41 (d, J = 8.8 Hz, 1H), 3.83–3.05 (m, 3H), 2.74 (t, J = 6.4 Hz, 2H), 2.40 (s, 3H), 1.98–1.87 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 143.8, 131.8, 129.2, 123.4, 122.1, 114.7, 41.9, 26.9, 22.0, 19.4. HR-MS (ESI): *m/z* calculated for $C_{10}H_{14}N_1S_1$ [M+H$^+$]: 180.0841, found: 180.0836.

The analytical data are consistent with those previously reported literature. [12]

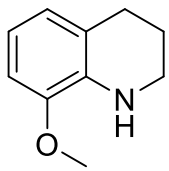


6-iodo-1,2,3,4-tetrahydroquinoline (2h): The procedure was followed using 6-iodoquinoline (127.5 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 100 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 80:1→50:1) yielded **2h** (41.4 mg, 32%, 90% purity). ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.15–7.05 (m, 2H), 6.32–6.22 (m, 1H), 5.87 (s, 1H), 3.18–3.12 (m, 2H), 2.62 (q, J = 6.0 Hz, 2H), 1.79–1.69 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ = 145.5, 137.2, 135.1, 123.5, 116.2, 75.4, 40.9, 26.8, 21.4. GC-MS m/z (relative intensity): 259 (100) [M^+], 260 (11), 258 (36), 132 (7), 131 (7), 130 (20). The analytical data are consistent with those previously reported literature.[13]



8-Methyl-1,2,3,4-tetrahydroquinoline (2i): The procedure was followed using 8-methylquinoline (70.1 μL, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (8.3 mg, 0.015 mmol), 120 ℃ for 24 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 80:1→50:1) yielded **2i** (57.5 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.98–6.83 (m, 2H), 6.65–6.58 (m, 1H), 3.44–3.39 (m, 2H), 2.84 (t, J = 6.4 Hz, 2H), 2.13 (s, 3H), 2.03–1.95 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 142.8, 127.9, 127.4, 121.2, 120.9, 116.5, 42.4, 27.4, 22.2, 17.2. HR-MS (ESI): *m/z* calculated for $C_{10}H_{14}N_1$ [$M+H^+$]: 148.1121, found: 148.1119.

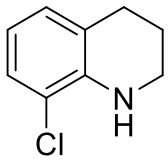
The analytical data are consistent with those previously reported literature. [9]



8-Methoxy-1,2,3,4-tetrahydroquinoline (2j): The procedure was followed using

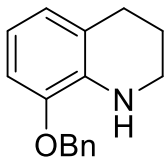
8-methoxyquinoline (79.4 μL, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2j** (65.2 mg, 80%). ^{1}H NMR (600 MHz, $CDCl_3$) δ = 6.67–6.62 (m, 2H), 6.62–6.58 (m, 1H), 4.25 (s, 1H), 3.85 (s, 3H), 3.38–3.33 (m, 2H), 2.81 (t, J = 6.4 Hz, 2H), 2.01-1.95 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 146.3, 134.6, 121.8, 121.4, 115.8, 107.4, 55.4, 41.6, 26.7, 22.2. HR-MS (ESI): *m/z* calculated for $C_{10}H_{14}N_1O_1$ [M+H$^+$]: 164.1070, found: 164.1069.

The analytical data are consistent with those previously reported literature. [14]



8-Chloro-1,2,3,4-tetrahydroquinoline (2k): The procedure was followed using 8-chloroquinoline (64.0 μL, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 100:1→80:1) yielded **2k** (56.1 mg, 67%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.11–7.04 (m, 1H), 6.90–6.83 (m, 1H), 6.52 (t, J = 7.7 Hz, 1H), 4.42 (s, 1H), 3.46–3.32 (m, 2H), 2.79 (t, J = 6.4 Hz, 2H), 2.00–1.88 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ = 140.7, 127.7, 126.8, 122.7, 118.0, 116.3, 41.8, 27.2, 21.7. HR-MS (ESI): *m/z* calculated for $C_9H_{11}Cl_1N_1$ [M+H$^+$]: 168.0575, found: 168.0572.

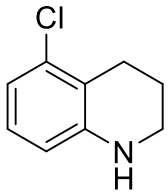
The analytical data are consistent with those previously reported literature. [11]



8-(Benzyloxy)-1,2,3,4-tetrahydroquinoline (2l): The procedure was followed using 8-(benzyloxy)quinoline (117.7 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2l** (89.7 mg, 75%). ^{1}H NMR

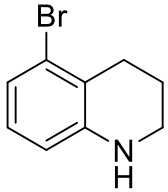
(400 MHz, $CDCl_3$) δ = 7.48–7.30 (m, 5H), 6.72–6.62 (m, 2H), 6.56 (t, *J* = 7.8 Hz, 1H), 5.06 (s, 2H), 4.30 (s, 1H), 3.37–3.29 (m, 2H), 2.80 (t, *J* = 6.4 Hz, 2H), 2.01–1.93 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 145.5, 137.4, 134.8, 128.6, 128.0, 127.7, 122.1, 121.6, 115.6, 108.9, 70.3, 41.5, 26.7, 22.1. HR-MS (ESI): *m/z* calculated for $C_{16}H_{18}N_1O_1$ [M+H$^+$]: 240.1383, found: 240.1380.

The analytical data are consistent with those previously reported literature. [15]



5-Chloro-1,2,3,4-tetrahydroquinoline (2m): The procedure was followed using 5-chloroquinoline (81.8 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2m** (59.1 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.88 (t, *J* = 8.0 Hz, 1H), 6.68 (d, *J* = 7.8 Hz, 1H), 6.37 (d, *J* = 8.0 Hz, 1H), 3.94 (s, 1H), 3.31–3.21 (m, 2H), 2.79 (t, *J* = 6.6 Hz, 2H), 1.96–1.92 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 146.4, 134.9, 127.1, 119.2, 117.5, 112.5, 41.4, 24.7, 21.9. HR-MS (ESI): *m/z* calculated for $C_9H_{11}Cl_1N_1$ [M+H$^+$]: 168.0574, found: 168.0573.

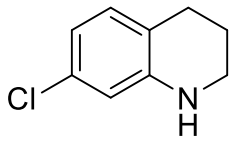
The analytical data are consistent with those previously reported literature. [16]



5-Bromo-1,2,3,4-tetrahydroquinoline (2n): The procedure was followed using 5-bromoquinoline (104.0 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 100 ℃ for 24 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2n** (71.0 mg, 67%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.89–6.76 (m, 2H), 6.44–6.38 (m, 1H), 3.92 (s, 1H), 3.31–

3.17 (m, 2H), 2.76 (t, J = 6.6 Hz, 2H), 2.01–1.89 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 146.5, 127.6, 126.0, 120.8, 120.7, 113.2, 41.5, 27.7, 22.2. HR-MS (ESI): *m/z* calculated for $C_9H_{11}Br_1N_1$ [M+H$^+$]: 212.0069, found: 212.0066.

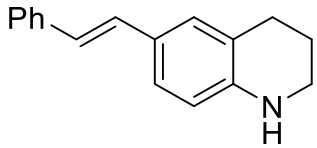
The analytical data are consistent with those previously reported literature. [12]



7-Chloro-1,2,3,4-tetrahydroquinoline (2o): The procedure was followed using 7-chloroquinoline (67.3 μL, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2o** (81.2 mg, 97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.89–6.77 (m, 2H), 6.38 (d, J = 8.4 Hz, 1H), 3.45 (s, 1H), 3.31–3.24 (m, 2H), 2.73 (t, J = 6.4 Hz, 2H), 2.00–1.91 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 143.3, 129.0, 126.5, 122.9, 121.2, 115.1, 41.9, 26.9, 21.8. HR-MS (ESI): *m/z* calculated for $C_9H_{11}Cl_1N_1$ [M+H$^+$]: 168.0575, found: 168.0581.

Ethanol as hydrogen source: The procedure was followed using 7-chloroquinoline (67.3 μL, 0.5 mmol), EtOH (0.1 mL) and **Mn-2** (6.2 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2o** (57.8 mg, 69%).

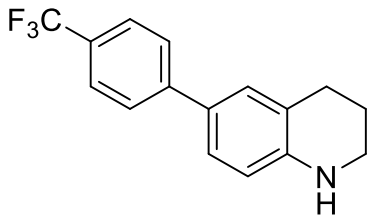
The analytical data are consistent with those previously reported literature. [17]



(*E*)-6-Styryl-1,2,3,4-tetrahydroquinoline (2p): The procedure was followed using (*E*)-6-styrylquinoline (115.6 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2p** (94 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.50–7.42 (m, 2H), 7.32 (t, J = 7.6 Hz, 2H), 7.22–7.09 (m, 3H),

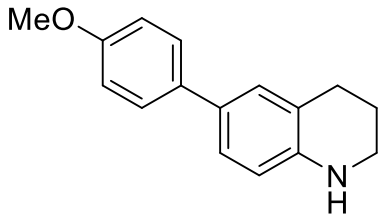
6.99 (d, J = 16.3 Hz, 1H), 6.87 (d, J = 16.3 Hz, 1H), 6.46 (d, J = 8.0 Hz, 1H), 3.99 (s, 1H), 3.39–3.30 (m, 2H), 2.79 (t, J = 6.3 Hz, 2H), 2.00–1.91 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 144.0, 138.2, 129.0, 128.6, 128.6, 127.9, 126.7, 126.0, 125.5, 124.3, 121.7, 114.5, 42.0, 27.0, 22.0. HR-MS (ESI): *m/z* calculated for $C_{17}H_{18}N_1$ [M+H$^+$]: 236.1434, found: 236.1429.

The analytical data are consistent with those previously reported literature. [11]

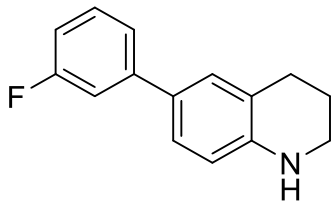


6-(4-(Trifluoromethyl)phenyl)-1,2,3,4-tetrahydroquinoline (2q): The procedure was followed using 6-(4-(trifluoromethyl)phenyl)quinoline (136.6 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2q** (118 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.66–7.57 (m, 4H), 7.25–7.21 (m, 2H), 6.55 (d, J = 8.0 Hz, 1H), 4.01 (s, 1H), 3.42–3.30 (m, 2H), 2.84 (t, J = 6.4 Hz, 2H), 2.02–1.94 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 145.1, 144.9 (d, $^5J_{C\text{-}F}$ = 1.4 Hz), 128.3, 128.0, 127.7(q, $^2J_{C\text{-}F}$ = 32 Hz), 125.6 (q, $^3J_{C\text{-}F}$ = 4 Hz), 124.6 (q, $^1J_{C\text{-}F}$ = 270 Hz), 126.2, 125.7, 121.6, 114.4, 41.9, 27.2, 22.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ = -62.13. HR-MS (ESI): *m/z* calculated for $C_{16}H_{15}F_3N_1$ [M+H$^+$]: 278.1151, found: 278.1148.

Ethanol as hydrogen source: The procedure was followed using 6-(4-(trifluoromethyl)phenyl)quinoline (136.6 mg, 0.5 mmol), EtOH (0.1 mL, 1.71 mmol) and **Mn-2** (6.2 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2q** (106.7 mg, 77%).

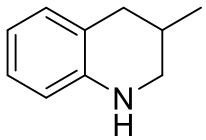


6-(4-Methoxyphenyl)-1,2,3,4-tetrahydroquinoline (2r): The procedure was followed using 6-(4-methoxyphenyl)quinoline (120.0 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 40:1→10:1) yielded **2r** (74.3 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.47–7.42 (m, 2H), 7.20–7.14 (m, 2H), 6.95–6.90 (m, 2H), 6.53 (d, J = 7.9 Hz, 1H), 3.83 (s, 3H), 3.39–3.29 (m, 2H), 2.82 (t, J = 6.4 Hz, 2H), 2.01–1.93 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.2, 143.8, 134.3, 129.8, 127.8, 127.3, 125.2, 121.7, 114.5, 114.1, 55.3, 42.1, 27.1, 22.3. HR-MS (ESI): *m/z* calculated for $C_{16}H_{18}N_1O_1$ [M+H$^+$]: 240.1383, found: 240.1378. The analytical data are consistent with those previously reported literature. [18]



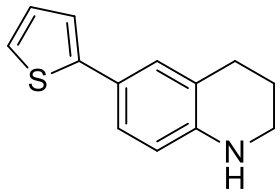
6-(3-Fluorophenyl)-1,2,3,4-tetrahydroquinoline (2s): The procedure was followed using 6-(3-fluorophenyl)quinoline (111.6 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2s** (97.4 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35–7.26 (m, 2H), 7.24–7.14 (m, 3H), 6.94–6.87 (m, 1H), 6.49 (d, J = 7.9 Hz, 1H), 3.68 (s, 1H), 3.35–3.26 (m, 2H), 2.80 (t, J = 6.4 Hz, 2H), 1.98–1.90 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.3 (d, $^{1}J_{C\text{-}F}$ = 245 Hz), 144.8, 143.9(d, $^{3}J_{C\text{-}F}$ = 8 Hz), 130.0 (d, $^{3}J_{C\text{-}F}$ = 9 Hz), 128.4 (d, $^{4}J_{C\text{-}F}$ = 2.2 Hz), 128.1, 125.5, 121.7 (d, $^{4}J_{C\text{-}F}$ = 2.5 Hz), 121.6, 114.4, 112.9 (d, $^{2}J_{C\text{-}F}$ = 22 Hz), 112. 5 (d, $^{2}J_{C\text{-}F}$ = 21 Hz), 42.0, 27.2, 22.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ = -113.61. HR-MS (ESI): *m/z* calculated for $C_{15}H_{15}F_1N_1$ [M+H$^+$]: 228.1183, found: 228.1179.

Ethanol as hydrogen source: The procedure was followed using 6-(3-fluorophenyl)quinoline (111.6 mg, 0.5 mmol), EtOH (0.1 mL) and **Mn-2** (6.2 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2s** (73.9 mg, 65%).



3-Methyl-1,2,3,4-tetrahydroquinoline (2t): The procedure was followed using 3-methylquinoline (67 μL, 0.5 mmol), *i*-PrOH (0.1 mL), and **Mn-1** (8.25 mg, 0.015 mmol), 120 ℃ for 24 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2t** (42.6 mg, 58%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.05–6.95 (m, 2H), 6.65 (t, J = 7.3 Hz, 1H), 6.51 (d, J = 7.9 Hz, 1H), 3.71 (s, 1H), 3.34–3.26 (m, 1H), 2.97–2.89 (m, 1H), 2.82 (dd, J = 16.0, 3.7 Hz, 1H), 2.47 (dd, J = 16.0, 10.3 Hz, 1H), 2.16–2.03 (m, 1H), 1.09 (d, J = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 144.4, 129.6, 126.8, 121.2, 117.0, 113.9, 48.9, 35.5, 27.2, 19.1. HR-MS (ESI): *m/z* calculated for $C_{10}H_{14}N_1$ [M+H$^+$]: 148.1121, found: 148.1119.

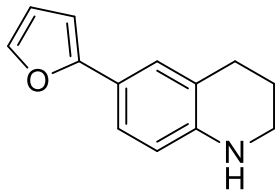
The analytical data are consistent with those previously reported literature. [9]



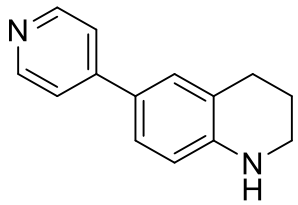
6-(Thiophen-2-yl)-1,2,3,4-tetrahydroquinoline (2u): The procedure was followed using 6-(thiophen-2-yl)quinoline (105.7 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2u** (105.6 mg, 98%).^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.28–7.20 (m, 2H), 7.17–7.10 (m, 2H), 7.06–7.00 (m, 1H), 6.44 (d, J = 8.0 Hz, 1H), 3.68 (s, 1H), 3.31–3.26 (m, 2H), 2.79 (t, J = 6.4 Hz, 2H), 1.98–1.90 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 145.6, 144.2, 127.8,

127.3, 124.8, 123.7, 122.6, 121.7, 120.8, 114.4, 42.0, 27.0, 22.0. HR-MS (ESI): *m/z* calculated for $C_{13}H_{14}N_1S_1$ [M+H$^+$]: 216.0841, found: 216.0839.

Ethanol as hydrogen source: The procedure was followed using 6-(thiophen-2-yl)quinoline (105.7 mg, 0.5 mmol), EtOH (0.1 mL) and **Mn-2** (6.2 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2u** (82.9 mg, 77%).

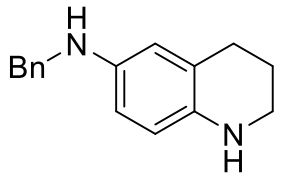


6-(Furan-2-yl)-1,2,3,4-tetrahydroquinoline (2v): The procedure was followed using 6-(furan-2-yl)quinoline (97.7 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **2v** (95.3 mg, 96%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.41–7.13 (m, 3H), 6.47–6.28 (m, 3H), 3.61 (s, 1H), 3.28–3.19 (m, 2H), 2.74 (t, *J* = 6.3 Hz, 2H), 1.94–1.83 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 155.1, 144.4, 140.6, 125.3, 122.9, 121.3, 120.3, 114.2, 111.5, 101.8, 42.0, 27.1, 22.1. HR-MS (ESI): *m/z* calculated for $C_{13}H_{14}N_1O_1$ [M+H$^+$]: 200.1070, found: 200.1068.

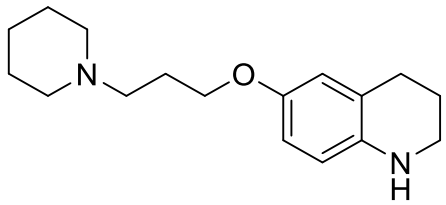


6-(Pyridin-4-yl)-1,2,3,4-tetrahydroquinoline (2w): The procedure was followed using 6-(pyridin-4-yl)quinoline (103.1 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (8.25 mg, 0.015 mmol), 120 ℃ for 24 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 5:1→1:1) yielded **2w** (71.3 mg, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.64–8.47 (m, 2H), 7.48–7.39 (m, 2H), 7.33–7.25 (m, 2H), 6.54 (d, *J* = 8.1 Hz, 1H), 4.09 (s, 1H), 3.42–3.30 (m, 2H), 2.83 (t, *J* = 6.3 Hz,

2H), 2.02–1.93 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 149.8, 148.5, 146.0, 128.0, 125.6, 125.5, 121.5, 120.3, 114.2, 41.9, 27.1, 21.8. HR-MS (ESI): *m/z* calculated for $C_{14}H_{15}N_2$ [M+H$^+$]: 211.1230, found: 211.1227.



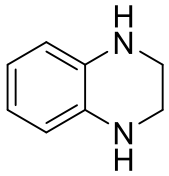
***N*-benzyl-1,2,3,4-tetrahydroquinolin-6-amine (2x)**: The procedure was followed using *N*-benzylquinolin-6-amine (117.1 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate/ Triethylamine: 10:1:0.1→6:3:0.1) yielded **2x** (64.3 mg, 54%). ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.38–7.26 (m, 4H), 7.23–7.17 (m, 1H), 6.36–6.12 (m, 3H), 4.98 (s, 2H), 4.31–3.93 (m, 2H), 3.21–2.86 (m, 2H), 2.65–2.45 (m, 2H), 1.77–1.68 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ = 141.6, 140.2, 137.3, 128.6, 127.7, 126.9, 121.7, 115.6, 114.3, 112.6, 48.2, 42.0, 27.4, 22.9. HR-MS (ESI): *m/z* calculated for $C_{16}H_{17}N_2$ [M$^+$]: 237.1386, found: 237.1382.



6-(3-(Piperidin-1-yl)propoxy)-1,2,3,4-tetrahydroquinoline (2y): The procedure was followed using 6-(3-(piperidin-1-yl)propoxy)quinoline (135.2 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate/ Triethylamine: 8:2:0.2→7:3:0.2) yielded **2y** (84.9mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.61–6.51 (m, 2H), 6.45–6.39 (m, 1H), 3.90 (t, *J* = 6.4 Hz, 2H), 3.57 (s, 1H), 3.27–3.19 (m, 2H), 2.73 (t, *J* = 6.5 Hz, 2H), 2.50–2.32 (m, 6H), 1.97–1.85 (m, 4H), 1.63–1.53 (m, 4H), 1.43 (q, *J* = 5.6, 5.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 151.2, 138.9, 122.9, 115.9, 115.5, 113.8, 67.3, 56.2, 54.6, 42.4, 27.2, 27.0, 26.0, 24.5, 22.5. HR-MS

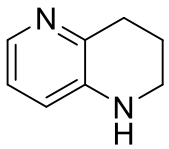
(ESI): *m/z* calculated for $C_{17}H_{27}N_2O_1$ [M+H$^+$]: 275.2118, found: 275.2114.

The analytical data are consistent with those previously reported literature. [5]



1,2,3,4-Tetrahydroquinoxaline (4a): The procedure was followed using quinoxaline (65.5 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **4a** (50.6 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.61–6.56 (m, 2H), 6.52–6.47 (m, 2H), 3.42 (s, 4H), 3.06 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 133.6, 118.9, 114.8, 41.4. HR-MS (ESI): *m/z* calculated for $C_8H_{11}N_2$ [M+H$^+$]: 135.0917, found: 135.0916.

The analytical data are consistent with those previously reported literature. [11]

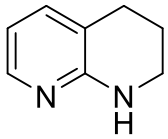


1,2,3,4-Tetrahydro-1,5-naphthyridine (4b): The procedure was followed using 1,5-naphthyridine (65.1 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 40:1→10:1) yielded **4b** (47.4 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.85 (dd, *J* = 4.7, 1.2 Hz, 1H), 6.88 (dd, *J* = 8.0, 4.7 Hz, 1H), 6.72 (dd, *J* = 8.0, 1.3 Hz, 1H), 3.81 (s, 1H), 3.34–3.25 (m, 2H), 2.93 (t, *J* = 6.5 Hz, 2H), 2.05–1.97 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 142.7, 141.0, 137.9, 121.9, 120.3, 41.5, 30.3, 21.8. HR-MS (ESI): *m/z* calculated for $C_8H_{11}N_2$ [M+H$^+$]: 135.0917, found: 135.0915.

Ethanol as hydrogen source: The procedure was followed using 1,5-naphthyridine (65.1 mg, 0.5 mmol), EtOH (0.1 mL) and **Mn-2** (6.2 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate:

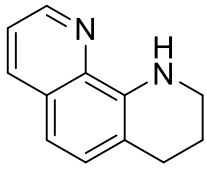
50:1→20:1) yielded **4b** (48.2 mg, 72%).

The analytical data are consistent with those previously reported literature. [11]



1,2,3,4-Tetrahydro-1,8-naphthyridine (4c): The procedure was followed using 1,8-naphthyridine (65.1 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 10:1→2:1) yielded **4c** (47.4 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.87–7.80 (m, 1H), 7.14–7.08 (m, 1H), 6.49–6.42 (m, 1H), 4.99 (s, 1H), 3.43–3.35 (m, 2H), 2.70 (t, *J* = 6.3 Hz, 2H), 1.94–1.86 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 156.3, 145.8, 136.2, 116.1, 112.5, 41.5, 26.7, 21.3. HR-MS (ESI): *m/z* calculated for $C_8H_{11}N_2$ [M+H$^+$]: 135.0917, found: 135.0916.

The analytical data are consistent with those previously reported literature. [12]



1,2,3,4-Tetrahydro-1,10-phenanthroline (4d): The procedure was followed using 1,10-phenanthroline (90.1 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **4d** (85.6 mg, 93%). ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.69 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.00 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.29 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.17 (d, *J* = 8.2 Hz, 1H), 6.98 (d, *J* = 8.2 Hz, 1H), 5.96 (s, 1H), 3.58–3.46 (m, 2H), 2.93 (t, *J* = 6.4 Hz, 2H), 2.04–1.95 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 146.9, 140.7, 137.5, 135.9, 129.1, 127.4, 120.6, 116.6, 113.1, 41.3, 27.1, 21.9. HR-MS (ESI): *m/z* calculated for $C_{12}H_{13}N_2$ [M+H$^+$]: 185.1073, found: 185.1071.

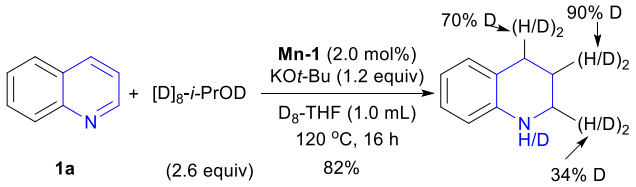
Ethanol as hydrogen source: The procedure was followed using 1,10-phenanthroline

(90.1 mg, 0.5 mmol), EtOH (0.1 mL) and **Mn-2** (6.2 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **4d** (74.3 mg, 81%).

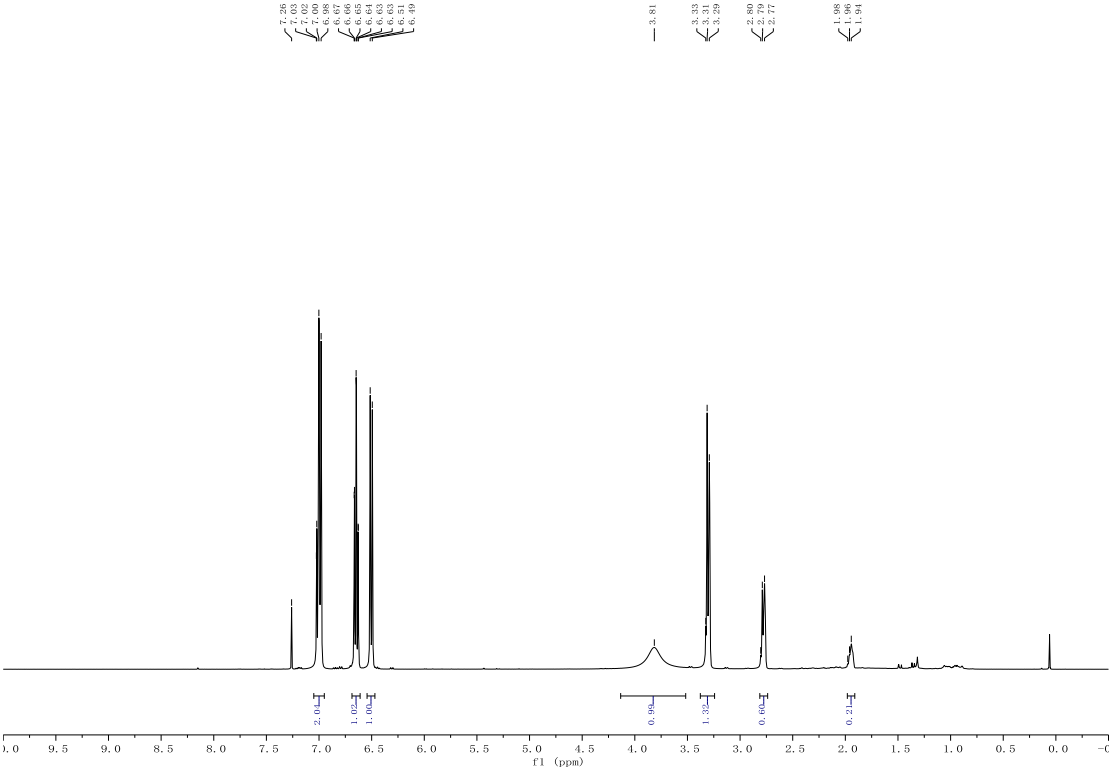
The analytical data are consistent with those previously reported literature. [12]

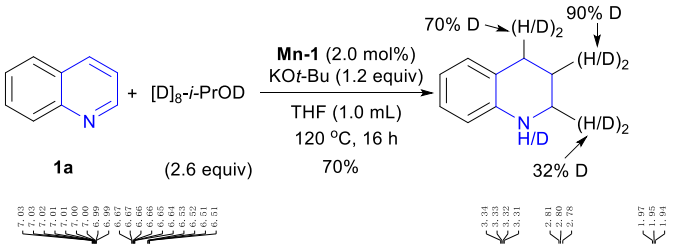
Experimental mechanistic studies

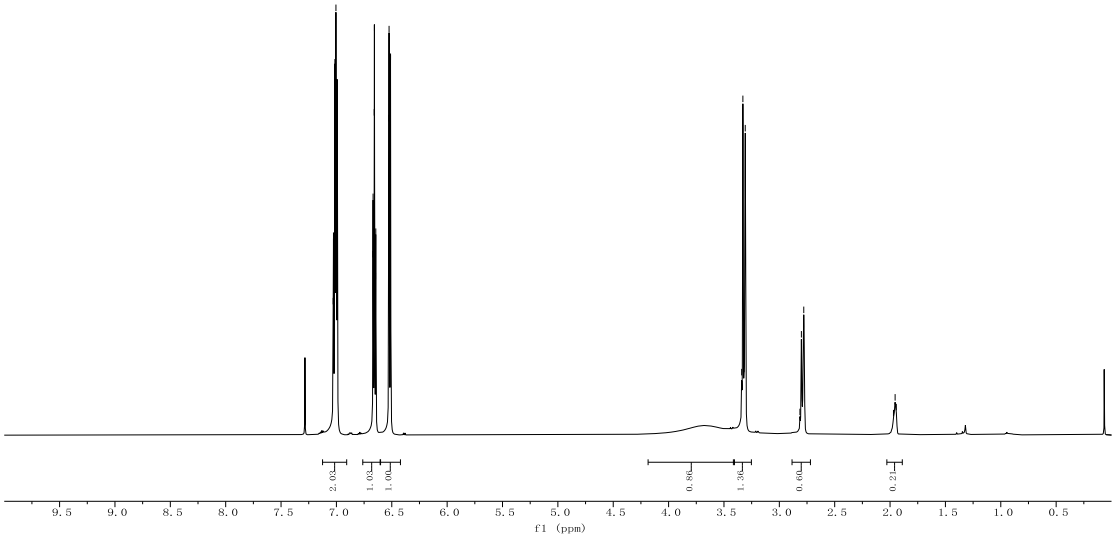
Transfer hydrogenation of 1a with D_8-*i*-PrOH



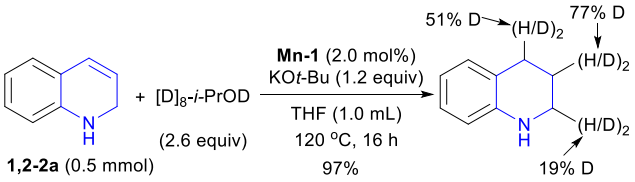
In glove box, a Schlenk sealed pressure tube (10.0 mL) containing a stirring bar was sequentially charged with **Mn-1** (2.0 mol%), KO*t*-Bu (0.6 mmol, 1.2 equiv.), D_8-THF (1.0 mL), **1a** (0.5 mmol, 1.0 equiv.) and D_8-*i*-Propanol (0.1 mL). Then the pressure tube was placed into a preheated aluminum block for 16 h. After the tube was cooled to ambient temperature, the reaction mixture was diluted with DCM (3.0 mL). The reaction mixture was purified by silica gel column chromatography to give the corresponding products.



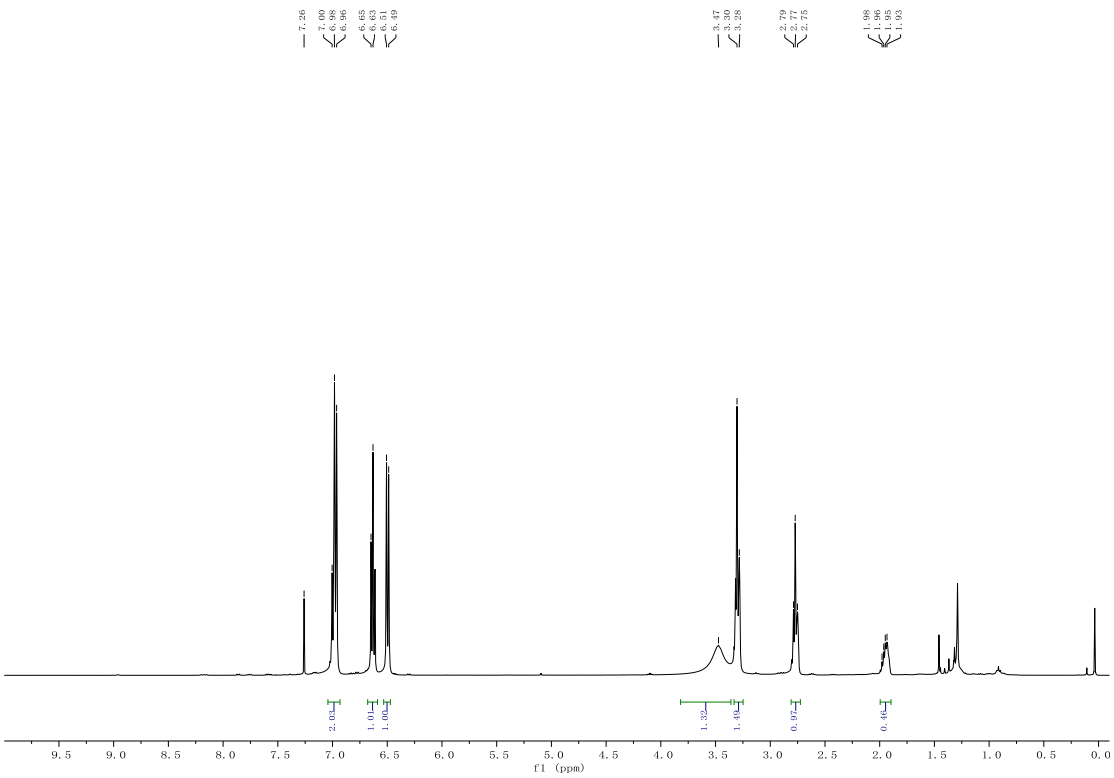




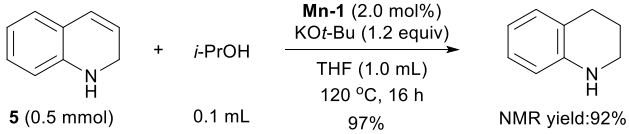
Transfer hydrogenation of 1,2-dihydroquinoline with D_8-*i*-PrOH



The procedure was followed using **1,2-2a** (65.5 mg, 0.5 mmol), D_8-*i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 80:1→40:1) yielded **2a** (65.5 mg, 97%).

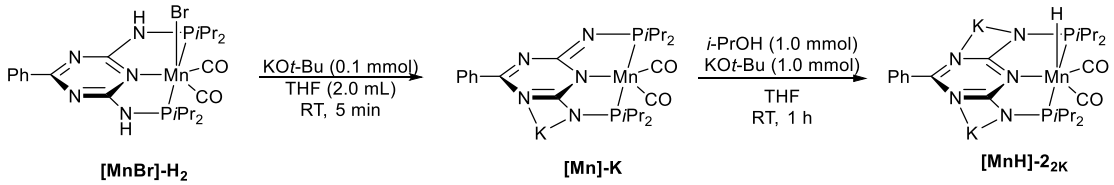


Transfer hydrogenation of 1,2-dihydroquinoline with *i*-PrOH



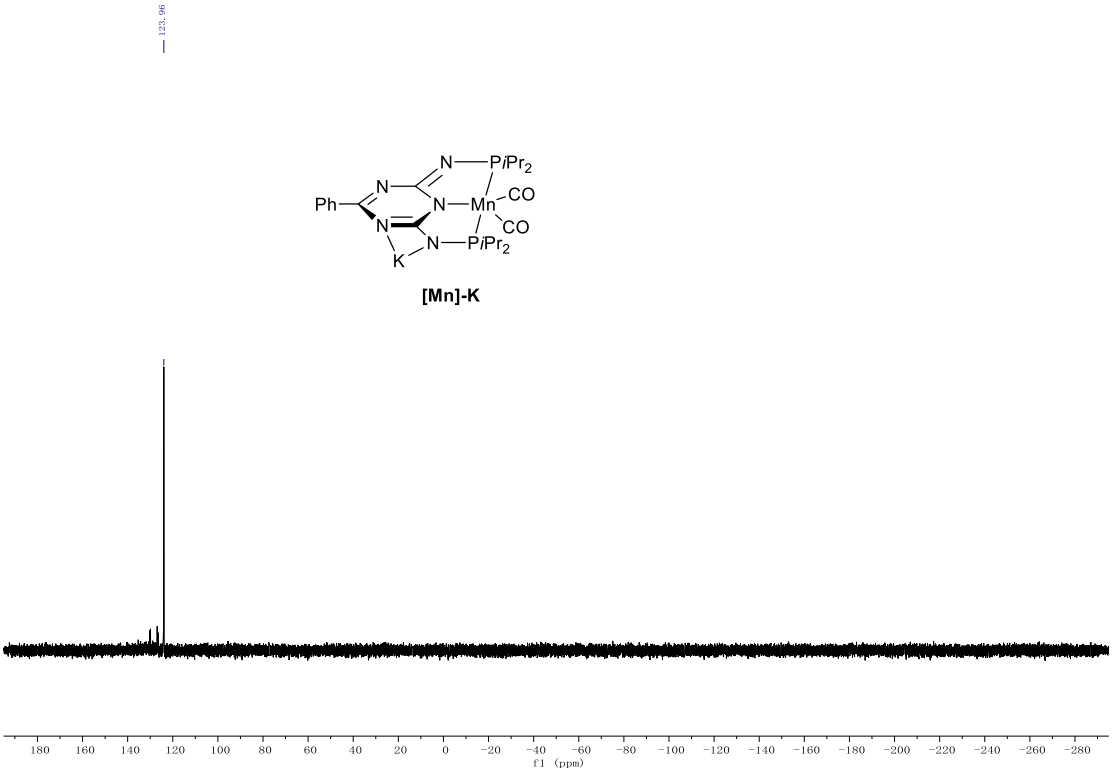
The procedure was followed using **1,2-2a** (65.5 mg, 0.5 mmol), *i*-PrOH (0.1 mL) and **Mn-1** (5.5 mg, 0.01 mmol), 120 ℃ for 16 h. The yield of **2a** was determined to be 92% by ^{1}H-NMR using CH_2Br_2 as internal standard.

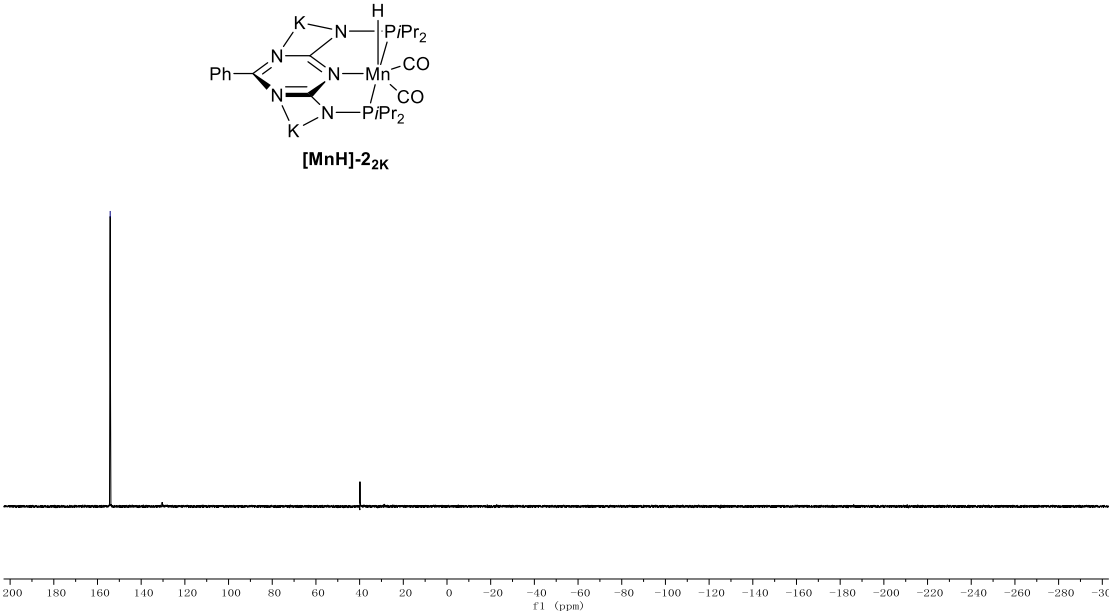
Determination of [MnH]-2_{2K}



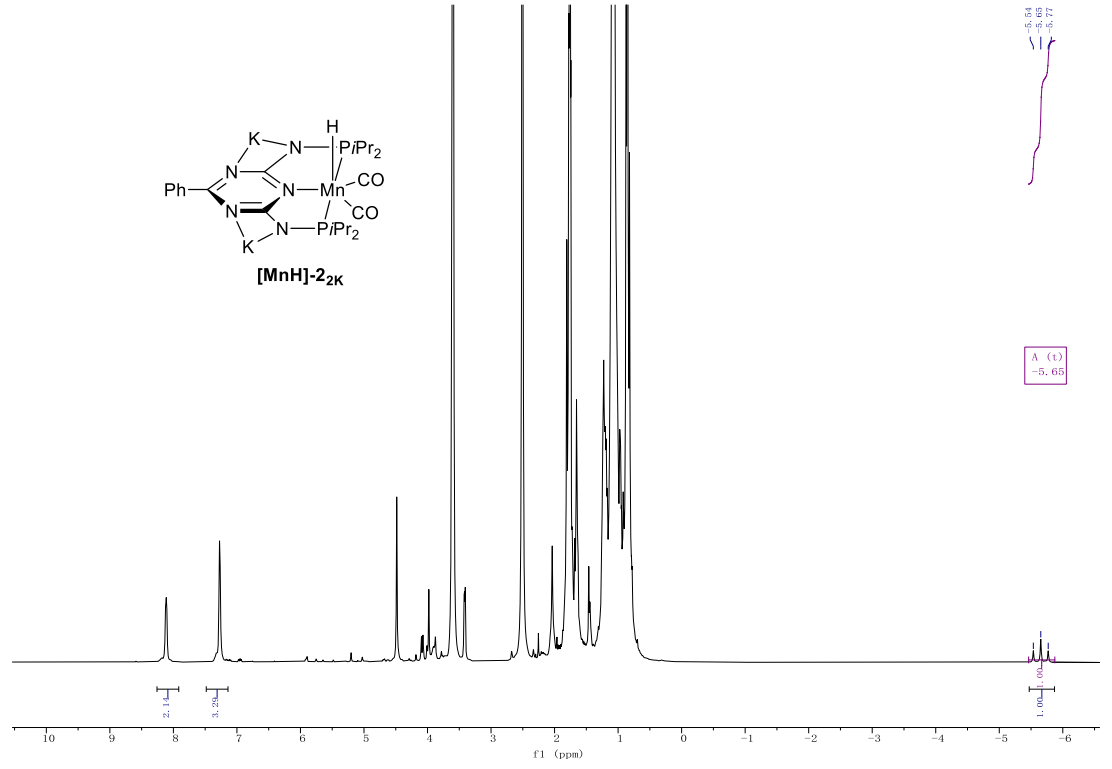
In glove box, a Schlenk sealed pressure tube (10.0 mL) containing a stirring bar was sequentially charged with **Mn-2** (31 mg, 0.05 mmol), KO*t*-Bu (11.2 mg, 0.1 mmol) and THF (2.0 mL). After generating the catalyst, an aliquot of the solution was transferred into a NMR-tube equipped with DMSO-d_6, and a ^{31}P NMR experiment

was conducted. Afterwards, *i*-PrOH (1.0 mmol) and KO*t*-Bu (112 mg, 1.0 mmol) was added to the reaction tube. The reaction mixture was stirred for one hour at room temperature. A color change from green to red could be observed. After the reaction time the red solution was transferred into a NMR-tube equipped with DMSO-d_6, ^{31}P NMR and ^{1}H NMR experiment was conducted.



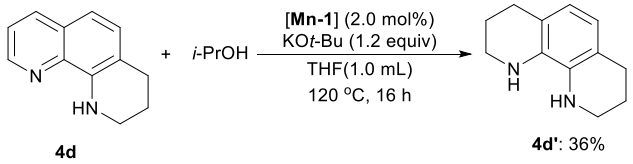


[MnH]-2$_{2K}$



[MnH]-2$_{2K}$

Transfer hydrogenation of 1,2,3,4-tetrahydro-1,10-phenanthroline

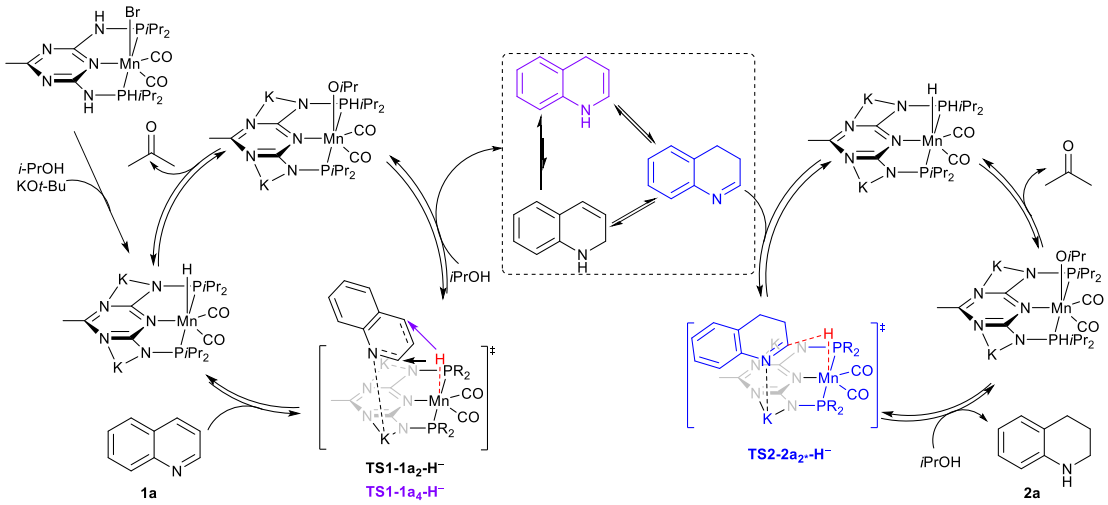


1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (4d'): The procedure was followed using 1,2,3,4-tetrahydro-1,10-phenanthroline (0.4 mmol), KO*t*-Bu (0.48 mmol), *i*-PrOH (0.08 mL) and **Mn-1** (4.4mg, 0.008 mmol), 120 ℃ for 16 h. Purification by column chromatography of Silica gel (Petroleum ether/ Ethyl acetate: 50:1→20:1) yielded **4d'** (27.8 mg, 37%). ^{1}H NMR (600 MHz, $CDCl_3$) δ = 6.47 (s, 2H), 3.39–3.26 (m, 4H), 3.58–3.10(m, 2H), 2.75 (t, J = 6.3 Hz, 4H), 1.95–1.86 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ = 132.9, 120.5, 119.2, 42.7, 27.0, 22.6.

GC-MS m/z (relative intensity): 188 (100) [M^+], 189 (13), 187 (40), 160 (14), 159 (29). The analytical data are consistent with those previously reported literature. [19]

Proposed mechanism cycle

Based on the experimental and DFT calculation studies, a mechanism for the Mn-catalysed transfer hydrogenation of quinoline (**1a**) was proposed (Scheme S1). The catalytically active species **MnH-1$_{2K}$** was generated in the presence of KO*t*-Bu and *i*-PrOH. Subsequently, hydride transfer from **MnH-1$_{2K}$** to the carbon of **1a** via nucleophilic attack, and then protonation of hydroquinoline anion intermediates by *i*-PrOH result in the formation of dihydroquinolines. The active species **MnH-1$_{2K}$** was regenerated through releasing acetone from **Mn-O*i*Pr**. Due to the free energy barrier for catalyst regeneration is higher than that of 1,2-, 3,4- and 1,4-dihydroquinoline formation, the isomerization of among these three dihydroquinolines can be occurred before catalyst regeneration. Once the intermediate 3,4-dihydroquinoline (**3,4-2a**) was formed, it is easily hydrogenated to furnish **2a** *via* an outer sphere hydrogen-transfer manner.



Scheme S1. Proposed mechanism cycle for manganese catalysed transfer hydrogenation of quinoline (**1a**)

DFT Calculations

Density functional theory calculations were performed with Gaussian 16 program[20] by using quinoline (**1a**) as model substrate and *i*PrOH as the hydrogen source. Herein, geometry optimizations and frequency calculations were performed at the M06L/def2-SVP[21] level. All optimized structures were characterized either as energy minimums without imaginary frequencies or transition states with only one imaginary mode, and the imaginary model connects the initial and the final states. The thermal correction to Gibbs free energy at 298 K from the frequency analysis was added to the total electronic energy calculated at M06L-SCRF(SMD)/def2-TZVP[21b, 21c] level under the consideration of solvation effect by using SMD solvation model[22] and THF as solvent.

Gibbs free energy profiles for Mn-5 as catalyst

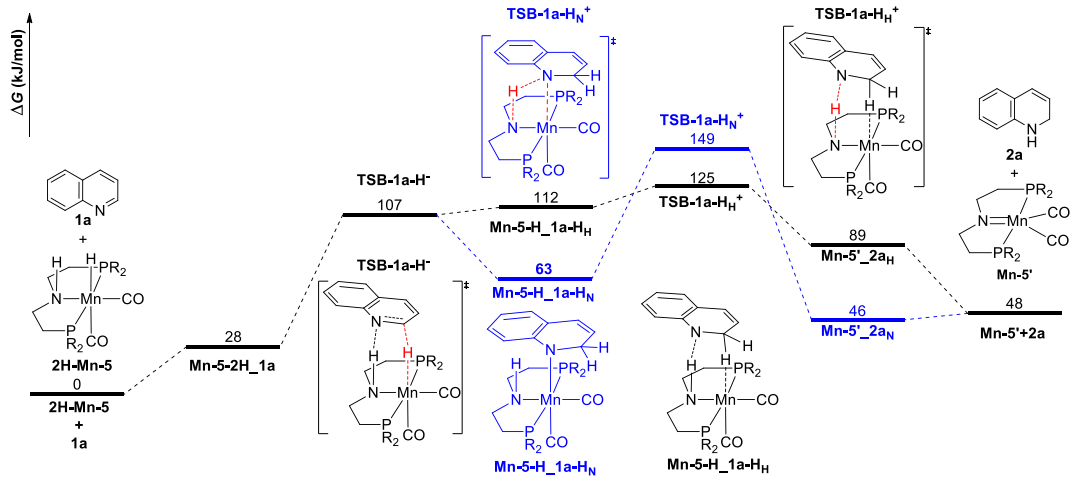


Figure S1. Gibbs free energy profile for amine complex of **2H-Mn-5** catalyzed quinoline (**1a**) hydrogenation to 1,2-dihydroquinoline (**2a**) and amido complex **Mn-5'** (R = *i*Pr)

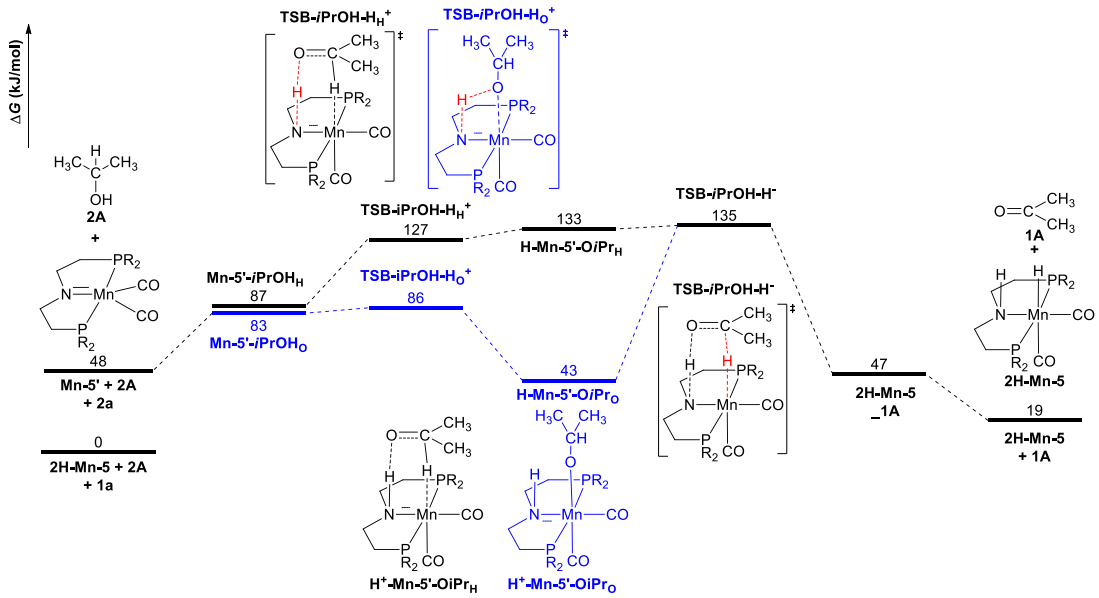
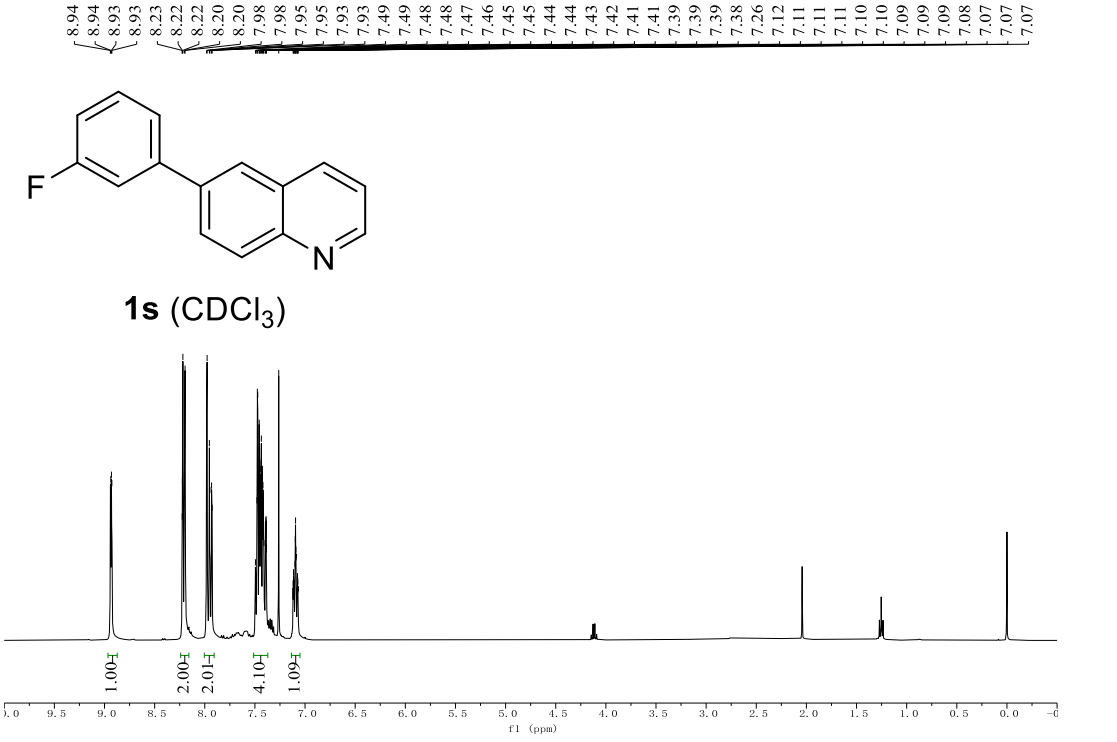


Figure S2. Gibbs free energy profile for dehydrogenation *i*-PrOH and regeneration of **2H-Mn-5** (R = *i*Pr)

NMR Spectra: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8.93
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8.22
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8.20
8.20
7.98
7.98
7.95
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7.93
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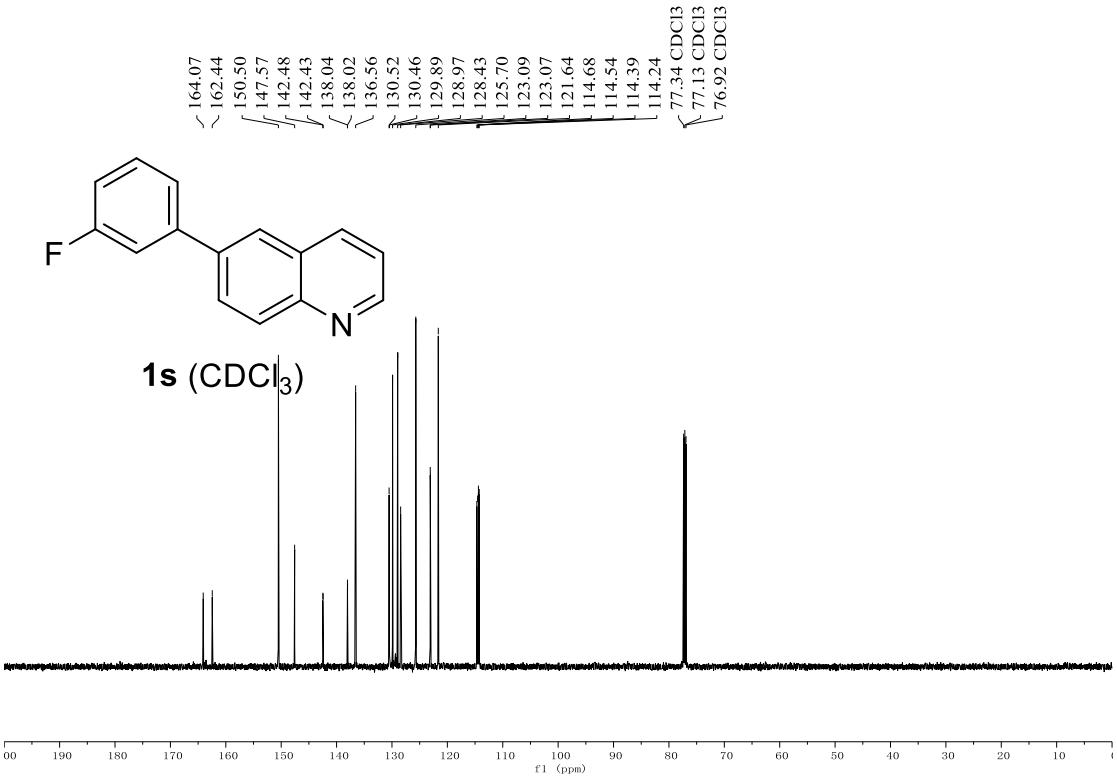
7.49
7.48
7.48
7.47
7.46
7.45
7.45
7.44
7.44
7.43
7.42
7.41
7.41
7.39
7.39
7.39
7.38
7.26
7.12
7.11
7.11
7.11
7.10
7.10
7.09
7.09
7.09
7.08
7.07
7.07
7.07
F
N
1s (CDCl3)
1.00
2.00
2.01
4.10
1.09
f1 (ppm)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162.44
150.50
147.57
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142.43
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138.02
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130.52
130.46
129.89
128.97
128.43
125.70
123.09
123.07
121.64
114.68
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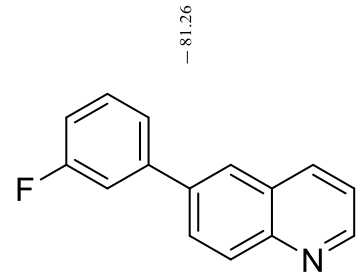
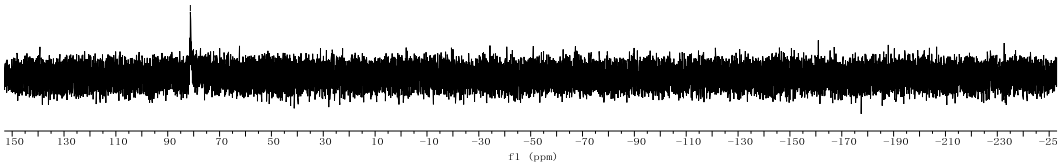
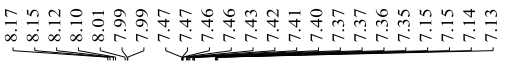
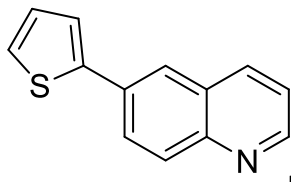
76.92 CDCl3
F
N
1s (CDCl3)
f1 (ppm)



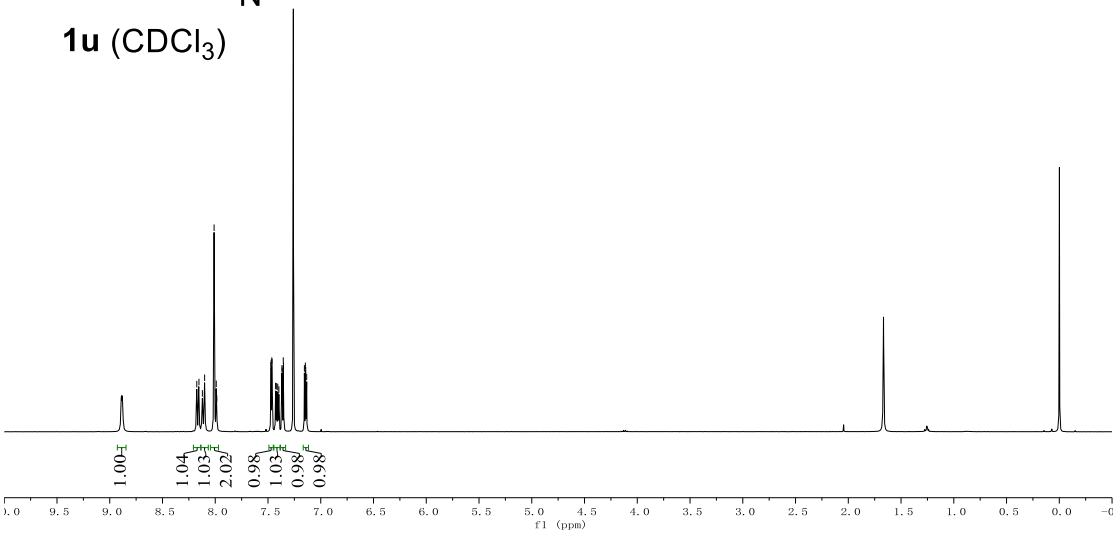
1s ($CDCl_3$)

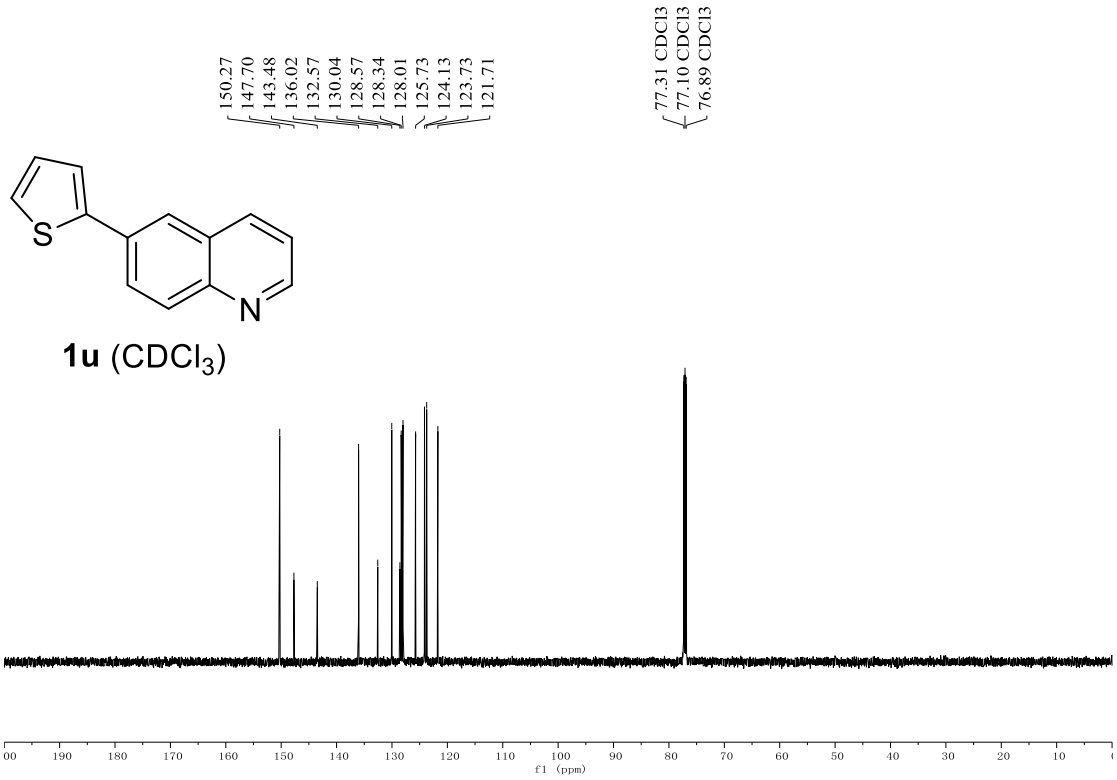




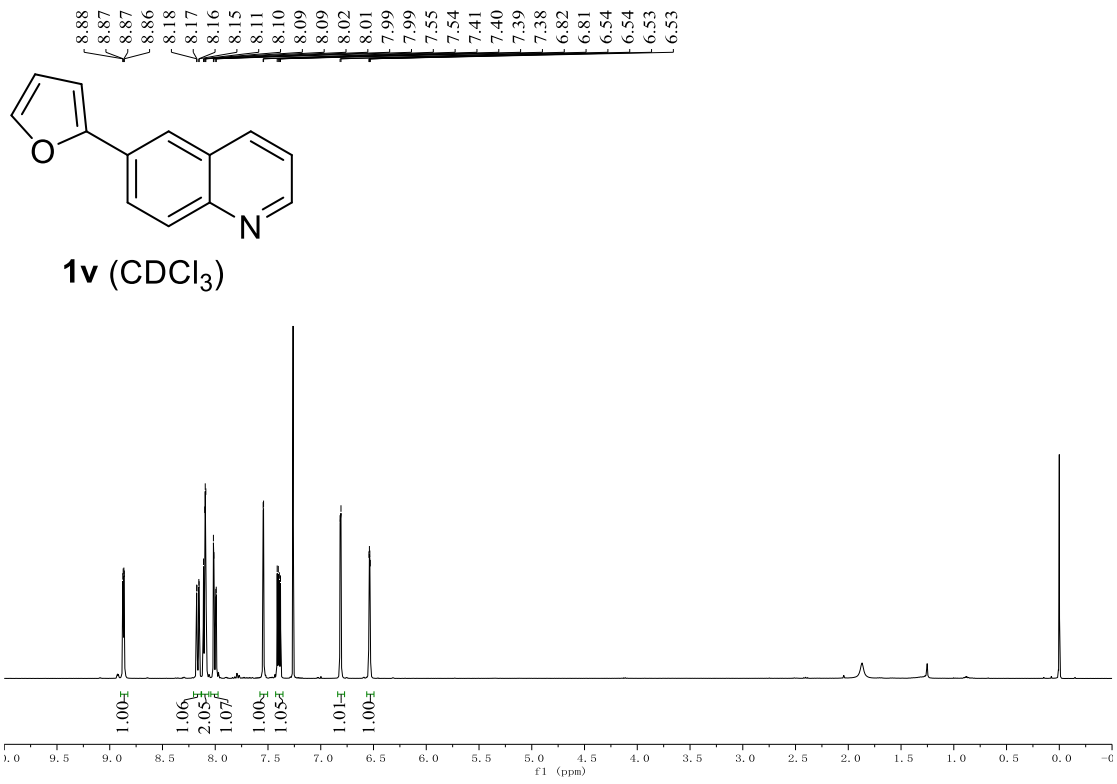


1u ($CDCl_3$)

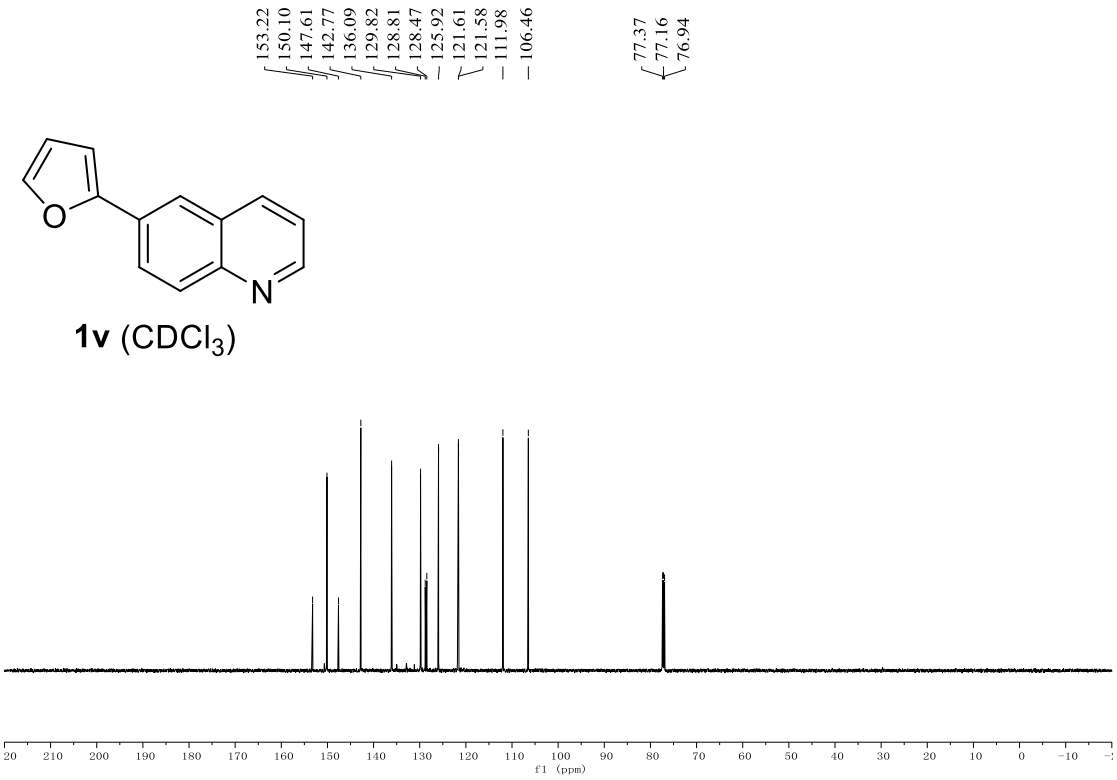




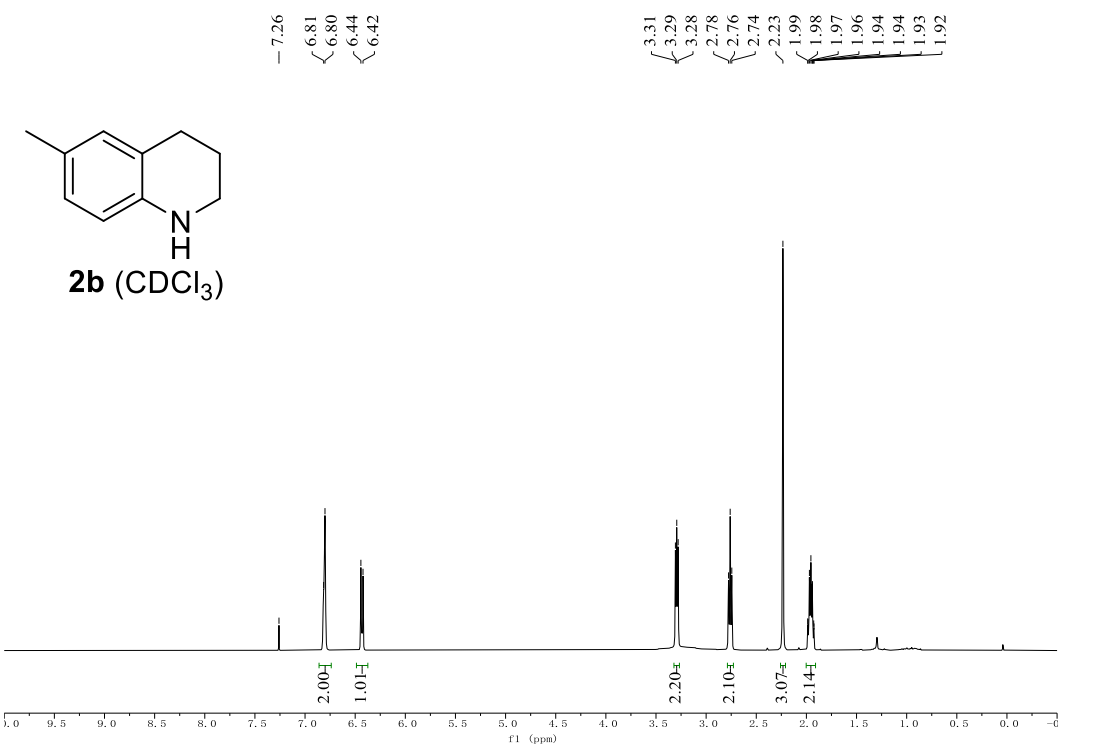
1u ($CDCl_3$)



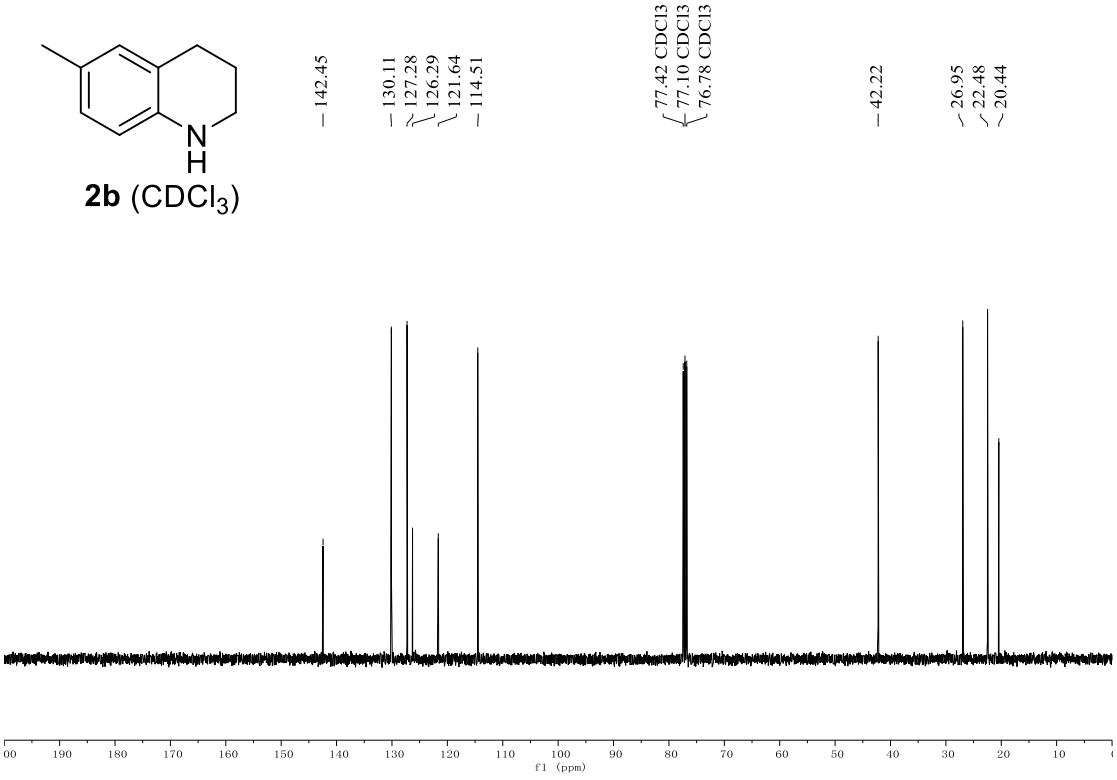
1v ($CDCl_3$)



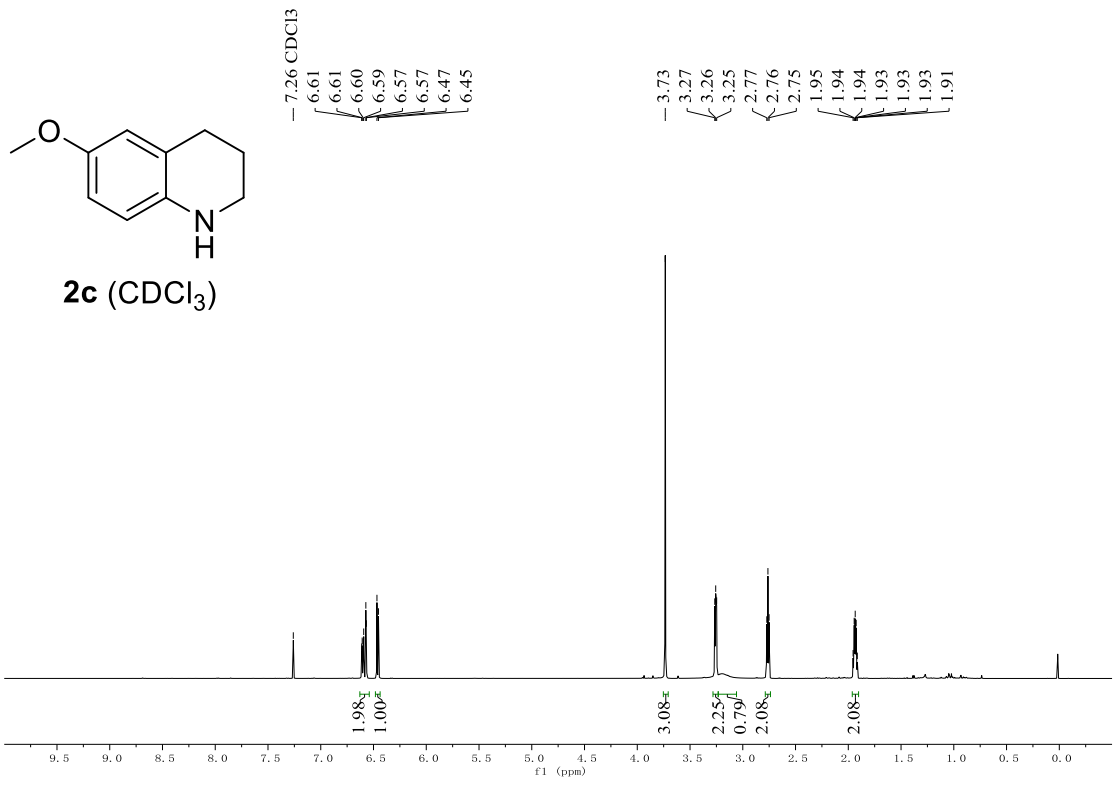
1v ($CDCl_3$)



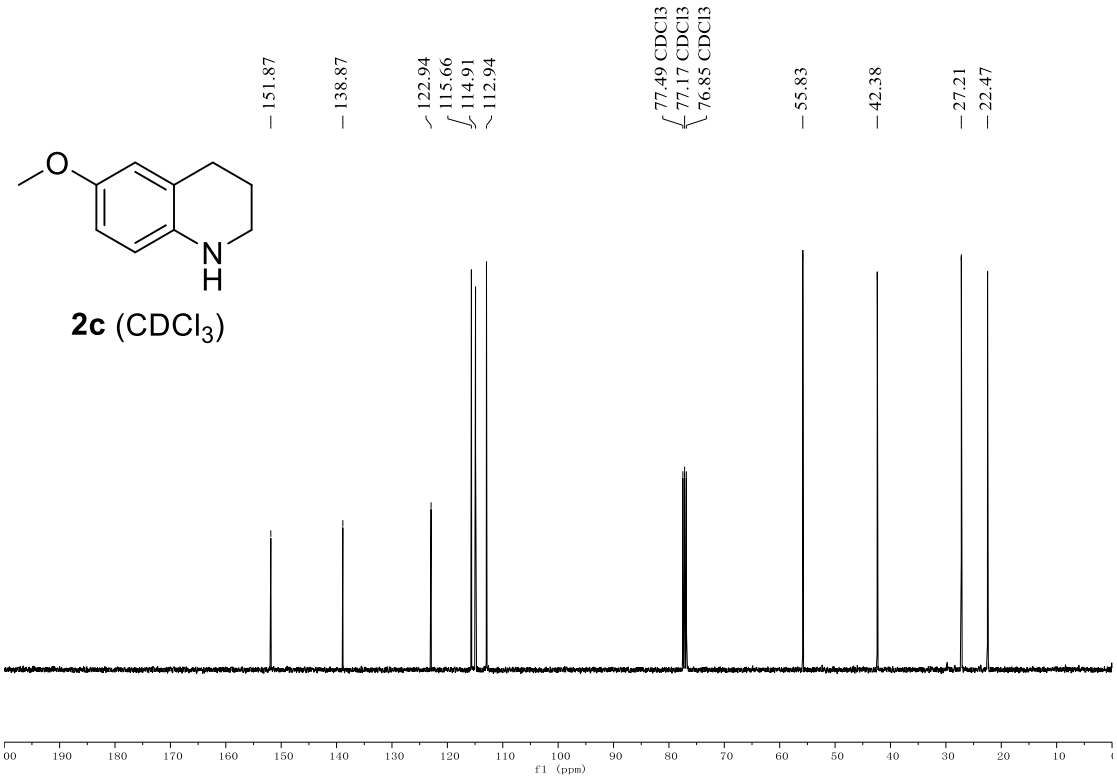
2b ($CDCl_3$)



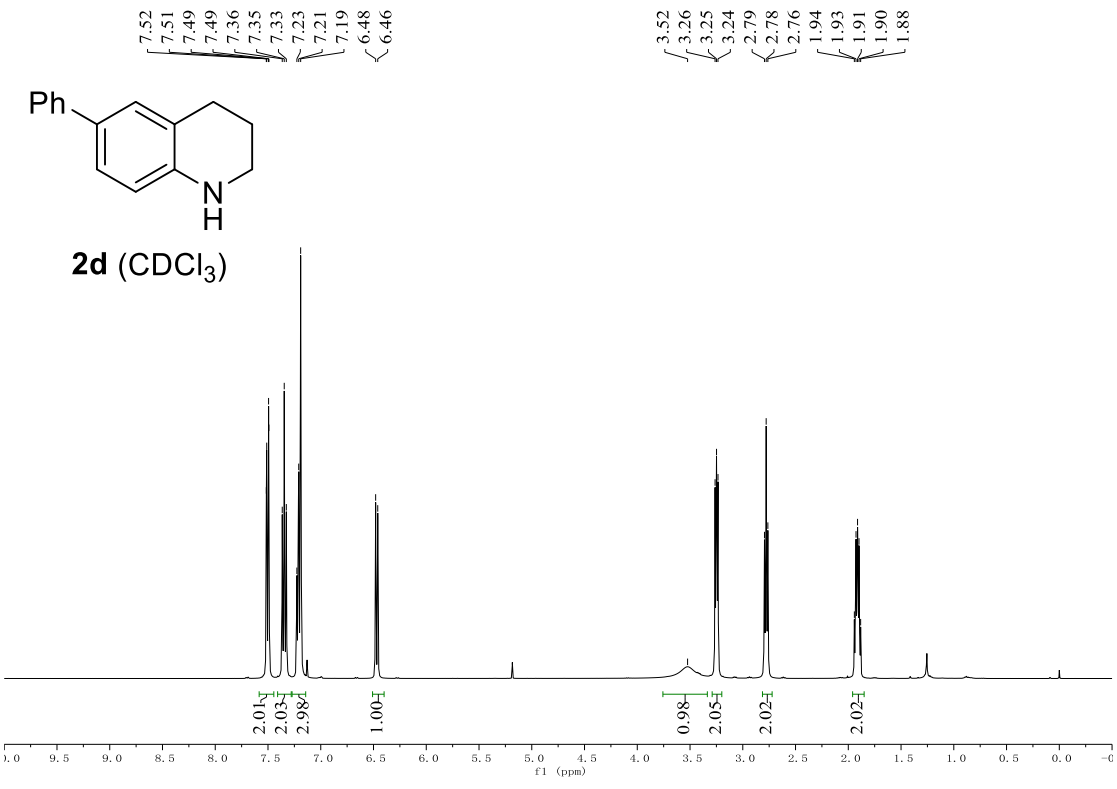
2b ($CDCl_3$)



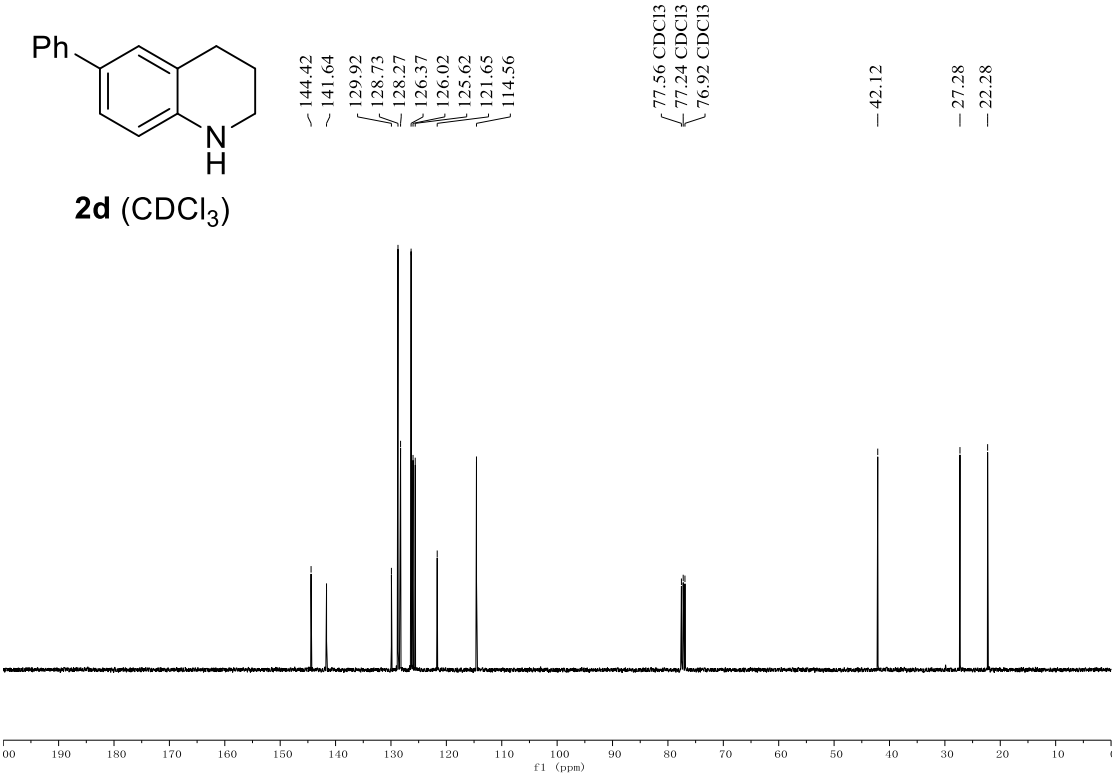
2c ($CDCl_3$)



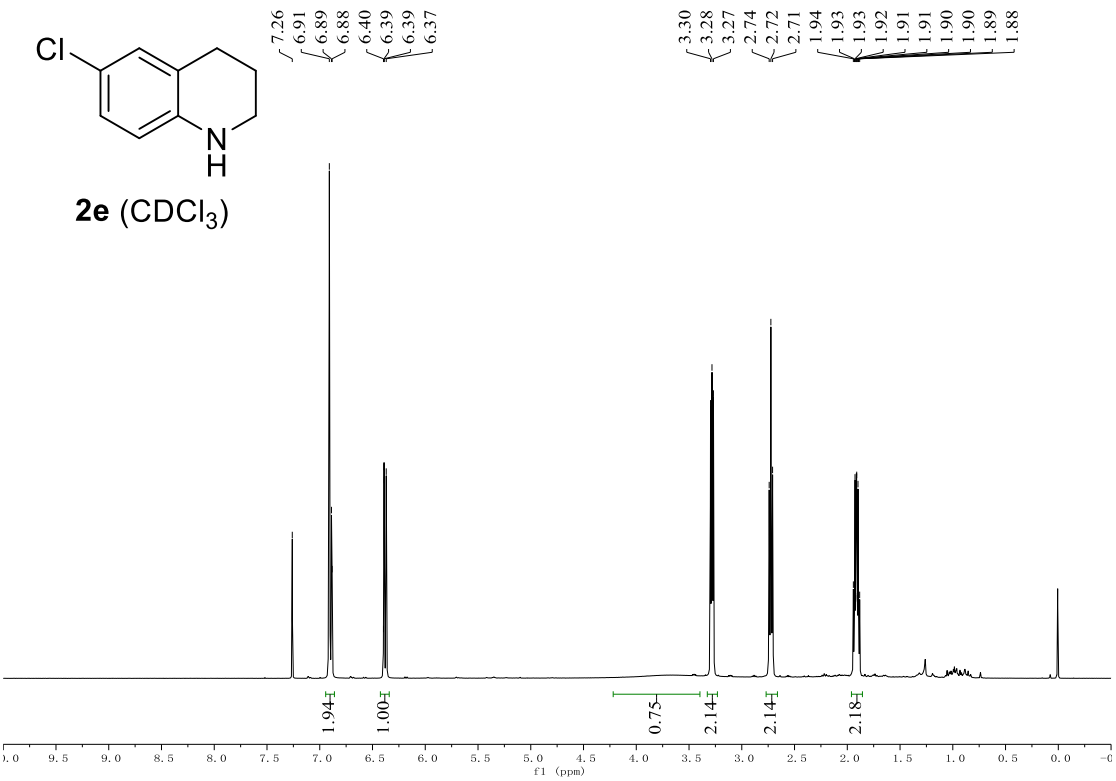
2c ($CDCl_3$)



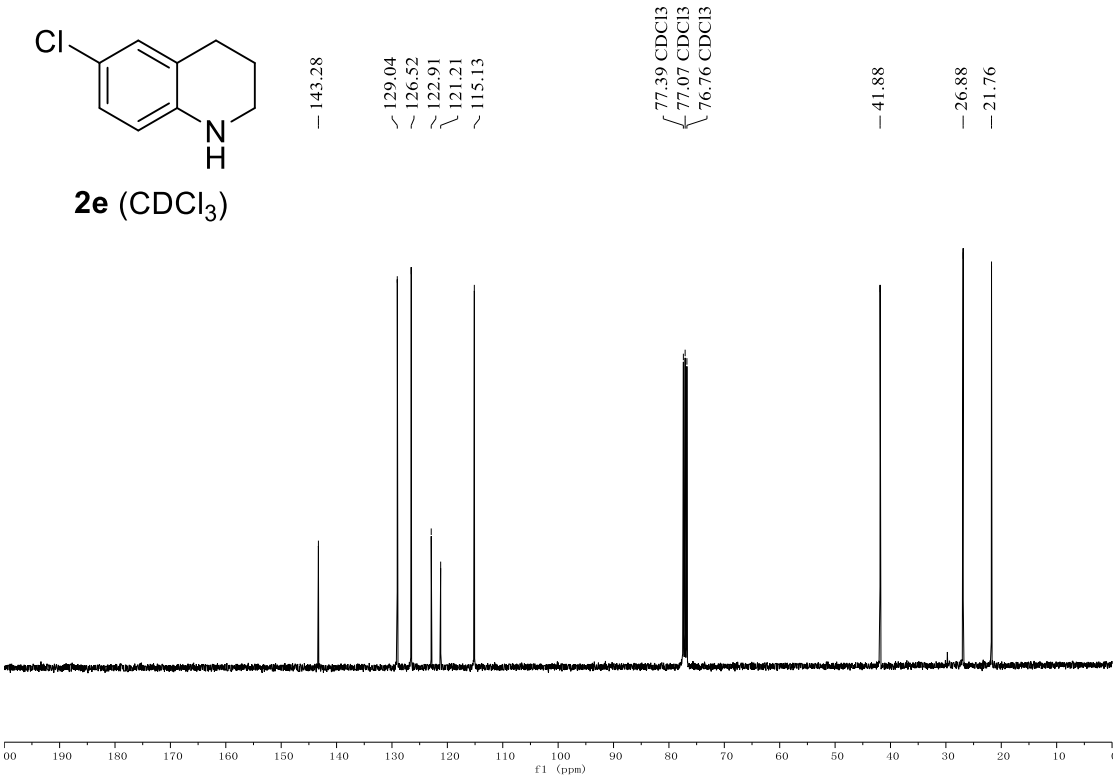
2d ($CDCl_3$)

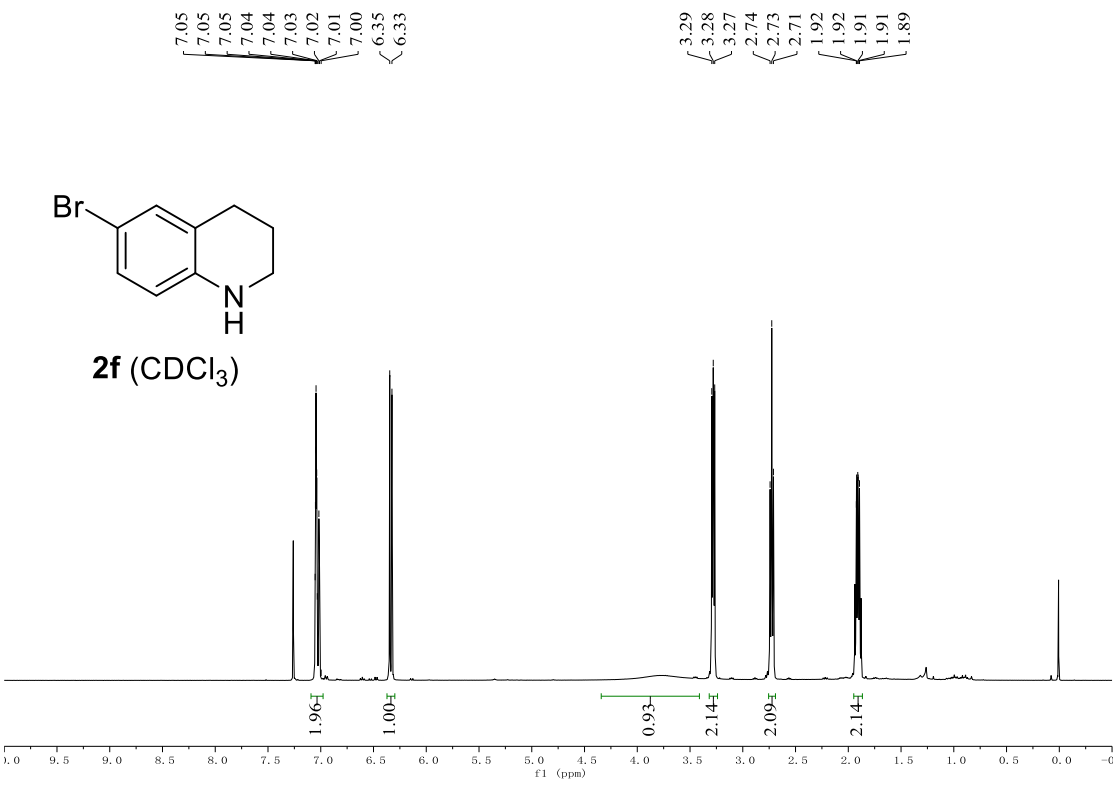


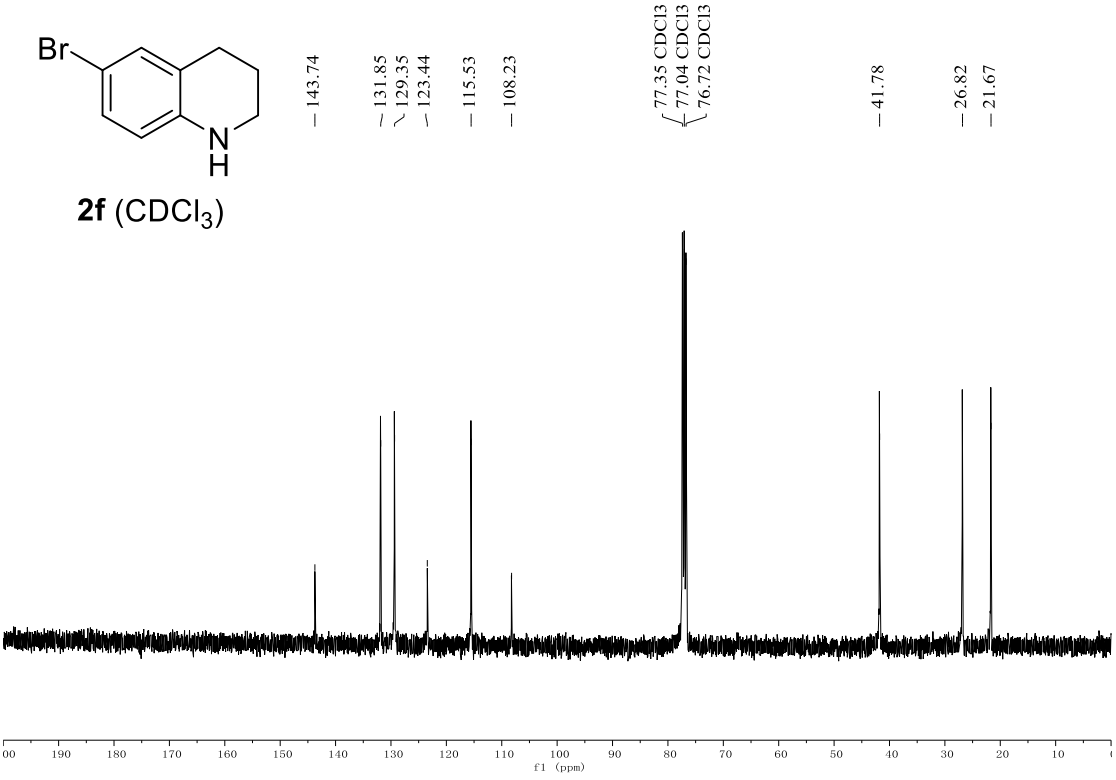
2d ($CDCl_3$)



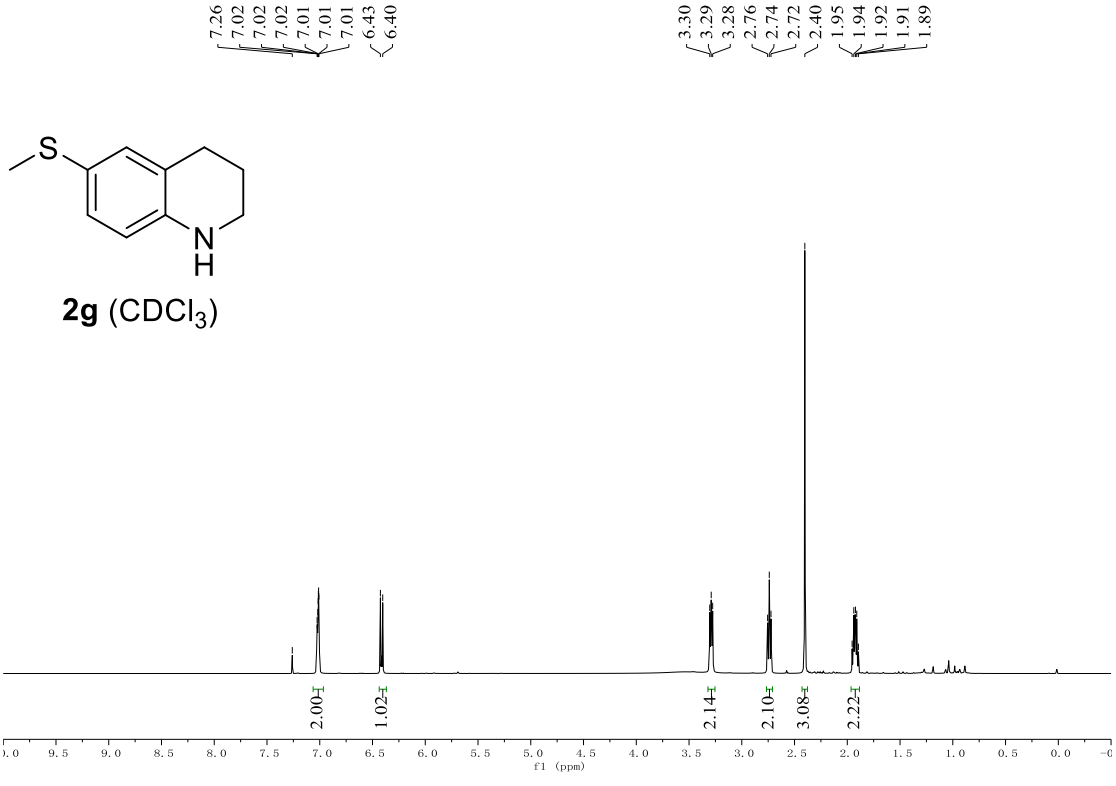
2e ($CDCl_3$)


Cl
N
H
2e (CDCl3)
143.28
129.04
126.52
122.91
121.21
115.13
77.39 CDCl3
77.07 CDCl3
76.76 CDCl3
41.88
26.88
21.76
f1 (ppm)

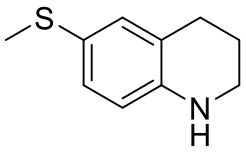

7.05
7.05
7.05
7.04
7.04
7.03
7.02
7.01
7.00
6.35
6.33
3.29
3.28
3.27
2.74
2.73
2.71
1.92
1.92
1.91
1.91
1.89
Br
N
H
2f (CDCl3)
1.96
1.00
0.93
2.14
2.09
2.14
f1 (ppm)



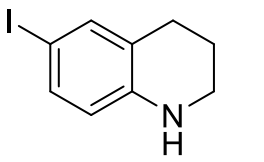
2f ($CDCl_3$)



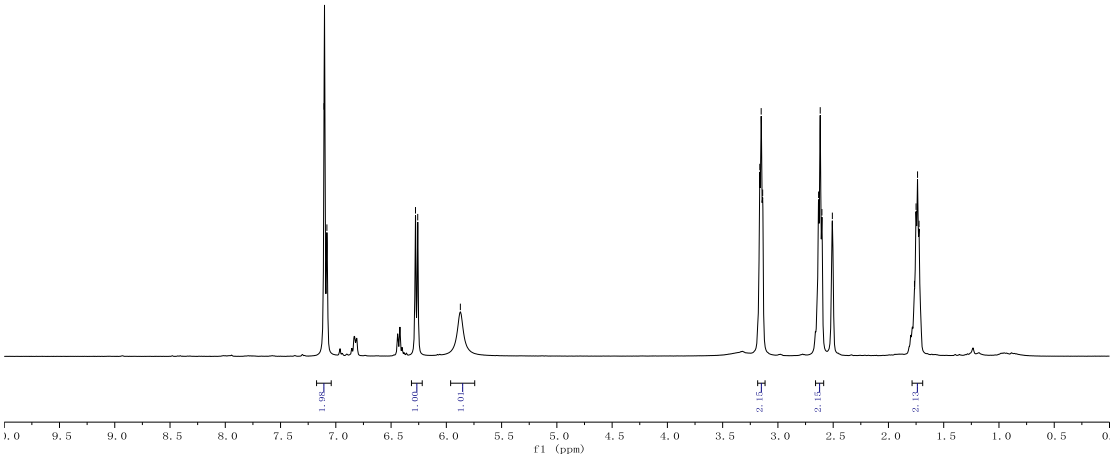
2g ($CDCl_3$)

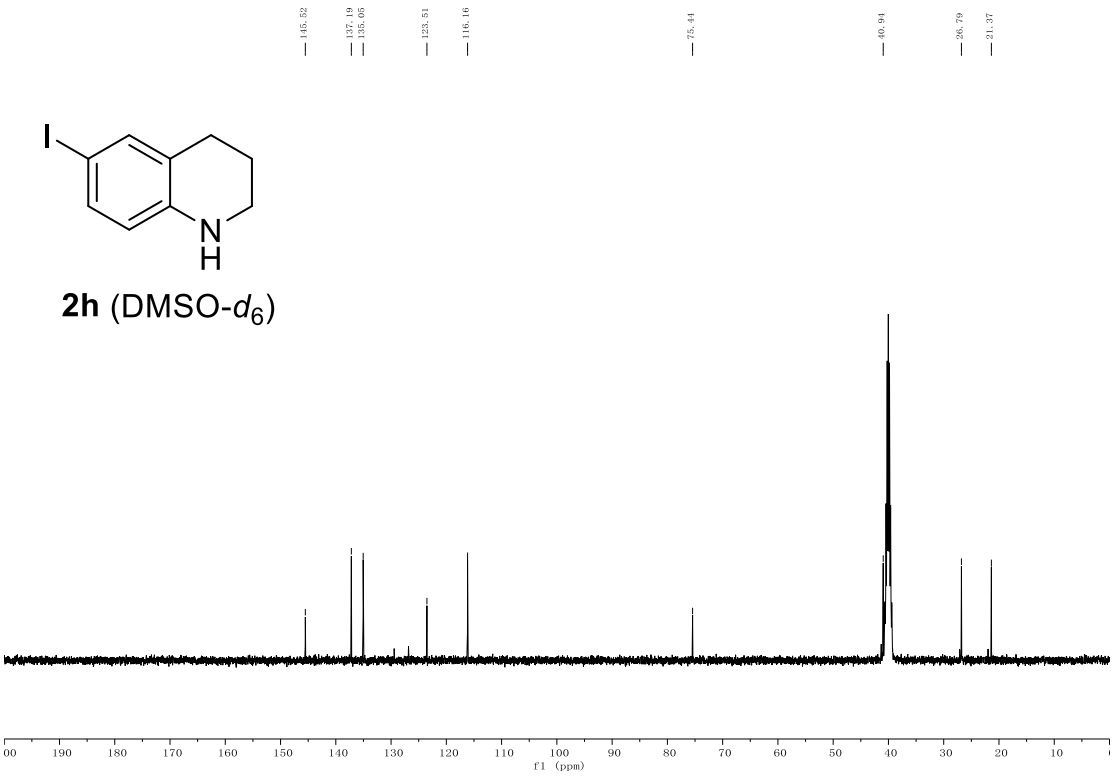


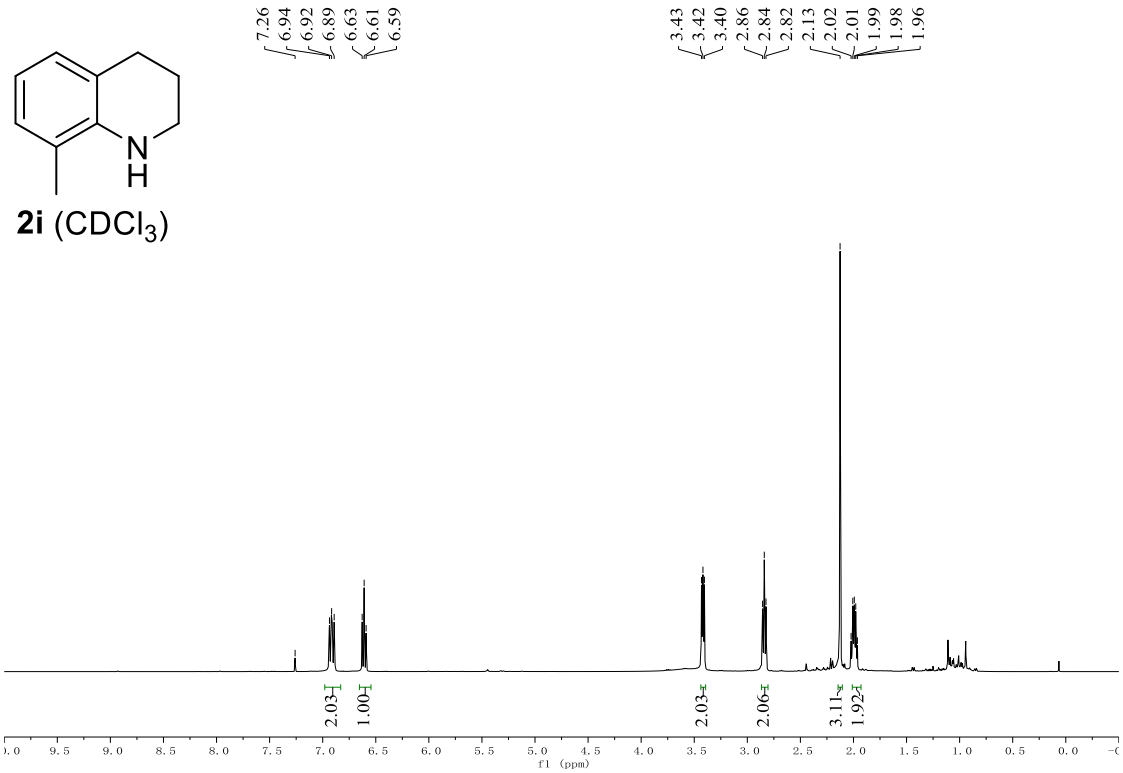
2g ($CDCl_3$)

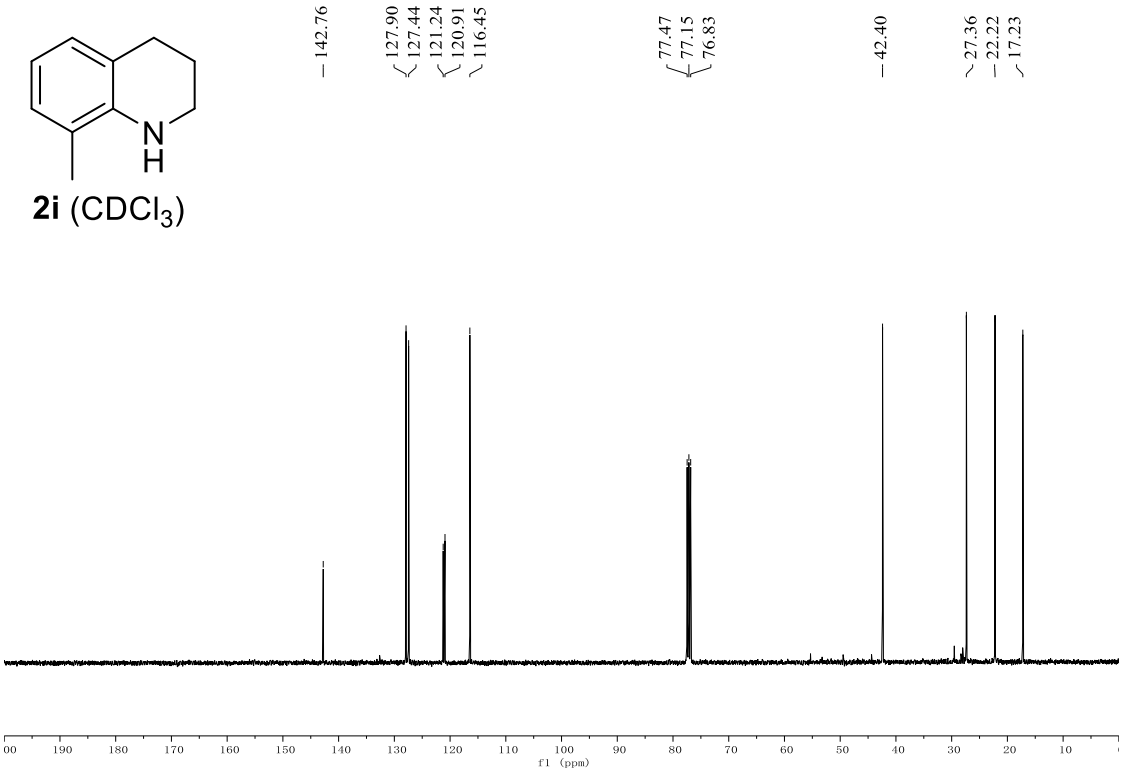


2h (DMSO-d_6)

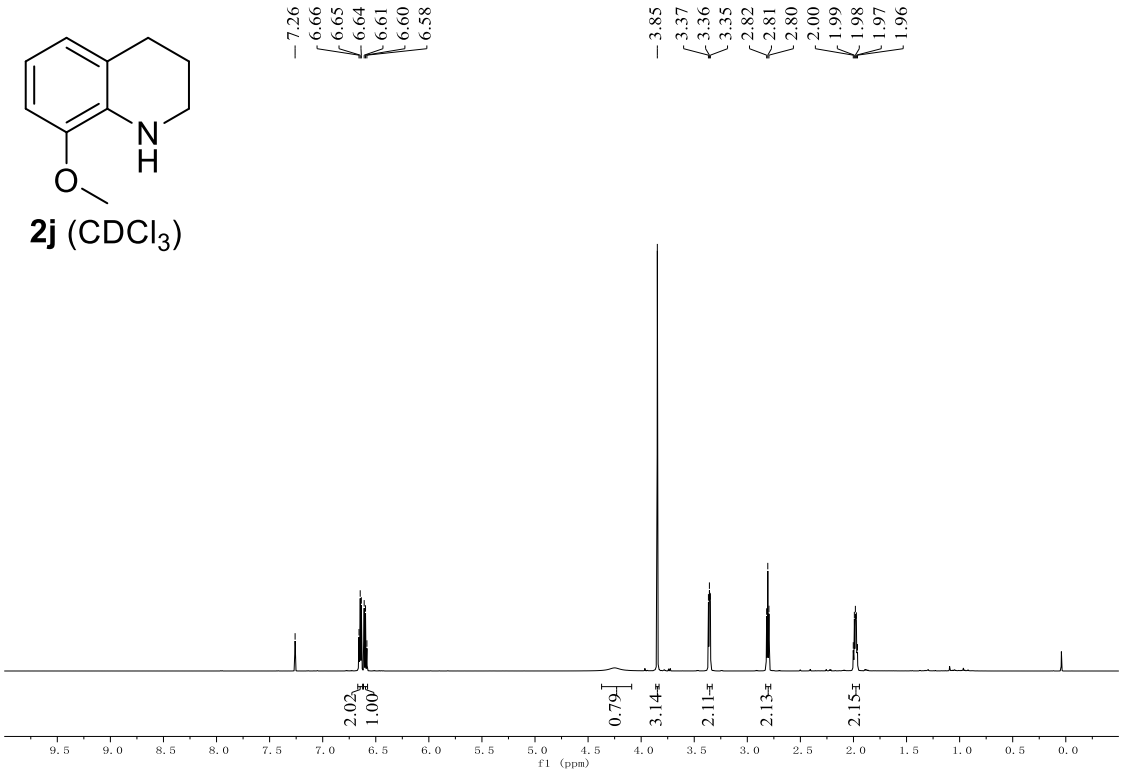



145.52
137.19
135.05
123.51
116.16
75.44
40.94
26.79
21.37
I
N
H
2h (DMSO-d6)
f1 (ppm)

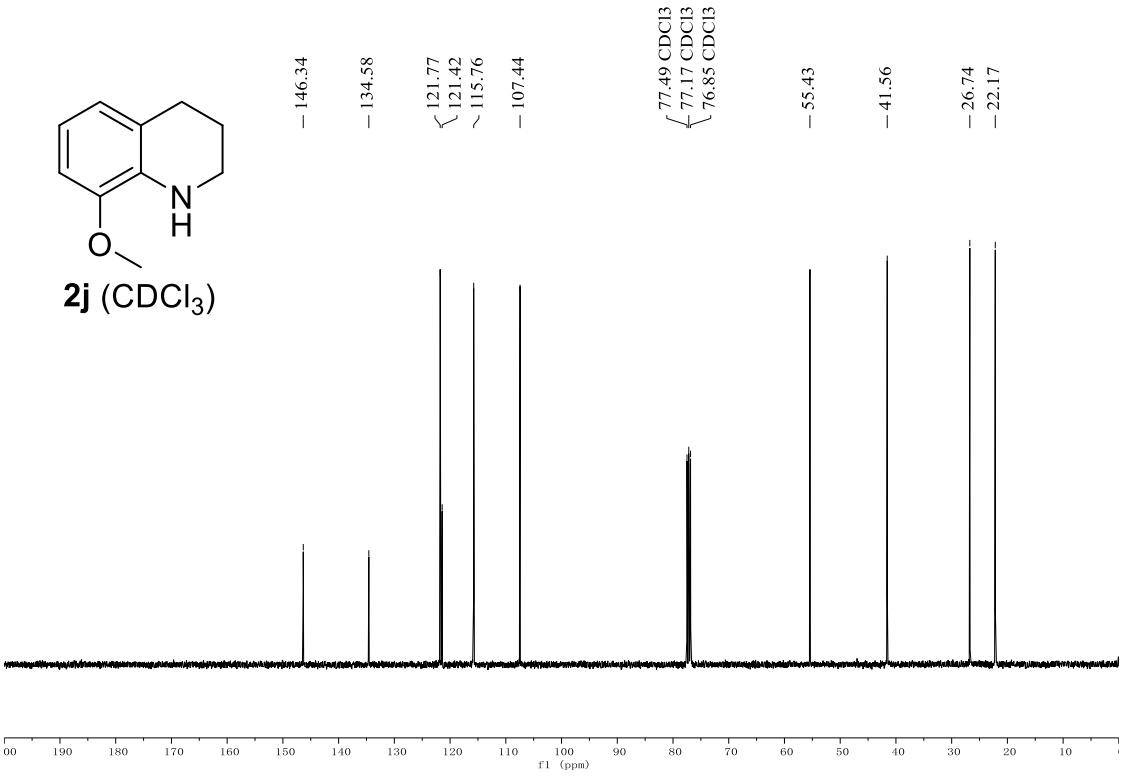

7.26
6.94
6.92
6.89
6.63
6.61
6.59
3.43
3.42
3.40
2.86
2.84
2.82
2.13
2.02
2.01
1.99
1.98
1.96
N
H
2i (CDCl3)
2.03
1.00
2.03
2.06
3.11
1.92
f1 (ppm)



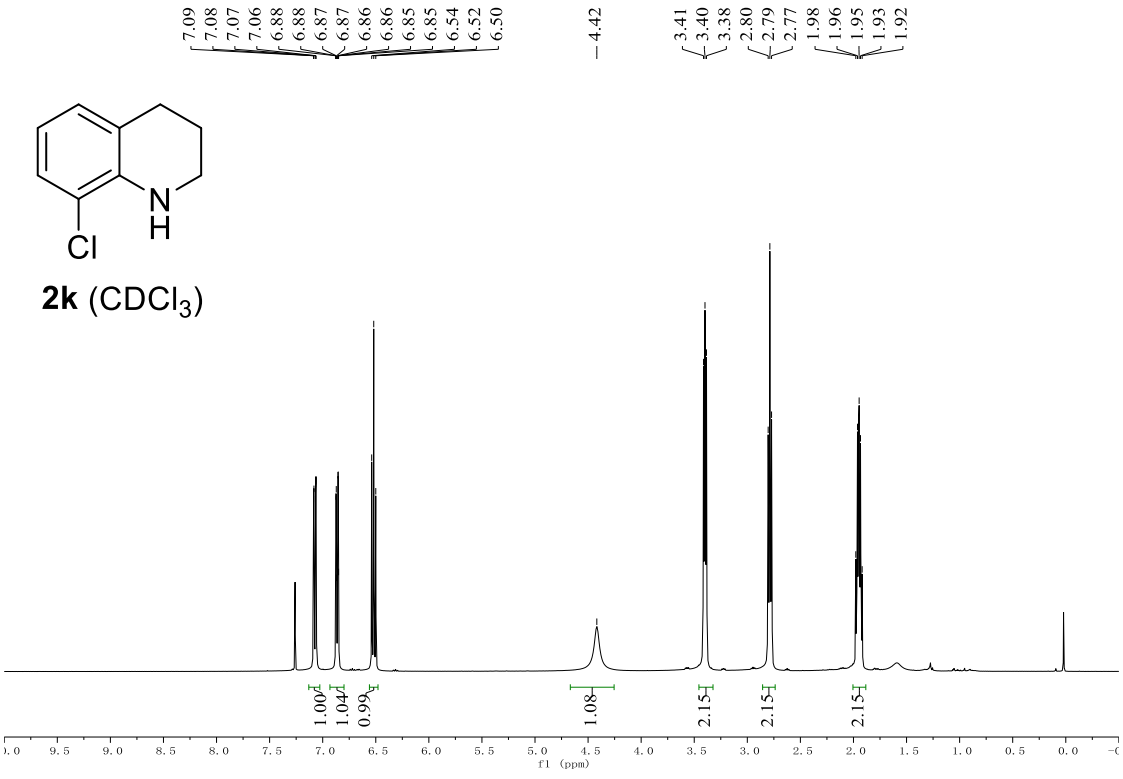
2i ($CDCl_3$)



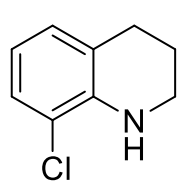
2j ($CDCl_3$)



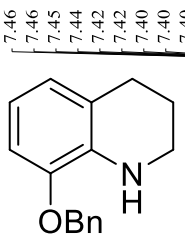
2j ($CDCl_3$)



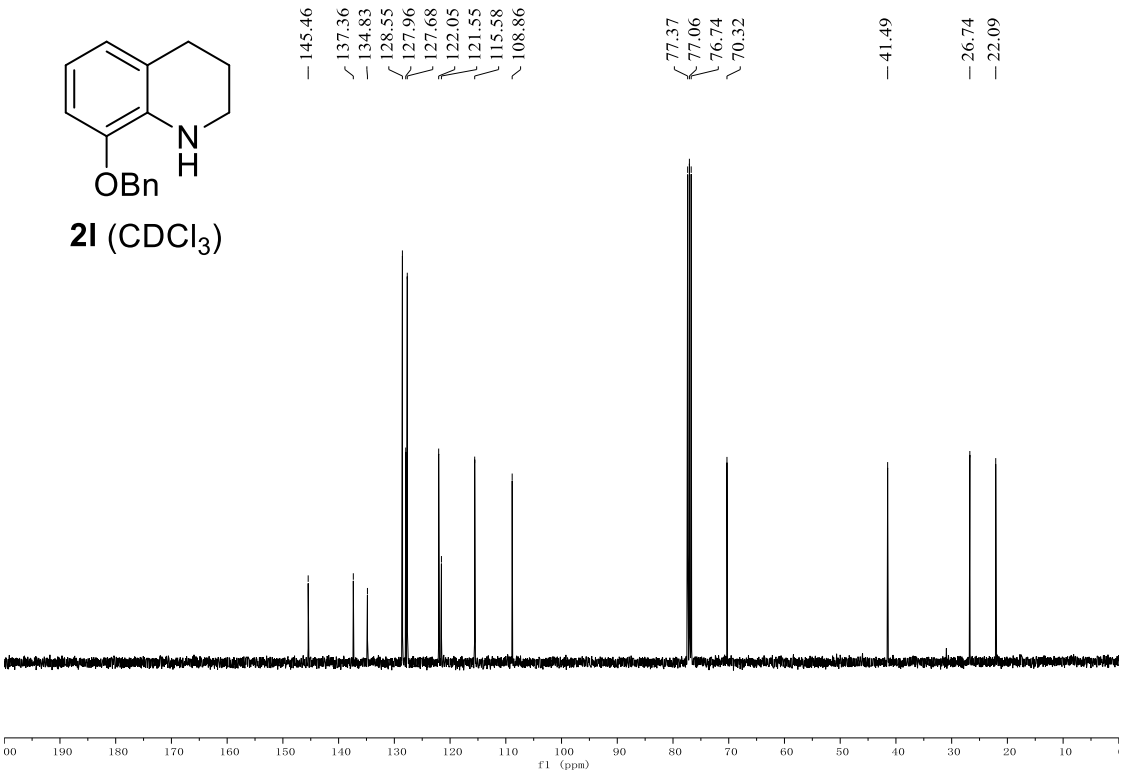
2k ($CDCl_3$)



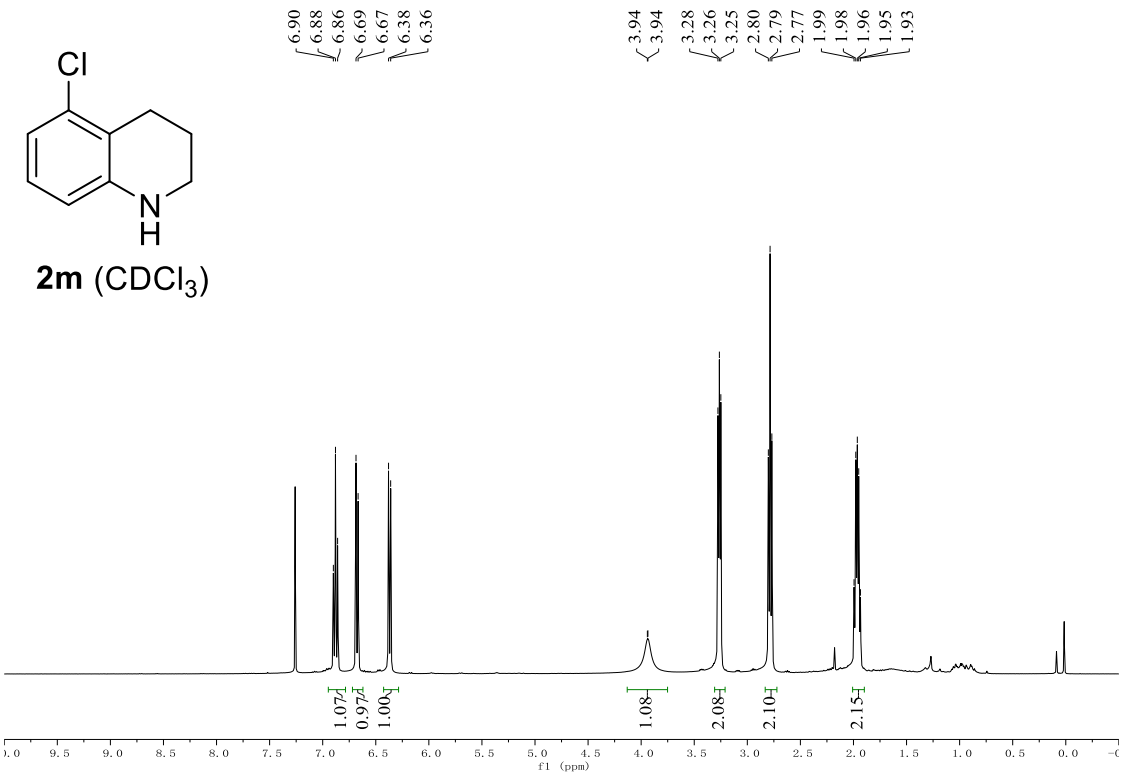
2k ($CDCl_3$)



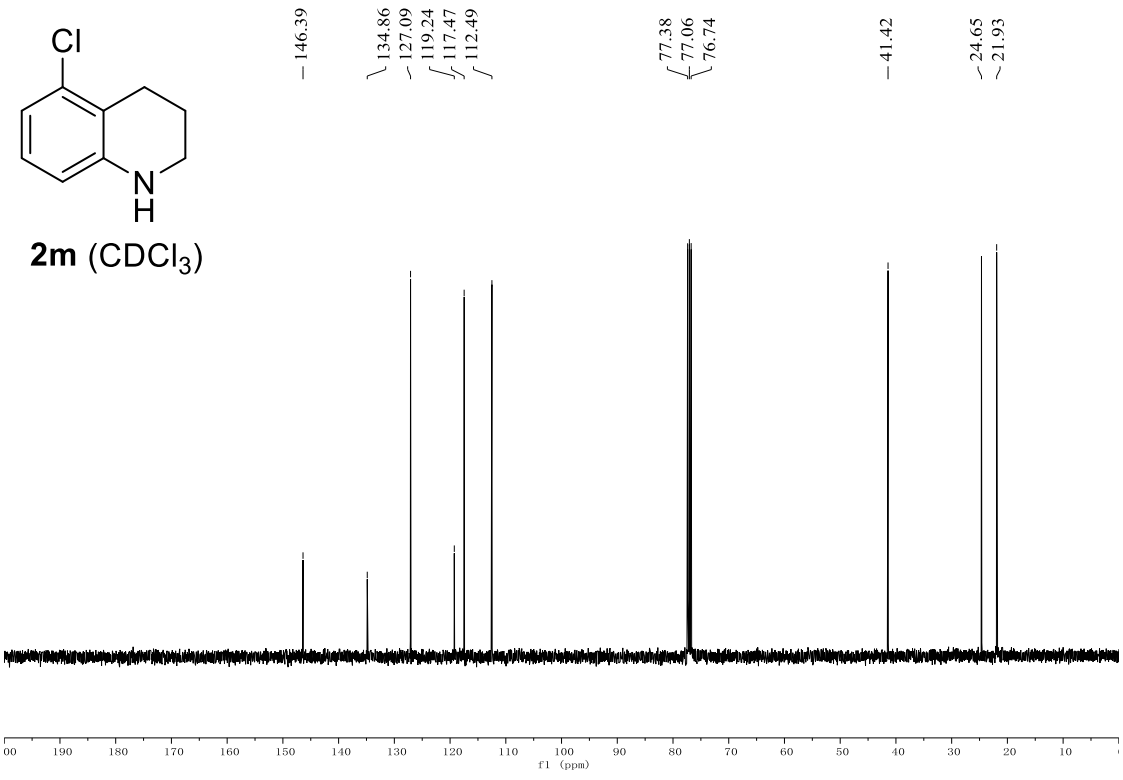
2l ($CDCl_3$)

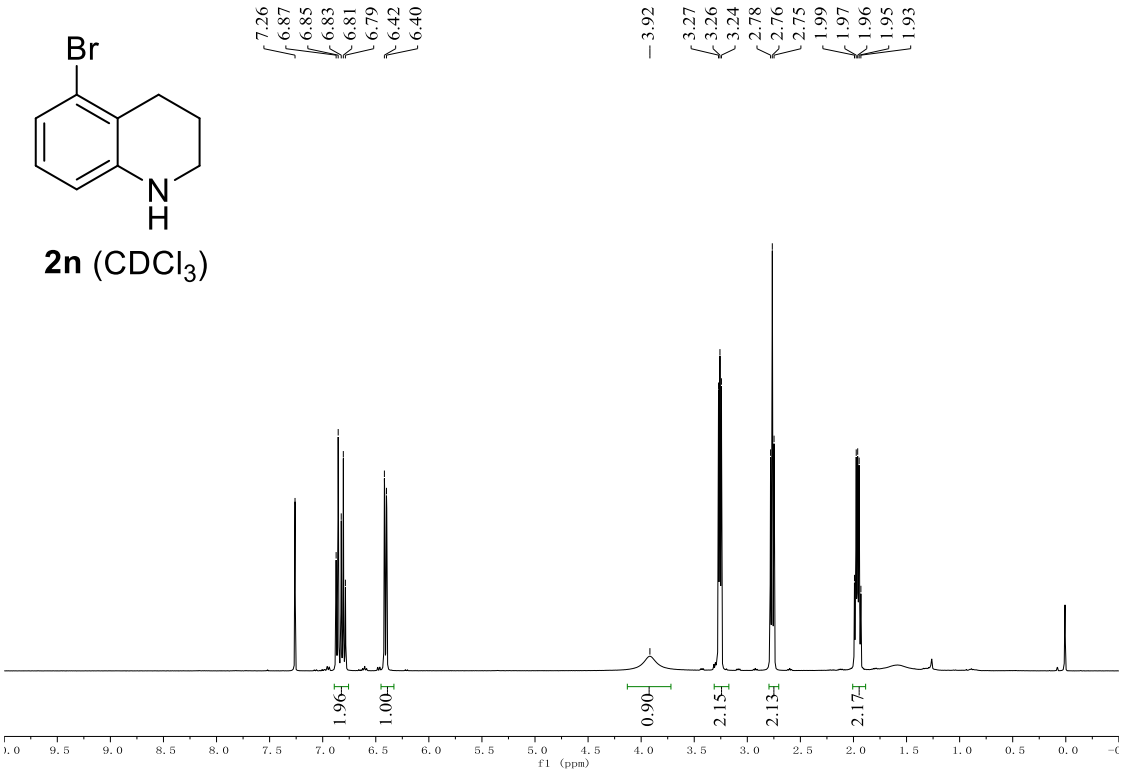


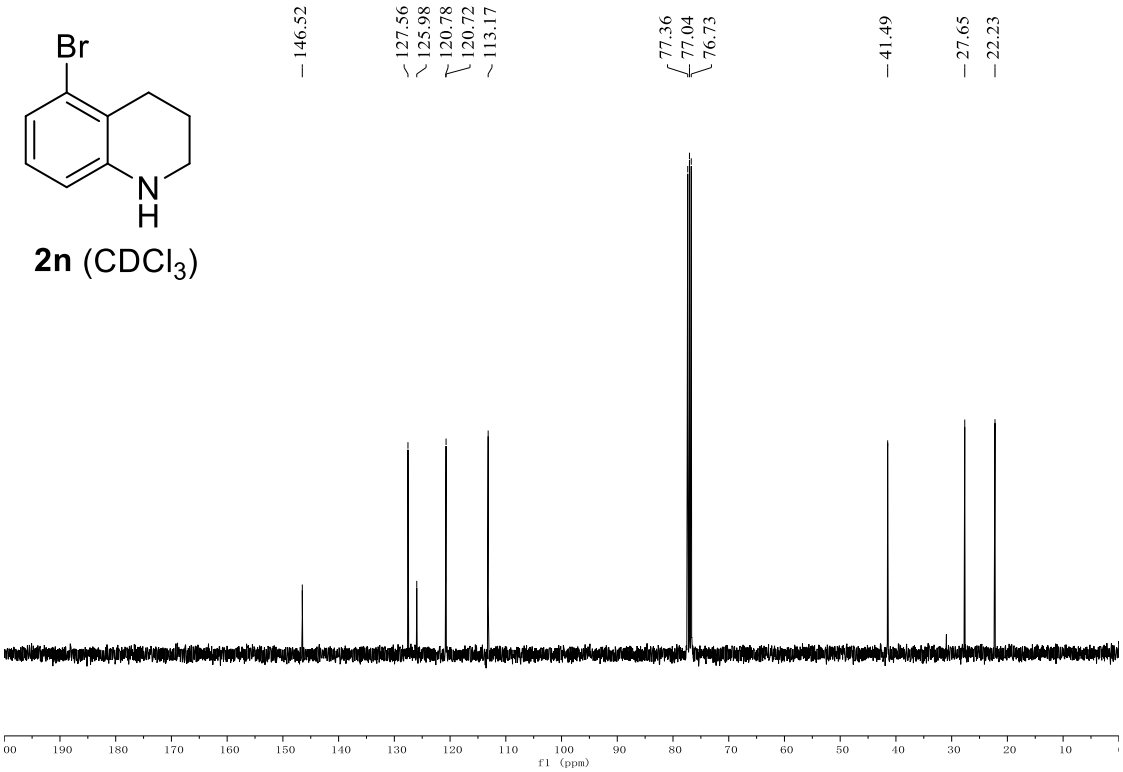
2l ($CDCl_3$)



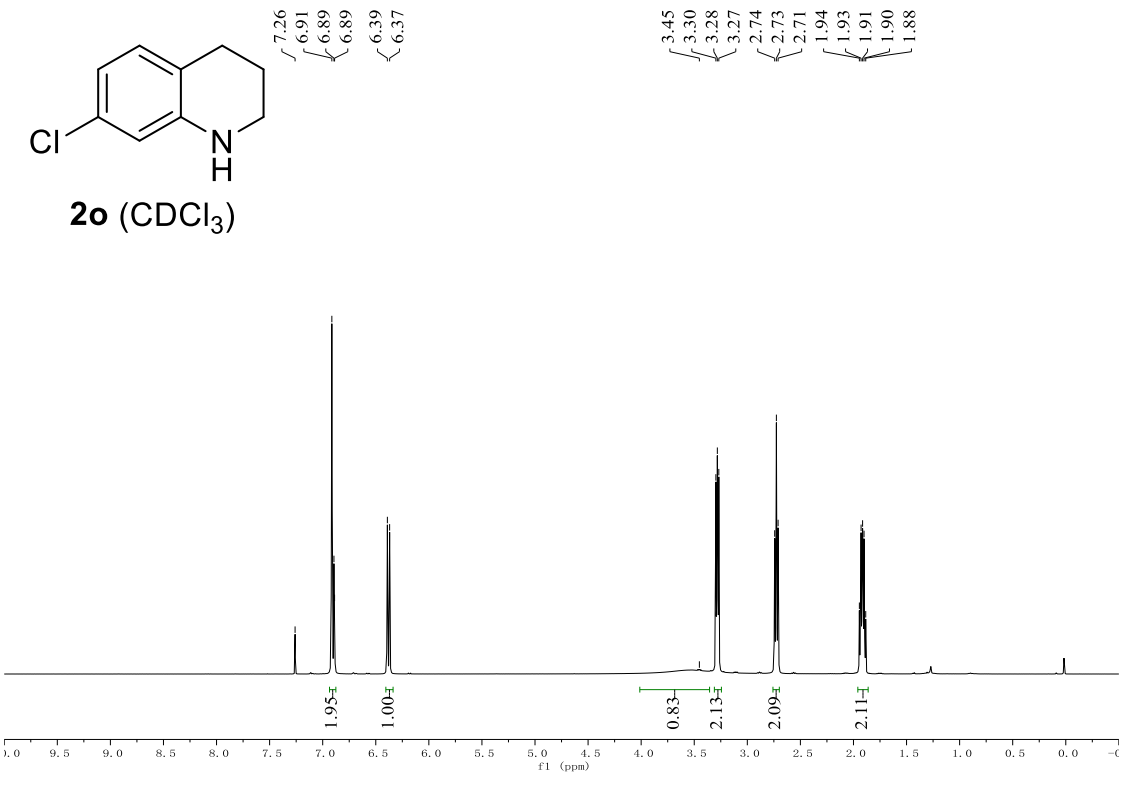
2m ($CDCl_3$)


Cl
N
H
2m (CDCl3)
146.39
134.86
127.09
119.24
117.47
112.49
77.38
77.06
76.74
41.42
24.65
21.93
f1 (ppm)

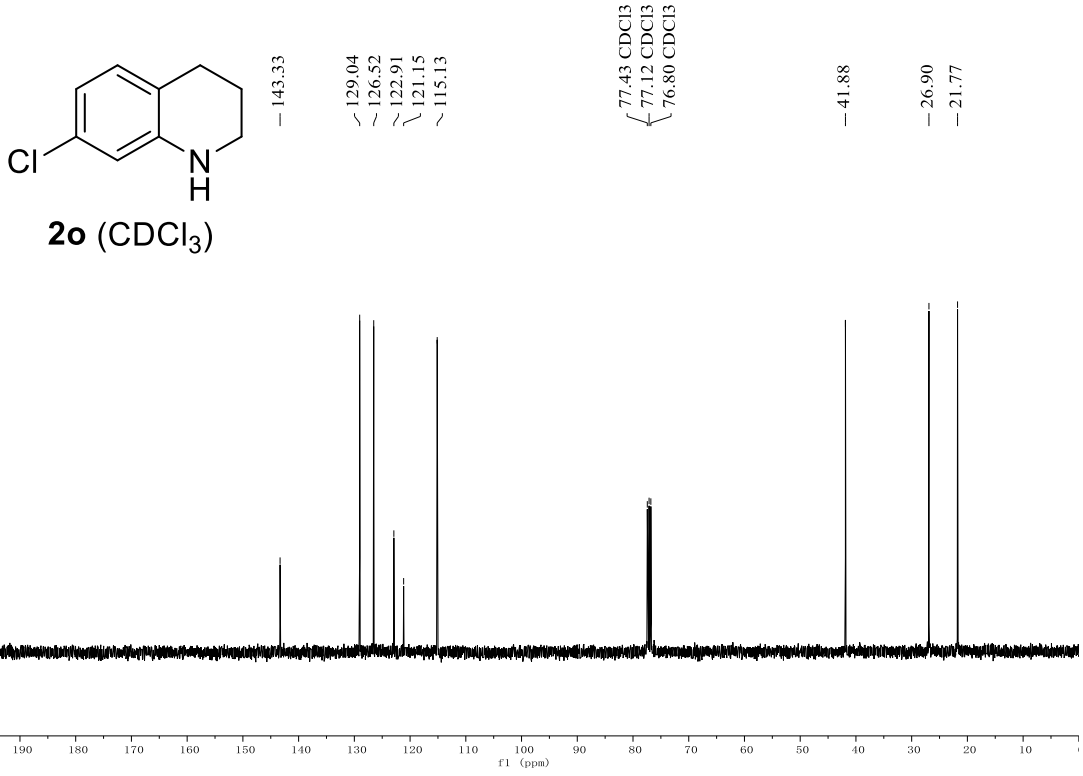

Br
N
H
2n (CDCl3)
7.26
6.87
6.85
6.83
6.81
6.79
6.42
6.40
3.92
3.27
3.26
3.24
2.78
2.76
2.75
1.99
1.97
1.96
1.95
1.93
1.96
1.00
0.90
2.15
2.13
2.17
f1 (ppm)

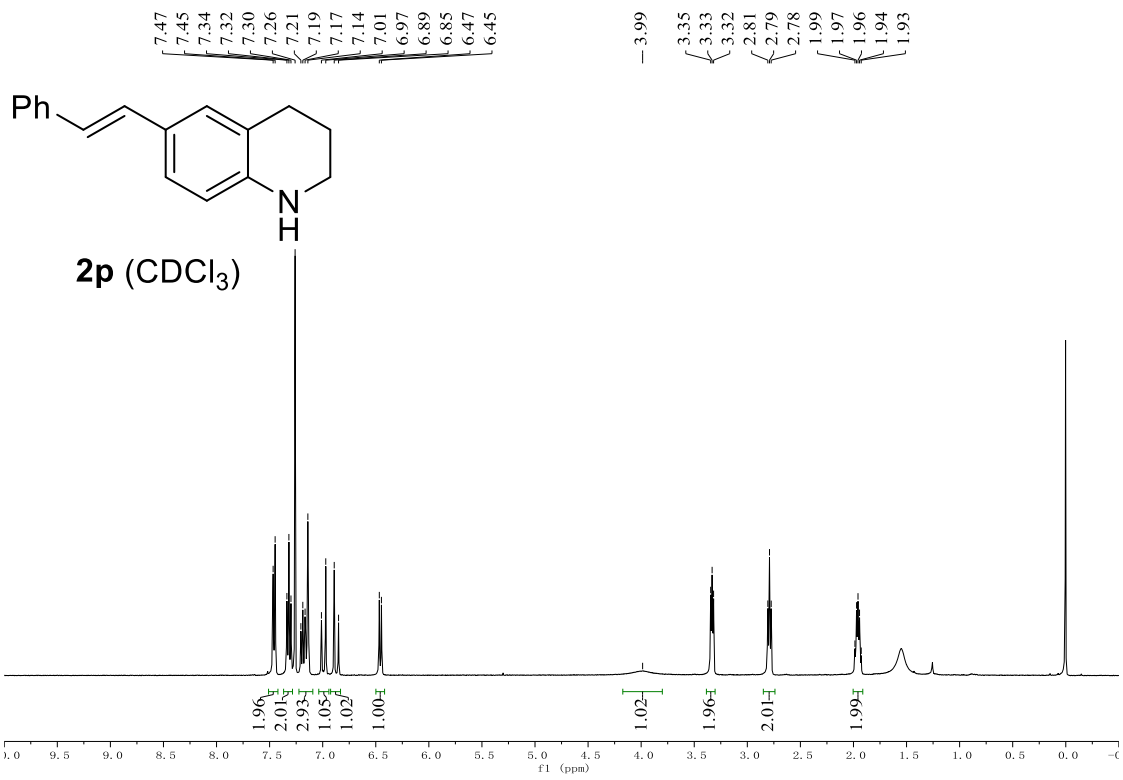


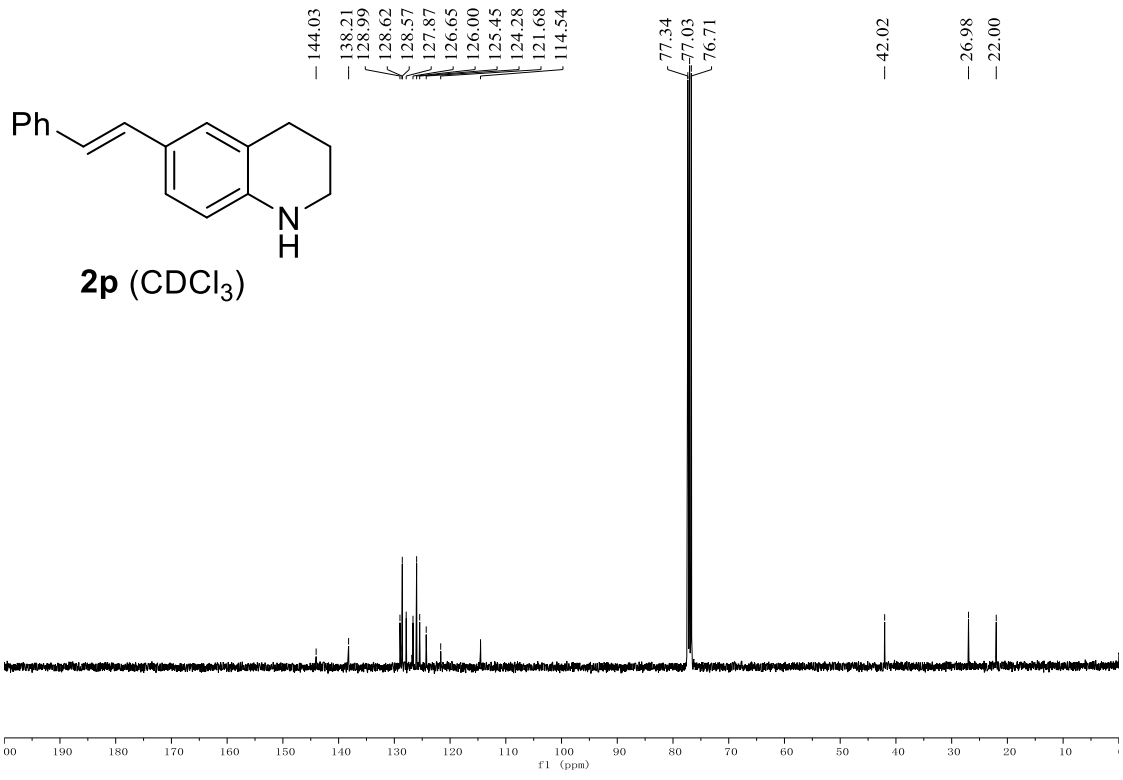
2n ($CDCl_3$)



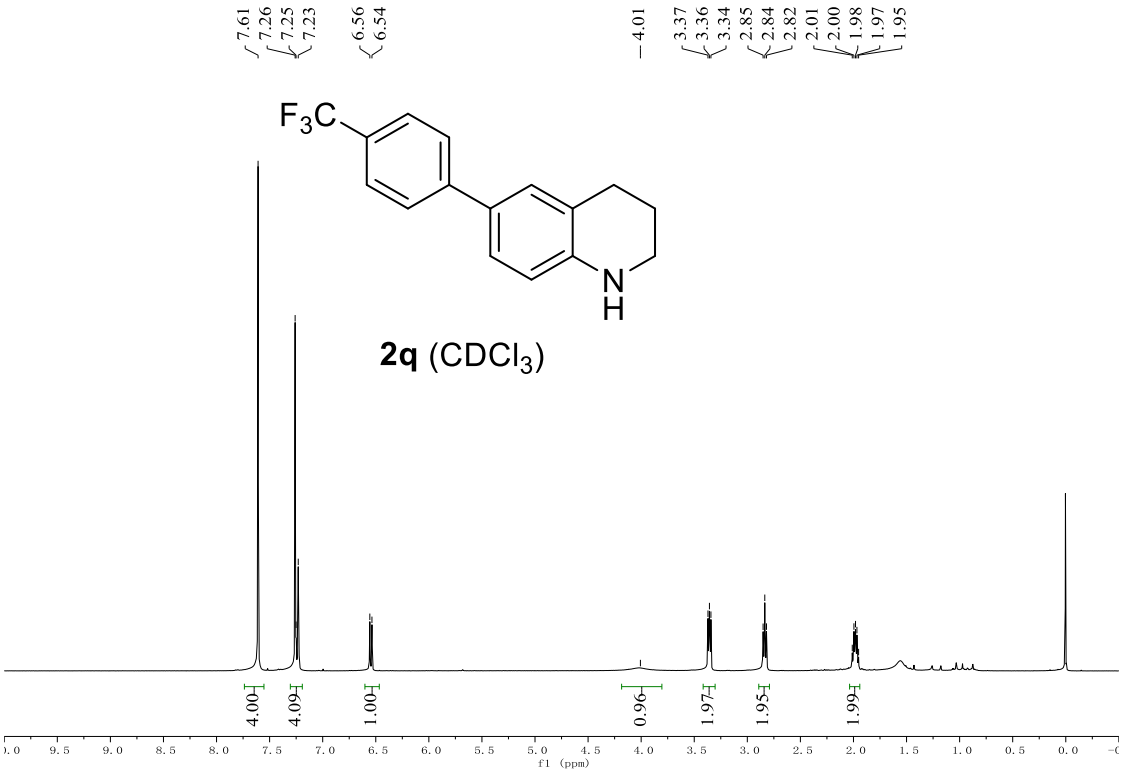
2o ($CDCl_3$)


143.33
129.04
126.52
122.91
121.15
115.13
77.43 CDCl3
77.12 CDCl3
76.80 CDCl3
41.88
26.90
21.77
Cl
N
H
2o (CDCl3)
f1 (ppm)

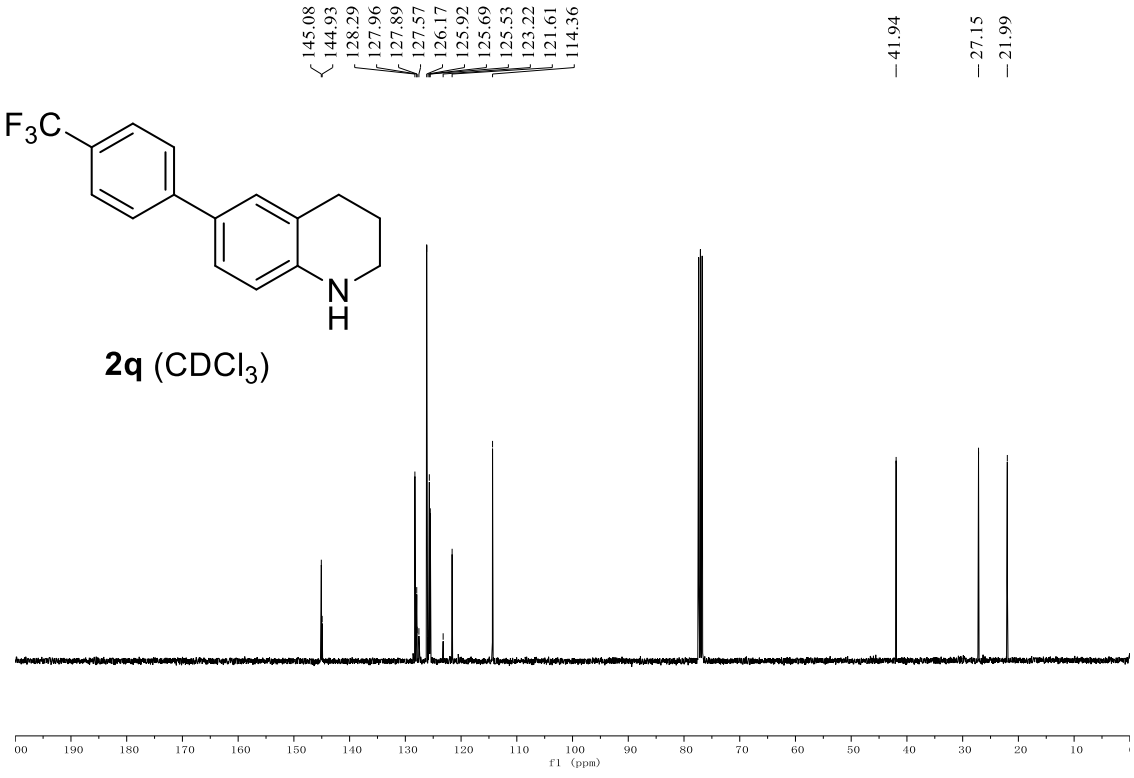

7.47
7.45
7.34
7.32
7.30
7.26
7.21
7.19
7.17
7.14
7.01
6.97
6.89
6.85
6.47
6.45
3.99
3.35
3.33
3.32
2.81
2.79
2.78
1.99
1.97
1.96
1.94
1.93
Ph
N
H
2p (CDCl3)
1.96
2.01
2.93
1.05
1.02
1.00
1.02
1.96
2.01
1.99
f1 (ppm)

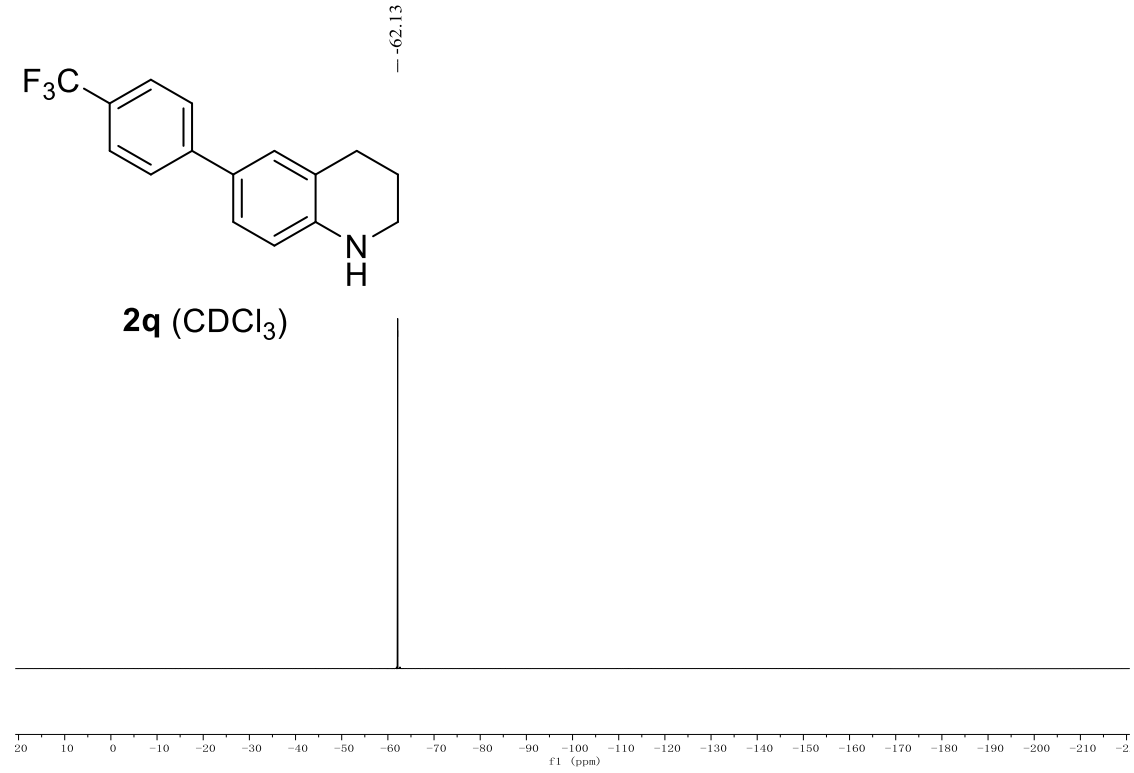


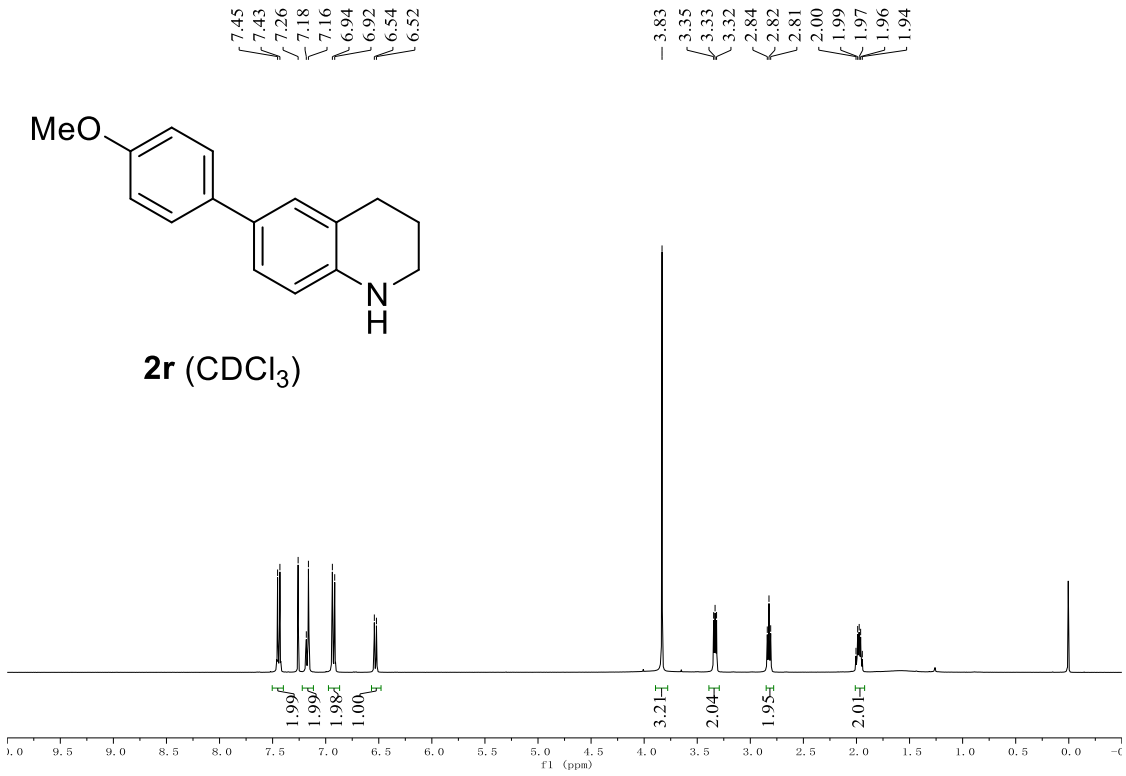
2p ($CDCl_3$)



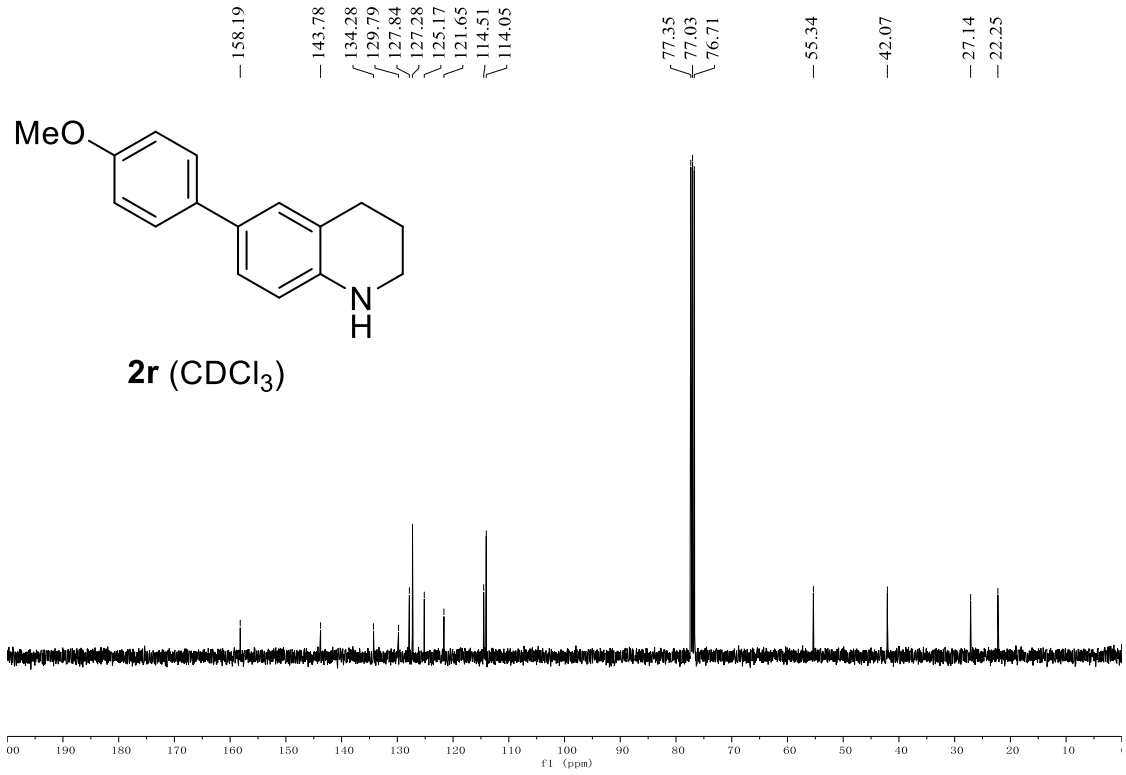
2q ($CDCl_3$)


145.08
144.93
128.29
127.96
127.89
127.57
126.17
125.92
125.69
125.53
123.22
121.61
114.36
41.94
27.15
21.99
F3C
N
H
2q (CDCl3)
f1 (ppm)

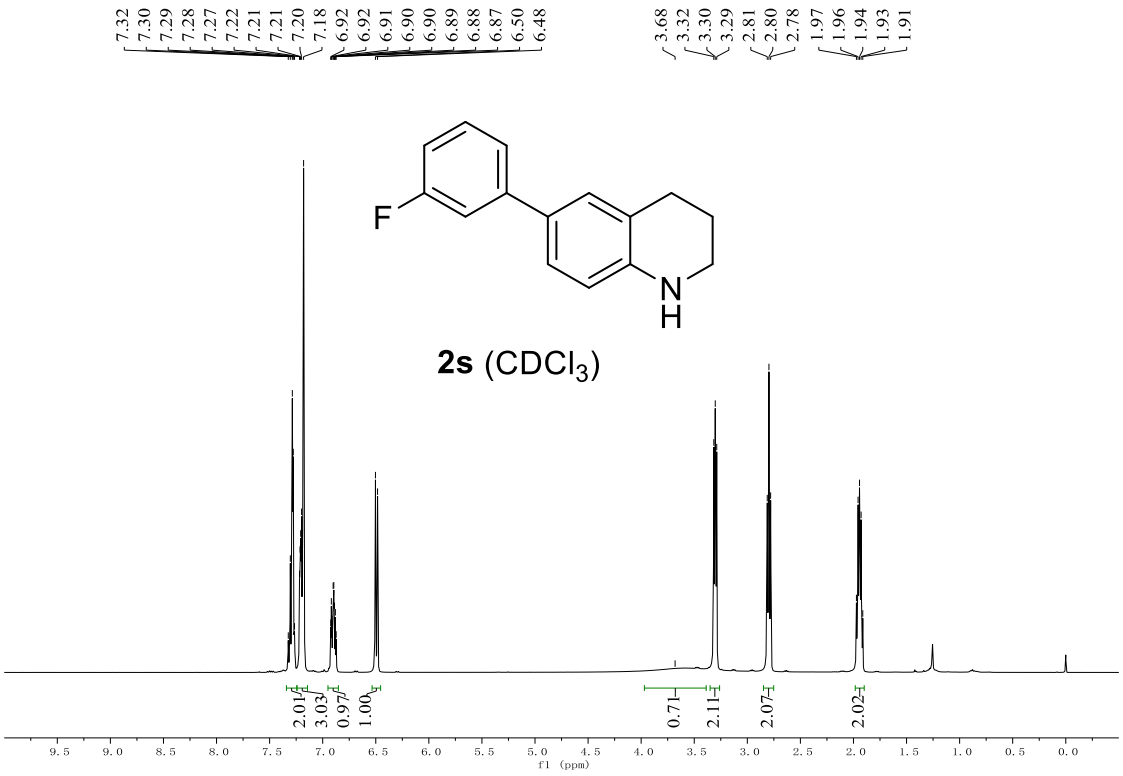

-62.13
F3C
N
H
2q (CDCl3)
f1 (ppm)

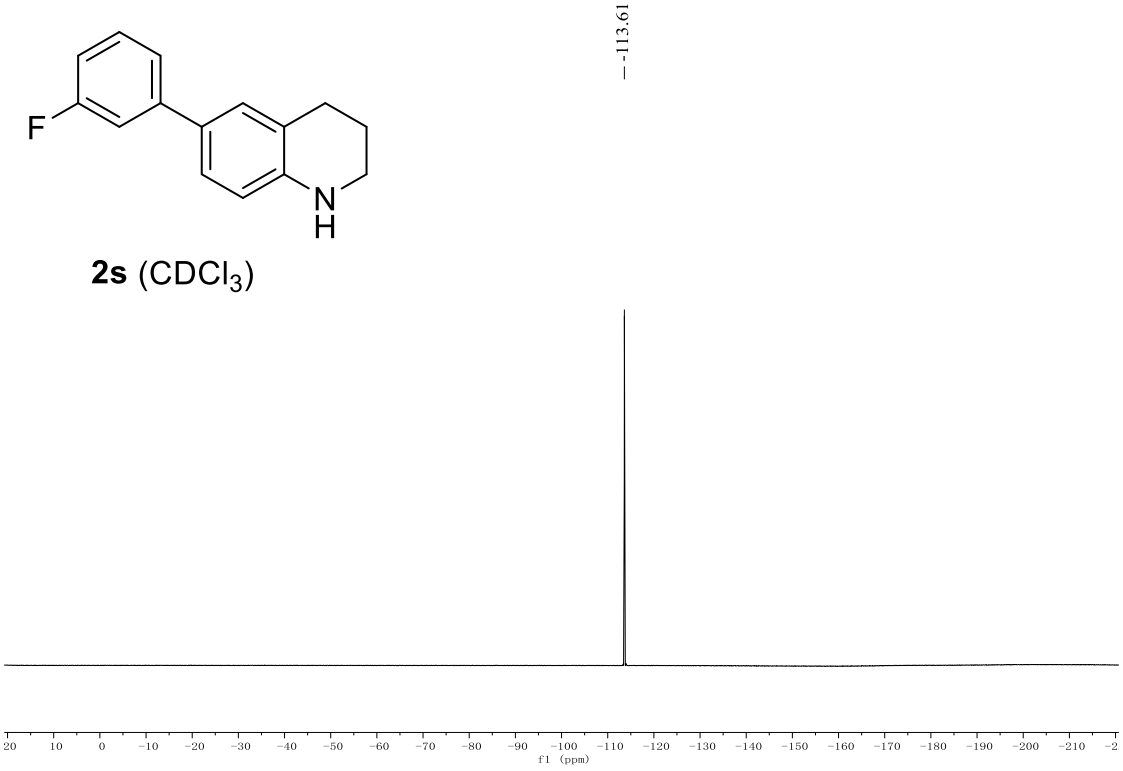


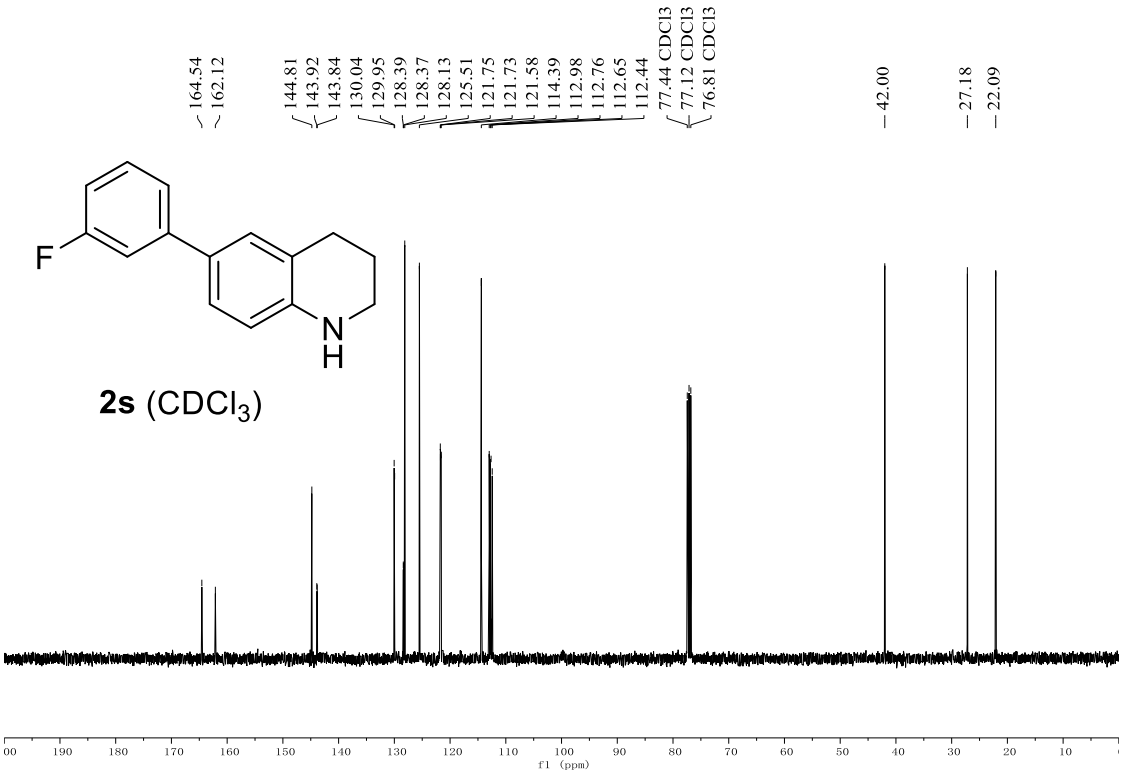
2r ($CDCl_3$)



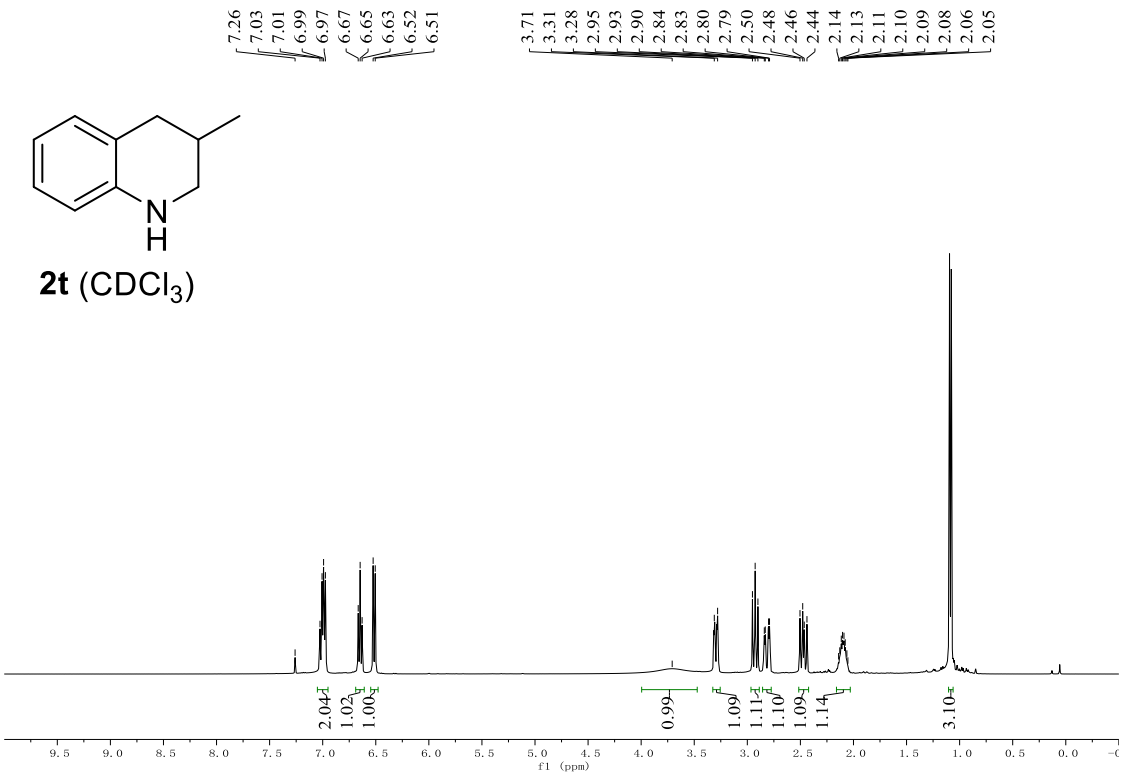
2r ($CDCl_3$)


7.32
7.30
7.29
7.28
7.27
7.22
7.21
7.21
7.20
7.18
6.92
6.92
6.91
6.90
6.90
6.89
6.88
6.87
6.50
6.48
3.68
3.32
3.30
3.29
2.81
2.80
2.78
1.97
1.96
1.94
1.93
1.91
F
N
H
2s (CDCl3)
2.01
3.03
0.97
1.00
0.71
2.11
2.07
2.02
f1 (ppm)

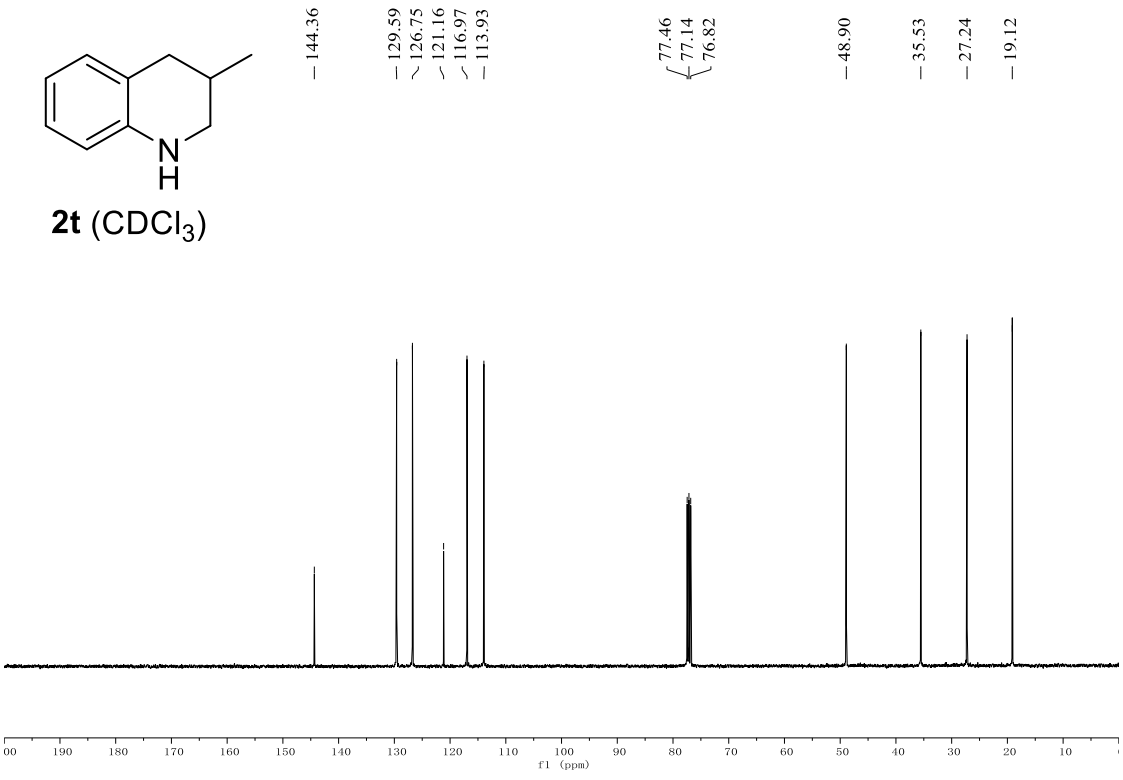

-113.61
F
N
H
2s (CDCl3)
f1 (ppm)



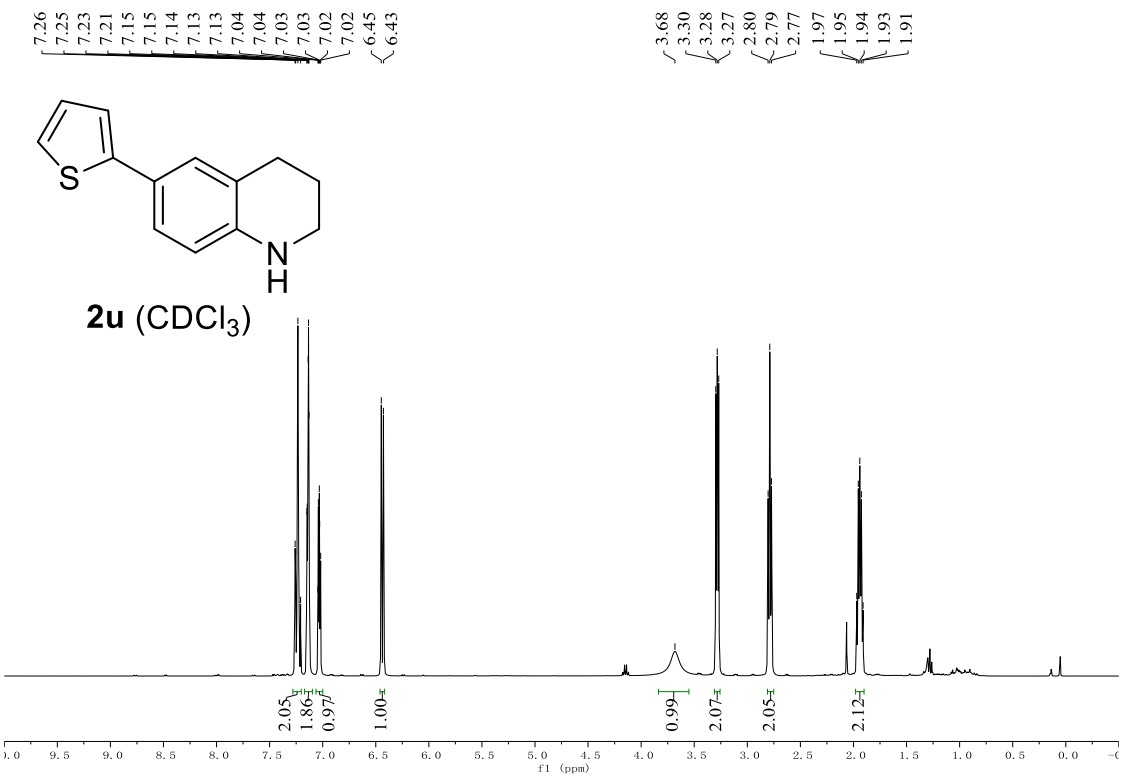
2s ($CDCl_3$)



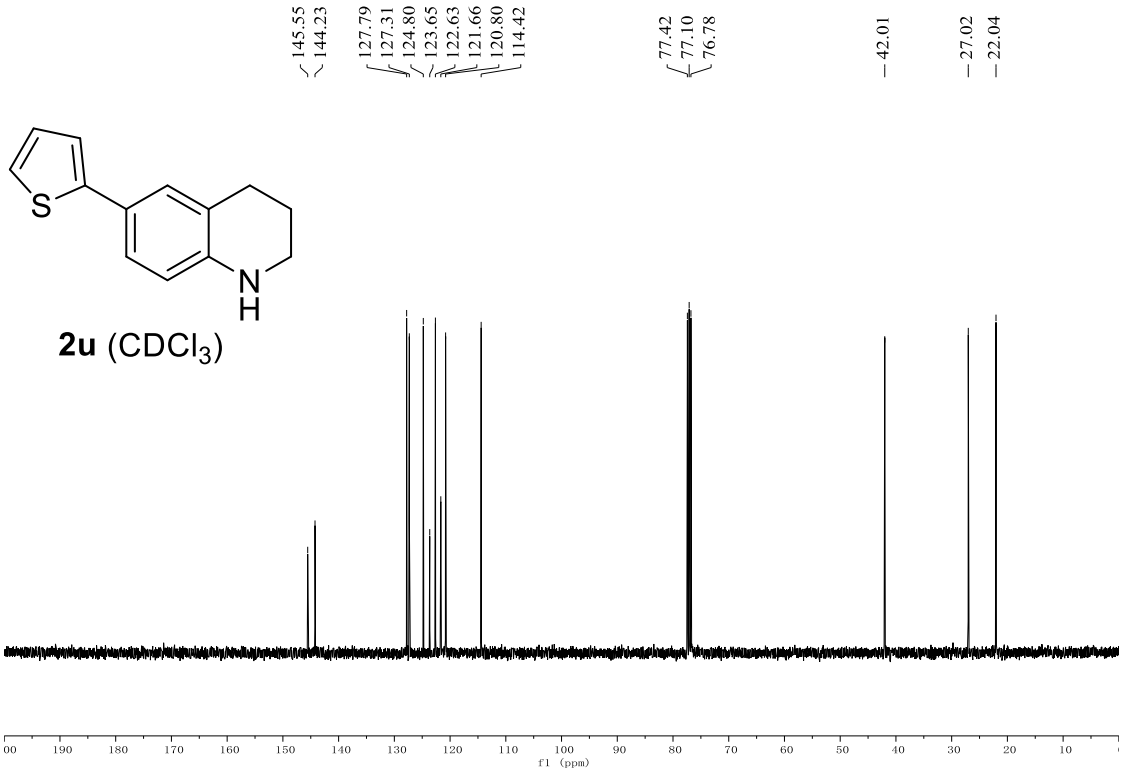
2t ($CDCl_3$)



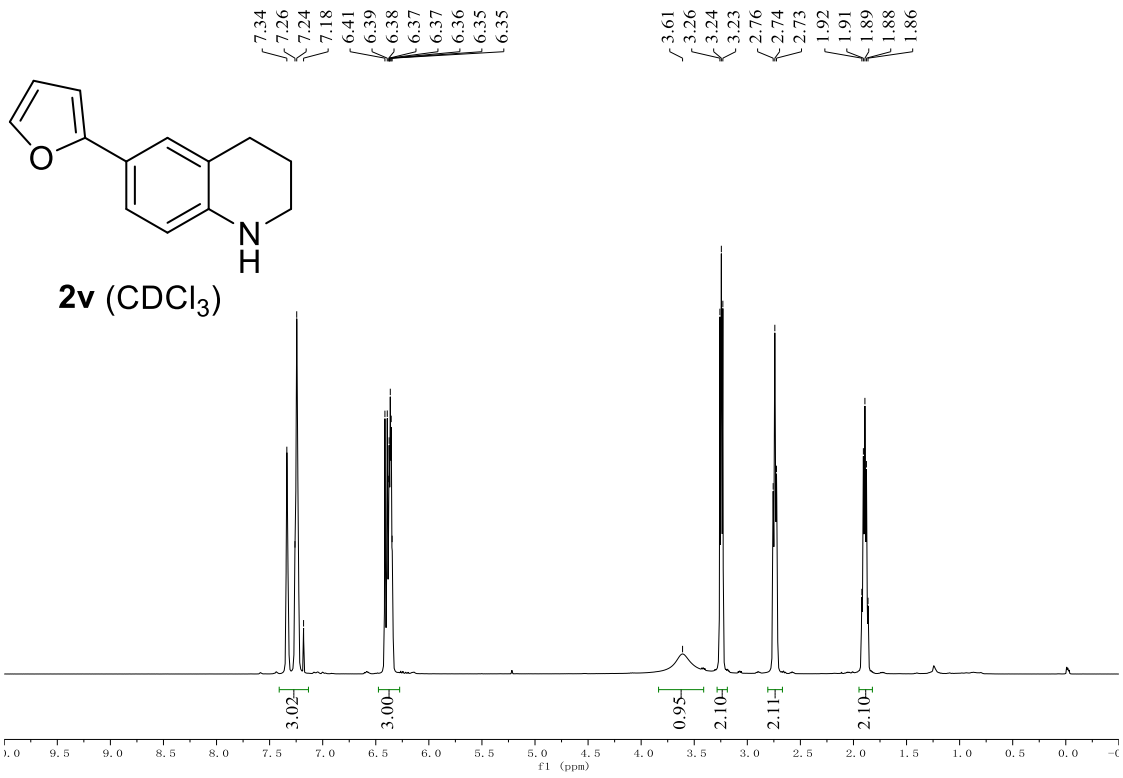
2t ($CDCl_3$)



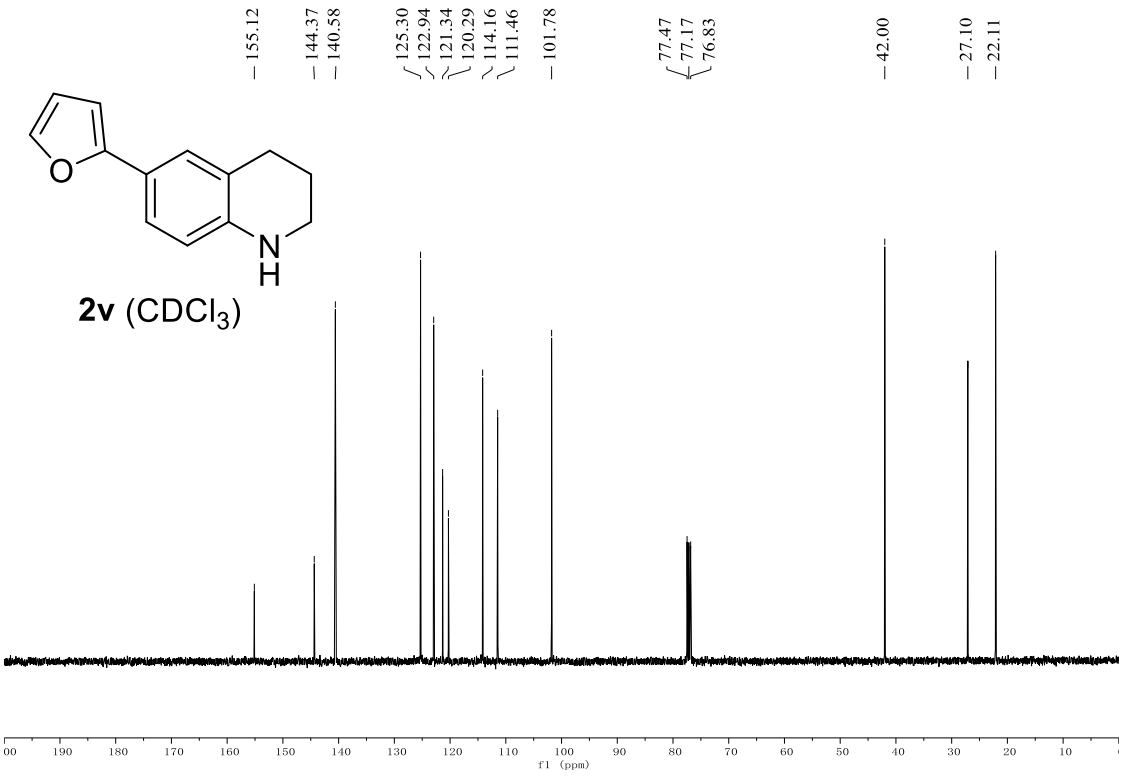
2u ($CDCl_3$)

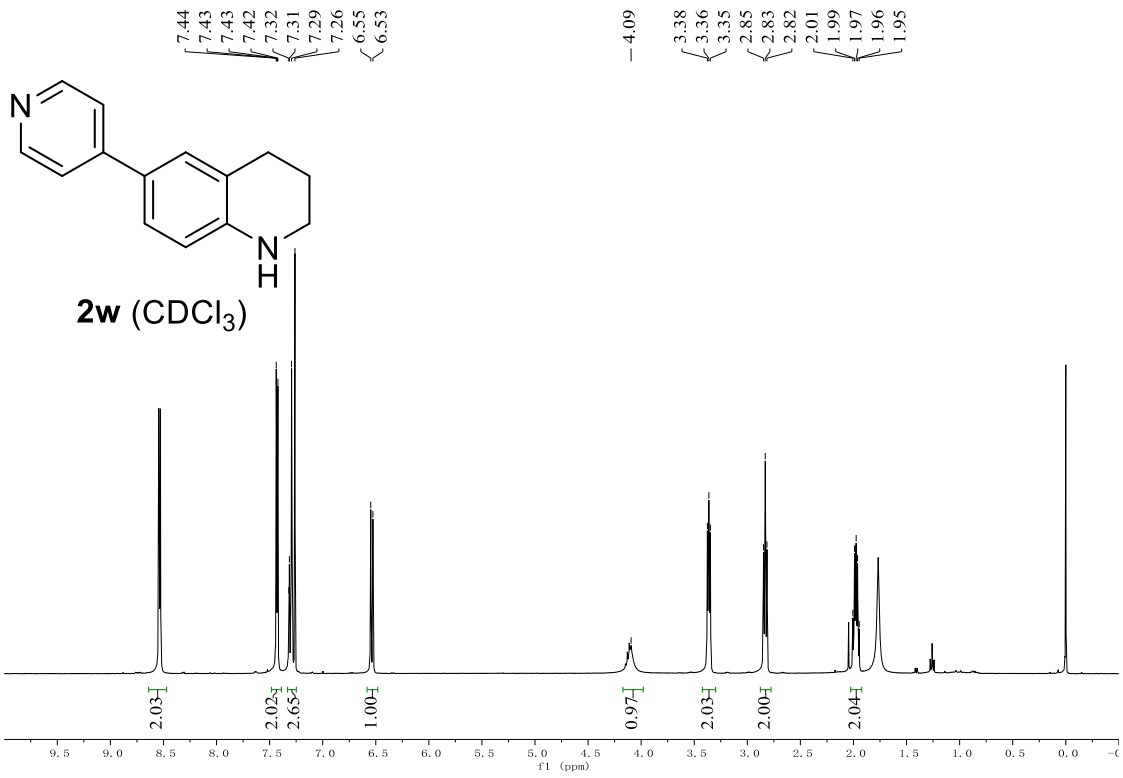


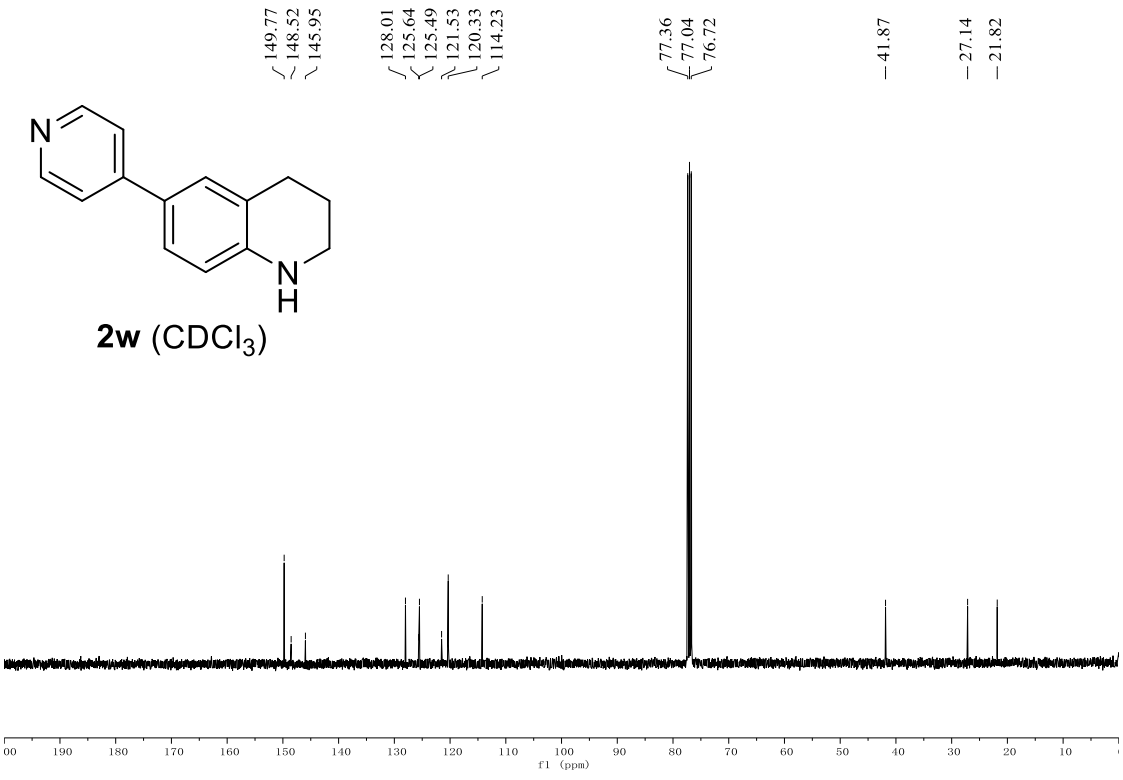
2u ($CDCl_3$)

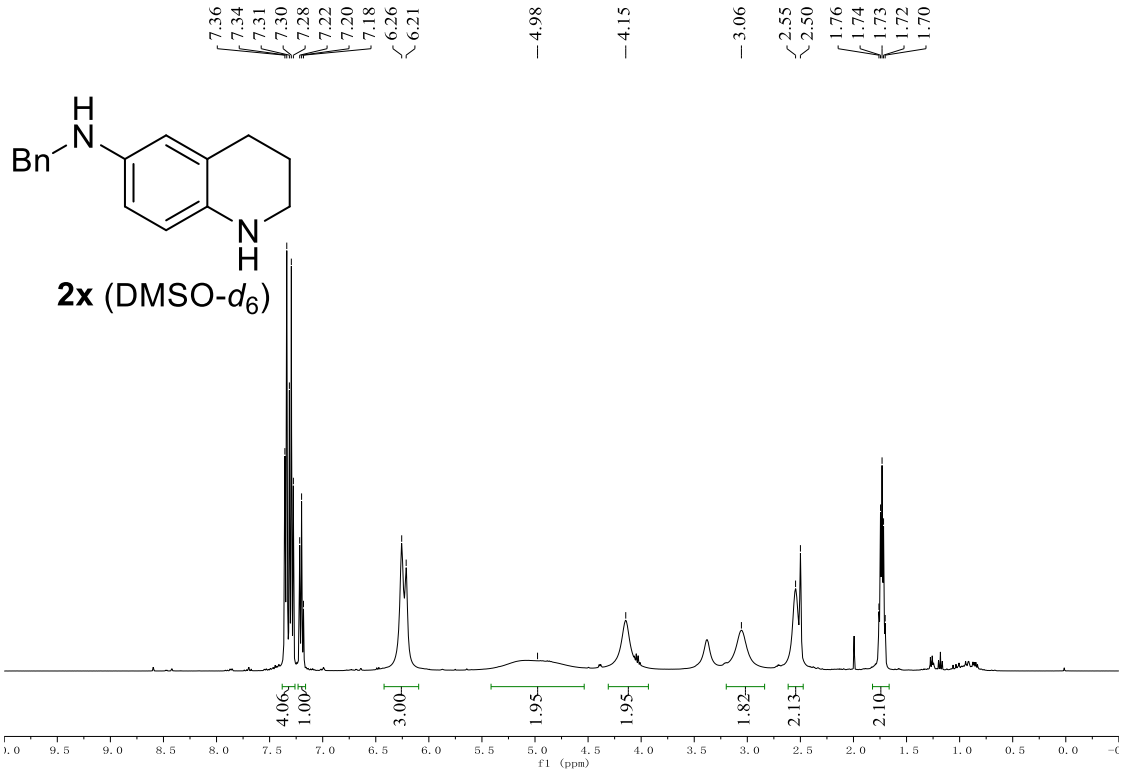


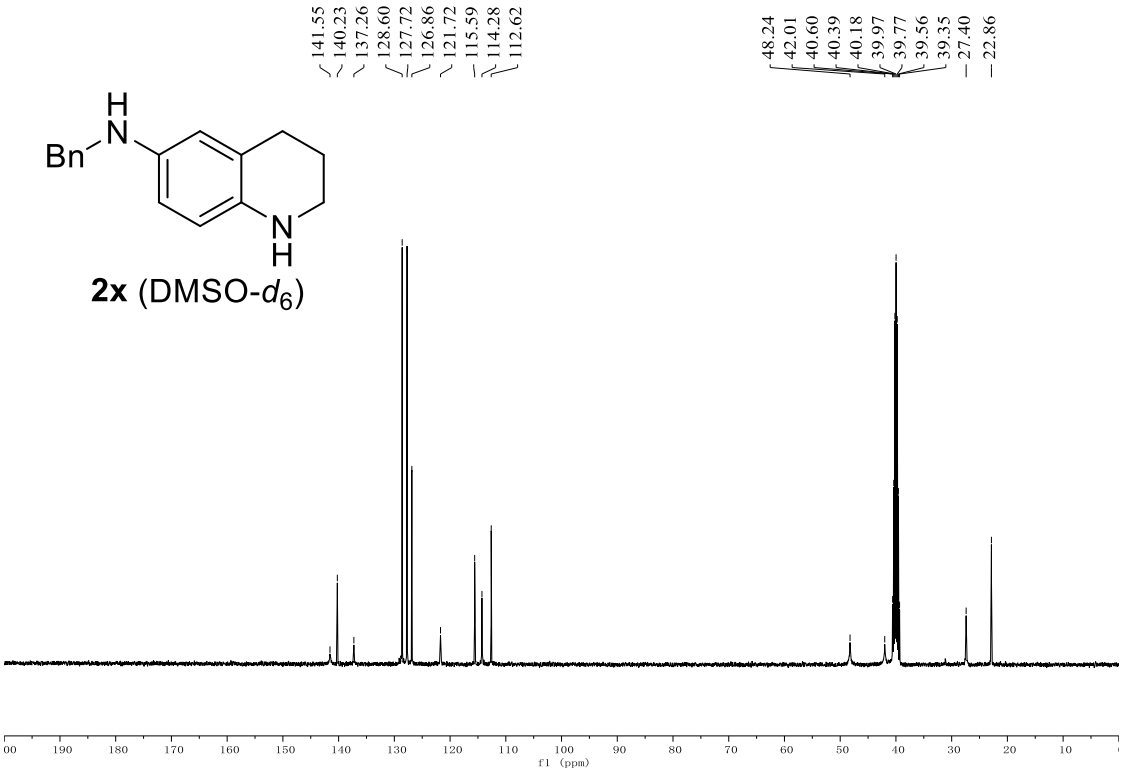
2v ($CDCl_3$)


155.12
144.37
140.58
125.30
122.94
121.34
120.29
114.16
111.46
101.78
77.47
77.17
76.83
42.00
27.10
22.11
O
N
H
2v (CDCl3)
f1 (ppm)

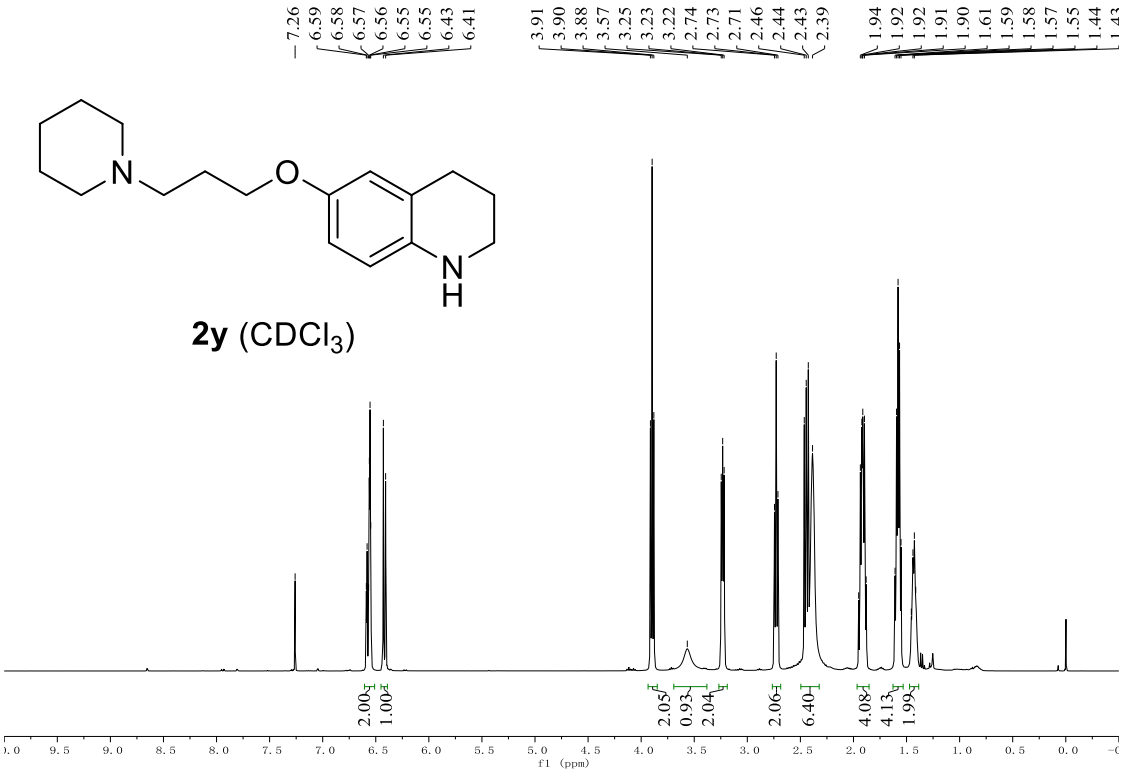

7.44
7.43
7.43
7.42
7.32
7.31
7.29
7.26
6.55
6.53
4.09
3.38
3.36
3.35
2.85
2.83
2.82
2.01
1.99
1.97
1.96
1.95
N
H
2w (CDCl3)
2.03
2.02
2.65
1.00
0.97
2.03
2.00
2.04
f1 (ppm)


149.77
148.52
145.95
128.01
125.64
125.49
121.53
120.33
114.23
77.36
77.04
76.72
41.87
27.14
21.82
N
N
H
2w (CDCl3)
f1 (ppm)

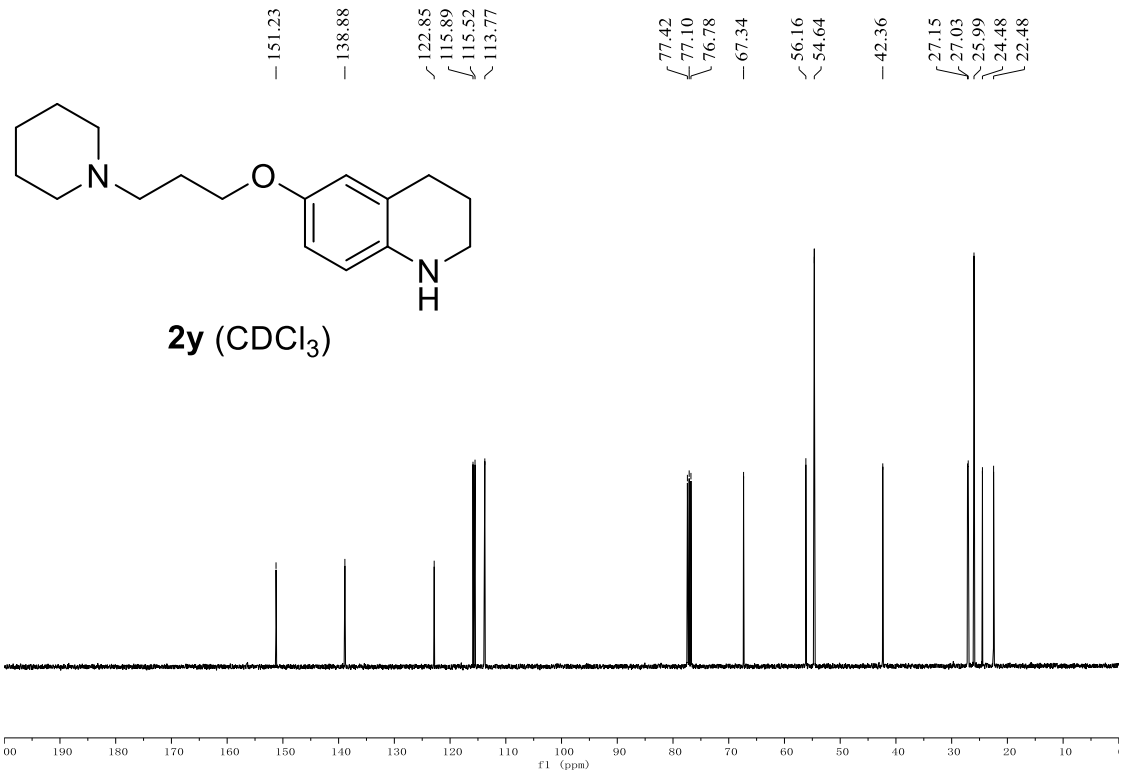

7.36
7.34
7.31
7.30
7.28
7.22
7.20
7.18
6.26
6.21
4.98
4.15
3.06
2.55
2.50
1.76
1.74
1.73
1.72
1.70
H
N
Bn
N
H
2x (DMSO-d6)
4.06
1.00
3.00
1.95
1.95
1.82
2.13
2.10
f1 (ppm)



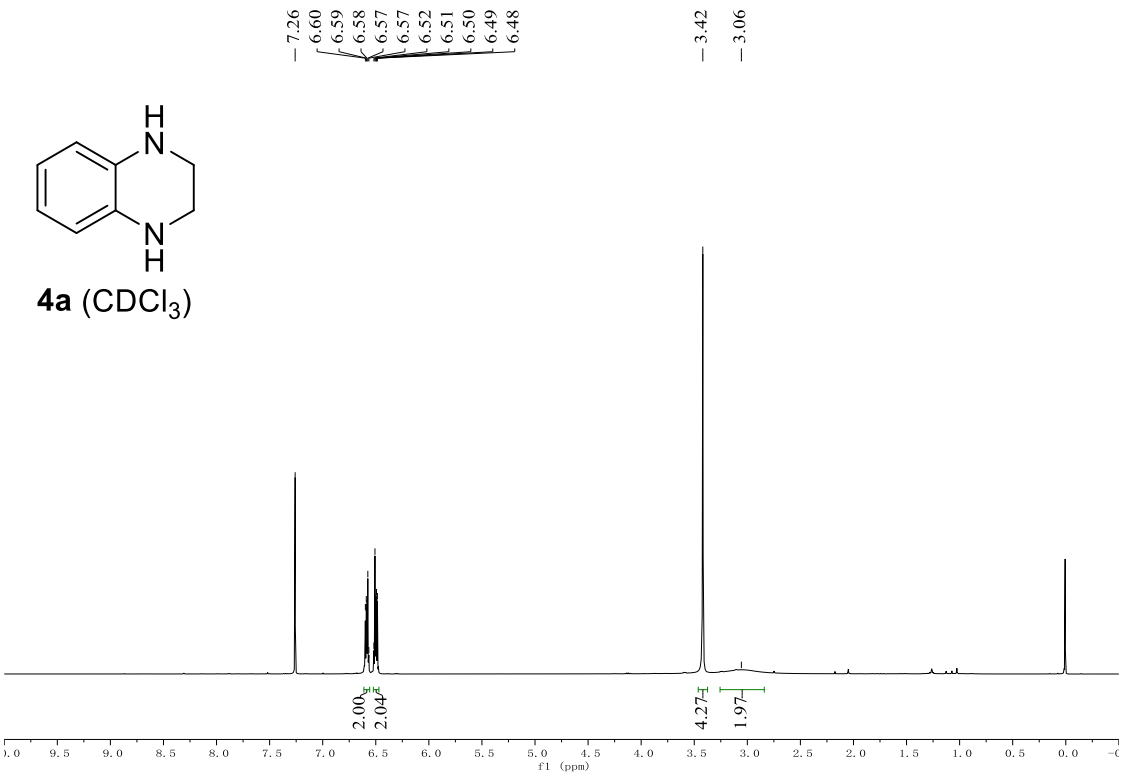
2x (DMSO-d_6)



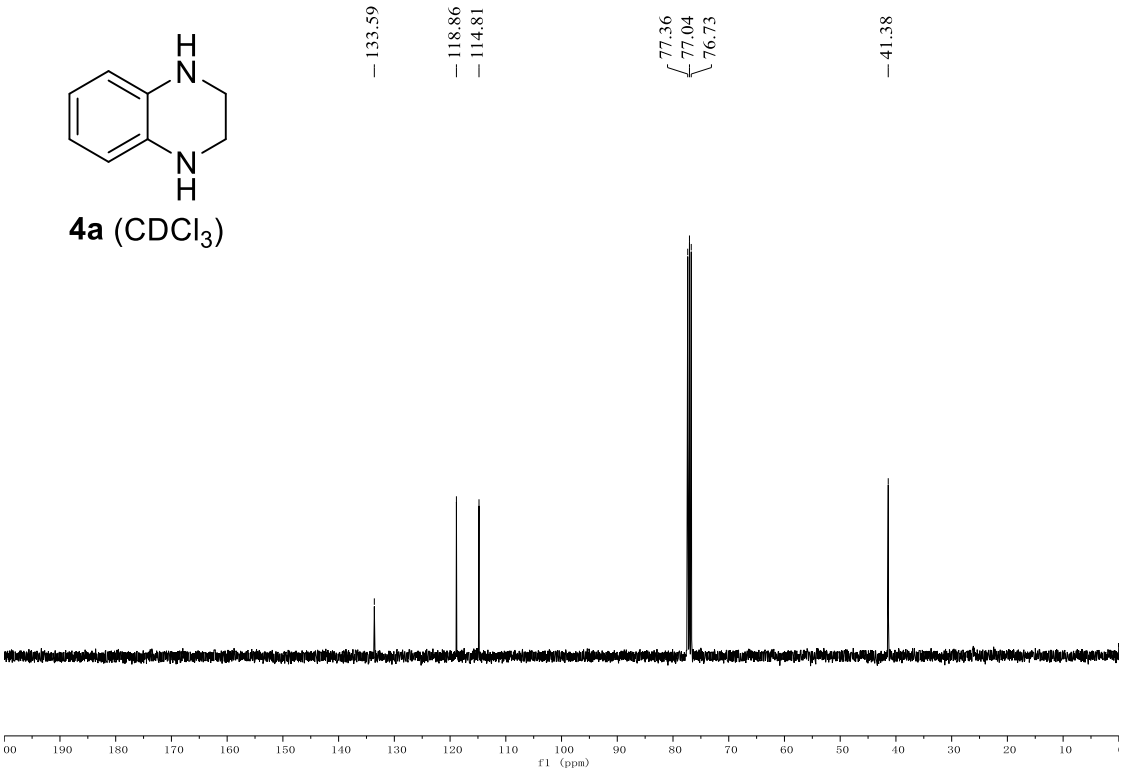
2y ($CDCl_3$)



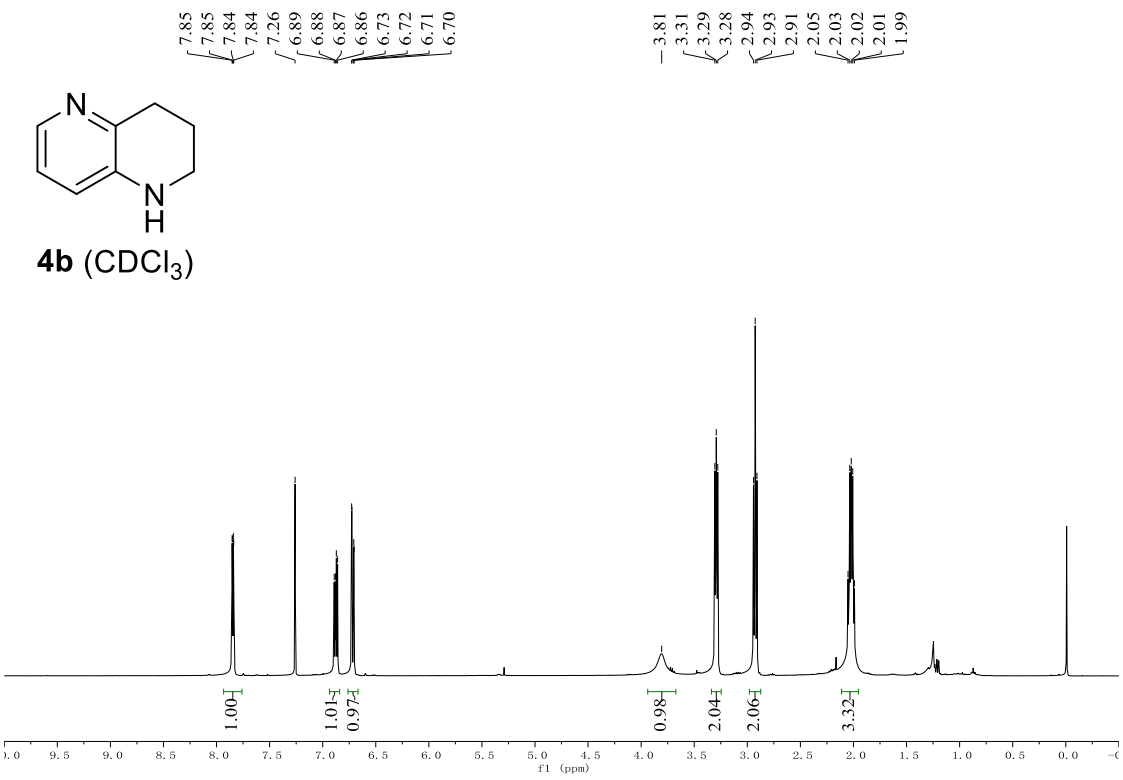
2y ($CDCl_3$)



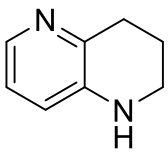
4a ($CDCl_3$)



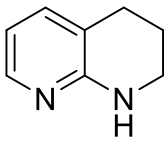
4a ($CDCl_3$)



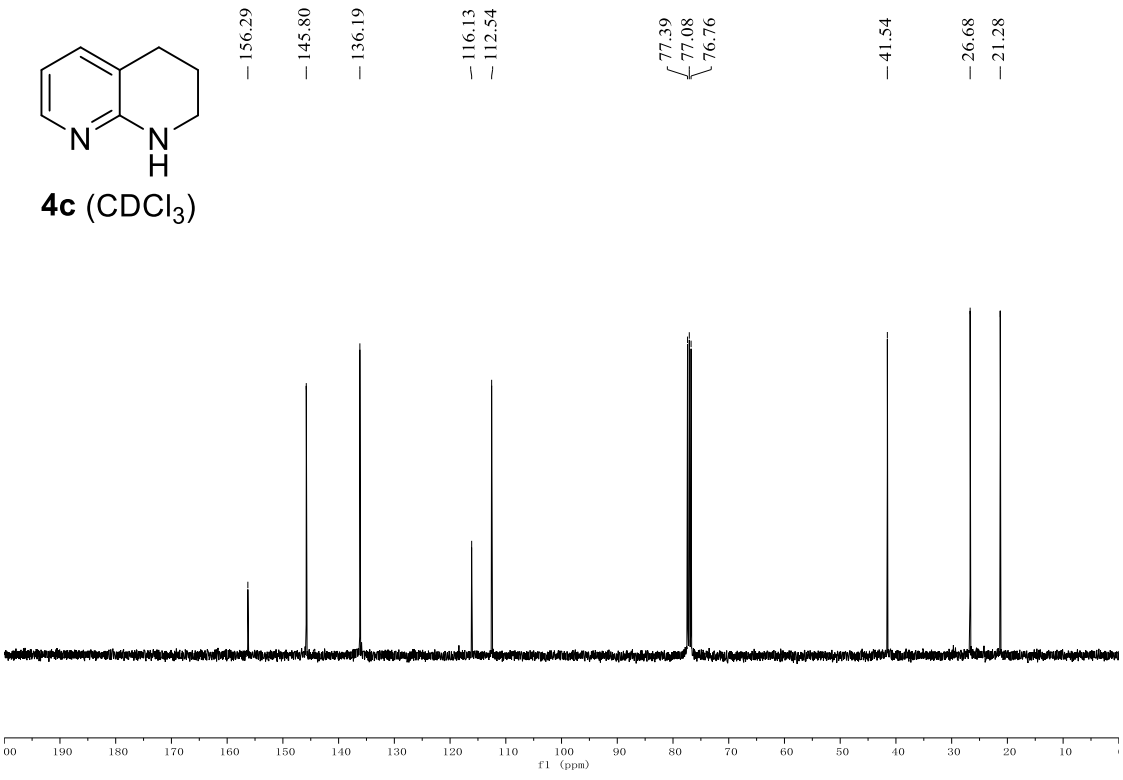
4b ($CDCl_3$)

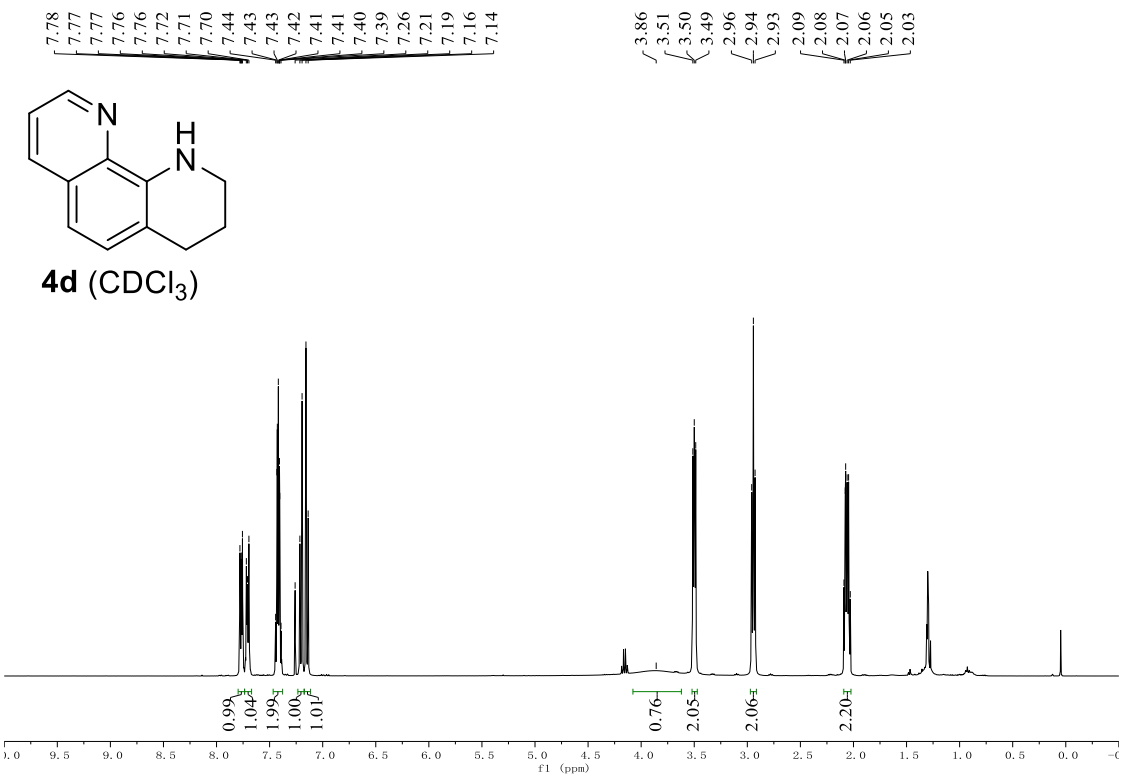


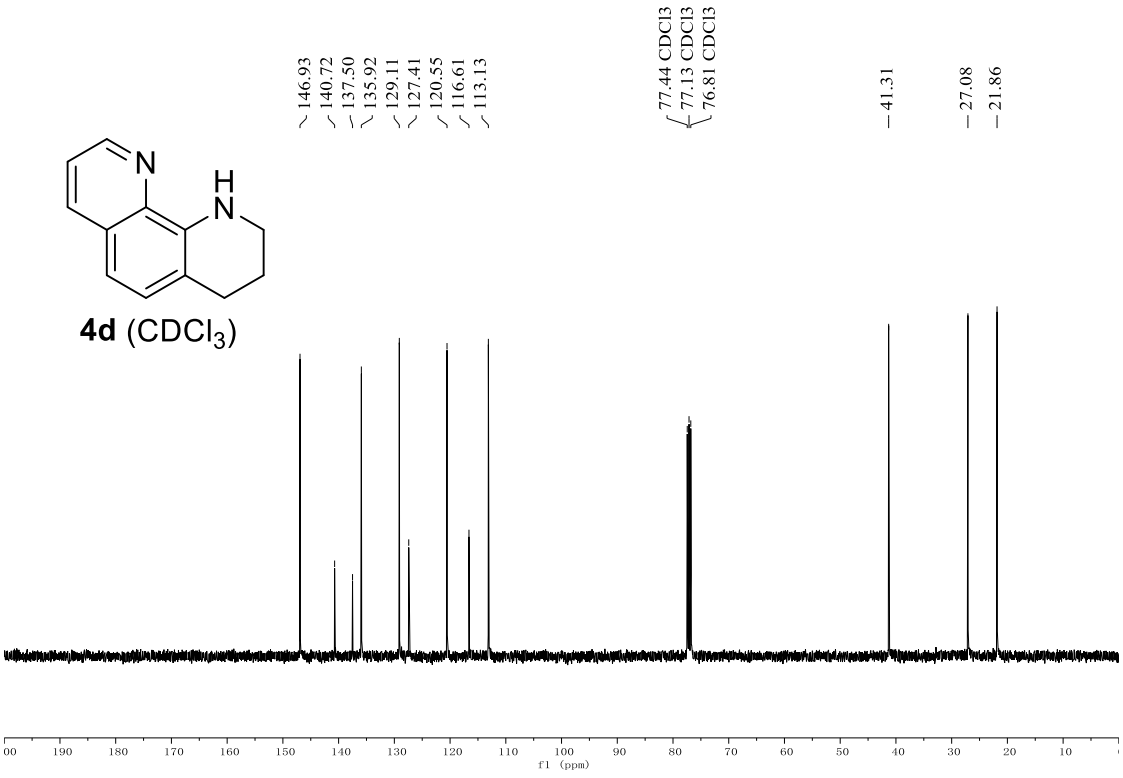
4b ($CDCl_3$)

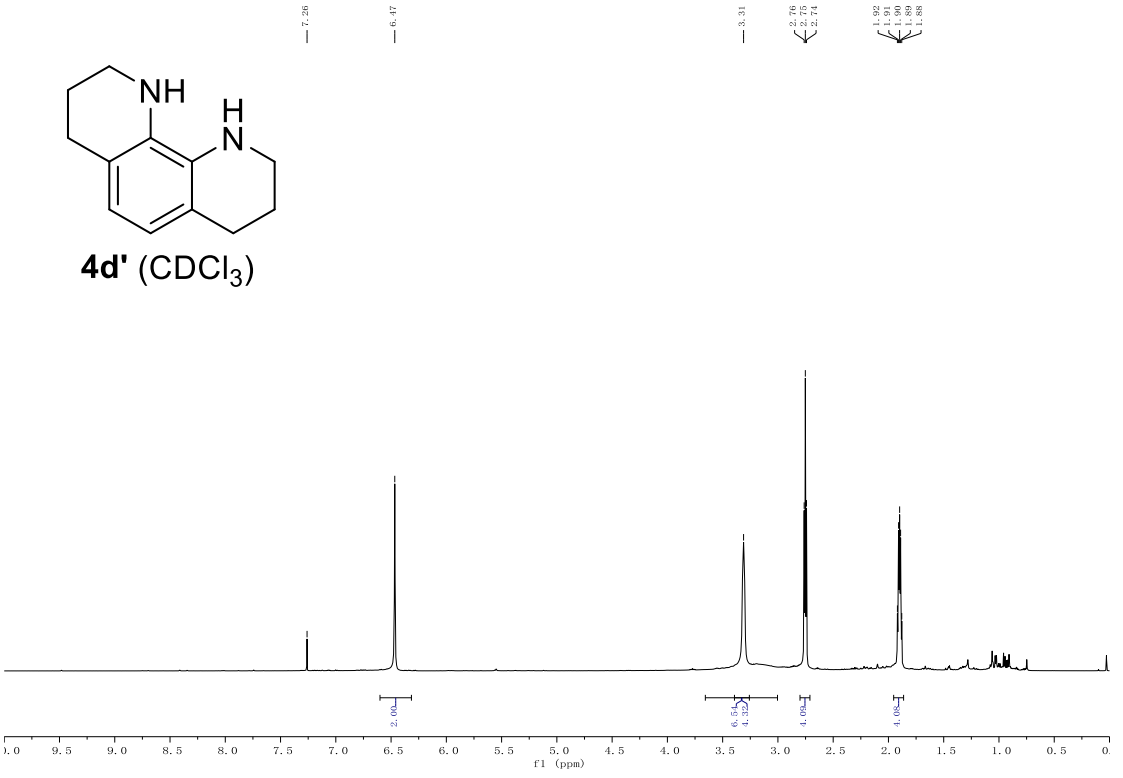


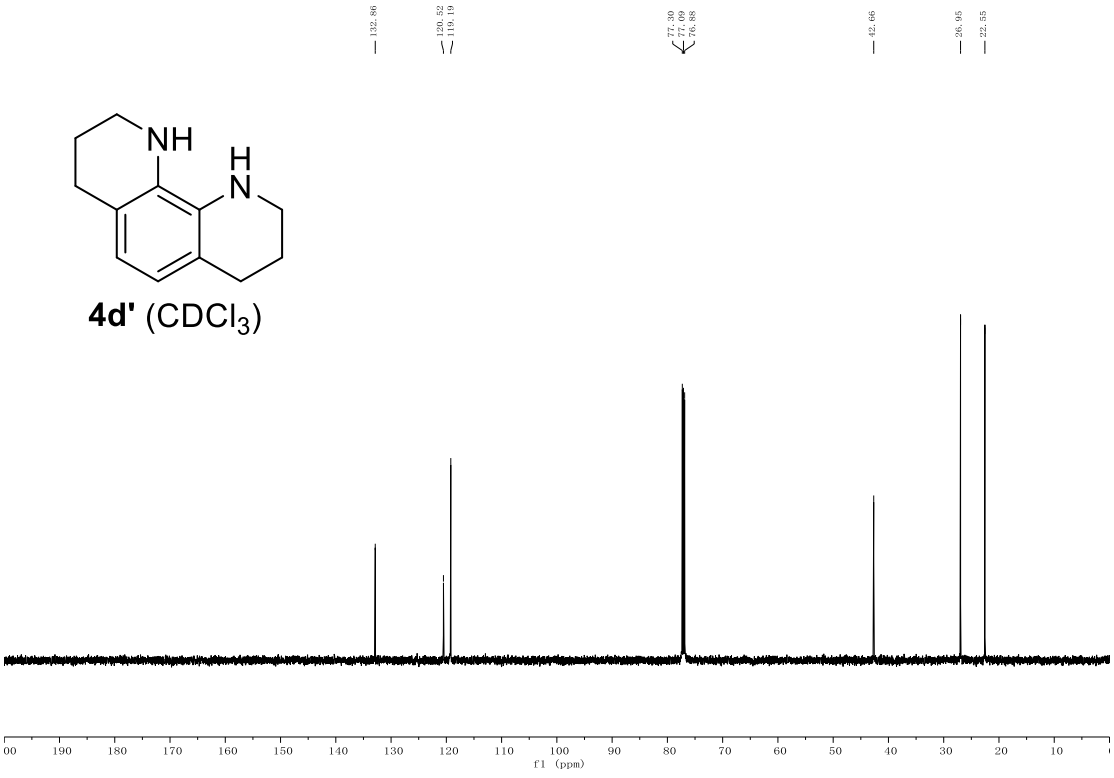
4c ($CDCl_3$)


156.29
145.80
136.19
116.13
112.54
77.39
77.08
76.76
41.54
26.68
21.28
4c (CDCl3)
f1 (ppm)


7.78
7.77
7.77
7.76
7.76
7.72
7.71
7.70
7.44
7.43
7.43
7.42
7.41
7.41
7.40
7.39
7.26
7.21
7.19
7.16
7.14
3.86
3.51
3.50
3.49
2.96
2.94
2.93
2.09
2.08
2.07
2.06
2.05
2.03
4d (CDCl3)
0.99
1.04
1.99
1.00
1.01
0.76
2.05
2.06
2.20
f1 (ppm)


146.93
140.72
137.50
135.92
129.11
127.41
120.55
116.61
113.13
77.44 CDCl3
77.13 CDCl3
76.81 CDCl3
41.31
27.08
21.86
4d (CDCl3)
f1 (ppm)


7.26
6.47
3.31
2.76
2.75
2.74
1.92
1.91
1.90
1.89
1.88
4d' (CDCl3)
2.00
6.54
4.32
4.09
4.08
f1 (ppm)


132.86
120.52
119.19
77.30
77.09
76.88
42.66
26.95
22.55
NH
H
N
4d' (CDCl3)
f1 (ppm)

Energetic Data and Cartesian Coordinates (xyz) for All Optimized Structures

Table S1. Computed Energetic Data for All Optimized Structures

Species	Imag	ZPE	H_{tot}_scrf	G_{tot}_scrf
1a	0	0.135818	-401.8799834	-401.9187374
1,2-2a	0	0.157746	-403.046004	-403.085090
3,4-2a	0	0.157962	-403.047590	-403.086812
1,4-2a	0	0.181818	-404.229637	-404.268844
1,2,3,4-2a	0	0.157746	-403.046004	-403.085090
2A	0	0.108088	-194.2926926	-194.3263296
1A	0	0.083236	-193.1228383	-193.1552853
MnH-1_{2K}	0	0.488981	-4163.025949	-4163.136707
MnH-1_{2K}.dis_CO	0	0.478742	-4049.604624	-4049.710589
MnH-1_{2K}.dis_P	0	0.488207	-4162.959635	-4163.068991
Mn-1_{K}	0	0.482424	-3562.462433	-3562.565492
MnH-1_{1K}_1a	0	0.625192	-4564.918652	-4565.045227
TS1-1a_2-H^-	1(-635.673)	0.623985	-4564.891994	-4565.016612
TS1-1a_3-H^-	1(-640.316)	0.624806	-4564.900712	-4565.024912
TS1-1a_4-H^-	1(-679.516)	0.647782	-4566.079892	-4566.204046
TS2-2a_2-H^-	1(-230.035)	0.647517	-4566.058396	-4566.184075
TS2-2a_3-H^-	1(-703.603)	0.647650	-4566.036851	-4566.161222
TS2-2a_4-H^-	1(-686.166)	0.647145	-4566.045682	-4566.171069
TS2-2a_2'-H^-	1(-703.612)	0.647345	-4566.043171	-4566.168096
TS2-2a_3'-H^-	1(-620.685)	0.623985	-4564.891994	-4565.016612
Mn-1_{1K}_1a-H	0	0.629068	-4564.906837	-4565.031328
Mn-OiPr$_O$-1_{2K}	0	0.580327	-4356.151789	-4356.270166
TS-1A-H^-	1(-442.935)	0.574537	-4356.143405	-4356.261907
MnH-1_{2K}_1A	0	0.57456	-4356.161621	-4356.283244
2H-Mn-5	0	0.5385	-2747.482145	-2747.574304
Mn-5'	0	0.516942	-2746.300553	-2746.392092
2H-Mn-5_1a	0	0.675464	-3149.371008	-3149.482214
TSB-1a-H_H^-	1(-610.087)	0.674426	-3149.344324	-3149.452218
Mn-5-H_1a-H_H	0	0.677433	-3149.342955	-3149.450523
Mn-5-H_1a-H_N	0	0.680257	-3149.349277	-3149.457881
TSB-1a-H_N^+	1(-1027.93)	0.674303	-3149.317761	-3149.425078
Mn-5'_2a$_N$	0	0.677045	-3149.350194	-3149.464419
TSB-1a-H_H^+	1(-932.978)	0.67311	-3149.338411	-3149.445639
Mn-5'_2a$_H$	0	0.677391	-3149.34752	-3149.459104
Mn-5'_iPrOH$_O$	0	0.627297	-2940.602085	-2940.705232
TSB-iPrOH-H_O^+	1(-743.22)	0.624301	-2940.602367	-2940.704028
H-Mn-5'-OiPr$_O$	0	0.629492	-2940.618583	-2940.720528
Mn-5'_iPrOH$_H$	0	0.628024	-2940.596619	-2940.703679
TSB-iPrOH-H_H^+	1(-984.169)	0.623919	-2940.588146	-2940.688507
H-Mn-5'-OiPr$_H$	0	0.627546	-2940.585406	-2940.686084
TSB-iPrOH-H^-	1(-600.265)	0.624429	-2940.583221	-2940.685283
2H-Mn-5_1A	0	0.623561	-2940.611466	-2940.71908

Table S2. The Cartesian Coordinates (xyz) for All Optimized Structures

1a

C	6.27146371	-0.42371054	0.20258571
C	5.55693910	-0.60414163	-0.96079085
C	4.30029457	-1.25862113	-0.93835738
C	3.77851754	-1.73183837	0.31026598
C	4.54033488	-1.52954113	1.48904333
C	5.75848568	-0.88999653	1.43461924
H	3.88113240	-1.12929571	-3.06654506
H	7.23956102	0.08154918	0.17682410
H	5.94849988	-0.24563252	-1.91683030
C	3.51548845	-1.47691490	-2.09607015
H	4.12377041	-1.89797266	2.42840135
H	6.33664860	-0.73972258	2.34938331
C	1.88834148	-2.54799051	-0.69512022
C	2.30715958	-2.12225541	-1.97849211
H	0.92530712	-3.06410641	-0.58899338
H	1.67545728	-2.30795027	-2.84946258
N	2.58148930	-2.36794687	0.40581005

1,2-2a

C	6.31514120	-0.40301654	0.22113238
C	5.56163500	-0.60342229	-0.93501376
C	4.32512272	-1.25278299	-0.89755871
C	3.82265703	-1.72015887	0.34502997
C	4.58452793	-1.51597357	1.50585975
C	5.81448697	-0.86474178	1.43856301
H	3.88833086	-1.12852880	-3.03898833
H	7.27914592	0.10617676	0.17348410
H	5.93248857	-0.25065953	-1.90189592
C	3.50970046	-1.48296819	-2.07587852
H	4.20257142	-1.87356725	2.46634633
H	6.38818911	-0.71844411	2.35719058
C	1.74163937	-2.61861686	-0.73624795
C	2.32331568	-2.10901845	-2.01245441
H	1.53566882	-3.70663120	-0.82832898
H	1.72890850	-2.26937588	-2.91502206
N	2.60985643	-2.35789584	0.39009947
H	2.29526302	-2.67559379	1.29580454
H	0.74106305	-2.16282441	-0.57445916

3,4-2a

C	-2.48007200	0.71959300	0.00003900
C	-1.25715900	1.39023400	-0.00000400
C	-0.04795800	0.69298900	-0.00004600
C	-0.07885800	-0.71450700	-0.00011800
C	-1.31028700	-1.38361100	-0.00000600
C	-2.50698900	-0.67503200	0.00006600
H	1.28471300	2.10994500	-0.86936300
H	-3.41263100	1.28870300	0.00008600
H	-1.23881400	2.48489700	0.00000500
C	1.26402000	1.43312900	-0.00006900
H	-1.29123000	-2.47550300	0.00000300
H	-3.46033400	-1.20816600	0.00012100
C	2.22128200	-0.93661000	0.00001300
C	2.50293300	0.53312200	0.00014900
H	3.15449500	0.74247700	0.86547300
N	1.08225100	-1.50833400	-0.00008200
H	1.28461900	2.11022500	0.86900600
H	3.15484900	0.74258400	-0.86487800
H	3.10711400	-1.59266000	-0.00001600

1,4-2a

C	-2.47846900	-0.71037500	-0.00004700
C	-1.25867700	-1.38622000	-0.00002100
C	-0.03533800	-0.71391300	0.00002700
C	-0.05573500	0.69778400	0.00004700
C	-1.28028300	1.38216900	0.00001700
C	-2.48241400	0.68383500	-0.00002200
H	-3.41708700	-1.26785100	-0.00008500
H	-1.24741700	-2.48068500	-0.00003900
C	1.26741600	-1.48303800	0.00007700
H	-1.27713800	2.47598500	0.00002400
H	-3.42593000	1.23448400	-0.00003800
C	2.35846600	0.75002700	-0.00005400
C	2.46602200	-0.58816500	-0.00006900
N	1.13916000	1.40068600	0.00005700
H	3.46189700	-1.03294500	-0.00015700
H	3.23166100	1.40428500	-0.00013900
H	1.10669800	2.40874700	-0.00001800
H	1.29366800	-2.16961700	0.86985600
H	1.29360800	-2.16983200	-0.86952900

1,2,3,4-2a

C	-2.58123800	0.69237000	-0.00005600
C	-1.36917100	1.37801600	-0.00009700
C	-0.13866400	0.71664900	-0.00005600
C	-0.12639500	-0.69197300	0.00000600
C	-1.35329000	-1.38746900	0.00005800
C	-2.56107700	-0.70412500	0.00004000
H	1.13363400	2.17859700	-0.86837300
H	-3.52686200	1.23757600	-0.00008500
H	-1.36630000	2.47310200	-0.00015200
C	1.14277500	1.49953300	-0.00006900
H	-1.33972100	-2.48161800	0.00011800
H	-3.49629700	-1.26958200	0.00007900
C	2.38241500	-0.83544700	-0.00008300
C	2.45592200	0.70177400	0.00019400

H 2.93629300 -1.21948700 0.87599500 H 3.05452100 1.00922100 0.86829400 N 1.05510900 -1.38818900 0.00004700 H 1.13348000 2.17883700 0.86804300 H 3.05499900 1.00946500 -0.86748600 H 2.93604200 -1.21919900 -0.87645300 H 0.98678400 -2.39554100 0.00007000	
2A C -0.00187997 0.04489746 0.35771399 H 0.00619659 0.08373572 1.46905181 C -1.32105728 -0.54117936 -0.08597122 H -2.15631620 0.08896422 0.24532521 H -1.36270013 -0.60111839 -1.18311457 H -1.46675359 -1.55083315 0.32007482 C 1.18455122 -0.78173029 -0.09981135 H 1.20799902 -0.84654440 -1.19758117 H 2.13574386 -0.33646913 0.22907415 H 1.14850440 -1.80412153 0.30238413 O 0.05352245 1.35937166 -0.17006954 H 0.89329463 1.74752020 0.09663173	**1A** C -0.98962179 1.86266121 1.24613524 H -1.37208115 2.88826333 1.21044933 H -1.32806191 1.38030015 2.17497759 H 0.10892310 1.88516052 1.29704218 C -0.98971558 -0.34961192 -0.03106975 H -1.32559450 -0.91227020 0.85241527 H -1.37431473 -0.83225032 -0.93580834 H 0.10886644 -0.40460603 -0.02802683 C -1.45183949 1.08284145 0.04234650 O -2.15175298 1.57676690 -0.81313980
MnH-1_{2K} Mn 1.68272736 0.91274884 -0.09674341 C 0.41176949 -1.57136934 -1.22127870 C -1.00480825 0.29922745 -1.30062418 N 0.21100904 -0.24159771 -1.01876731 N -0.53653061 -2.33714966 -1.87768919 N -1.97157732 -0.44117176 -1.95895655 C -1.65533059 -1.70603115 -2.22384252 N -1.30246967 1.54603511 -0.95779634 N 1.51638252 -2.17477966 -0.80154728 P -0.02454544 2.33133760 -0.11241420 P 2.58877469 -1.11240213 0.02800214 C 2.67780315 -1.95644098 1.70198109 H 1.59721442 -2.07675906 1.89839535 C 4.21391877 -1.58037734 -0.77386075 H 4.37199612 -2.65506822 -0.56086766 C 3.23909966 -1.06751273 2.79920824 H 3.15690983 -1.56108409 3.78080614 H 4.30219988 -0.82546977 2.64940002 H 2.69309275 -0.11636431 2.85213654 C 3.31727221 -3.33425274 1.69400530 H 4.41179623 -3.28276022 1.57977716 H 3.12552540 -3.86744579 2.63935192 H 2.92957405 -3.96674296 0.87833099 C 5.36023462 -0.77927948 -0.17677135 H 5.18294388 0.30166536 -0.29199842 H 5.49944353 -0.97293570 0.89641345 H 6.31393327 -1.01241173 -0.67611471 C 4.14824357 -1.40570824 -2.28274072 H 5.07095970 -1.77544469 -2.75857020 H 3.29784905 -1.94844140 -2.72282237 H 4.03630480 -0.35005617 -2.56540600 C -0.88667571 2.72593093 1.50734116 H -1.28848101 1.72347345 1.74046779	**Mn-1_{K}** Mn -0.01602802 -0.65918331 -0.02356993 C 1.23010719 2.05830548 -0.08318970 C -1.16026790 2.07569678 -0.03511524 N 0.01105536 1.35985922 -0.11449050 N 1.23037844 3.42430595 -0.05002451 N -1.15407473 3.43523435 0.02600318 C 0.06225491 4.02024769 0.00494962 N -2.35159615 1.46212046 -0.02013341 N 2.37514059 1.41969184 -0.09387204 P -2.23015864 -0.22094146 -0.15581539 P 2.22075137 -0.25664620 -0.18937051 C 2.98097766 -0.63482805 -1.85384522 H 2.20928696 -0.26417769 -2.55482239 C 3.43202873 -0.94019213 1.04302683 H 4.41728931 -0.90233162 0.54181150 C 3.17573037 -2.12308500 -2.09476491 H 3.98391350 -2.52754395 -1.46589791 H 2.27052625 -2.71435465 -1.89479154 H 3.46851497 -2.31055841 -3.13914936 C 4.25602975 0.15663809 -2.09753301 H 5.07260849 -0.18143745 -1.44068188 H 4.60271762 0.01871789 -3.13340561 H 4.10820159 1.22820027 -1.91521432 C 3.10527771 -2.38630039 1.39221882 H 2.18145139 -2.45037288 1.98522633 H 2.96517185

C	0.02589293	3.98355362	-0.99198396
H	-0.92987103	4.49619092	-0.77306023
C	0.06671767	3.10263812	2.62858301
H	-0.47149938	3.18515110	3.58640070
H	0.85438346	2.34698812	2.74802054
H	0.56238378	4.07018892	2.45653774
C	-2.05198025	3.69404402	1.39729406
H	-2.71828902	3.44763722	0.55410320
H	-2.66592493	3.68372621	2.31254784
H	-1.71429624	4.73351030	1.25885464
C	1.17653665	4.82647341	-0.46302255
H	2.14098968	4.32813784	-0.64741963
H	1.21189579	5.81024106	-0.95717313
H	1.10932338	5.00616385	0.61959908
C	0.12828403	3.80440297	-2.49837793
H	-0.70294580	3.20570990	-2.90049114
H	0.11975239	4.78147965	-3.00793371
H	1.06000633	3.29671527	-2.78440024
C	2.49850267	1.48932335	-1.57230878
O	3.08465632	1.91894202	-2.49967160
C	2.77616487	1.79173993	0.97808475
O	3.48062233	2.36339347	1.72165827
H	0.93756777	0.40011307	1.26993305
C	-2.65578280	-2.49702596	-3.01482482
H	-3.67974888	-2.14593209	-2.83406593
H	-2.46070451	-2.39271315	-4.09363486
H	-2.60181588	-3.56692890	-2.77649179
K	1.05724614	-4.46210777	-1.85116125
K	-3.57834485	1.66663687	-2.12123174

-3.02790670	0.51119130	H	3.91094302
-2.82849089	1.99797856	C	3.48643358
-0.05971956	2.28116927	H	4.21891363
-0.45609978	3.00073033	H	3.76205608
0.97251673	2.03231528	H	2.51195539
-0.03096122	2.79204603	C	-3.05492085
-0.56945972	-1.80153241	H	-2.29140979
-0.23327890	-2.52728384	C	-3.44134980
-0.91964749	1.07934941	H	-4.43639795
-0.88315446	0.59524640	C	-3.30874081
-2.05132933	-2.02863217	H	-3.62507596
-2.23763878	-3.06615439	H	-2.41795732
-2.66775641	-1.84127785	H	-4.11646594
-2.42654461	-1.38112227	C	-4.30925639
0.25803017	-2.03028829	H	-4.09714100
1.33457316	-1.97465414	H	-4.73795915
0.05272173	-3.02346194	H	-5.09478484
0.02635948	-1.29230923	C	-3.10612169
-2.37130857	1.40198953	H	-2.18718103
-2.43842020	2.00118044	H	-3.91369867
-2.83437528	1.98923844	H	-2.94895043
-2.99077145	0.50903755	C	-3.48711267
-0.08037837	2.34636431	H	-3.83373968
0.94503072	2.15673750	H	-4.16521680
-0.53405898	3.08524725	H	-2.49515648
-0.00865785	2.81675768	C	-0.01309966
-0.95969069	1.68795492	O	-0.01883270
-1.13257764	2.84715953	C	-0.03326297
-2.40309448	-0.35626020	O	-0.05551550
-3.54981393	-0.58871228	C	0.06096716
5.51722860	0.05449166	H	-0.51313596
5.93493398	-0.78567381	H	-0.41874898
5.87517519	0.97771249	H	1.08367952
5.90525374	0.01590467	K	-3.74799563
3.62711464	0.32248713		

MnH-1_{2K}-dis_CO			**MnH-1_{2K}-dis_P**		
Mn -1.14273700	0.12296800	0.00000000	Mn -0.13724500	-1.23708700	0.09134200
C 1.58842500	0.02693800	1.18171900	C 1.18785600	1.51970500	-0.31901300
C 1.58842500	0.02693800	-1.18171900	C -1.14193500	1.45781200	-0.65342600
N 0.89902600	0.12580700	0.00000000	N 0.03090800	0.78808900	-0.47094500
N 2.97227900	0.00170000	1.19102300	N 1.10467700	2.90015200	-0.15752900
N 2.97227900	0.00170000	-1.19102300	N -1.16540300	2.82089400	-0.85434300
C 3.56640700	0.01206900	0.00000000	C -0.04006300	3.45879400	-0.51012700

N	0.95646200	-0.04749500	-2.34435400
N	0.95646200	-0.04749500	2.34435400
P	-0.77065800	-0.04948900	-2.14816700
P	-0.77065800	-0.04948900	2.14816700
C	-1.21925600	-1.60969400	3.07745500
H	-0.54092800	-2.32846600	2.58354500
C	-1.21381700	1.33146600	3.33932700
H	-0.65359800	1.16561800	4.28088200
C	-2.64263800	-2.05608400	2.78494800
H	-2.83782100	-3.05699300	3.20251800
H	-3.39478100	-1.37464300	3.20970500
H	-2.81362400	-2.09093500	1.69976900
C	-0.89359400	-1.58561400	4.56080200
H	-1.55824100	-0.90934400	5.12126300
H	-1.00439000	-2.58427600	5.01484800
H	0.14072400	-1.25323000	4.74954300
C	-2.70533300	1.37318200	3.63324500
H	-3.29519800	1.36665700	2.70223700
H	-3.04256200	0.51796000	4.23577500
H	-2.97776600	2.28538600	4.18839500
C	-0.74612300	2.63655100	2.71257900
H	-0.92847600	3.49882400	3.37426600
H	0.32711500	2.61382200	2.46996300
H	-1.29029900	2.82383000	1.77179400
C	-1.21925600	-1.60969400	-3.07745500
H	-0.54092800	-2.32846600	-2.58354500
C	-1.21381700	1.33146600	-3.33932700
H	-0.65359800	1.16561800	-4.28088200
C	-2.64263800	-2.05608400	-2.78494800
H	-2.83782100	-3.05699300	-3.20251800
H	-2.81362400	-2.09093500	-1.69976900
H	-3.39478100	-1.37464300	-3.20970500
C	-0.89359400	-1.58561400	-4.56080200
H	0.14072400	-1.25323000	-4.74954300
H	-1.00439000	-2.58427600	-5.01484800
H	-1.55824100	-0.90934400	-5.12126300
C	-2.70533300	1.37318200	-3.63324500
H	-3.29519800	1.36665700	-2.70223700
H	-2.97776600	2.28538600	-4.18839500
H	-3.04256200	0.51796000	-4.23577500
C	-0.74612300	2.63655100	-2.71257900
H	0.32711500	2.61382200	-2.46996300
H	-0.92847600	3.49882400	-3.37426600
H	-1.29029900	2.82383000	-1.77179400
C	-2.89423600	0.19509600	0.00000000
O	-4.07895700	0.22156600	0.00000000
H	-1.18990900	-1.45798400	0.00000000
C	5.06619700	0.06479900	0.00000000
H	5.48662000	-0.41648300	-0.89260000
H	5.41476300	1.10964300	0.00000000
H	5.48662000	-0.41648300	0.89260000
K	3.02957000	-0.17898500	3.83411200
K	3.02957000	-0.17898500	-3.83411200

N	-2.32406700	0.83861200	-0.60906700
N	2.39283400	1.02238800	-0.22406000
P	-2.25344900	-0.74010100	0.01966400
P	3.04635900	-0.51814000	0.01430500
C	2.27235100	-1.66516600	-1.25543100
H	1.15441600	-1.54335500	-1.18085700
C	4.73375700	-0.14637500	-0.73613400
H	4.56711000	0.26505900	-1.74766000
C	2.56465300	-3.13439100	-0.99396700
H	1.86640000	-3.77566300	-1.55423000
H	3.58203800	-3.41468600	-1.30486400
H	2.45827300	-3.39178300	0.06942600
C	2.51409100	-1.25566700	-2.69980300
H	3.55939000	-1.42584700	-3.00089800
H	1.87969300	-1.83958700	-3.38497800
H	2.28432000	-0.19208900	-2.86052300
C	5.59563100	-1.39505300	-0.82499100
H	5.64968200	-1.91967500	0.14334900
H	5.22193900	-2.11716600	-1.56381800
H	6.62856000	-1.14675800	-1.11592100
C	5.41402700	0.92727900	0.09952600
H	6.41341300	1.17042800	-0.29492700
H	4.82555000	1.85587700	0.10855900
H	5.55663100	0.59085500	1.14233100
C	-3.36963700	-1.67209000	-1.15817400
H	-2.96847700	-1.30143500	-2.11794800
C	-3.31145000	-0.56675500	1.55795700
H	-4.29517000	-0.19999600	1.20932000
C	-3.18120700	-3.17955500	-1.13847100
H	-3.81334900	-3.65754600	-1.90333300
H	-2.13914200	-3.45144900	-1.34855800
H	-3.44595900	-3.63191700	-0.17134900
C	-4.83602600	-1.27954800	-1.07451300
H	-4.97817100	-0.18647900	-1.07288600
H	-5.39811500	-1.68073100	-1.93290100
H	-5.32334600	-1.67322400	-0.16884600
C	-3.49400500	-1.90392700	2.25752300
H	-2.52004600	-2.35114300	2.51242800
H	-4.05861200	-1.79075000	3.19648400
H	-4.03582200	-2.63539800	1.64097200
C	-2.73092700	0.47695300	2.49746000
H	-2.52750800	1.42735600	1.98019200
H	-3.42617700	0.68649500	3.32624100
H	-1.78716700	0.13657200	2.94523700
C	0.35261300	-0.70881600	1.70715000
O	0.67242000	-0.19906100	2.73277600
C	-0.33815200	-2.94696000	0.51275900
O	-0.48445000	-4.06982300	0.80841900
H	-0.68857000	-1.47108400	-1.43072400
C	-0.10405400	4.95754200	-0.50537000
H	-0.33834200	5.33111800	-1.51316500
H	-0.90052300	5.32286200	0.16005100
H	0.85178200	5.39267700	-0.19389700
K	2.32916200	1.91717400	2.26348700
K	-3.73014900	2.83633700	-1.42459700

MnH-1_{1K}_1a			
Mn	1.56269213		-0.98225018

TS1-$1a_2$-H^-			
Mn	1.56551059		-0.34817518

-0.04623242		C	0.54662726	-0.43506704		C	-0.87541169
1.55749672	1.20126410		C	-2.06461757	-0.06882454		C
-0.93121557			-0.25367232	-1.38749527			0.16185280
1.45951059		N	0.28889585	-0.63387828		N	-0.45524443
0.21995731	1.06573241		N	-0.83368105	-0.50505293		N
-0.32636333			2.38267771	-2.21289084			-2.33540651
1.88001023		N	-1.80099689	0.11685324		N	-2.73104728
0.54249249	2.17135849		C	-0.10417319	-0.51579293		C
-1.42299544			1.80493913	-3.05242839			-1.34349438
2.35500418		N	-1.33895827	-0.15686231		N	-1.03526155
-1.47751978	1.13968239		N	1.42803319	-0.82343658		N
1.61400235			2.11602359	-0.01354873			-3.01921707
0.64389468		P	-0.19684982	0.25576834		P	0.65388809
-2.34215346	0.19736853		P	1.67662862	-0.83763762		P
2.65598006			0.97807909	1.61778562			-2.55924547
-0.10362531		C	3.01749356	0.06083777		C	2.34152132
1.84598538	-1.73500088		H	-3.21268561	1.67435758		H
2.00585263			2.20079367	1.56901069			-2.89081184
-2.00610233		C	4.23642474	2.39854937		C	2.21731842
1.24429681	0.85836386		H	-3.80710777	-1.19063609		H
4.52522637			2.29628353	2.03790132			-4.79206034
0.68731948		C	3.46408964	-0.72522655		C	3.64190837
0.89179371	-2.83004658		H	-2.53150411	2.06916330		H
3.62462560			1.42822561	4.01815450			-2.92406384
-3.77894216		H	4.40717399	3.02719944		H	4.43612335
0.38128099	-2.58349357		H	-2.68220559	1.32314504		H
2.71722721			0.10587448	3.52192897			-1.44484288
-3.00379343		C	3.91264102	2.17369937		C	2.42958886
3.07047000	-1.63320747		H	-4.72800673	1.76695587		H
4.96114546			2.79802641	3.23270513			-5.13271207
-1.43881368		H	3.90866455	1.13288271		H	2.65624378
3.64052471	-2.57676260		H	-5.04560173	2.79788351		H
3.60113920			3.75294762	1.49359683			-5.22003616
-0.82655141		C	5.34074899	1.45980654		C	3.70244833
0.33055020	0.35077215		H	-3.65051049	-1.47587121		H
5.06296740			-0.72883100	3.93204394			-2.65466701
0.46119945		H	5.57592846	-1.88310331		H	4.32329104
0.49872889	-0.71107552		H	-3.79146798	-0.57851216		H
6.27293425			0.48354772	4.03937978			-4.38923976
0.91683737		C	3.99426944	-2.21959441		C	1.37231729
1.07922787	2.34995662		H	-3.75074087	-2.45350086		H
4.91164488			1.31110130	1.66088096			-4.56247743
2.91359070		H	3.20235761	-3.13919924		H	0.30419002
1.75318916	2.70469083		H	-3.86959520	-2.22543546		H
3.70784140			0.05162444	1.50188724			-2.80713591
2.61065193		C	-1.26014115	-2.99931844		C	0.77386726
-2.73450561	-1.29615081		H	3.03494149	0.44826846		H
-1.65030409			-1.71932849	0.16450507			2.56968763
-1.47578443		C	-0.09449591	1.24269590		C	0.89331880
-3.97294463	1.09842222		H	2.58152413	-2.45060625		H
-1.09021197			-4.44323992	0.30035476			3.50923257
1.00020721		C	-0.48894963	-2.35510092		C	2.16447701
-3.14346383	-2.53797503		H	3.25135964	1.01691470		H
-1.15663167			-3.18890164	2.13499980			3.95816056
-3.41527488		H	0.31598904	1.86281771		H	2.60875578
-2.43047212	-2.76156165		H	2.31481543	1.37714441		H
-0.02474722			-4.13681678	2.86296831			3.66947876

-2.44176707		C	-2.44417010	0.27650138		C	0.10852543
-3.64834574	-1.02934675		H	4.34478607	0.05725029		H
-2.96396534			-3.39740889	-0.86710759			4.19226380
-0.08997775		H	-3.18414365	-0.43206560		H	-0.05128572
-3.59273298	-1.84662078		H	4.98720398	0.93994887		H
-2.14310537			-4.70507231	0.72594282			4.92701213
-0.95297843		C	0.94692683	-0.64433123		C	2.35294032
-4.87187525	0.44889232		H	2.94627048	-2.67201467		H
1.95120733			-4.42716364	2.98826651			2.04919129
0.52114068		H	0.98726515	-2.71844249		H	2.48405981
-5.85494752	0.94339392		H	3.48570979	-3.62286030		H
0.74830811			-5.05099382	2.75307895			3.59198330
-0.61825239		C	0.17653661	-1.87650708		C	0.31176410
-3.77013391	2.58029126		H	1.79044260	-3.61156029		H
-0.57866808			-3.12100067	-0.74280132			1.53764816
3.04414733		H	0.16721513	-3.43596668		H	0.36858771
-4.73651891	3.10879964		H	2.37833803	-4.54097144		H
1.16104360			-3.31612787	0.85892812			0.85523548
2.75648042		C	2.55587644	-3.78866828		C	2.17960945
-1.74271932	1.22080262		O	-0.54533237	-2.08025657		O
3.26971571			-2.30614675	2.68815360			-0.63721793
1.96522049		C	2.42868997	-3.13538829		C	3.17688008
-1.87775621	-1.30141786		O	0.13706800	0.09834775		O
2.96941564			-2.46674098	4.23277020			0.46630266
-2.15787367		H	0.76534553	0.48790608		H	1.11657071
-0.38983289	-1.38621757		C	-0.00286711	1.22217951		C
-5.54538266			1.08053297	-3.84305913			2.18712829
-0.51713256		C	-4.81536853	3.52554042		C	-2.50783631
0.41988794	-1.49193844		C	2.54418915	3.68340846		C
-3.46703930			0.77039190	-1.46975969			1.62151112
-1.75191415		C	-2.85647370	3.44315219		C	-1.78443863
1.81849465	-0.98625141		C	0.28813925	3.00710812		C
-3.62635693			2.46495907	-3.15778960			-0.04377009
0.01045211		C	-4.94306934	2.85972645		C	-4.16065271
2.10681030	0.24079848		H	0.87737746	3.11739375		H
-3.11739469			-0.65831921	0.18612807			2.90463321
-3.35802941		H	-6.59420901	4.07167443		H	-4.63742673
0.82162101	-0.34766400		H	2.90393892	3.74841718		H
-5.27763077			-0.36762776	-2.24291131			3.54831270
-2.09515258		C	-2.68001850	4.03046992		C	-0.08917455
0.13961198	-2.75088993		H	1.92344742	3.67352500		H
-3.14858042			3.25445714	-3.41104673			-1.05550672
0.59573641		H	-5.52226910	2.53102655		H	-5.20743141
2.62999945	1.00619384		C	0.57978914	3.00688141		C
-0.86088778			1.55604116	0.45393786			-0.27998587
-2.09861958		C	-1.36817345	2.84045267		C	0.85448909
0.51509494	-2.90563638		H	0.98905683	3.38249879		H
0.18177268			1.86313829	1.19090586			-1.08457995
-2.23571125		H	-0.70788110	2.87206728		H	1.92026486
0.02443341	-3.62254405		N	1.18801574	3.51889849		N
-1.56716848			2.21588952	-0.83561096			-0.66203522
-1.19738034		C	-2.31942680	2.79259126		C	-4.51656343
2.65412152	3.20695373		H	-1.65016356	-0.05377269		H
-3.37302501			2.35704732	-5.08925036			-0.78032065
3.11205207		H	-2.04721195	0.29618719		H	-4.91363690
2.53593648	4.26675449		H	-1.91446196	-1.04530947		H
-2.21420430			3.72099286	-4.70443201			-2.50705308

2.96981902 K 0.14601787 4.17833026 -0.01807761 K -3.86879138 -0.93083831 1.46769290	0.60564659 K -1.41595241 -3.40860591 2.44203426 K -3.15366920 2.35891263 0.40207651
TS1-1a$_3$-H$^-$	**TS1-1a$_4$-H$^-$**
Mn -1.37634900 0.98191200 -0.19156700 C -0.51621000 -1.56049700 1.17893900 C 1.00956400 0.20989800 1.47003900 N -0.21970700 -0.22853900 1.04816400 N 0.32626700 -2.41071200 1.85799300 N 1.86213200 -0.62409200 2.15365100 C 1.45483500 -1.87892500 2.31310900 N 1.44909100 1.42978900 1.18937200 N -1.59631500 -2.09108400 0.61468800 P 0.37264000 2.34988300 0.23468900 P -2.62127100 -0.91838900 -0.09929000 C -3.23129600 -1.83029300 -1.62171600 H -2.27810500 -2.12382100 -2.09585800 C -4.08757200 -1.03110200 1.06103300 H -4.36374100 -2.10094900 1.04521300 C -3.96028200 -0.94508600 -2.62121000 H -4.19563800 -1.51125600 -3.53604700 H -4.91507700 -0.56769100 -2.22870800 H -3.36752800 -0.06990500 -2.91524400 C -4.00430200 -3.10342700 -1.31430000 H -5.01840000 -2.88530600 -0.94620400 H -4.12608000 -3.72064000 -2.21909200 H -3.50737400 -3.71770300 -0.54698700 C -5.27818800 -0.20060600 0.60919400 H -5.00922500 0.85615500 0.46618000 H -5.71686000 -0.56471200 -0.33038100 H -6.07803500 -0.22742600 1.36548600 C -3.66695200 -0.70072200 2.48515400 H -4.50024300 -0.89242700 3.17891100 H -2.81729900 -1.31627300 2.81103900 H -3.38812700 0.35492900 2.60108700 C 1.53352300 2.87563200 -1.14100100 H 2.02329300 1.90708300 -1.34335300 C 0.19157200 3.89956600 1.25671900 H 1.21437900 4.30837300 1.34206600 C 0.83517300 3.30063100 -2.42133500 H 1.57175900 3.53113400 -3.20834600 H 0.17227800 2.51433800 -2.80480600 H 0.21431200 4.19970800 -2.29034900 C 2.61473200 3.86046500 -0.72514400 H 3.09292600 3.58555300 0.22882400 H 3.40583700 3.92323100 -1.49085900 H 2.21948000 4.88051600 -0.59996500 C -0.69381400 4.92267900 0.56271500 H -1.70971600 4.53262400 0.40090600 H -0.79059400 5.83613800 1.16980400 H -0.29790400 5.22709100 -0.41754300 C -0.28142700 3.57821900 2.66542400 H 0.36598500 2.83061800 3.14415800 H -0.26662500 4.48585900 3.28883500 H -1.30996500 3.19537100 2.68027700 C -2.49360300 1.89994600 0.82400000 O -3.27771500 2.56548900 1.39268000	Mn -0.56829100 -1.30040500 -0.19521600 C -1.65950100 1.46836600 -0.60720600 C 0.54114400 1.22341400 -1.39920900 N -0.60560600 0.65485500 -0.89944300 N -1.66940800 2.79089300 -1.00087100 N 0.57893100 2.56005000 -1.73446700 C -0.53980700 3.24506500 -1.54340800 N 1.64695400 0.51831500 -1.56300300 N -2.71726100 1.02619200 0.06896700 P 1.45352100 -1.14830600 -1.21340200 P -2.54906500 -0.59178300 0.60393800 C -2.81278100 -0.36076400 2.45285600 H -2.13024600 0.48747100 2.63847800 C -4.16996500 -1.33531800 0.04167700 H -4.95651300 -0.78139800 0.58700100 C -2.33527800 -1.53240100 3.29518800 H -2.39945000 -1.29267500 4.36854300 H -2.93500900 -2.44057600 3.13418900 H -1.29513900 -1.80470900 3.07318000 C -4.20895300 0.08888200 2.85013100 H -4.94259600 -0.72922100 2.78023600 H -4.22844600 0.44045200 3.89414600 H -4.57436100 0.91577500 2.21987900 C -4.25980300 -2.80823300 0.40903600 H -3.45602700 -3.38729400 -0.06984900 H -4.18673000 -2.97872500 1.49273900 H -5.21605900 -3.24123000 0.07659100 C -4.40099000 -1.10854400 -1.44435400 H -5.40952100 -1.44575400 -1.73177900 H -4.30898300 -0.04623500 -1.71436000 H -3.68652300 -1.66695100 -2.06268400 C 3.06051000 -1.50860200 -0.33488200 H 3.03446700 -0.73307900 0.44860500 C 1.72147100 -1.86458100 -2.92215900 H 2.72252100 -1.50357900 -3.22096600 C 3.10304900 -2.85752000 0.36481100 H 4.02303600 -2.94640500 0.96419600 H 2.25332600 -3.00049300 1.04420200 H 3.10008600 -3.70034500 -0.34231100 C 4.30266400 -1.27129900 -1.17918600 H 4.25219000 -0.32585100 -1.74256500 H 5.20300000 -1.23673600 -0.54452400 H 4.46333800 -2.07539500 -1.91444400 C 1.71801200 -3.38502300 -2.92785800 H 0.77590800 -3.78974100 -2.52953400 H 1.82528100 -3.77102200 -3.95373200 H 2.54037500 -3.81261500 -2.33738600 C 0.72047600 -1.28918700 -3.91229000 H 0.74046800 -0.19049100 -3.91717300 H 0.95437300 -1.63158200 -4.93265000 H -0.30683000 -1.61006700 -3.69330400 C -1.28204700 -2.30521300 -1.46145900 O -1.73716400 -3.06575900 -2.23549500

C	-2.02955700	1.75097500	-1.63677300
O	-2.41645300	2.23012200	-2.63504000
H	-0.27082000	0.31228500	-1.40046300
C	5.29132800	-0.83152800	-1.16826900
C	4.29780200	-0.21870800	-1.91224600
C	2.95906900	-0.70972200	-1.90514700
C	2.68329000	-1.88455900	-1.11957500
C	3.70690600	-2.46708600	-0.35081300
C	4.99825700	-1.95243500	-0.35996400
H	6.31588900	-0.44916300	-1.21366600
H	4.53064300	0.65053400	-2.53606600
C	1.91293500	-0.13615700	-2.64896700
H	3.46047200	-3.35340800	0.24091600
H	5.78836000	-2.43557600	0.22012300
C	0.50391000	-1.89400700	-1.85049300
C	0.59362000	-0.59803400	-2.46871800
H	-0.45920800	-2.41805100	-1.91453200
H	-0.17239700	-0.33739700	-3.20354600
N	1.45084700	-2.49273300	-1.18051500
C	2.35714000	-2.77779800	3.10409200
H	3.41466100	-2.52615600	2.94666300
H	2.15680500	-2.65890000	4.17948600
H	2.19258000	-3.83513700	2.86011000
K	-0.23871400	-4.32193000	0.13510700
K	3.96930700	0.68721000	1.21763500
H	2.12066100	0.71260800	-3.30505400

C	-0.32685700	-2.71019500	0.83809700
O	-0.16114300	-3.61218000	1.56954400
H	0.20151500	-0.47357100	1.13274200
C	3.95491400	-0.86733100	3.15361000
C	2.58607100	-0.67589100	3.08969900
C	2.03932700	0.47096900	2.48320000
C	2.91165400	1.46004000	1.93209800
C	4.30861500	1.23131600	2.00036700
C	4.81926200	0.09245800	2.59597800
H	-0.03087300	0.05297800	2.97951000
H	4.36316900	-1.76659900	3.62013000
H	1.90151100	-1.43461300	3.48324400
C	0.61670800	0.65542100	2.33945200
H	4.97672400	1.99806600	1.59412000
H	5.90098700	-0.05885100	2.64220000
C	1.14060300	2.82053200	1.40437800
C	0.19841800	1.93097200	1.91459700
H	-0.85942200	2.20334600	1.91127200
N	2.45669000	2.61722700	1.35898700
C	-0.50729100	4.69561000	-1.92240200
H	-1.51512400	5.09079100	-2.10129700
H	-0.05878100	5.29211400	-1.11215300
H	0.10576400	4.85652300	-2.81781100
K	-4.16227700	3.14365300	-0.20102700
K	3.26354400	2.57208300	-1.25573600
H	0.79155500	3.78390600	1.00601200

TS2-2a$_2$-H$^-$

Mn	1.43549400	0.93959200	0.08929500
C	0.61829000	-1.56855300	-1.34562200
C	-0.90947500	0.19764000	-1.62877200
N	0.31054300	-0.24145600	-1.19843500
N	-0.23499700	-2.42569100	-2.00643500
N	-1.72562000	-0.61304800	-2.38398600
C	-1.32792300	-1.87418600	-2.52219600
N	-1.37956100	1.39613500	-1.29512900
N	1.70904400	-2.09344100	-0.80337700
P	-0.34927300	2.26080800	-0.24173500
P	2.66519400	-0.95328400	0.03553000
C	3.05174000	-1.92576600	1.60301500
H	2.06811700	-2.38917500	1.80755400
C	4.27512700	-1.03990100	-0.90516100
H	4.61143100	-2.08812800	-0.82270500
C	3.38701100	-1.03578800	2.78847000
H	3.57718900	-1.63586700	3.69279300
H	4.28364200	-0.42323000	2.61143200
H	2.57348000	-0.33211900	3.01187600
C	4.04769600	-3.06149000	1.42929600
H	5.07343400	-2.69095800	1.28248300
H	4.07252000	-3.70219800	2.32599200
H	3.80582000	-3.70022100	0.56571000
C	5.32380600	-0.12654900	-0.29039400
H	5.00116500	0.92523000	-0.31069700
H	5.54622000	-0.38156500	0.75685600
H	6.27300800	-0.18536800	-0.84549200
C	4.05201400	-0.75681000	-2.38218600
H	4.98828000	-0.90273600	-2.94320800
H	3.29753100	-1.43206500	-2.80871100

TS2-2a$_3$-H$^-$

Mn	-1.11632300	1.20563300	-0.14104500
C	-0.93809000	-1.63925400	0.83190400
C	0.94003900	-0.34496600	1.40692300
N	-0.32603100	-0.42384200	0.88460400
N	-0.37748900	-2.74791800	1.43230900
N	1.55229500	-1.45584400	1.94953600
C	0.84383100	-2.57327900	1.95012600
N	1.63039100	0.78131900	1.38340500
N	-2.09842100	-1.80757200	0.19692100
P	0.81444500	2.08368100	0.62899400
P	-2.69433300	-0.36600600	-0.52060200
C	-3.15014300	-0.96537800	-2.24766400
H	-2.23600700	-1.51157500	-2.53461500
C	-4.37438900	-0.26660800	0.30936900
H	-4.88726900	-1.20506700	0.02569000
C	-3.32501400	0.17232100	-3.24214600
H	-3.52172000	-0.22108100	-4.25189500
H	-4.16499600	0.83533200	-2.98698400
H	-2.43279900	0.80818300	-3.29898400
C	-4.29940400	-1.95813200	-2.30791000
H	-5.27387200	-1.47929100	-2.12541000
H	-4.36110300	-2.42544300	-3.30373000
H	-4.18498700	-2.77236800	-1.57438900
C	-5.19513900	0.91036800	-0.19286200
H	-4.67649300	1.86448300	-0.01738200
H	-5.41160600	0.84390600	-1.26846300
H	-6.16372000	0.96787500	0.32806600
C	-4.25255000	-0.26233500	1.82593200
H	-5.24617200	-0.36475800	2.29091600
H	-3.62187900	-1.08744900	2.19186400

H	3.72633600	0.27602400	-2.56268900	H	-3.81606600	0.67034900	2.20425900
C	-1.54504800	2.57961300	1.16961400	C	2.14449400	2.67036500	-0.54804500
H	-1.79754800	1.52990900	1.40212700	H	2.47574900	1.69925400	-0.95367500
C	-0.21408500	3.93426400	-1.05709500	C	0.84806600	3.36400500	1.98717000
H	-1.21077600	4.40364300	-0.95804000	H	1.91940800	3.53395900	2.19589500
C	-0.92332700	3.20845400	2.40532200	C	1.61400600	3.47932600	-1.71949800
H	-1.58949700	3.10906800	3.27915300	H	2.43169300	3.74388600	-2.40945400
H	0.04629100	2.76336000	2.66729300	H	0.86484900	2.91693800	-2.29176700
H	-0.75377400	4.28738700	2.26988900	H	1.13633300	4.42108300	-1.40875200
C	-2.82713000	3.29794400	0.77764800	C	3.34483300	3.33028500	0.11153900
H	-3.20227800	2.98030400	-0.20725900	H	3.70890400	2.76920300	0.98745500
H	-3.62653800	3.13010800	1.51986300	H	4.18312100	3.41620500	-0.59943900
H	-2.68188400	4.38755800	0.71719000	H	3.12129800	4.35125500	0.45864000
C	0.81544100	4.80189600	-0.34600100	C	0.22001000	4.67113500	1.52960000
H	1.83011100	4.40159700	-0.48279800	H	-0.83815300	4.53664100	1.26034700
H	0.81212200	5.82628500	-0.74973000	H	0.25756800	5.42807300	2.32856700
H	0.64323600	4.87563200	0.73736900	H	0.73093400	5.09941000	0.65449600
C	0.09123400	3.79838800	-2.54025200	C	0.22119900	2.83198200	3.26585900
H	-0.67382700	3.20518300	-3.05850900	H	0.69228100	1.89028400	3.58045300
H	0.13841800	4.79044000	-3.01616100	H	0.34501600	3.55949700	4.08350300
H	1.06249600	3.31309300	-2.71088900	H	-0.85624700	2.65285000	3.15564700
C	2.47862600	1.85626900	-1.00946700	C	-2.11610800	2.08699000	1.01569400
O	3.20697600	2.50954300	-1.66053200	O	-2.79642300	2.77192400	1.69047600
C	2.13544400	1.75869300	1.48711900	C	-1.52718300	2.37417300	-1.40048600
O	2.56344000	2.29464400	2.43955500	O	-1.78275600	3.12686500	-2.26176200
H	0.47964300	0.09333500	1.23875700	H	0.00364900	0.59077500	-1.37518300
C	-5.27119300	-1.15481100	0.63244200	C	5.51847100	-1.24954500	-1.33866300
C	-4.60457500	-0.48175800	1.66188500	C	4.57002400	-0.42763700	-1.96107000
C	-3.26272700	-0.73461100	1.95763900	C	3.19814200	-0.74621300	-1.98265400
C	-2.54042800	-1.66523800	1.16850700	C	2.78467800	-1.93933000	-1.30229800
C	-3.22204700	-2.32952100	0.12875200	C	3.73842400	-2.75189300	-0.67217400
C	-4.56942100	-2.09487700	-0.12994700	C	5.10162600	-2.42013900	-0.69830200
H	-3.07151400	-0.65369200	4.05433100	H	6.57888700	-0.98769300	-1.37874600
H	-6.33464200	-0.97300900	0.45390200	H	4.89248300	0.48621700	-2.47087800
H	-5.15326100	0.23100400	2.28740400	C	2.20078200	0.05086700	-2.63629300
C	-2.62246300	-0.14575500	3.18272700	H	3.40305800	-3.66597300	-0.17139400
H	-2.66395300	-3.04930500	-0.47626300	H	5.82995400	-3.08987100	-0.23317200
H	-5.07361600	-2.65098000	-0.92581400	C	0.48318200	-1.65725100	-2.17599600
C	-0.52166600	-1.23912000	2.22679800	C	0.85465500	-0.25519700	-2.56412500
C	-1.10111800	-0.28478800	3.23511200	H	0.38910500	-2.27225600	-3.10092500
H	0.49619500	-1.57111500	2.44999800	H	0.17848500	0.22154900	-3.27829900
H	-0.59311400	0.68423400	3.13646000	N	1.44697400	-2.22180700	-1.25821100
N	-1.20301200	-1.98044200	1.39110500	C	1.46927700	-3.77891800	2.58690400
C	-2.20711200	-2.76717500	-3.34598100	H	0.95440700	-4.03013200	3.52660900
H	-3.26397300	-2.47639800	-3.27329400	H	1.38719100	-4.66148900	1.93590400
H	-1.92688900	-2.69329100	-4.40745700	H	2.52571300	-3.60438000	2.82081700
H	-2.09297200	-3.82055900	-3.05948700	K	-2.67064000	-4.07822100	1.26698900
K	0.21106100	-4.05474000	0.08364300	K	3.98257400	-0.36096000	1.25790000
K	-3.88173400	0.66392000	-1.53517300	H	2.52581500	0.96539500	-3.13971500
H	-0.79120400	-0.65223400	4.22758500	H	-0.49756900	-1.68257700	-1.68458100
H	-2.92709100	0.90703500	3.29693000	H	1.16750300	-3.06781400	-0.77861900
TS2-2a$_4$-H$^-$				**TS2-2a$_2$'-H$^-$**			
Mn	0.53967200	-1.34000300	-0.03282500	Mn	-1.04083200	1.25289000	-0.17420800
C	1.58509600	1.27811300	1.00477000	C	-1.01634100	-1.54582400	0.91706700
C	-0.62417500	0.83618500	1.67043000	C	0.95247000	-0.35345100	1.39760500
N	0.55335400	0.39012000	1.12247700	N	-0.33916100	-0.36241300	0.93578500
N	1.52476000	2.52320500	1.59610100	N	-0.47923600	-2.68736400	1.48336000

N	-0.73184000	2.09961600	2.20437400	N	1.53002400	-1.49090900	1.91679900
C	0.36485200	2.84802200	2.16261400	C	0.76833800	-2.57691000	1.94171100
N	-1.70974800	0.07834800	1.68065800	N	1.70026800	0.73584900	1.33294800
N	2.68832700	0.97723500	0.32501700	N	-2.22667200	-1.64639900	0.37344400
P	-1.49712000	-1.45529600	0.95906900	P	0.93954700	2.05731400	0.55561900
P	2.59159100	-0.51123100	-0.50861900	P	-2.73455300	-0.22102000	-0.42702300
C	3.06054200	0.06053800	-2.24068600	C	-3.20418800	-0.93990700	-2.10249900
H	2.39211800	0.93348400	-2.34714900	H	-2.30222700	-1.53798300	-2.31894000
C	4.15079700	-1.35514800	0.08379700	C	-4.40345700	0.04662900	0.37948800
H	4.97068200	-0.66409400	-0.18641900	H	-4.96802400	-0.88535300	0.18674900
C	2.70955400	-0.92625500	-3.34209600	C	-3.34426700	0.09778900	-3.20413700
H	2.92842800	-0.49729700	-4.33293800	H	-3.51864600	-0.38946600	-4.17669300
H	3.28029900	-1.86363200	-3.26643100	H	-4.18852600	0.78248600	-3.03462800
H	1.64866700	-1.20509800	-3.32814600	H	-2.44862000	0.72387000	-3.30105400
C	4.48916000	0.56351900	-2.37371900	C	-4.38318900	-1.89870700	-2.07590100
H	5.21994400	-0.26000700	-2.37267600	H	-5.34280800	-1.37441200	-1.94565100
H	4.63110400	1.10827500	-3.32129200	H	-4.45678300	-2.45931400	-3.02173500
H	4.77185400	1.24414000	-1.55386100	H	-4.29803200	-2.63921800	-1.26390100
C	4.38107600	-2.68954700	-0.60720100	C	-5.15783900	1.21468100	-0.23496800
H	3.53955500	-3.37841200	-0.44105500	H	-4.58355200	2.14936100	-0.15245600
H	4.51491200	-2.58547600	-1.69358300	H	-5.38397000	1.05667000	-1.29912900
H	5.28457800	-3.18369800	-0.21710300	H	-6.11837100	1.37872600	0.27823600
C	4.15334300	-1.48677100	1.59903100	C	-4.26764800	0.18953400	1.88789400
H	5.13574200	-1.83924800	1.95112200	H	-5.26039000	0.18740100	2.36590200
H	3.94370000	-0.52521300	2.08876200	H	-3.67966300	-0.63183200	2.32460000
H	3.40676900	-2.21082100	1.94976000	H	-3.77625600	1.12974600	2.16937700
C	-3.11485100	-1.59824000	0.02922400	C	2.34482200	2.57753200	-0.57898700
H	-3.08824500	-0.66008700	-0.55346200	H	2.60819200	1.59090400	-0.99692000
C	-1.76899800	-2.55567100	2.44936200	C	1.01814700	3.34637500	1.90858800
H	-2.75071900	-2.23718700	2.84551800	H	2.09096400	3.42641700	2.16047100
C	-3.17067000	-2.74706400	-0.96383300	C	1.93193100	3.47536300	-1.73298300
H	-4.08575900	-2.68089900	-1.57384000	H	2.76827400	3.61000200	-2.43858300
H	-2.31561300	-2.74626200	-1.65172500	H	1.08330700	3.06740400	-2.29681800
H	-3.18795700	-3.72860800	-0.46743000	H	1.63614200	4.48041500	-1.39642400
C	-4.35200700	-1.56406200	0.91393300	C	3.58005700	3.10874000	0.13147600
H	-4.28617400	-0.80018200	1.70542700	H	3.85214900	2.50708000	1.01357200
H	-5.25428400	-1.35784200	0.31403100	H	4.44918200	3.12189600	-0.54766000
H	-4.52356400	-2.52695300	1.42010000	H	3.44158200	4.14247000	0.48457400
C	-1.82878600	-4.03453500	2.10200100	C	0.51793800	4.70154700	1.43500000
H	-0.91689600	-4.36905300	1.58610100	H	-0.53056800	4.65169600	1.10627500
H	-1.92240300	-4.64446000	3.01428400	H	0.56675500	5.44452200	2.24655900
H	-2.68622600	-4.28469100	1.46164000	H	1.10961000	5.10008600	0.59779800
C	-0.73434800	-2.26385800	3.52534900	C	0.29966700	2.87023100	3.16109100
H	-0.69325600	-1.19293600	3.76861900	H	0.65813500	1.88061800	3.47806500
H	-0.98319400	-2.80655500	4.45092100	H	0.47431500	3.57210300	3.99194600
H	0.27286900	-2.58303000	3.22536500	H	-0.78659100	2.80752700	3.01521400
C	1.17116000	-2.72423200	0.85865700	C	-1.98736300	2.33762500	0.84480800
O	1.57384200	-3.71138000	1.35763700	O	-2.64450700	3.13133500	1.41732200
C	0.25692100	-2.33205900	-1.46024700	C	-1.28882800	2.27538100	-1.59046500
O	0.05247700	-2.94809400	-2.44056000	O	-1.43291800	2.92984700	-2.55512400
H	-0.07847100	0.01726900	-1.09762200	H	-0.15657000	0.18819800	-1.34541600
C	-3.61733600	-0.25710600	-3.25251200	C	5.26419500	-1.01075900	-1.49843600
C	-2.25466500	-0.11233700	-2.98605900	C	4.13351000	-0.39133100	-2.05341800
C	-1.76094300	0.96430200	-2.24641700	C	2.85794700	-0.95021000	-1.98622400
C	-2.66858200	1.93023400	-1.76552000	C	2.70472600	-2.18542400	-1.28806500
C	-4.04105200	1.77319600	-2.01666300	C	3.84116300	-2.81130300	-0.72366200
C	-4.51284200	0.68697900	-2.75650500	C	5.10549300	-2.24561500	-0.85361000

H	0.31541400	0.65185300	-2.74133300	H	1.81416100	-0.49374600	-3.79244300
H	-3.97510400	-1.10950300	-3.83356100	H	6.25266000	-0.55979300	-1.60977100
H	-1.54140700	-0.86124400	-3.34488200	H	4.24996900	0.56093200	-2.58323400
C	-0.31240100	1.12468300	-1.97544800	C	1.68506400	-0.32952600	-2.70530300
H	-4.74250900	2.53770000	-1.65903400	H	3.71486800	-3.77402100	-0.21814000
H	-5.58392400	0.59222600	-2.95197400	H	5.97432600	-2.77203600	-0.44668000
C	-0.82227900	3.42802000	-1.00727000	C	0.32640700	-2.16941900	-1.76012700
C	0.09152500	2.38820600	-1.53680900	C	0.33990500	-0.88560700	-2.27947800
H	-0.73274000	4.35723400	-1.61692000	H	-0.58556400	-2.74913400	-1.62516900
H	1.15083600	2.66039800	-1.57001900	H	-0.47152500	-0.65755600	-2.97643200
N	-2.22979000	3.00850100	-0.97867600	N	1.47004600	-2.75016100	-1.20730500
C	0.29436200	4.18604600	2.83698500	C	1.37143600	-3.80146700	2.56538500
H	-0.73416800	4.56722100	2.86475500	H	0.91228900	-4.72290500	2.18251900
H	0.63470100	4.10458500	3.88090400	H	2.45596400	-3.84097200	2.39728700
H	0.93935700	4.92507400	2.34273500	H	1.22396100	-3.78958800	3.65642200
K	3.78181500	3.30291500	0.48650400	K	-2.80413200	-3.96075900	1.32281300
K	-3.35200700	2.05218500	1.46996600	K	3.98876500	-0.47749500	1.33991100
H	-2.84729000	3.80688900	-1.09611300	H	1.35376400	-3.54690400	-0.59481000
H	-0.54953500	3.75688400	0.02219500	H	1.69591600	0.76841600	-2.59226900
TS2-2a$_3$'-H$^-$							
Mn	1.18747900	1.10767500	0.27961000				
C	0.93840300	-1.39363800	-1.36868700				
C	-0.95389600	-0.00543700	-1.52744000				
N	0.35479100	-0.17391700	-1.15425500				
N	0.28254500	-2.38501300	-2.06777600				
N	-1.63036300	-0.98451300	-2.21540700				
C	-0.95916400	-2.10710300	-2.45253500				
N	-1.63061600	1.08900200	-1.20468500				
N	2.13307700	-1.69158000	-0.87507400				
P	-0.71757300	2.21114500	-0.29730100				
P	2.79189300	-0.48247800	0.13321600				
C	3.24789100	-1.53472300	1.62043700				
H	2.27448100	-2.02884100	1.80404900				
C	4.43102000	-0.18363700	-0.70777400				
H	4.90032600	-1.18289300	-0.76455400				
C	3.60693800	-0.75636700	2.87546300				
H	3.72063900	-1.43718300	3.73420600				
H	4.56047600	-0.21852600	2.77158600				
H	2.84698900	-0.01193900	3.14121700				
C	4.27968000	-2.61185500	1.31790900				
H	5.29563600	-2.19244800	1.25598100				
H	4.30795100	-3.37538200	2.11342500				
H	4.09447400	-3.11952700	0.35752400				
C	5.33760500	0.75111900	0.07664700				
H	4.85773000	1.72428300	0.25680300				
H	5.63015500	0.33752700	1.05233100				
H	6.26747300	0.94927900	-0.47876700				
C	4.20839400	0.29253700	-2.13526400				
H	5.16548000	0.33455000	-2.67808400				
H	3.54041000	-0.38471000	-2.68532500				
H	3.77376900	1.30073400	-2.16885000				
C	-2.04698500	2.78298700	0.89860100				
H	-2.42085700	1.79936500	1.22695000				
C	-0.62916900	3.63778500	-1.50522700				
H	-1.68286200	3.80937200	-1.79114800				
C	-1.53258700	3.52681600	2.12029300				
H	-2.34666300	3.69971600	2.84304300				

H	-0.73175000	2.98568800	2.64110300
H	-1.12556700	4.51568700	1.86370900
C	-3.21927400	3.50021500	0.24809200
H	-3.56391100	2.99133100	-0.66578400
H	-4.07442800	3.56478100	0.94155300
H	-2.96578800	4.53329700	-0.03506400
C	-0.06931000	4.90939200	-0.88859800
H	0.94492700	4.75867300	-0.49162600
H	-0.00229100	5.71021700	-1.64156100
H	-0.69534500	5.29274000	-0.06999500
C	0.11595200	3.23191800	-2.76724100
H	-0.28360700	2.30045400	-3.19242700
H	0.01970700	4.01554000	-3.53501000
H	1.18951400	3.08826300	-2.58599600
C	2.22777000	2.35295400	-0.41727900
O	2.96344100	3.20447400	-0.75937700
C	1.41577800	1.70497200	1.91552900
O	1.48563400	2.01902900	3.04710700
H	0.42196200	-0.20162100	1.22879600
C	-5.17434200	-0.62377000	1.54896300
C	-3.93384000	-0.15876500	1.97496000
C	-2.75539000	-0.91516800	1.76879700
C	-2.85826600	-2.16504600	1.10022900
C	-4.11666400	-2.60317700	0.68522000
C	-5.28142500	-1.85343000	0.89021700
H	-6.06745200	-0.02652400	1.75329100
H	-3.86447900	0.78489400	2.52314000
H	-4.18233100	-3.57632400	0.18596100
H	-6.25418800	-2.23884200	0.57633500
C	-0.44200100	-2.50301100	1.63288700
C	-0.34377800	-1.19350000	2.08527300
H	0.32592400	-3.20585300	1.97020700
H	0.35263900	-1.00619200	2.91174100
C	-1.69478100	-3.16696500	-3.21745300
H	-1.90339400	-2.82488300	-4.24147100
H	-1.11633300	-4.09621000	-3.28137700
H	-2.66988100	-3.38017700	-2.75422000
K	1.40942800	-4.14516800	-0.42992400
K	-3.98051400	-0.06020700	-1.32028300
N	-1.55166600	-0.46317800	2.22560700
C	-1.62897000	-3.01407600	0.88245100
H	-1.86710600	-4.04920800	1.19943400
H	-1.47212300	-3.10642400	-0.22034000
H	-1.46595000	0.51776600	2.46665600

Mn-1_{1K}_1a-H				**Mn-OiPr$_O$-1_{2K}**			
Mn	1.41550948		-0.86940884	Mn	0.51361272		-0.93265541
-0.19647340		C	0.55909845	-0.06613103		C	-1.36307884
1.56302834	1.33168297		C	1.17290120	-1.08318220		C
-0.92983912			-0.25356900	0.88138840			1.87997906
1.56658823		N	0.29341905	-1.03542396		N	-0.03934926
0.22275731	1.14692933		N	0.88979742	-0.90505217		N
-0.30731040			2.37117213	-1.76800300			2.45438963
2.02241373		N	-1.78044590	-1.41149302		N	0.51370717
0.52806330	2.29956685		C	3.12993693	-1.49706361		C
-1.40849248			1.79108075	-0.79576163			3.33391894
2.48562830		N	-1.35682688	-1.63076005		N	2.16152699
-1.46591158	1.23694668		N	1.69852535	-0.71928794		N

1.62832947			2.14050515	-2.30840303			0.26522231
0.80094001		P	-0.28818062	-0.89743740		P	2.49199558
-2.33425858	0.24102942		P	0.18080842	0.00062859		P
2.62001264			1.07658190	-1.72458930			-1.25986183
-0.07692222		C	2.98429324	-0.37566264		C	-2.79090538
2.12687540	-1.58860568		H	-1.55887887	1.13465543		H
1.96548206			2.46489989	-2.69753036			-0.57411136
-1.85758144		C	4.20574843	1.62400078		C	-2.43668273
1.13929561	0.89954901		H	-2.39669436	-1.67108138		H
4.46414910			2.21279973	-3.53392281			-2.35459243
0.92310426		C	3.52762996	-1.54865520		C	-2.17195809
1.34795445	-2.77555198		H	-2.56728051	2.08822155		H
3.69081188			2.01632902	-2.80181182			-2.69386586
-3.63516930		H	4.49208119	2.98372866		H	-2.04965595
0.86699368	-2.55703381		H	-3.56397575	1.63659963		H
2.84465213			0.55258823	-1.18455715			-2.21217594
-3.09983721		C	3.81020873	2.40962164		C	-4.25236675
3.36625027	-1.27892892		H	-1.84995583	0.83699750		H
4.86677302			3.11841101	-4.40073360			-2.86541040
-1.09633892		H	3.79674932	0.43705705		H	-4.86078041
4.06814047	-2.12811636		H	-1.78781512	1.75475747		H
3.44094862			3.89949280	-4.68776532			-1.15634381
-0.38944973		C	5.33665667	0.09765759		C	-1.96745658
0.36642885	0.24026649		H	-3.82613611	-1.44411075		H
5.07949973			-0.69342948	-0.87298516			-3.90341375
0.09770906		H	5.61445187	-1.53116091		H	-2.24395049
0.77713131	-0.74095274		H	-4.20942986	-0.45069237		H
6.24140369			0.39513791	-2.40389231			-4.50894446
0.86656706		C	3.96287164	-2.18976438		C	-2.11862238
0.70690138	2.33757794		H	-1.90461583	-3.07470071		H
4.86494728			0.88546032	-2.59331473			-2.55669942
2.94240009		H	3.13945824	-3.82491121		H	-2.48690785
1.27296295	2.79397296		H	-0.88210474	-3.23397949		H
3.72930570			-0.36290906	-1.03951642			-1.91124628
2.41773651		C	-1.46982935	-3.27857529		C	3.34923662
-2.86314266	-1.10925633		H	0.68352309	1.59335696		H
-1.92200205			-1.88450348	2.51506603			0.99074941
-1.35173394		C	0.00017972	2.24057212		C	3.96424851
-3.88170153	1.23479925		H	-0.46716330	-0.96965830		H
-1.00915983			-4.31261344	4.85519896			0.02228821
1.36321155		C	-0.81805541	-0.53099856		C	4.03582283
-3.38080106	-2.37954631		H	-0.49669266	2.26225670		H
-1.57573063			-3.52386435	4.34962407			-0.23521410
-3.16642632		H	-0.06331220	3.28504577		H	3.37154643
-2.68940102	-2.77388679		H	-1.37069564	2.33860960		H
-0.32186037			-4.35183355	4.94359943			-0.80981787
-2.23447759		C	-2.57864693	1.72262510		C	4.27579593
-3.78459835	-0.62405231		H	1.87952792	1.44810163		H
-3.00109016			-3.46282187	3.71900043			2.77799794
0.34077417		H	-3.40003041	1.14290304		H	4.77056581
-3.82892287	-1.35790495		H	2.11227842	2.40476334		H
-2.22376253			-4.81805654	5.07913704			1.70683044
-0.48850613		C	0.87918362	0.71127127		C	4.12206821
-4.88433230	0.50449259		H	-1.97491212	-0.80339085		H
1.87621751			-4.47180039	3.35637376			-2.51982870
0.29124845		H	1.02922699	-1.37068861		H	5.10292636
-5.78711359	1.11610457		H	-2.30490040	-1.18056872		H

0.44440848			-5.21179257	4.04055439			-2.30714460
-0.45060064		C	0.52651990	0.24005192		C	3.89495900
-3.54425173	2.62111095		H	-0.08459610	-2.43945436		H
-0.11826595			-2.81374679	3.92053051			1.00515235
3.12832825		H	0.56267251	-2.58735541		H	4.74300376
-4.45071253	3.24454699		H	-0.51782611	-2.99306918		H
1.54539139			-3.13626565	2.97500405			-0.45770918
2.58962549		C	2.61615559	-2.91232456		C	0.95112086
-1.82326181	0.63843354		O	-1.71295021	-1.57550786		O
3.44495313			-2.48771903	1.22417711			-2.27058399
1.13571928		C	2.02574242	-2.57682521		C	0.98887049
-1.53876618	-1.71500723		O	-2.38303349	0.85091274		O
2.40815561			-1.96540747	1.33542397			-3.32285683
-2.73622086		H	0.02708241	1.45348505		H	0.73669660
0.08489014	-1.31699375		C	1.70028060	1.73420154		C
-5.42227456			1.25524812	-1.21944579			4.71967141
-0.85331317		C	-4.69545590	-2.01942853		H	-1.28295858
0.51452557	-1.79133335		C	5.36481934	-1.12914252		H
-3.30887141			0.65440817	-0.49215157			5.18246254
-1.93556462		C	-2.56837382	-2.69896964		H	-2.20499856
1.58517742	-1.10494022		C	4.71532242	-2.49987129		C
-3.35387448			2.34928911	-0.07725505			1.11350249
-0.18107248		C	-4.72643837	2.24390516		C	-1.29316060
2.19000106	-0.06378594		H	2.05925376	2.21883026		H
-3.10962884			-0.56685774	-2.17495728			1.53482699
-3.74598579		H	-6.50687367	2.63315514		H	-1.13849132
1.15242286	-0.77603948		H	2.97497576	2.81476217		H
-5.21663143			-0.17954614	-1.50349984			2.37286619
-2.46097246		C	-2.56322004	1.18333947		C	0.36119195
0.00642821	-2.98924268		H	0.88961359	3.69367710		H
-2.83767896			3.07281785	0.65986808			1.81581880
0.45890690		H	-5.27375684	4.21387903		H	-0.46073047
2.80416038	0.65886014		C	0.42552140	4.26255129		H
-0.49194263			0.88770502	1.20281305			0.18171862
-1.99664064		C	-1.22405652	3.72875644		O	-0.34655525
0.14123254	-3.05473676		H	-0.07358702	1.63865600		K
0.39224023			1.38808814	3.03625297			3.95329706
-2.43169552		H	-0.64373659	-1.57884798		K	-3.95454513
-0.32727855	-3.85602549		N	1.97291148	0.10188835		
-1.25031083			1.79338358				
-1.20388010		C	-2.33130627				
2.64072198	3.30451337		H				
-3.38329875			2.43592866				
3.06291952		H	-2.20119841				
2.41036998	4.37230891		H				
-2.12190979			3.70865083				
3.16988448		K	-0.05061197				
4.01386433	-0.10660957		K				
-3.87408681	-0.60032836	1.06138679					
Mn-OiPr$_H$-1$_{2K}$				**TS-1A-H$^-$**			
Mn	-0.09214359		-1.13586817	Mn	1.27360558		-0.82802626
-0.07171347		C	-0.99137983	-0.26089894		C	0.38534710
1.54039212	-1.01793969		C	1.57732319	1.27058219		C
1.34120178			1.39986380	-0.88063605			-0.35043352
-0.63152590		N	0.12929482	1.75100225		N	0.20971423
0.78327971	-0.74809121		N	0.21935931	1.17481599		N
-0.87566482			2.89607351	-0.50903312			2.34663074

-1.22686996		N	1.47972183	1.98780128		N	-1.68066697
2.73720417	-0.91343190		C	0.36991578	2.61338150		C
0.34881948			3.39628513	-1.44751425			1.68426226
-1.18571426		N	2.42514110	2.65255208		N	-1.23632437
0.74868117	-0.20350109		N	-1.60814611	1.48947924		N
-2.20267912			1.01565813	1.37181787			2.19605372
-1.04368043		P	2.13636347	0.64782826		P	-0.28058391
-0.88170496	0.19553678		P	-2.35375881	0.28380235		P
-2.26576393			-0.61427005	2.35431158			1.16151847
-0.55292559		C	-3.52701324	-0.29917096		C	2.47909873
-0.54358955	0.81939217		H	2.13437870	-1.88849918		H
-3.00385296			0.14123170	1.40730755			2.25138658
1.51623734		C	-3.17940639	-2.12734887		C	4.01635790
-1.44999114	-1.94824627		H	1.42118732	0.51559323		H
-4.22663002			-1.11299013	4.24419914			2.49219247
-1.83870618		C	-3.76118093	0.36490007		C	3.11844127
-1.86849119	1.52722167		H	1.37973287	-3.04389301		H
-4.29943344			-1.70869793	2.96061345			1.92307608
2.47508398		H	-4.38033916	-3.98932367		H	4.20665137
-2.55475486	0.92865689		H	1.26878180	-2.92539108		H
-2.82620573			-2.39275213	2.69999084			0.37292598
1.76887317		C	-4.84223329	-3.17066272		C	3.08804472
0.10226077	0.40239632		H	3.51894900	-1.72097009		H
-5.50609954			-0.60876915	4.18590208			3.47856251
-0.11396895		H	-5.40272992	-1.64132060		H	2.86334831
0.46227414	1.28162286		H	4.15860452	-2.59064564		H
-4.69807361			0.94777899	2.72690014			4.03287534
-0.28862562		C	-3.14070695	-0.81559201		C	5.11123886
-2.96748470	-1.82576736		H	0.58535800	-0.12879045		H
-2.13547977			-3.36080214	4.89879801			-0.49029846
-2.02929480		H	-3.43410785	-0.04415977		H	5.24695608
-3.32821119	-0.83021684		H	0.81205938	-1.19544054		H
-3.82170317			-3.43188381	6.07946273			0.76314539
-2.55572036		C	-2.68099478	0.36499095		C	3.92617971
-0.97158163	-3.30249718		H	1.18446996	2.01532063		H
-3.25561704			-1.44823999	4.89211815			1.40621887
-4.11189147		H	-2.78043454	2.49579290		H	3.16452820
0.11670424	-3.40541922		H	1.82646079	2.47792594		H
-1.62457622			-1.22897972	3.68168496			0.14011278
-3.46337772		C	2.88468940	2.25293453		C	-1.57327454
-1.06781607	1.90588769		H	-2.94765679	-0.95011178		H
2.06954805			-0.72565845	-1.75508203			-2.05041825
2.56423734		C	3.37694178	-1.56402967		C	0.19536139
-1.80173629	-0.86642453		H	-3.99038135	1.07405163		H
4.35570188			-1.64604052	-0.70012026			-4.63794928
-0.36998810		C	3.17162132	0.99173037		C	-1.04588619
-2.51409346	2.27818622		H	-4.01972222	-1.89076677		H
3.42498873			-2.58720012	-1.76392103			-4.20360091
3.34687029		H	2.30462097	-2.70528474		H	-0.09304056
-3.16773770	2.10761649		H	-3.73033498	-2.35703488		H
4.02644641			-2.92565385	-0.89590135			-4.98276020
1.72027178		C	4.09478478	-1.37883495		C	-2.89055299
-0.17983723	2.14545002		H	-3.35581502	-0.31107309		H
3.81736830			0.88462118	-3.36422488			-2.51117375
2.13734134		H	4.54486961	0.21110282		H	-3.60326562
-0.38479782	3.12957145		H	-3.71716797	-1.06975252		H
4.88517481			-0.33717980	-2.76048572			-4.17534543

1.39207297		C	3.10196078	0.41668606		C	1.35249629
-3.29958382	-0.95118913		H	-4.66654603	0.34556347		H
2.24695147			-3.50534300	2.30474810			-4.17273438
-1.60709859		H	3.96991433	0.57740921		H	1.44716471
-3.82257200	-1.38189260		H	-5.71726115	0.66195540		H
2.88480407			-3.76982150	1.24901595			-4.66006712
0.01537451		C	3.44617214	-0.74687844		C	0.52430643
-1.19492813	-2.25980895		H	-3.81913138	2.54880892		H
3.75058176			-0.14064640	-0.33607101			-3.46029139
-2.24148812		H	4.16227065	3.13195481		H	0.85436455
-1.75007418	-2.88532228		H	-4.77436796	2.98667468		H
2.47009720			-1.24712733	1.34152830			-3.09704085
-2.76533573		C	0.09431612	2.69531161		C	2.52120504
-2.04510359	-1.55129920		O	-1.60924797	0.71466842		O
0.22577445			-2.64975631	3.38095737			-2.13144642
-2.54865259		C	-0.30730651	1.32417499		C	1.80362997
-2.60802629	0.89989777		O	-1.59143949	-1.76674655		O
-0.42705560			-3.56251158	2.07747118			-2.10531016
1.56634059		H	-0.29727238	-2.78491430		H	0.14354057
0.09607383	1.51732467		C	0.10480994	-1.22509486		C
0.48574092			4.87138952	-2.38517458			2.49972033
-1.41827833		H	1.37043525	3.49256936		H	-2.63484746
5.09364642	-2.02964779		H	1.97751327	4.42582971		H
-0.40368856			5.27792438	-1.95354237			3.47756219
-1.91233471		H	0.61421748	3.73456412		H	-3.33296212
5.40126196	-0.46117315		K	2.67038260	2.95844311		K
-2.97216512			3.01253537	-0.21174276			4.13539780
0.59167748		C	-0.58374587	-0.11274036		C	-1.10374700
0.88368986	2.39012052		C	1.13147392	-1.90335498		C
0.69330276			1.71164820	-2.22811626			0.69461566
2.61107638		H	0.50494775	-0.99187886		H	-3.17796792
2.38978285	3.45904355		H	1.00659283	-1.46050819		H
1.59734398			1.12835038	-2.27786666			-0.38282667
2.84142608		H	0.88738423	-0.80537028		H	-2.15451035
2.33967376	1.72775958		C	1.21296194	-0.02647277		C
-0.85303342			-0.05376339	-0.97742500			0.42238600
3.57151005		H	-0.01350154	-3.23120298		H	-1.09359986
-0.73928096	3.77506901		H	-0.66666419	-3.15261422		H
-1.04806845			0.53772165	-1.75798645			0.81047330
4.48029616		H	-1.74384749	-3.90890778		H	-0.00450041
-0.66772076	3.37734364		O	0.63500359	-3.69070421		O
-1.59488736			1.65309364	-0.74804115			2.32915286
2.05102186		K	3.88540929	-1.82067175		K	-3.11283661
2.85384445	0.15472064			-1.76705805	3.24157283		
MnH-1_{2K}_1A							
Mn	0.00342425		-1.28558943				
-0.34907007		C	-0.92833525				
1.53982247	-0.82391975		C				
1.40972949			1.34552553				
-0.65777683		N	0.18704036				
0.75658504	-0.71340900		N				
-0.81095928			2.90903650				
-0.96360935		N	1.55938203				
2.69352876	-0.91895344		C				
0.42574436			3.38533631				
-1.04407299		N	2.49749397				
0.65521325	-0.32290610		N				

-2.14428997			1.02115286
-0.75382396		P	2.16180498
-0.97789559	0.08482842		P
-2.14372324			-0.68282516
-0.52755056		C	-3.26407844
-0.81191660	0.97462837		H
-2.82330411			-0.01444864
1.59921617		C	-3.23719004
-1.24894067	-1.93185188		H
-4.23554258			-0.81117506
-1.75173742		C	-3.11701839
-2.11941150	1.73354486		H
-3.69177845			-2.09404021
2.67398451		H	-3.48216870
-2.98335901	1.15756601		H
-2.06609945			-2.32143387
1.98119358		C	-4.72099912
-0.45651348	0.72743196		H
-5.25354446			-1.25623533
0.18939251		H	-5.25925112
-0.30610433	1.67783193		H
-4.83670530			0.46134034
0.12840731		C	-3.34726635
-2.76577367	-1.93895357		H
-2.35819178			-3.23085202
-2.07410016		H	-3.76893348
-3.16580368	-1.00474105		H
-3.99042363			-3.11449753
-2.76215899		C	-2.73144406
-0.71286429	-3.26118307		H
-3.41668572			-0.99605976
-4.07588556		H	-2.65303284
0.38303649	-3.25026119		H
-1.74244570			-1.11831081
-3.51515124		C	2.78139692
-1.06345004	1.85404859		H
1.95895474			-0.56757054
2.39976157		C	3.49466486
-1.94494973	-0.81696256		H
4.41143751			-1.89836655
-0.19709147		C	2.86754937
-2.49539937	2.35620327		H
3.04147135			-2.52200637
3.44348016		H	1.94369319
-3.05791829	2.15562672		H
3.70286347			-3.04198651
1.89031786		C	4.06316174
-0.28983373	2.11024396		H
3.94777152			0.77451534
1.85561992		H	4.35886536
-0.34928259	3.17040134		H
4.91072396			-0.68649560
1.52590851		C	3.07800197
-3.40409651	-0.96423817		H
2.24788758			-3.50259056
-1.67804345		H	3.91360428
-4.01403131	-1.34262437		H

2.73704491 -3.85440751 -0.02228214 C 3.80033482 -1.34170205 -2.17858262 H 4.25031299 -0.34027170 -2.10342377 H 4.50269271 -1.97793015 -2.74011659 H 2.88838300 -1.24769264 -2.78763959 C 0.25332034 -1.81251884 -2.02982953 O 0.43526574 -2.22863558 -3.11555968 C -0.16252531 -2.93876602 0.25490538 O -0.25791661 -4.02352175 0.69172079 H -0.24600481 -0.83453194 1.22936594 C 0.56197536 4.86751854 -1.23176158 H 1.50132409 5.12395356 -1.73802943 H -0.27849199 5.27448977 -1.80705129 H 0.56962667 5.37837816 -0.25573388 K -3.19742133 3.18387911 0.27521008 C -1.10290676 1.77340889 2.86543635 C 0.29922865 1.94697161 2.38969128 H 1.02023448 1.91239464 3.21920973 H 0.51482195 1.06550456 1.75444607 H 0.42888698 2.86284198 1.80092074 C -1.34018310 0.60625446 3.76877524 H -1.06705418 -0.30542665 3.20551007 H -0.67666984 0.63745906 4.64490938 H -2.38624958 0.54636260 4.08959747 O -2.01802647 2.49304421 2.48277021 K 4.19834251 2.46995113 -0.96044998	
2H-Mn-5	**Mn-5'**
P 0.32159337 0.11048416 -2.20074844 P 0.32159337 0.11048416 2.20074844 C 1.94633111 -0.78129739 -2.41792726 C 1.94633111 -0.78129739 2.41792726 H 2.74631301 -0.02096992 -2.42905740 H 2.74631301 -0.02096992 2.42905740 H 2.02104907 -1.31971617 -3.37483152 H 2.02104907 -1.31971617 3.37483152 C 2.14635720 -1.71435180 -1.23856266 C 2.14635720 -1.71435180 1.23856266 H 3.15911255 -2.16324459 -1.24858814 H 3.15911255	P 0.38696289 0.13985825 -2.23784688 P 0.38696289 0.13985825 2.23784688 C 2.04182818 -0.64038920 -2.44213276 C 2.04182818 -0.64038920 2.44213276 H 2.75355427 0.19288671 -2.55874678 H 2.75355427 0.19288671 2.55874678 H 2.11985992 -1.25938880 -3.35055929 H 2.11985992 -1.25938880 3.35055929 C 2.36890106 -1.42300976 -1.18182950 C 2.36890106 -1.42300976 1.18182950 H 3.46965565 -1.44978520 -1.04232584 H 3.46965565 -1.44978520 1.04232584 H 2.08931051 -2.49189865

-2.16324459	1.24858814	H	1.42535646	-1.30597728	H	2.08931051	-2.54898382
-2.49189865	1.30597728	N	-1.26869847	1.73022076	-0.86210592	-2.54898382	H
1.42535646	0.00000000	C	0.47582475	1.90601778	-0.97012744	1.26869847	N
1.62129606	3.35931364	C	0.00000000	0.47582475	1.62129606	0.00000000	C
0.71750412	1.77400955	2.95917464	C	-3.35931364	H	1.39309252	0.71750412
2.11255633	2.98355209	H	-2.95917464	H	1.66590961	1.39309252	2.11255633
2.00956471	2.44157803	H	1.66590961	-2.98355209	C	-0.75822092	2.00956471
-1.07847909	3.07039970	C	-2.44157803	C	-0.79055031	-0.75822092	-1.07847909
-0.73010323	3.44598788	C	-0.79055031	-3.07039970	C	-0.83530082	-0.73010323
-2.34416519	2.22787131	C	-3.44598788	C	-0.72011071	-0.83530082	-2.34416519
-2.24714478	3.34947030	C	-0.72011071	-2.22787131	O	0.89668326	-2.24714478
3.23601260	0.00000000	H	-3.34947030	O	-2.46315432	-0.28198616	-1.32570769
1.68006677	0.00000000	H	-0.42528977	-4.03805442	H	-0.28198616	-0.43433074
-1.32570769	4.03805442	C	-4.44600748	H	-0.42528977	-2.14649272	-0.51671991
-0.43433074	4.44600748	C	-2.22185666	-3.33639172	C	-2.14649272	-0.24270488
-0.51671991	3.33639172	H	-3.27235369	C	-2.22185666	-2.14246222	0.28398772
-0.24270488	3.27235369	H	-2.31665277	-4.08740049	H	-2.14246222	0.28398772
4.08740049	H	-2.61258159	0.84839889	-3.36382825	H	-2.31665277	-0.11795742
-2.42353203	H	0.84839889	3.36382825	H	-2.61258159	-0.11795742	-2.61400672
-0.52020825	2.42353203	H	-2.80873508	-2.28196088	H	-2.61400672	-1.30847229
-3.71824479	H	-0.52020825	2.28196088	H	-2.80873508	-1.30847229	-2.88291201
-0.69427165	3.71824479	C	-0.66937863	2.60385935	-4.02737417	H	-2.88291201
3.15581342	C	-0.66937863	2.60385935	-0.69427165	4.02737417	C	-3.15581342
H	-1.62261352	2.22595116	-0.27578973	3.54983478	H	-1.62261352	2.56774504
C	-0.27578973	2.22595116	-3.54983478	H	2.85630261	-2.56774504	H
-0.82403727	2.84805051	-1.27789970	2.68227441	2.09683382	H	-0.82403727	2.98656370
H	-1.27789970	2.84805051	-2.09683382	H	2.68227441	-2.98656370	H
-0.45724771	3.54658062	-0.37971115	2.92839269	3.68170559	H	-0.45724771	1.47724161
H	-0.37971115	3.54658062	-3.68170559	C	2.92839269	-1.47724161	H
1.26594889	4.82319804	C	0.06059404	0.68508115	1.26594889	3.83569842	2.94059939
H	0.06059404	-4.82319804	H	1.53540787	3.83569842	-2.94059939	C
0.58539932	4.97655238	H	0.97489578	1.53540787	0.58539932	1.74589159	4.45700150
C	0.97489578	-4.97655238	H	-0.20487573	1.74589159	-4.45700150	H
5.25941090	H	-0.20487573	1.66820315	0.78712495	-5.25941090	H	0.94638885
0.78712495	-5.25941090	H	4.75984467	H	1.66820315	0.88177909	2.16979086
0.88177909	2.16979086	0.94638885	-4.75984467	H	5.41951214	H	0.88177909
0.04375153	1.61095286	2.16979086	-5.41951214	H	5.02824753	H	0.04375153
-1.48097986	-3.09388728	1.61095286	-5.02824753	H	2.70951670	H	-1.25986746
1.41204750	2.69844601	-2.12960851	1.23494455	H	4.79344440	H	1.41204750
0.14645993	-2.81147821						

2.69844601	-4.79344440		H	2.06975360		H	-1.48097986
-1.38988591			-2.70284331	-3.09388728	-2.70951670	H	0.14645993
4.09446315		H	-1.04411395	-2.81147821	-2.06975360		H
-2.61235745	2.36514326		H	-1.25986746			-2.12960851
0.28580220			-2.64461865	-1.23494455	C 0.58663502		2.10604753
3.54681960		H	-1.38988591	0.00000000		Mn	0.26721717
-2.70284331	-4.09446315		H	0.38009876	0.00000000		C
0.28580220			-2.64461865	-1.49208668			0.61731112
-3.54681960		H	-1.04411395	0.00000000		O	-2.65769084
-2.61235745	-2.36514326		C	0.74956265	0.00000000		
-1.50994713			1.00168397				
0.00000000		Mn	-0.05742550				
-0.00120624	0.00000000		C				
-0.99303598			-1.51772797				
0.00000000		O	-1.65957863				
-2.48631220	0.00000000		H				
0.86502062			1.36362295				
0.00000000		H	2.51025208				
-0.14676720	0.00000000						
2H-Mn-5_1a				**TSB-1a-H_H^-**			
P	-0.80167737		1.73991167	P	-0.89186666		1.78340090
0.13513448		C	-1.57639812	-0.22379601	C	-1.55820970	1.22814078
1.33804259	-1.50939725		C	-1.86351080	C	-0.44365241	0.57367720
-0.50410081			0.81620835	-2.65438530	H	-2.05116243	2.02899015
-2.44338469		H	-2.13183031	-2.43333555	H	-2.33512242	0.47677979
2.17727279	-1.95234885		H	-1.64570644	H	-0.84538284	0.08486418
-2.31585312			0.54173895	-3.56356803	H	0.29811566	1.31659443
-1.32786255		H	-0.95334390	-2.99591341	N	0.24125339	-0.40414762
0.39517131	-3.36542511		H	-1.79883397	C	1.27653786	-1.16236017
0.17717401			1.62421594	-2.50906559	C	1.96931201	-2.10948116
-2.76073411		N	0.29072525	-1.54827677	H	1.99490734	-0.44344269
-0.19178694	-1.73583822		C	-2.93851025	H	0.84071205	-1.71895634
1.30415267			-0.83949616	-3.36085148	H	1.24337683	-2.86449954
-2.57041825		C	2.07608758	-1.19889834	H	2.78372540	-2.66565334
-1.83674402	-1.73059293		H	-2.03783146	P	2.51387355	-1.15293307
1.97332672			-0.05293958	-0.05433247	Mn	0.95881744	0.49595287
-2.95925907		H	0.84265115	0.03038028	C	1.98553969	1.67208567
-1.33113874	-3.44949049		H	-0.79669470	O	2.65826694	2.46649175
1.39528622			-2.64586945	-1.34215448	C	1.38398442	1.06041931
-1.41155443		H	2.88225675	1.65319544	O	1.66826163	1.42437688
-2.31794244	-2.30541036		P	2.72862685	C	-2.35166244	1.50984118
2.66305323			-0.98077717	0.89351490	C	-3.66953530	2.05259428
-0.18648338		Mn	1.15730898	0.36427048	C	-2.08203716	1.95870946
0.64965229	0.09321618		C	2.32020434	H	-2.41161445	0.41048642
2.05480088			1.92398909	0.89635903	H	-3.93442559	1.64418038
-0.77140783		O	2.66733990	-0.62130695	H	-4.49068254	1.78214763
2.78210093	-1.29399743		C	1.04568639	H	-3.66968811	3.15139619
1.71104912			1.15071566	0.28791039	H	-1.12312329	1.58296113
1.68880842		O	2.06118266	2.70543178	H	-2.07646512	3.05623318
1.45597560	2.76475382		C	2.41143909	H	-2.87384883	1.58916087
-2.13635166			1.13435180	2.98978783	C	-0.73773195	3.64479122
1.29053208		C	-3.52886704	-0.30287186	C	-0.33074549	4.16123708
1.68359141	1.02691887		C	-1.67480460	C	0.22753403	4.13367190
-1.73934038			1.26125535	0.77070702	H	-1.74736464	4.03294517
2.75117794		H	-2.13009415	-0.07197015	H	-1.06084117	3.92127277
0.05818791	1.03841354		H	-2.45975255	H	-0.23800663	5.25750901
-3.86494545			1.52425617	-1.65191487	H	0.64776050	3.76818690

-0.00889693		H	-4.26630993
1.18810151	1.67890041		H
-3.59921393			2.76152385
1.24036146		H	-0.72767682
0.87276227	2.93622026		H
-1.76960994			2.30721040
3.09437312		H	-2.43733206
0.69902243	3.39155388		C
-0.85942116			3.60356500
0.28119591		C	-0.54039562
4.30211521	-1.03255650		C
0.10665017			4.05568515
1.36945746		H	-1.89042204
3.86919220	0.58077944		H
-1.27928402			4.10280872
-1.82085048		H	-0.51847200
5.39271273	-0.88629480		H
0.45072799			4.01360577
-1.41263639		H	-0.03367761
3.52736325	2.32241240		H
1.14793411			3.87927355
1.06082494		H	-0.00391480
5.13322087	1.56447469		C
2.74477901			-2.41558870
1.00763553		C	3.23927692
-1.99852186	2.38340233		C
3.49291178			-3.63495437
0.49214777		H	1.67329913
-2.67045851	1.10255258		H
2.72362666			-1.10524640
2.76127040		H	3.08213796
-2.80842480	3.11190346		H
4.31976306			-1.78854956
2.37746642		H	3.11764575
-3.99555869	-0.47606580		H
4.57024341			-3.44029348
0.37759713		H	3.40303824
-4.47095622	1.20301921		C
4.46235872			-0.57128037
-0.49856073		C	4.93153749
0.47431486	0.50705229		C
4.70931574			-0.08592847
-1.91929253		H	5.03538258
-1.50436706	-0.34229804		H
4.70841669			0.20784158
1.54893998		H	6.01852602
0.62782889	0.42727734		H
4.44692519			1.44291101
0.31729062		H	4.47225929
-0.84072124	-2.68252920		H
4.12787417			0.82179855
-2.14019182		H	5.76922881
0.17928742	-2.05190278		H
0.33617127			-0.53007312
0.88033701		C	-5.95204297
-1.24989828	-0.97322303		C
-5.46502085			-1.64180435
-1.98515286		H	0.00535164	3.73074364
1.76811265		H	1.26180606	3.84588574
0.53352799		H	0.20037706	5.23151215
0.84160240		C	2.64882484	-2.48445128
1.25536105		C	3.30316396	-1.96955177
2.52903772		C	3.30659762	-3.76750782
0.77005352			H	1.59711436
-2.71277101	1.49844927		H	2.86205479
-1.02664361	2.88151095		H	3.19295852
-2.70731227	3.33771238		H	4.38385848
-1.81007959	2.39567463		H	2.77786784
-4.22770243	-0.07572596		H	4.35151594
-3.60799286	0.46171853		H	3.32965149
-4.51460647	1.57797115		C	4.31181278
-0.72375991	-0.35142710		C	4.75545409
0.41507413	0.56104695		C	4.61463664
-0.39159440	-1.80495555		H	4.87999763
-1.63384091	-0.08194297		H	4.47547827
0.26891827	1.61213449		H	5.84935042
0.52887181	0.52264165		H	4.31908637
1.37144565	0.24359869		H	4.39353949
-1.21953053	-2.49300864		H	4.06012143
0.49602885	-2.14245215		H	5.68329295
-0.15682041	-1.92200584		H	-0.18131120
-0.68018378	0.74952014		C	-5.88081068
-1.48430599	-0.21480574		C	-5.15506754
-1.59211373	0.96065460		C	-3.75704798
-1.74736097	0.94046864		C	-3.06174098
-1.80594713	-0.31431006		C	-3.83459417
-1.70491097	-1.50029315		C	-5.20706997
-1.54366814	-1.44867985		H	-3.46131411
-1.86329800	3.10119046		H	-6.96518675
-1.36029709	-0.18610627		H	-5.66282306
-1.55118464	1.92951151		C	-2.96246353
-1.85441903	2.12693945		H	-3.30868386
-1.76400835	-2.45764686		H	-5.77607006
-1.46626436	-2.37900585		C	-0.97301155
-1.93584209	0.72989910		C	-1.61043754
-1.94961728	2.03746512		H	-0.03982437
-2.51194411	0.66419354		H	-0.98176829
-2.01492673	2.93000214		N	-1.72137577
-1.99094455	-0.40324611		H	-0.48958680
-1.07966676	-1.47653758			

0.25404205 C -4.09949847 -1.98453189 0.41166785 C -3.22589958 -1.91882041 -0.72181354 C -3.76076428 -1.52097032 -1.97288991 C -5.09288400 -1.19203879 -2.09379813 H -4.17381016 -2.44262627 2.53499483 H -7.00560130 -0.98536420 -1.08531066 H -6.12427512 -1.69145012 1.12501160 C -3.53654488 -2.38696081 1.64766322 H -3.08268912 -1.48487504 -2.82907986 H -5.49230679 -0.88599743 -3.06339480 C -1.42188397 -2.58683556 0.53447608 C -2.19911131 -2.69572757 1.71126774 H -0.35106159 -2.81436909 0.57740353 H -1.72727453 -3.00260009 2.64616995 N -1.89904975 -2.21330853 -0.63434683 H -0.35917039 -0.91927691 -1.40607453	
Mn-5-H_1a-H_H P -0.93467099 1.76932331 0.05691967 C -1.56095847 1.45727286 -1.65798549 C -0.42489509 0.93199658 -2.51149875 H -2.04847259 2.33130092 -2.11290586 H -2.33514640 0.67720710 -1.56957127 H -0.80821896 0.56664434 -3.48392275 H 0.31010853 1.72397611 -2.73953401 N 0.25983021 -0.14896953 -1.78904003 C 1.29233005 -0.80264024 -2.60067143 C 1.99450395 -1.86765649 -1.78126102 H 2.00605255 -0.03329922 -2.94198945 H 0.84777967 -1.24434315 -3.51276941 H 1.27160384 -2.66367699 -1.53069773 H 2.80899311 -2.34901959 -2.34442137 P 2.54147555 -1.12492287 -0.17428692 Mn 0.94631642 0.47406398 0.14624340 C 1.95703969 1.77401663 -0.46820398 O 2.62118108 2.64981142 -0.88113877 C 1.34901369 0.80410754 1.84260299 O 1.62637111 1.02364049 2.95708031 C -2.40193412 1.30809153 1.09837777 C -3.72124022 1.89753062 0.62515724 C -2.16286647 1.55586553 2.57869570 H -2.44650545 0.21908959 0.94358108 H -3.96415227 1.62098928 -0.41036420 H -4.54546239 1.51944938 1.24868659 H -3.74170402 2.99631438 0.70015551 H -1.20012206 1.15261873 2.92502317 H -2.18761606 2.62901152 2.82512178 H -2.95321245 1.07404297 3.17389855 C -0.79651829 3.62028745	**Mn-5-H_1a-H_N** P 2.41028792 -0.56250848 0.47044809 C 2.27594970 -0.63401960 2.32623867 C 1.31435724 0.43693644 2.80813226 H 3.25024863 -0.53145347 2.82412617 H 1.91157544 -1.63324659 2.60577564 H 1.07782259 0.29627771 3.88015593 H 1.77702613 1.43482605 2.72286067 N 0.08316557 0.45512278 2.00315522 C -0.86298680 1.48550792 2.44454415 H -0.35469264 2.46308097 2.38674203 H -1.13779783 1.33599079 3.50605254 Mn 0.52246063 0.57593225 -0.14547725 C 1.31920825 2.10830053 0.18024437 O 1.86756417 3.12745455 0.38602053 C 0.93455374 0.80648891 -1.85233554 O 1.22728535 1.03636541 -2.95969087 C 2.59558960 -2.34415517 -0.03129211 C 3.57030633 -3.14476355 0.81645496 C 2.92881142 -2.44256857 -1.51312258 H 1.57397200 -2.73793205 0.11336422 H 3.29776469 -3.16740533 1.88071572 H 3.60212362

0.26767906	C	-0.38018756	4.34633159	-4.19066748	0.47566021		H
-1.00282127	C	0.14580999	3.94983407	4.59983196			-2.75951110
1.41934759	H	-1.81488033	3.95520162	0.74442318		H	2.27412252
0.53975379	H	-1.09781213	4.22159405	-1.81103414	-2.13150475		H
-1.82491883	H	-0.30352199	5.42679318	3.97098247			-2.14976749
-0.80949149	H	0.60706709	4.01811532	-1.71642298		H	2.81443310
-1.35732950	H	-0.08498872	3.39593421	-3.47810988	-1.86596476		C
2.33928101		H	1.18825097	4.10569406			0.16136405
3.71742608	1.15837200		H	0.12608682		C	4.58499706
0.09986250			5.02309293	1.15394783	1.17602396		C
1.65756306		C	2.69994825	4.14393562			0.79641510
-2.62210976	0.93657040	C	3.34675657	-1.25869392		H	4.79500766
-2.28432383	2.27168446	C	3.37785046	-0.70381114	0.13258464		H
-3.81162636	0.27310052	H	1.65126987	4.73384230			0.70403801
-2.90020956	1.13848517	H	2.89447085	2.16649437		H	5.55609064
-1.40662552	2.75421526	H	3.24402926	1.57372924	0.87383307		H
-3.13049060	2.96701258	H	4.42573027	3.89590400			2.00387781
-2.09547740	2.16547272	H	2.85532420	1.28309158		H	3.75374044
-4.15449135	-0.63008317	H	4.42032321	0.14307631	-2.04950288		H
-3.59418161	-0.00678958	H	3.41177495	3.55412793			1.72391245
-4.66545766	0.96656290	C	4.32659586	-1.28776979		H	5.17754318
-0.62107382	-0.41472766	C	4.76368956	1.06132347	-1.52751585		C
0.37449757	0.65470924	C	4.61072750	-2.08569148			1.45159265
-0.07396047	-1.80563690	H	4.90872038	1.55419000		H	-0.38903942
-1.55304849	-0.28761629	H	4.50115139	-0.45093981	2.10936635		C
0.06547976	1.67444835		H	-1.53719940			-3.13950454
5.85505981			0.51086486	2.54664294		C	-0.78351379
0.62213565		H	4.31015147	-2.41332765	1.62490173		C
1.36084673	0.49045893		H	-1.22072069			-2.14900039
4.39026464			-0.79408710	0.29717019		C	-2.45417247
-2.60588920	H	4.04428535	0.84741852	-2.80532215	-0.07562980		C
-2.00404662	H	5.67579876	0.18696186	-3.19896169			-3.51136833
-1.89573796	H	-0.25832212	-0.89717089	0.87071468		C	-2.77548381
0.68832147		C	-5.81975741	-3.67094385	2.19255044		H
-1.62391604	-0.61868820	C	-5.13231857	-1.12888252			-3.31645000
-1.86345790	0.56402061		C	3.54663590		H	0.23303690
-3.73201511			-1.94707806	-2.12542864	1.88648191		C
0.59165316		C	-2.97301541	-2.88613292			-2.68966290
-1.79498016	-0.62136368	C	-3.70788364	-1.45221384		H	-4.14274680
-1.56358610	-1.81726212	C	-5.08938189	-3.96130448	0.54402809		H
-1.47754879	-1.81066969	H	-3.52937442	-3.37553434			-4.23339399
-2.37135345	2.72713450		H	2.90993873		C	-2.05373128
-6.90938832	-1.55775200	-0.62522497	H	-2.16318963	-2.36513865		C
-5.67992199			-1.98654284	-0.68545947			-1.70229164
1.50439314		C	-2.98444862	-1.96751415		H	-2.34231027
-2.18810829	1.79510925		H	-2.08011539	-3.41801030		H
-3.14405596	-1.46237347	-2.74982927	H	-0.40494471			-0.85474283
-5.61948236	-1.29674562	-2.75012582	C	-2.60826041		N	-0.52961547
-0.90155181			-1.94910242	-1.34178083	-0.55825932		P
0.51711126		C	-1.63158128	-1.55356917			1.59869763
-2.19316643	1.77771839		H	-0.21233246		H	-2.58092097
-0.02878405			-2.62324492	0.46804443	1.64702136		H
0.41937297		H	-1.05176760	-2.82868921			2.20784476
-2.36027916	2.69089696		N	1.84975729		C	-3.00283143
-1.62820469	-1.89182035	-0.67026908	H	0.86604260	-1.10822037		H
-0.48116634	-0.87141612	-1.56285838		-2.89013322			-0.20644781
				-0.88210281		C	-1.67736548

				3.41880798	-0.63179753	H	-2.74019584
				3.57469513	-0.89578005	C	-0.82639464
				3.74155137	-1.85459743	H	-1.03061955
				4.76448852	-2.20503502	H	0.24629162
				3.68736905	-1.62109076	H	-1.00573424
				3.06193691	-2.69814069	C	-1.34193175
				4.35169223	0.52231560	H	-0.29138213
				4.25870143	0.83217962	H	-1.48513535
				5.39780308	0.21211042	H	-1.97795771
				4.19357841	1.40458028	C	-4.35875100
				1.32927507	-0.59922705	H	-4.51587440
				2.41137051	-0.73498550	H	-5.16062329
				0.82367644	-1.15856277	H	-4.52067832
				1.09769362	0.46218005	C	-2.88223782
				1.04580484	-2.61332739	H	-3.61208001
				0.40732056	-3.13315531	H	-3.08912569
				2.08412934	-2.91830633	H	-1.88474493
				0.77866705	-2.99259565	H	-3.88481652
				-3.04643623	-1.72492838	H	0.05010524
				-2.49680358	-2.25738492		
TSB-1a-H$_N^+$				**Mn-5'_2a$_N$**			
P	2.65169820		-0.55377182	P	2.66001092		-0.72162236
0.35403503	C	2.42629685	-0.94748033	0.06831397	C	2.46756748	
2.14422600	C	1.48125915	0.06215584	-1.45075637	1.75027444	C	1.60675453
2.76909418	H	3.38452523	-1.00119917	-0.52066611	2.58315107	H	3.43093393
2.68639360	H	1.98044714	-1.95610397	-1.67876591	2.23450186	H	1.94225673
2.18440685	H	1.14750549	-0.30949607	-2.40973463	1.60524537	H	1.11244110
3.76146036	H	2.01628493	1.00732270	-1.10255971	3.39121685	H	2.23842953
2.98797062	N	0.33705777	0.31550516	0.21012076	3.13331984	N	0.61226747
1.91114716	C	-0.50786767	1.33031560	0.16676600	1.77328041	C	-0.41569828
0.69408984	2.52636721	H	0.08103670	2.26595686	2.65663978	H	0.00537725
2.64170646	H	-0.77733490	1.03711734	1.47936724	3.32276085	H	-0.75021478
-0.09958333	3.56427524	Mn	0.52631626	0.34381548	3.36157604	Mn	0.77476542
0.52328825	-0.20525995	C	1.35187649	1.78765615	-0.11353241	C	1.53040926
1.71338532	-0.72919466	O	1.88838542	2.72842871	-1.17404385	O	2.05641738
2.53007481	-1.18334846	C	0.43762893	-0.12202177	-1.83269514	C	0.12152335
-0.32933810	-1.92318360	O	0.41137049	-0.39606536	-0.34420436	-1.50240331	O
2.91965685	-3.05726580	C	3.42039256	-2.14805416	-0.95070977	-2.39816061	C
4.09145338	-0.29902443	C	4.85775053	-2.39872657	-2.22908697	-0.99430206	C
2.95656773	0.13292458	C	3.24236045	-2.30332947	-3.09212393	-0.55297673	C
1.97830719	-1.80337353	H	2.80741543	-2.92239926	-1.94093138	-2.48959323	H
4.04697719	0.19290552	H	5.00200448	-2.29417516	-2.77506936	-0.79058792	H
4.12031588	1.21811781	H	5.15353873	-3.42511081	-3.36169336	0.51222430	H
5.05459526	-0.13219985	H	5.57155934	-1.72835706	-4.03248956	-1.12448233	H
2.19858619	-0.36747346	H	2.19434139	-2.20452404	-2.58778504	-0.72730178	H
3.93493759	-2.11704654	H	3.80956432	-1.55241257	-1.21146272	-2.80057290	H
	-2.37136806	H	3.59742383	-3.29114043			
	-2.13368532	C	4.13129358	0.59537932			

0.37283014	C	3.94577767	1.82676320
1.25000402	C	4.60701329	0.93886332
-1.03242830	H	4.91985854	-0.01005736
0.85313539	H	3.89190387	1.56584941
2.31522813	H	4.80979173	2.49781737
1.13185354	H	3.05174026	2.41303353
1.00049144	H	4.90541509	0.04748386
-1.60042981	H	3.84733456	1.46979029
-1.61929657	H	5.48959752	1.59404479
-0.98131341	C	-1.77578263	1.62410471
1.74307265	H	-0.15407808	-0.83370868
1.47804875	C	-4.00358567	-1.63403643
2.15410305	C	-2.62496258	-1.49868599
1.99907313	C	-1.98370479	-1.88707339
0.80897490	C	-2.76946318	-2.52142765
-0.19936039	C	-4.15291457	-2.63945154
-0.02623244	C	-4.78013507	-2.18596770
1.13330629	H	-4.47306127	-1.32037120
3.09030424	H	-2.01865778	-1.09205609
2.81270228	C	-2.08063133	-2.98081653
-1.39109896	H	-4.74191566	-3.10370403
-0.82339195	H	-5.86029557	-2.29097105
1.25424410	C	-0.74201624	-3.09732482
-1.37291598	C	-0.00258465	-2.76712506
-0.11073195	H	-0.18629300	-3.45136751
-2.24602449	H	1.02428877	-2.49310507
-0.35718964	N	-0.62470898	-1.66240841
0.60691902	P	-1.44474825	1.55335734
-0.07357147	H	-2.55178592	0.87501002
1.95138739	H	-2.20321204	2.59617828
2.03456067	C	-3.06174720	0.89675544
-0.74714169	H	-3.25125842	0.04942415
-0.07012077	C	-1.48244654	3.36397231
-0.53912917	H	-2.51807327	3.66458267
-0.29897113	C	-1.26379302	3.57888335
-2.02913342	H	-1.31792162	4.65016614
-2.27507516	H	-0.27948783	3.22162243
-2.36135339	H	-2.02455696	3.07025193
-2.63708454	C	-0.57070300	4.23055012
0.31891048	H	0.49354764	4.01493899
0.16864285	H	-0.71941254	5.29001797
0.06077261	H	-0.78728466	4.13396579
1.39203784	C	-4.23899175	1.84919835
-0.60897245	H	-4.18991911	2.68500500
-1.32382786	H	-5.17818401	1.31215217
-0.81272299	H	-4.32761249	2.27509089
0.40199580	C	-2.93933732	0.32622034
-2.15047964	H	-3.88307065	-0.16046208
-2.44229700	H	-2.72285164	1.09379298
-2.90868524	H	-2.14751342	-0.43093667
-2.21540839	H	0.06215889	-3.68238872
0.52768301	H	-2.66665593	-3.23328910
-2.27991322			

-1.56270162	-2.81455320	H	2.77035769
-2.86452648	-3.05752377	C	4.31976072
0.12934986	0.18411691	C	4.20290258
1.35038367	1.08682135	C	4.90425173
0.50801732	-1.16826683	H	4.99279566
-0.60243566	0.66960749	H	3.80553164
1.10963688	2.08261173		H
5.18875214			1.81704160
1.23320517		H	3.54394064
2.11078194	0.64178432		H
5.20961677			-0.36670344
-1.75634311	H	4.19819488	1.09429956
-1.77410721	H	5.80213886	1.12951302
-1.03134142	C	-1.61307725	1.22923730
1.89532533		H	-2.86342706
-2.01058347	2.83266570		C
-5.07942489	-1.02706364	-0.30111419	C
-4.38086371			-1.31979341
0.86925681		C	-3.15336635
-2.00016816	0.81456892		C
-2.62917627	-2.37579416	-0.44983789	C
-3.34329735	-2.05599092	-1.60763633	C
-4.56652865	-1.38659329	-1.54782185	H
-6.03618022	-0.50268759	-0.23168433	H
-4.78924271			-1.03060648
1.84263576		C	-1.37257305
-3.10334841	-0.46437040	H	-2.91362568
-2.33808235	-2.57253491	H	-5.11222992
-1.14894428	-2.46298528	C	-0.69806972
-3.37629822	0.66403850		C
-1.16253379			-2.94750452
2.01425729		H	0.23917722
-3.93921257	0.62940935		H
-0.40846203			-2.26577846
2.46365466		N	-2.45901242
-2.30897036	1.95598071	P	-1.06143186
1.80398951	0.23661118		H
-2.32740965			0.41513024
1.69560374	H	-2.15442173	2.00623861
2.45855628	C	-2.59135694	1.59002368
-0.79136254	H	-2.76884060	0.50746584
-0.64802628	C	-0.83032507	3.63925071
0.49572546	H	-1.71966639	3.96590143
1.06735521	C	-0.76741962	4.43215119
-0.80050300	H	-0.51294402	5.48228712
-0.59090496	H	0.00269638	4.04534884
-1.48369603	H	-1.72460910	4.43595767
-1.33777621	C	0.40896426	3.88208718
1.34698619		H	1.32296975
3.60440664	0.80110841		H
0.49555086			4.94737072
1.60978832		H	0.40168073
3.31199696	2.28685243		C
-3.79888367			2.34473545
-0.25954558	H	-3.67651044	3.43562623
-0.35237340	H	-4.70072392	2.07378760
-0.83031027	H	-4.00812692	2.11839118

				0.79645771	C	-2.38460874	1.81675388
				-2.28257134	H	-3.20217549	1.34379354
				-2.84736198	H	-2.38721837	2.88295452
				-2.54805843	H	-1.44537840	1.38526160
				-2.65151961	H	-0.97769922	-3.42284325
				-1.43209997	H	-1.19800415	-3.82245743
				2.69574320			
TSB-1a-H_H^+				**Mn-5'_2a$_H$**			
P	-0.75213722		1.89267943	P	-0.87766124		1.81975997
-0.26818685		C	-1.55785744	-0.07541423		C	-1.61629741
1.26321505	-1.80822492		C	1.29925571	-1.68369323		C
-0.59414569			0.33420817	-0.53939220			0.61523507
-2.51887727		H	-1.92623974	-2.50326442		H	-2.10907702
2.06300307	-2.46609882		H	2.12040966	-2.22464900		H
-2.44383062			0.69152624	-2.40625280			0.57156618
-1.48860127		H	-1.13549039	-1.43764473		H	-1.01599730
-0.24696515	-3.29305069		H	-0.00271358	-3.29427097		H
0.18049815			0.90846515	0.06402354			1.36616798
-3.06455439		N	0.04032858	-3.06039948		N	0.30914324
-0.56419760	-1.55210284		C	-0.20824739	-1.65274377		C
0.83777392			-1.57712666	1.10798748			-1.09954359
-2.24278865		C	1.53962256	-2.47753339		C	1.91478958
-2.46933106	-1.23706612		H	-2.04700811	-1.61248224		H
1.57337917			-1.08926418	1.78236851			-0.52907842
-2.91153628		H	0.19116637	-3.15430614		H	0.45533908
-2.19019540	-2.90369576		H	-1.68416649	-3.16187946		H
0.78465756			-3.06382223	1.24010669			-2.79960149
-0.69400925		H	2.22167771	-1.16772181		H	2.67809151
-3.18754441	-1.71831466	P	2.36370847	-2.60115665	-2.18132259		P
-1.39906858	0.02447650		Mn	2.60280601			-1.08736997
0.97874872			0.42214355	-0.19463871		Mn	1.03766357
0.03308733		C	2.04603055	0.56918972	0.00963647		C
1.39120249	-0.95524832		O	2.05876273			1.84890834
2.74070654			2.04125317	-0.57457199		O	2.72381085
-1.64210147		C	1.59035906	2.69997018	-1.03430173		C
1.11172072	1.55544665		O	1.41512356			0.95447494
2.01452126			1.56889007	1.71234046		O	1.69206494
2.54468137		C	-2.16385729	1.23778663	2.81443579		C
1.86327229	0.94113923		C	-2.26055110			1.42171489
-3.43914870			2.52527664	1.11289091		C	-3.61691675
0.44345575		C	-1.76070398	1.97229969	0.69844212		C
2.36519709	2.31765640		H	-1.93709380			1.76181616
-2.36183476			0.78176312	2.55824121		H	-2.31038464
1.01840056		H	-3.80111337	0.32295410	1.02732194		H
2.09823511	-0.50244886		H	-3.92143737			1.65463515
-4.24573842			2.38240351	-0.30861912		H	-4.39384794
1.17880969		H	-3.32324826	1.61129887	1.38995761		H
3.61168705	0.30558257		H	-3.64890706			3.07244130
-0.82577692			1.91041231	0.73271027		H	-0.95002913
2.67635243		H	-1.62825040	1.39535485	2.87291333		H
3.45839108	2.33169486		H	-1.96523658			2.84753403
-2.54466095			2.13018762	2.73839394		H	-2.68488725
3.05336003		C	-0.39503996	1.31010023	3.22760269		C
3.71046123	-0.50779561		C	-0.77719861			3.68125004
-0.02483506			4.07344787	-0.06634981		C	-0.37261301
-1.93825577		C	0.67998566	4.25209184	-1.41772387		C
4.17000336	0.46991939		H	0.16824275			4.15409906

-1.34081691		4.22455488	1.03227814	H	-1.79912973
-0.25473541	H	-0.82925337	4.03226085	0.16925024	H
3.86592671	-2.65636075	H	-1.09390068		4.02301366
0.19265646		5.14986236	-2.21366801	H	-0.29914226
-2.00664523	H	0.87819365	5.34824396	-1.35701941	H
3.54556750	-2.27543335	H	0.61305484		3.88439357
0.47907670		3.86950875	-1.73643127	H	-0.03490136
1.50719473	H	1.66374608	3.69315759	2.00819626	H
3.75822603	0.20226499	H	1.21334645		3.92399813
0.76962616		5.26655364	0.78160804	H	0.09574541
0.45324268	C	2.51508395	5.24480354	1.15796826	C
-2.53901333	1.49970057	C	2.78489255		-2.41441280
3.35569501		-1.94060866	1.11046645	C	3.44526989
2.61762467	C	2.98102724	-1.92426999	2.39008860	C
-3.94299448	1.14384907	H	3.44426525		-3.68874729
1.47621071		-2.60953712	0.60352201	H	1.72979309
1.86634881	H	3.06168959	-2.64581536	1.34360243	H
-0.91216694	2.86921525	H	3.03038860		-0.97369098
3.25519203		-2.54404265	2.75111852	H	3.31584767
3.53189544	H	4.42602478	-2.66605273	3.19221787	H
-1.93537175	2.36212250	H	4.52980749		-1.79366154
2.31856489		-4.44608702	2.25902996	H	2.93133421
0.42684537	H	3.99713830	-4.12461534	-0.26442175	H
-3.94844273	0.71982610	H	4.49571840		-3.52469341
3.01500462		-4.57251376	0.32199251	H	3.44849472
2.04588872	C	4.14085324	-4.45527656	1.39327524	C
-1.20842121	-0.52150850	C	4.35984288		-0.66590290
4.81505355		-0.03783567	-0.65696023	C	4.94869539
0.18652292	C	4.28718983	0.37796181	0.28540558	C
-1.08081575	-2.03057661	H	4.47080658		-0.20806145
4.63839124		-2.14500112	-2.10426558	H	4.92807263
-0.20670823	H	4.65399512	-1.60858245	-0.54593119	H
-0.02947509	1.27189551	H	4.81549748		0.13495662
5.90148262		-0.06615288	1.34704700	H	6.02889638
0.01443677	H	4.45285003	0.48452184	0.10509621	H
0.92369230	-0.19994635	H	4.49550928		1.36411577
3.89624973		-1.95080856	0.11996358	H	4.16100605
-2.57598945	H	3.78488613	-0.97905164	-2.82307983	H
-0.18066277	-2.41333432	H	3.86954953		0.69413015
5.35040951		-0.98617303	-2.29043135	H	5.51403550
-2.29756559	H	-0.34576314	0.05131779	-2.33901211	H
-0.61267246	1.10539290	C	-0.34012793		-1.04322221
-5.85642235		-1.23599112	1.18532417	C	-5.84082413
-0.51446688	C	-5.28155430	-1.78503958	-0.68017925	C
-1.20827034	0.75128794	C	-5.28141499		-1.92731027
-3.90092889		-1.36907984	0.58833099	C	-3.89603603
0.93125832	C	-3.05019052	-1.96648186	0.77542538	C
-1.57778959	-0.20081574	C	-3.03701772		-1.87391076
-3.66046904		-1.61704381	-0.35223839	C	-3.60853984
-1.47830310	C	-5.02897649	-1.72761438	-1.62786382	C
-1.44464435	-1.62689904	H	-4.99163551		-1.68285080
-3.89907803		-1.22488045	-1.78397308	H	-3.92586052
3.11556178	H	-6.93278940	-2.12165722	2.96029908	H
-1.10546205	-0.63978494	H	-6.92416989		-1.75445661
-5.90616496		-1.05040096	-0.80807137	H	-5.92623947
1.63651126	C	-3.26792850	-1.99854925	1.46945839	C
-1.32908062	2.22710493	H	-3.27475698		-2.05535266

-3.02375736			-1.79379638	2.08349504		H	-2.94937817
-2.35071264		H	-5.46553034	-1.65823897	-2.49848652		H
-1.47855547	-2.62888555		C	-5.41034705			-1.57071932
-1.05865574			-1.56437033	-2.78723457		C	-1.00512777
1.15672965		C	-1.92687478	-1.95275963	1.08104999		C
-1.41318748	2.34963623		H	-1.93861504			-2.03555846
-0.30111393			-2.35475137	2.23658315		H	-0.28425222
1.33505106		H	-1.44430803	-2.79884811	1.12412405		H
-1.36808039	3.33009984		N	-1.48793761			-2.07888858
-1.70714182			-1.75485548	3.23127994		N	-1.67480356
-0.08503089		H	-0.88072837	-1.92670355	-0.19316307		H
-1.20414727	-0.96058641			-1.09505867	-1.50338152	-0.93082532	
Mn-5'_iPrOH$_O$				**Mn-5'_iPrOH$_H$**			
P	-2.27710058		-0.15892966	P	2.26800468		0.32150691
-0.12811145		P	2.26816442	-0.06953585		P	-2.26796404
-0.24622033	-0.21411592		C	0.32256854	-0.06739975		C
-2.46470652			-0.08490490	2.40070223			-0.50182028
-1.96481811		C	2.37739148	-1.71372251		C	-2.40261361
-0.18550824	-2.05822433		H	-0.50073991	-1.71148670		H
-2.44398795			0.98814739	2.33098418			-1.58553898
-2.22593352		H	2.38909747	-1.51883060		H	-2.33345805
0.88709842	-2.31931118		H	-1.58450053	-1.51662194		H
-3.42699995			-0.48109388	3.36130108			-0.32230351
-2.32503271		H	3.30598179	-2.22128881		H	-3.36360880
-0.62246770	-2.45706220		C	-0.32077424	-2.21814674		C
-1.26260071			-0.77135742	1.19787639			-0.09720886
-2.59109169		C	1.12401021	-2.54174844		C	-1.20036859
-0.82421379	-2.63367188		H	-0.09670687	-2.54063577		H
-1.26673512			-0.59121014	1.08707481			-0.79592895
-3.68811518		H	1.09337151	-3.39633436		H	-1.09065872
-0.64828682	-3.73095480		H	-0.79545486	-3.39534403		H
-1.36488131			-1.87724034	1.34664423			0.90266871
-2.48603510		H	1.18286369	-3.00084538		H	-1.34918424
-1.93325461	-2.52678140		N	0.90322875	-2.99959396		N
-0.04750328			-0.27198039	-0.00088230			-0.12385065
-1.98856210		C	3.23987719	-1.71107680		C	-3.14770038
1.26189195	0.29540670		C	-0.88250070	1.05695316		C
-3.25117645			1.33203442	3.14828133			-0.88397794
0.44111911		H	2.57858624	1.05393716		H	-2.40282715
2.06889118	-0.06315463		H	-1.69517232	1.13709541		H
-2.60756588			2.17129115	2.40316601			-1.69637489
0.12667610		C	3.33182424	1.13467677		C	-3.40340244
-1.66955224	0.35543619		C	1.80001506	-0.15121712		C
-3.34113232			-1.57645783	3.40400123			1.79846923
0.46762808		C	3.28562518	-0.15432344		C	-3.24548050
-2.86515160	-0.58508044		C	2.54852151	-1.46740614		C
-3.36699623			-2.75520197	3.24521423			2.54708330
-0.49437441		O	0.03728692	-1.47034347		O	0.00160141
0.11994525	3.03982495		H	0.51613449	3.07016412		H
-4.36489264			-1.16151847	4.42856609			1.38183543
0.52658333		H	4.36619173	-0.10773149		H	-4.42811763
-1.27718861	0.36251306		C	1.38385819	-0.10365792		C
-2.92250897			-2.02314739	3.20077995			2.74617720
1.86451568		C	2.95999826	1.02233600		C	-3.19862675
-2.07993960	1.77646215		H	2.74767493	1.02520572		H
-2.79592097			-1.19103358	3.20975551			2.24569130
2.56958091		H	2.90021209	1.99799683		H	-3.20702128

-1.23231728	2.47216852		H	2.24724821	2.00090039		H
-1.97004823			-2.56936037	2.24613664			3.28168213
1.83941422		H	1.98413051	0.93957770		H	-2.24375501
-2.58426899	1.80113049		H	3.28264046	0.94157450		H
-3.67542375			-2.70513235	3.99605064			3.50656430
2.28793672		H	3.70172934	1.03597576		H	-3.99346304
-2.78706861	2.17767166		C	3.50850340	1.03949923		C
3.37281674			1.39170926	-3.39397266			-0.34364988
1.80472251		C	-3.38748105	2.45807646		C	3.39606103
1.38861400	1.95542626		H	-0.34536209	2.45488367		H
4.08248814			0.65685646	-4.21200004			0.39217530
2.21536750		H	-4.10616588	2.46844017		H	4.21437426
0.64041143	2.32361113		H	0.39015384	2.46455850		H
2.41515754			1.26074640	-2.50554402			0.12390143
2.32843184		H	-2.43467558	2.90209808		H	2.50822711
1.21829848	2.47730773		H	0.12248253	2.89978437		H
3.76334794			2.38570751	-3.70062078			-1.16144367
2.07225391		H	-3.76784255	3.12694024		H	3.70302992
2.37173578	2.27206587		C	-1.16333684	3.12338030		C
4.58792531			1.39405056	-4.42571180			-1.45597494
-0.39627724		C	-4.60047593	0.46260945		C	4.42551628
1.49144388	-0.24362881		H	-1.45789515	0.45834934		H
4.51047105			1.38025113	-4.26738897			-1.96367034
-1.49219059		H	-4.52057587	-0.49820650		H	4.26609773
1.55660089	-1.33726617		H	-1.96534801	-0.50240923		H
5.28535407			0.59389844	-5.19044403			-0.67902655
-0.10301362		H	-5.28383086	0.30630673		H	5.19043649
0.66027038	-0.01049233		H	-0.68124236	0.30150401		H
5.07016414			2.34431162	-4.86509759			-2.19635805
-0.11904714		H	-5.09897065	1.14850254		H	4.86520085
2.41113601	0.09938951		H	-2.19857964	1.14372789		H
3.93502190			-3.66817997	-3.91153964			3.42403148
-0.20477438		H	2.27242297	-1.48771729		H	-2.21944321
-3.28419570	-0.66110780		H	2.92637218	-1.59240205		H
3.63101824			-2.62615389	-3.49170358			1.93498347
-1.60014713		H	-4.01718649	-2.34475457		H	3.91166219
-3.54927633	-0.09691592		H	3.42228336	-1.49125700		H
-3.75431786			-2.49020014	3.49032932			1.93343960
-1.48763987		H	-2.36936913	-2.34793003		H	2.21923566
-3.19710266	-0.62507673		C	2.92541146	-1.59438121		C
0.02668146			-0.01040376	0.00095646			0.53036902
1.87591578		Mn	-0.00443597	1.89948118		Mn	0.00012563
-0.26140976	0.11331587		C	0.56203138	0.11445973		C
-0.03442028			-2.00032953	0.00047904			2.30309279
0.24209788		O	-0.04052910	0.04637527		O	0.00067405
-3.17412234	0.27398741		H	3.46678936	-0.10420655		H
-1.25864615			3.24379988	0.00116270			-2.32550868
-0.83017187		H	0.05498330	0.47629509		H	-0.00012448
1.36260700	-1.51724527		C	-1.97202862	-1.54010236		C
-0.21133087			3.15131430	0.00049301			-3.27772774
-0.46921605		O	0.22417101	-0.11755391		O	0.00227639
1.81106204	-0.62124936		C	-2.95324999	-1.48995896		C
0.65540863			4.06974729	1.25241339			-4.06395941
-1.30823401		H	0.31735894	0.22680800		H	1.31139287
5.11327378	-1.23838437		H	-4.29872194	1.29980346		H
1.70310513			4.03128206	1.26418952			-5.01289141
-0.97378561		H	0.63099436	-0.32953371		H	2.16147077

3.78134427	-2.36866692	C		-3.51456081	-0.05561981	C	
-0.17060111	3.48062825			-1.25393569	-4.06092680		
1.00411999	H	0.85557517		0.22483360	H	-1.26689041	
3.38801535	1.39084464	H		-5.01008436	-0.33109653	H	
-0.51691445	4.50509580			-1.31556677	-4.29503969		
1.19751882	H	-0.79887569		1.29783845	H	-2.16120307	
2.78643617	1.57958268			-3.50956677	-0.05955536		
TSB-iPrOH-H_O^+				**TSB-iPrOH-H_H^+**			
P	-2.30482239	-0.13447475		P	0.26801158	-0.00501917	
-0.13078181	P	2.26640772	-0.17932175	2.27504955	P	0.26975833	
-0.25137805	C	-2.50084736	0.54524226	-0.01630435	-2.27475561	C	
-1.83974180	C	2.35289589	0.43815040	-0.37796776	-1.72880415		
-1.99316535	H	-2.50571467	1.64485974	2.41854982	C	-0.37576863	
-1.74220233	H	2.38811585	1.53802920	-1.74093865	-2.41018644	H	
-1.91662434	H	-3.45906146	0.26412279	-1.47608052	-1.66167538		
-2.30566875	H	3.26878680	0.12368272	2.32716532	H	-1.47397749	
-2.51696350	C	-1.30143963	0.11404456	-1.67363961	-2.32005278	H	
-2.66716389	C	1.08942505	0.02965733	-0.15253614	-2.21268875		
-2.73001802	H	-1.30105411	0.66508485	3.38100275	H	-0.14928939	
-3.63225894	H	1.05489604	0.54537417	-2.22958916	-3.36997693	C	
-3.71367803	H	-1.40048267	-0.95682078	0.12619534	-2.52276185		
-2.95078153	H	1.12428851	-1.05550321	1.22633449	C	0.12764057	
-2.97617436	N	-0.07716478	0.35411180	-2.52873655	-1.21355637	H	
-1.93413405	C	3.24865048	1.12026777	-0.36144442	-3.51643985		
0.65564073	C	-3.33596565	1.05632584	1.20281560	H	-0.35945953	
0.89511375	H	2.59209610	1.99596863	-3.52256140	-1.18551336	H	
0.51587099	H	-3.06593832	2.02947385	1.21414082	-2.70959798		
0.44842572	C	3.33943870	-1.70144793	1.28793106	H	1.21573147	
-0.17340255	C	-3.33977349	-1.68983187	-2.71529711	-1.27322160	N	
-0.14178396	C	3.20239840	-2.58829662	-0.19092974	-1.77805367		
-1.40279145	C	-3.11651824	-2.56386838	0.00436972	C	-0.90952273	
-1.36735182	O	0.07271811	-0.69590971	1.01514624	-3.28710971	C	
3.00891172	H	-4.38345932	-1.33527808	-0.91156830	1.03129078		
-0.19058527	H	4.37848906	-1.32365396	3.28209979	H	-1.76463983	
-0.13744208	C	-3.15605898	-2.46357692	1.14155841	-2.60686051	H	
1.15590615	C	3.06412581	-2.48923099	-1.76690687	1.15376814		
1.10319042	H	-3.37647464	-1.85412824	2.60141051	C	1.82553049	
2.04413302	H	3.06880248		0.03217108	-3.31459487	C	
-1.86603360	2.00730772	H	-2.12860101	1.82334350	0.04835350		
-2.83948570	1.26316295	H	2.08557777	3.31538391	C	2.62638348	
-2.98626679	1.06013191	H	-3.82686467	-1.26122831	-3.27542967	C	
-3.33542241	1.18490211	H	3.82175912	2.62396508	-1.24538338		
-3.27561803	1.23944701	C	3.37209811	3.28309126	O	0.71610227	
0.84865298	2.14661682	C	-2.90707492	3.14817231	-0.00762812	H	
1.09153403	2.35376127	H	4.09507443	1.45182058	0.19225927		
0.04513601	2.35542398	H		4.34815577	H	1.45438759	
-3.07311330	0.13206010			0.17075658	-4.34823761	C	
2.86535575	H	2.41610758	0.56755893	2.70977626	1.23509935		
2.60978737	H	-1.84051258	1.32608095	2.95109604	C	2.71153802	
2.46169634	H	3.74151097	1.74400354	1.22083272	-2.95555020	H	
2.66992905	H	-3.47594000	1.85502056	2.16292510	2.18137071		
2.90618961	C	4.60354434	1.42212578	2.85696394	H	2.16433034	
0.03365000	C	-4.84184785	0.89916300	2.16724221	-2.86489427	H	
0.75139468	H	4.53991556	1.68447900	3.22964474	1.06637617		
-1.03145870	H	-5.16983249	0.84744387	1.99930912	H	3.23186083	
-0.29737675	H	5.30212270	0.57609445	1.05605928	-2.00329615	H	
0.12677187	H	-5.21352095	-0.00065219	3.48454816	1.37805891		

1.26410004	H	5.07731424	2.27357532	3.71939270	H	3.48595353	
0.54629188	H	-5.35820425	1.75624227	1.36104316	-3.72470980	C	
1.20987635	H	3.85875134		-0.36503141	2.40392491		
-3.46663695	-1.30882593	H	2.17783878	-3.58554873	C	-0.36749907	
-2.96841954	-1.51945601	H	3.48318122	2.42178250	3.57323322	H	
-2.07629523	-2.33350336	H	-3.77012177	0.45874842	2.37766931		
-3.44771976	-1.31210134	H	-3.36469251	-4.31484363	H	0.45536892	
-2.04422885	-2.30322084	H	-2.08725061	2.39967688	4.30370278	H	
-2.93490136	-1.44594812	C	0.04147801	-0.00773217	2.92183439		
-0.51515629	1.85361313	Mn	-0.01116993	-2.68446259	H	-0.00901188	
-0.28789939	0.09048472	C	-0.02956052	2.93451419	2.66966475	H	
-2.01532087	-0.17418659	O	-0.01039888	-1.15620793	3.02797813		
-3.17703391	-0.34465499	H	-1.37826480	-4.02687762	H	-1.15920930	
2.94339365	0.56989233	H	0.03001654	3.04837930	4.00996645	C	
1.54767641	-1.10450758	C	-0.27298611	-1.39113097	0.31834073		
3.03143265	0.48752823	O	0.26535449	-4.54990305	C	-1.39265791	
1.85632832	-0.07279409	C	0.03922756	0.34065861	4.54849586	H	
4.21009305	-0.41443953	H	-0.36329335	-1.90529392	-0.63024145		
5.14894178	-0.00829930	H	1.12795305	-4.34294707	H	-1.90962541	
4.32805663	-0.52799321	H	-0.38747528	-0.60736775	4.34597545	H	
4.06807377	-1.41807029	C	0.28755161	-0.56425486	0.10310371		
3.20866401	1.88307224	H	1.36830231	-5.24548261	H	-0.56517634	
3.41521084	1.84853700	H		0.12584177	5.24347431	H	
-0.19647724	4.04471003			-2.10251837	0.95867947		
2.40788473	H	0.14511309	2.29934274	-5.09326448	H	-2.10142260	
2.48459050				0.98489586	5.09067203	H	
				3.49981729	-1.17883108		
				-3.93969628	H	3.01556152	
				-1.46932277	-2.26870930	H	
				2.05205018	-2.13576954		
				-3.61018379	H	3.49541010	
				-1.16095885	3.94970813	H	
				2.04843515	-2.11865781		
				3.61909343	H	3.01602768	
				-1.45702001	2.27821608	C	
				0.56378538	1.98979054		
				-0.00476705	Mn	0.37627359	
				0.21613456	-0.00038959	C	
				2.08833813	-0.10484365		
				0.00096162	O	3.22452891	
				-0.39944631	0.00196421	H	
				-1.80596005	0.25187866		
				-0.00156830	H	-1.34942777	
				-1.74482035	0.00359799	C	
				-2.86837843	-0.31718477		
				-0.00060171	O	-2.67813812	
				-1.63714438	0.00231036	C	
				-3.60383519	0.18180827		
				1.24519352	H	-3.62647307	
				1.27963550	1.33395566	H	
				-4.64411315	-0.17411684		
				1.20108131	H	-3.17074446	
				-0.24460377	2.15947412	C	
				-3.60327791	0.17639590		
				-1.24888110	H	-4.64379233	
				-0.17865998	-1.20331845	H	
				-3.62525773	1.27380671		

							-1.34279993	H	-3.17024516
							-0.25459138	-2.16104334	
H-Mn-5'-OiPr$_O$							**H-Mn-5'-OiPr$_H$**		
P	-2.29478671		-0.13876840				P	2.27718804	-0.16261253
-0.15030803	P	2.25287020	-0.19226785				0.04221880	P	-2.27515708
-0.21578569	C	-2.45982885	-0.12357715				-0.16878806	0.04055583	C
-1.99723027	C	2.35662567	-0.17366306				2.41172246		0.49897014
-2.06585164	H	-2.39289324	0.93911886				1.76192852	C	-2.41282856
-2.28856796	H	2.28979724	0.89093050				0.49269397	1.76014346	H
-2.34783697	H	-3.43382805	-0.49079917				2.30753375		1.59601275
-2.35479195	H	3.31282762	-0.55362915				1.68720435	H	-2.31178644
-2.45630128	C	-1.30262240	-0.87993426				1.59002259	1.68553265	H
-2.62415469	C	1.16806545	-0.91195552				3.37548267		0.28708468
-2.65477511	H	-1.31709264	-0.76723039				2.24935996	H	-3.37639907
-3.72612775	H	1.15344369	-0.80701022				0.27821199	2.24680604	C
-3.75751337	H	-1.37574358	-1.96296392				1.22562371		-0.01194357
-2.42273873	H	1.22301321	-1.99506493				2.56079127	C	-1.22596170
-2.44676878	N	-0.05397720	-0.38221205				-0.01496241	2.55994615	H
-2.05948480	C	3.20144933	1.33297568				1.20661510		0.46488045
0.25315567	C	-3.27782368	1.36502364				3.55913815	H	-1.20892774
0.34330802	H	2.48154527	2.10873804				0.46207300	3.55823002	H
-0.05710846	H	-2.61601601	2.18844555				1.28073146		-1.10162026
0.02581198	C	3.34923665	-1.59706997				2.73131490	H	-1.27834367
0.34142305	C	-3.37219437	-1.54981968				-1.10473201	2.73063419	N
0.43966665	C	3.28410150	-2.81056587				-0.00033871		0.31212283
-0.57483049	C	-3.34861146	-2.75814064				1.82321966	C	-3.31072148
-0.48511272	O	0.02946344	0.14713255				0.98155104	-1.00054682	C
3.02646614	H	-4.40185515	-1.14520211				3.30934979		0.99156674
0.44675646		H	4.38037415				-0.99786908	H	-2.64239256
-1.19608180	0.31037526	C	-3.00161708				1.84126902	-1.14983126	H
-1.95391525	1.86255204	C	3.02150767				2.63845286		1.84947402
-1.99083748	1.77782716	H	-2.94307839				-1.14608816	C	-3.30338597
-1.10441315	2.55519878	H	2.99702312				-1.73452164	0.01514495	C
-1.13730538	2.46771841	H	-2.02763169				3.31000132		-1.72524946
-2.46085318	1.89138835	H	2.04072743				0.01668584	C	-3.26713364
-2.48254486	1.83866359	H	-3.74565038				-2.51824502	1.31893758	C
-2.65760851	2.26548988	H	3.76759190				3.27502819		-2.50957323
-2.70366315	2.16030341	C	3.41345261				1.32014939	O	0.00249992
1.44070661	1.75526449	C	-3.45593228				-0.63337822	-3.11651669	H
1.45441325	1.85208048	H	4.18755549				4.34414076		-1.35849846
0.74191629	2.10942571		H				-0.12889432	H	-4.33847349
-4.20580474			0.73402061				-1.37077306	-0.13127101	C
2.21449249	H	2.49646584	1.24621440				2.94811650		-2.62623324
2.32984758	H	-2.52257005	1.27134987				-1.15991666	C	-2.93820619
2.40408630	H	3.75739273	2.45204736				-2.63500184	-1.16081650	H
2.02064822	H	-3.81500412	2.45457073				2.85033348		-2.09002587
2.13742232	C	4.50380236	1.52655214				-2.11189747	H	-2.84125915
-0.50661107	C	-4.60793183	1.51315920				-2.09897468	-2.11298101	H
-0.38017588	H	4.36504444	1.56564213				1.99896825		-3.14851483
-1.59575160	H	-4.49933767	1.57019668				-0.98449202	H	-1.98774930
-1.47189125	H	5.23472383	0.73039103				-3.15459100	-0.98452209	H
-0.29196800	H	-5.29961890	0.68562618				3.71970457		-3.39903989
-0.15700646	H	4.97951816	2.47475915				-1.29570568	H	-3.70756020
-0.21195600	H	-5.11382341	2.43730286				-3.41000839	-1.29675937	C
-0.06136282	H	3.95324386	-3.60116907				-3.61627599		0.40926132
-0.20294941	H	2.27300446	-3.24217314				-2.37661090	C	3.61633936
-0.60439180	H	3.59439442	-2.58969381				0.42154260	-2.37455078	H

-1.60575358	H	-4.00911223	-3.54566418
-0.09182159	H	-3.69729340	-2.53027587
-1.50216682	H	-2.34330191	-3.19771876
-0.55510165	C	0.00928866	0.02932599
1.86347237	Mn	-0.02287807	-0.22766903
0.11066629	C	-0.03814152	-1.97111261
0.31342396	O	-0.03453134	-3.14324374
0.41048273	H	-1.22168376	3.27398532
-0.54422323	H	-0.03629899	0.65598929
-2.07908660	C	-0.16406908	2.99816480
-0.27769680	O	0.12830713	1.70765032
-0.66817816	C	0.70782186	3.98259555
-1.05312705	H	0.41908701	5.02856436
-0.86689140	H	1.77011711	3.87908227
-0.77794771	H	0.62797665	3.79644782
-2.13412452	C	-0.03552618	3.21721088
1.22169058	H	0.98002104	2.96575069
1.56751242	H	-0.24141283	4.26007248
1.50887642	H	-0.73357603	2.57371124
1.77563986			

-4.33491182			-0.42296394
-2.33038105		H	4.33723742
-0.40878223	-2.32915708		H
-2.71551561			0.05514726
-2.89745062		H	2.71653131
0.06546578	-2.89568942		H
-4.07317080			1.18474355
-3.00909187		H	4.07107518
1.19886868	-3.00631845		C
-4.57121644			1.46174023
-0.29872905		C	4.56855291
1.47479215	-0.29581250		H
-4.35854644			2.00261954
0.63362676		H	4.35442985
2.01404357	0.63715198		H
-5.25254479			0.63137456
-0.05324371		H	5.25244256
0.64622583	-0.05137565		H
-5.13304255			2.14946498
-0.94889772		H	5.12815315
2.16489431	-0.94538442		H
-3.93547267			-3.38959989
1.24785182		H	-2.26255887
-2.90996656	1.53222411		H
-3.60001011			-1.93122001
2.18584866		H	3.94581779
-3.37905715	1.24926352		H
3.60564790			-1.92189611
2.18748265		H	2.27137281
-2.90411821	1.53260048		C
0.00207793			-0.47089070
-1.95985877		Mn	0.00126943
-0.26167986	-0.18976904		C
0.00367910			-1.97118235
0.15745396		O	0.00589334
-3.10356488	0.46696575		H
-0.00040702			1.85513075
-0.23636824		H	-0.00144809
1.40517908	1.77452064		C
-0.00245635			2.96774968
0.29068050		O	-0.00108838
2.85437621	1.60473024		C
1.24319092			3.66659472
-0.26383128		H	1.33410308
3.61001699	-1.36036087		H
1.19339650			4.72981442
0.01575985		H	2.15655927
3.26973792	0.19822461		C
-1.25225258			3.66084168
-0.26166903		H	-1.20766917
4.72388339	0.01946425		H
-1.34385233			3.60534491
-1.35820367		H	-2.16317072
3.25859824	0.20055979		

TSB-iPrOH-H$^-$			
P	0.03811411		0.20224584
2.26717572	P	0.04095698	0.20301890

2H-Mn-5_1A			
P	-2.30774658		-0.27573254
-0.13794045		P	2.09212190

-2.26443094	C	1.76993319	-0.43643528	-0.28098669	-0.09639988	C	2.42084993
C	1.76722167	-0.44964019	-2.41281353	H	1.71115454	-1.53657899	-1.80326658
C	2.34141659	2.35155149	H	1.69984379	0.42532125	-1.80270062	H
-1.54857320	-2.32995679	H	2.25150772	-2.44967808	1.63030338	-0.19608513	3.38108258
H	2.25092571	-1.64232394	H	2.37076367	-0.22178908	-3.37505531	C
2.57247789	1.52347503	-1.70510733	H	0.06559719	1.23302085	C	2.57294724
-3.45251086	0.32634555	0.05670224	-1.22888354	H	3.58716506	-2.29171032	H
3.29147546	-0.37624658	1.23785911	H	3.58562601	0.12029466	-2.26618130	C
-0.38970364	-1.23195200	H	2.70337603	-1.31511442	0.12023134	1.16089978	1.26431875
H	2.70831153	-2.66861333	C	1.14990847	1.15127800	-1.26561554	N
1.86005414	0.04204712	-2.66016737	H	-0.29355515	0.00335363	C	-0.98241729
-1.30943855	0.67597065	-0.92353326	-3.34542119	C	-0.97612797	-3.62690074	H
1.17311622	-0.92878321	3.35289887	H	-1.14461037	0.57837860	-3.62908646	H
-1.79542163	-2.69867213	H	-1.12751954	-1.37194844	-0.95286298	-1.80743110	2.71269053
C	0.02479502	-2.92052660	H	1.15285383	1.77917211	-3.28354731	C
0.00841296	-1.03792043	-2.88874707	N	1.78106315	3.28235690	C	1.32983099
-0.07776417	0.34311769	2.56088294	-3.25076448	C	1.30860525	-1.92044423	C
2.81110456	2.57095849	3.25300742	O	1.09301219	0.94807309	C	-3.12198085
0.62918641	-0.00101938	H	-3.09702361	1.00210677	-0.14542176	1.42972891	0.97914118
H	2.23649751	4.32044268	H	-0.12683586	1.42566693	1.93999690	0.53370170
H	-4.32129221	C	-1.16817520	2.67404211	-2.60130496	1.91767655	2.89993619
C	-1.14740011	2.68100829	0.60930565	C	3.33631509	-2.90842844	H
-2.11492091	2.13085706	-1.67005398	0.01359690	C	2.78842447	H	-2.09818573
2.14456151	-3.54816058	-1.67213549	-2.79917299	H	-0.98211338	3.19352100	-0.20296702
C	3.31716428	1.95142749	H	-0.96149794	3.20178190	-2.56011814	-1.22057536
C	-1.96062609	H	-1.32125875	3.44868474	-3.42333692	-2.49123704	3.66667257
H	-1.29227765	3.45452659	-1.47899052	O	-0.13253668	-3.67788795	C
-2.35453069	-0.34335902	-1.55422299	2.82008275	H	-3.65506065	C	-2.35490809
-0.35981990	-4.55059625	-1.20758539	3.65378404	H	-2.30036251	0.50649476	-0.19392281
H	4.33363581	-4.35218739	H	-2.31123213	0.49501694	-1.19843385	0.08352393
C	4.34552271	H	-2.88519030	-0.01133539	-3.39493495	-2.55284064	-2.75154885
H	-2.88512625	-0.03836295	1.02876162	C	3.08044039	2.74616963	H
-2.98211638	-1.10692422	-2.49008475	1.27080648	H	-4.13848621	H	-2.97724600
-1.12600547	-3.50765522	-1.99433889	4.13982734	C	-0.26673062	-1.37838715	1.96897570
H	3.06326500	-4.60745136	C	-0.26005764	-1.36723298	-1.88277841	2.18664593
H	4.62054967	H	0.65898766	-2.40203768	-3.02763750	-1.93121560	-4.39529318
H	0.67172836	1.05180140	H	2.10896784	-1.91257584	4.41568433	H
-0.00435386	-3.00392534	1.21044917	H	-0.53447987	-5.26546560	H	-0.00824761
-4.14620422	-3.35704363	-0.51617338	5.27342292	H	-0.91331350	1.03220451	H
3.85475263	-2.04706353	-5.19625572	H	-0.90193752	-3.26146764	1.39931834	C
-2.03804248	5.21204362	H	1.25532867	2.45349819	0.99093072	3.43734088	-3.91233956
H	1.55143607	2.42105657	C	-2.70260019	2.94584222	-2.24551081	H
2.19359862	0.84725609	2.43901187	H	1.97585065	-3.59577466	H	1.22525390
2.97062550	0.15902648	3.44911833	3.91125743	H	2.17441408	2.92225258	H
-3.10167610	1.99285128	3.60444041	H	1.53289060	-0.07342524	2.88991481	H
2.95401532	2.24769351	C	-1.96196205	1.37372886	0.84532247	0.48525305	-0.00027789
Mn	-0.19820397	2.56415637	H	-1.61111692			

0.27161548	0.00090224	C	0.18597898
1.98708769	0.00138687	O	0.50734226
3.11763077	-0.00009797	H	-0.33951745
-1.57926335	-0.01106000	H	1.79893988
-1.33824567	0.00459144	C	0.28103108
-3.06287291	-0.01698666	O	1.53818271
-2.93821057	-0.03519157	C	-0.35369998
-3.60043799	1.25245670	H	-1.43188800
-3.40209899	1.32658662	H	-0.21545975
-4.69399365	1.24912138	H	0.16268607
-3.22381780	2.14297646	C	-0.38890635
-3.60989530	-1.26414949	H	-0.26237867
-4.70476804	-1.24948046	H	-1.46641728
-3.40120727	-1.31643735	H	0.11131374
-3.25060882	-2.17089129		

0.82215920	2.55917468		H
2.74724704			1.90989971
2.95382910		H	-3.09223809
1.68880484	3.03305210		C
4.29055949			1.36159127
0.73015862		C	-4.59803747
1.16511554	0.80448369		H
4.56168452			1.42260529
-0.33490176		H	-4.89977180
1.25046801	-0.25048147		H
4.91916102			0.58238825
1.18769326		H	-5.15384202
0.32132295	1.24109810		H
4.58898723			2.31415950
1.19656563		H	-4.95332573
2.07176148	1.31819156		H
4.05067780			-3.37326685
-1.11070876		H	2.33624762
-3.03353533	-1.36698369		H
3.57619244			-2.02280690
-2.14364887		H	-4.15953145
-3.30943264	-1.47576414		H
-3.61250468			-1.89997554
-2.38648714		H	-2.43194906
-2.95525255	-1.57478320		C
-0.12422920			-1.20509151
1.70225483		Mn	-0.10935421
-0.64446983	0.03001360		C
-0.09223800			-2.29945760
-0.63081583		O	-0.08093217
-3.41276707	-1.00900209		H
-0.13578954			0.90217752
0.58895141		H	-0.04324195
1.33384655	-1.65825935		C
0.65022276			3.84629004
-0.24227630		O	0.53463126
3.22837169	-1.28596552		C
-0.45279190			3.89743819
0.76992598		H	-0.37589845
2.97543732	1.37372457		H
-0.38705692			4.76029852
1.44477891		H	-1.43207082
3.87030113	0.27680089		C
1.92084539			4.56629896
0.10765297		H	1.74933206
5.65310812	0.06549945		H
2.22646507			4.34780077
1.14187940		H	2.72921984
4.30932025	-0.58688930		

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