Supporting Information

Rhodium-Catalyzed Regioselective Silylation of Alkyl C-H Bonds for the Synthesis of 1,4-Diols

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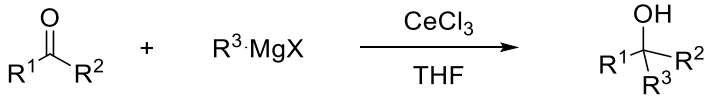
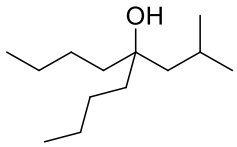
Materials and Methods

All silylation reactions were assembled in an N_2-filled glovebox using oven-dried glassware and were stirred with Teflon-coated magnetic stirring bars. $[Ir(cod)OMe]_2$ was obtained as a gift from Johnson Matthey and was used as received. 3,4,7,8-Tetramethyl-1,10-phenanthroline (Me_4phen) was purchased from Aldrich and was used as received. Diethylsilane (Et_2SiH_2) was purchased from Alfa Aesar and was used as received. Ethyl, *n*-propyl, *n*-butyl and cyclohexyl magnesium chloride were purchased from Acros and were used as received. Other Grignard reagents were prepared from the corresponding alkyl bromides with magnesium turnings. Norbornene (nbe), Xantphos, *tert*-butyl hydroperoxide (5-6 M in decane, stored over molecular sieves), tetra-*n*-butylammonium fluoride (TBAF) and anhydrous dimethylformamide (DMF) were purchased from Aldrich and were used as received. RhCl(Xantphos) was synthesized by literature procedures.[1] Diethyl ether and tetrahydrofuran (THF) were degassed by purging with nitrogen and then dried with a solvent purification system containing activated alumina. All other solvents and reagents were used as received. Reaction temperatures above 23 °C refer to temperatures of an aluminum heating block, which were either controlled by an electronic temperature modulator or controlled manually and monitored using a standard alcohol thermometer. NMR spectra were recorded on Bruker AVQ-400, AVB-400, AV-500, DRX-500 and AV-600 instruments. Chemical shifts (δ) are reported in ppm relative to the residual solvent signal. Data for ^{1}H NMR spectra are reported as follows: chemical shift (multiplicity, coupling constants, number of hydrogens). Abbreviations are as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad). GC-MS data were obtained on an Agilent 6890-N GC system containing an Alltech EC-1 capillary column and an Agilent 5973 mass selective detector. High-resolution mass spectral data were obtained from the University of California, Berkeley Mass Spectrometry Laboratory. Elemental analysis was conducted at the Micro Analytical Facility in the College of Chemistry. IR spectra were recorded with a Bruker Vertex 80 FTIR spectrometer, the spectra were reported in cm^{-1}.

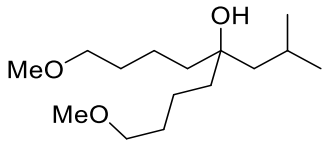
General procedure for the synthesis of substrates



A suspension of $CeCl_3$ (6.0 mmol) in 15 mL of anhydrous THF was stirred at room temperature for 3 h. The suspension was cooled to 0 °C, and a Grignard reagent (5.0 mmol) was added. The resulting mixture was stirred at 0 °C for 1 h before a solution of ketone (5.0 mmol) in 3.0 mL of THF was added. After 30 min at 0 °C, the reaction was quenched by adding 1 mL of water. The mixture was filtered through Celite, dried over Na_2SO_4 and concentrated. The crude product was further purified by column chromatography on silica gel with EtOAc/hexanes mixture as eluent.

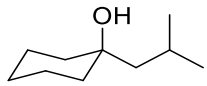


Alcohol 1a: Following the general procedure, 5-nonanone (5.0 mmol) was allowed to react with *iso*-butyl magnesium bromide. The crude product was purified by column chromatography on silica gel to give 792 mg (79% yield) of alcohol **1a** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.76 (hept, J = 6.6 Hz, 1H), 1.42 (t, J = 3.9 Hz, 4H), 1.37 – 1.18 (m, 11H), 0.95 (d, J = 6.6 Hz, 6H), 0.90 (t, J = 7.0 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 75.22, 48.11, 39.54, 25.99, 24.97, 23.91, 23.47, 14.28. EI-HR calcd for $C_{12}H_{24}O$ (M^+) 200.2140, found 200.2136.

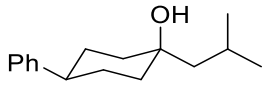


Alcohol 1b: To a cooled solution of ethyl isovalerate (5.0 mmol) in 10 mL of THF at 0 °C was added dropwise 4-methoxybutyl magnesium bromide (12.0 mmol). The resulting mixture was stirred at 0 °C for 1 h. Water (2 mL) was added, and the mixture was filtered through Celite. The filtrate was dried and concentrated. The crude product

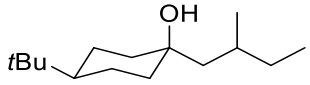
was purified by column chromatography on silica gel to give 936 mg (72% yield) of alcohol **1b** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.36 (t, *J* = 6.5 Hz, 4H), 3.31 (s, 6H), 1.74 (hept, *J* = 6.6 Hz, 1H), 1.58 – 1.47 (m, 5H), 1.47 – 1.40 (m, 4H), 1.37 – 1.28 (m, 6H), 0.93 (d, *J* = 6.6 Hz, 7H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 75.07, 72.83, 58.66, 47.94, 39.52, 30.23, 24.91, 23.89, 20.40. EI-HR calcd for $C_{15}H_{32}O_3$ (M^+) 260.2351, found 260.2348.



Alcohol 1c: Following the general procedure, cyclohexanone (5.0 mmol) was allowed to react with *iso*-butyl magnesium bromide. The crude product was purified by column chromatography on silica gel to give 604 mg (78% yield) of alcohol **1c** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.82 (hept, *J* = 6.4 Hz, 1H), 1.63 – 1.19 (m, 13H), 0.95 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 72.25, 51.15, 38.11, 25.96, 25.14, 23.53, 22.42. EI-HR calcd for $C_{10}H_{20}O$ (M^+) 156.1514, found 156.1510.

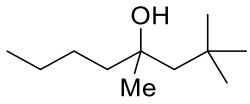


Alcohol 1d: Following the general procedure, 4-phenyl cyclohexanone (5.0 mmol) was allowed to react with *iso*-butyl magnesium bromide. The crude product was purified by column chromatography on silica gel to give 928 mg (80% yield) of alcohol **1d** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.21 (m, 5H), 2.58 – 2.41 (m, 1H), 1.99 – 1.69 (m, 7H), 1.53 (td, *J* = 13.3, 3.6 Hz, 2H), 1.45 (d, *J* = 5.8 Hz, 2H), 1.33 (s, 1H), 1.03 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.42, 128.45, 126.98, 126.06, 71.27, 53.30, 44.18, 37.85, 29.41, 25.21, 23.69. EI-HR calcd for $C_{16}H_{24}O$ (M^+) 232.1827, found 232.1823.

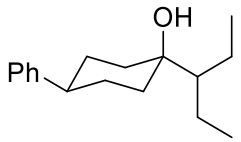


Alcohol 1e: Following the general procedure, 4-tert-butyl cyclohexanone (5.0 mmol)

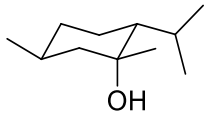
was allowed to react with 2-methylbutyl magnesium bromide. The crude product was purified by column chromatography on silica gel to give 847 mg (75% yield) of alcohol **1e** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.74 – 1.62 (m, 2H), 1.62 – 1.50 (m, 3H), 1.47 – 1.11 (m, 10H), 0.94 (d, *J* = 6.6 Hz, 3H), 0.89 – 0.82 (m, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 71.51, 51.04, 48.04, 38.33, 37.82, 32.53, 31.68, 29.97, 27.71, 22.61, 22.58, 21.99, 11.62. EI-HR calcd for $C_{15}H_{30}O$ (M^+) 226.2297, found 226.2293.



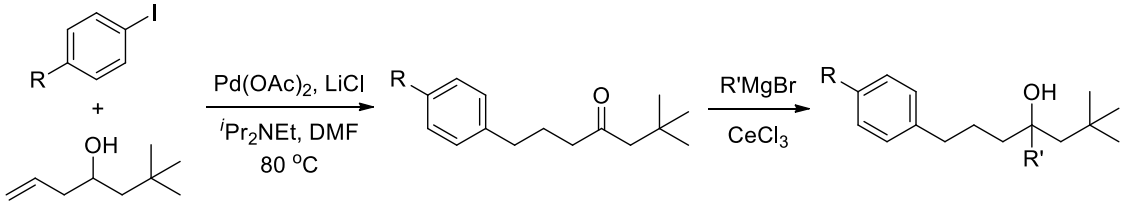
Alcohol 1f: Following the general procedure, 2-hexanone (5.0 mmol) was allowed to react with 2,2-dimethylpropyl magnesium bromide. The crude product was purified by column chromatography on silica gel to give 645 mg (74% yield) of alcohol **1f** as a colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.50 – 1.42 (m, 4H), 1.34 – 1.26 (m, 5H), 1.23 (s, 3H), 1.02 (s, 9H), 0.91 (t, *J* = 6.5 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 74.46, 53.84, 44.84, 31.75, 31.50, 28.47, 26.46, 23.44, 14.25. EI-HR calcd for $C_{11}H_{24}O$ (M^+) 172.1827, found 172.1823.



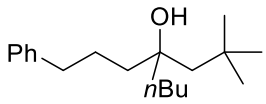
Alcohol 1h: Following the general procedure, 4-phenyl cyclohexanone (5.0 mmol) was allowed to react with 3-pentyl magnesium bromide. The crude product was purified by column chromatography on silica gel to give 1.01 g (82% yield) of alcohol **1h** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (t, *J* = 7.4 Hz, 2H), 7.29 (d, *J* = 7.3 Hz, 2H), 7.23 (t, *J* = 7.1 Hz, 1H), 2.50 (tt, *J* = 14.5, 5.0 Hz, 1H), 1.91 (ddd, *J* = 16.1, 13.2, 3.4 Hz, 2H), 1.84 – 1.71 (m, 5H), 1.70 – 1.54 (m, 4H), 1.28 (tt, *J* = 14.5, 7.3 Hz, 2H), 1.12 – 1.07 (m, 1H), 1.04 (t, *J* = 7.4 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.42, 128.38, 126.92, 125.99, 73.92, 53.53, 44.18, 34.58, 29.39, 22.36, 14.13. EI-HR calcd for $C_{17}H_{26}O$ (M^+) 246.1984, found 246.1981.



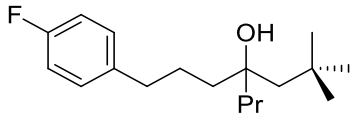
Alcohol 1t: Following the general procedure, (-)-methone (5.0 mmol) was allowed to react with methyl magnesium bromide. The crude product was purified by column chromatography on silica gel to give 697 mg (82% yield) of alcohol **1t** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.18 – 2.08 (m, 1H), 1.80 – 1.72 (m, 1H), 1.70 – 1.61 (m, 1H), 1.57 (d, *J* = 13.5 Hz, 1H), 1.50 (dd, *J* = 13.3, 3.2 Hz, 1H), 1.41 – 1.24 (m, 3H), 1.22 (s, 3H), 1.08 – 0.95 (m, 2H), 0.92 – 0.82 (m, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 73.26, 50.85, 50.61, 35.35, 29.01, 28.35, 26.24, 23.96, 22.46, 21.04, 18.38. EI-HR calcd for $C_{11}H_{22}O$ (M^+) 170.1671, found 170.1667.



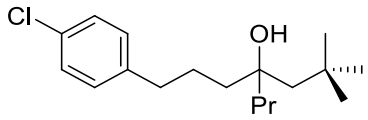
The literature procedure[2] was used with slight modifications. Into a 20 mL screw-capped vial was placed $Pd(OAc)_2$ (0.15 mmol, 0.030 equiv), LiCl (15 mmol. 3.0 equiv) and dried DMF (5.0 mL). The solution was magnetically stirred to afford a yellow suspension. Diisopropylethylamine (7.5 mmol. 1.5 equiv), the homoallylic alcohol (6.0 mmol, 1.2 equiv) and the aryl iodide (5.0 mmol, 1.0 equiv) were added successively. The vial was capped with a Teflon-lined screw cap and placed in a preheated aluminum block at 80 °C. After 18 h, the reaction mixture was poured into 50 mL of H_2O and extracted with ether (20 mL x 3). The combined ether extracts were washed successively with aq. HCl (30 mL, 1N), H_2O (30 mL), saturated brine (30 mL) and H_2O (30 mL). The solution was dried over $MgSO_4$, filtered and evaporated to give the crude ketone product. The crude product was used without further purification. Reaction of the ketone product with a Grignard reagent according to the general procedure for the Grignard reaction provided the tertiary alcohol.



Alcohol **1g**: Following the general procedure, iodobenzene (716 mg, 3.00 mmol) was coupled with 6,6-dimethyl-1-hepten-4-ol. The Grignard reaction of the resulting ketone with *n*-butylmagnesium bromide provided 530 mg (64%) of alcohol **1g** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.18 (m, 5H), 2.63 (t, *J* = 7.2 Hz, 2H), 1.72 – 1.48 (m, 6H), 1.47 (s, 2H), 1.37 – 1.19 (m, 5H), 1.05 (s, 9H), 0.93 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.62, 128.54, 128.42, 125.87, 76.27, 51.30, 40.46, 40.36, 36.55, 31.83, 31.57, 26.12, 26.07, 23.39, 14.28. EI-HR calcd for $C_{19}H_{32}O$ (M^+) 276.2453, found 276.2448.

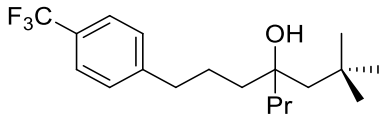


Alcohol **1j**: Following the general procedure, 4-fluoroiodobenzene (1.11 g, 5.00 mmol) was coupled with 6,6-dimethyl-1-hepten-4-ol. The Grignard reaction of the resulting ketone with *n*-propylmagnesium bromide provided 882 mg (63%) of alcohol **1j** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (t, *J* = 8.6 Hz, 2H), 6.96 (t, *J* = 8.6 Hz, 2H), 2.56 (t, *J* = 7.3 Hz, 2H), 1.67 – 1.40 (m, 8H), 1.35 – 1.19 (m, 3H), 1.01 (s, 9H), 0.89 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.31 (d, *J* = 244.4 Hz), 138.16 (d, *J* = 2.5 Hz), 129.81 (d, *J* = 7.5 Hz), 115.09 (d, *J* = 21.4 Hz), 76.22, 51.30, 43.04, 40.25, 35.69, 31.80, 31.54, 26.10, 17.19, 14.71. EI-HR calcd for $C_{18}H_{29}FO$ (M^+) 280.2202, found 280.2198.

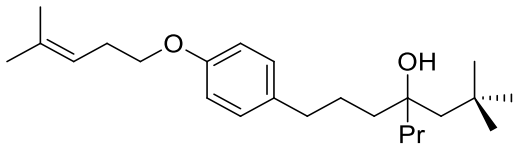


Alcohol **1k**: Following the general procedure, 4-chloroiodobenzene (1.19 g, 5.00 mmol) was coupled with 6,6-dimethyl-1-hepten-4-ol. The Grignard reaction of the resulting ketone with *n*-propylmagnesium bromide provided 1.07 g (72%) of alcohol **1k** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 (d, *J* = 7.3 Hz, 2H), 7.13 (d, *J* = 7.3 Hz, 2H), 2.59 (t, *J* = 6.9 Hz, 2H), 1.68 – 1.43 (m, 8H), 1.35 – 1.21 (m, 3H) (s, 3H), 1.04

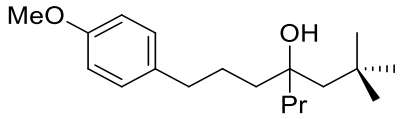
(d, *J* = 1.2 Hz, 9H), 0.92 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.00, 131.53, 129.87, 128.48, 76.21, 51.30, 43.02, 40.29, 35.86, 31.81, 31.55, 25.86, 17.22, 14.72. EI-HR calcd for $C_{18}H_{29}ClO$ (M^+) 296.1907, found 296.1903.



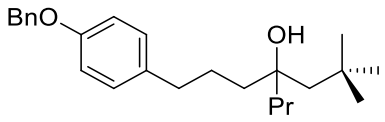
Alcohol **1l**: Following the general procedure, 4-trifluoromethyliodobenzene (1.36 g, 5.00 mmol) was coupled with 6,6-dimethyl-1-hepten-4-ol. The Grignard reaction of the resulting ketone with *n*-propylmagnesium bromide provided 957 mg (58%) of alcohol **1l** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.5 Hz, 2H), 7.29 (td *J* = 7.5 Hz, 2H), 2.65 (t, *J* = 7.3 Hz, 2H), 1.70 – 1.39 (m, 8H), 1.26 (s, 3H), 1.01 (s, 9H), 0.89 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.72, 128.83, 128.15 (q, *J* = 32.6 Hz), 125.24 (q, *J* = 3.6 Hz), 124.41(q, *J* = 272.4 Hz), 76.20, 51.30, 43.02, 40.31, 36.37, 31.79, 31.55, 25.71, 17.25, 14.70. EI-HR calcd for $C_{19}H_{29}F_3O$ (M^+) 330.2171, found 330.2168.



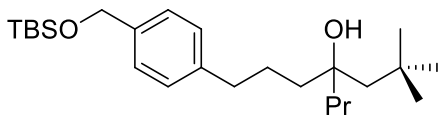
Alcohol **1m**: Following the general procedure, 1-iodo-4-((4-methylpent-3-en-1-yl)oxy)benzene (906 mg, 3.00 mmol) was coupled with 6,6-dimethyl-1-hepten-4-ol. The Grignard reaction of the resulting ketone with *n*-propylmagnesium bromide provided 561 mg (52%) of alcohol **1m** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.09 (d, *J* = 8.1 Hz, 2H), 6.82 (d, *J* = 8.2 Hz, 2H), 5.22 (s, 1H), 3.91 (t, *J* = 7.0 Hz, 2H), 2.63 – 2.40 (m, 4H), 1.73 (s, 3H), 1.65 (s, 3H), 1.61 – 1.34 (m, 8H), 1.35 – 1.21 (m, 2H), 1.20 – 1.09 (br, 1H), 1.02 (s, 9H), 0.89 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.22, 134.59, 134.45, 129.34, 119.77, 114.47, 76.27, 67.76, 51.29, 43.04, 40.39, 35.64, 31.81, 31.54, 28.43, 26.28, 25.90, 18.00, 17.18, 14.73. EI-HR calcd for $C_{24}H_{40}O2$ (M^+) 360.3028, found 360.3024.



Alcohol **1n**: Following the general procedure, 4-methoxyiodobenzene (1.17 g, 5.00 mmol) was coupled with 6,6-dimethyl-1-hepten-4-ol. The Grignard reaction of the resulting ketone with *n*-propylmagnesium bromide provided 978 mg (67%) of alcohol **1n** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.11 (d, J = 8.4 Hz, 2H), 6.83 (d, J = 8.5 Hz, 2H), 3.79 (s, 3H), 2.54 (t, J = 7.2 Hz, 2H), 1.69 – 1.37 (m, 8H), 1.34 – 1.20 (m, 3H), 1.02 (s, 9H), 0.90 (t, J = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.78, 134.70, 129.37, 113.79, 76.25, 55.35, 51.28, 43.03, 40.37, 35.62, 31.80, 31.53, 26.28, 17.17, 14.72. EI-HR calcd for $C_{19}H_{32}O_2$ (M^+) 292.2402, found 292.2398.

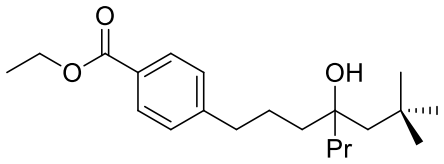


Alcohol **1o**: Following the general procedure, 4-benzyloxyiodobenzene (1.55 g, 5.00 mmol) was coupled with 6,6-dimethyl-1-hepten-4-ol. The Grignard reaction of the resulting ketone with *n*-propylmagnesium bromide provided 1.20 g (65%) of alcohol **1o** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, J = 7.3 Hz, 2H), 7.40 (t, J = 7.4 Hz, 2H), 7.34 (t, J = 7.1 Hz, 1H), 7.12 (d, J = 8.4 Hz, 2H), 6.92 (d, J = 8.5 Hz, 2H), 5.06 (s, 2H), 2.56 (t, J = 7.0 Hz, 2H), 1.69 – 1.38 (m, 8H), 1.34 – 1.20 (m, 3H), 1.04 (s, 9H), 0.91 (t, J = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.04, 137.32, 135.00, 129.40, 128.66, 127.99, 127.58, 114.78, 76.26, 70.13, 51.28, 43.04, 40.38, 35.65, 31.81, 31.54, 26.26, 17.17, 14.73. EI-HR calcd for $C_{25}H_{36}O_2$ (M^+) 368.2715, found 368.2711.

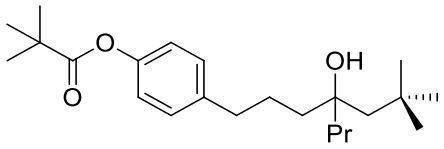


Alcohol **1p**: Following the general procedure, *tert*-butyl((4-iodobenzyl)oxy)dimethylsilane (1.39 g, 4.00 mmol) was coupled with 6,6-dimethyl-1-hepten-4-ol. The Grignard reaction of the resulting ketone with *n*-propylmagnesium bromide provided 1.10 g (68%) of alcohol **1p** as a colorless oil. ^{1}H NMR (500 MHz,

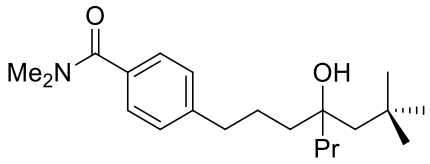
$CDCl_3$) δ 7.27 (d, *J* = 7.5 Hz, 2H), 7.18 (d, *J* = 7.6 Hz, 2H), 4.75 (s, 2H), 2.61 (t, *J* = 7.2 Hz, 2H), 1.77 – 1.40 (m, 8H), 1.38 – 1.22 (m, 3H), 1.03 (s, 9H), 0.98 (s, 9H), 0.92 (t, *J* = 7.2 Hz, 3H), 0.13 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.22, 138.93, 128.36, 126.25, 76.27, 65.00, 51.30, 43.05, 40.43, 36.24, 31.82, 31.55, 26.11, 18.56, 17.19, 14.74, -5.08. EI-HR calcd for $C_{25}H_{44}OSi$ ($[M-H_2O]^+$) 388.3161, found 388.3157.



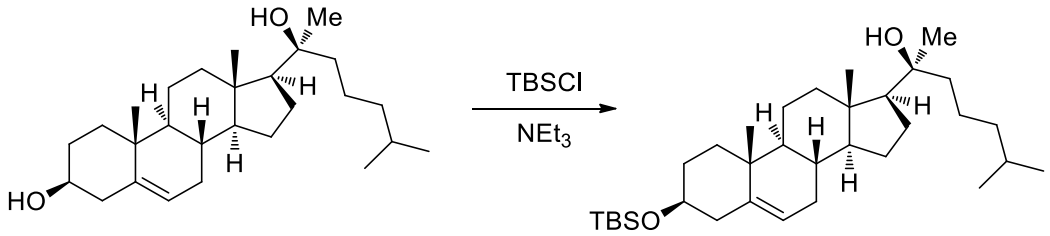
Alcohol **1q**: Following the general procedure, 4-ethyloxycarbonyliodobenzene (828 mg, 3.00 mmol) was coupled with 6,6-dimethyl-1-hepten-4-ol. The Grignard reaction of the resulting ketone with *n*-propylmagnesium bromide at 0 °C provided 521 mg (52%) of alcohol **1q** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 8.0 Hz, 2H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.67 (t, *J* = 7.5 Hz, 2H), 1.71 – 1.21 (m, 13H), 1.02 (s, 9H), 0.90 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.82, 148.02, 129.75, 128.52, 128.19, 76.17, 60.90, 51.28, 42.99, 40.31, 36.53, 31.79, 31.53, 25.59, 17.21, 14.70, 14.47. EI-HR calcd for $C_{21}H_{34}O_3$ (M^+) 334.2508, found 334.2504.



Alcohol **1r**: Following the general procedure, 4-pivolyliodobenzene (912 mg, 3.00 mmol) was coupled with 6,6-dimethyl-1-hepten-4-ol. The Grignard reaction of the resulting ketone with *n*-propylmagnesium bromide at 0 °C provided 586 mg (54%) of alcohol **1r** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17 (d, *J* = 7.6 Hz, 2H), 6.96 (d, *J* = 7.5 Hz, 2H), 2.58 (t, *J* = 7.0 Hz, 2H), 1.67 – 1.40 (m, 8H), 1.37 – 1.22 (m, 12H), 1.02 (s, 9H), 0.89 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.37, 149.20, 139.89, 129.31, 121.30, 76.23, 51.28, 43.00, 40.41, 39.14, 35.92, 31.80, 31.54, 27.27, 26.00, 17.21, 14.72. EI-HR calcd for $C_{23}H_{36}O_2$ ($[M-H_2O]^+$) 344.2715, found 344.2711.



Alcohol **1s**: Following the general procedure, 4-dimethylaminocarbonyliodobenzene (825 mg, 3.00 mmol) was coupled with 6,6-dimethyl-1-hepten-4-ol. The Grignard reaction of the resulting ketone with *n*-propylmagnesium bromide at 0 °C provided 539 mg (54%) of alcohol **1s** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.15 (d, *J* = 8.2 Hz, 2H), 7.00 (d, *J* = 8.3 Hz, 2H), 3.05 (s, 3H), 3.00 (s, 3H), 2.56 (t, *J* = 7.1 Hz, 2H), 1.66 – 1.34 (m, 9 H), 1.31 – 1.18 (m, 2H), 1.01 (s, 9H), 0.88 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.21, 149.59, 139.42, 129.16, 121.58, 76.20, 51.24, 42.96, 40.41, 36.77, 36.51, 35.89, 31.78, 31.51, 26.00, 17.18, 14.69. EI-HR calcd for $C_{21}H_{35}NO_2$ (M^+) 333.2668, found 333.2664.



Alcohol **1u'**: To a solution of diol (804 mg, 2.00 mmol) in 10 mL of anhydrous dichloromethane and triethylamine (404 mg, 4.00 mmol) was added dropwise a solution of TBSCl (360 mg, 2.40 mmol) in 5 mL of dichloromethane. The solution was stirred at room temperature for 2 hours. The reaction mixture was concentrated and purified by silica gel chromatography to afford 972 mg of mono-protected diol **1u'** (94% yield) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.31 (m, 1H), 3.56 – 3.45 (m, 1H), 2.34 – 2.23 (m, 1H), 2.19 (dd, *J* = 13.1, 2.7 Hz, 1H), 2.12 (t, *J* = 12.2 Hz, 1H), 1.99 (d, *J* = 14.6 Hz, 1H), 1.86 – 1.63 (m, 6H), 1.58 – 1.39 (m, 9H), 1.34 – 1.25 (m, 6H), 1.20 – 1.13 (m, 4H), 1.02 (s, 3H), 0.95 – 0.86 (m, 20H), 0.08 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.59, 121.10, 75.28, 72.63, 57.67, 56.93, 50.13, 44.20, 42.81, 42.67, 40.15, 39.64, 37.39, 36.61, 32.09, 31.84, 31.35, 27.96, 26.46, 25.97, 23.81, 22.77, 22.61, 22.39, 22.05, 20.93, 19.46, 18.30, 13.63, -4.56. EI-HR calcd for $C_{33}H_{60}O_2Si$ (M^+)

516.4363, found 516.4358.

General procedure for Ir-catalyzed silylation of alcohols:

In an N_2-filled glovebox, 0.50 mmol of the alcohol was weighed into a one-dram screw-capped vial. A stir bar was added, and the substrate was dissolved in Et_2O (1.0 mL). The resulting solution was treated first with $[Ir(cod)OMe]_2$ (0.50 μmol, 0.10 mol %, unless otherwise specified) and then neat Et_2SiH_2 (0.75 mmol). The vial was capped with a Teflon-lined screw cap, and the resulting solution was stirred in the glovebox at room temperature until complete conversion to the corresponding diethyl(hydrido)silyl ether was observed, as determined by GC (generally 1-2 h) (CAUTION: H_2 evolution!).

General procedure for Ru-catalyzed silylation of alcohols:

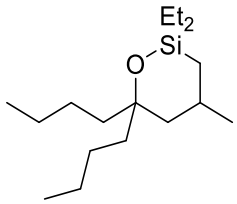
In an N_2-filled glovebox, 0.50 mmol of the alcohol was weighed into a one-dram screw-capped vial. A stir bar was added, and the substrate was dissolved in PhH (1.0 mL). The resulting solution was treated first with $RuCl_2(PPh_3)_3$ (2.5 μmol, 0.50 mol %, unless otherwise specified) and then neat Et_2SiH_2 (0.75 mmol). The vial was capped with a Teflon-lined screw cap, and the resulting solution was stirred at 50 °C until complete conversion to the corresponding diethyl(hydrido)silyl ether was observed, as determined by GC (generally 3-5 h) (CAUTION: H_2 evolution!).

General procedure for Rh-catalyzed intramolecular aliphatic silylation:

In an N_2-filled glovebox, the crude reaction mixture containing the diethyl(hydrido)silyl ether (ca. 0.50 mmol) and solvent was placed under high-vacuum for 0.5 h (the stir bar was temporarily removed during this operation to prevent bumping). The stir bar was replaced, and the concentrated diethyl(hydrido)silyl ether was then sequentially treated with norbornene (0.60 mmol, 1.2 equiv), RhCl(Xantphos) (0.020 mmol, 4.0 mol %) and THF (1.0 mL). The Teflon-lined screw cap was replaced, and the vial was then removed from the glovebox, placed in a pre-heated aluminum block at 100 °C for 16 h.

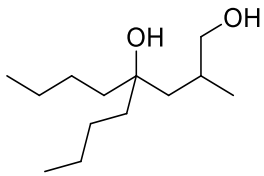
General procedure for Tamao-Fleming oxidation of oxasilolanes:

To an ice-cooled (0 °C) stirred solution of KH (120 mg, 3.0 mmol, 6.0 equiv) in 5.0 mL of NMP was added *tert*-butyl hydroperoxide (0.55 mL, 5.0 ~ 6.0 M in decane stored over molecular sieves) dropwise. The mixture was allowed to warm to RT and kept for 10 min. The crude reaction mixture containing the silolane (ca. 0.5 mmol) in 1.0 mL of THF was then added. After stirring at RT for 10 min, 2.5 mL of TBAF solution (2.5 mmol, 1.0 M solution in THF) was added. The resulting mixture was stirred for 14 h at RT. The reaction was carefully quenched with aq. Na_2SO_3 (saturated, 5 mL), and the resulting mixture was extracted with EtOAc (30 mL, then 2 x 15 mL). The combined organic layers were washed (30 mL of saturated Na_2SO_3, 30 mL of brine, 30 mL of 0.1 N HCl, then 30 mL of brine), dried over $MgSO_4$, filtered through Celite, and concentrated by rotary evaporation. The crude diol was further purified by column chromatography on silica gel with EtOAc/hexanes mixture as eluent.

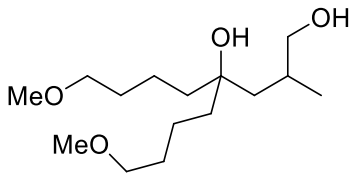


Oxasilolane 3a: In an N_2-filled glovebox, 5-*iso*butylnonan-5-ol (200 mg, 1.00 mmol) and Et_2SiH_2 (132 mg, 1.50 mmol) were weighed in a 20 mL screw-capped vial. A stir bar was added, followed by THF (1.0 mL). The resulting solution was treated with $[Ir(cod)OMe]_2$ (0.6 mg, 1.0 μmol, 0.1 mol %). The vial was capped with a Teflon-lined screw cap, and the resulting solution was stirred in the glovebox at room temperature for 15 h, at which point GC analysis indicated full conversion to diethyl(hydrido)silyl ether. The volatile materials were removed by placing the reaction mixture directly under high vacuum for 0.5 h (the stir bar was temporarily removed during this operation to prevent bumping). The stir bar was replaced, and the concentrated diethyl(hydrido)silyl ether was then sequentially treated with norbornene (113 mg, 1.20 mmol), RhCl(Xantphos) (29 mg, 0.040 mmol, 4.0 mol %) and THF (3.0 mL). The Teflon-lined screw cap was replaced, and the resulting solution was stirred in a pre-

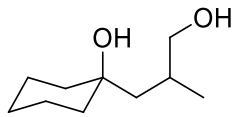
heated aluminum block at 100 °C for 16 h. The reaction mixture was then cooled to room temperature, and the solvent was removed by rotary evaporation. The resulting residue was purified by Kugelrohr distillation (25 mTorr, 75 °C) to give 267 mg (94%) of oxasilolane **3a** as colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.97 – 1.78 (m, 1H), 1.54 (dd, *J* = 18.5, 7.4 Hz, 1H), 1.46 – 1.37 (m, 4H), 1.36 – 1.21 (m, 8H), 1.16 (dd, *J* = 14.7, 8.7 Hz, 1H), 1.10 – 1.03 (m, 1H), 0.97 (d, *J* = 6.3 Hz, 3H), 0.96 – 0.88 (m, 12H), 0.66 (d, *J* = 14.3 Hz, 1H), 0.61 – 0.52 (m, 3H), 0.52 – 0.42 (m, 1H), 0.18 (t, *J* = 13.5 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 76.79, 45.65, 41.79, 38.90, 27.48, 26.37, 25.71, 24.11, 23.40, 23.34, 18.26, 14.17, 14.13, 8.03, 7.04, 6.84, 6.50. EI-HR calcd for $C_{17}H_{36}OSi$ (M^+) 284.2535, found 284.2531.



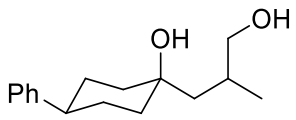
Diol 4a: Following the general procedure, 5-*iso*butylnonan-5-ol (200 mg, 1.00 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.10 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 166 mg (77% overall yield) of **4a** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.78 (s, 1H), 3.58 (dd, *J* = 10.5, 3.4 Hz, 1H), 3.34 – 3.21 (dd, *J* = 10.5, 3.4 Hz, 1H), 1.94 (d, *J* = 3.4 Hz, 1H), 1.63 – 1.38 (m, 6H), 1.32 (dd, *J* = 14.6, 7.0 Hz, 6H), 1.25 – 1.08 (m, 2H), 0.92 (t, *J* = 7.5 Hz, 6H), 0.89 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 74.43, 69.27, 46.08, 40.65, 37.70, 31.19, 26.43, 25.59, 23.32, 23.31, 19.71, 14.16, 14.14. ESI-HR calcd for $C_{13}H_{28}O_2Na$ ($[M+Na]^+$) 239.1982, found 239.1978.



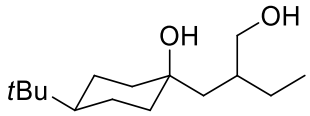
Diol 4b: Following the general procedure, 5-isobutyl-1,9-dimethoxynonan-5-ol (130 mg, 0.500 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.20 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 99 mg (72% overall yield) of **4b** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.59 (d, *J* = 10.4 Hz, 1H), 3.40 (dd, *J* = 8.2, 4.1 Hz, 4H), 3.34 (s, 6H), 3.29 (d, *J* = 8.6 Hz, 1H), 1.94 (br, 2H), 1.64 -1.54 (m, 5H), 1.52 - 1.44 (m, 3H), 1.42 – 1.36 (m, 1H), 1.34 – 1.18 (m, 2H), 0.89 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 74.26, 72.77, 72.61, 69.29, 58.57, 45.91, 45.89, 40.51, 37.94, 31.26, 30.07, 30.05, 20.78, 20.12, 19.69. ESI-HR calcd for $C_{15}H_{32}O_4Na$ ($[M+Na]^+$) 299.2193, found 299.2189.



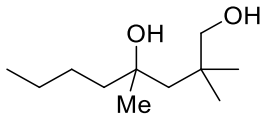
Diol 4c: Following the general procedure, 1-isobutyl-1-cyclohexanol (78 mg, 0.50 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.10 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 65 mg (75% overall yield) of **4c** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.80 (br, 2H), 3.58 (dd, *J* = 10.5, 3.5 Hz, 1H), 3.31 (t, *J* = 9.6 Hz, 1H), 1.94 (t, *J* = 24.7 Hz, 1H), 1.67 (s, 1H), 1.64 – 1.38 (m, 10H), 1.34 – 1.26 (m, 1H), 0.90 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 71.40, 69.22, 48.18, 40.05, 35.98, 30.85, 25.84, 22.58, 22.23, 19.73. ESI-HR calcd for $C_{10}H_{20}O_2Na$ ($[M+Na]^+$) 195.1356, found 195.1352.



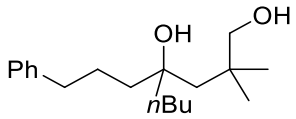
Diol 4d: Following the general procedure, 1-isobutyl-4-phenylcyclohexanol (116 mg, 0.500 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.25 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 94 mg (76% overall yield) of **4d** as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.24 (m, 4H), 7.21 (t, *J* = 6.7 Hz, 1H), 3.81 (s, 2H), 3.65 (dd, *J* = 10.2, 3.2 Hz, 1H), 3.38 (t, *J* = 9.6 Hz, 1H), 2.56 – 2.43 (m, 1H), 2.17 – 1.97 (m, 2H), 1.94 – 1.70 (m, 5H), 1.64 (dd, *J* = 14.6, 8.7 Hz, 1H), 1.59 – 1.48 (m, 2H), 1.42 (td, *J* = 13.4, 3.7 Hz, 1H), 0.94 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.35, 128.43, 126.97, 126.05, 70.24, 69.36, 50.99, 44.21, 39.84, 35.87, 31.06, 29.48, 29.26, 19.80. ESI-HR calcd for $C_{16}H_{24}O_2Na$ ($[M+Na]^+$) 271.1669, found 271.1667.



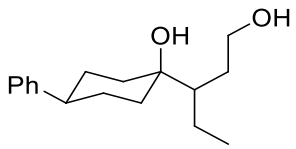
Diol 4e: Following the general procedure, 4-(tert-butyl)-1-(2-methylbutyl)cyclohexanol (113 mg, 0.500 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.25 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 104 mg (86% overall yield) of **4e** as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.68 (dd, *J* = 10.5, 3.3 Hz, 1H), 3.58 (br, 2H), 3.36 (d, *J* = 10.0 Hz, 1H), 1.95 (dd, *J* = 13.0, 2.6 Hz, 1H), 1.76 (s, 1H), 1.70 (d, *J* = 10.4 Hz, 1H), 1.62 (s, 2H), 1.56 – 1.45 (m, 2H), 1.41 – 1.23 (m, 4H), 1.23 – 1.13 (m, 2H), 0.97 (dd, *J* = 19.6, 7.9 Hz, 1H), 0.91 (t, *J* = 7.5 Hz, 3H), 0.88 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 70.49, 67.73, 48.18, 47.96, 40.24, 37.66, 35.93, 32.43, 27.59, 26.54, 22.63, 22.38, 11.72. ESI-HR calcd for $C_{15}H_{30}O_2Na$ ($[M+Na]^+$) 265.2138, found 265.21384.



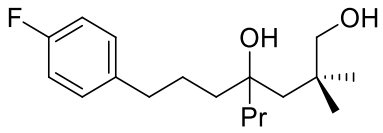
Diol 4f: Following the general procedure, 2,2,4-trimethyloctan-4-ol (86 mg, 0.50 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.10 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 62 mg (66% overall yield) of **4f** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.01 (br, 2H), 3.46 (d, *J* = 11.1 Hz, 1H), 3.37 (d, *J* = 11.0 Hz, 1H), 1.57 (d, *J* = 15.1 Hz, 1H), 1.55 – 1.47 (m, 2H), 1.44 (d, *J* = 15.1 Hz, 1H), 1.35 – 1.28 (m, 4H), 1.27 (s, 3H), 1.00 (s, 3H), 0.95 (s, 3H), 0.91 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 73.98, 71.04, 50.65, 44.90, 36.43, 28.55, 28.20, 27.03, 26.60, 23.28, 14.14. ESI-HR calcd for $C_{11}H_{24}O_2Na$ ($[M+Na]^+$) 211.1669, found 211.1665.



Diol 4g: Following the general procedure, 2,2-dimethyl-4-(3-phenylpropyl)octan-4-ol (138 mg, 0.500 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.20 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 105 mg (72% overall yield) of **4g** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.5 Hz, 2H), 7.22 (t, *J* = 6.2 Hz, 3H), 3.55 (br, 2H), 3.42 (s, 2H), 2.62 (t, *J* = 6.7 Hz, 2H), 1.67 – 1.58 (m, 3H), 1.59 – 1.44 (m, 5H), 1.35 – 1.25 (m, 2H), 1.25 – 1.15 (m, 2H), 0.96 (s, 6H), 0.92 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.36, 128.44, 128.37, 125.86, 75.98, 71.15, 48.52, 40.15, 40.00, 36.45, 36.36, 27.89, 27.87, 26.10, 26.09, 23.23, 14.17. ESI-HR calcd for $C_{19}H_{32}O_2Na$ ($[M+Na]^+$) 315.2295, found 315.2291.

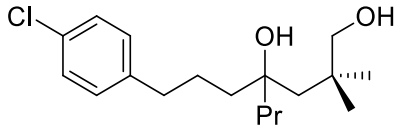


Diol 4h: Following the general procedure, 1-(pentan-3-yl)-4-phenylcyclohexanol (123 mg, 0.500 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.10 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 91 mg (74% overall yield) of **4h** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.10 (m, 5H), 3.83 (dt, *J* = 6.3, 5.7 Hz, 1H), 3.73 – 3.18 (br, 2H), 3.68 – 3.59 (m, 1H), 2.48 (dd, *J* = 16.2, 7.7 Hz, 1H), 2.00 – 1.59 (m, 10H), 1.45 (dt, *J* = 14.1, 4.0 Hz, 1H), 1.40 – 1.31 (m, 1H), 1.31 – 1.19 (m, 1H), 0.98 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.38, 128.40, 126.94, 126.02, 72.75, 61.71, 49.96, 44.14, 36.15, 33.22, 31.03, 29.48, 29.32, 22.79, 13.38. ESI-HR calcd for $C_{17}H_{26}O_2Na$ ($[M+Na]^+$) 285.1825, found 285.1821.

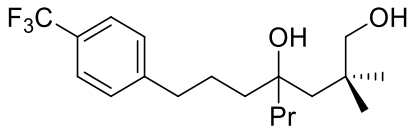


Diol 4j: Following the general procedure, 1-(4-fluorophenyl)-6,6-dimethyl-4-propylheptan-4-ol (140 mg, 0.500 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.20 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 110 mg (74% overall yield) of **4j** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.14 (dd, *J* = 8.1, 5.6 Hz, 2H), 6.98 (t, *J* = 8.6 Hz, 2H), 3.82 (br, 2H), 3.40 (q, *J* = 11.1 Hz, 2H), 2.58 (t, *J* = 6.8 Hz, 2H), 1.64 – 1.42 (m, 8H), 1.25 (td, *J* = 14.8, 7.1 Hz, 2H), 0.97 (s, 3H), 0.96 (s, 3H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.24 (d, *J* = 244 Hz), 137.94 (d, *J* = 2.5 Hz), 129.71 (d, *J* = 7.5 Hz), 115.04 (d, *J* = 21.4 Hz), 75.81, 71.10, 48.59, 42.71, 39.95, 36.41,

35.53, 27.89, 27.77, 26.12, 17.21, 14.58. ESI-HR calcd for $C_{18}H_{29}FO_2Na$ ([M+Na]$^+$) 319.2044, found 319.2040.

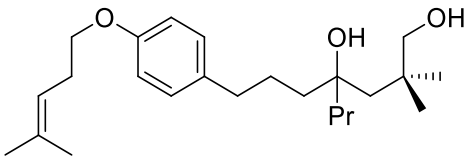


Diol 4k: Following the general procedure, 1-(4-chlorophenyl)-6,6-dimethyl-4-propylheptan-4-ol (148 mg, 0.500 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.20 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 131 mg (84% overall yield) of **4k** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.3 Hz, 2H), 7.12 (d, *J* = 8.2 Hz, 2H), 3.83 (br, 2H), 3.40 (q, *J* = 11.0 Hz, 2H), 2.57 (t, *J* = 6.7 Hz, 2H), 1.62 – 1.42 (m, 8H), 1.24 (dt, *J* = 15.0, 7.0 Hz, 2H), 0.97 (s, 3H), 0.96 (s, 3H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.78, 131.48, 129.77, 128.42, 75.76, 71.10, 48.60, 42.69, 39.98, 36.41, 35.70, 27.93, 27.74, 25.88, 17.25, 14.59. ESI-HR calcd for $C_{18}H_{29}ClO_2Na$ ([M+Na]$^+$) 335.1748, found 335.1744.

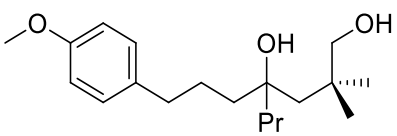


Diol 4l: Following the general procedure, 1-(4-trifluoromethylphenyl)-6,6-dimethyl-4-propylheptan-4-ol (165 mg, 0.500 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.20 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 106 mg (61% overall yield) of **4l** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.9 Hz, 2H), 7.30 (d, *J* = 7.8 Hz, 2H), 3.75 (br, 2H), 3.41 (q, *J* = 11.0 Hz, 2H), 2.66 (t, *J* = 6.9 Hz, 2H), 1.66 – 1.46

(m, 8H), 1.23 (dt, *J* = 34.4, 17.1 Hz, 2H), 0.98 (s, 3H), 0.97 (s, 3H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.49, 128.71, 128.18 (q, *J* = 32.8 Hz), 124.38 (q, *J* = 273 Hz), 125.26 (q, *J* = 273 Hz), 75.73, 71.11, 48.61, 42.67, 40.01, 36.39, 36.19, 27.92, 27.68, 25.71, 17.26, 14.55. ESI-HR calcd for $C_{19}H_{29}F_3O_2Na$ ($[M+Na]^+$) 369.2012, found 369.2008.

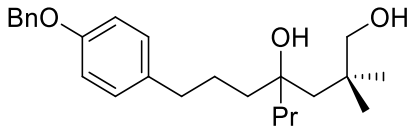


Diol 4m: Following the general procedure, 6,6-dimethyl-1-(4-((4-methylpent-3-en-1-yl)oxy)phenyl)-4-propylheptan-4-ol (108 mg, 0.300 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.20 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 69 mg (61% overall yield) of **4m** as a colorless oil. This compound contained ~15% inseparable impurities. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.10 (d, *J* = 8.3 Hz, 2H), 6.84 (d, *J* = 8.4 Hz, 2H), 5.28 – 5.16 (m, 1H), 3.94 (t, *J* = 15.3 Hz, 2H), 3.42 (d, *J* = 2.4 Hz, 2H), 3.18 (s, 2H), 2.55 (s, 2H), 2.49 (dd, *J* = 13.6, 6.7 Hz, 2H), 1.75 (s, 3H), 1.68 (s, 3H), 1.58 – 1.50 (m, 7H), 1.29 – 1.23 (m, 3H), 0.98 (s, 3H), 0.97 (s, 3H), 0.91 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.18, 134.39, 134.29, 129.25, 119.66, 114.42, 76.08, 71.15, 67.69, 48.41, 42.73, 40.07, 36.44, 35.45, 28.33, 27.93, 27.80, 26.29, 25.81, 17.91, 17.19, 14.59. ESI-HR calcd for $C_{24}H_{38}O_2Na$ ($[M+Na]^+$) 399.2870, found 399.2866.



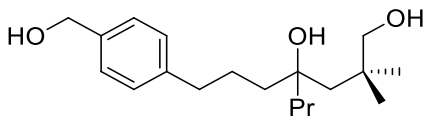
Diol 4n: Following the general procedure, 1-(4-methoxyphenyl)-6,6-dimethyl-4-propylheptan-4-ol (146 mg, 0.500 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.20 mol %) as catalyst at room

temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 129 mg (84% overall yield) of **4n** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.12 (d, *J* = 8.3 Hz, 2H), 6.85 (d, *J* = 8.4 Hz, 2H), 3.81 (s, 3H), 3.65 (br, 2H), 3.45 – 3.35 (m, 2H), 2.55 (s, 2H), 1.65 – 1.44 (m, 8H), 1.31 – 1.18 (m, 2H), 0.98 (d, *J* = 1.8 Hz, 3H), 0.96 (s, 3H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.74, 134.47, 129.29, 113.76, 75.95, 71.12, 55.29, 48.51, 42.72, 40.06, 36.43, 35.46, 27.92, 27.80, 26.32, 17.20, 14.60. ESI-HR calcd for $C_{19}H_{32}O_3Na$ ($[M+Na]^+$) 331.2244, found 331.2240.

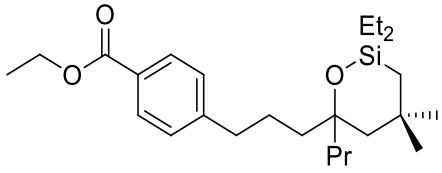


Diol 4o: Following the general procedure, 1-(4-benzyloxyphenyl)-6,6-dimethyl-4-propylheptan-4-ol (184 mg, 0.500 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.20 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 167 mg (87% overall yield) of **4o** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.2 Hz, 2H), 7.42 (t, *J* = 7.4 Hz, 2H), 7.36 (t, *J* = 7.1 Hz, 1H), 7.14 (d, *J* = 8.3 Hz, 2H), 6.94 (d, *J* = 8.4 Hz, 2H), 5.08 (s, 2H), 3.72 (br, 2H), 3.48 – 3.38 (m, 2H), 2.57 (s, 2H), 1.64 – 1.46 (m, 8H), 1.33 – 1.22 (m, 2H), 1.00 (s, 3H), 0.99 (s, 3H), 0.93 (t, *J* = 7.1 Hz, 3H).

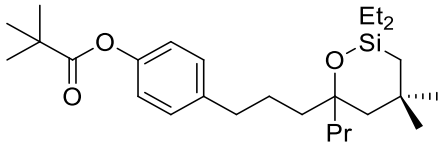
^{13}C NMR (126 MHz, $CDCl_3$) δ 157.02, 137.24, 134.80, 129.34, 128.62, 127.96, 127.53, 114.76, 75.97, 71.14, 70.08, 48.54, 42.74, 40.08, 36.45, 35.51, 27.95, 27.83, 26.31, 17.22, 14.63. ESI-HR calcd for $C_{25}H_{36}O_3Na$ ($[M+Na]^+$) 407.2557, found 407.2553.



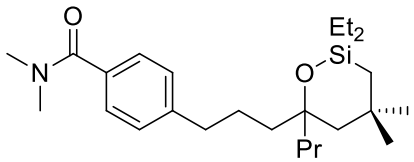
Diol 4p: Following the general procedure, 1-(4-(((tert-butyldimethylsilyl)oxy)methyl)phenyl)-6,6-dimethyl-4-propylheptan-4-ol (102 mg, 0.250 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.20 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 48 mg (62% overall yield) of **4p** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.9 Hz, 2H), 7.17 (d, *J* = 7.8 Hz, 2H), 4.62 (s, 2H), 3.50 (br, 2H), 3.37 (q, *J* = 11.0 Hz, 2H), 2.59 (t, *J* = 6.7 Hz, 2H), 1.65 – 1.41 (m, 8H), 1.30 – 1.18 (m, 2H), 0.95 (s, 3H), 0.95 (s, 3H), 0.90 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.72, 138.52, 128.56, 127.20, 75.82, 71.07, 64.95, 48.64, 42.66, 39.98, 36.39, 36.04, 27.91, 27.75, 26.00, 17.24, 14.61. ESI-HR calcd for $C_{19}H_{30}O_2Na$ ($[M+Na]^+$) 331.2244, found 331.2240.



Oxasilolane 4q: Following the general procedure, ethyl 4-(4-hydroxy-6,6-dimethyl-4-propylheptyl)benzoate (84 mg, 0.25 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $RuCl_2(PPh_3)_3$ (0.50 mol %) as catalyst at 50 °C for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Purification by preparative TLC gave 96 mg (92% overall yield) of **4q** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.9 Hz, 2H), 7.24 (d, *J* = 7.8 Hz, 2H), 4.36 (q, *J* = 7.0 Hz, 2H), 2.61 (d, *J* = 7.1 Hz, 2H), 1.70 – 1.16 (m, 13H), 1.04 (s, 3H), 1.00 (s, 3H), 0.93 – 0.82 (m, 9H), 0.62 – 0.43 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.88, 148.36, 129.69, 128.54, 128.08, 76.86, 60.88, 48.64, 44.58, 41.68, 36.62, 34.32, 34.28, 31.41, 25.62, 23.17, 17.40, 14.85, 14.49, 8.54, 8.50, 6.86, 6.82. ESI-HR calcd for $C_{25}H_{42}O_3Si$ (M^+) 418.2903, found 418.2900.

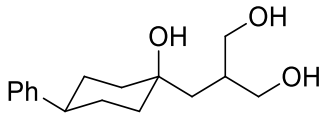


Oxasilolane 4r: Following the general procedure, ethyl 4-(4-hydroxy-6,6-dimethyl-4-propylheptyl)phenyl pivalate (91 mg, 0.25 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $RuCl_2(PPh_3)_3$ (0.50 mol %) as catalyst at 50 °C for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Purification by preparative TLC gave 100 mg (90% overall yield) of **4r** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 8.0 Hz, 2H), 2.56 (t, *J* = 6.6 Hz, 2H), 1.73 – 1.13 (m, 23H), 1.04 (s, 3H), 1.01 (s, 3H), 0.96 – 0.90 (m, 4H), 0.87 (t, *J* = 7.1 Hz, 3H), 0.64 – 0.43 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.38, 149.14, 140.22, 129.32, 121.22, 48.63, 44.63, 41.84, 39.16, 36.03, 34.39, 34.29, 31.43, 27.29, 26.02, 23.20, 17.39, 14.87, 8.56, 8.53, 6.87, 6.84. ESI-HR calcd for $C_{27}H_{46}O_3Si$ (M^+) 446.3216, found 446.3212.

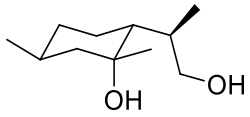


Oxasilolane 4s: Following the general procedure, 4-(4-hydroxy-6,6-dimethyl-4-propylheptyl)-N,N-dimethylbenzamide (83 mg, 0.25 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $RuCl_2(PPh_3)_3$ (0.50 mol %) as catalyst at 50 °C for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Purification by preparative TLC gave 98 mg (94% overall yield) of **4s** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 (d, *J* = 7.9 Hz, 2H), 7.03 (d, *J* = 8.2 Hz, 2H), 3.12 (s, 3H), 3.03 (s, 3H), 2.55 (t, *J* = 6.2 Hz, 2H), 1.75 – 1.17 (m, 11H), 1.07 (s, 2H), 1.05 (s, 3H), 0.98 – 0.90 (m, 6H), 0.88 (t, *J* = 7.1 Hz, 3H), 0.65 – 0.44 (m, 6H).

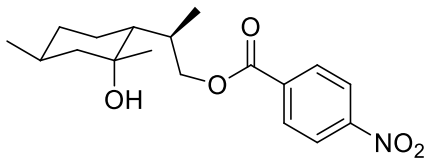
^{13}C NMR (126 MHz, $CDCl_3$) δ 155.18, 149.46, 139.67, 129.09, 121.43, 76.86, 48.51, 44.53, 41.80, 36.70, 36.45, 35.93, 34.30, 34.18, 31.32, 25.95, 23.10, 17.28, 14.78, 8.45, 8.42, 6.78, 6.74. ESI-HR calcd for $C_{25}H_{43}NO_2Si$ (M^+) 417.3063, found 417.3060.



Triol 6d: Following the general procedure, compound **5d** (72 mg, 0.20 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.50 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 38 mg (72% overall yield) of **6d** as a white solid. ^{1}H NMR (500 MHz, CD_3OD) δ 7.32 – 7.09 (m, 5H), 4.95 – 4.82 (br, 3H), 3.61 (dd, *J* = 10.6, 6.2 Hz, 2H), 3.55 (dd, *J* = 10.6, 6.2 Hz, 2H), 2.55 – 2.41 (m, 1H), 2.10 – 1.97 (m, 1H), 1.97 – 1.80 (m, 4H),1.67 (d, *J* = 9.9 Hz, 2H), 1.58 – 1.41 (m, 4H). ^{13}C NMR (126 MHz, CD_3OD) δ 149.67, 130.17, 128.72, 127.75, 71.87, 66.34, 46.36, 46.01, 40.83, 39.43, 31.39. ESI-HR calcd for $C_{16}H_{24}NaO_3$ ($[M+Na]^+$) 287.1618, found 287.1614.



Diol 4t: Following the general procedure, (*1R,2R,5S*)-2-isopropyl-1,5-dimethylcyclohexanol (170 mg, 1.00 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.20 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 153 mg (82% overall yield) of **4t** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.92 (s, 2H), 3.42 (t, *J* = 10.8 Hz, 1H), 3.33 (dd, *J* = 10.9, 3.4 Hz, 1H), 2.39 – 2.29 (m, 1H), 1.87 – 1.76 (m, 2H), 1.65 (dt, *J* = 22.6, 7.3 Hz, 1H), 1.55 – 1.42 (m, 2H), 1.25 (s, 3H), 1.24 – 1.17 (m, 1H), 1.05 (t, *J* = 23.1Hz, 1H), 0.92 – 0.81 (m, 7H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 71.26, 63.54, 51.62, 50.01, 35.50, 33.60, 29.09, 27.89, 22.30, 20.45, 18.34. ESI-HR calcd for $C_{11}H_{22}O_2Na$ ($[M+Na]^+$) 209.1512, found 209.1508.



Protected diol 5t: A mixture of **4t** (150 mg, 0.600 mmol), 4-nitrobenzoyl chloride (134 mg, 0.720 mmol), NEt_3 (165 µL, 1.60 mmol), DMAP (3.7 mg, 0.030 mmol) in 5 mL of anhydrous CH_2Cl_2 was stirred at room temperature for 14 h. The crude reaction mixture was concentrated and directly purified by column chromatography to afford the product as a white solid (149 mg, 74%). Single crystal suitable for X-ray crystallography was obtained by slow diffusion of hexane to a solution of the product in EtOAc at room temperature. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.8 Hz, 2H), 8.24 (d, *J* = 8.9 Hz, 2H), 4.89 (dd, *J* = 10.8, 4.2 Hz, 1H), 4.09 (dd, *J* = 10.7, 9.3 Hz, 1H), 2.57 – 2.40 (m, 1H), 1.85 – 1.65 (m, 5H), 1.48 (ddd, *J* = 26.1, 13.0, 3.2 Hz, 1H), 1.35 (s, 3H), 1.31 – 1.20 (m, 2H), 1.14 (d, *J* = 6.9 Hz, 3H), 0.96 – 0.86 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.94, 150.43, 135.91, 130.61, 123.53, 72.45, 69.25, 50.37, 50.24, 35.31, 31.46, 29.10, 28.04, 22.18, 21.60, 18.44. ESI-HR calcd for $C_{18}H_{25}NO_5$ $[M]^+$ 335.1733, found 335.1738.

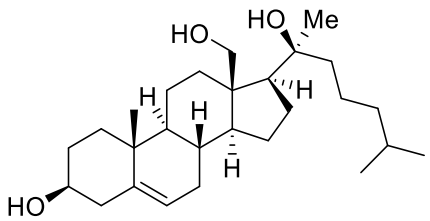
Crystal data and structure refinement for 6d:

A colorless plate 0.050 x 0.040 x 0.020 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 10 seconds per frame using a scan width of 2.0°. Data collection was 98.5% complete to 67.000° in θ. A total of 5741 reflections were collected covering the indices, -7<=*h*<=7, -8<=*k*<=8, -21<=*l*<=21. 5741 reflections were found to be symmetry independent, with an R_{int} of 0.0473. Indexing and unit cell refinement indicated a primitive, triclinic lattice. The space group was found to be P 1 (No. 1). The data were integrated using the Bruker SAINT software program and scaled using the TWINABS software program. Solution by iterative methods (SHELXT-2014) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were

placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. Absolute stereochemistry was unambiguously determined to be *R* at C4, C9, C22, and C27, and *S* at C1, C6, C19, and C24, respectively.

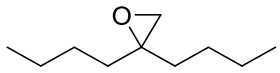
Empirical formula	$C_{18}H_{25}NO_5$	
Formula weight	335.39	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P 1	
Unit cell dimensions	a = 6.5555(3) Å	α= 88.767(2)°.
	b = 7.2872(3) Å	β= 87.077(2)°.
	c = 17.9836(7) Å	γ = 88.171(2)°.
Volume	857.37(6) $Å^3$	
Z	2	
Density (calculated)	1.299 Mg/m^3	
Absorption coefficient	0.776 mm^{-1}	
F(000)	360	
Crystal size	0.050 x 0.040 x 0.020 mm^3	
Theta range for data collection	2.461 to 68.734°.	
Index ranges	-7<=h<=7, -8<=k<=8, -21<=l<=21	
Reflections collected	5741	
Independent reflections	5741 [R(int) = 0.0473]	
Completeness to theta = 67.000°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.808	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	5741 / 3 / 442
Goodness-of-fit on F^2	1.011
Final R indices [I>2sigma(I)]	R1 = 0.0403, wR2 = 0.1077
R indices (all data)	R1 = 0.0464, wR2 = 0.1120
Absolute structure parameter	-0.13(11)
Extinction coefficient	n/a
Largest diff. peak and hole	0.212 and -0.168 e.$Å^{-3}$



Triol 4u: Following the general procedure, compound **1v'** (103 mg, 0.200 mmol) was converted to the corresponding diethyl(hydrido)silyl ether with $[Ir(cod)OMe]_2$ (0.50 mol %) as catalyst at room temperature for 14 h. The subsequent cyclization was conducted with RhCl(Xantphos) at 100 °C for 15 h to provide the intermediate oxasilolane. Tamao-Fleming oxidation and purification by silica gel chromatography gave 38 mg (44% overall yield) of **4u** as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.35 (d, *J* = 4.4 Hz, 1H), 3.69 (d, *J* = 11.7 Hz, 1H), 3.58 (d, *J* = 11.8 Hz, 1H), 3.56 – 3.49 (m, 1H), 2.84 (br, 3H), 2.59 (d, *J* = 12.6 Hz, 1H), 2.27 (dt, *J* = 22.9, 9.8 Hz, 2H), 1.99 (d, *J* = 9.0 Hz, 1H), 1.92 – 1.79 (m, 3H), 1.68 (dd, *J* = 27.5, 9.3 Hz, 2H), 1.62 – 1.45 (m, 9H), 1.39 (s, 3H), 1.33 – 1.24 (m, 4H), 1.15 (t, *J* = 13.3 Hz, 4H), 1.04 (s, 3H), 0.98 (d, *J* = 6.7 Hz, 1H), 0.89 (d, *J* = 6.5 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.96, 121.31, 74.83, 71.75, 58.96, 57.41, 56.29, 50.21, 47.00, 44.11, 42.23, 39.60, 37.24, 36.57, 34.46, 32.09, 31.88, 31.60, 27.91, 26.98, 23.43, 22.75, 22.60, 22.48, 22.32, 20.63, 19.48. ESI-HR calcd for $C_{27}H_{46}O_3Na$ ($[M+Na]^+$) 441.3339, found 441.3336.

Synthesis of materials and complexes for studies of the reaction mechanism



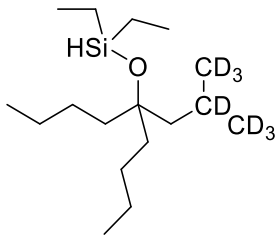
Synthesis of Dibutyl Oxirane

Trimethylsulfoxonium iodide (4.4 g, 20 mmol) was added to a 50 mL two necked round bottom flask fitted with a stir bar. The flask was sealed with two septa and purged with N_2. 15 mL DMSO from an Aldrich Sure/Seal bottle was added through a septum. The flask was placed under a positive pressure of N_2, and one septum was removed. A 60% dispersion of NaH in oil (800 mg, 20 mmol) was added portionwise to the solution with vigorous stirring. When no more H_2 evolution was observed, the septum was replaced. 5-Nonanone (2 mL, 11.6 mmol) was added through the septum. The solution was stirred for 18 h. The solution was diluted with Et_2O, washed with water, and washed with brine. The organic layer was dried with sodium sulfate, filtered, and concentrated under reduced pressure. The resulting oil was purified by column chromatography (1:10, Et_2O to hexane) to yield 1.43 g (79% yield) of a colorless oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 2.57 (s, 2H), 1.68 – 1.45 (m, 4H), 1.38 – 1.27 (m, 8H), 0.91 (t, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 59.72, 52.81, 34.09, 27.19, 23.01, 14.19.

HRMS (EI +) Calc for $C_{10}H_{20}O$ $[M]^+$ 156.1514 found 156.1516



Synthesis of 2a-*d*$_7$

In an N_2 filled glovebox, Mg metal (242 mg, 9.96 mmol), I_2 (1 crystal), and 8 mL of Et_2O was added to a 25 mL round bottom flask containing a stir bar. In a separate flask, a solution of 1,2-dibromoethane (0.085 mL) in 2 mL of Et_2O was prepared. These solutions were removed from glovebox. Under a flow of nitrogen, the solution of 1,2-dibromoethane was added, by syringe, to the stirring suspension of Mg metal. Evolution of gas was observed. As gas evolution slowed, a solution of isopropylbromide-*d*$_7$ (0.80

mL, 8.5 mmol) in 4 mL of Et_2O was added dropwise to the activated Mg metal suspension. This solution was stirred for 2 h at room temperature, at which point little solid remained. CuI (1 g, 5 mmol) was added to a 50 mL round bottom flask fitted with a stir bar. This flask was evacuated and refilled with nitrogen, followed by 20 mL of THF. This suspension was stirred at -20 °C. The solution of Grignard reagent was canula transferred to the CuI suspension. A solution of dibutyloxirane (320 mg, 2.0 mmol) in 5 mL THF was added dropwise to the stirring solution of isopropylcuprate. The resulting solution was stirred for 1 h and then allowed to come to room temperature. The solution was diluted with Et_2O, washed with water, washed with brine, dried with sodium sulfate, filtered, and concentrated under reduced pressure. The resulting oil was purified by column chromatography (1:5, Et_2O to hexane) to yield a colorless oil, which contained unreacted epoxide starting material. This material was brought into a nitrogen filled glovebox and treated with 2 mL of a 4 M solution of [Ir(COD)(OMe)] followed by diethylsilane (0.1 mL, 0.8 mmol) at room temperature. Hydrogen evolution was observed. After 3 h, the volatiles were evaporated under reduced pressure and the resulting oil was purified by column chromatography (1:20, Et_2O to hexane) to yield 97 mg of **2a-*d*$_7$** (17%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 4.43 (p, *J* = 2.3 Hz, 1H), 1.46 – 1.42 (m, 4H), 1.38 – 1.22 (m, 10H), 0.99 (t, *J* = 7.9 Hz, 6H), 0.90 (t, *J* = 7.0 Hz, 6H), 0.66 (dq, *J* = 8.1, 2.1 Hz, 4H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 74.65, 37.05, 34.11, 27.92, 22.98, 14.25, 6.91, 5.80.

Synthesis of (H)Si(Et)$_2$(OAd)

In a N_2-filled glovebox, 1-adamantyl alcohol (76 mg, 0.50 mmol) was weighed into a 4 mL vial, fitted with a stir bar. To this vial, 1 mL of a 6 mM solution of $[Ir(cod)OMe]_2$ in Et_2O was added, followed by Et_2SiH_2 (0.1 mL, 0.8 mmol). The vial was capped with a Teflon-lined screw cap, and the resulting solution was stirred in the glovebox at room temperature for 15 h. Hydrogen evolution was observed. Complete conversion to the corresponding diethyl(hydrido)silyl ether was determined by GC-MS. Solvent and excess silane were removed by placing the vial under high vacuum for 1 h.

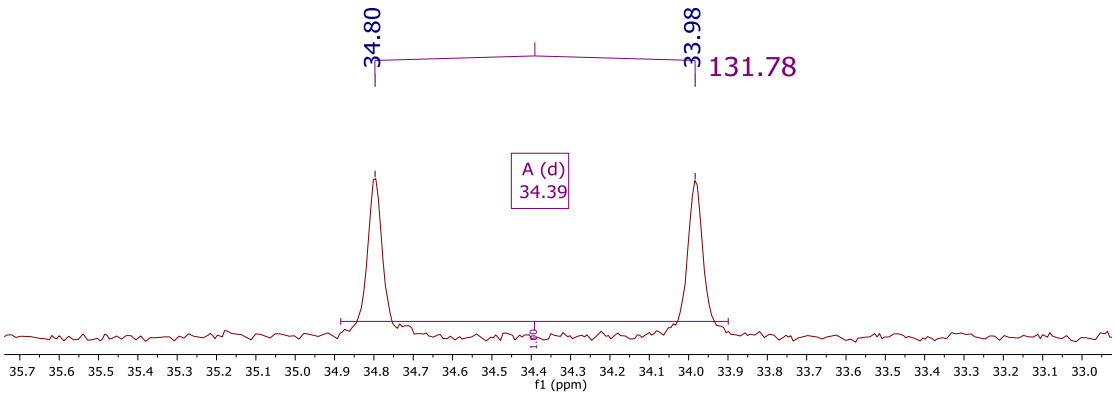
^{1}H NMR (500 MHz, Benzene-d_6) δ 4.92 – 4.85 (m, 1H), 2.03 – 1.92 (m, 3H), 1.84 (d, J = 3.1 Hz, 6H), 1.48 (t, J = 3.1 Hz, 6H), 1.07 (t, J = 7.9 Hz, 6H), 0.68 (dq, J = 10.5, 4.8 Hz, 4H).

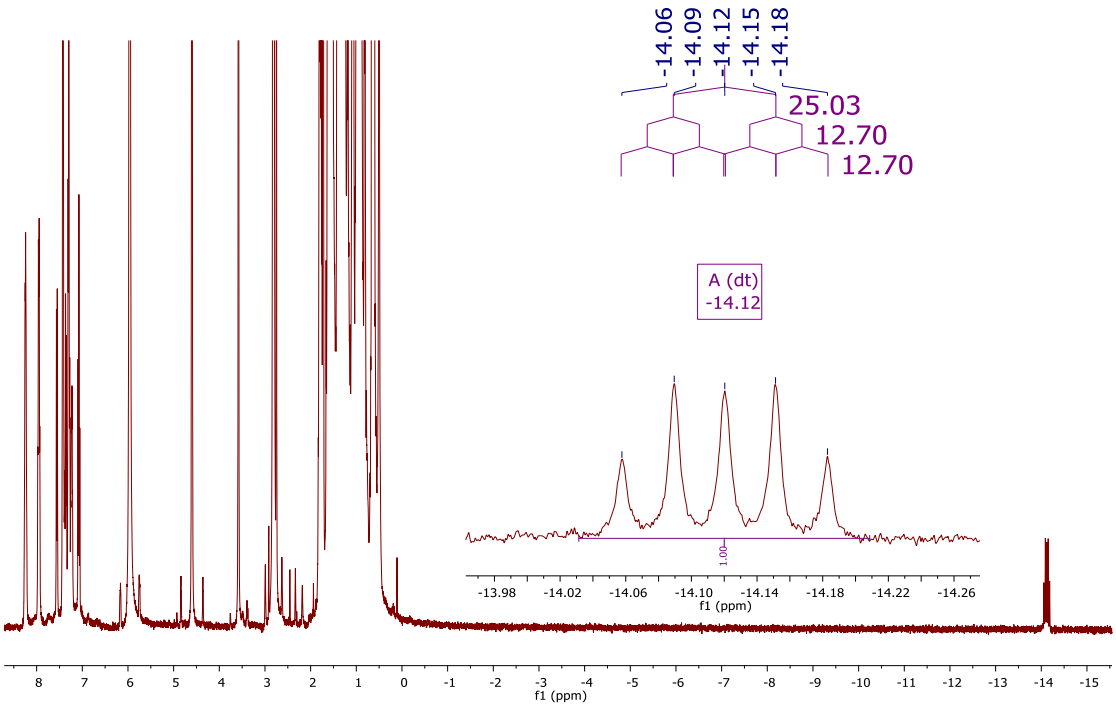
^{13}C NMR (126 MHz, $CDCl_3$) δ 71.19, 45.88, 36.49, 31.29, 7.49, 7.23.

Observations of the Soluble Precatalyst and Resting State

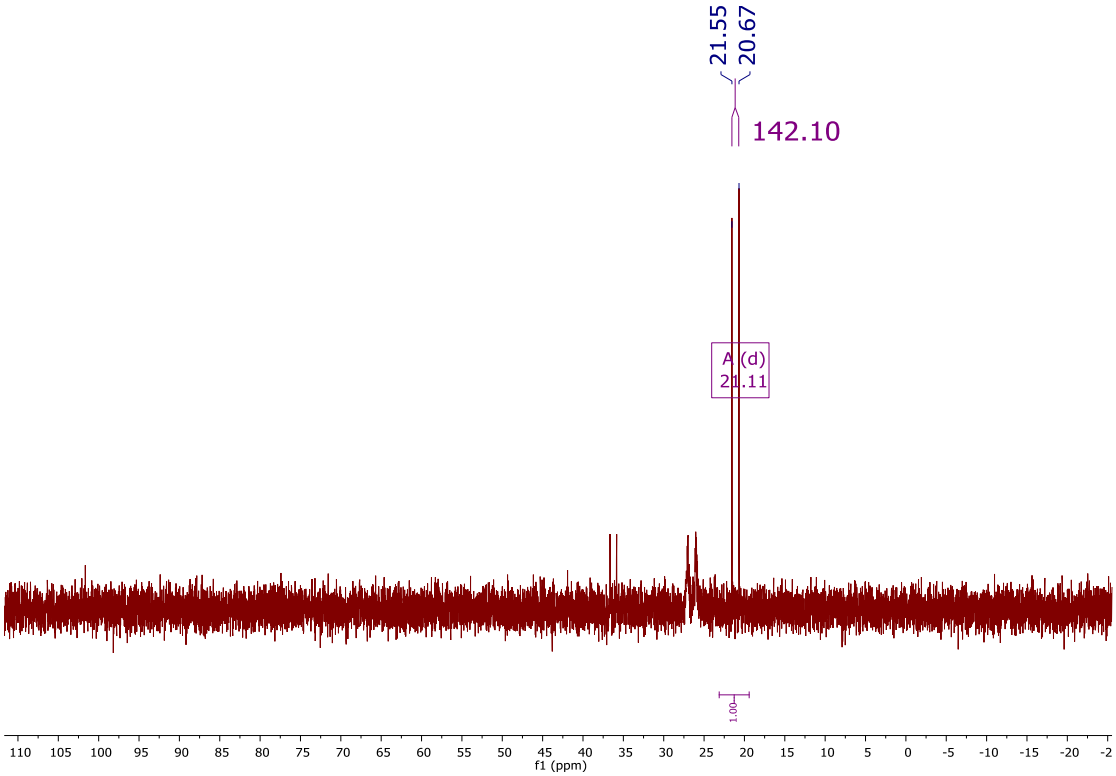
In an N_2-filled glovebox, 5-*iso*butylnonan-5-ol (25 mg) and Et_2SiH_2 (25 uL) were weighed in a 4 mL screw-capped vial. 0.25 mL of a 12 mM solution of $[Ir(cod)OMe]_2$ in Et_2O was then added. The vial was capped with a Teflon-lined screw cap, and the resulting solution was stirred in the glovebox at room temperature for 2 h, at which point GC analysis indicated full conversion to diethyl(hydrido)silyl ether. The volatile materials were evaporated by placing the reaction mixture directly under high vacuum for 0.5 h. The concentrated diethyl(hydrido)silyl ether was then sequentially treated with norbornene (30 mg, 0.3 mmol), RhCl(Xantphos) (7.2 mg, 0.010 mmol) and THF-d_8 (0.75 mL). This solution was a brick red suspension but was observed to form a clear solution after 10 m (ca.). This solution was transferred to a J-Young NMR tube and analyzed by ^{1}H and ^{31}P NMR spectroscopy. The J-Young tube was placed in a pre-heated aluminum block at 100 °C for 1 h. Upon heating the solution turned red. The solution was then cooled to room temperature, and was analyzed by ^{1}H and ^{31}P NMR spectroscopy.

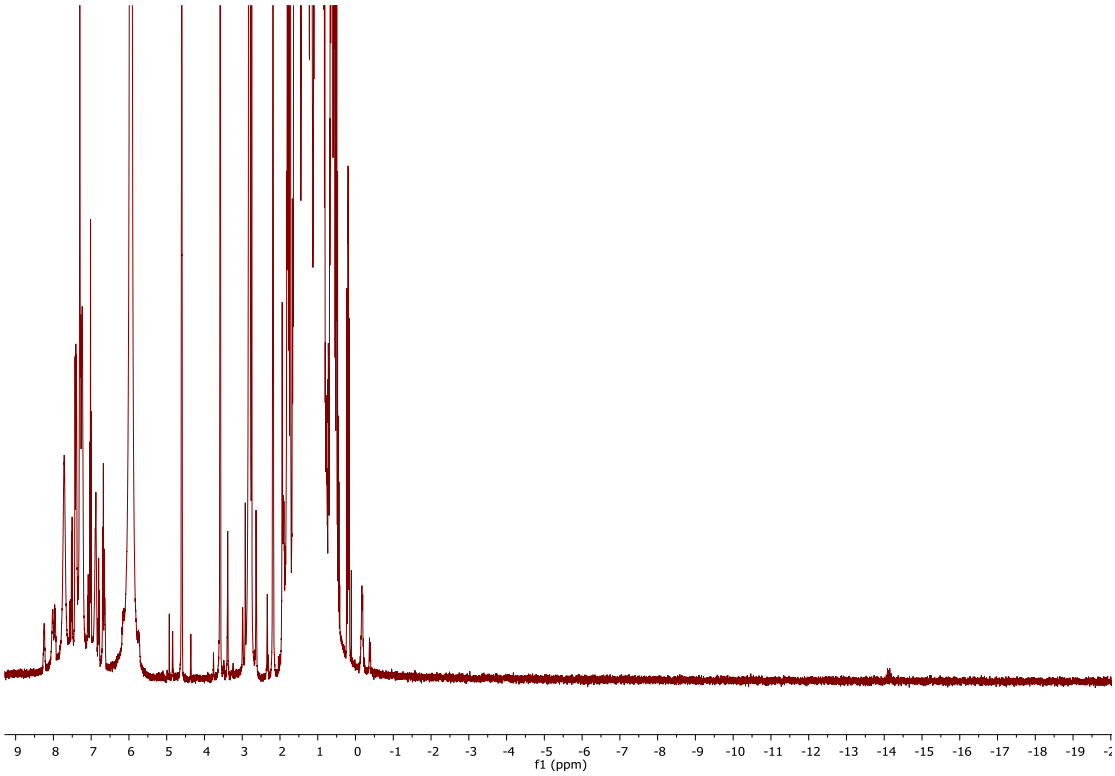
Before Heating:

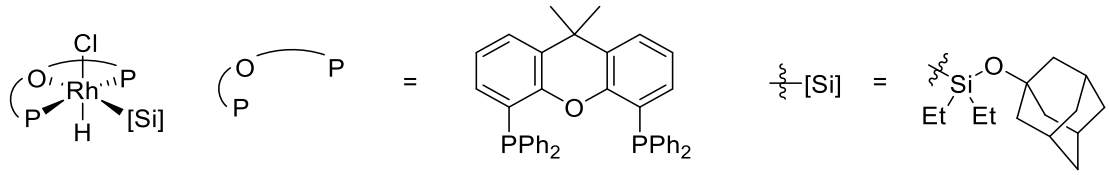




After heating:







Synthesis of (Xantphos)Rh(Cl)(H)(SiEt$_2$OAd) (8)

In a N_2-filled glovebox, (Xantphos)Rh(Cl) (72 mg, 0.10 M) was weighed into a 20 mL vial. A stir bar was added. 5 mL of a 0.2 M solution of **2v** in THF was added. The resulting solution was stirred in the glovebox at room temperature for 24 h. Pentane was carefully added to form a separate phase above the solution and then allowed to diffuse into the solution over 2 d at -28 °C. A white precipitate formed which was filtered, washed with Et_2O and dried under vacuum yielding 42 mg (0.044 mmol, 44%) of white solid. The solid was dissolved in THF and crystallized by slow diffusion of pentane.

^{1}H NMR (600 MHz, Benzene-d_6) δ 8.35 (dq, J = 30.9, 5.6, Hz, 8H), 7.27 – 7.19 (m, 2H), 7.14 – 7.05 (m, 10H), 7.05 – 6.98 (m, 4H), 6.73 (t, J = 7.7 Hz, 2H), 1.91 (d, J = 4.2 Hz, 3H), 1.61 (apparent doublet, 6 H), 1.43 (s, 6H), 1.33 (s, 3H), 1.30 (t, J = 7.6

Hz, 6H), 0.95 (s, 3H), 0.93 (d, 7.6 Hz, 2H), 0.91 (d, 7.6 Hz, 2H), -13.49 (dt, *J* = 25.5, 14.0 Hz, 1H).

Observation of Rh hydride in THF-d_8: ^{1}H NMR (400 MHz, THF-d_8) δ -14.02 (dt, *J* = 25.3, 14.2 Hz, 1H).

^{13}C NMR (151 MHz, Benzene-d_6) δ 152.9 (t, *J* = 6.7 Hz), 135.0 (t, *J* = 5.8 Hz), 134.6 (t, *J* = 7.0 Hz), 133.5, 133.1 (t, *J* = 22.4 Hz), 132.0 (t, *J* = 2.6 Hz), 130.0, 129.6, 127.2, 123.9, 72.7, 45.0, 36.2, 34.7, 34.4, 31.0, 27.4, 17.5, 9.1.

^{31}P NMR (243 MHz, Benzene-d_6) δ 34.7 (d, *J* = 131.4 Hz).

Elemental analysis (%) calcd for $C_{58}H_{70}ClO_2P_2RhSi$ [M+pentane]: C 67.79, H 6.23, found: C 67.89, 6.27

IR (neat, cm–1) ν 3051, 2905, 2849, 2116, 1435, 1087, 692.

HRMS (ESI +) Calc for $C_{53}H_{58}O_2P_2RhSi$ $[M-Cl]^+$ 919.2736 found 919.2731

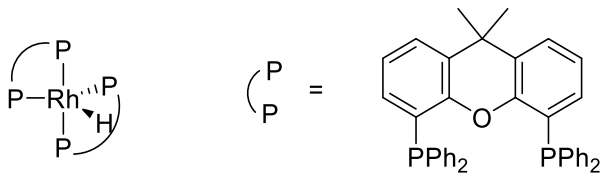
X-Ray structural data for Complex 8:

A yellow prism 0.050 x 0.040 x 0.040 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 10 seconds per frame using a scan width of 2.0°. Data collection was 98.8% complete to 67.000° in θ. A total of 69005 reflections were collected covering the indices, -13<=*h*<=10, -19<=*k*<=19, -32<=*l*<=32. 17750 reflections were found to be symmetry independent, with an R_{int} of 0.0913. Indexing and unit cell refinement indicated a primitive, triclinic lattice. The space group was found to be P -1 (No. 2). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT-2014) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014.

Empirical formula	$C_{54}H_{59}Cl_2O_2P_2RhSi$

Formula weight	1003.85	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.5444(5) Å	α= 95.114(3)°.
	b = 16.0589(7) Å	β= 92.970(3)°.
	c = 26.8374(14) Å	γ = 90.036(3)°.
Volume	4948.9(4) $Å^3$	
Z	4	
Density (calculated)	1.347 Mg/m^3	
Absorption coefficient	4.931 mm^{-1}	
F(000)	2088	
Crystal size	0.050 x 0.040 x 0.040 mm^3	
Theta range for data collection	2.763 to 69.312°.	
Index ranges	-13<=h<=10, -19<=k<=19, -32<=l<=32	
Reflections collected	69005	
Independent reflections	17750 [R(int) = 0.0913]	
Completeness to theta = 67.000°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.616	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17750 / 12 / 1126	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.1059, wR2 = 0.2772	
R indices (all data)	R1 = 0.1193, wR2 = 0.2935	
Extinction coefficient	n/a	

Largest diff. peak and hole 5.911 and -1.528 e.Å^{-3}



Synthesis of (Xantphos)$_2$Rh(H)

In a N_2-filled glovebox, (Xantphos)Rh(Cl) (14 mg, 0.020 mmol) and Xantphos (12 mg, 0.021 mmol) was weighed into a 4 mL vial. 1 mL of a 0.2 M solution of **2v** in THF was added. The resulting solution was kept in the glovebox at room temperature for 24 h. Red crystals, suitable for x-ray diffraction, formed in an otherwise colorless solution. The solvent was removed by pipette, and the remaining solids were washed with 2 mL of Et_2O and 2 mL of pentane and dried under vacuum yielding 18 mg (0.014 mmol, 73%) of red crystalline solids.

Elemental analysis (%) calcd for $C_{78}H_{65}O_2P_4Rh$: C 74.28, H 5.20, found: C 74.36, 5.31

IR (neat, cm–1) ν 3058, 2973, 2156, 1584, 1431, 1398, 1221, 913, 743, 694

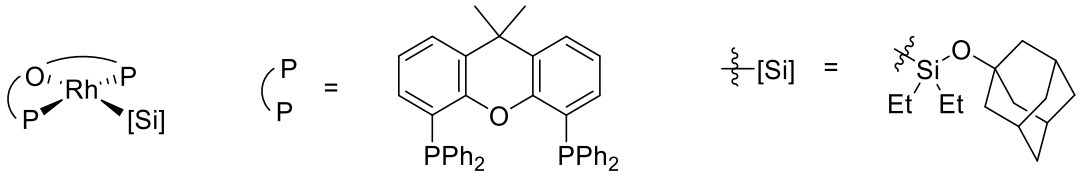
X-Ray structure data for Complex 9:

A yellow prism 0.050 x 0.030 x 0.030 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 40 mm and exposure time was 10 seconds per frame using a scan width of 2.0°. Data collection was 98.1% complete to 25.000° in θ. A total of 26276 reflections were collected covering the indices, -20<=*h*<=20, -20<=*k*<=21, -22<=*l*<=22. 5321 reflections were found to be symmetry independent, with an R_{int} of 0.0597. Indexing and unit cell refinement indicated a C-centered, monoclinic lattice. The space group was found to be C 2/c (No. 15). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT 2014) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-

hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2016). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2016.

Empirical formula	$C_{78}H_{65}O_2P_4Rh$
Formula weight	1260.18
Temperature/K	100.15
Crystal system	monoclinic
Space group	C2/c
a/Å	17.6304(6)
b/Å	18.1797(6)
c/Å	18.7127(6)
α/°	90
β/°	96.862(1)
γ/°	90
Volume/Å^3	5954.7(3)
Z	4
ρ_{calc}g/cm^3	1.4055
μ/mm^{-1}	0.445
F(000)	2610.1
Crystal size/mm^3	0.05 × 0.03 × 0.03
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	3.22 to 50.76
Index ranges	$-20 \leq h \leq 20$, $-20 \leq k \leq 21$, $-22 \leq l \leq 22$
Reflections collected	26276
Independent reflections	5321 [R_{int} = 0.0597, R_{sigma} = 0.0633]
Data/restraints/parameters	5321/0/386

Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0452, wR_2 = 0.0990
Final R indexes [all data]	R_1 = 0.0676, wR_2 = 0.1098
Largest diff. peak/hole / e $Å^{-3}$	1.39/-0.80

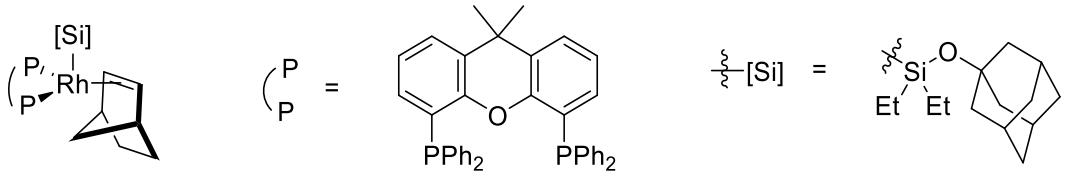


Synthesis of (Xantphos)Rh(SiEt$_2$OAd)

In a N_2-filled glovebox, (Xantphos)Rh(Cl)(H)(SiEt$_2$OAd) (10 mg, 0.01 mmol) was weighed into a 4 mL vial. A stir bar was added. LiHMDS (2 mg, 0.01 mmol) was weighed into a separate 4 mL vial. THF-d_8 (600 uL) was added to the LiHMDS. When the LiHMDS was fully dissolved, this solution was added to vial containing complex **8**. After stirring at room temperature for 15 m, the solution was observed to turn a red. This solution was transferred to a J-Young tube, and NMR analysis was performed directly on this mixture. Isolation was attempted by slow diffusion of pentane, leading to precipitation of the complex. NMR spectroscopy of the isolated red solid indicated the same material was present as in the crude reaction mixture but with additional impurities. Repeated attempts at precipitation, crystallization and washing only produced more impurities and eventually eliminated any red products and gave an orange solid that produced no signal in the ^{31}P NMR spetrum.

^{1}H NMR (400 MHz, THF-d_8) δ 7.87 (qd, J = 5.3, 2.7 Hz, 8H), 7.57 (dd, J = 7.7, 1.6 Hz, 2H), 7.34 – 7.25 (m, 14H), 7.09 (t, J = 7.6 Hz, 2H), 1.73 (s, 6H), 1.65 (s, 6H), 1.36 (apparent doublet, J = 2.9 Hz, 6H), 1.33 (s, 3H), 0.81 (t, J = 7.7 Hz, 6H), 0.51 – 0.39 (m, 2H), 0.23 – 0.13 (m, 2H).

^{31}P NMR (162 MHz, THF-d_8) δ 32.6 (d, J = 193.4 Hz).



Synthesis of (Xantphos)Rh(SiEt$_2$OAd)(nbe)

In a N_2-filled glovebox, (Xantphos)Rh(Cl)(H)(SiEt$_2$OAd) (38 mg, 0.040 mmol) was weighed into a 4 mL vial. A stir bar was added. LiHMDS (34 mg, 0.20 mmol) and norbornene (4 mg, 0.04 mmol) were weighed into a separate 4 mL vial. C_6D_6 (600 uL) was added to the vial containing LiHMDS and norbornene. When the LiHMDS was dissolved, this solution was added to vial containing complex **8**. After stirring at room temperature for 1 h, the solution was observed to turn red. This solution was transferred to a J-Young tube and NMR analyses showed that complex **8** was fully consumed. Inside of a N_2-filled glovebox, the solution was transferred to a 20 mL vial. The product was crystallized by slow diffusion of pentane at -30 °C. Reddish orange crystals formed after several days, along with a larger amount of orange powder. This powder was observed to decompose instantaneously upon removal of solvent, though the crystalline material could be removed from solvent without immediate decomposition. The powder was removed as a suspension in Et_2O, and the remaining crystals were washed with pentane. The resulting solids had a mass of 9.5 mg (24%). A few crystals were removed from the vial and dissolved in C_6D_6 (600 uL) for NMR analysis.

^{1}H NMR (500 MHz, Benzene-d_6) δ 8.03 (s, 8H), 7.22 – 7.16 (m, 2H), 7.08 (m, 12H), 6.93 (d, J = 7.6 Hz, 2H), 6.74 (t, J = 7.7 Hz, 2H), 2.62 (s, 2H), 2.03 (s, 2H), 1.94 (s, 3H), 1.74 (s, 6H), 1.47 (s, 6H), 1.46 – 1.33 (m, 2H), 1.23 – 0.98 (m, 14H), 0.98 – 0.88 (m, 2H), 0.85 (t, J = 7.1 Hz, 3H), 0.57 (t, J = 7.8 Hz, 1H).

^{31}P NMR (202 MHz, Chloroform-d) δ 21.47 (d, J = 143.0 Hz).

X-Ray structural data for Complex 11:

A yellow blade 0.070 x 0.040 x 0.020 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 40 mm and exposure time was 10

seconds per frame using a scan width of 0.5°. Data collection was 100.0% complete to 25.000° in □. A total of 127076 reflections were collected covering the indices, -22<=*h*<=22, -15<=*k*<=15, -30<=*l*<=30. 11400 reflections were found to be symmetry independent, with an R_{int} of 0.0545. Indexing and unit cell refinement indicated a primitive, monoclinic lattice. The space group was found to be P 21/c (No. 14). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT-2014) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2016). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2016.

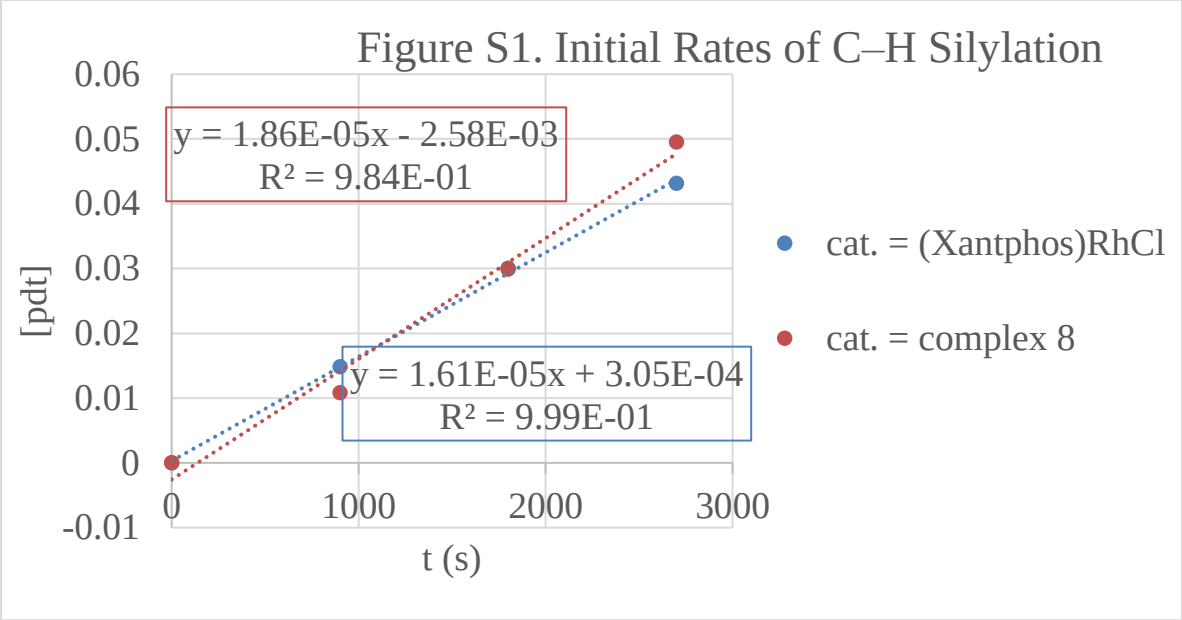
Empirical formula	$C_{66}H_{73}O_2P_2RhSi$	
Formula weight	1091.18	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 18.4691(15) Å	□= 90°.
	b = 13.1762(10) Å	□= 95.478(4)°.
	c = 25.638(2) Å	□ = 90°.
Volume	6210.6(9) $Å^3$	
Z	4	
Density (calculated)	1.167 Mg/m^3	
Absorption coefficient	0.386 mm^{-1}	
F(000)	2296	
Crystal size	0.070 x 0.040 x 0.020 mm^3	
Theta range for data collection	1.108 to 25.377°.	

Index ranges	-22<=h<=22, -15<=k<=15, -30<=l<=30
Reflections collected	127076
Independent reflections	11400 [R(int) = 0.0545]
Completeness to theta = 25.000°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928 and 0.852
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11400 / 0 / 653
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0418, wR2 = 0.1018
R indices (all data)	R1 = 0.0531, wR2 = 0.1088
Extinction coefficient	n/a
Largest diff. peak and hole	0.915 and -0.523 e.$Å^{-3}$

Details of Kinetic Analyses

Test of Kinetic Competence

The silylation of **2a** was conducted in diglyme with a total volume of 0.40 mL. The concentrations of each reagent under the standard conditions for catalytic silylation were: 0.2 M silane, 0.4 M norbornene, and 8 mM catalyst. To determine the catalytic competence of each pre-catalyst, the reaction was conducted three times, with (Xantphos)Rh(Cl) as precatalyst, complex **8** as precatalyst, and complex **9** as precatalyst. The rate of the reaction was determined by the method of initial rates at 120 °C, monitored by GC analysis with dodecane as the internal standard. No product was observed when complex **9** was used as precatalyst for the silylation reaction.



Determination of Experimental Rate Law

Silylation of **2a** was conducted in diglyme with a total volume of 0.40 mL. The concentrations of each reagent under the standard conditions for catalytic silylation were: 0.16 M silane, 0.4 M norbornene, 8 mM catalyst (**8**). To determine the rate dependence on one reagent, the concentration of that reagent was varied, while the concentration of the other reagents and the total volume (0.40 mL) were held constant. The concentration of the silane was varied between 0.04 and 0.32 M. The concentration of the catalyst (**8**) was varied between 2 and 16 mM. The concentration of norbornene was varied between 0.4 M and 3 M. The rate law of the reaction was determined by the method of initial rates at 120 °C monitored by GC analysis with dodecane as the internal standard.

Figure S2. Dependence of Rate of Silylation on [norbornene]

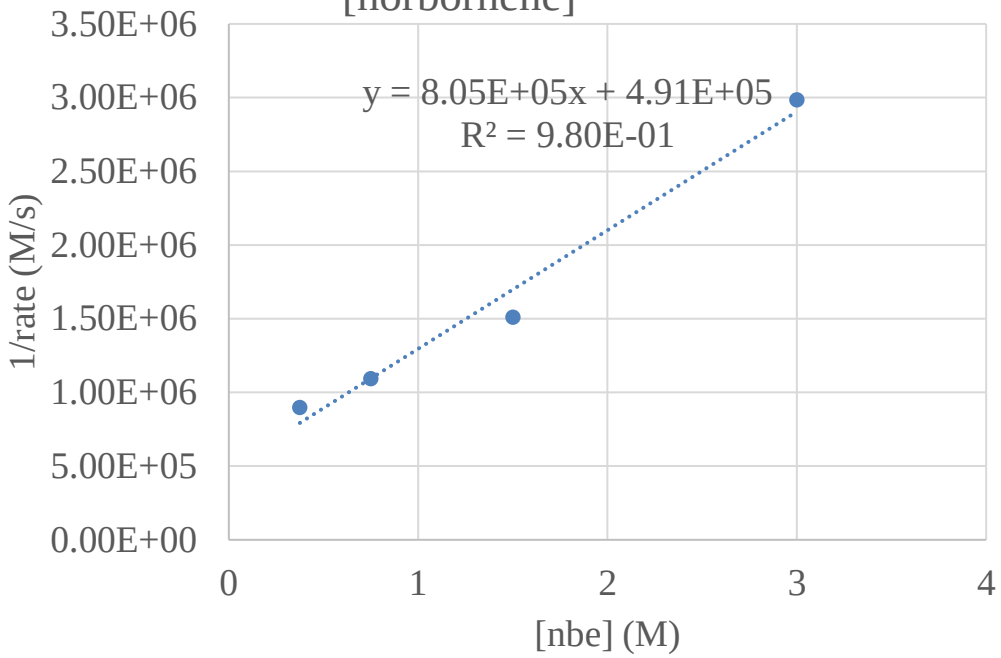
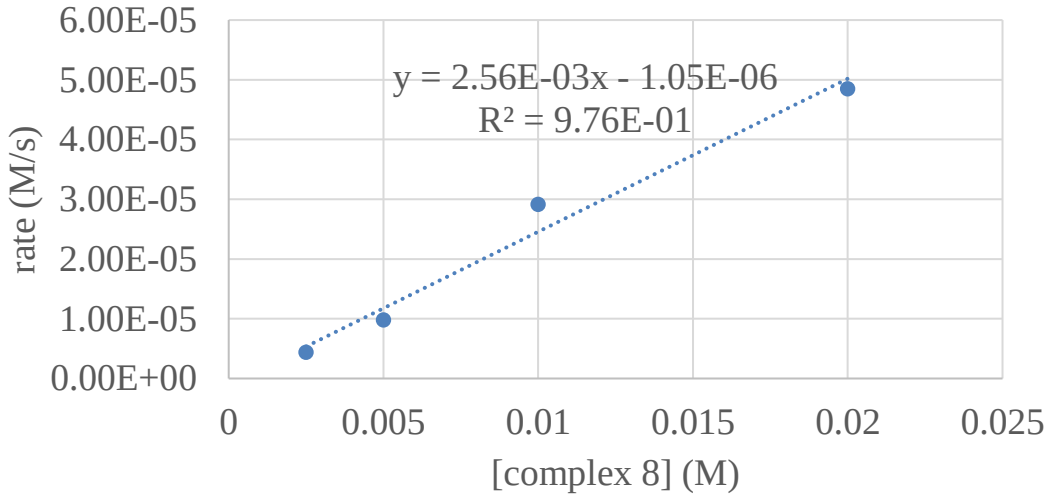
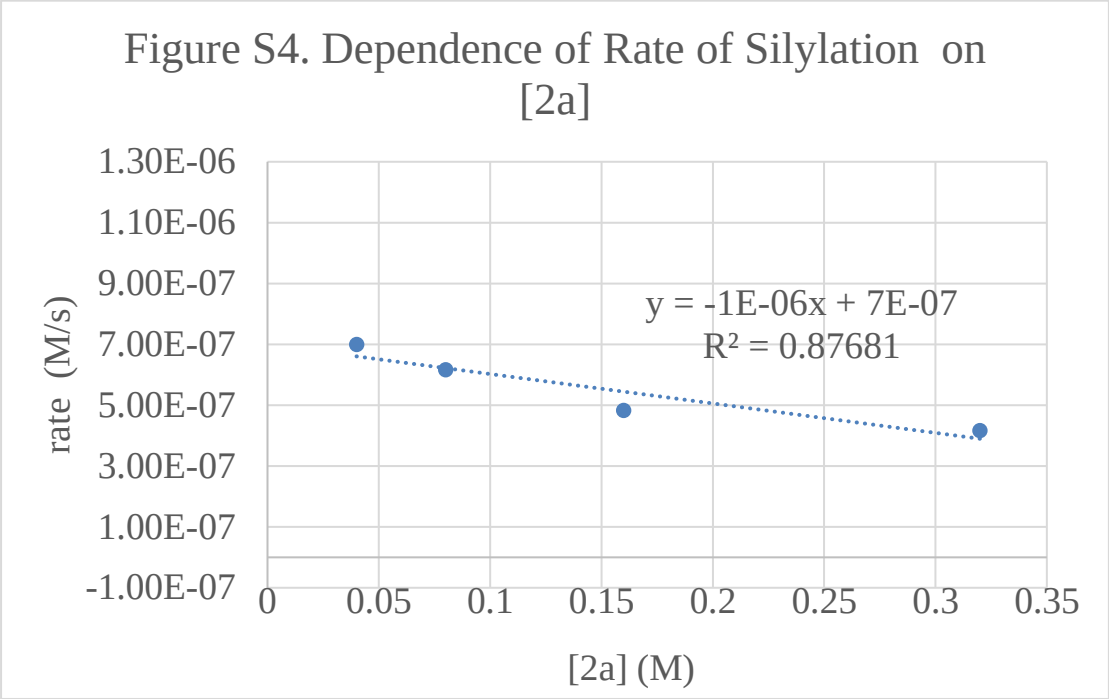


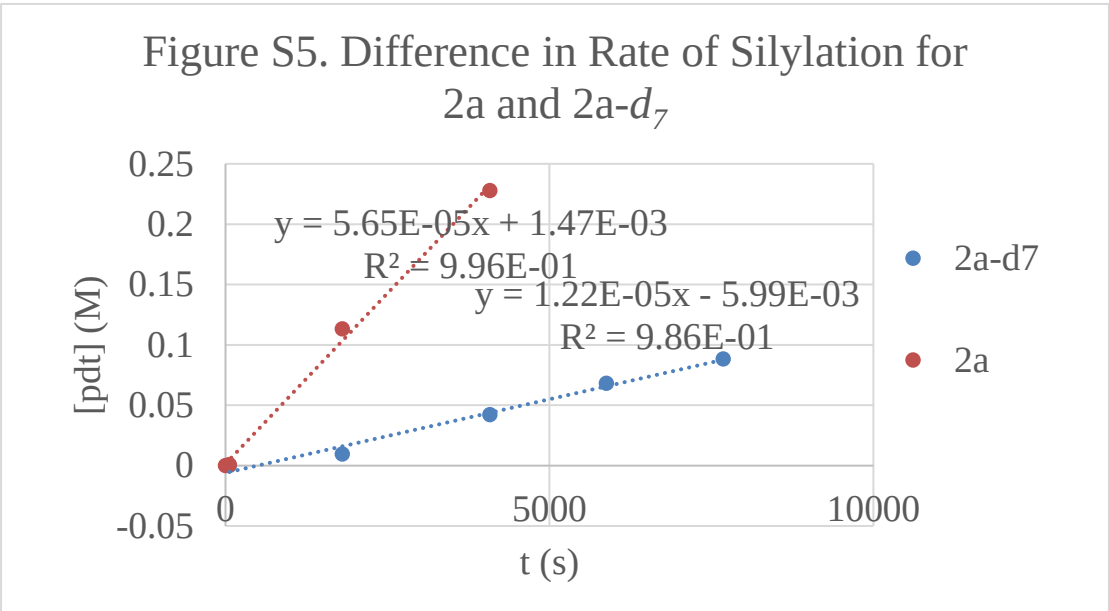
Figure S3. Dependence of Rate of Silylation on [complex 8]





Determination of the Kinetic Isotope Effect

The silylation of **2a-*d*$_7$** was conducted in THF with a total volume of 0.40 mL. The concentrations of each reagent under the standard conditions were 0.2 M **2a-*d*$_7$**, 0.4 M norbornene and 8 mM catalyst. The silylation of **2a** was conducted under the same conditions. The initial rate of the reactions of **2a** and **2a-*d*$_7$** at 100 °C were monitored by GC analysis with dodecane as the internal standard. The kinetic isotope effect (k_H/k_D) was determined to be 4.6±0.5.



Computational Details

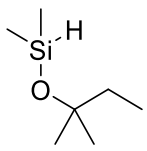
DFT calculations were performed with the Gaussian 09 software package. B3LYP functionals (with gd3 dispersion correction), and LANL2DZ basis set for Rh and 6-31g(d,p) basis set for all other atoms was applied for geometry optimizations. The M06 functional, and LANL2TZ basis set for Rh and 6-31++g** basis set for all other atoms, and SMD THF solvent correction was applied to single point energy calculations. Thermal corrections from the geometry optimizations were added to the energies found in single point energy calculations to find values for Gibbs free energy. Cartesian coordinates and Gibbs energy are given. Single point energy calculations were not performed for geometry comparisons

Non-metal containing molecules:

H2

G° = -1.170194856 Hartrees

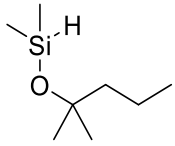
H	0.00000000	0.00000000	0.37139600
H	0.00000000	0.00000000	-0.37139600



G° = -641.9037591 Hartrees

Si	-1.77358500	-0.05367000	0.22958100
O	-0.23774800	-0.37602900	-0.32713600
C	1.05411200	-0.02734100	0.20341600
C	1.07997300	1.44910300	0.62443100
C	1.34974000	-0.93837700	1.40285700
C	-2.86833200	-1.42064800	-0.44581100
C	-2.38021200	1.62848400	-0.36022500
H	2.06570300	1.73361400	1.00345200
H	0.83713600	2.09386100	-0.22580000
H	0.35579000	1.63852500	1.42377800
H	2.33199300	-0.72571100	1.83516800
H	0.59904200	-0.79271700	2.18516900
H	1.32354500	-1.98711200	1.09196900
H	-2.83087700	-1.43726300	-1.54031600
H	-2.54255200	-2.40108900	-0.08479900
H	-3.91213300	-1.27552900	-0.14572900

H	-1.75843300	2.44037100	0.02907300
H	-2.35774200	1.68460300	-1.45413000
H	-3.41167800	1.80879900	-0.03547300
C	2.02056500	-0.29592400	-0.96889100
C	3.50804900	-0.05470100	-0.69315000
H	1.69063700	0.32829200	-1.80800200
H	1.86355800	-1.33539900	-1.27970200
H	3.88367600	-0.69403500	0.11217400
H	3.71107500	0.98520100	-0.41704200
H	-1.79978100	-0.07336900	1.72468100
H	4.09984800	-0.27500400	-1.58727300



G° = -681.1608613 Hartrees

Si	-2.20647500	-0.06178300	0.09229900
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C	0.58786300	0.12717100	0.47302400
C	0.49692000	1.65710800	0.56987300
C	0.72408100	-0.49753900	1.86842200
C	-3.15078400	-1.60697900	-0.40156500
C	-2.75853900	1.40920700	-0.94556700
H	1.40067700	2.07844900	1.01911900
H	0.36771200	2.09615700	-0.42409800
H	-0.34985100	1.95751300	1.19602900
H	1.61645800	-0.13314200	2.38598300
H	-0.14673000	-0.24876900	2.48216900
H	0.78697100	-1.58670800	1.78600300
H	-2.94887200	-1.86410400	-1.44689400
H	-2.85794400	-2.46164900	0.21613300
H	-4.23121200	-1.46077700	-0.29234200
H	-2.22231000	2.32178300	-0.66789500
H	-2.57334800	1.22238100	-2.00910100
H	-3.83119600	1.59701700	-0.81904400
C	1.73077400	-0.31220000	-0.46434500
C	3.15686700	0.06825800	-0.04839100
C	4.19776000	-0.42595600	-1.05961500
H	1.51538500	0.10370200	-1.45696600
H	1.65922700	-1.40223300	-0.56825800
H	3.38510500	-0.35219000	0.93868000
H	3.24331400	1.15738000	0.05280100
H	5.21340400	-0.14998000	-0.75775100
H	4.01542100	0.00108800	-2.05240900
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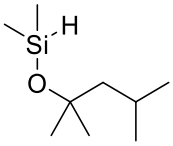

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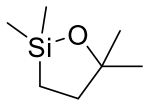
C	-0.27607	-0.29009	-1.65506
C	-0.41336	-1.92224	0.27267
C	3.5162	0.11853	1.56599
C	3.00718	1.13852	-1.30395
H	-1.19499	-0.6728	-2.10824
H	-0.16688	0.76266	-1.93332
H	0.55972	-0.85264	-2.08392
H	-1.32812	-2.38616	-0.10024
H	0.43811	-2.48133	-0.12712
H	-0.3983	-2.00961	1.36284
H	3.33116	1.10903	1.99526
H	3.25638	-0.62829	2.32256
H	4.58877	0.03556	1.35783
H	2.43935	1.00909	-2.23038
H	2.83354	2.15884	-0.9446
H	4.07223	1.04454	-1.54646
C	-1.40617	0.43936	0.51002
C	-2.81578	0.49309	-0.11434
C	-3.65418	1.53492	0.64609
H	-1.00001	1.45744	0.49914
H	-1.48971	0.15868	1.56863
H	-2.71775	0.84533	-1.15068
H	-4.64312	1.65558	0.19079
H	-3.16449	2.51464	0.65569
H	-3.80281	1.22726	1.68845
H	2.73512	-1.49254	-0.54667
C	-3.55732	-0.85194	-0.14155
H	-3.09294	-1.56985	-0.8229
H	-3.58329	-1.30523	0.85664
H	-4.59286	-0.71438	-0.4718

Three products



G° = -640.730435119 Hartrees

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6	1.93055	-1.43968	-0.09
6	2.46821	0.90678	-0.83414
6	-2.16855	-1.55865	-0.40052
6	-2.22632	1.53192	-0.38299
1	2.8902	-1.50868	0.43335
1	1.21155	-2.08058	0.43042
1	2.05491	-1.82693	-1.10514
1	3.39666	0.94714	-0.25439
1	2.69791	0.52444	-1.83313
1	2.0752	1.92236	-0.93821
1	-2.48179	-1.59303	-1.44955
1	-1.56568	-2.45084	-0.20187
1	-3.07177	-1.61463	0.21831
1	-3.1614	1.51849	0.18878
1	-1.67844	2.4419	-0.11665
1	-2.48543	1.59767	-1.4453
6	1.07083	0.54267	1.2687
6	-0.33222	0.01746	1.65822
1	1.0484	1.63906	1.2302
1	1.84529	0.26435	1.99292
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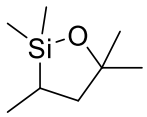
1	-0.80733	0.64939	2.41416



G° = -679.986495477 Hartrees

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6	-2.02671	-0.387	1.64527
6	1.58821	-0.08493	0.07409
6	-0.49981	1.15693	-0.654
6	2.65119	-0.11497	1.1713
6	2.18765	-0.52078	-1.27064
6	0.90792	1.30731	-0.0285
1	-3.04514	-0.04556	1.42776
1	-2.09936	-1.3538	2.15486
1	-1.57326	0.32425	2.34357
1	-2.81924	-1.3413	-1.42782
1	-1.2231	-1.78389	-2.06105
1	-1.93242	-2.70056	-0.72337
1	3.44435	0.61211	0.96617
1	2.19944	0.12278	2.13877
1	3.10016	-1.11043	1.23842
1	2.54776	-1.55076	-1.19658
1	3.02541	0.12478	-1.55545
1	1.43982	-0.48119	-2.06899
1	1.54127	2.0075	-0.58762
1	0.80265	1.71755	0.98554
1	-0.39381	1.0325	-1.74072
6	-1.41319	2.35897	-0.38404
1	-0.98234	3.29036	-0.77252
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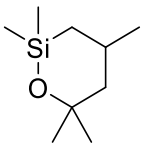

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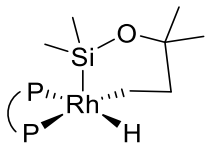
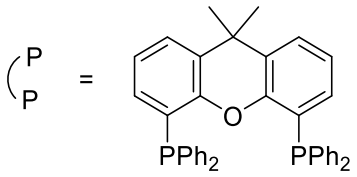
C	-1.67398	-2.24345	-0.93498
C	-1.26654	-1.50386	1.42856
C	2.81573	-0.10648	-1.30288
C	2.12957	-0.02577	1.70016
H	-2.75576	-2.31004	-0.77916
H	-1.48318	-2.02625	-1.98994
H	-1.22512	-3.21287	-0.69977
H	-2.3332	-1.58822	1.66146
H	-0.78334	-2.4594	1.65061
H	-0.83454	-0.74819	2.08982
H	3.31949	-1.07332	-1.19862
H	2.42738	-0.03886	-2.32419
H	3.56875	0.67915	-1.1723
H	1.36174	0.15993	2.45841

H	2.55886	-1.01411	1.89648
H	2.9228	0.71779	1.84248
C	-1.6761	0.21755	-0.41296
C	-1.02657	1.46315	0.22477
C	0.4245	1.65028	-0.28129
H	-2.73875	0.1816	-0.1409
H	-1.63716	0.33432	-1.5051
H	-1.00005	1.32412	1.31519
H	0.89344	2.50681	0.22018
H	0.39381	1.89661	-1.3527
C	-1.87664	2.71031	-0.05607
H	-2.89117	2.60715	0.34626
H	-1.42388	3.6026	0.3899
H	-1.96028	2.88406	-1.13594

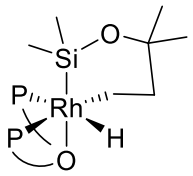


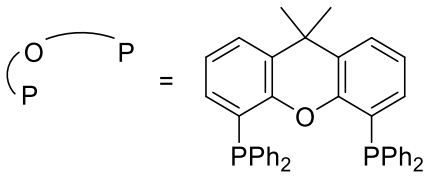


G° = -3014.135723 Hartrees

Rh	-0.53495900	1.33972400	0.56962500
P	1.83484200	0.86003800	0.38376300
P	-1.50365000	-0.94771600	0.53205500
Si	-1.00141500	2.07705600	-1.55004400
C	4.82460900	4.39846100	0.94023600
C	5.26049000	3.07960200	1.09736900
C	4.36246000	2.02400400	0.94995300
C	3.01218100	2.26948100	0.64344900
C	2.58542800	3.59460100	0.49458800
C	3.48683400	4.65227400	0.63928300
C	3.27790400	-1.94425500	3.80643100
C	3.73331500	-2.18521800	2.51009100
C	3.31666500	-1.37012000	1.45554900
C	2.43240700	-0.30813300	1.68658200
C	1.96990100	-0.08171000	2.99188100
C	2.39515100	-0.88870100	4.04481000
C	-0.29720200	-2.85982800	4.58888400
C	0.09800500	-3.48372700	3.40524500
C	-0.25985100	-2.94259500	2.16910100
C	-1.00954000	-1.76234500	2.10758600
C	-1.37887800	-1.12176900	3.30359300
C	-1.03597900	-1.67500000	4.53582600
C	-6.14473500	-1.25127500	0.42323500
C	-5.44328200	-1.97989800	1.38510200
C	-4.05204700	-1.88186900	1.46452200
C	-3.34814000	-1.04200700	0.58979800
C	-4.06227400	-0.30075900	-0.36573300
C	-5.44994400	-0.41354600	-0.45225200
O	-2.58099500	2.64372300	-1.66233500
H	5.52455300	5.22119500	1.05678400
H	6.29969700	2.87318000	1.33797300
H	4.71114000	1.00391400	1.07759900
H	1.54323700	3.79261300	0.27680100
H	3.13776700	5.67406100	0.51969400
H	3.60137700	-2.57975400	4.62587100
H	4.41761000	-3.00679000	2.31601400
H	3.68705700	-1.56186300	0.45374400
H	1.26939800	0.72731900	3.18258200
H	2.01965600	-0.70665900	5.04664700
H	-0.02238800	-3.28829100	5.54848200
H	0.68783000	-4.39494000	3.44102300
H	0.04337000	-3.44075400	1.25455300
H	-1.95396800	-0.19984400	3.26417500
H	-1.34094300	-1.17931500	5.45323500
H	-7.22616900	-1.33199300	0.35881400
H	-5.97582600	-2.63236500	2.07151600
H	-3.53935600	0.38189100	-1.02889700
H	-5.98685900	0.16743700	-1.19616500
H	-3.51716600	-2.46713200	2.20498700
C	3.24101000	-1.06896100	-3.60931500
C	3.75023100	0.18398800	-3.25813800
C	3.40304200	0.78272300	-2.04575400
C	2.51068200	0.14374100	-1.17374800
C	2.00356200	-1.09449200	-1.57364500
O	1.09156800	-1.68242200	-0.71877100
C	0.06756700	-2.37155600	-1.33392200
C	-1.20814300	-2.23293700	-0.77932200
C	-2.23803400	-2.98295400	-1.37152800
C	-1.98922800	-3.77606600	-2.49031400
C	-0.71219100	-3.83544400	-3.05139800
C	0.34795400	-3.13364600	-2.47414400

C	1.79786900	-3.15242600	-2.97215100
C	2.35966300	-1.74302100	-2.75783200
C	2.60817900	-4.13342100	-2.07807200
C	1.90337600	-3.60116000	-4.43589300
C	-0.96818800	0.69736200	-2.84670400
C	0.19413700	3.41244000	-2.17526200
C	-3.26005800	3.59891300	-0.83265100
C	-2.34766500	2.23555000	1.19348000
C	-3.08732600	4.98938300	-1.46199100
C	-4.74389200	3.20474800	-0.86105800
C	-2.73241700	3.60640600	0.62911800
H	3.53827700	-1.51896800	-4.54993700
H	4.43222600	0.69387200	-3.93180200
H	3.81697700	1.74900300	-1.77990600
H	-3.24417000	-2.92491400	-0.97606200
H	-2.80182700	-4.33962700	-2.93862500
H	-0.54796200	-4.43502900	-3.93981700
H	3.66053700	-4.14077200	-2.38050700
H	2.55405200	-3.83816400	-1.02653200
H	2.20801400	-5.14827100	-2.17165900
H	2.94764900	-3.61169500	-4.75993200
H	1.52630900	-4.62017500	-4.55777900
H	1.33922500	-2.93947900	-5.09971500
H	-0.07570600	3.70529200	-3.19708600
H	0.17286400	4.30622700	-1.54546900
H	1.22168600	3.03285000	-2.18800400
H	0.04381700	0.29789600	-2.96437400
H	-1.63191200	-0.13410000	-2.60006000
H	-1.28465800	1.11324000	-3.81088000
H	-3.59989000	5.75188900	-0.86499200
H	-2.02819600	5.25536200	-1.52021500
H	-3.50077400	5.00223500	-2.47524500
H	-5.06762400	3.05649500	-1.89603700
H	-5.36019900	3.98979800	-0.41053600
H	-4.91304700	2.28001700	-0.30697200
H	-3.52917400	4.06645500	1.23454400
H	-1.87000700	4.27948500	0.69784700
H	-2.09666000	2.35888500	2.26195000
H	-3.20293400	1.55680100	1.13913800
H	-0.08803800	2.83283300	0.74298800





G° = -3014.130476 Hartrees

Rh	0.26627000	-0.91005000	-0.65042900
P	-1.87049600	-0.42887300	0.31923300
P	1.75661500	0.69039200	0.46604300
Si	0.76704500	-2.96095200	0.23780000
C	-5.15588300	-3.66713200	-0.34467200
C	-5.00700700	-3.09877800	0.91939600
C	-4.04084700	-2.11291400	1.14093000
C	-3.20430800	-1.69363500	0.09866500
C	-3.36186600	-2.27101500	-1.17200000
C	-4.33257500	-3.24480100	-1.39295100
C	-2.67005000	0.68408400	4.75908100
C	-3.32744100	1.41506100	3.76828300
C	-3.09164600	1.14290400	2.41982300
C	-2.18897300	0.13689100	2.04701100
C	-1.51153400	-0.57262300	3.05048400
C	-1.75796600	-0.30862000	4.39662200
C	0.48309400	2.29725900	4.64484400
C	0.00129200	2.91255000	3.48942200
C	0.40340300	2.46097000	2.23206200
C	1.29143000	1.38330400	2.11322600
C	1.75271000	0.75431600	3.28179900
C	1.35938400	1.21571000	4.53661600
C	6.30711900	-0.15033800	0.97312200
C	5.74643100	0.96420700	1.60345800
C	4.38422600	1.23186800	1.47195100
C	3.56331700	0.39311800	0.69663300
C	4.13296800	-0.73099200	0.08654700
C	5.49642600	-1.00033000	0.22084200
O	1.76646400	-3.88321500	-0.75192500
H	-5.90544200	-4.43487300	-0.51427100
H	-5.64182800	-3.42003000	1.74049100
H	-3.94044700	-1.67968200	2.12990300
H	-2.70746500	-1.96480900	-1.98202300

H	-4.44006400	-3.68207500	-2.38162200
H	-2.85738500	0.89573800	5.80797100
H	-4.02854300	2.19822400	4.04372000
H	-3.61285800	1.71764600	1.66224400
H	-0.78819200	-1.33127200	2.76892100
H	-1.22357600	-0.86579500	5.16007000
H	0.16887100	2.65081500	5.62240500
H	-0.69338100	3.74390200	3.56388100
H	0.02520800	2.95438500	1.34198600
H	2.43049000	-0.09041200	3.20999500
H	1.73361900	0.72468300	5.43067400
H	7.36747800	-0.36027800	1.08147300
H	6.36826600	1.62047900	2.20597400
H	3.50136000	-1.40537500	-0.47446400
H	5.91682400	-1.88131700	-0.25542000
H	3.95382800	2.07876900	1.99728700
C	-3.41938100	3.17604400	-2.22515500
C	-4.34319500	2.37185500	-1.54905000
C	-3.91813700	1.26382000	-0.81681500
C	-2.55374400	0.94573700	-0.73213500
C	-1.67359000	1.74263700	-1.46949700
O	-0.33942700	1.38202500	-1.47472200
C	0.58024500	2.41367600	-1.40955100
C	1.70371500	2.22481600	-0.59771200
C	2.64978500	3.25977900	-0.58509000
C	2.43536300	4.42722800	-1.31690600
C	1.27174900	4.59314700	-2.07436800
C	0.31737500	3.57589900	-2.14210100
C	-0.95880100	3.59651300	-2.99627200
C	-2.05723400	2.86566600	-2.20973800
C	-1.37564400	5.02500800	-3.37396700
C	-0.67944800	2.78586900	-4.29437900
C	-0.74619000	-4.03628200	0.63179000
C	1.75478800	-2.83983000	1.85932500
C	1.90446500	-3.83743800	-2.17466200
C	1.60159500	-1.20315200	-2.30813900
C	2.95276700	-4.90993800	-2.50452400
C	0.57999200	-4.18376100	-2.87213800
C	2.44295900	-2.45238000	-2.60575300
H	-3.77446900	4.03613900	-2.78218500
H	-5.40082700	2.61283400	-1.59753100
H	-4.64103300	0.63988300	-0.30037500
H	3.55382000	3.15575500	0.00313900
H	3.17669500	5.22024100	-1.29266100
H	1.12112300	5.51777000	-2.62062600
H	-2.27175700	5.01281800	-3.99990500
H	-1.57827600	5.63368200	-2.48763200
H	-0.59236900	5.51341200	-3.95965900
H	-1.57983100	2.74606600	-4.91595200
H	0.12436100	3.25888600	-4.86755400
H	-0.37694800	1.76211500	-4.05910200
H	1.95820300	-3.84668800	2.24376300
H	2.71143600	-2.33390000	1.70829200
H	1.20050000	-2.28980000	2.62737400
H	-1.38089900	-3.58788800	1.40332800
H	-1.36743900	-4.18721300	-0.25485500
H	-0.41167000	-5.01638600	0.99268400
H	3.16309500	-4.94145900	-3.57892100
H	3.88444000	-4.69971500	-1.97004400
H	2.59460900	-5.89406700	-2.18776100
H	-0.59797100	-1.88550500	-1.52227100
H	0.20933400	-5.14818500	-2.51063800
H	0.72572200	-4.25080700	-3.95613400
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H	2.63739400	-2.50708600	-3.68838500
H	3.43162000	-2.36220800	-2.13924300
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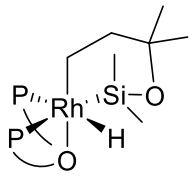

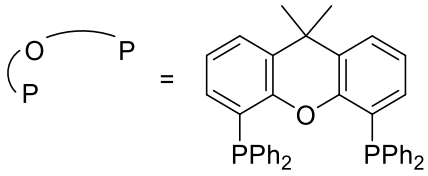

G° = -3014.122092 Hartrees

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P	-1.40529300	-1.04273300	0.70207300
Si	-2.16458400	1.76871500	-1.48746200
C	4.53211100	4.62208600	0.94320700
C	5.09509500	3.39536100	1.30185900
C	4.36095400	2.21740800	1.15775900
C	3.05261500	2.25072900	0.64610600
C	2.49154900	3.48973100	0.29935300
C	3.22942500	4.66550100	0.44310600
C	4.10893100	-1.99982300	3.58195500
C	4.38753400	-2.21878200	2.23338800
C	3.77439100	-1.43731400	1.25052000
C	2.87235500	-0.42464500	1.60683000
C	2.57581000	-0.23436700	2.96747500
C	3.19552300	-1.00696800	3.94589500
C	0.88189700	-3.47431100	3.94888800
C	1.14931600	-3.70831300	2.60060600
C	0.45812200	-3.00463300	1.61313200
C	-0.51191100	-2.05624200	1.96343200
C	-0.75556200	-1.80799800	3.32500500
C	-0.07067200	-2.51818300	4.30890600
C	-5.83113600	-1.46021300	2.07537900
C	-4.94668700	-2.52140400	2.29048500
C	-3.61491300	-2.41368100	1.89215900
C	-3.15139900	-1.24476800	1.26134300
C	-4.04288500	-0.18198600	1.05976600
C	-5.37546700	-0.29238000	1.46401400
O	-3.35887000	2.59684400	-0.61417500
H	5.10359600	5.53874700	1.05936400
H	6.10635500	3.35382400	1.69722500
H	4.80416800	1.27141400	1.45275600
H	1.47571200	3.52120700	-0.08137400
H	2.78075000	5.61673800	0.17075300
H	4.58851600	-2.60633900	4.34497200
H	5.08776500	-2.99655800	1.94045800
H	4.01071200	-1.61521300	0.20718900
H	1.85312200	0.52331200	3.25895800
H	2.95399700	-0.84504100	4.99219300
H	1.42153800	-4.02325800	4.71492200
H	1.90398200	-4.43398300	2.31318800
H	0.67330200	-3.20105300	0.56748900
H	-1.50136300	-1.07306300	3.61505600
H	-0.27970200	-2.32334500	5.35717800
H	-6.86734100	-1.54381900	2.39123600
H	-5.29227000	-3.43043400	2.77500800
H	-3.70635100	0.73268300	0.58670500
H	-6.04925700	0.54369700	1.30143700
H	-2.92890700	-3.23115500	2.09140300
C	3.33730600	-1.20440100	-3.61989700
C	4.28403500	-0.49309900	-2.87617500
C	3.92222000	0.14355400	-1.68877100
C	2.60281700	0.07793100	-1.21869300
C	1.67960600	-0.59513900	-2.02407100
O	0.35211500	-0.59361800	-1.61812800
C	-0.36296000	-1.77089400	-1.79927000
C	-1.28224000	-2.12754900	-0.80781600
C	-2.02155700	-3.29763200	-1.02483100
C	-1.81451400	-4.06405900	-2.17142700
C	-0.87149000	-3.67775400	-3.12838800
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C	0.85296900	-1.91553700	-3.98731300
C	2.00220900	-1.25966200	-3.21010300
C	1.35699300	-2.97317500	-4.97920700
C	0.10881800	-0.79559200	-4.77033600
C	-3.16178500	0.40015900	-2.35474200
C	-1.59541500	2.90012700	-2.90964800
C	-3.15139500	3.67268800	0.31110800
C	-1.08182500	2.40758700	1.30653000
C	-3.48544100	4.98353100	-0.41724700
C	-4.14994300	3.45212700	1.45829900
C	-1.70046100	3.73187700	0.85141500
H	3.64529300	-1.70193400	-4.53287800
H	5.31089500	-0.44042400	-3.22524900
H	4.66574800	0.68274900	-1.11034200
H	-2.76404500	-3.60488400	-0.29674800
H	-2.39514400	-4.96848600	-2.32572300

H	-0.73163800	-4.29000600	-4.01226900
H	2.02753500	-2.52270500	-5.71579500
H	1.89048500	-3.78196100	-4.47080100
H	0.52303100	-3.40426400	-5.53907300
H	0.78578400	-0.32871100	-5.49288500
H	-0.74724300	-1.21541000	-5.30809600
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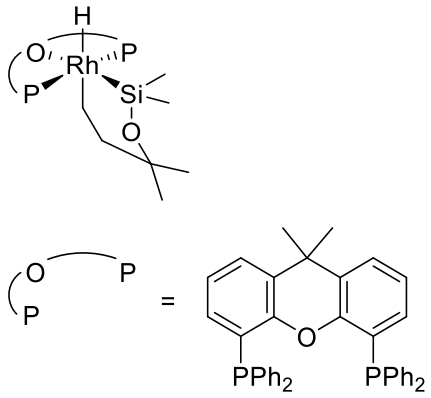
H	-2.43958300	3.20497600	-3.54039500
H	-1.10382600	3.79996800	-2.52608700
H	-0.86559000	2.37769700	-3.54072700
H	-2.53004500	-0.15105200	-3.06008600
H	-3.58905600	-0.32217600	-1.65581000
H	-3.98159000	0.85612400	-2.92297500
H	-3.35982400	5.84783700	0.24470000
H	-2.82909600	5.11071600	-1.28293900
H	-4.51979000	4.96236900	-0.77384600
H	0.12669700	2.27324800	-0.89770700
H	-5.15579100	3.32542600	1.04602700
H	-4.15750400	4.30784000	2.14173700
H	-3.90306500	2.55628200	2.03355500
H	-1.71714000	4.43778200	1.69674300
H	-1.05296100	4.18916600	0.09232000
H	-0.16328100	2.62945500	1.86276300
H	-1.76374200	1.88018700	1.98440400



G° = -3014.122180 Hartrees

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P	2.27357300	0.01548400	0.31708200
Si	-0.10721700	-2.65995400	0.79562700
C	-5.14765800	-1.61417700	-2.94157300
C	-5.07412800	-0.23300600	-2.75581100
C	-4.19684600	0.30407600	-1.81070600
C	-3.37681600	-0.53807000	-1.04611300
C	-3.43285000	-1.92487400	-1.26076300
C	-4.32276800	-2.45699700	-2.19338600
C	-4.68873000	-0.54905700	4.18128500
C	-3.35402200	-0.13685300	4.22749800
C	-2.62713400	0.02192600	3.04959900
C	-3.22970000	-0.21835800	1.80563600
C	-4.57144000	-0.62345000	1.76440500
C	-5.29404500	-0.79215000	2.94856200
C	4.59051400	-0.35209600	4.34366800
C	5.30825600	-0.27359600	3.14892500
C	4.63427800	-0.17898700	1.93068200
C	3.22971600	-0.16149700	1.89008100
C	2.51851300	-0.24382600	3.09609500
C	3.19495800	-0.33605600	4.31293800
C	4.85121800	-1.74292800	-3.12489500
C	4.87683400	-2.34531700	-1.86590700
C	4.16493400	-1.78519700	-0.80522700
C	3.42215200	-0.60623400	-0.98416100
C	3.40899600	-0.00634200	-2.25302800
C	4.11688000	-0.57078000	-3.31363400
O	-0.61350700	-3.62684100	-0.49139200
H	-5.83412200	-2.03076300	-3.67329100
H	-5.70161900	0.43115800	-3.34376000
H	-4.15846700	1.37899300	-1.67369600
H	-2.75483200	-2.58552100	-0.72907400
H	-4.35103600	-3.53126500	-2.34944800
H	-5.25095800	-0.68346700	5.10113200
H	-2.87429300	0.04936100	5.18440300
H	-1.58044200	0.30976100	3.07699100
H	-5.05479700	-0.81367700	0.81251900
H	-6.33037100	-1.11498200	2.90289500
H	5.11610000	-0.42982200	5.29125100
H	6.39446600	-0.28863100	3.16182900
H	5.20886400	-0.13264900	1.01148500
H	1.43313700	-0.23705600	3.06070200
H	2.62834700	-0.40284800	5.23742800
H	5.39936800	-2.18355800	-3.95254300
H	5.44608000	-3.25676900	-1.70750700
H	2.83854800	0.90225200	-2.41588200
H	4.09133900	-0.09444600	-4.28955600
H	4.18842200	-2.26960900	0.16486500
C	-2.35224300	4.67279600	-0.23537500
C	-3.45458400	3.99850600	0.29145600
C	-3.41253700	2.61640000	0.45116700
C	-2.26263800	1.88486300	0.11652500
C	-1.15391200	2.60108600	-0.35572700
O	0.02147800	1.90377200	-0.61347400
C	1.22146500	2.57970300	-0.42470400
C	2.33995100	1.85112800	0.00655800
C	3.54081400	2.55524800	0.18051700
C	3.61280000	3.92485900	-0.04828100
C	2.48267700	4.61878900	-0.48151400
C	1.27215200	3.95634200	-0.69238000
C	0.02095400	4.61564600	-1.27380700
C	-1.18756100	3.98392100	-0.58245900
C	0.04430900	6.14400700	-1.12863400
C	-0.05233300	4.25781800	-2.78667500
C	-1.38397300	-3.08963500	2.12336300
C	1.55756700	-3.33268400	1.41739100
C	0.00602500	-3.74834300	-1.78494200
C	0.07409400	-1.14157000	-1.87859600
C	0.96522300	-4.94885400	-1.74117200
C	-1.12242800	-4.04314800	-2.78289300
C	0.77602000	-2.46773000	-2.19269200
H	-2.40691500	5.74586000	-0.37784800
H	-4.34826900	4.55039800	0.56588400
H	-4.27381200	2.08980500	0.84930900

H	4.42333900	2.02342300	0.51619000
H	4.54862400	4.45314700	0.10571900
H	2.55381300	5.68455500	-0.66541700
H	-0.85165300	6.58628000	-1.57174700
H	0.10241300	6.45013600	-0.07989400
H	0.89699300	6.56968600	-1.66369000
H	-0.95934100	4.68010400	-3.23122900
H	0.81924000	4.66174100	-3.31199100
H	-0.07112000	3.17460400	-2.93342900
H	1.44705800	-4.39210200	1.67774500
H	2.32946900	-3.25543300	0.64815600
H	1.90341000	-2.78985000	2.30151900
H	-1.21533200	-2.50363300	3.03159600
H	-2.40983900	-2.90170500	1.79672300
H	-1.29513700	-4.15398500	2.37115800
H	1.45367300	-5.08864600	-2.71202100
H	1.74260500	-4.79666700	-0.98815000
H	0.41860500	-5.86339000	-1.48972700
H	-1.74690100	-4.85997300	-2.40661600
H	-0.70784000	-4.33941100	-3.75218900
H	-1.75263900	-3.16630500	-2.93577000
H	0.98003700	-2.56527200	-3.27157400
H	1.75937200	-2.48979700	-1.71243300
H	0.61004000	-0.33688200	-2.40117000
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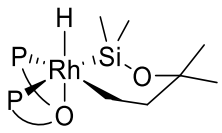

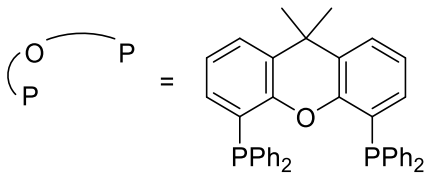

G° = -3014.110061Hartrees

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P	-2.06526800	0.28759400	-0.37230300
Si	2.13765800	-2.03934100	-1.20552000
C	5.67765300	2.04054800	-2.35884700
C	5.69233400	1.75019400	-0.99546800
C	4.49747100	1.51618800	-0.30910500
C	3.26972700	1.57013300	-0.98024000
C	3.26733000	1.84510600	-2.35862700
C	4.45826800	2.08484300	-3.04019800
C	-0.35398800	5.44334600	-0.72441500
C	0.53522100	5.23362400	0.33195300
C	1.14143700	3.98943200	0.50342700
C	0.86047600	2.93471700	-0.37595300
C	-0.03080000	3.15656900	-1.43625300
C	-0.63191800	4.40305300	-1.61130600
C	-3.43181100	4.45437300	1.22474700
C	-2.33154100	3.78354200	1.76544800
C	-1.96706500	2.53222800	1.27806400
C	-2.69597200	1.92229000	0.24259200
C	-3.80321600	2.59790500	-0.28679100
C	-4.16524200	3.85659800	0.20115400
C	-5.22874100	-1.17501200	-3.44175600
C	-5.08141700	-1.88147700	-2.24844800
C	-4.17399900	-1.44994100	-1.27832200
C	-3.40104500	-0.30010800	-1.48826400
C	-3.53402500	0.38558700	-2.70939100
C	-4.44911400	-0.03830600	-3.67099200
O	1.66916800	-3.59423300	-0.73591000
H	6.60787000	2.21909000	-2.89027100
H	6.63549300	1.69515800	-0.45909300
H	4.53882100	1.25582500	0.74094500
H	2.32675200	1.85330200	-2.90215100
H	4.43495500	2.29384400	-4.10585000
H	-0.83484700	6.40921100	-0.84846200
H	0.75256800	6.03866800	1.02859200
H	1.81642500	3.84391200	1.33890100
H	-0.27067800	2.33291100	-2.10257100
H	-1.33313500	4.55371700	-2.42684100
H	-3.71238200	5.43449900	1.59960300
H	-1.74677300	4.24108700	2.55766600
H	-1.10229400	2.03057200	1.70220000
H	-4.39399300	2.14537200	-1.07525400
H	-5.02828600	4.36500800	-0.22022400
H	-5.93483900	-1.51349400	-4.19437400
H	-5.66807300	-2.77819600	-2.07017100
H	-2.91150700	1.25359200	-2.91098700
H	-4.54256700	0.50968200	-4.60419600
H	-4.05695000	-2.02777600	-0.36930500
C	2.03106400	0.15111300	4.26772600
C	2.78585700	1.21581300	3.76836100

C	2.68622400	1.58919000	2.42894300
C	1.82075300	0.91543700	1.54970500
C	1.06301400	-0.12784600	2.10408900
O	0.14167300	-0.79714300	1.29910900
C	-1.09366800	-1.02136500	1.90634000
C	-2.25310700	-0.65578900	1.21749000
C	-3.47307000	-0.85491700	1.88455300
C	-3.50325800	-1.40850100	3.16252400
C	-2.31507900	-1.72906400	3.82782900
C	-1.07994600	-1.52559600	3.21045400
C	0.29861500	-1.75782500	3.84125300
C	1.15396100	-0.54756900	3.43612400
C	0.21266000	-1.92278700	5.36392600
C	0.93502600	-3.03912600	3.22873800
C	3.52102100	-1.81655800	0.08208500
C	3.00179800	-2.08253500	-2.89541400
C	0.55730800	-4.35603800	-1.20857200
C	-0.85448500	-2.24263100	-1.75671000
C	1.12796500	-5.62690900	-1.85383000
C	-0.28494000	-4.72221400	0.02342200
C	-0.26988200	-3.56812700	-2.24284800
H	2.13343600	-0.13138400	5.30954000
H	3.46267500	1.75138400	4.42707900
H	3.29338900	2.40870500	2.06213500
H	-4.39709700	-0.54501300	1.40753000
H	-4.45580700	-1.56315300	3.66026800
H	-2.36020600	-2.11994400	4.83820200
H	1.20601300	-2.09305000	5.78793400
H	-0.22649300	-1.04369000	5.84570900
H	-0.39296900	-2.79680800	5.61859900
H	1.93094500	-3.19847700	3.65417200
H	0.31287900	-3.90924400	3.46109800
H	1.03437800	-2.97233100	2.14357900
H	3.78124300	-2.85356700	-2.92509200
H	2.29370700	-2.26849700	-3.70822100
H	3.47209400	-1.10920200	-3.08019300
H	4.19697400	-0.99591800	-0.16264200
H	3.13781700	-1.66331800	1.09507000
H	4.10018000	-2.74705200	0.08497500
H	0.32785000	-6.29327700	-2.19551800
H	1.75198900	-5.36187400	-2.71306800
H	1.75102000	-6.16656100	-1.13391100
H	0.56287700	-0.37906100	-2.56686400
H	0.32924100	-5.28089200	0.73653800
H	-1.14904100	-5.33716900	-0.25214800
H	-0.64461600	-3.81946300	0.52357000
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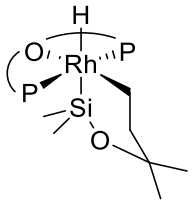

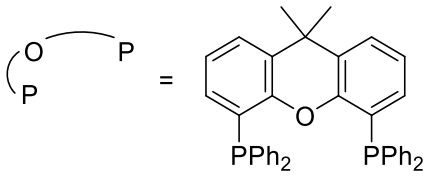

G° = -3014.085681 Hartrees

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Si	0.23283900	-1.31773600	-2.22692100
C	-6.08362700	-1.95540900	-1.27950400
C	-6.18018000	-1.21694200	-0.09641800
C	-5.03992900	-0.65077300	0.47295000
C	-3.78590000	-0.80727900	-0.14310400
C	-3.70023600	-1.55989000	-1.31840700
C	-4.84022300	-2.12927700	-1.88786900
C	-3.11749700	-0.15267600	5.09626900
C	-2.85948000	1.07144700	4.47664300
C	-2.62559800	1.13048100	3.10171800
C	-2.65299300	-0.03725800	2.32974400
C	-2.91776600	-1.26521500	2.95729300
C	-3.14566600	-1.32156600	4.33171000
C	3.17765500	0.95774400	4.91964300
C	3.50101700	1.90177500	3.94685300
C	3.21704400	1.65199100	2.59970500
C	2.59497800	0.45748300	2.21902000
C	2.25973900	-0.48312200	3.20674500
C	2.55702700	-0.23865500	4.54442800
C	5.90778100	-2.59683800	-0.58470500
C	6.05857300	-1.49450300	0.26099500
C	4.95553800	-0.70541000	0.58497200
C	3.68928600	-0.99544600	0.04577300

C	3.54323400	-2.11413000	-0.78716200
C	4.64910800	-2.90753700	-1.09948700
O	0.65408500	-2.97343800	-2.24694700
H	-6.97309700	-2.40011000	-1.71686200
H	-7.14413600	-1.08825100	0.38808400
H	-5.12376800	-0.10563500	1.40787500
H	-2.73300100	-1.70135200	-1.77788500
H	-4.75135500	-2.71149000	-2.80068800
H	-3.29602200	-0.19599300	6.16682400
H	-2.83737300	1.98536700	5.06384100
H	-2.41220500	2.08631100	2.63433000
H	-2.94810200	-2.17871000	2.36939600
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H	3.97339500	2.83835600	4.23029200
H	3.47308000	2.39887900	1.85586000
H	1.73980100	-1.39343600	2.92348000
H	2.29188100	-0.97500000	5.29778400
H	6.76652400	-3.21599400	-0.82894400
H	7.03237100	-1.25633300	0.67975500
H	2.57331300	-2.37532100	-1.19340000
H	4.51535700	-3.77175200	-1.74343800
H	5.07706400	0.12210600	1.27713300
C	-2.47011800	4.30495100	-1.07252600
C	-3.57033800	3.74488700	-0.42101500
C	-3.50208500	2.44428200	0.06959100
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C	-1.21765200	2.31812900	-0.64062400
O	-0.03372600	1.60107000	-0.71310600
C	1.17816800	2.25679200	-0.89273700
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C	3.56983300	2.21510200	-0.72548300
C	3.62187300	3.45226900	-1.36418900
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C	-0.07458900	5.57209400	-2.27353300
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C	1.67597700	-0.50086700	-3.18493100
C	-1.14570200	-1.07279600	-3.55466200
C	0.07447000	-4.02589900	-1.46886900
C	0.06430000	-2.54303200	0.71846000
C	-0.93627900	-4.76560900	-2.36225700
C	1.23186000	-4.97447200	-1.11382200
C	-0.65049200	-3.55624100	-0.17600100
H	-2.55655500	5.30074400	-1.49137900
H	-4.48968100	4.31414100	-0.32513100
H	-4.37598800	1.99578500	0.52884900
H	4.48872400	1.71573700	-0.43852500
H	4.58100900	3.91921400	-1.56532200
H	2.50529100	5.04436200	-2.26119800
H	-1.00040500	5.93927000	-2.72280900
H	0.07141200	6.07425600	-1.31276600
H	0.73077700	5.86999800	-2.94884100
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H	0.49011800	3.65590500	-4.18152800
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H	-0.69049100	-1.05595900	-4.55271200
H	-1.89602100	-1.86922800	-3.56480100
H	-1.67711900	-0.12311100	-3.41065900
H	1.39793300	0.53154200	-3.43412300
H	2.62609500	-0.46043400	-2.64902000
H	1.83992400	-1.03269500	-4.13063900
H	-1.38050700	-5.62076400	-1.84014200
H	-1.74364100	-4.08986800	-2.66106500
H	-0.44048400	-5.12459400	-3.26901000
H	1.77420400	-5.24217800	-2.02563200
H	0.86206000	-5.89186200	-0.64354000
H	1.93626700	-4.49750800	-0.42729100
H	-0.83368700	-4.47400800	0.40672400
H	-1.64577900	-3.17622600	-0.43141800
H	-0.39945500	-2.53919500	1.71072900
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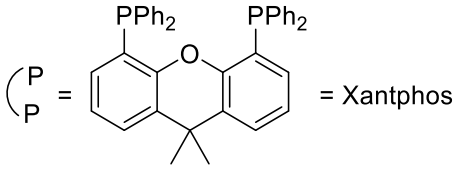
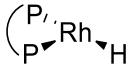
H	-0.06862300	-0.00273600	1.65755000

For the following complexes



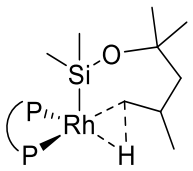


G° = -2,371.799286 Hartrees

6	-2.41478	3.83906	-1.0833
6	-3.53257	3.03105	-1.28946
6	-3.48682	1.68219	-0.94703
6	-2.32167	1.1082	-0.41722

6	-1.19812	1.94017	-0.27573
8	0.00001	1.36778	0.17048
6	1.19814	1.94017	-0.27573
6	2.32169	1.1082	-0.41723
6	3.48684	1.6822	-0.94704
6	3.53259	3.03107	-1.28945
6	2.4148	3.83907	-1.0833
6	1.23068	3.31149	-0.55941
6	0.00001	4.14601	-0.20539
6	-1.23067	3.31149	-0.55942
1	-2.46961	4.89186	-1.33438
1	-4.43933	3.45619	-1.70889
1	-4.35715	1.05366	-1.10608
1	4.35717	1.05368	-1.1061
1	4.43934	3.45622	-1.70888
1	2.46962	4.89187	-1.33436
6	0.	4.37178	1.33433
6	0.	5.51373	-0.90337
6	-4.71769	-2.71966	-3.26907
6	-5.3715	-2.2855	-2.11426
6	-4.64843	-1.67893	-1.0849
6	-3.26241	-1.50107	-1.20536
6	-2.60943	-1.95614	-2.36088
6	-3.33522	-2.55512	-3.38998
1	-5.28166	-3.1937	-4.06762
1	-6.44455	-2.42203	-2.01152
1	-5.16124	-1.35279	-0.18483
1	-1.53002	-1.84574	-2.42984
1	-2.82126	-2.90412	-4.28132
6	-4.79077	-1.17203	3.92785
6	-4.94212	-0.00588	3.17654
6	-4.19304	0.18442	2.01245
6	-3.27797	-0.79089	1.59062
6	-3.11862	-1.95346	2.36443
6	-3.87658	-2.14639	3.51822
1	-5.37483	-1.31748	4.83226
1	-5.64404	0.76011	3.49498
1	-4.31979	1.09805	1.44126
1	-2.38486	-2.6953	2.06101
1	-3.74448	-3.05126	4.10472
6	4.79052	-1.17196	3.928
6	3.87635	-2.14632	3.51834
6	3.11847	-1.95342	2.36448
6	3.27789	-0.79087	1.59065
6	4.19293	0.18445	2.01252
6	4.94193	-0.00583	3.17667
1	5.37452	-1.31739	4.83245
1	3.74421	-3.05117	4.10485
1	2.38472	-2.69526	2.06103
1	4.31973	1.09805	1.44131
1	5.64384	0.76017	3.49513
6	4.71787	-2.71977	-3.2689
6	3.3354	-2.5553	-3.38986
6	2.60955	-1.95627	-2.36082
6	3.26247	-1.50109	-1.20532
6	4.6485	-1.67887	-1.08481
6	5.37162	-2.28548	-2.1141
1	5.28188	-3.19384	-4.0674
1	2.82147	-2.90439	-4.28118
1	1.53013	-1.84593	-2.42982
1	5.16127	-1.35265	-0.18475
1	6.44468	-2.42195	-2.01132
1	-0.89043	4.93428	1.63337
1	-0.00002	3.41912	1.87043
1	0.89045	4.93425	1.63338
1	-0.87571	6.09713	-0.6076
1	0.87571	6.09713	-0.6076
1	0.	5.41269	-1.99278
45	0.00002	-0.97795	0.26725
15	-2.22534	-0.68076	0.07772
15	2.22534	-0.68074	0.07769
1	0.00006	-2.52857	0.24628

TS-OxAdd-δ



G° = -3091.01117 Hartrees

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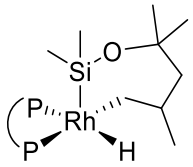
14	1.69281	0.64319	-1.7041
6	4.51308	-4.3422	1.0022
6	3.35139	-4.73384	1.67315
6	2.18763	-3.97277	1.55804
6	2.17499	-2.8046	0.77817
6	3.3481	-2.4118	0.11753
6	4.50721	-3.18346	0.22363
6	-1.29176	-2.08069	4.78804

6	-2.04373	-2.42771	3.66441	6	-2.25436	1.16506	-1.22923
6	-1.47968	-2.36712	2.39036	6	-2.75109	2.08593	-2.16311
6	-0.14958	-1.95695	2.2244	6	-3.44947	1.64821	-3.28936
6	0.5969	-1.59304	3.36009	6	-3.69399	0.2881	-3.49136
6	0.03091	-1.66098	4.63248	6	-3.23294	-0.6607	-2.57358
6	-3.79236	0.62895	3.95606	6	-3.52077	-2.16558	-2.62223
6	-4.36071	0.49033	2.6898	6	-2.24801	-2.8777	-2.15121
6	-3.60626	0.76063	1.54583	6	-4.65695	-2.46992	-1.60446
6	-2.27043	1.16857	1.65671	6	-3.96301	-2.62802	-4.01708
6	-1.70365	1.29221	2.9353	6	1.1291	2.20951	-2.62992
6	-2.45978	1.02992	4.0756	6	1.12402	-0.77384	-2.82104
6	-1.41234	6.24913	0.33226	6	4.53393	1.26935	-1.5376
6	-2.56358	5.50346	0.60579	6	3.45109	2.76715	0.35731
6	-2.52045	4.11023	0.57131	6	2.45102	2.08623	1.30335
6	-1.32545	3.44259	0.25522	6	5.70759	0.29819	-1.74271
6	-0.17685	4.19955	-0.00801	6	4.63202	2.40972	-2.56413
6	-0.21844	5.59523	0.02676	6	4.58305	1.80543	-0.08756
8	3.36562	0.49009	-1.80093	1	-2.26758	-4.56702	-3.49112
1	5.41874	-4.93587	1.09132	1	-0.22962	-5.59099	-2.55063
1	3.35153	-5.63101	2.28617	1	1.01016	-4.48007	-0.73531
1	1.28696	-4.28257	2.07982	1	-2.57987	3.14618	-2.01286
1	3.35863	-1.49582	-0.46471	1	-3.81574	2.37357	-4.00964
1	5.40785	-2.87247	-0.29865	1	-4.25289	-0.02828	-4.36496
1	-1.73631	-2.1303	5.77796	1	-4.86146	-3.54524	-1.57669
1	-3.07768	-2.74003	3.7775	1	-4.37748	-2.14691	-0.59793
1	-2.07677	-2.64038	1.52788	1	-5.57373	-1.94484	-1.89232
1	1.62932	-1.27505	3.24277	1	-4.18775	-3.69798	-4.0158
1	0.62355	-1.38665	5.50092	1	-4.87934	-2.11419	-4.31991
1	-4.38004	0.41749	4.8449	1	-3.19119	-2.43566	-4.76816
1	-5.39588	0.17542	2.58822	1	1.49121	-1.74582	-2.48421
1	-4.06452	0.65954	0.56739	1	0.03254	-0.82452	-2.87674
1	-0.66415	1.59287	3.03763	1	1.51114	-0.59401	-3.83114
1	-2.00291	1.12152	5.05616	1	0.03706	2.21743	-2.70543
1	-1.44754	7.33454	0.36379	1	1.43988	3.1551	-2.18337
1	-3.49395	6.009	0.84964	1	1.53754	2.1656	-3.64703
1	0.74827	3.68529	-0.23449	1	6.67008	0.80439	-1.61605
1	0.6821	6.16682	-0.17994	1	5.64708	-0.51997	-1.01881
1	-3.41483	3.53632	0.79549	1	5.66411	-0.12981	-2.74824
6	-1.75434	-4.07703	-2.67126	1	2.49538	0.59421	0.93352
6	-0.599	-4.65488	-2.14256	1	4.59448	1.99696	-3.57645
6	0.09551	-4.03299	-1.1062	1	5.57302	2.95712	-2.44452
6	-0.35371	-2.81744	-0.56614	1	3.80965	3.1206	-2.46069
6	-1.53696	-2.28968	-1.09962	1	5.5522	2.30865	0.01945
8	-1.99367	-1.09754	-0.56718	1	4.61267	0.94164	0.58765
6	-2.50204	-0.19151	-1.47765	1	2.9043	3.09468	-0.53376

1	2.97369	1.80573	2.22908
1	1.66918	2.79118	1.59976
6	4.0292	4.03616	1.00932
1	4.60342	3.78335	1.90911
1	4.69929	4.56796	0.32289
1	3.23083	4.72548	1.30655

Rhodacycle-δ



G° = -3091.028934 Hartrees

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14	2.02438	0.35889	-1.64433
6	3.43961	-5.25148	0.86204
6	2.2167	-5.39269	1.52209
6	1.25839	-4.38123	1.44362
6	1.51155	-3.20998	0.7102
6	2.74507	-3.07579	0.05419
6	3.6985	-4.09315	0.1276
6	-1.93457	-2.23268	4.63715
6	-2.68148	-2.36697	3.46622
6	-2.06115	-2.27932	2.21902
6	-0.68214	-2.05251	2.13146
6	0.06025	-1.89223	3.31481
6	-0.56093	-1.99038	4.55847
6	-3.75548	0.97741	3.8614
6	-4.29106	1.12382	2.58115
6	-3.45	1.34911	1.48947
6	-2.06213	1.42065	1.66813
6	-1.5318	1.25622	2.95671
6	-2.3732	1.04495	4.04707
6	-0.33417	6.39745	0.58104
6	-1.40026	5.7917	1.24884
6	-1.57574	4.40798	1.18732
6	-0.68125	3.60955	0.45858
6	0.39092	4.22835	-0.20309
6	0.56051	5.61181	-0.14814
8	3.65979	-0.00777	-1.70485
1	4.18633	-6.03827	0.92358
1	2.00755	-6.28909	2.09934
1	0.30956	-4.50179	1.95724
1	2.97812	-2.17328	-0.4987
1	4.64757	-3.97006	-0.38655
1	-2.42094	-2.30795	5.60555
1	-3.75252	-2.53865	3.52061
1	-2.65239	-2.39177	1.31716
1	1.13087	-1.71424	3.25648
1	0.0275	-1.8791	5.46504
1	-4.41073	0.80176	4.70981
1	-5.36561	1.06807	2.42968
1	-3.87704	1.47632	0.49989
1	-0.45594	1.28881	3.10566
1	-1.94747	0.90915	5.03591
1	-0.199	7.47411	0.63269
1	-2.09959	6.39626	1.81969
1	1.09778	3.62107	-0.7522
1	1.39778	6.07127	-0.66572
1	-2.41011	3.95198	1.70937
6	-2.40937	-3.50465	-2.94452
6	-1.42561	-4.3345	-2.40274
6	-0.67083	-3.92183	-1.3054
6	-0.89042	-2.66557	-0.71995
6	-1.90923	-1.88144	-1.26859
8	-2.12736	-0.65081	-0.67845
6	-2.40081	0.38441	-1.55097
6	-1.89549	1.64281	-1.20903
6	-2.16037	2.7019	-2.08844
6	-2.88331	2.48135	-3.26155
6	-3.38325	1.21244	-3.56234
6	-3.16312	0.13686	-2.69655
6	-3.74781	-1.27122	-2.85323
6	-2.6736	-2.25476	-2.37855
6	-4.97261	-1.38874	-1.9016
6	-4.20221	-1.55661	-4.29087
6	1.72101	1.94372	-2.65558
6	1.29402	-0.99979	-2.74735
6	4.86887	0.52858	-1.15674
6	3.72337	2.3211	0.42442
6	2.41612	1.9253	1.13263
6	5.8287	-0.6691	-1.07236
6	5.42103	1.56582	-2.14847
6	4.70643	1.13514	0.25744
1	-2.96803	-3.83802	-3.81211
1	-1.23567	-5.30577	-2.8495
1	0.11268	-4.56499	-0.92288
1	-1.78939	3.69471	-1.86005

1	-3.06807	3.30755	-3.94133
1	-3.9544	1.0681	-4.47269
1	-5.3924	-2.39883	-1.94893
1	-4.68475	-1.18338	-0.86688
1	-5.7475	-0.6716	-2.19189
1	-4.641	-2.55525	-4.36492
1	-4.97743	-0.8492	-4.59746
1	-3.36944	-1.48899	-4.99705
1	1.45376	-2.00639	-2.35543
1	0.21743	-0.85964	-2.88699
1	1.77704	-0.93849	-3.72993
1	0.65144	2.16236	-2.73623
1	2.23029	2.8305	-2.27229
1	2.10311	1.75817	-3.66702
1	6.82081	-0.36314	-0.7243
1	5.43116	-1.41634	-0.37828
1	5.93007	-1.13413	-2.05755
1	2.49112	-0.43641	0.69854
1	5.53507	1.10709	-3.13496
1	6.39633	1.94111	-1.82014
1	4.7436	2.41771	-2.24969
1	5.71311	1.45114	0.55961
1	4.41628	0.3331	0.94393
1	3.46554	2.70895	-0.56855
1	2.67714	1.537	2.13493
1	1.82148	2.82969	1.29111
6	4.40291	3.48552	1.17244
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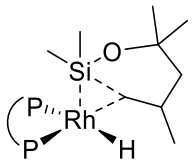

TS-RedElim-δ

G° = -3091.018353 Hartrees

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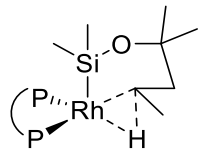
15	-0.78925	1.84089	0.30089
14	2.38128	0.58658	-1.53228
6	2.82612	-5.55136	0.68218
6	1.63279	-5.57111	1.40614
6	0.79794	-4.45174	1.41223
6	1.15739	-3.2901	0.71145
6	2.36079	-3.2765	-0.01103
6	3.1834	-4.40401	-0.02932
6	-2.56686	-2.34731	4.41344
6	-3.19879	-2.34586	3.17052
6	-2.45061	-2.2154	1.99787
6	-1.06054	-2.0667	2.05867
6	-0.43361	-2.04394	3.31674
6	-1.17848	-2.1981	4.48349
6	-3.66733	1.34704	3.91571
6	-4.1799	1.79273	2.6957
6	-3.33696	1.9434	1.59398
6	-1.9739	1.63368	1.69858
6	-1.46967	1.1756	2.92404
6	-2.30973	1.04384	4.02927
6	0.72267	6.22576	0.77391
6	0.01539	5.6231	1.8146
6	-0.48672	4.32741	1.67172
6	-0.28066	3.60991	0.48493
6	0.44031	4.22493	-0.55415
6	0.92949	5.52314	-0.41542
8	3.76533	-0.37569	-1.54137
1	3.47332	-6.42402	0.67277
1	1.34597	-6.4587	1.96336
1	-0.1365	-4.48676	1.96252
1	2.66177	-2.38499	-0.55213
1	4.10925	-4.37754	-0.59631
1	-3.15066	-2.45735	5.32286
1	-4.27814	-2.45136	3.10804
1	-2.95586	-2.234	1.03896
1	0.64455	-1.91881	3.37547
1	-0.67726	-2.19548	5.44761
1	-4.32475	1.22916	4.77251
1	-5.23656	2.02768	2.60134
1	-3.74057	2.29946	0.6513
1	-0.42017	0.9075	3.00348
1	-1.90828	0.67523	4.96719
1	1.11116	7.23366	0.888
1	-0.15281	6.16242	2.74263
1	0.62506	3.68534	-1.47689
1	1.48185	5.97847	-1.23245
1	-1.04004	3.87772	2.48879
6	-2.52517	-3.10691	-3.14064
6	-1.55936	-3.97997	-2.63756
6	-0.82548	-3.65091	-1.49871
6	-1.03488	-2.42973	-0.83837

6	-2.01875	-1.59131	-1.36782
8	-2.22612	-0.39023	-0.71858
6	-2.48794	0.68675	-1.53983
6	-1.92104	1.90574	-1.15758
6	-2.22638	3.02636	-1.94208
6	-3.01826	2.89234	-3.08377
6	-3.5326	1.64782	-3.45476
6	-3.28444	0.51495	-2.67409
6	-3.86106	-0.88348	-2.91399
6	-2.78082	-1.89107	-2.50267
6	-5.08207	-1.06909	-1.9685
6	-4.31675	-1.08067	-4.36622
6	2.65238	2.10332	-2.66532
6	1.24342	-0.43295	-2.69007
6	5.03264	-0.19864	-0.90255
6	4.19969	1.88556	0.41647
6	2.65868	1.81336	0.28329
6	5.59968	-1.60624	-0.67219
6	5.95184	0.56819	-1.86951
6	4.89617	0.51957	0.45631
1	-3.07876	-3.38216	-4.03167
1	-1.37257	-4.92403	-3.14034
1	-0.07026	-4.33768	-1.13809
1	-1.83774	4.00061	-1.67023
1	-3.23754	3.7667	-3.68919
1	-4.13923	1.56836	-4.34995
1	-5.49207	-2.0788	-2.07422
1	-4.79342	-0.9212	-0.92424
1	-5.86485	-0.34381	-2.21391
1	-4.74799	-2.07588	-4.50329
1	-5.09797	-0.36131	-4.62628
1	-3.48572	-0.96122	-5.06751
1	1.15401	-1.4772	-2.38624
1	0.23611	-0.00813	-2.74531
1	1.68126	-0.40256	-3.69674
1	1.68154	2.49937	-2.98999
1	3.22429	2.92781	-2.23091
1	3.17107	1.76633	-3.57041
1	6.62118	-1.55838	-0.2799
1	4.98058	-2.15394	0.04249
1	5.61347	-2.15899	-1.61683
1	2.26961	-0.72376	0.80977
1	6.04075	0.00843	-2.80513
1	6.9526	0.70157	-1.44411
1	5.54456	1.55316	-2.11051
1	5.90719	0.6368	0.86729
1	4.34478	-0.13219	1.14504
1	4.57751	2.43938	-0.45265
1	2.26963	1.66802	1.31986
1	2.28783	2.78972	-0.02333
6	4.56509	2.7151	1.66059
1	5.64324	2.91088	1.7099
1	4.04168	3.67747	1.65692
1	4.27731	2.18112	2.5748

TS-OxAdd-γ-2°



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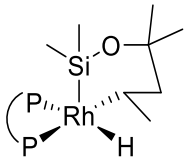
14	-0.96546	1.5705	-1.87883
6	4.05686	5.06346	0.53474
6	4.7457	3.85021	0.63196
6	4.0515	2.64489	0.54418
6	2.65966	2.63459	0.34877
6	1.97876	3.85395	0.26634
6	2.67346	5.06295	0.35586
6	3.31802	-0.93645	4.1509
6	3.86748	-1.32038	2.92752
6	3.40395	-0.75332	1.73839
6	2.37931	0.20175	1.75994
6	1.82448	0.57287	2.99536
6	2.29425	0.01313	4.18136
6	-0.14688	-2.2756	4.8433
6	0.43138	-2.95507	3.77022
6	0.05134	-2.66142	2.4601
6	-0.91466	-1.67895	2.20733
6	-1.47757	-0.98406	3.29309
6	-1.10322	-1.2869	4.60112
6	-6.02499	-1.75511	0.39462
6	-5.28194	-2.43266	1.36485
6	-3.89828	-2.26359	1.43346
6	-3.24115	-1.40471	0.53767
6	-3.99654	-0.71831	-0.42608
6	-5.37897	-0.90118	-0.5009
8	-2.58598	1.99227	-2.08135

1	4.5979	6.00299	0.60578
1	5.82172	3.84476	0.7827
1	4.58938	1.7053	0.6322
1	0.90008	3.83961	0.14629
1	2.13152	6.00228	0.28798
1	3.67864	-1.37939	5.07494
1	4.66236	-2.06081	2.89512
1	3.84684	-1.05509	0.79481
1	1.01876	1.30217	3.02656
1	1.84778	0.30458	5.12699
1	0.15155	-2.50907	5.86131
1	1.18693	-3.71401	3.95084
1	0.50879	-3.19811	1.63663
1	-2.22934	-0.22087	3.11059
1	-1.55684	-0.74967	5.42953
1	-7.10166	-1.89007	0.34056
1	-5.7786	-3.09862	2.06528
1	-3.50627	-0.03128	-1.10987
1	-5.94914	-0.36412	-1.25325
1	-3.32786	-2.80176	2.18379
6	3.56417	-1.29335	-3.32223
6	3.89501	0.0531	-3.15437
6	3.40926	0.77538	-2.06384
6	2.5548	0.17096	-1.12924
6	2.22076	-1.17082	-1.35129
8	1.32893	-1.74843	-0.46712
6	0.42272	-2.62509	-1.03497
6	-0.9013	-2.55861	-0.58484
6	-1.80922	-3.4693	-1.14909
6	-1.40061	-4.36352	-2.13731
6	-0.08001	-4.36746	-2.59104
6	0.86106	-3.49511	-2.03936
6	2.3406	-3.41981	-2.43088
6	2.72361	-1.93576	-2.40816
6	3.17633	-4.15109	-1.34214
6	2.61561	-4.0704	-3.79286
6	-0.78971	0.07333	-3.01925
6	0.13265	2.94416	-2.59473
6	-3.35156	3.09786	-1.58094
6	-2.46482	2.46346	0.79643
6	-3.23993	4.2539	-2.5857
6	-4.80649	2.60839	-1.52149
6	-2.89714	3.57317	-0.17453
1	3.96607	-1.83934	-4.16843
1	4.54536	0.54105	-3.87413
1	3.68636	1.81645	-1.94302
1	-2.84585	-3.45803	-0.83387
1	-2.11979	-5.05448	-2.56694
1	0.21034	-5.05479	-3.378
1	4.24413	-4.08038	-1.57423
1	3.00836	-3.70821	-0.35682
1	2.89573	-5.20847	-1.2972
1	3.67893	-4.00959	-4.04019
1	2.35695	-5.13255	-3.77245
1	2.04405	-3.58857	-4.59164
1	-0.14739	3.12729	-3.63936
1	0.04206	3.88378	-2.04402
1	1.18586	2.64608	-2.57236
1	0.24124	-0.29237	-3.03338
1	-1.4378	-0.75319	-2.71823
1	-1.06188	0.37086	-4.03903
1	-3.82418	5.11822	-2.25095
1	-2.19821	4.56548	-2.69794
1	-3.61195	3.93885	-3.56531
1	-5.07549	2.14031	-2.47322
1	-5.48826	3.44487	-1.33649
1	-4.94155	1.87481	-0.72414
1	-3.74539	4.12699	0.2553
1	-2.08618	4.30761	-0.28078
1	-3.15222	1.6197	0.69832
1	-0.98174	2.66693	0.53896
6	-2.46595	2.9395	2.25278
1	-1.81423	3.81098	2.39154
1	-3.47722	3.22538	2.5764
1	-2.10872	2.15778	2.93264

Rhodacycle-γ-2°



G° = -3,051.780473 Hartrees

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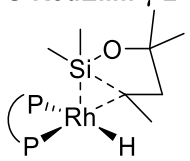
15	-1.41692	-1.0526	0.53002
14	-1.05636	1.88798	-1.71108
6	4.5885	4.65301	0.89225
6	5.07865	3.37163	1.15892
6	4.24632	2.26165	1.02348

6	2.90778	2.41512	0.62172
6	2.42626	3.70406	0.36032
6	3.26216	4.81564	0.49246
6	3.32151	-1.70093	3.8997
6	3.83659	-1.93638	2.62486
6	3.4025	-1.17256	1.53924
6	2.44212	-0.16807	1.71732
6	1.91791	0.04983	3.00084
6	2.36041	-0.7048	4.08501
6	-0.10178	-2.9955	4.54909
6	0.39948	-3.50224	3.35008
6	0.00787	-2.94883	2.13024
6	-0.88752	-1.87244	2.09564
6	-1.36805	-1.35113	3.30948
6	-0.98725	-1.91566	4.52581
6	-6.03697	-1.59964	0.35219
6	-5.31697	-2.28109	1.33457
6	-3.93405	-2.11233	1.43734
6	-3.25667	-1.24464	0.56825
6	-3.99058	-0.55374	-0.41041
6	-5.36871	-0.73932	-0.52162
8	-2.66873	2.34777	-1.87535
1	5.23723	5.51788	0.99964
1	6.10933	3.23639	1.47497
1	4.638	1.27163	1.23466
1	1.39253	3.83153	0.06326
1	2.87136	5.80791	0.28547
1	3.65819	-2.29659	4.74336
1	4.58103	-2.71315	2.47197
1	3.81916	-1.35774	0.55434
1	1.15747	0.81195	3.15197
1	1.93785	-0.53055	5.06942
1	0.20129	-3.43304	5.49596
1	1.10068	-4.3314	3.35999
1	0.40037	-3.36049	1.20756
1	-2.06699	-0.52034	3.30029
1	-1.38172	-1.51093	5.45372
1	-7.11145	-1.7365	0.26891
1	-5.82766	-2.95387	2.01799
1	-3.49111	0.13988	-1.08014
1	-5.91913	-0.19804	-1.28527
1	-3.38584	-2.66617	2.19158
6	3.41987	-0.9984	-3.54504
6	3.87028	0.27882	-3.20075
6	3.46602	0.88227	-2.00853
6	2.57638	0.22079	-1.15084
6	2.13383	-1.04483	-1.54041
8	1.22906	-1.65679	-0.69559
6	0.24754	-2.40003	-1.31832
6	-1.04138	-2.31797	-0.78335
6	-2.02542	-3.11972	-1.38481
6	-1.72303	-3.90813	-2.49371
6	-0.43542	-3.91482	-3.03284
6	0.58214	-3.16142	-2.4442
6	2.04126	-3.12725	-2.91431
6	2.54418	-1.69491	-2.70572
6	2.87134	-4.06678	-1.99417
6	2.19297	-3.587	-4.37059
6	-0.92603	0.45794	-2.94544
6	0.07045	3.2563	-2.39464
6	-3.39408	3.32741	-1.11624
6	-2.4354	2.16815	1.0286
6	-3.28318	4.67551	-1.8446
6	-4.85897	2.86649	-1.11637
6	-2.87377	3.46444	0.33799
1	3.75832	-1.4496	-4.47103
1	4.54987	0.80486	-3.86436
1	3.83147	1.86939	-1.74804
1	-3.03887	-3.107	-1.00459
1	-2.50188	-4.51136	-2.95021
1	-0.22909	-4.51484	-3.91212
1	3.92816	-4.04019	-2.27951
1	2.78987	-3.76003	-0.94767
1	2.50926	-5.09648	-2.08036
1	3.24301	-3.55985	-4.67422
1	1.85867	-4.62134	-4.48808
1	1.61645	-2.95514	-5.05256
1	-0.20477	3.48968	-3.43025
1	0.00548	4.17585	-1.80599
1	1.11506	2.92512	-2.38549
1	0.10155	0.08775	-3.01099
1	-1.57283	-0.38372	-2.68964
1	-1.21926	0.82586	-3.93616
1	-3.83487	5.45484	-1.30717
1	-2.23734	4.98611	-1.91977
1	-3.69024	4.59353	-2.85728
1	-5.16963	2.62392	-2.13735
1	-5.51179	3.65596	-0.72957
1	-4.99045	1.98123	-0.49202
1	-3.69174	3.93415	0.91002

1	-2.04207	4.17906	0.36393
1	-3.23895	1.4316	0.94198
1	-0.20091	2.8178	0.48522
6	-2.17514	2.43366	2.51946
1	-1.50078	3.28581	2.66287
1	-3.11177	2.66137	3.05411
1	-1.72534	1.57463	3.03563

TS-RedElim-γ-2°



G° = -3,051.750275 Hartrees

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14	1.93757	2.13685	0.9877
6	-4.08164	5.17815	-0.69168
6	-4.74446	3.9786	-0.96234
6	-4.0542	2.76764	-0.90556
6	-2.68512	2.73911	-0.59133
6	-2.03088	3.94754	-0.32092
6	-2.72465	5.15847	-0.36673
6	-4.09133	-1.33334	-3.62237
6	-4.12039	-1.77497	-2.30053
6	-3.45393	-1.06072	-1.30119
6	-2.73368	0.09535	-1.62102
6	-2.69421	0.52392	-2.95928
6	-3.37877	-0.17581	-3.9489
6	-1.19565	-3.77281	-3.73556
6	-0.89319	-4.36972	-2.51027
6	-0.21584	-3.64755	-1.5271
6	0.15501	-2.31446	-1.75501
6	-0.1624	-1.72026	-2.98445
6	-0.82507	-2.44817	-3.9719
6	5.52771	-2.50996	-1.35971
6	4.51843	-3.02075	-2.1756
6	3.18535	-2.66934	-1.94922
6	2.84786	-1.78553	-0.91479
6	3.87398	-1.25042	-0.11554
6	5.2005	-1.62618	-0.32835
8	3.58044	1.95314	1.45355
1	-4.61983	6.12086	-0.73576
1	-5.80045	3.98398	-1.21768
1	-4.58294	1.8419	-1.10784
1	-0.97417	3.93672	-0.08221
1	-2.19968	6.08524	-0.15312
1	-4.61558	-1.88824	-4.39513
1	-4.66695	-2.67663	-2.0391
1	-3.50595	-1.40903	-0.27682
1	-2.12841	1.41465	-3.21898
1	-3.34898	0.17582	-4.97657
1	-1.72471	-4.33482	-4.50006
1	-1.18184	-5.3997	-2.31921
1	0.02659	-4.12216	-0.5817
1	0.09571	-0.67898	-3.15713
1	-1.07491	-1.97139	-4.91418
1	6.56309	-2.79208	-1.52839
1	4.76318	-3.70244	-2.98547
1	3.64792	-0.52907	0.66585
1	5.9796	-1.21195	0.30374
1	2.40896	-3.09023	-2.57837
6	-3.22222	-0.19139	3.85183
6	-3.56995	1.07224	3.36999
6	-3.19691	1.47351	2.08778
6	-2.4507	0.61931	1.25984
6	-2.11024	-0.6292	1.78602
8	-1.34414	-1.45151	0.98515
6	-0.38471	-2.18698	1.653
6	0.85618	-2.29913	1.02395
6	1.82776	-3.07845	1.66747
6	1.5588	-3.65994	2.90751
6	0.32003	-3.48126	3.52664
6	-0.6856	-2.7406	2.89911
6	-2.09945	-2.50768	3.44104
6	-2.48773	-1.07477	3.05747
6	-3.06729	-3.4844	2.71481
6	-2.18762	-2.74843	4.95409
6	1.26703	0.95327	2.33288
6	1.27878	3.84117	1.52826
6	4.54901	2.72437	0.74258
6	2.60216	2.56247	-0.96625
6	5.09443	3.80504	1.68685
6	5.69198	1.79898	0.30818
6	3.83331	3.37097	-0.47497
6	2.98011	1.54687	-2.05797
1	-3.52705	-0.48328	4.85065
1	-4.1384	1.75069	3.99884
1	-3.47303	2.46023	1.73706

1	2.80233	-3.21141	1.21366
1	2.3255	-4.25107	3.39917
1	0.14169	-3.92635	4.49931
1	-4.09852	-3.30513	3.03621
1	-3.01512	-3.35253	1.63067
1	-2.80191	-4.52115	2.94641
1	-3.21005	-2.59489	5.31
1	-1.92203	-3.78117	5.19502
1	-1.52162	-2.07981	5.50735
1	0.24021	3.73825	1.86164
1	1.85725	4.21985	2.37899
1	1.30605	4.5953	0.73514
1	0.17697	0.89488	2.34008
1	1.67258	-0.05706	2.26539
1	1.6021	1.3831	3.28621
1	5.81205	4.45361	1.17093
1	4.27578	4.42452	2.06417
1	5.59549	3.34208	2.54276
1	-0.01893	2.51464	-1.22432
1	6.0653	1.24437	1.17533
1	6.51937	2.37741	-0.11726
1	5.35809	1.08168	-0.44164
1	4.53896	3.50226	-1.30694
1	3.50384	4.37655	-0.19204
1	1.92075	3.29103	-1.40607
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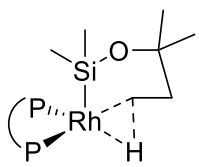

TS-OxAdd-γ-1°

G° = -3,012.502916 Hartrees

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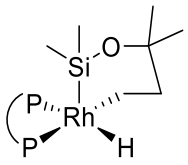
14	-0.87967	1.88789	-1.63156
6	4.63371	4.52358	0.84433
6	5.16315	3.22916	0.82682
6	4.31853	2.1321	0.6673
6	2.93296	2.31371	0.51627
6	2.41246	3.61175	0.54854
6	3.25837	4.71236	0.7084
6	3.32831	-1.67367	3.91168
6	3.73763	-2.01538	2.62285
6	3.28783	-1.28156	1.5231
6	2.41707	-0.19836	1.70013
6	2.00299	0.13134	3.00047
6	2.458	-0.59725	4.09733
6	-0.2272	-2.59966	4.68192
6	0.19529	-3.2597	3.52722
6	-0.20522	-2.80894	2.26899
6	-1.03091	-1.68361	2.15142
6	-1.43222	-1.00863	3.31856
6	-1.04191	-1.47035	4.57445
6	-6.20358	-1.05391	0.65363
6	-5.49244	-1.88815	1.52005
6	-4.09683	-1.87585	1.51821
6	-3.39407	-1.01962	0.65543
6	-4.11601	-0.17535	-0.20299
6	-5.51227	-0.20076	-0.20828
8	-2.45362	2.48583	-1.7372
1	5.29227	5.37843	0.97103
1	6.23249	3.07587	0.94343
1	4.7328	1.12793	0.66525
1	1.33866	3.74398	0.46147
1	2.84037	5.71505	0.72975
1	3.67736	-2.24674	4.766
1	4.41231	-2.85341	2.46905
1	3.62279	-1.55455	0.52797
1	1.3196	0.96285	3.15243
1	2.11882	-0.3351	5.09472
1	0.08461	-2.95701	5.65913
1	0.84282	-4.12823	3.60334
1	0.12671	-3.33371	1.38004
1	-2.0689	-0.1309	3.23906
1	-1.37104	-0.94645	5.46765
1	-7.28994	-1.06672	0.65431
1	-6.02412	-2.55418	2.19423
1	-3.58741	0.51009	-0.85946
1	-6.05619	0.4576	-0.87937
1	-3.55346	-2.53558	2.18726
6	3.19815	-1.2924	-3.55526
6	3.69755	-0.01855	-3.2748
6	3.34773	0.64039	-2.09547
6	2.46546	0.04653	-1.18056

6	1.96451	-1.21836	-1.51242
8	1.05097	-1.77718	-0.63823
6	0.02179	-2.48284	-1.23345
6	-1.26223	-2.31194	-0.70199
6	-2.29709	-3.05372	-1.29482
6	-2.04461	-3.88389	-2.38584
6	-0.75732	-3.98946	-2.91645
6	0.30558	-3.28891	-2.3412
6	1.76288	-3.34189	-2.81312
6	2.32454	-1.92362	-2.66459
6	2.55565	-4.278	-1.85743
6	1.88929	-3.86923	-4.24853
6	-0.8964	0.49561	-2.90724
6	0.32863	3.21034	-2.25896
6	-3.07591	3.62262	-1.12268
6	-2.16159	2.72113	1.14714
6	-2.89746	4.83123	-2.05351
6	-4.56906	3.2806	-1.00882
6	-2.49726	3.9459	0.2815
1	3.49477	-1.79085	-4.47139
1	4.37252	0.4611	-3.97726
1	3.75351	1.6242	-1.88833
1	-3.3089	-2.95824	-0.91887
1	-2.86006	-4.44271	-2.83526
1	-0.58781	-4.6212	-3.78128
1	3.61235	-4.30354	-2.14345
1	2.4872	-3.92993	-0.82327
1	2.1536	-5.29527	-1.90583
1	2.93848	-3.90363	-4.5548
1	1.5067	-4.89099	-4.31972
1	1.33994	-3.242	-4.95683
1	0.04584	3.51156	-3.27502
1	0.33447	4.10079	-1.62515
1	1.34975	2.81702	-2.29097
1	0.08938	0.03229	-3.00049
1	-1.61678	-0.28513	-2.65377
1	-1.17197	0.91527	-3.88205
1	-3.37288	5.72266	-1.62949
1	-1.83691	5.04781	-2.20584
1	-3.34942	4.62511	-3.02848
1	-4.93553	2.91117	-1.97135
1	-5.14773	4.16729	-0.72985
1	-4.74079	2.51078	-0.25409
1	-3.24292	4.57455	0.78731
1	-1.60368	4.5736	0.16391
1	-2.07325	3.01698	2.19868
1	-2.96125	1.97904	1.08645
1	-0.67385	2.76054	0.93563



Rhodacycle-γ-1°

G° = -3,012.523660 Hartrees

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15	-1.50365	-0.94772	0.53206
14	-1.00141	2.07706	-1.55004
6	4.82461	4.39846	0.94024
6	5.26049	3.0796	1.09737
6	4.36246	2.024	0.94995
6	3.01218	2.26948	0.64345
6	2.58543	3.5946	0.49459
6	3.48683	4.65227	0.63928
6	3.2779	-1.94426	3.80643
6	3.73332	-2.18522	2.51009
6	3.31666	-1.37012	1.45555
6	2.43241	-0.30813	1.68658
6	1.9699	-0.08171	2.99188
6	2.39515	-0.8887	4.04481
6	-0.2972	-2.85983	4.58888
6	0.09801	-3.48373	3.40525
6	-0.25985	-2.9426	2.1691
6	-1.00954	-1.76235	2.10759
6	-1.37888	-1.12177	3.30359
6	-1.03598	-1.675	4.53583
6	-6.14473	-1.25128	0.42324
6	-5.44328	-1.9799	1.3851
6	-4.05205	-1.88187	1.46452
6	-3.34814	-1.04201	0.5898
6	-4.06227	-0.30076	-0.36573
6	-5.44994	-0.41355	-0.45225
8	-2.581	2.64372	-1.66234
1	5.52455	5.22119	1.05678
1	6.2997	2.87318	1.33797
1	4.71114	1.00391	1.0776
1	1.54324	3.79261	0.2768
1	3.13777	5.67406	0.51969

1	3.60138	-2.57975	4.62587
1	4.41761	-3.00679	2.31601
1	3.68706	-1.56186	0.45374
1	1.2694	0.72732	3.18258
1	2.01966	-0.70666	5.04665
1	-0.02239	-3.28829	5.54848
1	0.68783	-4.39494	3.44102
1	0.04337	-3.44075	1.25455
1	-1.95397	-0.19984	3.26418
1	-1.34094	-1.17932	5.45324
1	-7.22617	-1.33199	0.35881
1	-5.97583	-2.63237	2.07152
1	-3.53936	0.38189	-1.0289
1	-5.98686	0.16744	-1.19617
1	-3.51717	-2.46713	2.20499
6	3.24101	-1.06896	-3.60932
6	3.75023	0.18399	-3.25814
6	3.40304	0.78272	-2.04575
6	2.51068	0.14374	-1.17375
6	2.00356	-1.09449	-1.57365
8	1.09157	-1.68242	-0.71877
6	0.06757	-2.37156	-1.33392
6	-1.20814	-2.23294	-0.77932
6	-2.23803	-2.98295	-1.37153
6	-1.98923	-3.77607	-2.49031
6	-0.71219	-3.83544	-3.0514
6	0.34795	-3.13365	-2.47414
6	1.79787	-3.15243	-2.97215
6	2.35966	-1.74302	-2.75783
6	2.60818	-4.13342	-2.07807
6	1.90338	-3.60116	-4.43589
6	-0.96819	0.69736	-2.8467
6	0.19414	3.41244	-2.17526
6	-3.26006	3.59891	-0.83265
6	-2.34767	2.23555	1.19348
6	-3.08733	4.98938	-1.46199
6	-4.74389	3.20475	-0.86106
6	-2.73242	3.60641	0.62912
1	3.53828	-1.51897	-4.54994
1	4.43223	0.69387	-3.9318
1	3.81698	1.749	-1.77991
1	-3.24417	-2.92491	-0.97606
1	-2.80183	-4.33963	-2.93863
1	-0.54796	-4.43503	-3.93982
1	3.66054	-4.14077	-2.38051
1	2.55405	-3.83816	-1.02653
1	2.20801	-5.14827	-2.17166
1	2.94765	-3.6117	-4.75993
1	1.52631	-4.62018	-4.55778
1	1.33923	-2.93948	-5.09971
1	-0.07571	3.70529	-3.19709
1	0.17286	4.30623	-1.54547
1	1.22169	3.03285	-2.188
1	0.04382	0.2979	-2.96437
1	-1.63191	-0.1341	-2.60006
1	-1.28466	1.11324	-3.81088
1	-3.59989	5.75189	-0.86499
1	-2.0282	5.25536	-1.52022
1	-3.50077	5.00223	-2.47525
1	-5.06762	3.05649	-1.89604
1	-5.3602	3.9898	-0.41054
1	-4.91305	2.28002	-0.30697
1	-3.52917	4.06646	1.23454
1	-1.87001	4.27949	0.69785
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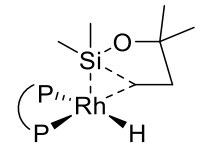
1	-3.20293	1.5568	1.13914
1	-0.08804	2.83283	0.74299



TS-RedElim-γ-1°

G° = -3,012.508932 Hartrees

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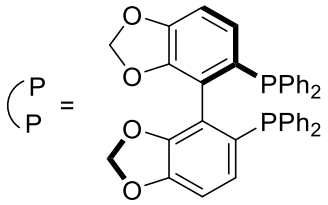
15	1.14511	-1.37136	-0.54661
14	1.8642	2.09204	0.99437
6	-4.2208	4.9075	-1.25487
6	-4.85353	3.66537	-1.15133
6	-4.09936	2.51107	-0.94996
6	-2.69694	2.57495	-0.85211
6	-2.07638	3.82458	-0.955
6	-2.83223	4.98301	-1.15475
6	-4.19144	-1.83681	-3.23456
6	-4.08591	-2.1408	-1.87835
6	-3.37005	-1.30348	-1.01819
6	-2.7338	-0.15917	-1.51152
6	-2.83744	0.13346	-2.88278
6	-3.56831	-0.69007	-3.73444

6	-1.11557	-4.07804	-3.56964
6	-0.70483	-4.61788	-2.34902
6	-0.03482	-3.82106	-1.42052
6	0.21942	-2.47057	-1.69926
6	-0.20735	-1.93339	-2.92158
6	-0.86216	-2.73589	-3.85558
6	5.60857	-2.04604	-1.72973
6	4.59397	-2.4764	-2.5846
6	3.25256	-2.32096	-2.22534
6	2.90444	-1.72477	-1.00528
6	3.9369	-1.28697	-0.15458
6	5.27501	-1.45359	-0.50924
8	3.43507	2.69047	1.32313
1	-4.80808	5.80767	-1.41343
1	-5.93498	3.59505	-1.22806
1	-4.60318	1.55309	-0.86885
1	-0.99708	3.88574	-0.8824
1	-2.32974	5.94293	-1.23359
1	-4.7537	-2.48728	-3.89834
1	-4.56691	-3.02993	-1.48042
1	-3.31935	-1.54813	0.03506
1	-2.35479	1.0228	-3.27975
1	-3.64755	-0.44061	-4.78903
1	-1.63856	-4.69885	-4.2916
1	-0.90374	-5.66116	-2.11976
1	0.28811	-4.24893	-0.47662
1	-0.03794	-0.88087	-3.13092
1	-1.1975	-2.30444	-4.79315
1	6.65048	-2.16896	-2.01081
1	4.84248	-2.94101	-3.53474
1	3.69813	-0.8119	0.79159
1	6.05396	-1.10956	0.16506
1	2.4777	-2.66983	-2.89947
6	-2.76621	0.24447	3.9944
6	-3.15328	1.44775	3.40134
6	-2.91246	1.6869	2.0482
6	-2.25628	0.72957	1.25923
6	-1.86409	-0.44997	1.89898
8	-1.17561	-1.36854	1.13169
6	-0.18112	-2.06572	1.7827
6	0.99716	-2.27451	1.06211
6	1.98975	-3.051	1.67636
6	1.81375	-3.51773	2.97987
6	0.65164	-3.21781	3.69457
6	-0.37974	-2.48555	3.0995
6	-1.72032	-2.13211	3.75282
6	-2.11844	-0.74015	3.24333
6	-2.78589	-3.14976	3.25673
6	-1.6468	-2.18817	5.2851
6	1.68459	0.85712	2.41767
6	0.77315	3.59679	1.38297
6	4.17308	3.31409	0.27032
6	2.70332	1.71191	-0.96065
6	4.307	4.80999	0.57522
6	5.55656	2.64894	0.22704
6	3.39879	3.07464	-1.05274
1	-2.97358	0.07851	5.04558
1	-3.65152	2.20563	3.99821
1	-3.22099	2.62798	1.60918
1	2.91193	-3.26614	1.14966
1	2.59546	-4.10824	3.44812
1	0.55241	-3.56475	4.71716
1	-3.77081	-2.89579	3.66185
1	-2.8504	-3.14646	2.16514
1	-2.52184	-4.16192	3.58022
1	-2.61841	-1.95204	5.72744
1	-1.38485	-3.19448	5.62263
1	-0.90535	-1.4856	5.67661
1	-0.28047	3.32106	1.48398
1	1.11664	4.04751	2.32232
1	0.8511	4.3553	0.59769
1	0.63267	0.6155	2.59312
1	2.22158	-0.08178	2.26827
1	2.08864	1.3345	3.31838
1	4.84274	5.32894	-0.22805
1	3.31568	5.26069	0.68062
1	4.85245	4.96027	1.51189
1	0.24054	2.51888	-1.20375
1	6.02389	2.71406	1.21419
1	6.20995	3.13748	-0.50429
1	5.47001	1.59082	-0.03848
1	4.09348	3.10907	-1.90203
1	2.65938	3.8688	-1.21563
1	2.25333	1.47072	-1.94552
1	3.44081	0.93503	-0.76536

For the following complexes



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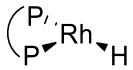

G° = -2,556.892631 Hartrees

6	0.30736	1.55157	0.13437
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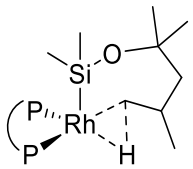
6	0.34138	3.56859	-1.24617
6	1.19621	3.01138	-2.17281
6	1.62844	1.69845	-1.92027
6	1.22728	0.97077	-0.79118
8	-0.94407	3.62252	0.611
8	-0.23252	4.81294	-1.25018
1	1.51169	3.55631	-3.05488
1	2.29799	1.23668	-2.63641
15	1.71136	-0.81157	-0.64872
6	-1.52876	-0.29456	3.6296
6	-0.55299	0.67298	3.72332
6	0.01982	1.24311	2.58853
6	-0.31399	0.8635	1.30315
6	-1.32504	-0.1384	1.18627
6	-1.90692	-0.68768	2.33166
1	-1.98156	-0.73042	4.51262
15	-1.6954	-0.79012	-0.50435
1	-2.67227	-1.44785	2.22825
8	0.93649	2.19399	2.96136
8	-0.01524	1.24135	4.85023
6	1.02135	2.1188	4.38889
1	0.87085	3.11632	4.81537
1	1.9978	1.70601	4.67234
6	-1.10438	4.84878	-0.11064
1	-2.1427	4.93487	-0.45334
1	-0.82629	5.69049	0.53426
6	5.97741	-1.05279	-2.54018
6	5.61001	0.0764	-1.80395
6	4.33103	0.1709	-1.25851
6	3.39253	-0.86224	-1.43921
6	3.76935	-1.98302	-2.18981
6	5.05311	-2.07888	-2.73239
1	6.97445	-1.12599	-2.96561
1	6.31801	0.88733	-1.65668
1	4.05725	1.06879	-0.71603
1	3.04288	-2.77389	-2.34625
1	5.32501	-2.95738	-3.31083
6	2.67604	-1.3405	3.88508
6	3.25769	-0.28444	3.17835
6	2.98069	-0.11072	1.82293
6	2.13138	-1.00217	1.15089
6	1.56229	-2.06564	1.86405
6	1.82661	-2.22962	3.22443
1	2.88374	-1.46794	4.94382
1	3.92517	0.40869	3.68363
1	3.41208	0.7355	1.30141
1	0.89648	-2.74353	1.33699
1	1.36584	-3.04928	3.76811
6	-5.28689	-3.69526	0.07353
6	-5.54037	-2.39774	-0.37475
6	-4.49234	-1.48966	-0.53969
6	-3.17226	-1.87156	-0.26081
6	-2.9258	-3.18669	0.17718
6	-3.97544	-4.08846	0.35064
1	-6.10542	-4.39799	0.20064
1	-6.55775	-2.08879	-0.59828
1	-4.70498	-0.48662	-0.89294
1	-1.90318	-3.49601	0.38576
1	-3.76804	-5.09796	0.69404
6	-3.19886	3.00198	-2.72774
6	-3.61789	2.77636	-1.41268
6	-3.18577	1.64167	-0.72599
6	-2.34838	0.70872	-1.35752
6	-1.93456	0.94076	-2.67612
6	-2.35503	2.0845	-3.35692
1	-3.52436	3.89342	-3.25649
1	-4.27473	3.48849	-0.91999
1	-3.48129	1.48755	0.30775
1	-1.25491	0.23382	-3.14498
1	-2.01544	2.26434	-4.37273
45	0.09106	-2.09584	-1.3529
1	1.2429	-3.13883	-1.74663

TS-OxAdd-δ



G° = -3276.099906 Hartrees

6	1.91862	0.64752	1.27142
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6	1.98959	0.25999	3.68419
6	0.80207	0.92593	3.90495
6	0.16207	1.46492	2.77528
6	0.69289	1.35656	1.47796
8	3.7186	-0.54328	2.46958
8	2.81607	-0.34739	4.59354
1	0.37859	1.0186	4.89836
1	-0.78793	1.96846	2.91202
15	-0.38606	1.77199	0.03356
6	4.05887	0.01471	-2.46818
6	4.35878	1.03862	-1.59714
6	3.6465	1.21585	-0.41376
6	2.57936	0.41934	-0.04742
6	2.23515	-0.63325	-0.94781
6	2.98289	-0.82123	-2.11512
1	4.62229	-0.13591	-3.3818
15	0.75293	-1.66445	-0.51622
1	2.73148	-1.63468	-2.78425
8	4.15958	2.28314	0.27976
8	5.34251	1.98804	-1.69519
6	5.17598	2.84677	-0.55711
1	6.1183	2.90012	-0.00059
1	4.85627	3.83942	-0.89711
6	3.79068	-1.05181	3.80672
1	3.55184	-2.12389	3.80093
1	4.78818	-0.86302	4.21309
6	-3.06795	5.38983	1.20016
6	-1.77923	5.31158	1.73445
6	-0.95592	4.23022	1.42051
6	-1.41469	3.20527	0.57572
6	-2.71923	3.27968	0.06504
6	-3.53472	4.37187	0.36764
1	-3.7073	6.23421	1.44209
1	-1.41486	6.09212	2.39678
1	0.03694	4.17113	1.85578
1	-3.11066	2.46839	-0.54059
1	-4.54203	4.41575	-0.03663
6	2.39521	3.72587	-3.15904
6	2.28423	4.32323	-1.89982
6	1.46082	3.75961	-0.92548
6	0.72969	2.5942	-1.20032
6	0.83588	2.01336	-2.46976
6	1.66705	2.56982	-3.44263
1	3.04437	4.16124	-3.91325
1	2.83841	5.23151	-1.67746
1	1.39402	4.22835	0.04948
1	0.27451	1.11073	-2.67936
1	1.74975	2.09685	-4.41676
6	-0.00775	-4.40074	-4.2014
6	0.2442	-4.97401	-2.95483
6	0.52981	-4.16808	-1.85008
6	0.55453	-2.77183	-1.97427
6	0.2881	-2.20449	-3.23341
6	0.02151	-3.00997	-4.33852
1	-0.22654	-5.02979	-5.05926
1	0.2253	-6.05405	-2.83856
1	0.7343	-4.6298	-0.88977
1	0.29375	-1.1256	-3.34854
1	-0.17587	-2.5513	-5.3033
6	2.5498	-4.52019	2.70583
6	3.37577	-4.01775	1.69538
6	2.85642	-3.15872	0.72702
6	1.5014	-2.79321	0.75213
6	0.68221	-3.29817	1.77179
6	1.20189	-4.15773	2.74238
1	2.95576	-5.18937	3.45958
1	4.42648	-4.29305	1.66313
1	3.50654	-2.76204	-0.04583
1	-0.36231	-3.01481	1.80538
1	0.55431	-4.53952	3.52657
45	-1.21964	-0.37292	0.19892
14	-2.7926	-0.43239	-1.46162
8	-4.25976	0.22421	-0.97104
6	-5.23544	-0.06217	0.03756
6	-5.25136	1.12382	1.01144
6	-6.57314	-0.13022	-0.72128
6	-2.45392	0.59684	-3.01671
6	-3.08661	-2.2201	-2.04782
1	-5.9723	0.96041	1.82003
1	-4.26192	1.28184	1.44546
1	-5.52914	2.0369	0.47754

1	-7.42379	-0.19848	-0.03453
1	-6.68806	0.76673	-1.33616
1	-6.58755	-1.00164	-1.38402
1	-3.33805	0.55874	-3.66395
1	-2.24282	1.64384	-2.78337
1	-1.60681	0.19277	-3.57965
1	-3.08821	-2.94006	-1.22657
1	-4.05454	-2.27821	-2.56102
1	-2.30721	-2.52482	-2.75093
6	-5.04686	-1.41098	0.78789
6	-2.55243	-1.65779	1.50696
1	-4.8644	-2.1979	0.04646
1	-6.0319	-1.63723	1.21552
1	-1.93003	-1.72668	2.40666
1	-2.52734	-0.19381	1.06901
1	-2.43729	-2.5861	0.93688
6	-4.02885	-1.54474	1.94292
1	-4.13317	-0.66801	2.59604
6	-4.39451	-2.78205	2.78556
1	-3.69441	-2.91106	3.61834
1	-5.40538	-2.70376	3.20348
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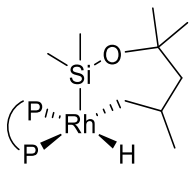
Rhodacycle-δ



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6	-2.87429	0.69132	-3.40591
6	-1.90311	1.31724	-2.60524
6	-1.7559	1.04407	-1.23757
8	-4.47419	-1.46121	-1.0601
8	-4.70645	-0.97432	-3.31774
1	-2.96838	0.9096	-4.46331
1	-1.24908	2.04327	-3.07341
15	-0.32547	1.78372	-0.32333
6	-2.61733	-1.41183	3.47798
6	-3.55263	-0.52674	2.99107
6	-3.49699	-0.06403	1.67858
6	-2.49764	-0.41342	0.79118
6	-1.4976	-1.30757	1.28755
6	-1.58761	-1.79164	2.59656
1	-2.66917	-1.79402	4.49079
15	-0.03721	-1.67141	0.20643
1	-0.84721	-2.49216	2.96005
8	-4.56202	0.76713	1.43733
8	-4.64657	0.00169	3.62479
6	-5.2222	0.93361	2.69678
1	-6.28938	0.71852	2.58041
1	-5.05598	1.9556	3.06074
6	-5.20794	-1.78602	-2.24597
1	-5.0513	-2.84311	-2.48997
1	-6.27116	-1.56695	-2.08873
6	0.27799	5.92607	-2.39227
6	-1.0176	5.48286	-2.11255
6	-1.21758	4.24193	-1.51078
6	-0.12673	3.42174	-1.16836
6	1.16437	3.86585	-1.48308
6	1.36614	5.11101	-2.08352
1	0.43401	6.89365	-2.86095
1	-1.87379	6.09978	-2.37086
1	-2.23137	3.89272	-1.34812
1	2.01153	3.22562	-1.27235
1	2.37671	5.43579	-2.3139
6	-2.0866	2.73007	3.89852
6	-2.64607	3.35047	2.77884
6	-2.13794	3.0949	1.50472
6	-1.05032	2.22691	1.33047
6	-0.49068	1.61902	2.464
6	-1.00683	1.86058	3.73641
1	-2.49005	2.92257	4.88849
1	-3.48182	4.03539	2.8957
1	-2.60231	3.57312	0.65183
1	0.33786	0.9323	2.33556
1	-0.56803	1.36578	4.59762
6	2.39168	-5.11483	2.18175
6	1.77103	-5.32932	0.95159
6	0.99243	-4.32727	0.36719
6	0.82456	-3.09132	1.00747
6	1.47337	-2.87914	2.23581
6	2.23878	-3.88362	2.82417
1	2.99722	-5.89543	2.63302
1	1.89303	-6.27849	0.43752
1	0.52546	-4.5121	-0.59309
1	1.39187	-1.91906	2.72997
1	2.72701	-3.69764	3.77651

6	-2.16848	-3.55486	-3.47673
6	-2.50039	-3.98013	-2.18673
6	-1.86109	-3.42191	-1.08093
6	-0.86586	-2.4465	-1.25198
6	-0.53317	-2.03228	-2.54888
6	-1.18658	-2.57936	-3.65457
1	-2.67673	-3.97891	-4.33793
1	-3.26255	-4.74096	-2.04151
1	-2.14132	-3.73199	-0.07881
1	0.21647	-1.262	-2.69548
1	-0.93337	-2.23545	-4.65286
45	1.45589	0.18741	-0.46018
14	3.07687	1.12745	0.91412
8	4.61192	1.3599	0.27768
6	5.73335	0.51919	0.00623
6	6.51811	1.22629	-1.10954
6	6.60527	0.44229	1.27158
6	2.70211	2.8891	1.50791
6	3.24624	0.07872	2.49605
1	7.43651	0.68119	-1.35213
1	5.91248	1.31123	-2.01537
1	6.78411	2.23696	-0.78617
1	7.52598	-0.12018	1.08165
1	6.87434	1.45102	1.59933
1	6.06588	-0.0508	2.0848
1	3.35008	3.09949	2.36753
1	2.93512	3.62339	0.7332
1	1.66546	3.03593	1.8183
1	2.30749	0.06636	3.06003
1	3.53243	-0.95368	2.28349
1	4.01104	0.52981	3.13966
6	5.31484	-0.89963	-0.42432
6	2.8555	-1.29738	-1.03485
1	4.93922	-1.44125	0.4531
1	6.23593	-1.42095	-0.71574
1	2.26638	-1.72686	-1.86404
1	2.43398	1.25419	-1.0858
1	2.92548	-2.08746	-0.27668
6	4.26943	-0.99655	-1.56469
1	4.24527	-0.04337	-2.10538
6	4.69878	-2.08447	-2.56876
1	5.69279	-1.87801	-2.9855
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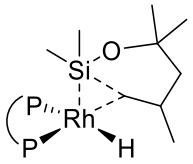

TS-RedElim-δ

G° = -3276.114716 Hartrees

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C	3.21991	0.73198	3.09864
C	2.1693	1.52389	3.50994
C	1.21621	1.86298	2.53353
C	1.31221	1.43351	1.20284
O	4.43688	-0.49849	1.64566
O	4.2707	0.25066	3.83632
H	2.07948	1.86085	4.53614
H	0.37157	2.47331	2.83235
P	-0.11092	1.70747	0.05832
C	3.20659	-1.1785	-3.09771
C	3.88868	-0.08976	-2.60348
C	3.58663	0.44903	-1.35468
C	2.57508	-0.02931	-0.54462
C	1.8344	-1.14208	-1.05439
C	2.17034	-1.69217	-2.29524
H	3.44951	-1.61219	-4.06081
P	0.3512	-1.71823	-0.1009
H	1.61536	-2.54291	-2.67047
O	4.43024	1.49902	-1.09014
O	4.92688	0.60404	-3.16973
C	5.168	1.71792	-2.29747
H	6.23631	1.77439	-2.06672
H	4.81086	2.63796	-2.77846
C	5.03421	-0.57499	2.94474
H	5.00181	-1.61307	3.29648
H	6.06415	-0.20232	2.89496
C	-1.95412	5.88126	0.99916
C	-0.59875	5.66483	1.2555
C	-0.0291	4.41509	1.00859
C	-0.81111	3.35798	0.51424
C	-2.17349	3.58478	0.26473
C	-2.7376	4.83909	0.50069
H	-2.39683	6.85439	1.19219
H	0.01744	6.46772	1.65067
H	1.02247	4.25939	1.22674
H	-2.79526	2.7724	-0.09762
H	-3.79433	4.99473	0.30317

C	1.85823	2.63601	-4.06288
C	2.1386	3.45614	-2.96595
C	1.55831	3.19168	-1.72579
C	0.68168	2.1078	-1.56875
C	0.39814	1.29916	-2.67555
C	0.98678	1.55643	-3.91371
H	2.31654	2.83896	-5.0266
H	2.8082	4.30505	-3.07665
H	1.79451	3.83154	-0.8833
H	-0.26545	0.45342	-2.54869
H	0.76846	0.90932	-4.75797
C	-1.05331	-5.55042	-2.33473
C	-0.43091	-5.68542	-1.09367
C	0.02877	-4.55873	-0.40666
C	-0.14154	-3.27795	-0.95006
C	-0.79664	-3.15121	-2.18765
C	-1.23322	-4.2776	-2.88273
H	-1.4058	-6.42851	-2.86792
H	-0.29786	-6.67066	-0.6556
H	0.51619	-4.68246	0.5539
H	-0.97315	-2.16266	-2.60217
H	-1.7331	-4.1589	-3.83954
C	2.44101	-3.02987	3.84879
C	2.97682	-3.41801	2.61699
C	2.35105	-3.03594	1.43116
C	1.1663	-2.2826	1.46087
C	0.63675	-1.89803	2.70096
C	1.27349	-2.26605	3.88765
H	2.93564	-3.31618	4.7727
H	3.88862	-4.00796	2.5795
H	2.78988	-3.30868	0.47616
H	-0.25254	-1.27684	2.73404
H	0.86258	-1.9455	4.84035
Rh	-1.42997	-0.12652	0.30214
Si	-3.51891	-0.57915	-0.88641
O	-4.83308	0.36959	-0.43918
C	-5.70689	0.33068	0.68886
C	-5.43166	1.59455	1.52064
C	-7.1372	0.37429	0.13192
C	-2.99301	0.37784	-2.45964
C	-4.2161	-2.17035	-1.68104
H	-6.08828	1.6486	2.39616
H	-4.39167	1.62292	1.85371
H	-5.60482	2.47935	0.90037
H	-7.87885	0.40623	0.93792
H	-7.26321	1.26123	-0.49596
H	-7.32729	-0.50929	-0.48523
H	-3.91377	0.52023	-3.04033
H	-2.55084	1.35465	-2.26085
H	-2.29848	-0.20232	-3.07589
H	-3.43752	-2.9189	-1.85761
H	-4.97857	-2.6383	-1.04965
H	-4.68092	-1.9306	-2.64429
C	-5.52055	-0.9534	1.52324
C	-3.04281	-1.60958	0.97627
H	-5.8584	-1.811	0.92703
H	-6.19896	-0.89333	2.38382
H	-2.09338	-1.71133	1.5345
H	-2.49192	0.93112	0.77824
H	-3.21207	-2.61435	0.58232
C	-4.09605	-1.21269	2.03053
H	-3.73363	-0.33073	2.56731
C	-4.16825	-2.34359	3.07334
H	-4.06539	-3.28867	2.58227
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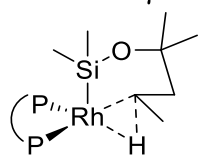
TS-OxAdd-γ-2°



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6	2.26424	-1.36467	-3.47079
6	1.21779	-1.67729	-2.58377
6	1.2175	-1.2794	-1.24175
8	4.49515	0.44089	-1.35903
8	4.45369	-0.20963	-3.58665
1	2.24255	-1.67482	-4.50909
1	0.38363	-2.25142	-2.96675
15	-0.25977	-1.61246	-0.16344
6	2.97255	0.90908	3.33608
6	3.64399	-0.16744	2.8006
6	3.40136	-0.59947	1.49871
6	2.45975	-0.01971	0.66958
6	1.75746	1.10393	1.20545
6	2.02623	1.54086	2.50697

1	3.17065	1.25818	4.34288
15	0.39305	1.82919	0.1885
1	1.49855	2.40035	2.90173
8	4.22915	-1.65291	1.20091
8	4.62355	-0.93781	3.37245
6	4.93577	-1.95421	2.40937
1	6.0131	-1.94996	2.21098
1	4.60339	-2.92785	2.79052
6	5.18944	0.53779	-2.60738
1	5.23562	1.58941	-2.91534
1	6.19299	0.10979	-2.50066
6	-2.56095	-4.88835	-2.55832
6	-1.64105	-5.28543	-1.58745
6	-0.91993	-4.3314	-0.8658
6	-1.1182	-2.96465	-1.09882
6	-2.05293	-2.57522	-2.07264
6	-2.76202	-3.52748	-2.80245
1	-3.12464	-5.63248	-3.1138
1	-1.4871	-6.34116	-1.38215
1	-0.22487	-4.66294	-0.10349
1	-2.24198	-1.51805	-2.22863
1	-3.48529	-3.20527	-3.54605
6	1.69716	-3.68445	3.51785
6	2.14037	-4.01558	2.23427
6	1.57139	-3.40414	1.1171
6	0.52864	-2.47697	1.26793
6	0.09301	-2.15001	2.55961
6	0.67615	-2.74539	3.67882
1	2.14912	-4.15236	4.38791
1	2.93776	-4.74211	2.10254
1	1.95117	-3.63092	0.12579
1	-0.69301	-1.41112	2.68156
1	0.33551	-2.47463	4.67391
6	-0.91556	5.71288	2.39031
6	-0.19128	5.8235	1.20325
6	0.25384	4.67943	0.5361
6	-0.02662	3.40457	1.04624
6	-0.77941	3.30492	2.23214
6	-1.20729	4.44727	2.90593
1	-1.25928	6.60473	2.90619
1	0.0304	6.80365	0.79037
1	0.81126	4.78592	-0.38778
1	-1.03947	2.32416	2.6229
1	-1.78134	4.34827	3.82271
6	2.54481	2.99171	-3.75435
6	3.11794	3.36033	-2.53331
6	2.48689	3.02519	-1.33539
6	1.26186	2.34068	-1.3502
6	0.69132	1.97677	-2.57791
6	1.33343	2.29724	-3.77458
1	3.04475	3.24018	-4.68618
1	4.06045	3.90103	-2.51418
1	2.95069	3.28003	-0.38712
1	-0.23902	1.41652	-2.58164
1	0.89379	1.99551	-4.72054
45	-1.5646	0.28036	0.13949
14	-3.38808	-0.9155	0.95679
8	-4.8442	-0.63916	0.15051
6	-5.26461	0.55556	-0.51496
6	-5.05394	0.3671	-2.02507
6	-6.7658	0.68702	-0.21783
6	-3.45212	-2.79345	1.18523
6	-3.50923	-0.1992	2.73603
1	-5.40982	1.23845	-2.58516
1	-3.99643	0.21602	-2.25812
1	-5.60086	-0.51897	-2.36134
1	-7.2052	1.53927	-0.74756
1	-7.28393	-0.2252	-0.52769
1	-6.9262	0.82065	0.8565
1	-4.31976	-3.03742	1.81012
1	-3.55992	-3.31717	0.23299
1	-2.55541	-3.17433	1.6847
1	-4.50372	-0.41873	3.14513
1	-2.76856	-0.66431	3.39728
1	-3.35812	0.88408	2.7693
6	-4.53504	1.80433	0.04019
6	-3.023	1.9891	-0.19646
1	-4.73233	1.80641	1.11821
1	-5.05743	2.68633	-0.36044
1	-2.60321	0.50736	-0.97403
1	-2.62635	2.49141	0.69018
6	-2.72589	2.8802	-1.41001
1	-3.27985	3.8281	-1.33891
1	-1.66411	3.12864	-1.48287
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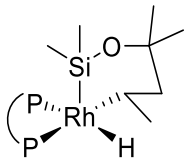
Rhodacycle-γ-2°



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6	-3.6507	-0.20508	-2.67343
6	-2.86134	0.7239	-3.31498
6	-1.85981	1.33981	-2.54369
6	-1.65346	1.03969	-1.18992
8	-4.34032	-1.49407	-0.95133
8	-4.67744	-0.95581	-3.18364
1	-3.00203	0.96327	-4.3626
1	-1.23052	2.07938	-3.02433
15	-0.2108	1.78071	-0.29817
6	-2.27678	-1.52201	3.50469
6	-3.25311	-0.65316	3.07223
6	-3.26039	-0.16537	1.76785
6	-2.28868	-0.47246	0.83505
6	-1.24943	-1.35415	1.2724
6	-1.27533	-1.8618	2.57524
1	-2.27786	-1.92339	4.5114
15	0.16644	-1.67825	0.11778
1	-0.50781	-2.55372	2.89565
8	-4.35383	0.64328	1.58422
8	-4.33428	-0.16397	3.75772
6	-4.96048	0.77836	2.87399
1	-6.02892	0.55226	2.79972
1	-4.78889	1.79532	3.24952
6	-5.10418	-1.81779	-2.1183
1	-4.91154	-2.86016	-2.3984
1	-6.16839	-1.64855	-1.91638
6	0.37779	5.94874	-2.32068
6	-0.91735	5.49149	-2.06244
6	-1.11489	4.24231	-1.4771
6	-0.02172	3.42585	-1.13275
6	1.26968	3.88688	-1.42127
6	1.46889	5.14056	-2.0044
1	0.53147	6.9228	-2.77645
1	-1.77536	6.10468	-2.32353
1	-2.12792	3.88568	-1.32696
1	2.11829	3.25219	-1.19925
1	2.47969	5.47818	-2.21456
6	-1.94609	2.74057	3.9304
6	-2.52458	3.34071	2.8089
6	-2.02564	3.07736	1.53283
6	-0.92827	2.22157	1.35876
6	-0.35495	1.62883	2.49202
6	-0.85994	1.87942	3.76715
1	-2.34088	2.9414	4.92224
1	-3.36857	4.01537	2.92597
1	-2.50363	3.54068	0.67909
1	0.47314	0.94428	2.36232
1	-0.40738	1.39758	4.62857
6	2.69822	-5.19701	1.82333
6	2.04774	-5.3468	0.59897
6	1.23651	-4.32561	0.09792
6	1.06549	-3.13253	0.81642
6	1.74509	-2.9856	2.03715
6	2.5421	-4.01037	2.54326
1	3.32827	-5.9928	2.20982
1	2.17075	-6.26053	0.02444
1	0.74645	-4.4628	-0.85879
1	1.66099	-2.06108	2.59225
1	3.05164	-3.8736	3.4928
6	-2.13211	-3.48124	-3.50709
6	-2.3579	-3.98133	-2.22044
6	-1.67195	-3.44551	-1.13171
6	-0.73629	-2.41489	-1.31773
6	-0.51796	-1.92066	-2.60918
6	-1.21416	-2.44813	-3.69807
1	-2.67485	-3.89098	-4.35404
1	-3.07301	-4.78455	-2.06458
1	-1.86591	-3.81994	-0.1311
1	0.17042	-1.09745	-2.76093
1	-1.04662	-2.04206	-4.69094
45	1.62199	0.22498	-0.46537
14	3.13138	1.07713	1.08101
8	4.73742	1.05537	0.60075
6	5.36338	0.19711	-0.35877
6	5.51927	0.99243	-1.66322
6	6.75006	-0.12727	0.21772
6	2.8718	2.887	1.58097
6	3.13759	0.09643	2.71851
1	5.95375	0.37636	-2.45758
1	4.5495	1.36339	-1.99867
1	6.17149	1.85468	-1.49072

1	7.34251	-0.72175	-0.48636
1	7.28788	0.80098	0.43243
1	6.65043	-0.68789	1.15253
1	3.52913	3.11248	2.42931
1	3.13644	3.56573	0.76638
1	1.84333	3.10174	1.88384
1	2.16835	0.03942	3.22466
1	3.51147	-0.91749	2.56021
1	3.83528	0.60865	3.39277
6	4.57781	-1.12364	-0.53325
6	3.16082	-1.13091	-1.12657
1	4.53431	-1.58552	0.46197
1	5.21212	-1.78963	-1.14262
1	2.61766	1.35249	-0.94388
1	2.77997	-2.12746	-0.88037
6	3.14724	-1.02371	-2.66221
1	3.92401	-1.66987	-3.10445
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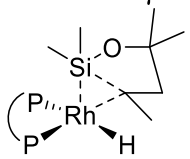
1	3.32567	-0.01146	-3.03274

TS-RedElim-γ-2°



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6	-3.80363	0.23418	-2.71373
6	-2.84828	1.05485	-2.08883
6	-2.20218	0.69597	-0.89912
8	-3.9416	-2.54351	-0.48704
8	-4.96465	-1.94159	-2.4812
1	-4.28601	0.52374	-3.64003
1	-2.60958	2.00104	-2.55756
15	-0.81987	1.74042	-0.24241
6	-1.21013	-2.24554	3.52576
6	-2.44401	-1.66618	3.336
6	-2.79868	-1.11245	2.10939
6	-1.95221	-1.06479	1.01538
6	-0.65742	-1.64559	1.19873
6	-0.32822	-2.22308	2.43017
1	-0.93368	-2.70218	4.46893
15	0.59795	-1.46744	-0.16029
1	0.63661	-2.69294	2.56031
8	-4.09666	-0.66239	2.16877
8	-3.49579	-1.57701	4.21192
6	-4.49364	-0.79904	3.5381
1	-5.45591	-1.31838	3.58727
1	-4.55266	0.19509	4.00106
6	-4.88799	-2.9621	-1.47588
1	-4.54455	-3.89678	-1.93457
1	-5.87251	-3.08996	-1.00865
6	-1.56941	5.67936	-2.6321
6	-2.23939	5.47236	-1.42581
6	-2.0169	4.30824	-0.68716
6	-1.10835	3.34072	-1.13852
6	-0.43195	3.56338	-2.34881
6	-0.66674	4.71867	-3.09401
1	-1.74392	6.5854	-3.20553
1	-2.93715	6.21783	-1.05463
1	-2.54824	4.16514	0.24694
1	0.28953	2.82946	-2.69461
1	-0.13518	4.87293	-4.02882
6	-2.16748	2.82589	4.07752
6	-3.13119	2.50294	3.11872
6	-2.74533	2.15456	1.82386
6	-1.38717	2.1341	1.4704
6	-0.42831	2.46832	2.435
6	-0.81498	2.80847	3.73187
1	-2.46975	3.0903	5.08691
1	-4.18678	2.52666	3.37588
1	-3.5003	1.87966	1.09507
1	0.61976	2.45309	2.16646
1	-0.05827	3.05647	4.4705
6	3.92843	-4.63854	0.6768
6	3.15839	-4.73019	-0.48211
6	2.13206	-3.81463	-0.72511
6	1.86341	-2.77776	0.18308
6	2.67861	-2.67108	1.32436
6	3.68227	-3.60408	1.58094
1	4.72044	-5.35649	0.86853
1	3.34987	-5.52006	-1.20305
1	1.54551	-3.91415	-1.63041
1	2.545	-1.84212	2.008
1	4.2889	-3.50471	2.47604
6	-1.71221	-3.21258	-3.8009
6	-1.70334	-3.91225	-2.59019
6	-1.01423	-3.40031	-1.49224

6	-0.31045	-2.19011	-1.59772
6	-0.31202	-1.50241	-2.81828
6	-1.01605	-2.00815	-3.91301
1	-2.26291	-3.60437	-4.65122
1	-2.23798	-4.85408	-2.50063
1	-1.03114	-3.93092	-0.5452
1	0.21509	-0.55489	-2.89391
1	-1.02699	-1.45689	-4.8486
45	1.26514	0.85007	-0.5546
14	3.21152	1.51485	0.74146
8	4.89403	1.24708	0.79038
6	5.52988	0.16083	0.12341
6	6.78158	0.71274	-0.57633
6	5.96092	-0.87599	1.17107
6	3.19704	3.40261	0.87224
6	2.65181	0.76854	2.42226
1	7.36023	-0.09813	-1.03266
1	6.52106	1.42978	-1.35636
1	7.41422	1.22239	0.15689
1	6.41229	-1.7539	0.69503
1	6.68762	-0.43682	1.86152
1	5.0981	-1.21241	1.74853
1	3.93046	3.72931	1.61858
1	3.45886	3.8555	-0.08843
1	2.20697	3.7755	1.15053
1	1.64175	0.35316	2.43474
1	3.36565	-0.00082	2.7299
1	2.70102	1.56449	3.17691
6	4.51442	-0.45289	-0.88399
6	3.43498	0.55213	-1.30741
1	4.03299	-1.32524	-0.436
1	5.05412	-0.81542	-1.77114
1	1.54466	2.34548	-0.92306
1	2.71362	-0.01366	-1.92299
6	3.96902	1.6961	-2.18662
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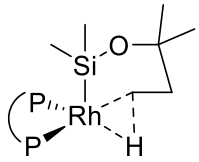

TS-OxAdd-γ-1°

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6	-1.02263	-1.78458	2.54829
6	-1.07375	-1.35471	1.21698
8	-4.45316	0.14657	1.4391
8	-4.32373	-0.5523	3.6489
1	-2.00425	-1.89086	4.49265
1	-0.1477	-2.31598	2.90095
15	0.40896	-1.56297	0.1143
6	-2.98372	0.86681	-3.27136
6	-3.5999	-0.25634	-2.76555
6	-3.33505	-0.71291	-1.47639
6	-2.42155	-0.11085	-0.6319
6	-1.7838	1.06499	-1.13364
6	-2.07292	1.52424	-2.42317
1	-3.19709	1.2302	-4.26993
15	-0.46235	1.84045	-0.10197
1	-1.58609	2.4191	-2.7917
8	-4.10091	-1.82072	-1.21278
8	-4.53379	-1.06309	-3.36312
6	-4.81112	-2.10964	-2.42222
1	-5.88677	-2.13805	-2.21425
1	-4.4591	-3.06483	-2.83044
6	-5.13345	0.15484	2.69902
1	-5.26192	1.19098	3.03439
1	-6.10014	-0.35198	2.5945
6	2.89008	-4.8784	2.26682
6	1.99837	-5.25082	1.26081
6	1.22254	-4.28723	0.612
6	1.33611	-2.93386	0.95424
6	2.24573	-2.56848	1.96111
6	3.0086	-3.53151	2.61881
1	3.49628	-5.62929	2.76553
1	1.90923	-6.29396	0.97043
1	0.55186	-4.59849	-0.17993
1	2.3736	-1.51722	2.1992
1	3.7102	-3.22658	3.38996
6	-1.45102	-3.47869	-3.69787
6	-1.86157	-3.93083	-2.44054
6	-1.32234	-3.36932	-1.28321
6	-0.34057	-2.36989	-1.36963
6	0.06501	-1.92413	-2.63505

6	-0.49008	-2.47004	-3.79301
1	-1.88172	-3.90756	-4.59826
1	-2.61006	-4.71465	-2.36039
1	-1.67965	-3.69227	-0.3102
1	0.80383	-1.13156	-2.70328
1	-0.17509	-2.10617	-4.76661
6	0.54878	5.79676	-2.33028
6	-0.31418	5.84718	-1.23492
6	-0.65762	4.67816	-0.55139
6	-0.13426	3.4419	-0.9533
6	0.75034	3.40486	-2.04723
6	1.07965	4.57002	-2.73777
1	0.81377	6.70812	-2.85852
1	-0.72338	6.79903	-0.90794
1	-1.32746	4.73502	0.29957
1	1.18997	2.45726	-2.34909
1	1.76085	4.52148	-3.58243
6	-2.62368	2.86295	3.87332
6	-3.27891	3.11025	2.66316
6	-2.6501	2.81406	1.4537
6	-1.3477	2.29151	1.44508
6	-0.69358	2.05278	2.66187
6	-1.33213	2.33229	3.87092
1	-3.12129	3.07891	4.81446
1	-4.28308	3.52586	2.66166
1	-3.1757	2.96816	0.51614
1	0.3049	1.62406	2.64858
1	-0.82513	2.12838	4.80945
45	1.58506	0.42143	-0.02699
14	3.49428	-0.55808	-0.91056
8	4.93034	-0.19811	-0.1018
6	5.26677	0.96811	0.65701
6	5.13118	0.62587	2.14887
6	6.73435	1.27057	0.32327
6	3.70179	-2.40767	-1.25116
6	3.55175	0.2745	-2.64042
1	5.42176	1.4758	2.7764
1	4.10156	0.35198	2.39605
1	5.77249	-0.22708	2.38963
1	7.11449	2.10902	0.91705
1	7.3488	0.38852	0.5257
1	6.83511	1.51825	-0.7381
1	3.85507	-2.97648	-0.33178
1	2.8281	-2.82252	-1.76482
1	4.57791	-2.5526	-1.89452
1	4.53456	0.08623	-3.09139
1	2.79248	-0.1472	-3.30925
1	3.40119	1.3576	-2.59826
6	4.39749	2.18714	0.26569
6	2.90076	2.15402	0.60362
1	4.52427	2.32689	-0.81444
1	4.84721	3.07185	0.74018
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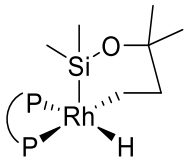

Rhodacycle-γ-1°

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6	-2.67069	0.70408	-3.39203
6	-1.76533	1.36553	-2.54389
6	-1.61447	1.03372	-1.18956
8	-4.12415	-1.68601	-1.18433
8	-4.36564	-1.10295	-3.41815
1	-2.77018	0.96977	-4.43802
1	-1.16584	2.16498	-2.96298
15	-0.24408	1.81775	-0.22455
6	-2.34893	-1.70886	3.38622
6	-3.32795	-0.85283	2.93451
6	-3.28823	-0.3231	1.64699
6	-2.26515	-0.57397	0.75386
6	-1.21995	-1.43395	1.21534
6	-1.29366	-1.98799	2.49754
1	-2.3878	-2.14446	4.37783
15	0.26659	-1.6502	0.13122
1	-0.52057	-2.66647	2.83339
8	-4.39558	0.45959	1.43563
8	-4.45544	-0.41918	3.58151
6	-5.08127	0.51672	2.69148
1	-6.12999	0.23646	2.54748
1	-4.99063	1.52771	3.10843
6	-4.80318	-2.01608	-2.40138
1	-4.5397	-3.03836	-2.69656

1	-5.88482	-1.90927	-2.25596
6	0.10116	6.08295	-2.08804
6	-1.16363	5.56047	-1.80325
6	-1.28675	4.2829	-1.26088
6	-0.14754	3.50479	-0.9851
6	1.1118	4.02912	-1.30349
6	1.23639	5.31121	-1.84454
1	0.19663	7.0794	-2.51016
1	-2.05541	6.14505	-2.01154
1	-2.27769	3.87579	-1.09255
1	1.99274	3.42066	-1.1422
1	2.22325	5.69943	-2.0796
6	-1.99269	2.4604	4.05213
6	-2.6434	3.04703	2.96336
6	-2.14669	2.87678	1.67118
6	-0.9803	2.12992	1.44869
6	-0.33141	1.55346	2.54967
6	-0.83519	1.71025	3.84096
1	-2.3872	2.58657	5.05625
1	-3.54141	3.63899	3.11963
1	-2.68381	3.3189	0.84173
1	0.55642	0.95598	2.38043
1	-0.32495	1.24302	4.67802
6	2.94778	-4.96687	1.99376
6	2.38078	-5.16375	0.73496
6	1.5296	-4.2027	0.18409
6	1.23697	-3.02385	0.88554
6	1.82792	-2.82956	2.14447
6	2.66559	-3.79489	2.69969
1	3.60931	-5.71569	2.41954
1	2.59989	-6.06755	0.1735
1	1.10106	-4.37355	-0.79656
1	1.64042	-1.91345	2.68973
1	3.10792	-3.62297	3.67675
6	-1.60871	-3.59283	-3.65636
6	-1.98172	-4.04625	-2.38725
6	-1.42635	-3.46757	-1.24692
6	-0.47388	-2.44324	-1.36335
6	-0.09461	-2.004	-2.63925
6	-0.66579	-2.57113	-3.7797
1	-2.05194	-4.03451	-4.54428
1	-2.70976	-4.84664	-2.28575
1	-1.73838	-3.80173	-0.2621
1	0.63991	-1.21136	-2.7404
1	-0.37609	-2.21137	-4.76244
45	1.59659	0.31717	-0.4983
14	3.22472	1.14867	0.91615
8	4.77762	1.11706	0.28817
6	5.33127	0.19579	-0.66157
6	5.40389	0.9122	-2.01781
6	6.74375	-0.12536	-0.15488
6	3.00435	2.94697	1.47252
6	3.34434	0.15878	2.54007
1	5.83329	0.25922	-2.78604
1	4.40649	1.22202	-2.33862
1	6.02809	1.80672	-1.9297
1	7.27798	-0.77515	-0.85669
1	7.31415	0.79977	-0.02894
1	6.69073	-0.62774	0.81623
1	3.7122	3.15388	2.28413
1	3.20819	3.6537	0.6647
1	1.99408	3.13898	1.84851
1	2.41644	0.14868	3.12099
1	3.65946	-0.87079	2.36142
1	4.1147	0.64581	3.15096
6	4.50869	-1.10824	-0.75174
6	3.0791	-1.00257	-1.28821
1	4.49373	-1.56633	0.24623
1	5.08534	-1.7984	-1.38807
1	3.10541	-0.68048	-2.3399
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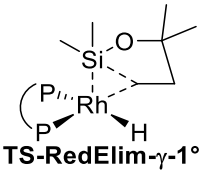

TS-RedElim-γ-1°

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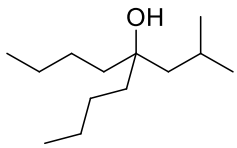
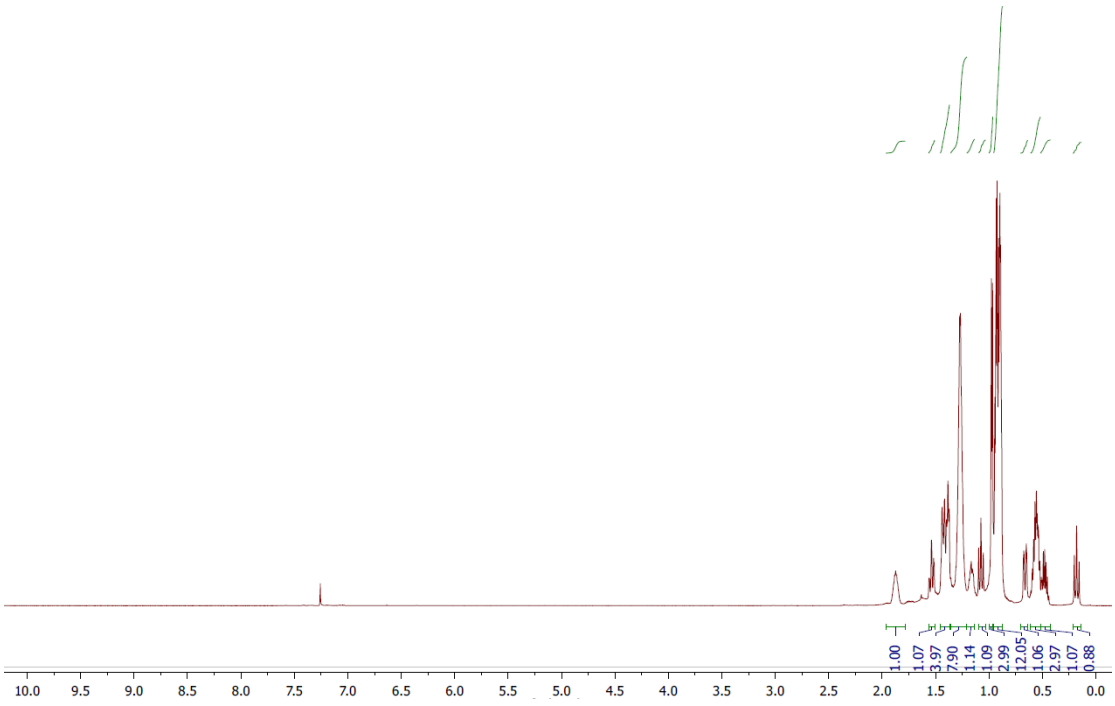
References

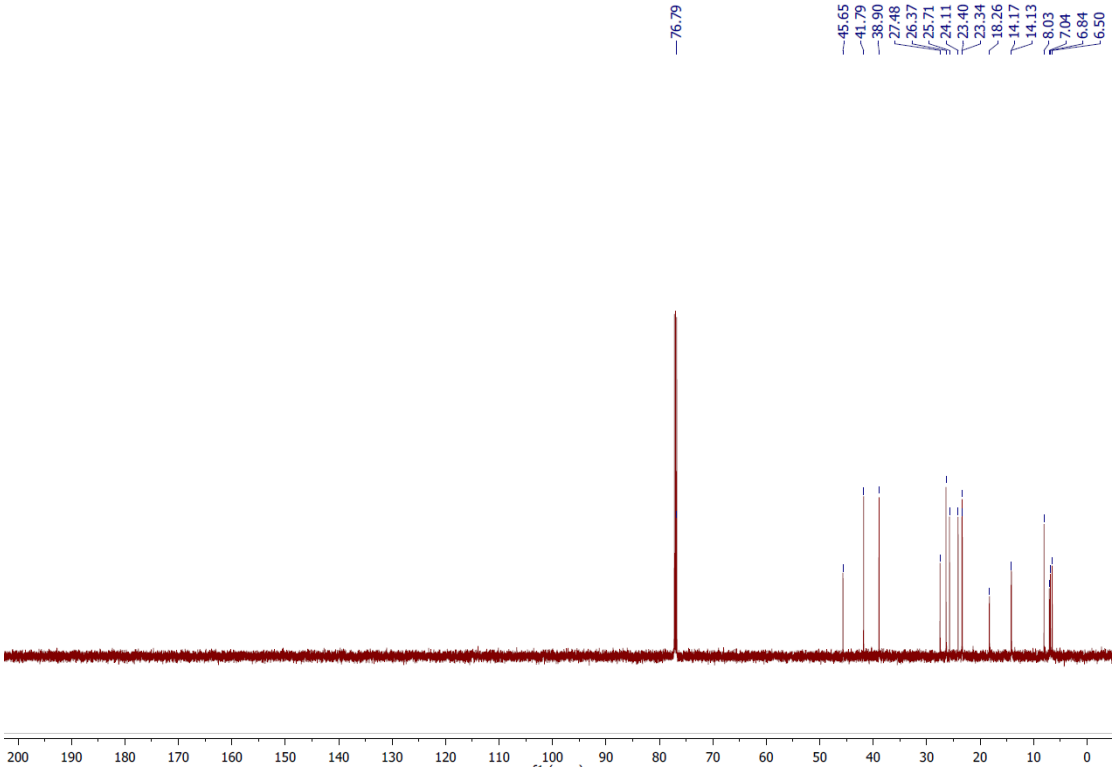
1 Esteruelas, M. A.; Oliván, M.; Vélez, A. *Inorg. Chem.* **2013**, *52*, 5339.

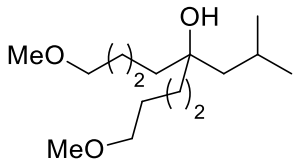
2 Qadir, M.; Priestley, R. E.; Rising, T.; Gelbrich, T.; Coles, S. J.; Hursthouse, M. B.; Sheldrake, P. W.; Whittall, N.; Hii, K. K. *Tetrahedron Lett.* **2003**, *44*, 3675.

Copies of NMR spectra





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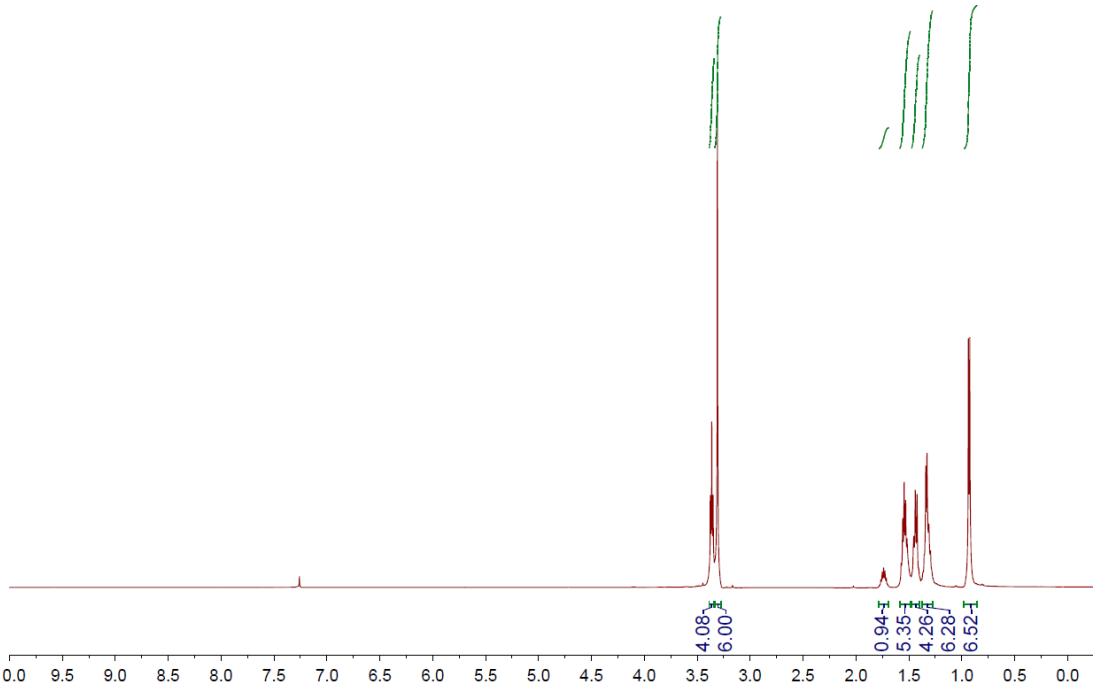
MeO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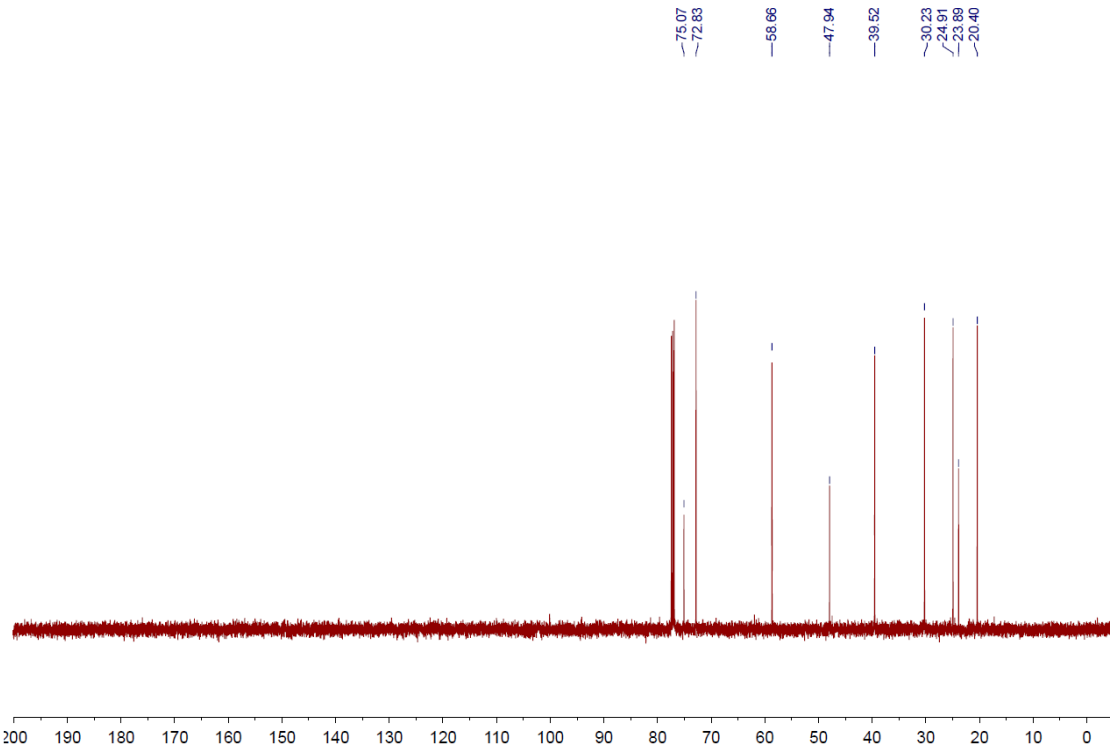
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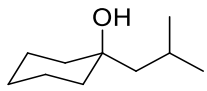
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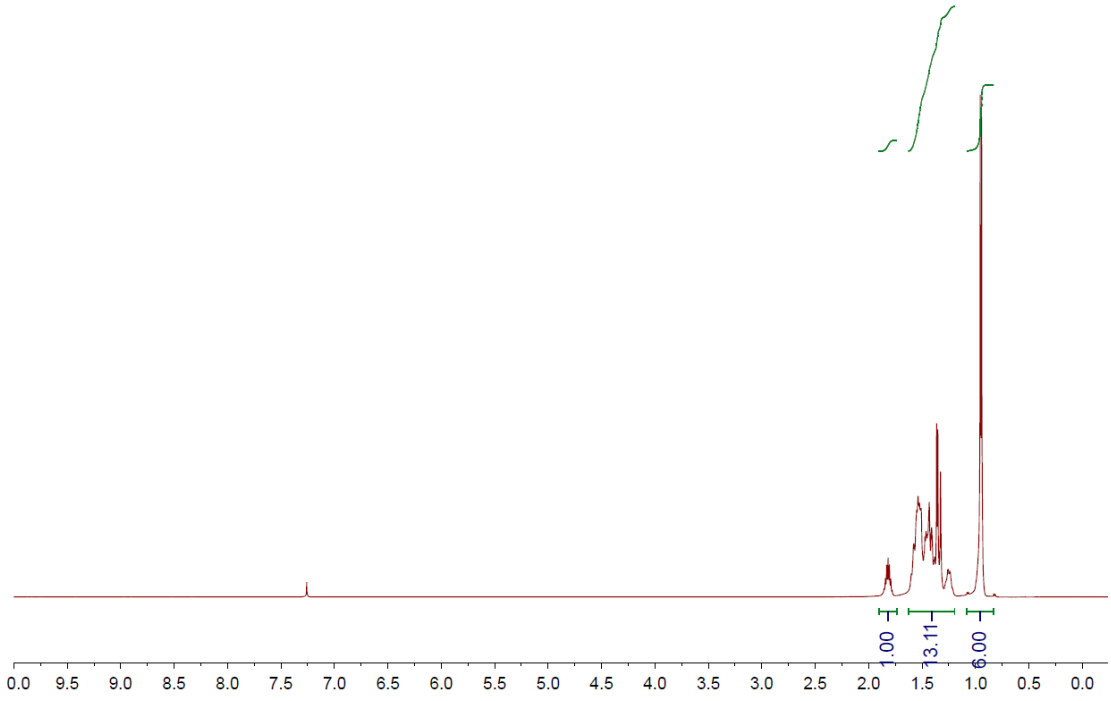
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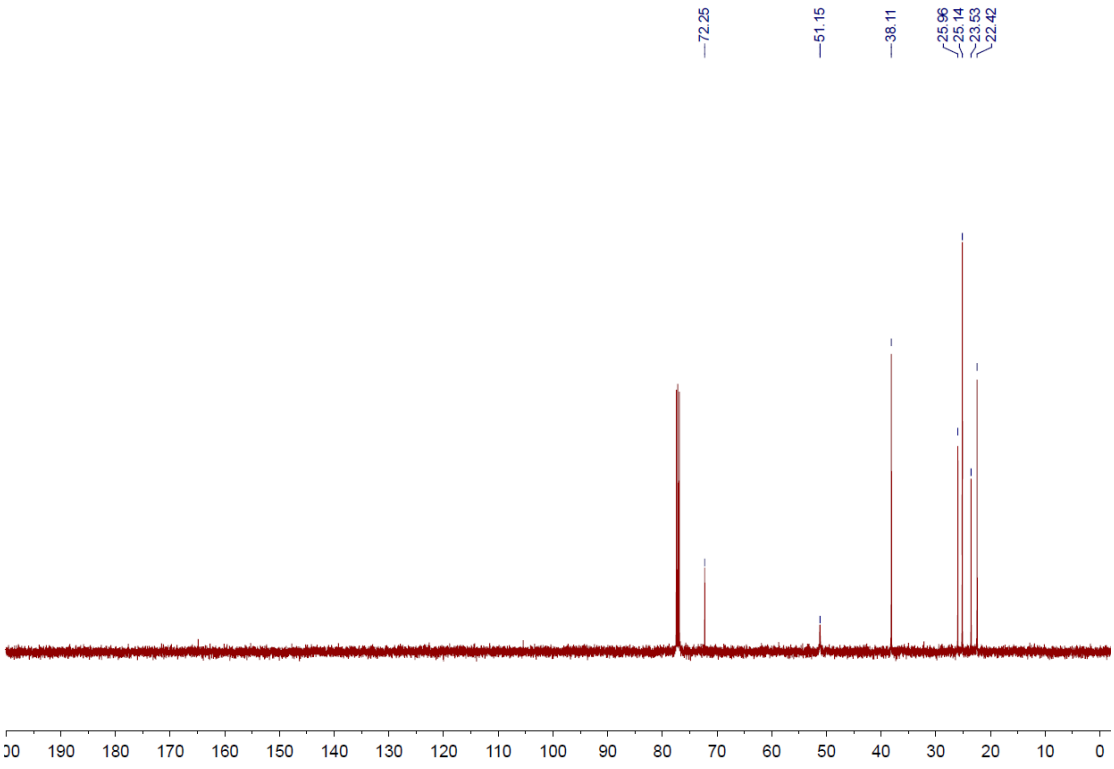
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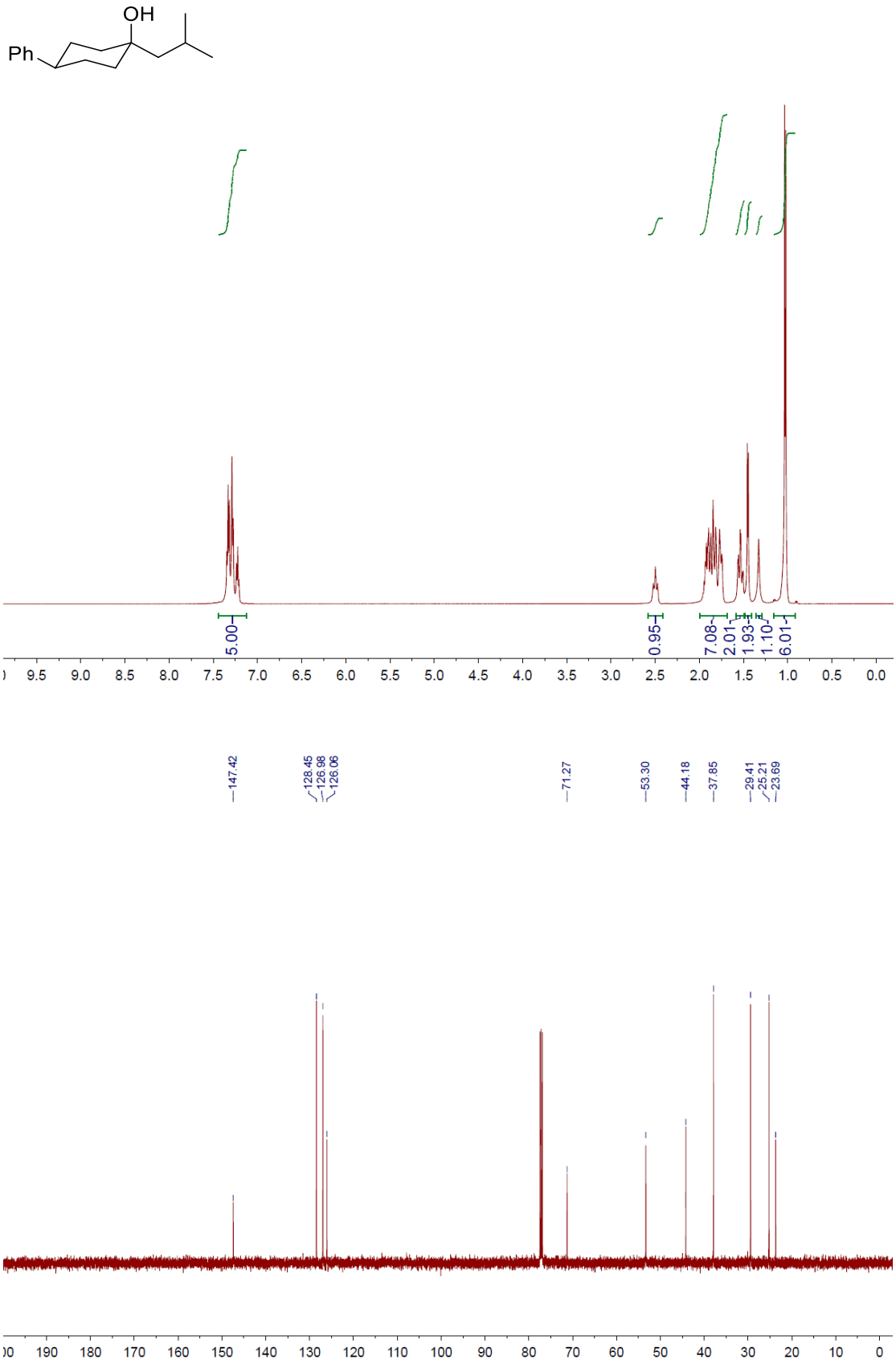
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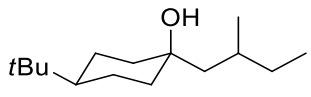
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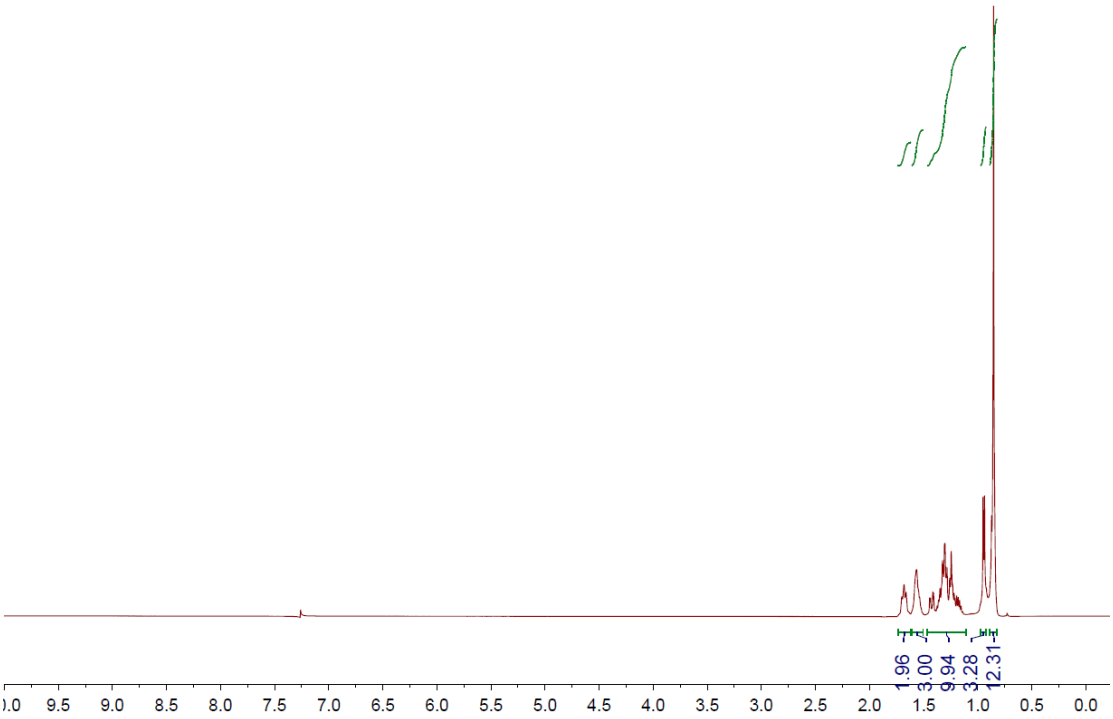
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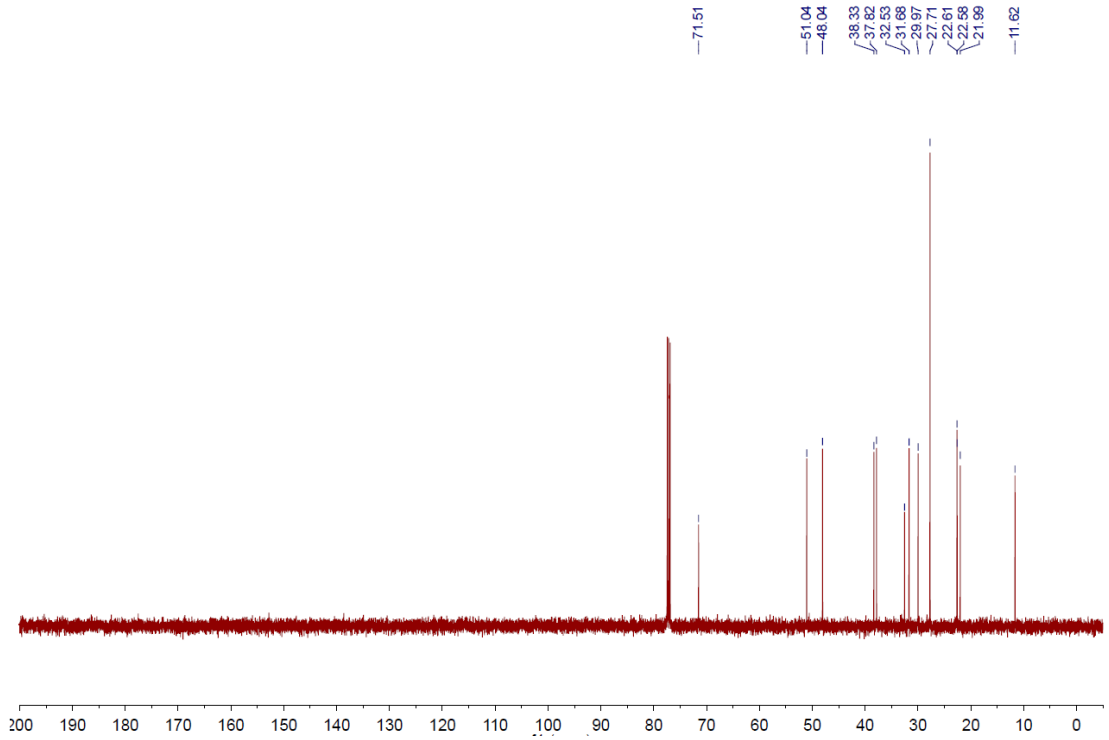
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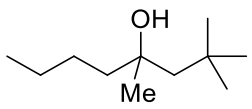
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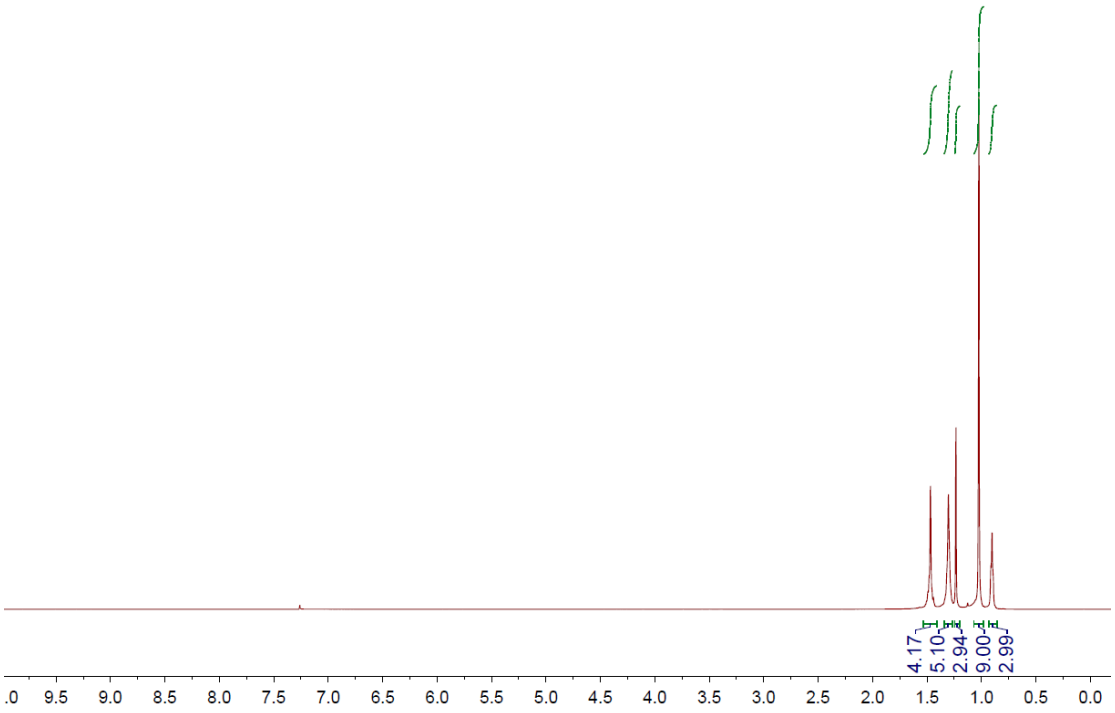
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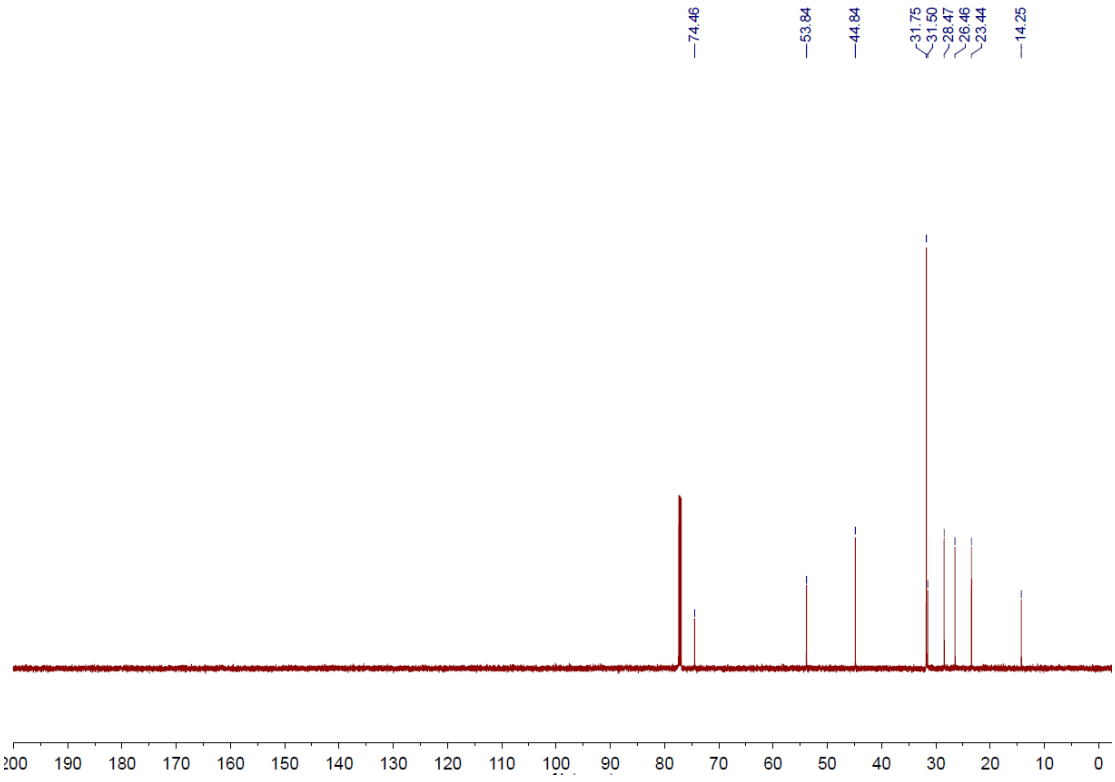
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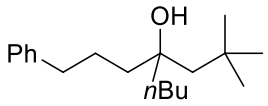
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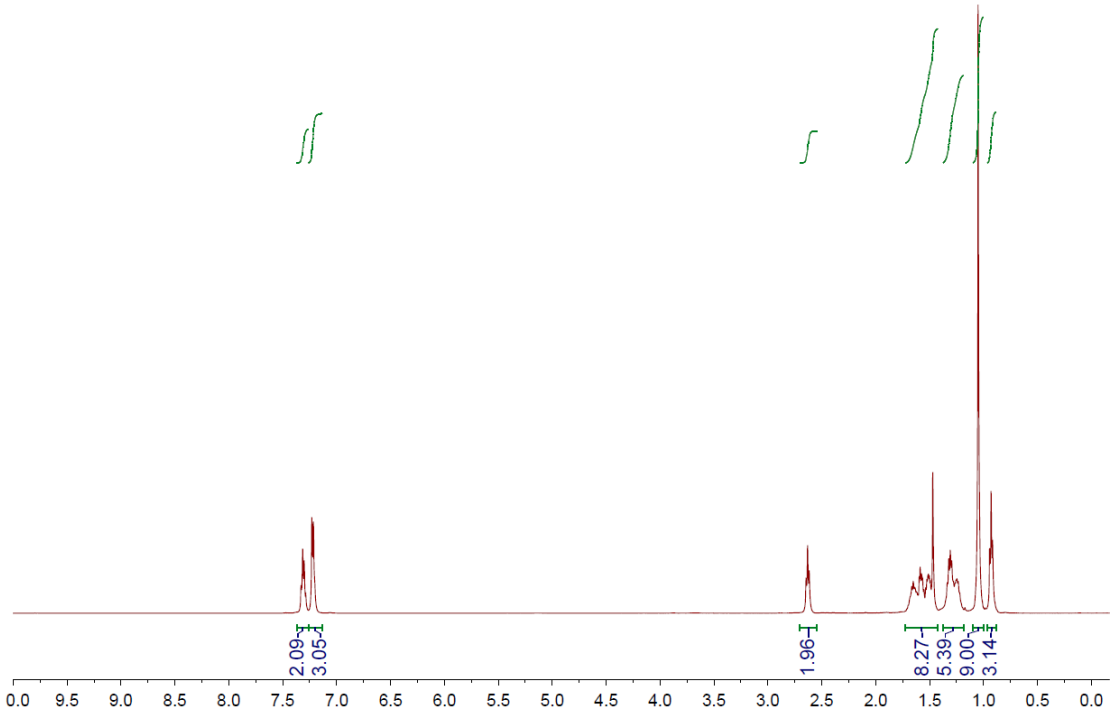
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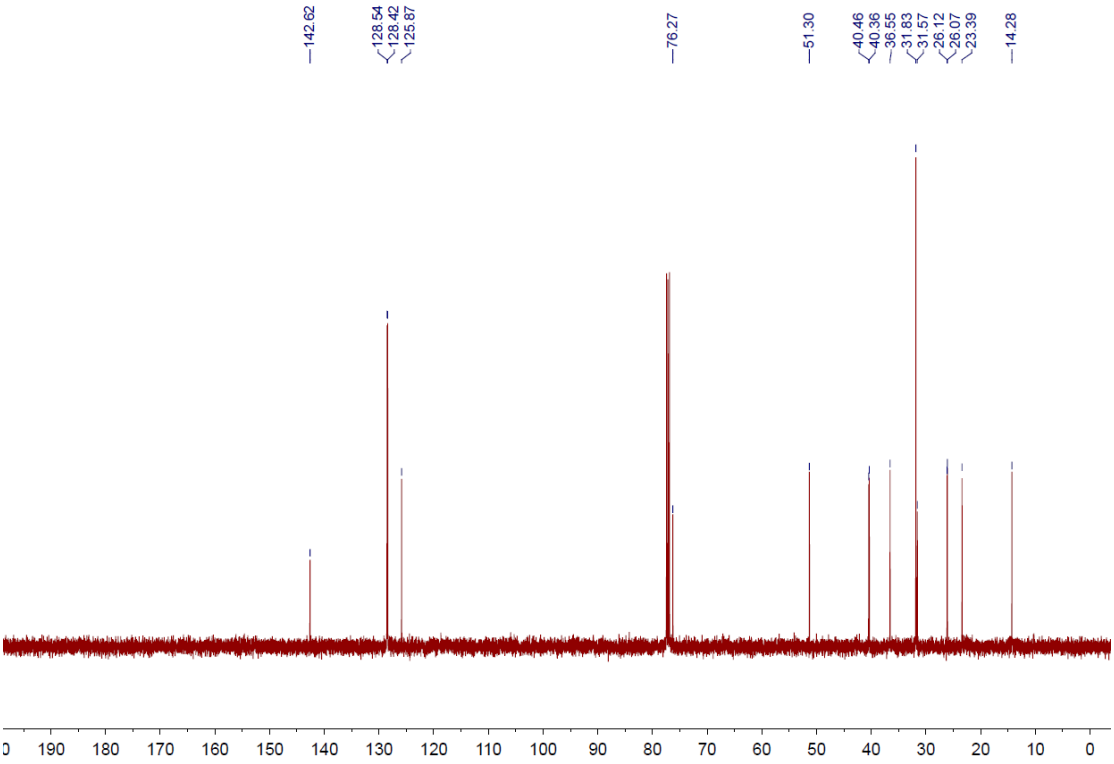
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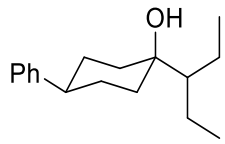
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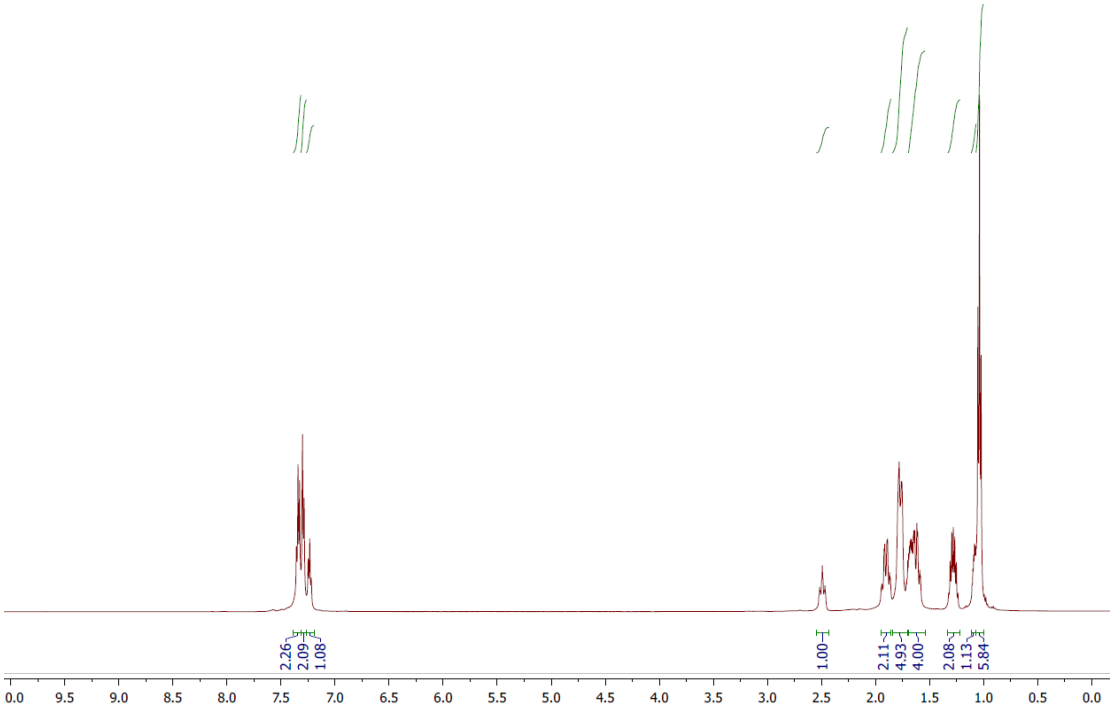
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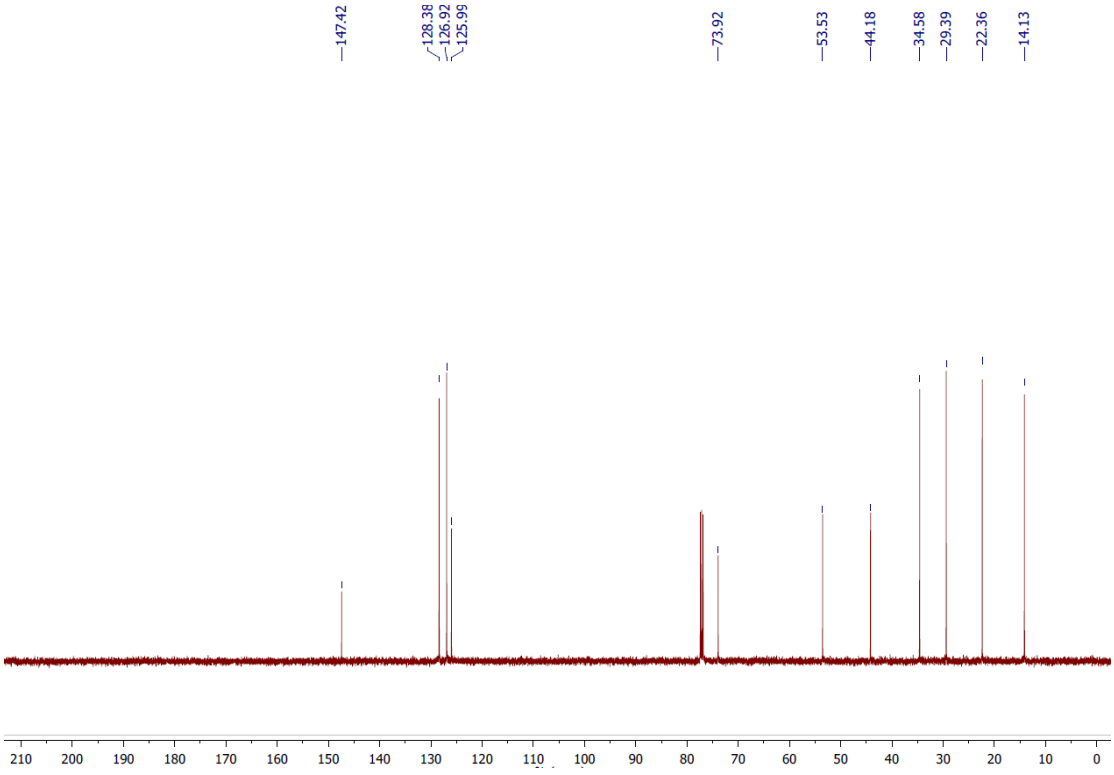
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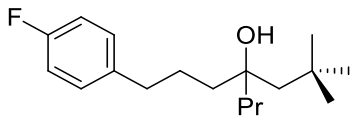
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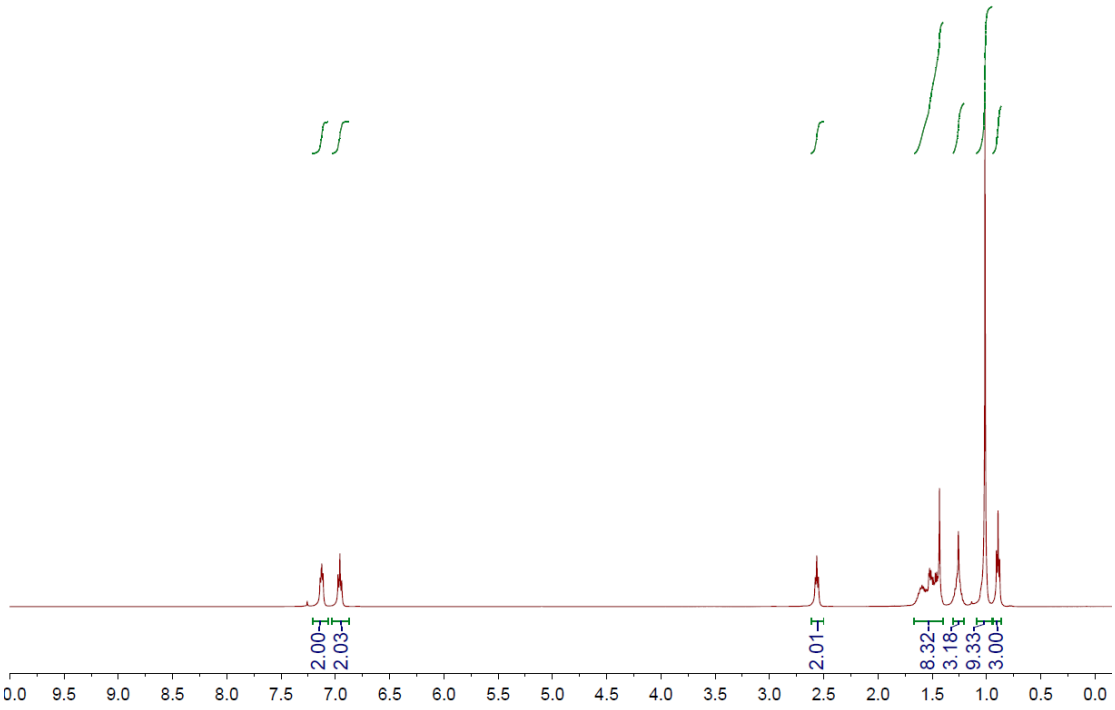
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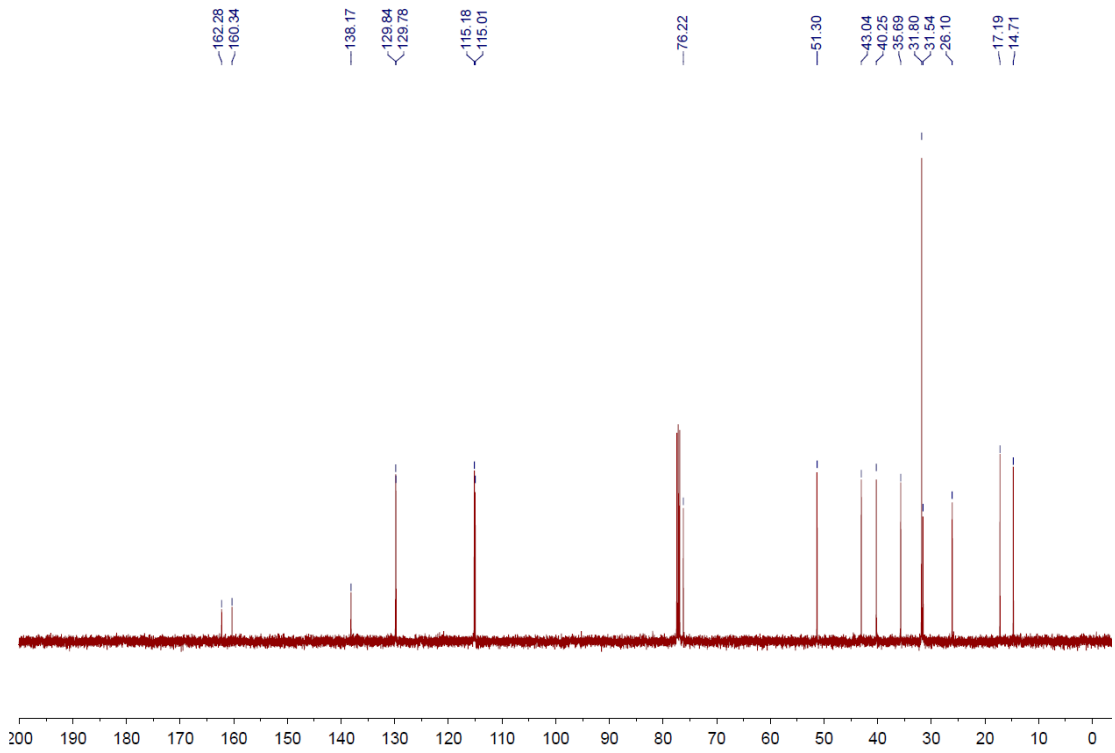
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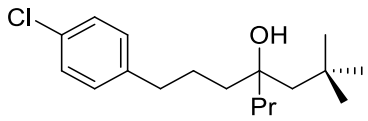
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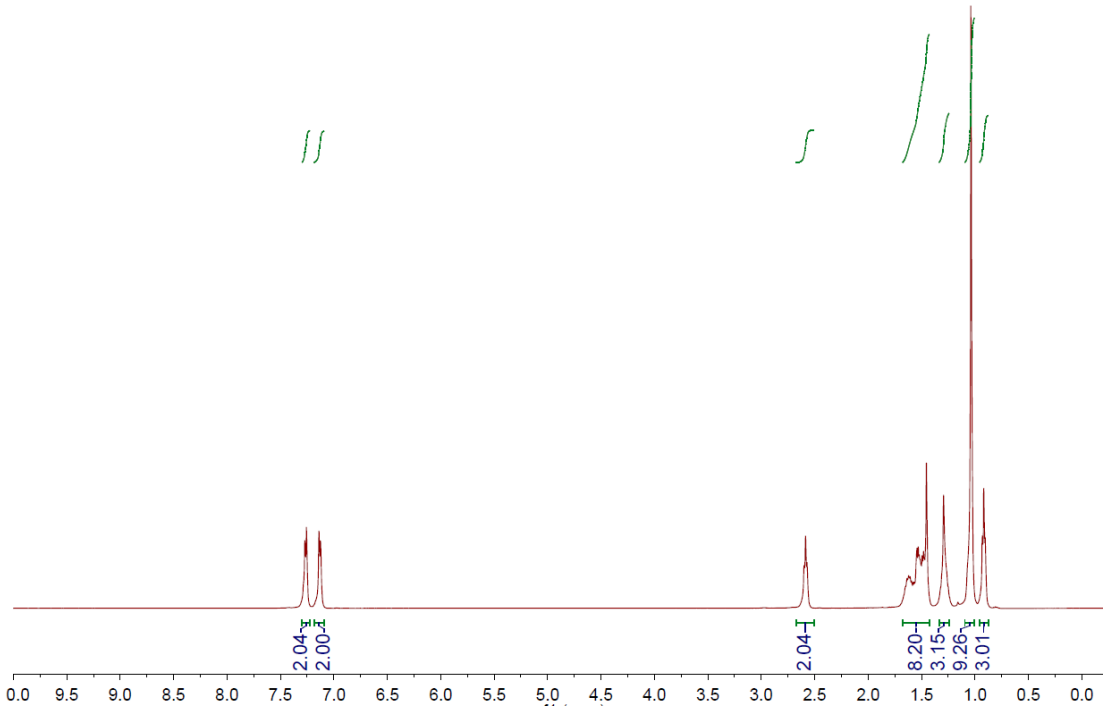
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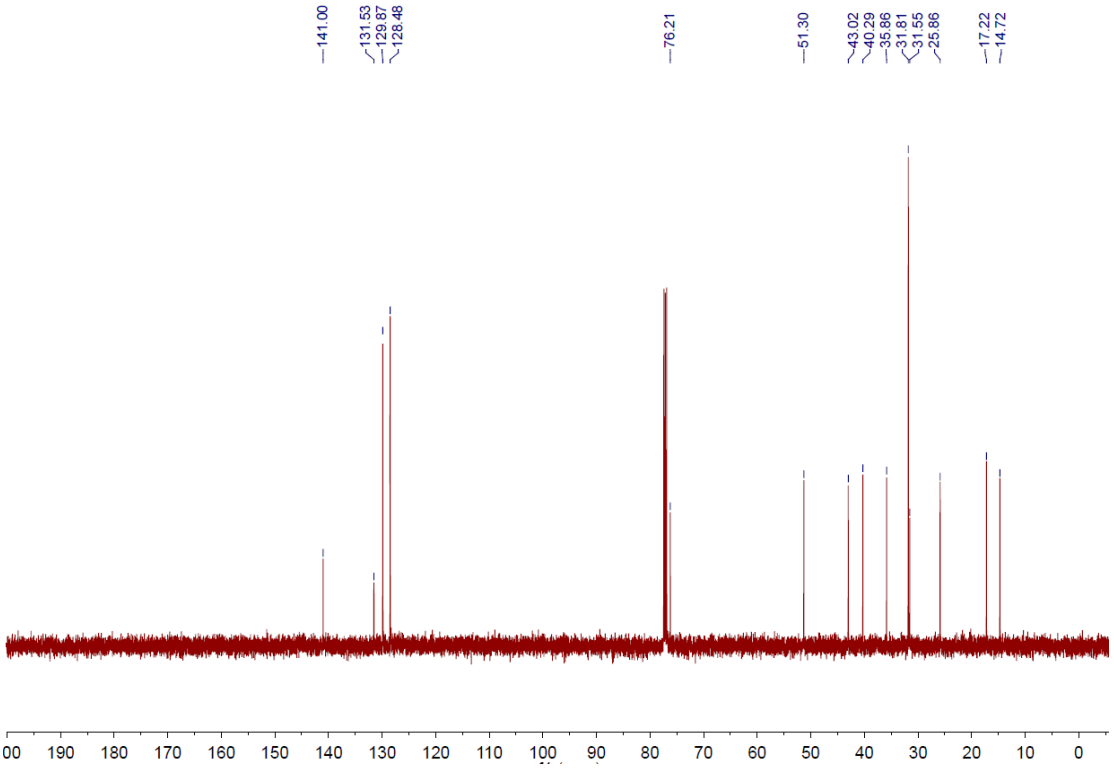
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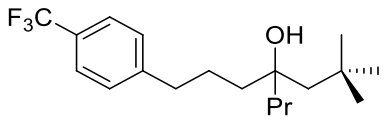
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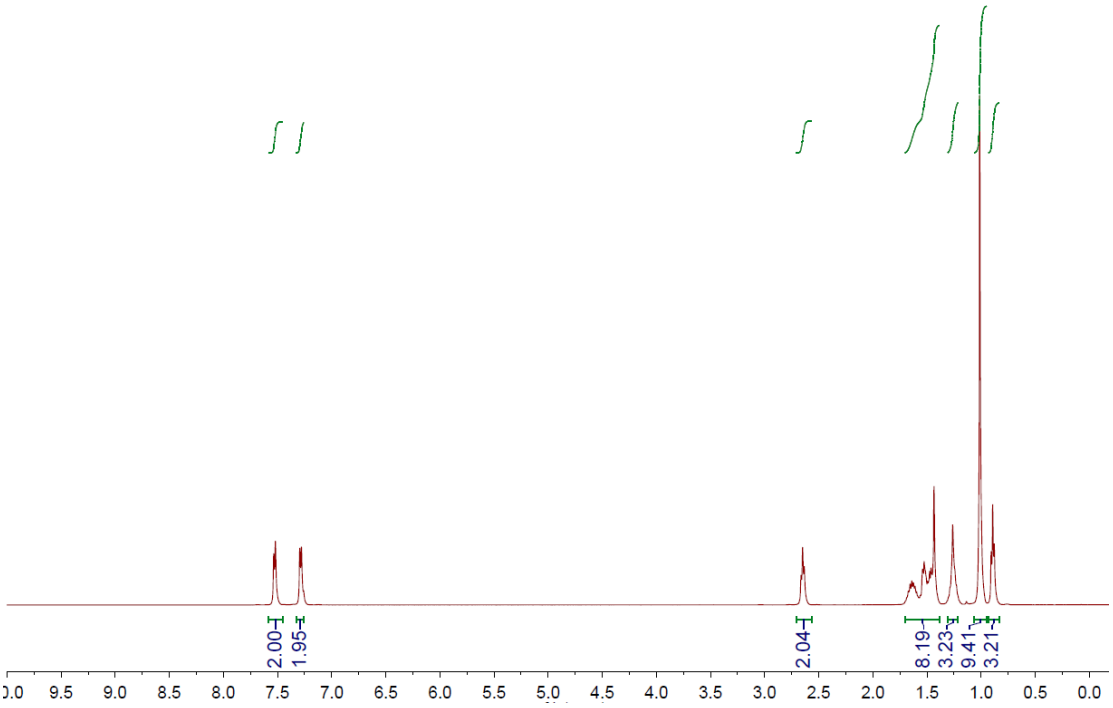
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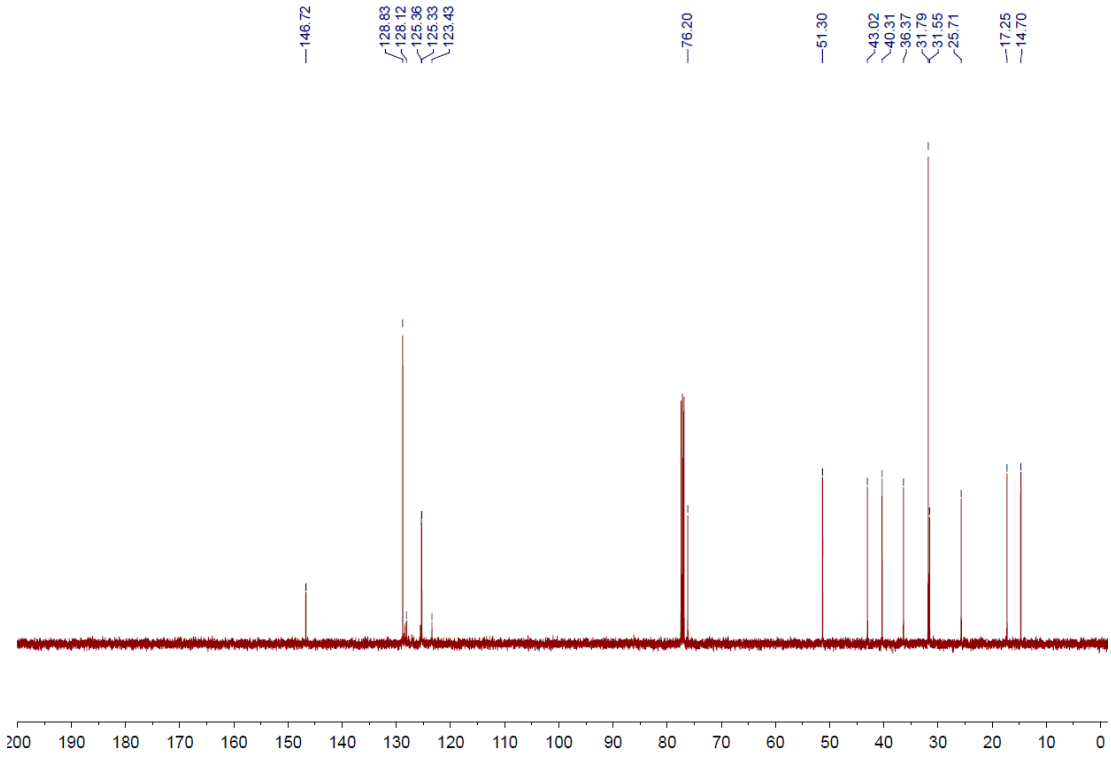
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36.37
31.79
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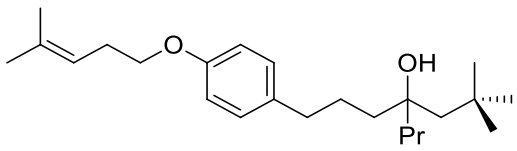
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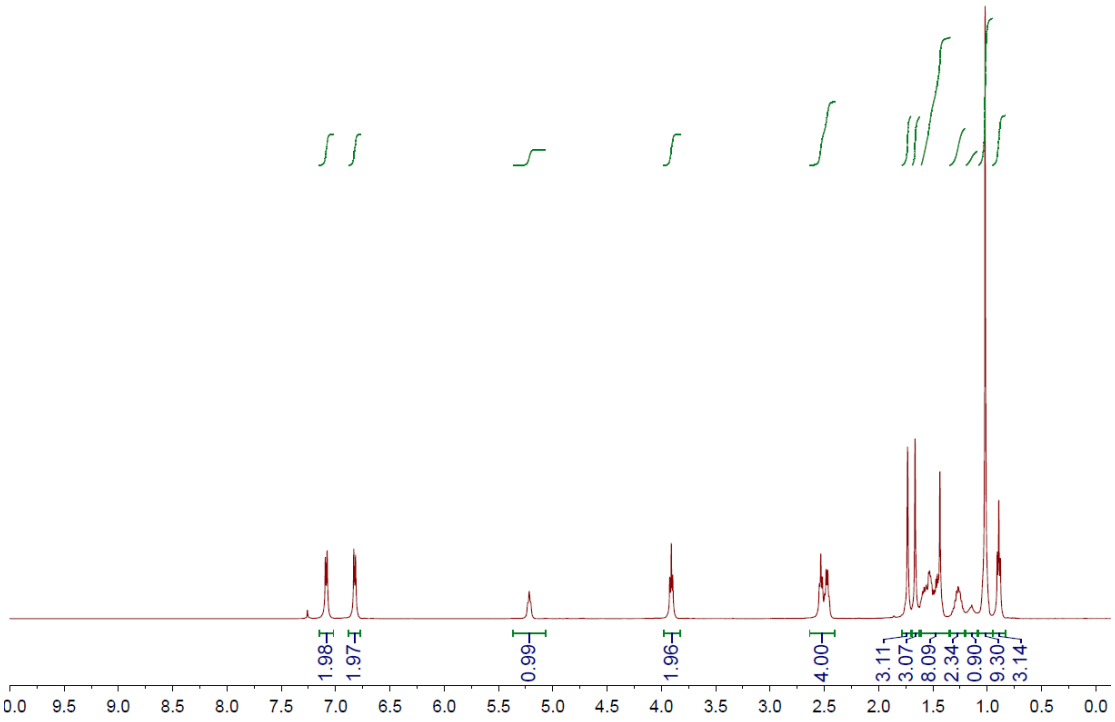
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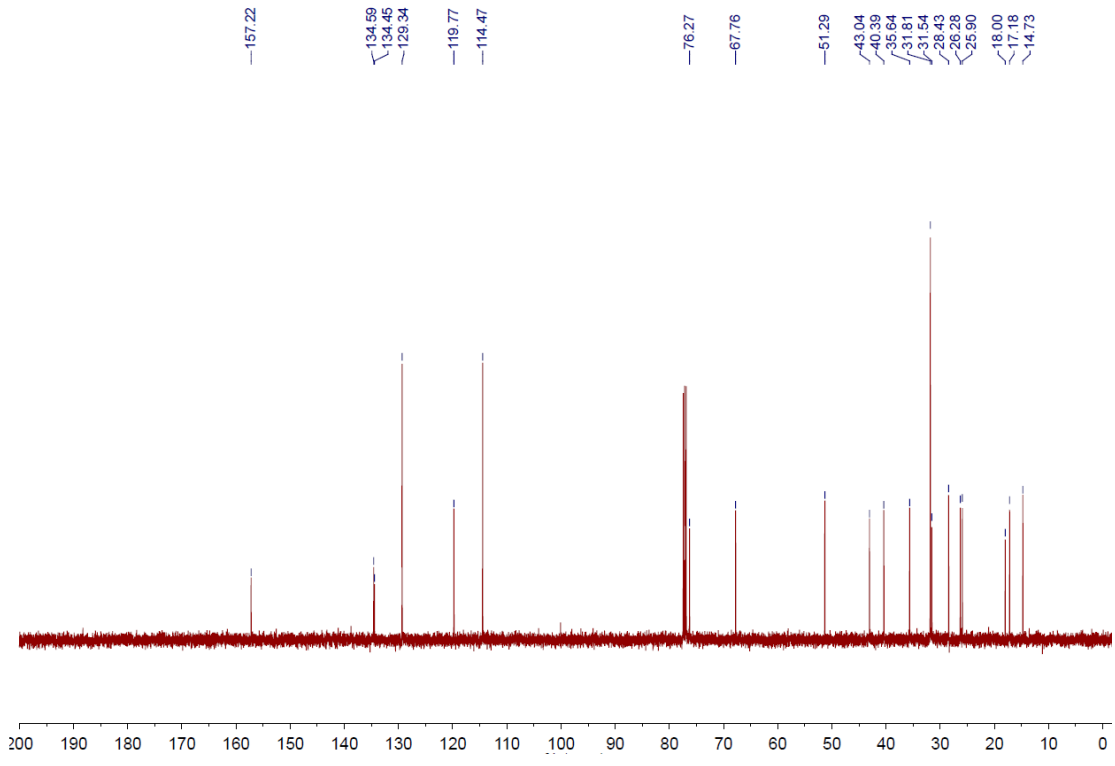
8.09
2.34
0.90
9.30
3.14
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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17.18
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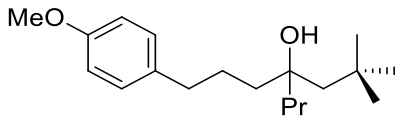
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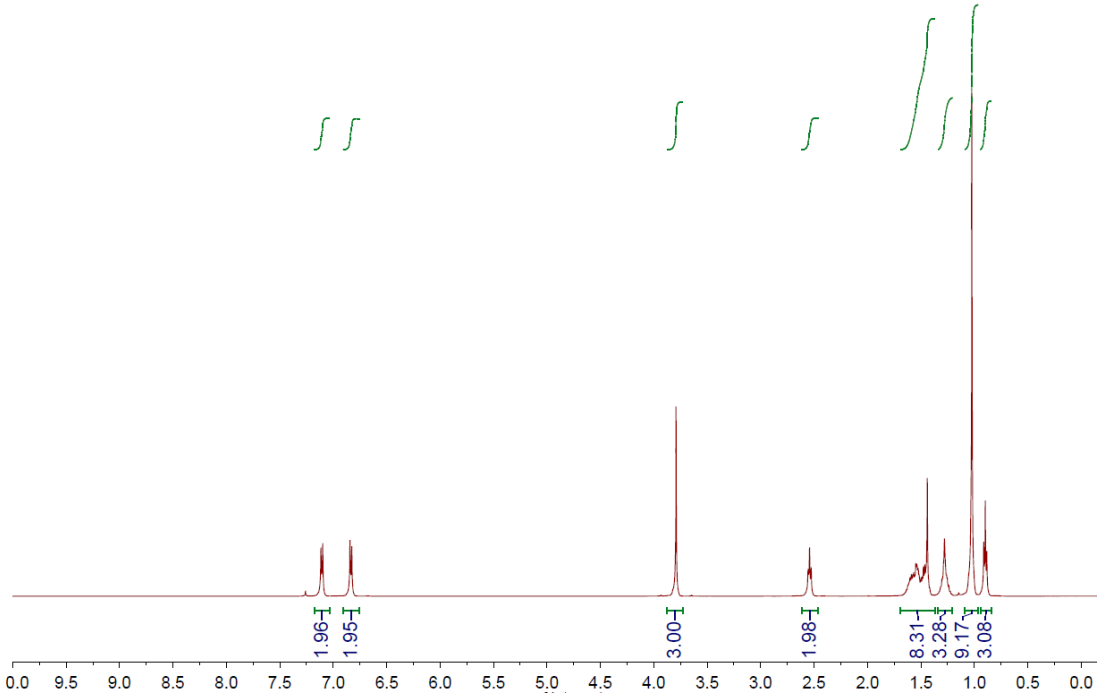
Pr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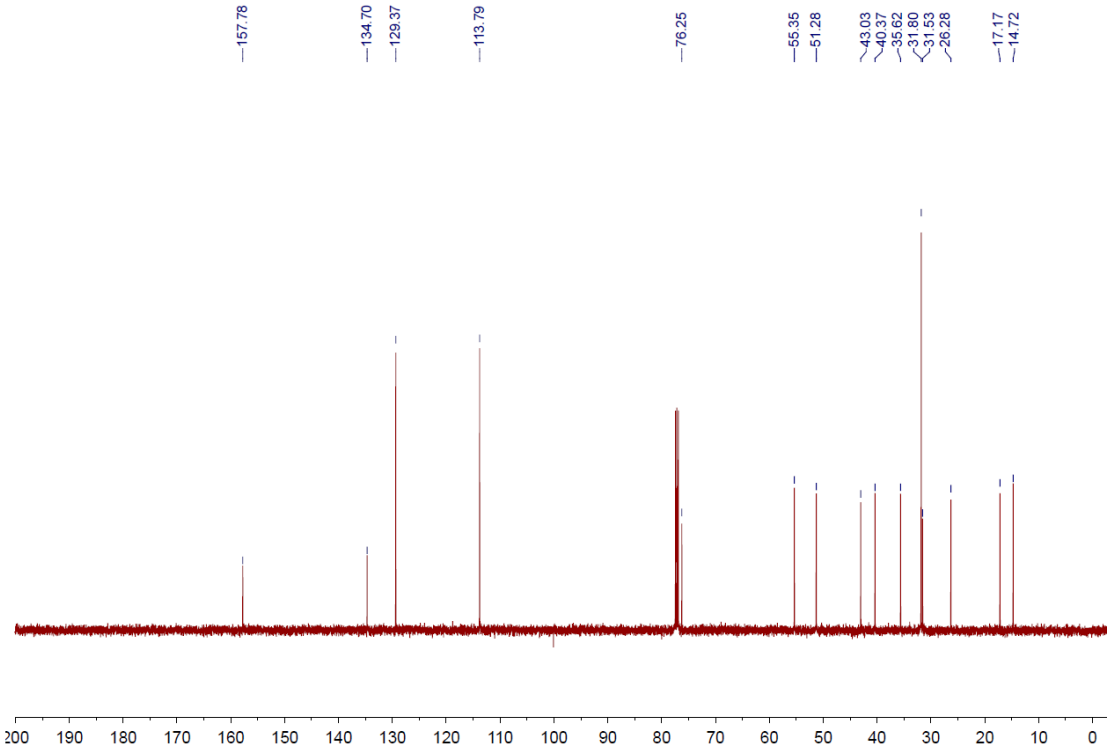
3.28
9.17
3.08
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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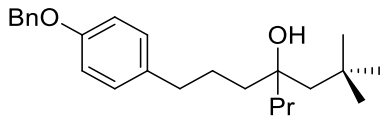
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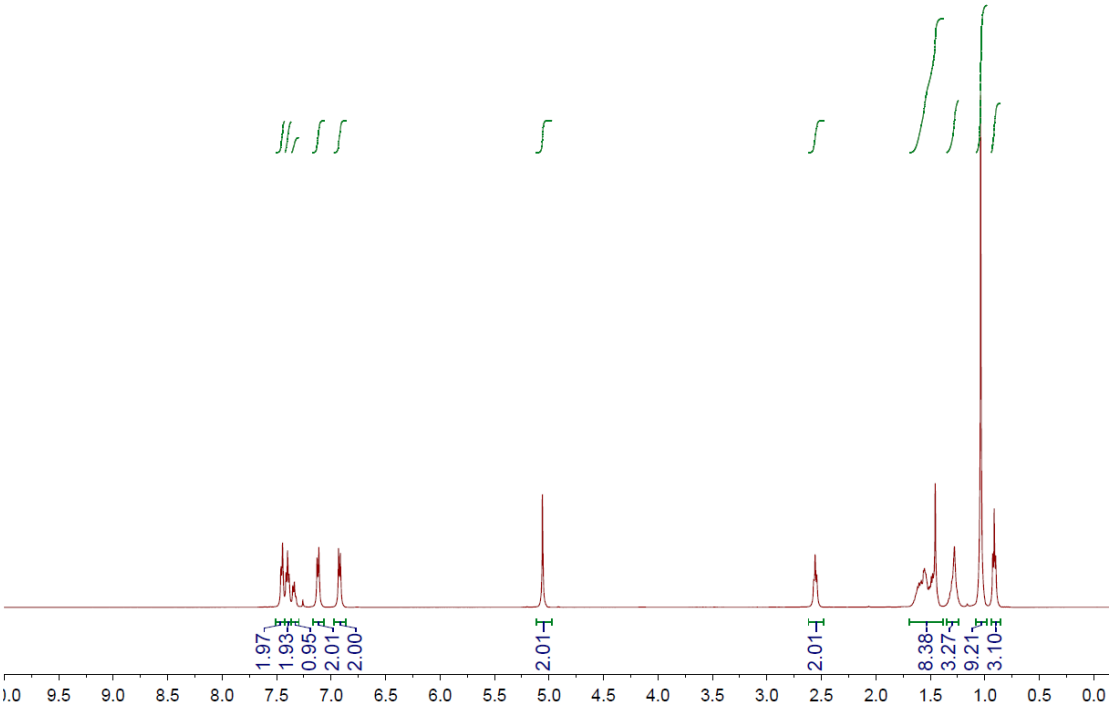
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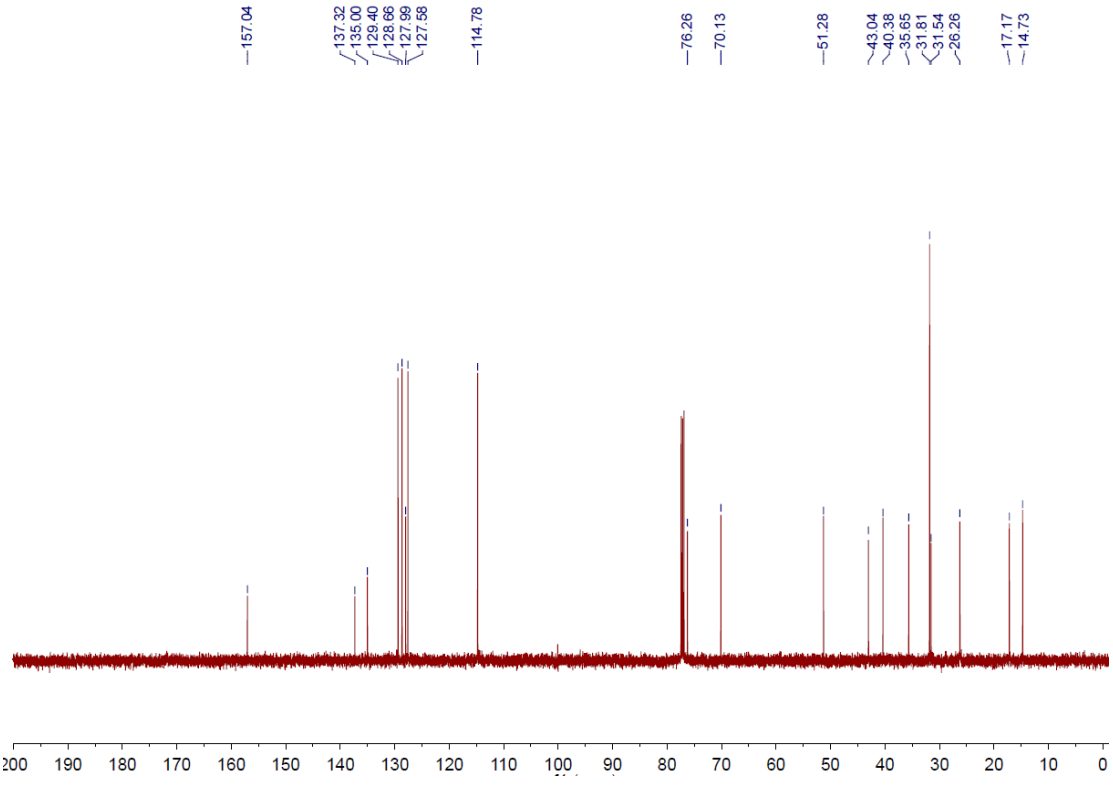
1.0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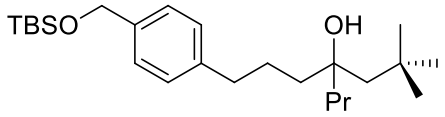
17.17
14.73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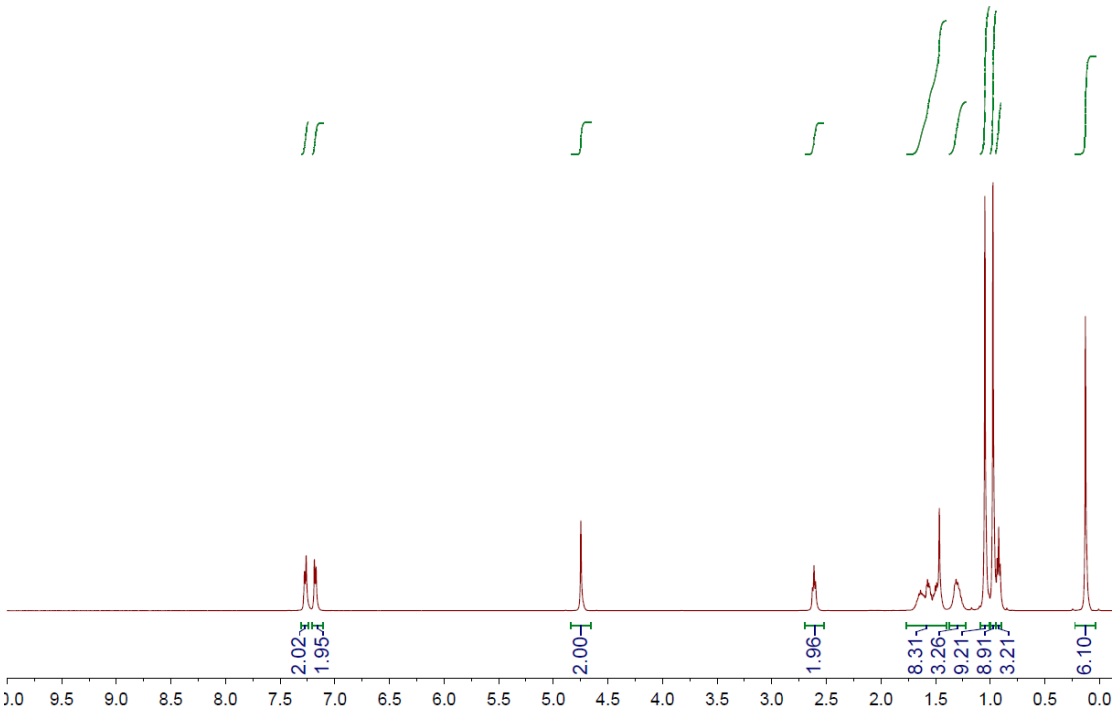
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3.21
6.10
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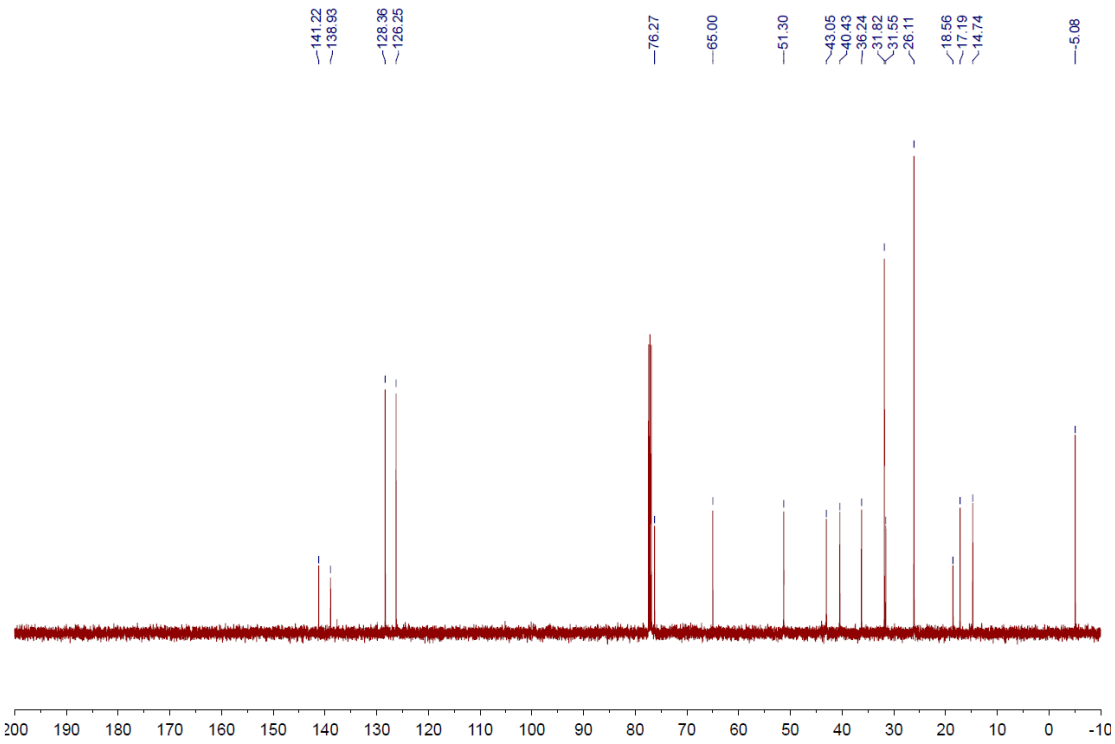
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65.00
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36.24
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14.74
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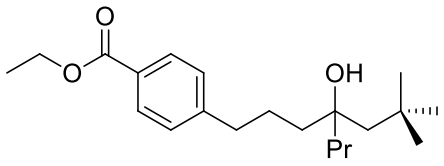
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OH
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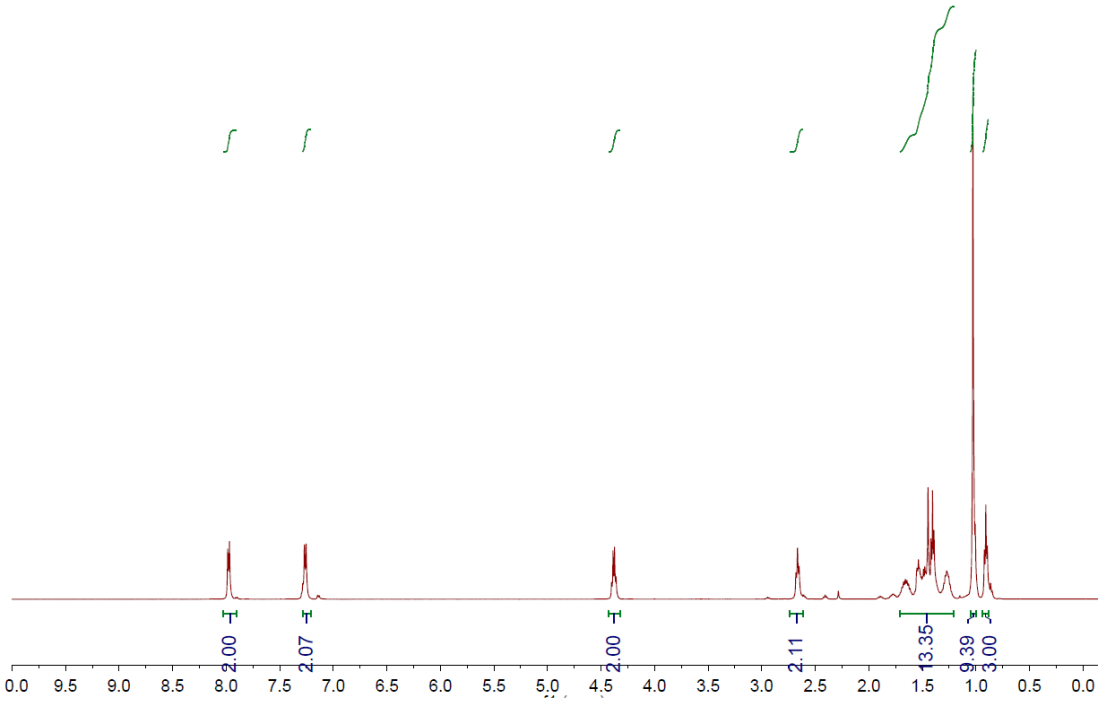
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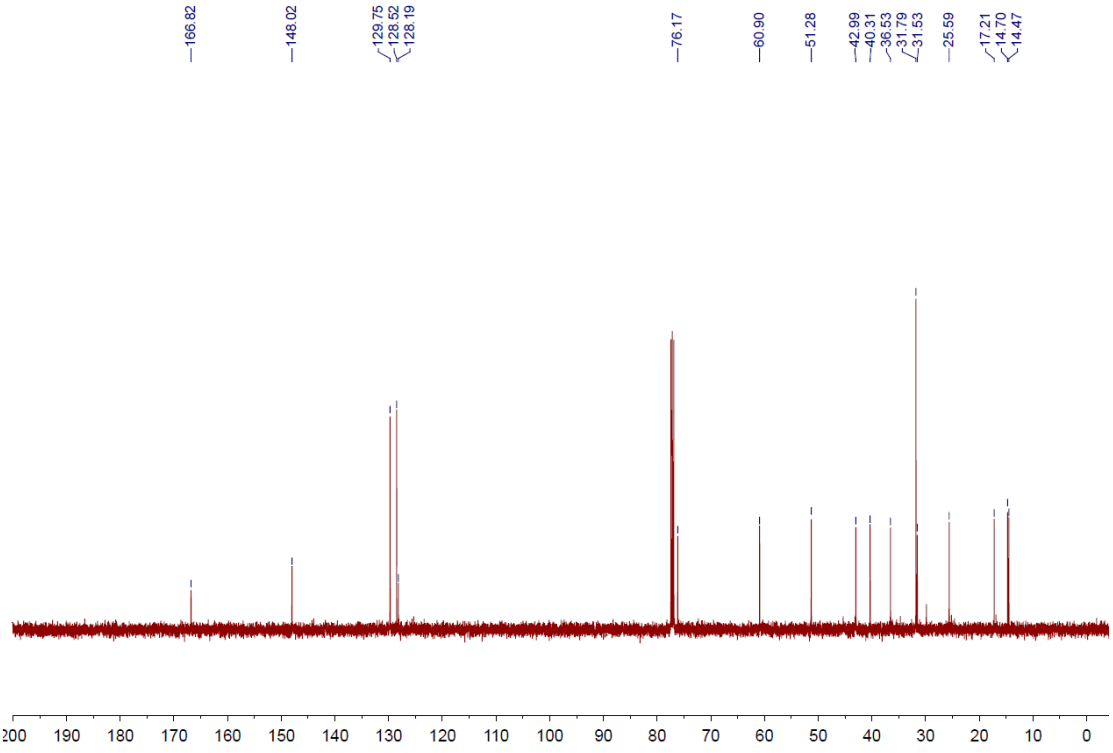
9.39
3.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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128.19
76.17
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42.99
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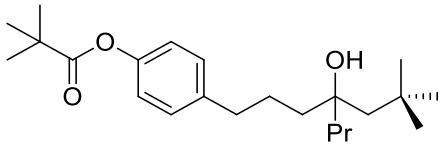
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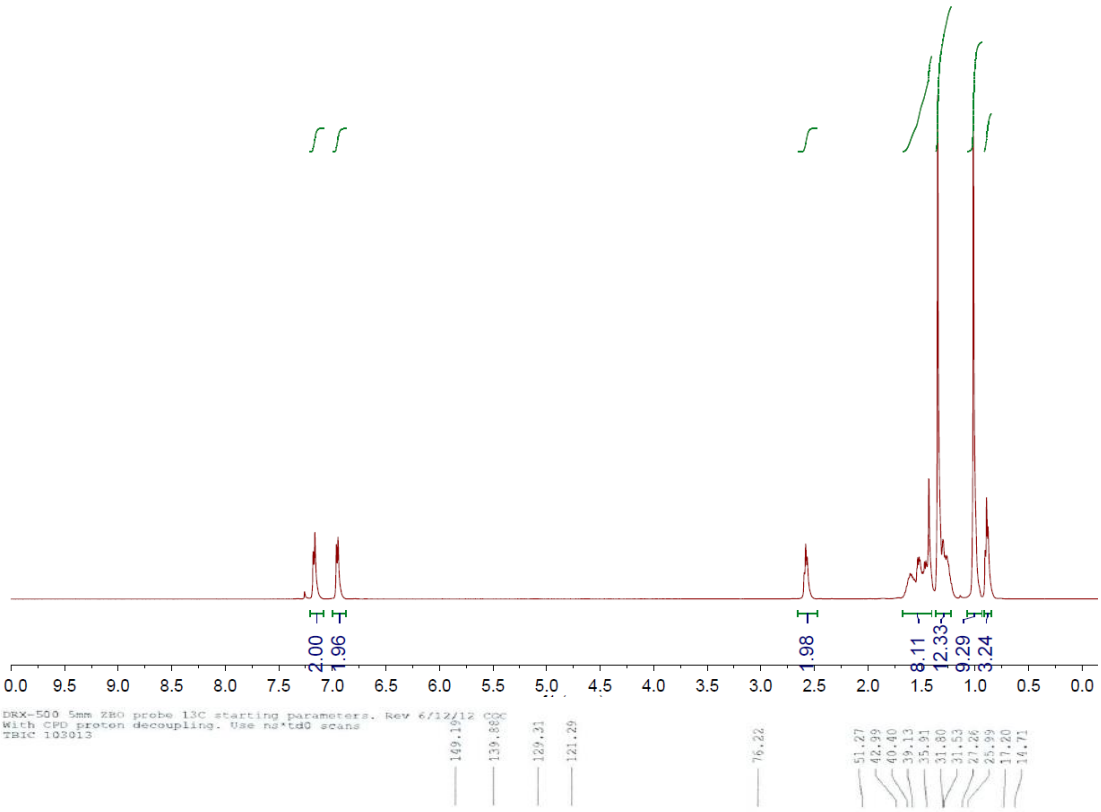
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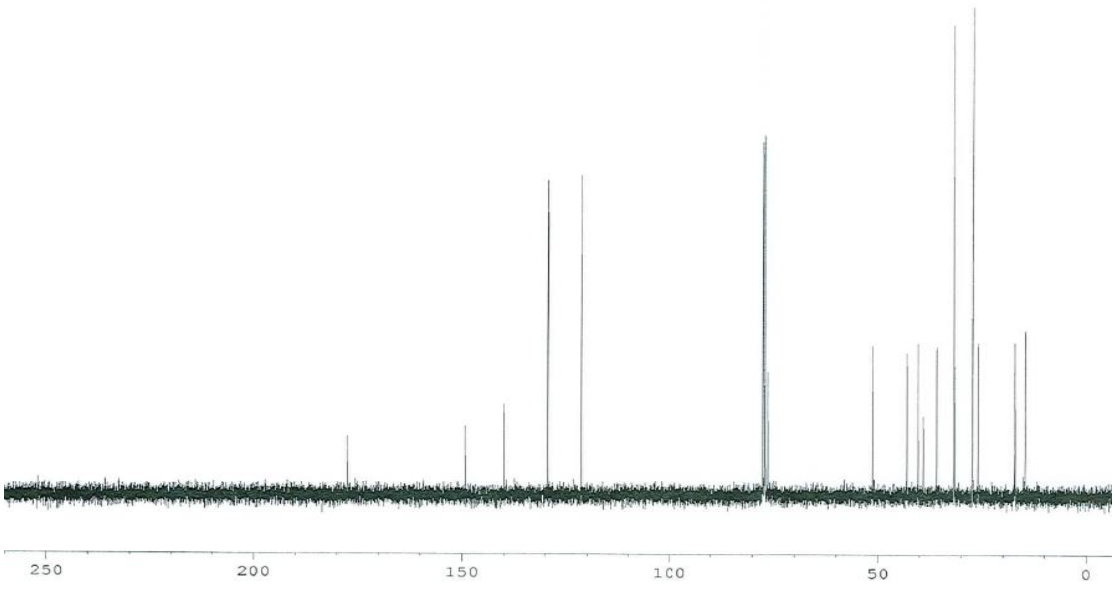
1.98
8.11
12.33
9.29
3.24
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
DRX-500 5mm ZBO probe 13C starting parameters. Rev 6/12/12 CQC
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
149.19
139.88
129.31
121.29
76.22
51.27
42.99
40.40
39.13
35.91
31.80
31.53
27.26
25.99
17.20
14.71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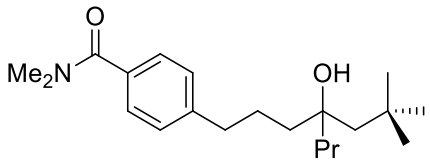
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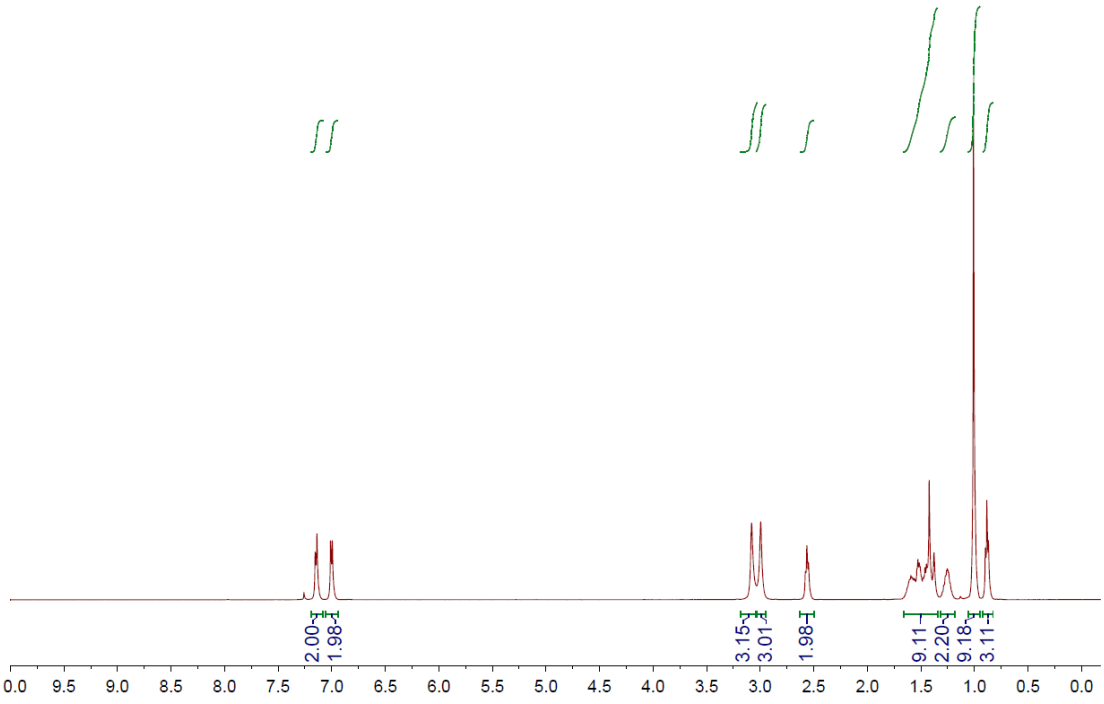
OH
Pr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9.11
2.20
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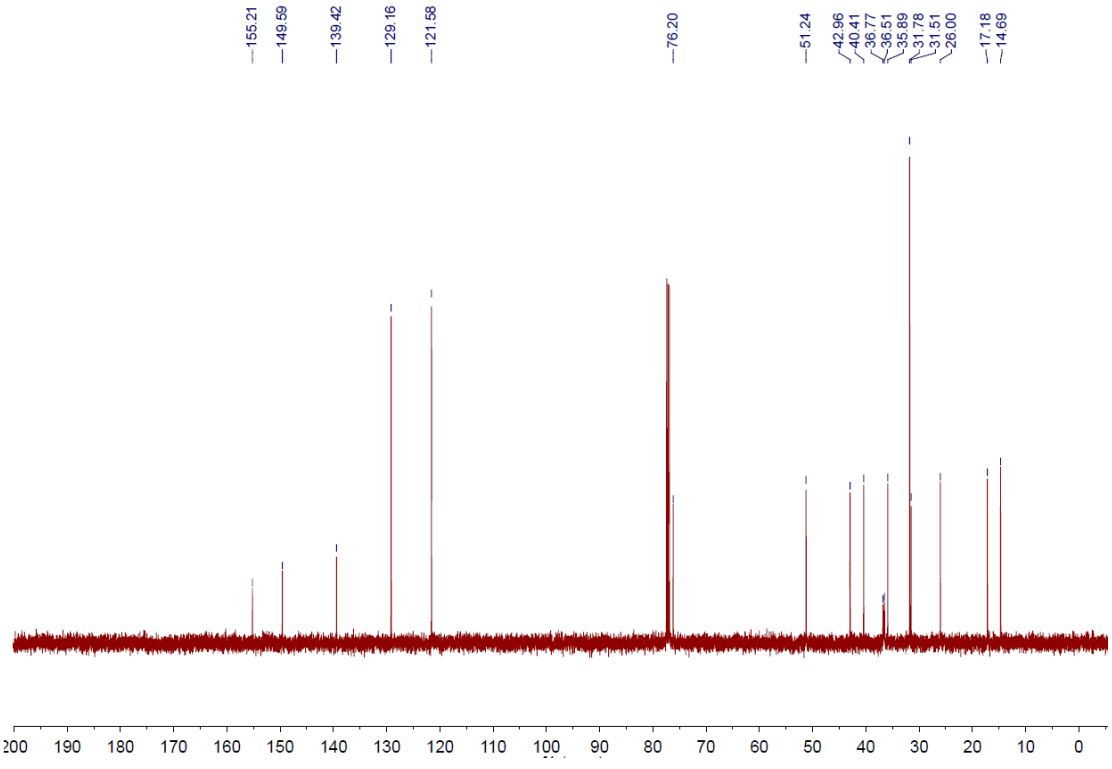
3.11
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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42.96
40.41
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31.51
26.00
17.18
14.69
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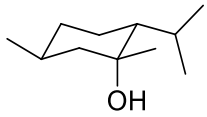
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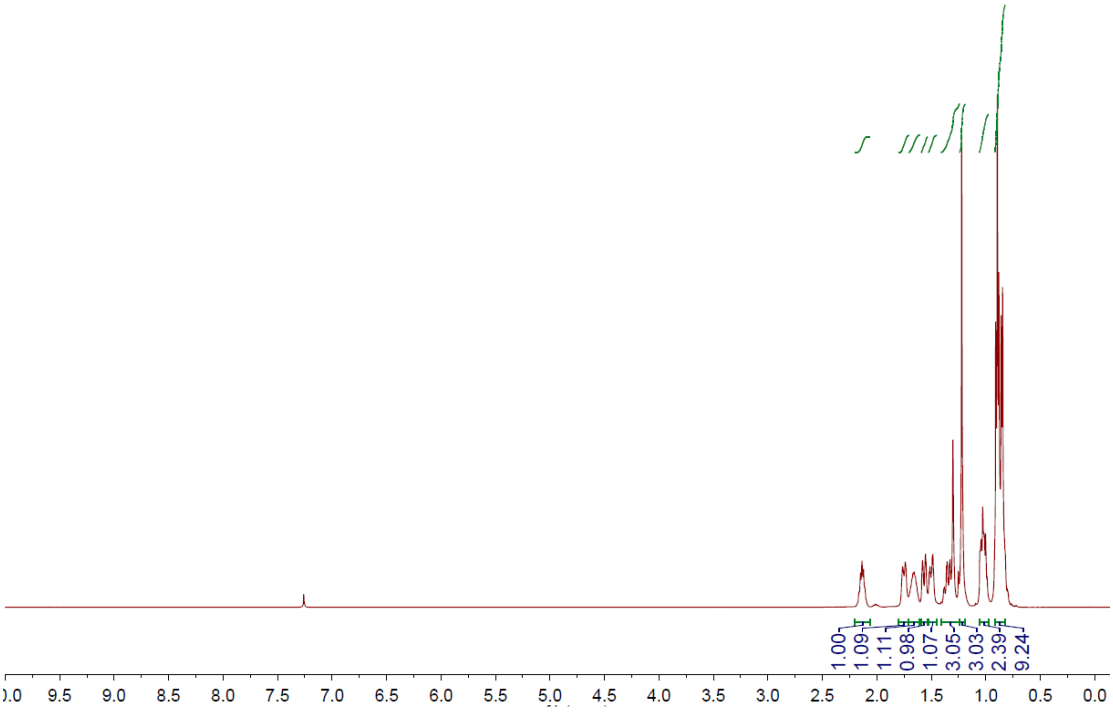
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1.07
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2.39
9.24
9.5
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8.0
7.5
7.0
6.5
6.0
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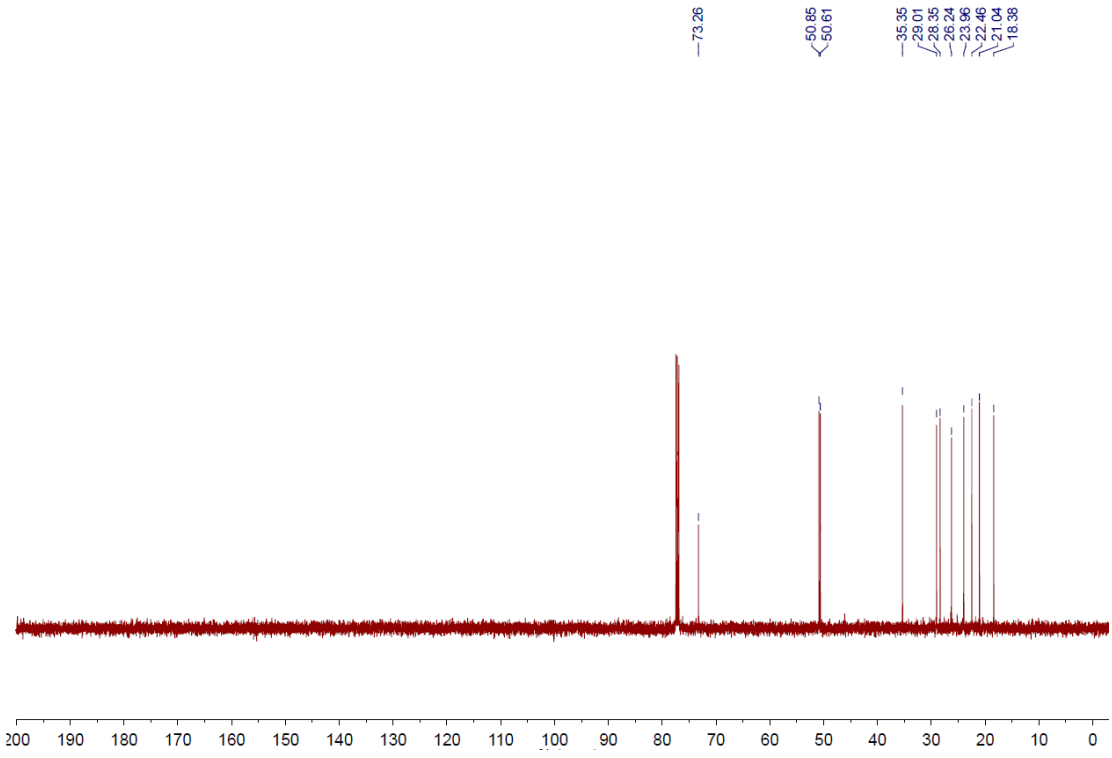
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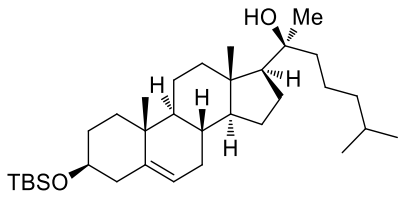
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Me
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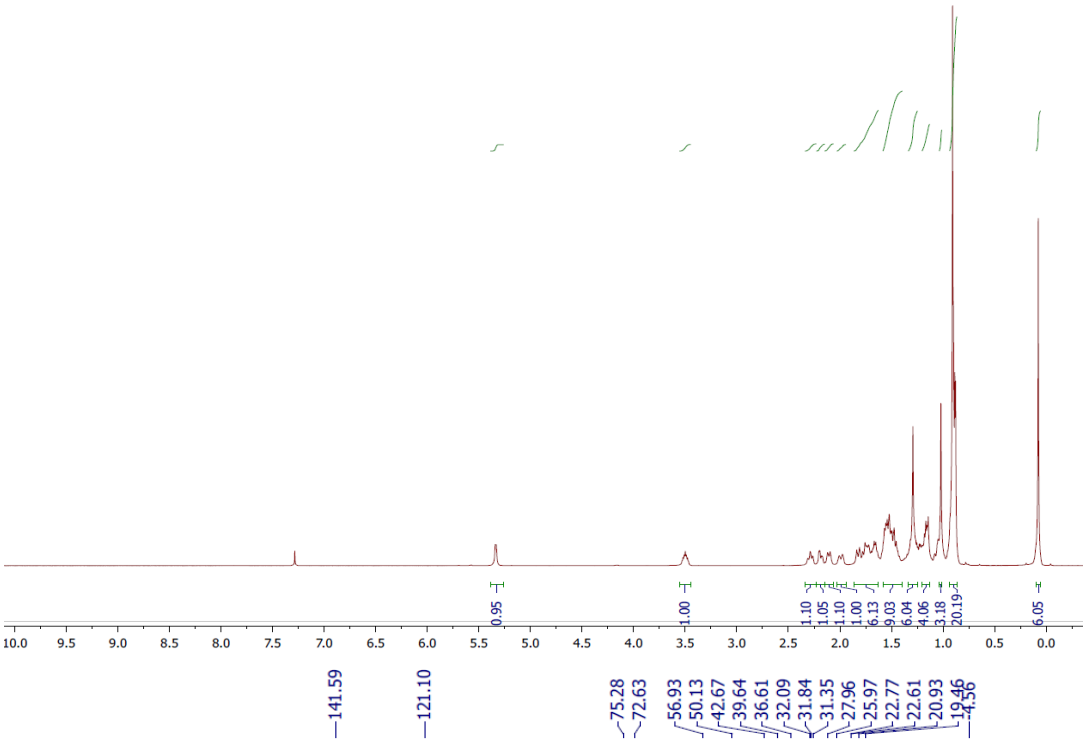
H
H
H
TBSO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4.06
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6.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.5
4.0
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3.0
2.5
2.0
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1.0
0.5
0.0

141.59
121.10
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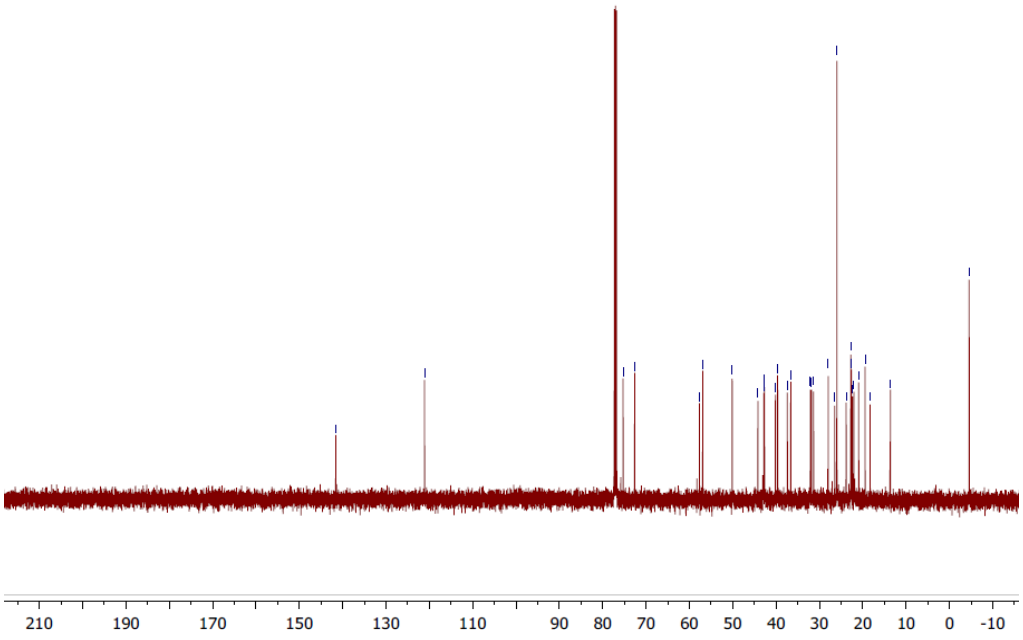
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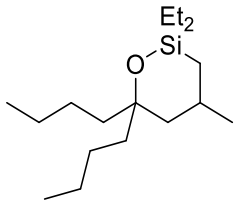
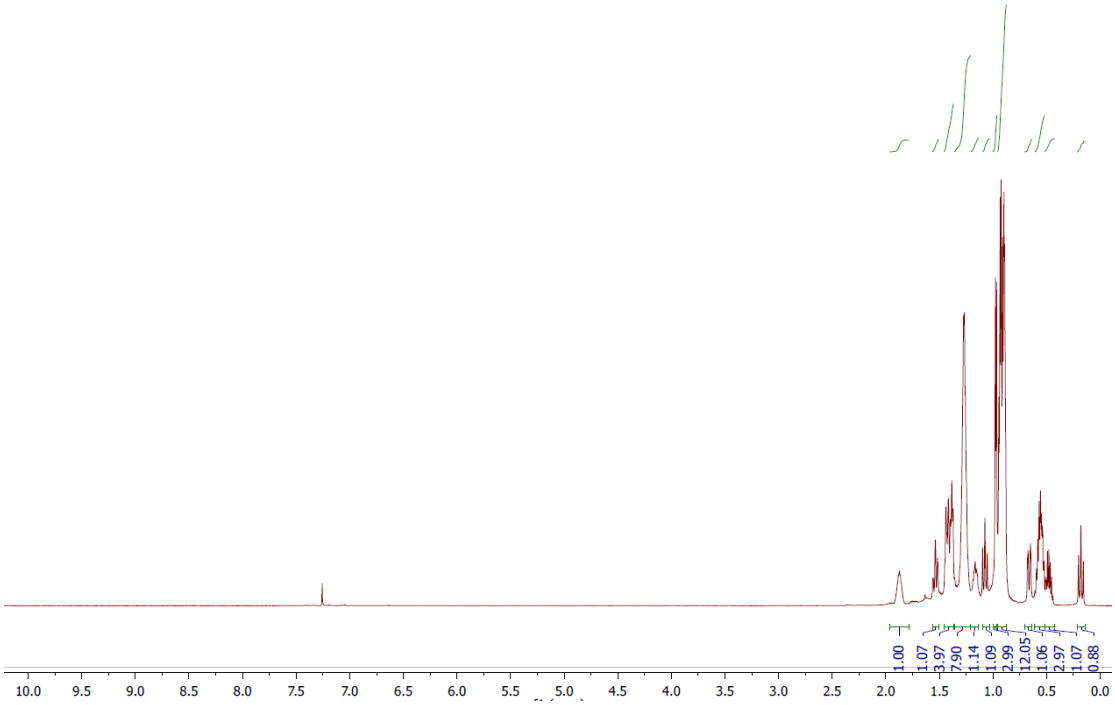
-10


Et2
Si
O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12.05
1.06
2.97
1.07
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10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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2.0
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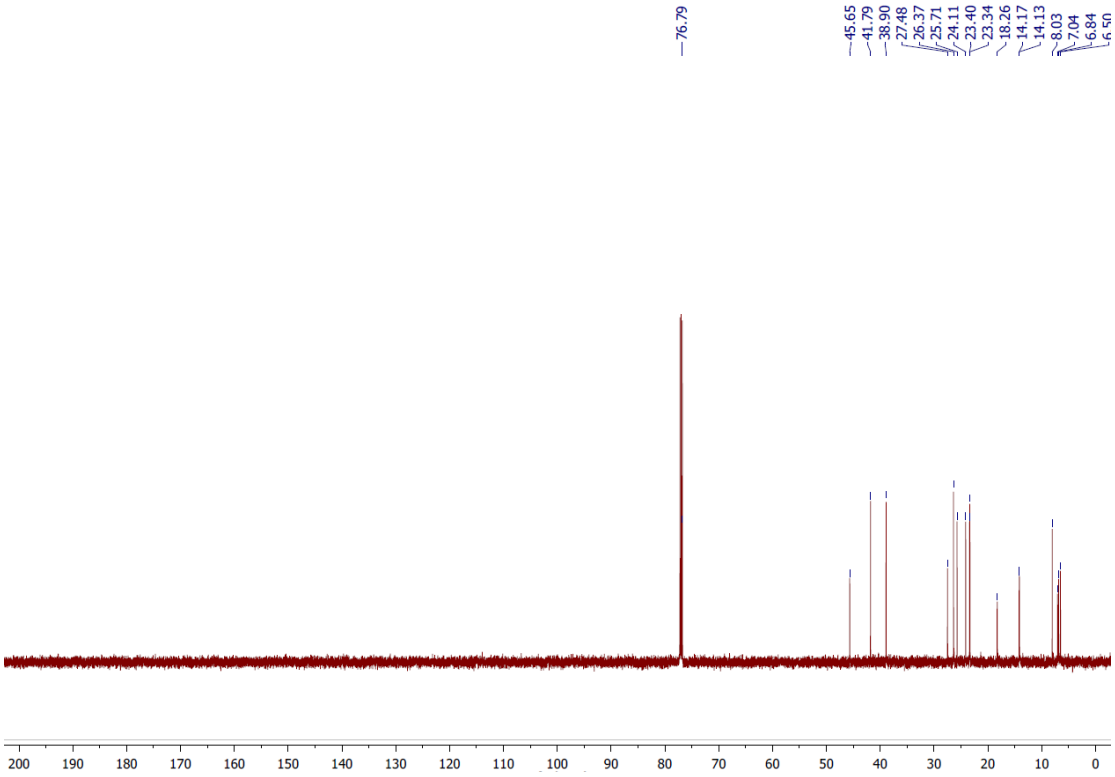
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24.11
23.40
23.34
18.26
14.17
14.13
8.03
7.04
6.84
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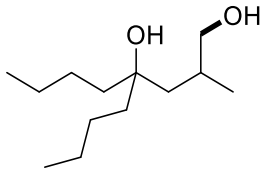
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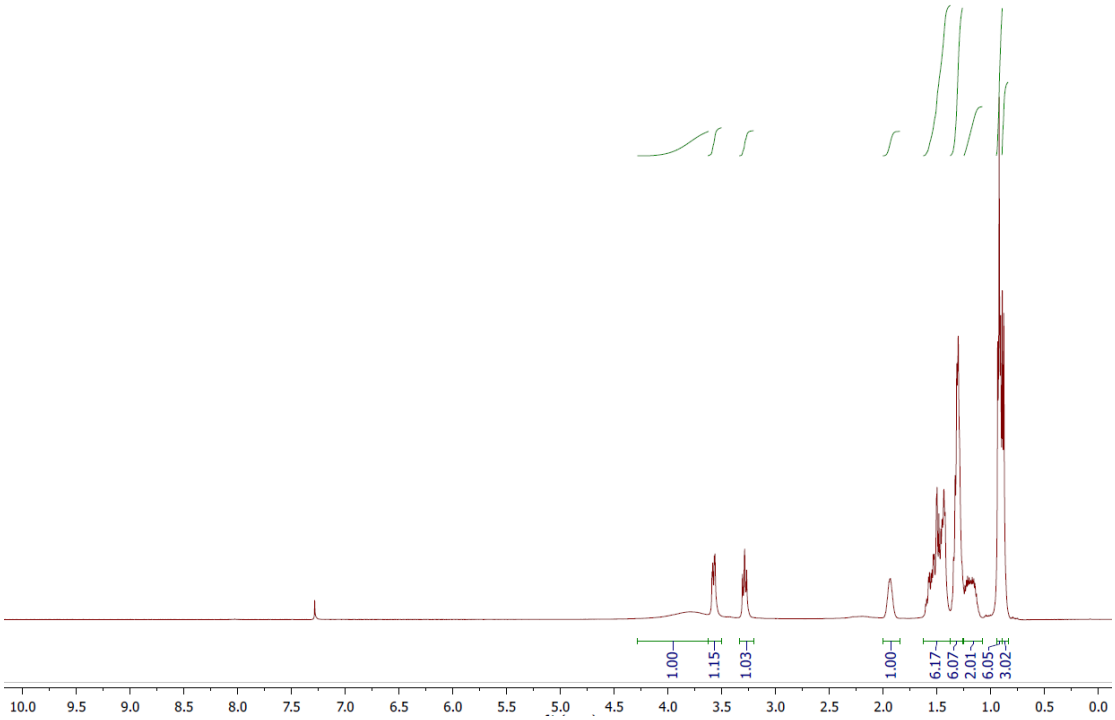
OH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1.00
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6.07
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6.05
3.02
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9.5
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8.5
8.0
7.5
7.0
6.5
6.0
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3.0
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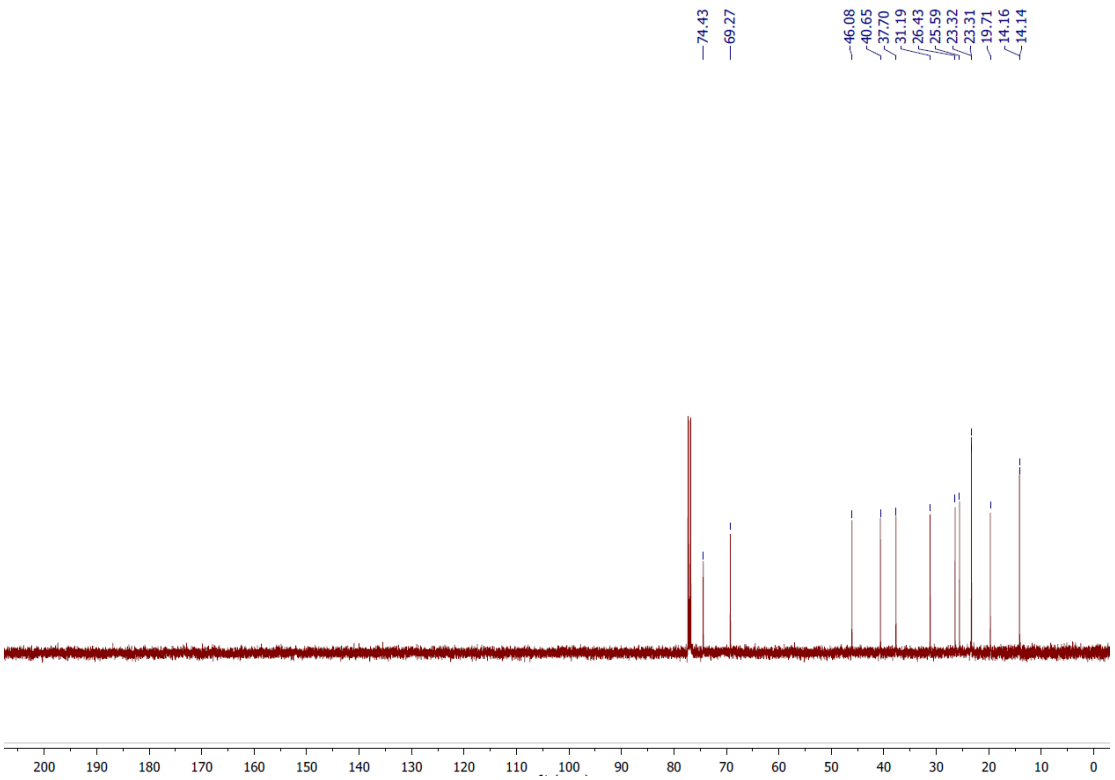
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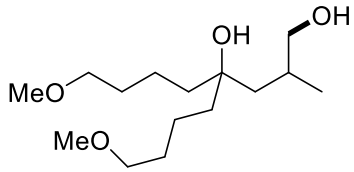
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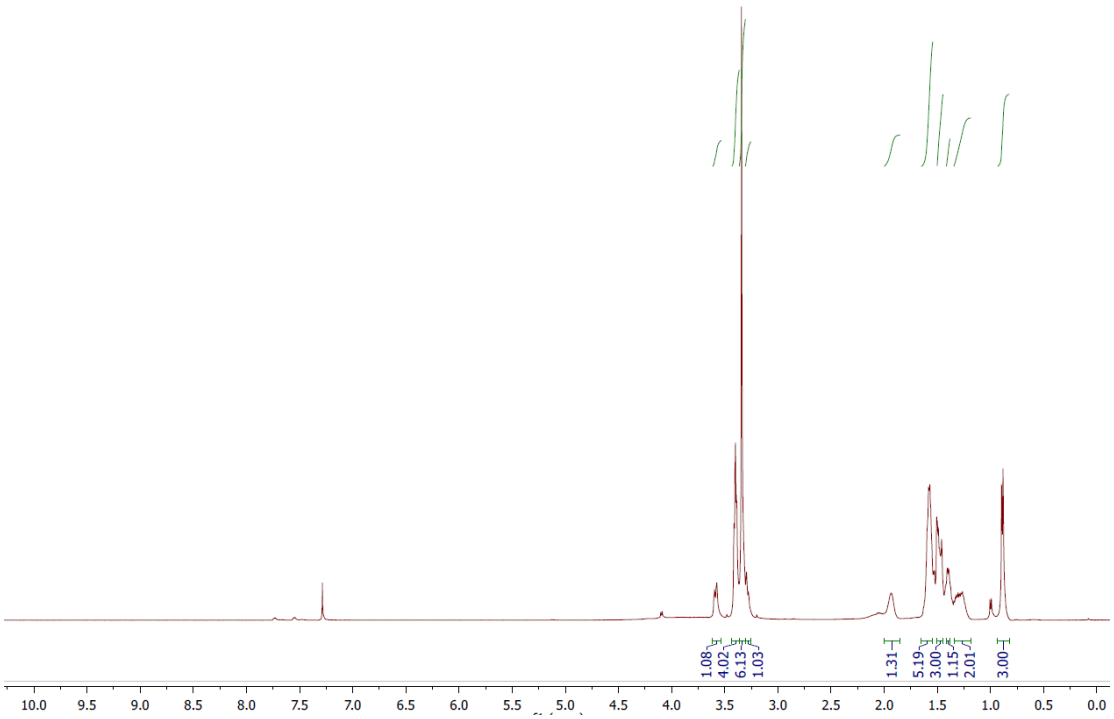
OH
MeO
MeO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1.03
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5.19
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3.00
10.0
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9.0
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8.0
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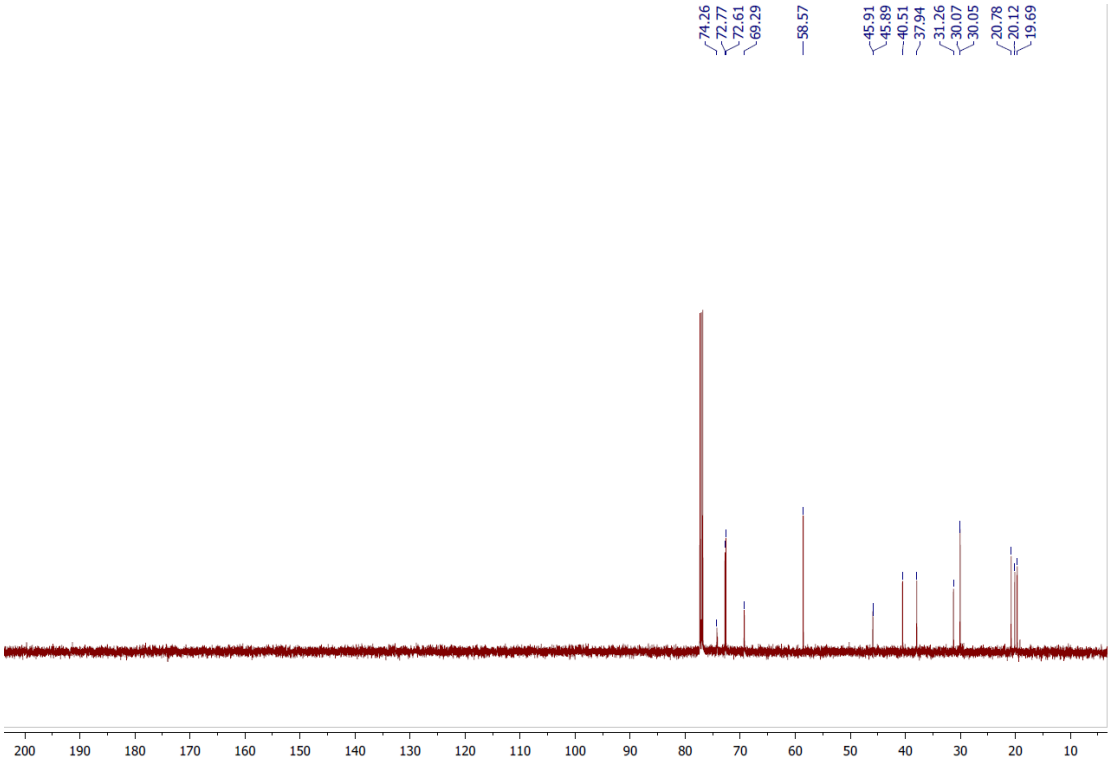
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31.26
30.07
30.05
20.78
20.12
19.69
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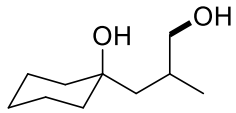
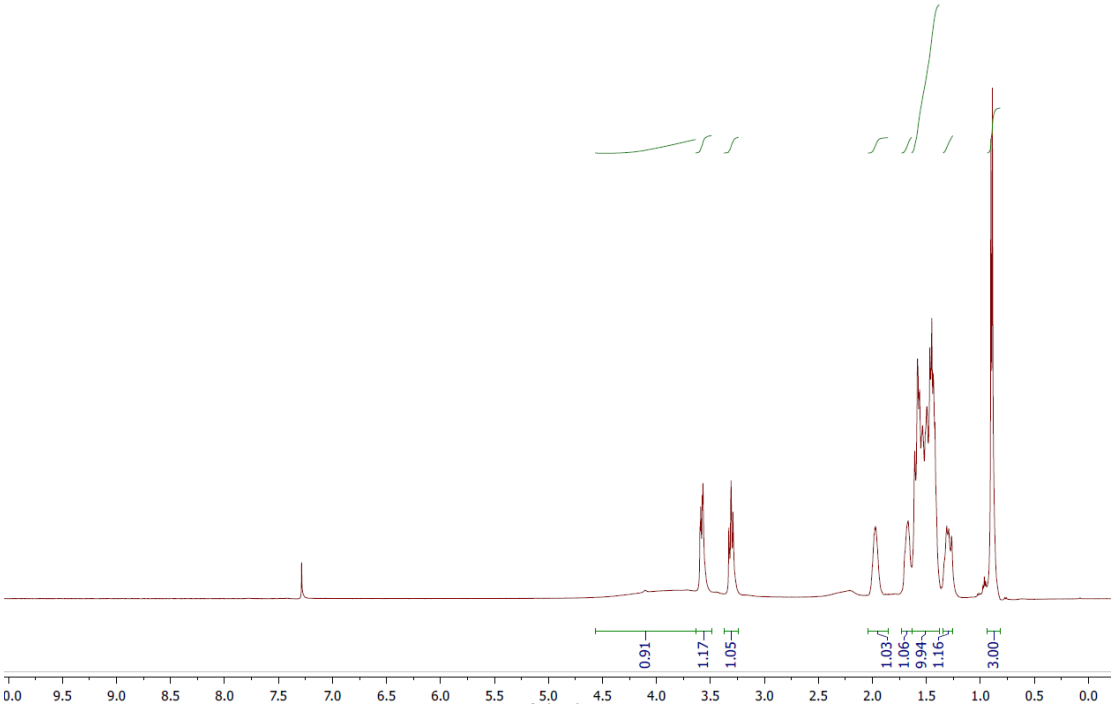

OH
OH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1.03
1.06
9.94
1.16
3.00
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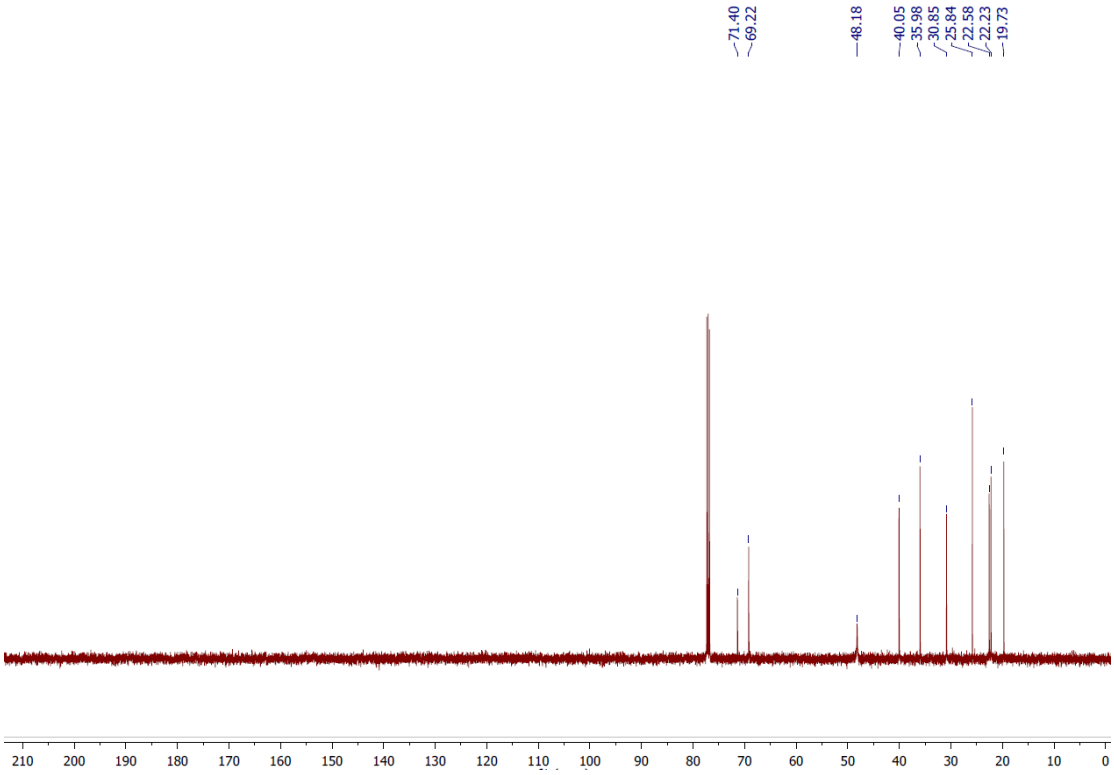
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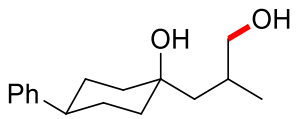
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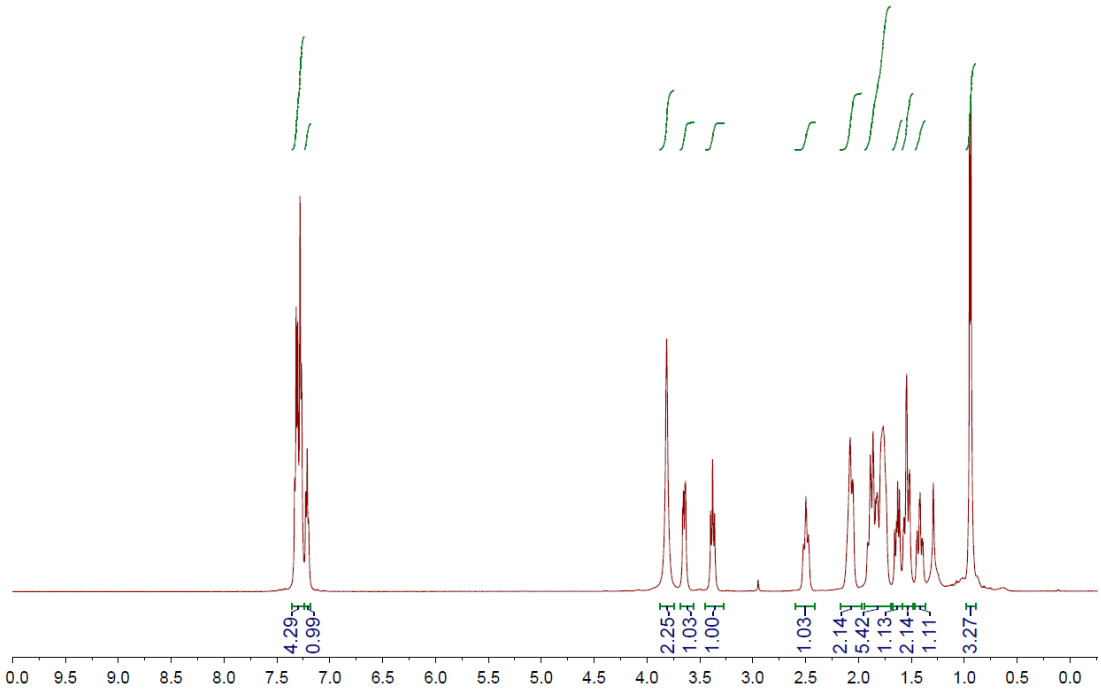
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3.27
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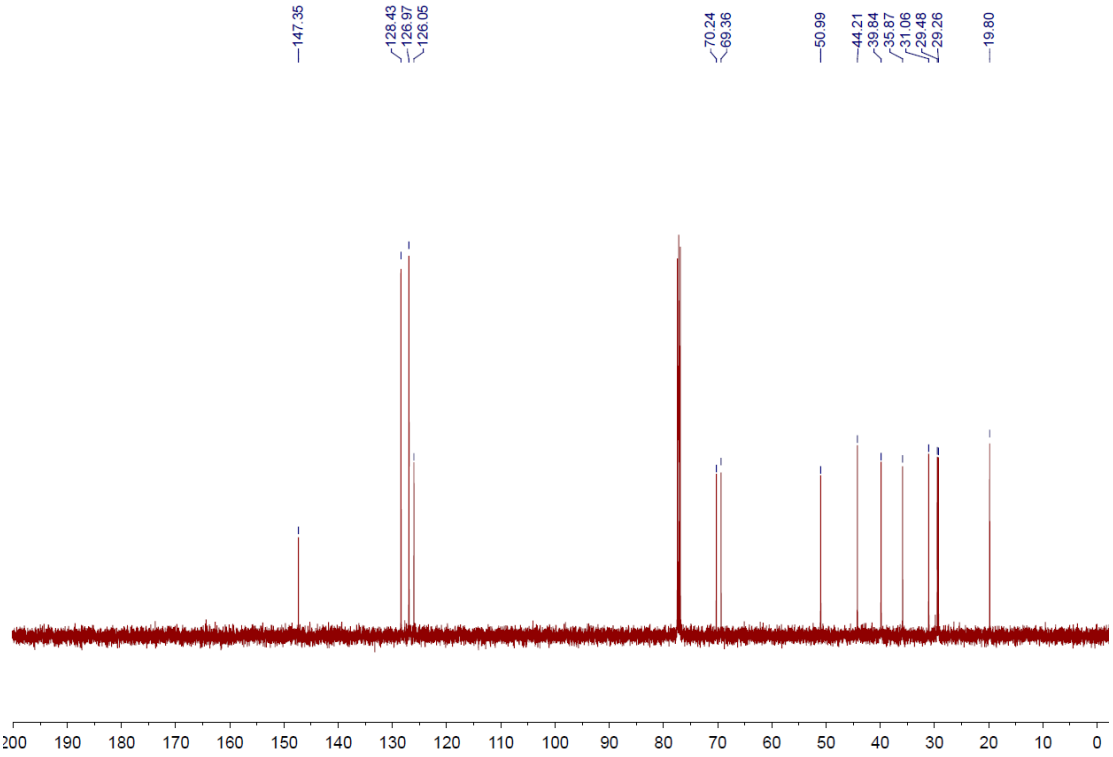
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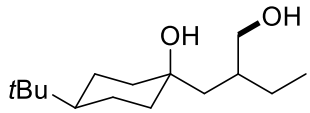
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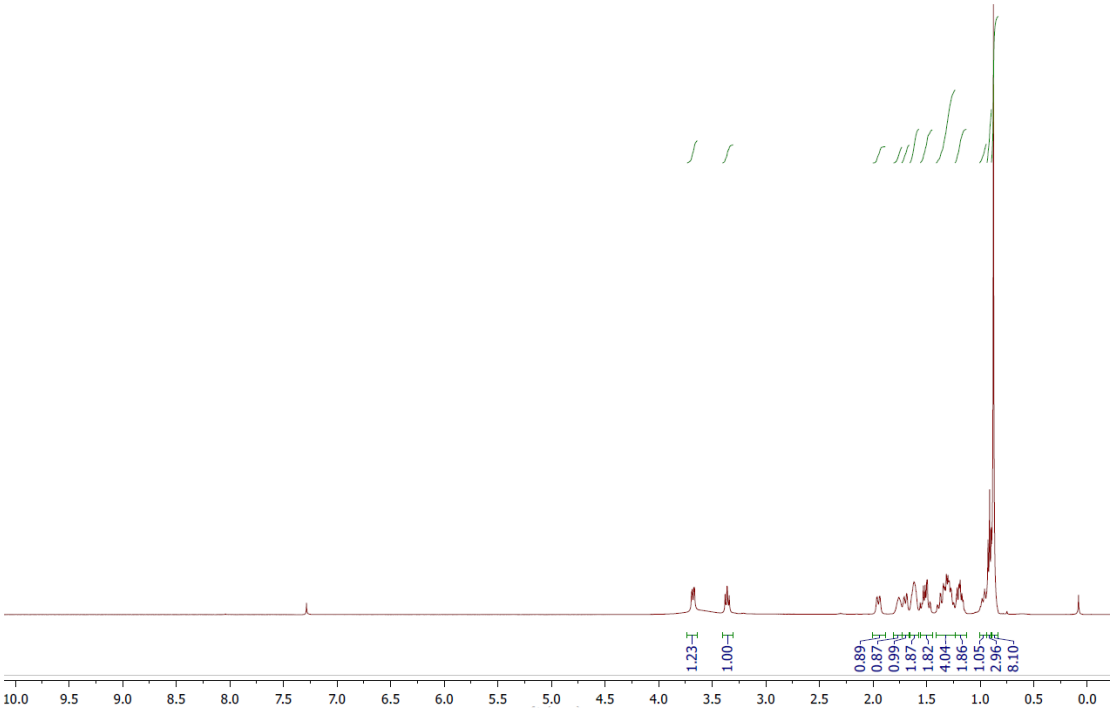
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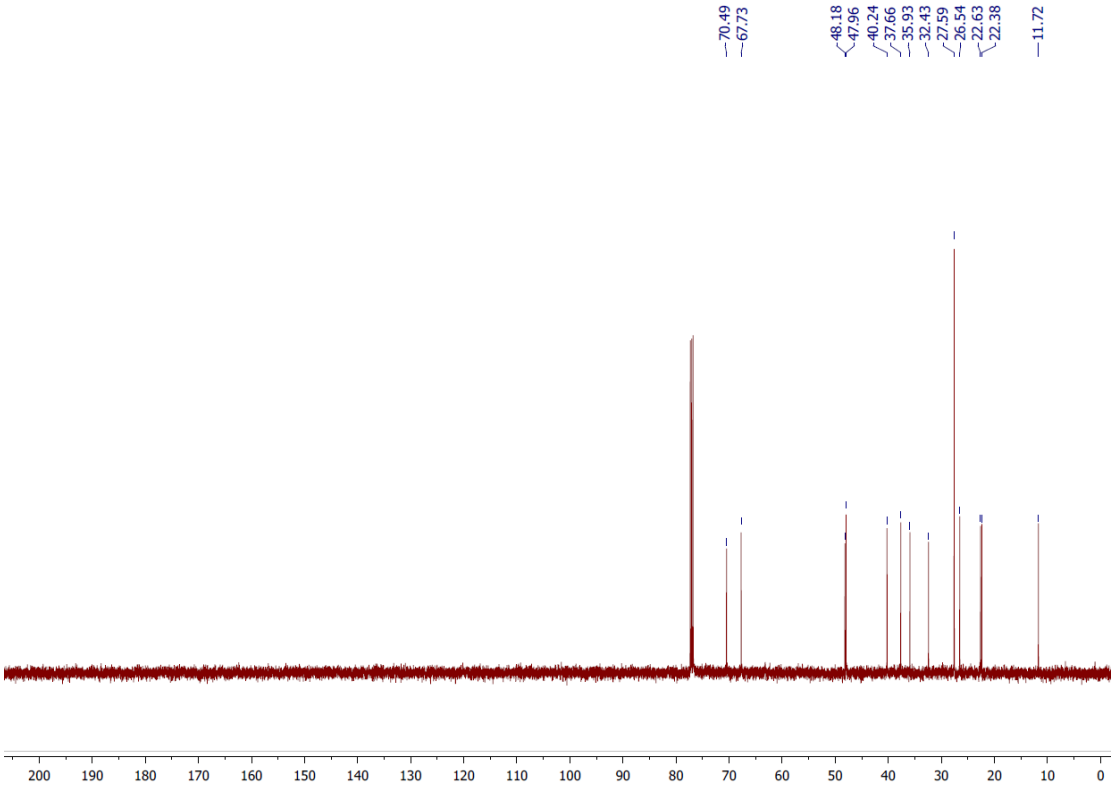
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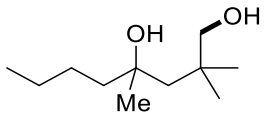
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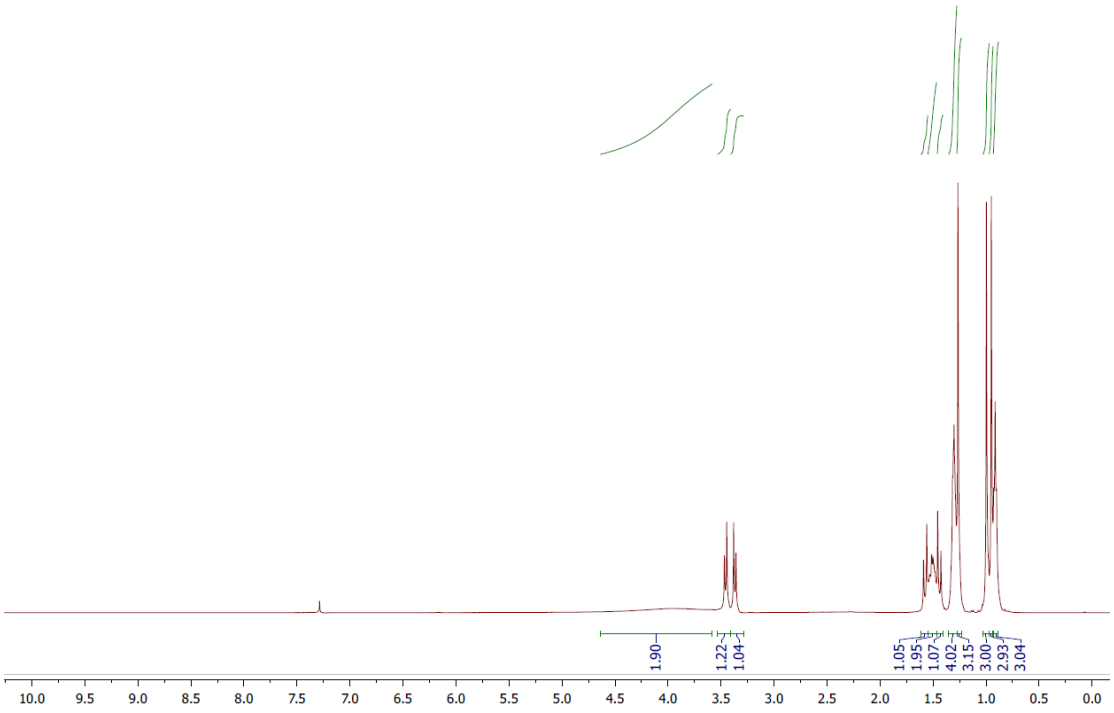
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9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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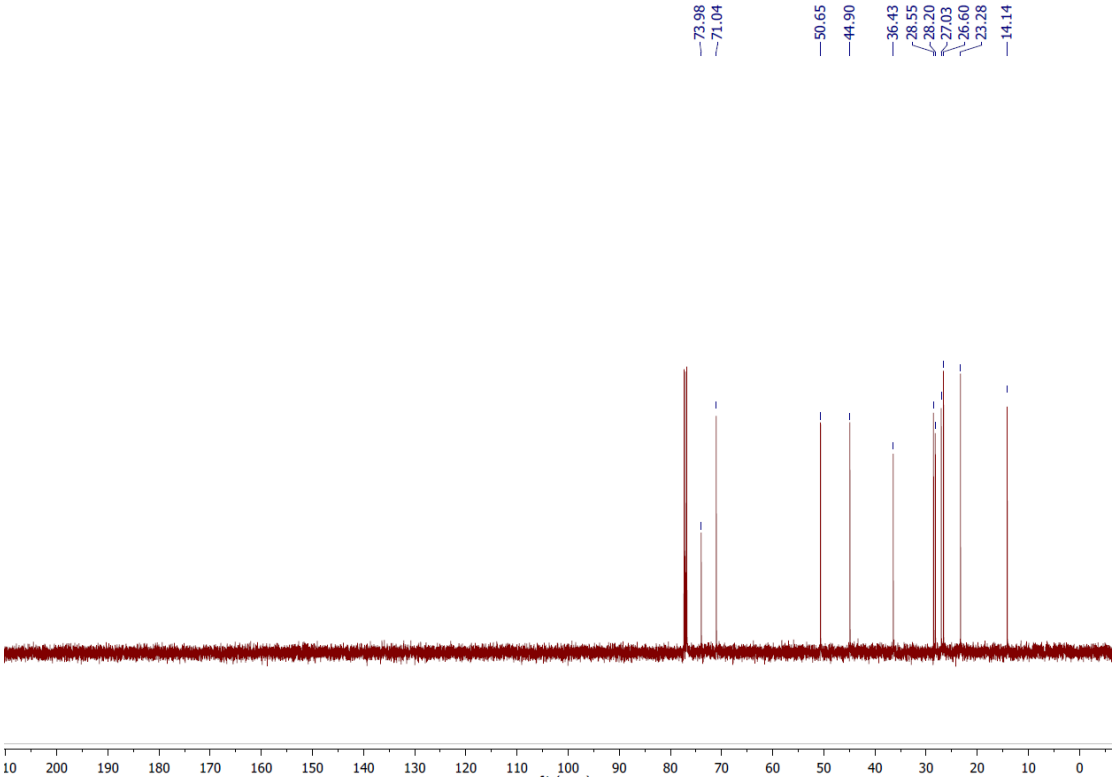
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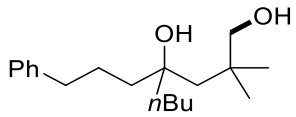
0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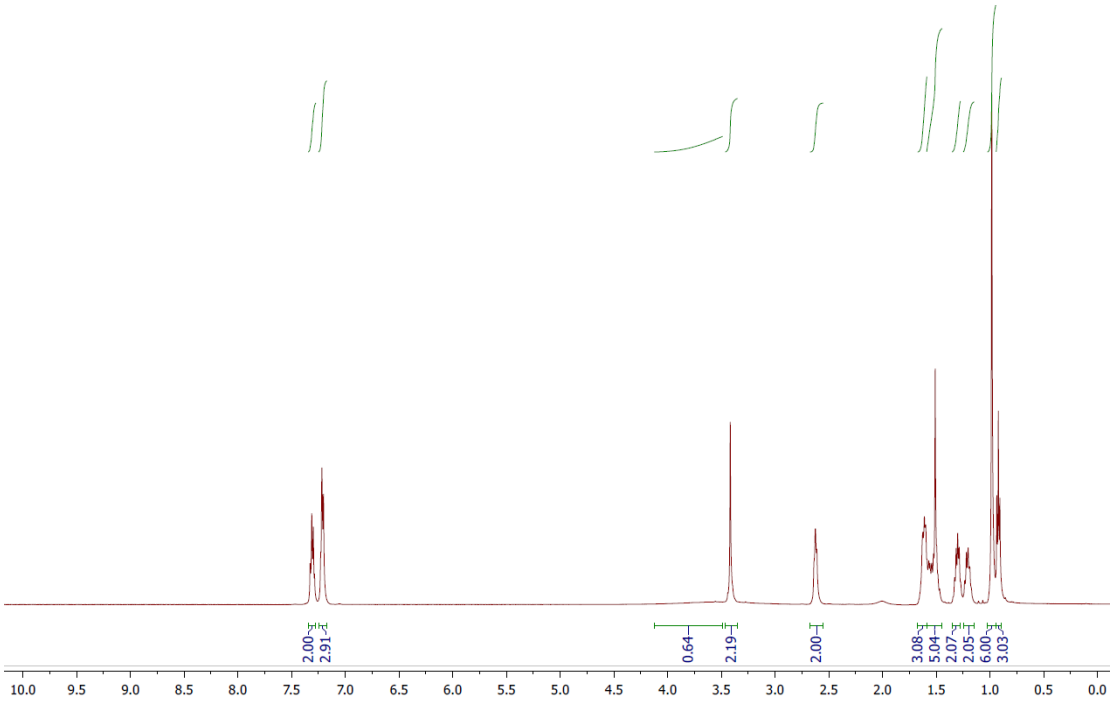
Ph
nBu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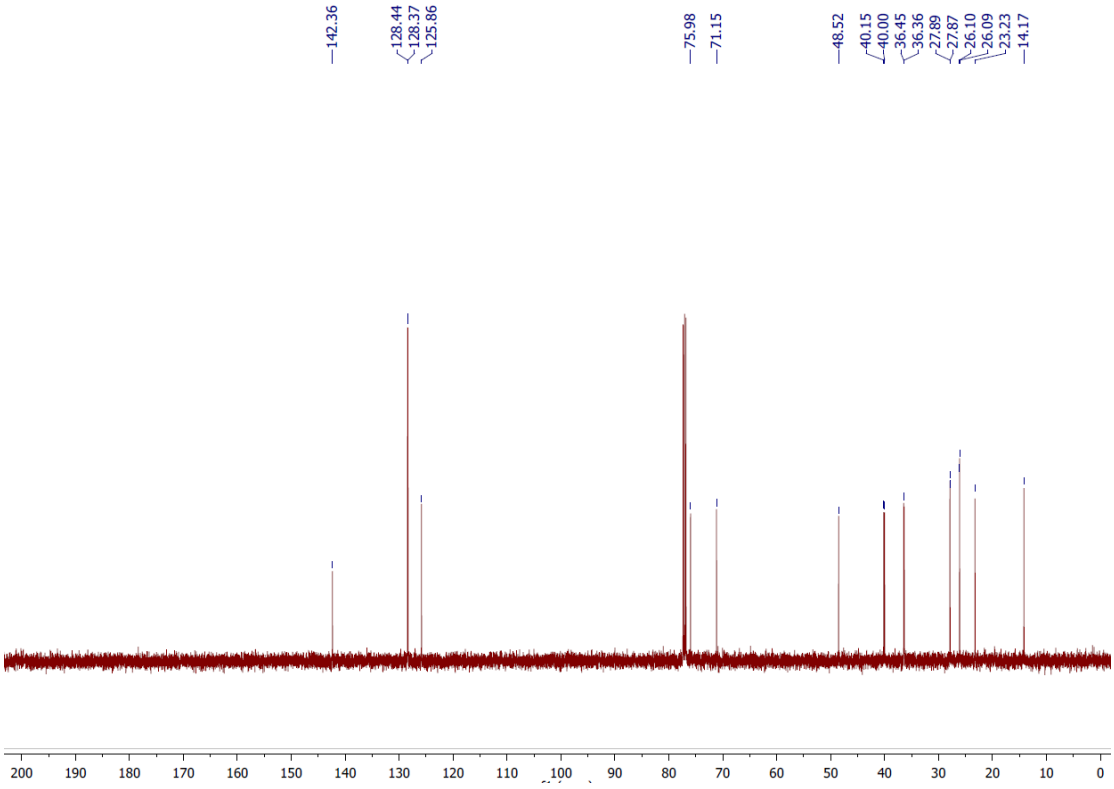
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26.09
23.23
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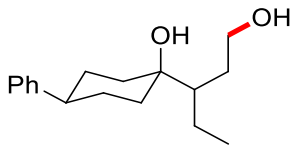
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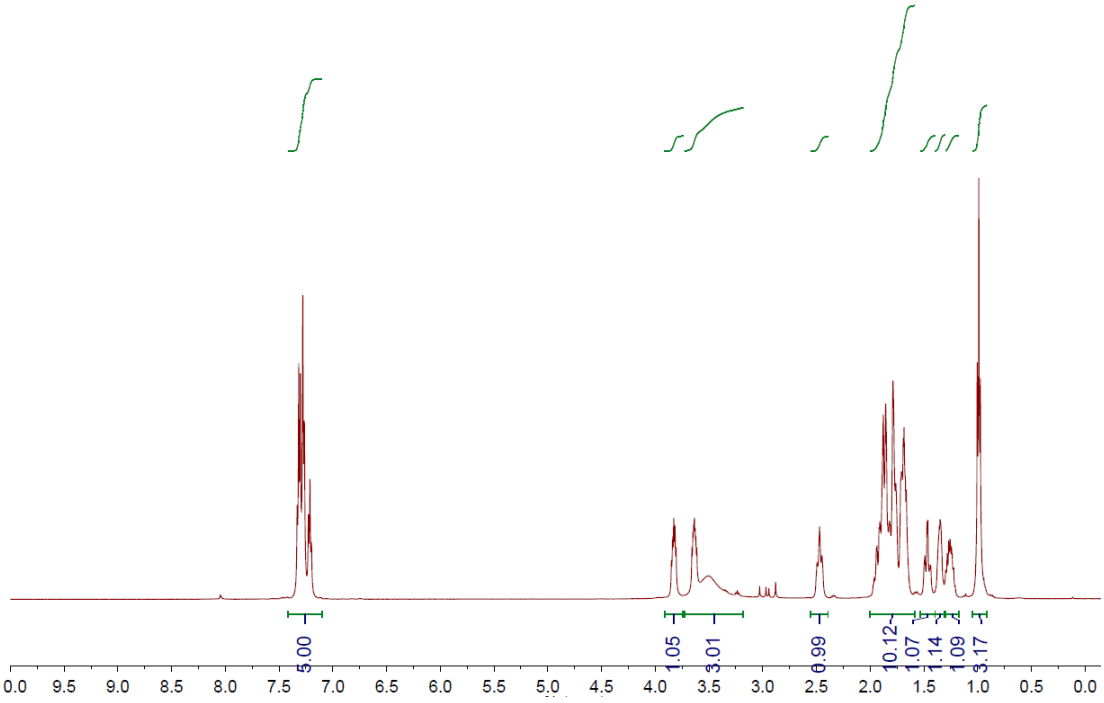
OH
Ph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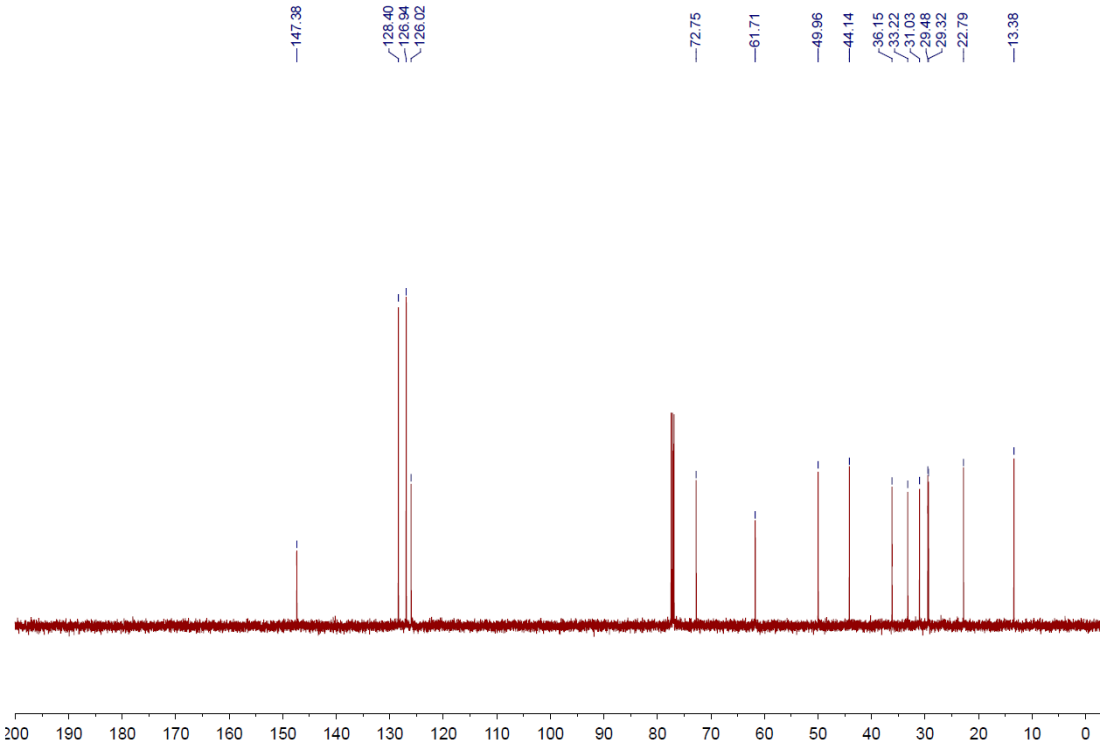
3.01
0.99
10.12
1.07
1.14
1.09
3.17
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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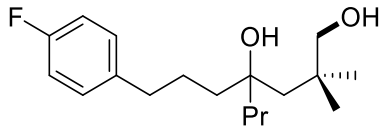
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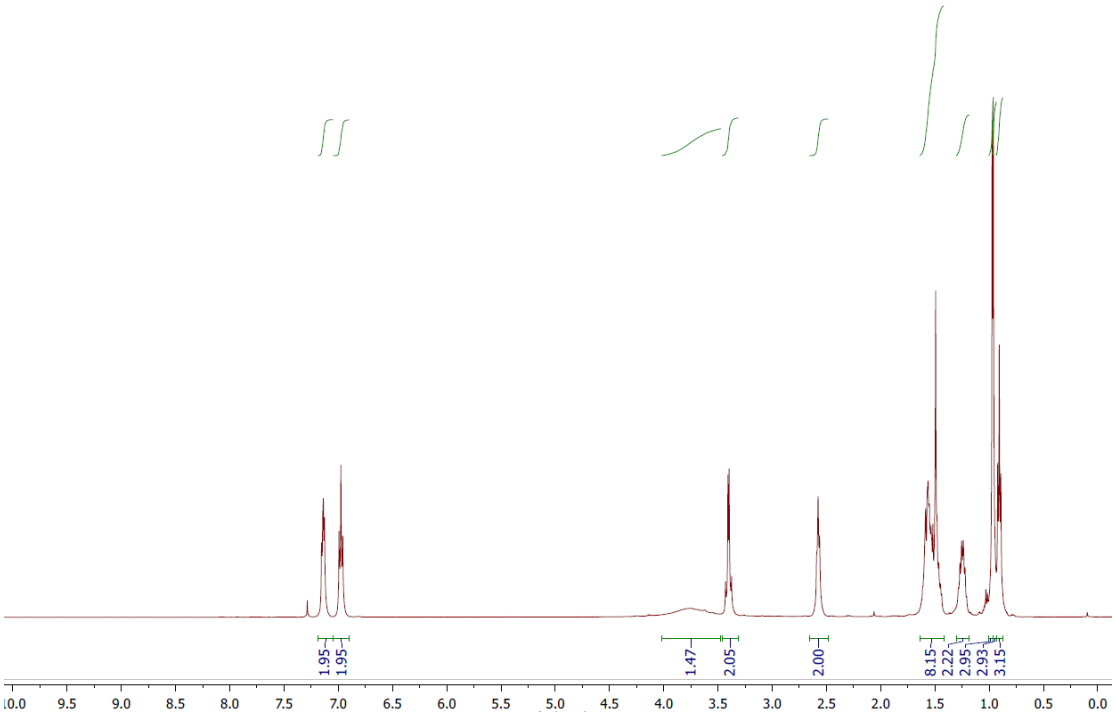
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9.5
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8.5
8.0
7.5
7.0
6.5
6.0
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5.0
4.5
4.0
3.5
3.0
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2.0
1.5
1.0
0.5
0.0


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137.95
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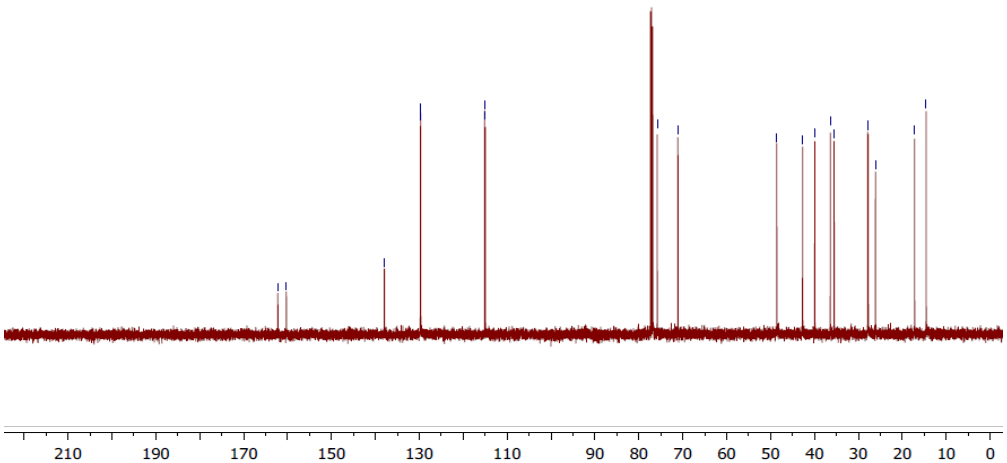
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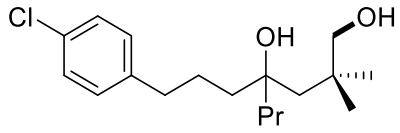
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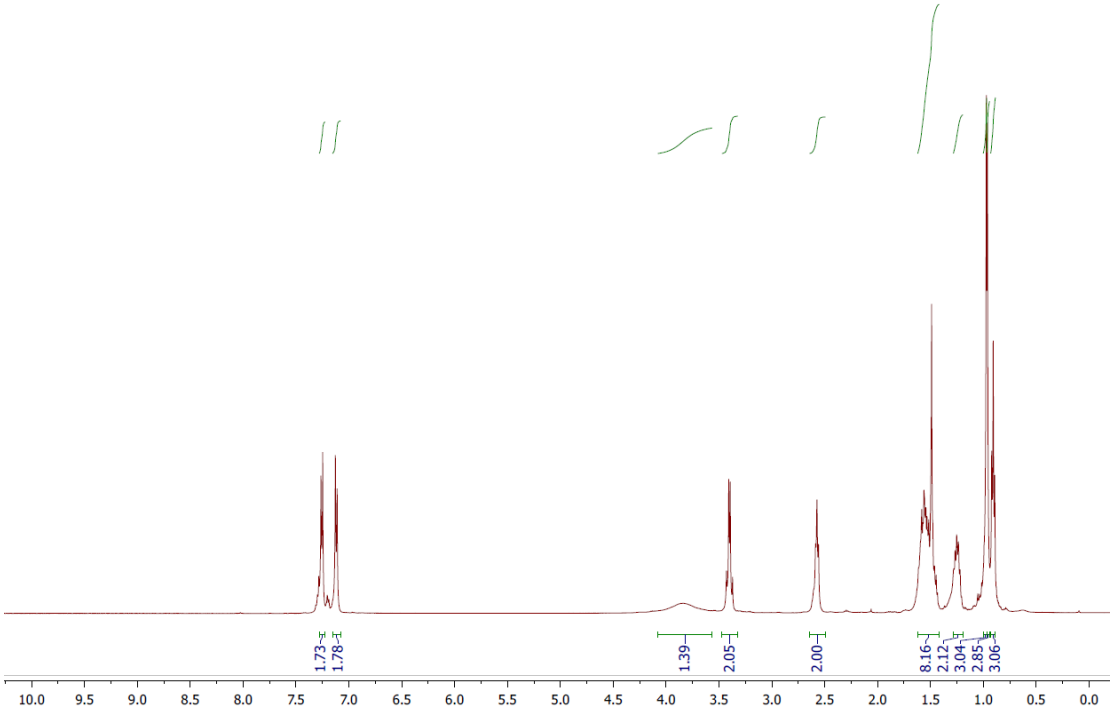
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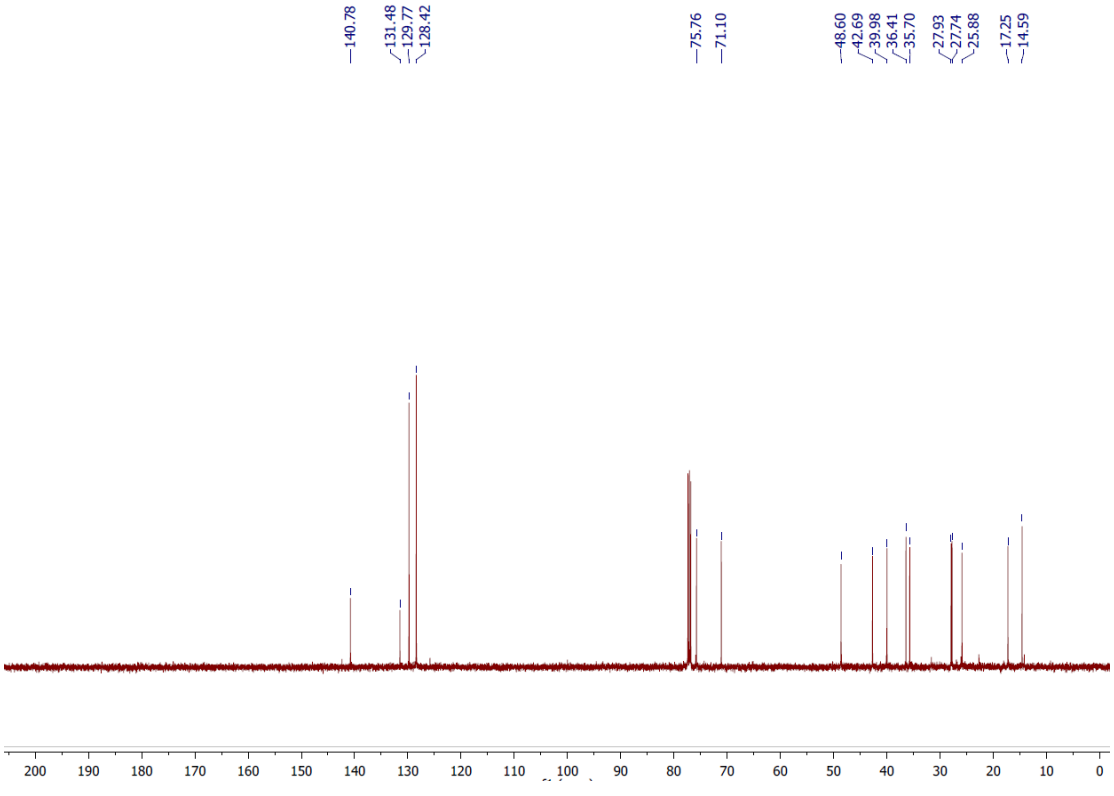
2.85
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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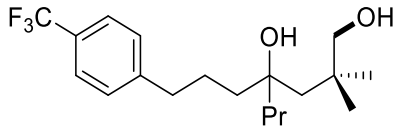
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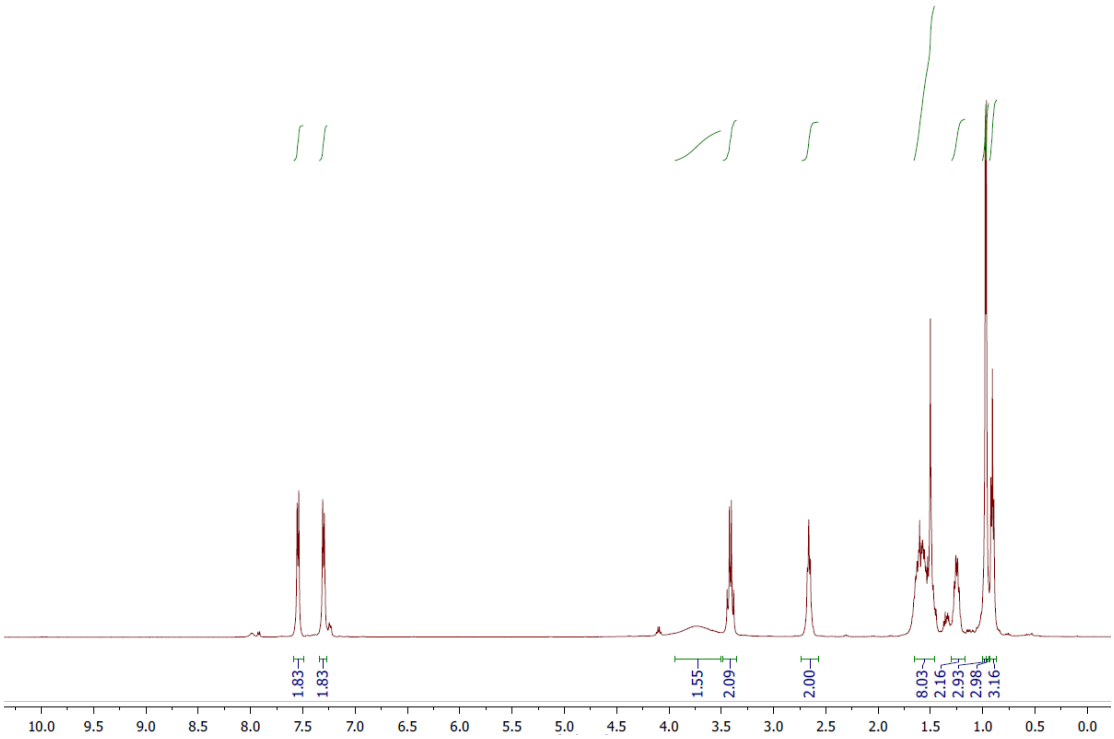
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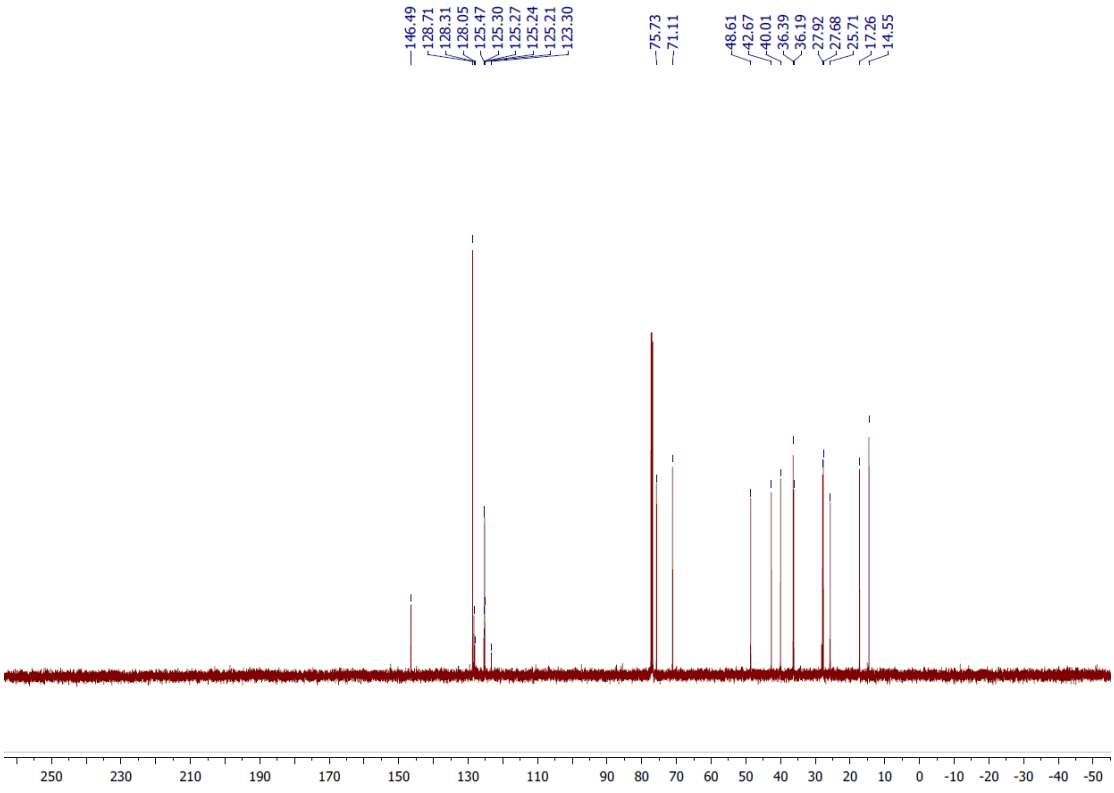
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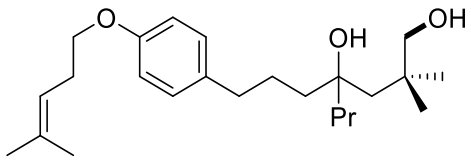
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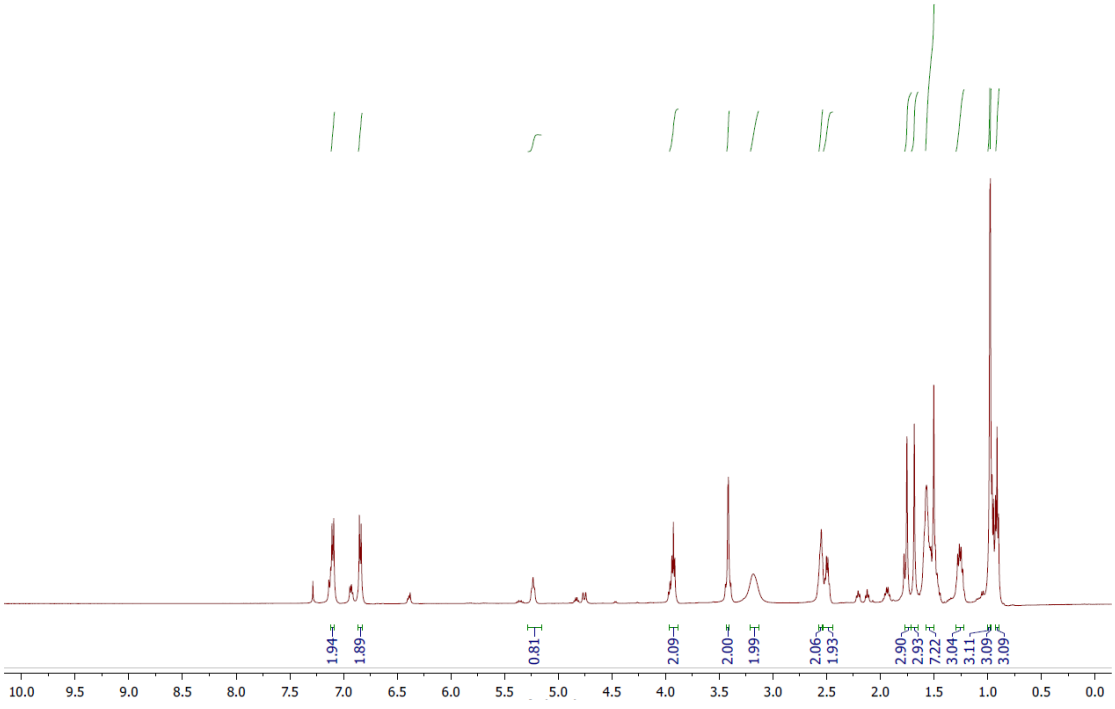
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3.09
3.09
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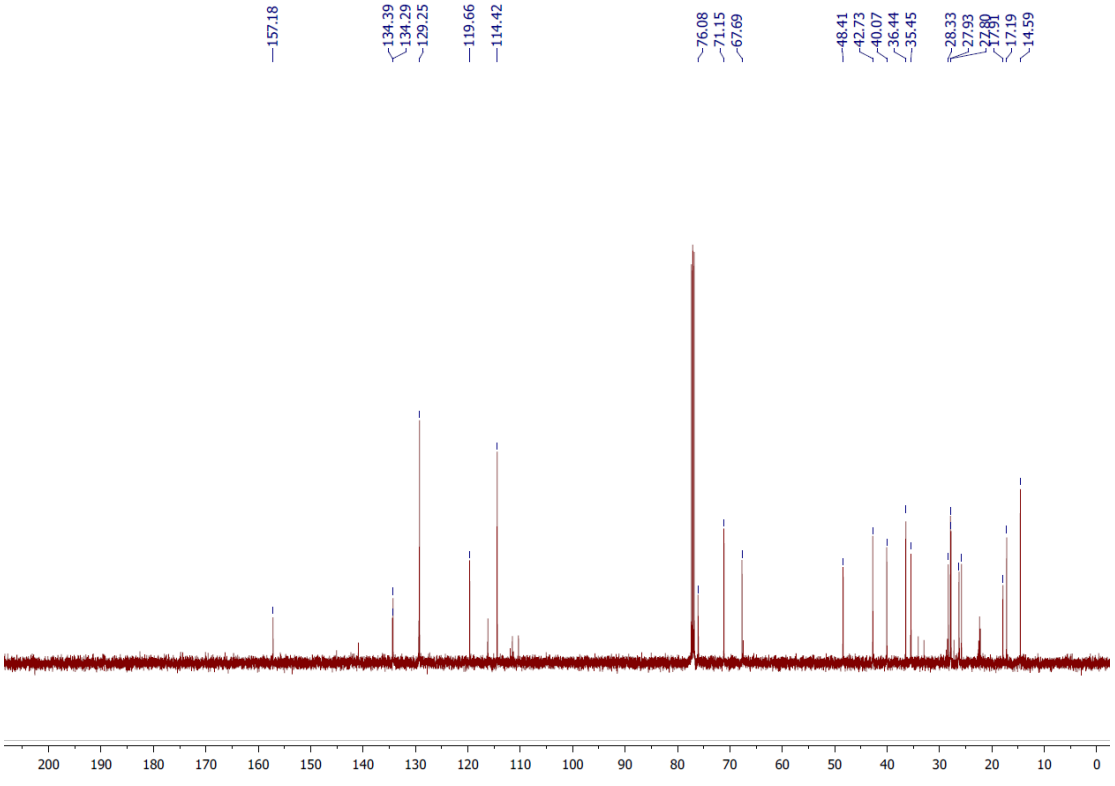
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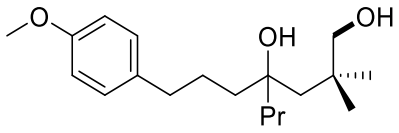
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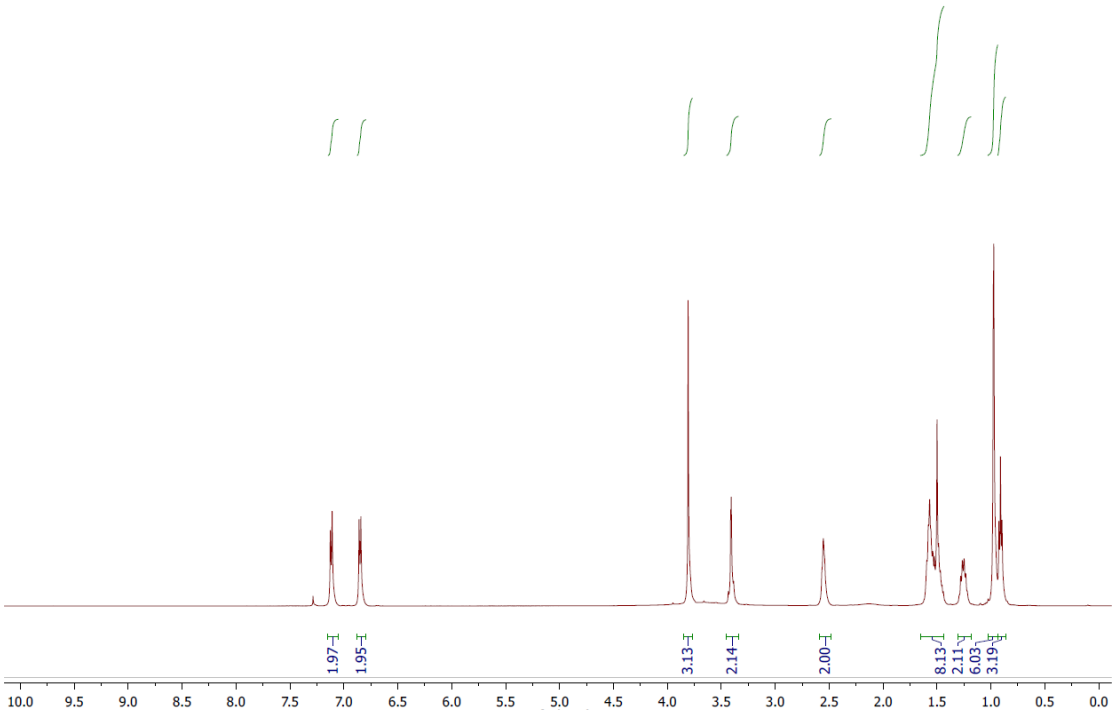
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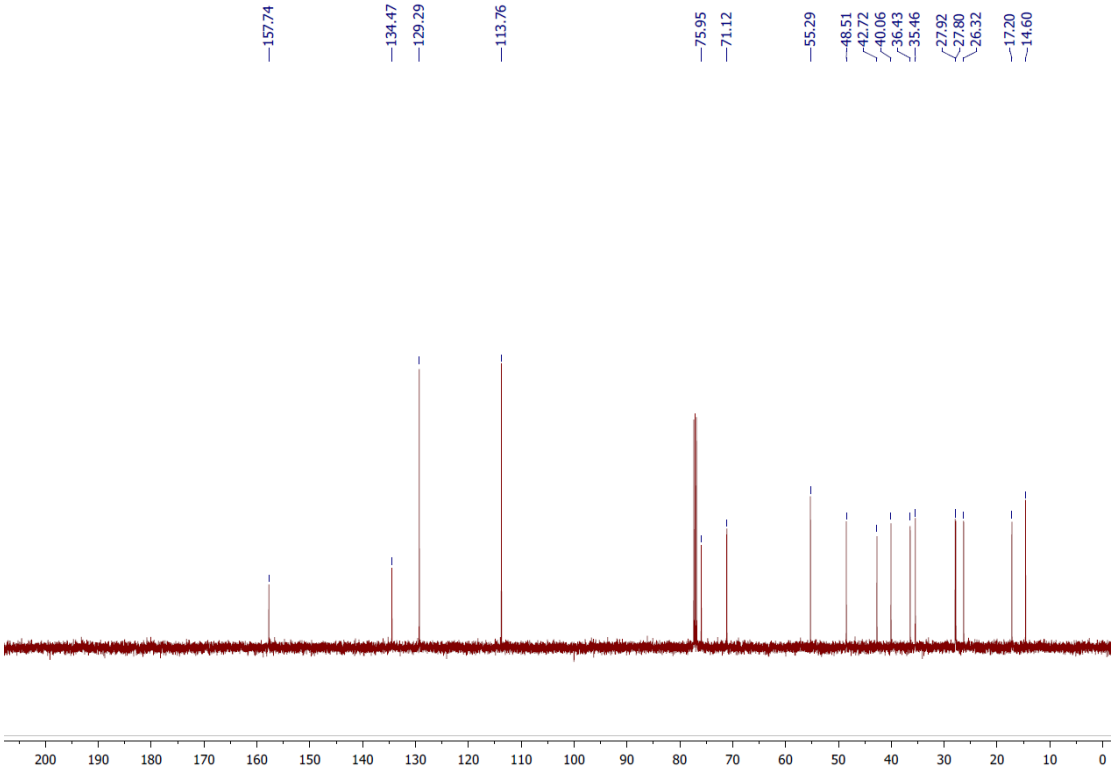
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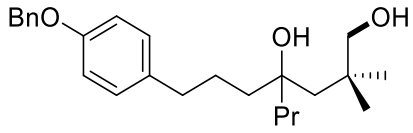
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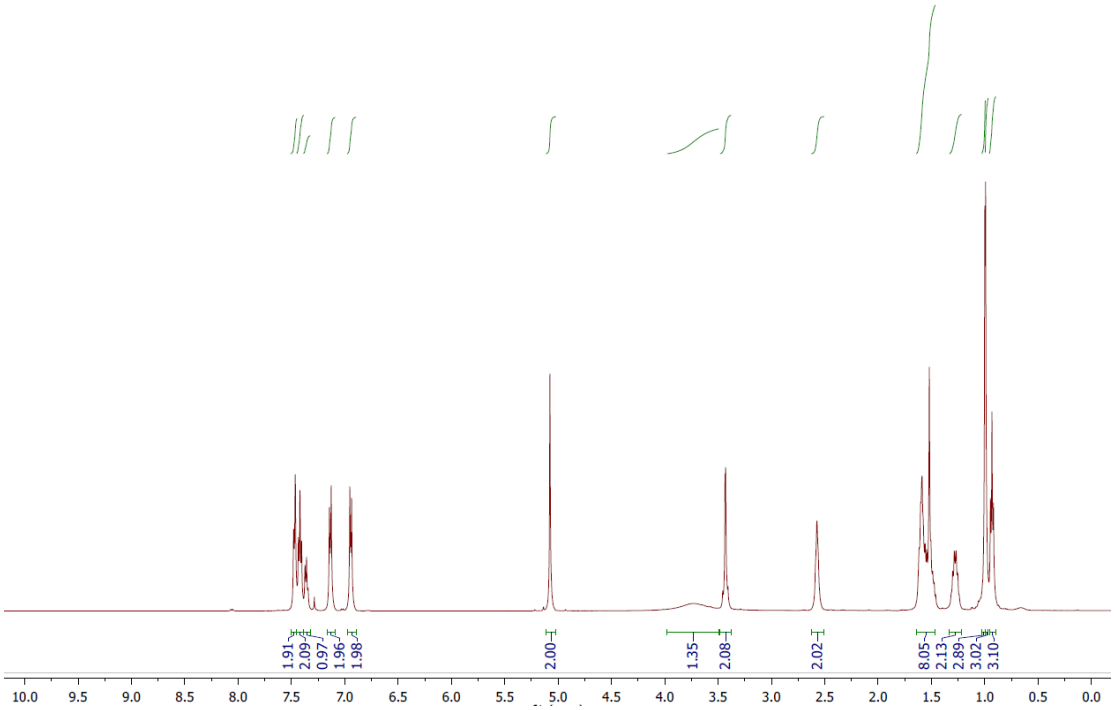
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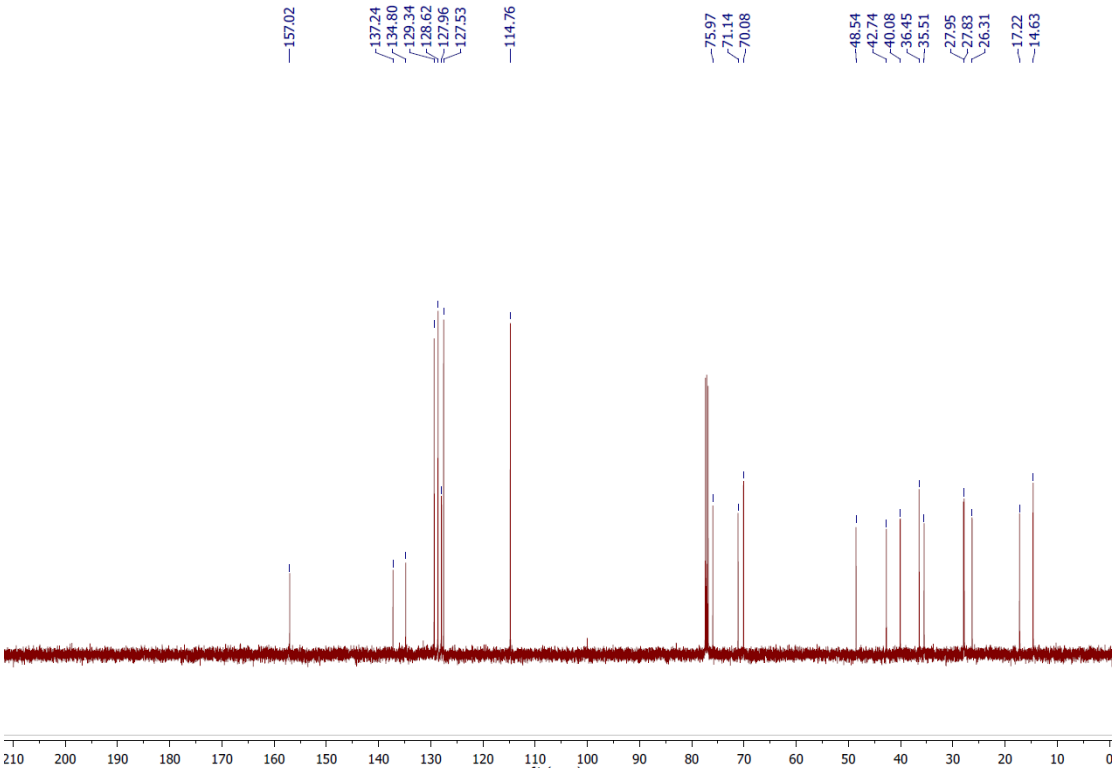
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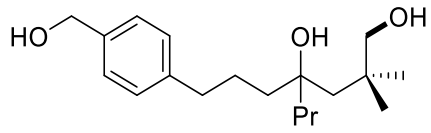
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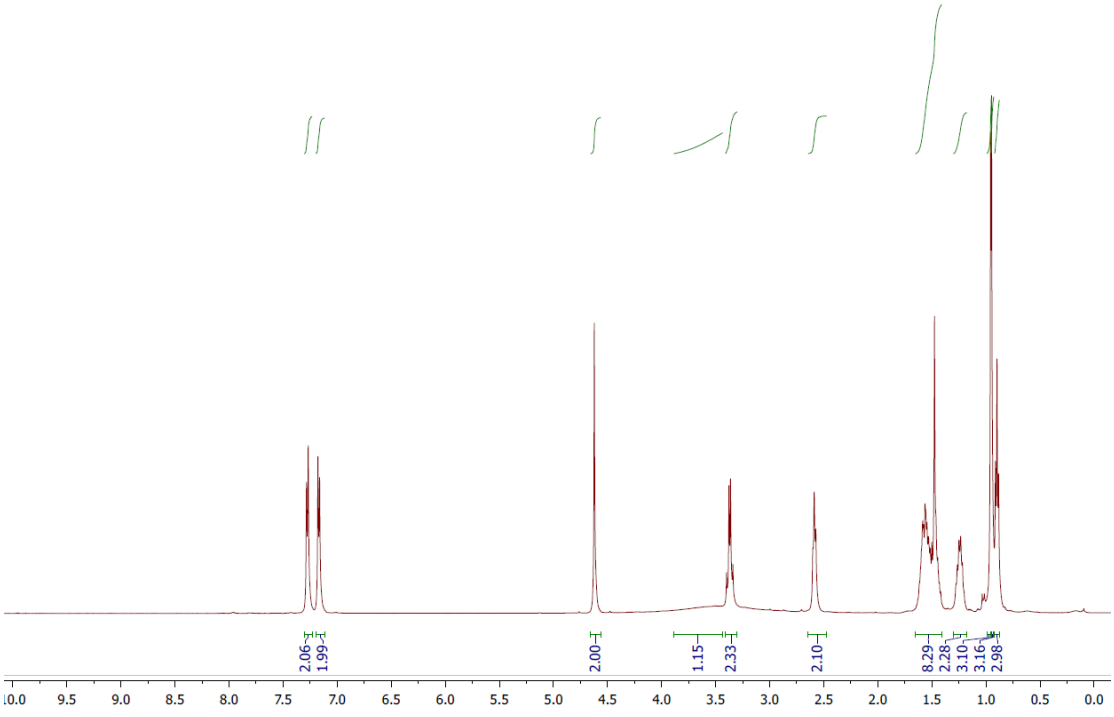
OH
Pr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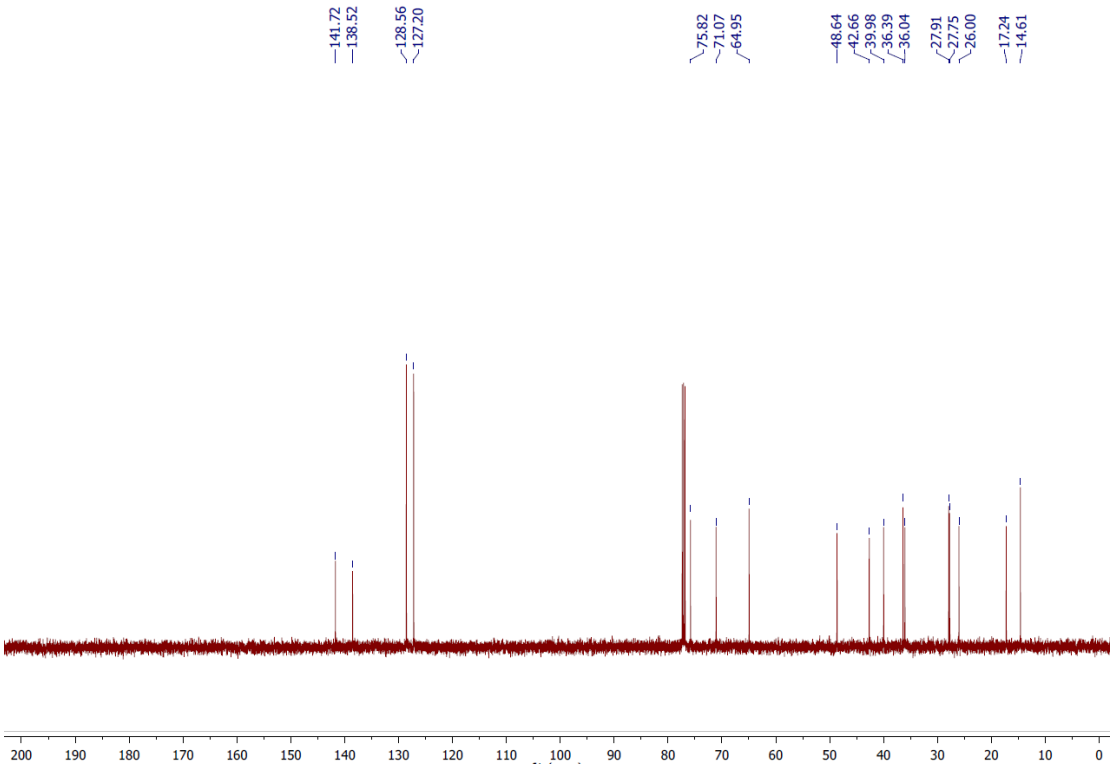
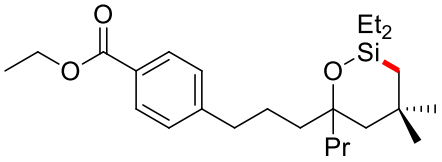
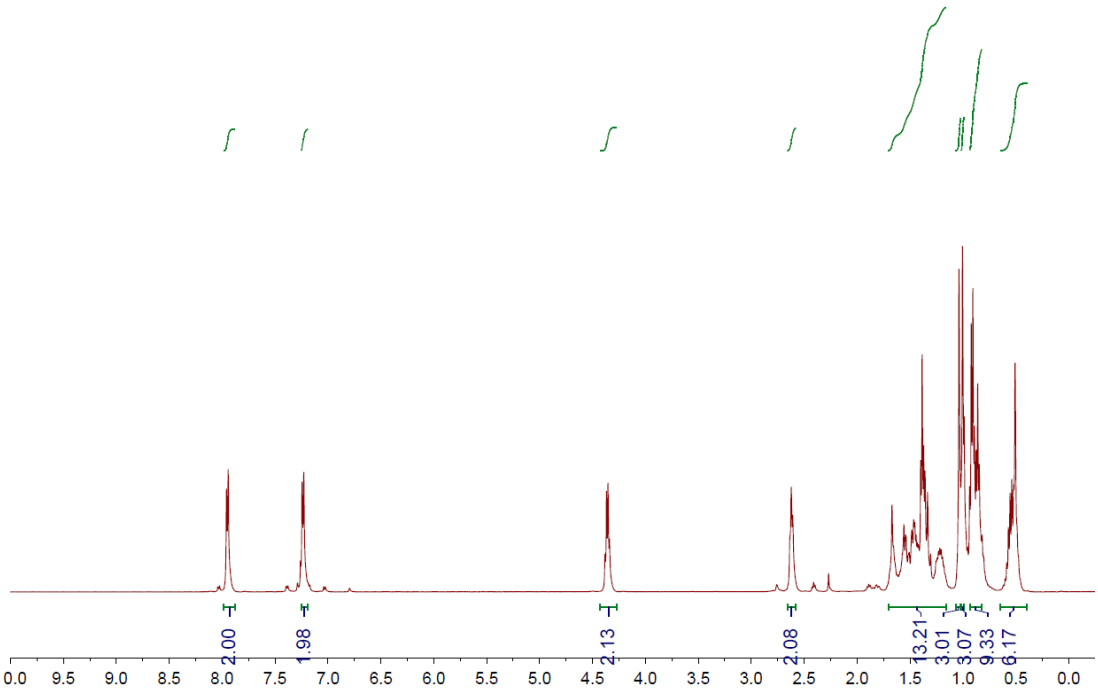
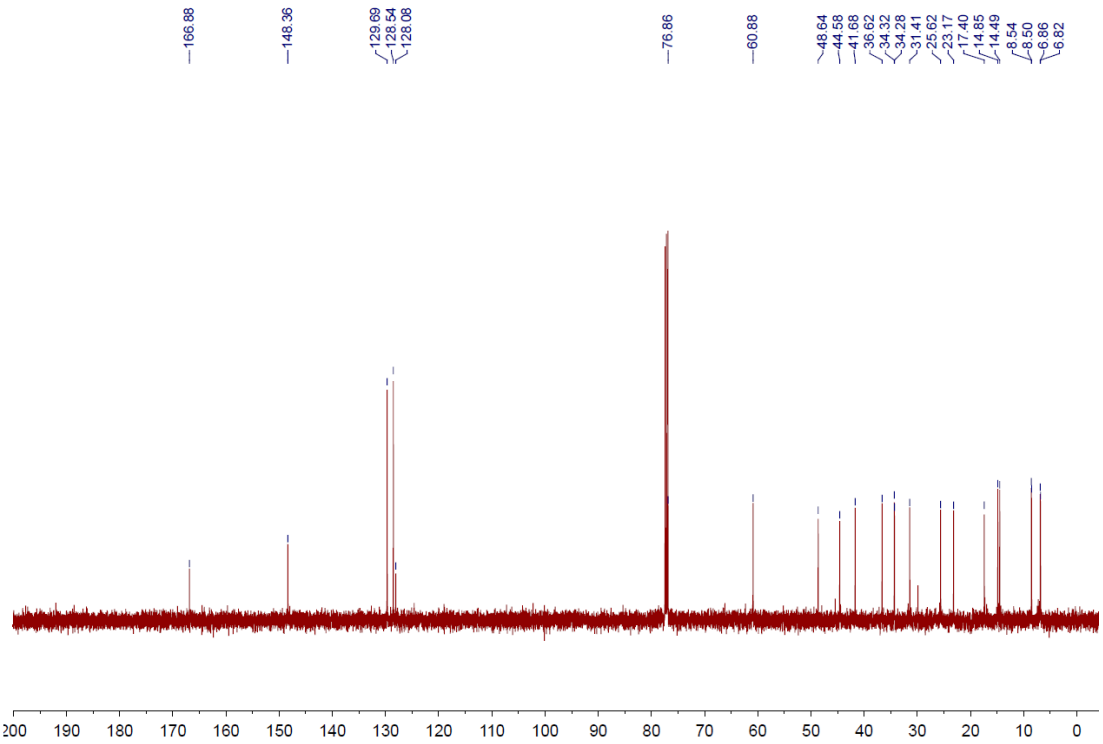
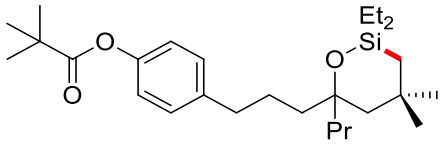
3.16
2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

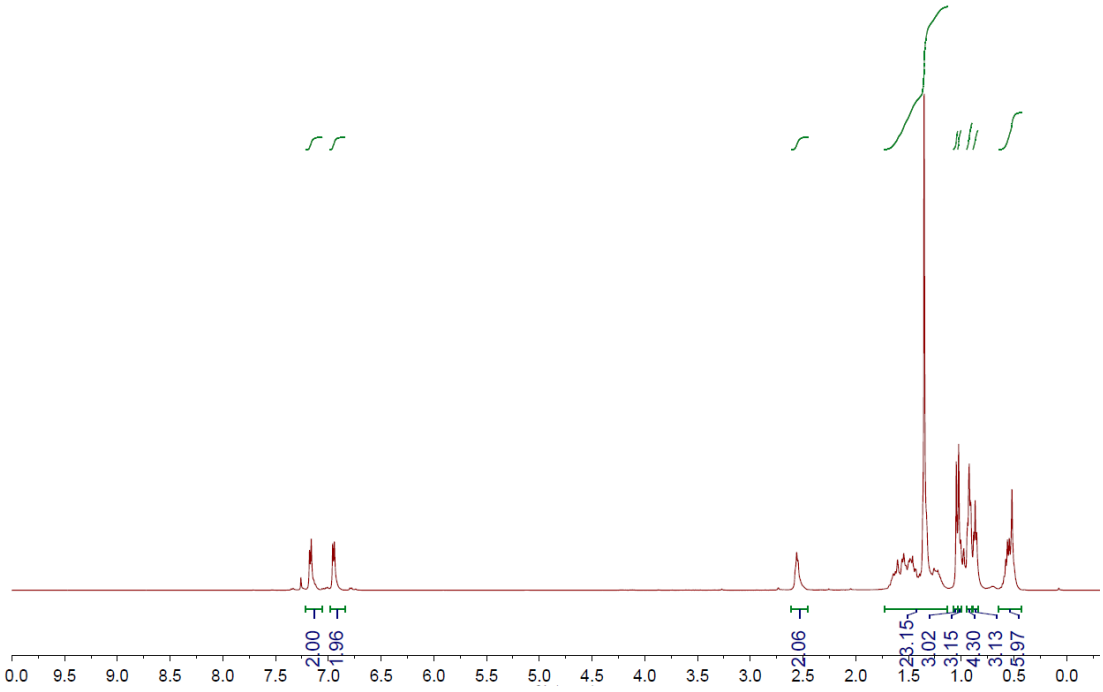

141.72
138.52
128.56
127.20
75.82
71.07
64.95
48.64
42.66
39.98
36.39
36.04
27.91
27.75
26.00
17.24
14.61
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

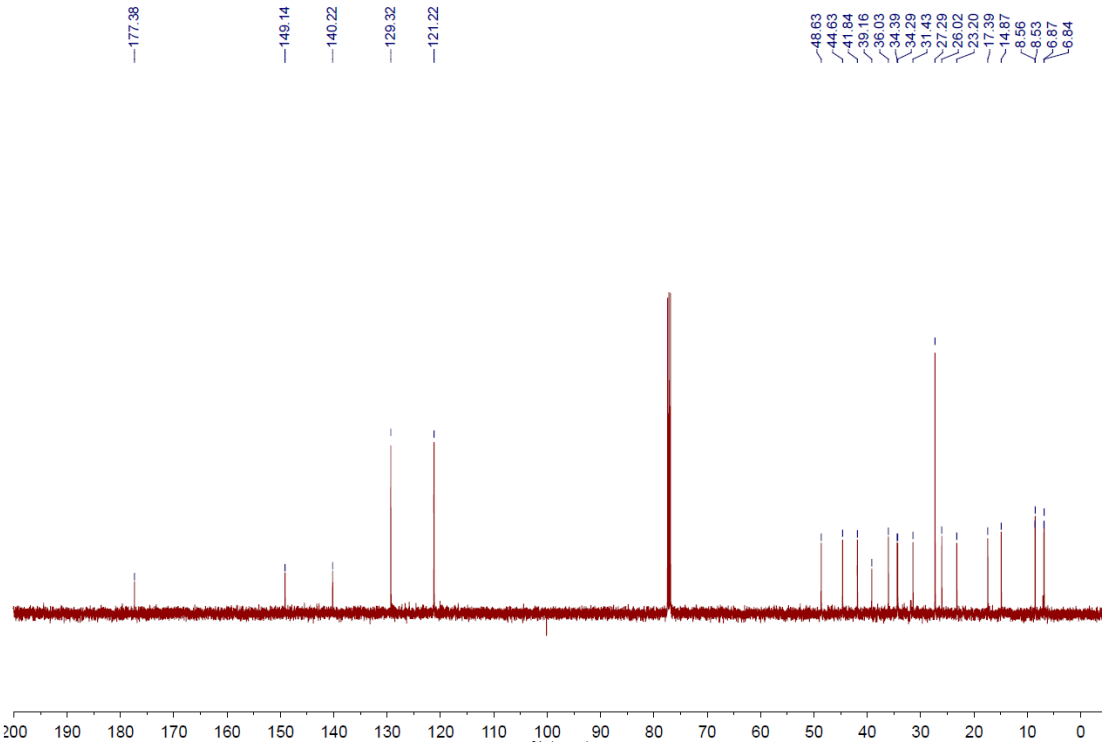

O
O
Et2
Si
O
Pr

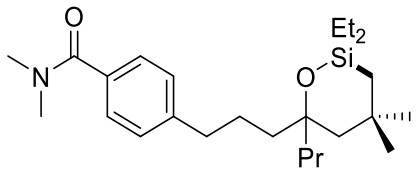

2.00
1.98
2.13
2.08
13.21
3.01
3.07
9.33
6.17
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

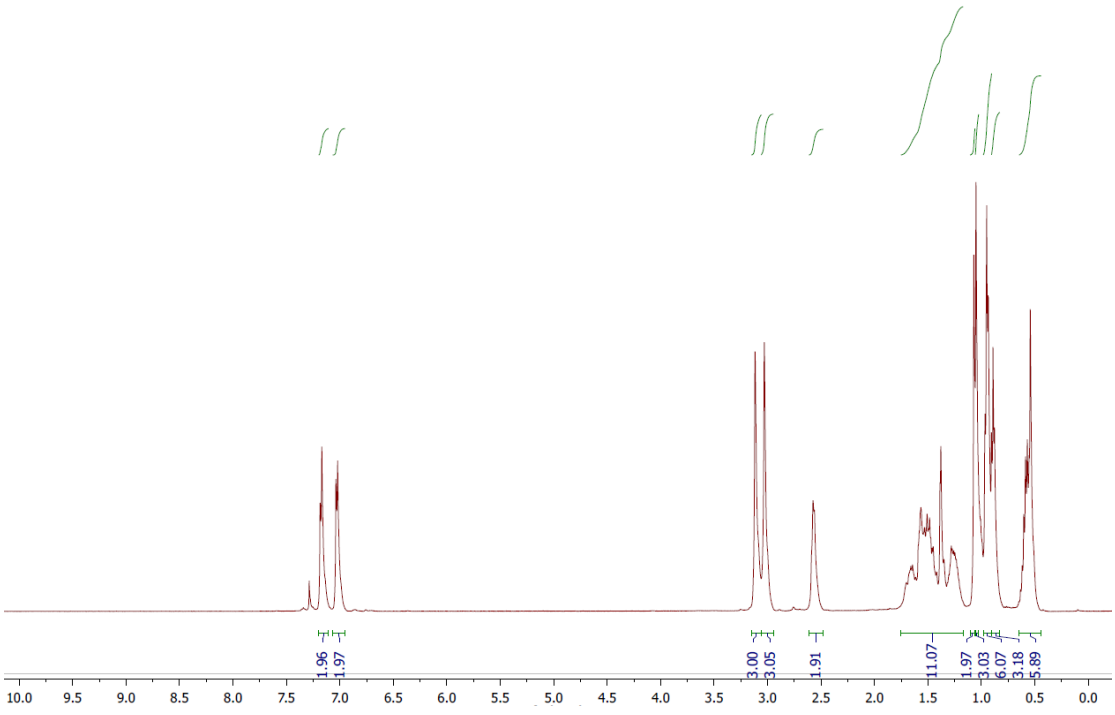

166.88
148.36
129.69
128.54
128.08
76.86
60.88
48.64
44.58
41.68
36.62
34.32
34.28
31.41
25.62
23.17
17.40
14.85
14.49
8.54
8.50
6.86
6.82
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

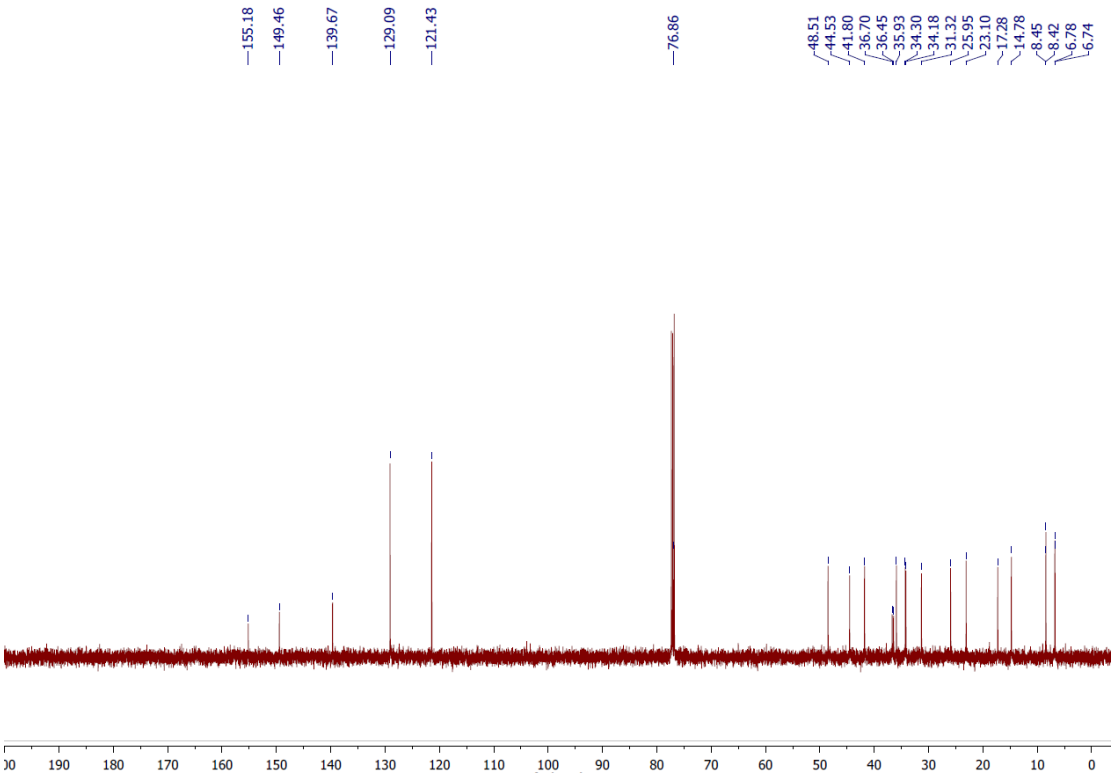

Et2
Si
O
O
O
Pr

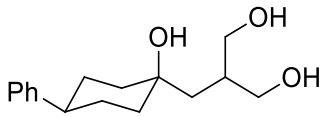

2.00
1.96
2.06
23.15
3.02
3.15
4.30
3.13
5.97
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

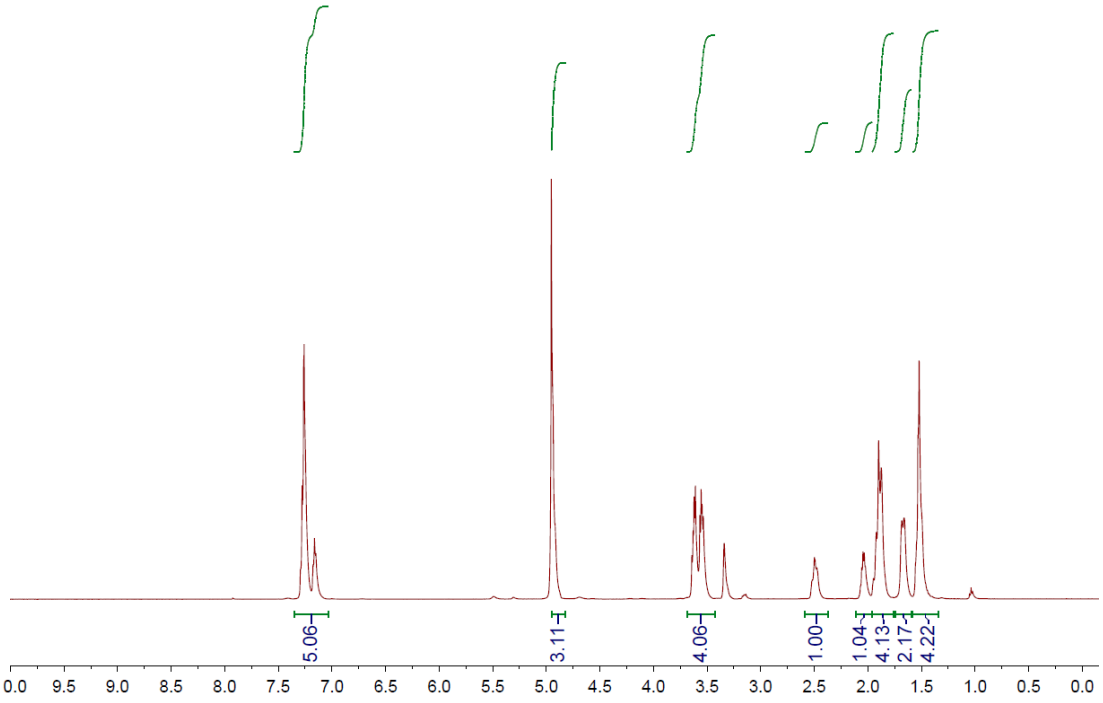

177.38
149.14
140.22
129.32
121.22
48.63
44.63
41.84
39.16
36.03
34.39
34.29
31.43
27.29
26.02
23.20
17.39
14.87
8.56
8.53
6.87
6.84
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

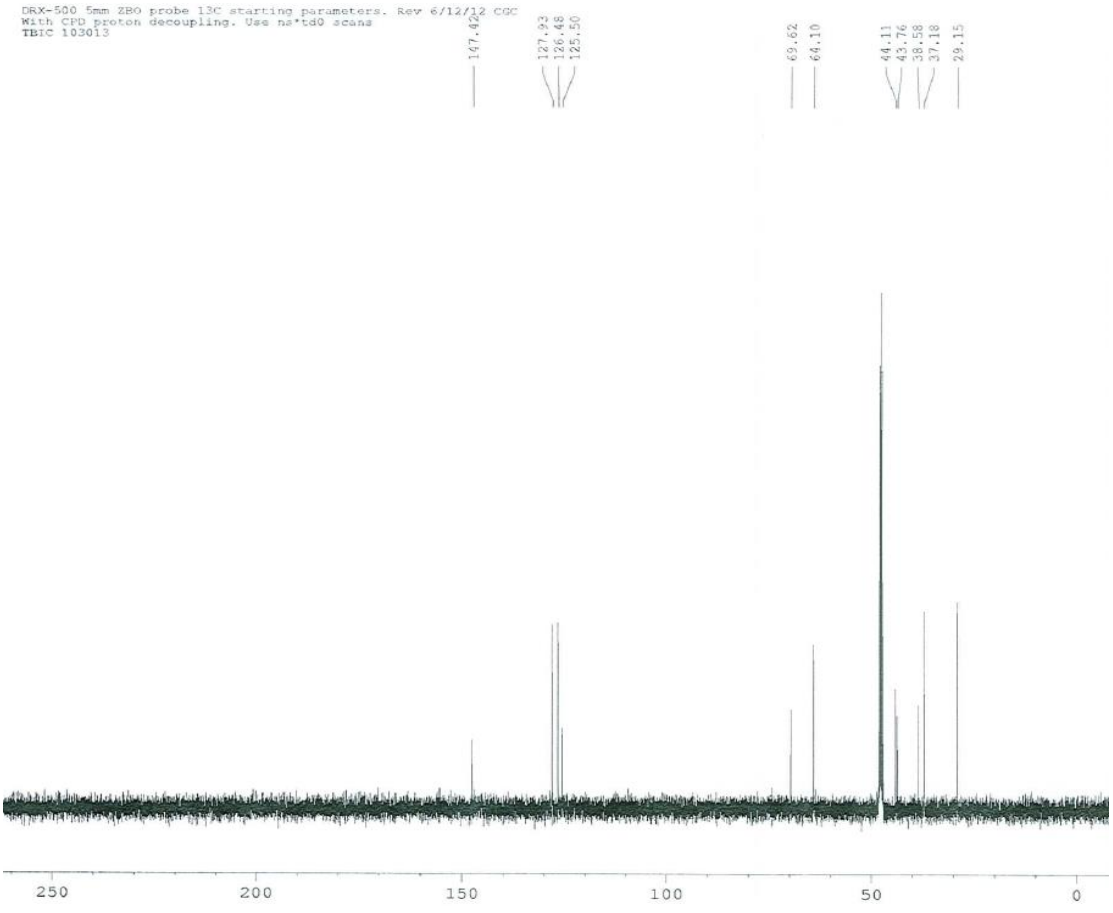

O
N
Et2
Si
O
Pr

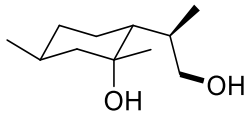

1.96
1.97
3.00
3.05
1.91
11.07
1.97
3.03
6.07
3.18
5.89
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

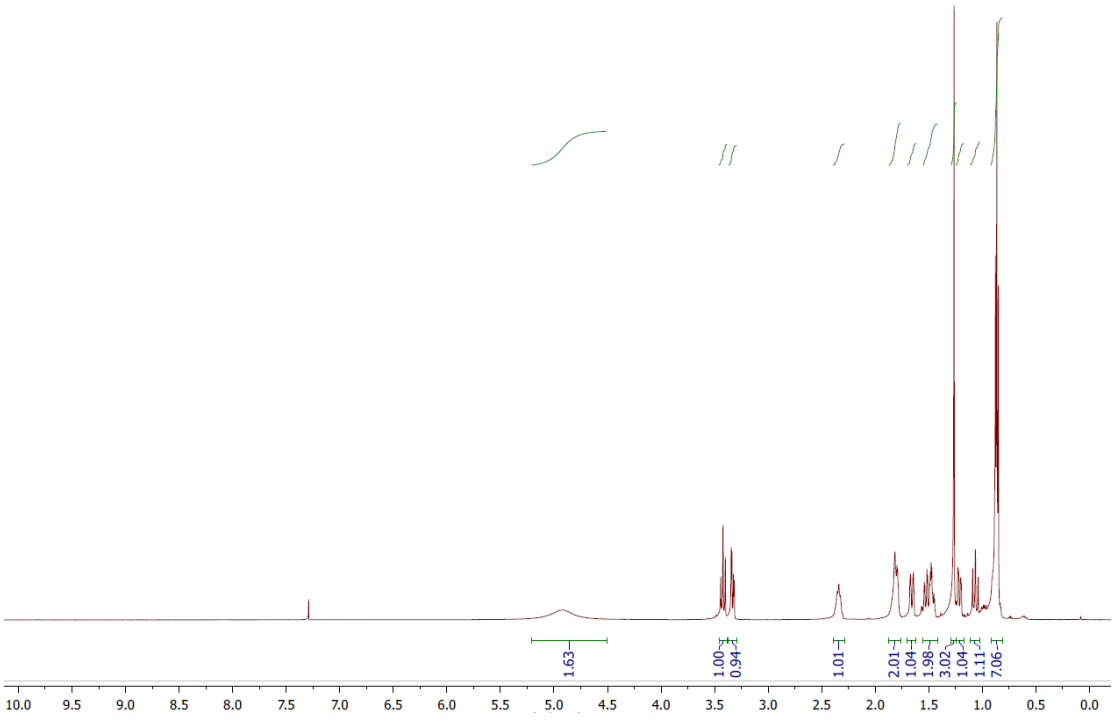

155.18
149.46
139.67
129.09
121.43
76.86
48.51
44.53
41.80
36.70
36.45
35.93
34.30
34.18
31.32
25.95
23.10
17.28
14.78
8.45
8.42
6.78
6.74
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

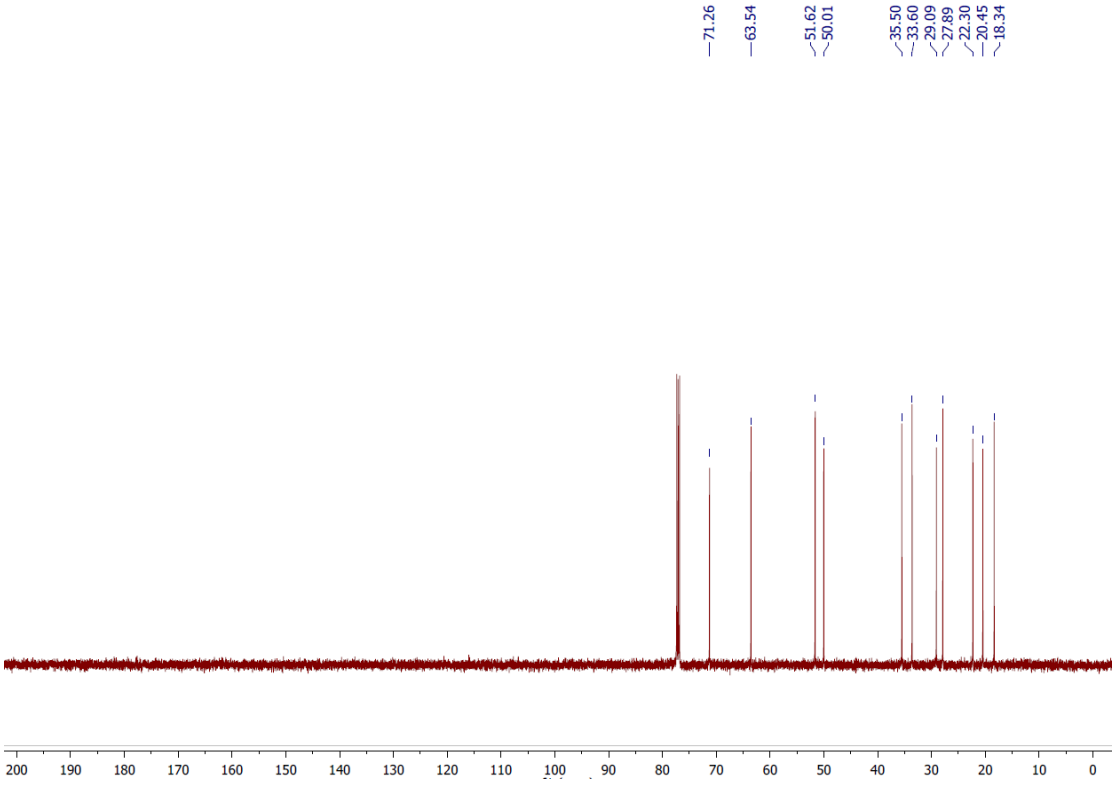

OH
OH
Ph
OH

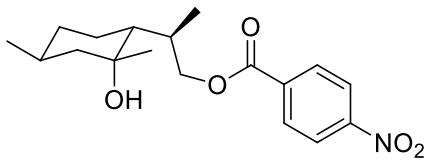

5.06
3.11
4.06
1.00
1.04
4.13
2.17
4.22
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

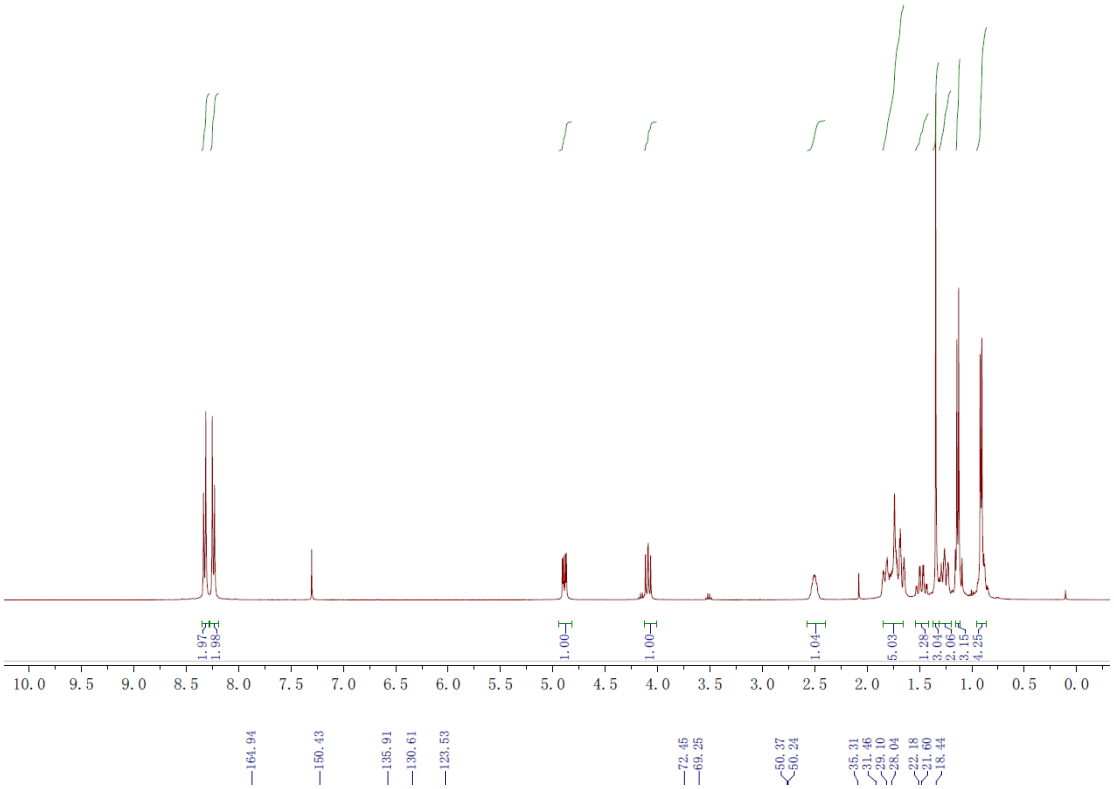

DRX-500 5mm ZBO probe 13C starting parameters. Rev 6/12/12 CGC
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
147.42
127.93
126.48
125.50
69.62
64.10
44.11
43.76
38.58
37.18
29.15
250 200 150 100 50 0

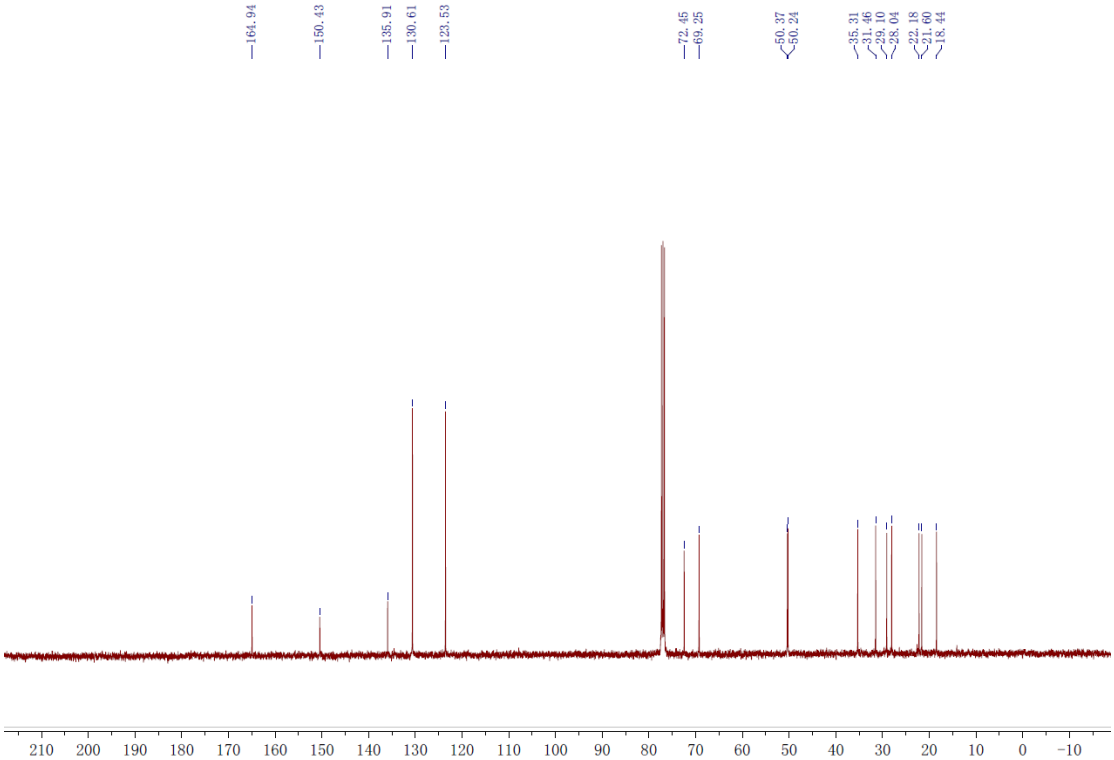

OH
OH

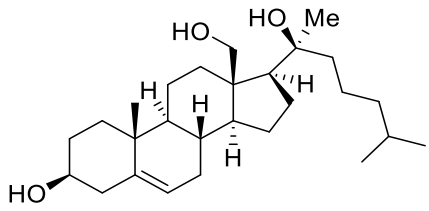

1.63
1.00
0.94
1.01
2.01
1.04
1.98
3.02
1.04
1.11
7.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

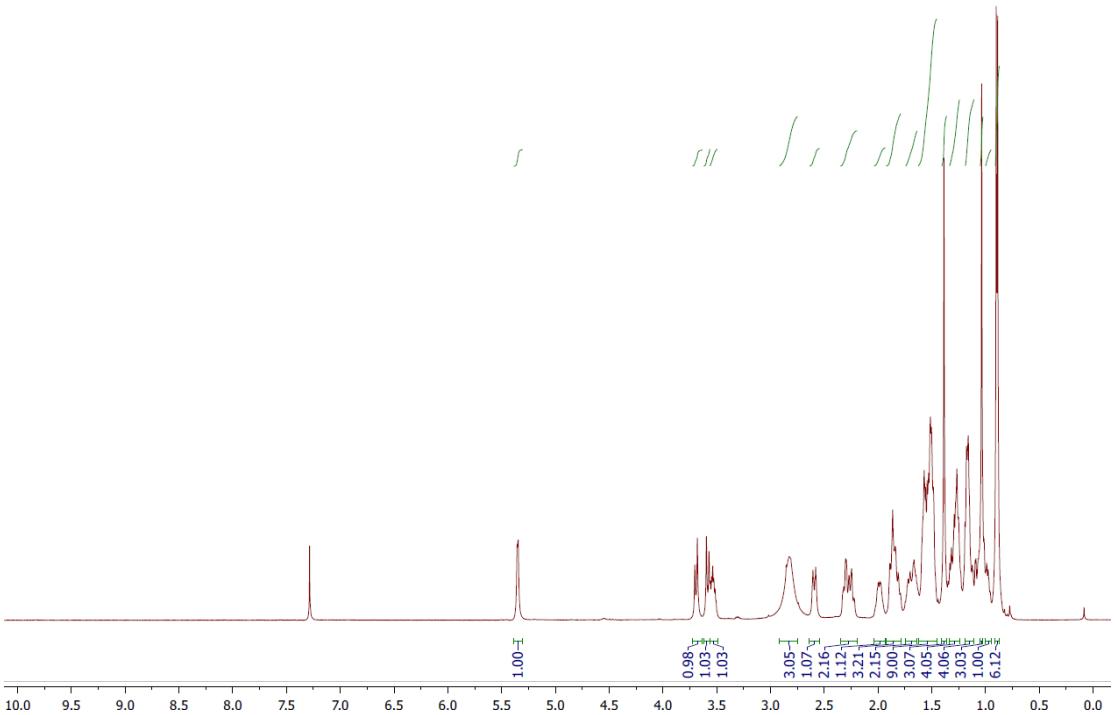

71.26
63.54
51.62
50.01
35.50
33.60
29.09
27.89
22.30
20.45
18.34
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


O
O
OH
NO2

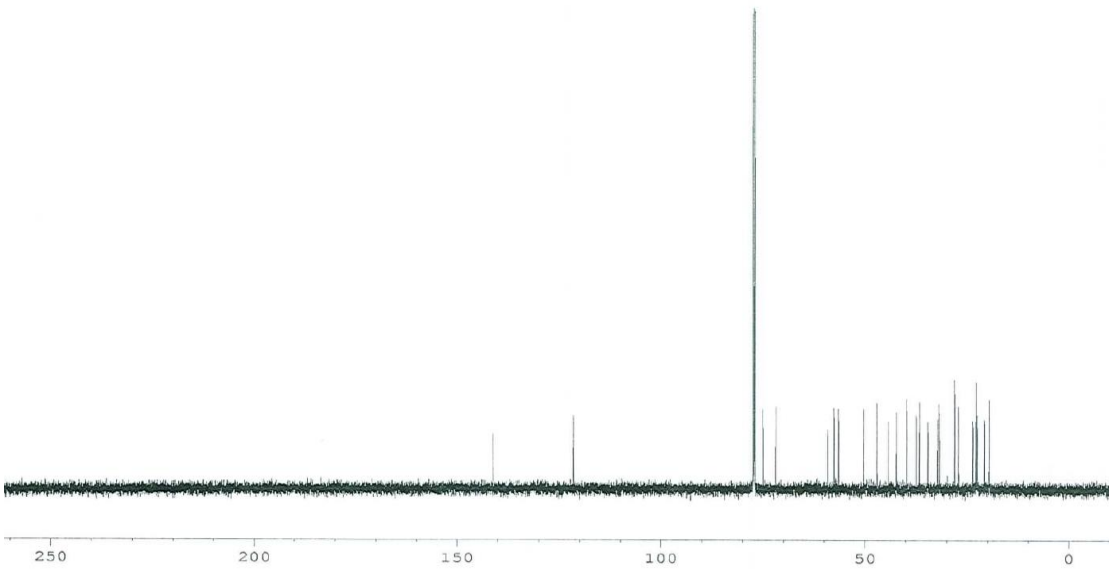

1.97
1.98
1.00
1.00
1.04
5.03
1.28
3.04
2.06
3.15
4.25
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

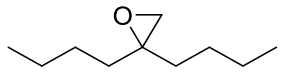

164.94
150.43
135.91
130.61
123.53
72.45
69.25
50.37
50.24
35.31
31.46
29.10
28.04
22.18
21.60
18.44
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

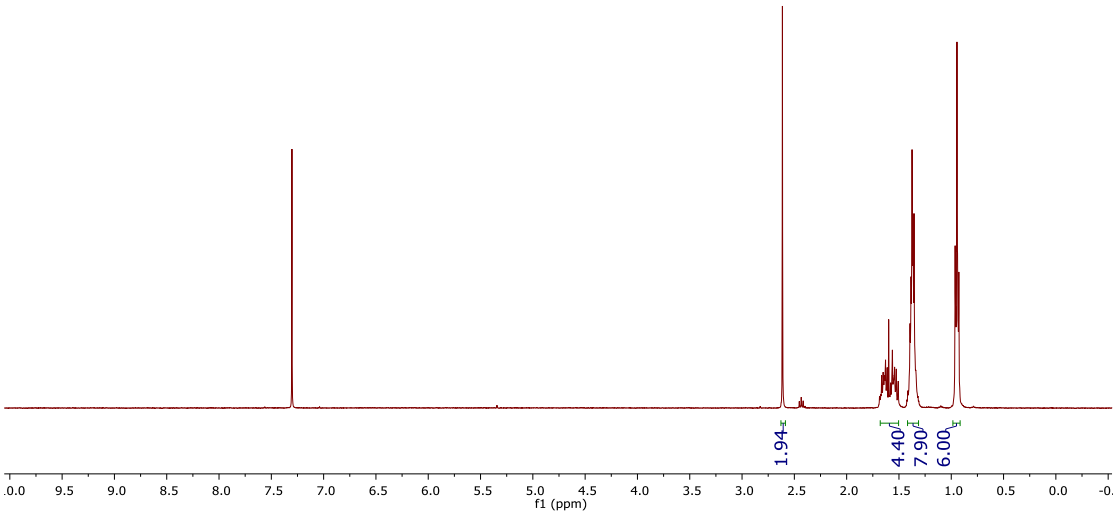

HO
HO
Me
H
H
H
H
HO

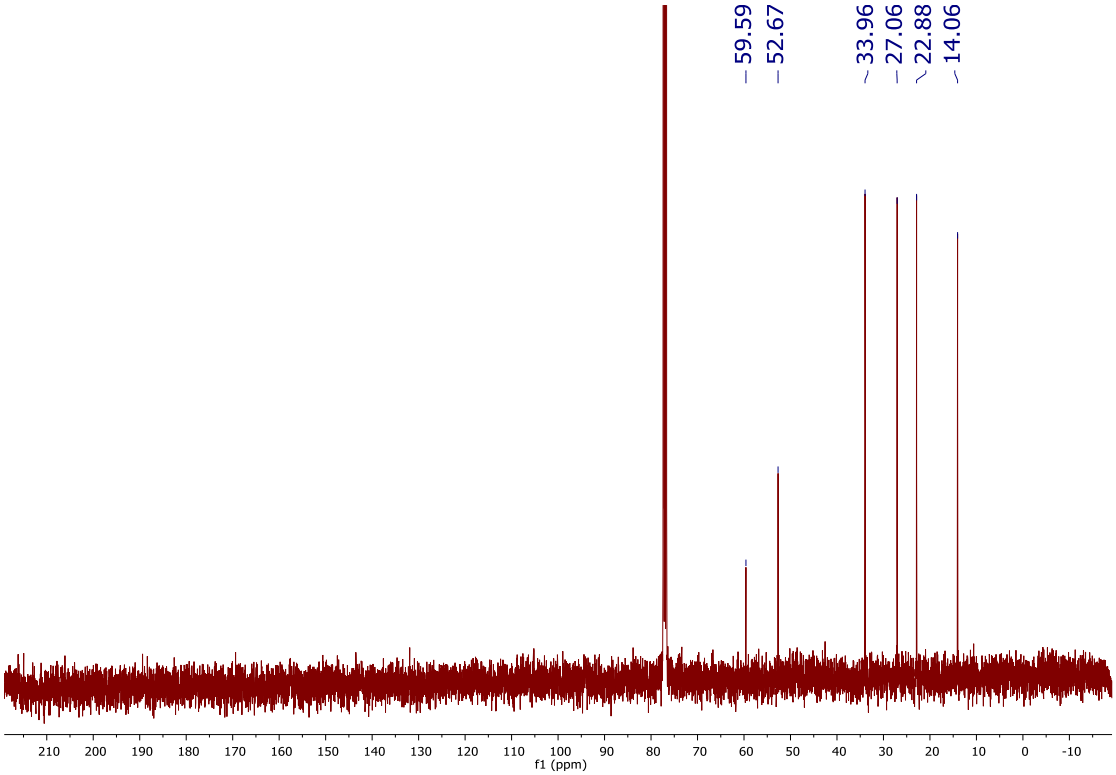

1.00
0.98
1.03
1.03
3.05
1.07
2.16
1.12
3.21
2.15
9.00
3.07
4.05
4.06
3.03
1.00
6.12
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

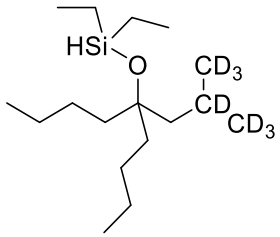

DRX-500 5mm ZBO probe 13C starting parameters. Rev 6/12/12 CGC
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
141.05
121.40
74.92
71.84
59.05
57.50
56.39
50.31
47.09
44.21
42.32
39.69
37.33
36.67
34.56
32.18
31.97
31.69
28.00
27.07
23.52
22.84
22.69
22.57
22.41
20.73
19.57

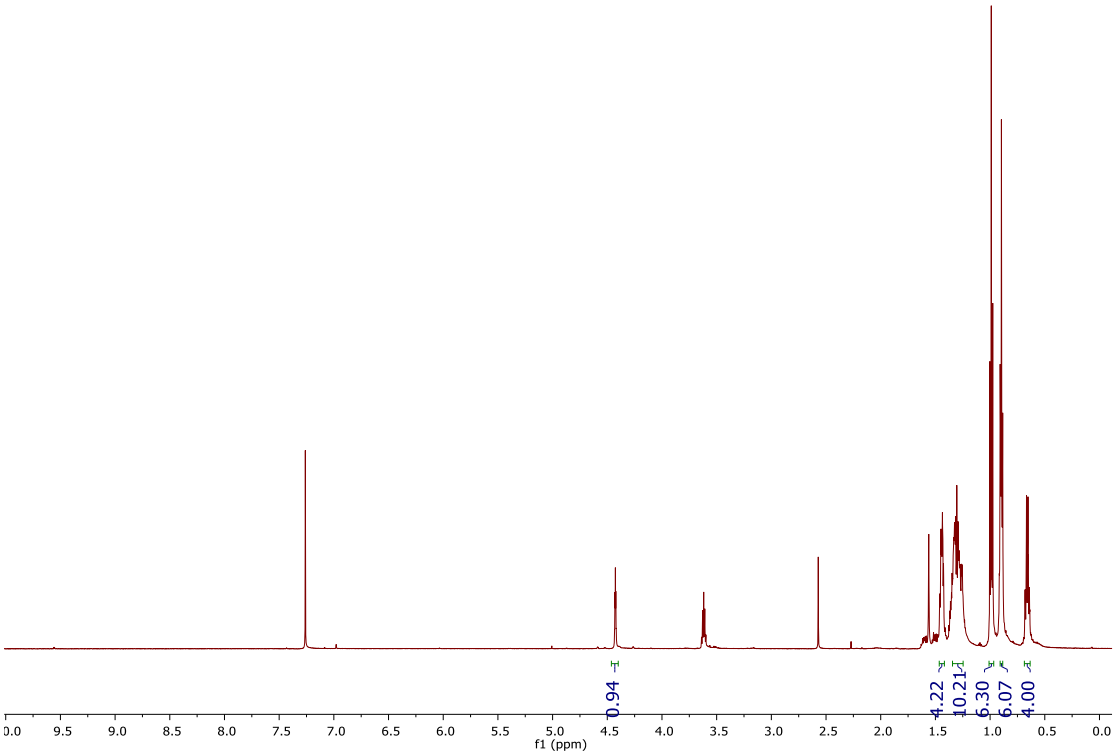

250
200
150
100
50
0

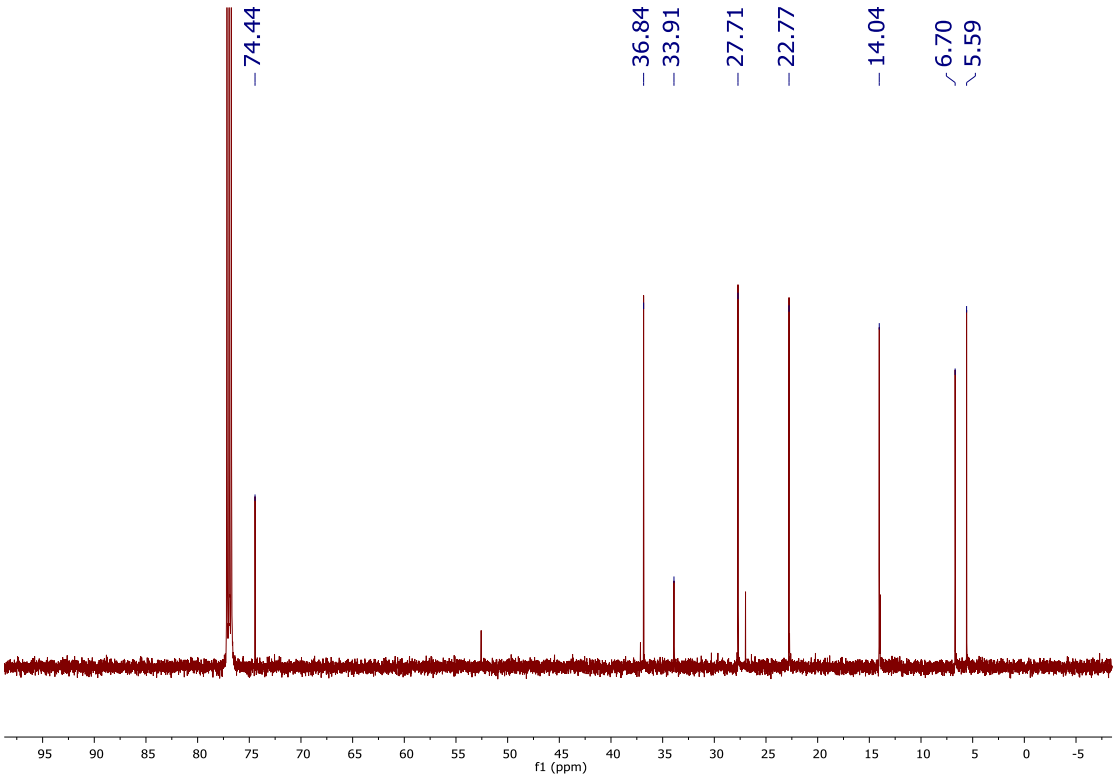


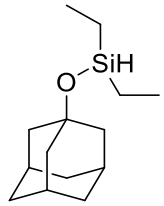

1.94
4.40
7.90
6.00
f1 (ppm)

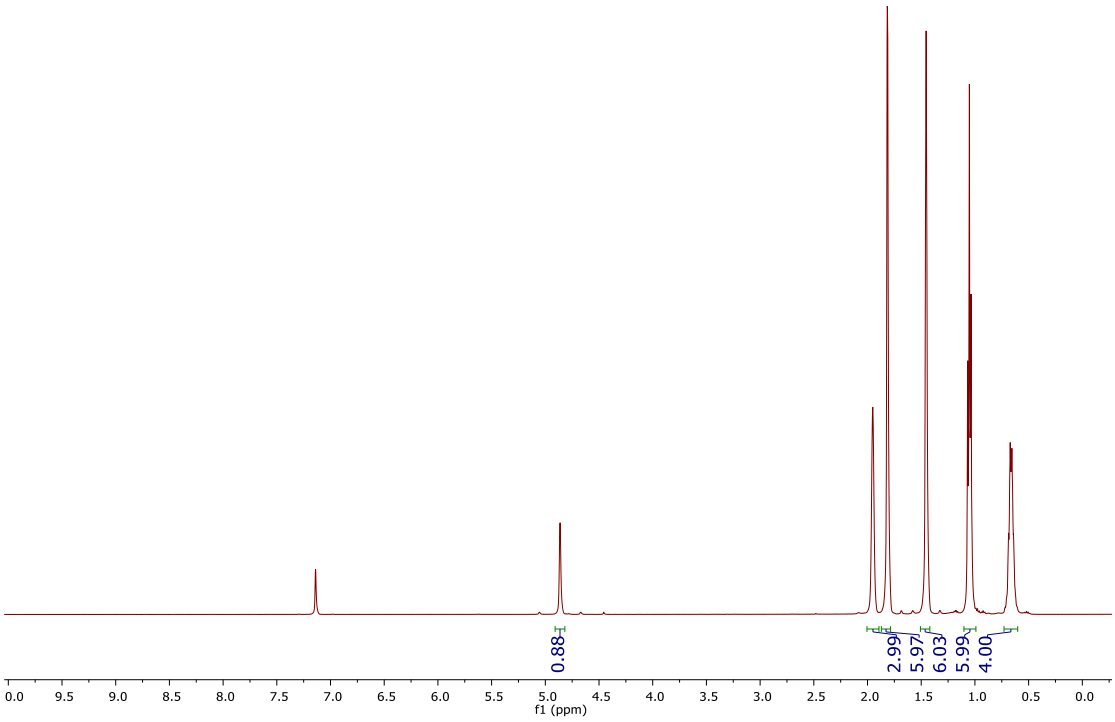

59.59
52.67
33.96
27.06
22.88
14.06
f1 (ppm)

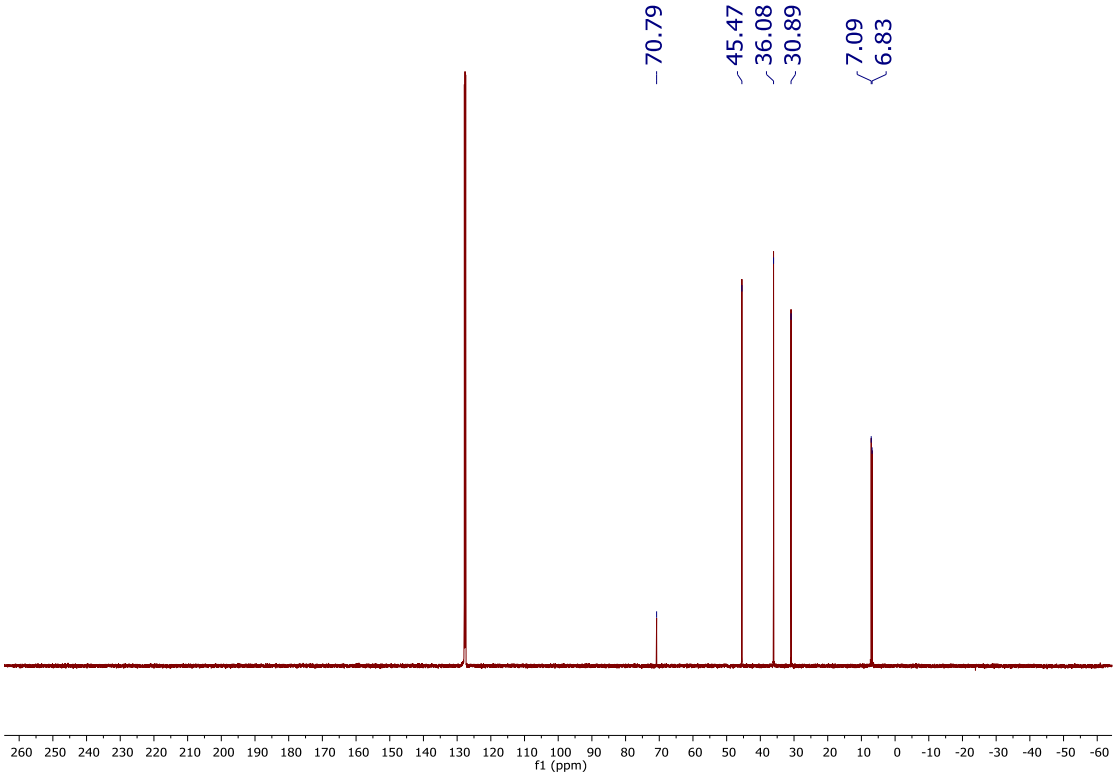

HSi
O
CD3
CD
CD3

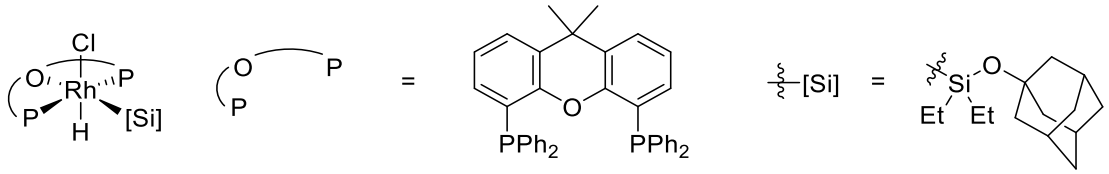

0.94
4.22
10.21
6.30
6.07
4.00
f1 (ppm)

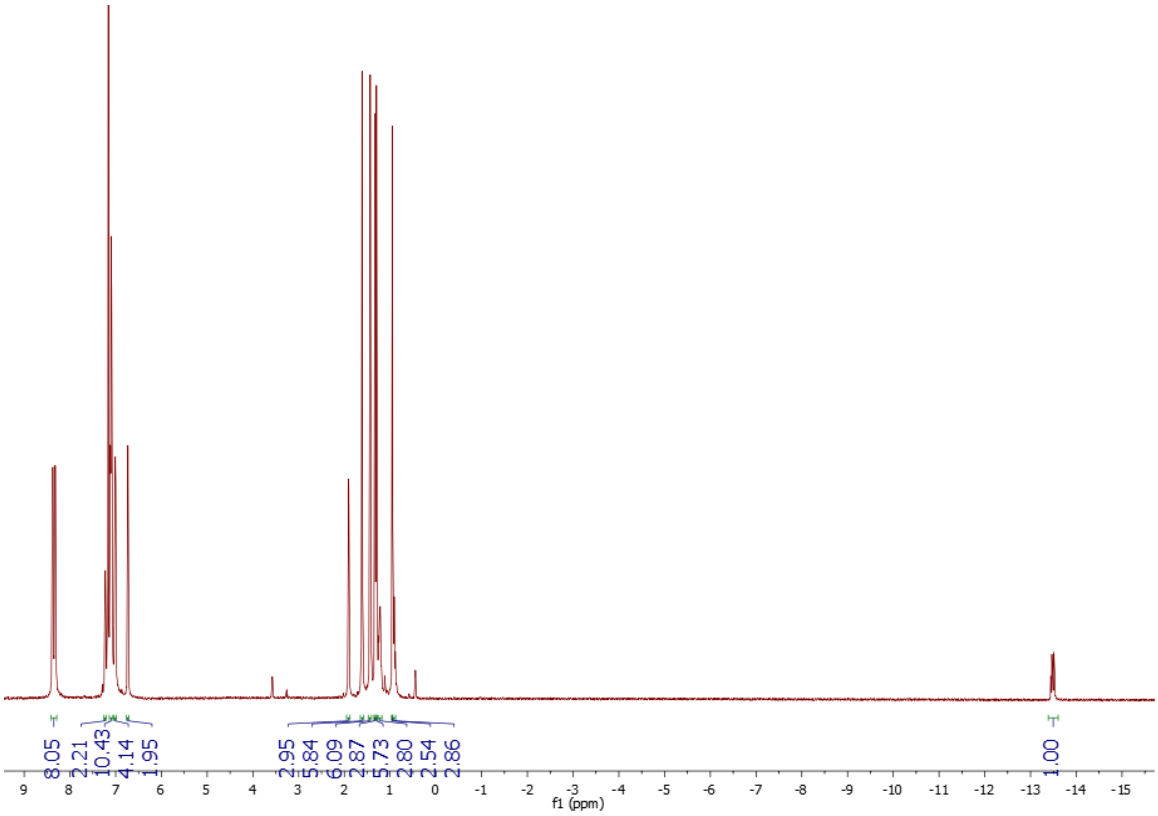

74.44
36.84
33.91
27.71
22.77
14.04
6.70
5.59
f1 (ppm)

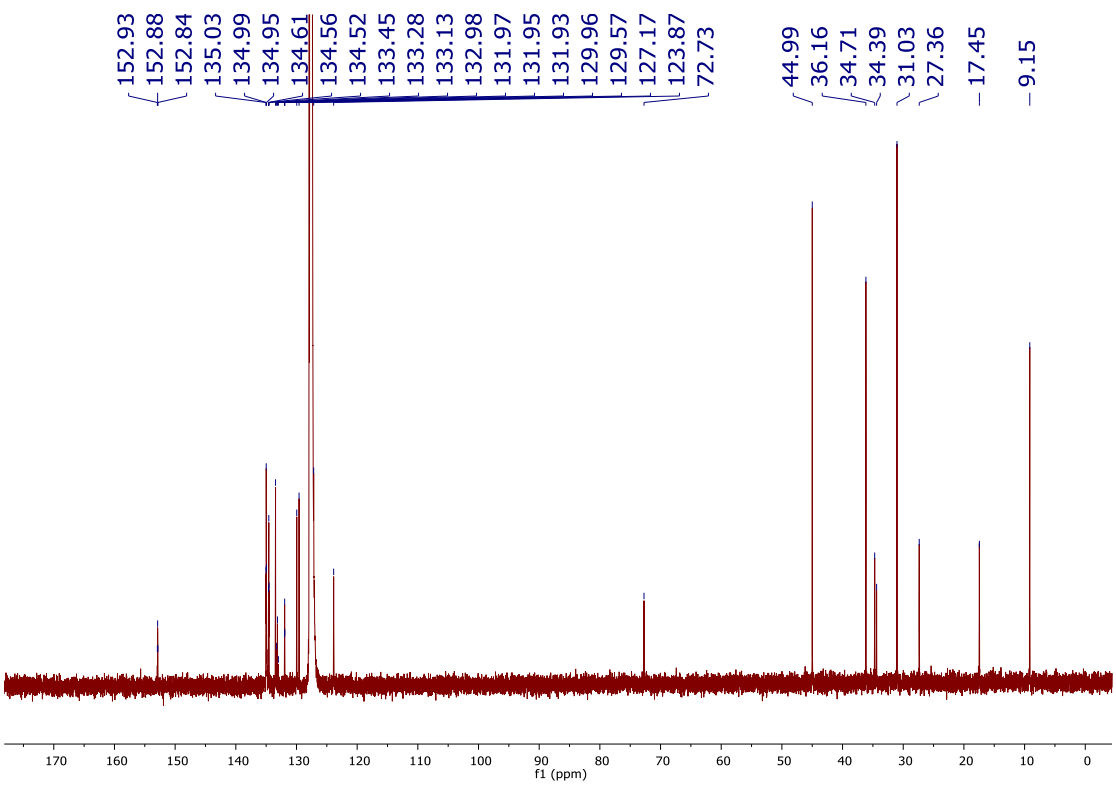

SiH
O

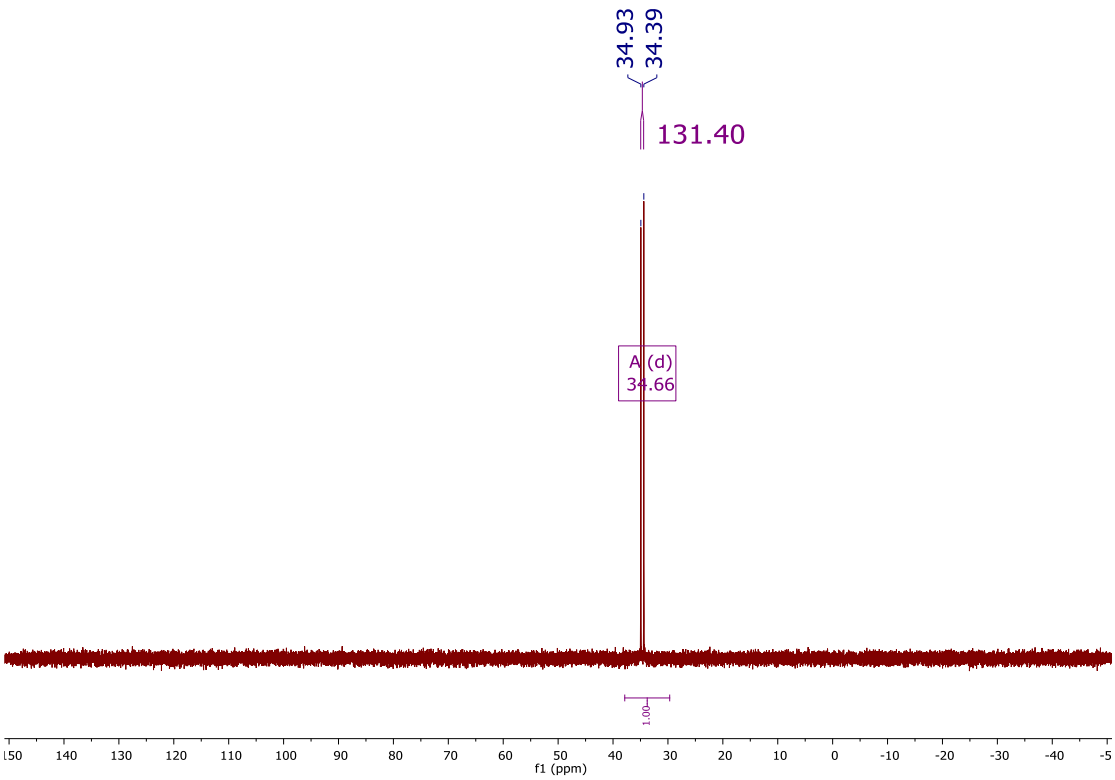

0.88
2.99
5.97
6.03
5.99
4.00
f1 (ppm)


70.79
45.47
36.08
30.89
7.09
6.83
f1 (ppm)

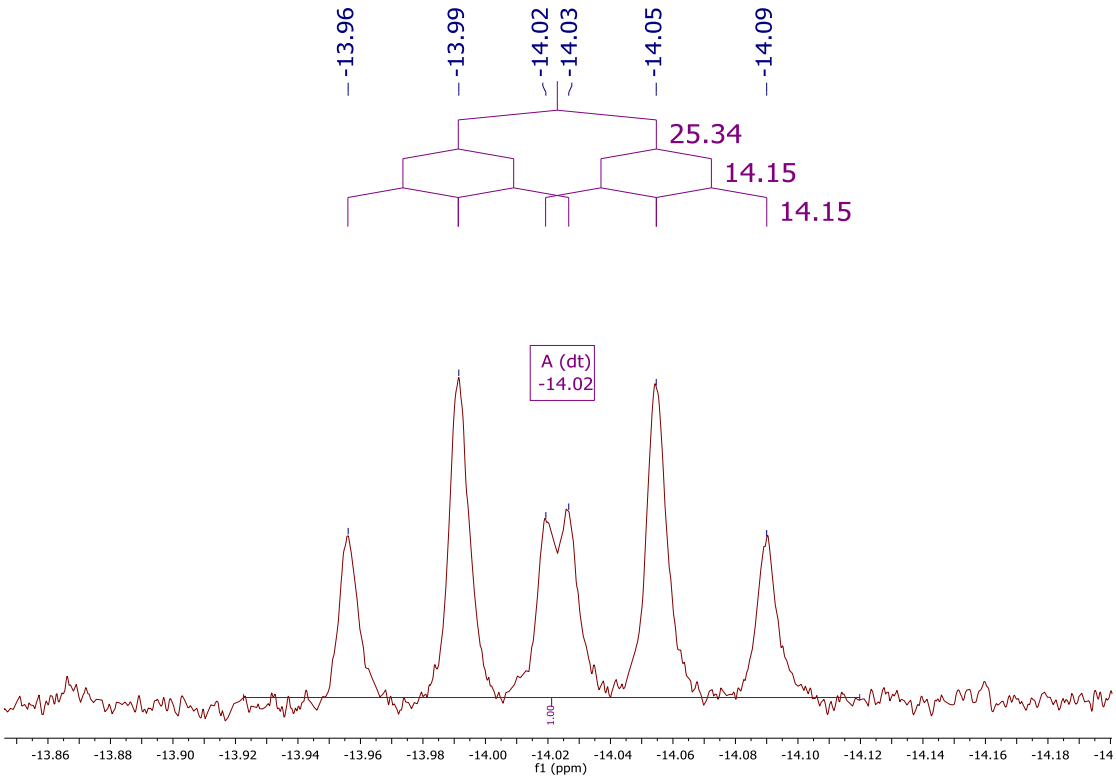

Cl
O
Rh
P
P
H
[Si]
O
P
P
=
O
PPh2
PPh2
[Si]
=
Si
O
Et
Et

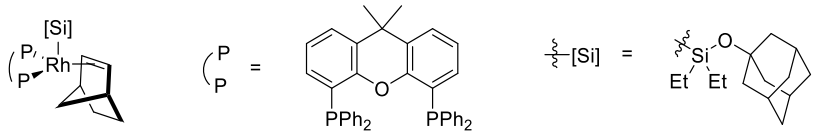

8.05
2.21
10.43
4.14
1.95
2.95
5.84
6.09
2.87
5.73
2.80
2.54
2.86
1.00
f1 (ppm)

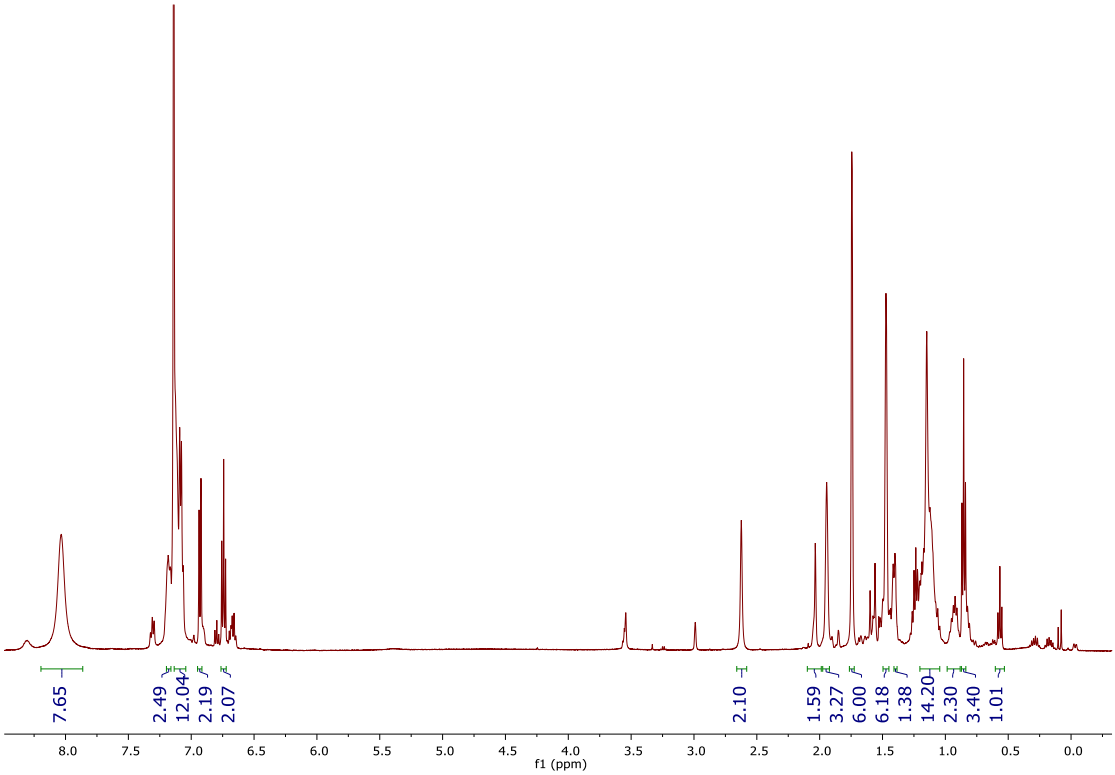

152.93
152.88
152.84
135.03
134.99
134.95
134.61
134.56
134.52
133.45
133.28
133.13
132.98
131.97
131.95
131.93
129.96
129.57
127.17
123.87
72.73
44.99
36.16
34.71
34.39
31.03
27.36
17.45
9.15
f1 (ppm)

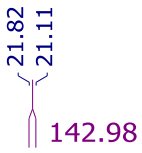

34.93
34.39
131.40
A (d)
34.66
1.00
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -5
f1 (ppm)

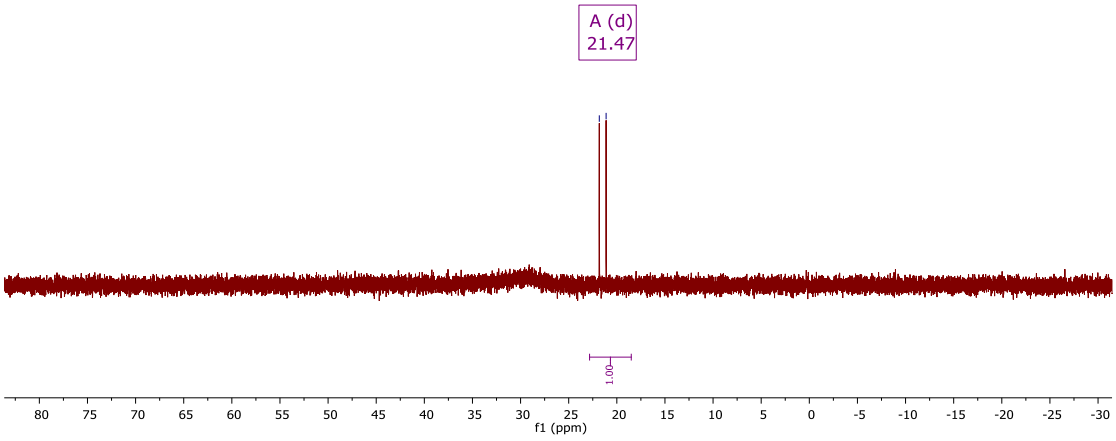
In THF:

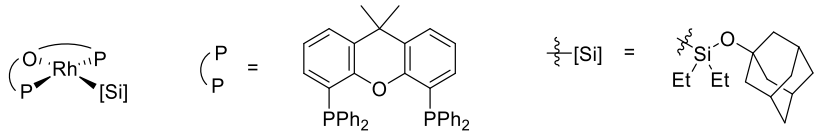

-13.96
-13.99
-14.02
-14.03
-14.05
-14.09
25.34
14.15
14.15
A (dt)
-14.02
1.00
-13.86 -13.88 -13.90 -13.92 -13.94 -13.96 -13.98 -14.00 -14.02 -14.04 -14.06 -14.08 -14.10 -14.12 -14.14 -14.16 -14.18 -14
f1 (ppm)

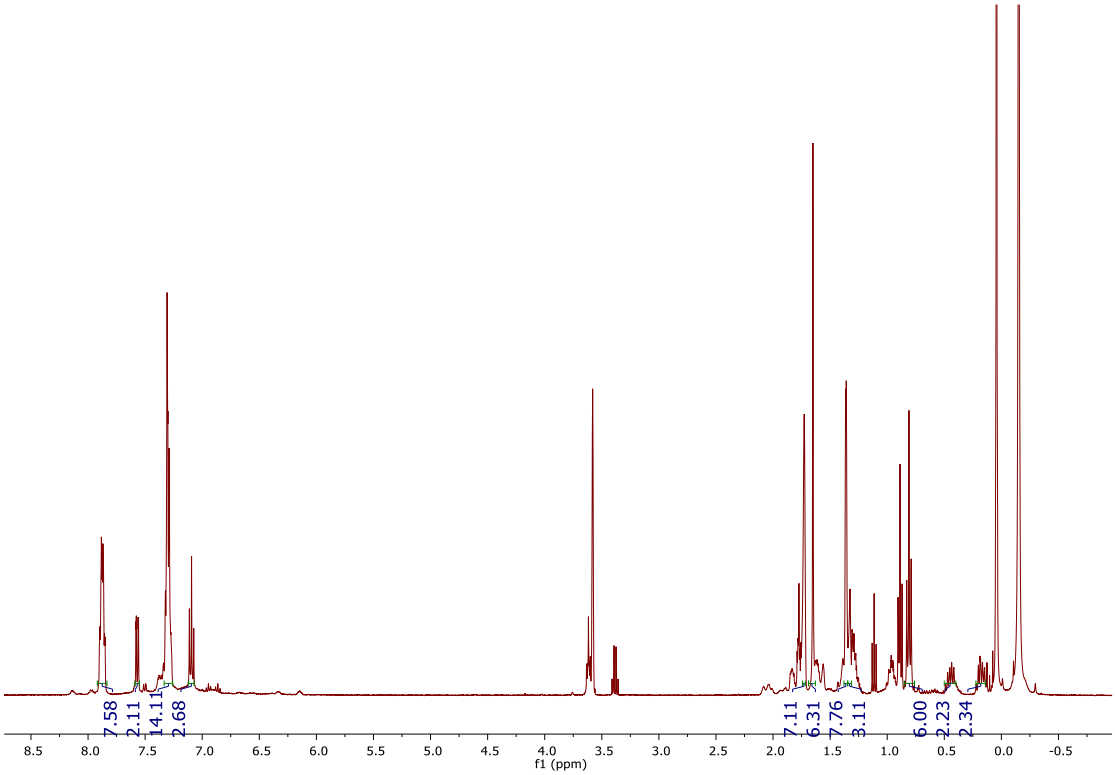

[Si]
P
Rh
P
=
O
PPh2
PPh2
[Si] =
Si
O
Et
Et

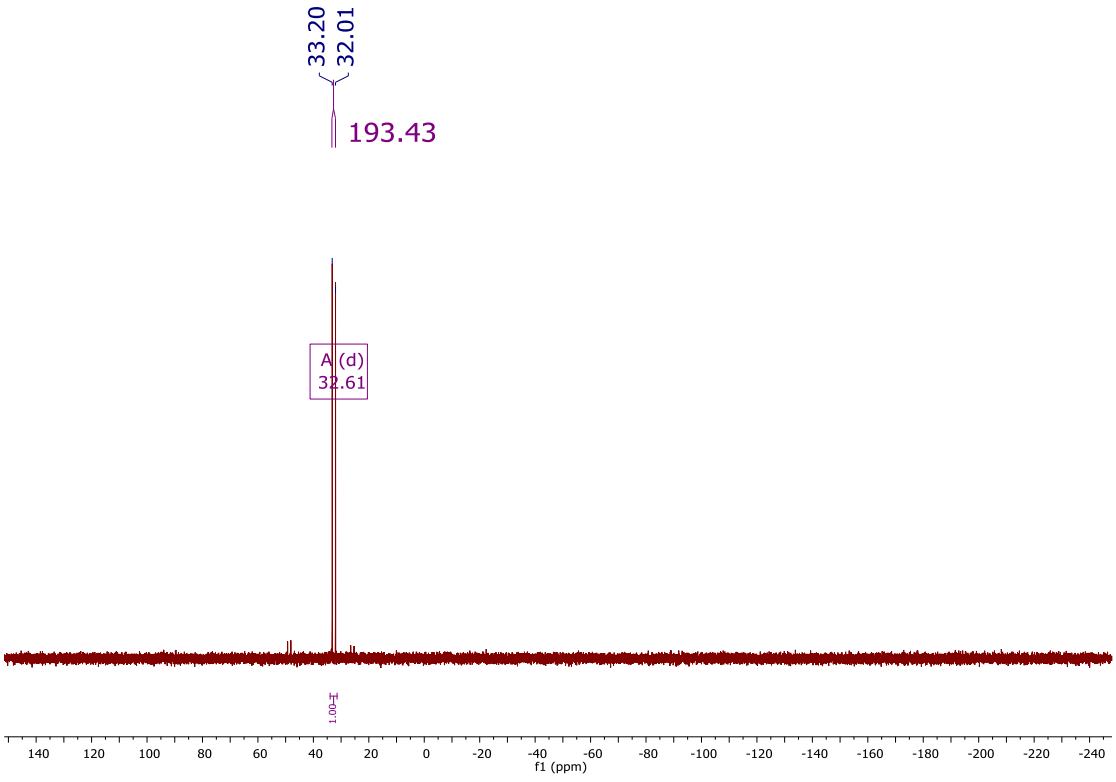

7.65
2.49
12.04
2.19
2.07
2.10
1.59
3.27
6.00
6.18
1.38
14.20
2.30
3.40
1.01
f1 (ppm)


21.82
21.11
142.98


A (d)
21.47
1.00
f1 (ppm)


O
Rh
P
P
[Si]
=
PPh2
PPh2
[Si]
=
Si
O
Et
Et


7.58
2.11
14.11
2.68
7.11
6.31
7.76
3.11
6.00
2.23
2.34
f1 (ppm)


33.20
32.01
193.43
A (d)
32.61
1.00
f1 (ppm)