Supporting Information

Total Synthesis of Nahuoic Acid A via a Putative Biogenetic Intramolecular Diels-Alder (IMDA) Reaction

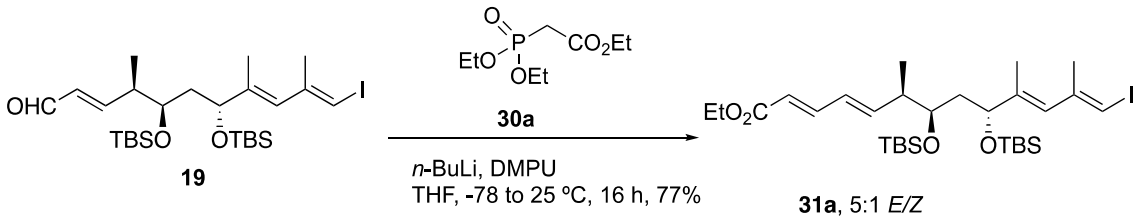
Lucía Guillade, Paula Mora, Pedro Villar, Rosana Alvarez,* and Angel R. de Lera*

Departamento de Química Orgánica, Facultade de Química, CINBIO and IIS Galicia Sur, Universidade de Vigo, 36310 Vigo, Spain

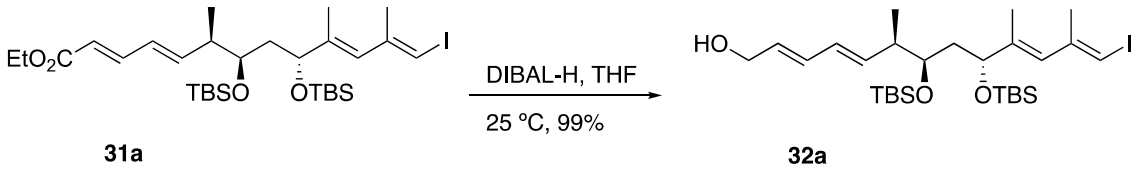
I. GENERAL EXPERIMENTAL PROCEDURES

All reagents were commercial compounds of the highest purity available. All reactions were carried out under an atmosphere of argon, and those not involving aqueous reagents were carried out in oven-dried glassware. All solvents and anhydrous solutions were transferred thought syringes and cannules previously dried in the oven for at least 12 h and kept in a dessicator with KOH. All solvent used in the reactions were purified following the general procedures described in the literature and CH_2Cl_2, MeOH, toluene and THF were dried using a Puresolv^{TM} solvent purification system. Flash column chromatography was carried out using Merck Kieselgel 60 (230-400 mesh) or Silicycle SiliaFlash® P60 (230-400 mesh) under pressure. Analytical thin layer chromatography (TLC) was performed on aluminium plates with Merck Kieselgel 60 F_{254} and visualized by UV irradiation (254 nm) or by staining with solution of phosphomolibdic acid (in EtOH). HPLC separations were carried out using a Waters 1525 Binary Pump and a Waters 2487 Dual Absorbance Detector, and a Synergi MAX-RP column, C18-silica gel, 4 µm, 250 x 4.6 mm. UV/Vis spectra were recorded on a Cary 100 Bio spectrophotometer. Infrared spectra were obtained on a JASCO IR 4200 spectrophotometer from a thin film deposited into NaCl glass. High-resolution mass spectra were taken on a VG Austospec instrument. ^{1}H NMR and ^{13}C-NMR spectra were recorded in $CDCl_3$, C_6D_6 and CD_2Cl_2, at ambient temperature on a Bruker AMX-400 at 400.13 and 100.1, respectively, with residual protic solvent as the internal reference ($CHCl_3$, δ_H = 7.24 ppm, δ_C = 77.2 ppm; C_6D_6, δ_H = 7.26 ppm, δ_C = 128.0 ppm; CD_2Cl_2, δ_H = 5.32 ppm, δ_C = 54.0 ppm); chemical shifts (δ) are given in parts per million (ppm), and coupling constants (*J*) are given in Hertz (Hz). The proton spectra are reported as follows: δ (multiplicity, coupling constant *J*, number of protons, assignment). DEPT135, HSQC, HMBC and COSY are used to aid in the assignment of signals in the ^{13}C NMR spectra. Different NOESY and NOE experiments were also performed in selected cases.

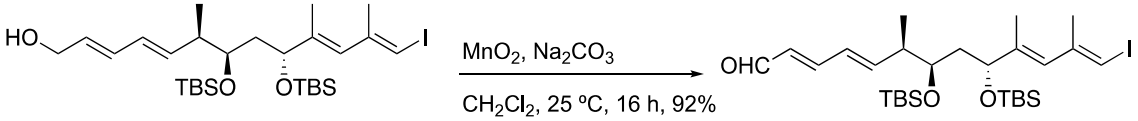
II. Experimental SECTION



Ethyl (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-Butyldimethylsilyloxy)-13-iodo-6,10,12-trimethyltrideca-2,4,10,12-tetraenoate 31a. General procedure for the Horner-Wadsworth-Emmons olefination. To a cooled (0 °C) solution of ethyl 2-(diethoxyphosphoryl)acetate **30a** (0.07 mL, 0.34 mmol) in THF (1 mL), *n*-BuLi (0.21 mL, 1.51 M, 0.32 mmol) and DMPU (0.2 mL, 1.9 mmol) were added dropwise. After stirring for 30 min at 0 °C, the reaction mixture was cooled down to -78 °C and a solution of (2*E*,4*R*,5*R*,7*R*,8*E*,10*E*)-5,7-bis(*tert*-butyldimethylsilyloxy)-11-iodo-4,8,10-trimethylundeca-2,8,10-trienal **19** (0.11 g, 0.19 mmol) in THF (0.9 mL) was added. The mixture was allowed to reach room temperature overnight. The reaction mixture was cooled down to 0 °C and a saturated aqueous solution of NH_4Cl (3.0 mL) was added. The aqueous layer was extracted with Et_2O (3x). The combined organic layers were washed with H_2O (2x), brine (2x), dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 70:30 hexane/CH_2Cl_2) to afford 0.081 g (77%) of a colorless oil, for the major isomer, which was identified as ethyl (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-6,10,12-trimethyltrideca-2,4,10,12-tetraenoate **31a**. **Molecular formula:** $C_{30}H_{55}IO_4Si_2$. **MW:** 662.84 g/mol. **$[\alpha]_D^{20}$** 16.0° (*c* 0.54, CH_2Cl_2). **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 7.25 (dd, *J* = 15.6, 10.0 Hz, 1H, H_3), 6.23 – 6.06 (m, 2H, H_4 + H_5), 6.02 – 6.01 (m, 1H, H_{13}), 5.79 (d, *J* = 15.6 Hz, 1H, H_2), 5.77 (s, 1H, H_{11}), 4.20 (q, *J* = 7.1 Hz, 2H, $COO\underline{CH_2}CH_3$), 4.05 (dd, *J* = 8.4, 3.5 Hz, 1H, H_9), 3.72 (app. dt, *J* = 7.2, 4.0 Hz, 1H, H_7), 3.51 – 3.43 (m, 1H, H_6), 1.91 (d, *J* = 0.7 Hz, 3H, CH_3), 1.70 – 1.63 (m, 1H, H_{8A}), 1.66 (d, *J* = 1.3 Hz, 3H, CH_3), 1.38 (ddd, *J* = 14.1, 6.9, 3.7 Hz, 1H, H_{8B}), 1.29 (t, *J* = 7.1 Hz, 3H, $OCH_2\underline{CH_3}$), 1.01 (d, *J* = 6.9 Hz, 3H, CH_3), 0.89 (s, 9H, $SiC(CH_3)_3$), 0.88 (s, 9H, $SiC(CH_3)_3$), 0.07 (s, 3H, $SiCH_3$), 0.05 (s, 3H, $SiCH_3$), 0.04 (s, 3H, $SiCH_3$), -0.04 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 167.5 (s), 146.8 (d), 145.2 (d), 144.4 (s), 141.2 (s), 128.0 (d), 126.2 (d), 119.8 (d), 80.0 (d), 75.9 (d), 73.7 (d), 60.4 (t), 42.5 (d), 41.6 (t), 26.0 (q, 3x), 26.1 (q, 3x), 25.2 (q), 18.3 (s, 2x), 14.5 (q), 13.9 (q), 13.4 (q), -3.8 (q), -4.0 (q, 2x), -4.7 (q) ppm. **MS** (ESI^+): *m/z* 663 ($[M+H]^+$, 30), 531 (100), 399 (49). **HRMS** (ESI^+): Calcd. for $C_{30}H_{56}IO_4Si_2$ ($[M+H]^+$), 663.2756; found, 663.2726. **IR** (NaCl): ν 2954 (m, C-H), 2930 (m, C-H), 2857 (w, C-H), 1716 (s, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 258 nm.

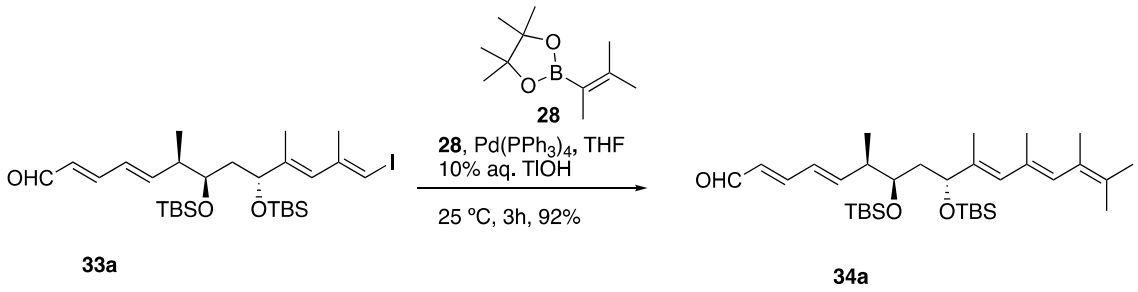


(2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-Butyldimethylsilyloxy)-13-iodo-6,10,12-trimethyltrideca-2,4,10,12-tetraen-1-ol 32a. General procedure for the reduction of esters with DIBAL-H. To a cooled (-78 °C) solution of ethyl (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-6,10,12-trimethyltrideca-2,4,10,12-tetraenoate **31a** (0.08 g, 0.12 mmol) in THF (1.3 mL), DIBAL-H (0.31 mL, 1 M, 0.31 mmol) was added dropwise. The reaction mixture was stirred for 7h at -78 °C. Then, a mixture of an aqueous saturated solution of Rochelle's salt and Et_2O (20 mL, 1:1 *v/v*) was added and the reaction mixture was stirred at room temperature until a clear solution was obtained. The aqueous layer was extracted with Et_2O (3x). The combined organic layers were washed with brine (2x), dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 90:10 hexane/EtOAc) to afford 0.08 g (99%) of a colorless oil, which was identified as (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-6,10,12-trimethyltrideca-2,4,10,12-tetraen-1-ol **32a**. **Molecular formula:** $C_{28}H_{53}IO_3Si_2$. **MW:** 620.80 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 6.22 (dd, *J* = 15.1, 10.5 Hz, 1H, H_3), 6.00 (dd, *J* = 15.8, 10.4 Hz, 1H, H_4), 6.01 – 6.00 (m, 1H, H_{13}), 5.79 – 5.70 (m, 2H, H_5 + H_2), 5.77 (s, 1H, H_{11}), 4.17 (app. t, *J* = 5.4 Hz, 2H, H_1), 4.05 (dd, *J* = 8.1, 4.0 Hz, 1H, H_9), 3.67 (app. dt, *J* = 7.6, 4.3 Hz, 1H, H_7), 2.42 – 2.35 (m, 1H, H_6), 1.91 (d, *J* = 0.7 Hz, 3H, CH_3), 1.71 – 1.63 (m, 1H, H_{8A}), 1.66 (d, *J* = 1.3 Hz, 3H, CH_3), 1.40 (ddd, *J* = 14.1, 6.9, 4.0 Hz, 1H, H_{8B}), 0.98 (d, *J* = 6.9 Hz, 3H, CH_3), 0.89 (s, 9H, $SiC(CH_3)_3$), 0.88 (s, 9H, $SiC(CH_3)_3$), 0.06 (s, 6H, $SiCH_3$), 0.05 (s, 3H, $SiCH_3$), 0.04 (s, 3H, $SiCH_3$), -0.03 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 144.5 (s), 141.3 (s), 138.0 (d), 132.4 (d), 129.9 (d), 129.0 (d), 126.1 (d), 79.9 (d), 76.0 (d), 74.0 (d), 63.7 (t), 41.9 (d), 41.6 (t), 26.1 (q, 3x), 26.0 (q, 3x), 25.2 (q), 18.3 (s, 2x), 14.3 (q), 13.4 (q), -3.8 (q), -4.0 (q, 2x), -4.7 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{28}H_{52}IO_2Si_2$ ($[M+H-OH]^+$), 603.2545; found, 603.2531. **IR** (NaCl): ν 3500 – 3100 (br, O-H), 2953 (m, C-H), 2931 (m, C-H), 2856 (w, C-H) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 231 nm.

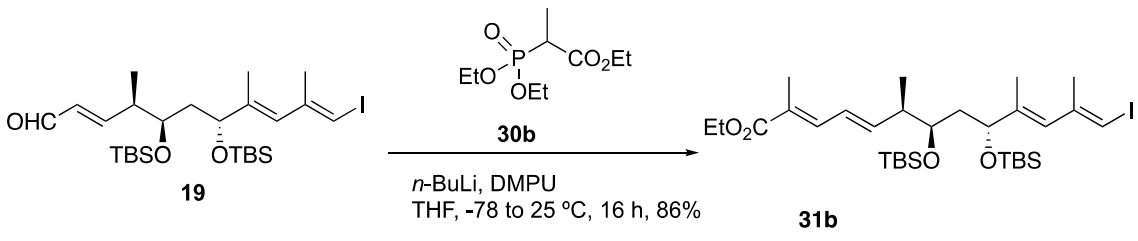


32a **33a**

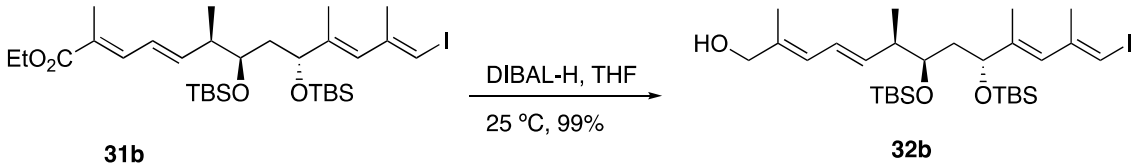
(2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-Butyldimethylsilyloxy)-6,10,12-trimethyltrideca-2,4,10,12-tetraenal 33a. General procedure for the oxidation of allylic alcohols. To a cooled (0 °C) solution of (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-6,10,12-trimethyltrideca-2,4,10,12-tetraen-1-ol **32a** (0.07 g, 0.13 mmol) in CH_2Cl_2 (1.2 mL), Na_2CO_3 (0.23 g, 2.32 mmol) and MnO_2 (0.22 g, 2.32 mmol) were added. After stirring the reaction mixture for 18h at 25 °C, the suspension was filtered through a pad of Celite® washing with CH_2Cl_2. The solvent was concentrated under vacuum to afford 0.067 g (92%) of a yellow oil, which was identified as (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-6,10,12-trimethyltrideca-2,4,10,12-tetraenal **33a**, and was used in the next step without further purification.



(2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-Butyldimethylsilyloxy)-6,10,12,14,15-pentamethylhexadeca-2,4,10,12,14-pentaenal 34a. General procedure for the Suzuki-Miyaura cross-coupling. To a solution of $Pd(PPh_3)_4$ (0.002 g, 0.002 mmol) in THF (5 mL), a solution of (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-6,10,12-trimethyltrideca-2,4,10,12-tetraenal **33a** (0.07 g, 0.11 mmol) in THF (4 mL) was added and the resulting mixture was stirred at room temperature for 15 min. Then, a solution of 4,4,5,5-tetramethyl-2-(3-methylbut-2-en-2-yl)-1,3,2-dioxaborolane **28** (0.023 g, 0.12 mmol) in THF (4 mL) and a 10% aqueous solution of TlOH (1 mL, 0.45 mmol) were added, and the resulting mixture was stirred for 3 h. The reaction mixture was diluted with Et_2O (10 mL) and washed with $NaHCO_3$ (20 mL). The aqueous layer was extracted with Et_2O (3x). The combined organic layers were dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (C18-silica gel, 80:20 acetonitrile/H_2O), to afford 0.06 g (92%) of a colorless oil, which was identified as (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-6,10,12,14,15-pentamethylhexadeca-2,4,10,12,14-pentaenal **34a**. **Molecular formula:** $C_{33}H_{60}O_3Si_2$. **MW:** 561.01 g/mol. **$[\alpha]_D^{22}$** -6.77° (*c* 0.86, MeOH). **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 9.54 (d, *J* = 8.0 Hz, 1H, CHO), 7.08 (dd, *J* = 15.3, 10.0 Hz, 1H, H_3), 6.40 – 6.20 (m, 2H, H_4 + H_5), 6.08 (dd, *J* = 15.3, 8.0 Hz, 1H, H_2), 5.81 (s, 1H, H_{11}), 5.75 (s, 1H, H_{13}), 4.06 (dd, *J* = 8.1, 4.3 Hz, 1H, H_9), 3.80 – 3.72 (m, 1H, H_7), 2.57 – 2.49 (m, 1H, H_6), 1.77 – 1.74 (m, 1H, H_{8A}), 1.74 (s, 3H, CH_3), 1.72 (s, 3H, CH_3), 1.70 (s, 3H, CH_3), 1.63 (s, 3H, CH_3), 1.62 (s, 3H, CH_3), 1.48 – 1.41 (m, 1H, H_{8B}), 1.05 (d, *J* = 6.8 Hz, 3H, CH_3), 0.90 (s, 9H, $SiC(CH_3)_3$), 0.89 (s, 9H, $SiC(CH_3)_3$), 0.09 (s, 3H, $SiCH_3$), 0.07 (s, 3H, $SiCH_3$), 0.04 (s, 3H, CH_3), 0.00 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, C_6D_6): δ 192.5 (d), 151.2 (d), 148.0 (d), 138.1 (s), 133.2 (d), 132.6 (s), 131.1 (d), 130.5 (d), 128.7 (d), 127.9 (s), 126.8 (s), 77.2 (d), 74.1 (d), 42.8 (d), 42.0 (t), 26.2 (q, 3x), 26.1 (q, 3x), 22.2 (q), 20.1 (q), 18.9 (q), 18.7 (q), 18.5 (s), 18.4 (s), 13.8 (q), 13.4 (q), -3.8 (q, 2x), -3.9 (q), -4.6 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{33}H_{61}O_3Si_2$ ($[M+H-OH]^+$), 561.4154; found, 561.4157. **IR** (NaCl): ν 2930 (s, C-H), 2858 (s, C-H), 1687 (s, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 271 nm.



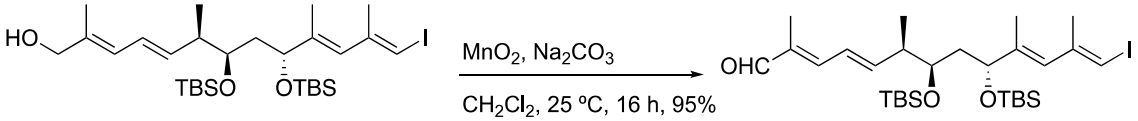
Ethyl (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-Butyldimethylsilyloxy)-13-iodo-2,6,10,12-tetramethyltrideca-2,4,10,12-tetraenoate 31b. Following the general procedure for the Horner-Wadsworth-Emmons olefination, the reaction of a solution of ethyl 2-(diethoxyphosphoryl)propanoate **30b** (0.13 mL, 0.61 mmol) in THF (1.8 mL), *n*-BuLi (0.37 mL, 1.55 M, 0.57 mmol) and DMPU (0.41 mL, 3.37 mmol), followed by the addition of a solution of (2*E*,4*R*,5*R*,7*R*,8*E*,10*E*)-5,7-bis(*tert*-butyldimethylsilyloxy)-11-iodo-4,8,10-trimethylundeca-2,8,10-trienal **19** (0.2 g, 0.34 mmol) in THF (1.5 mL) afforded, after purification by flash-column chromatography (silica gel, 80:20 hexane/CH_2Cl_2), 0.2 g (86%) of a colorless oil, which was identified as ethyl (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-2,6,10,12-tetramethyl trideca-2,4,10,12-tetraenoate **31b**. **Molecular formula:** $C_{31}H_{57}IO_4Si_2$. **MW:** 676.87 g/mol. **$[\alpha]_D^{21}$** 7.16° (*c* 0.39, CH_2Cl_2). **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 7.15 (d, *J* = 11.2 Hz, 1H, H_3), 6.30 (dd, *J* = 15.3, 11.2 Hz, 1H, H_4), 6.11 (dd, *J* = 15.3, 6.8 Hz, 1H, H_5), 6.02 (s, 1H, H_{13}), 5.78 (s, 1H, H_{11}), 4.21 (q, *J* = 7.1 Hz, 2H, $O\underline{CH_2}CH_3$), 4.06 (dd, *J* = 8.1, 3.4 Hz, 1H, H_9), 3.72 (app. dt, *J* = 7.0, 3.9 Hz, 1H, H_7), 2.55 – 2.42 (m, 1H, H_6), 1.92 (s, 6H, 2xCH_3), 1.72 – 1.64 (m, 1H, H_{8A}), 1.66 (s, 3H, CH_3), 1.45 - 1.35 (m, 1H, H_{8B}), 1.30 (t, *J* = 7.1 Hz, 3H, $O\underline{CH_2}CH_3$), 1.03 (d, *J* = 6.9 Hz, 3H, CH_3), 0.89 (s, 9H, $SiC(CH_3)_3$), 0.88 (s, 9H, $SiC(CH_3)_3$), 0.07 (s, 3H, $SiCH_3$), 0.06 (s, 3H, $SiCH_3$), 0.05 (s, 3H, $SiCH_3$), -0.03 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 168.8 (s), 145.2 (d), 144.5 (s), 141.2 (s), 138.7 (d), 126.1 (d), 125.7 (d), 125.6 (s), 79.9 (d), 76.0 (d), 73.9 (d), 60.6 (t), 42.8 (d), 41.6 (t), 26.1 (q, 3x), 26.0 (q, 3x), 25.2 (q), 18.3 (s, 2x), 14.5 (q), 14.2 (q), 13.4 (q), 12.7 (q), -3.8 (q), -4.0 (q), -4.0 (q), -4.7 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{31}H_{58}IO_4Si_2$ ($[M+H]^+$), 677.2913; found, 677.2927. **IR** (NaCl): ν 2954 (m, C-H), 2930 (m, C-H), 2857 (w, C-H), 1707 (s, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 262 nm.



31b **32b**

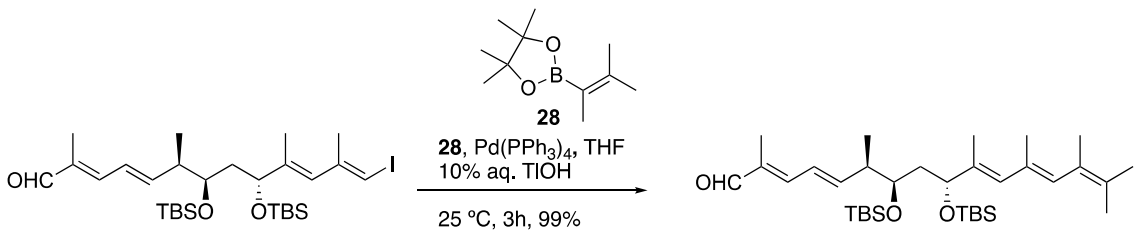
(2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-Butyldimethylsilyloxy)-13-iodo-2,6,10,12-tetramethyltrideca-2,4,10,12-tetraen-1-ol 32b. Following the general procedure for the reduction of esters with DIBAL-H, the reaction of ethyl (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-2,6,10,12-tetramethyltrideca-2,4,10,12-tetraenoate **31b** (0.2 g, 0.29 mmol) and DIBAL-H (0.73 mL, 1 M, 0.73 mmol) in THF (3.2 mL) afforded, after purification by flash-column chromatography (silica gel, 90:10 hexane/EtOAc), 0.2 g (99%) of a colorless oil, which was identified as (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-2,6,10,12-tetramethyltrideca-2,4,10,12-tetraen-1-ol **32b**. **Molecular formula:** $C_{29}H_{55}IO_3Si_2$. **MW:** 634.86 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 6.21 (ddd, *J* = 15.2, 10.6, 1.2 Hz, 1H, H_4), 6.02 (d, *J* = 10.6 Hz, 1H, H_3), 6.02 – 6.00 (m, 1H, H_{13}), 5.78 (s, 1H, H_{11}), 5.73 (dd, *J* = 15.2, 7.0 Hz, 1H, H_5), 4.08 – 4.04 (m, 3H, H_1 + H_9), 3.68 (app. dt, *J* = 7.7, 4.4 Hz, 1H, H_7), 2.45 – 2.37 (m, 1H, H_6), 1.92 (d, *J* = 0.7 Hz, 3H, CH_3), 1.77 (s, 3H, CH_3), 1.71 – 1.65 (m, 1H, H_{8A}), 1.67 (d, *J* = 1.3 Hz, 3H, CH_3), 1.42 (ddd, *J* = 14.1, 6.3, 4.1 Hz, 1H,

H_{8B}), 0.99 (d, *J* = 6.9 Hz, 3H, CH_3), 0.89 (s, 9H, $SiC(CH_3)_3$), 0.89 (s, 9H, $SiC(CH_3)_3$), 0.07 (s, 6H, $SiCH_3$), 0.06 (s, 3H, $SiCH_3$), 0.04 (s, 3H, $SiCH_3$), -0.03 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 144.5 (s), 141.3 (s), 137.5 (d), 135.1 (s), 126.1 (d), 125.7 (d), 125.5 (d), 79.8 (d), 76.0 (d), 74.1 (d), 68.9 (t), 42.3 (d), 41.6 (t), 26.1 (q, 3x), 26.0 (q, 3x), 25.2 (q), 18.3 (s, 2x), 14.5 (q), 14.2 (q), 13.4 (q), -3.8 (q), -4.0 (q, 2x), -4.7 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{29}H_{54}IO_2Si_2$ ($[M+H-OH]^+$), 617.2702; found, 617.2693. **IR** (NaCl): ν 3500 – 3100 (br, O-H), 2954 (s, C-H), 2930 (s, C-H), 2857 (m, C-H), 1253 (m) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 239 nm.



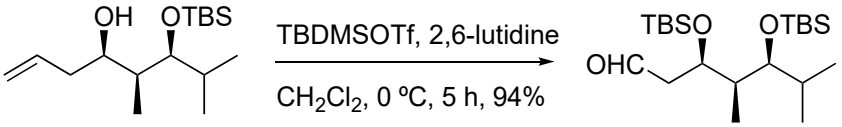
32b **33b**

(2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-Butyldimethylsilyloxy)-13-iodo-2,6,10,12-tetramethyltrideca-2,4,10,12-tetraenal 33b. Following the general procedure for the oxidation of allylic alcohols, the reaction of (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-2,6,10,12-tetramethyltrideca-2,4,10,12-tetraen-1-ol **32b** (0.07 g, 0.10 mmol), MnO_2 (0.2 g, 1.98 mmol) and Na_2CO_3 (0.21 g, 1.98 mmol) in CH_2Cl_2 (0.9 mL), afforded 0.067 g (95%) of a colorless oil, identified as (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-2,6,10,12-tetramethyl trideca-2,4,10,12-tetraenal **33b**, which was used in the next step without further purification. **Molecular formula:** $C_{29}H_{53}IO_3Si_2$. **MW:** 632.81 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 9.43 (s, 1H, CHO), 6.82 (d, *J* = 10.9 Hz, 1H, H_3), 6.49 (ddd, *J* = 15.3, 11.0, 1.2 Hz, 1H, H_4), 6.28 (dd, *J* = 15.3, 6.8 Hz, 1H, H_5), 6.03 – 6.02 (m, 1H, H_{13}), 5.79 (s, 1H, H_{11}), 4.07 (dd, *J* = 8.3, 3.7 Hz, 1H, H_9), 3.76 (app. dt, *J* = 7.5, 4.3 Hz, 1H, H_7), 2.61 – 2.48 (m, 1H, H_6), 1.92 (d, *J* = 0.7 Hz, 3H, CH_3), 1.83 (s, 3H, CH_3), 1.75 – 1.68 (m, 1H, H_{8A}), 1.68 (d, *J* = 1.3 Hz, 3H, CH_3), 1.42 (ddd, *J* = 14.1, 6.8, 3.8 Hz, 1H, H_{8B}), 1.06 (d, *J* = 6.9 Hz, 3H, CH_3), 0.90 (s, 9H, $SiC(CH_3)_3$), 0.89 (s, 9H, $SiC(CH_3)_3$), 0.08 (s, 3H, $SiCH_3$), 0.06 (s, 3H, $SiCH_3$), 0.05 (s, 3H, $SiCH_3$), -0.02 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 195.3 (d), 149.4 (d), 148.1 (d), 144.4 (s), 141.1 (s), 136.5 (s), 126.2 (d), 125.5 (d), 80.1 (d), 76.0 (d), 73.7 (d), 43.0 (d), 41.7 (t), 26.0 (q, 3x), 26.0 (q, 3x), 25.1 (q), 18.3 (s, 2x), 13.9 (q), 13.4 (q), 9.6 (q), -3.9 (q), -4.0 (q, 2x), -4.7 (q) ppm. **MS** (ESI^+): *m/z* 633 ($[M+H]^+$, 22), 501 (100), 373 (22). **HRMS** (ESI^+): Calcd. for $C_{29}H_{54}IO_3Si_2$ ($[M+H]^+$), 633.2651; found, 633.2643. **IR** (NaCl): ν 2954 (s, C-H), 2930 (s, C-H), 2857 (m, C-H), 1682 (s, C=O), 1635 (m) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 277 nm.



33b **34b**

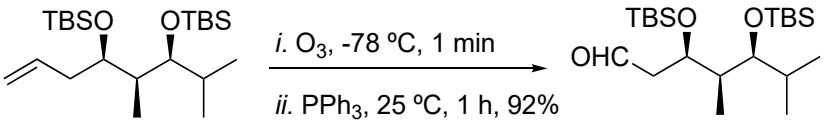
(2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-Butyldimethylsilyloxy)-2,6,10,12,14,15-hexamethylhexadeca-2,4,10,12,14-pentaenal 34b. Following the general procedure for the Suzuki-Miyaura cross-coupling, the reaction of $Pd(PPh_3)_4$ (0.002 g, 0.002 mmol) in THF (5 mL), a solution of (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-13-iodo-2,6,10,12-tetramethyltrideca-2,4,10,12-tetraenal **33b** (0.062 g, 0.1 mmol) in THF (4 mL), a solution of 4,4,5,5-tetramethyl-2-(3-methylbut-2-en-2-yl)-1,3,2-dioxaborolane **28** (0.023 g, 0.12 mmol) in THF (4 mL) and a 10% aqueous solution of TlOH (0.9 mL, 0.39 mmol) afforded, after purification by flash-column chromatography (silica gel, 97:3 hexane/Et_3N), 0.06 g (99%) of a colorless oil, which was identified as (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-2,6,10,12,14,15-hexamethylhexadeca-2,4,10,12,14-pentaenal **34b**. **Molecular formula:** $C_{34}H_{62}O_3Si_2$. **MW:** 575.04 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 9.42 (s, 1H, CHO), 6.82 (d, *J* = 10.8 Hz, 1H, H_3), 6.49 (ddd, *J* = 15.3, 11.0, 1.2 Hz, 1H, H_4), 6.29 (dd, *J* = 15.3, 7.0 Hz, 1H, H_5), 5.82 (s, 1H, H_{11}), 5.75 (s, 1H, H_{13}), 4.07 (dd, *J* = 8.0, 4.3 Hz, 1H, H_9), 3.76 (ddd, *J* = 6.4, 5.0, 3.3 Hz, 1H, H_7), 2.59 – 2.52 (m, 1H, H_6), 1.82 (d, *J* = 1.0 Hz, 3H, CH_3), 1.78 – 1.73 (m, 1H, H_{8A}), 1.74 (d, *J* = 1.3 Hz, 3H, CH_3), 1.72 (s, 3H, CH_3), 1.70 (s, 3H, CH_3), 1.64 (d, *J* = 1.2 Hz, 3H, CH_3), 1.61 (s, 3H, CH_3), 1.47 (ddd, *J* = 14.1, 6.5, 4.5 Hz, 1H, H_{8B}), 1.07 (d, *J* = 6.9 Hz, 3H, CH_3), 0.91 (s, 9H, $SiC(CH_3)_3$), 0.90 (s, 9H, $SiC(CH_3)_3$), 0.09 (s, 3H, $SiCH_3$), 0.07 (s, 3H, $SiCH_3$), 0.04 (s, 3H, $SiCH_3$), 0.00 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 195.3 (d), 149.6 (d), 148.8 (d), 137.8 (s), 136.3 (s), 132.4 (d), 132.3 (s), 130.0 (d), 128.0 (s), 126.2 (s), 125.4 (d), 76.8 (d), 73.7 (d), 42.9 (d), 41.6 (t), 26.1 (q, 6x), 22.2 (q), 20.3 (q), 18.8 (q), 18.6 (q), 18.3 (s), 18.2 (s), 13.7 (q), 13.2 (q), 9.5 (q), -4.0 (q, 2x), -4.1 (q), -4.7 (q) ppm. **MS** (ESI^+): *m/z* 575 ($[M+H]^+$, 57), 443 (100), 311 (18). **HRMS** (ESI^+): Calcd. for $C_{34}H_{63}O_3Si_2$ ($[M+H]^+$), 575.4310; found, 575.4309. **IR** (NaCl): ν 2954 (s, C-H), 2930 (s, C-H), 2857 (m, C-H), 1684 (C=O), 1635 (m) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 277 nm.



44 **44A**

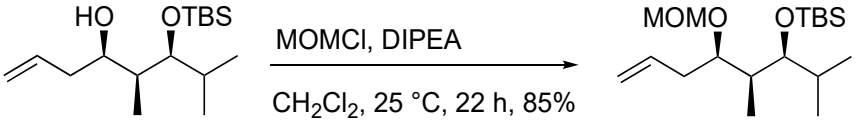
(4*R*,5*S*,6*S*)-4,6-Bis[(*tert*-butyldimethylsilyl)oxy]-5,7-dimethyloct-1-ene 44A. General procedure for the protection of alcohols as *tert*-butyldimethylsilyl ethers. To a cooled (0 ºC) solution of (4*R*,5*S*,6*S*)-6-[(*tert*-butyldimethylsilyl)oxy]-5,7-dimethyloct-1-en-4-ol **44** (0.11 g, 0.37 mmol), in CH_2Cl_2 (3.3 mL), 2,6-lutidine (0.07 mL, 0.62 mmol) and TBDMSOTf (0.13 mL, 0.55 mmol) were added. After stirring for 5.5h at the same temperature, the reaction mixture was quenched with a saturated aqueous solution of NH_4Cl (3.0 mL) and the aqueous layer was extracted with CH_2Cl_2 (3x). The combined organic layers were washed with brine, dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, hexane), to afford 0.14 g (94%) of a colorless oil, which was identified as (4*R*,5*S*,6*S*)-4,6-bis[(*tert*-butyldimethylsilyl)oxy]-5,7-dimethyloct-1-ene **44A**. **Molecular formula:** $C_{22}H_{48}O_2Si_2$. **MW:** 400.79 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 5.86 – 5.70 (m, 1H, H_2), 5.08 –

4.99 (m, 2H, 2H1), 3.68 (app. q, *J* = 6.0 Hz, 1H, H4), 3.46 (app. t, *J* = 4.7 Hz, 1H, H6), 2.36 – 2.21 (m, 2H, 2H3), 1.84 – 1.74 (m, 1H, H7), 1.72 – 1.63 (m, 1H, H5), 0.92 (s, 9H, ^{t}Bu), 0.90 (s, 9H, ^{t}Bu), 0.89 (s, 3H, CH3), 0.86 (d, *J* = 1.2 Hz, 3H, CH3), 0.83 (d, *J* = 6.8 Hz, 3H, CH3), 0.06 (s, 6H, 2xSiCH3), 0.05 (s, 3H, SiCH3), 0.04 (s, 3H, SiCH3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 135.1 (d), 117.0 (t), 77.1 (d), 73.0 (d), 40.0 (d), 39.8 (t), 32.0 (d), 26.4 (q, 3x), 26.1 (q, 3x), 20.4 (q), 18.8 (s), 18.3 (s), 17.6 (q), 10.6 (q), -3.2 (q), -3.3 (q), -3.8 (q), -4.3 (q) ppm. **MS** (ESI^+): *m/z* 401 ($[M+H]^+$, 54), 269 (100). **HRMS** (ESI^+): Calcd. for $C_{22}H_{49}O_2Si_2$ ($[M+H]^+$), 401.3266; found, 401.3260. **IR** (NaCl): ν 2956 (m, C-H), 2932 (m, C-H), 2858 (w, C-H) cm^{-1}.



44A **16**

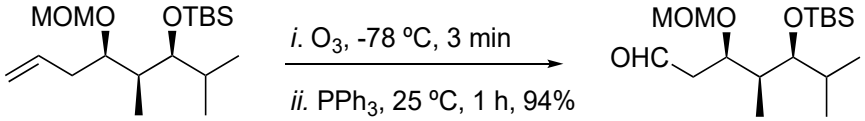
(3*R*,4*S*,5*S*)-3,5-Bis[(*tert*-butyldimethylsilyl)oxy]-4,6-dimethylheptanal 16. General procedure for the ozonolysis of olefins. To a cooled (-78 °C) solution of (4*R*,5*S*,7*S*)-4,6-bis[(*tert*-butyldimethylsilyl)oxy]-5,7-dimethyloct-1-ene **44A** (0.09 g, 0.23 mmol) in CH_2Cl_2 (10.0 mL), O_3 was bubbled in an ozone generator reactor for 3 min (I = 0.5 A, flow = 1 mL/min), until a blue ozone color in the CH_2Cl_2 solution was observed. The reaction mixture was quenched with PPh_3 (0.09 g, 0.35 mmol) and stirred at 25 °C for 1 h. The solvent was evaporated and the residue was purified by flash-column chromatography (C18-silica gel, acetonitrile) to afford 0.07 g (92%) of a colorless oil, which was identified as (3*R*,4*S*,5*S*)-3,5-bis[(*tert*-butyldimethylsilyl)oxy]-4,6-dimethylheptanal **16**. **Molecular formula:** $C_{21}H_{46}O_3Si_2$. **MW:** 402.77 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 9.82 (dd, *J* = 2.8, 2.1 Hz, 1H, H1), 4.12 (app. q, *J* = 5.5 Hz, 1H, H3), 3.54 (app. t, *J* = 4.2 Hz, 1H, H5), 2.68 – 2.55 (m, 2H, 2H2), 1.88 – 1.79 (m, 1H, H6), 1.79 – 1.70 (m, 1H, H4), 0.93 – 0.90 (m, 6H, 2xCH3), 0.91 (s, 9H, ^{t}Bu), 0.88 (s, 9H, ^{t}Bu), 0.86 (d, *J* = 6.8 Hz, 3H, CH3), 0.07 (s, 3H, SiCH3), 0.06 (s, 3H, SiCH3), 0.05 (s, 3H, SiCH3), 0.04 (s, 3H, SiCH3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 202.5 (d), 76.3 (d), 70.1 (d), 49.2 (t), 41.7 (d), 32.7 (d), 26.4 (q, 3x), 26.0 (q, 3x), 19.7 (q), 18.7 (s), 18.2 (s), 18.1 (q), 11.6 (q), -3.3 (q), -3.4 (q), -4.2 (q), -4.3 (q) ppm.



44 **48**

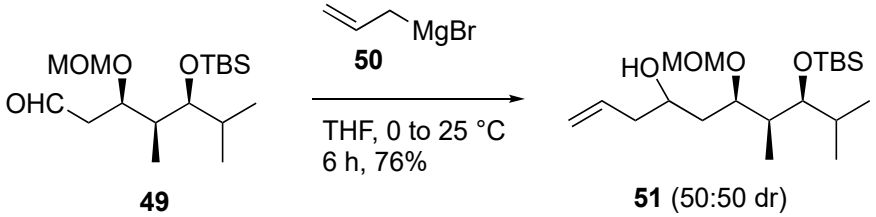
(4*R*,5*S*,6*S*)-6-[(*tert*-Butyldimethylsilyl)oxy]-4-methoxymethoxy-5,7-dimethyloct-1-ene 48. To a cooled (0 °C) solution of (4*R*,5*S*,6*S*)-6-[(*tert*-butyldimethylsilyl)oxy]-5,7-dimethyloct-1-en-4-ol **44** (0.028 g, 0.1 mmol) in CH_2Cl_2 (0.5 mL), DIPEA (0.06 mL, 0.34 mmol) and MOMCl (0.022 mL, 0.29 mmol) were added. After stirring for 14 h at 25 °C, the reaction mixture was cooled down to 0 °C and a saturated aqueous solution of NH_4Cl (3.0 mL) was added. The aqueous layer was extracted with Et_2O (3x). The combined organic layers were washed with brine, dried (Na_2SO_4) and the solvent was

evaporated. The residue was purified by flash-column chromatography (silica gel, 95:5 hexane/EtOAc) to afford 0.027 g (85%) of a colorless oil, which was identified as (4*R*,5*S*,6*S*)-6-[(*tert*-butyldimethylsilyl)oxy]-4-methoxymethoxy-5,7-dimethyloct-1-ene **48**. **Molecular formula:** $C_{18}H_{38}O_3Si$. **MW:** 330.58 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 5.88 – 5.71 (m, 1H, H_2), 5.14 – 4.97 (m, 2H, H_{1A} + H_{1B}), 4.68 (d, *J* = 6.9 Hz, 1H, -O$\underline{CH}_{2A}$O-), 4.60 (d, *J* = 6.9 Hz, 1H, -OCH$_{2B}$O-), 3.56 (app. q, *J* = 5.6 Hz, 1H, H_4), 3.50 (app. t, *J* = 4.4 Hz, 1H, H_6), 3.38 (s, 3H, OCH_3), 2.42 – 2.30 (m, 2H, $2H_3$), 1.88 – 1.72 (m, 2H, H_7 + H_5), 0.93 (d, *J* = 7.0 Hz, 3H, CH_3), 0.91 (s, 9H, ^{t}Bu), 0.89 (d, *J* = 7.3 Hz, 3H, CH_3), 0.84 (d, *J* = 6.8 Hz, 3H, CH_3), 0.06 (s, 6H, 2xSiCH_3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 135.1 (d), 117.3 (t), 96.1 (t), 79.0 (d), 77.1 (d), 56.0 (q), 38.8 (d), 36.8 (t), 32.4 (d), 26.4 (q, 3x), 19.9 (q), 18.7 (s), 17.8 (q), 10.9 (q), -3.35 (q, 2x) ppm. **HRMS** (ESI^+): Calcd. for $C_{18}H_{38}NaO_3Si$ ($[M+Na]^+$), 353.24824; found, 353.2486. **IR** (NaCl): ν 2955 (m, C-H), 2932 (m, C-H), 2858 (w, C-H), 1468 (w) cm^{-1}.



48 **49**

(3*R*,4*S*,5*S*)-5-[(*tert*-Butyldimethylsilyl)oxy]-3-(methoxymethoxy)-4,6-dimethylheptanal 49. Following the general procedure for the ozonolysis of olefins, the reaction of (4*R*,5*S*,6*S*)-[(*tert*-butyldimethylsilyl)oxy]-4-methoxymethoxy-5,7-dimethyloct-1-ene **48** (0.25 g, 0.76 mmol) in CH_2Cl_2 (7.0 mL), bubbled with O_3 and followed by the addition of PPh_3 (0.3 g, 1.14 mmol) afforded, after purification by flash-column chromatography (silica gel, 70:30 hexane/EtOAc), 0.24 g (94%) of a colorless oil, which was identified as (3*R*,4*S*,5*S*)-5-[(*tert*-butyldimethylsilyl)oxy]-3-(methoxymethoxy)-4,6-dimethylheptanal **49**. **Molecular formula:** $C_{17}H_{36}O_4Si$. **MW:** 332.56 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 9.80 (dd, *J* = 2.7, 1.9 Hz, 1H, H_1), 4.66 (d, *J* = 7.0 Hz, 1H, -O$\underline{CH}_{2A}$O-), 4.62 (d, *J* = 7.0 Hz, 1H, -OCH$_{2B}$O-), 4.03 (app. dt, *J* = 6.6, 5.2 Hz, 1H, H_3), 3.54 (app. t, *J* = 4.1 Hz, 1H, H_5), 3.33 (s, 3H, OCH_3), 2.69 – 2.62 (m, 2H, $2H_2$), 1.91 – 1.78 (m, 2H, H_4 + H_6), 0.95 (d, *J* = 7.0 Hz, 3H, CH_3), 0.91 (s, 9H, ^{t}Bu), 0.90 (d, *J* = 6.7 Hz, 3H, CH_3), 0.86 (d, *J* = 6.8 Hz, 3H, CH_3), 0.07 (s, 6H, 2xSiCH_3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 201.8 (d), 96.6 (t), 76.5 (d), 75.8 (d), 56.0 (q), 47.2 (t), 39.9 (d), 33.0 (d), 26.3 (q, 3x), 19.3 (q), 18.6 (s), 18.1 (q), 11.7 (q), -3.3 (q), -3.6 (q). **MS** (ESI^+): *m/z* 355 ($[M+H]^+$, 100), 317 (15), 301 (30), 287 (41), 279 (48), 269 (32), 255 (27). **HRMS** (ESI^+): Calcd. for $C_{17}H_{36}NaO_4Si$ ($[M+Na]^+$), 355.2275; found, 355.2275. **IR** (NaCl): ν 2956 (m, C-H), 2933 (m, C-H), 2891 (m, C-H), 1727 (s, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 223 nm.

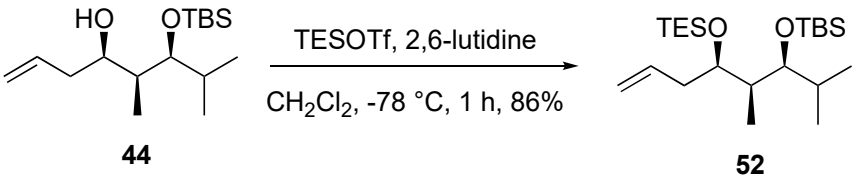


49 **51** (50:50 dr)

(4*S*,6*R*,7*S*,8*S*)-8-[(*tert*-Butyldimethylsilyl)oxy]-6-(methoxymethoxy)-7,9-dimethyldec-1-en-4-ol and (4*R*,6*R*,7*S*,8*S*)-8-[(*tert*-butyldimethylsilyl)oxy]-6-(methoxymethoxy)-7,9-dimethyldec-1-en-4-ol 51. To a cooled (0 °C) solution of (3*R*,4*S*,5*S*)-5-[(*tert*-butyldimethylsilyl)oxy]-3-(methoxymethoxy)-4,6-dimethylheptanal **49** (0.11 g, 0.33 mmol) in THF (1.0 mL), allylmagnesium bromide **50** (0.5 mL, 2 M in THF, 1.0 mmol) was slowly added. After stirring the resulting suspension at 25 °C for 6 h, the reaction mixture was quenched with H_2O (1 mL) and the solvent was evaporated under reduced pressure. The aqueous layer was diluted with EtOAc (2 mL) and a saturated aqueous solution of $NaHCO_3$ was added. The aqueous layer was extracted with EtOAc (3x), the combined organic layers were washed with $NaHCO_3$ (1x), brine and dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 90:10 hexane/EtOAc) to afford 0.083 g (70%) of a colorless oil, which was identified as a ca. 1:1 mixture of diastereomers **51**, which were separated by flash-column chromatography.

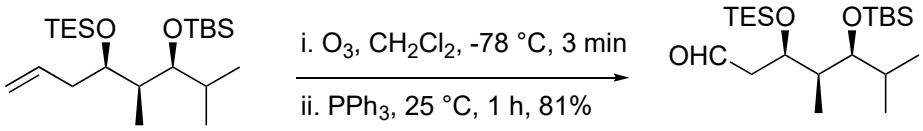
Diastereomer 1. Molecular formula: $C_{20}H_{42}O_4Si$. **MW:** 374.64 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 5.94 – 5.76 (m, 1H, H_2), 5.20 – 5.02 (m, 2H, $2H_1$), 4.64 (s, 2H, -O$\underline{CH_2}$O-), 3.90 (app. p, *J* = 6.8, 6.3 Hz, 1H, H_4), 3.70 (app. q, *J* = 6.4 Hz, 1H, H_6), 3.50 (dd, *J* = 4.5, 3.2 Hz, 1H, H_8), 3.40 (s, 3H, OCH_3), 2.29 – 2.20 (m, 2H, $2H_3$), 1.89 – 1.77 (m, 2H, H_7 + H_9), 1.64 – 1.59 (m, 3H, $2H_5$ + OH), 0.92 (d, *J* = 7.1 Hz, 3H, CH_3), 0.90 (s, 9H, ^{t}Bu), 0.88 (d, *J* = 6.9 Hz, 3H, CH_3), 0.85 (d, *J* = 6.8 Hz, 3H, CH_3), 0.06 (s, 3H, $SiCH_3$), 0.05 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 135.3 (d), 117.5 (t), 97.3 (t), 78.9 (d), 76.2 (d), 67.3 (d), 56.2 (q), 42.2 (t), 39.3 (d), 39.0 (t), 33.5 (d), 26.3 (q, 3x), 19.0 (q), 18.7 (q + s), 11.8 (q), -3.4 (q), -3.6 (q) ppm. **MS** (ESI^+): *m/z* 397 ($[M+Na]^+$, 100), 343 (63). **HRMS** (ESI^+): Calcd. for $C_{20}H_{42}NaO_4Si$ ($[M+Na]^+$), 397.2745; found, 397.2738. **IR** (NaCl): ν 3600 – 3100 (br, O-H), 2955 (m, C-H), 2856 (m, C-H), 1467 (m) cm^{-1}.

Diastereomer 2. Molecular formula: $C_{20}H_{42}O_4Si$. **MW:** 374.64 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 5.91 – 5.77 (m, 1H, H_2), 5.17 – 5.06 (m, 2H, $2H_1$), 4.68 (d, *J* = 6.6 Hz, 1H, -O$\underline{CH_{2A}}$O-), 4.62 (d, *J* = 6.6 Hz, 1H, -O$\underline{CH_{2B}}$O-), 3.79 (app. dtd, *J* = 9.0, 6.3, 3.0 Hz, 1H, H_4), 3.71 (app. dt, *J* = 8.5, 4.4 Hz, 1H, H_6), 3.62 (app. t, *J* = 3.8 Hz, 1H, H_8), 3.40 (s, 3H, OCH_3), 2.25 (app. t, *J* = 6.4 Hz, 2H, $2H_3$), 1.91 – 1.81 (m, 2H, H_7 + H_9), 1.76 – 1.59 (m, 3H, $2H_5$ + OH), 0.91 – 0.89 (m, 6H, 2xCH_3), 0.91 (s, 9H, ^{t}Bu), 0.83 (d, *J* = 6.8 Hz, 3H, CH_3), 0.07 (s, 3H, $SiCH_3$), 0.06 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 134.9 (d), 117.7 (t), 95.7 (t), 80.3 (d), 75.7 (d), 70.3 (d), 56.1 (q), 42.3 (t), 38.1 (t), 38.0 (d), 33.2 (d), 26.2 (q, 3x), 18.8 (q), 18.5 (s), 17.5 (q), 11.9 (q), -3.3 (q), -3.8 (q) ppm. **MS** (ESI^+): *m/z* 397 ($[M+Na]^+$, 46), 343 (100), 211 (15). **HRMS** (ESI^+): Calcd. for $C_{20}H_{42}NaO_4Si$ ($[M+Na]^+$), 397.2745; found, 397.2739.



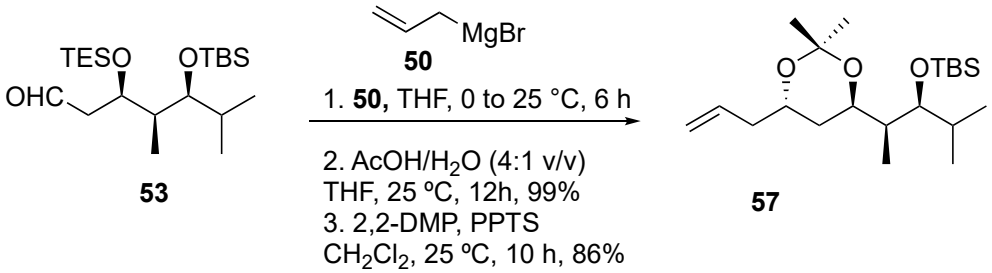
44 **52**

(4*R*,5*S*,6*S*)-6-[(*tert*-Butyldimethylsilyl)oxy)-4-[(triethylsilyl)oxy]-5,7-dimethyloct-1-ene 52. To a cooled (-78 °C) solution of (4*R*,5*S*,6*S*)-6-[(*tert*-butyldimethylsilyl)oxy]-5,7-dimethyloct-1-en-4-ol **44** (0.05 g, 0.19 mmol) in CH_2Cl_2 (1.9 mL), 2,6-lutidine (0.04 mL, 0.47 mmol) and TESOTf (0.06 mL, 0.28 mmol) were added. After stirring for 30 min at the same temperature, the reaction mixture was quenched with H_2O (2.0 mL) and the aqueous layer was extracted with CH_2Cl_2 (3x). The combined organic layers were dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, hexane) to afford 0.07 g (95%) of a colorless oil, which was identified as (4*R*,5*S*,6*S*)-6-[(*tert*-butyldimethylsilyl)oxy)-4-[(triethylsilyl)oxy]-5,7-dimethyloct-1-ene **52**. **Molecular formula:** $C_{22}H_{48}O_2Si_2$. **MW:** 400.79 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 5.87 – 5.72 (m, 1H, H_2), 5.09 – 5.00 (m, 2H, $2H_1$), 3.70 (app. q, J = 5.5 Hz, 1H, H_4), 3.47 (app. t, J = 4.7 Hz, 1H, H_6), 2.37 – 2.21 (m, 2H, $2H_3$), 1.83 – 1.75 (m, 1H, H_7), 1.72 – 1.63 (m, 1H, H_5), 0.96 (t, J = 7.9 Hz, 9H, 3xSi$CH_2\underline{CH_3}$), 0.91 (s, 9H, ^{t}Bu), 0.89 (d, J = 6.9 Hz, 3H, CH_3), 0.88 (d, J = 6.9 Hz, 3H, CH_3), 0.84 (d, J = 6.8 Hz, 3H, CH_3), 0.60 (q, J = 8.1 Hz, 6H, 3xSi$\underline{CH_2}CH_3$), 0.05 (s, 6H, Si($\underline{CH_3}$)$_2$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 135.2 (d), 117.1 (t), 77.2 (d), 73.4 (d), 40.3 (d), 39.9 (t), 32.3 (d), 26.4 (q, 3x), 20.3 (q), 18.7 (s), 17.8 (q), 10.6 (q), 7.2 (q, 3x), 5.5 (t, 3x), -3.2 (q), -3.4 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{22}H_{49}O_2Si_2$ ($[M+H]^+$), 401.3266; found, 401.3263. **IR** (NaCl): ν 2956 (m, C-H), 2933 (m, C-H), 2881 (m, C-H), 1465 (m) cm^{-1}.



52 **53**

(3*R*,4*S*,5*S*)-5-[(*tert*-Butyldimethylsilyl)oxy]-4,6-dimethyl-3-[(triethylsilyl)oxy]heptanal 53. Following the general procedure for the ozonolysis of olefins, the reaction of (4*R*,5*S*,6*S*)-6-[(*tert*-butyldimethylsilyl)oxy)-4-[(triethylsilyl)oxy]-5,7-dimethyloct-1-ene **52** (0.06 g, 0.16 mmol) in CH_2Cl_2 (9.0 mL), bubbled with O_3 and followed by the addition of PPh_3 (0.06 g, 0.24 mmol) afforded, after purification by flash-column chromatography (silica gel-C18, 90:10 CH_3CN/H_2O), 0.05 g (81%) of a colorless oil identified as (3*R*,4*S*,5*S*)-5-[(*tert*-butyldimethylsilyl)oxy]-4,6-dimethyl-3-[(triethylsilyl)oxy]heptanal **53**. **Molecular formula:** $C_{21}H_{46}O_3Si_2$. **MW:** 402.77 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 9.82 (t, J = 2.3 Hz, 1H, H_1), 4.14 (app. q, J = 5.8 Hz, 1H, H_3), 3.53 (app. t, J = 4.1 Hz, 1H, H_5), 2.66 – 2.57 (m, 2H, H_2), 1.88 – 1.77 (m, 1H, H_6), 1.78 – 1.70 (m, 1H, H_4), 0.95 (t, J = 7.9 Hz, 9H, 3xSi$CH_2\underline{CH_3}$), 0.92 (d, J = 7.1 Hz, 3H, CH_3), 0.91 (s, 9H, ^{t}Bu), 0.89 (d, J = 7.1 Hz, 3H, CH_3), 0.86 (d, J = 6.8 Hz, 3H, CH_3), 0.60 (q, J = 7.9 Hz, 6H, 3xSi$\underline{CH_2}CH_3$), 0.06 (s, 3H, $SiCH_3$), 0.05 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 202.5 (d), 76.3 (d), 70.2 (d), 49.3 (t), 41.8 (d), 33.0 (d), 26.3 (q, 3x), 19.5 (q), 18.7 (s), 18.3 (q), 11.6 (q), 7.1 (q, 3x), 5.3 (t, 3x), -3.3 (q), -3.5 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{21}H_{47}O_3Si_2$ ($[M+H]^+$), 403.3058; found, 403.3062. **IR** (NaCl): ν 2957 (m, C-H), 2934 (m, C-H), 2882 (m, C-H), 1710 (s, C=O) cm^{-1}.

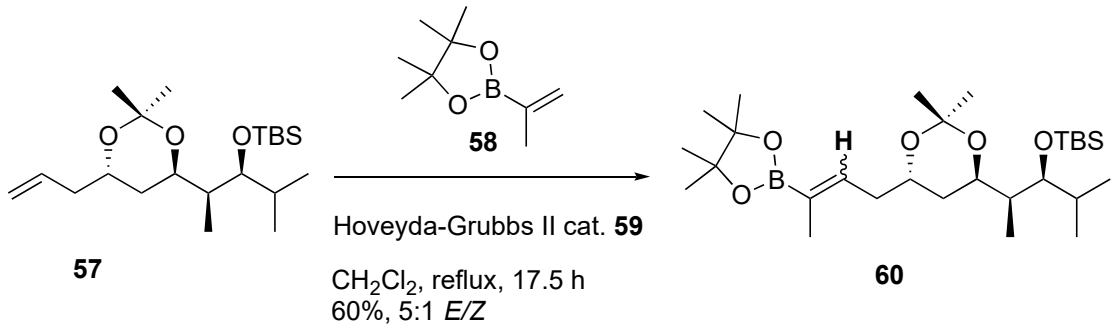


Dioxolane (4*S*,6*R*,7*S*,8*S*)-57. To a cooled (0 °C) solution of (3*R*,4*S*,5*S*)-5-[(*tert*-butyldimethylsilyl)oxy]-4,6-dimethyl-3-[(triethylsilyl)oxy]heptanal **53** (0.05 g, 0.12 mmol) in THF (0.5 mL), allylmagnesium bromide **50** (0.18 mL, 2 M in THF, 0.37 mmol) was slowly added. The resulting suspension was stirred at 25 °C for 6 h. The reaction mixture was quenched with H_2O (1 mL) and the solvent was evaporated under reduced pressure. The aqueous layer was diluted with EtOAc (1 mL) and a saturated aqueous solution of $NaHCO_3$ was added. The aqueous layer was extracted with EtOAc (3x). The combined organic layers were washed with $NaHCO_3$ (1x), brine and dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by column chromatography (silica gel-Diol, 98:2 hexane/EtOAc) to afford 0.04 g (76%) of a colorless oil, which was identified as a ca. 1:1 mixture of diastereomers, which could not be separated by flash-column chromatography.

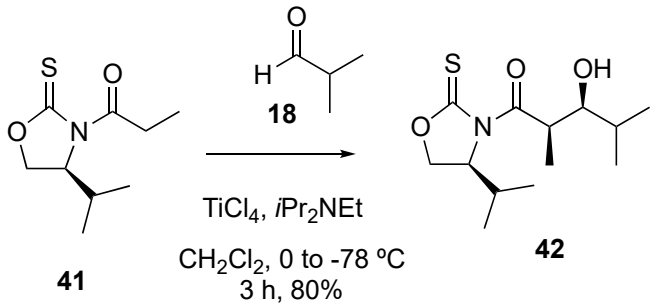
To a solution of the mixture obtained above (0.04 g, 0.1 mmol) in THF (1.0 mL), a 4 : 1 mixture of AcOH and H_2O (0.93 mL : 0.23 mL) was added and the reaction was stirred at 25 °C for 12 h. The reaction mixture was poured into an aqueous saturated solution of $NaHCO_3$ (12.1 mL) and the aqueous layer was extracted with Et_2O (3x). The combined organic layers were dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by column chromatography (silica gel, 90:10 hexane/EtOAc) to afford 0.032 g (99%) of a colorless oil, which was identified as a ca. 1:1 mixture of diastereomers **55** and **56**, which were separated by flash-column chromatography.

To a solution of diol (*S*)-**55** (0.015 g, 0.04 mmol) in CH_2Cl_2 (0.4 mL), 2,2-dimethoxypropane (0.014 mL, 0.11 mmol) and PPTS (0.001, 0.005 mmol) were added and the reaction mixture was stirred for 10 h at 25 °C. A saturated aqueous solution of $NaHCO_3$ was added and the resulting mixture was stirred for 30 min. The aqueous layer was extracted with EtOAc (3x), the combined organic layers were washed with $NaHCO_3$ (2x), brine (2x) and dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 95:5 hexane/EtOAc) to afford 0.014 g (86%) of a colorless oil, which was identified as dioxolane (4*S*,6*R*,7*S*,8*S*)-**57**. **Molecular formula:** $C_{21}H_{42}O_3Si$. **MW:** 370.65 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 5.81 (app. ddt, *J* = 17.1, 10.2, 6.8 Hz, 1H, H_2), 5.15 – 4.97 (m, 2H, $2H_1$), 3.86 – 3.79 (m, 1H, H_4), 3.70 – 3.62 (m, 1H, H_6), 3.37 (app. dd, *J* = 6.0, 2.3 Hz, 1H, H_8), 2.35 – 2.14 (m, 2H, $2H_3$), 1.80 – 1.69 (m, 1H, H_9), 1.67 – 1.58 (m, 3H, H_7 + $2H_5$), 1.33 (s, 3H, CH_3), 1.32 (s, 3H, CH_3), 0.92 (d, *J* = 6.9 Hz, 3H, CH_3), 0.90 (s, 9H, ^{t}Bu), 0.89 (d, *J* = 5.9 Hz, 3H, CH_3), 0.86 (d, *J* = 6.8 Hz, 3H, CH_3), 0.07 (s, 3H, $SiCH_3$), 0.05 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 134.8 (d), 116.9

(t), 100.5 (s), 76.4 (d), 68.7 (d), 66.5 (d), 41.4 (d), 40.4 (t), 37.2 (t), 33.4 (d), 26.3 (q, 3x), 24.9 (q), 24.6 (q), 19.5 (q), 19.4 (q), 18.7 (s), 10.6 (q), -3.6 (q), -3.7 (q) ppm.

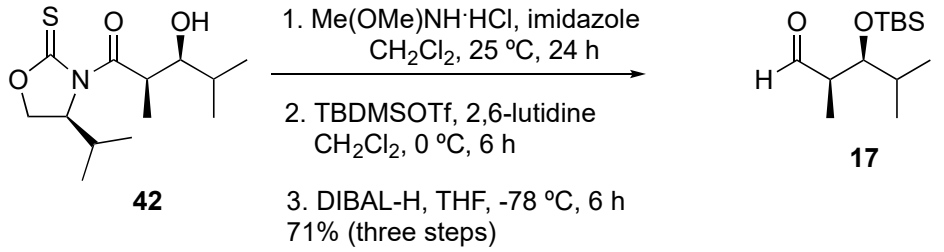


Dioxaborolane (*Z*,4*S*,6*R*,7*S*,8*S*)-60. In a sealed tube, HG-II catalyst **59** (0.001 g, 0.002 mmol) was introduced and dissolved in degassed CH_2Cl_2 (0.2 mL). To this mixture, dioxolane (4*S*,6*R*,7*S*,8*S*)-**57** (0.015 g, 0.04 mmol) and 4,4,5,5-tetramethyl-2-(prop-1-en-2-yl)-1,3,2-dioxaborolane **58** in CH_2Cl_2 (0.2 mL) were added. After stirring the resulting mixture at 50 °C for 18 h, the solvent was removed under reduced pressure. The residue was purified by flash-column chromatography (C18-silica gel, acetonitrile) to afford 0.015 g (60%) of a colorless oil, which was identified as a 5:1 *Z/E* mixture of isomers **60**, which could not be separated by flash-column chromatography. Data for the major isomer: **Molecular formula:** $C_{28}H_{55}BO_5Si$. **MW:** 510.64 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 6.30 (app. td, *J* = 6.7, 1.5 Hz, 1H, H_2), 3.93 – 3.80 (m, 1H, H_4), 3.72 – 3.61 (m, 1H, H_6), 3.37 (app. dd, *J* = 5.9, 2.3 Hz, 1H, H_8), 2.42 – 2.24 (m, 2H, $2H_3$), 1.77 – 1.70 (m, 1H, H_9), 1.69 (app. d, *J* = 1.5 Hz, 3H, C_1-CH_3), 1.67 – 1.59 (m, 3H, H_7 + $2H_5$), 1.34 (s, 3H, CH_3), 1.32 (s, 3H, CH_3), 1.26 (s, 12H, 4xCH_3), 0.92 (d, *J* = 7.0 Hz, 3H, CH_3), 0.91 (s, 9H, ^{t}Bu), 0.88 (d, *J* = 6.5 Hz, 3H, CH_3), 0.86 (d, *J* = 6.2 Hz, 3H, CH_3), 0.07 (s, 3H, $SiCH_3$), 0.05 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 141.3 (d), 100.5 (s), 83.3 (s), 77.2 (s, 2x), 76.4 (d), 68.7 (d), 66.4 (d), 41.3 (d), 37.4 (t), 35.5 (t), 33.4 (d), 26.3 (q, 3x), 25.0 (q, 2x), 24.9 (q, 2x), 24.6 (q, 2x), 19.4 (q, 2x), 18.7 (s), 14.4 (q), 10.6 (q), -3.5 (q), -3.6 (q) ppm.



(2*R*,3*S*)-3-Hydroxy-1-((*S*)-4-isopropyl-2-thioxo-oxazolidin-3-yl)-2,4-dimethylpentan-1-one 42. General procedure for the diastereoselective aldol reaction. To a cooled (0 °C) solution of (*S*)-1-(4-isopropyl-2-thioxo-3-oxazolidinyl)propan-1-one **41** (1.18 g, 5.89 mmol) in CH_2Cl_2 (60.0 mL), $TiCl_4$ (6.48 mL, 1M in CH_2Cl_2, 6.48 mmol) was added dropwise. The reaction mixture was stirred for 5 min and cooled down to -78 °C before the addition of DIPEA (1.1 mL, 6.48 mmol). After stirring for 2h at -78 °C, a solution of isobutyraldehyde **18** (0.25 g, 3.47 mmol) in CH_2Cl_2 (11.0 mL)

was added and the reaction mixture was stirred for 1h at -78 °C. The reaction mixture was quenched with a saturated aqueous solution of NH_4Cl (0.5 mL), diluted with CH_2Cl_2 and allowed to reach room temperature. The aqueous layer was extracted with CH_2Cl_2 (3x), the combined organic layers were washed with brine, dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 70:30 hexane/EtOAc), to afford 0.86 g (80%) of a yellow oil, which was identified as (2*R*,3*S*)-3-hydroxy-1-((*S*)-4-isopropyl-2-thioxo-3-oxazolidinyl)-2,4-dimethylpentan-1-one **42**. **Molecular formula:** $C_{13}H_{23}NO_3S$. **MW:** 273.39 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 5.07 (qd, *J* = 7.0, 2.9 Hz, 1H, H_2), 4.73 (ddd, *J* = 6.4, 5.0, 3.9 Hz, 1H, $H_{4'}$), 4.40 – 4.36 (m, 2H, $2H_{5'}$), 3.65 (dt, *J* = 8.4, 3.0 Hz, 1H, H_3), 2.67 (d, *J* = 3.6 Hz, 1H, OH), 2.38 – 2.26 (m, 1H, $\underline{CH}(CH_3)_2$), 1.77 – 1.65 (m, 1H, H_4), 1.18 (d, *J* = 7.0 Hz, 3H, CH_3), 1.04 (d, *J* = 6.6 Hz, 3H, CH_3), 0.94 (d, *J* = 6.9 Hz, 3H, CH_3), 0.93 (d, *J* = 6.9 Hz, 3H, CH_3), 0.89 (d, *J* = 6.9 Hz, 3H, CH_3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 185.9 (s), 179.0 (s), 76.8 (d), 67.4 (t), 63.4 (d), 39.8 (d), 31.3 (d), 29.1 (d), 19.4 (q), 19.0 (q), 18.5 (q), 15.0 (q), 10.2 (q) ppm. **MS** (ESI^+): *m/z* 296 ($[M+23]^+$, 30), 274 ($[M+1]^+$, 100), 256 (21). **HRMS** (ESI^+): Calcd. for $C_{13}H_{24}NO_3S$ ($[M+H]^+$), 274.1471; found, 274.1474. **IR** (NaCl): ν 3600-3300 (br, O-H), 2963 (w, C-H), 2875 (w, C-H), 1694 (s, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 270 nm.

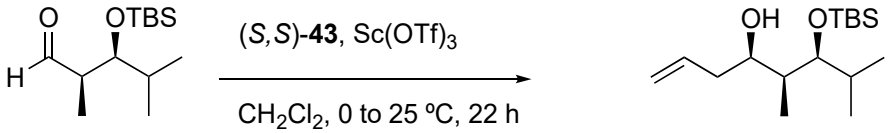


(2*R*,3*S*)-3-((*tert*-Butyldimethylsilyl)oxy)-2,4-dimethylpentanal 17. <u>General procedure for the formation of Weinreb amides</u>. To a solution of (2*R*,3*S*)-3-hydroxy-1-((*S*)-4-isopropyl-2-thioxo-oxazolidin-3-yl)-2,4-dimethylpentan-1-one **42** (0.8 g, 2.94 mmol) in CH_2Cl_2 (17.5 mL), Me(OMe)NH·HCl (0.72 g, 7.34 mmol) and imidazole (1.0 g, 14.7 mmol) were added. The suspension was stirred for 20h at room temperature. The reaction mixture was quenched at 0 °C with a saturated aqueous solution of NH_4Cl (8.0 mL). The aqueous layer was extracted with Et_2O (4x), the combined organic layers were washed with brine, dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 70:30 hexane/EtOAc), to afford a mixture of (3*S*)-3-hydroxy-*N*-methoxy-*N*,2,4-trimethylpentanamide and (*S*)-4-isopropyloxazolidine-2-thione, which could not be separated by flash-column chromatography, and the product was used in the next step without further purification.

<u>General procedure for the protection of alcohols as silyl ethers</u>. To a cooled (0 °C) solution of the product obtained above (0.81 g, 5.03 mmol) (0.37 + 0.45 g of the amide and the thione calculated by ^{1}H-NMR), in CH_2Cl_2 (45 mL), 2,6-lutidine (1 mL, 8.56 mmol) and TBDMSOTf (1.73 mL, 7.55 mmol) were added. After stirring for 5.5h at the same temperature, the reaction mixture was quenched with a saturated aqueous solution of NH_4Cl (12.0 mL) and the aqueous layer was extracted with CH_2Cl_2 (3x). The

combined organic layers were washed with brine, dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 80:20 hexane/EtOAc), to afford a mixture of (3*S*)-3-((*tert*-butyldimethylsilyl)oxy)-*N*-methoxy-*N*,2,4-trimethylpentanamide and (*S*)-3-(*tert*- butyldimethylsilyl)-4-isopropyloxazolidine-2-thione, which could not be separated by flash-column chromatography, and the product was used in the next step without further purification.

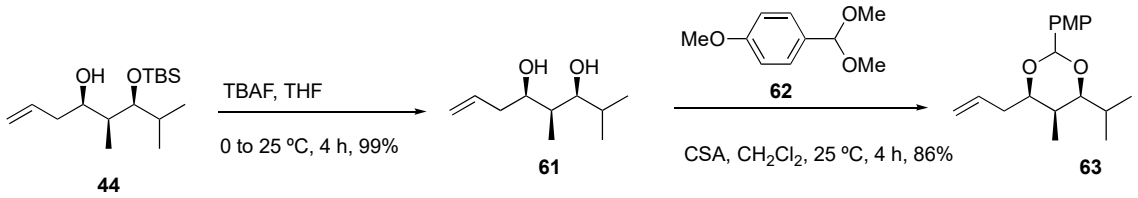
General procedure for the reduction of Weinreb amides. To a cooled (-78 °C) solution of the reaction product obtained above (1.4 g, 5.06 mmol) (0.6 + 0.8 g of the amide and the protected thione calculated by ^{1}H-NMR) in THF (45 mL), DIBAL-H (7.6 mL, 1M in hexane, 7.6 mmol) was added dropwise. The reaction mixture was stirred for 3h at -78 °C and then MeOH (2 mL) was added dropwise and the mixture was stirred for 5 min. The reaction mixture was poured into Et_2O and Rochelle's salt (1:1, 40 mL) at -15 °C. The mixture was warmed up to room temperature and stirred for 30 min. The aqueous layer was extracted with Et_2O (3x). The combined organic layers were washed with brine, dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 90:10 hexane/EtOAc), to afford 0.69 g (71%) of a yellow oil, which was identified as (2*R*,3*S*)-3-((*tert*-butyldimethylsilyl)oxy)-2,4-dimethylpentanal **17**. **Molecular formula:** $C_{13}H_{28}O_2Si$. **MW:** 244.45 g/mol. **$[\alpha]_D^{21}$** -37.2° (*c* 0.25, CH_2Cl_2). **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 9.79 (s, 1H, CHO), 3.90 (app. t, *J* = 5.0 Hz, 1H, H_3), 2.55 – 2.43 (m, 1H, H_2), 1.80 (app. oct., *J* = 6.8 Hz, 1H, H_4), 1.09 (d, *J* = 7.0 Hz, 3H, CH_3), 0.92 (d, *J* = 6.8 Hz, 3H, CH_3), 0.89 (d, *J* = 5.7 Hz, 3H, CH_3), 0.89 (s, 9H, ^{t}Bu), 0.07 (s, 3H, $SiCH_3$), 0.01 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 205.7 (d), 76.6 (d), 50.8 (d), 32.3 (d), 26.1 (q, 3x), 19.9 (s), 18.4 (q, 2x), 8.7 (q), -3.9 (q), -4.0 (q) ppm. **MS** (ESI^+): *m/z* 283 ($[M+K]^+$, 15), 267 ($[M+Na]^+$, 51), 245 ($[M+H]^+$, 74), 187 (100). **HRMS** (ESI^+): Calcd. for $C_{13}H_{29}IO_2Si$ ($[M+H]^+$), 245.1931; found, 245.1931. **IR** (NaCl): ν 2957 (w, C-H), 2927 (m, C-H), 2856 (m, C-H), 1728 (s, C=O) cm^{-1}.



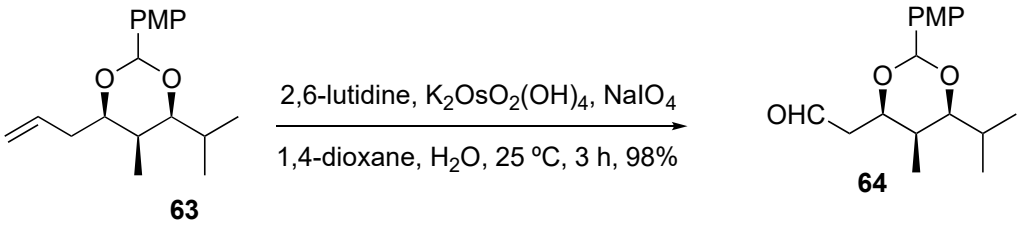
17 **44**

(4*R*,5*S*,6*S*)-6-[(*tert*-Butyldimethylsilyl)oxy]-5,7-dimethyloct-1-en-4-ol 44. To a cooled (0 °C) solution of (2*R*,3*S*)-3-[(*tert*-butyldimethylsilyl)oxy]-2,4-dimethylpentanal **17** (0.54 g, 2.22 mmol) in CH_2Cl_2 (22.2 mL), (*S,S*)-Leighton's reagent **43** (1.48 g, 2.69 mmol) and $Sc(OTf)_3$ were added. The reaction mixture was stirred at 0 °C for 1h and then at 25 °C for 22h. The reaction was quenched with TBAF (2.22 mmol, 1 M in THF, 2.2 mL) and stirred for 30 min at 25 °C. The solvent was removed under reduced pressure. The residue was purified by flash-column chromatography (silica gel, 90:10 hexane/EtOAc) to afford 0.66 g (99%) of a colorless oil, which was identified as (4*R*,5*S*,6*S*)-6-[(*tert*-butyldimethylsilyl)oxy]-5,7-dimethyloct-1-en-4-ol **44**. **Molecular formula:** $C_{16}H_{34}O_2Si$. **MW:** 286.53 g/mol. **$[\alpha]_D^{22}$** -1.24° (*c* 0.5, CH_2Cl_2) **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 5.90 – 5.74 (m, 1H, H_2), 5.22 – 5.04 (m, 2H, $2H_1$), 3.67 (app.

dt, *J* = 8.0, 3.9 Hz, 1H, H_4), 3.57 (dd, *J* = 4.9, 3.5 Hz, 1H, H_6), 2.33 – 2.14 (m, 2H, $2H_3$), 1.93 (d, *J* = 3.1 Hz, 1H, OH), 1.89 – 1.80 (m, 1H, H_7), 1.68 (ddq, *J* = 10.8, 7.0, 3.8 Hz, 1H, H_5), 0.94 (d, *J* = 7.0 Hz, 3H, CH_3), 0.9 (d, *J* = 7.0 Hz, 3H, CH_3), 0.91 (s, 9H, ^{t}Bu), 0.88 (d, *J* = 6.9 Hz, 3H, CH_3), 0.08 (s, 3H, $SiCH_3$), 0.08 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 135.5 (d), 117.8 (t), 79.6 (d), 73.7 (d), 40.0 (d), 39.8 (t), 32.9 (d), 26.3 (q, 3x), 19.3 (q), 18.7 (q), 18.6 (s), 9.0 (q), -3.3 (q), -3.9 (q) ppm. **MS** (ESI^+): *m/z* 309 ($[M+Na]^+$, 11), 287 ($[M+H]^+$, 100). **HRMS** (ESI^+): Calcd. for $C_{16}H_{35}O_2Si$ ($[M+H]^+$), 287.2401; found, 287.2400. **IR** (NaCl): ν 3600-3100 (br, O-H), 2957 (m, C-H), 2931 (m, C-H), 2857 (w, C-H) cm^{-1}.

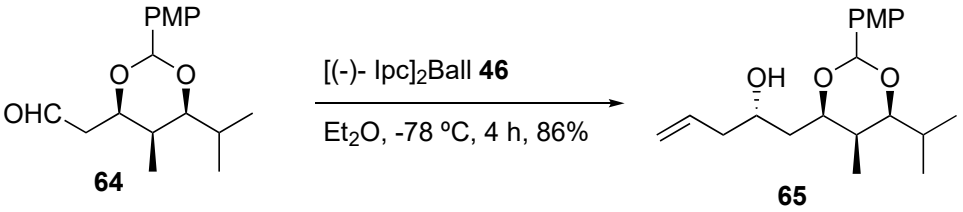


Cyclic acetal (4*R*,5*S*,6*S*)-63. To a cooled (0 °C) solution of (4*R*,5*S*,6*S*)-6-((*tert*-butyldimethylsilyl)oxy)-5,7-dimethyloct-1-en-4-ol **44** (0.3 g, 1.05 mmol) in THF (13.6 mL), TBAF (1.4 mL, 1.39 mmol) was added and the reaction mixture was stirred at 25 °C for 4h. EtOAc (5 mL) was added to the reaction mixture and the organic layer was washed with a saturated aqueous solution of $NaHCO_3$ (10 mL). The aqueous layer was extracted with Et_2O (3x) and the combined organic layers were washed with brine and dried and the solvent was evaporated to obtain a colorless oil of *syn*-1,3-diol **61**, which was used in the next step without further purification. To a solution of the residue obtained above (0.2 g, 1.16 mmol) in CH_2Cl_2 (9.2 mL), *p*-anisaldehyde dimethylacetal **62** (0.4 mL, 2.32 mmol) and CSA (0.013 g, 0.06 mmol) were added and the reaction mixture was stirred at 25 °C for 4h. The reaction mixture was quenched with a saturated aqueous solution of $NaHCO_3$ (5 mL) and the aqueous layer was extracted with CH_2Cl_2 (3x). The combined organic layers were washed with water (2x), brine and dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 95:5 hexane/EtOAc) to afford 0.29 g (86%) of a colorless oil, which was identified as cyclic acetal (4*R*,5*S*,6*S*)-**63**. **Molecular formula:** $C_{18}H_{26}O_3$. **MW:** 290.40 g/mol. **$[\alpha]_D^{19}$** 8.4° (*c* 0.31, CH_2Cl_2). **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 7.44 (d, *J* = 8.6 Hz, 2H, ArH), 6.89 (d, *J* = 8.6 Hz, 2H, ArH), 5.93 – 5.76 (m, 1H, H_2), 5.46 (s, 1H, ArCH(OR)(OR')), 5.21 – 5.03 (m, 2H, $2H_1$), 3.84 (td, *J* = 7.2, 2.2 Hz, 1H, H_4), 3.80 (s, 3H, OCH_3), 3.28 (dd, *J* = 9.9, 2.1 Hz, 1H, H_6), 2.55 – 2.42 (m, 1H, H_{3A}), 2.31 – 2.17 (m, 1H, H_{3B}), 1.90 – 1.80 (m, 1H, H_7), 1.64 (qt, *J* = 6.8, 2.2 Hz, 1H, H_5), 1.03 (d, *J* = 6.4 Hz, 3H, CH_3), 0.96 (d, *J* = 6.8 Hz, 3H, CH_3), 0.85 (d, *J* = 6.8 Hz, 3H, CH_3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 159.9 (s), 134.6 (d), 131.9 (s), 127.5 (d, 2x), 117.2 (t), 113.7 (d, 2x), 101.5 (d), 87.3 (d), 80.9 (d), 55.5 (q), 37.3 (t), 32.4 (d), 29.4 (d), 20.1 (q), 17.6 (q), 5.7 (q) ppm. **MS** (ESI^+): *m/z* 329 ($[M+K]^+$, 20), 291 ($[M+H]^+$, 100). **HRMS** (ESI^+): Calcd. for $C_{18}H_{27}O_3$ ($[M+H]^+$), 291.1955; found, 291.1942. **IR** (NaCl): ν 2960 (s, C-H), 2912 (m, C-H), 2872 (m, C-H), 1617 (w), 1517 (m) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 224 nm.



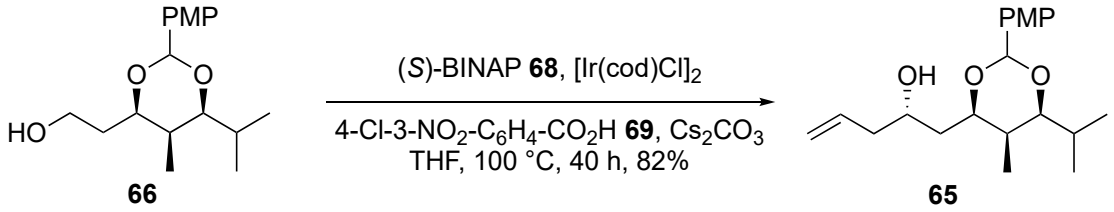
63 **64**

Aldehyde (3*R*,4*S*,5*S*)-64. To a solution of (4*R*,5*S*,6*S*)-**63** (0.15 g, 0.52 mmol) in a 1,4-dioxane/H_2O mixture (3.2 mL, 3:1 v/v), 2,6-lutidine (0.12 mL, 1.0 mmol), $K_2OsO_2(OH)_4$ (0.008 g, 0.01 mmol) and $NaIO_4$ (0.44 g, 2.1 mmol) were sequentially added. After stirring the white suspension at 25 °C for 3h, the solvent was evaporated and the reaction mixture was diluted with CH_2Cl_2 (2 mL) and water (2 mL). The aqueous layer was extracted with CH_2Cl_2 (3x). The combined organic layers were washed with brine and dried (Na_2SO_4) and the solvent was evaporated to afford a dark oil. The residue was purified by flash-column chromatography (silica gel, 90:10 hexane/EtOAc) to afford 0.15 g (98%) of a brown oil, which was identified as aldehyde (3*R*,4*S*,5*S*)-**64**. **Molecular formula:** $C_{17}H_{24}O_4$. **MW:** 292.38 g/mol. **$[\alpha]_D^{22}$** -4.02° (*c* 0.40, CH_2Cl_2).**^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 9.85 (br s, 1H, CHO), 7.41 (d, *J* = 8.6 Hz, 2H, ArH), 6.88 (d, *J* = 8.6 Hz, 2H, ArH), 5.52 (s, 1H, ArCH(OR)(OR')), 4.43 (ddd, *J* = 8.8, 4.4, 2.3 Hz, 1H, H_3), 3.80 (s, 3H, OCH_3), 3.37 (dd, *J* = 9.9, 2.1 Hz, 1H, H_5), 2.85 (ddd, *J* = 16.8, 8.8, 1.9 Hz, 1H, H_{2A}), 2.48 (ddd, *J* = 16.8, 4.4, 1.9 Hz, 1H, H_{2B}), 1.89 – 1.80 (m, 1H, H_6), 1.68 (app. qt, *J* = 6.9, 2.3 Hz, 1H, H_4), 1.04 (d, *J* = 6.4 Hz, 3H, CH_3), 0.97 (d, *J* = 6.9 Hz, 3H, CH_3), 0.86 (d, *J* = 6.8 Hz, 3H, CH_3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 201.0 (d), 160.0 (s), 131.4 (s), 127.5 (d, 2x), 113.7 (d, 2x), 101.6 (d), 87.0 (d), 76.0 (d), 55.5 (q), 47.0 (t), 32.9 (d), 29.4 (d), 20.0 (q), 17.5 (q), 6.2 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{17}H_{25}O_4$ ($[M+H]^+$), 293.1747; found, 293.1736. **IR** (NaCl): ν 2964 (m, C-H), 2913 (m, C-H), 2872 (w, C-H), 1726 (s, C=O), 1616 (w), 1247 (s) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 224 nm.

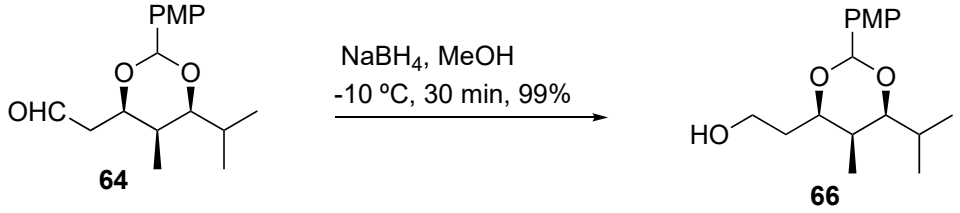


64 **65**

Homoallylic alcohol (4*S*,6*R*,7*S*,8*S*)-65. **Procedure A**. To a cooled (-78 °C) solution of (-)-Ipc_2Ball **46** (0.55 mL, 1M in pentane, 0.55 mmol) in Et_2O (0.5 mL), (3*R*,4*S*,5*S*)-**64** (0.08 g, 0.28 mmol) in Et_2O (1.2 mL) was added and the resulting mixture was stirred for 4h. The reaction mixture was quenched with a 30% aqueous solution of H_2O_2 (0.7 mL) and then stirred with an aqueous solution of NaOH (1.4 mL, 1M) for 2h. The layers were separated and the aqueous layer was extracted with EtOAc (3x). The combined organic layers were dried (Na_2SO_4) and filtered and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 90:20 hexane/EtOAc) to afford 0.08 g (87%) of a colorless oil, which was isolated as a 1:0.06 mixture of (4*S*,6*R*,7*S*,8*S*)-**65** and (4*R*,6*R*,7*S*,8*S*)-**65** diastereomers.

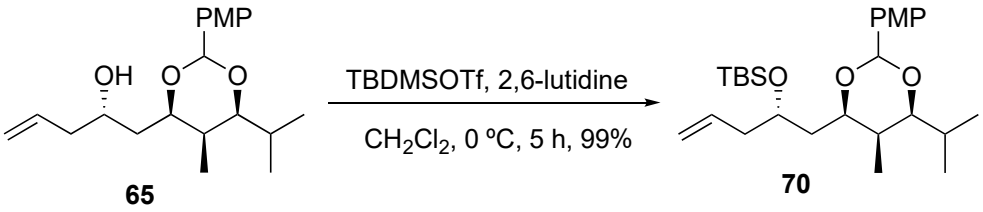


Procedure B. To an oven-dried sealed tube kept under inert atmosphere and charged with alcohol (3*R*,4*S*,5*S*)-**66** (0.1 g, 0.34 mmol), $[Ir(cod)Cl]_2$ (0.006 g, 0.009 mmol), (*S*)-BINAP **68** (0.011 g, 0.02 mmol), Cs_2CO_3 (0.022 g, 0.07 mmol) and 4-chloro-3-nitrobenzoic acid **69** (0.007 g, 0.034 mmol), was added THF (1.7 mL) followed by allyl acetate **67** (0.37 mL, 3.4 mmol). The reaction mixture was stirred at 100 °C for 40h at which point it was saturated with silica gel, and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 90:20 hexane/EtOAc) to afford 0.09 g (82%) of a colorless oil, which was identified as allylic alcohol (4*S*,6*R*,7*S*,8*S*)-**65**. **Molecular formula:** $C_{20}H_{30}O_4$. **MW:** 334.46 g/mol. **$[\alpha]_D^{20}$** 20.4° (*c* 0.11, CH_2Cl_2). **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 7.42 (d, *J* = 8.7 Hz, 2H, ArH), 6.88 (d, *J* = 8.7 Hz, 2H, ArH), 5.91 – 5.77 (m, 1H, H_2), 5.50 (s, 1H, ArCH(OR)(OR')), 5.17 – 5.12 (m, 2H, $2H_1$), 4.14 (app. dt, *J* = 10.3, 2.1 Hz, 1H, H_6), 3.98 – 3.92 (m, 1H, H_4), 3.80 (s, 3H, OCH_3), 3.33 (dd, *J* = 9.9, 2.0 Hz, 1H, H_8), 2.40 – 2.28 (m, 1H, H_{3A}), 2.25 – 2.15 (m, 1H, H_{3B}), 1.96 – 1.87 (m, 1H, H_{5A}), 1.87 – 1.78 (m, 1H, H_9), 1.57 (app. qt, *J* = 7.0, 2.2 Hz, 1H, H_7), 1.44 (ddd, *J* = 15.0, 9.1, 2.1 Hz, 1H, H_{5B}), 1.03 (d, *J* = 6.4 Hz, 3H, CH_3), 0.95 (d, *J* = 6.8 Hz, 3H, CH_3), 0.84 (d, *J* = 6.8 Hz, 3H, CH_3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 159.9 (s), 134.9 (d), 131.9 (s), 127.4 (d, 2x), 118.4 (t), 113.7 (d, 2x), 101.4 (d), 87.4 (d), 77.7 (d), 67.6 (d), 55.5 (q), 42.6 (t), 40.1 (t), 33.8 (d), 29.3 (d), 20.0 (q), 17.5 (q), 6.2 (q) ppm. **MS** (ESI^+): *m/z* 357 ($[M+Na]^+$, 57), 335 ($[M+H]^+$, 57), 199 (100). **HRMS** (ESI^+): Calcd. for $C_{20}H_{31}O_4$ ($[M+H]^+$), 335.2217; found, 335.2204. **IR** (NaCl): ν 3500 – 3100 (br, O-H), 2958 (m, C-H), 1516 (m) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 274, 224 nm.



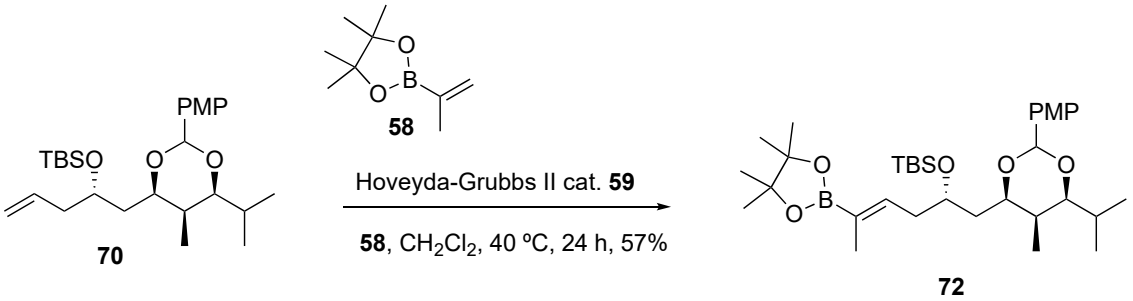
Alcohol (3*R*,4*S*,5*S*)-66. To a cooled (-10 °C) solution of aldehyde (3*R*,4*S*,5*S*)-**64** (0.16 g, 0.55 mmol) in MeOH (8.9 mL), $NaBH_4$ (0.04 g, 1.1 mmol) was added and the reaction was stirred at the same temperature for 30 min. A saturated aqueous solution of $NaHCO_3$ (5 mL) was added and the resulting solution was stirred for 5 min at 0 °C. The aqueous layer was extracted with CH_2Cl_2 (3x) and the combined organic layers were washed with brine and dried (Na_2SO_4), and the solvent was evaporated to afford 0.16 g (99%) of a colourless oil identified as alcohol (3*R*,4*S*,5*S*)-**66**, which was used in the next step without further purification. **Molecular formula:** $C_{17}H_{26}O_4$. **MW:** 294.39 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 7.41 (d, *J* = 8.7 Hz, 2H, ArH), 6.88 (d, *J* = 8.7 Hz, 2H, ArH), 5.50 (s, 1H, ArCH(OR)(OR')), 4.05 (app. dt, *J* = 9.9, 2.7 Hz, 1H,

H_3), 3.86 – 3.81 (m, 2H, $2H_1$), 3.80 (s, 3H, OCH_3), 3.32 (dd, *J* = 9.9, 2.1 Hz, 1H, H_5), 2.03 (dddd, *J* = 14.9, 10.0, 7.1, 5.1 Hz, 1H, H_{2A}), 1.89 – 1.80 (m, 1H, H_6), 1.64 – 1.55 (m, 2H, H_{2B} + H_5), 1.03 (d, *J* = 6.4 Hz, 3H, CH_3), 0.98 (d, *J* = 6.9 Hz, 3H, CH_3), 0.85 (d, *J* = 6.8 Hz, 3H, CH_3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 160.0 (s), 131.7 (s), 127.4 (d, 2x), 113.8 (d, 2x), 101.6 (d), 87.4 (d), 80.6 (d), 61.3 (t), 55.5 (q), 35.5 (t), 33.5 (d), 29.3 (d), 20.0 (q), 17.5 (q), 6.2 (q) ppm. **MS** (ESI^+): *m/z* 317 ($[M+Na]^+$, 100), 295 ($[M+H]^+$, 59), 277 (11). **HRMS** (ESI^+): Calcd. for $C_{17}H_{27}O_4$ ($[M+H]^+$), 295.1904; found, 295.1905. **IR** (NaCl): ν 3600 – 3100 (br, O-H), 2960 (m, C-H), 2874 (m, C-H) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 225 nm.



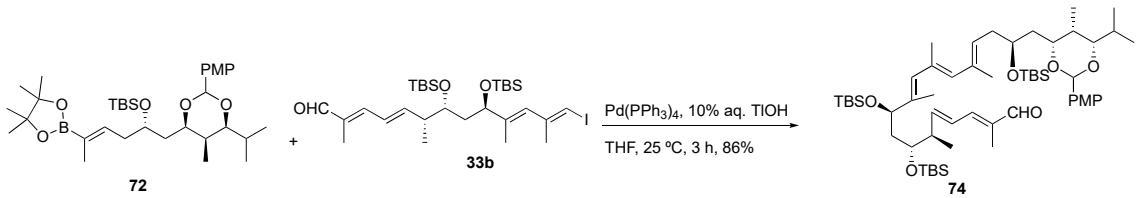
65 **70**

Protected allylic alcohol (4*S*,6*R*,7*S*,8*S*)-70. To a cooled (-78 °C) solution of allylic alcohol (4*S*,6*R*,7*S*,8*S*)-**65** (0.05 g, 0.15 mmol), in CH_2Cl_2 (1.3 mL), 2,6-lutidine (0.03 g, 0.25 mmol) and TBDMSOTf (0.05 mL, 0.22 mmol) were added. After stirring for 30 min at the same temperature, the reaction mixture was quenched with H_2O (2.0 mL) and the aqueous layer was extracted with CH_2Cl_2 (3x). The combined organic layers were dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 95:5 hexane/EtOAc), to afford 0.06 g (99%) of a colorless oil, which was identified as the protected allylic alcohol (4*S*,6*R*,7*S*,8*S*)-**70**. **Molecular formula:** $C_{26}H_{44}O_4Si$. **MW:** 448.72 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 7.43 (d, *J* = 8.6 Hz, 2H, ArH), 6.88 (d, *J* = 8.6 Hz, 2H, ArH), 5.90 – 5.76 (m, 1H, H_2), 5.43 (s, 1H, Ar<u>CH</u>(OR)(OR'), 5.09 – 4.98 (m, 2H, $2H_1$), 4.08 – 3.98 (m, 1H, H_4), 3.98 (app. dt, *J* = 10.2, 2.1 Hz, 1H, H_6), 3.80 (s, 3H, OCH_3), 3.27 (dd, *J* = 9.9, 2.1 Hz, 1H, H_8), 2.34 – 2.17 (m, 2H, $2H_3$), 1.87 – 1.72 (m, 2H, H_{5A} + H_9), 1.52 (app. qt, *J* = 6.9, 2.2 Hz, 1H, H_7), 1.38 (ddd, *J* = 14.2, 10.0, 2.1 Hz, 1H, H_{5B}), 1.03 (d, *J* = 6.4 Hz, 3H, CH_3), 0.93 (d, *J* = 6.3 Hz, 3H, CH_3), 0.92 (s, 9H, ^{t}Bu), 0.85 (d, *J* = 6.8 Hz, 3H, CH_3), 0.08 (s, 3H, $SiCH_3$), 0.07 (s, 3H, CH_3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 159.8 (s), 134.8 (d), 132.1 (s), 127.4 (d, 2x), 117.2 (t), 113.7 (d, 2x), 101.3 (d), 87.5 (d), 77.0 (d), 68.0 (d), 55.5 (q), 43.0 (t), 40.5 (t), 33.9 (d), 29.4 (d), 26.1 (q, 3x), 20.0 (q), 18.3 (s), 17.5 (q), 6.2 (q), -4.0 (q), -4.4 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{26}H_{45}O_4Si$ ($[M+H]^+$), 449.3082; found, 449.3060. **IR** (NaCl): ν 2955 (m, C-H), 2930 (m, C-H), 2857 (w, C-H), 1517 (m), 1250 (s) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 272, 225 nm.



70 **72**

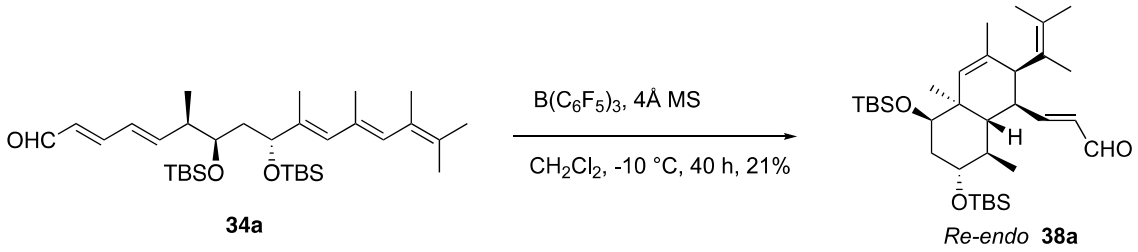
Dioxoborolane (*Z*,4*S*,6*R*,7*S*,8*S*)-72. In a Schlenk tube, a solution of **70** (0.05 g, 0.12 mmol) and isopropenyl boronic acid pinacol ester **58** (0.22 mL, 1.2 mmol) in degassed CH_2Cl_2 (1 mL) was stirred at 25 °C. A solution of 2nd generation Hoveyda-Grubbs catalyst **59** (0.004 g, 0.006 mmol) in CH_2Cl_2 (0.2 mL) was added. After heating the resulting solution up to 45 °C for 1h, it was freeze-pump-thawed (liquid nitrogen) to remove solvated ethylene under high vacuum. A further portion of HG-II catalyst (0.0018 g, 0.003 mmol) was added and the reaction mixture was heated at 45 °C for 1h. The reaction mixture was freeze-pump-thawed (liquid nitrogen) and then a final portion of HG-II catalyst (0.0018 g, 0.003 mmol) was added. The reaction mixture was then heated to 45 °C for 24h. After this time, the reaction mixture was concentrated under vacuum washing with CH_2Cl_2 and then concentrated under reduced pressure (ca. 0.2 mm Hg) to remove the excess of pinacol ester. The residue was purified by flash-column chromatography (silica gel, 98:2 hexane/EtOAc) to afford 0.04 g (57%) of a yellow oil, which was identified as dioxoborolane (*Z*,4*S*,6*R*,7*S*,8*S*)-**72**. **Molecular formula:** $C_{33}H_{57}BO_6Si$. **MW:** 588.71 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 7.43 (d, *J* = 8.6 Hz, 2H, ArH), 6.88 (d, *J* = 8.6 Hz, 2H, ArH), 6.36 (tq, *J* = 7.1, 1.7 Hz, 1H, H_2), 5.43 (s, 1H, ArCH(OR)(OR')), 4.07 – 4.02 (m, 1H, H_4), 4.00 (app. dt, *J* = 9.8, 2.2 Hz, 1H, H_6), 3.80 (s, 3H, OCH_3), 3.27 (dd, *J* = 9.8, 2.0 Hz, 1H, H_8), 2.38 – 2.29 (m, 2H, $2H_3$), 1.88 – 1.75 (m, 2H, H_{5A} + H_9), 1.68 (d, *J* = 1.6 Hz, 3H, CH_3), 1.53 (app. qt, *J* = 6.9, 2.1 Hz, 1H, H_7), 1.41 (ddd, *J* = 14.1, 9.7, 2.3 Hz, 1H, H_{5B}), 1.26 (s, 12H, 4xCH_3), 1.03 (d, *J* = 6.4 Hz, 3H, CH_3), 0.92 (d, *J* = 6.3 Hz, 3H, CH_3), 0.92 (s, 9H, $SiCH_3$), 0.85 (d, *J* = 6.8 Hz, 3H, CH_3), 0.08 ($SiCH_3$), 0.07 ($SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 159.8 (s), 142.2 (d + s, 2x), 132.1 (s), 127.4 (d, 2x), 113.7 (d, 2x), 101.2 (d), 87.5 (d), 83.3 (s, 2x), 77.2 (d), 68.4 (d), 55.5 (q), 41.2 (t), 38.0 (t), 33.8 (d), 29.4 (d), 26.2 (q, 3x), 24.9 (q, 4x), 20.0 (q), 18.3 (s), 17.5 (q), 14.3 (q), 6.3 (q), -3.9 (q), -4.3 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{33}H_{58}O_6Si$ ($[M+H]^+$), 589.4096; found, 589.4087. **IR** (NaCl): ν 2955 (m, C-H), 2930 (m, C-H), 2858 (w, C-H), 1517 (m), 1371 (s) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 272 nm.



All-*trans*-(6*R*,7*R*,9*R*,17*S*,4'*S*,5'*S*,6'*R*)-7,9,17-tris[(*tert*-butyldimethylsilyl)oxy]-18-[5'-methyl-2'-(*para*-methoxyphenylmethyl)-4'-(prop-2-yl)]-2,6,10,12,14-pentamethyl-decaoct-2,4,10,12,14-pentaenal 74. To a solution of $Pd(PPh_3)_4$ (0.003 g, 0.003 mmol) in THF (2 mL), a solution of (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis((*tert*-butyldimethylsilyl)oxy)-13-iodo-2,6,10,12-tetramethyltrideca-2,4,10,12-tetraenal **33b** (0.037 g, 0.059 mmol) in THF (2.5 mL) was added and the resulting mixture was stirred at 25 °C for 15 min. Then, a solution of (*Z*,4*S*,6*R*,7*S*,8*S*)-**72** (0.035 g, 0.059 mmol) in THF (2 mL) was added followed by the addition of a 10% aqueous solution of TlOH (0.52 mL, 0.24 mmol). The reaction mixture was stirred at 25 °C for 3h and then diluted with Et_2O. The organic layer was washed with a saturated aqueous solution of $NaHCO_3$

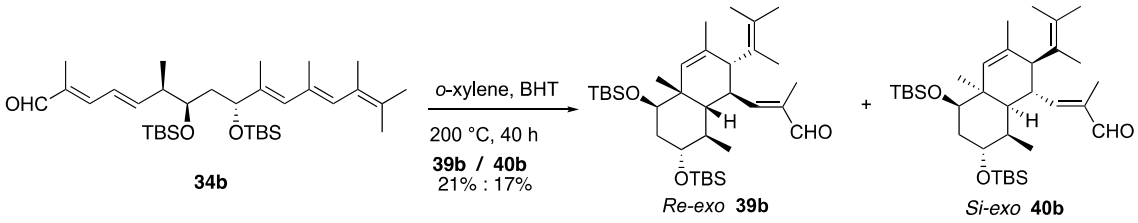
(8 mL) and the aqueous layer was extracted with Et_2O. The combined organic layers were dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 98:2 hexane/EtOAc) to afford 0.05 g (86%) of a yellow oil, which was identified as all-*trans*-(6*R*,7*R*,9*R*,17*S*,4'*S*,5'*S*,6'*R*)-7,9,17-tris[(*tert*-butyldimethylsilyl)oxy]-18-[5'-methyl-2'-(*para*-methoxyphenylmethyl)-4'-(prop-2-yl)]-2,6,10,12,14-pentamethyl-decaoct-2,4,10,12,14-pentaenal **74**. **Molecular formula:** $C_{56}H_{98}O_7Si_3$. **MW:** 967.65 g/mol. **$[\alpha]_D^{23}$** -13.6° (*c* 0.05, MeOH). **^{1}H-NMR** (400.13 MHz, CD_2Cl_2): δ 9.40 (s, 1H, CHO), 7.40 (d, *J* = 8.6 Hz, 2H, ArH), 6.87 (d, *J* = 8.8 Hz, 2H, ArH), 6.84 (d, *J* = 12.5 Hz, 1H, H_3), 6.52 (ddd, *J* = 15.2, 11.0, 1.2 Hz, 1H, H_4), 6.31 (dd, *J* = 15.3, 7.0 Hz, 1H, H_5), 5.85 (s, 1H, H_{13}), 5.76 (s, 1H, H_{11}), 5.43 (s, 1H, ArCH(OR)(OR')), 5.40 (t, *J* = 7.4 Hz, 1H, H_{15}), 4.10 (dd, *J* = 7.9, 4.6 Hz, 1H, H_9), 4.06 – 4.01 (m, 1H, H_{17}), 4.00 (app. dt, *J* = 10.2, 2.2 Hz, 1H, $H_{6'}$), 3.79 (s, 3H, OCH_3), 3.80 – 3.75 (m, 1H, H_7), 3.29 (dd, *J* = 9.8, 2.0 Hz, 1H, $H_{4'}$), 2.62 – 2.54 (m, 1H, H_6), 2.33 (app. t, *J* = 6.4 Hz, 2H, $2H_{16}$), 1.89 (d, *J* = 1.1 Hz, 3H, CH_3), 1.83 – 1.76 (m, 2H, $H_{5'}$ + H_{8A}), 1.80 (d, *J* = 1.0 Hz, 3H, CH_3), 1.77 – 1.73 (m, 6H, 2xCH_3), 1.57 – 1.50 (m, 1H, H_{22}), 1.49 – 1.40 (m, 2H, H_{18} + H_{8B}), 1.08 (d, *J* = 6.8 Hz, 3H, CH_3), 1.01 (d, *J* = 6.4 Hz, 3H, CH_3), 0.92 (s, 9H, ^{t}Bu), 0.91 (s, 21H, 2x ^{t}Bu + CH_3), 0.85 (d, *J* = 6.9 Hz, 3H, CH_3), 0.10 (s, 3H, $SiCH_3$), 0.09 (s, 6H, 2x$SiCH_3$), 0.08 (s, 3H, $SiCH_3$), 0.06 (s, 3H, $SiCH_3$), 0.02 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, CD_2Cl_2): δ 195.3 (d), 160.4 (s), 149.6 (d), 149.1 (d), 138.5 (s), 136.8 (s), 134.7 (s), 134.3 (d), 132.7 (s), 132.6 (s), 131.3 (d), 127.9 (d, 2x), 126.7 (d), 125.9 (d), 113.9 (d, 2x), 101.8 (d), 87.8 (d), 77.7 (d), 77.3 (d), 74.2 (d), 69.1 (d), 55.8 (q), 43.2 (d), 42.1 (t), 41.3 (t), 37.8 (t), 34.3 (d), 29.8 (d), 26.32 (q, 3x), 26.27 (q, 6x), 20.1 (q), 19.2 (q), 18.6 (s), 18.63 (s), 18.59 (s), 17.74 (q), 17.70 (q), 13.9 (q), 13.3 (q), 9.7 (q), 6.4 (q), -3.78 (q), -3.81 (q), -3.83 (q), -3.86 (q), -4.3 (q), -4.5 (q) ppm. **MS** (ESI^+): *m/z* 836 ($[M+H-OTBS]^+$, 100). **IR** (NaCl): ν 2954 (m, C-H), 2859 (m, C-H), 1685 (s, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 273, 226 nm.

INTRAMOLECULAR DIELS-ALDER REACTIONS



(*E*)-3-((1'*S*,2'*S*,4'a*R*,5'*R*,7'*R*,8'*R*,8'a*R*)-5',7'-bis(*tert*-Butyldimethylsilyloxy)-3',4'a,8'-trimethyl-2'-(3''-methylbut-2''-en-2''-yl)-1',2',4'a,5',6',7',8',8'a-octahydronaphthalen-1'-yl)acrylaldehyde 38a. In a round bottomed flask, powdered 4Å molecular sieves (0.01 g) activated under vacuum and tris(pentafluorophenyl)borane (0.005 g, 0.009 mmol) were introduced and then CH_2Cl_2 (1.5 mL) was added. A solution of (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-6,10,12,14,15-pentamethyl hexadeca-2,4,10,12,14-pentaenal **34a** (0.05 g, 0.09 mmol) in THF (3 mL) was added and the reaction mixture was stirred at -10 °C for 40h. The solution was then quenched with a saturated aqueous solution of $NaHCO_3$ (5 mL). The

aqueous layer was extracted with CH_2Cl_2 (3x), the combined organic layers were washed with brine and dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 60:40 hexane/CH_2Cl_2) to afford 0.01 g (21%) of a colourless oil, which was identified as the titled compound **38a**. **Molecular formula:** $C_{33}H_{60}O_3Si_2$. **MW:** 561.00 g/mol. **$[\alpha]_D^{22}$** -96.8° (*c* 0.36, MeOH). **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 9.43 (d, *J* = 8.0 Hz, 1H, CHO), 6.91 (dd, *J* = 15.4, 10.7 Hz, 1H, H_3), 6.00 (dd, *J* = 15.4, 8.0 Hz, 1H, H_2), 5.28 (s, 1H, $H_{4'}$), 3.62 (app. t, *J* = 3.0 Hz, 1H, $H_{5'}$), 3.50 (app. td, *J* = 10.1, 6.2 Hz, 1H, $H_{7'}$), 3.24 (d, *J* = 7.0 Hz, 1H, $H_{2'}$), 2.89 (app. ddd, *J* = 11.4, 11.0, 7.1 Hz, 1H, $H_{1'}$), 2.24 (app. t, *J* = 11.5 Hz, 1H, $H_{8'a}$), 1.82 – 1.70 (m, 2H, $2H_{6'}$), 1.66 (s, 3H, CH_3), 1.64 (s, 3H, CH_3), 1.50 (s, 3H, CH_3), 1.50 – 1.47 (m, 1H, $H_{8'}$), 1.41 (s, 3H, CH_3), 0.98 (s, 3H, CH_3), 0.97 (d, *J* = 6.4 Hz, 3H, CH_3), 0.89 (s, 9H, $SiC(CH_3)_3$), 0.86 (s, 9H, $SiC(CH_3)_3$), 0.09 (s, 3H, $SiCH_3$), 0.05 (s, 3H, $SiCH_3$), 0.02 (s, 3H, CH_3), 0.01 (s, 3H, CH_3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 194.2 (d), 166.5 (d), 134.8 (d), 131.9 (s), 129.5 (d), 128.7 (s), 125.7 (s), 76.9 (d), 73.7 (d), 47.4 (d), 44.1 (d), 41.9 (s), 40.1 (d), 39.7 (d), 38.5 (t), 26.1 (q, 3x), 26.0 (q, 3x), 22.0 (q), 21.2 (q, 3x), 19.0 (q), 18.2 (s), 18.1 (s), 16.7 (q), -3.6 (q), -4.1 (q), -4.7 (q), -4.6 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{33}H_{61}O_3Si_2$ ($[M+H]^+$), 561.4154; found, 561.4138. **IR** (NaCl): ν 2929 (m, C-H), 2858 (w, C-H), 1689 (C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 289 nm.



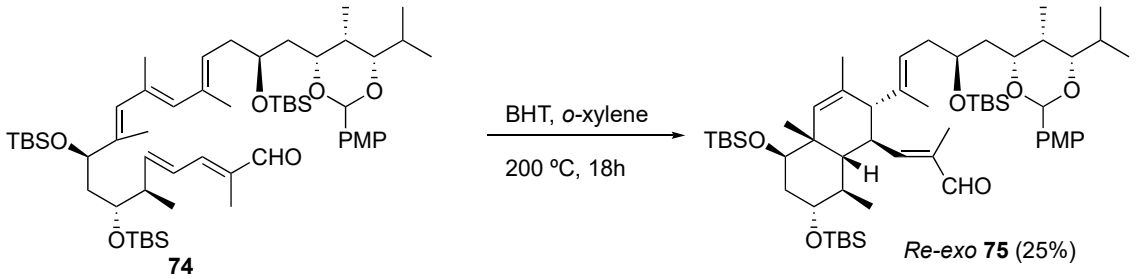
(*E*)-3-((1'*S*,2'*R*,4'a*S*,5'*R*,7'*R*,8'*R*,8'a*R*)-5',7'-bis(*tert*-Butyldimethylsilyloxy)-3',4'a,8'-trimethyl-2'-(3''-methylbut-2''-en-2''-yl)-1',2',4'a,5',6',7',8',8'a-octahydronaphthalen-1'-yl)-2-methylacrylaldehyde 39b and **(*E*)-3-((1'*R*,2'*S*,4'a*R*,5'*R*,7'*R*,8'*R*,8'a*S*)-5',7'-bis(*tert*-Butyldimethylsilyloxy)-3',4'a,8'-trimethyl-2'-(3''-methylbut-2''-en-2''-yl)-1',2',4'a,5',6',7',8',8'a-octahydronaphthalen-1'-yl)-2-methylacrylaldehyde 40b**.

To a solution of (2*E*,4*E*,6*R*,7*R*,9*R*,10*E*,12*E*)-7,9-bis(*tert*-butyldimethylsilyloxy)-2,6,10,12,14,15-hexamethylhexadeca-2,4,10,12,14-pentaenal **34b** (0.048 g, 0.083 mmol) in *o*-xylene (7 mL), BHT (0.002 g, 0.008 mmol) was added and the reaction mixture was stirred in a Schlenk tube at 200 °C for 40h. The solvent was evaporated and the residue was purified by flash-column chromatography (silica gel basified with hexane/Et_3N 97:3, then, 80:20 hexane/CH_2Cl_2) followed by HPLC purification (silica gel, Spherisorb 5µm, 250x10 mm, 89.55:9.95:0.5 hexane/CH_2Cl_2/EtOAc, flow rate = 2 mL/min; t_R = 23 min **39b**, t_R = 42 min **40b**) to afford 0.01 g (21%) of **39b** and 0.008 g (17%) of **40b**, as colorless solids.

Data for *Re-exo* 39b. **Molecular formula:** $C_{34}H_{62}O_3Si_2$. **MW:** 575.04 g/mol. **$[\alpha]_D^{20}$** -36.5° (*c* 0.1, MeOH). **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 9.38 (s, 1H, CHO), 6.26 (d, *J* = 9.7 Hz, 1H, H_3), 5.43 (s, 1H, $H_{4'}$), 4.03 (dd, *J* = 10.1, 3.6 Hz, 1H, $H_{5'}$), 3.82 – 3.77 (m, 1H, $H_{7'}$), 3.14 (app. q, *J* = 9.7 Hz, 1H, $H_{1'}$), 3.02 (d, *J* = 9.1 Hz, 1H, $H_{2'}$), 1.84 (ddd, *J* = 13.7, 10.7, 3.3 Hz, 1H, $H_{6'A}$), 1.77 – 1.69 (m, 1H, $H_{8'}$), 1.61 (s, 3H, CH_3), 1.56 (s, 3H, CH_3), 1.59 – 1.54 (m, 1H, $H_{6'B}$), 1.51 (s, 3H, CH_3), 1.53 – 1.50 (m, 1H, $H_{8'a}$), 1.48 (s, 3H, CH_3), 1.45 (s, 3H, CH_3), 1.08 (s, 3H, CH_3), 1.07 (d, *J* = 6.8 Hz, 3H, CH_3), 0.91 (s,

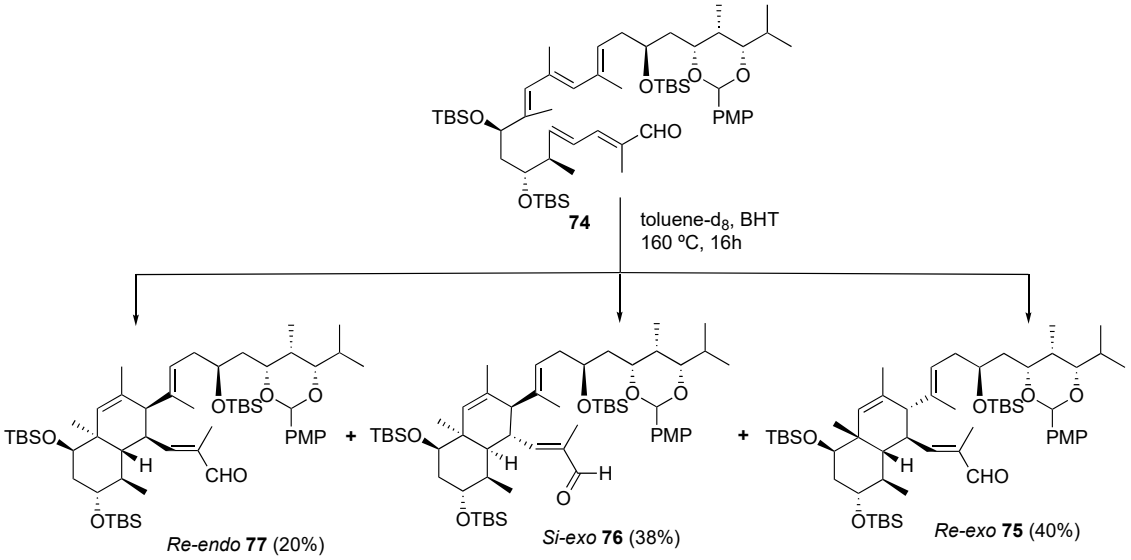
9H, $SiC(CH_3)_3$), 0.85 (s, 9H, $SiC(CH_3)_3$), 0.05 (s, 3H, $SiCH_3$), 0.04 (s, 3H, $SiCH_3$), 0.02 (s, 3H, $SiCH_3$), 0.02 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 196.0 (d), 161.5 (d), 139.5 (s), 134.6 (d), 131.5 (s), 128.0 (s), 126.9 (s), 74.6 (d), 72.3 (d), 50.5 (d), 47.0 (d), 40.8 (d), 39.9 (s), 39.3 (d), 36.0 (t), 26.6 (q, 3x), 26.1 (q, 3x), 23.6 (q), 22.5 (q), 21.4 (q), 21.1 (q), 20.5 (q), 18.8 (s), 18.3 (s), 14.5 (q), 10.8 (q), -4.0 (q), -4.3 (q, 2x), -4.7 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{34}H_{63}O_3Si_2$ ($[M+H]^+$), 575.4310; found, 575.4292. **IR** (NaCl): ν 2953 (s, C-H), 2858 (s, C-H), 1688 (m, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 232 nm.

Data for *Si-exo* 40b. **Molecular formula:** $C_{34}H_{62}O_3Si_2$. **MW:** 575.04 g/mol. **$[\alpha]_D^{22}$** -18.7° (*c* 0.05, MeOH). **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 9.36 (s, 1H, CHO), 6.34 (d, *J* = 11.6 Hz, 1H, H_3), 5.16 (s, 1H, $H_{4'}$), 3.75 (app. dt, *J* = 10.9, 4.3 Hz, 1H, $H_{7'}$), 3.74 – 3.71 (m, 1H, $H_{5'}$), 3.62 (q, *J* = 11.1 Hz, 1H, $H_{1'}$), 3.08 (d, *J* = 9.0 Hz, 1H, $H_{2'}$), 2.14 – 2.07 (m, 1H, $H_{8'}$), 1.94 (dt, *J* = 13.7, 3.5 Hz, 1H, $H_{6'A}$), 1.80 (td, *J* = 11.2, 10.7, 3.6 Hz, 2H, $H_{6'B}$ + H_{8a}), 1.71 (s, 3H, CH_3), 1.57 (s, 3H, CH_3), 1.51 (s, 3H, CH_3), 1.47 (s, 3H, CH_3), 1.42 (s, 3H, CH_3), 1.12 (s, 3H, CH_3), 0.89 (d, J = 6.5 Hz, 3H, CH_3), 0.92 (s, 9H, $SiC(CH_3)_3$), 0.84 (s, 9H, $SiC(CH_3)_3$), 0.07 (s, 6H, 2x$SiCH_3$), 0.01 (s, 3H, $SiCH_3$), -0.05 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 196.0 (d), 161.5 (d), 139.5 (d), 134.6 (s), 131.5 (s), 128.0 (s), 126.9 (s), 74.6 (d), 72.3 (d), 50.5 (d), 47.0 (d), 40.8 (d), 39.9 (s), 39.3 (d), 36.0 (t), 26.6 (q, 3x), 26.1 (q, 3x), 23.6 (q), 22.5 (q), 21.4 (q), 21.1 (q), 20.5 (q), 18.8 (s), 18.3 (s), 14.5 (q), 10.8 (q), -4.0 (q), -4.3 (q, 2x), -4.7 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{34}H_{63}O_3Si_2$ ($[M+H]^+$), 575.4310; found, 575.4296. **IR** (NaCl): ν 2931 (s, C-H), 2859 (s, C-H), 1686 (m, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 239 nm.



Octahydronaphthalene *Re-exo* 75. In a Schlenk tube, a solution of **74** (0.037 g, 0.038 mmol) in *o*-xylene (3.5 mL) and BHT (1 mg, 0.004 mmol) was stirred for 18h at 200 °C. The solvent was evaporated and the residue was purified by flash-column chromatography (silica gel, 97:3 hexane/EtOAc) followed by HPLC (C12-silica gel, Synergy MAX-RP, 250 x 4.6 mm, 4 µm, 100% MeOH, flow rate = 2 mL/min, t_R = 19 min) to afford 0.01 g (25%) of a white solid, which was identified as *Re-exo* **75**. **Molecular formula:** $C_{56}H_{98}O_7Si_3$. **MW:** 967.65 g/mol. **$[\alpha]_D^{23}$** -8.52° (*c* 0.1, MeOH). **^{1}H-NMR** (400.13 MHz, CD_2Cl_2): δ 9.36 (s, 1H, CHO), 7.37 (d, *J* = 8.6 Hz, 2H, ArH), 6.86 (d, *J* = 8.8 Hz, 2H, ArH), 6.25 (d, *J* = 9.4 Hz, 1H, H_3), 5.45 (s, 1H, H_{11}), 5.40 (s, 1H, Ar<u>CH</u>(OR)(OR')), 5.18 (t, *J* = 6.1 Hz, H_{15}), 4.04 – 3.89 (m, 3H, H_9 + H_{17} + H_{19}), 3.79 (s, 4H, OCH_3 + H_7), 3.27 (dd, *J* = 9.8, 1.8 Hz, 1H, H_{21}), 3.12 (q, *J* = 9.5 Hz, 1H, H_4), 2.43 (d, *J* = 8.0 Hz, 1H, H_{13}), 2.23 (ddd, *J* = 14.8, 8.2, 3.8 Hz, 1H, H_{16A}), 2.11 – 1.97 (m, 1H, H_{16B}), 1.90 – 1.61 (m, 5H, H_{18A} + H_6 + $2H_8$ + H_{22}), 1.60 (s, 3H, CH_3), 1.53 (s, 4H, CH_3 + H_5), 1.50 (s, 4H, CH_3 + H_{20}), 1.38 – 1.24 (m, 1H, H_{18B}), 1.07 (s, 3H, CH_3), 1.07 (d, *J* = 6.9 Hz, 3H, CH_3), 1.00 (d, *J* = 6.4 Hz, 3H, CH_3), 0.92 (s, 9H, $SiC(CH_3)_3$), 0.89 (s, 9H, $SiC(CH_3)_3$), 0.88 (s, 3H, CH_3), 0.87 (s, 9H, $SiC(CH_3)_3$), 0.85 (m, 3H, CH_3), 0.07 (s, 3H, $SiCH_3$), 0.05 (s, 6H, 2xCH_3), 0.05 – 0.03 (m, 9 H, 3x$SiCH_3$)

ppm. **^{13}C-NMR** (100.16 MHz, CD_2Cl_2): δ 195.9 (d), 161.0 (d), 160.3 (s), 139.9 (s), 136.5 (s), 135.1 (s), 132.7 (d), 131.1 (s), 127.9 (d, 2x), 125.3 (d), 113.8 (d, 2x), 101.7 (d), 87.8 (d), 77.7 (d), 74.8 (d), 73.2 (d), 68.7 (d), 55.8 (q), 55.3 (d), 50.4 (d), 40.9 (t), 40.4 (d), 39.9 (s), 37.4 (t), 36.7 (t), 34.2 (d), 30.7 (d), 29.8 (d), 26.8 (q, 3x), 26.3 (q, 6x), 24.1 (q), 22.2 (q), 21.9 (q), 20.1 (q), 19.0 (s), 18.6 (s), 18.5 (s), 17.7 (d), 13.0 (q), 11.2 (q), 6.4 (q), -3.8 (q), -3.9 (q), -4.1 (q), -4.1 (q), -4.3 (q), -4.4 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{56}H_{99}O_7Si_3$ ($[M+H]^+$), 967.6693; found, 967.6676. **IR** (NaCl): ν 2953 (s, C-H), 2858 (s, C-H), 1687 (m, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 226 nm.



Octahydronaphthalene *Re-exo* 75, **Octahydronaphthalene *Si-exo* 76 and Octahydronaphthalene *Re-endo* 77**.

Procedure A: To a solution of **74** (6 mg, 0.006 mmol) in CD_3OD (0.75 mL), BHT (1 mg, 0.001 mmol) was added and the reaction mixture was stirred in a sealed NMR tube for 14h at 170 °C. The solvent was evaporated and the residue was purified by column chromatography (silica gel, 95:5 hexane/EtOAc) followed by HPLC (C12-silica gel, Synergy MAX-RP, 250 x 4.6 mm, 4 μm, 100% MeOH, flow rate = 2 mL/min) to afford 2.3 mg (40%) of the *Re-exo* **75** (t_R = 20 min), 2.2 mg (37%) of the *Si-exo* **76** (t_R = 22 min) and 1.5 mg (20%) of the *Re-endo* **77** (t_R = 25 min) diastereomers (1:1:0.5 d.r.).

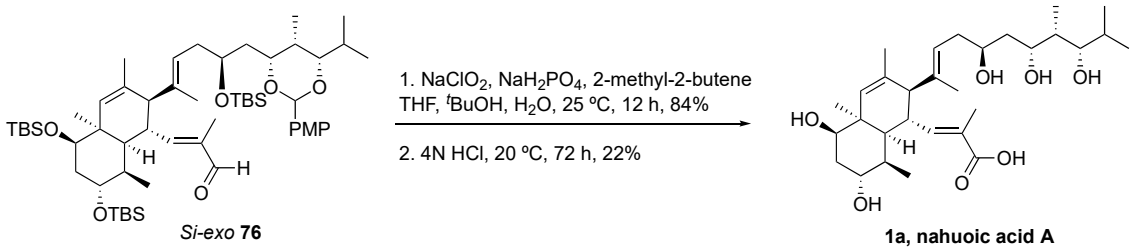
Procedure B: To a solution of **74** (6 mg, 0.006 mmol) in toluene-d_8 (0.75 mL), BHT (0.01 mL, 0.1 M in MeOH, 0.001 mmol) and $Eu(fod)_3$ (1 mg, 0.001 mmol) were added and the reaction mixture was stirred in a sealed NMR tube for 16h at 160 °C. An aqueous saturated solution of $NaHCO_3$ was added and the reaction mixture was stirred for 30 min at room temperature. The aqueous layer was extracted with Et_2O (3x) and the combined organic layers were washed with brine, dried (Na_2SO_4) and the solvent was evaporated. The residue was purified by flash-column chromatography (silica gel, 95:5 hexane/EtOAc) followed by HPLC (C-18-silica gel, Synergy MAX-RP, 250 x 4.6 mm, 4 μm, 100% MeOH, flow rate = 2 mL/min) to afford 2.3 mg (40%) of the *Re-exo* **75** (t_R = 20 min), 2.2 mg (37%) of the *Si-exo* **76** (t_R = 22 min) and 1.5 mg (20%) of the *Re-endo* **77** (t_R = 25 min) diastereomers (1:1:0.5 d.r.).

Data for *Si-exo* 76. **Molecular formula:** $C_{56}H_{98}O_7Si_3$. **MW:** 967.65 g/mol. **^{1}H-NMR** (400.13 MHz, CD_2Cl_2): δ 9.35 (s, 1H, CHO), 7.39 (d, J = 8.7 Hz, 2H, ArH), 6.87 (d, J = 8.6 Hz, 2H, ArH), 6.33 (d, J = 11.6 Hz, 1H, H_3), 5.41 (s, 1H, ArCH(OR)(OR')), 5.22 – 5.12 (m, 2H, H_{11} + H_{15}), 3.94 – 3.87 (m, 2H, H_9 + H_{19}), 3.79 (s, 4H, OCH_3), 3.78 – 3.74

(m, 2H, H_7 + H_{17}), 3.67 (app. q, *J* = 10.4 Hz, 1H, H_4), 3.28 (app. d, *J* = 9.5 Hz, 1H, H_{21}), 2.60 (d, *J* = 9.0 Hz, 1H, H_{13}), 2.24 – 1.99 (m, 3H, CH_2 + H_6), 1.99 – 1.92 (m, 1H, CH_2), 1.83 – 1.76 (m, 3H, CH_2 + H_{20} + H_5), 1.73 (s, 3H, CH_3), 1.67 – 1.62 (m, 1H, CH_2), 1.54 – 1.49 (m, 4H, CH_3 + H_{22}), 1.41 (s, 3H, CH_3), 1.23 – 1.16 (m, 1H, CH_2), 1.12 (s, 3H, CH_3), 1.00 (d, *J* = 6.4 Hz, 3H, CH_3), 0.93 (s, 9H, $SiC(CH_3)_3$), 0.92 – 0.89 (m, 3H, CH_3), 0.90 (s, 9H, $SiC(CH_3)_3$), 0.88 (d, *J* = 2.1 Hz, 3H, CH_3), 0.86 (d, *J* = 2.1 Hz, 3H, CH_3), 0.85 (s, 9H, $SiC(CH_3)_3$), 0.09 (s, 3H, $SiCH_3$), 0.08 (s, 3H, $SiCH_3$), 0.05 (s, 3H, $SiCH_3$), 0.04 (s, 3H, $SiCH_3$), 0.03 (s, 3H, $SiCH_3$), -0.04 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, CD_2Cl_2): δ 195.8 (d), 163.0 (d), 160.3 (s), 136.7 (s), 133.7 (d), 132.8 (s), 128.6 (s), 128.1 (s), 127.9 (d, 2x), 126.0 (d), 113.8 (d, 2x), 101.7 (d), 87.8 (d), 77.6 (d), 77.1 (d), 69.6 (d), 68.8 (d), 59.5 (d), 55.8 (q), 52.4 (d), 43.0 (s), 42.0 (t), 40.9 (t), 39.9 (d), 37.2 (t), 34.0 (d), 30.7 (d), 29.8 (d), 28.8 (q), 26.8 (q, 3x), 26.3 (q, 3x), 26.2 (q, 3x), 22.0 (q), 20.1 (q), 19.4 (q), 19.1 (s), 18.51 (s), 18.49 (s), 17.7 (q), 14.2 (q), 10.8 (q), 6.4 (q), -3.4 (q), -3.7 (q), -3.9 (q), -4.3 (q), -4.4 (q), -4.5 (q) ppm.

Data for *Re-endo* 77. **Molecular formula:** $C_{56}H_{98}O_7Si_3$. **MW:** 967.65 g/mol. **^{1}H-NMR** (400.13 MHz, CD_2Cl_2): δ 9.38 (s, 1H, CHO), 7.38 (d, *J* = 8.8 Hz, 2H, ArH), 6.86 (d, *J* = 8.8 Hz, 2H, ArH), 6.57 (d, *J* = 11.1 Hz, 1H, H_3), 5.40 (s, 1H, ArCH(OR)(OR')), 5.31 (s, 1H, H_{11}), 5.14 (app. t, *J* = 7.0 Hz, 1H, H_{15}), 3.98 – 3.91 (m, 2H, H_{17} + H_{19}), 3.79 (s, 3H, OCH_3), 3.66 (app. t, *J* = 2.4 Hz, 1H, H_9), 3.52 (app. td, *J* = 10.1, 5.9 Hz, 1H, H_7), 3.28 (dd, *J* = 9.9, 2.0 Hz, 1H, H_{21}), 3.26 – 3.20 (m, 1H, H_4), 2.53 (d, *J* = 6.3 Hz, 1H, H_{13}), 2.27 – 2.12 (m, 3H, CH_2 + H_5), 1.86 – 1.74 (m, 3H, H_{20} + CH_2), 1.73 (d, *J* = 1.2 Hz, 3H, CH_3), 1.72 – 1.66 (m, 1H, CH_2), 1.63 (s, 3H, CH_3), 1.52 – 1.47 (m, 2H, H_6 + H_{22}), 1.49 (s, 3H, CH_3), 1.29 – 1.19 (m, 1H, CH_2), 1.03 (s, 3H, CH_3), 1.00 (d, *J* = 6.4 Hz, 3H, CH_3), 0.94 (d, *J* = 6.3 Hz, 3H, CH_3), 0.90 (s, 9H, $SiC(CH_3)_3$), 0.89 – 0.96 (m, 6H, 2xCH_3), 0.90 (s, 9H, $SiC(CH_3)_3$), 0.86 (s, 9H, $SiC(CH_3)_3$), 0.10 (s, 3H, $SiCH_3$), 0.07 (s, 3H, $SiCH_3$), 0.06 (s, 3H, $SiCH_3$), 0.05 (s, 3H, $SiCH_3$), 0.04 (s, 3H, $SiCH_3$), 0.02 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, CD_2Cl_2): δ 195.8 (d), 162.1 (d), 160.3 (s), 136.1 (s), 135.5 (d), 135.5 (s), 132.7 (s), 131.7 (s), 127.9 (d, 2x), 126.5 (d), 113.8 (d, 2x), 101.7 (d), 87.8 (d), 77.5 (d), 77.3 (d), 74.3 (d), 68.7 (d), 55.8 (q), 55.3 (d), 42.6 (s), 41.0 (t), 40.3 (d), 40.2 (d), 39.8 (d), 39.0 (t), 37.4 (t), 34.2 (d), 30.7 (q), 29.8 (d), 26.3 (q, 3x), 26.3 (q, 3x), 26.2 (q, 3x), 22.2 (q), 22.0 (d), 20.1 (q), 19.0 (q), 18.51 (s), 18.48 (s), 18.46 (s), 17.7 (q), 9.3 (q), 6.4 (q), 5.7 (q) -3.4 (q), -3.90 (q), -3.92 (q), -4.3 (q), -4.4 (q), -4.5 (q) ppm.

Nahuoic acid A (1a).



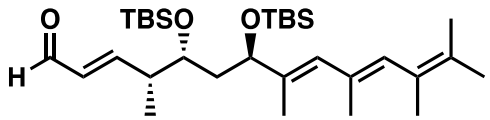
Si-exo **76** **1a, nahuoic acid A**

Octahydronaphthalene Carboxylic Acid 78. A solution of $NaClO_2$ (0.005 g, 0.052 mmol) and NaH_2PO_4 (0.007 g, 0.052 mmol) in H_2O (0.18 mL) was added dropwise for 10 minutes to a rapidly stirred solution of octahydronaphtalene **76** (0.01 g, 0.01 mmol) and 2-methyl-2-butene (0.036 mL, 0.34 mmol) in THF (0.53 mL) and *tert*-butanol (0.53 mL). The resultant solution was stirred for 12h at 25 °C. After that, a saturated aqueous solution of NH_4Cl was added and the aqueous layer was extracted with CH_2Cl_2 (3x). The combined organic layers were washed with brine, dried (Na_2SO_4) and the solvent

was evaporated. The residue was purified by flash-column chromatography (silica gel, 90:10 hexane/EtOAc) to afford 0.008 g (84%) of a white solid, which was identified as **78**, which was used in the next step without further purification.

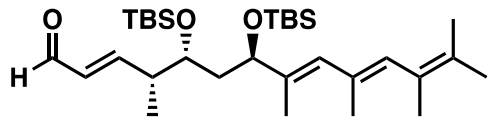
To a solution of protected nahuoic acid A **78** (7 mg, 0.007 mmol) in THF (0.50 mL) was added HCl (4N, 0.50 mL). The resulting mixture was stirred for 72 h at 20 ºC; then it was neutralized with a saturated aqueous solution of $NaHCO_3$ and acidified with an aqueous solution of TFA 1M until pH 1. The resulting solution was concentrated *in vacuo* and then lyophilized to remove H_2O. Salts were filtered through a pad of Celite washing with EtOAc and the solvent was removed under reduced pressure. The residue was then purified by HPLC (C12-silica gel, Synergi Max RP, 250 x 10 mm, 4 μm) with a linear gradient elution from 30% MeCN in water to 100% MeCN over 30 min, with a flow rate of 2.5 mL/min, to afford 0.8 mg (22% yield) of a white solid, which was identified as nahuoic acid A **1a**.[1] **Molecular formula:** $C_{30}H_{50}O_7$. **MW:** 522.72 g/mol. $\mathbf{[\alpha]_D^{21}}$ -6.58º (0.005, CH_2Cl_2). **^{1}H-NMR** (400.13 MHz, DMSO-d_6): δ 6.41 (d, *J* = 11.2 Hz, 1H, H_3), 5.15 (s, 1H, H_{11}), 4.98 (br s, 1H, H_{15}), 4.39 (br s, 1H, C7-O<u>H</u>), 4.33 (br d, *J* = 4.1 Hz, 1H, C21-O<u>H</u>), 4.31-4.25 (m, 2H, C17-O<u>H</u> + C19-O<u>H</u>), 4.24 (d, *J* = 5.8 Hz, 1H, C7-O<u>H</u>), 3.78 (d, *J* = 9.4 Hz, 1H, H_{19}), 3.62 – 3.53 (m, 2H, H_{17} + H_4), 3.52 – 3.46 (m, 2H, H_7 + H_4), 3.15 – 3.10 (m, 1H, H_{21}), 2.23 (d, *J* = 9.2 Hz, 1H, H_{13}), 2.11 – 1.99 (m, 1H, H_{16b}), 1.97 – 1.84 (m, 3H, H_6 + H_{16a} + H_{8eq}), 1.67 – 1.61 (m, 2H, H_{8ax} + H_{22}), 1.59 (s, 3H, CH_3), 1.53 (d, *J* = 12.6 Hz, 1H, H_5), 1.47 (s, 3H, CH_3), 1.45 – 1.41 (m, 2H, H_{18b} + H_{20}), 1.40 (s, 3H, CH_3), 1.28 – 1.12 (m, 1H, H_{18a}), 1.02 (s, 3H, CH_3), 0.87 (s, 3H, CH_3), 0.84 (d, *J* = 6.5 Hz, 3H, CH_3), 0.77 (d, *J* = 6.9 Hz, 3H, CH_3), 0.77 (d, *J* = 6.9 Hz, 3H, CH_3) ppm. **^{13}C NMR** (100.16 MHz, DMSO-d_6): δ 169.2 (s), 148.9 (d), 135.1 (s), 132.7 (s), 132.4 (d), 125.4 (d), 124.4 (s), 78.7 (d), 72.8 (d), 70.0 (d), 67.1 (d), 66.3 (d), 56.8 (d), 50.1 (d), 41.7 (t), 41.2 (s), 40.2 (t), 39.6 (d), 38.9 (d), 37.1 (t), 36.1 (d), 30.4 (d), 27.7 (q), 21.7 (q), 19.6 (q), 18.5 (q), 18.2 (q), 13.1 (q), 12.4 (q), 7.2 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{30}H_{51}O_7$ ($[M+H]^+$) 523.3629; found, 523.3630. **IR** (NaCl): ν 3412 (br, O-H), 2923 (m, C-H), 2855 (m, C-H), 1680 (m, C=O).

III. INTRAMOLECULAR DIELS-ALDER REACTIONS



MODEL 1

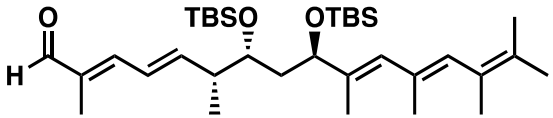
	Code	Conditions	Scale (mg)	comments
Lewis acid	**LG367**	Me_2AlCl (1.5 equiv), DCM (0.058M) -78°C → -20°C, 18 h	6	possible Prins product (?)
	LG370	Me_2AlCl (1.2 equiv), tol (0.058M) -10°C, 16 h	9	possible Prins product (?)
	LG377	Me_2AlCl (1.2 equiv), tol (0.058M) -78°C, 24 h	10	possible Prins product (?)
	LG379	Me_2AlCl (1.2 equiv), tol (0.058M) -78°C → -40°C, 40 h	1	**Total conversion to *Re*-endo**
	LG440	$B(C_6F_5)_3$ (10 mol%), DCM (0.076M) -78°C, 43 h	14	100% SM



MODEL 1

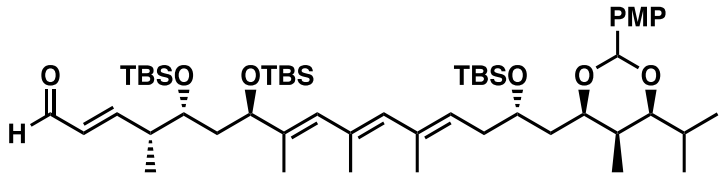
	Code	Conditions	Scale (mg)	comments
	LG442	$B(C_6F_5)_3$ (10 mol%), DCM (0.076M) -40°C, 40 h	13	100% SM
	LG446	$B(C_6F_5)_3$ (10 mol%), DCM (0.076M) -15°C, 26 h	13	SM + unidentified product
	LG451	$B(C_6F_5)_3$ (0.5 equiv), DCM (0.076M) -10°C, 24 h	13	**DA adducts could be formed, but the low mass unabled their characterization**

Lewis acid	**LG495**	$B(C_6F_5)_3$ (10 mol%), DCM (0.031M) -78°C → -10°C, 24 h	13	Complex mixture of diastereoisomers: issues to separate them by flash-column chromatography. Major product was ***Re*-endo**
	LG508	$B(C_6F_5)_3$ (10 mol%), DCM (0.016M) -78°C → -10°C, 28 h	90	
	LG551	$B(C_6F_5)_3$ (10 mol%), DCM (0.02M) -78°C → -10°C, 28 h	180	
Thermal cond.	**LG654**	BHT (10 mol%), tol (0.01M) 140°C → 180°C, 5 d	5	Mixture of DA adducts: ***Re*-exo/*Si*-exo/*Re*-endo (1.0/0.7/1.0) + sm (0.2)**
	LG683	BHT (10 mol%), *o*-xylene (0.01M) 200°C, 40 h	34	DA adducts were finally purified by FCC: ***Re*-exo/*Si*-exo/*Re*-endo: 32%/32%/17%**
	LG835	BHT (10 mol%), CD_3OD, 160°C, 14 h	8	**ratio *Re*-exo/*Si*-exo/*Re*-endo: 0.7/1/1** (from ^{1}H-NMR)



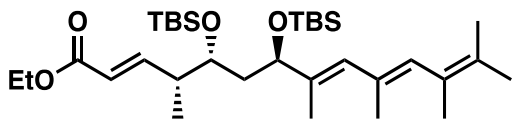
MODEL 2

	Code	Conditions	Scale (mg)	comments
Lewis acid	**LG664**	$B(C_6F_5)_3$ (10 mol%), DCM (0.02 M) -10°C, 28 h	50	Complex mixture of aldehydes → separation by FCC but need for HPLC
ther	**LG689**	BHT (10 mol%), *o*-xylene (0.01 M) 200°C, 40 h	48	Separation of 3 peaks by HPLC → **isolated** ***Re*-exo 39b/*Si*-exo 40b** **21%/17%**



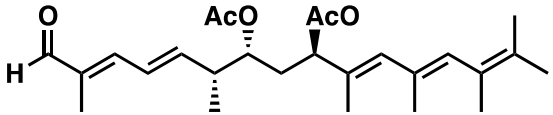
MODEL 3

	Code	Conditions	Scale (mg)	comments
Lewis acid	**LG667**	Me_2AlCl (1.2 equiv), tol (0.06M) -78°C → -40°C, 40 h	25	starting material (SM)
	LG669	Me_2AlCl (1.2 equiv), tol (0.06M) -78°C → -10°C, 48 h	20	**No SM**. Prins byproducts?
	LG679	$B(C_6F_5)_3$ (10 mol%), DCM (0.02 M) -10°C, 28 h	50	SM + byproducts (don't look like DA adducts)
	LG682	$B(C_6F_5)_3$ (10 mol%), DCM (0.02 M) rt, 3 d	30	Not clear if DA occurred. PMP deprotection
ther	**LG690**	BHT (10 mol%), *m*-xylene (0.01 M) 200°C, 40 h	42	HPLC purification: no DA adducts were isolated



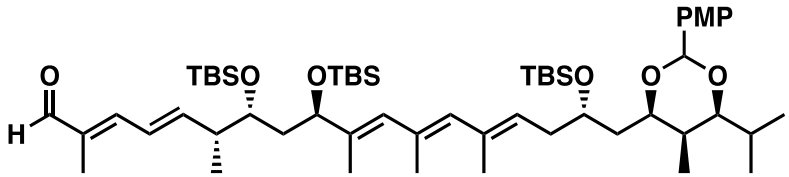
MODEL 4

	Code	Conditions	Scale (mg)	comments
thermal	**LG386**	BHT (10 mol%), tol (0.029 M), 165°C, 40 h	13	Decomposition
	LG388	BHT (10 mol%), tol (0.023 M), 80°C →110 °C, 40 h	10	Decomposition
	LG394	BHT (10 mol%), tol (0.011 M) 115°C, 40 h	5	Decomposition



MODEL 5

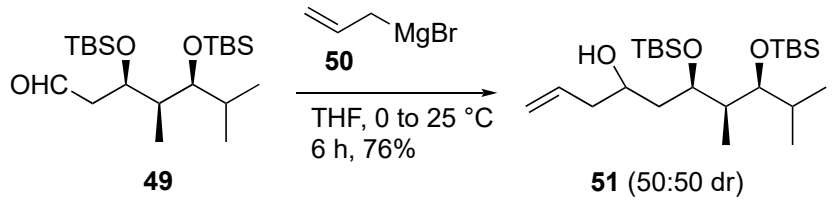
	Code	Conditions	Scale (mg)	comments
thermal	**LG811**	BHT (10 mol%), *m*-xylene (0.012 M) 200°C, 24 h	21	Decomposition
	LG814	BHT (10 mol%), tol (0.021 M) 80°C →150°C, 40 h	7	Degradation increases when raising T, reaction did not finish
	LG823	BHT (10 mol%), MeOH (0.031 M) 80°C, 20 h	10	Mixture of 2 products (cyclization cmp., unidentified + SM)
	LG829	BHT (10 mol%), MeOH (0.010 M) 80°C, 40 h	9	Same as in LG823: **no IMDA product**



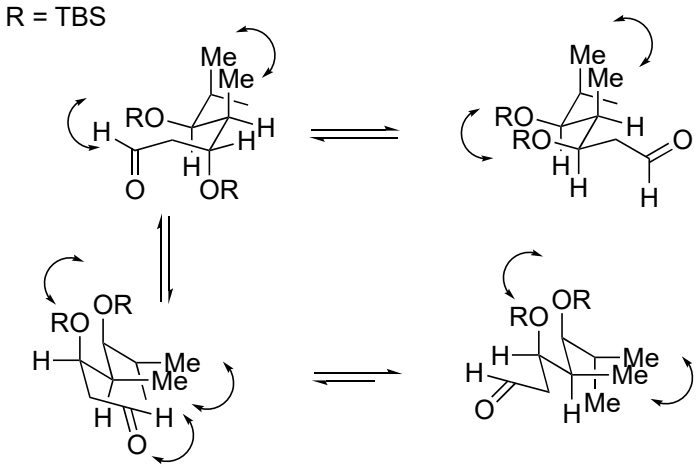
	Code	Conditions	Scale (mg)	comments
Thermal cond.	**LG776**	BHT (10 mol%), tol (0.004 M) 180°C, 18 h	3	Mixture of products that **could be DA adducts**
	LG778	BHT (10 mol%), tol (0.004M) 200°C, 40 h	37	HPLC conditions for separation were found
	LG804	BHT (10 mol%), tol (0.004M) 200°C, 18 h	31	***Re*-exo 75** and ***Re*-endo 77** adducts isolated
	LG834	BHT (10 mol%), CD_3OD (0.008 M) 80°C →170°C, 40 h	6	Reaction followed by ^{1}H-NMR. HPLC purification ***Re*-exo 75/*Si*-exo 76/*Re*-endo 77** **yieldS not determined**
	LG853	BHT (10 mol%), MeOH (0.008 M) 170°C, 27 h	41	***Re*-exo 75/*Si*-exo 76/*Re*-endo 77 17%/10%/9%** But *Si-exo* was obtained more pure
Lewis acid	**LG831**	$Eu(fod)_3$ (10 mol%), BHT, tol (0.008 M) 160°C, 17 h	6	Reaction followed by ^{1}H-NMR. HPLC purification ***Re*-exo 75/*Si*-exo 76/*Re*-endo 77** **40%/35%/23%**
	LG849	$Eu(fod)_3$ (10 mol%), BHT, tol (0.008 M) 160°C, 18 h	38	***Re*-exo 75/*Si*-exo 76/*Re*-endo 77 (32%/27%/14%)**

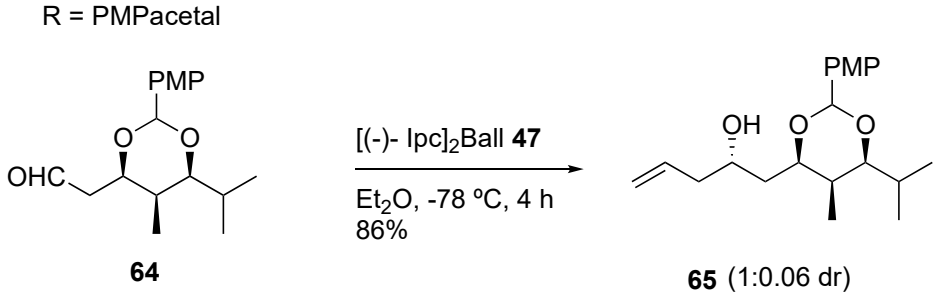
	LG867	$Eu(fod)_3$ (10 mol%), BHT, tol (0.008 M) 160°C, 24 h	38	***Re*-exo 75/*Si*-exo 76/*Re*-endo 77 (19%/12%/10%)**

IV. ADDITION OF ALLYL ORGANOMETALS TO ALDEHYDES

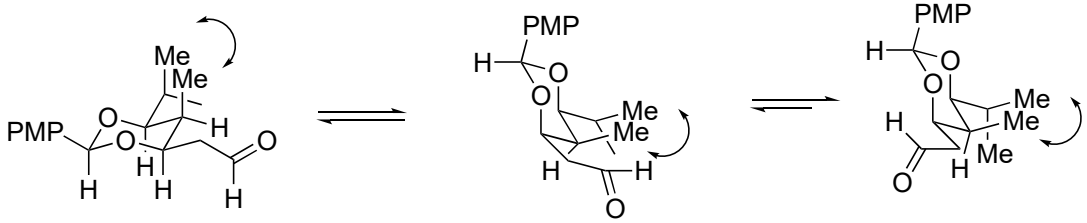


49 **51** (50:50 dr)





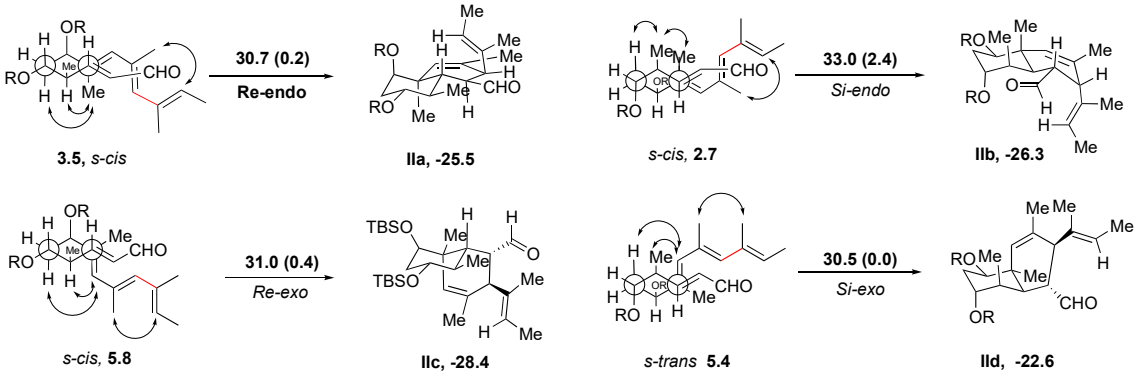
64 **65** (1:0.06 dr)



Scheme 1. Conformation of protected diols and structural destabilization by *syn*-pentane interactions.[2]

V. COMPUTATIONAL STUDIES

All calculations were carried out with the Gaussian 09 suite of programs.[3] Three different functionals were employed in the model system calculation for comparison, namely ωB97X-D,[4] M06-2X,[5] and B3LYP,[6] with Grimme's empirical dispersion correction (B3LYP-D3).[7] Each geometry was optimized at the ωB97XD/Def2SVP level,using the Def2SVP Ahlrichs basis set.[8] Minima and transition states were individually characterized by the analysis of the number of imaginary frequencies obtained through the computation of the normal mode vibrational analysis. To approach the effect of the reaction medium the SMD model,[9] which includes a solute surface area-dispersion term with toluene, DCM or MeOH as solvent, was used during the geometry optimization and single point calculations; thus solvent effects and corrections to the Gibbs energy were taken into account. IRC calculations[10] from every optimized TS was followed to their respective adjacent minima on the potential energy surface. To improve the quality of the computed energies, triple ζ computations, single point calculations were carried out over the optimized structures at the Def2TZVP basis set of Ahlrichs. Furthermore, the frequencies lower than 100 cm^{-1} were corrected using the anharmonic approximation proposed by Grimme,[11] using the software Goodvibes developed by Paton and coworkers[12] in order to obtain the corresponding Gibbs free energies.



Scheme 2. Representation of the four alternative transition states for the IMDA reaction of tetraenal model system computed using ωB97X-D.[4]).

Comparison of Functionals:

Three different functionals were used over the model system in order to evaluate their accuracy for these kind of intramolecular cyclization reactions. It was found that ωB97X-D[4] has the better agreement with experimental results. Furthermore, M06-2X[5] functional gives slightly worse results in terms of selectivity (the values obtained have bigger differences between ΔΔG of transition states than ωB97X-D[4]). Finally, in this case, B3LYP,[6] performed poorly. The values obtained suggest a complete selectivity for the *Si-Exo* approach which is not observed in the experiments.

Table 1: Results obtained using different functionals. All values are given in kcal/mol.

Structure	***Method***					
	ωB97X-D		M06-2X		B3LYP-D3	
	ΔG	ΔΔG	ΔG	ΔΔG	ΔG	ΔΔG
Re-Endo	30.7	0.2	28.9	0.0	28.1	1.0
Re-Exo	31.0	0.4	29.6	0.7	28.9	1.8
Si-Endo	33.0	2.4	32.5	3.6	30.3	3.1
Si-Exo	30.5	0.0	29.6	0.8	27.1	0.0

Model and solvent comparison:

Calculations were carried out for different model systems (model **I** with R= H and **II** with R= Me) and different solvents (toluene and MeOH). The energy values for both model systems are quite similar when the same solvent is used in the calculation. Specifically, in the case of using toluene as solvent the values for system II predict a slight decrease in energy barrier for *Re-Exo* approach and a similar increase for the corresponding *Re-Endo* approach. In any case, the expected result would be a mixture of diastereomers for both models. When methanol was used as solvent significant changes where observed in both the energy barriers and in the predicted selectivity. The barriers decreased in both cases and the difference between transition state energies increased, thus suggesting an improved selectivity.

Table 2: Energy values obtained for both model systems **I** and **II** using toluene and MeOH as solvent. All energies are given in kcal/mol.

Structure	***System Comparison***							
	I Toluene		**I** MeOH		**II** Toluene		**II** MeOH	
	ΔG	ΔΔG	ΔG	ΔΔG	ΔG	ΔΔG	ΔG	ΔΔG
Re-Endo	30.7	0.2	27.3	1.1	31.5	0.5	28.2	1.1
Re-Exo	31.0	0.4	28.8	2.6	31.2	0.2	27.7	0.6
Si-Endo	33.0	2.4	29.7	3.5	33.5	2.5	30.1	2.9
Si-Exo	30.5	0.0	26.2	0.0	31.0	0.0	27.2	0.0

Energy values:

System I, Toluene, ωB97X-D

Structure	SCF (Def2SVP)	SCF+ZPVE (Def2SVP)	H (Def2SVP)	T·S (Def2SVP)	G (Def2SVP)	ΔG (Def2SVP)	G Anhar (au)	G Anhar (kcal)	ΔG Anar	SCF (Def2TZVP)	G (Def2TZVP)	ΔG (Def2TZVP)	ΔΔG (Def2TZVP)
lineal-scis-scis	-1242536.7	-1242033.4	-1242002.6	83.0	-1242085.7	0.0	-1979.377	-1242078.9	0.0	-1243617.2	-1243159.4	0.0	
lineal-scis-stran	-1242535.7	-1242032.3	-1242001.5	83.8	-1242085.3	0.4	-1979.376	-1242078.1	0.8	-1243616.3	-1243158.7	0.7	
lineal-strans-scis	-1242536.7	-1242033.1	-1242002.4	82.5	-1242084.9	0.8	-1979.376	-1242078.4	0.5	-1243617.2	-1243158.9	0.5	
lineal-strans-strans	-1242534.8	-1242031.1	-1242000.4	83.0	-1242083.4	2.3	-1979.373	-1242076.5	2.4	-1243615.4	-1243157.1	2.3	
pp_Reendo	-1242534.2	-1242031.3	-1242000.4	83.0	-1242083.4	2.3	-1979.374	-1242076.7	2.2	-1243613.3	-1243155.9	3.5	
pp_Reexo	-1242532.5	-1242029.2	-1241998.4	82.3	-1242080.7	5.0	-1979.370	-1242074.4	4.5	-1243611.6	-1243153.6	5.8	
pp_Siendo	-1242534.4	-1242031.5	-1242000.6	83.8	-1242084.4	1.3	-1979.374	-1242077.3	1.6	-1243613.8	-1243156.7	2.7	
pp_Siexo	-1242533.9	-1242029.9	-1241999.4	81.8	-1242081.2	4.5	-1979.371	-1242074.9	4.0	-1243613.0	-1243154.0	5.4	
TSReendo	-1242511.7	-1242008.0	-1241978.4	79.2	-1242057.6	28.0	-1979.334	-1242051.9	27.1	-1243588.6	-1243128.7	30.7	0.2
TSReexo	-1242510.8	-1242007.7	-1241977.8	79.9	-1242057.7	28.0	-1979.334	-1242051.9	27.1	-1243587.4	-1243128.4	31.0	0.4
TSSiendo	-1242508.8	-1242005.0	-1241975.3	80.3	-1242055.5	30.1	-1979.330	-1242049.3	29.7	-1243586.0	-1243126.5	33.0	2.4
TSSiexo	-1242511.5	-1242007.5	-1241977.8	79.7	-1242057.5	28.1	-1979.333	-1242051.5	27.4	-1243588.8	-1243128.9	30.5	0.0
pf_Reendo	-1242575.9	-1242068.9	-1242039.8	77.1	-1242116.9	-31.2	-1979.430	-1242111.9	-32.9	-1243649.0	-1243184.9	-25.5	
pf_Reexo	-1242578.0	-1242071.6	-1242042.3	78.9	-1242121.2	-35.5	-1979.435	-1242115.4	-36.4	-1243650.5	-1243187.8	-28.4	
pf_Siendo	-1242576.1	-1242069.2	-1242039.9	78.1	-1242118.0	-32.3	-1979.431	-1242112.6	-33.7	-1243649.2	-1243185.7	-26.3	
pf_Siexo	-1242570.4	-1242064.1	-1242034.6	80.1	-1242114.7	-29.0	-1979.424	-1242108.3	-29.3	-1243644.1	-1243182.0	-22.6	

System I, Methanol, ωB97X-D

Structure	SCF (Def2SVP)	SCF+ZPVE (Def2SVP)	H (Def2SVP)	T·S (Def2SVP)	G (Def2SVP)	ΔG (Def2SVP)	G Anhar (au)	G Anhar (kcal)	ΔG Anar	SCF (Def2TZVP)	G (Def2TZVP)	ΔG (Def2TZVP)	ΔΔG (Def2TZVP)
lineal-scis-scis	-1242539.0	-1242036.4	-1242005.8	82.3	-1242088.1	0.4	-1979.381	-1242081.6	0.3	-1243620.1	-1243162.7	0.4	
lineal-scis-stran	-1242538.2	-1242035.5	-1242004.8	82.8	-1242087.7	0.8	-1979.380	-1242080.8	1.2	-1243619.5	-1243162.0	1.1	
lineal-strans-scis	-1242538.9	-1242036.6	-1242005.8	82.7	-1242088.5	0.0	-1979.382	-1242081.9	0.0	-1243620.0	-1243163.1	0.0	
lineal-strans-strans	-1242537.5	-1242034.4	-1242003.9	82.2	-1242086.1	2.4	-1979.378	-1242079.5	2.5	-1243618.7	-1243160.7	2.4	
pp_Reendo	-1242537.1	-1242035.4	-1242004.6	82.6	-1242087.1	1.3	-1979.380	-1242080.7	1.2	-1243617.0	-1243160.6	2.5	
pp_Reexo	-1242534.8	-1242032.4	-1242001.7	81.9	-1242083.7	4.8	-1979.375	-1242077.4	4.5	-1243614.5	-1243157.1	6.0	
pp_Siendo	-1242538.1	-1242035.8	-1242005.1	82.4	-1242087.5	1.0	-1979.380	-1242081.0	0.9	-1243617.9	-1243160.9	2.2	
pp_Siexo	-1242537.1	-1242034.4	-1242003.9	82.1	-1242086.0	2.5	-1979.378	-1242079.5	2.5	-1243616.3	-1243158.7	4.4	
TSReendo	-1242516.8	-1242014.0	-1241984.3	79.0	-1242063.4	25.1	-1979.343	-1242057.7	24.2	-1243594.9	-1243135.8	27.3	1.1
TSReexo	-1242514.8	-1242012.6	-1241982.8	79.3	-1242062.2	26.3	-1979.342	-1242056.6	25.4	-1243592.5	-1243134.3	28.8	2.6
TSSiendo	-1242514.3	-1242011.2	-1241981.6	79.5	-1242061.2	27.3	-1979.339	-1242055.2	26.8	-1243592.6	-1243133.4	29.7	3.5
TSSiexo	-1242517.0	-1242014.2	-1241984.5	80.0	-1242064.4	24.0	-1979.345	-1242058.5	23.5	-1243595.4	-1243136.9	26.2	0.0
pf_Reendo	-1242578.0	-1242071.9	-1242042.9	76.6	-1242119.6	-31.1	-1979.434	-1242114.7	-32.8	-1243651.6	-1243188.3	-25.2	
pf_Reexo	-1242573.1	-1242067.8	-1242038.4	79.2	-1242117.6	-29.1	-1979.429	-1242111.5	-29.6	-1243647.3	-1243185.8	-22.7	
pf_Siendo	-1242578.2	-1242072.1	-1242042.9	77.6	-1242120.5	-32.0	-1979.435	-1242115.3	-33.3	-1243651.7	-1243188.8	-25.7	
pf_Siexo	-1242572.4	-1242067.0	-1242037.6	78.9	-1242116.5	-28.0	-1979.428	-1242110.6	-28.7	-1243646.5	-1243184.7	-21.6	

System II, Toluene, ωB97X-D

Structure	SCF (Def2SVP)	SCF+ZPVE (Def2SVP)	H (Def2SVP)	T·S (Def2SVP)	G (Def2SVP)	ΔG (Def2SVP)	G Anhar (au)	G Anhar (kcal)	ΔG Anar	SCF (Def2TZVP)	G (Def2TZVP)	ΔG (Def2TZVP)	ΔΔG (Def2TZVP)
lineal-scis-scis	-1267184.5	-1266663.6	-1266632.0	85.1	-1266717.1	0.0	-2018.629	-1266710.0	0.0	-1268290.6	-1267816.1	0.0	
lineal-scis-stran	-1267182.5	-1266662.1	-1266630.1	86.3	-1266716.5	0.6	-2018.628	-1266709.0	1.0	-1268288.8	-1267815.3	0.8	
lineal-strans-scis	-1267184.6	-1266663.5	-1266631.9	85.1	-1266717.0	0.1	-2018.629	-1266709.9	0.1	-1268290.7	-1267816.0	0.0	
lineal-strans-strans	-1267182.4	-1266661.5	-1266629.7	85.5	-1266715.2	1.9	-2018.626	-1266708.0	2.0	-1268288.6	-1267814.2	1.9	
TSReendo	-1267158.4	-1266637.2	-1266606.6	81.3	-1266687.9	29.2	-2018.584	-1266681.9	28.1	-1268261.1	-1267784.6	31.5	0.5
TSReexo	-1267159.7	-1266638.4	-1266607.9	80.4	-1266688.3	28.8	-2018.586	-1266682.7	27.3	-1268261.9	-1267784.9	31.2	0.2
TSSiendo	-1267155.9	-1266634.3	-1266603.7	82.6	-1266686.3	30.8	-2018.581	-1266679.5	30.4	-1268258.8	-1267782.5	33.5	2.5
TSSiexo	-1267159.3	-1266637.8	-1266607.2	80.9	-1266688.2	28.9	-2018.585	-1266682.4	27.6	-1268261.9	-1267785.0	31.0	0.0

System II, Methanol, ωB97X-D

Structure	SCF (Def2SVP)	SCF+ZPVE (Def2SVP)	H (Def2SVP)	T·S (Def2SVP)	G (Def2SVP)	ΔG (Def2SVP)	G Anhar (au)	G Anhar (kcal)	ΔG Anar	SCF (Def2TZVP)	G (Def2TZVP)	ΔG (Def2TZVP)	ΔΔG (Def2TZVP)
lineal-scis-scis	-1267186.8	-1266667.1	-1266635.4	85.1	-1266720.5	0.0	-2018.635	-1266713.5	0.0	-1268293.5	-1267820.2	0.0	
lineal-scis-stran	-1267184.8	-1266665.4	-1266633.5	85.7	-1266719.2	1.3	-2018.632	-1266711.9	1.5	-1268291.7	-1267818.8	1.4	
lineal-strans-scis	-1267186.6	-1266666.9	-1266635.2	85.4	-1266720.5	0.0	-2018.635	-1266713.4	0.1	-1268293.3	-1267820.1	0.1	
lineal-strans-strans	-1267184.6	-1266664.6	-1266632.9	85.2	-1266718.1	2.4	-2018.631	-1266711.0	2.4	-1268291.3	-1267817.8	2.4	
TSReendo	-1267164.1	-1266643.7	-1266613.2	80.8	-1266694.0	26.5	-2018.594	-1266688.2	25.3	-1268267.9	-1267791.9	28.2	1.1
TSReexo	-1267164.4	-1266644.4	-1266613.8	81.2	-1266695.0	25.5	-2018.596	-1266689.1	24.3	-1268267.7	-1267792.5	27.7	0.6
TSSiendo	-1267162.3	-1266641.5	-1266611.0	81.1	-1266692.1	28.4	-2018.591	-1266686.0	27.4	-1268266.3	-1267790.1	30.1	2.9
TSSiexo	-1267164.8	-1266644.6	-1266613.9	81.3	-1266695.2	25.3	-2018.596	-1266689.3	24.2	-1268268.5	-1267793.0	27.2	0.0

System I, Toluene, M06-2X

Structure	SCF (Def2SVP)	SCF+ZPVE (Def2SVP)	H (Def2SVP)	T·S (Def2SVP)	G (Def2SVP)	ΔG (Def2SVP)	G Anhar (au)	G Anhar (kcal)	ΔG Anar	SCF (Def2TZVP)	G (Def2TZVP)	ΔG (Def2TZVP)	ΔΔG (Def2TZVP)
lineal-scis-scis	-1242316.9	-1241815.0	-1241784.0	82.9	-1241867.0	0.6	-1979.029	-1241860.5	0.3	-1243445.3	-1242988.8	0.4	
lineal-scis-stran	-1242316.3	-1241814.2	-1241783.3	83.5	-1241866.8	0.8	-1979.028	-1241859.9	0.9	-1243444.7	-1242988.2	0.9	
lineal-strans-scis	-1242317.3	-1241815.1	-1241784.2	83.4	-1241867.6	0.0	-1979.030	-1241860.8	0.0	-1243445.6	-1242989.2	0.0	
lineal-strans-strans	-1242315.8	-1241813.5	-1241782.6	83.9	-1241866.4	1.2	-1979.027	-1241859.4	1.5	-1243444.1	-1242987.7	1.5	
pp_Reendo	-1242314.6	-1241813.0	-1241782.1	83.5	-1241865.6	2.0	-1979.026	-1241858.8	2.0	-1243442.0	-1242986.1	3.0	
pp_Reexo	-1242312.7	-1241810.8	-1241779.9	82.8	-1241862.7	4.9	-1979.022	-1241856.2	4.6	-1243439.7	-1242983.3	5.9	
pp_Siendo	-1242314.3	-1241812.3	-1241781.4	83.5	-1241864.9	2.7	-1979.025	-1241858.0	2.8	-1243441.5	-1242985.2	4.0	
pp_Siexo	-1242314.2	-1241811.6	-1241780.8	82.2	-1241863.0	4.5	-1979.023	-1241856.7	4.1	-1243440.9	-1242983.5	5.7	
TSReendo	-1242293.4	-1241791.1	-1241761.4	79.4	-1241840.8	26.8	-1978.988	-1241835.1	25.8	-1243418.7	-1242960.3	28.9	0.0
TSReexo	-1242292.8	-1241790.7	-1241760.8	79.4	-1241840.3	27.3	-1978.988	-1241834.7	26.1	-1243417.7	-1242959.6	29.6	0.7
TSSiendo	-1242289.7	-1241787.2	-1241757.4	80.0	-1241837.4	30.2	-1978.982	-1241831.3	29.5	-1243415.2	-1242956.7	32.5	3.6
TSSiexo	-1242292.6	-1241790.1	-1241760.2	79.6	-1241839.9	27.7	-1978.987	-1241834.0	26.8	-1243418.1	-1242959.5	29.6	0.8
pf_Reendo	-1242353.2	-1241847.5	-1241818.3	77.4	-1241895.7	-28.1	-1979.077	-1241890.6	-29.8	-1243475.1	-1243012.5	-23.4	
pf_Reexo	-1242355.8	-1241850.7	-1241821.4	78.3	-1241899.7	-32.1	-1979.083	-1241894.2	-33.4	-1243477.1	-1243015.6	-26.4	
pf_Siendo	-1242353.2	-1241847.8	-1241818.3	78.8	-1241897.0	-29.5	-1979.078	-1241891.5	-30.7	-1243475.2	-1243013.5	-24.3	
pf_Siexo	-1242348.0	-1241842.7	-1241813.2	79.7	-1241892.9	-25.3	-1979.071	-1241886.7	-25.9	-1243470.5	-1243009.2	-20.0	

System I, Toluene, B3LYP-D3

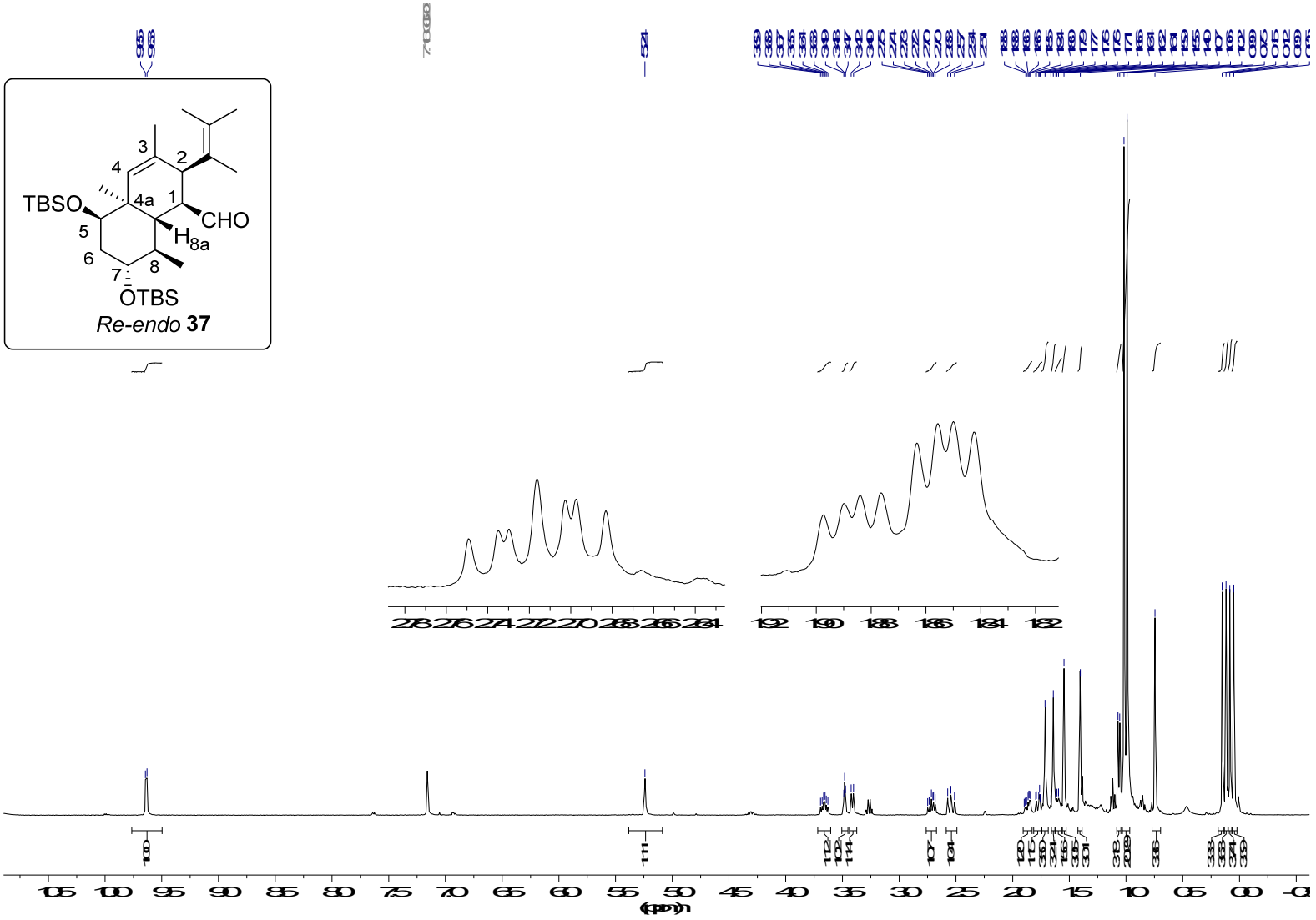
Structure	SCF (Def2SVP)	SCF+ZPVE (Def2SVP)	H (Def2SVP)	T·S (Def2SVP)	G (Def2SVP)	ΔG (Def2SVP)	G Anhar (au)	G Anhar (kcal)	ΔG Anar	SCF (Def2TZVP)	G (Def2TZVP)	ΔG (Def2TZVP)	ΔΔG (Def2TZVP)
lineal-scis-scis	-1242864.5	-1242365.6	-1242334.6	84.2	-1242418.8	0.0	-1979.9	-1242411.6	0.0	-1243976.4	-1243523.5	0.0	
lineal-scis-stran	-1242864.1	-1242365.1	-1242334.0	84.7	-1242418.6	0.2	-1979.9	-1242411.2	0.5	-1243975.9	-1243523.0	0.5	
lineal-strans-scis	-1242865.1	-1242365.9	-1242335.0	83.4	-1242418.4	0.4	-1979.9	-1242411.6	0.0	-1243976.9	-1243523.4	0.1	
lineal-strans-strans	-1242864.7	-1242365.2	-1242334.4	83.3	-1242417.6	1.2	-1979.9	-1242410.7	0.9	-1243976.3	-1243522.4	1.1	
pp_Reendo	-1242862.1	-1242363.2	-1242332.3	82.7	-1242415.1	3.7	-1979.9	-1242408.6	3.1	-1243972.5	-1243519.0	4.5	
pp_Reexo	-1242860.6	-1242361.4	-1242330.7	82.2	-1242412.9	5.9	-1979.9	-1242406.6	5.0	-1243970.7	-1243516.7	6.9	
pp_Siendo	-1242862.6	-1242363.8	-1242332.8	83.6	-1242416.4	2.4	-1979.9	-1242409.5	2.1	-1243973.3	-1243520.3	3.3	
pp_Siexo	-1242862.6	-1242362.7	-1242332.0	81.8	-1242413.8	5.0	-1979.9	-1242407.7	4.0	-1243972.6	-1243517.7	5.8	
TSReendo	-1242842.7	-1242343.4	-1242313.5	79.8	-1242393.3	25.5	-1979.9	-1242387.4	24.2	-1243950.7	-1243495.4	28.1	1.0
TSReexo	-1242841.5	-1242342.4	-1242312.5	80.0	-1242392.4	26.4	-1979.9	-1242386.6	25.0	-1243949.5	-1243494.6	28.9	1.8
TSSiendo	-1242840.0	-1242340.7	-1242310.7	80.6	-1242391.4	27.4	-1979.9	-1242385.0	26.6	-1243948.2	-1243493.3	30.3	3.1
TSSiexo	-1242843.3	-1242343.9	-1242314.0	80.2	-1242394.2	24.6	-1979.9	-1242388.2	23.5	-1243951.5	-1243496.4	27.1	0.0
pf_Reendo	-1242891.9	-1242388.9	-1242359.8	77.6	-1242437.4	-18.6	-1979.9	-1242432.1	-20.5	-1243996.1	-1243536.3	-12.8	
pf_Reexo	-1242893.7	-1242391.4	-1242362.1	78.5	-1242440.6	-21.8	-1979.9	-1242435.0	-23.4	-1243997.6	-1243539.0	-15.4	
pf_Siendo	-1242892.1	-1242389.4	-1242360.0	78.3	-1242438.3	-19.5	-1979.9	-1242432.8	-21.2	-1243996.4	-1243537.1	-13.5	
pf_Siexo	-1242885.9	-1242383.7	-1242354.2	79.6	-1242433.8	-15.0	-1979.9	-1242427.6	-16.0	-1243991.1	-1243532.8	-9.3	

VI. REFERENCES

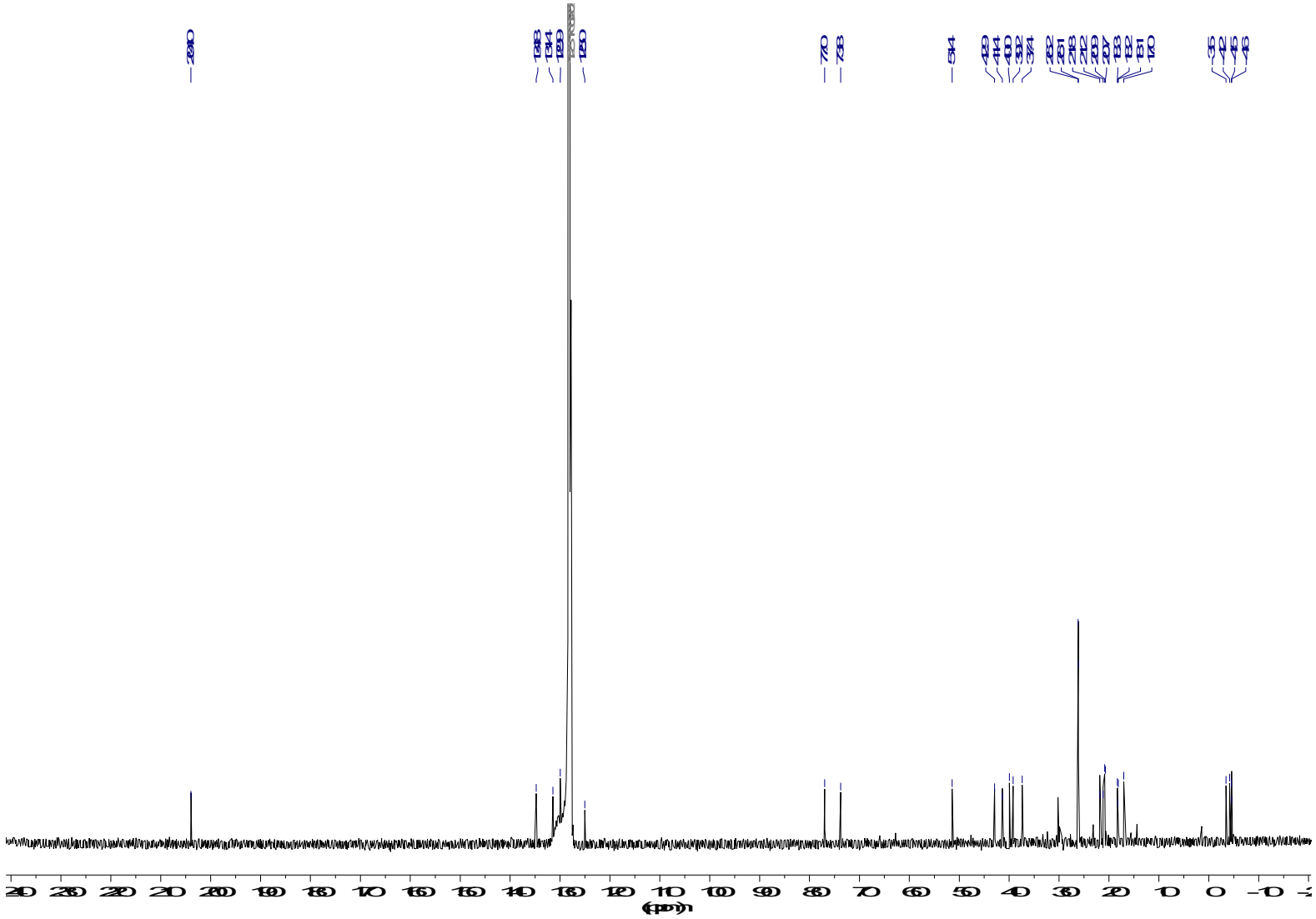
1. D. E. Williams, D. S. Dalisay, F. Li, J. Amphlett, W. Maneerat, M. A. G. Chavez, Y. A. Wang, T. Matainaho, W. Yu, P. J. Brown, C. H. Arrowsmith, M. Vedadi and R. J. Andersen, *Org. Lett.*, **2013**, *15*, 414-417.
2. G. Stork and S. D. Rychnovsky, *J. Am. Chem. Soc*., **1987**, *109*, 1565-1567.
3. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision B.01, in *Gaussian 09, Revision B.01, Gaussian, Inc., Wallingford CT*, Wallingford CT2009.
4. J.-D. Chai and M. Head-Gordon, *PhysChemChemPhys*, **2008**, *10*, 6615-6620.
5. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc*., **2008**, *120*, 215-241.
6. A. D. Becke, Phys. Rev. A., 1988, 38; C. Lee, W. Yang and R. G. Parr, P*hys. Rev. B: Cond. Matter*, **1988**, *37*, 785-789.
7. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys*., **2010**, *132*, 154104-154119.
8. (a) F. Weigend and R. Ahlrichs, Phys. Chem. Chem. Phys., **2005**, *7*, 3297-3305; (b) F. Weigend, *Phys. Chem. Chem. Phys*., **2006**, *8*, 1057-1065.
9. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, **2009**, *113*, 6378-6396.
10. (a) K. Fukui, *Acc. Chem. Res.*, **1981**, *14*, 363-368; (b) C. González and H. B. Schlegel, *J. Phys. Chem*., **1990**, *94*, 5523-5527; (c) H. P. Hratchian and H. B. Schlegel, in *Theory and Applications of Computational Chemistry*, ed. C. E. Dykstra, G. Frenking, K. S. Kim and G. E. Scuseria, Elsevier, Amsterdam 2005, pp. 195-249.
11. S. Grimme, *Chem. - Eur. J*., **2012**, *18*, 9955-9964.
12. G. Luchini, J. Alegre-Requena, I. Funes-Ardoiz and R. Paton, *F1000Research* **2020**, 9.

VII. NMR SPECTRA:

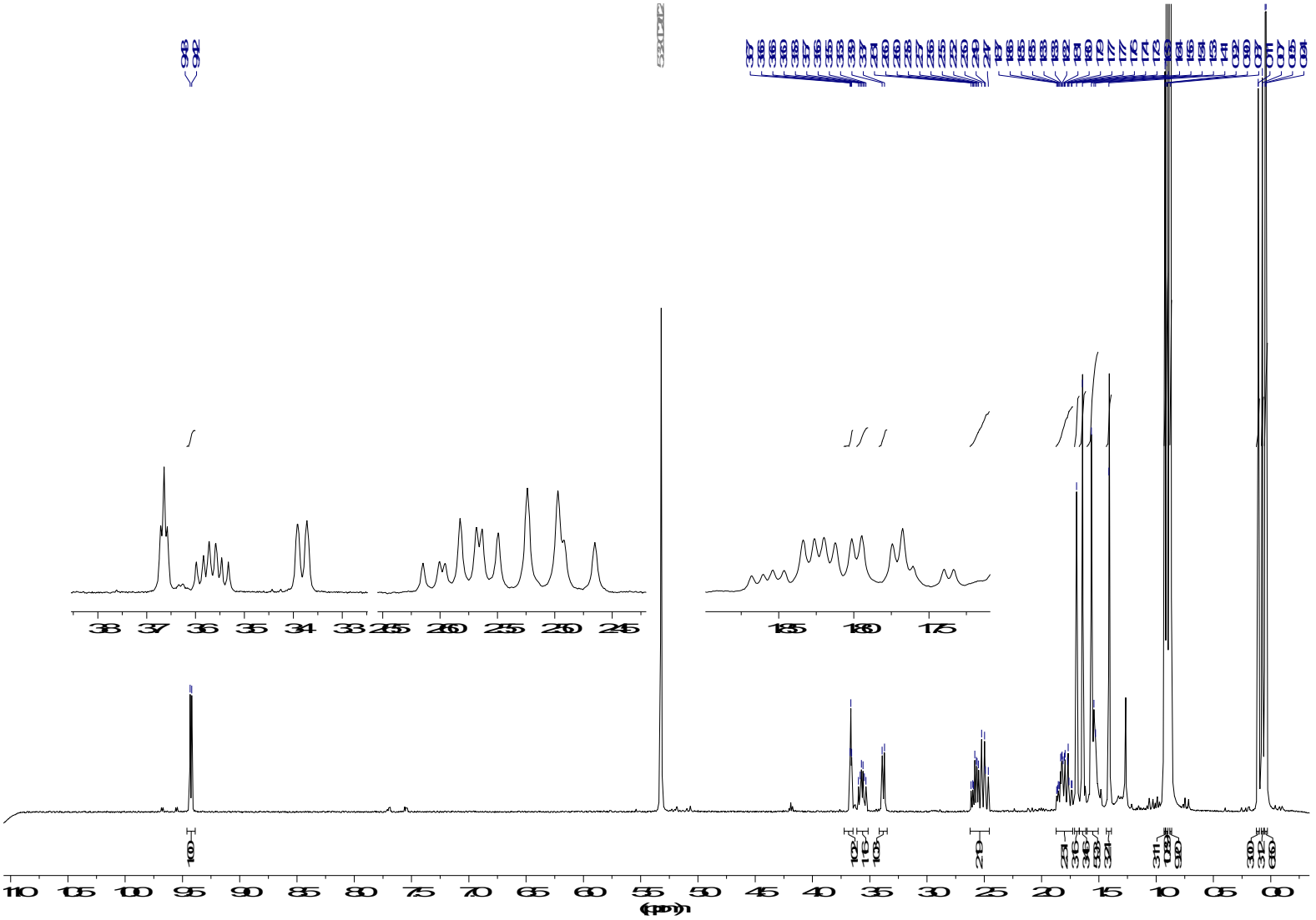
^{1}H-NMR (400.13 MHz, C_6D_6)



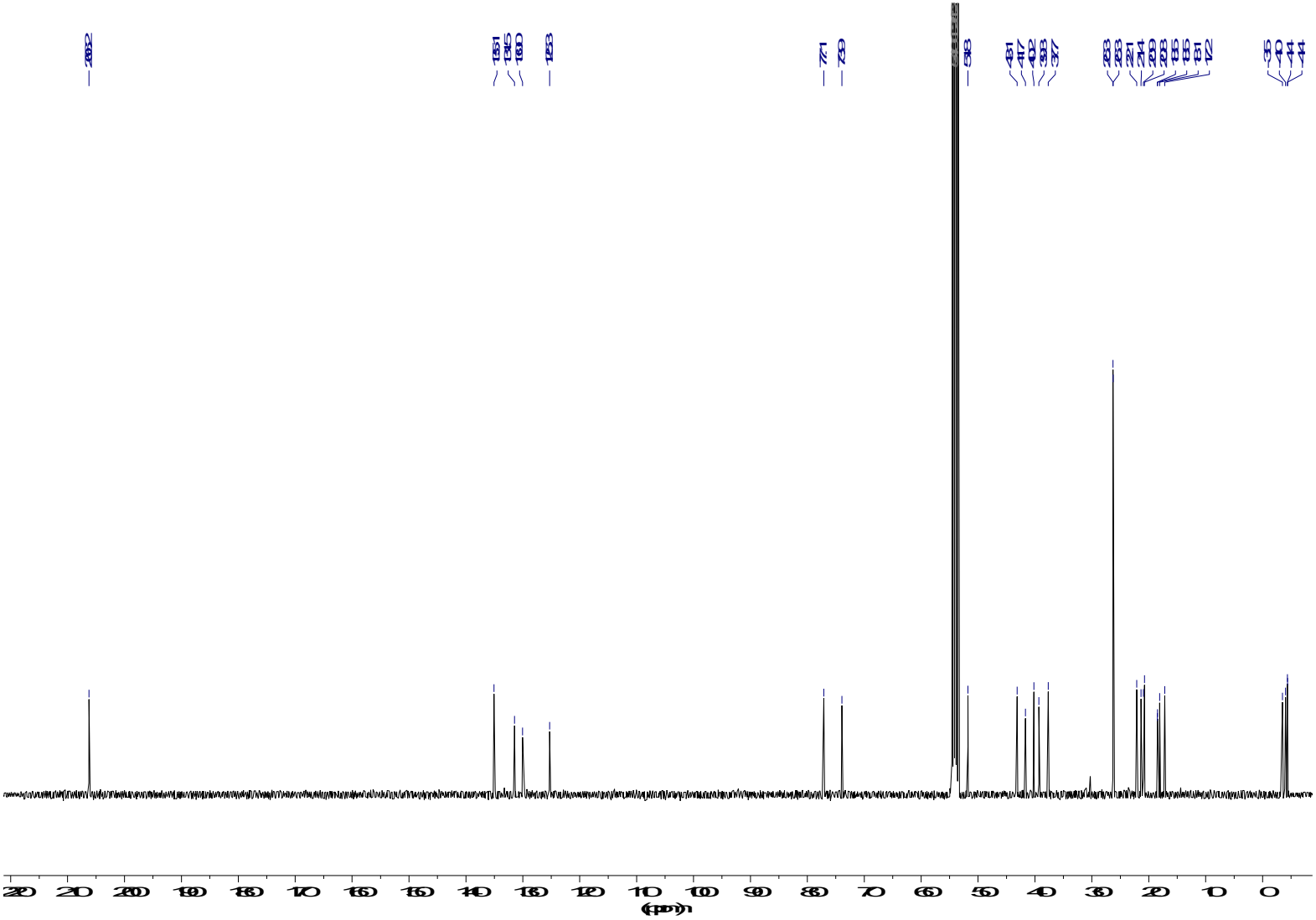
^{13}C-NMR (100.13 MHz, C_6D_6)



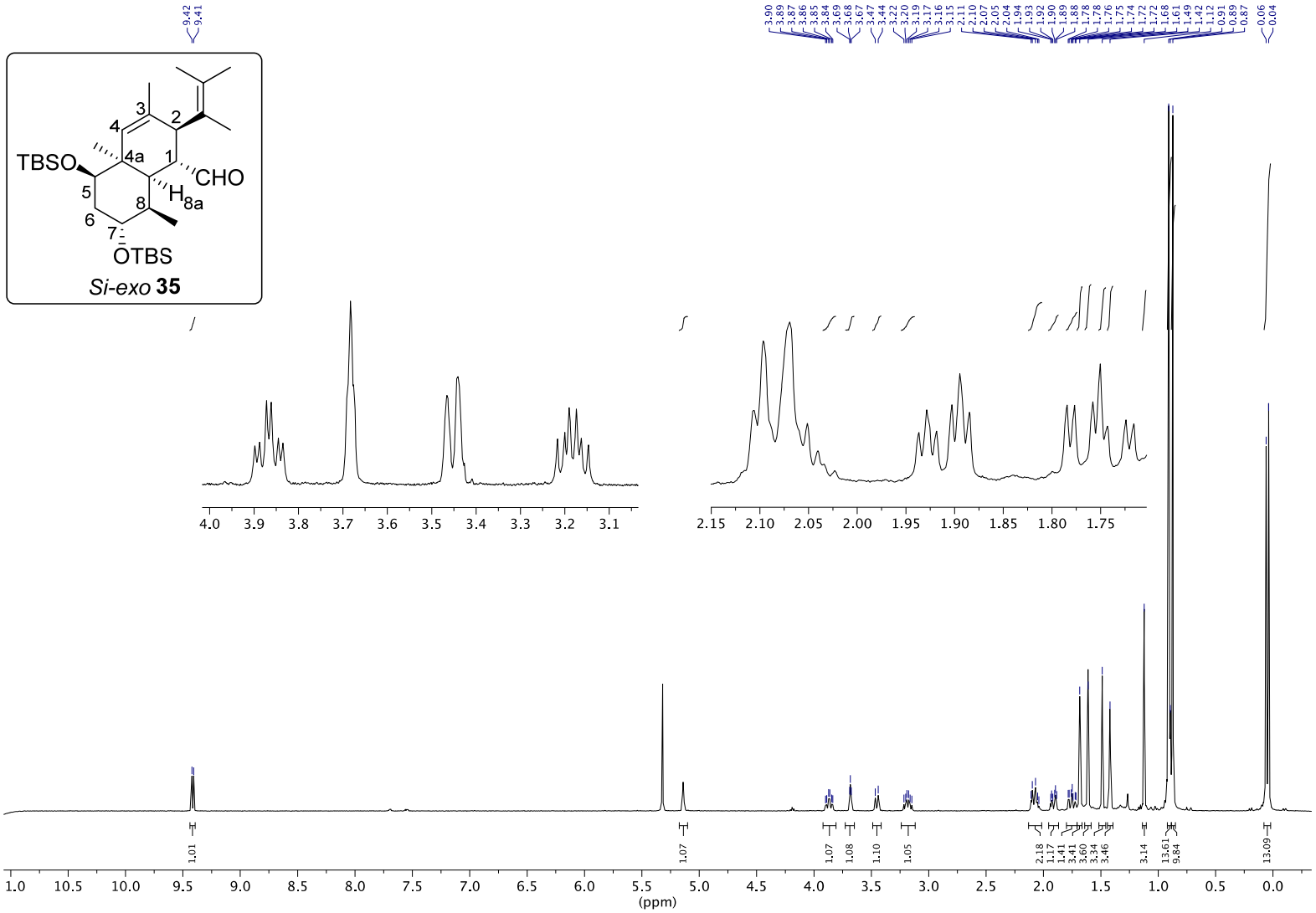
^{1}H-NMR (400.13 MHz, CD_2Cl_2)



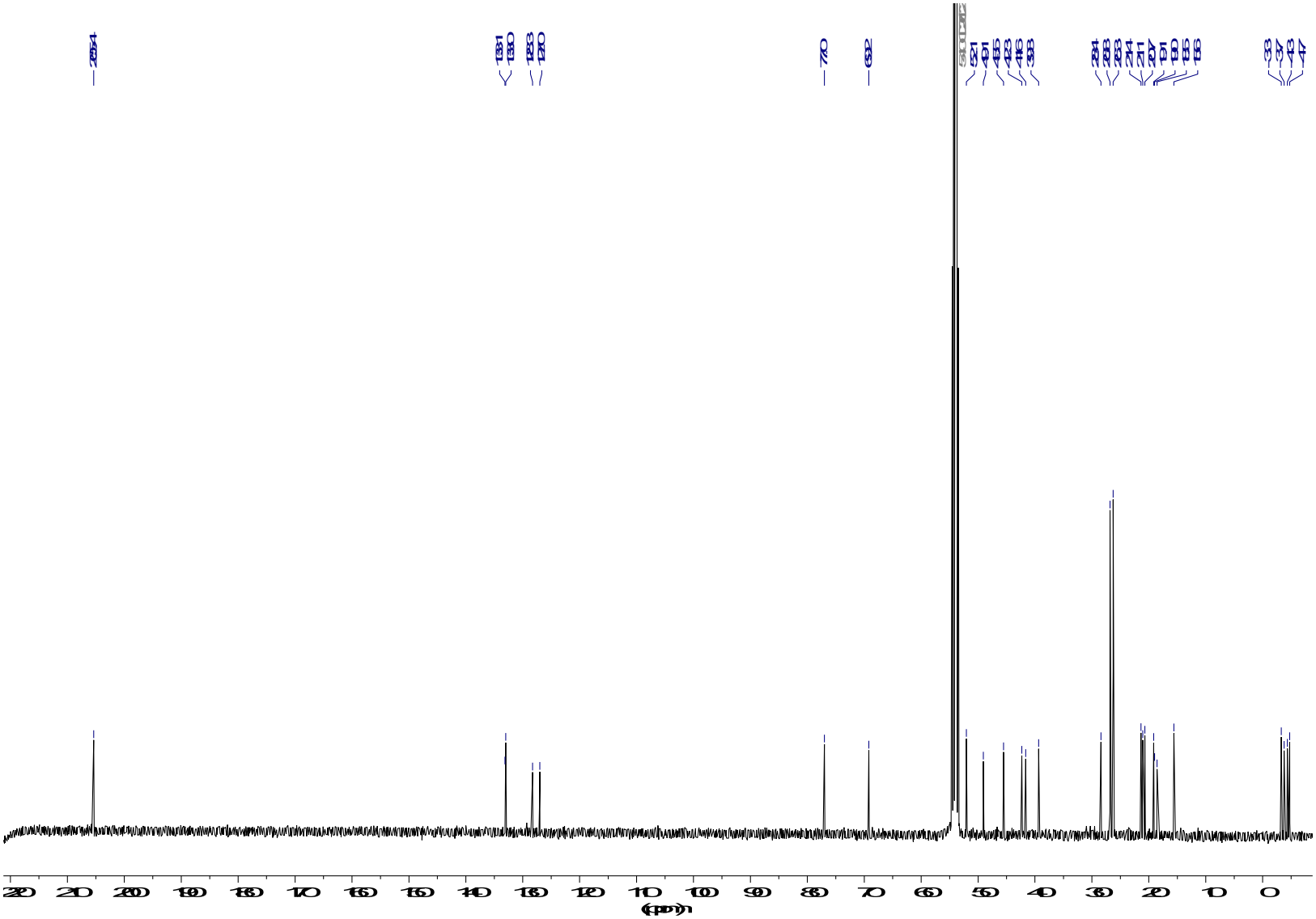
^{13}C-NMR (100.13 MHz, CD_2Cl_2)



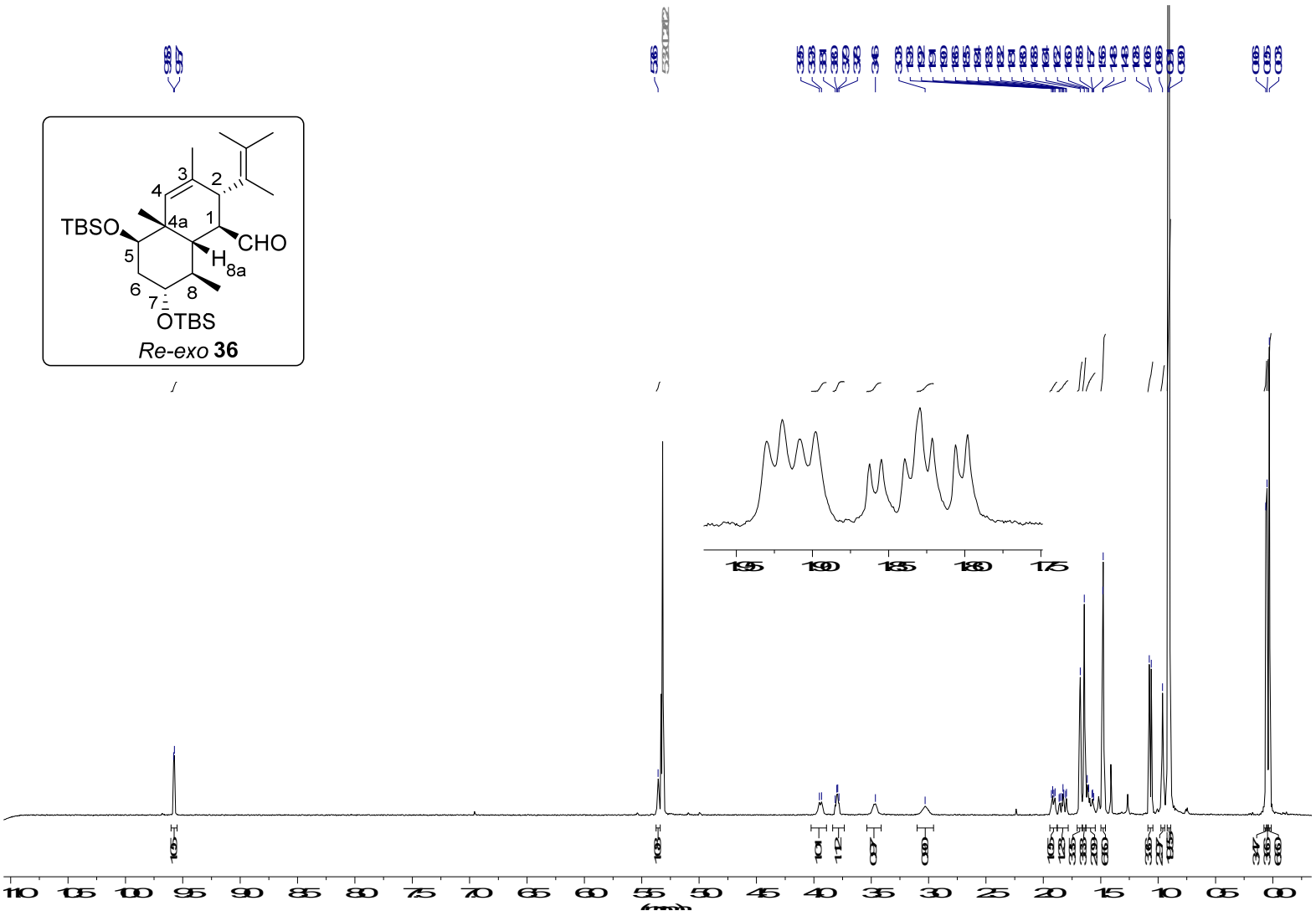
^{1}H-NMR (400.13 MHz, CD_2Cl_2)



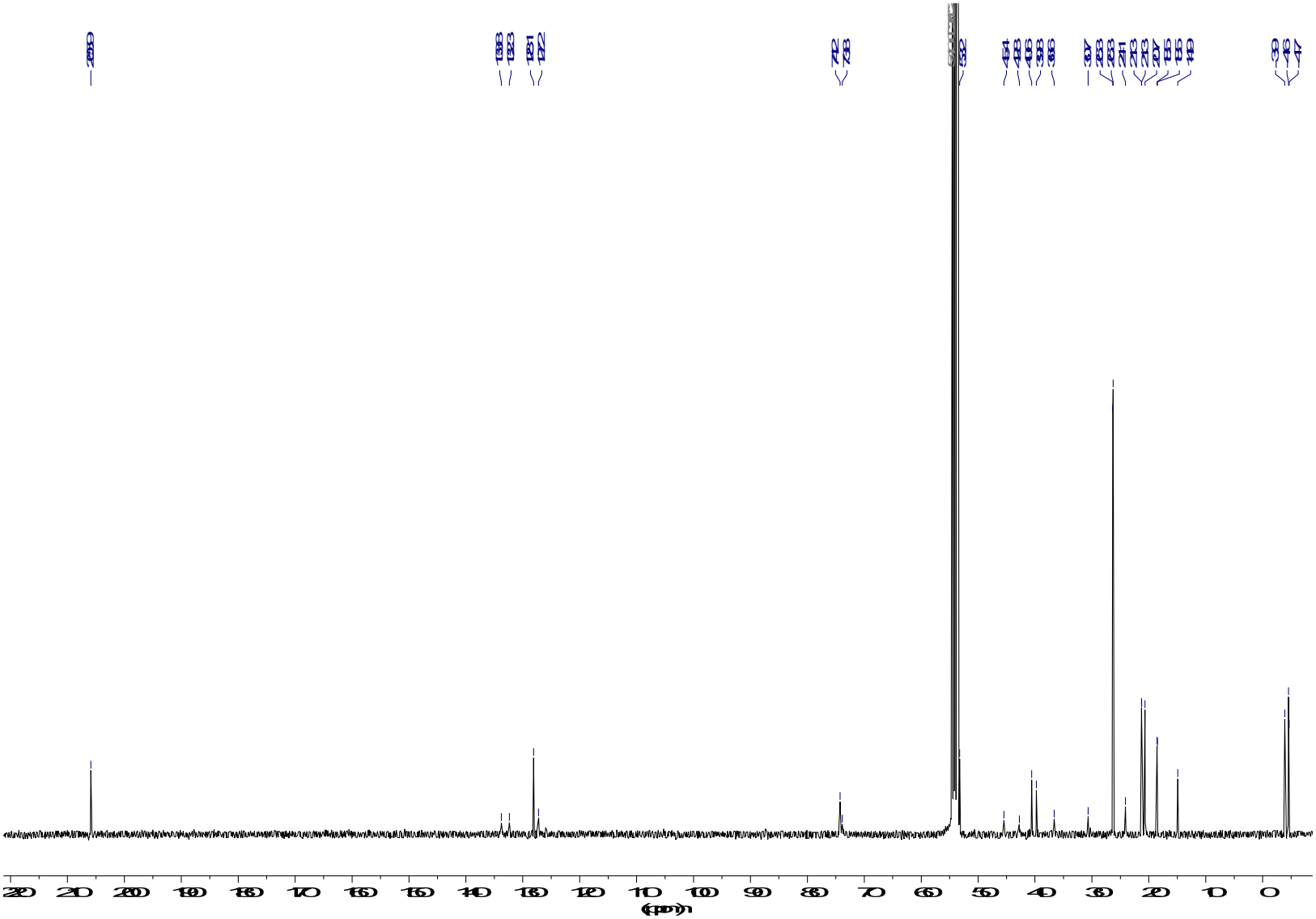
^{13}C-NMR (100.13 MHz, CD_2Cl_2)



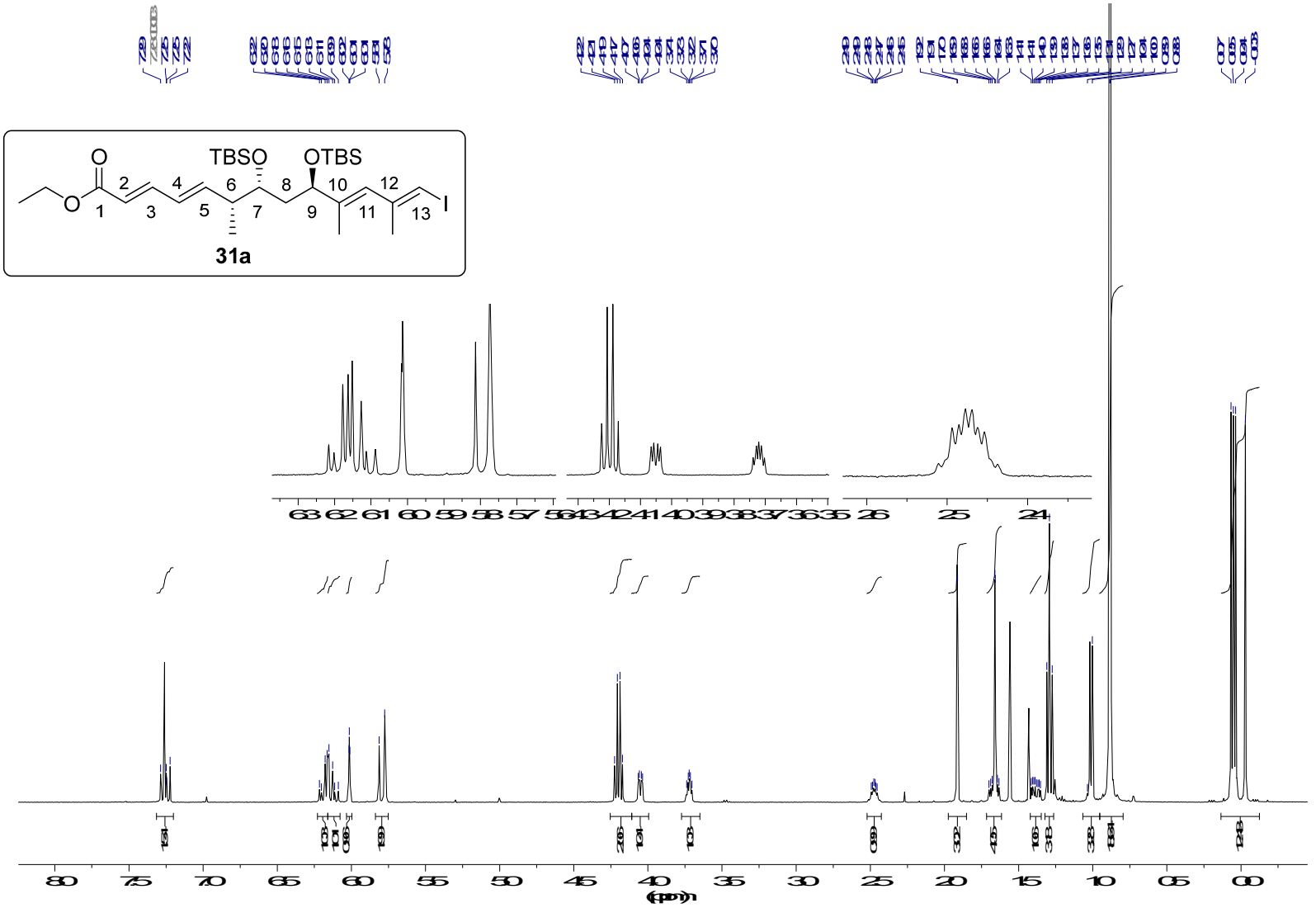
^{1}H-NMR (400.13 MHz, CD_2Cl_2)



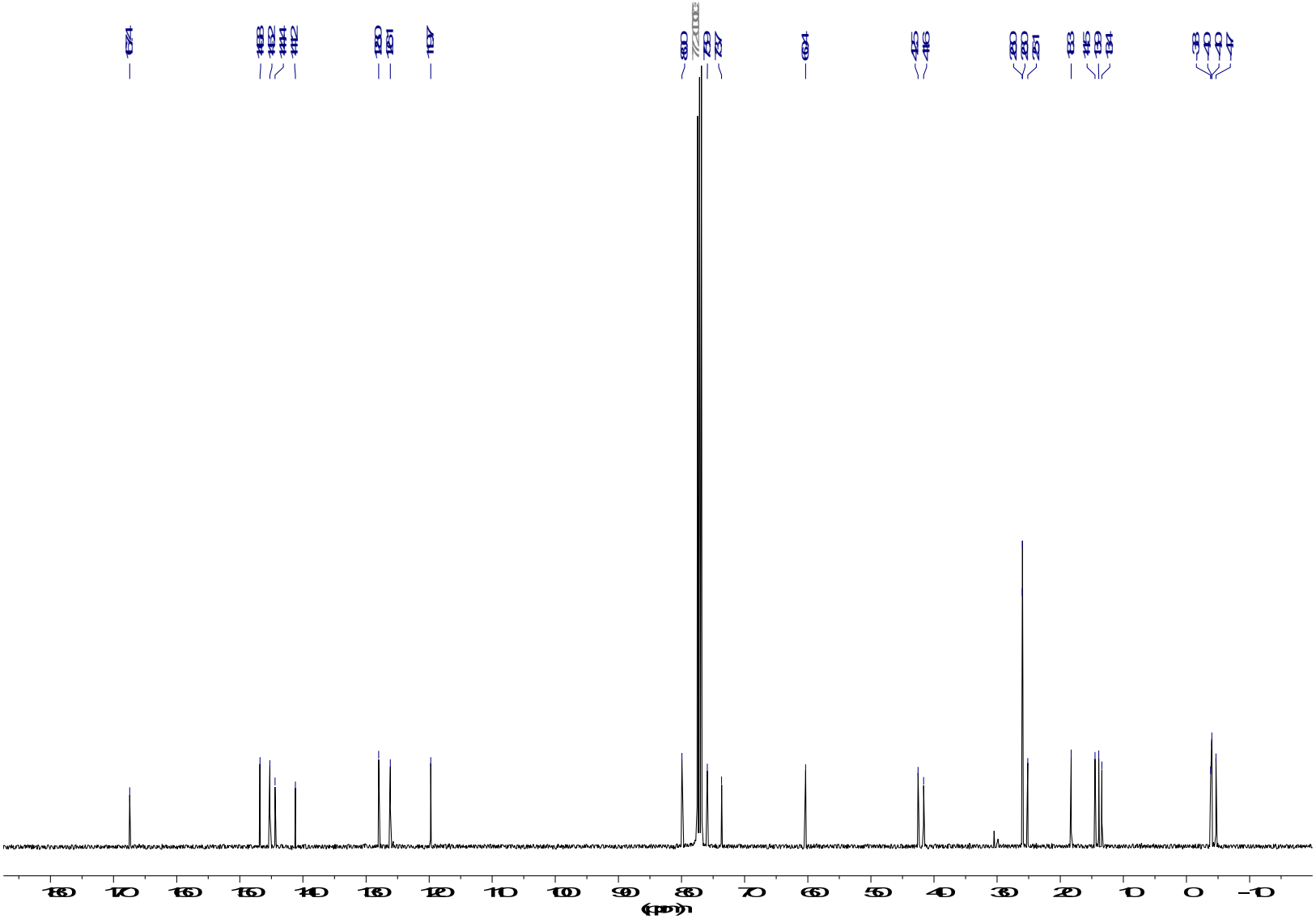
^{13}C-NMR (100.13 MHz, CD_2Cl_2)



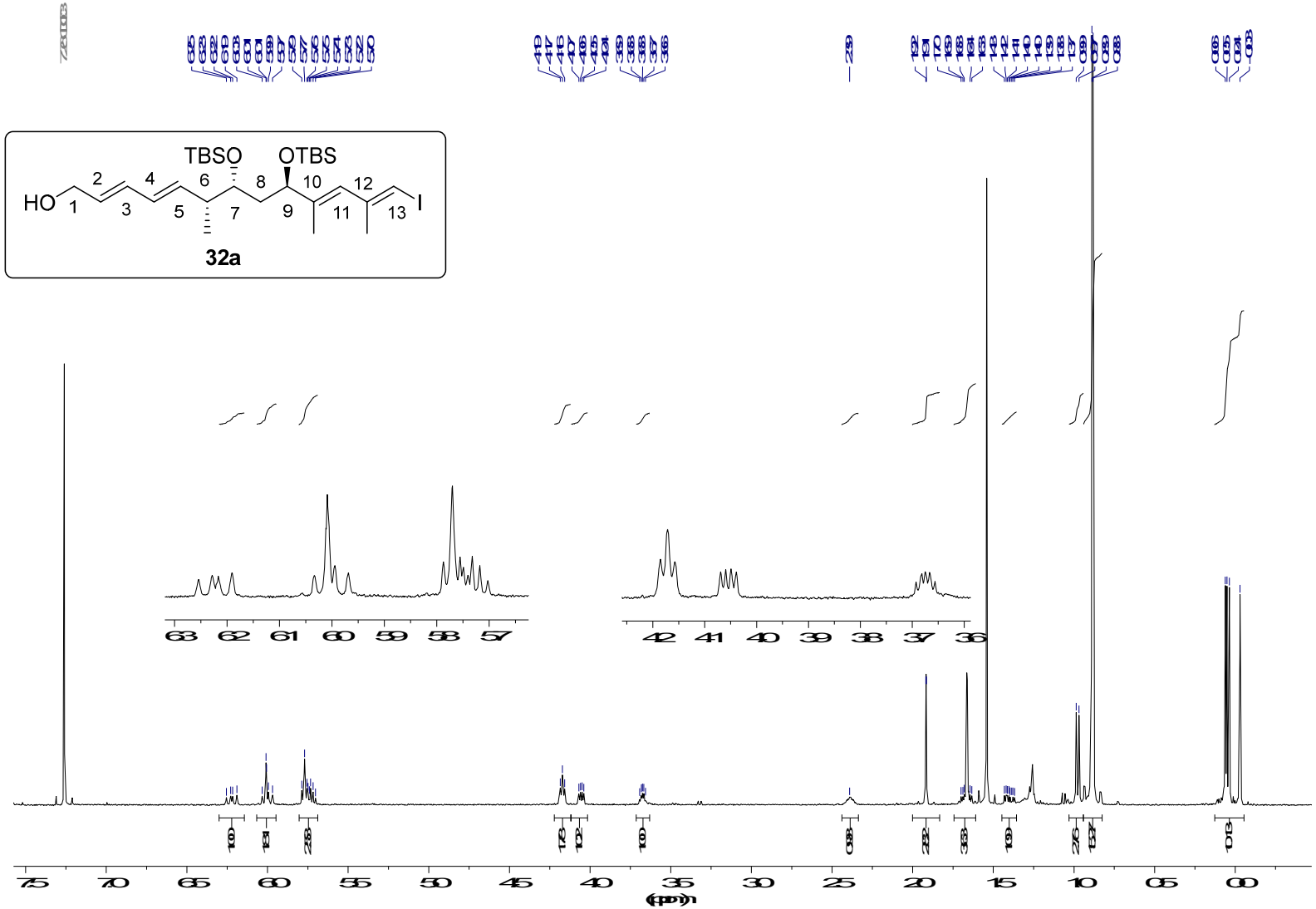
^{1}H-NMR (400.13 MHz, $CDCl_3$)



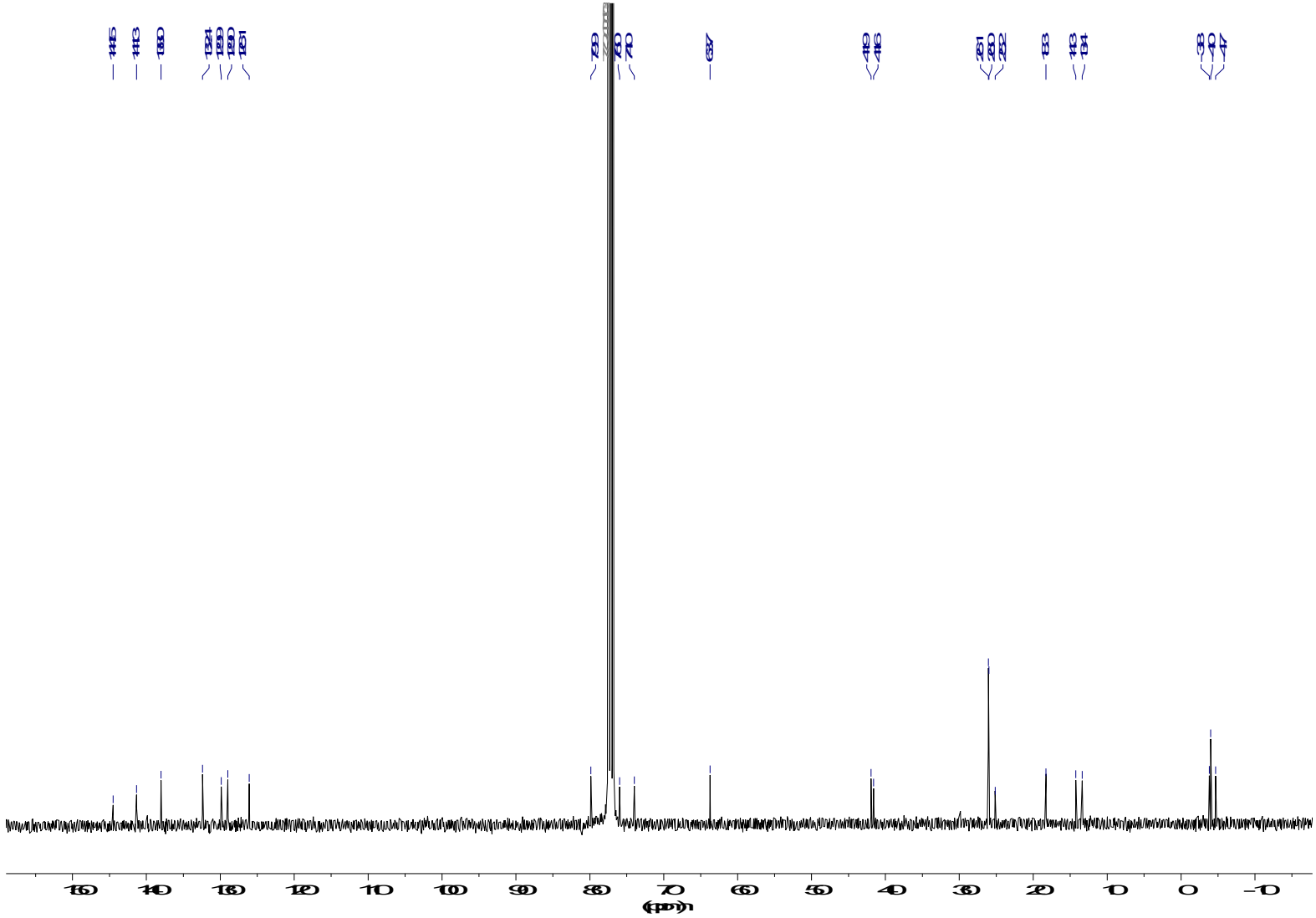
^{13}C-NMR (100.13 MHz, $CDCl_3$)



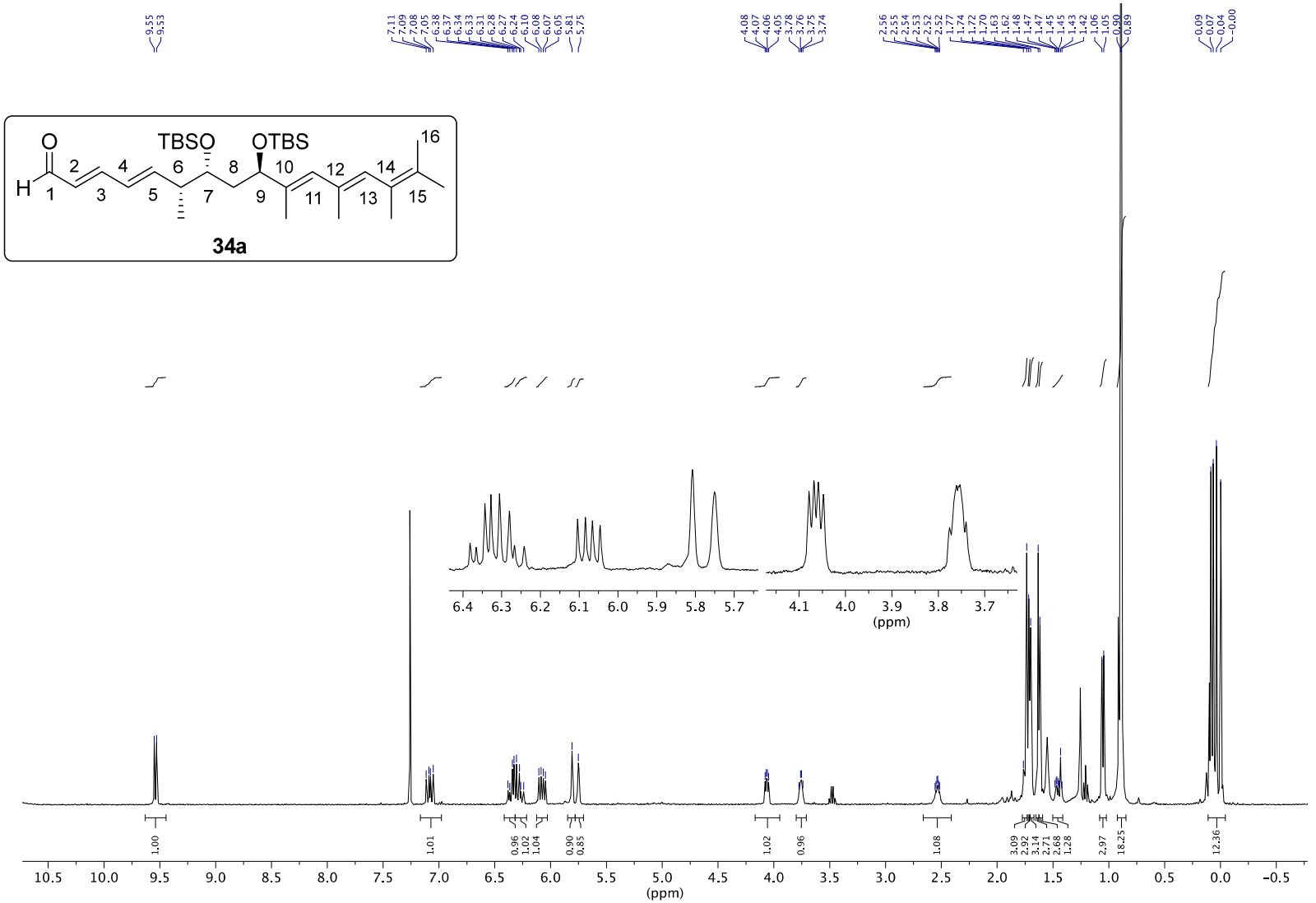
^{1}H-NMR (400.13 MHz, $CDCl_3$)



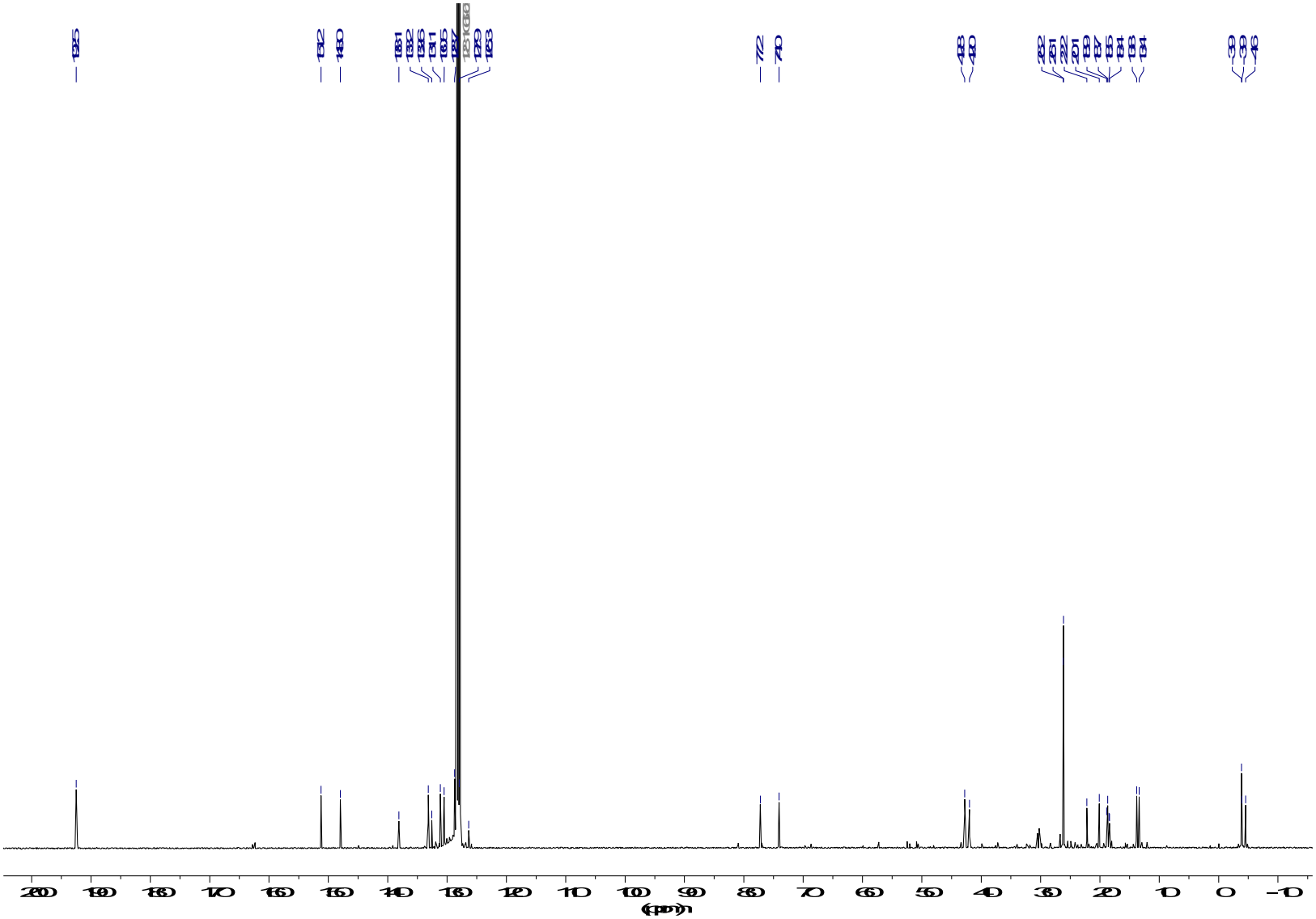
^{13}C-NMR (100.13 MHz, $CDCl_3$)



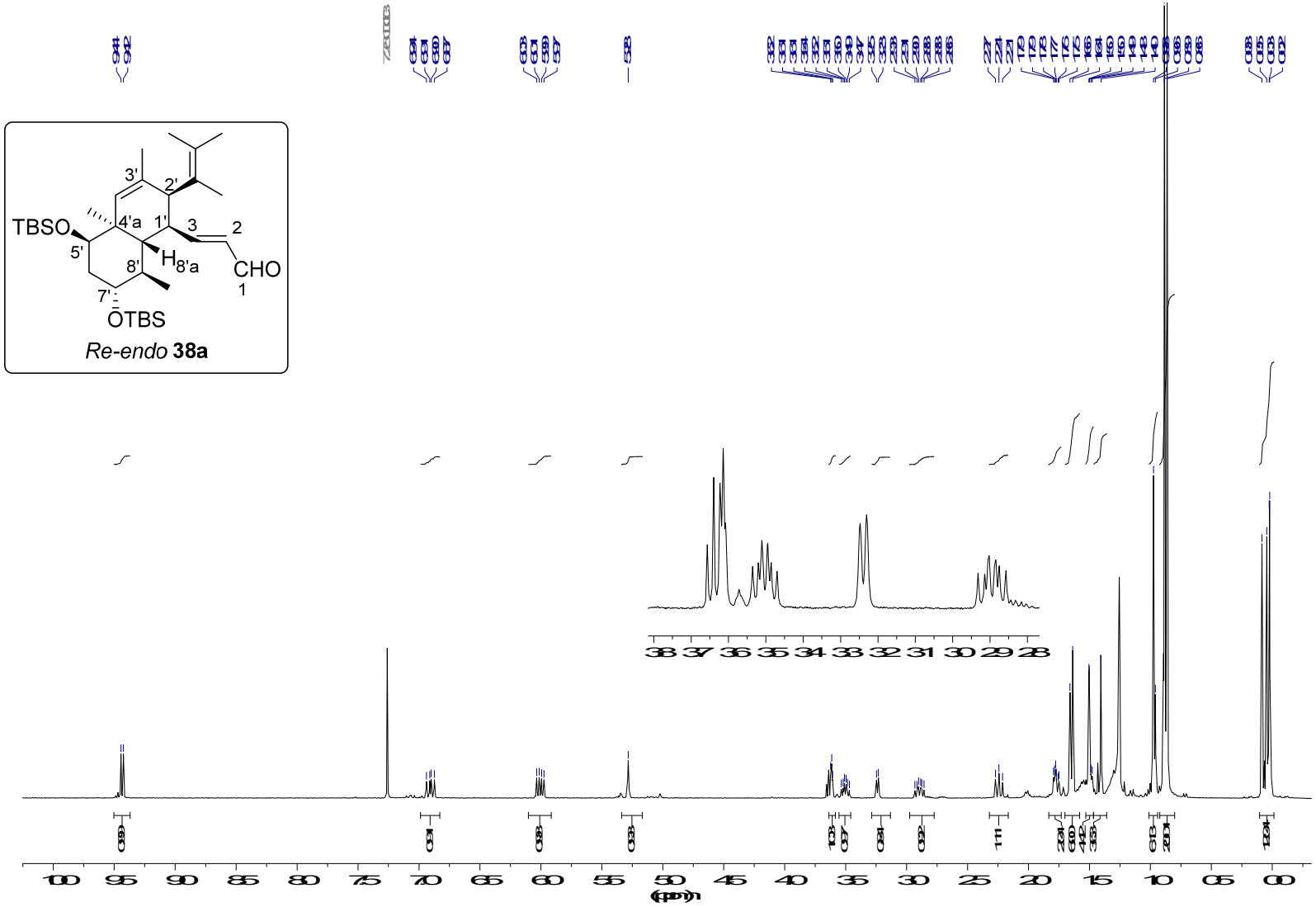
^{1}H-NMR (400.13 MHz, $CDCl_3$)



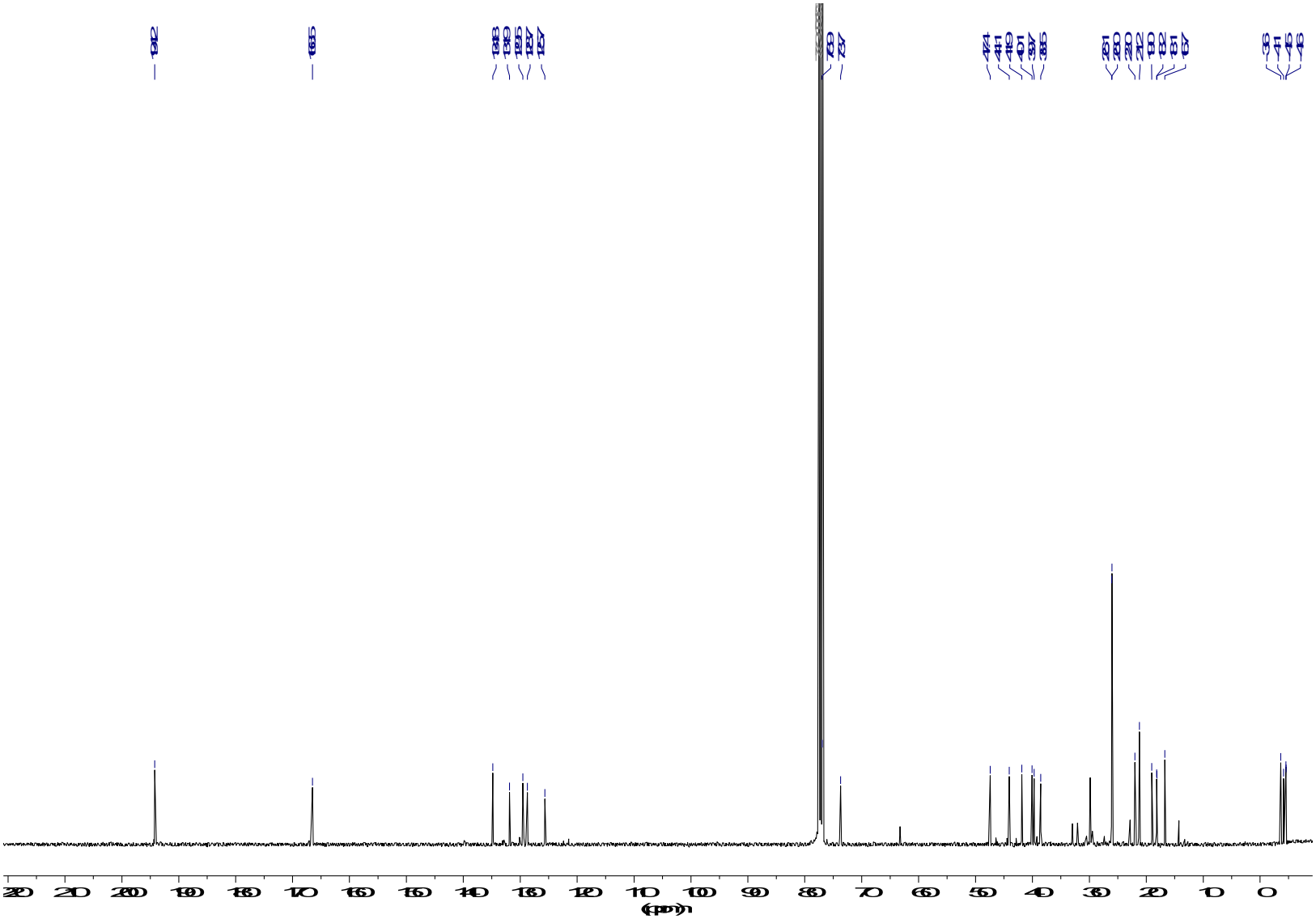
^{13}C-NMR (100.13 MHz, $CDCl_3$)



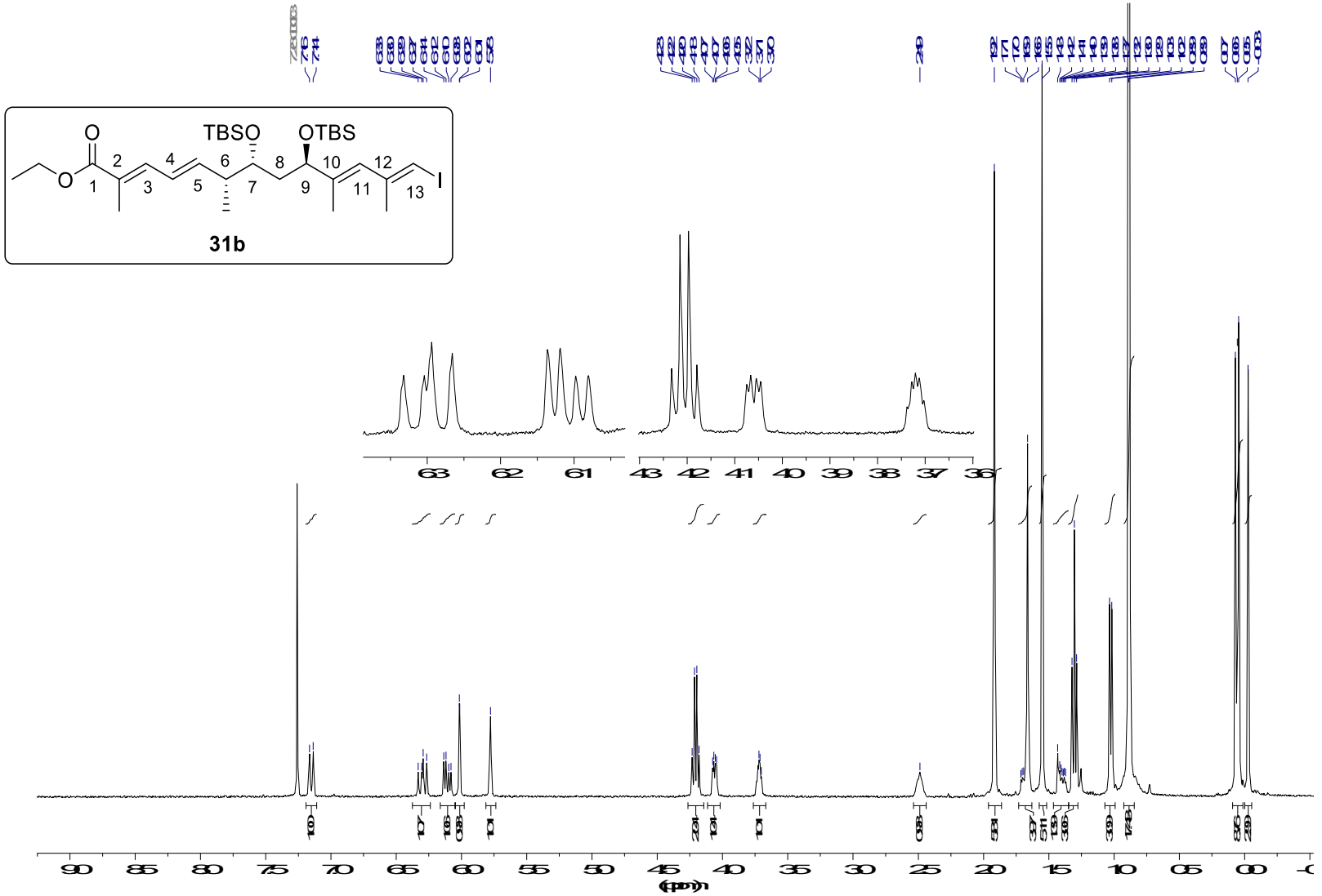
^{1}H-NMR (400.13 MHz, $CDCl_3$)



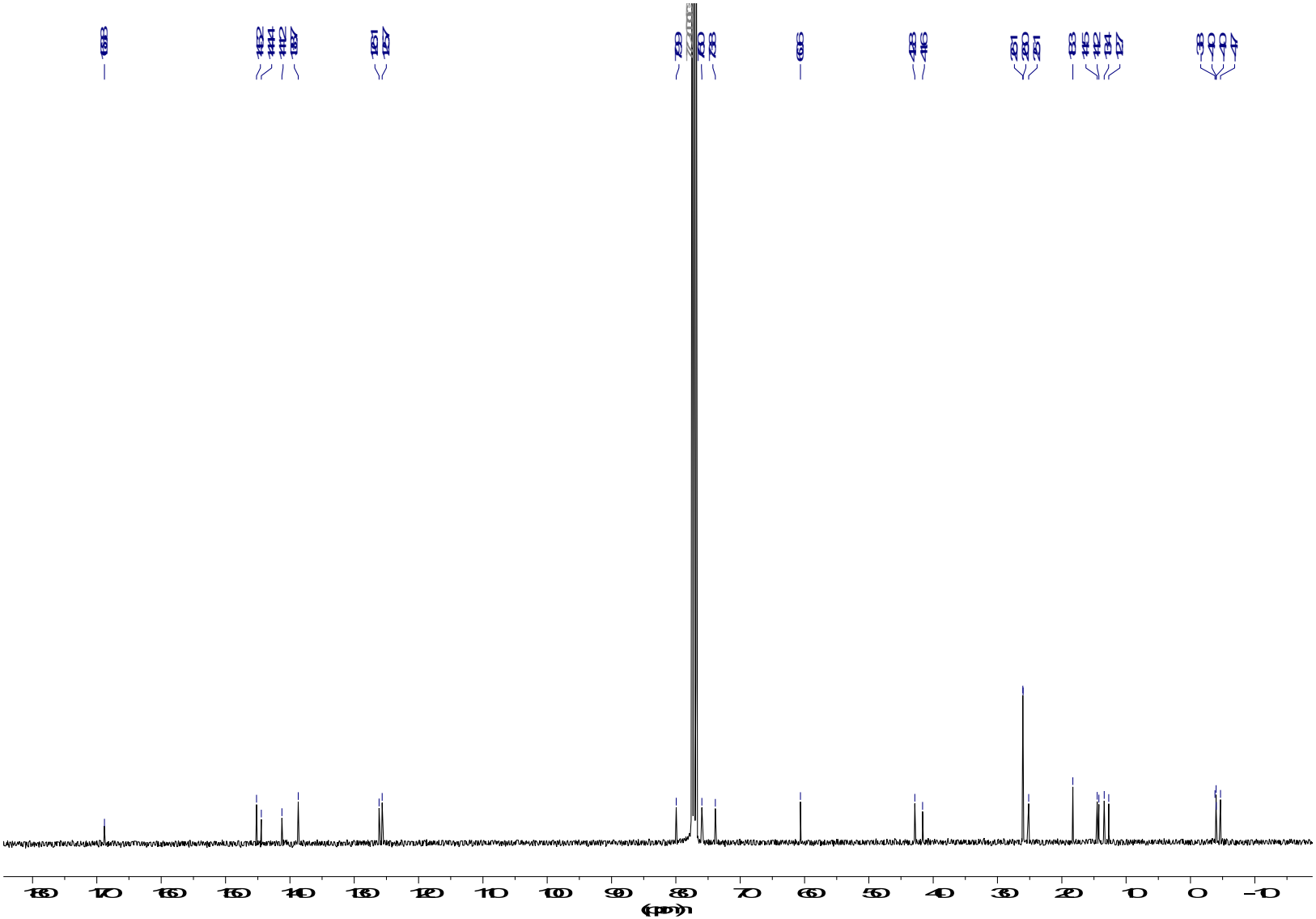
^{13}C-NMR (100.13 MHz, $CDCl_3$)



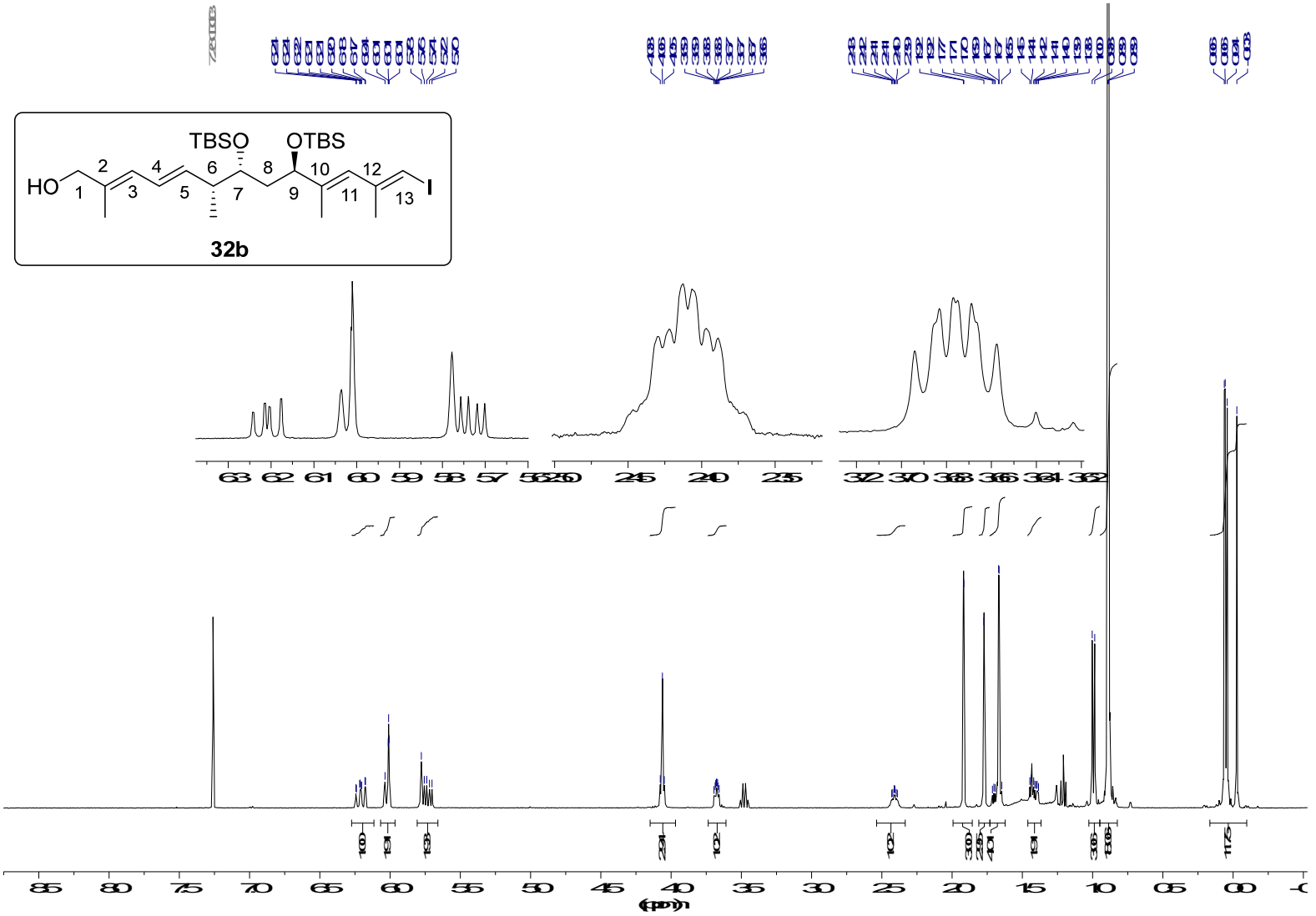
^{1}H-NMR (400.13 MHz, $CDCl_3$)



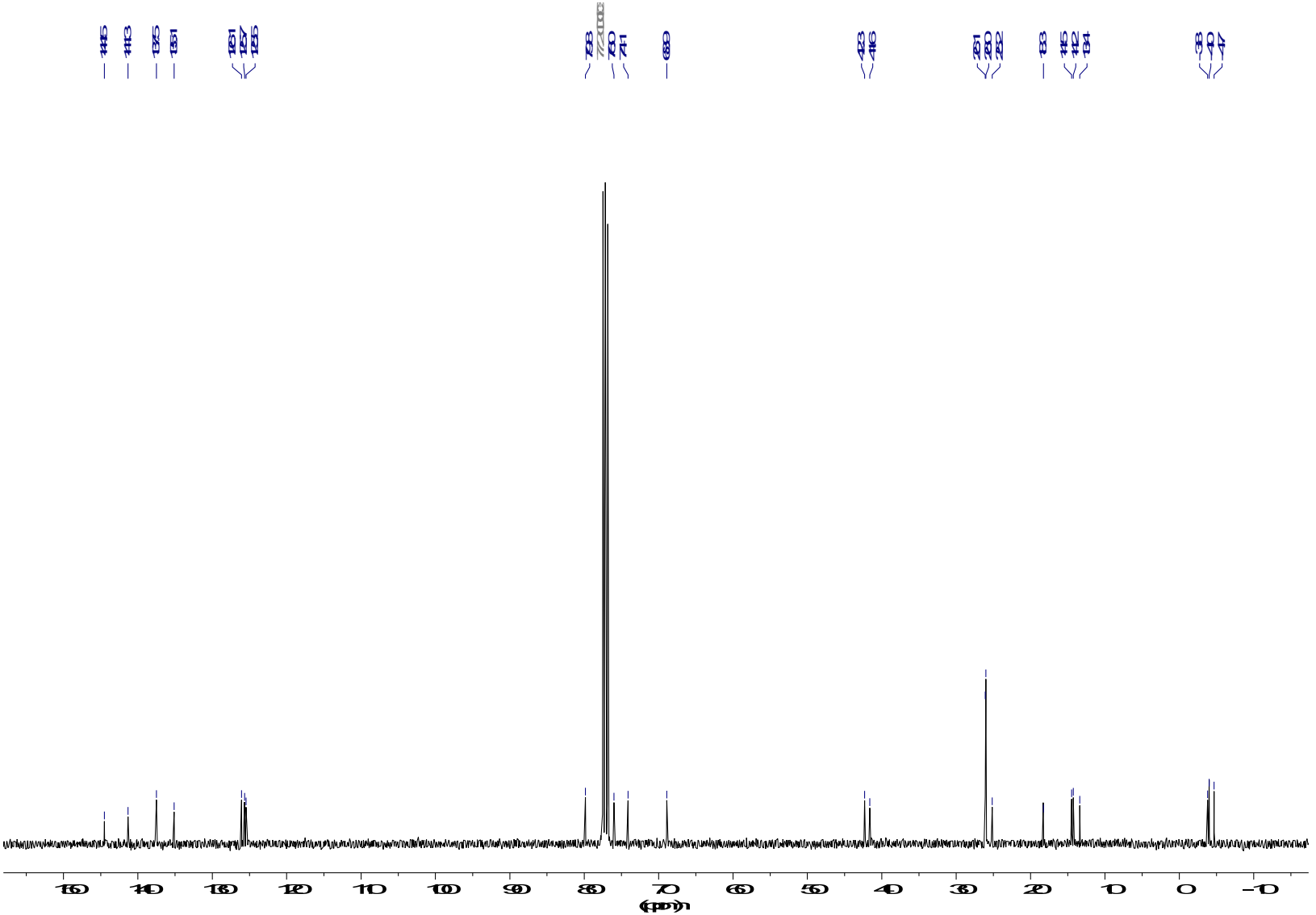
^{13}C-NMR (100.13 MHz, $CDCl_3$)



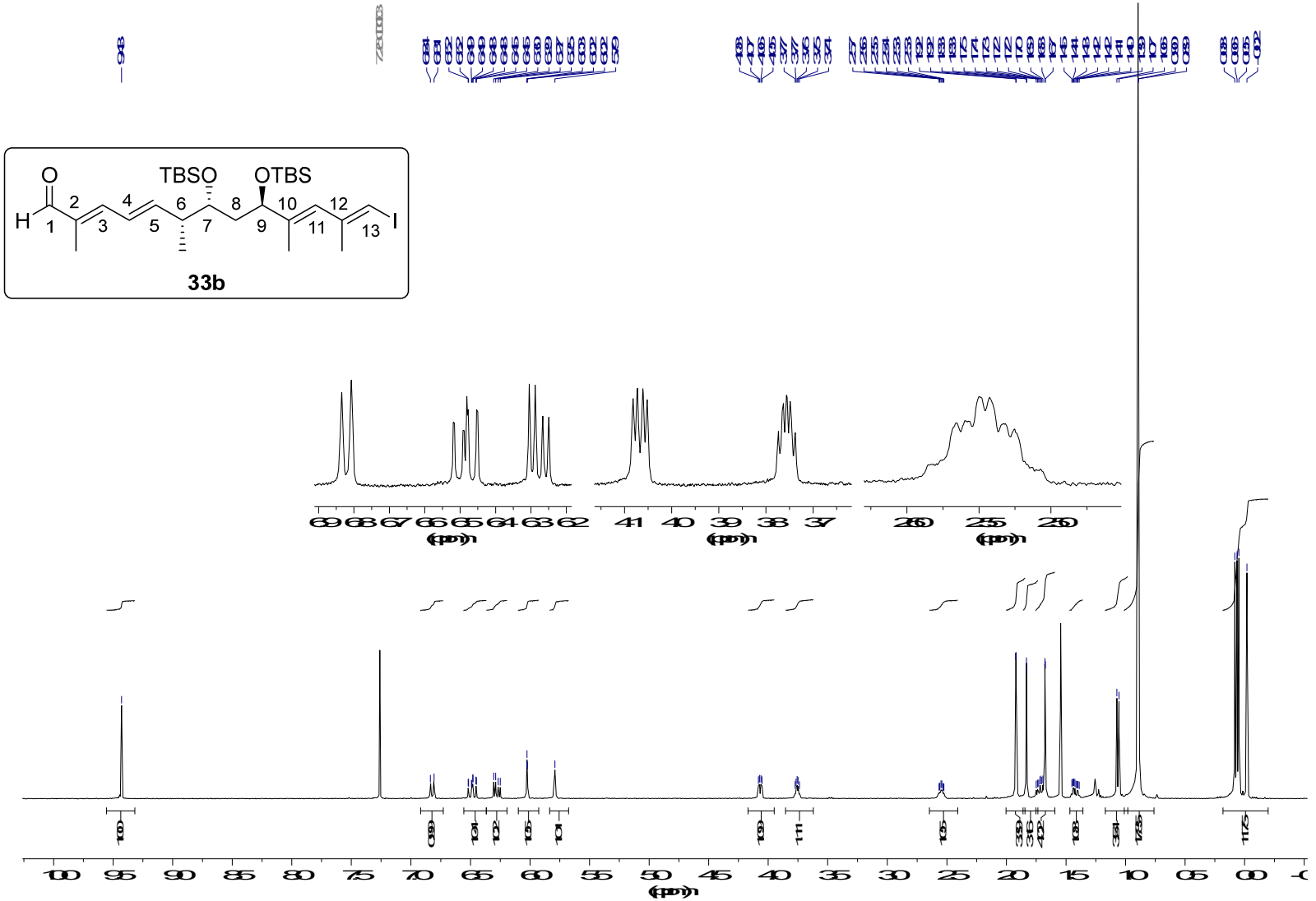
^{1}H-NMR (400.13 MHz, $CDCl_3$)



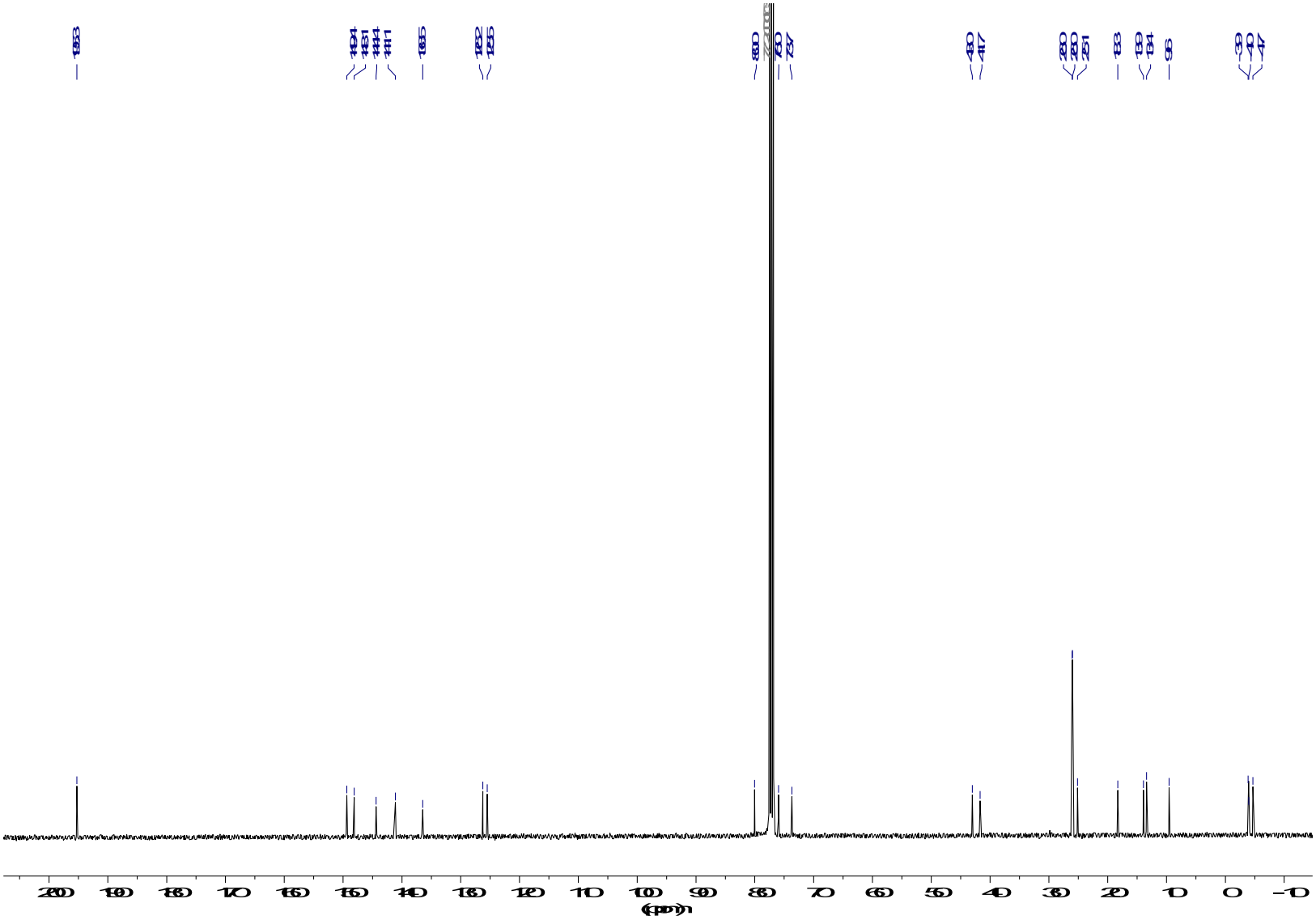
^{13}C-NMR (100.13 MHz, $CDCl_3$)



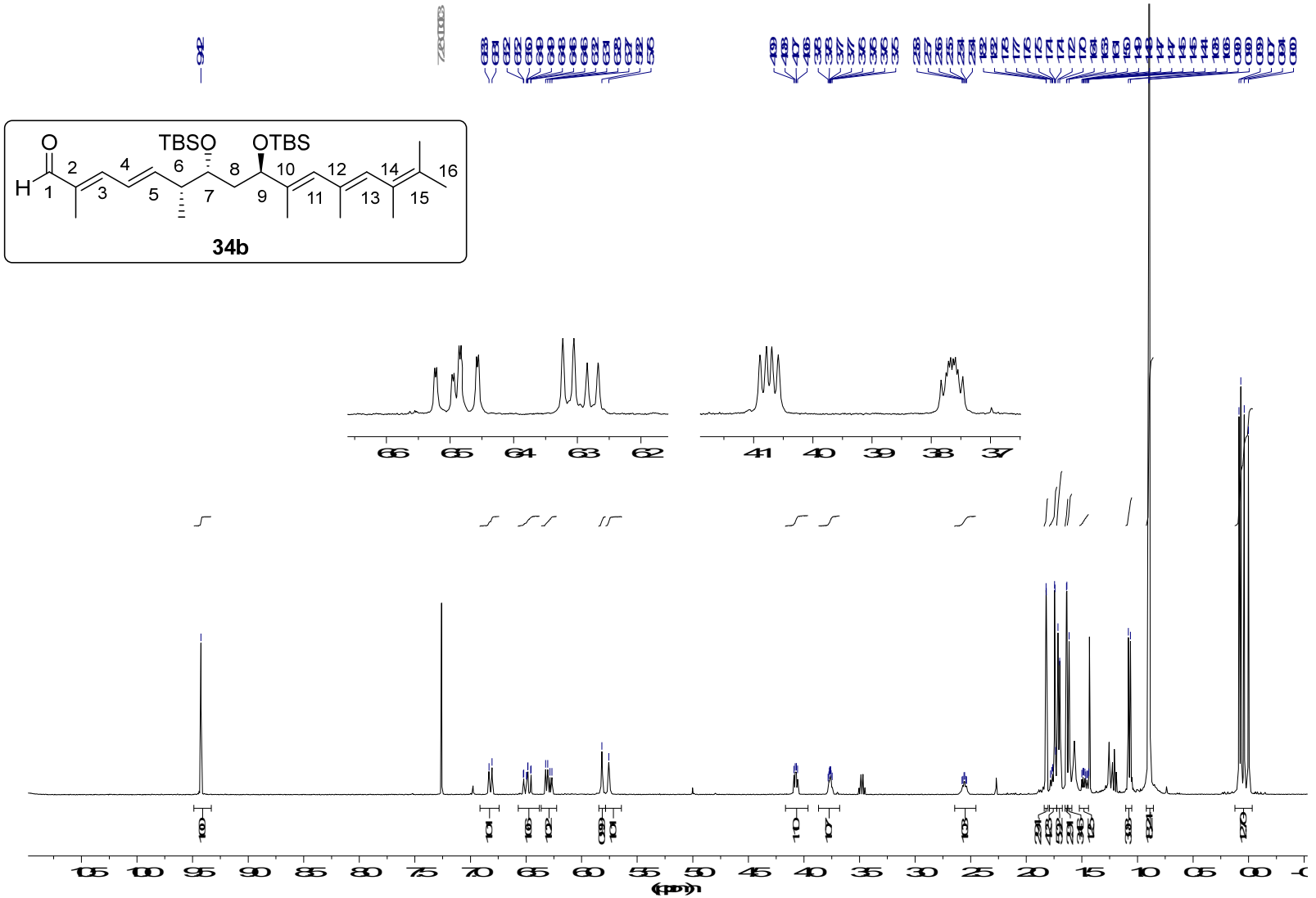
^{1}H-NMR (400.13 MHz, $CDCl_3$)



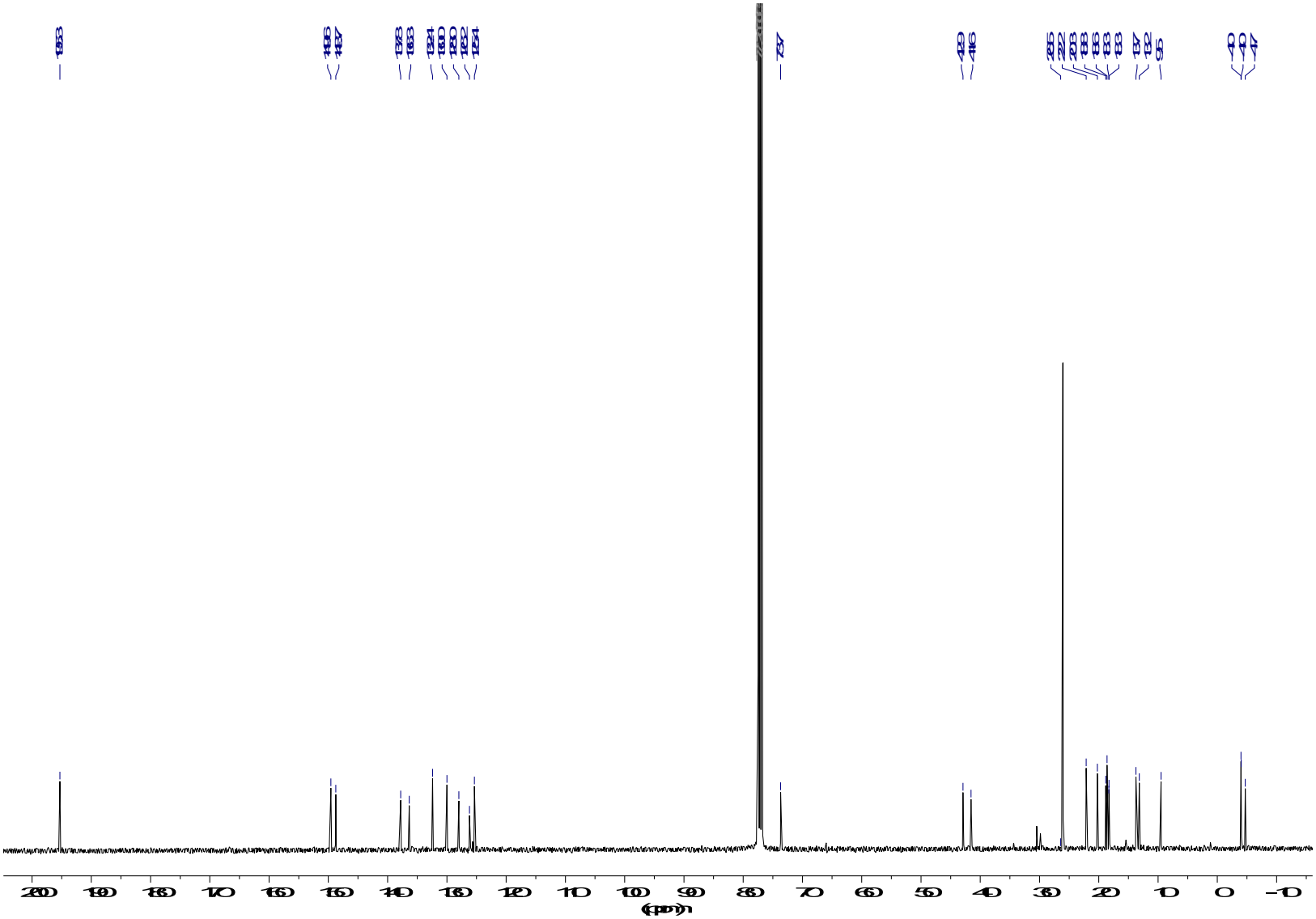
^{13}C-NMR (100.13 MHz, $CDCl_3$)



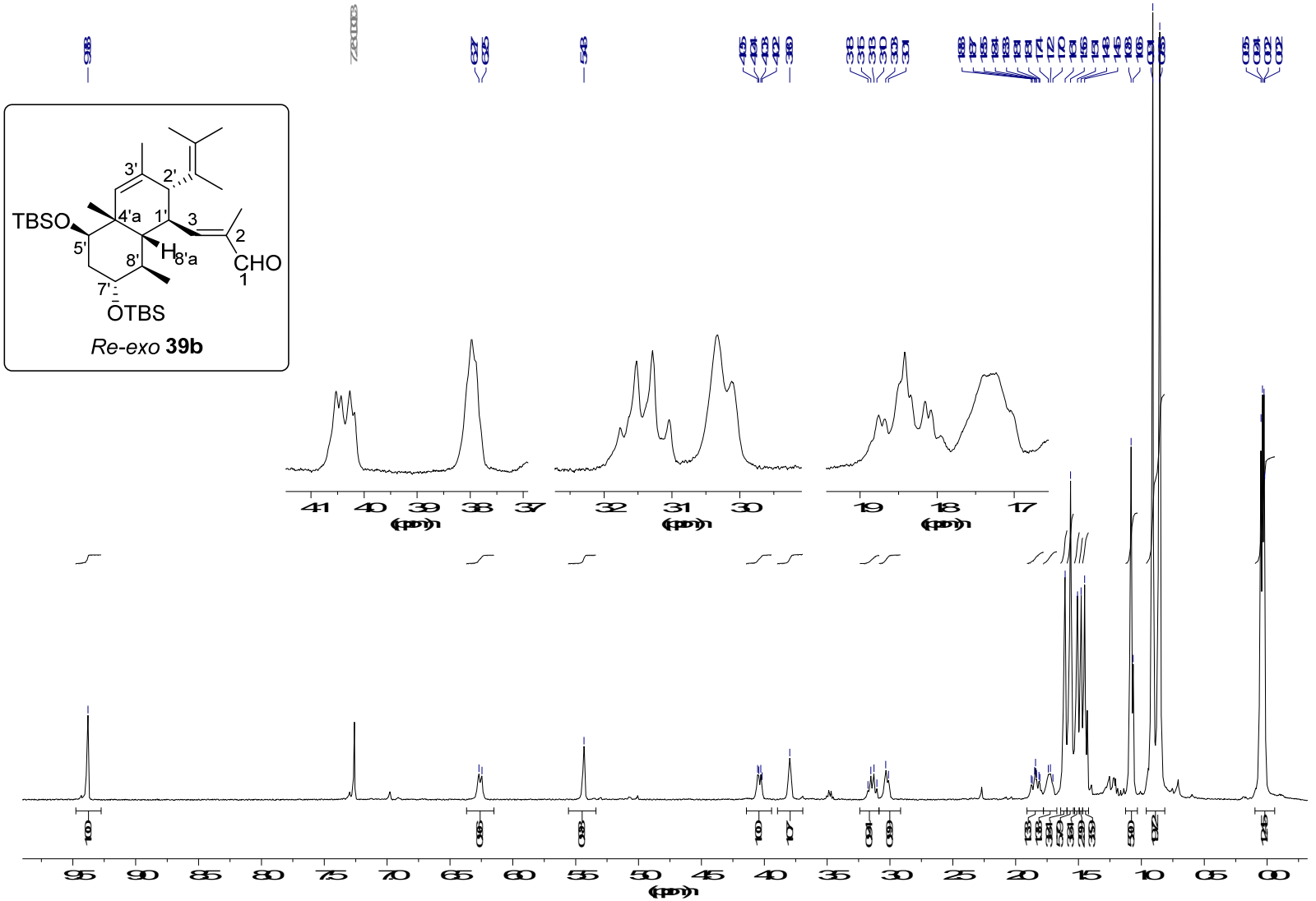
^{1}H-NMR (400.13 MHz, $CDCl_3$)



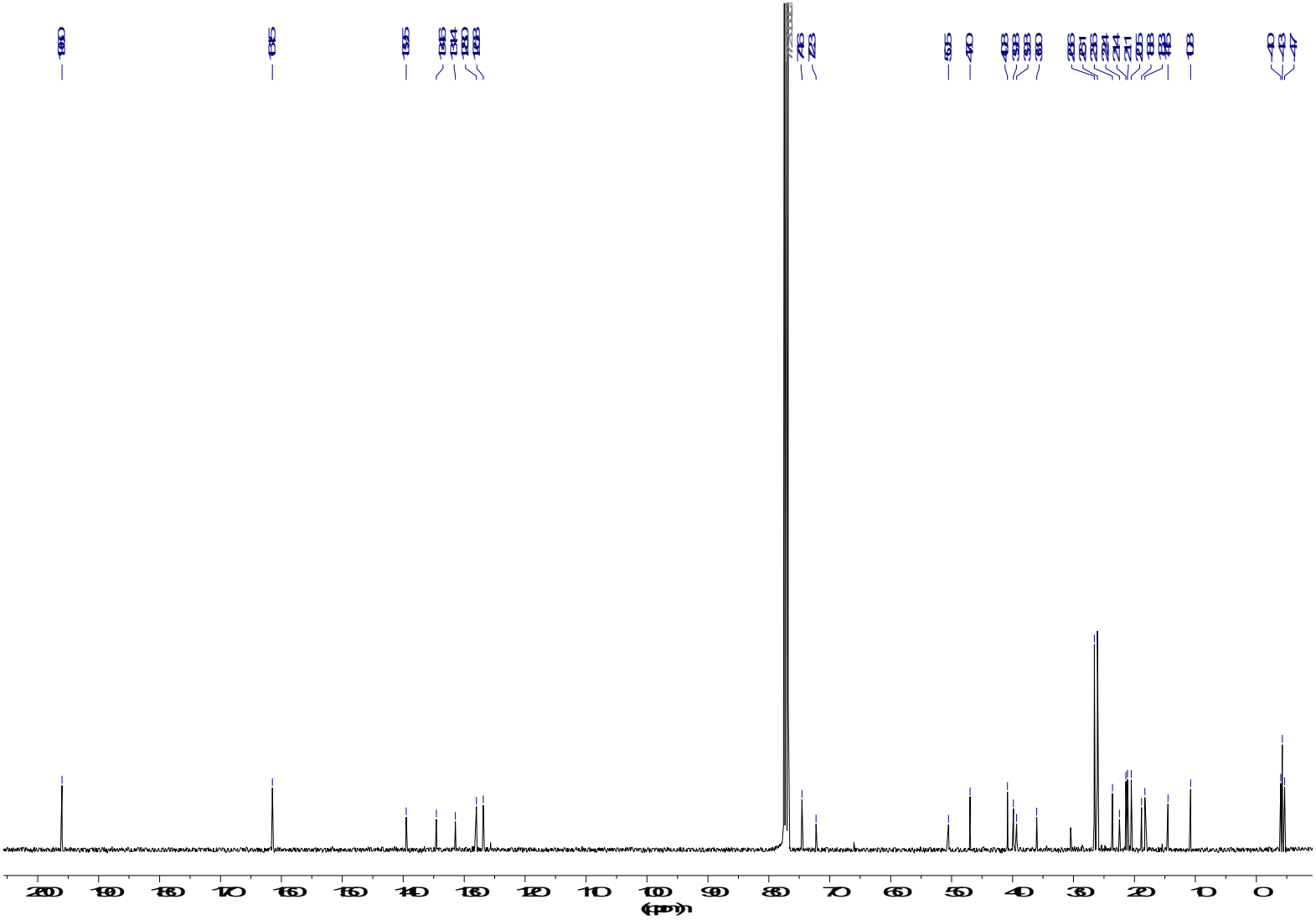
^{13}C-NMR (100.13 MHz, $CDCl_3$)



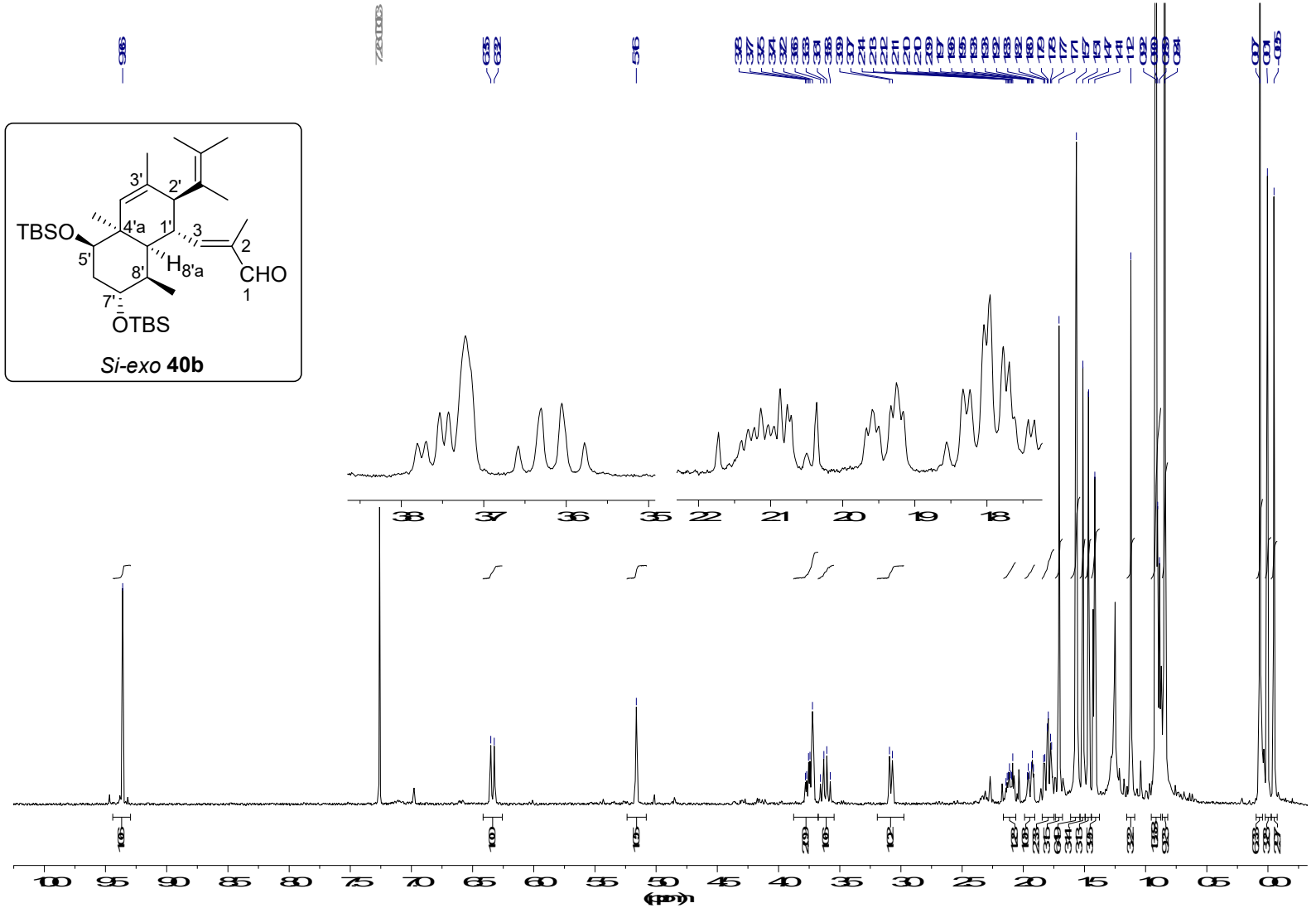
^{1}H-NMR (400.13 MHz, $CDCl_3$)



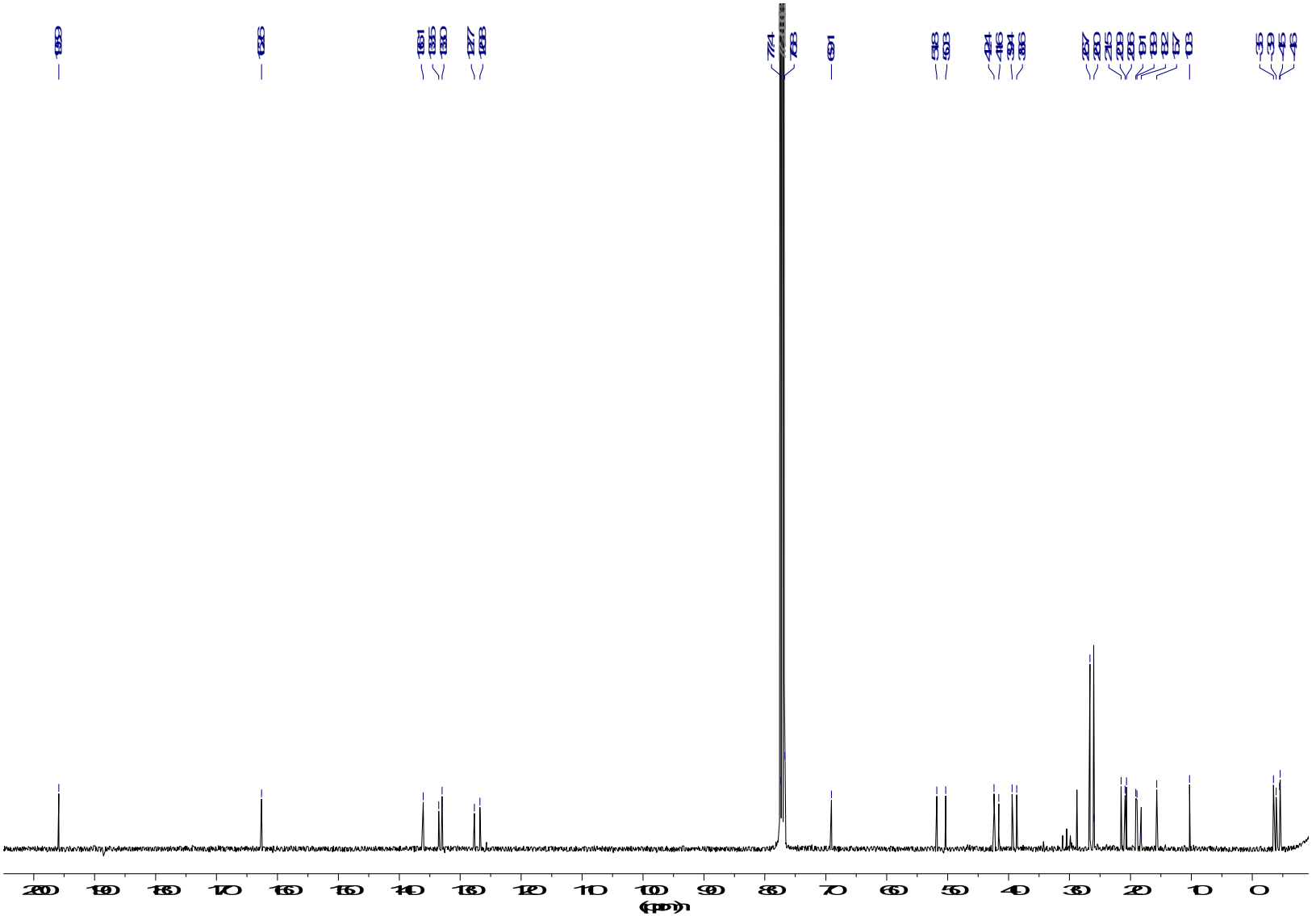
^{13}C-NMR (100.13 MHz, $CDCl_3$)



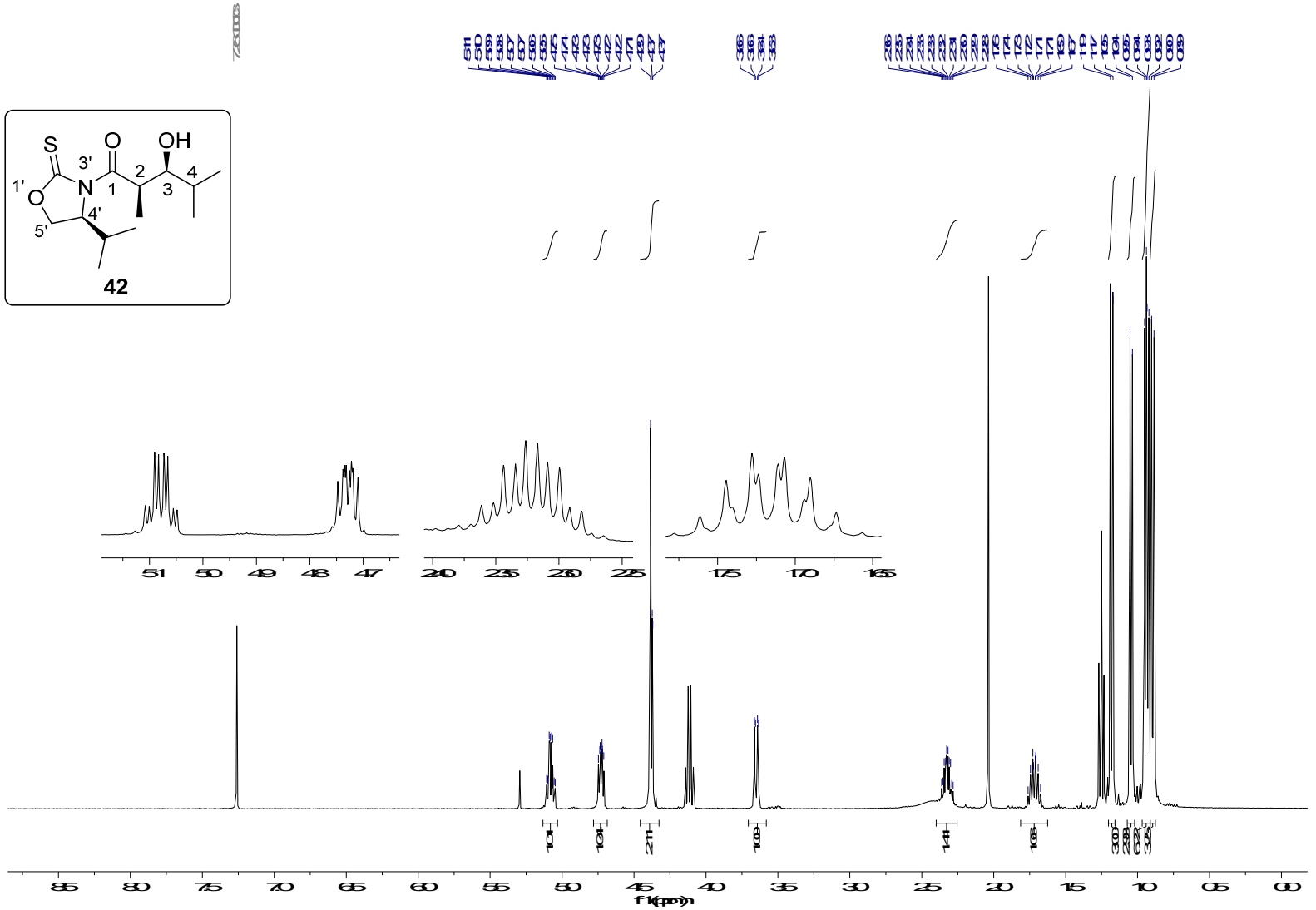
^{1}H-NMR (400.13 MHz, $CDCl_3$)



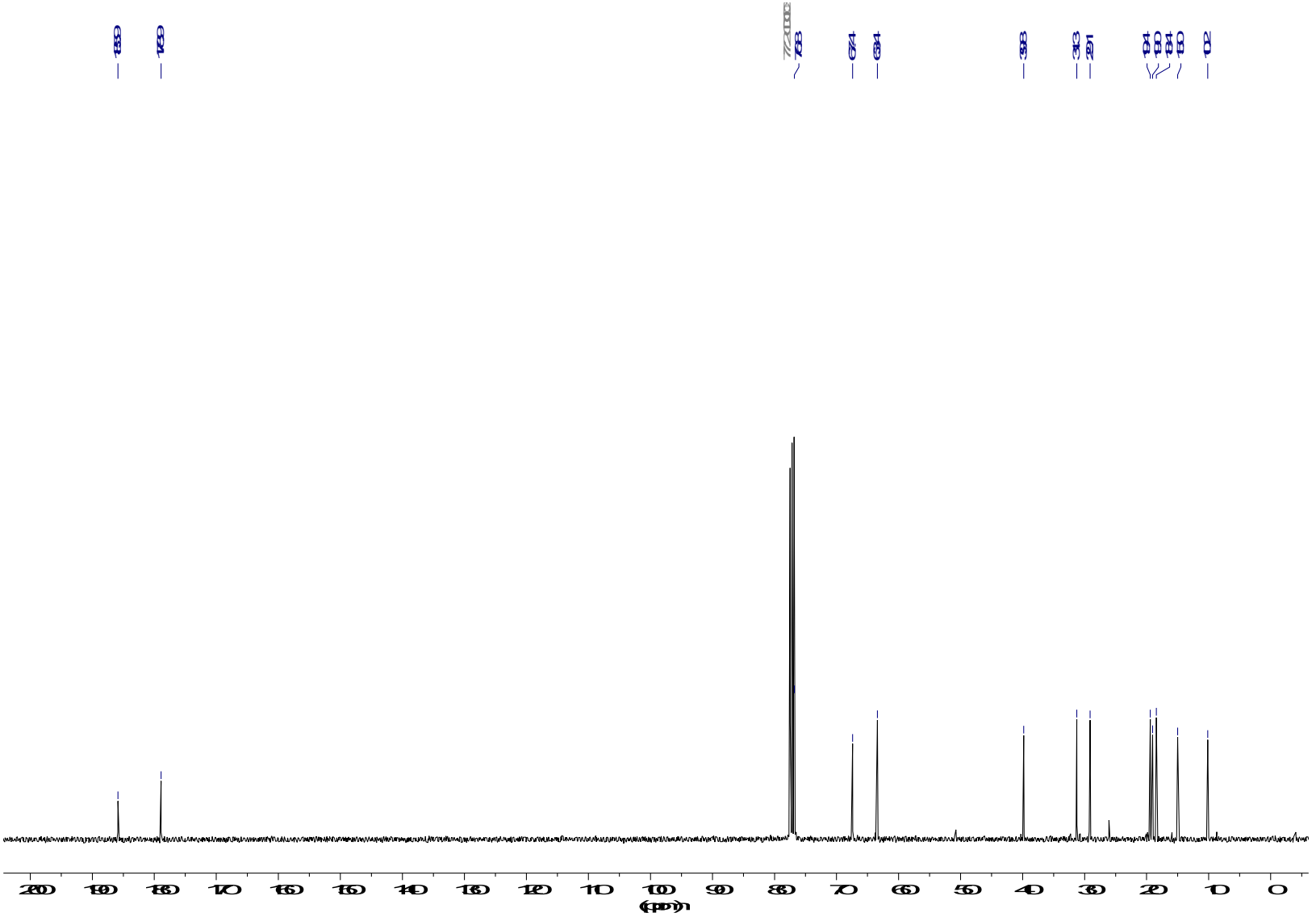
^{13}C-NMR (100.13 MHz, $CDCl_3$)



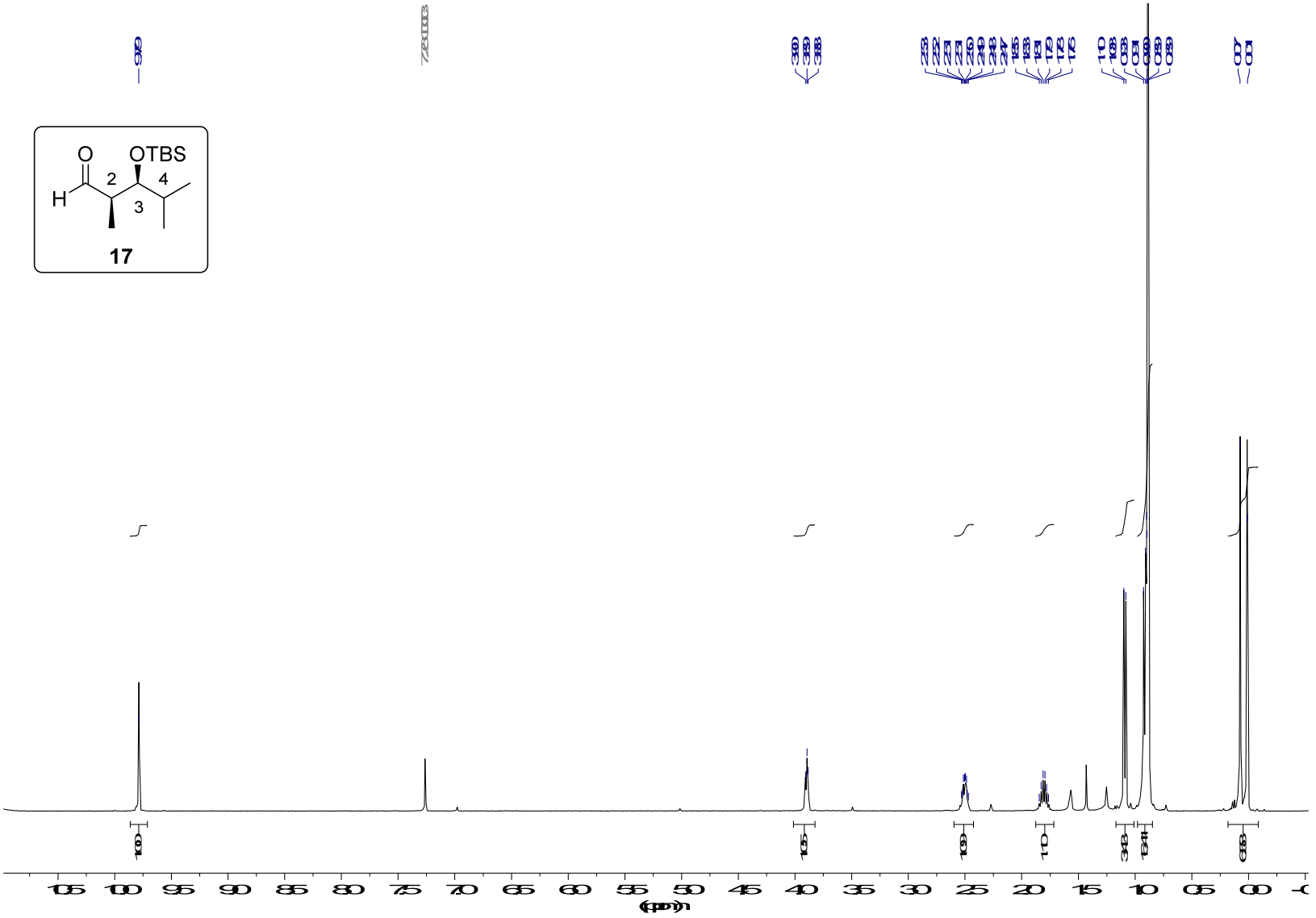
^{1}H-NMR (400.13 MHz, $CDCl_3$)



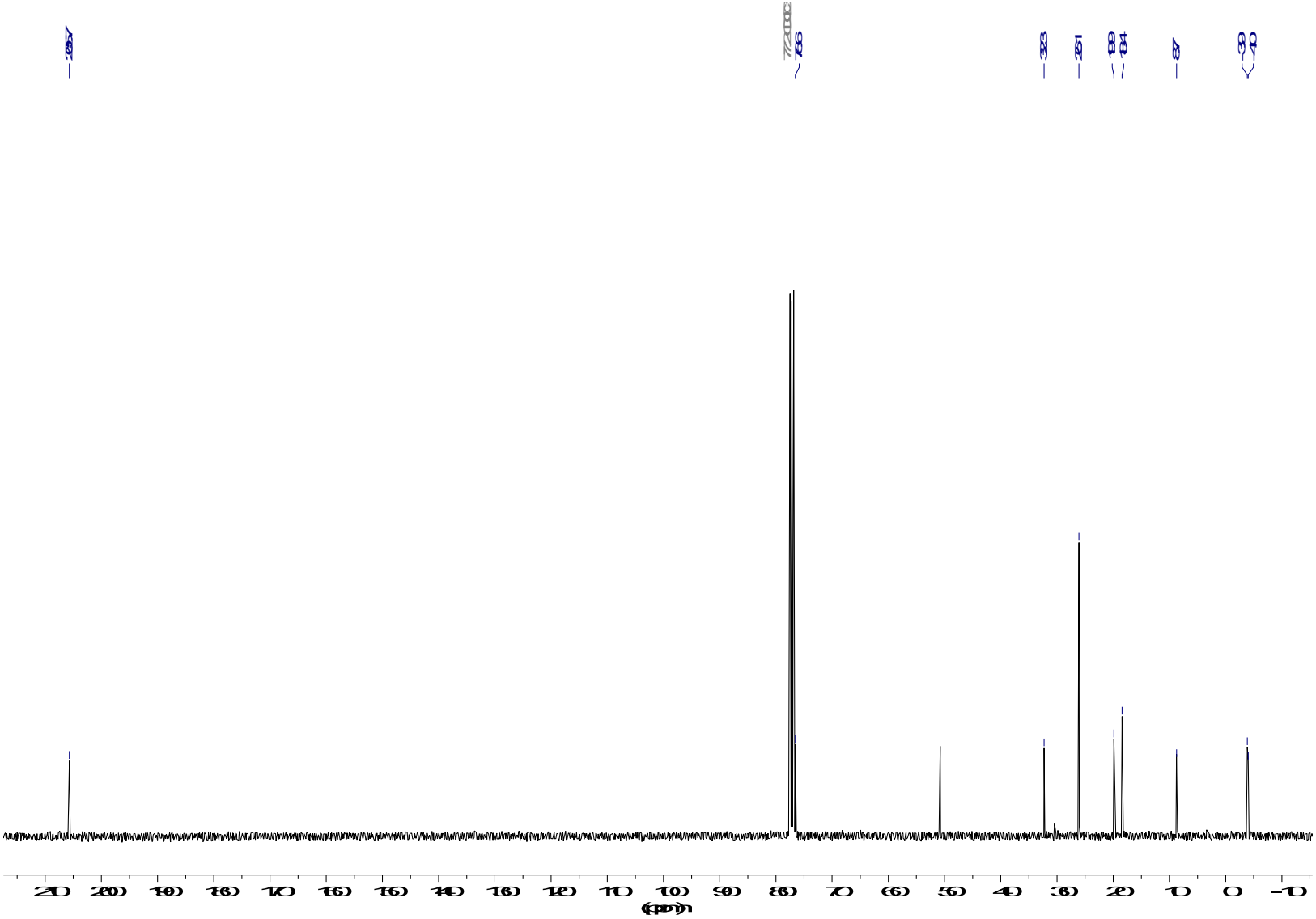
^{13}C-NMR (100.13 MHz, $CDCl_3$)



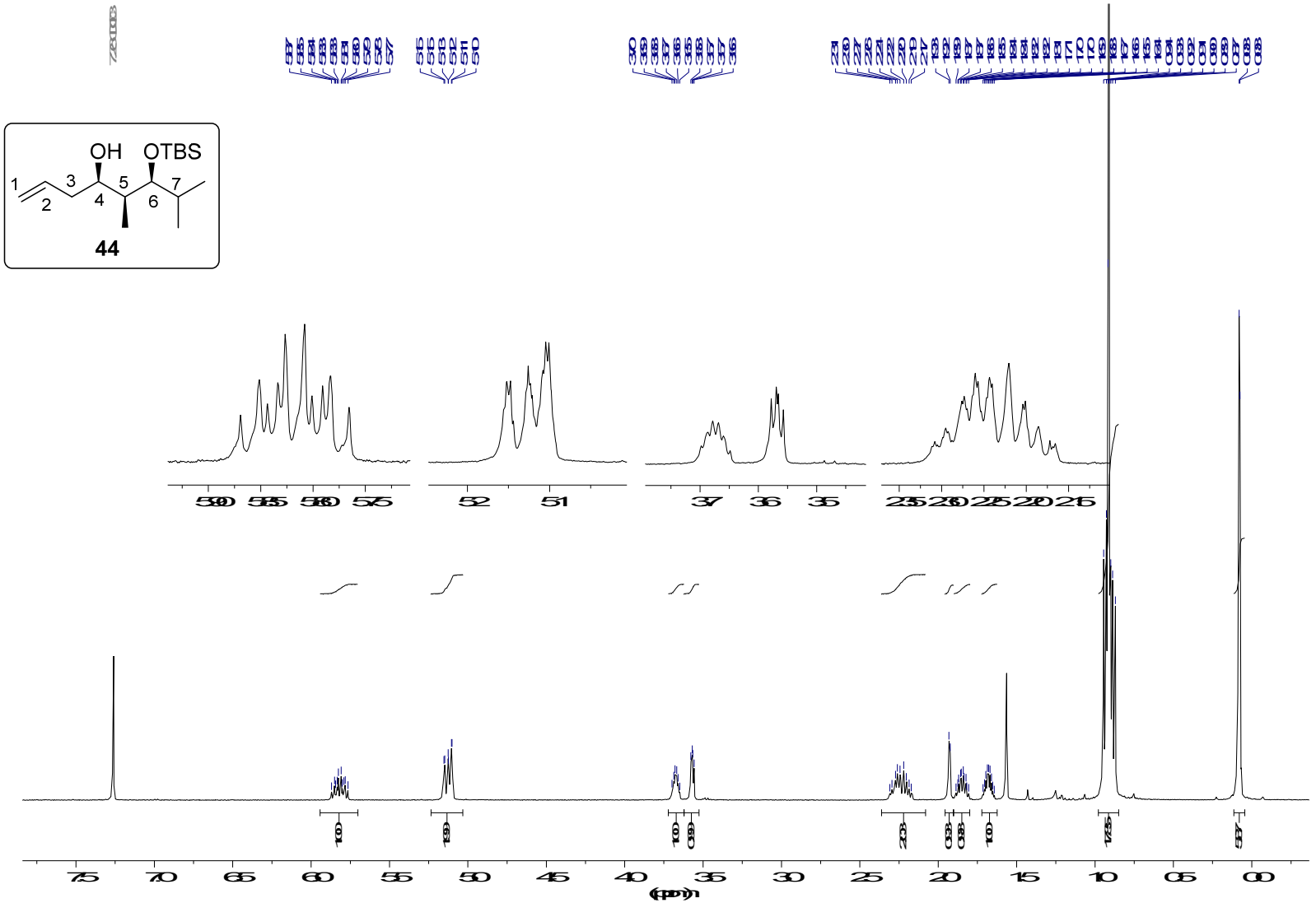
^{1}H-NMR (400.13 MHz, $CDCl_3$)



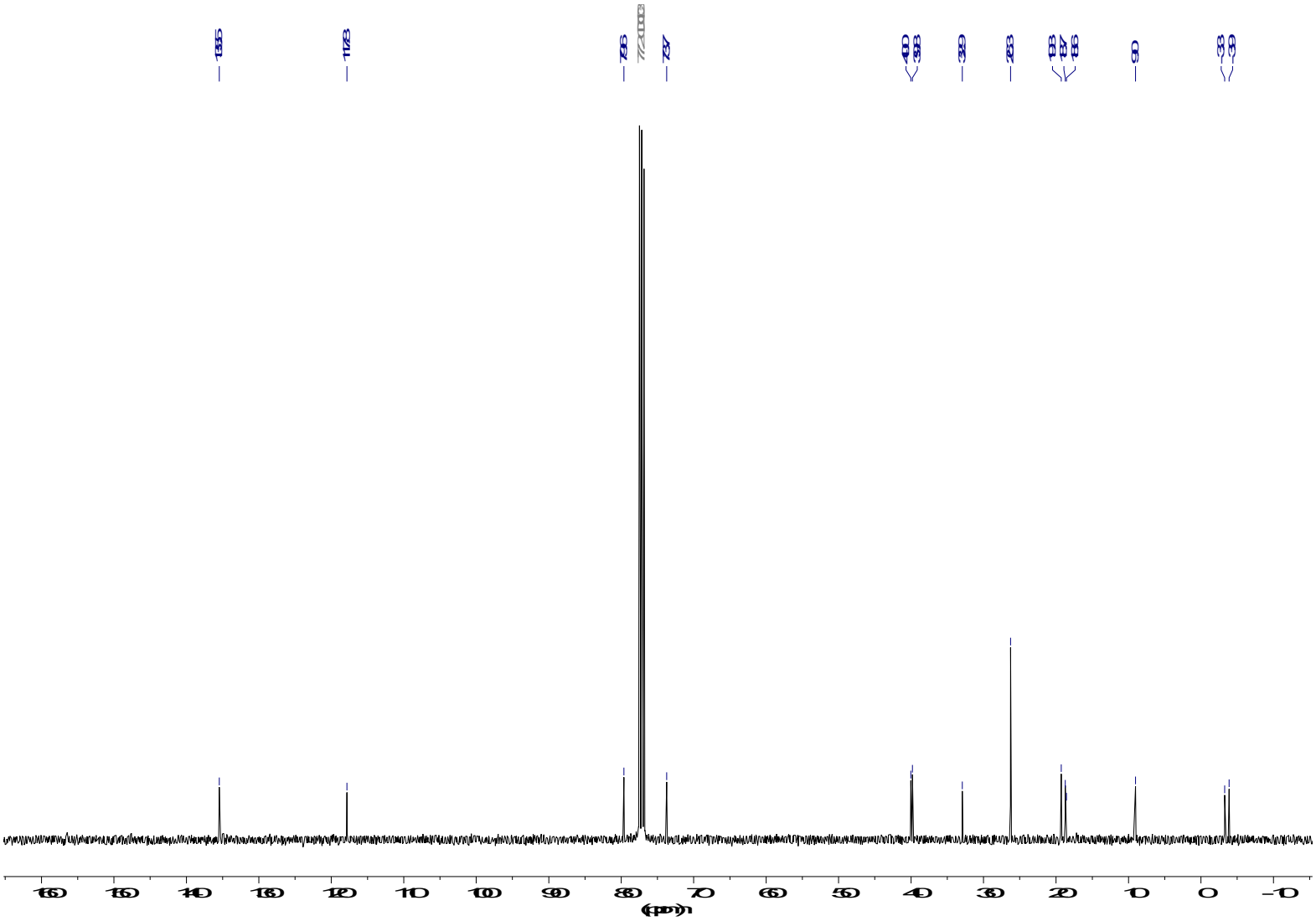
^{13}C-NMR (100.13 MHz, $CDCl_3$)



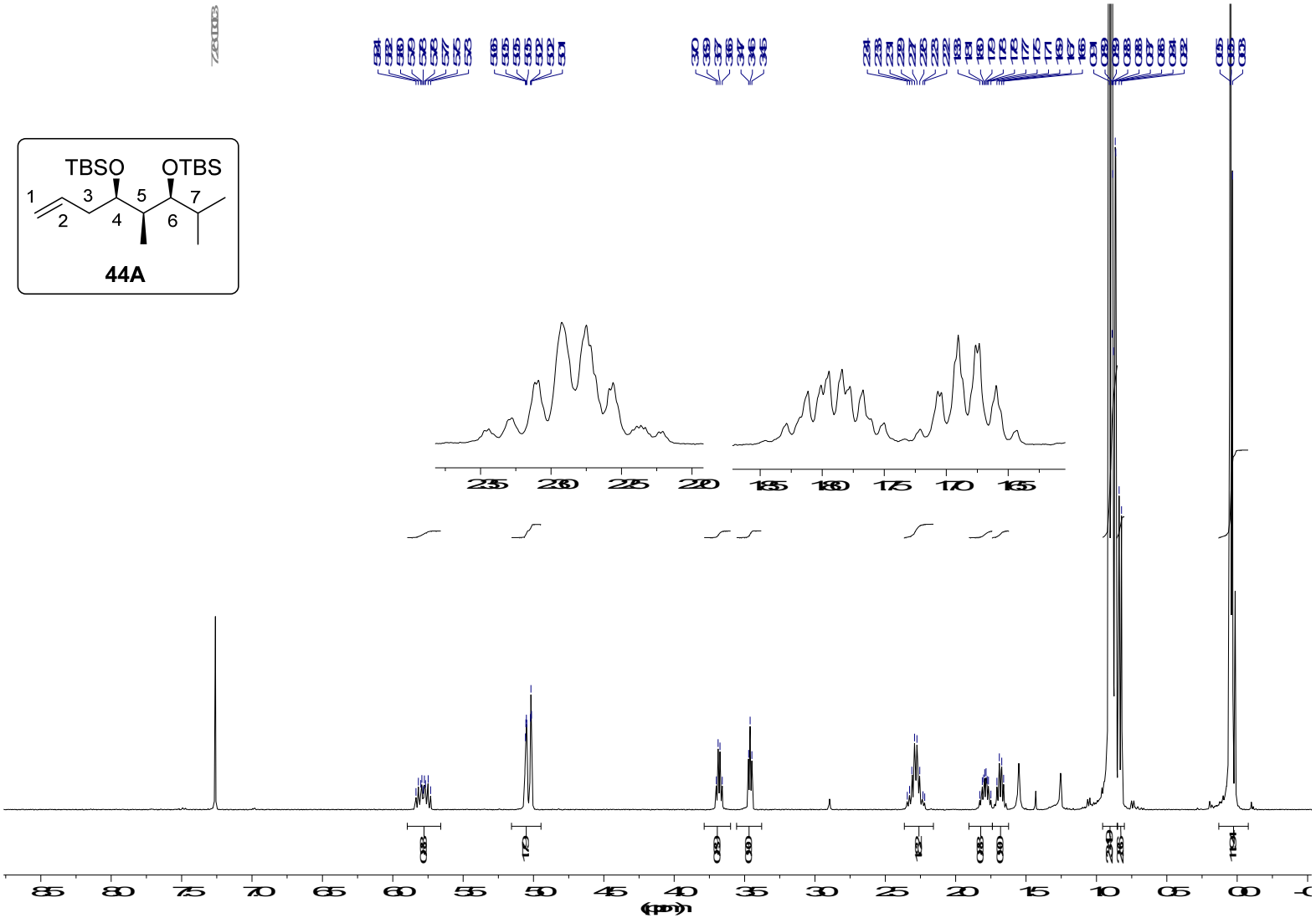
^{1}H-NMR (400.13 MHz, $CDCl_3$)



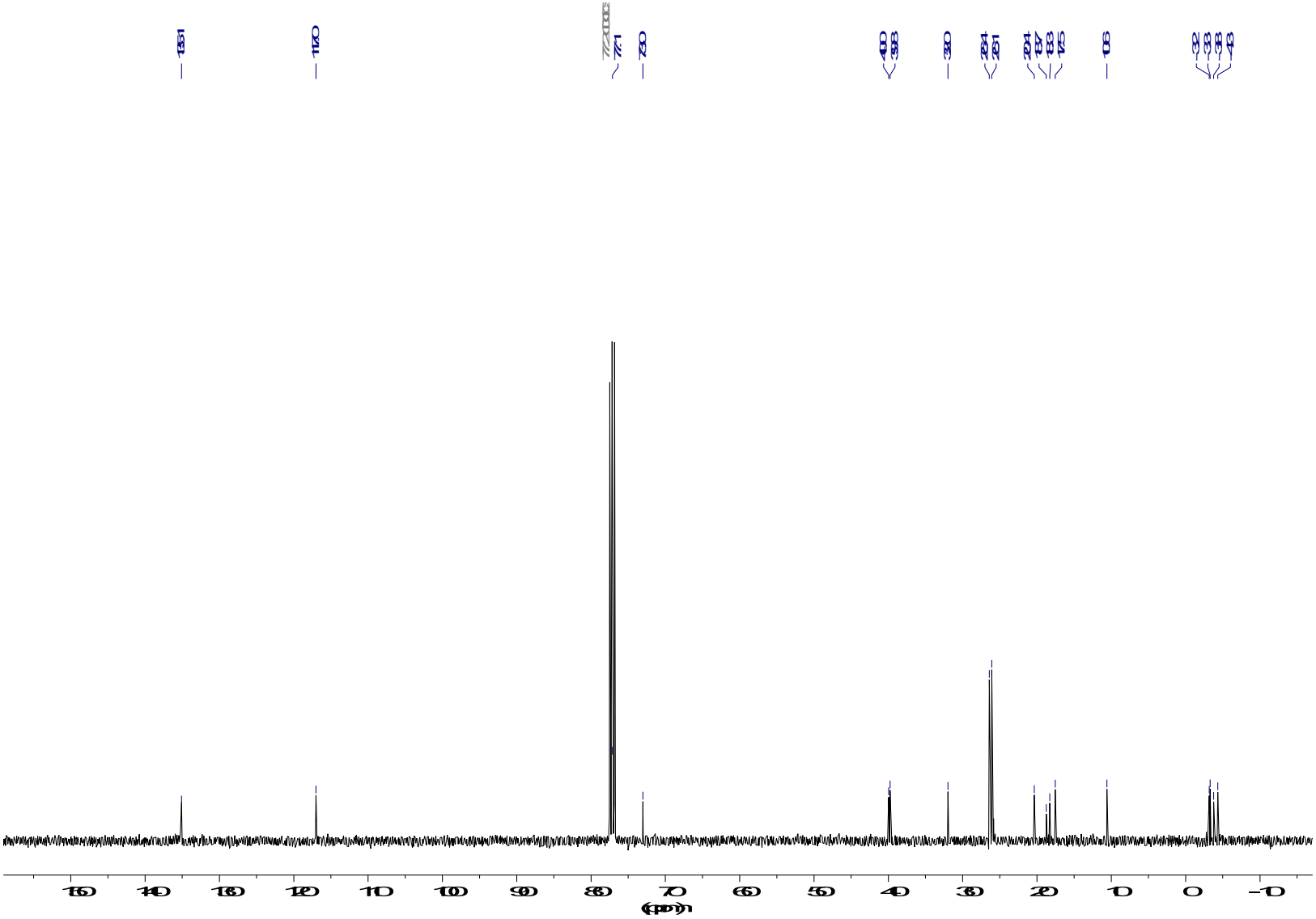
^{13}C-NMR (100.13 MHz, $CDCl_3$)



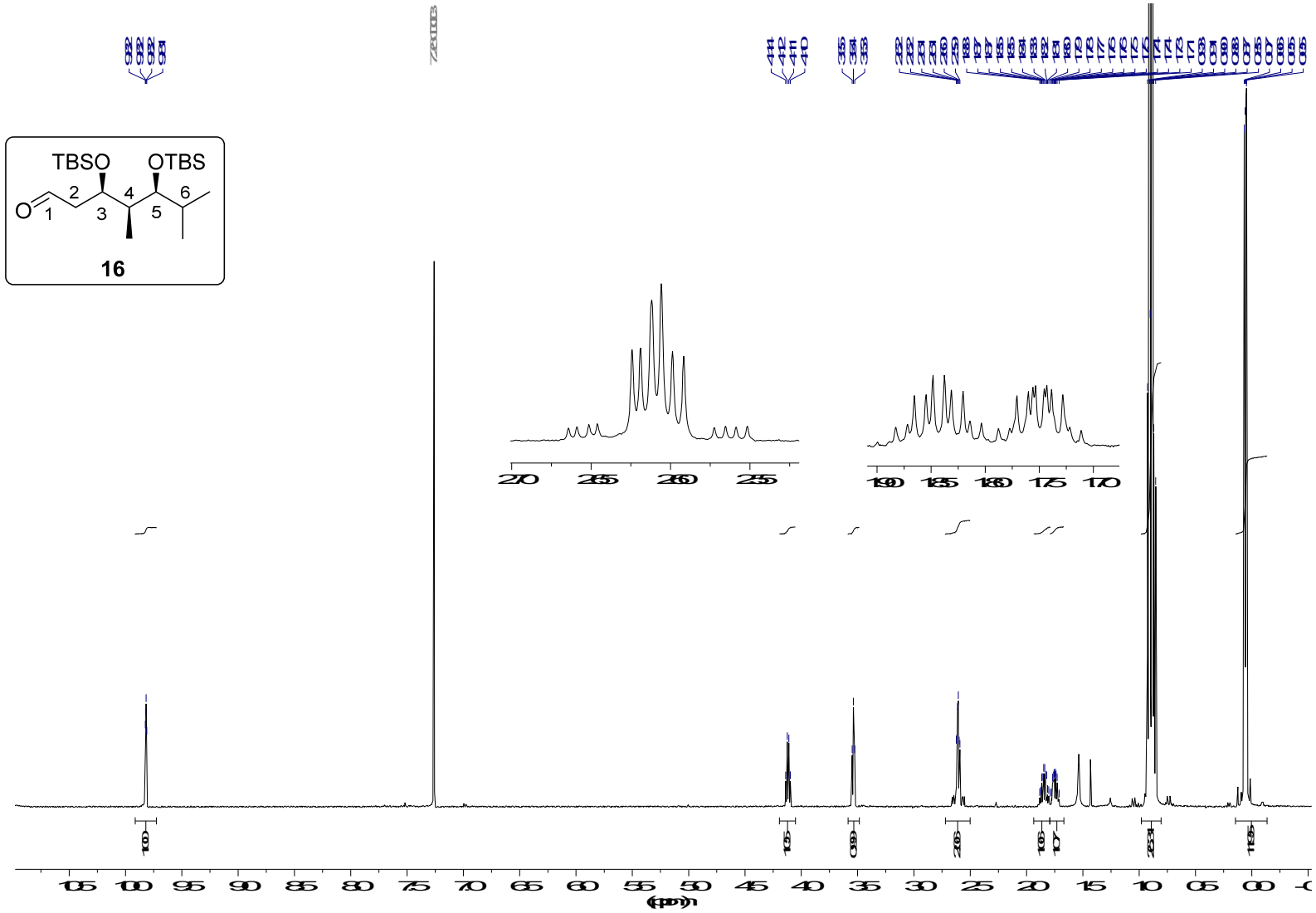
^{1}H-NMR (400.13 MHz, $CDCl_3$)



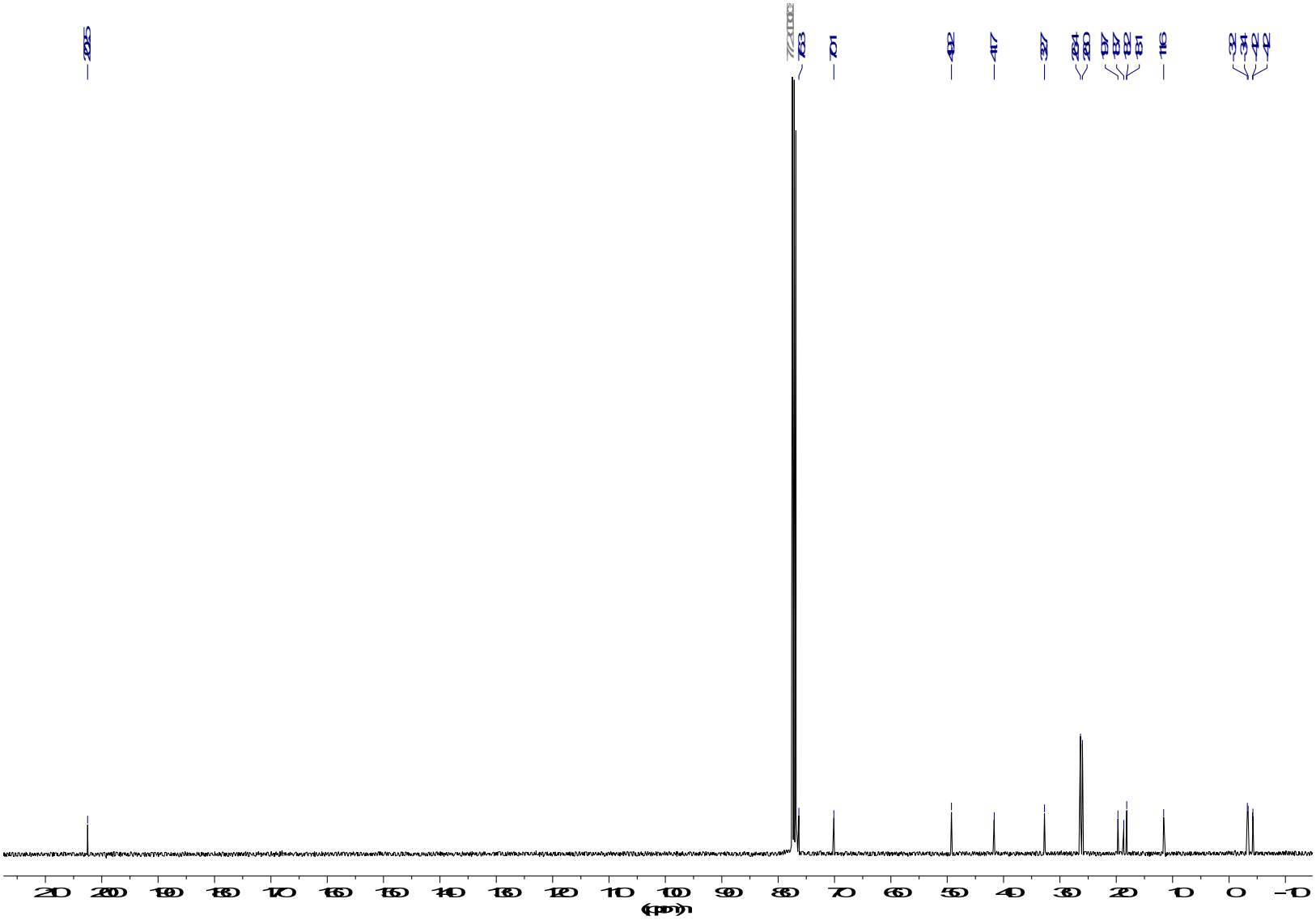
^{13}C-NMR (100.13 MHz, $CDCl_3$)



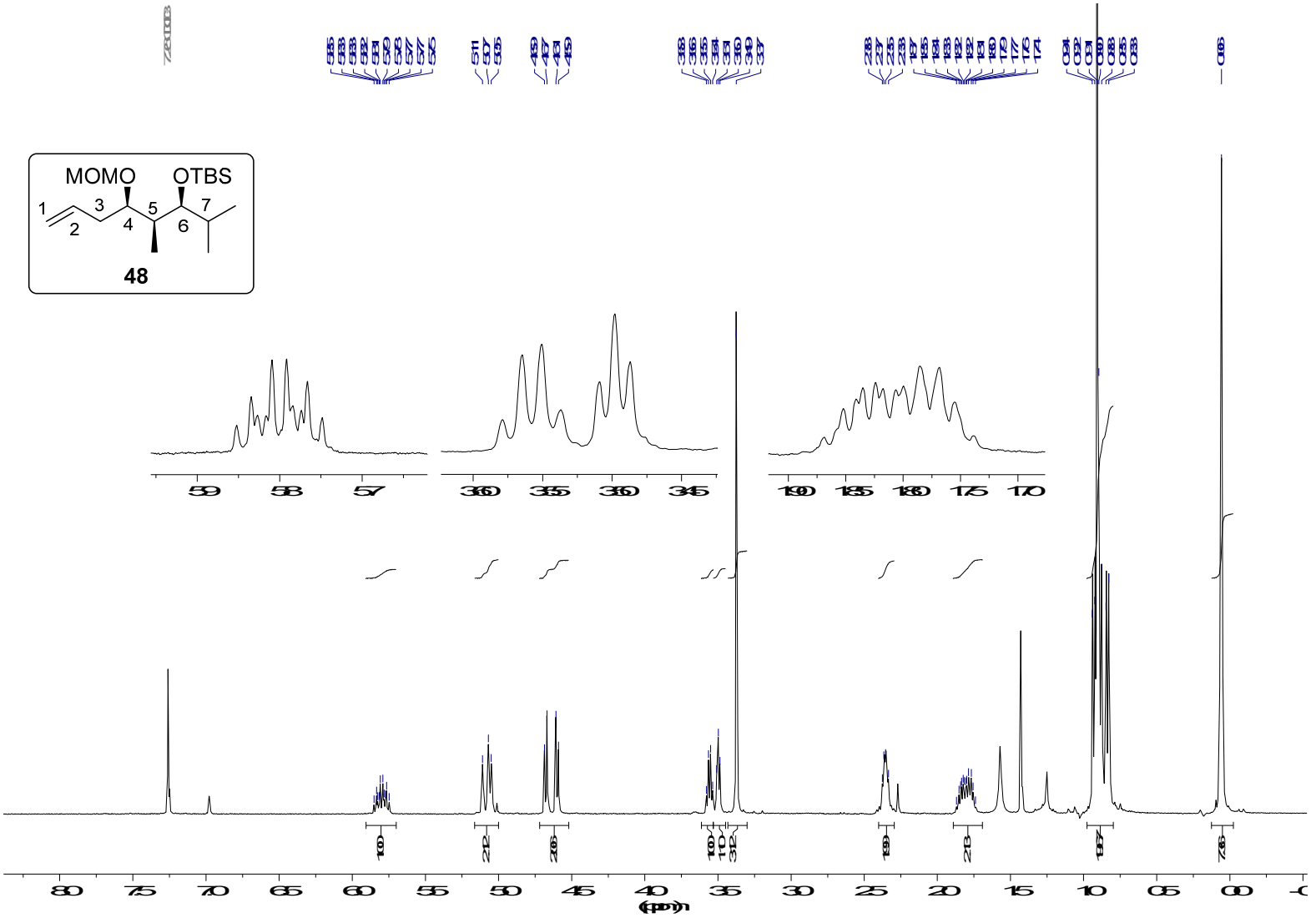
^{1}H-NMR (400.13 MHz, $CDCl_3$)



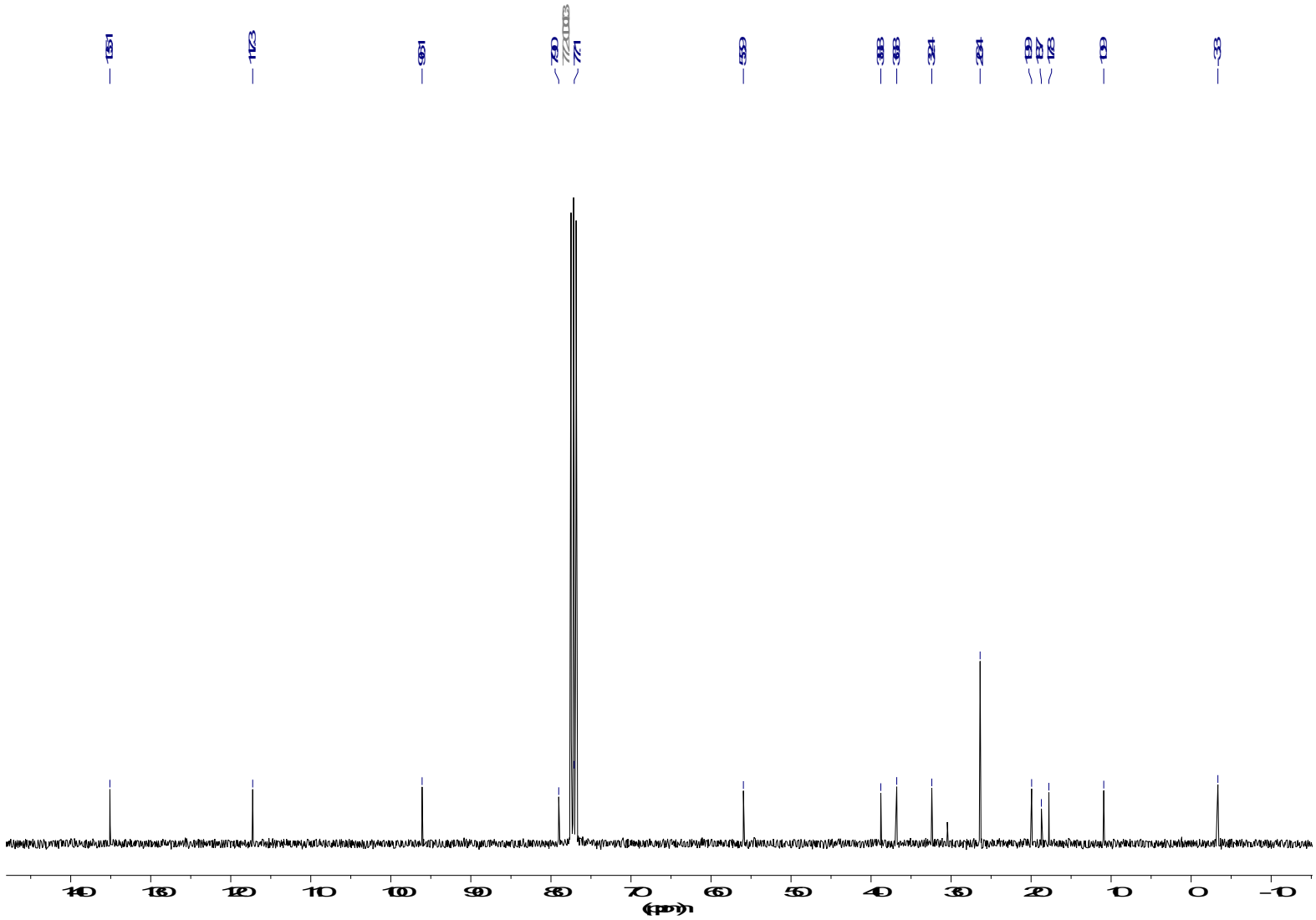
^{13}C-NMR (100.13 MHz, $CDCl_3$)



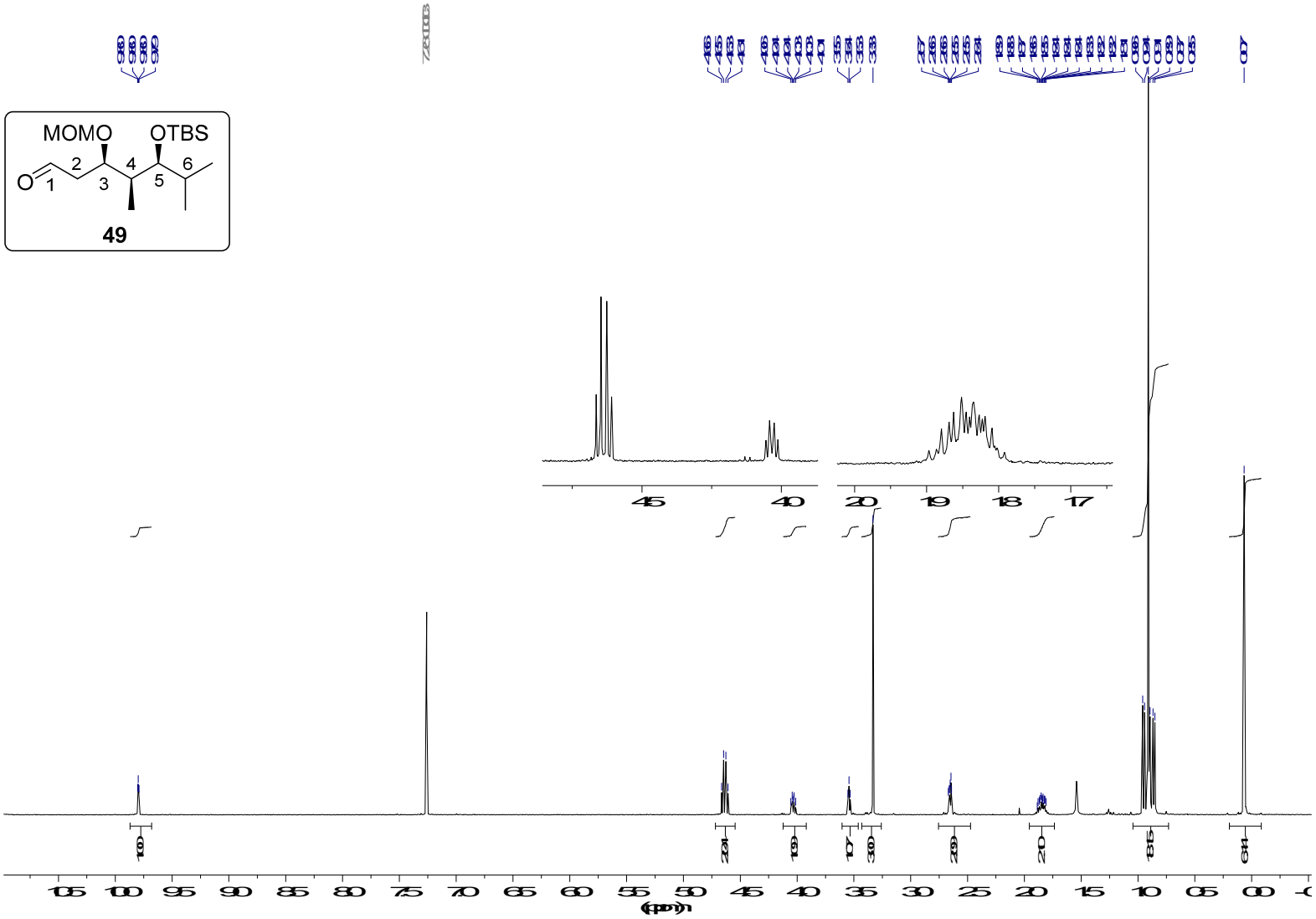
^{1}H-NMR (400.13 MHz, $CDCl_3$)



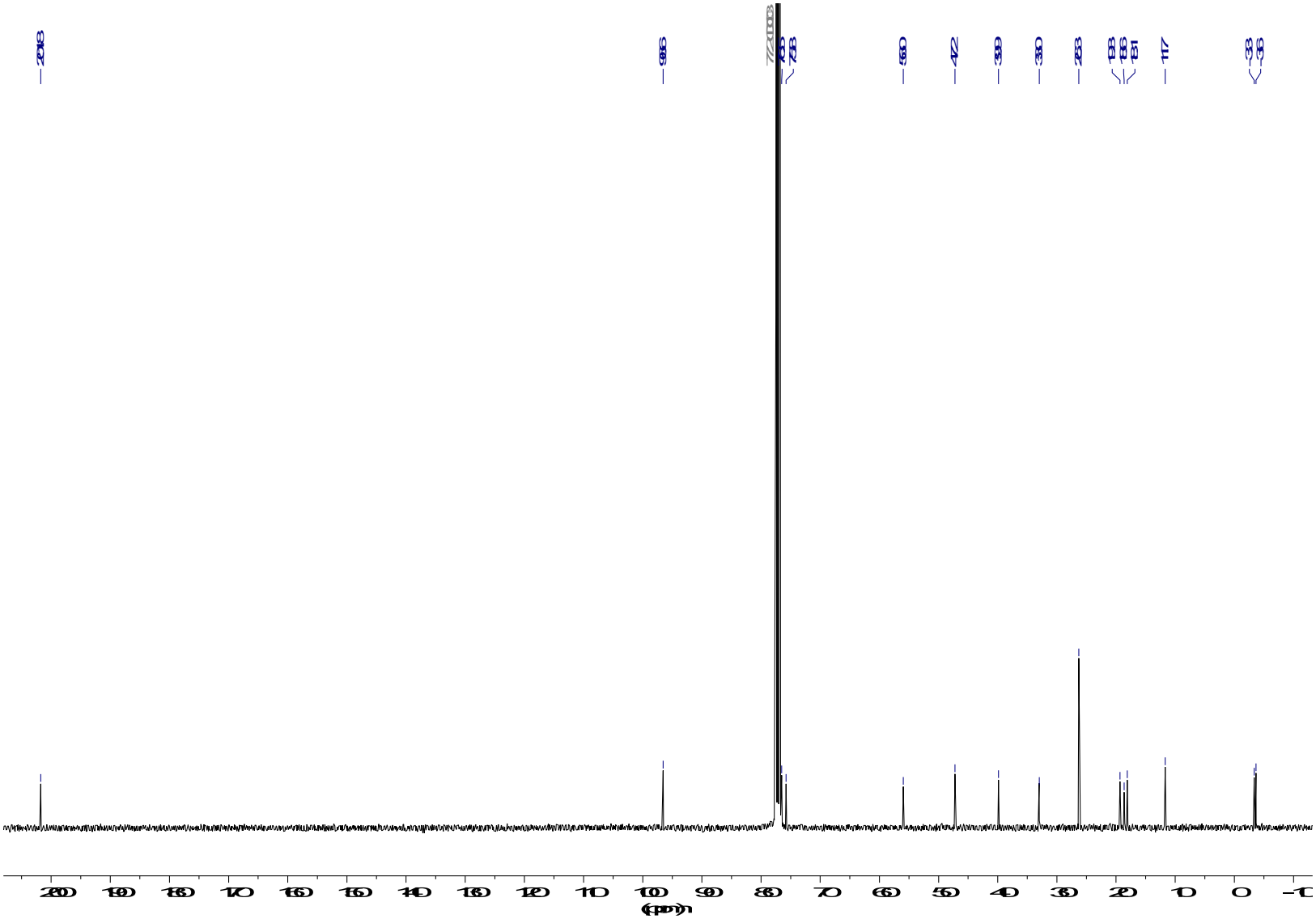
^{13}C-NMR (100.13 MHz, $CDCl_3$)



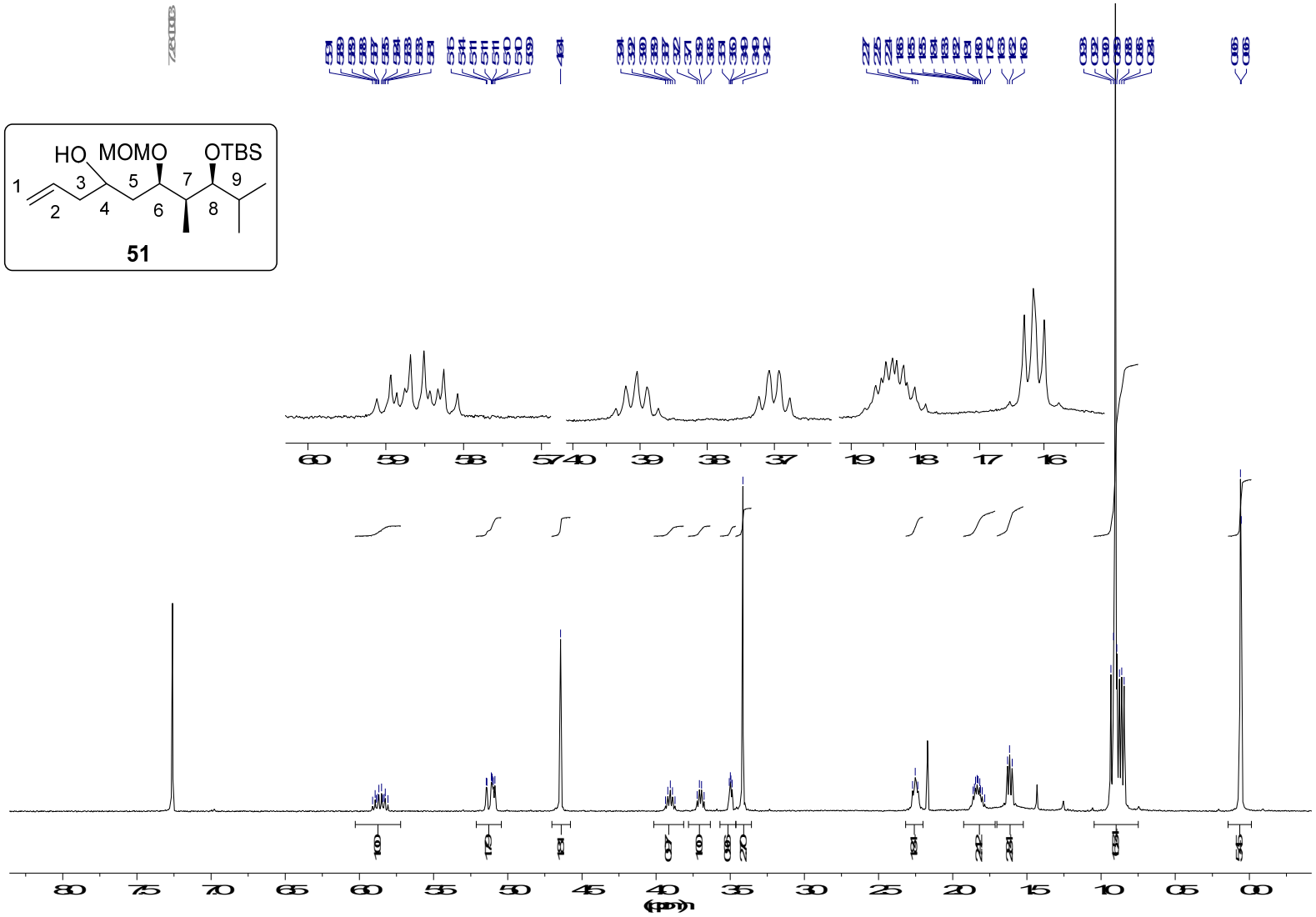
^{1}H-NMR (400.13 MHz, $CDCl_3$)



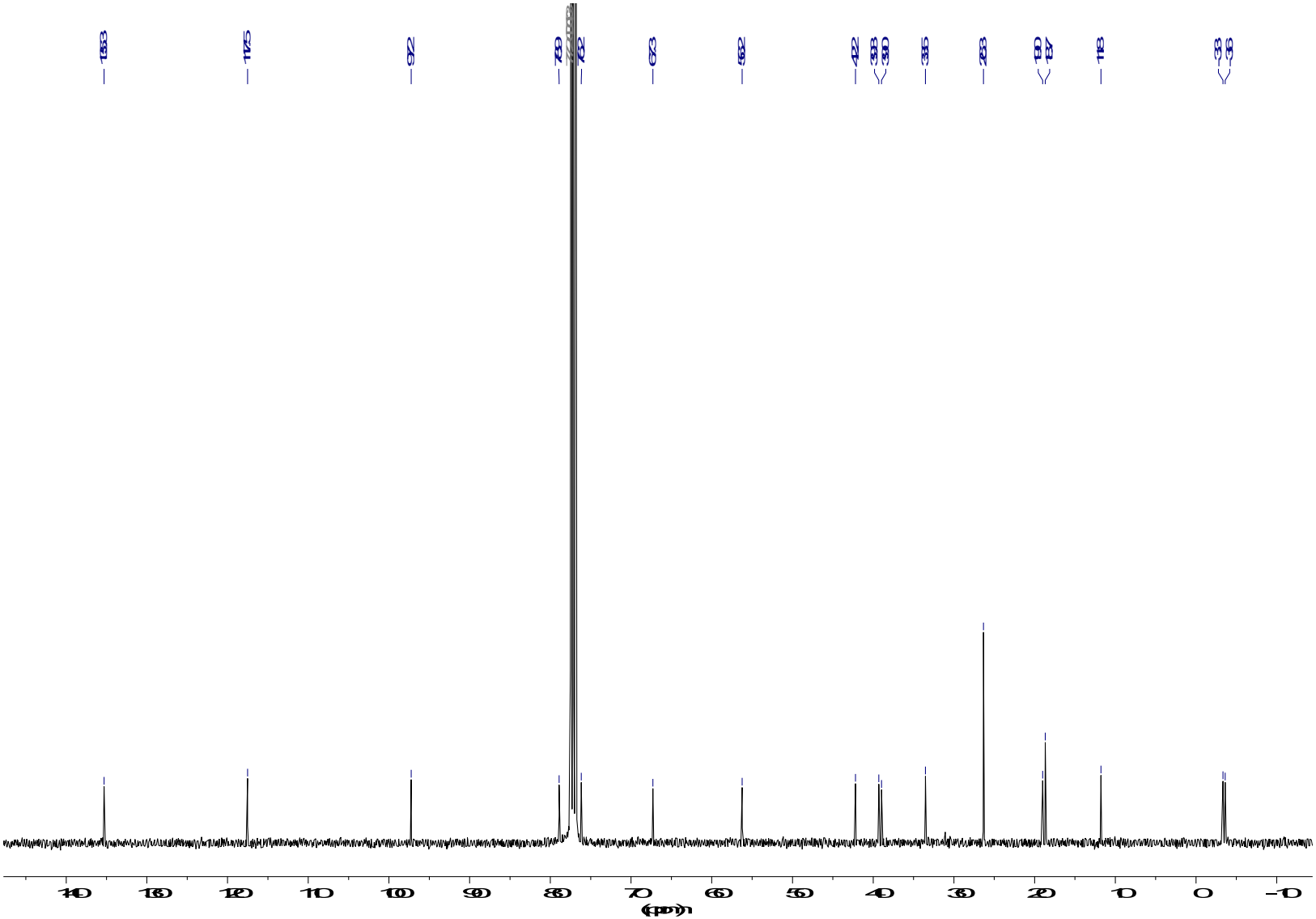
^{13}C-NMR (100.13 MHz, $CDCl_3$)



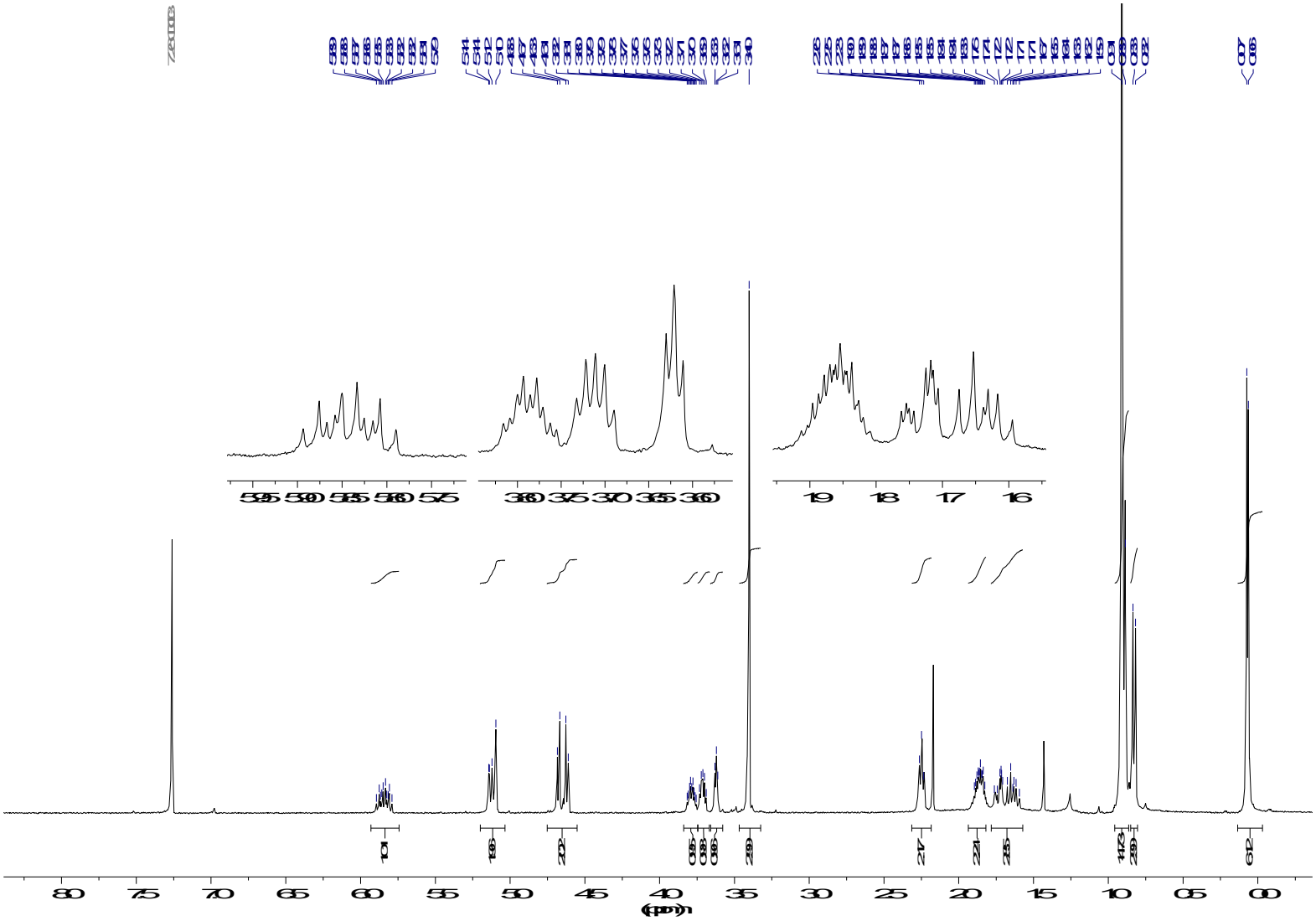
Diastereoisomer 1. ^{1}H-NMR (400.13 MHz, $CDCl_3$)



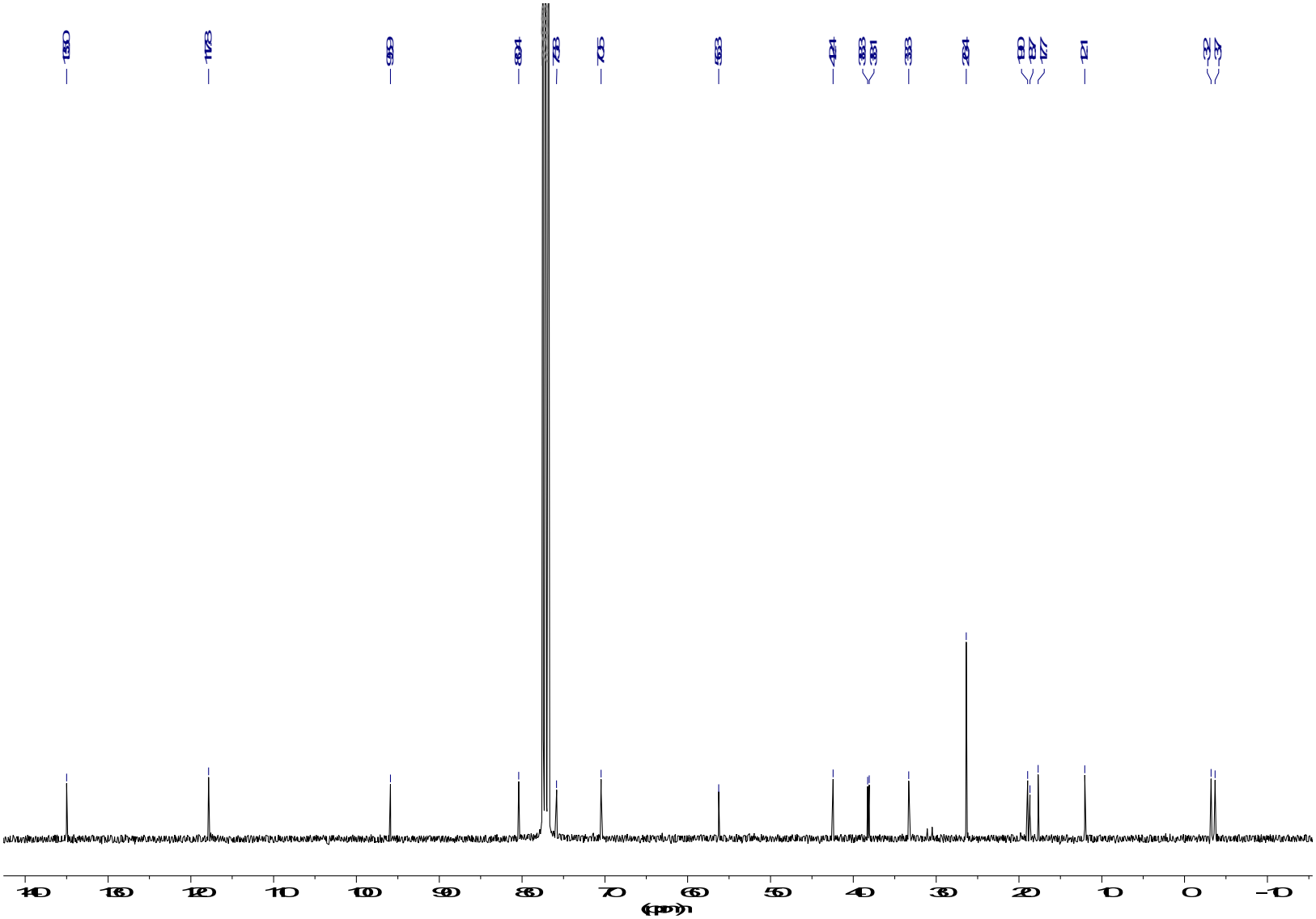
^{13}C-NMR (100.13 MHz, $CDCl_3$)



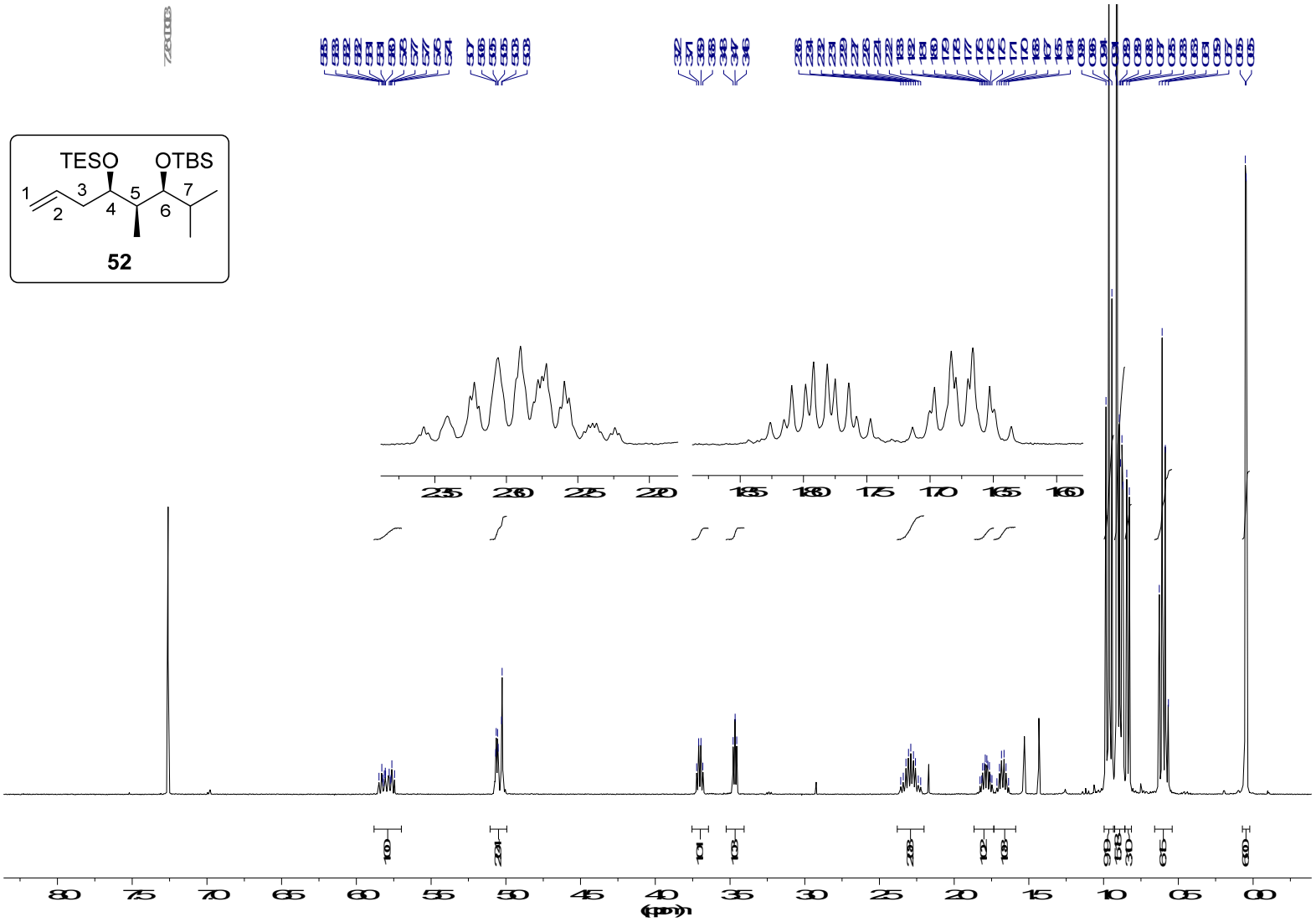
Diastereoisomer 2. ^{1}H-NMR (400.13 MHz, $CDCl_3$)



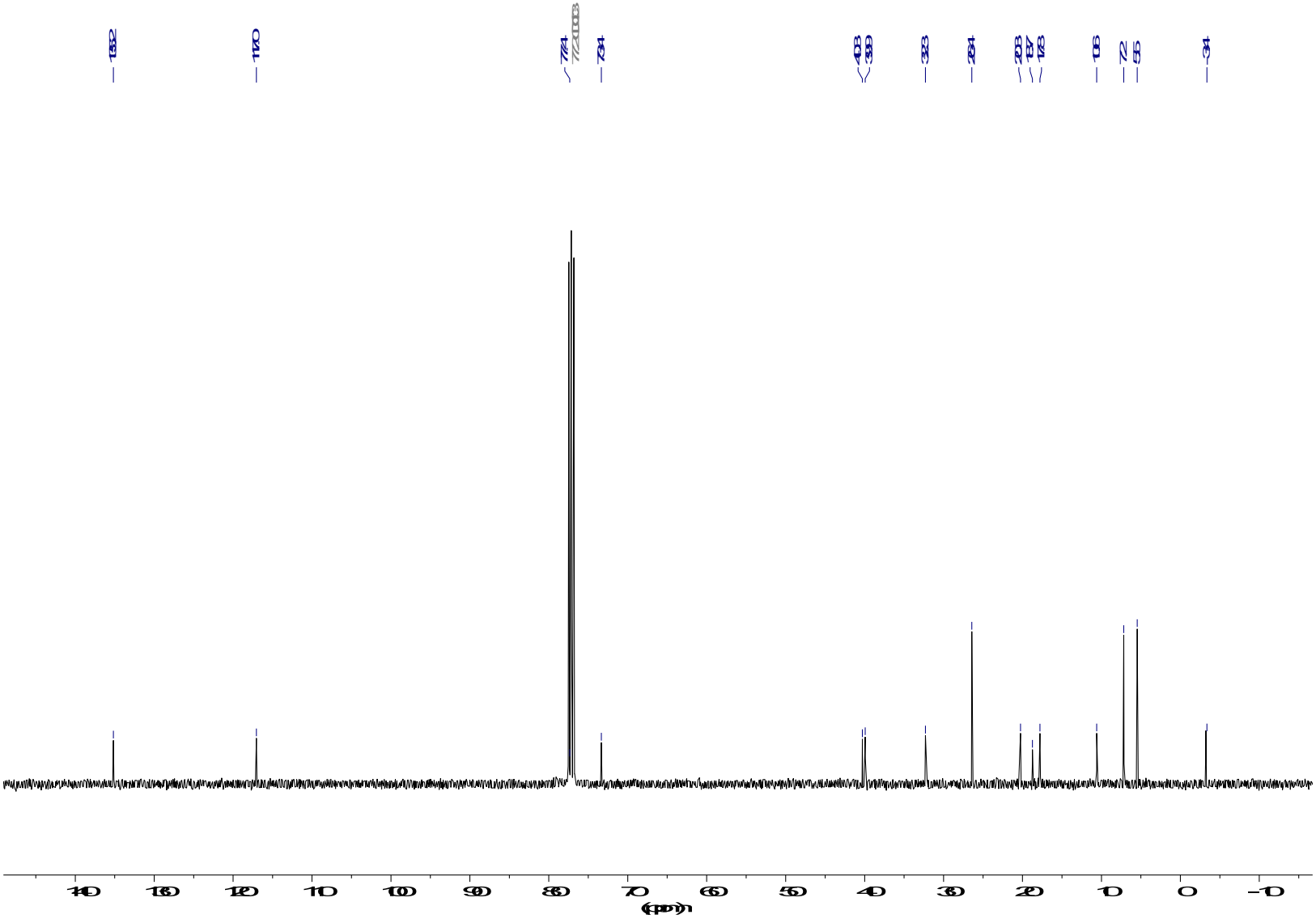
^{13}C-NMR (100.13 MHz, $CDCl_3$)



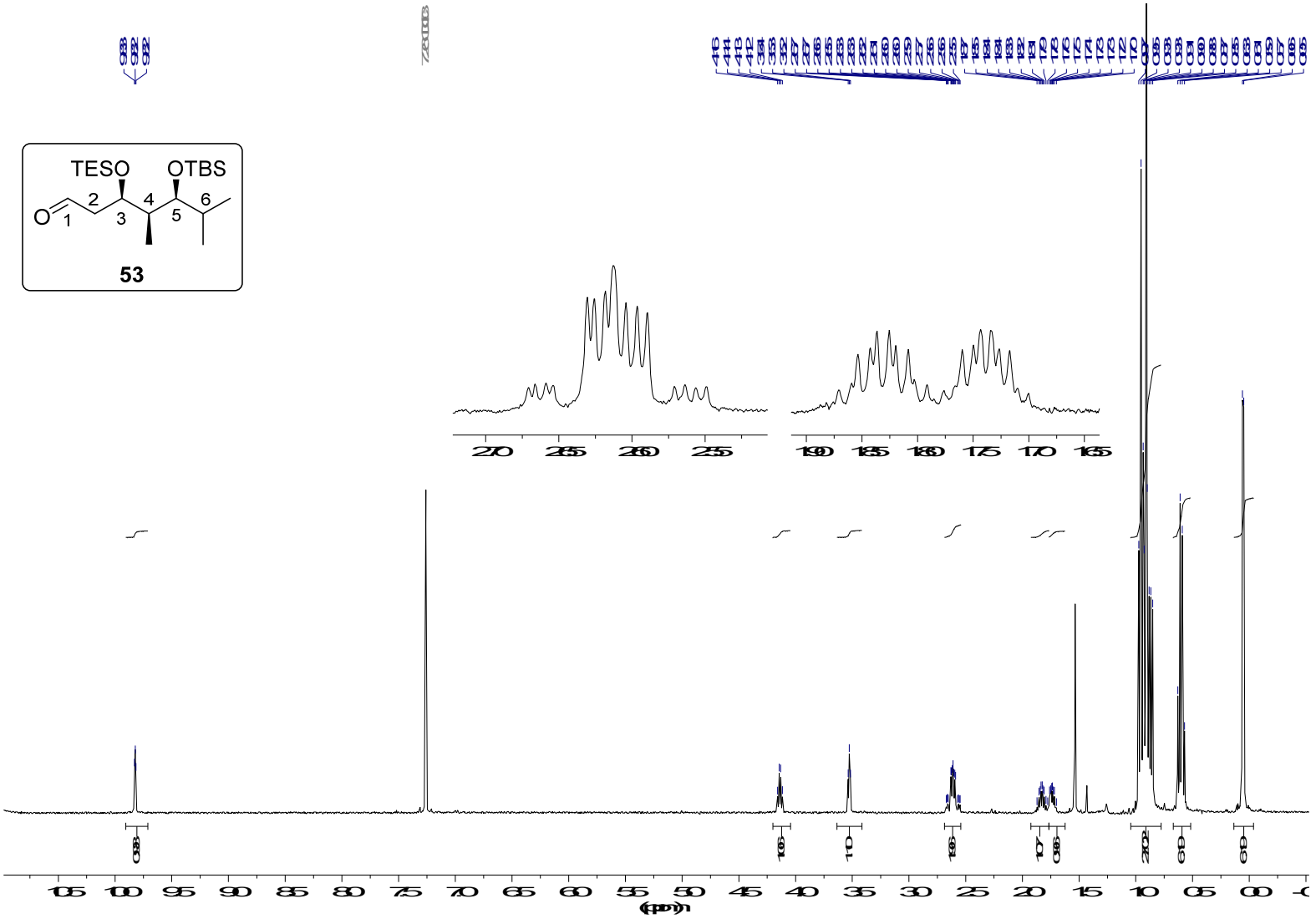
^{1}H-NMR (400.13 MHz, $CDCl_3$)



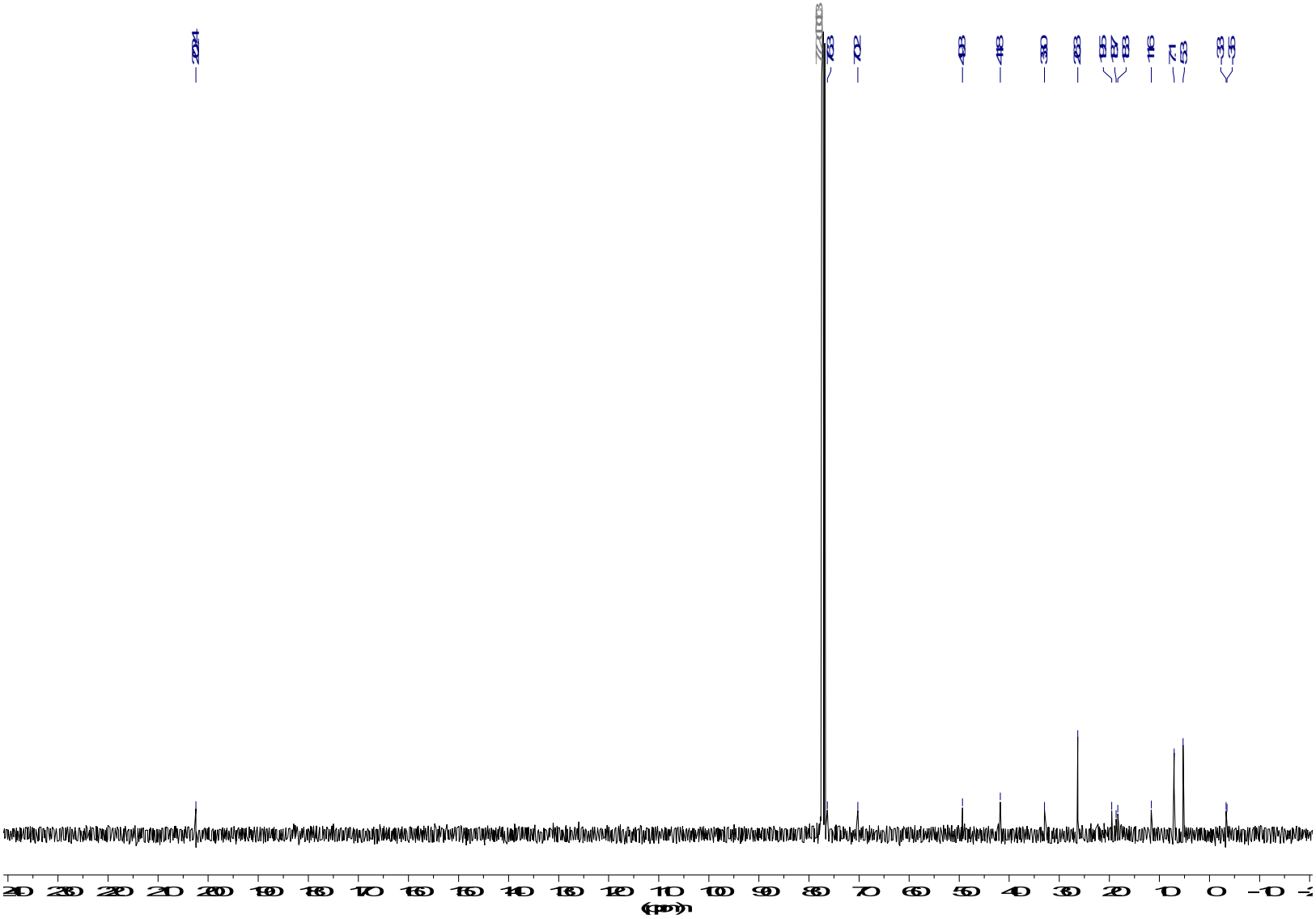
^{13}C-NMR (100.13 MHz, $CDCl_3$)



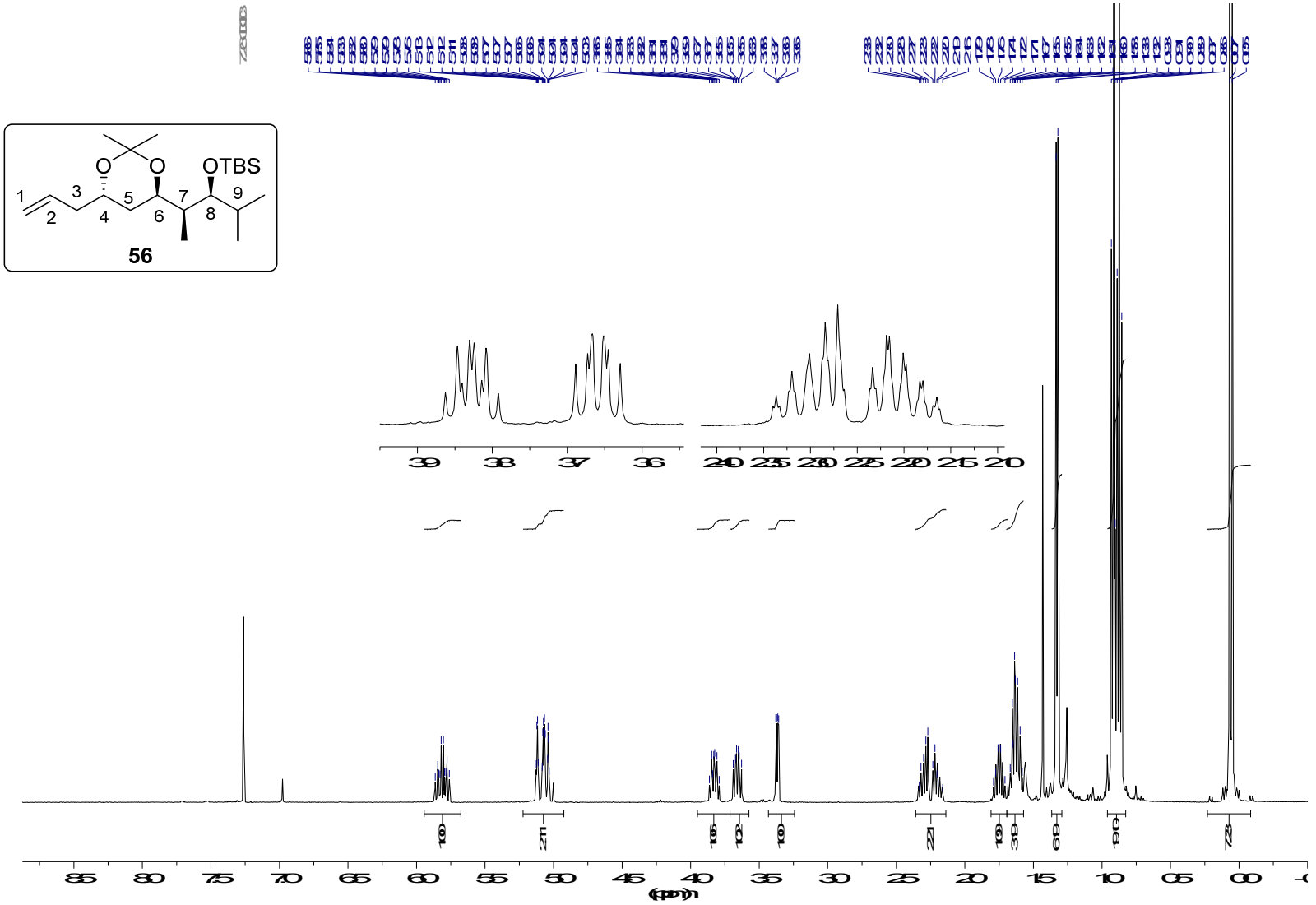
^{1}H-NMR (400.13 MHz, $CDCl_3$)



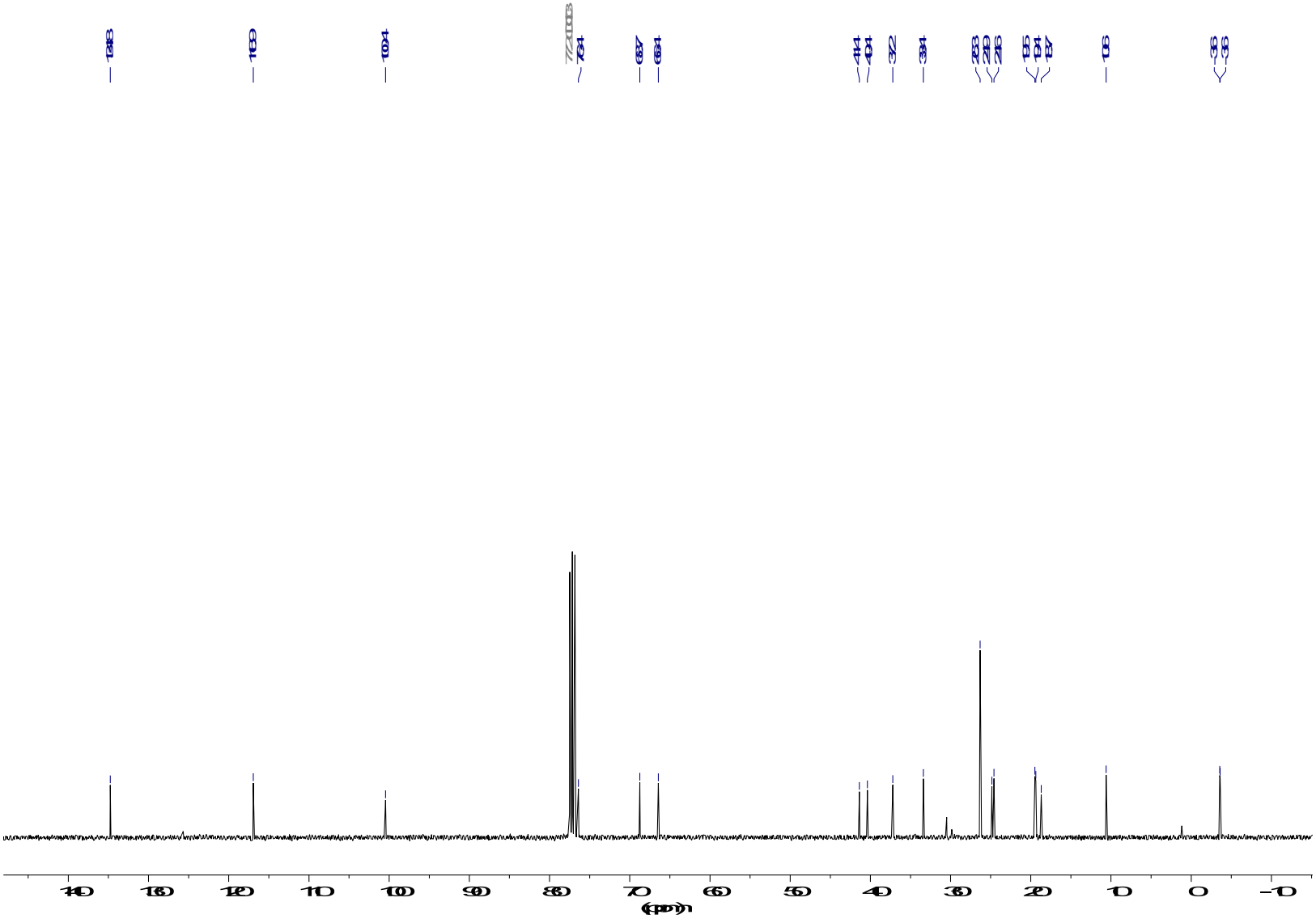
^{13}C-NMR (100.13 MHz, $CDCl_3$)



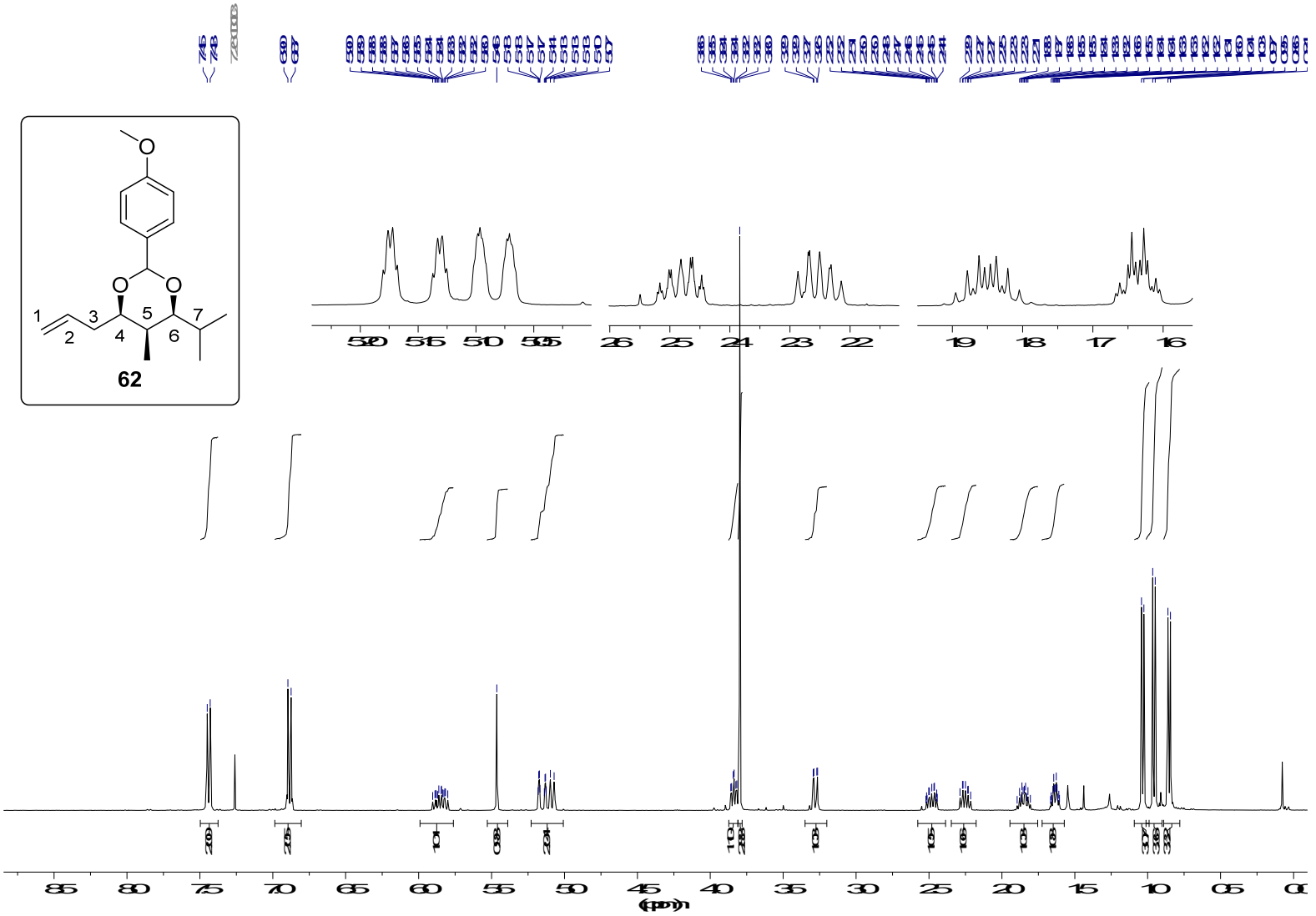
^{1}H-NMR (400.13 MHz, $CDCl_3$)



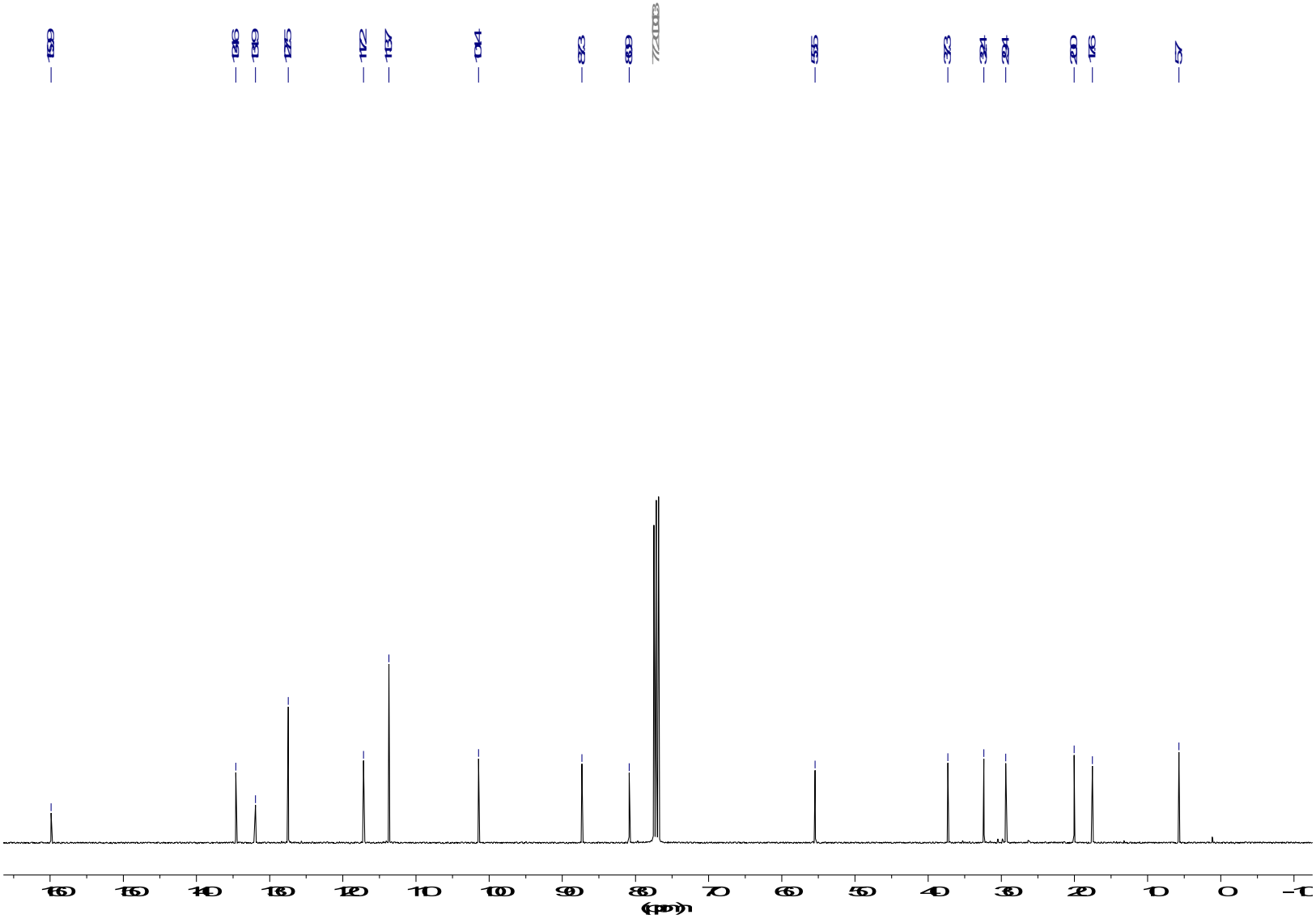
^{13}C-NMR (100.13 MHz, $CDCl_3$)



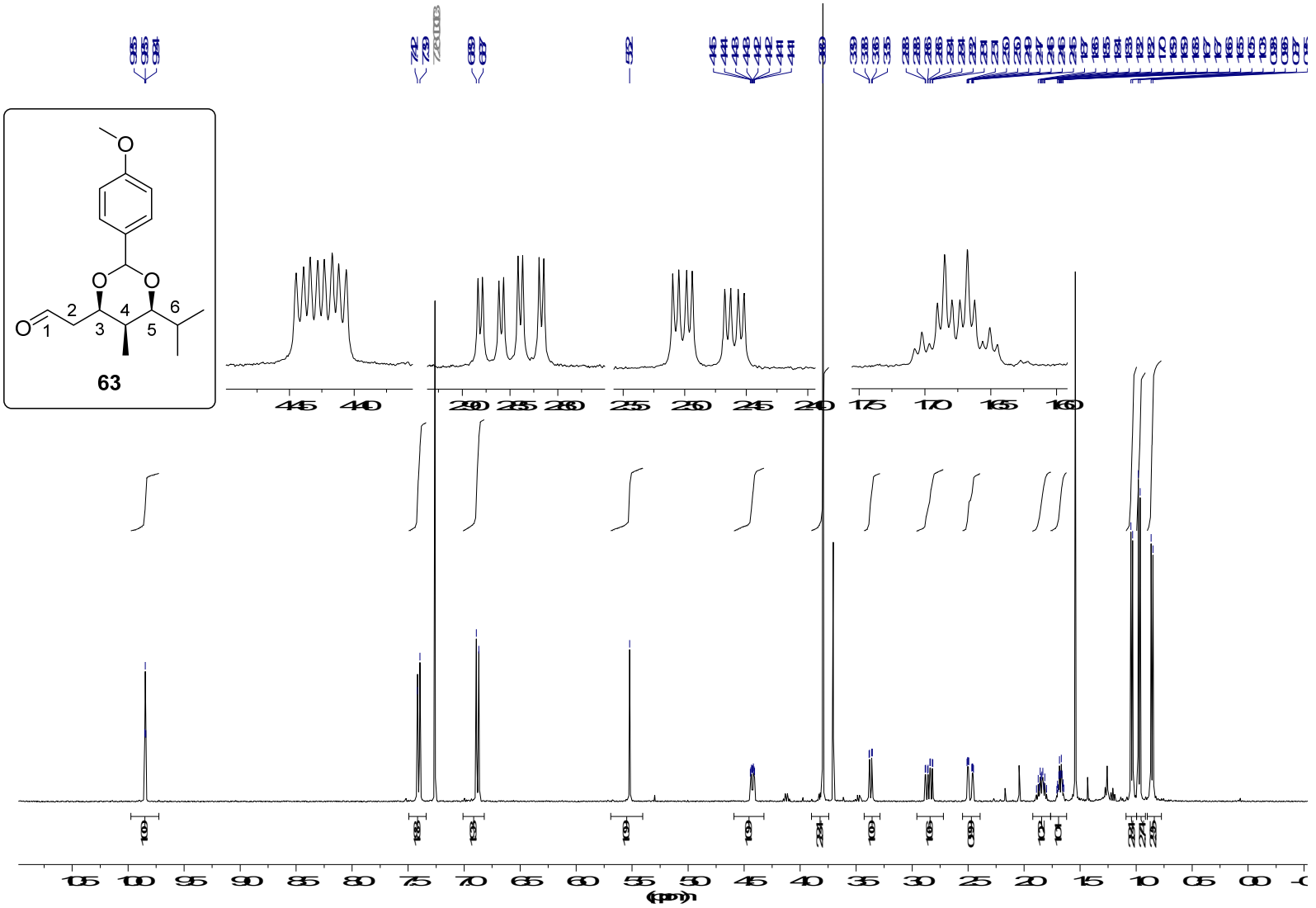
^{1}H-NMR (400.13 MHz, $CDCl_3$)



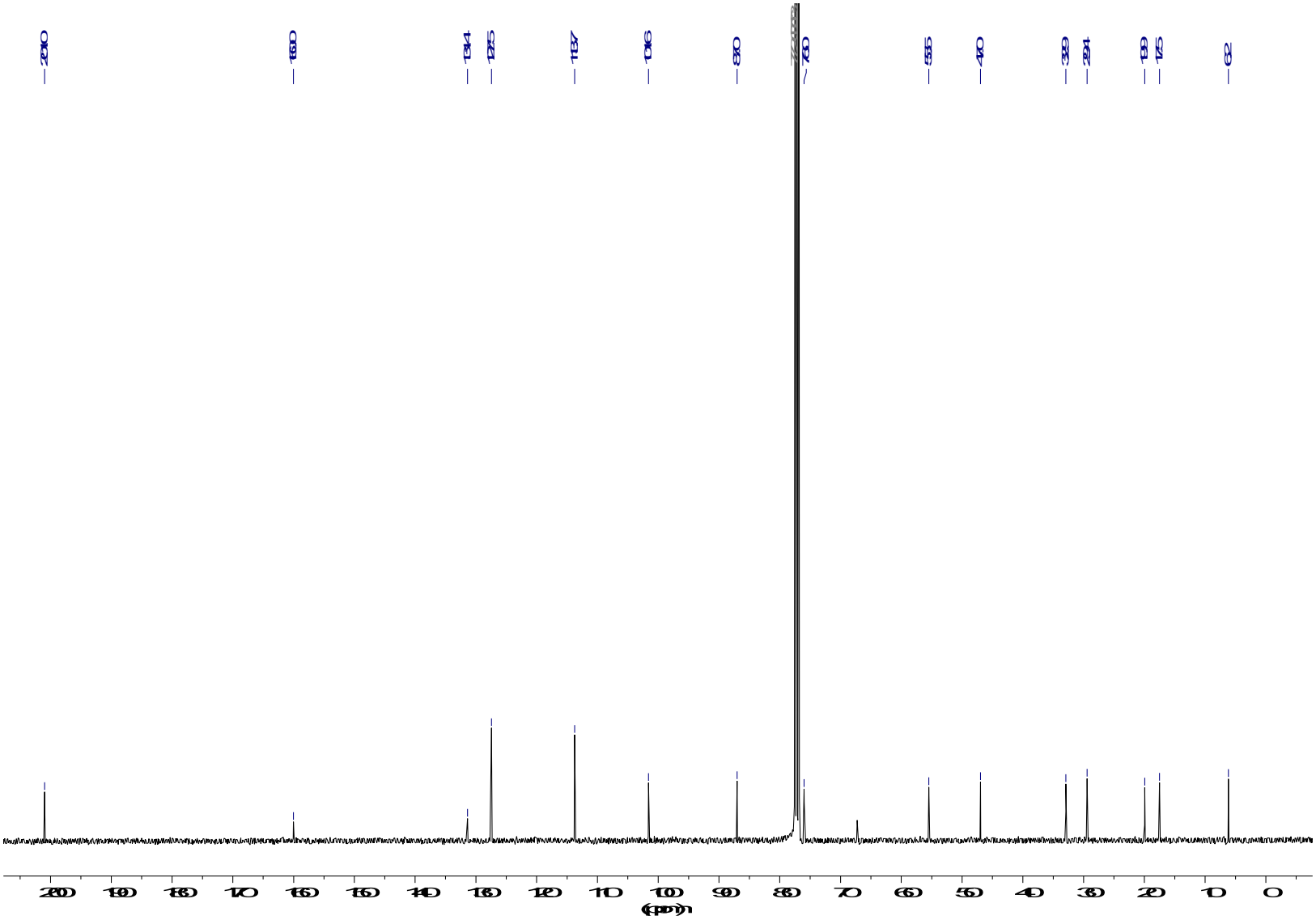
^{13}C-NMR (100.13 MHz, $CDCl_3$)



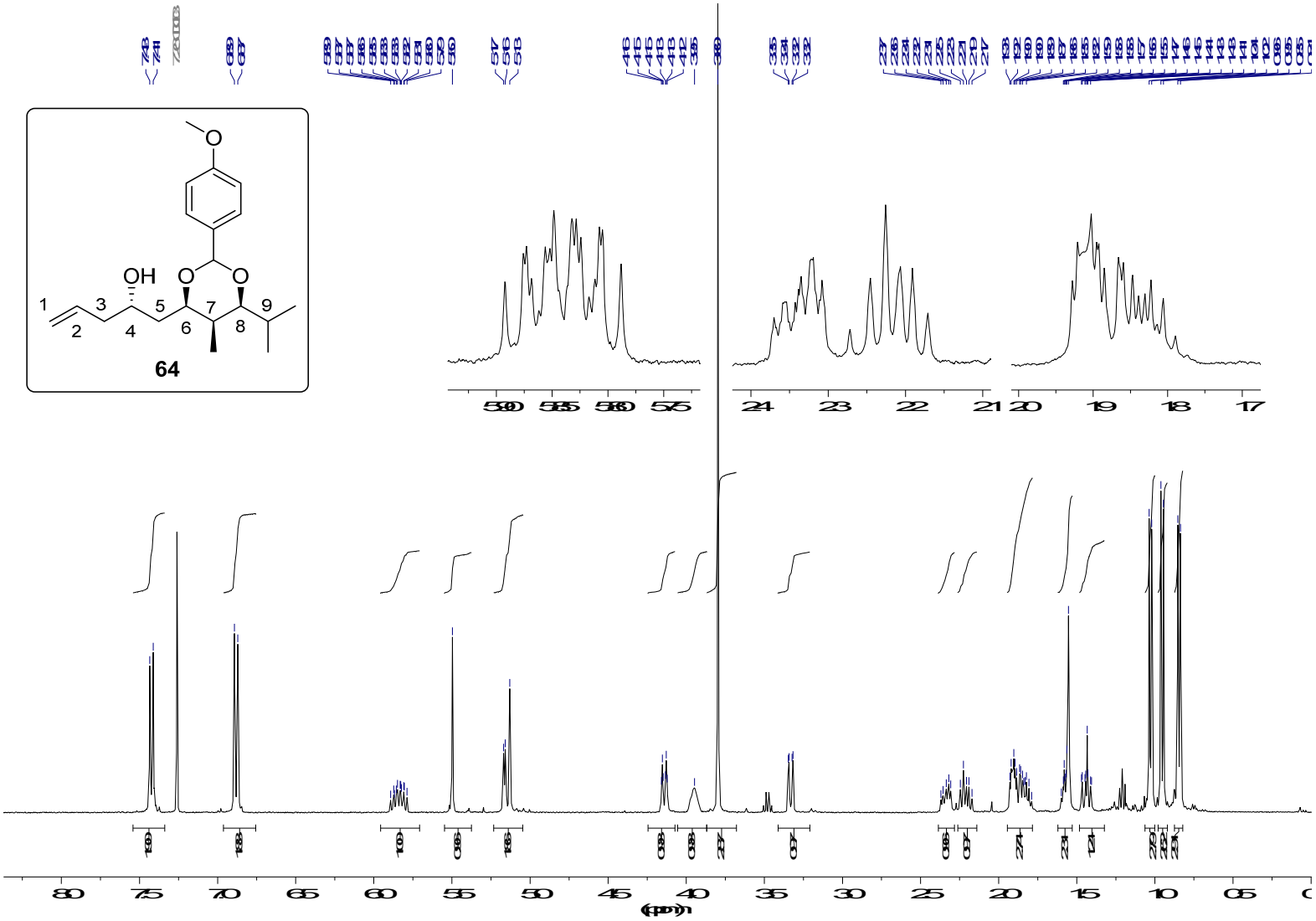
^{1}H-NMR (400.13 MHz, $CDCl_3$)



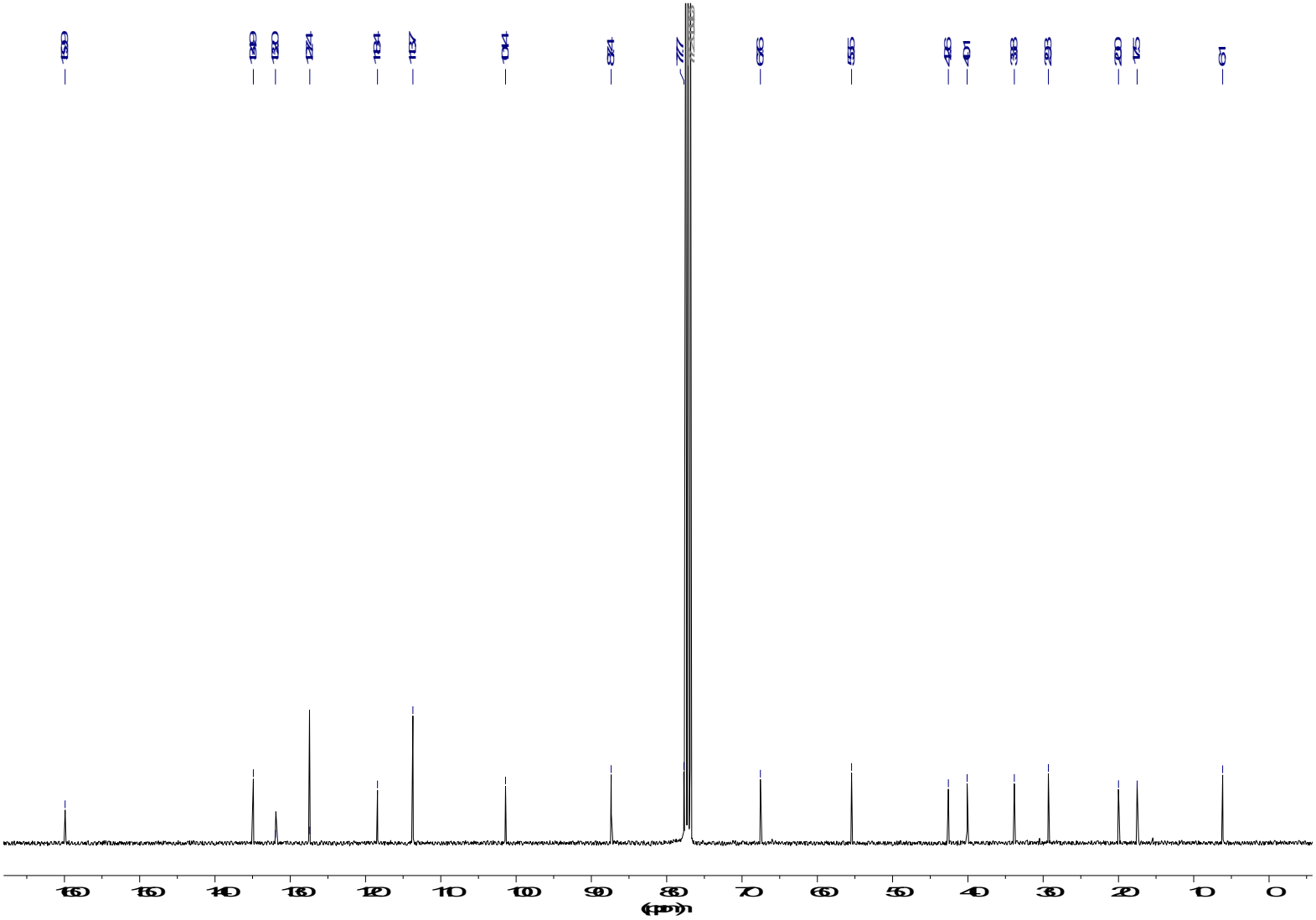
^{13}C-NMR (100.13 MHz, $CDCl_3$)



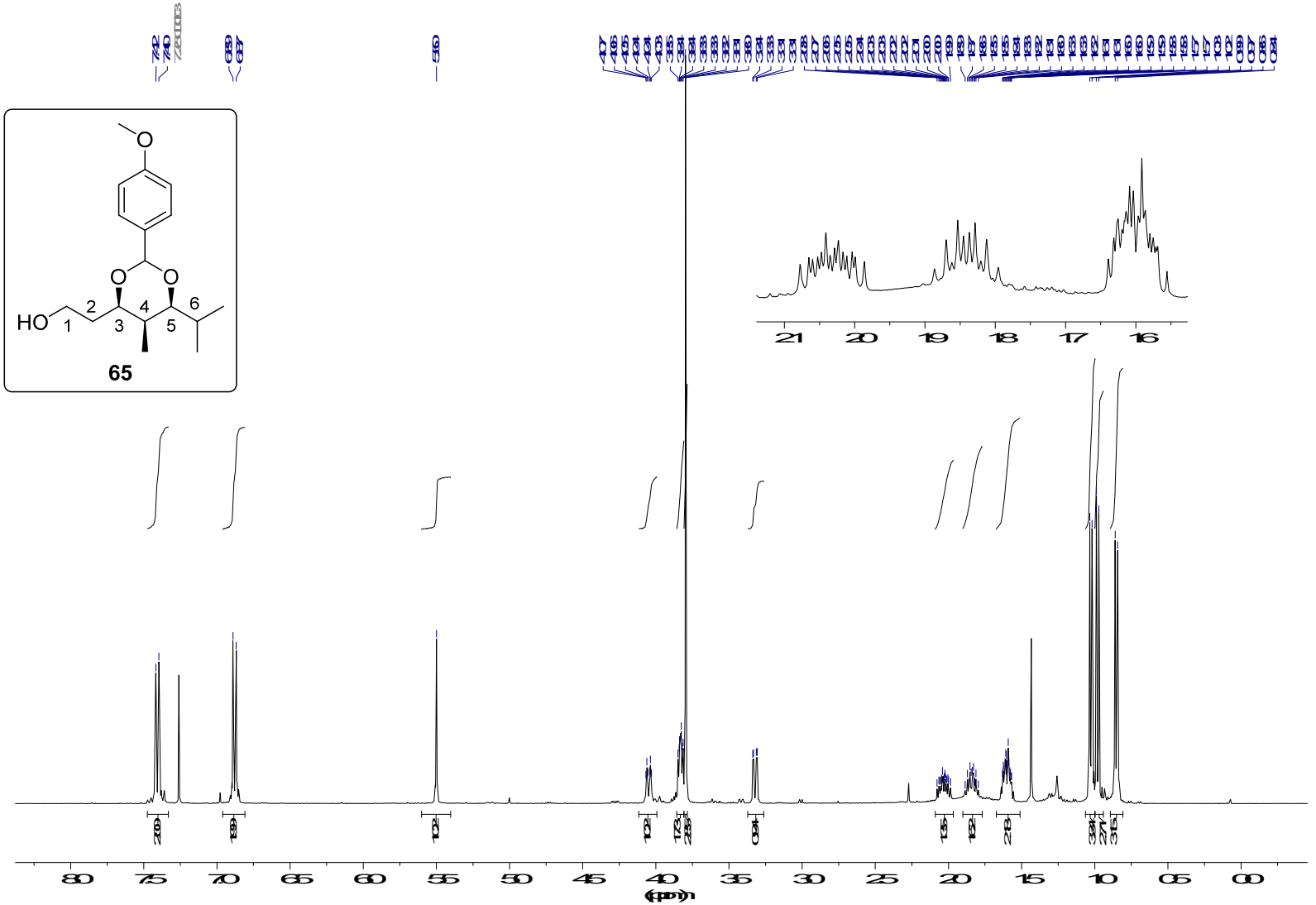
^{1}H-NMR (400.13 MHz, $CDCl_3$)



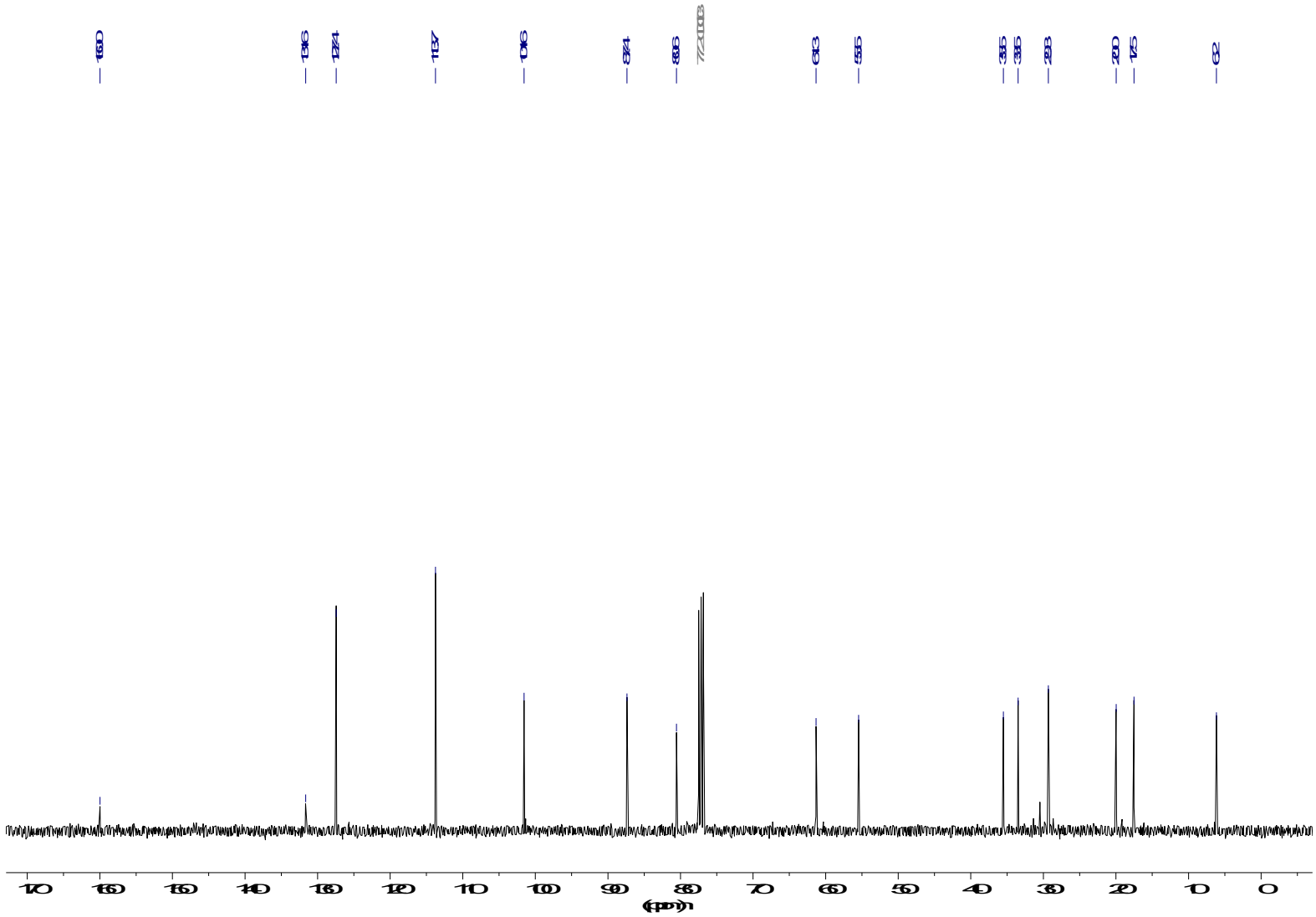
^{13}C-NMR (100.13 MHz, $CDCl_3$)



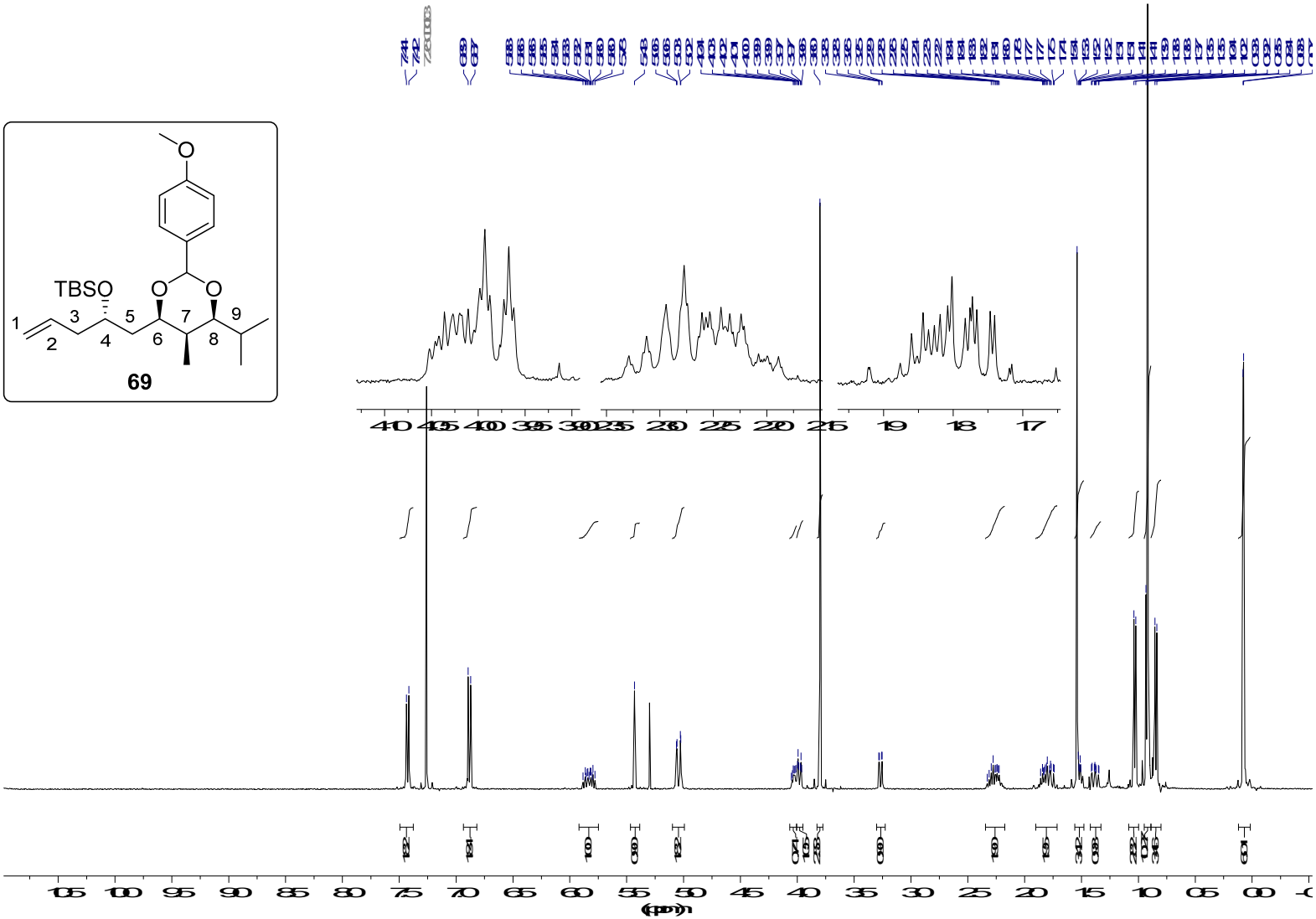
^{1}H-NMR (400.13 MHz, $CDCl_3$)



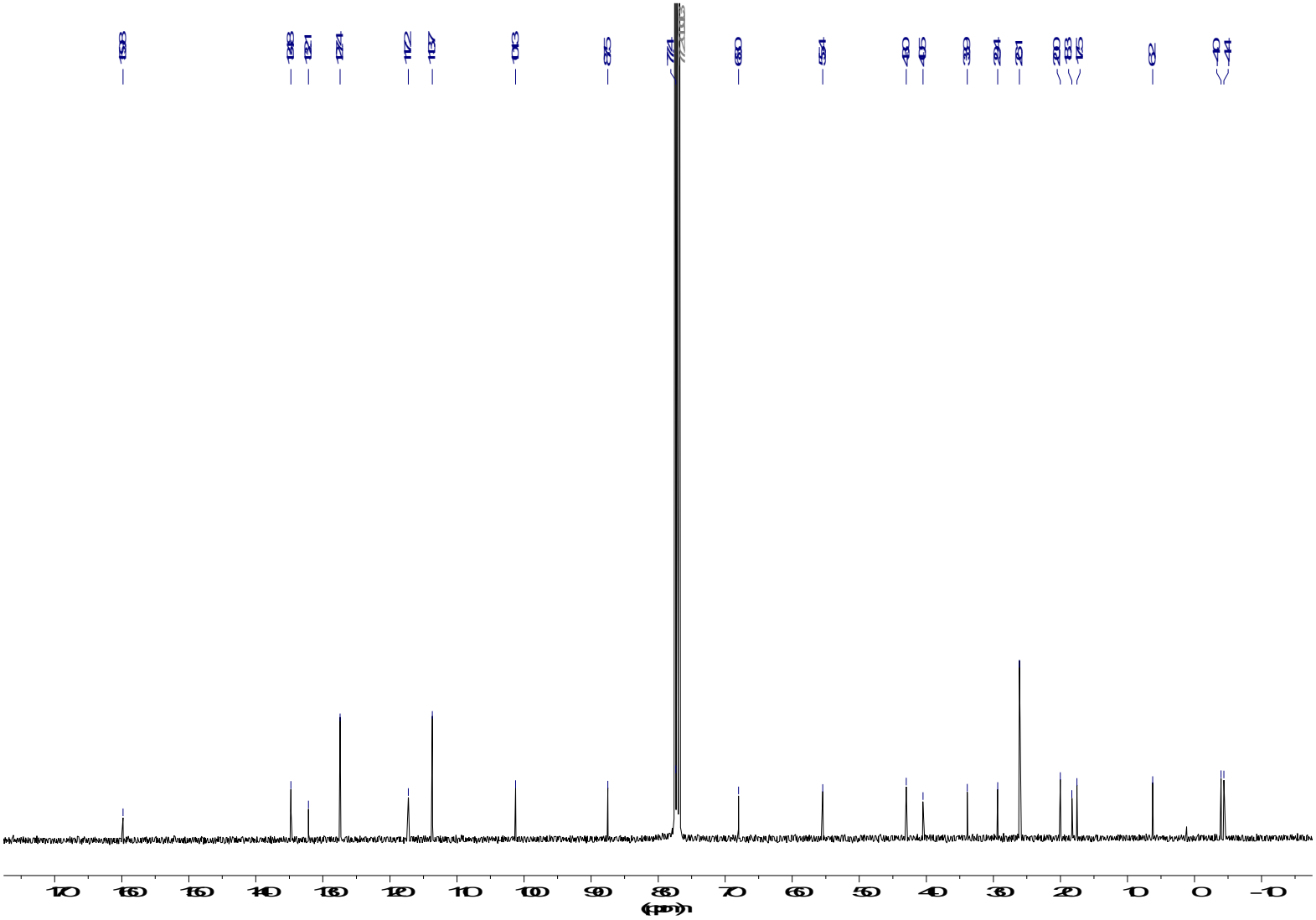
^{13}C-NMR (100.13 MHz, $CDCl_3$)



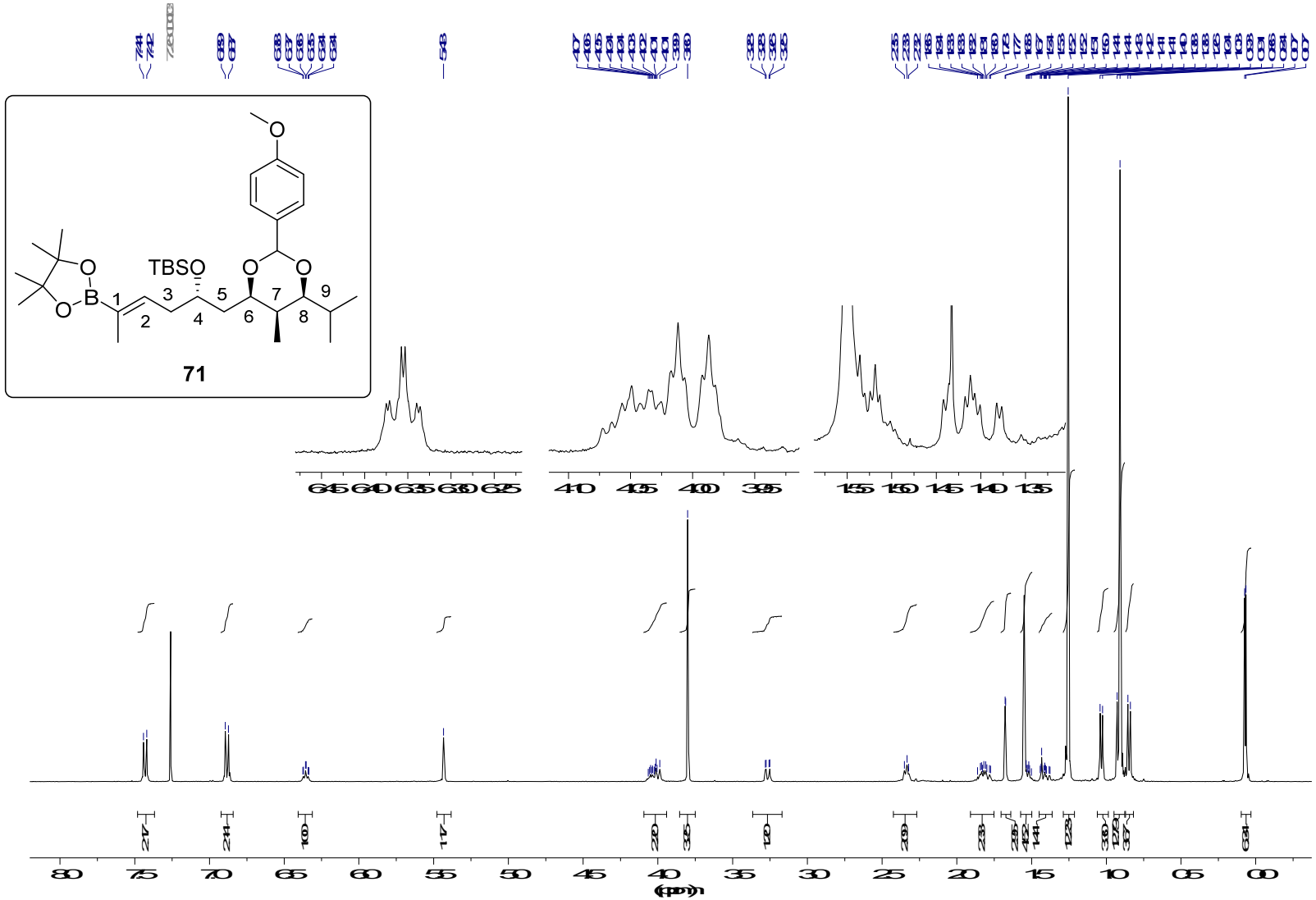
^{1}H-NMR (400.13 MHz, $CDCl_3$)



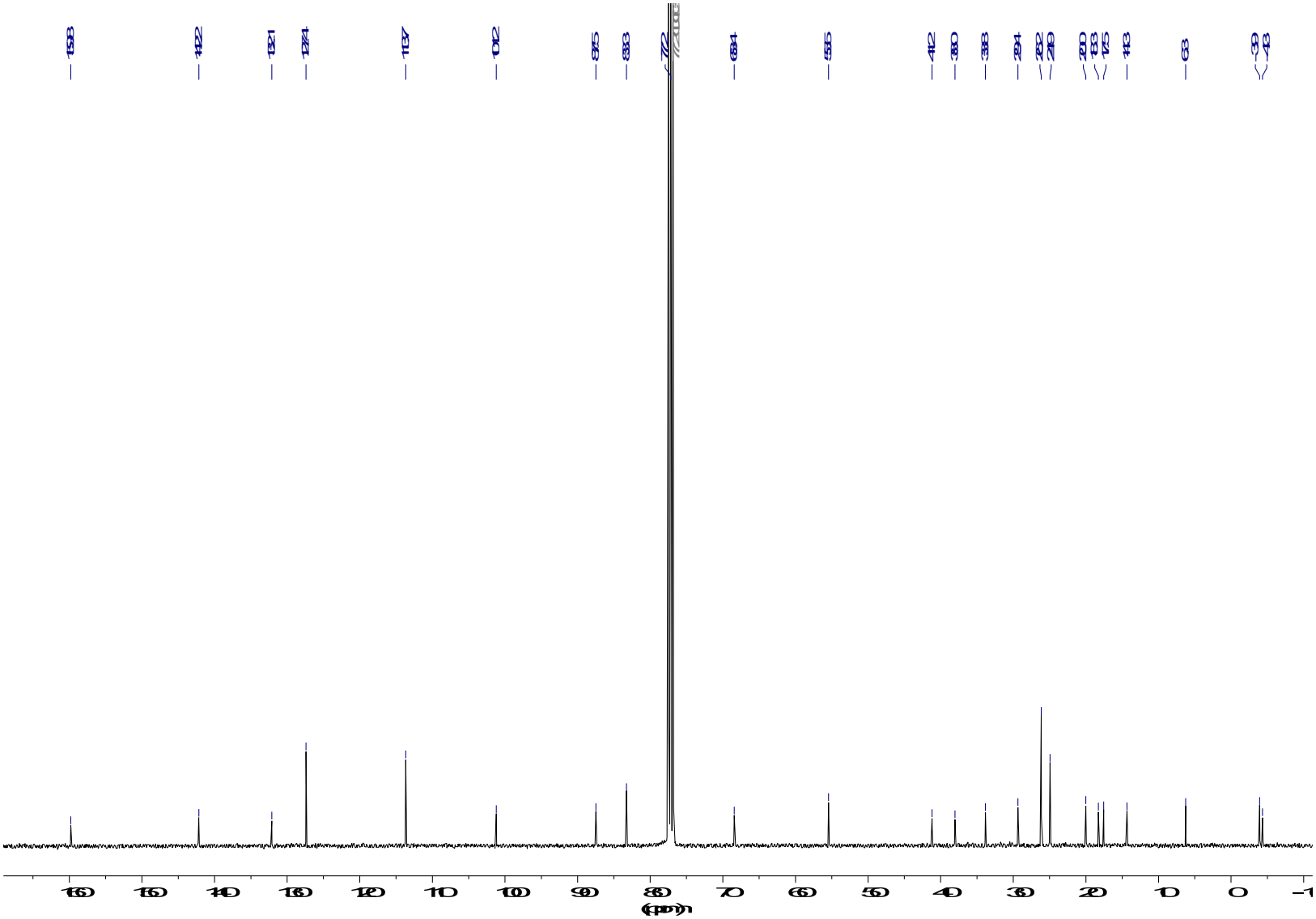
^{13}C-NMR (100.13 MHz, $CDCl_3$)



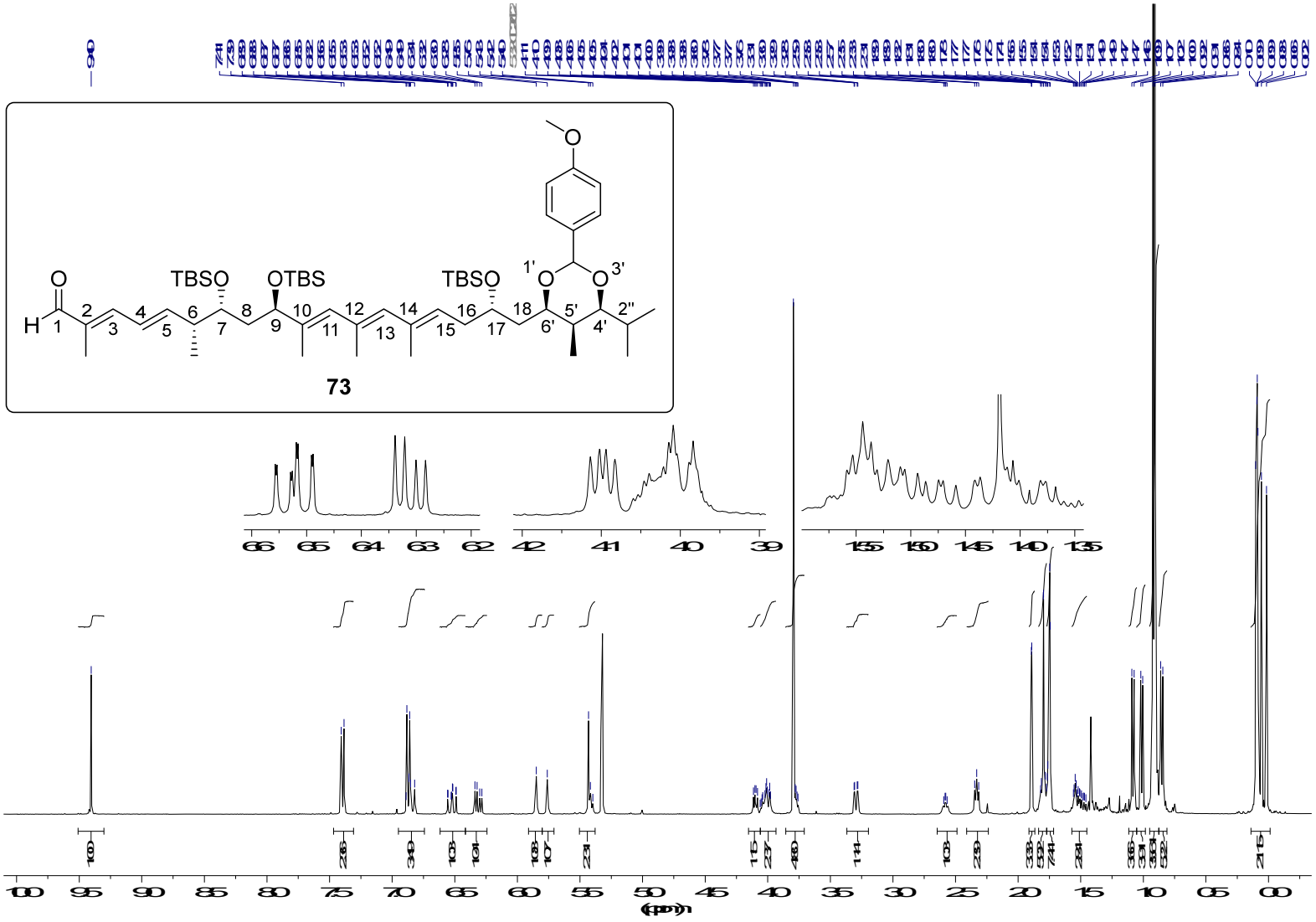
^{1}H-NMR (400.13 MHz, $CDCl_3$)



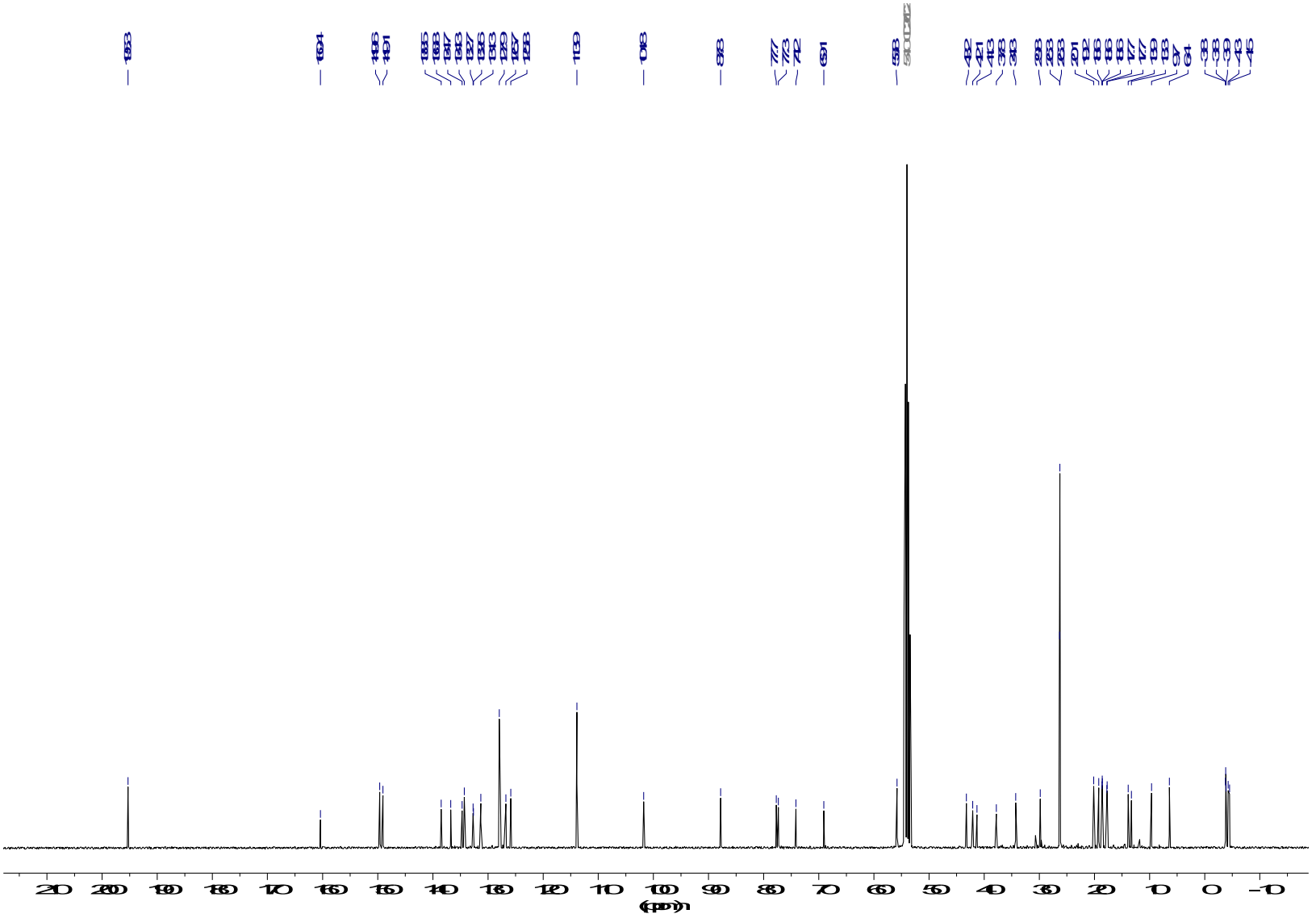
^{13}C-NMR (100.13 MHz, $CDCl_3$)



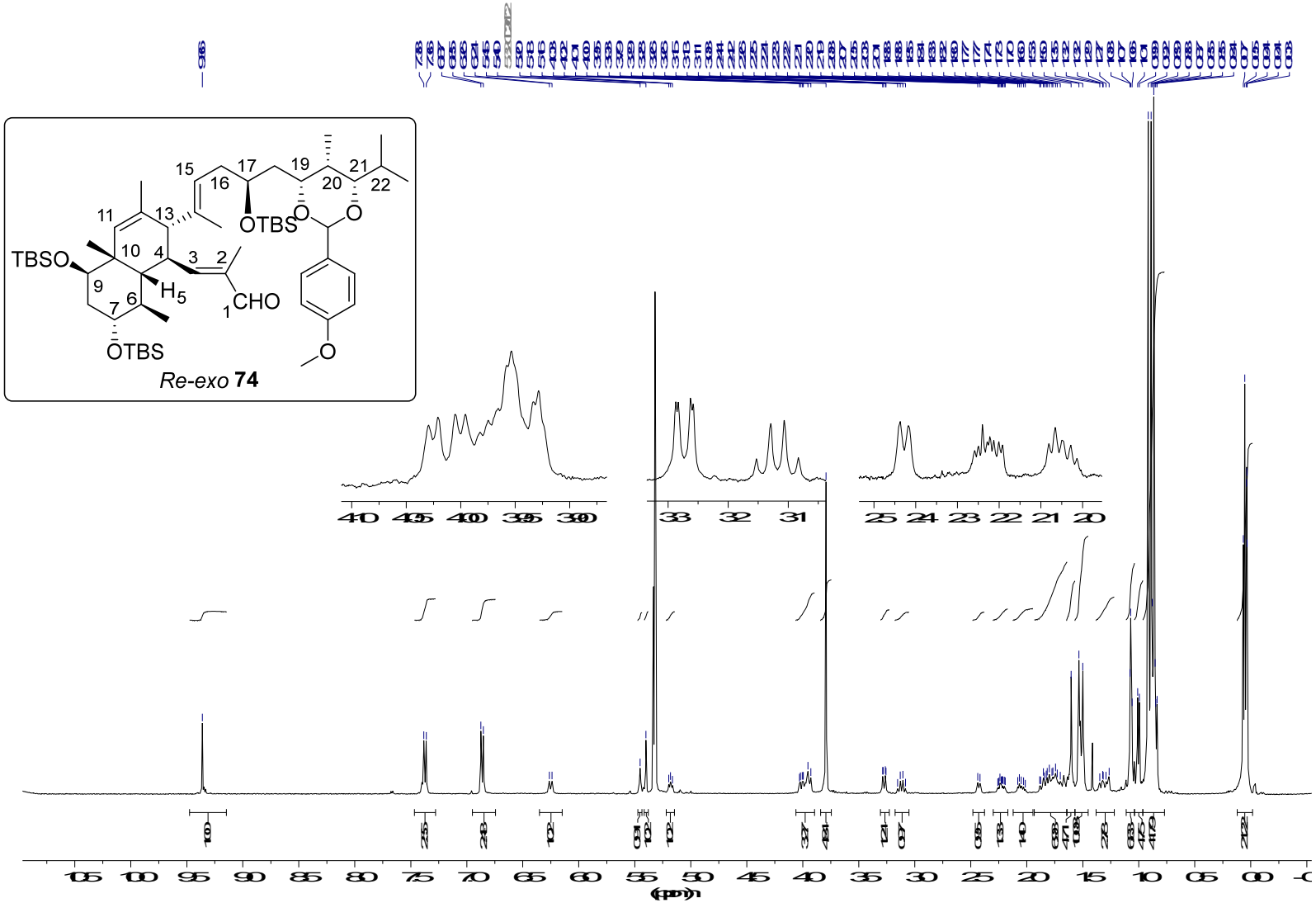
^{1}H-NMR (400.13 MHz, CD_2Cl_2)



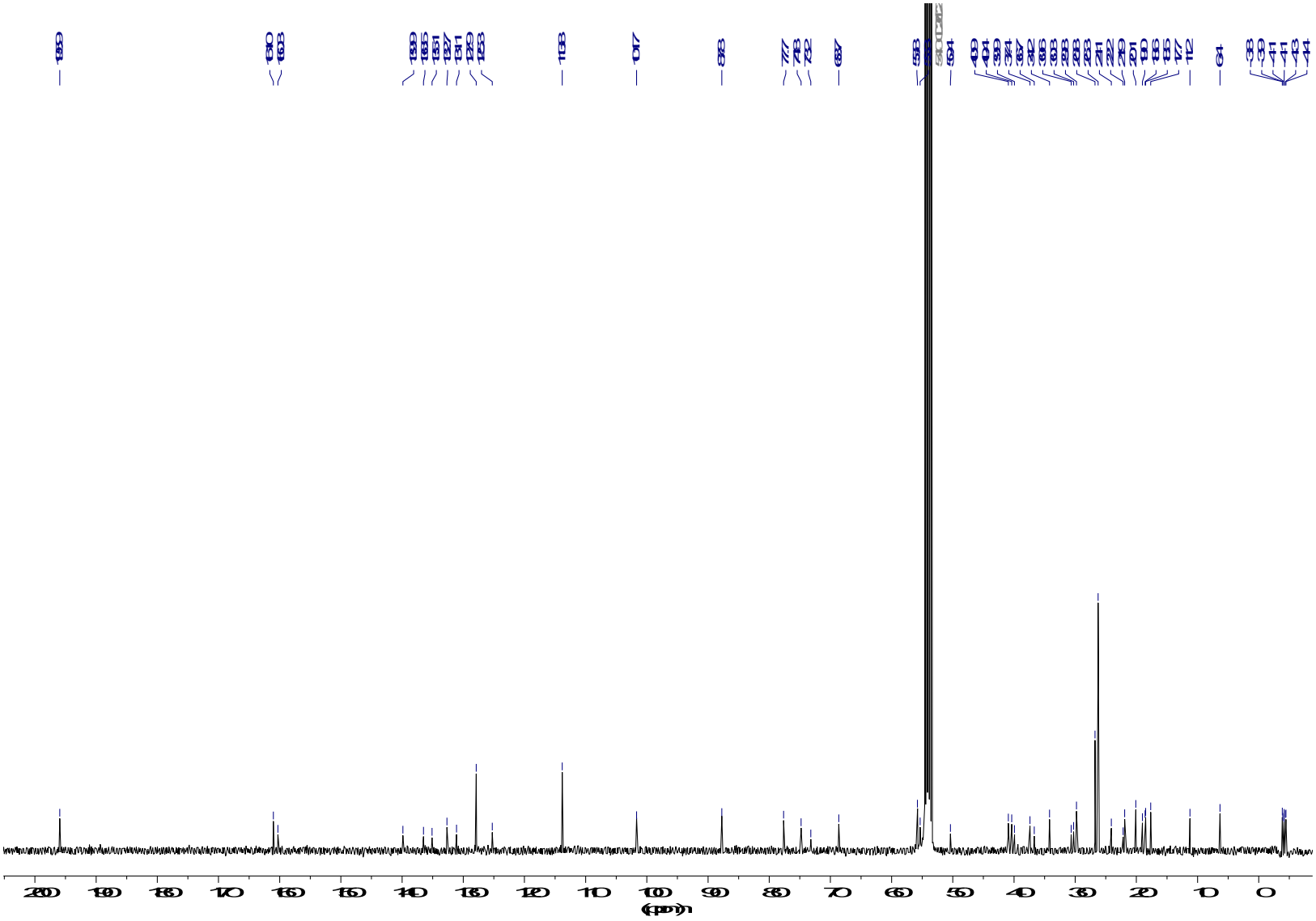
^{13}C-NMR (400.13 MHz, CD_2Cl_2)



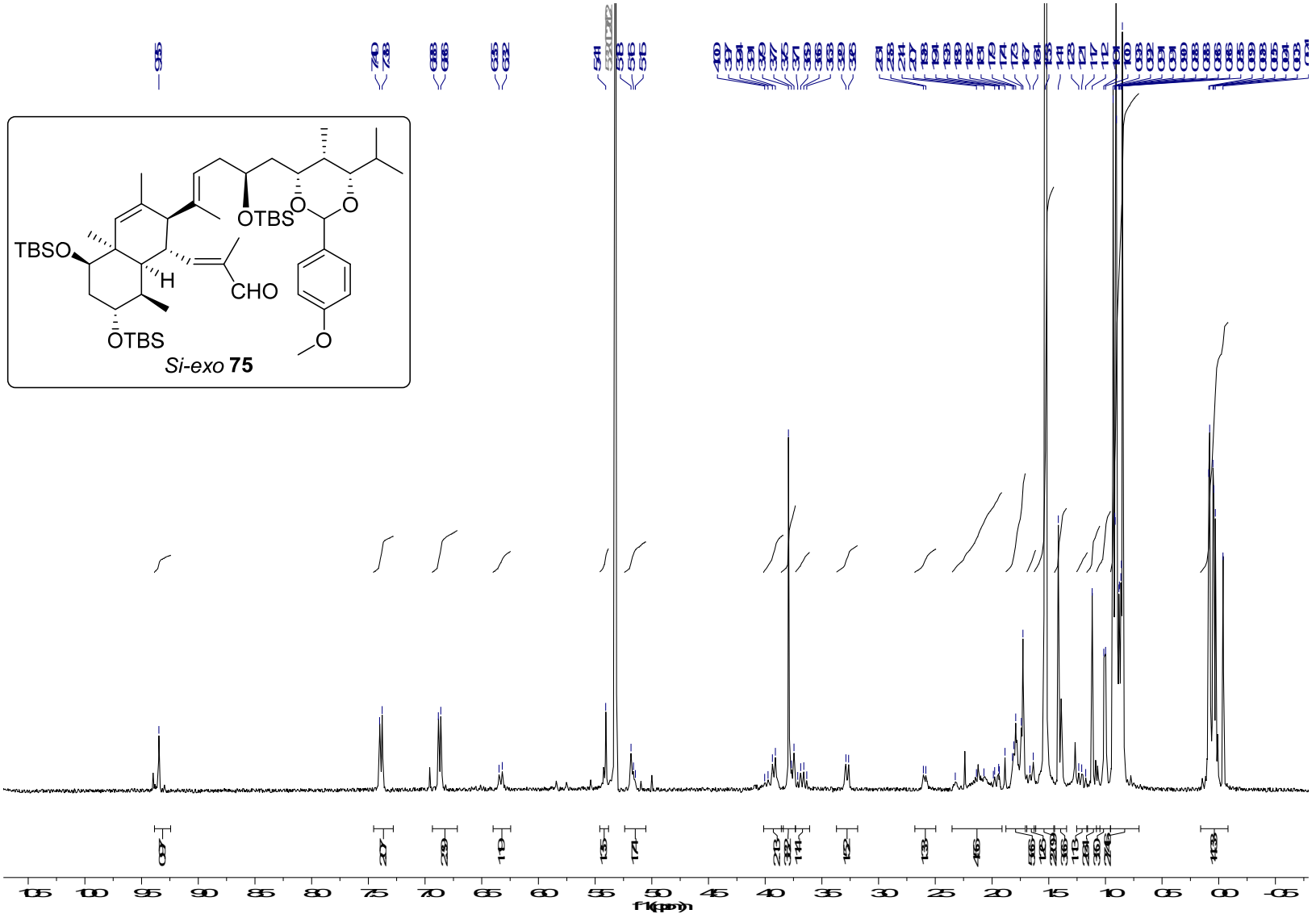
^{1}H-NMR (400.13 MHz, CD_2Cl_2)



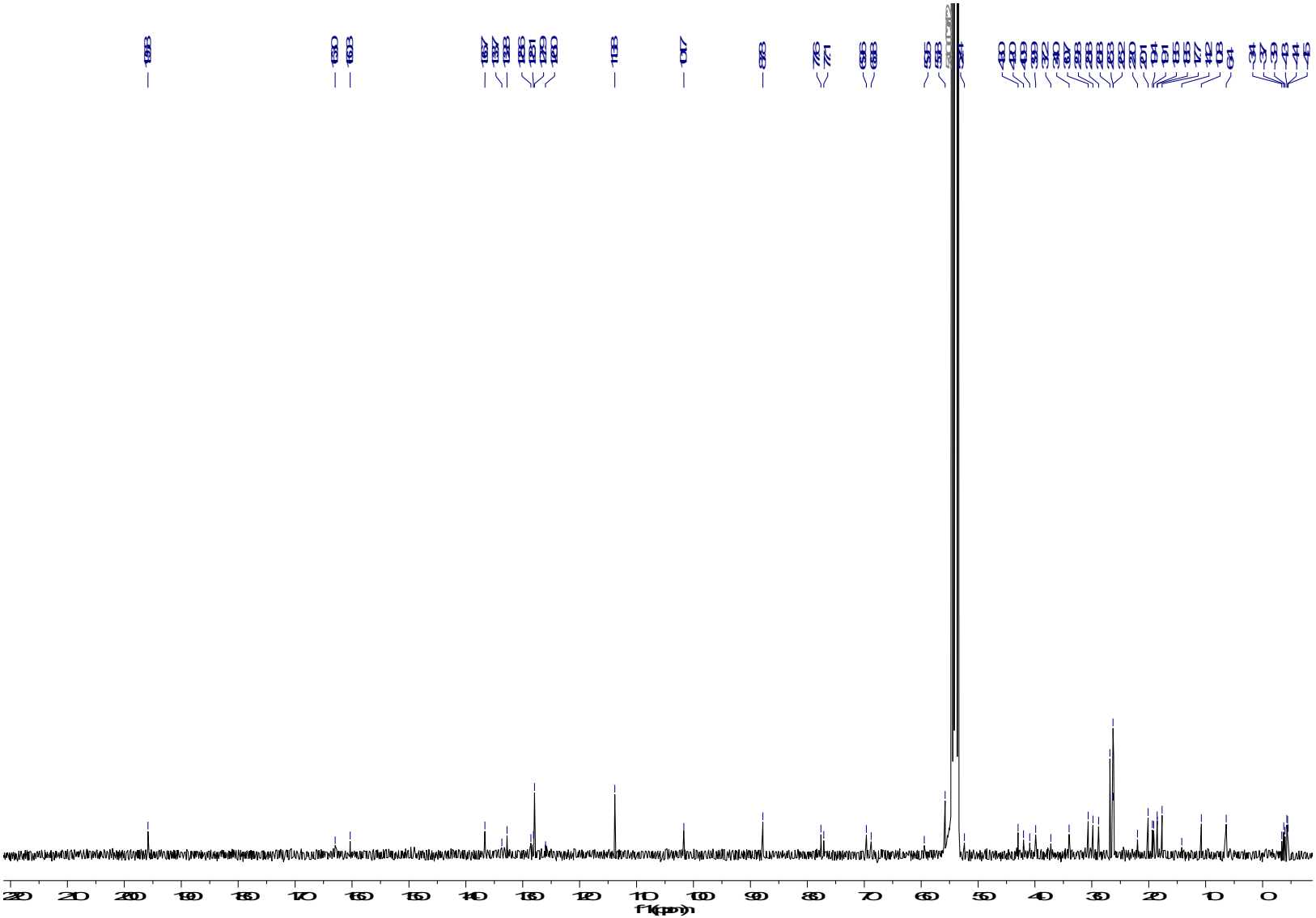
^{13}C-NMR (400.13 MHz, CD_2Cl_2):



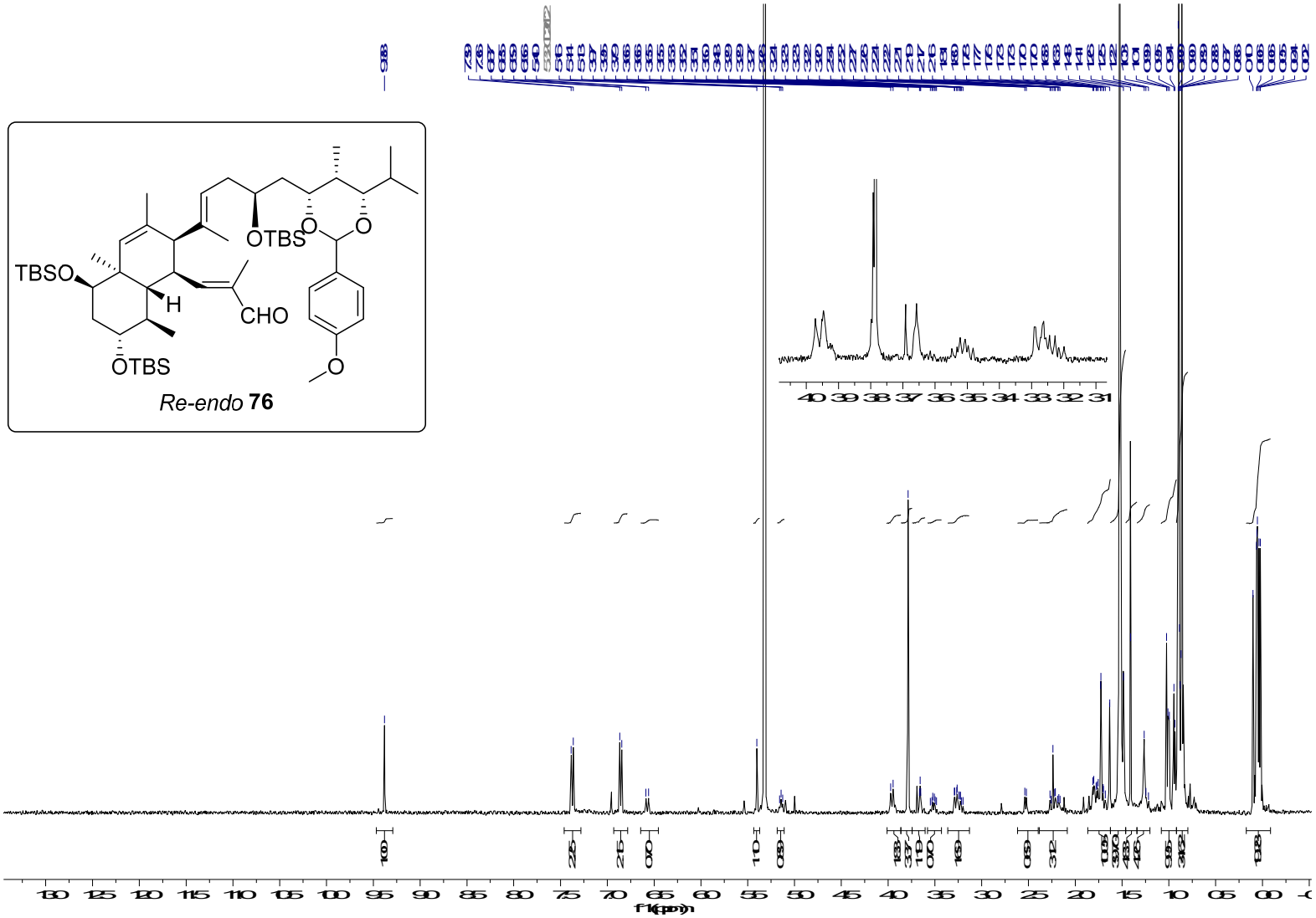
^{1}H-NMR (400.13 MHz, CD_2Cl_2)



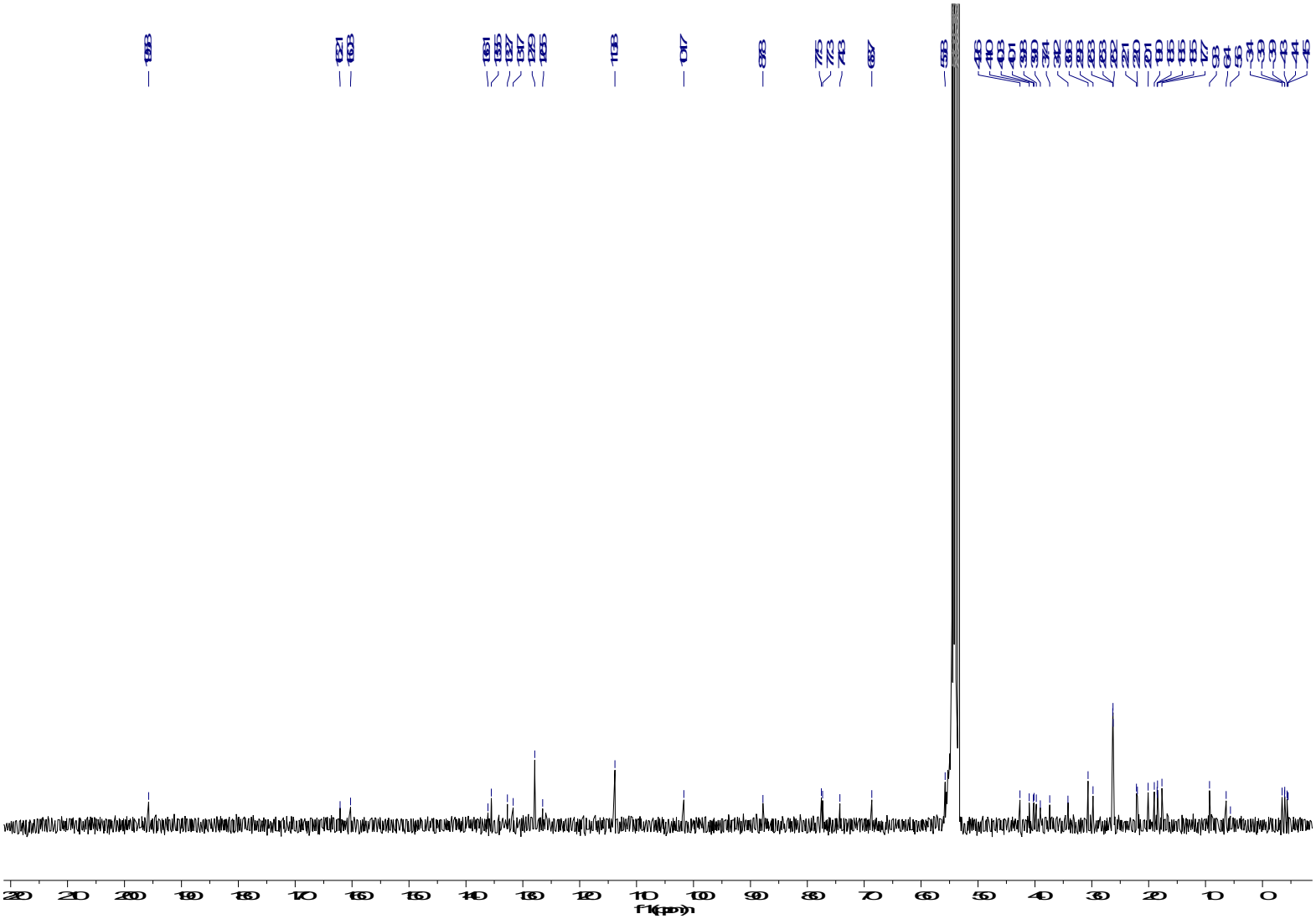
^{13}C-NMR (400.13 MHz, CD_2Cl_2):



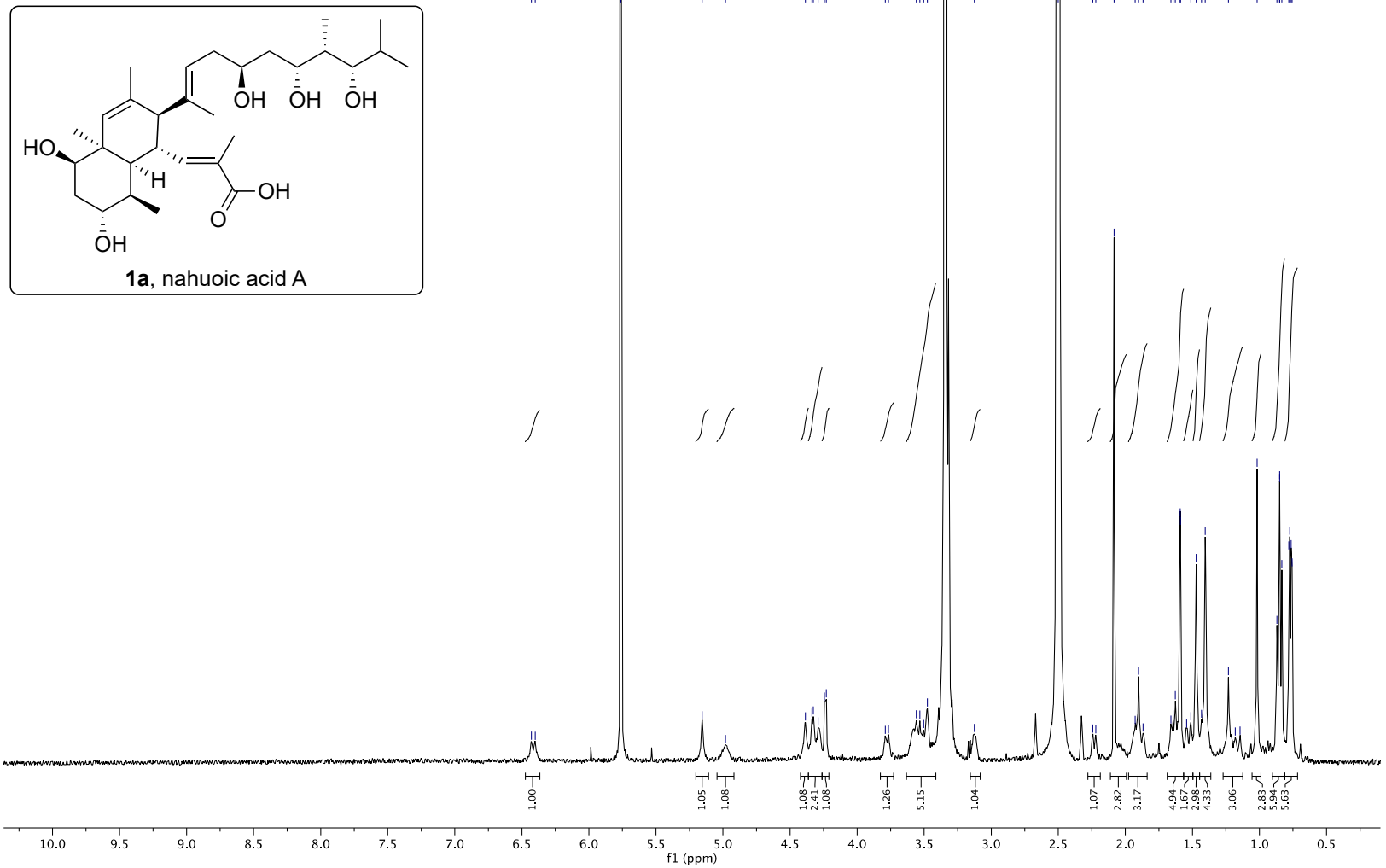
^{1}H-NMR (400.13 MHz, CD_2Cl_2)



^{13}C-NMR (400.13 MHz, CD_2Cl_2):

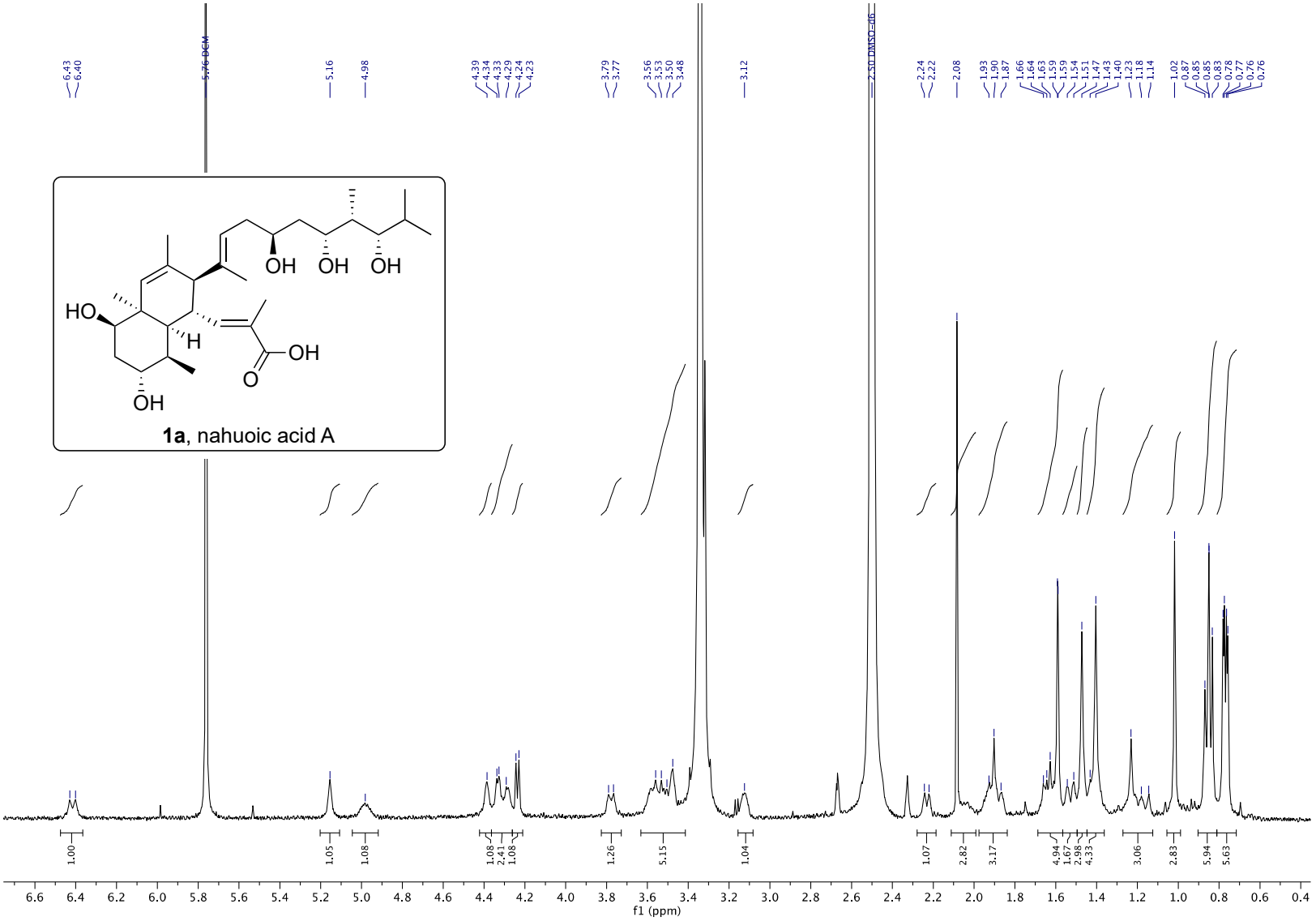


^{1}H-NMR (400.13 MHz, DMSO-d_6)

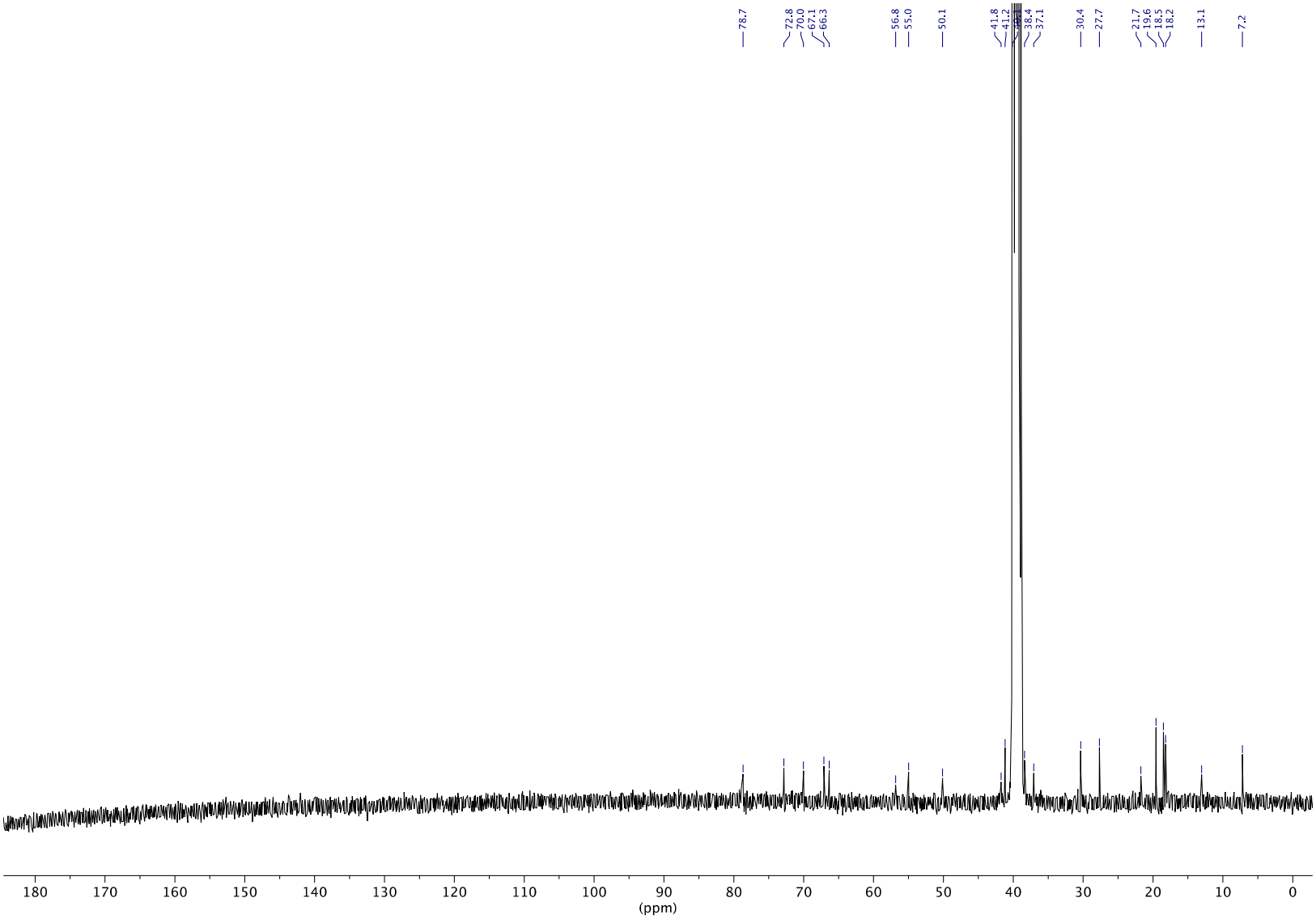


1a, nahuoic acid A

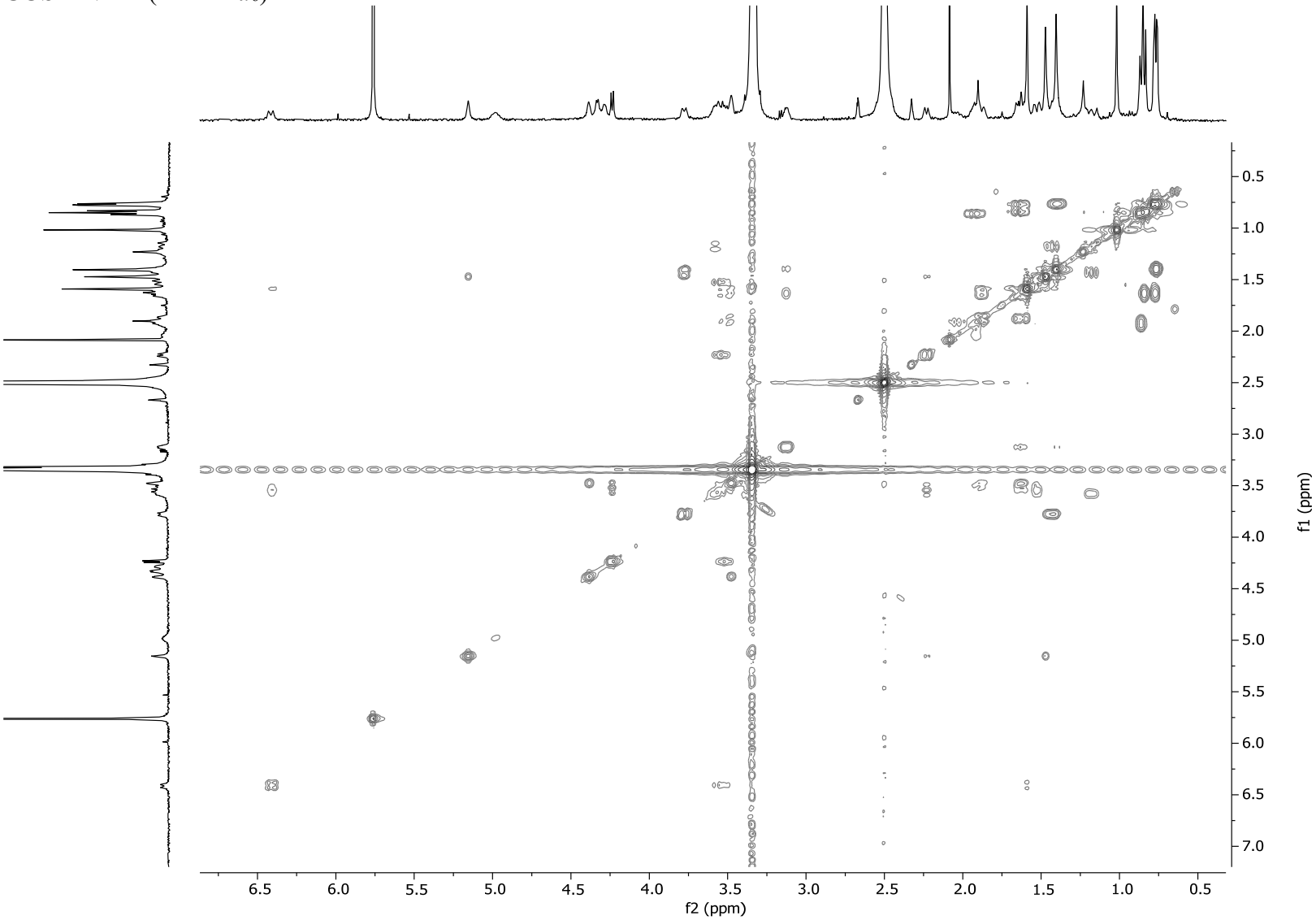
Expanded ^{1}H-NMR (400.13 MHz, DMSO-d_6)



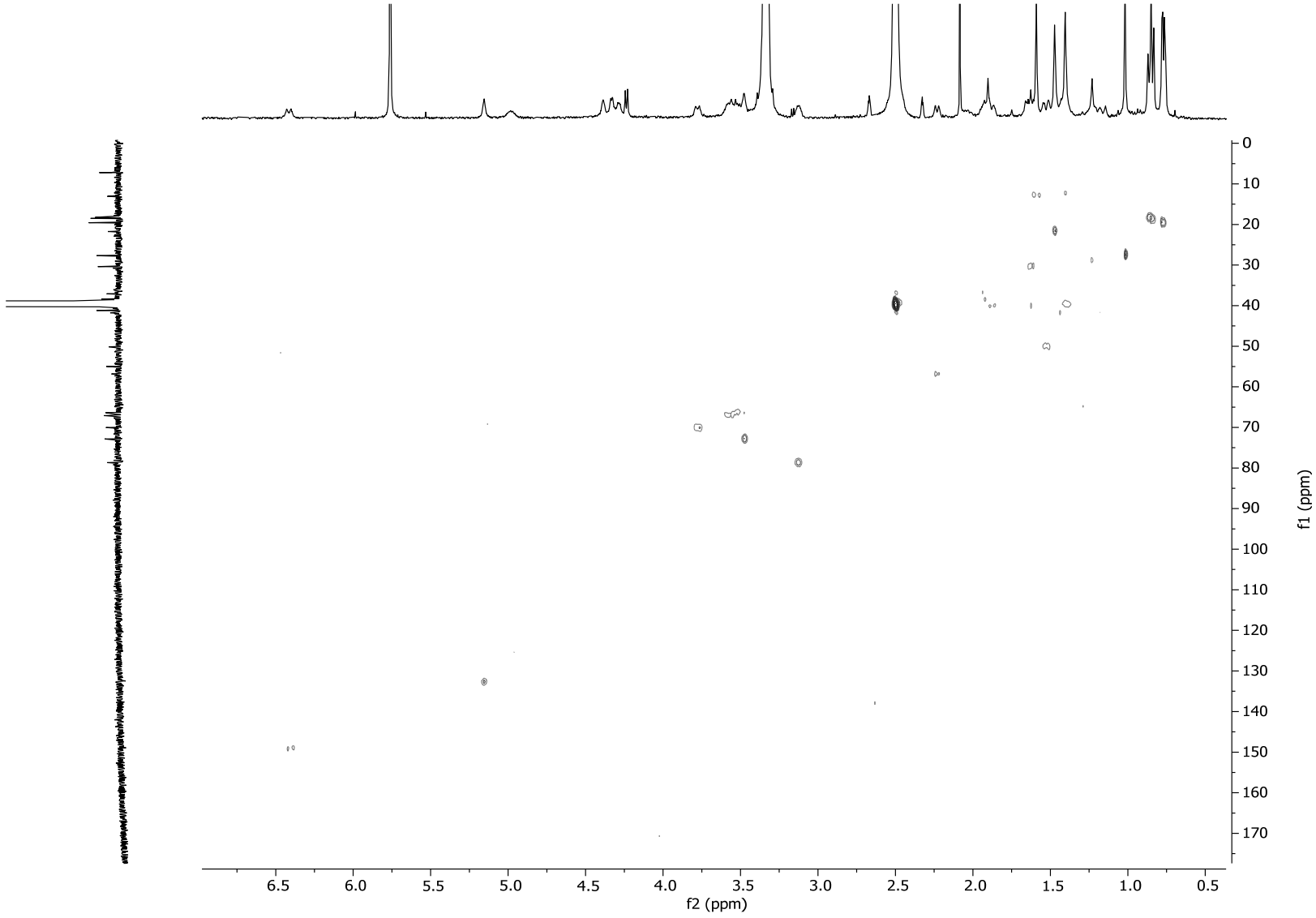
^{13}C-NMR (400.13 MHz, DMSO-d_6):



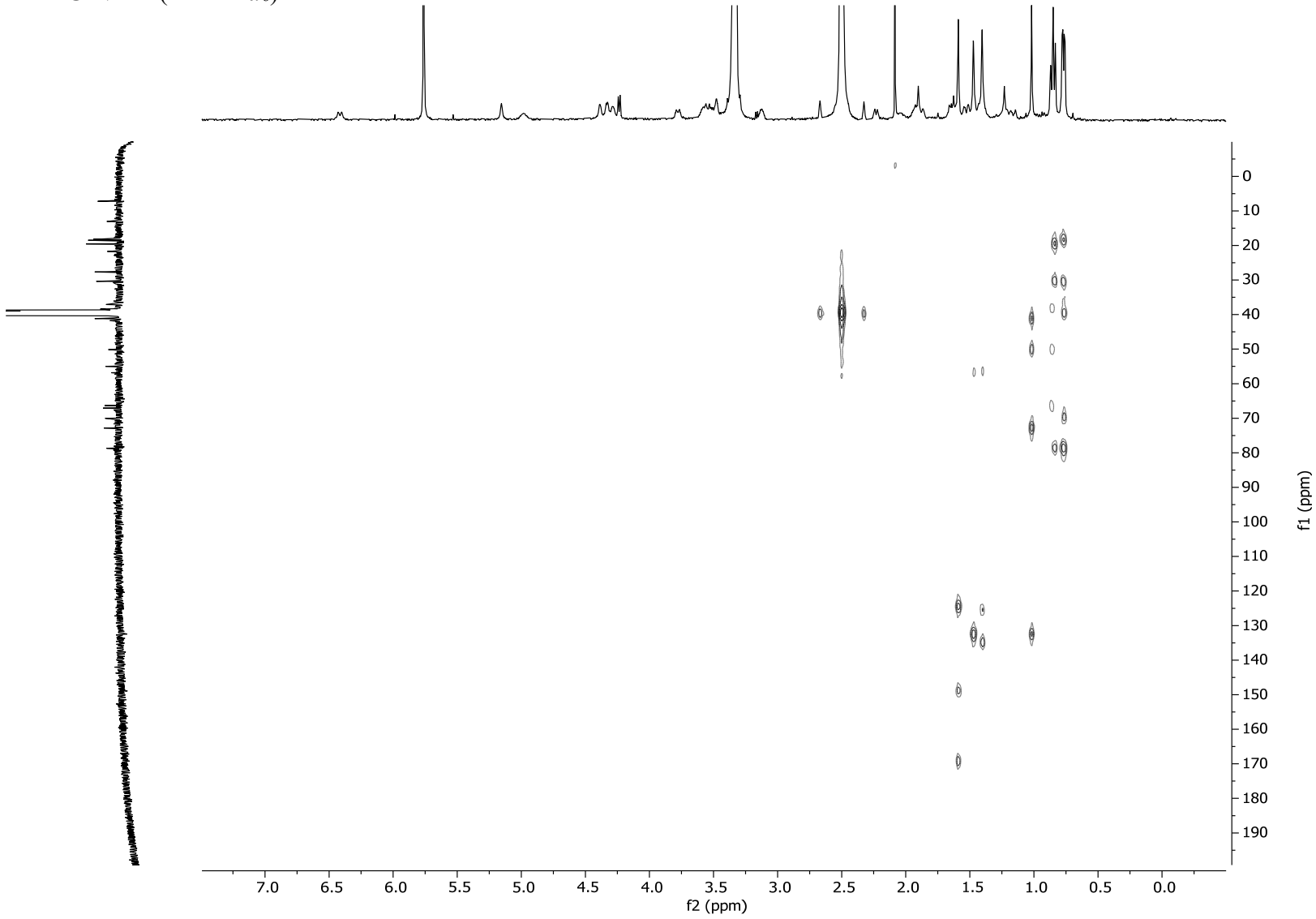
COSY-NMR (DMSO-d_6):



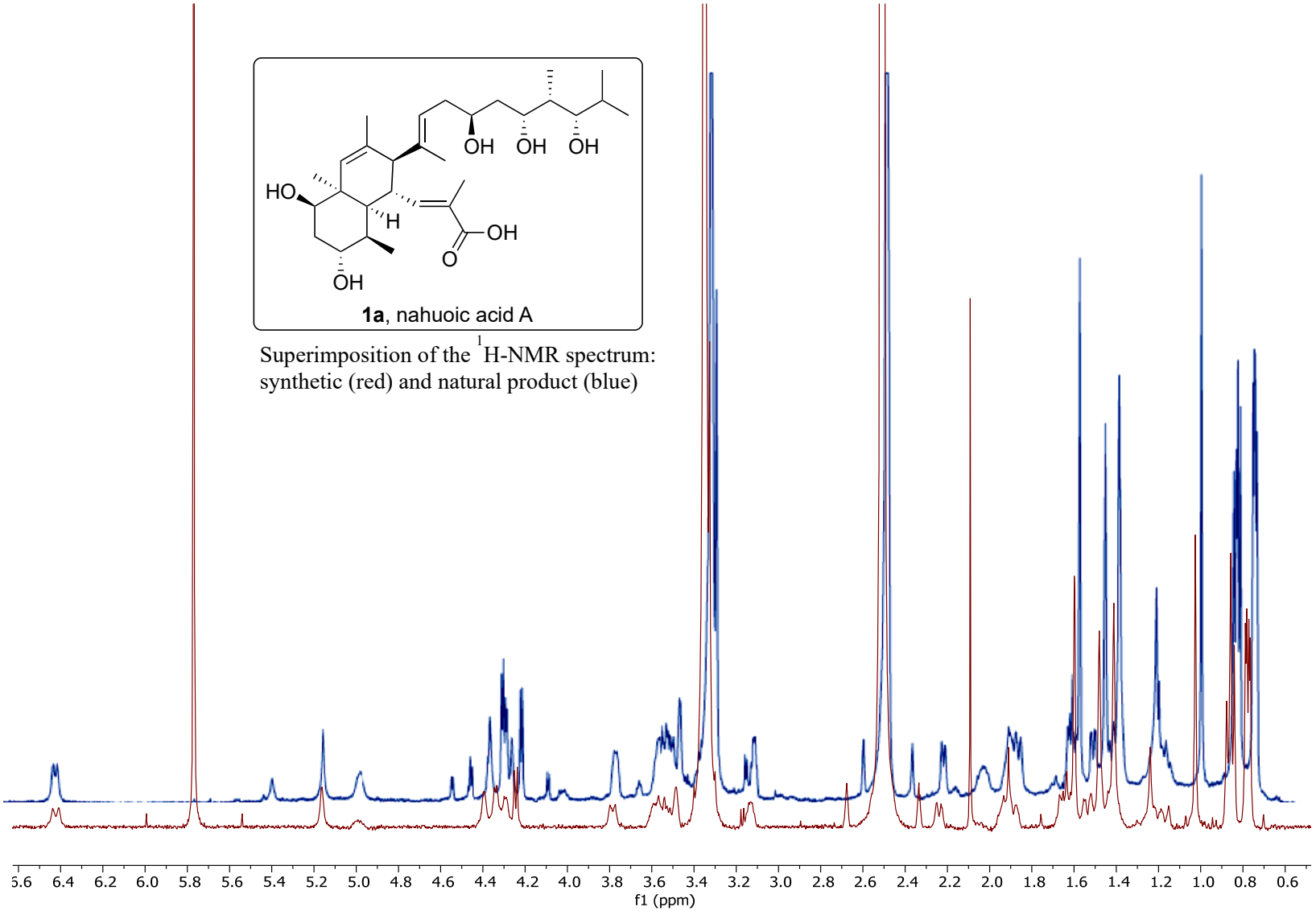
HSQC-NMR (DMSO-d_6):



HMBC-NMR (DMSO-d_6):



The superimposition of ^{1}H-NMR spectrum of synthetic nahuoic acid **1a** and natural product:



Superimposition of the ^{1}H-NMR spectrum: synthetic (red) and natural product (blue)

XYZ COORDINATES

System I, Toluene, ωB97X-D

lineal_scis-scis_S1_tol_wB97XD
SCF Energy: -1980.10664907
Num. Imaginary Frequencies: 0

C	0.662255	0.327605	0.522003
C	-0.331950	-0.096354	1.602286
C	-1.776961	0.107370	1.148530
C	-2.765602	0.223928	2.333680
C	-4.106332	0.637782	1.807166
C	2.058505	-0.226445	0.740153
C	-5.267037	-0.023048	1.915518
C	4.963739	-1.196903	0.096160
C	3.810812	-1.879560	-0.079443
C	2.510541	-1.179355	-0.096092
H	0.293569	-0.073585	-0.438341
H	-0.131298	0.495245	2.508913
H	-1.819751	1.064187	0.591958
H	-4.111325	1.583267	1.246518
H	4.888714	-0.103726	0.142716
H	1.815422	-1.525334	-0.873387
H	-5.357618	-0.978920	2.438516
C	-6.482808	0.502514	1.280618
O	-7.549628	-0.064786	1.262128
C	2.820682	0.340405	1.903780
H	3.303983	1.292532	1.634590
H	2.147934	0.559106	2.746790
H	3.607631	-0.344385	2.249045
C	3.726348	-3.363777	-0.326432
H	3.384052	-3.898545	0.575456
H	2.985014	-3.574533	-1.114450
H	4.690580	-3.794552	-0.628397
C	6.344145	-1.721462	0.160187
C	7.343734	-0.924948	-0.640199
H	7.100674	-0.964815	-1.714877
H	8.377644	-1.270313	-0.512742
H	7.306492	0.137952	-0.348564
C	6.650535	-2.795978	0.912317
C	7.982293	-3.455353	1.090464
H	8.293221	-3.427411	2.148335
H	8.781652	-2.999122	0.491582
H	7.923747	-4.521246	0.813083
H	-6.356094	1.500522	0.785388
H	-0.189610	-1.159811	1.845665
O	-2.153393	-0.963969	0.320851
O	0.686267	1.740896	0.491689
H	-2.398660	1.074063	2.937913
C	-2.793608	-1.028903	3.200251
H	-1.805379	-1.224525	3.640186
H	-3.508819	-0.923221	4.029383
H	-3.077511	-1.909996	2.606512
Si	-2.698509	-1.044218	-1.265667
C	-2.637018	-3.855204	-1.176640
H	-2.112090	-3.775470	-0.211146
H	-3.168070	-4.823767	-1.187339
H	-1.875175	-3.893959	-1.972020
C	-3.626672	-2.697497	-1.380986
C	-4.710656	-2.763495	-0.295490
H	-4.274494	-2.696920	0.712345
H	-5.450777	-1.952874	-0.390986
H	-5.263876	-3.717239	-0.360625
C	-4.282899	-2.817421	-2.765499
H	-5.029137	-2.024836	-2.938557
H	-4.808522	-3.784176	-2.860356
H	-3.545420	-2.768951	-3.583631
C	-3.822885	0.404840	-1.666522
H	-4.807851	0.299962	-1.186654
H	-3.982395	0.474982	-2.754981
H	-3.387493	1.363025	-1.341547
H	-0.497983	-1.817440	-2.159472
C	-1.230193	-1.043901	-2.439533
H	-0.706951	-0.075293	-2.447900
H	-1.554100	-1.245126	-3.473829
Si	0.852734	2.718213	-0.868597
C	-0.837018	2.957227	-1.651697
H	-1.567272	3.338560	-0.920641
H	-1.225812	2.010168	-2.056043
H	-0.794076	3.672815	-2.489129
C	2.010565	1.915684	-2.106024
H	1.644017	0.919426	-2.402089
H	2.083083	2.523028	-3.023021
H	3.025734	1.784368	-1.700462
C	1.533396	4.366112	-0.213726
C	0.479008	5.039182	0.678765
H	-0.426547	5.312525	0.113326
H	0.172739	4.385367	1.511210
H	0.881017	5.969464	1.118470
C	2.801555	4.105251	0.612053
H	2.583433	3.482671	1.492870
H	3.232128	5.056907	0.971558
H	3.583035	3.596092	0.024046
C	1.870350	5.287348	-1.396517
H	2.231300	6.266001	-1.033142
H	2.663249	4.865575	-2.035403
H	0.993767	5.483394	-2.036094
H	5.834221	-3.248051	1.487006

lineal_scis-strans_S1_tol_wB97XD
SCF Energy: -1980.10508731
Num. Imaginary Frequencies: 0

C	0.651854	0.217643	0.526886
C	-0.372997	-0.113385	1.611009
C	-1.800703	0.168954	1.145273
C	-2.783375	0.374668	2.323564
C	-4.093717	0.862137	1.783715
C	2.011051	-0.410342	0.776766
C	-5.294420	0.278699	1.900493
C	4.849874	-1.540660	0.183559
C	3.672077	-2.187850	0.024533
C	2.413759	-1.413886	-0.025562
H	0.267630	-0.190944	-0.424215
H	-0.139629	0.487858	2.503307
H	-1.781604	1.113088	0.566411
H	-4.037888	1.795193	1.205379
H	4.786717	-0.447709	0.191546
H	1.703761	-1.742581	-0.796992
H	-5.447047	-0.659080	2.441529
C	-6.472374	0.867553	1.250007
O	-7.572912	0.368621	1.237666
C	2.794088	0.144993	1.932298
H	3.349916	1.049229	1.638894
H	2.126279	0.442206	2.754846
H	3.524826	-0.580944	2.315436
C	3.480996	-3.674474	-0.158098
H	3.194917	-4.159764	0.790457
H	2.653627	-3.858565	-0.861572
H	4.366377	-4.185201	-0.551300
C	6.231985	-2.034968	0.330745
C	6.500798	-3.474400	0.697790
H	6.494899	-4.134176	-0.184615
H	5.741153	-3.852259	1.396420
H	7.479006	-3.591802	1.182671
C	7.224599	-1.132465	0.171345
C	8.701250	-1.348971	0.259133
H	9.184976	-1.082561	-0.695824
H	8.981593	-2.384489	0.492782
H	9.148238	-0.692599	1.024908
H	-6.281202	1.845381	0.735653
H	-0.298735	-1.176924	1.882710
O	-2.240951	-0.895788	0.340804
O	0.759516	1.625573	0.452601
H	-2.364292	1.212415	2.910883
C	-2.893438	-0.854733	3.216874
H	-1.920910	-1.102521	3.665420
H	-3.603121	-0.686187	4.040344
H	-3.230090	-1.729151	2.641095
Si	-2.787287	-0.974598	-1.245465
C	-2.912846	-3.780396	-1.098253
H	-2.384659	-3.715747	-0.133388
H	-3.506469	-4.711967	-1.090509
H	-2.154504	-3.885382	-1.891031
C	-3.823705	-2.564321	-1.328437
C	-4.910270	-2.535345	-0.244016
H	-4.471043	-2.473049	0.762724
H	-5.597024	-1.681555	-0.359947
H	-5.523346	-3.453036	-0.287804
C	-4.485505	-2.669318	-2.711486
H	-5.177583	-1.832886	-2.902329
H	-5.073859	-3.600978	-2.787330
H	-3.745981	-2.686636	-3.529036
C	-3.810953	0.537322	-1.682121
H	-4.801161	0.510444	-1.202470
H	-3.964246	0.592863	-2.772311
H	-3.312089	1.471144	-1.378252
H	-0.639081	-1.908900	-2.114577
C	-1.319635	-1.096259	-2.413437
H	-0.735918	-0.163248	-2.439440
H	-1.653360	-1.297928	-3.444517
Si	1.000601	2.550719	-0.932808
C	-0.664570	2.890778	-1.731759
H	-1.372258	3.329953	-1.010985
H	-1.114569	1.968144	-2.129050
H	-0.566901	3.592200	-2.576608
C	2.102779	1.636088	-2.142793
H	1.672859	0.656363	-2.406986
H	2.211634	2.208268	-3.078625
H	3.108538	1.453470	-1.733829
C	1.792404	4.165161	-0.319995
C	0.782791	4.935842	0.544880
H	-0.098845	5.254030	-0.034745
H	0.427669	4.329688	1.393835
H	1.245992	5.848763	0.960125
C	3.034595	3.840288	0.522207
H	2.768289	3.261102	1.419162
H	3.529795	4.769376	0.856686
H	3.780920	3.259640	-0.044932
C	2.199608	5.025915	-1.526009
H	2.626035	5.987121	-1.187861
H	2.964636	4.531475	-2.146533
H	1.342526	5.264169	-2.177560
H	6.926966	-0.103367	-0.065469

lineal_strans-scis_S1_tol_wB97XD
SCF Energy: -1980.10661749
Num. Imaginary Frequencies: 0

C	0.576998	0.440664	0.711409
C	-0.508386	0.131211	1.740446
C	-1.916497	0.229945	1.157591
C	-2.996082	0.411483	2.253806

C	-4.305119	0.736406	1.600827
C	1.969463	0.128531	1.234143
C	-5.450456	0.044579	1.674728
C	4.681605	-1.919452	-0.219199
C	4.065102	-1.299905	0.816166
C	2.710721	-0.772814	0.561604
H	0.394017	-0.191270	-0.174882
H	-0.404821	0.840686	2.576543
H	-1.944516	1.131356	0.515019
H	-4.297138	1.638222	0.972556
H	4.101029	-2.018515	-1.146264
H	2.252133	-1.177226	-0.349022
H	-5.551371	-0.873349	2.260072
C	-6.630965	0.480421	0.917270
O	-7.676297	-0.123666	0.864548
C	2.371296	0.906778	2.459400
H	1.836076	1.867505	2.473923
H	2.107188	0.372693	3.387472
H	3.445288	1.123856	2.492525
C	4.666625	-1.204605	2.194910
H	5.151962	-0.232758	2.376844
H	3.892043	-1.330586	2.964783
H	5.431635	-1.979527	2.342621
C	6.019736	-2.540527	-0.272336
C	6.054254	-3.860168	-1.002788
H	5.443528	-4.612244	-0.476609
H	7.066821	-4.266711	-1.119583
H	5.619611	-3.750212	-2.010250
C	7.100590	-1.936452	0.259130
C	8.514777	-2.424883	0.292372
H	9.178774	-1.734257	-0.254320
H	8.644290	-3.427624	-0.135784
H	8.886091	-2.454283	1.330436
H	-6.497836	1.444087	0.359650
H	-0.357855	-0.885430	2.134488
O	-2.192662	-0.925167	0.406530
O	0.467746	1.808477	0.371924
H	-2.699784	1.320542	2.808959
C	-3.055223	-0.765467	3.219742
H	-2.100781	-0.886199	3.751527
H	-3.838760	-0.619182	3.977923
H	-3.261167	-1.702907	2.682914
Si	-2.635884	-1.142847	-1.199000
C	-2.486589	-3.934253	-0.901059
H	-2.031761	-3.769198	0.088822
H	-2.981124	-4.921815	-0.879252
H	-1.671054	-3.995558	-1.639848
C	-3.499726	-2.832951	-1.250298
C	-4.650440	-2.863681	-0.234216
H	-4.284940	-2.710573	0.792207
H	-5.409026	-2.090203	-0.434965
H	-5.166220	-3.839884	-0.265366
C	-4.058281	-3.073914	-2.661696
H	-4.817078	-2.324008	-2.939058
H	-4.544234	-4.064038	-2.719967
H	-3.269889	-3.055019	-3.432204
C	-3.772717	0.233463	-1.782130
H	-4.790548	0.124654	-1.378321
H	-3.842940	0.228012	-2.882203
H	-3.395323	1.225844	-1.487281
H	-0.341046	-1.859646	-1.897309
C	-1.097106	-1.153779	-2.275194
H	-0.639155	-0.154034	-2.313364
H	-1.339581	-1.438505	-3.312079
Si	0.850787	2.574218	-1.077989
C	-0.756379	2.901805	-1.991438
H	-1.445720	3.512357	-1.386390
H	-1.270588	1.958697	-2.233957
H	-0.581936	3.430421	-2.942565
C	1.977701	1.505532	-2.129893
H	1.498184	0.552906	-2.405598
H	2.224584	2.027407	-3.069286
H	2.919993	1.267508	-1.613857
C	1.697531	4.205515	-0.592877
C	0.830281	4.941929	0.439344
H	-0.163207	5.198797	0.036345
H	0.675613	4.334605	1.344609
H	1.311796	5.887741	0.746082
C	3.072103	3.900303	0.021422
H	2.992256	3.227475	0.889368
H	3.557111	4.830630	0.367311
H	3.753173	3.428365	-0.704855
C	1.878018	5.089600	-1.836334
H	2.403543	6.024746	-1.572538
H	2.476564	4.592290	-2.617608
H	0.912793	5.375488	-2.284736
H	6.947370	-0.950369	0.711040

lineal_strans-strans_S1_tol_wB97XD
SCF Energy: -1980.10362298
Num. Imaginary Frequencies: 0

C	0.612633	0.793087	0.693495
C	-0.400101	0.319668	1.735115
C	-1.804327	0.183138	1.148561
C	-2.908393	0.219303	2.233719
C	-4.245864	0.301340	1.562559
C	2.051749	0.627875	1.151263
C	-5.263024	-0.566106	1.655571
C	4.549070	-1.907489	0.151683
C	4.197336	-0.734190	0.734127
C	2.803352	-0.299168	0.524648
H	0.473783	0.170164	-0.206488

H	-0.408319	1.040723	2.567542
H	-1.971517	1.051166	0.481433
H	-4.378248	1.167284	0.898737
H	3.770013	-2.379270	-0.459028
H	2.290976	-0.860972	-0.266058
H	-5.220264	-1.465913	2.275154
C	-6.487190	-0.359002	0.870943
O	-7.418337	-1.128286	0.831855
C	2.466007	1.506122	2.306588
H	3.246843	2.226800	2.024646
H	1.612215	2.094409	2.668986
H	2.852648	0.916802	3.151001
C	5.138561	0.162985	1.498135
H	4.988316	1.207883	1.191931
H	4.973919	0.118152	2.585971
H	6.188006	-0.078926	1.304754
C	5.799730	-2.688760	0.182838
C	6.803285	-2.505767	1.297762
H	7.541361	-1.719162	1.071836
H	7.365203	-3.430863	1.484888
H	6.304321	-2.231286	2.237563
C	5.971511	-3.608845	-0.791415
C	7.133139	-4.525653	-1.002997
H	6.807521	-5.579730	-0.992072
H	7.928506	-4.406500	-0.255460
H	7.582215	-4.351970	-1.995415
H	-6.504557	0.592142	0.277384
H	-0.089956	-0.658540	2.131978
O	-1.888347	-1.020006	0.427332
O	0.331578	2.148147	0.404534
H	-2.770787	1.182179	2.759386
C	-2.782321	-0.919802	3.237759
H	-1.824677	-0.866520	3.774813
H	-3.584608	-0.878180	3.989290
H	-2.829943	-1.895170	2.731954
Si	-2.257666	-1.359696	-1.175511
C	-1.669014	-4.077816	-0.763613
H	-1.266916	-3.803912	0.224944
H	-1.999466	-5.130441	-0.708231
H	-0.839345	-4.035478	-1.487814
C	-2.838096	-3.167948	-1.171928
C	-3.988795	-3.344190	-0.170717
H	-3.673608	-3.090036	0.852232
H	-4.859155	-2.714631	-0.416019
H	-4.337701	-4.392139	-0.165018
C	-3.322721	-3.549922	-2.579423
H	-4.185417	-2.942179	-2.897953
H	-3.643933	-4.606417	-2.602765
H	-2.532144	-3.435599	-3.339413
C	-3.592207	-0.207255	-1.820793
H	-4.582637	-0.459525	-1.412960
H	-3.652663	-0.271313	-2.919600
H	-3.380008	0.844242	-1.569910
H	0.130223	-1.740252	-1.816005
C	-0.715392	-1.170623	-2.232288
H	-0.405891	-0.117453	-2.312011
H	-0.894549	-1.532902	-3.257863
Si	0.514494	2.946270	-1.066570
C	-1.122841	2.883301	-1.983549
H	-1.947876	3.257677	-1.357064
H	-1.369838	1.854405	-2.287345
H	-1.093480	3.493174	-2.901304
C	1.848852	2.129583	-2.100727
H	1.633606	1.061007	-2.261223
H	1.908269	2.602621	-3.094666
H	2.841034	2.197467	-1.628986
C	0.964873	4.736352	-0.616406
C	-0.197807	5.377118	0.157179
H	-1.109367	5.454681	-0.457422
H	-0.449542	4.801205	1.062175
H	0.066924	6.400804	0.477314
C	2.221365	4.738526	0.266382
H	2.050056	4.196229	1.208069
H	2.513081	5.772726	0.522654
H	3.084034	4.272161	-0.237387
C	1.235945	5.538874	-1.898211
H	1.475156	6.589085	-1.653168
H	2.090683	5.135357	-2.465300
H	0.364010	5.555204	-2.572759
H	5.172878	-3.699756	-1.538141

pp_Reendo_S1_tol_wB97XD
SCF Energy: -1980.10255488
Num. Imaginary Frequencies: 0

C	0.080682	0.669049	-1.523153
C	-1.079586	-0.335889	-1.433908
C	-1.447452	-0.933721	-0.068672
C	-0.427676	-1.926264	0.535065
C	0.738478	-1.205704	1.163143
C	1.475849	0.062665	-1.607942
C	1.834536	-1.788250	1.672183
C	4.206507	-1.212484	-0.782067
C	3.865758	0.093242	-0.719480
C	2.461462	0.528397	-0.823045
C	4.841302	1.212928	-0.458300
C	5.546120	-1.823408	-0.635024
C	5.893792	-2.808430	-1.722768
C	6.324588	-1.538845	0.424701
C	7.681978	-2.079215	0.748166
C	1.643557	-0.987540	-2.669887
C	2.878423	-0.972123	2.301397
O	3.865755	-1.404692	2.850174

O	-2.685429	-1.586541	-0.246149
O	-0.039383	1.589881	-0.472016
H	-0.060425	1.179918	-2.500053
H	-1.980953	0.201926	-1.765324
H	-0.937516	-1.160105	-2.149674
H	-1.554856	-0.099021	0.651499
H	0.657493	-0.114177	1.239920
H	2.000860	-2.870021	1.638552
H	3.401287	-1.930887	-0.972890
H	2.191739	1.349019	-0.149390
H	4.752609	1.575416	0.580377
H	5.883233	0.904633	-0.614242
H	4.626263	2.070602	-1.115487
H	5.966449	-2.301023	-2.699295
H	6.838636	-3.338059	-1.544424
H	5.098364	-3.566388	-1.820620
H	8.081204	-2.756675	-0.018707
H	8.404098	-1.255502	0.876544
H	2.685887	-1.055644	-3.010386
H	1.347915	-1.987808	-2.310445
H	1.009521	-0.764675	-3.543790
H	2.686803	0.131628	2.253118
C	-1.081772	-2.840255	1.581566
H	-1.472156	-2.252689	2.427324
H	-1.912793	-3.404488	1.140091
H	-0.346443	-3.552952	1.981433
H	-0.047826	-2.570011	-0.278902
H	7.660292	-2.624313	1.706613
Si	-0.275999	3.250969	-0.634646
Si	-4.162644	-0.999613	0.308344
C	-0.491611	3.847523	1.152389
C	1.217273	4.016175	-1.470549
H	2.119623	3.958374	-0.842493
H	1.438162	3.494647	-2.416504
H	1.038888	5.076369	-1.713543
C	-1.800318	3.557020	-1.683533
H	-1.650321	3.189960	-2.712194
H	-2.690531	3.054814	-1.274765
H	-2.020764	4.634690	-1.754582
C	-5.446853	-2.181607	-0.433769
C	-4.195227	-1.009497	2.184654
H	-3.365026	-0.410459	2.593368
H	-5.130312	-0.563720	2.561540
H	-4.112692	-2.026387	2.598285
C	-4.393869	0.770902	-0.273099
H	-3.601402	1.412085	0.146017
H	-4.362996	0.859940	-1.369936
H	-5.357582	1.178327	0.073789
C	0.712657	3.389983	1.990154
H	0.612669	3.737732	3.033611
H	0.795404	2.292089	2.012593
H	1.664371	3.790125	1.604133
C	-1.776376	3.244860	1.741157
H	-2.676120	3.580193	1.200291
H	-1.755661	2.143253	1.713773
H	-1.898793	3.546575	2.796532
C	-0.581903	5.381059	1.172733
H	-1.430189	5.755101	0.575848
H	-0.724782	5.746957	2.204934
H	0.335313	5.853170	0.784404
C	-5.072418	-3.627435	-0.072949
H	-5.040473	-3.787885	1.017218
H	-5.815560	-4.333506	-0.484791
H	-4.087588	-3.901656	-0.481260
C	-6.837673	-1.852192	0.129749
H	-7.602232	-2.511923	-0.317779
H	-6.885238	-1.994114	1.221721
H	-7.139270	-0.813795	-0.086820
C	-5.458676	-2.025722	-1.962173
H	-4.462177	-2.205413	-2.396255
H	-6.156950	-2.748969	-2.419981
H	-5.784237	-1.019139	-2.271301
H	5.910938	-0.855638	1.174024

pp_Reexo_S1_tol_wB97XD
SCF Energy: -1980.09986280
Num. Imaginary Frequencies: 0

C	0.255286	0.728356	-1.407258
C	-0.771838	-0.390446	-1.209444
C	-1.251977	-0.721966	0.211872
C	-0.174247	-1.174180	1.223835
C	0.646855	-0.025323	1.731296
C	1.735739	0.380884	-1.252243
C	1.944210	-0.087067	2.062522
C	4.432122	-0.960028	-0.337854
C	3.586102	-1.371547	-1.306556
C	2.191669	-0.878784	-1.367625
C	3.929192	-2.382044	-2.372333
C	5.832591	-1.359309	-0.080307
C	6.723055	-0.200723	0.293263
C	6.224438	-2.647189	-0.113213
C	7.589343	-3.206884	0.142844
C	2.620643	1.585092	-1.102684
C	2.640253	1.097102	2.569150
O	3.833073	1.172115	2.763918
O	-2.210740	-1.746294	0.070395
O	-0.074826	1.813398	-0.561011
H	0.159921	1.052368	-2.465481
H	-1.679821	-0.095042	-1.758208
H	-0.433835	-1.323060	-1.683146
H	-1.723297	0.187331	0.632115
H	0.115216	0.921909	1.888350

H	2.534807	-0.995853	1.910533
H	4.060201	-0.201946	0.358904
H	1.463293	-1.671662	-1.571161
H	5.013547	-2.510643	-2.489239
H	3.497809	-3.370760	-2.138589
H	3.507153	-2.072697	-3.341687
H	6.780303	0.528205	-0.532098
H	6.294851	0.332406	1.158126
H	7.745970	-0.501585	0.553144
H	7.923780	-3.816025	-0.713662
H	8.351722	-2.437102	0.321756
H	2.563143	2.002834	-0.085671
H	3.670902	1.352960	-1.318533
H	2.292429	2.384196	-1.784969
H	1.976504	1.979271	2.763541
C	-0.812183	-1.855951	2.444705
H	-1.473810	-1.162492	2.988070
H	-1.405426	-2.725909	2.135067
H	-0.031622	-2.191803	3.142581
H	0.491192	-1.903307	0.733652
H	7.578042	-3.880066	1.016732
Si	-3.874942	-1.593986	0.262467
Si	-0.854656	3.234648	-1.019753
C	-4.560395	-3.265733	-0.314024
C	-4.302665	-1.235469	2.054324
H	-3.797392	-0.318640	2.399816
H	-5.386522	-1.067381	2.165796
H	-4.014975	-2.055215	2.730193
C	-4.508781	-0.164112	-0.775024
H	-5.609520	-0.113842	-0.742872
H	-4.132265	0.790095	-0.371916
H	-4.203584	-0.237879	-1.830009
C	-1.417625	4.014338	0.617760
C	-2.296632	2.836572	-2.152506
H	-2.805362	3.761166	-2.470923
H	-1.947215	2.331268	-3.068046
H	-3.045012	2.186577	-1.676152
C	0.328883	4.355239	-1.947725
H	1.213162	4.618179	-1.347092
H	0.680017	3.871809	-2.874093
H	-0.172282	5.291547	-2.243365
C	-0.191148	4.261053	1.509289
H	0.358106	3.327072	1.707008
H	0.516634	4.971674	1.053141
H	-0.496412	4.683318	2.483173
C	-2.387253	3.068480	1.341791
H	-2.735444	3.520133	2.287613
H	-3.283007	2.848088	0.738021
H	-1.906794	2.110099	1.593497
C	-2.125497	5.348115	0.332705
H	-2.455364	5.818931	1.275686
H	-1.464021	6.068820	-0.174825
H	-3.022295	5.215318	-0.294562
C	-3.845316	-4.394970	0.443775
H	-4.232904	-5.379562	0.126370
H	-2.761223	-4.383736	0.253215
H	-3.996003	-4.322307	1.533490
C	-6.069526	-3.331449	-0.033923
H	-6.293276	-3.265001	1.043266
H	-6.622988	-2.524104	-0.541780
H	-6.488033	-4.287798	-0.394847
C	-4.307724	-3.423492	-1.821281
H	-4.848666	-2.665532	-2.411064
H	-3.236638	-3.337822	-2.064432
H	-4.650330	-4.414002	-2.170278
H	5.455513	-3.397209	-0.329362

pp_Siendo_S1_tol_wB97XD
SCF Energy: -1980.10293333
Num. Imaginary Frequencies: 0

C	-0.769730	0.725823	0.687805
C	-1.218762	-0.127899	1.875516
C	-0.993039	-1.643332	1.788353
C	0.365745	-2.220503	2.255673
C	1.466989	-2.116319	1.243874
C	0.718363	0.994027	0.573461
C	2.783423	-2.045373	1.494595
C	3.769879	0.925486	-0.125889
C	2.736842	0.906135	-0.997593
C	1.345710	0.667012	-0.572634
C	2.888463	1.101770	-2.486297
C	5.207959	1.133857	-0.398307
C	5.871307	2.102860	0.547796
C	5.846658	0.441240	-1.358192
C	7.295738	0.485363	-1.727366
C	1.338081	1.716737	1.734460
C	3.755845	-2.160631	0.399319
O	4.951446	-2.260611	0.550022
O	-1.256167	-2.091204	0.481473
O	-1.431027	1.975433	0.809560
H	-1.094273	0.199747	-0.226478
H	-0.806098	0.271248	2.815064
H	-2.307541	0.028904	1.933821
H	-1.724389	-2.080748	2.496862
H	1.139996	-2.210251	0.202502
H	3.194208	-1.968172	2.505866
H	3.537506	0.778855	0.933109
H	0.721856	0.199686	-1.346068
H	3.852030	1.555791	-2.751301
H	2.813893	0.138827	-3.020561
H	2.080831	1.743483	-2.873041
H	5.739252	1.766130	1.589954

H	6.948218	2.216569	0.369408
H	5.406093	3.099857	0.475455
H	7.864511	1.252734	-1.185470
H	7.769310	-0.490638	-1.527888
H	1.838972	1.018765	2.426559
H	2.096920	2.440917	1.402643
H	0.567292	2.259343	2.300119
H	3.299411	-2.189915	-0.623471
C	0.743439	-1.777149	3.664188
H	1.541978	-2.408168	4.080060
H	1.096587	-0.735322	3.683824
H	-0.120718	-1.854105	4.342026
H	0.166037	-3.310060	2.292868
H	7.415888	0.676860	-2.806676
Si	-2.540155	-3.074713	0.012548
Si	-2.293677	2.702557	-0.438846
C	-2.350776	-3.217192	-1.869447
C	-4.152500	-2.257405	0.512072
H	-4.236011	-2.195531	1.609685
H	-4.234397	-1.235156	0.111251
H	-5.021389	-2.833333	0.153734
C	-2.386226	-4.734198	0.872523
H	-1.457406	-5.256020	0.592902
H	-2.383018	-4.605802	1.967687
H	-3.234683	-5.393514	0.627489
C	-1.215112	2.865160	-1.965752
H	-1.727082	3.445106	-2.751362
H	-0.260540	3.363473	-1.736930
H	-0.983684	1.874984	-2.389928
C	-2.806716	4.392492	0.255120
C	-3.776462	1.625626	-0.847170
H	-4.450773	1.513563	0.016405
H	-4.359649	2.036720	-1.687084
H	-3.439752	0.620716	-1.148493
C	-1.552984	5.255069	0.466971
H	-1.823520	6.228399	0.914155
H	-0.832217	4.767981	1.142638
H	-1.032940	5.465626	-0.481618
C	-3.524389	4.195120	1.598959
H	-4.442485	3.594278	1.491855
H	-2.877442	3.688331	2.331327
H	-3.820607	5.169866	2.026348
C	-3.751267	5.092113	-0.734349
H	-3.282724	5.244549	-1.720769
H	-4.682413	4.523138	-0.890150
H	-4.038776	6.088938	-0.355003
C	-0.918460	-3.657637	-2.208320
H	-0.177559	-2.918308	-1.866656
H	-0.661260	-4.626035	-1.748918
H	-0.798218	-3.772170	-3.300259
C	-2.626965	-1.851675	-2.517119
H	-2.469569	-1.901123	-3.609186
H	-3.664261	-1.518152	-2.352499
H	-1.954550	-1.072136	-2.123305
C	-3.350113	-4.253221	-2.407250
H	-3.279831	-4.322919	-3.507187
H	-3.156597	-5.260753	-2.004708
H	-4.393410	-3.990146	-2.165669
H	5.252954	-0.283814	-1.925207

pp_Siexo_S1_tol_wB97XD
SCF Energy: -1980.10217620
Num. Imaginary Frequencies: 0

C	-0.008977	0.816722	0.469614
C	-0.525901	0.148960	1.752541
C	-0.999061	-1.301995	1.615224
C	0.085822	-2.382332	1.365160
C	0.600420	-2.378293	-0.040467
C	1.495273	0.841057	0.222059
C	1.868651	-2.552751	-0.441780
C	4.489585	0.019766	0.200717
C	3.868665	0.771028	1.140060
C	2.392009	0.759690	1.220237
C	4.528450	1.619258	2.200662
C	5.910204	-0.157653	-0.152558
C	6.962679	0.792780	0.363026
C	6.196722	-1.182289	-0.986464
C	7.530938	-1.605856	-1.510784
C	1.838618	1.075995	-1.221488
C	2.185097	-2.576533	-1.872725
O	3.297538	-2.680677	-2.338781
O	-1.979032	-1.373033	0.602858
O	-0.447576	2.164674	0.407290
H	-0.455018	0.255878	-0.373703
H	0.191650	0.222396	2.581543
H	-1.405406	0.725885	2.071009
H	-1.445493	-1.562681	2.595178
H	-0.174443	-2.264980	-0.808636
H	2.702187	-2.664083	0.257267
H	3.828100	-0.590553	-0.420587
H	2.005818	0.710003	2.244483
H	5.556882	1.319784	2.427377
H	4.535677	2.683367	1.909295
H	3.952350	1.559798	3.137926
H	6.593345	1.828439	0.364283
H	7.268967	0.551039	1.393630
H	7.868609	0.768954	-0.256820
H	8.365088	-0.980389	-1.165635
H	7.746759	-2.644831	-1.209041
H	2.871931	1.417149	-1.363556
H	1.703274	0.159569	-1.820521
H	1.158944	1.834740	-1.639796

H	1.295178	-2.490310	-2.548288
C	1.162373	-2.409976	2.442586
H	1.750259	-3.337969	2.387834
H	1.859911	-1.566731	2.343401
H	0.709496	-2.366302	3.445154
H	-0.476587	-3.332662	1.433778
H	7.532172	-1.601545	-2.613902
Si	-3.430772	-2.233123	0.669346
Si	-1.818656	2.712521	-0.398495
C	-4.070267	-2.256426	-1.119027
C	-4.607132	-1.374936	1.850650
H	-4.830429	-0.341269	1.546335
H	-5.561067	-1.922270	1.924133
H	-4.174457	-1.337796	2.864265
C	-3.123087	-3.972511	1.307466
H	-4.078579	-4.509685	1.423479
H	-2.484210	-4.565877	0.634632
H	-2.646292	-3.952028	2.301364
C	-3.342719	2.042878	0.465159
H	-3.255826	0.947147	0.513777
H	-3.429655	2.419612	1.496458
H	-4.272607	2.288388	-0.072126
C	-1.801238	2.103728	-2.176540
H	-1.635543	1.015317	-2.226276
H	-2.765173	2.307814	-2.670372
H	-1.010016	2.586468	-2.771349
C	-1.697311	4.603391	-0.302899
C	-2.861041	5.229939	-1.086117
H	-3.842330	4.920295	-0.689352
H	-2.819840	6.332282	-1.026729
H	-2.832337	4.961239	-2.154972
C	-1.765440	5.045880	1.166739
H	-0.969129	4.578367	1.767212
H	-1.645664	6.141183	1.247234
H	-2.731862	4.789786	1.630609
C	-0.359781	5.057755	-0.906793
H	-0.267756	4.776785	-1.968693
H	-0.263820	6.156981	-0.851860
H	0.494587	4.618000	-0.369390
C	-4.514512	-0.851024	-1.550858
H	-5.336221	-0.464961	-0.926387
H	-3.686759	-0.127599	-1.501736
H	-4.875982	-0.866624	-2.594549
C	-2.953868	-2.740951	-2.056615
H	-3.328397	-2.824929	-3.092133
H	-2.107013	-2.037459	-2.067302
H	-2.565209	-3.731901	-1.769364
C	-5.267453	-3.217512	-1.204282
H	-6.082717	-2.928756	-0.520090
H	-5.687242	-3.218102	-2.225697
H	-4.983874	-4.256069	-0.969323
H	5.354011	-1.794318	-1.331348

TSReendo_S1_tol_wB97XD
SCF Energy: -1980.06679774
Num. Imaginary Frequencies: 1

C	0.069086	0.798959	-1.503635
C	-1.181589	-0.073622	-1.523099
C	-1.393269	-0.871106	-0.245494
C	-0.242773	-1.842985	0.054820
C	1.060251	-1.100560	0.353909
C	1.386697	0.011819	-1.380162
C	2.203967	-1.848442	0.669113
C	4.145287	-0.964706	-0.832645
C	3.796110	0.381552	-0.697983
C	2.480075	0.792128	-0.962197
C	4.734709	1.420858	-0.130868
C	5.380269	-1.662640	-0.485078
C	5.633838	-2.897596	-1.317108
C	6.142063	-1.305907	0.573435
C	7.362727	-1.983133	1.101716
C	1.557327	-1.040039	-2.471546
C	3.094397	-1.428642	1.725434
O	3.934583	-2.116360	2.280744
O	-2.604762	-1.582490	-0.360307
O	-0.041244	1.727761	-0.456190
H	0.121085	1.323050	-2.481398
H	-2.050492	0.584586	-1.673073
H	-1.169920	-0.772365	-2.372684
H	-1.442112	-0.157708	0.601245
H	0.904272	-0.215696	0.982124
H	2.304326	-2.883542	0.326107
H	3.492842	-1.564652	-1.457424
H	2.228242	1.796881	-0.613155
H	4.714291	1.438952	0.971503
H	5.775766	1.242247	-0.436811
H	4.444757	2.424207	-0.475253
H	5.610281	-2.662434	-2.393095
H	6.597824	-3.374032	-1.100808
H	4.846328	-3.647590	-1.131791
H	7.730211	-2.799885	0.467422
H	8.180996	-1.256293	1.233965
H	2.455518	-0.837303	-3.072823
H	1.634288	-2.070109	-2.094320
H	0.703791	-1.024722	-3.163109
H	2.938052	-0.362576	2.044398
C	-0.605551	-2.737707	1.246049
H	-0.723142	-2.137991	2.163645
H	-1.549157	-3.267195	1.057227
H	0.180331	-3.482033	1.434735
H	-0.107064	-2.493314	-0.827304
H	7.146858	-2.398217	2.100081

Si	-0.451362	3.356069	-0.583954
Si	-4.030773	-1.147585	0.420867
C	-0.607545	3.917934	1.220040
C	0.910258	4.264071	-1.501690
H	1.852853	4.287625	-0.932765
H	1.117315	3.777798	-2.469457
H	0.619261	5.305251	-1.715981
C	-2.056270	3.541477	-1.536624
H	-1.943744	3.170532	-2.568761
H	-2.886248	2.990011	-1.069047
H	-2.350300	4.601728	-1.604612
C	-5.324422	-2.365559	-0.243404
C	-3.812648	-1.291722	2.279179
H	-2.978752	-0.658702	2.623774
H	-4.717548	-0.949706	2.807676
H	-3.602670	-2.324539	2.597036
C	-4.448156	0.637250	0.012612
H	-3.658032	1.304310	0.394333
H	-4.545734	0.805064	-1.071110
H	-5.391881	0.945720	0.491445
C	0.698383	3.600205	1.965247
H	0.625994	3.913236	3.021947
H	0.921631	2.522095	1.950707
H	1.562959	4.126975	1.529339
C	-1.768928	3.164438	1.886622
H	-2.737138	3.397277	1.414259
H	-1.622113	2.073285	1.840245
H	-1.851354	3.442383	2.952343
C	-0.875559	5.429862	1.267856
H	-1.805413	5.703661	0.742401
H	-0.980519	5.771599	2.312847
H	-0.052930	6.009445	0.817730
C	-4.824164	-3.802118	-0.026974
H	-4.660824	-4.027377	1.039690
H	-5.564302	-4.530343	-0.404321
H	-3.876010	-3.982529	-0.556419
C	-6.653335	-2.164082	0.500686
H	-7.424680	-2.849811	0.107010
H	-6.557896	-2.367834	1.579691
H	-7.042909	-1.138798	0.386404
C	-5.531701	-2.119675	-1.745730
H	-4.587780	-2.212317	-2.306045
H	-6.241726	-2.855175	-2.164426
H	-5.945386	-1.117878	-1.946031
H	5.821780	-0.447196	1.165042

TSReexo_S1_tol_wB97XD
SCF Energy: -1980.06533679
Num. Imaginary Frequencies: 1

C	-0.026647	1.147773	-1.388303
C	-0.825805	-0.150775	-1.399123
C	-0.889619	-0.841296	-0.041260
C	0.483098	-1.231872	0.528812
C	1.371681	-0.016921	0.767527
C	1.466926	0.963376	-1.059127
C	2.665758	-0.213704	1.260442
C	4.287760	-0.135431	-0.662077
C	3.413246	-0.581114	-1.648036
C	2.132622	-0.013059	-1.819100
C	3.690903	-1.825777	-2.466322
C	5.525104	-0.778572	-0.186803
C	6.636073	0.189748	0.131987
C	5.589789	-2.107775	0.029027
C	6.740569	-2.904191	0.554330
C	2.099071	2.290841	-0.688395
C	3.313967	0.810288	2.060593
O	4.378953	0.700067	2.638315
O	-1.692642	-1.993140	-0.169031
O	-0.605605	2.019804	-0.446577
H	-0.075070	1.596964	-2.401982
H	-1.853814	0.083772	-1.714701
H	-0.429878	-0.862501	-2.138274
H	-1.343494	-0.130987	0.678479
H	0.841880	0.858891	1.164857
H	3.112230	-1.208958	1.292783
H	4.212692	0.904197	-0.362577
H	1.496232	-0.591389	-2.496421
H	4.767179	-2.011555	-2.582195
H	3.247186	-2.728183	-2.014339
H	3.251963	-1.721011	-3.469793
H	6.824726	0.867025	-0.716363
H	6.337650	0.808859	0.993317
H	7.581558	-0.305846	0.385944
H	6.950062	-3.762306	-0.105552
H	7.665470	-2.322009	0.657523
H	1.614959	2.739271	0.187879
H	3.175529	2.252185	-0.508945
H	1.946291	2.984795	-1.532405
H	2.737519	1.770588	2.132674
C	0.304962	-2.015144	1.833492
H	-0.169312	-1.387880	2.606233
H	-0.329395	-2.896594	1.668955
H	1.272296	-2.354494	2.229571
H	0.980705	-1.892508	-0.202807
H	6.496894	-3.324513	1.544829
Si	-3.276712	-2.116698	0.384981
Si	-1.601789	3.340970	-0.751646
C	-3.861731	-3.810975	-0.235706
C	-3.313843	-1.999073	2.257564
H	-2.861796	-1.053055	2.597402
H	-4.351378	-2.013516	2.629721
H	-2.767482	-2.823847	2.740380

C	-4.298443	-0.703889	-0.311972
H	-5.349662	-0.775535	0.011924
H	-3.910140	0.257986	0.060502
H	-4.282633	-0.678553	-1.412518
C	-2.195495	3.853390	0.975327
C	-3.015182	2.831670	-1.875191
H	-3.691865	3.681658	-2.061983
H	-2.635731	2.499889	-2.855804
H	-3.613327	2.011082	-1.450556
C	-0.613308	4.692443	-1.596687
H	0.212353	5.058707	-0.967253
H	-0.179959	4.325327	-2.541624
H	-1.255633	5.551980	-1.848968
C	-0.977440	4.074622	1.885618
H	-0.382239	3.154640	1.994916
H	-0.309443	4.862818	1.501578
H	-1.300576	4.384772	2.895215
C	-3.071040	2.735968	1.563366
H	-3.383887	2.988269	2.592077
H	-3.988874	2.577224	0.974267
H	-2.527605	1.778228	1.609497
C	-3.010935	5.151742	0.878611
H	-3.385097	5.448658	1.874409
H	-2.407546	5.990608	0.495130
H	-3.889802	5.042600	0.221718
C	-2.870039	-4.889108	0.228006
H	-3.192152	-5.886619	-0.120921
H	-1.859887	-4.704486	-0.168657
H	-2.795075	-4.937498	1.326781
C	-5.257193	-4.115128	0.330326
H	-5.253359	-4.171982	1.431060
H	-5.999954	-3.354809	0.036594
H	-5.623066	-5.087643	-0.044541
C	-3.919125	-3.798741	-1.770958
H	-4.662482	-3.078519	-2.149887
H	-2.943505	-3.538574	-2.211445
H	-4.204111	-4.794152	-2.156093
H	4.683108	-2.691013	-0.163778

TSSiendo_S1_tol_wB97XD
SCF Energy: -1980.06210263
Num. Imaginary Frequencies: 1

C	-0.652205	0.743275	0.607246
C	-1.343833	0.020146	1.753930
C	-1.031848	-1.468636	1.778837
C	0.449108	-1.777337	2.036932
C	1.349491	-1.296031	0.894942
C	0.881860	0.705959	0.632510
C	2.744482	-1.452817	0.981367
C	3.784764	0.771080	-0.064717
C	2.788133	0.894398	-1.036689
C	1.439755	0.866897	-0.653924
C	3.082081	0.922852	-2.518240
C	5.228266	0.617292	-0.202349
C	6.010986	1.109168	0.992039
C	5.788771	-0.045858	-1.239370
C	7.228170	-0.374037	-1.454080
C	1.474509	1.425525	1.839573
C	3.490007	-2.016575	-0.116009
O	4.631257	-2.447903	-0.072100
O	-1.404835	-2.042623	0.544755
O	-1.061368	2.096016	0.613867
H	-0.970656	0.243396	-0.324832
H	-1.079397	0.485923	2.715363
H	-2.428884	0.158172	1.628724
H	-1.604923	-1.929060	2.607479
H	0.929538	-1.625968	-0.060421
H	3.264597	-1.402259	1.942819
H	3.485690	1.000226	0.951842
H	0.728924	0.775038	-1.483322
H	4.012404	1.466229	-2.738610
H	3.185572	-0.090632	-2.940097
H	2.261866	1.416136	-3.059924
H	5.802122	0.471617	1.867803
H	7.095868	1.099799	0.830222
H	5.721602	2.137271	1.260651
H	7.905117	0.092274	-0.727048
H	7.364432	-1.466428	-1.393874
H	2.235348	0.844570	2.376691
H	1.933617	2.376844	1.530481
H	0.685720	1.676834	2.561037
H	2.907216	-2.066701	-1.075764
C	0.873177	-1.420077	3.458532
H	1.912990	-1.718233	3.654203
H	0.783921	-0.348793	3.679819
H	0.241164	-1.958674	4.181779
H	0.512498	-2.877331	1.955751
H	7.546974	-0.072034	-2.465246
Si	-2.767342	-2.986466	0.261414
Si	-2.098803	2.778630	-0.521430
C	-2.764013	-3.246225	-1.617919
C	-4.300385	-2.075736	0.848148
H	-4.236866	-1.861444	1.927870
H	-4.441452	-1.117605	0.323861
H	-5.206560	-2.683835	0.693167
C	-2.601268	-4.595927	1.209525
H	-1.672072	-5.125236	0.946246
H	-2.581319	-4.407353	2.295670
H	-3.448465	-5.272898	1.012954
C	-1.299805	2.758437	-2.220137
H	-1.905869	3.323484	-2.947424
H	-0.291098	3.199459	-2.200220

H	-1.213512	1.729046	-2.604704
C	-2.383141	4.545004	0.107703
C	-3.682962	1.772905	-0.593146
H	-4.223665	1.775394	0.366127
H	-4.364853	2.153436	-1.371006
H	-3.449151	0.726929	-0.851207
C	-1.051268	5.310739	0.075301
H	-1.180089	6.329400	0.482955
H	-0.278086	4.806198	0.676162
H	-0.662155	5.417138	-0.950392
C	-2.906266	4.491076	1.551166
H	-3.873435	3.966467	1.620177
H	-2.197979	3.975580	2.217830
H	-3.059986	5.511534	1.945411
C	-3.410737	5.256195	-0.785779
H	-3.078776	5.316757	-1.835365
H	-4.390128	4.750287	-0.772768
H	-3.574680	6.291599	-0.437631
C	-1.489289	-3.999936	-2.027362
H	-0.579848	-3.456794	-1.725557
H	-1.442612	-5.005574	-1.579169
H	-1.452216	-4.129607	-3.123700
C	-2.793171	-1.878675	-2.317824
H	-2.767460	-2.003834	-3.414974
H	-3.707272	-1.311491	-2.077571
H	-1.926528	-1.260918	-2.033036
C	-3.999688	-4.060979	-2.029829
H	-4.005867	-4.228984	-3.121453
H	-4.021085	-5.053074	-1.549546
H	-4.939951	-3.544728	-1.775670
H	5.123219	-0.444388	-2.006773

TSSiexo_S1_tol_wB97XD
SCF Energy: -1980.06642898
Num. Imaginary Frequencies: 1

C	-0.504729	0.777160	0.274022
C	-0.916892	0.129233	1.588424
C	-0.739487	-1.384852	1.554035
C	0.718580	-1.846374	1.411502
C	1.354655	-1.400360	0.099369
C	0.984856	0.656181	-0.067863
C	2.709037	-1.664439	-0.146884
C	3.999741	0.634237	-0.107968
C	3.263105	1.144970	0.959650
C	1.858765	1.168404	0.908330
C	3.895404	1.542592	2.276501
C	5.396126	0.225692	-0.176006
C	6.155378	-0.159196	1.070242
C	5.917310	0.077708	-1.418102
C	7.283884	-0.381944	-1.797711
C	1.226704	0.863644	-1.553958
C	3.195495	-1.991236	-1.464503
O	4.326832	-2.359278	-1.738260
O	-1.487691	-1.907963	0.476373
O	-0.861957	2.144544	0.267563
H	-1.054090	0.237788	-0.518100
H	-0.367748	0.564087	2.437482
H	-1.981734	0.351857	1.756411
H	-1.111556	-1.793587	2.513788
H	0.691323	-1.573793	-0.757417
H	3.403597	-1.859570	0.672507
H	3.524392	0.679588	-1.082259
H	1.379916	1.476908	1.843038
H	4.087155	0.674941	2.928461
H	4.847839	2.070659	2.136563
H	3.224025	2.217897	2.826570
H	6.568363	0.710321	1.603894
H	5.499703	-0.693737	1.772105
H	6.990534	-0.831810	0.836781
H	7.974803	-0.461736	-0.948397
H	7.218159	-1.370031	-2.283229
H	1.512139	1.907764	-1.756782
H	2.005005	0.219489	-1.978516
H	0.306405	0.652675	-2.117588
H	2.429072	-1.897908	-2.280845
C	1.535740	-1.569521	2.670232
H	2.523706	-2.048996	2.622723
H	1.695911	-0.495633	2.838761
H	1.021078	-1.975128	3.555305
H	0.642236	-2.944829	1.314355
H	7.729415	0.304199	-2.535935
Si	-2.878959	-2.843086	0.613137
Si	-2.206868	2.770414	-0.528264
C	-3.442551	-3.105459	-1.179391
C	-4.156849	-1.919488	1.631806
H	-4.454968	-0.968489	1.163243
H	-5.065292	-2.527114	1.774800
H	-3.761721	-1.689125	2.635109
C	-2.449554	-4.454508	1.471820
H	-3.324381	-5.121100	1.543363
H	-1.650737	-4.995886	0.941148
H	-2.099436	-4.266609	2.500344
C	-3.745663	1.840923	0.013906
H	-3.619121	0.766975	-0.198297
H	-3.949857	1.953965	1.089986
H	-4.635519	2.179384	-0.541449
C	-2.010471	2.552788	-2.382188
H	-2.022000	1.485116	-2.655869
H	-2.842191	3.031986	-2.924399
H	-1.068698	2.986974	-2.751603
C	-2.237267	4.597662	-0.021825
C	-3.460043	5.290502	-0.641971

H	-4.407499	4.840509	-0.302234
H	-3.486084	6.357307	-0.356554
H	-3.446209	5.250682	-1.743607
C	-2.310705	4.696464	1.509590
H	-1.457761	4.190481	1.987725
H	-2.298819	5.753524	1.830315
H	-3.234567	4.246027	1.908104
C	-0.950463	5.277159	-0.515422
H	-0.875906	5.268400	-1.615097
H	-0.923176	6.334083	-0.195072
H	-0.051841	4.782567	-0.114129
C	-3.643734	-1.739873	-1.854183
H	-4.428117	-1.145232	-1.358225
H	-2.715860	-1.146120	-1.848593
H	-3.950984	-1.869275	-2.907236
C	-2.368481	-3.896266	-1.942091
H	-2.661080	-4.024991	-2.999401
H	-1.394992	-3.381209	-1.927014
H	-2.220794	-4.903652	-1.520584
C	-4.765665	-3.886373	-1.195022
H	-5.574020	-3.341973	-0.679934
H	-5.100150	-4.059398	-2.233336
H	-4.669353	-4.875172	-0.717003
H	5.262227	0.312340	-2.263842

pf_Reendo_S1_tol_wB97XD
SCF Energy: -1980.16914127
Num. Imaginary Frequencies: 0

C	0.467760	0.614610	-1.793887
C	-1.035348	0.391776	-1.702045
C	-1.406209	-0.487998	-0.513855
C	-0.631131	-1.823304	-0.470590
C	0.885005	-1.513944	-0.540633
C	1.232539	-0.726959	-1.835441
C	1.881188	-2.680946	-0.391817
C	3.341414	-2.137316	-0.219132
C	3.663978	-1.045580	-1.213648
C	2.707438	-0.423203	-1.905201
C	5.118675	-0.699699	-1.361379
C	3.686216	-1.715243	1.217401
C	4.458927	-2.740693	2.004113
C	3.341002	-0.504369	1.682479
C	3.593222	0.067039	3.043747
C	0.874942	-1.484988	-3.129630
C	1.638462	-3.626624	0.758479
O	1.695452	-4.828107	0.661415
O	-2.790436	-0.742661	-0.532371
O	0.896887	1.349769	-0.673823
H	0.693628	1.165660	-2.727041
H	-1.539196	1.366494	-1.606325
H	-1.416142	-0.074981	-2.622571
H	-1.129835	0.058689	0.409580
H	1.085057	-0.824673	0.295400
H	1.863193	-3.309466	-1.295199
H	4.004033	-2.988084	-0.454648
H	2.995689	0.351330	-2.627281
H	5.540709	-0.355538	-0.403193
H	5.704741	-1.581100	-1.671778
H	5.273918	0.093211	-2.106952
H	5.472498	-2.850770	1.581152
H	4.564489	-2.487525	3.066703
H	3.991271	-3.736172	1.941709
H	4.131081	-0.616645	3.714028
H	4.184328	0.995316	2.971399
H	1.142659	-0.876036	-4.007925
H	1.442844	-2.423139	-3.204449
H	-0.191546	-1.732318	-3.214360
H	1.468229	-3.145321	1.751150
C	-1.073948	-2.596372	0.770070
H	-0.708900	-2.117134	1.693517
H	-2.170945	-2.619526	0.814321
H	-0.739280	-3.641818	0.763365
H	-0.935150	-2.407757	-1.355391
H	2.644345	0.340576	3.533515
Si	1.435516	2.932776	-0.544639
Si	-3.963954	0.089493	0.337899
C	0.665923	3.547551	1.080935
C	3.308778	2.946851	-0.479561
H	3.693277	2.277109	0.305173
H	3.728719	2.604980	-1.438992
H	3.700066	3.959478	-0.288187
C	0.845382	3.925513	-2.023670
H	1.326478	3.579869	-2.953107
H	-0.245025	3.857317	-2.162968
H	1.103706	4.990361	-1.904134
C	-5.533719	-0.961237	0.140266
C	-3.432684	0.232219	2.133271
H	-2.473027	0.767052	2.222744
H	-4.174272	0.803560	2.715059
H	-3.313026	-0.753844	2.608814
C	-4.201955	1.810401	-0.374197
H	-3.329939	2.449186	-0.163440
H	-4.342830	1.778496	-1.465992
H	-5.082152	2.305974	0.067618
C	1.142540	2.642738	2.227019
H	0.682109	2.949501	3.183369
H	0.871398	1.589889	2.048607
H	2.234961	2.690586	2.361487
C	-0.862606	3.452788	0.967068
H	-1.261670	4.114500	0.180740
H	-1.179534	2.423760	0.734418
H	-1.346930	3.744436	1.916131

C	1.080471	4.998886	1.360005
H	0.747862	5.685549	0.564265
H	0.633187	5.356073	2.304767
H	2.173261	5.104832	1.458640
C	-5.229631	-2.416419	0.526909
H	-4.872629	-2.503943	1.566372
H	-6.139444	-3.037369	0.441897
H	-4.462710	-2.854992	-0.129518
C	-6.641471	-0.408873	1.050577
H	-7.574313	-0.985262	0.917130
H	-6.370018	-0.472886	2.116896
H	-6.878305	0.644843	0.827983
C	-5.998566	-0.911723	-1.323577
H	-5.211216	-1.257755	-2.012198
H	-6.879377	-1.561820	-1.472356
H	-6.289998	0.106240	-1.629452
H	2.823040	0.167958	0.987643

pf_Reexo_S1_tol_wB97XD
SCF Energy: -1980.17246419
Num. Imaginary Frequencies: 0

C	0.444026	1.380205	1.175600
C	0.466808	-0.129494	1.346811
C	0.233029	-0.811392	0.008916
C	-1.129189	-0.416925	-0.568728
C	-1.294413	1.120854	-0.669971
C	-0.909532	1.884740	0.622707
C	-2.731453	1.490810	-1.091622
C	-3.808241	1.269420	-0.003096
C	-3.283123	1.472104	1.405785
C	-1.991179	1.712988	1.664532
C	-4.318023	1.515843	2.497979
C	-4.567743	-0.040129	-0.230756
C	-5.564547	0.033170	-1.356486
C	-4.346516	-1.133942	0.511738
C	-4.969545	-2.489488	0.385690
C	-0.757038	3.397568	0.365949
C	-2.821923	2.850160	-1.748686
O	-3.751288	3.611531	-1.664662
O	0.287200	-2.211224	0.171006
O	1.475750	1.758944	0.291828
H	0.588477	1.861437	2.163892
H	1.437262	-0.441200	1.761506
H	-0.315114	-0.447303	2.055168
H	1.020270	-0.471301	-0.692263
H	-0.608970	1.463881	-1.466445
H	-2.973179	0.848648	-1.958198
H	-4.549226	2.073867	-0.161732
H	-1.696257	1.914489	2.702346
H	-5.015776	2.352264	2.322329
H	-4.926981	0.600353	2.530424
H	-3.857311	1.661015	3.485697
H	-6.424653	0.658387	-1.062272
H	-5.128943	0.513583	-2.248111
H	-5.949638	-0.947671	-1.663168
H	-5.489454	-2.768717	1.317290
H	-5.693809	-2.565868	-0.436368
H	-0.052241	3.595258	-0.454067
H	-1.718570	3.876898	0.139171
H	-0.368849	3.894833	1.269207
H	-1.954788	3.088122	-2.416707
C	-1.366655	-1.116415	-1.904087
H	-0.721962	-0.699174	-2.696569
H	-1.142871	-2.187448	-1.810516
H	-2.411935	-1.039715	-2.237284
H	-1.868280	-0.800482	0.148358
H	-4.190860	-3.253466	0.222595
Si	1.589606	-3.167069	-0.291685
Si	2.979572	2.380810	0.710599
C	1.116945	-4.911923	0.284615
C	1.816425	-3.077315	-2.153521
H	1.934957	-2.031361	-2.480532
H	2.723647	-3.619539	-2.466565
H	0.960567	-3.503173	-2.699877
C	3.157332	-2.537346	0.527629
H	4.023001	-3.173287	0.279940
H	3.386892	-1.521576	0.166677
H	3.065363	-2.498645	1.624095
C	3.937594	2.395264	-0.927543
C	3.795750	1.285871	1.998433
H	4.794973	1.669227	2.262835
H	3.201625	1.265230	2.926992
H	3.913006	0.247626	1.651549
C	2.770545	4.102140	1.426646
H	2.310071	4.796940	0.707364
H	2.130628	4.074874	2.323913
H	3.741208	4.523808	1.734961
C	3.132761	3.173548	-1.979612
H	2.150955	2.709184	-2.159721
H	2.958637	4.219423	-1.678208
H	3.674868	3.197315	-2.941851
C	4.138327	0.950336	-1.409986
H	4.647751	0.934786	-2.389970
H	4.758701	0.364445	-0.712442
H	3.176287	0.426238	-1.529207
C	5.304660	3.065521	-0.723261
H	5.883190	3.059860	-1.664158
H	5.205950	4.117396	-0.409094
H	5.913632	2.545113	0.034458
C	-0.271945	-5.266337	-0.269201
H	-0.570229	-6.279832	0.054039
H	-1.038618	-4.560271	0.085328

H	-0.292773	-5.257478	-1.371416
C	2.151682	-5.925403	-0.227277
H	2.185817	-5.960605	-1.328463
H	3.169262	-5.698445	0.132154
H	1.903477	-6.943094	0.123434
C	1.075547	-4.946441	1.820052
H	2.066206	-4.754354	2.263423
H	0.375300	-4.197917	2.223684
H	0.745484	-5.938556	2.176861
H	-3.610159	-1.048351	1.319839

pf_Siendo_S1_tol_wB97XD
SCF Energy: -1980.16939499
Num. Imaginary Frequencies: 0

C	1.142607	-0.207488	0.754674
C	0.818796	0.816474	1.842574
C	-0.683888	1.068058	1.961427
C	-1.474333	-0.231454	2.196052
C	-1.081328	-1.234407	1.092260
C	0.429722	-1.558391	1.008302
C	-1.921328	-2.519249	1.025143
C	-1.725554	-3.203641	-0.362776
C	-0.262863	-3.242210	-0.757608
C	0.665496	-2.488990	-0.157138
C	0.082610	-4.190266	-1.872392
C	-2.610025	-2.611621	-1.467358
C	-3.933154	-3.307828	-1.648732
C	-2.191421	-1.580066	-2.216775
C	-2.912997	-0.889417	-3.331858
C	1.033141	-2.260341	2.240679
C	-3.373245	-2.207684	1.289184
O	-4.035089	-2.711343	2.162275
O	-1.149359	1.647841	0.760857
O	2.535188	-0.383434	0.652653
H	0.733938	0.184441	-0.196580
H	1.226773	0.475750	2.806333
H	1.324806	1.763690	1.601762
H	-0.868797	1.747803	2.815707
H	-1.310030	-0.689038	0.162271
H	-1.611857	-3.228241	1.807971
H	-2.050641	-4.251915	-0.242531
H	1.709461	-2.581594	-0.474347
H	-0.141499	-5.231361	-1.584471
H	-0.509975	-3.973952	-2.775879
H	1.147629	-4.132334	-2.139032
H	-4.415797	-3.524398	-0.682163
H	-4.646653	-2.736525	-2.256793
H	-3.778796	-4.284526	-2.139311
H	-3.949864	-1.227844	-3.461054
H	-2.929831	0.198752	-3.163971
H	0.406518	-3.104296	2.563659
H	2.024214	-2.661611	1.986389
H	1.172306	-1.591863	3.098809
H	-3.823373	-1.439819	0.610235
C	-1.414310	-0.712148	3.645720
H	-1.896362	-1.693974	3.763241
H	-0.391296	-0.795683	4.034191
H	-1.953545	-0.006030	4.296409
H	-2.523537	0.048711	2.002750
H	-2.386955	-1.048830	-4.288313
Si	-1.510891	3.260950	0.472405
Si	3.443836	0.260691	-0.611320
C	-2.119565	3.261594	-1.325463
C	0.019263	4.322595	0.702820
H	0.413023	4.218411	1.727453
H	0.825298	4.049412	0.004052
H	-0.213483	5.389641	0.552925
C	-2.836836	3.822875	1.675292
H	-3.696143	3.133938	1.678793
H	-2.442630	3.872109	2.703581
H	-3.207900	4.829564	1.422265
C	2.970106	-0.570115	-2.226950
H	3.467122	-0.080152	-3.080253
H	3.240117	-1.637448	-2.245217
H	1.883162	-0.498557	-2.396192
C	5.245794	-0.085487	-0.132659
C	3.076948	2.096003	-0.764914
H	3.293421	2.644887	0.164512
H	3.664967	2.554348	-1.576703
H	2.012290	2.244943	-1.009546
C	5.424297	-1.591251	0.115484
H	6.467360	-1.814802	0.402669
H	4.770103	-1.947494	0.926077
H	5.199618	-2.188453	-0.783373
C	5.587857	0.685889	1.151141
H	5.524650	1.776618	1.005655
H	4.911102	0.416945	1.977564
H	6.619056	0.459463	1.476307
C	6.176227	0.363709	-1.269679
H	5.982402	-0.187302	-2.204538
H	6.076072	1.439886	-1.488080
H	7.232108	0.184391	-0.999206
C	-3.453981	2.504260	-1.405747
H	-3.360025	1.471906	-1.031813
H	-4.245750	3.002074	-0.822685
H	-3.807199	2.451149	-2.451266
C	-1.078863	2.558924	-2.211092
H	-1.411111	2.545837	-3.264701
H	-0.103089	3.072009	-2.186644
H	-0.918046	1.516473	-1.894797
C	-2.316503	4.706234	-1.808818
H	-2.703404	4.719111	-2.843352

H	-3.039955	5.258316	-1.186020
H	-1.371995	5.274332	-1.808001
H	-1.181152	-1.201722	-2.020979

pf_Siexo_S1_tol_wB97XD
SCF Energy: -1980.16027496
Num. Imaginary Frequencies: 0

C	-0.583489	0.695392	0.230812
C	-0.861734	0.037974	1.573750
C	-0.475271	-1.435761	1.519714
C	1.023295	-1.584792	1.237635
C	1.388240	-0.888530	-0.101223
C	0.890633	0.578506	-0.236279
C	2.910504	-1.034650	-0.396449
C	3.756627	0.273714	-0.353627
C	3.136236	1.360787	0.517556
C	1.803839	1.490036	0.549521
C	4.050517	2.342673	1.193540
C	5.212073	-0.043065	-0.046501
C	5.511098	-0.698070	1.280159
C	6.155932	0.221321	-0.962877
C	7.624004	-0.056364	-0.871033
C	0.900940	1.010471	-1.716571
C	3.105315	-1.709198	-1.732338
O	3.530910	-2.825088	-1.881171
O	-1.206541	-2.077332	0.496713
O	-0.964715	2.050870	0.259375
H	-1.182226	0.146641	-0.519509
H	-0.307459	0.557280	2.370735
H	-1.932166	0.136199	1.808494
H	-0.688840	-1.907399	2.498156
H	0.835063	-1.463769	-0.863239
H	3.326005	-1.741328	0.333024
H	3.755024	0.693182	-1.376351
H	1.343602	2.314168	1.102804
H	4.704504	1.862950	1.938557
H	4.718366	2.823588	0.459819
H	3.475770	3.130208	1.701812
H	6.496411	-0.411041	1.673161
H	4.762261	-0.425370	2.037419
H	5.500479	-1.797849	1.196090
H	7.919698	-0.511291	0.083921
H	7.936366	-0.742408	-1.675930
H	0.507750	2.032392	-1.808665
H	1.907934	1.009011	-2.153911
H	0.268610	0.341603	-2.323684
H	2.802508	-1.096173	-2.621598
C	1.837506	-1.188401	2.470185
H	2.904568	-1.406881	2.335228
H	1.752033	-0.122099	2.718424
H	1.500106	-1.769594	3.343194
H	1.196915	-2.661579	1.069013
H	8.208596	0.869039	-1.004786
Si	-2.575838	-3.032269	0.686719
Si	-2.411076	2.647048	-0.359705
C	-3.295906	-3.161656	-1.064717
C	-3.771431	-2.211762	1.880110
H	-4.083605	-1.211843	1.540689
H	-4.679707	-2.823577	2.006605
H	-3.315880	-2.100065	2.877874
C	-2.068153	-4.700629	1.375603
H	-2.938500	-5.355590	1.542838
H	-1.370407	-5.221996	0.701558
H	-1.560659	-4.576260	2.346647
C	-3.858509	1.785122	0.469270
H	-3.856763	0.714650	0.207161
H	-3.823319	1.869026	1.566547
H	-4.819937	2.200696	0.125614
C	-2.508485	2.311034	-2.204005
H	-2.395056	1.234644	-2.411707
H	-3.490335	2.614504	-2.602855
H	-1.731398	2.845706	-2.771567
C	-2.355475	4.503659	0.025044
C	-3.578356	5.196514	-0.595363
H	-4.527566	4.789781	-0.208864
H	-3.569953	6.276444	-0.363262
H	-3.595146	5.100747	-1.693385
C	-2.363991	4.707923	1.547753
H	-1.519220	4.192117	2.031116
H	-2.285445	5.781737	1.795205
H	-3.293385	4.334989	2.008283
C	-1.069547	5.105222	-0.562746
H	-1.022893	4.991218	-1.658202
H	-1.014685	6.187024	-0.345433
H	-0.170097	4.632019	-0.139655
C	-3.753697	-1.769004	-1.524977
H	-4.576922	-1.378691	-0.904789
H	-2.928234	-1.039816	-1.488507
H	-4.119246	-1.803256	-2.566697
C	-2.214759	-3.682270	-2.023973
H	-2.613459	-3.757388	-3.051434
H	-1.341282	-3.012550	-2.051463
H	-1.856911	-4.685067	-1.739414
C	-4.493143	-4.124215	-1.065136
H	-5.293128	-3.793326	-0.382199
H	-4.935683	-4.191288	-2.074939
H	-4.201529	-5.145385	-0.770086
H	5.829169	0.684904	-1.902409

System I, Methanol, ωB97X-D

lineal_scis-scis_S1_MeOH_wB97XD
SCF Energy: -1980.11032021
Num. Imaginary Frequencies: 0

C	0.659929	0.354392	0.535792
C	-0.334913	-0.071944	1.614721
C	-1.780714	0.121279	1.159450
C	-2.766029	0.249489	2.345719
C	-4.108194	0.636912	1.809088
C	2.050352	-0.217256	0.745748
C	-5.256091	-0.050624	1.915115
C	4.934772	-1.233365	0.096204
C	3.771214	-1.898980	-0.082054
C	2.481102	-1.179492	-0.092214
H	0.286678	-0.026447	-0.429655
H	-0.140291	0.519493	2.522986
H	-1.833870	1.066563	0.586897
H	-4.126191	1.575549	1.238807
H	4.877347	-0.139225	0.150728
H	1.775552	-1.516709	-0.864190
H	-5.331479	-1.003235	2.447357
C	-6.460964	0.438975	1.250302
O	-7.515496	-0.167806	1.204645
C	2.827405	0.339208	1.905162
H	3.345507	1.270984	1.627352
H	2.159779	0.586357	2.744875
H	3.592255	-0.365887	2.260654
C	3.662494	-3.380022	-0.338554
H	3.326362	-3.916332	0.564994
H	2.906538	-3.573207	-1.117139
H	4.616049	-3.824247	-0.656091
C	6.308661	-1.776584	0.153009
C	7.319472	-0.972957	-0.626320
H	7.075400	-0.981054	-1.701876
H	8.348649	-1.336273	-0.509121
H	7.294574	0.082577	-0.307257
C	6.601044	-2.871596	0.882418
C	7.925445	-3.548399	1.050322
H	8.224948	-3.558373	2.112039
H	8.734898	-3.080752	0.473754
H	7.857537	-4.604848	0.739778
H	-6.360611	1.434522	0.755158
H	-0.185437	-1.133591	1.864027
O	-2.157071	-0.968233	0.343910
O	0.701984	1.772061	0.520984
H	-2.407918	1.118769	2.926698
C	-2.777916	-0.981583	3.243447
H	-1.785672	-1.154101	3.684441
H	-3.491409	-0.859215	4.072074
H	-3.059821	-1.884142	2.680433
Si	-2.688855	-1.021825	-1.259096
C	-2.667756	-3.837722	-1.193305
H	-2.156379	-3.784058	-0.218060
H	-3.211861	-4.798870	-1.228536
H	-1.893287	-3.872273	-1.976672
C	-3.638172	-2.663258	-1.393737
C	-4.740058	-2.730684	-0.326342
H	-4.322287	-2.700757	0.691682
H	-5.460789	-1.901357	-0.414414
H	-5.311117	-3.671700	-0.423977
C	-4.277250	-2.756010	-2.788567
H	-5.011295	-1.951252	-2.959204
H	-4.812338	-3.715868	-2.903584
H	-3.527920	-2.702822	-3.595575
C	-3.792738	0.442412	-1.646936
H	-4.792251	0.327298	-1.200082
H	-3.915653	0.542485	-2.738058
H	-3.360485	1.385559	-1.277130
H	-0.478707	-1.808943	-2.110048
C	-1.207791	-1.040147	-2.411754
H	-0.687013	-0.070389	-2.430626
H	-1.525779	-1.260757	-3.444252
Si	0.869082	2.736798	-0.860310
C	-0.821181	2.980541	-1.631195
H	-1.546531	3.363136	-0.895796
H	-1.211301	2.033330	-2.033580
H	-0.773918	3.697943	-2.467218
C	2.018428	1.907527	-2.085407
H	1.633194	0.915878	-2.374127
H	2.096169	2.510680	-3.005074
H	3.032698	1.771729	-1.677845
C	1.570825	4.379696	-0.216300
C	0.532934	5.065071	0.686083
H	-0.381187	5.334044	0.132261
H	0.236641	4.422841	1.531813
H	0.945648	5.998616	1.109466
C	2.850522	4.116573	0.591010
H	2.646690	3.505428	1.483984
H	3.293086	5.069208	0.933961
H	3.618105	3.595469	-0.004938
C	1.896043	5.292091	-1.409369
H	2.269310	6.270087	-1.055722
H	2.675961	4.860249	-2.057799
H	1.010570	5.489362	-2.036357
H	5.778904	-3.330547	1.443925

lineal_scis-strans_S1_MeOH_wB97XD
SCF Energy: -1980.10905207
Num. Imaginary Frequencies: 0

C	0.643130	0.244750	0.556061
C	-0.388090	-0.074191	1.637547
C	-1.813874	0.197972	1.160817
C	-2.800550	0.413809	2.333552

C	-4.113799	0.865877	1.776136
C	1.989765	-0.411642	0.799195
C	-5.300986	0.250544	1.892980
C	4.811720	-1.565951	0.188349
C	3.626158	-2.195827	0.010974
C	2.377516	-1.404775	-0.024361
H	0.253224	-0.141948	-0.400228
H	-0.163387	0.535321	2.526641
H	-1.802125	1.131515	0.567006
H	-4.073817	1.788049	1.180828
H	4.764170	-0.472106	0.222962
H	1.664412	-1.706950	-0.803964
H	-5.435115	-0.681898	2.448888
C	-6.471748	0.792152	1.208097
O	-7.558736	0.244989	1.169733
C	2.776716	0.104909	1.970555
H	3.358002	1.000757	1.699354
H	2.108729	0.398467	2.794887
H	3.488880	-0.643747	2.346054
C	3.418579	-3.675091	-0.208864
H	3.128825	-4.180223	0.728394
H	2.587947	-3.830717	-0.915529
H	4.298967	-4.185765	-0.614199
C	6.187110	-2.084379	0.323630
C	6.434795	-3.534256	0.664197
H	6.418205	-4.177760	-0.230137
H	5.668713	-3.914142	1.355166
H	7.411930	-3.674175	1.145846
C	7.192843	-1.192740	0.177940
C	8.665972	-1.434597	0.258088
H	9.151598	-1.150119	-0.690952
H	8.930482	-2.479864	0.466633
H	9.123170	-0.801681	1.037839
H	-6.311830	1.768125	0.690135
H	-0.311743	-1.133781	1.926062
O	-2.248237	-0.884350	0.364737
O	0.785579	1.655085	0.493434
H	-2.396686	1.274836	2.896580
C	-2.893023	-0.791119	3.261760
H	-1.916994	-1.009773	3.718118
H	-3.605861	-0.606266	4.079273
H	-3.221746	-1.690099	2.718711
Si	-2.776739	-0.937563	-1.239442
C	-2.911878	-3.747443	-1.116158
H	-2.402902	-3.701828	-0.139261
H	-3.507502	-4.678023	-1.135135
H	-2.136786	-3.840153	-1.894205
C	-3.815470	-2.525948	-1.345809
C	-4.923016	-2.509477	-0.282269
H	-4.507539	-2.475674	0.736603
H	-5.599298	-1.646242	-0.394188
H	-5.542096	-3.421584	-0.359238
C	-4.453158	-2.612826	-2.741588
H	-5.139208	-1.771430	-2.933935
H	-5.041850	-3.542857	-2.838472
H	-3.698547	-2.620533	-3.545402
C	-3.794396	0.578846	-1.661902
H	-4.803067	0.528140	-1.223945
H	-3.901029	0.666356	-2.755844
H	-3.313306	1.502721	-1.303904
H	-0.611849	-1.862312	-2.071967
C	-1.295532	-1.057420	-2.385440
H	-0.721461	-0.118522	-2.414118
H	-1.622872	-1.272356	-3.416232
Si	1.010544	2.563155	-0.917828
C	-0.665897	2.936942	-1.666954
H	-1.345695	3.385875	-0.925478
H	-1.139739	2.021918	-2.053656
H	-0.571909	3.640089	-2.511161
C	2.059390	1.604898	-2.139070
H	1.590080	0.638353	-2.385403
H	2.160599	2.170522	-3.080049
H	3.069925	1.402447	-1.750480
C	1.866457	4.154441	-0.332908
C	0.905105	4.960102	0.554784
H	0.014013	5.295031	-0.000645
H	0.559463	4.374023	1.422351
H	1.406059	5.864130	0.945770
C	3.124805	3.799931	0.473011
H	2.873655	3.244747	1.390095
H	3.660770	4.717568	0.775787
H	3.831758	3.185175	-0.108668
C	2.261401	4.995224	-1.557082
H	2.722508	5.947230	-1.237791
H	2.994926	4.475156	-2.194805
H	1.391854	5.249920	-2.185717
H	6.910690	-0.154316	-0.038317

lineal_strans-scis_S1_MeOH_wB97XD
SCF Energy: -1980.11007459
Num. Imaginary Frequencies: 0

C	0.577663	0.499774	0.736894
C	-0.518222	0.200715	1.757779
C	-1.918077	0.264980	1.150163
C	-3.014141	0.496043	2.219642
C	-4.312565	0.763107	1.525083
C	1.962123	0.154851	1.259334
C	-5.441789	0.042187	1.607898
C	4.634968	-1.919614	-0.227927
C	4.028884	-1.308970	0.820165
C	2.684777	-0.751541	0.571754
H	0.388030	-0.114116	-0.159431

H	-0.435879	0.928689	2.580297
H	-1.947928	1.128001	0.458908
H	-4.309478	1.631491	0.852505
H	4.052859	-1.991440	-1.156895
H	2.219220	-1.130620	-0.346499
H	-5.533351	-0.848642	2.235969
C	-6.596385	0.402483	0.789209
O	-7.619922	-0.252995	0.718633
C	2.378280	0.898496	2.501452
H	1.850337	1.861877	2.554635
H	2.118319	0.338429	3.415244
H	3.454340	1.107718	2.531278
C	4.628889	-1.248339	2.201438
H	5.134353	-0.289823	2.398399
H	3.849900	-1.368817	2.967974
H	5.377350	-2.041436	2.340113
C	5.963009	-2.561751	-0.294301
C	5.978706	-3.857792	-1.066764
H	5.347790	-4.613997	-0.570360
H	6.984819	-4.280181	-1.185666
H	5.554408	-3.706762	-2.073539
C	7.053033	-1.993967	0.260320
C	8.457729	-2.509684	0.280500
H	9.137128	-1.806401	-0.230426
H	8.572070	-3.495262	-0.190482
H	8.820943	-2.588219	1.319183
H	-6.485955	1.342519	0.197239
H	-0.361983	-0.803486	2.181669
O	-2.179251	-0.933823	0.451332
O	0.500375	1.877756	0.411074
H	-2.736778	1.442156	2.718884
C	-3.074958	-0.617569	3.258192
H	-2.124533	-0.695569	3.805350
H	-3.867057	-0.425321	3.997270
H	-3.275657	-1.592232	2.788285
Si	-2.574973	-1.191877	-1.170957
C	-2.440805	-3.976317	-0.777384
H	-2.022420	-3.789488	0.225338
H	-2.937094	-4.963252	-0.749572
H	-1.597915	-4.054446	-1.483277
C	-3.438894	-2.883906	-1.191268
C	-4.625534	-2.885905	-0.216490
H	-4.298974	-2.718631	0.821519
H	-5.369454	-2.109617	-0.459720
H	-5.146767	-3.859769	-0.248629
C	-3.948777	-3.164844	-2.613780
H	-4.695238	-2.421120	-2.938271
H	-4.434283	-4.156316	-2.659942
H	-3.133418	-3.167271	-3.355985
C	-3.699420	0.163422	-1.813981
H	-4.732963	0.042738	-1.455375
H	-3.715706	0.144766	-2.916305
H	-3.346835	1.161162	-1.507344
H	-0.258421	-1.926832	-1.764678
C	-1.004587	-1.239848	-2.194149
H	-0.549194	-0.240294	-2.260810
H	-1.221034	-1.570210	-3.223530
Si	0.852609	2.609702	-1.072973
C	-0.759644	2.844449	-1.999179
H	-1.483929	3.427846	-1.408267
H	-1.219824	1.871704	-2.233010
H	-0.597822	3.369404	-2.954943
C	2.023007	1.549583	-2.081817
H	1.585903	0.561361	-2.297049
H	2.225163	2.037032	-3.050216
H	2.985446	1.390328	-1.572017
C	1.637014	4.278913	-0.616890
C	0.708044	5.038510	0.342460
H	-0.273961	5.248143	-0.112895
H	0.531559	4.474309	1.272253
H	1.152819	6.010453	0.622878
C	2.989629	4.033844	0.069173
H	2.887144	3.402256	0.966293
H	3.440525	4.990742	0.388571
H	3.710075	3.542157	-0.604582
C	1.851603	5.112122	-1.889667
H	2.335008	6.074890	-1.643819
H	2.501816	4.598155	-2.617130
H	0.900694	5.344782	-2.396302
H	6.917947	-1.021178	0.746462

lineal_strans-strans_S1_MeOH_wB97XD
SCF Energy: -1980.10785519
Num. Imaginary Frequencies: 0

C	0.605987	0.888758	0.701047
C	-0.400450	0.397711	1.741129
C	-1.790639	0.199616	1.138238
C	-2.911753	0.240011	2.204845
C	-4.235417	0.227343	1.506142
C	2.050827	0.683894	1.121062
C	-5.203804	-0.695328	1.618118
C	4.457437	-1.935877	0.159541
C	4.161837	-0.702029	0.641110
C	2.761682	-0.261312	0.474061
H	0.440793	0.305791	-0.219793
H	-0.444061	1.130590	2.562073
H	-1.979088	1.031819	0.433888
H	-4.398489	1.055657	0.803447
H	3.629722	-2.454661	-0.340100
H	2.213648	-0.824569	-0.292097
H	-5.123777	-1.563951	2.278073
C	-6.404195	-0.597587	0.791893

O	-7.280640	-1.441992	0.755098
C	2.529210	1.558221	2.251828
H	3.081800	2.436416	1.881297
H	1.678547	1.943276	2.832470
H	3.189138	1.019781	2.944492
C	5.163705	0.254367	1.243370
H	4.898603	1.289927	0.989045
H	5.203396	0.190428	2.342351
H	6.175246	0.076553	0.861849
C	5.698484	-2.732433	0.184955
C	6.819768	-2.391436	1.137571
H	7.486360	-1.613345	0.732392
H	7.442398	-3.269131	1.356982
H	6.426331	-2.019516	2.094183
C	5.753295	-3.801149	-0.642093
C	6.872893	-4.773748	-0.828971
H	6.531004	-5.803893	-0.630241
H	7.743523	-4.572469	-0.190706
H	7.217111	-4.762289	-1.877248
H	-6.476597	0.320654	0.161113
H	-0.062838	-0.561462	2.162512
O	-1.825140	-1.037048	0.457384
O	0.349772	2.263458	0.463231
H	-2.825525	1.235282	2.677505
C	-2.754926	-0.835793	3.272712
H	-1.809243	-0.710445	3.819194
H	-3.571214	-0.783616	4.008629
H	-2.758647	-1.843027	2.829304
Si	-2.144590	-1.403792	-1.161417
C	-1.484355	-4.099359	-0.687478
H	-1.118476	-3.806609	0.310452
H	-1.783405	-5.161675	-0.631420
H	-0.635735	-4.035649	-1.387874
C	-2.668999	-3.230254	-1.137360
C	-3.842064	-3.432229	-0.167079
H	-3.564443	-3.172098	0.865998
H	-4.719914	-2.823319	-0.438558
H	-4.164222	-4.489265	-0.169454
C	-3.103176	-3.643858	-2.552541
H	-3.975494	-3.066307	-2.900565
H	-3.389584	-4.710870	-2.570891
H	-2.296312	-3.510988	-3.292144
C	-3.503735	-0.306349	-1.840894
H	-4.494407	-0.602756	-1.463468
H	-3.523760	-0.369966	-2.941448
H	-3.340399	0.750306	-1.576124
H	0.269177	-1.720939	-1.722886
C	-0.582053	-1.190138	-2.178022
H	-0.304167	-0.129907	-2.281110
H	-0.727614	-1.590592	-3.195010
Si	0.459099	3.049167	-1.032019
C	-1.173735	2.858734	-1.931084
H	-2.018633	3.186768	-1.304995
H	-1.346843	1.809127	-2.213808
H	-1.186097	3.454836	-2.858602
C	1.842447	2.304514	-2.052842
H	1.680283	1.225132	-2.207038
H	1.877621	2.777261	-3.048326
H	2.826967	2.434880	-1.576678
C	0.793427	4.866175	-0.592298
C	-0.413273	5.443280	0.163909
H	-1.323343	5.452996	-0.457773
H	-0.637084	4.868671	1.077770
H	-0.214800	6.486363	0.470001
C	2.042092	4.959711	0.297123
H	1.899001	4.431624	1.252560
H	2.271135	6.015029	0.531339
H	2.933259	4.532549	-0.191944
C	1.022199	5.667622	-1.883205
H	1.186812	6.735077	-1.650014
H	1.908154	5.314465	-2.436116
H	0.157768	5.613367	-2.565681
H	4.875036	-3.988385	-1.273136

pp_Reendo_S1_MeOH_wB97XD
SCF Energy: -1980.10731464
Num. Imaginary Frequencies: 0

C	0.063674	0.654785	-1.449346
C	-1.070965	-0.381474	-1.428041
C	-1.463924	-1.037034	-0.097676
C	-0.500755	-2.115023	0.444083
C	0.729364	-1.517078	1.067795
C	1.478493	0.094622	-1.506316
C	1.858544	-2.189932	1.346777
C	4.288859	-1.050669	-0.754124
C	3.856367	0.220126	-0.586420
C	2.430053	0.577238	-0.687777
C	4.747716	1.380594	-0.220651
C	5.659056	-1.591943	-0.629133
C	6.035363	-2.555391	-1.727207
C	6.447609	-1.280623	0.417973
C	7.836202	-1.758597	0.706797
C	1.702658	-0.919408	-2.591908
C	2.937753	-1.532397	2.075955
O	3.948066	-2.088256	2.471482
O	-2.736153	-1.624213	-0.307843
O	-0.120479	1.554945	-0.385730
H	-0.058330	1.180553	-2.419874
H	-1.971902	0.154482	-1.762854
H	-0.888101	-1.169903	-2.174307
H	-1.536757	-0.246547	0.673549
H	0.659479	-0.473349	1.399418

H	2.000262	-3.239465	1.066516
H	3.540232	-1.802253	-1.025594
H	2.117611	1.364235	0.006660
H	4.646014	1.631082	0.849444
H	5.808764	1.175227	-0.415611
H	4.455121	2.279668	-0.786120
H	6.045225	-2.045339	-2.705164
H	7.016992	-3.023831	-1.578353
H	5.284493	-3.360123	-1.800865
H	8.251025	-2.406252	-0.077378
H	8.519104	-0.901499	0.832715
H	2.744011	-0.919169	-2.943368
H	1.470944	-1.941299	-2.246024
H	1.048096	-0.717841	-3.455017
H	2.770098	-0.448340	2.285365
C	-1.181992	-2.988603	1.512288
H	-1.488634	-2.381723	2.378937
H	-2.073032	-3.483423	1.105063
H	-0.487060	-3.762417	1.869180
H	-0.199388	-2.773060	-0.389870
H	7.862445	-2.316421	1.658332
Si	-0.294626	3.229931	-0.569782
Si	-4.171115	-0.959468	0.296107
C	-0.505393	3.853192	1.208693
C	1.235642	3.930176	-1.393782
H	2.125278	3.853124	-0.749591
H	1.448999	3.391408	-2.332111
H	1.088857	4.992535	-1.649396
C	-1.791769	3.572279	-1.641691
H	-1.656364	3.137701	-2.646105
H	-2.712612	3.149777	-1.211319
H	-1.939776	4.657057	-1.771191
C	-5.533430	-2.044356	-0.455125
C	-4.163240	-1.028202	2.169074
H	-3.286398	-0.495648	2.572732
H	-5.061179	-0.534279	2.575769
H	-4.140095	-2.061654	2.548395
C	-4.292155	0.832515	-0.239408
H	-3.430324	1.396452	0.152739
H	-4.304071	0.941706	-1.334906
H	-5.204398	1.303219	0.162635
C	0.697143	3.407123	2.055433
H	0.601110	3.784962	3.089280
H	0.772130	2.309327	2.111460
H	1.651095	3.788464	1.655651
C	-1.794429	3.274796	1.812229
H	-2.690592	3.591425	1.254312
H	-1.779771	2.172693	1.827086
H	-1.919322	3.616989	2.855411
C	-0.584720	5.387685	1.195740
H	-1.433076	5.753199	0.593519
H	-0.720691	5.775812	2.221188
H	0.334174	5.844668	0.792751
C	-5.255083	-3.519140	-0.125999
H	-5.213269	-3.701060	0.960596
H	-6.054431	-4.163073	-0.535267
H	-4.301419	-3.859289	-0.559914
C	-6.891552	-1.632636	0.133820
H	-7.704434	-2.230236	-0.316668
H	-6.934067	-1.792771	1.223665
H	-7.122443	-0.571445	-0.058351
C	-5.555717	-1.857873	-1.979963
H	-4.581535	-2.099087	-2.435862
H	-6.310146	-2.521593	-2.439569
H	-5.812457	-0.824568	-2.264791
H	6.027183	-0.613603	1.178723

pp_Reexo_S1_MeOH_wB97XD
SCF Energy: -1980.10361472
Num. Imaginary Frequencies: 0

C	0.290274	0.725504	-1.412386
C	-0.741818	-0.392331	-1.234880
C	-1.246255	-0.736034	0.175041
C	-0.188131	-1.204287	1.201358
C	0.610846	-0.061484	1.748141
C	1.769751	0.374051	-1.259729
C	1.923691	-0.094998	2.026557
C	4.470674	-0.934274	-0.338784
C	3.616273	-1.382635	-1.285176
C	2.222299	-0.889312	-1.353805
C	3.947508	-2.436610	-2.311588
C	5.872387	-1.321424	-0.069535
C	6.752449	-0.150919	0.294312
C	6.278096	-2.606425	-0.085401
C	7.648274	-3.148214	0.180542
C	2.659001	1.579382	-1.136313
C	2.589702	1.080307	2.570493
O	3.794872	1.182538	2.729871
O	-2.209677	-1.759367	0.004889
O	-0.034724	1.803526	-0.551392
H	0.199368	1.064358	-2.465119
H	-1.639993	-0.087453	-1.794307
H	-0.396247	-1.319944	-1.714095
H	-1.726321	0.164847	0.599039
H	0.048319	0.847305	1.999065
H	2.537595	-0.971904	1.798706
H	4.102196	-0.148191	0.328028
H	1.492764	-1.685426	-1.538767
H	5.030331	-2.559432	-2.451046
H	3.534867	-3.417895	-2.020296
H	3.496343	-2.178426	-3.282824
H	6.804271	0.571706	-0.537287

H	6.317442	0.388017	1.153043
H	7.777679	-0.439674	0.559575
H	7.988765	-3.763545	-0.669339
H	8.403090	-2.369502	0.354341
H	2.639871	1.996421	-0.116443
H	3.702767	1.348310	-1.385697
H	2.308828	2.378061	-1.807905
H	1.915920	1.930654	2.832991
C	-0.844237	-1.896715	2.407512
H	-1.511806	-1.206104	2.946299
H	-1.434034	-2.764944	2.085795
H	-0.072534	-2.241764	3.111384
H	0.490362	-1.924205	0.715438
H	7.639428	-3.815236	1.059465
Si	-3.877355	-1.551941	0.203914
Si	-0.829571	3.228074	-1.001819
C	-4.604488	-3.238003	-0.272174
C	-4.270471	-1.085762	1.976232
H	-3.717145	-0.177985	2.269040
H	-5.345000	-0.860106	2.078492
H	-4.019895	-1.886285	2.689257
C	-4.479178	-0.171246	-0.909770
H	-5.580490	-0.117890	-0.897562
H	-4.102554	0.796551	-0.540763
H	-4.153991	-0.296530	-1.954061
C	-1.471922	3.944886	0.634761
C	-2.210779	2.837202	-2.205354
H	-2.700182	3.767906	-2.536820
H	-1.814014	2.338971	-3.105412
H	-2.980706	2.185223	-1.767556
C	0.380781	4.391519	-1.835125
H	1.245234	4.621569	-1.192851
H	0.758267	3.951975	-2.773132
H	-0.113966	5.341952	-2.095338
C	-0.287130	4.207936	1.576930
H	0.284423	3.287304	1.778714
H	0.413101	4.951544	1.162709
H	-0.643077	4.597534	2.547726
C	-2.440739	2.956634	1.301747
H	-2.860730	3.393391	2.225643
H	-3.289152	2.697701	0.646898
H	-1.935693	2.019863	1.584032
C	-2.207733	5.263709	0.349701
H	-2.579740	5.707576	1.290550
H	-1.551736	6.011007	-0.126100
H	-3.080138	5.115494	-0.308111
C	-3.902956	-4.346052	0.528207
H	-4.336780	-5.332412	0.283284
H	-2.826155	-4.391850	0.301311
H	-4.011137	-4.202771	1.616090
C	-6.107862	-3.248966	0.045140
H	-6.302270	-3.125670	1.123170
H	-6.650788	-2.449853	-0.486756
H	-6.559364	-4.209724	-0.261275
C	-4.394004	-3.479969	-1.774699
H	-4.928638	-2.737534	-2.389560
H	-3.327610	-3.438572	-2.050890
H	-4.771832	-4.477586	-2.062858
H	5.519868	-3.369077	-0.295935

pp_Siendo_S1_MeOH_wB97XD
SCF Energy: -1980.10877030
Num. Imaginary Frequencies: 0

C	-0.730283	0.763875	0.700280
C	-1.210799	-0.093883	1.871431
C	-1.008819	-1.611179	1.770743
C	0.344188	-2.210408	2.227408
C	1.441474	-2.123918	1.214297
C	0.764340	0.996941	0.596214
C	2.760848	-2.042483	1.462422
C	3.813192	0.894060	-0.114648
C	2.777314	0.877319	-0.985339
C	1.381226	0.672722	-0.557798
C	2.927648	1.040540	-2.478043
C	5.255998	1.064200	-0.390871
C	5.948305	2.005153	0.563356
C	5.875350	0.370017	-1.364725
C	7.322621	0.393726	-1.744484
C	1.403178	1.679403	1.771676
C	3.713090	-2.166067	0.363530
O	4.922948	-2.227616	0.502520
O	-1.290599	-2.042320	0.458316
O	-1.358818	2.037042	0.826394
H	-1.062184	0.266664	-0.226142
H	-0.803870	0.284841	2.822011
H	-2.299240	0.072963	1.916059
H	-1.740995	-2.042752	2.479397
H	1.121809	-2.241839	0.172806
H	3.174042	-1.938841	2.470456
H	3.582711	0.777920	0.948248
H	0.744227	0.232373	-1.335952
H	3.888638	1.492069	-2.757663
H	2.854488	0.064963	-2.988796
H	2.115948	1.669381	-2.877346
H	5.797057	1.669443	1.603332
H	7.029302	2.084438	0.389609
H	5.516002	3.017332	0.493741
H	7.914249	1.126350	-1.179189
H	7.775972	-0.600451	-1.591121
H	1.910226	0.956997	2.433145
H	2.160683	2.412666	1.455357
H	0.646701	2.204753	2.372306

H	3.256303	-2.239947	-0.652433
C	0.733437	-1.782826	3.637048
H	1.527523	-2.426632	4.042437
H	1.095321	-0.744076	3.664095
H	-0.130895	-1.858914	4.314451
H	0.130123	-3.297866	2.256031
H	7.435469	0.622866	-2.817485
Si	-2.572848	-3.059334	0.029822
Si	-2.292402	2.701198	-0.420456
C	-2.446561	-3.173926	-1.859395
C	-4.179617	-2.283375	0.599727
H	-4.212897	-2.224440	1.700317
H	-4.304091	-1.264298	0.201501
H	-5.045070	-2.885301	0.276884
C	-2.335838	-4.718131	0.866924
H	-1.400016	-5.205755	0.550439
H	-2.301263	-4.593819	1.962181
H	-3.171796	-5.400247	0.640777
C	-1.277634	2.777204	-1.994631
H	-1.833691	3.299644	-2.790768
H	-0.323263	3.304899	-1.840576
H	-1.050867	1.763337	-2.362555
C	-2.761349	4.425684	0.214813
C	-3.788035	1.605446	-0.689360
H	-4.422253	1.551371	0.209649
H	-4.406654	1.968086	-1.526555
H	-3.462539	0.583336	-0.941070
C	-1.493146	5.282248	0.351484
H	-1.742229	6.279810	0.756225
H	-0.759264	4.822772	1.033629
H	-0.995307	5.438360	-0.619484
C	-3.445282	4.300894	1.584832
H	-4.368945	3.701288	1.531913
H	-2.783930	3.830343	2.329664
H	-3.724019	5.298588	1.969385
C	-3.725563	5.089117	-0.780784
H	-3.280709	5.191291	-1.784575
H	-4.664485	4.521070	-0.886623
H	-3.994619	6.104617	-0.438400
C	-1.028032	-3.609658	-2.257687
H	-0.271759	-2.872813	-1.943005
H	-0.752884	-4.582001	-1.816882
H	-0.951912	-3.714034	-3.354987
C	-2.749192	-1.801879	-2.481181
H	-2.643169	-1.844302	-3.580170
H	-3.776889	-1.468429	-2.264194
H	-2.058496	-1.024669	-2.114331
C	-3.463749	-4.205984	-2.370913
H	-3.430598	-4.265807	-3.473603
H	-3.256331	-5.216582	-1.982474
H	-4.497608	-3.944393	-2.090012
H	5.263343	-0.328566	-1.946580

pp_Siexo_S1_MeOH_wB97XD
SCF Energy: -1980.10721462
Num. Imaginary Frequencies: 0

C	-0.567060	0.597029	0.591791
C	-1.212907	-0.084648	1.800509
C	-1.757669	-1.513553	1.616694
C	-0.833827	-2.694579	2.013193
C	0.214473	-3.023220	0.999920
C	0.778404	0.024726	0.152999
C	1.488097	-3.376039	1.245778
C	3.818249	-0.016747	-0.436890
C	3.232647	-0.270000	0.758917
C	1.832240	0.140118	0.982236
C	3.910269	-0.901229	1.956111
C	5.164031	-0.331802	-0.952197
C	6.023189	-1.358575	-0.258319
C	5.546378	0.302213	-2.084003
C	6.835920	0.185674	-2.831777
C	0.799009	-0.592506	-1.214792
C	2.382724	-3.698418	0.141971
O	3.563864	-3.974808	0.273178
O	-2.217452	-1.720882	0.299003
O	-0.456830	1.972596	0.927367
H	-1.264219	0.493701	-0.255945
H	-0.520447	-0.048105	2.655296
H	-2.063523	0.559304	2.070999
H	-2.603244	-1.597821	2.325110
H	-0.126734	-3.018626	-0.041310
H	1.911144	-3.405583	2.253993
H	3.210490	0.547590	-1.151462
H	1.634966	0.570704	1.973433
H	4.070394	-1.980305	1.811323
H	4.888100	-0.446775	2.169549
H	3.286783	-0.783146	2.854351
H	6.432342	-0.980811	0.690796
H	5.435545	-2.258514	-0.026525
H	6.872303	-1.668355	-0.880944
H	7.555323	-0.503386	-2.369575
H	6.655759	-0.152640	-3.866655
H	0.830507	0.188158	-1.995688
H	1.664066	-1.250662	-1.371577
H	-0.123089	-1.168723	-1.385939
H	1.918629	-3.683829	-0.872409
C	-0.318807	-2.579261	3.442460
H	0.090419	-3.538268	3.792717
H	0.476300	-1.823109	3.532135
H	-1.134399	-2.296787	4.125497
H	-1.517508	-3.565189	1.966645
H	7.321755	1.172937	-2.912750

Si	-3.806795	-1.434142	-0.215506
Si	-0.272940	3.215784	-0.208242
C	-3.737318	-1.610634	-2.103507
C	-4.336641	0.285160	0.310218
H	-3.604274	1.050173	0.006797
H	-5.307718	0.544523	-0.143488
H	-4.458922	0.342449	1.404216
C	-4.921426	-2.715732	0.573399
H	-5.981145	-2.516862	0.344831
H	-4.679297	-3.732682	0.225112
H	-4.811757	-2.699189	1.670580
C	-1.450311	2.915241	-1.636109
H	-1.136570	2.042536	-2.230925
H	-2.480602	2.739910	-1.287852
H	-1.463870	3.785459	-2.313047
C	1.488364	3.267430	-0.847862
H	1.706549	2.369241	-1.447544
H	1.643380	4.145375	-1.496763
H	2.222094	3.313512	-0.027493
C	-0.714313	4.782356	0.769620
C	-0.530548	6.019653	-0.122252
H	-1.167700	5.981743	-1.021417
H	-0.801834	6.936880	0.430973
H	0.513265	6.137562	-0.456309
C	-2.176958	4.696648	1.231989
H	-2.356869	3.806208	1.855895
H	-2.445790	5.583653	1.833641
H	-2.875852	4.655230	0.380365
C	0.205363	4.893802	1.995528
H	1.266590	4.975825	1.708095
H	-0.044790	5.793609	2.586228
H	0.105898	4.021540	2.661283
C	-3.022515	-0.395064	-2.713463
H	-3.560516	0.545035	-2.511074
H	-1.997303	-0.285344	-2.325707
H	-2.949194	-0.501430	-3.810896
C	-2.979171	-2.891629	-2.482483
H	-2.976961	-3.026653	-3.579113
H	-1.929050	-2.857596	-2.151324
H	-3.439439	-3.792153	-2.043077
C	-5.172988	-1.684826	-2.647866
H	-5.770561	-0.801051	-2.367690
H	-5.163026	-1.734405	-3.751494
H	-5.706028	-2.578711	-2.284996
H	4.827890	1.006092	-2.523658

TSReendo_S1_MeOH_wB97XD
SCF Energy: -1980.07495138
Num. Imaginary Frequencies: 1

C	0.085472	0.810227	-1.435838
C	-1.122878	-0.114052	-1.508183
C	-1.345781	-0.913429	-0.236071
C	-0.170795	-1.843284	0.094421
C	1.107567	-1.072061	0.434491
C	1.431273	0.081643	-1.242929
C	2.256799	-1.833302	0.712936
C	4.276777	-0.666939	-0.645761
C	3.794146	0.627275	-0.452034
C	2.448893	0.916692	-0.743141
C	4.592359	1.738291	0.196643
C	5.540484	-1.288813	-0.257241
C	6.519250	-0.596502	0.654498
C	5.723002	-2.558889	-0.696508
C	6.871722	-3.477106	-0.452354
C	1.719284	-0.929933	-2.347224
C	3.169257	-1.492579	1.755799
O	4.039538	-2.235164	2.227582
O	-2.530775	-1.672282	-0.387697
O	-0.122373	1.745424	-0.404184
H	0.166900	1.326411	-2.414081
H	-2.010810	0.507257	-1.698164
H	-1.040091	-0.813011	-2.353818
H	-1.452148	-0.207969	0.610711
H	0.927240	-0.238482	1.123496
H	2.376191	-2.824245	0.260383
H	3.680112	-1.311991	-1.280567
H	2.100519	1.880067	-0.363556
H	4.786843	1.544659	1.262010
H	5.563142	1.890041	-0.294788
H	4.039037	2.685792	0.132018
H	6.977534	0.281900	0.177694
H	6.017859	-0.252973	1.570330
H	7.330881	-1.267783	0.960393
H	7.724529	-3.002431	0.049598
H	6.544184	-4.332378	0.163904
H	2.595270	-0.622068	-2.937528
H	1.907753	-1.948782	-1.979752
H	0.873682	-0.998994	-3.044303
H	3.025637	-0.469550	2.184110
C	-0.529606	-2.750662	1.278128
H	-0.682806	-2.155374	2.193443
H	-1.453811	-3.308669	1.074454
H	0.273286	-3.474305	1.477029
H	0.016590	-2.484580	-0.785056
H	7.225387	-3.902471	-1.405809
Si	-0.572815	3.363100	-0.622811
Si	-3.983821	-1.259439	0.376511
C	-0.829293	3.991828	1.147191
C	0.812913	4.260408	-1.509210
H	1.721240	4.332986	-0.890479
H	1.079330	3.732839	-2.440404
H	0.506162	5.282347	-1.786153

C	-2.134038	3.448136	-1.653113
H	-1.956842	3.035771	-2.660296
H	-2.962607	2.886099	-1.195254
H	-2.458826	4.494243	-1.778968
C	-5.229821	-2.527090	-0.285264
C	-3.774071	-1.375808	2.235397
H	-2.953044	-0.722545	2.573718
H	-4.690838	-1.041000	2.748333
H	-3.552009	-2.402108	2.566924
C	-4.437734	0.502549	-0.073185
H	-3.669987	1.197656	0.304350
H	-4.524966	0.643559	-1.161726
H	-5.396987	0.790824	0.387681
C	-1.124088	5.499284	1.109591
H	-2.027969	5.730426	0.521726
H	-1.291437	5.885363	2.131156
H	-0.287242	6.072096	0.676956
C	-2.011206	3.249843	1.790154
H	-2.955964	3.436118	1.254018
H	-1.845955	2.160145	1.813093
H	-2.155173	3.583555	2.833567
C	0.442424	3.736355	1.971300
H	0.314920	4.112462	3.002334
H	0.676750	2.661970	2.037596
H	1.322445	4.245179	1.544632
C	-4.689106	-3.946236	-0.051907
H	-4.509247	-4.150473	1.016502
H	-5.413426	-4.699062	-0.412046
H	-3.742034	-4.113908	-0.588890
C	-5.440867	-2.301993	-1.790317
H	-4.494539	-2.372207	-2.351242
H	-6.127717	-3.062985	-2.202767
H	-5.882817	-1.314388	-2.000705
C	-6.566640	-2.358187	0.453103
H	-7.317144	-3.066907	0.058989
H	-6.468498	-2.553967	1.533506
H	-6.981946	-1.343636	0.332808
H	4.921051	-2.989606	-1.308756

TSReexo_S1_MeOH_wB97XD
SCF Energy: -1980.07177805
Num. Imaginary Frequencies: 1

C	-0.004590	1.171749	-1.342969
C	-0.798171	-0.128200	-1.409098
C	-0.887351	-0.852224	-0.071649
C	0.472875	-1.269280	0.508006
C	1.378992	-0.074177	0.783299
C	1.484041	0.985801	-0.988641
C	2.670248	-0.323628	1.270670
C	4.342620	-0.054424	-0.654735
C	3.461683	-0.509479	-1.626467
C	2.165623	0.036760	-1.769327
C	3.746945	-1.742918	-2.457368
C	5.605590	-0.664563	-0.209142
C	6.706264	0.331252	0.060812
C	5.706264	-1.991788	0.009702
C	6.889052	-2.760458	0.502284
C	2.097429	2.302786	-0.553660
C	3.346663	0.624626	2.109779
O	4.407570	0.428891	2.702491
O	-1.698592	-2.000217	-0.239554
O	-0.612935	2.016584	-0.391172
H	-0.030021	1.647901	-2.343542
H	-1.819075	0.116102	-1.739566
H	-0.383239	-0.815282	-2.161233
H	-1.351411	-0.164129	0.661108
H	0.865776	0.787413	1.229724
H	3.098933	-1.327125	1.218112
H	4.232514	0.972161	-0.321149
H	1.536368	-0.537187	-2.456520
H	4.824316	-1.906339	-2.598892
H	3.333233	-2.654134	-1.994815
H	3.280395	-1.645183	-3.449052
H	6.900970	0.950724	-0.829777
H	6.399618	1.016426	0.868192
H	7.651000	-0.140479	0.359892
H	7.116658	-3.592154	-0.185281
H	7.795871	-2.151364	0.612804
H	1.593430	2.712127	0.330429
H	3.169591	2.271385	-0.350925
H	1.951484	3.025781	-1.373955
H	2.831118	1.610113	2.218878
C	0.270850	-2.064737	1.802730
H	-0.197885	-1.436392	2.578053
H	-0.377720	-2.934430	1.628474
H	1.229902	-2.428024	2.198691
H	0.971517	-1.925537	-0.227194
H	6.666368	-3.220938	1.479933
Si	-3.297371	-2.087635	0.310184
Si	-1.608300	3.341926	-0.722445
C	-3.871712	-3.815487	-0.222116
C	-3.342306	-1.868506	2.171208
H	-2.870416	-0.915377	2.461144
H	-4.384936	-1.838756	2.528611
H	-2.822178	-2.681774	2.700808
C	-4.302158	-0.719572	-0.483281
H	-5.361953	-0.788096	-0.186766
H	-3.930357	0.261616	-0.146675
H	-4.251183	-0.749551	-1.582842
C	-2.327801	3.780887	0.976788
C	-2.928332	2.848721	-1.957175
H	-3.601372	3.697685	-2.162316

H	-2.471854	2.553256	-2.916513
H	-3.540727	2.007292	-1.598150
C	-0.577650	4.730311	-1.442944
H	0.192754	5.082737	-0.739366
H	-0.072108	4.396199	-2.364133
H	-1.214260	5.589371	-1.711935
C	-1.183388	3.983067	1.982012
H	-0.594277	3.062286	2.119463
H	-0.490519	4.780850	1.667413
H	-1.585369	4.269360	2.970597
C	-3.232984	2.637121	1.459991
H	-3.623226	2.853097	2.470860
H	-4.102106	2.492609	0.797950
H	-2.688893	1.679557	1.514563
C	-3.147872	5.075084	0.863198
H	-3.601389	5.331623	1.837476
H	-2.525236	5.931753	0.556997
H	-3.970998	4.981654	0.135224
C	-2.884769	-4.868886	0.304223
H	-3.217846	-5.884240	0.022718
H	-1.875283	-4.723935	-0.111978
H	-2.801070	-4.845678	1.403333
C	-5.269269	-4.086197	0.356241
H	-5.266896	-4.084747	1.458645
H	-6.008577	-3.339394	0.021688
H	-5.635938	-5.076536	0.031155
C	-3.926846	-3.888690	-1.755757
H	-4.665059	-3.185669	-2.175009
H	-2.949664	-3.660344	-2.211911
H	-4.216732	-4.903072	-2.084453
H	4.809371	-2.597042	-0.161136

TSSiendo_S1_MeOH_wB97XD
SCF Energy: -1980.07093030
Num. Imaginary Frequencies: 1

C	-0.607187	0.725667	0.634699
C	-1.348300	0.027158	1.763797
C	-1.120055	-1.476553	1.762920
C	0.340456	-1.865590	2.023083
C	1.282646	-1.415070	0.900719
C	0.923287	0.592345	0.659712
C	2.669716	-1.637154	1.029869
C	3.829859	0.591236	-0.087489
C	2.820821	0.719720	-1.041596
C	1.477318	0.723560	-0.632919
C	3.082229	0.729399	-2.528876
C	5.267942	0.409646	-0.245786
C	6.075283	0.886639	0.938124
C	5.801419	-0.252987	-1.298941
C	7.233824	-0.592455	-1.541706
C	1.559758	1.271948	1.867539
C	3.426977	-2.191779	-0.044106
O	4.569482	-2.659708	0.032666
O	-1.518733	-2.014913	0.515798
O	-0.922288	2.109004	0.664473
H	-0.955158	0.276378	-0.311598
H	-1.060821	0.454156	2.736889
H	-2.423003	0.228386	1.636375
H	-1.719769	-1.919616	2.579968
H	0.880058	-1.725319	-0.068478
H	3.162361	-1.590085	2.006149
H	3.547942	0.808950	0.937265
H	0.753808	0.645819	-1.452442
H	4.011905	1.262307	-2.777367
H	3.168835	-0.290829	-2.937802
H	2.253063	1.221459	-3.057671
H	5.838055	0.274036	1.824610
H	7.158410	0.829093	0.773376
H	5.826261	1.929152	1.191698
H	7.927981	-0.140665	-0.821619
H	7.364171	-1.687413	-1.502753
H	2.316200	0.659935	2.375222
H	2.040252	2.216496	1.568221
H	0.795474	1.523368	2.614966
H	2.885517	-2.228260	-1.022095
C	0.769647	-1.554602	3.453986
H	1.780007	-1.934299	3.662800
H	0.759152	-0.481335	3.683341
H	0.083673	-2.049145	4.159173
H	0.349370	-2.966083	1.922400
H	7.533228	-0.281319	-2.556120
Si	-2.967817	-2.836636	0.230349
Si	-1.933075	2.851269	-0.473605
C	-3.031249	-2.996364	-1.659243
C	-4.403674	-1.840808	0.907550
H	-4.306314	-1.710331	1.998111
H	-4.466917	-0.841353	0.449576
H	-5.358030	-2.361539	0.723928
C	-2.892970	-4.498800	1.090491
H	-2.053700	-5.109545	0.721357
H	-2.758054	-4.361493	2.176435
H	-3.824633	-5.069220	0.943367
C	-1.168217	2.718697	-2.179702
H	-1.763951	3.284422	-2.915227
H	-0.139094	3.110622	-2.198934
H	-1.141656	1.669868	-2.518007
C	-2.040592	4.648762	0.121589
C	-3.594098	1.985098	-0.474700
H	-4.098435	2.050104	0.502180
H	-4.263871	2.415545	-1.237276
H	-3.458644	0.919546	-0.721731
C	-0.642939	5.285293	0.071012

H	-0.677185	6.323279	0.448317
H	0.081453	4.731556	0.690307
H	-0.244775	5.323789	-0.956132
C	-2.565352	4.680830	1.565176
H	-3.576474	4.249044	1.646273
H	-1.907723	4.122934	2.250720
H	-2.623328	5.721550	1.931838
C	-2.997389	5.433034	-0.789511
H	-2.659720	5.438378	-1.839080
H	-4.019406	5.019886	-0.768212
H	-3.063806	6.486442	-0.462784
C	-1.777971	-3.730410	-2.160046
H	-0.854494	-3.189051	-1.898690
H	-1.699510	-4.747551	-1.742457
H	-1.803558	-3.829104	-3.260272
C	-3.085352	-1.594949	-2.287302
H	-3.088550	-1.665090	-3.389987
H	-3.994476	-1.046191	-1.992397
H	-2.214830	-0.983269	-1.998175
C	-4.284880	-3.788728	-2.060978
H	-4.347187	-3.880842	-3.160247
H	-4.277020	-4.810925	-1.647932
H	-5.211846	-3.297106	-1.722088
H	5.117811	-0.636145	-2.059400

TSSiexo_S1_MeOH_wB97XD
SCF Energy: -1980.07517006
Num. Imaginary Frequencies: 1

C	-0.444536	0.781467	0.263657
C	-0.916848	0.128209	1.554216
C	-0.821196	-1.391533	1.491314
C	0.609978	-1.925437	1.335052
C	1.280470	-1.466682	0.044119
C	1.042078	0.585700	-0.061048
C	2.619579	-1.815863	-0.205782
C	4.068827	0.485681	-0.064441
C	3.330464	0.938451	1.023762
C	1.924669	1.006987	0.951403
C	3.945238	1.231575	2.375480
C	5.459134	0.056146	-0.146549
C	6.218968	-0.378626	1.082088
C	5.980208	-0.029279	-1.396776
C	7.349443	-0.460520	-1.799371
C	1.315846	0.838281	-1.534593
C	3.090755	-2.108396	-1.520914
O	4.216769	-2.529629	-1.806565
O	-1.606414	-1.860678	0.407976
O	-0.719838	2.173788	0.285301
H	-1.008922	0.304643	-0.556223
H	-0.360686	0.509346	2.424376
H	-1.971145	0.402641	1.710418
H	-1.208987	-1.795753	2.444799
H	0.620455	-1.569807	-0.826876
H	3.302932	-2.051793	0.613601
H	3.595955	0.574142	-1.037388
H	1.447548	1.275417	1.899195
H	4.119378	0.313315	2.958982
H	4.904145	1.759571	2.289510
H	3.268763	1.866504	2.965735
H	6.610324	0.473402	1.658176
H	5.569611	-0.958050	1.753706
H	7.071027	-1.018718	0.819150
H	8.029630	-0.624058	-0.953450
H	7.290905	-1.395625	-2.382575
H	1.619541	1.884874	-1.695973
H	2.095828	0.200727	-1.964759
H	0.403507	0.656643	-2.120477
H	2.345963	-1.951458	-2.340126
C	1.430093	-1.746933	2.609446
H	2.402809	-2.254466	2.539525
H	1.620108	-0.690017	2.843304
H	0.894039	-2.186157	3.465020
H	0.476433	-3.013652	1.192378
H	7.803240	0.291341	-2.465656
Si	-3.054476	-2.713319	0.601314
Si	-2.039354	2.864488	-0.524757
C	-3.691359	-2.953034	-1.169505
C	-4.232547	-1.701879	1.650623
H	-4.476502	-0.736161	1.180611
H	-5.175033	-2.248392	1.819323
H	-3.791337	-1.496752	2.640145
C	-2.682594	-4.339189	1.454954
H	-3.597730	-4.939413	1.587246
H	-1.957505	-4.940654	0.883969
H	-2.258424	-4.160624	2.457094
C	-3.614037	1.989351	-0.008707
H	-3.531716	0.913420	-0.232711
H	-3.823741	2.101273	1.066555
H	-4.480260	2.375984	-0.570476
C	-1.812355	2.663058	-2.373890
H	-1.841362	1.597764	-2.655769
H	-2.626458	3.167814	-2.920120
H	-0.855687	3.082806	-2.721939
C	-1.997328	4.682975	0.011236
C	-3.179732	5.430662	-0.623810
H	-4.150034	5.013091	-0.307757
H	-3.168697	6.494343	-0.324981
H	-3.145200	5.401471	-1.725430
C	-2.098783	4.766947	1.541918
H	-1.273299	4.229282	2.035200
H	-2.057301	5.819735	1.874731
H	-3.045030	4.342802	1.916103

C	-0.676861	5.319186	-0.449929
H	-0.578855	5.314462	-1.547869
H	-0.619330	6.372216	-0.120134
H	0.197638	4.793302	-0.033455
C	-3.879403	-1.583241	-1.839766
H	-4.613213	-0.958860	-1.304589
H	-2.933678	-1.019865	-1.892137
H	-4.247794	-1.707515	-2.874078
C	-2.678421	-3.780379	-1.975605
H	-3.027902	-3.910584	-3.015687
H	-1.691328	-3.292124	-2.017762
H	-2.536186	-4.787134	-1.550123
C	-5.038402	-3.691311	-1.125674
H	-5.803687	-3.122165	-0.572547
H	-5.424658	-3.849621	-2.148654
H	-4.951493	-4.683680	-0.652963
H	5.324804	0.252309	-2.229115

pf_Reendo_S1_MeOH_wB97XD
SCF Energy: -1980.17246850
Num. Imaginary Frequencies: 0

C	0.405965	0.635131	-1.769537
C	-1.080837	0.322894	-1.682929
C	-1.395584	-0.568859	-0.489048
C	-0.556289	-1.863926	-0.452205
C	0.944726	-1.487538	-0.534365
C	1.245516	-0.659888	-1.814917
C	1.975977	-2.630639	-0.440112
C	3.433357	-2.064535	-0.300039
C	3.695467	-0.917304	-1.249433
C	2.705022	-0.288030	-1.887558
C	5.138397	-0.537323	-1.431858
C	3.828663	-1.709630	1.141517
C	4.630223	-2.767118	1.853223
C	3.501218	-0.521122	1.671971
C	3.795303	-0.007110	3.047320
C	0.927426	-1.419687	-3.120314
C	1.786666	-3.596521	0.696221
O	1.865806	-4.800620	0.568699
O	-2.773600	-0.888934	-0.499534
O	0.785665	1.403552	-0.644041
H	0.606932	1.196222	-2.701757
H	-1.643299	1.264574	-1.594902
H	-1.426938	-0.172777	-2.602079
H	-1.145778	-0.007105	0.432333
H	1.136325	-0.820448	0.322684
H	1.940284	-3.241226	-1.354989
H	4.100791	-2.888837	-0.604433
H	2.952252	0.526993	-2.579067
H	5.606502	-0.273223	-0.469651
H	5.715279	-1.382171	-1.844792
H	5.248089	0.319408	-2.112692
H	5.632232	-2.843393	1.396164
H	4.762078	-2.566530	2.924414
H	4.171784	-3.763719	1.750613
H	4.335848	-0.725730	3.678269
H	4.398332	0.914910	2.994925
H	1.139185	-0.774389	-3.987822
H	1.561100	-2.312507	-3.218673
H	-0.119507	-1.742380	-3.197475
H	1.635110	-3.149202	1.704043
C	-0.944350	-2.663815	0.790478
H	-0.578239	-2.180359	1.710942
H	-2.038465	-2.734691	0.861337
H	-0.571883	-3.696536	0.764762
H	-0.835225	-2.459229	-1.338570
H	2.861659	0.263801	3.567635
Si	1.021593	3.076738	-0.624814
Si	-3.917452	-0.102000	0.468120
C	0.796472	3.563150	1.196458
C	2.748865	3.437223	-1.253724
H	3.513399	2.918837	-0.652875
H	2.851668	3.097434	-2.297626
H	2.968912	4.517192	-1.234369
C	-0.245980	3.909131	-1.726536
H	-0.133873	3.584681	-2.774094
H	-1.277177	3.686541	-1.409976
H	-0.113068	5.003488	-1.705756
C	-5.542976	-1.001992	0.082991
C	-3.427995	-0.263553	2.270721
H	-2.415416	0.138948	2.438057
H	-4.117566	0.311298	2.910646
H	-3.438115	-1.310857	2.611173
C	-3.988766	1.713548	0.007174
H	-3.038644	2.212700	0.257157
H	-4.176881	1.856538	-1.068567
H	-4.787916	2.228924	0.565476
C	1.697777	2.688121	2.079323
H	1.611579	2.989056	3.139131
H	1.414785	1.626425	2.012601
H	2.760983	2.771230	1.800408
C	-0.669393	3.345390	1.602014
H	-1.354904	4.001627	1.041775
H	-0.987977	2.303103	1.433796
H	-0.811013	3.563598	2.675848
C	1.170598	5.041570	1.381087
H	0.565363	5.706607	0.742512
H	1.003713	5.353855	2.427727
H	2.231881	5.229381	1.149664
C	-5.354227	-2.513173	0.286389
H	-5.047694	-2.757464	1.316917
H	-6.300168	-3.049774	0.090470

H	-4.592849	-2.923293	-0.395790
C	-6.642206	-0.490195	1.026827
H	-7.606438	-0.978064	0.796254
H	-6.411922	-0.705569	2.083171
H	-6.797181	0.597628	0.932848
C	-5.948688	-0.729948	-1.373745
H	-5.165467	-1.044649	-2.082754
H	-6.868822	-1.285986	-1.629177
H	-6.152435	0.338560	-1.551656
H	2.965776	0.182701	1.024161

pf_Reexo_S1_MeOH_wB97XD
SCF Energy: -1980.16457851
Num. Imaginary Frequencies: 0

C	0.134107	1.322816	1.215400
C	0.685977	-0.080694	1.415191
C	0.667903	-0.836324	0.098704
C	-0.748960	-0.950217	-0.471399
C	-1.485589	0.413394	-0.537573
C	-1.333388	1.299539	0.730495
C	-2.980758	0.140749	-0.888282
C	-4.039415	0.430401	0.218844
C	-3.458664	0.321322	1.621937
C	-2.207149	0.747301	1.833781
C	-4.345424	-0.132405	2.746327
C	-5.307623	-0.386139	-0.035403
C	-6.523659	0.431331	-0.369850
C	-5.276110	-1.724762	0.031705
C	-6.394514	-2.697659	-0.179615
C	-1.750118	2.751098	0.428821
C	-3.365084	0.893069	-2.129846
O	-3.721930	0.373300	-3.163762
O	1.209436	-2.133603	0.273664
O	0.937946	2.005016	0.274076
H	0.142461	1.858975	2.183994
H	1.715891	-0.021334	1.798106
H	0.087158	-0.628337	2.160572
H	1.277834	-0.268868	-0.629191
H	-1.024025	0.977052	-1.368592
H	-3.083538	-0.920853	-1.136862
H	-4.336742	1.490069	0.120581
H	-1.809662	0.753614	2.855577
H	-5.294969	0.428806	2.750287
H	-4.613186	-1.196051	2.654399
H	-3.853535	0.016543	3.718683
H	-6.767405	1.118799	0.457913
H	-6.324073	1.063603	-1.252629
H	-7.414417	-0.174256	-0.582015
H	-6.554926	-3.304818	0.727365
H	-7.348675	-2.217153	-0.435564
H	-1.157086	3.169146	-0.397227
H	-2.811184	2.831218	0.156192
H	-1.590912	3.383271	1.316869
H	-3.301624	2.006360	-2.054303
C	-0.692127	-1.614029	-1.848154
H	-0.078064	-1.010114	-2.537133
H	-0.240162	-2.613601	-1.780576
H	-1.683972	-1.730159	-2.308141
H	-1.309037	-1.604374	0.222208
H	-6.144832	-3.406653	-0.986809
Si	2.778421	-2.531815	-0.220639
Si	2.132853	3.137894	0.649996
C	2.994631	-4.333634	0.331088
C	2.920004	-2.338810	-2.080005
H	2.664474	-1.310014	-2.382571
H	3.954488	-2.529315	-2.410507
H	2.255142	-3.028550	-2.623043
C	4.001530	-1.374003	0.601531
H	5.037063	-1.638217	0.330269
H	3.826071	-0.341156	0.259510
H	3.919475	-1.391749	1.699525
C	3.024703	3.410225	-1.002442
C	3.272876	2.451891	1.970197
H	4.073757	3.174005	2.200606
H	2.718876	2.267281	2.905527
H	3.745493	1.506313	1.662250
C	1.320972	4.700914	1.289487
H	0.659080	5.159839	0.538322
H	0.717790	4.481438	2.186004
H	2.079595	5.446623	1.579230
C	1.999840	3.786981	-2.083312
H	1.264450	2.982903	-2.245037
H	1.443366	4.703274	-1.825759
H	2.506791	3.971689	-3.047616
C	3.745321	2.116663	-1.413108
H	4.231520	2.240259	-2.397613
H	4.531534	1.837307	-0.693087
H	3.047437	1.266954	-1.495084
C	4.049795	4.544192	-0.848403
H	4.601381	4.696992	-1.793500
H	3.568569	5.502463	-0.592550
H	4.796667	4.325153	-0.067135
C	1.852475	-5.185523	-0.243789
H	1.969916	-6.242327	0.056974
H	0.869124	-4.844918	0.117329
H	1.831346	-5.159673	-1.345817
C	4.341289	-4.865372	-0.183213
H	4.390092	-4.867939	-1.284546
H	5.192000	-4.270012	0.188306
H	4.499347	-5.905795	0.153630
C	2.964241	-4.406574	1.865408
H	3.801131	-3.852041	2.320501

H	2.027433	-3.995541	2.275802
H	3.042827	-5.455234	2.204770
H	-4.311496	-2.188155	0.281641

pf_Siendo_S1_MeOH_wB97XD
SCF Energy: -1980.17270475
Num. Imaginary Frequencies: 0

C	1.133067	-0.226258	0.771527
C	0.794552	0.801447	1.850914
C	-0.709329	1.048408	1.958757
C	-1.496169	-0.254276	2.185987
C	-1.087840	-1.256421	1.087306
C	0.424056	-1.580110	1.021333
C	-1.924964	-2.543313	1.004222
C	-1.718255	-3.211130	-0.390067
C	-0.249506	-3.258582	-0.758772
C	0.674117	-2.513452	-0.139919
C	0.108238	-4.206854	-1.869500
C	-2.577436	-2.593707	-1.500227
C	-3.902689	-3.275710	-1.715492
C	-2.136867	-1.555270	-2.228731
C	-2.832721	-0.850058	-3.351619
C	1.009597	-2.277179	2.265593
C	-3.372831	-2.231941	1.259218
O	-4.032585	-2.730836	2.145268
O	-1.171158	1.630536	0.752694
O	2.533384	-0.392848	0.684949
H	0.739837	0.155676	-0.189504
H	1.191095	0.466207	2.821668
H	1.298715	1.750071	1.611554
H	-0.902185	1.727461	2.810153
H	-1.305479	-0.715915	0.152275
H	-1.619155	-3.259278	1.782317
H	-2.055837	-4.256884	-0.289286
H	1.722213	-2.615162	-0.442180
H	-0.130411	-5.246249	-1.587074
H	-0.468823	-3.985995	-2.782323
H	1.178162	-4.155664	-2.118812
H	-4.402147	-3.505968	-0.760264
H	-4.601015	-2.688015	-2.325942
H	-3.745851	-4.245649	-2.218875
H	-3.878771	-1.158737	-3.483918
H	-2.816196	0.239450	-3.192428
H	0.368545	-3.109582	2.591080
H	1.996645	-2.699867	2.025918
H	1.148242	-1.601722	3.118773
H	-3.832780	-1.474592	0.580900
C	-1.443438	-0.732125	3.636902
H	-1.904466	-1.724889	3.751034
H	-0.422513	-0.791432	4.035713
H	-2.004046	-0.034262	4.278513
H	-2.545983	0.019433	1.984573
H	-2.305973	-1.031922	-4.304181
Si	-1.519071	3.259488	0.485983
Si	3.422969	0.265497	-0.599291
C	-2.091530	3.283371	-1.323331
C	0.012587	4.302580	0.762244
H	0.388858	4.171419	1.790464
H	0.824084	4.038531	0.066112
H	-0.216606	5.373129	0.631262
C	-2.867136	3.796270	1.671984
H	-3.730100	3.112328	1.637247
H	-2.491949	3.815585	2.708566
H	-3.224200	4.811590	1.432712
C	2.939325	-0.582290	-2.199928
H	3.436557	-0.098888	-3.057149
H	3.209952	-1.649792	-2.205954
H	1.851768	-0.506586	-2.365010
C	5.231120	-0.061805	-0.131835
C	3.029468	2.092670	-0.741313
H	3.254068	2.640696	0.186885
H	3.604545	2.555088	-1.560402
H	1.960018	2.230292	-0.971973
C	5.435950	-1.566425	0.102812
H	6.487007	-1.775186	0.372378
H	4.802878	-1.941492	0.922744
H	5.205122	-2.160634	-0.796591
C	5.575288	0.707184	1.152885
H	5.488322	1.797448	1.015954
H	4.916950	0.420834	1.989161
H	6.615132	0.497533	1.462198
C	6.143695	0.409086	-1.274778
H	5.948592	-0.139160	-2.211156
H	6.023245	1.484885	-1.485010
H	7.204688	0.244056	-1.014197
C	-3.419128	2.519573	-1.445822
H	-3.327889	1.478416	-1.094461
H	-4.224401	2.999731	-0.866069
H	-3.750817	2.486777	-2.499309
C	-1.028161	2.609701	-2.205081
H	-1.335983	2.631444	-3.266141
H	-0.053302	3.120946	-2.138358
H	-0.872723	1.555382	-1.925668
C	-2.290293	4.736798	-1.779557
H	-2.658882	4.767704	-2.820733
H	-3.028127	5.270129	-1.157058
H	-1.349426	5.310531	-1.749213
H	-1.127504	-1.184940	-2.012169

pf_Siexo_S1_MeOH_wB97XD
SCF Energy: -1980.16353213
Num. Imaginary Frequencies: 0

C	-0.572277	0.685203	0.245921
C	-0.862609	-0.010685	1.566138
C	-0.477848	-1.483221	1.479149
C	1.019390	-1.627888	1.189448
C	1.392977	-0.892476	-0.126832
C	0.904540	0.582043	-0.214353
C	2.908452	-1.041169	-0.423083
C	3.774360	0.262792	-0.329747
C	3.154128	1.316485	0.580455
C	1.821950	1.453934	0.611599
C	4.071826	2.260965	1.303685
C	5.223449	-0.082095	-0.027341
C	5.514077	-0.783987	1.276821
C	6.170584	0.196658	-0.937172
C	7.635414	-0.100579	-0.851307
C	0.927878	1.066963	-1.678819
C	3.149105	-1.626743	-1.786407
O	3.925262	-2.528989	-2.009588
O	-1.217276	-2.111519	0.446160
O	-0.959541	2.043471	0.311499
H	-1.165892	0.166283	-0.528340
H	-0.312093	0.481328	2.383348
H	-1.934448	0.083136	1.795890
H	-0.688505	-1.974001	2.447368
H	0.844975	-1.436899	-0.914776
H	3.329739	-1.770846	0.280942
H	3.781693	0.723253	-1.334157
H	1.374694	2.254902	1.209009
H	4.715624	1.743392	2.032240
H	4.747837	2.767636	0.594573
H	3.499953	3.031403	1.841314
H	6.502018	-0.519900	1.679686
H	4.765686	-0.533397	2.041798
H	5.492837	-1.880056	1.153320
H	7.926132	-0.579415	0.093779
H	7.939941	-0.770397	-1.673262
H	0.547103	2.096661	-1.739675
H	1.935646	1.067662	-2.114314
H	0.288384	0.427844	-2.309579
H	2.577309	-1.161672	-2.625633
C	1.830792	-1.274062	2.436956
H	2.900696	-1.472110	2.292890
H	1.728033	-0.221101	2.732392
H	1.498607	-1.896793	3.282922
H	1.192004	-2.700011	0.990862
H	8.229876	0.821328	-0.966333
Si	-2.624181	-3.022097	0.665828
Si	-2.410524	2.629858	-0.332973
C	-3.394841	-3.097735	-1.066924
C	-3.753571	-2.180766	1.902782
H	-4.045664	-1.169197	1.580689
H	-4.673759	-2.771880	2.043092
H	-3.264419	-2.096979	2.887326
C	-2.144773	-4.714991	1.309101
H	-3.032748	-5.338718	1.502631
H	-1.495876	-5.251053	0.598162
H	-1.594606	-4.618401	2.260178
C	-3.855564	1.796820	0.521239
H	-3.868529	0.722518	0.276422
H	-3.806997	1.899393	1.616667
H	-4.813037	2.222967	0.178510
C	-2.493577	2.251272	-2.167006
H	-2.383871	1.169395	-2.346854
H	-3.473432	2.551829	-2.573658
H	-1.711169	2.773549	-2.739183
C	-2.341974	4.494504	0.009231
C	-3.557045	5.174472	-0.640610
H	-4.510710	4.776256	-0.255929
H	-3.548912	6.259566	-0.432321
H	-3.560855	5.052582	-1.736295
C	-2.365316	4.739377	1.525732
H	-1.525988	4.237468	2.034214
H	-2.287142	5.819687	1.744539
H	-3.299756	4.379201	1.986379
C	-1.050227	5.078558	-0.583445
H	-0.987194	4.921598	-1.672892
H	-1.003341	6.168322	-0.406476
H	-0.152405	4.630317	-0.129115
C	-3.829773	-1.685796	-1.489612
H	-4.622057	-1.286354	-0.835949
H	-2.987600	-0.974648	-1.468692
H	-4.228688	-1.694696	-2.519982
C	-2.361782	-3.633345	-2.069789
H	-2.801525	-3.692142	-3.081778
H	-1.476334	-2.980699	-2.131151
H	-2.013989	-4.645515	-1.805244
C	-4.617249	-4.028049	-1.042687
H	-5.382272	-3.688539	-0.324666
H	-5.096227	-4.062539	-2.037797
H	-4.342975	-5.062092	-0.776363
H	5.849551	0.689457	-1.863996

System II, Toluene, ωB97X-D

lineal_scis-scis_S2_tol_wB97XD
SCF Energy: -2019.38540036
Num. Imaginary Frequencies: 0

C	0.483887	0.422728	0.486905
C	-0.461633	-0.100855	1.567125
C	-1.925410	0.039801	1.151446
C	-2.893366	0.033669	2.359465

C	-4.267279	0.395768	1.882390
C	1.912557	-0.062356	0.652962
C	-5.385596	-0.336606	1.976073
C	4.855282	-0.855226	-0.084286
C	3.732049	-1.580552	-0.271816
C	2.395751	-0.953960	-0.231763
H	0.116900	0.041857	-0.482229
H	-0.274940	0.462151	2.494756
H	-2.036395	1.020554	0.648559
H	-4.339663	1.368559	1.375578
H	4.734924	0.230932	0.014362
H	1.702520	-1.305048	-1.008310
H	-5.409911	-1.323207	2.446651
C	-6.643065	0.151076	1.394210
O	-7.676120	-0.475158	1.364624
C	2.670775	0.498025	1.822233
H	3.104364	1.480673	1.579819
H	2.006373	0.653612	2.685526
H	3.496300	-0.160240	2.126739
C	3.731645	-3.053531	-0.581826
H	3.370232	-3.638193	0.281023
H	3.044955	-3.268301	-1.417021
H	4.731375	-3.421818	-0.848323
C	6.259900	-1.322912	-0.115611
C	7.097667	-0.572815	-1.125917
H	6.831718	-0.869785	-2.154657
H	8.178316	-0.713298	-0.998617
H	6.895655	0.508609	-1.053981
C	6.741133	-2.290767	0.698439
C	8.159248	-2.800076	0.648713
H	8.729114	-2.458833	1.530578
H	8.711770	-2.499868	-0.249696
H	8.163420	-3.902163	0.685170
H	-6.584140	1.180095	0.952712
H	-0.254983	-1.163953	1.761116
O	-2.255379	-1.006608	0.273485
O	0.430467	1.835291	0.515928
C	5.919614	-2.949123	1.775419
H	4.975477	-2.426155	1.973319
H	5.680554	-3.993792	1.511110
H	6.495618	-2.990796	2.715222
H	-2.563122	0.870019	3.002807
C	-2.829867	-1.263618	3.156017
H	-1.823392	-1.422761	3.568411
H	-3.533477	-1.246225	4.001474
H	-3.072624	-2.126811	2.519274
Si	-2.832302	-1.032614	-1.303760
C	-2.612556	-3.835489	-1.376864
H	-2.067158	-3.780034	-0.421059
H	-3.088439	-4.830922	-1.430758
H	-1.871324	-3.785647	-2.190897
C	-3.670653	-2.726910	-1.490998
C	-4.719491	-2.914902	-0.385642
H	-4.260707	-2.878546	0.613617
H	-5.506361	-2.144396	-0.418176
H	-5.219618	-3.894015	-0.491164
C	-4.356487	-2.807223	-2.863984
H	-5.150214	-2.050283	-2.973776
H	-4.829736	-3.795740	-3.000885
H	-3.645411	-2.671561	-3.695569
C	-4.042048	0.371812	-1.600807
H	-5.006168	0.190540	-1.101986
H	-4.235448	0.488143	-2.679756
H	-3.648651	1.334520	-1.237920
H	-0.611947	-1.628819	-2.282919
C	-1.395615	-0.888469	-2.507927
H	-0.931227	0.109403	-2.482664
H	-1.734033	-1.060632	-3.542866
Si	0.524167	2.873356	-0.806112
C	-1.189705	3.060294	-1.550117
H	-1.922436	3.383430	-0.793954
H	-1.542987	2.110220	-1.979131
H	-1.195339	3.804203	-2.363578
C	1.695457	2.178290	-2.094997
H	1.370551	1.178672	-2.426289
H	1.721853	2.825404	-2.986952
H	2.723254	2.079269	-1.712799
C	1.135308	4.525937	-0.096660
C	0.070937	5.103560	0.849328
H	-0.862419	5.351414	0.318408
H	-0.178355	4.399911	1.659853
H	0.435069	6.034824	1.318924
C	2.436432	4.298404	0.686524
H	2.273967	3.628875	1.544630
H	2.826220	5.255600	1.076551
H	3.227686	3.856448	0.058636
C	1.392446	5.512971	-1.245946
H	1.712350	6.492906	-0.849128
H	2.188474	5.161113	-1.922205
H	0.489845	5.689620	-1.854179

lineal_scis-strans_S2_tol_wB97XD
SCF Energy: -2019.38215210
Num. Imaginary Frequencies: 0

C	0.465642	0.290968	0.458606
C	-0.510104	-0.066416	1.578596
C	-1.962032	0.156031	1.157396
C	-2.914865	0.323334	2.365966
C	-4.261228	0.752911	1.867165
C	1.857625	-0.274595	0.671382
C	-5.432150	0.120734	2.025391
C	4.748961	-1.284037	-0.036409

C	3.587388	-1.963545	-0.118765
C	2.287305	-1.259874	-0.136655
H	0.069416	-0.147879	-0.473742
H	-0.272372	0.552994	2.457273
H	-1.999779	1.099058	0.577514
H	-4.262860	1.684397	1.283610
H	4.674241	-0.194097	0.041954
H	1.576986	-1.634234	-0.887385
H	-5.527968	-0.819966	2.574302
C	-6.654241	0.657353	1.412330
O	-7.733196	0.113815	1.438826
C	2.655096	0.319845	1.798175
H	3.185165	1.230103	1.476518
H	2.002452	0.616642	2.632613
H	3.406792	-0.387461	2.175739
C	3.487354	-3.464436	-0.225910
H	2.734752	-3.845300	0.482920
H	3.155661	-3.769438	-1.233478
H	4.436921	-3.969849	-0.009844
C	6.127669	-1.835784	-0.080289
C	6.466949	-2.789394	-1.212796
H	5.636216	-2.868316	-1.926487
H	6.694410	-3.807678	-0.856348
H	7.345038	-2.440963	-1.779044
C	7.056783	-1.443422	0.819837
C	8.479012	-1.937106	0.798024
H	9.168253	-1.119698	0.521386
H	8.647835	-2.767896	0.101636
H	8.785187	-2.274033	1.802466
H	-6.520346	1.639632	0.888378
H	-0.385343	-1.123283	1.857851
O	-2.383324	-0.927539	0.367868
O	0.511937	1.701137	0.361732
C	6.765179	-0.490550	1.948429
H	5.787127	0.000182	1.867617
H	6.786064	-1.022658	2.915468
H	7.540011	0.292262	2.006113
H	-2.513723	1.180071	2.938289
C	-2.944629	-0.906714	3.264626
H	-1.949583	-1.110806	3.684825
H	-3.636415	-0.766406	4.108371
H	-3.260165	-1.796551	2.700613
Si	-2.977484	-1.030531	-1.199750
C	-2.982214	-3.839524	-1.051498
H	-2.426557	-3.753318	-0.103907
H	-3.536704	-4.794589	-1.025948
H	-2.245934	-3.913449	-1.868173
C	-3.949234	-2.661945	-1.250607
C	-5.000631	-2.678670	-0.131777
H	-4.532416	-2.600155	0.860722
H	-5.725192	-1.853718	-0.223565
H	-5.576815	-3.620603	-0.158491
C	-4.650397	-2.793879	-2.611830
H	-5.382113	-1.986630	-2.779027
H	-5.202074	-3.748942	-2.670145
H	-3.937560	-2.780516	-3.452834
C	-4.075359	0.438269	-1.602553
H	-5.050399	0.369331	-1.096808
H	-4.260124	0.490586	-2.688018
H	-3.607391	1.391003	-1.308284
H	-0.821709	-1.875742	-2.139467
C	-1.545083	-1.092526	-2.415404
H	-1.001949	-0.136111	-2.460613
H	-1.903991	-1.309066	-3.434939
Si	0.678245	2.616224	-1.041386
C	-1.024301	2.907697	-1.778155
H	-1.714985	3.334161	-1.033659
H	-1.465032	1.970557	-2.150990
H	-0.977566	3.604445	-2.631175
C	1.755046	1.713896	-2.283126
H	1.338518	0.721495	-2.519989
H	1.814205	2.277682	-3.228453
H	2.779736	1.559479	-1.911069
C	1.454120	4.256540	-0.478309
C	0.459180	5.015783	0.413273
H	-0.449606	5.307137	-0.137819
H	0.148471	4.412968	1.281828
H	0.916408	5.943901	0.800528
C	2.733462	3.971768	0.321716
H	2.512959	3.401986	1.236869
H	3.220250	4.916485	0.623164
H	3.470903	3.397916	-0.263659
C	1.797020	5.109971	-1.709268
H	2.212226	6.085425	-1.399109
H	2.550923	4.625173	-2.350644
H	0.911625	5.319172	-2.332308

lineal_strans-scis_S2_tol_wB97XD
SCF Energy: -2019.38545024
Num. Imaginary Frequencies: 0

C	0.372040	0.452148	0.714060
C	-0.711894	0.135246	1.742089
C	-2.120422	0.224743	1.158847
C	-3.201802	0.393640	2.255339
C	-4.512769	0.712957	1.603457
C	1.768813	0.163200	1.239396
C	-5.654312	0.014701	1.675677
C	4.489297	-1.886546	-0.217203
C	3.893500	-1.220532	0.800066
C	2.526311	-0.721596	0.563070
H	0.198713	-0.186803	-0.169070
H	-0.614925	0.844905	2.578752

H	-2.154858	1.128486	0.520004
H	-4.509915	1.616698	0.977899
H	3.884205	-2.053796	-1.119111
H	2.069104	-1.138144	-0.342668
H	-5.749991	-0.905630	2.258132
C	-6.837530	0.446733	0.920269
O	-7.879935	-0.162303	0.866646
C	2.150392	0.941531	2.471260
H	1.588964	1.886891	2.496837
H	1.902023	0.389459	3.393229
H	3.217310	1.188649	2.508290
C	4.558134	-1.038870	2.138235
H	4.961775	-0.022168	2.266349
H	3.844784	-1.212754	2.956893
H	5.397555	-1.738084	2.253571
C	5.826311	-2.518090	-0.249190
C	5.766887	-3.986328	-0.607185
H	5.399258	-4.585115	0.243464
H	6.730696	-4.402349	-0.926666
H	5.051241	-4.145220	-1.430292
C	6.977273	-1.845465	-0.016938
C	8.337329	-2.495683	-0.007715
H	8.910835	-2.218380	-0.909462
H	8.308259	-3.590330	0.053671
H	8.920898	-2.132457	0.854346
H	-6.709564	1.412632	0.365295
H	-0.553899	-0.880389	2.135911
O	-2.387538	-0.929279	0.402813
O	0.246572	1.816490	0.365445
C	7.033084	-0.359531	0.218915
H	6.090229	0.147875	-0.022158
H	7.286482	-0.132476	1.268967
H	7.832182	0.087861	-0.395950
H	-2.912115	1.302175	2.814871
C	-3.253402	-0.788047	3.215881
H	-2.298324	-0.904840	3.747408
H	-4.038076	-0.650445	3.974518
H	-3.452930	-1.724396	2.674736
Si	-2.829364	-1.141413	-1.203895
C	-2.666895	-3.932833	-0.916136
H	-2.215980	-3.769516	0.075815
H	-3.156199	-4.923107	-0.900044
H	-1.848784	-3.986621	-1.652667
C	-3.684835	-2.835452	-1.263794
C	-4.837870	-2.875854	-0.250704
H	-4.475929	-2.723638	0.777112
H	-5.600401	-2.106199	-0.451153
H	-5.347946	-3.854910	-0.286019
C	-4.238627	-3.073917	-2.677477
H	-5.000116	-2.326475	-2.954144
H	-4.719905	-4.066028	-2.740549
H	-3.448325	-3.048691	-3.445836
C	-3.971564	0.232947	-1.781027
H	-4.988620	0.120102	-1.376434
H	-4.043036	0.230635	-2.881035
H	-3.596302	1.225448	-1.483684
H	-0.529575	-1.841013	-1.905085
C	-1.290357	-1.138395	-2.279515
H	-0.839656	-0.135211	-2.311913
H	-1.530487	-1.419082	-3.318029
Si	0.642125	2.583632	-1.080494
C	-0.960879	2.922656	-1.996956
H	-1.650081	3.531139	-1.389674
H	-1.477427	1.982675	-2.246948
H	-0.782158	3.457052	-2.944025
C	1.766771	1.513303	-2.133445
H	1.288921	0.558794	-2.405081
H	2.007991	2.033800	-3.075093
H	2.712114	1.278839	-1.621483
C	1.498419	4.208912	-0.590870
C	0.630924	4.951983	0.436314
H	-0.357880	5.217093	0.027211
H	0.465602	4.345497	1.340286
H	1.118170	5.893684	0.746634
C	2.867328	3.894067	0.031213
H	2.777271	3.224253	0.900340
H	3.358066	4.821254	0.377444
H	3.548464	3.414882	-0.690309
C	1.692568	5.091244	-1.833516
H	2.222392	6.023116	-1.566725
H	2.292947	4.589665	-2.610627
H	0.732166	5.383154	-2.288340

lineal_strans-strans_S2_tol_wB97XD
SCF Energy: -2019.38205611
Num. Imaginary Frequencies: 0

C	0.361213	0.681347	0.774918
C	-0.714987	0.258405	1.773031
C	-2.104335	0.186800	1.142866
C	-3.234534	0.248618	2.200512
C	-4.550657	0.404539	1.500971
C	1.764225	0.532284	1.342417
C	-5.607826	-0.417157	1.556147
C	4.487348	-1.749537	0.247800
C	3.970084	-0.773278	1.028098
C	2.590556	-0.345113	0.739389
H	0.278008	0.024507	-0.107894
H	-0.723035	0.981474	2.603863
H	-2.215749	1.073394	0.488941
H	-4.628922	1.288954	0.853241
H	3.853398	-2.120339	-0.567686
H	2.164576	-0.863910	-0.128044

H	-5.617615	-1.329738	2.158224
C	-6.806494	-0.140088	0.753992
O	-7.770069	-0.866058	0.683741
C	2.038800	1.379388	2.558672
H	3.052728	1.793706	2.579694
H	1.337591	2.225512	2.587524
H	1.897341	0.802063	3.487727
C	4.775398	-0.120702	2.120220
H	4.872201	0.959770	1.933413
H	4.305533	-0.241356	3.108350
H	5.792344	-0.528892	2.170647
C	5.818385	-2.398191	0.379188
C	6.126527	-3.088983	1.696561
H	7.075224	-2.747597	2.140387
H	6.203129	-4.181234	1.565170
H	5.331497	-2.912832	2.433451
C	6.677202	-2.428378	-0.662566
C	8.007033	-3.131556	-0.608739
H	8.161868	-3.732206	-1.520671
H	8.116362	-3.799530	0.255130
H	8.833484	-2.400071	-0.574810
H	-6.770948	0.821804	0.178891
H	-0.460954	-0.730523	2.183863
O	-2.217450	-0.998518	0.396304
O	0.108191	2.024109	0.413427
C	6.396420	-1.743907	-1.973913
H	5.511173	-1.095420	-1.940585
H	7.256210	-1.120900	-2.273262
H	6.252963	-2.484324	-2.780315
H	-3.069116	1.193243	2.750743
C	-3.184687	-0.915620	3.182279
H	-2.239785	-0.916750	3.743911
H	-4.002928	-0.853704	3.914960
H	-3.262645	-1.877160	2.654248
Si	-2.573147	-1.276386	-1.221883
C	-2.126124	-4.030594	-0.880725
H	-1.733566	-3.806792	0.124141
H	-2.507851	-5.067098	-0.865399
H	-1.279310	-4.006583	-1.585663
C	-3.240633	-3.052834	-1.284625
C	-4.420495	-3.202421	-0.313539
H	-4.115781	-2.996712	0.723443
H	-5.253076	-2.522648	-0.556036
H	-4.820757	-4.231257	-0.348908
C	-3.711343	-3.368087	-2.713255
H	-4.536407	-2.709728	-3.030900
H	-4.082366	-4.406483	-2.776334
H	-2.899183	-3.269621	-3.452416
C	-3.834851	-0.039729	-1.858955
H	-4.846803	-0.256565	-1.485099
H	-3.869016	-0.063648	-2.960496
H	-3.579229	0.991258	-1.565872
H	-0.193239	-1.750276	-1.836538
C	-1.003415	-1.123573	-2.240971
H	-0.648448	-0.082334	-2.259599
H	-1.176915	-1.425691	-3.286662
Si	0.454731	2.808170	-1.036067
C	-1.141805	2.933444	-2.015511
H	-1.922267	3.464702	-1.447511
H	-1.531056	1.933632	-2.263325
H	-0.992299	3.468513	-2.967289
C	1.737984	1.860138	-2.022683
H	1.379958	0.855975	-2.300324
H	1.966027	2.393781	-2.960191
H	2.677085	1.735128	-1.462985
C	1.087198	4.533873	-0.550741
C	0.095552	5.182389	0.427003
H	-0.900491	5.319574	-0.025140
H	-0.032093	4.574443	1.336062
H	0.452982	6.180861	0.736531
C	2.458054	4.398450	0.129153
H	2.413930	3.738525	1.009375
H	2.819804	5.384286	0.472133
H	3.219775	3.992001	-0.555576
C	1.222344	5.412499	-1.803747
H	1.623206	6.406678	-1.536964
H	1.910372	4.975601	-2.546521
H	0.252689	5.576751	-2.301010

TSReendo_S2_tol_wB97XD
SCF Energy: -2019.34380654
Num. Imaginary Frequencies: 1

C	-0.068679	0.854646	-1.441062
C	-1.218714	-0.145368	-1.481173
C	-1.415753	-0.898894	-0.175718
C	-0.192799	-1.737852	0.221034
C	1.025239	-0.869087	0.542366
C	1.313916	0.218489	-1.204673
C	2.215334	-1.517572	0.902370
C	4.130378	-0.409490	-0.477569
C	3.626364	0.892450	-0.410558
C	2.286773	1.130829	-0.754270
C	4.400662	2.069720	0.142522
C	5.410007	-0.954782	-0.037867
C	6.228219	-0.239235	1.013574
C	5.806716	-2.148254	-0.563638
C	7.114251	-2.805735	-0.225685
C	1.665781	-0.839769	-2.244455
C	3.033104	-1.057359	2.001873
O	3.878141	-1.710323	2.589423
O	-2.544846	-1.732462	-0.309358
O	-0.338557	1.815741	-0.453001

H	-0.012889	1.334259	-2.441242
H	-2.141454	0.408634	-1.709910
H	-1.085890	-0.878369	-2.290877
H	-1.575735	-0.156280	0.631123
H	0.770744	0.004436	1.154343
H	2.407718	-2.540880	0.561884
H	3.564108	-1.087556	-1.097704
H	1.899574	2.109082	-0.458499
H	4.404153	2.087467	1.243867
H	5.446009	2.074021	-0.192553
H	3.943395	3.010880	-0.195133
H	6.946441	0.473600	0.576173
H	5.582084	0.315359	1.702579
H	6.791832	-0.947442	1.632537
H	7.792046	-2.179123	0.364857
H	6.935807	-3.740513	0.334457
H	2.568400	-0.553986	-2.804574
H	1.840439	-1.840833	-1.823064
H	0.857183	-0.948290	-2.980332
H	2.801763	-0.006325	2.326271
C	-0.525349	-2.612364	1.436044
H	-0.741378	-1.988119	2.318765
H	-1.405743	-3.236692	1.232429
H	0.317297	-3.269070	1.692632
H	0.047284	-2.408384	-0.623187
H	7.641024	-3.092824	-1.150923
Si	-0.905444	3.382299	-0.700404
Si	-4.043306	-1.414953	0.387487
C	-1.200590	4.032519	1.055723
C	0.397113	4.371837	-1.619861
H	1.301340	4.537881	-1.013795
H	0.704689	3.848532	-2.540415
H	0.006737	5.357663	-1.920658
C	-2.474444	3.341844	-1.726919
H	-2.275319	2.928276	-2.729388
H	-3.262621	2.731221	-1.260673
H	-2.874498	4.358950	-1.870461
C	-5.172046	-2.785929	-0.279214
C	-3.902733	-1.461172	2.258201
H	-3.156477	-0.730668	2.610895
H	-4.862832	-1.195334	2.730112
H	-3.603135	-2.452823	2.630756
C	-4.619949	0.298915	-0.118953
H	-3.926531	1.060502	0.273569
H	-4.673635	0.413749	-1.212585
H	-5.616133	0.523180	0.296313
C	4.965478	-2.928446	-1.546683
H	5.413885	-3.910708	-1.751117
H	3.947224	-3.109882	-1.165273
H	4.864384	-2.408490	-2.513240
C	-1.617232	5.509968	0.994751
H	-2.544349	5.656673	0.416238
H	-1.802979	5.901892	2.010482
H	-0.835522	6.141144	0.541120
C	-2.312234	3.207918	1.722897
H	-3.275737	3.312646	1.198010
H	-2.057447	2.136290	1.754402
H	-2.470954	3.540987	2.763919
C	0.094395	3.893160	1.871472
H	-0.056432	4.261931	2.901585
H	0.421321	2.843795	1.936465
H	0.923099	4.475515	1.436553
C	-4.530437	-4.152288	0.007528
H	-4.385053	-4.323166	1.086844
H	-5.173836	-4.968152	-0.367904
H	-3.548708	-4.246490	-0.481483
C	-5.342344	-2.611937	-1.796195
H	-4.371449	-2.615743	-2.316733
H	-5.948434	-3.435098	-2.215096
H	-5.855641	-1.669556	-2.047761
C	-6.544471	-2.705853	0.406573
H	-7.223179	-3.479346	0.005002
H	-6.473110	-2.869534	1.494202
H	-7.034028	-1.730847	0.245896

TSReexo_S2_tol_wB97XD
SCF Energy: -2019.34582864
Num. Imaginary Frequencies: 1

C	-0.076138	1.053345	-1.427784
C	-1.058330	-0.112739	-1.433195
C	-1.218985	-0.778569	-0.071564
C	0.079084	-1.370977	0.497252
C	1.166792	-0.325787	0.723437
C	1.378115	0.646440	-1.134041
C	2.416047	-0.772194	1.167033
C	4.050249	-0.627477	-0.804141
C	3.132430	-1.066193	-1.758486
C	1.887015	-0.424799	-1.888136
C	3.344203	-2.317123	-2.584841
C	5.235721	-1.295289	-0.287975
C	5.249817	-2.804907	-0.173458
C	6.257251	-0.568599	0.243869
C	7.437495	-1.250825	0.883033
C	2.255261	1.842357	-0.795043
C	3.268576	0.012620	2.030470
O	4.295031	-0.377792	2.560718
O	-2.183668	-1.800848	-0.191359
O	-0.502963	1.991160	-0.465246
H	-0.081299	1.519486	-2.435008
H	-2.042393	0.267048	-1.747307
H	-0.773775	-0.877358	-2.170653
H	-1.560808	-0.005511	0.644476

H	0.812011	0.621112	1.151672
H	2.678267	-1.829850	1.081810
H	3.954899	0.406581	-0.507018
H	1.173661	-0.955823	-2.526383
H	4.408553	-2.522907	-2.759376
H	2.900927	-3.211180	-2.116056
H	2.865688	-2.201086	-3.568794
H	4.253350	-3.231931	-0.337212
H	5.938094	-3.285292	-0.888875
H	5.560558	-3.110335	0.836876
H	7.753808	-2.155883	0.344768
H	8.303469	-0.576123	0.948684
H	2.739160	1.777426	0.188888
H	3.046497	1.976241	-1.548256
H	1.647887	2.754115	-0.773525
H	2.911861	1.062131	2.212190
C	-0.214539	-2.101069	1.812764
H	-0.576194	-1.395691	2.579258
H	-0.982087	-2.872699	1.665368
H	0.690011	-2.583875	2.208292
H	0.456916	-2.112507	-0.228902
H	7.178124	-1.551745	1.913302
Si	-3.765037	-1.707474	0.372695
Si	-1.375139	3.405971	-0.736099
C	-4.543474	-3.360650	-0.137542
C	-3.775025	-1.467589	2.234257
H	-3.204020	-0.567707	2.515477
H	-4.804037	-1.325236	2.603172
H	-3.336513	-2.323404	2.770003
C	-4.630736	-0.238193	-0.411930
H	-5.691395	-0.194898	-0.114765
H	-4.160764	0.697525	-0.069242
H	-4.585958	-0.264537	-1.511657
C	-1.947620	3.924477	0.996394
C	-2.810138	3.073894	-1.897831
H	-3.393895	3.994296	-2.063470
H	-2.446813	2.740562	-2.883955
H	-3.496810	2.304413	-1.514345
C	-0.256385	4.691109	-1.522397
H	0.557271	5.005466	-0.850057
H	0.202726	4.297160	-2.444183
H	-0.827983	5.590684	-1.803423
C	6.330733	0.931046	0.280099
H	5.417562	1.446151	-0.040442
H	6.565330	1.262055	1.304205
H	7.151968	1.286400	-0.366133
C	-0.734748	3.969679	1.938664
H	-1.045117	4.276162	2.953374
H	-0.248453	2.985308	2.020025
H	0.026789	4.690797	1.599549
C	-2.601481	5.313186	0.929328
H	-3.468917	5.332184	0.248734
H	-2.965070	5.617977	1.926691
H	-1.893116	6.086982	0.591353
C	-2.964560	2.901507	1.525358
H	-3.883061	2.880873	0.916594
H	-2.545617	1.882172	1.540638
H	-3.264608	3.150020	2.558771
C	-3.672177	-4.512814	0.385866
H	-3.588467	-4.502063	1.485051
H	-4.108059	-5.487488	0.101984
H	-2.653262	-4.466907	-0.028168
C	-4.619946	-3.435554	-1.670172
H	-3.627292	-3.314784	-2.132359
H	-5.020292	-4.413939	-1.991068
H	-5.282567	-2.660087	-2.087934
C	-5.956275	-3.471409	0.455622
H	-6.433803	-4.417290	0.143381
H	-5.943465	-3.462326	1.557731
H	-6.613594	-2.651416	0.121566

TSSiendo_S2_tol_wB97XD
SCF Energy: -2019.33972685
Num. Imaginary Frequencies: 1

C	0.717013	0.733531	-0.578354
C	1.366947	0.071777	-1.783516
C	1.177887	-1.437412	-1.780128
C	-0.287930	-1.862432	-1.933431
C	-1.149598	-1.455430	-0.731970
C	-0.803966	0.555217	-0.465022
C	-2.535466	-1.695602	-0.767638
C	-3.617666	0.398058	0.532695
C	-2.537678	0.578454	1.403128
C	-1.241613	0.649574	0.876192
C	-2.657475	0.589466	2.912148
C	-5.016307	0.108944	0.803874
C	-5.440610	-0.442600	2.145744
C	-5.906967	0.270910	-0.217333
C	-7.381257	0.025667	-0.073369
C	-1.564176	1.253116	-1.587656
C	-3.232565	-2.345318	0.314221
O	-4.351938	-2.829770	0.256581
O	1.679279	-1.968739	-0.573134
O	0.999107	2.118293	-0.613169
H	1.162879	0.267648	0.318077
H	0.979406	0.507233	-2.717256
H	2.442944	0.303041	-1.752674
H	1.726889	-1.859405	-2.644701
H	-0.666323	-1.784004	0.193572
H	-3.089173	-1.634579	-1.709624
H	-3.415948	0.648648	-0.497639
H	-0.442323	0.600639	1.624574

H	-3.532689	1.156878	3.253859
H	-2.732571	-0.424859	3.334430
H	-1.767673	1.059806	3.354975
H	-5.659188	0.349426	2.880320
H	-6.331553	-1.074718	2.056419
H	-4.656956	-1.082289	2.567518
H	-7.717036	-0.097974	0.962342
H	-7.947291	0.862344	-0.514449
H	-2.333731	0.628236	-2.059952
H	-2.055812	2.163376	-1.211265
H	-0.872063	1.572934	-2.378075
H	-2.632247	-2.418413	1.262033
C	-0.838241	-1.532248	-3.318257
H	-1.834585	-1.971054	-3.469096
H	-0.914924	-0.453471	-3.505870
H	-0.179068	-1.955281	-4.092433
H	-0.259292	-2.964289	-1.858230
H	-7.668340	-0.879353	-0.637401
Si	3.133084	-2.787857	-0.370531
Si	2.062503	2.895444	0.433290
C	3.283256	-2.994876	1.509652
C	4.539156	-1.770933	-1.086745
H	4.386643	-1.600191	-2.165329
H	4.631559	-0.786796	-0.601370
H	5.502557	-2.295075	-0.976367
C	3.038606	-4.431593	-1.268114
H	2.186878	-5.035177	-0.917258
H	2.911717	-4.275140	-2.352143
H	3.958000	-5.023532	-1.130460
C	1.422711	2.796478	2.195560
H	2.032917	3.418014	2.871522
H	0.378077	3.136802	2.268309
H	1.471585	1.763595	2.577177
C	2.118386	4.682052	-0.201068
C	3.735708	2.047186	0.355296
H	4.185817	2.101046	-0.648232
H	4.445112	2.490394	1.073003
H	3.625638	0.983722	0.623843
C	-5.489431	0.701196	-1.602914
H	-4.698918	0.049294	-2.009397
H	-6.338299	0.656570	-2.299121
H	-5.104412	1.733566	-1.621704
C	0.726684	5.314362	-0.044514
H	0.719984	6.341781	-0.450555
H	-0.043448	4.738207	-0.581500
H	0.420369	5.379731	1.012202
C	2.514372	4.680819	-1.685411
H	3.518407	4.254182	-1.844081
H	1.803902	4.098213	-2.291733
H	2.531775	5.711697	-2.082158
C	3.147222	5.489142	0.605173
H	2.905161	5.516348	1.680417
H	4.166029	5.080970	0.501362
H	3.178696	6.535860	0.253650
C	3.271743	-1.609412	2.173903
H	3.324870	-1.705547	3.272993
H	4.130685	-0.993782	1.860651
H	2.351106	-1.054111	1.932995
C	4.596194	-3.716902	1.848744
H	4.694560	-3.848197	2.941003
H	4.645713	-4.720892	1.396187
H	5.479679	-3.151765	1.509036
C	2.093302	-3.816472	2.028872
H	1.131548	-3.338209	1.785328
H	2.077806	-4.833801	1.605592
H	2.145703	-3.921110	3.127261

TSSiexo_S2_tol_wB97XD
SCF Energy: -2019.34515425
Num. Imaginary Frequencies: 1

C	-0.664339	0.763649	0.329796
C	-1.129040	0.105506	1.621079
C	-0.964590	-1.409712	1.574796
C	0.493766	-1.884269	1.489984
C	1.190880	-1.437623	0.209530
C	0.834528	0.632202	0.040531
C	2.555939	-1.701327	0.031891
C	3.829804	0.567647	0.078642
C	3.081669	1.101528	1.127225
C	1.679984	1.137140	1.045263
C	3.696235	1.517984	2.445596
C	5.217355	0.136053	0.061939
C	5.831288	-0.443483	1.318632
C	5.910628	0.092191	-1.110008
C	7.310121	-0.460095	-1.156845
C	1.133434	0.840394	-1.436229
C	3.119259	-2.038490	-1.253288
O	4.261871	-2.418910	-1.452424
O	-1.671212	-1.912718	0.460188
O	-1.008597	2.134815	0.326042
H	-1.190379	0.238580	-0.487160
H	-0.605617	0.525002	2.493845
H	-2.196984	0.336927	1.754192
H	-1.380956	-1.826224	2.512769
H	0.567744	-1.603480	-0.678140
H	3.203224	-1.898892	0.888509
H	3.360468	0.615126	-0.893873
H	1.178373	1.453105	1.966115
H	3.680176	0.704710	3.190910
H	4.737002	1.849519	2.333763
H	3.126954	2.356490	2.874015
H	6.593178	0.214181	1.769512

H	5.071647	-0.641364	2.084075
H	6.315974	-1.406445	1.099193
H	7.910263	-0.185069	-0.277669
H	7.269917	-1.562683	-1.199642
H	1.499734	1.862526	-1.620908
H	1.873409	0.143768	-1.848842
H	0.216740	0.702850	-2.027379
H	2.407323	-1.942214	-2.117184
C	1.259665	-1.618697	2.782955
H	2.234840	-2.125824	2.785383
H	1.441526	-0.547645	2.948368
H	0.694035	-2.000875	3.647118
H	0.411174	-2.981689	1.385211
H	7.846516	-0.118049	-2.053903
Si	-3.075354	-2.835957	0.525135
Si	-2.319678	2.784322	-0.505623
C	-3.575674	-3.051337	-1.292311
C	-4.380660	-1.922351	1.517791
H	-4.648615	-0.955585	1.063511
H	-5.301436	-2.521308	1.609172
H	-4.022519	-1.723538	2.541501
C	-2.692899	-4.470707	1.361353
H	-3.577641	-5.127219	1.392812
H	-1.884984	-5.011153	0.843648
H	-2.371493	-4.308243	2.403495
C	-3.887400	1.872604	-0.019043
H	-3.770043	0.798968	-0.237845
H	-4.122360	1.978688	1.051476
H	-4.755156	2.229144	-0.597585
C	-2.069065	2.578828	-2.354530
H	-2.087039	1.513630	-2.637629
H	-2.876685	3.074122	-2.918272
H	-1.110163	3.002702	-2.690450
C	-2.341035	4.607940	0.014561
C	5.392712	0.546905	-2.443953
H	5.946687	1.439877	-2.781523
H	5.569497	-0.240405	-3.193680
H	4.326028	0.799106	-2.463234
C	-3.534620	5.322775	-0.636634
H	-4.498149	4.884134	-0.328764
H	-3.554056	6.387781	-0.344039
H	-3.488352	5.290576	-1.737638
C	-2.459812	4.695502	1.543809
H	-1.628315	4.174619	2.043227
H	-2.444196	5.749726	1.873594
H	-3.400997	4.253902	1.910395
C	-1.030515	5.273373	-0.433733
H	-0.922571	5.272790	-1.530678
H	-0.998347	6.327073	-0.103339
H	-0.151566	4.762650	-0.009744
C	-3.751966	-1.668392	-1.938078
H	-4.554767	-1.086669	-1.456526
H	-2.825207	-1.075441	-1.881834
H	-4.019051	-1.769688	-3.005075
C	-2.475562	-3.823565	-2.036658
H	-2.731140	-3.925805	-3.106395
H	-1.503474	-3.309454	-1.974656
H	-2.342150	-4.841165	-1.635383
C	-4.897783	-3.829695	-1.375167
H	-5.723320	-3.298578	-0.873614
H	-5.196218	-3.973710	-2.428789
H	-4.818364	-4.831326	-0.921407

System II, Methanol, ωB97X-D

lineal_scis-scis_S2_MeOH_wB97XD
SCF Energy: -2019.38894180
Num. Imaginary Frequencies: 0

C	0.486250	0.440441	0.492964
C	-0.457471	-0.090298	1.571547
C	-1.922329	0.044266	1.158009
C	-2.884253	0.055909	2.370270
C	-4.258010	0.398460	1.885226
C	1.912738	-0.053482	0.650774
C	-5.364719	-0.355465	1.977118
C	4.843950	-0.870668	-0.087961
C	3.714656	-1.586015	-0.282708
C	2.383120	-0.949034	-0.237959
H	0.115636	0.078144	-0.480680
H	-0.273538	0.467537	2.503039
H	-2.041112	1.013408	0.637590
H	-4.340248	1.364971	1.369646
H	4.734165	0.216190	0.018907
H	1.683097	-1.294310	-1.011312
H	-5.375876	-1.339004	2.455596
C	-6.610329	0.102625	1.366983
O	-7.630038	-0.559795	1.307599
C	2.681194	0.499085	1.817838
H	3.147241	1.465423	1.567385
H	2.017585	0.680443	2.677166
H	3.487085	-0.178838	2.133497
C	3.700031	-3.056073	-0.605542
H	3.335284	-3.644621	0.253486
H	3.008112	-3.255570	-1.440359
H	4.695266	-3.433588	-0.877175
C	6.244894	-1.349764	-0.119542
C	7.094347	-0.592079	-1.114955
H	6.836268	-0.876700	-2.149682
H	8.173514	-0.739845	-0.980960
H	6.895076	0.489355	-1.032597
C	6.714930	-2.333136	0.683689

C	8.129098	-2.852989	0.631436
H	8.697708	-2.528945	1.520808
H	8.687458	-2.544403	-0.260893
H	8.122534	-3.955597	0.654386
H	-6.577547	1.129067	0.929159
H	-0.244234	-1.152587	1.765757
O	-2.257366	-1.021188	0.294281
O	0.443663	1.857425	0.538481
C	5.884761	-3.000041	1.748693
H	4.945064	-2.471549	1.955204
H	5.636202	-4.037718	1.466221
H	6.460752	-3.063620	2.687475
H	-2.558253	0.910920	2.989996
C	-2.809772	-1.220139	3.199710
H	-1.798915	-1.363466	3.607684
H	-3.506776	-1.179376	4.050131
H	-3.059717	-2.105316	2.595595
Si	-2.829041	-1.021948	-1.295918
C	-2.648478	-3.831175	-1.366495
H	-2.122039	-3.795517	-0.398481
H	-3.137336	-4.819424	-1.440596
H	-1.888723	-3.782400	-2.163444
C	-3.687998	-2.706451	-1.491746
C	-4.760199	-2.886320	-0.407301
H	-4.322719	-2.875944	0.602828
H	-5.530066	-2.098335	-0.444067
H	-5.277130	-3.854480	-0.536138
C	-4.351342	-2.770658	-2.876743
H	-5.130570	-1.999829	-2.996178
H	-4.837097	-3.751864	-3.025624
H	-3.623272	-2.640937	-3.694470
C	-4.021341	0.396261	-1.578433
H	-4.999324	0.205643	-1.110421
H	-4.181907	0.544208	-2.659149
H	-3.628553	1.341666	-1.172250
H	-0.602002	-1.635805	-2.243365
C	-1.381573	-0.895614	-2.484139
H	-0.917170	0.102417	-2.463819
H	-1.716024	-1.079296	-3.518684
Si	0.526407	2.888973	-0.800584
C	-1.190717	3.068811	-1.528541
H	-1.919376	3.387948	-0.766634
H	-1.539045	2.115784	-1.954909
H	-1.199172	3.814538	-2.340688
C	1.693424	2.179721	-2.083366
H	1.358470	1.180729	-2.407445
H	1.716924	2.824726	-2.977256
H	2.722488	2.084812	-1.702115
C	1.148704	4.539931	-0.098442
C	0.097403	5.121529	0.859579
H	-0.845859	5.359353	0.341503
H	-0.137274	4.425854	1.682075
H	0.466035	6.058497	1.314846
C	2.462507	4.316677	0.664855
H	2.318095	3.655094	1.533102
H	2.858428	5.277326	1.040885
H	3.242616	3.868821	0.027116
C	1.388469	5.522427	-1.255530
H	1.715340	6.503540	-0.866387
H	2.173419	5.166193	-1.942695
H	0.476163	5.695959	-1.850190

lineal_scis-strans_S2_MeOH_wB97XD
SCF Energy: -2019.38586780
Num. Imaginary Frequencies: 0

C	0.467131	0.333891	0.467952
C	-0.510197	-0.021351	1.587652
C	-1.962200	0.181487	1.157157
C	-2.918147	0.374763	2.358593
C	-4.266226	0.762528	1.836890
C	1.852025	-0.251423	0.673690
C	-5.424382	0.105846	2.007879
C	4.713073	-1.328819	-0.033668
C	3.537843	-1.987391	-0.110945
C	2.252539	-1.256457	-0.126295
H	0.065519	-0.085656	-0.469700
H	-0.282274	0.606416	2.463238
H	-2.010798	1.104749	0.549325
H	-4.281147	1.671910	1.220972
H	4.657217	-0.237674	0.044598
H	1.526726	-1.626290	-0.864722
H	-5.503878	-0.817377	2.589039
C	-6.638064	0.587555	1.353477
O	-7.706318	0.003775	1.371842
C	2.669134	0.342901	1.786934
H	3.221551	1.234114	1.447963
H	2.026452	0.666163	2.620030
H	3.408691	-0.372853	2.173358
C	3.402866	-3.485883	-0.215900
H	2.625242	-3.845048	0.477477
H	3.083459	-3.784040	-1.229489
H	4.333996	-4.016501	0.020263
C	6.082636	-1.901586	-0.077170
C	6.397388	-2.901233	-1.176583
H	5.571303	-2.971775	-1.897101
H	6.582230	-3.916129	-0.786965
H	7.294889	-2.604228	-1.741733
C	7.029254	-1.487314	0.796561
C	8.443218	-2.004900	0.775869
H	9.134908	-1.224570	0.411069
H	8.579091	-2.894826	0.148146
H	8.773468	-2.258748	1.796871

H	-6.531738	1.553297	0.803551
H	-0.375900	-1.073586	1.881549
O	-2.375922	-0.931515	0.392974
O	0.533197	1.748321	0.384286
C	6.768499	-0.485776	1.890508
H	5.810291	0.040381	1.790420
H	6.769076	-0.985350	2.875308
H	7.574042	0.266901	1.923773
H	-2.533221	1.261372	2.894640
C	-2.929594	-0.817092	3.308006
H	-1.930255	-0.989053	3.732822
H	-3.620515	-0.646860	4.147239
H	-3.240681	-1.737467	2.791078
Si	-2.948706	-1.038630	-1.192918
C	-2.984094	-3.847859	-1.001575
H	-2.453460	-3.761831	-0.039021
H	-3.547758	-4.798175	-0.984477
H	-2.225447	-3.932722	-1.796543
C	-3.934506	-2.663398	-1.235957
C	-5.014788	-2.658831	-0.144654
H	-4.575334	-2.586004	0.862036
H	-5.722962	-1.821935	-0.259332
H	-5.603774	-3.592991	-0.184194
C	-4.604049	-2.805034	-2.612204
H	-5.322175	-1.991249	-2.806325
H	-5.164070	-3.755682	-2.671714
H	-3.870270	-2.807919	-3.435098
C	-4.031126	0.432998	-1.611959
H	-5.017550	0.362401	-1.128283
H	-4.187586	0.487668	-2.701999
H	-3.564980	1.380560	-1.298977
H	-0.776139	-1.904424	-2.065899
C	-1.498315	-1.134184	-2.380163
H	-0.960244	-0.176404	-2.451636
H	-1.847144	-1.389820	-3.394471
Si	0.695191	2.648475	-1.040405
C	-1.004526	2.906063	-1.785821
H	-1.705819	3.329882	-1.049658
H	-1.424300	1.955596	-2.148946
H	-0.957757	3.594321	-2.646036
C	1.794559	1.737484	-2.253174
H	1.375926	0.745613	-2.490155
H	1.867261	2.298747	-3.199371
H	2.813816	1.590933	-1.862160
C	1.452474	4.297516	-0.479842
C	0.450280	5.046442	0.412379
H	-0.466906	5.317382	-0.135417
H	0.153467	4.446745	1.288636
H	0.895192	5.984789	0.790073
C	2.740100	4.033356	0.314384
H	2.536921	3.466226	1.235998
H	3.214903	4.986889	0.608258
H	3.481586	3.466326	-0.272647
C	1.778059	5.151302	-1.715310
H	2.181999	6.133141	-1.409191
H	2.534926	4.673322	-2.358704
H	0.886285	5.345258	-2.334344

lineal_strans-scis_S2_MeOH_wB97XD
SCF Energy: -2019.38871900
Num. Imaginary Frequencies: 0

C	0.375305	0.526457	0.736095
C	-0.715471	0.212185	1.757693
C	-2.116228	0.258028	1.150416
C	-3.215442	0.473840	2.219728
C	-4.516922	0.725427	1.525039
C	1.766743	0.206583	1.256041
C	-5.637335	-0.009148	1.607252
C	4.441455	-1.880096	-0.231716
C	3.859229	-1.218121	0.797080
C	2.502779	-0.686567	0.565478
H	0.194639	-0.092069	-0.158827
H	-0.643074	0.940563	2.580772
H	-2.157298	1.121082	0.459852
H	-4.524191	1.594254	0.853025
H	3.832516	-2.021078	-1.135989
H	2.035647	-1.079801	-0.345936
H	-5.717948	-0.901460	2.234723
C	-6.796349	0.337599	0.788914
O	-7.811716	-0.330400	0.718044
C	2.169448	0.954403	2.500472
H	1.603502	1.894523	2.573150
H	1.946860	0.372814	3.410691
H	3.235881	1.208292	2.518875
C	4.523018	-1.071595	2.139875
H	4.943524	-0.064481	2.286711
H	3.803422	-1.245625	2.953371
H	5.349553	-1.787708	2.247285
C	5.765871	-2.537622	-0.275440
C	5.676737	-3.994985	-0.671086
H	5.287146	-4.606560	0.161050
H	6.634609	-4.425517	-0.989866
H	4.965193	-4.115968	-1.504517
C	6.930779	-1.894927	-0.023669
C	8.276755	-2.573698	-0.028423
H	8.862625	-2.273848	-0.915072
H	8.225060	-3.669304	-0.008527
H	8.860038	-2.252031	0.850448
H	-6.697562	1.279338	0.197600
H	-0.545316	-0.790102	2.180796
O	-2.361663	-0.943461	0.450430
O	0.275805	1.902455	0.406960

C	7.018874	-0.417406	0.252026
H	6.089459	0.119924	0.022438
H	7.272304	-0.225642	1.309005
H	7.832182	0.026566	-0.346746
H	-2.950354	1.422805	2.720242
C	-3.262418	-0.641760	3.256844
H	-2.311085	-0.708429	3.803940
H	-4.056920	-0.460494	3.996119
H	-3.450716	-1.618255	2.785603
Si	-2.752697	-1.203698	-1.172649
C	-2.584987	-3.987018	-0.784625
H	-2.169668	-3.797182	0.218809
H	-3.069167	-4.980017	-0.759232
H	-1.740672	-4.053409	-1.490017
C	-3.596071	-2.906022	-1.196983
C	-4.783290	-2.924641	-0.223162
H	-4.459583	-2.756291	0.815550
H	-5.536192	-2.156590	-0.464861
H	-5.292938	-3.904520	-0.258281
C	-4.101427	-3.190209	-2.620470
H	-4.857386	-2.455545	-2.943603
H	-4.573843	-4.187858	-2.669271
H	-3.285713	-3.180193	-3.362226
C	-3.892312	0.139398	-1.814376
H	-4.924203	0.007348	-1.455060
H	-3.909135	0.120943	-2.916693
H	-3.550242	1.140779	-1.507628
H	-0.426310	-1.908566	-1.764677
C	-1.181117	-1.231455	-2.194744
H	-0.738780	-0.226114	-2.261444
H	-1.392632	-1.564867	-3.224168
Si	0.626770	2.638501	-1.075530
C	-0.986883	2.863877	-2.001737
H	-1.717704	3.434830	-1.406730
H	-1.436838	1.888219	-2.243585
H	-0.829987	3.398138	-2.953153
C	1.804566	1.588490	-2.086475
H	1.380486	0.592754	-2.292597
H	1.991550	2.073217	-3.059289
H	2.773498	1.446350	-1.583998
C	1.401112	4.311898	-0.617333
C	0.459907	5.071365	0.330091
H	-0.516754	5.279400	-0.137298
H	0.272942	4.507729	1.258242
H	0.900072	6.044091	0.615036
C	2.747428	4.073647	0.083376
H	2.636683	3.448916	0.984154
H	3.194124	5.033476	0.399849
H	3.475062	3.577580	-0.579409
C	1.626006	5.141482	-1.890672
H	2.100246	6.108278	-1.642775
H	2.288401	4.628716	-2.607879
H	0.680023	5.366149	-2.410009

lineal_strans-strans_S2_MeOH_wB97XD
SCF Energy: -2019.38545067
Num. Imaginary Frequencies: 0

C	0.344557	0.864531	0.781857
C	-0.714216	0.405762	1.783043
C	-2.080842	0.209615	1.128865
C	-3.239509	0.268856	2.153915
C	-4.538189	0.257395	1.409991
C	1.760032	0.713523	1.312006
C	-5.521313	-0.651338	1.506862
C	4.398675	-1.698108	0.307788
C	3.938475	-0.619481	0.984775
C	2.551272	-0.201705	0.716633
H	0.252442	0.230672	-0.115254
H	-0.786562	1.154723	2.587381
H	-2.236747	1.036396	0.410597
H	-4.667307	1.073761	0.686601
H	3.711883	-2.152967	-0.417154
H	2.089510	-0.757801	-0.108986
H	-5.474057	-1.508377	2.184913
C	-6.693045	-0.554951	0.640377
O	-7.578964	-1.388805	0.592020
C	2.113004	1.598535	2.482361
H	2.935631	2.289115	2.247327
H	1.252693	2.214974	2.776739
H	2.419062	1.011964	3.361297
C	4.809242	0.168918	1.928348
H	4.761780	1.241332	1.688772
H	4.492668	0.058276	2.977047
H	5.861071	-0.135975	1.856031
C	5.723372	-2.354234	0.445271
C	6.171326	-2.747721	1.842547
H	7.123197	-2.272663	2.130304
H	6.317984	-3.837532	1.921807
H	5.421288	-2.470316	2.595339
C	6.463423	-2.650074	-0.647799
C	7.784294	-3.367581	-0.571400
H	7.842281	-4.149748	-1.346957
H	7.974012	-3.839707	0.401223
H	8.615669	-2.669162	-0.773298
H	-6.733118	0.351416	-0.010112
H	-0.403262	-0.547279	2.237920
O	-2.100107	-1.033093	0.457964
O	0.076624	2.218182	0.454780
C	6.056630	-2.269247	-2.046800
H	5.193699	-1.591402	-2.082074
H	6.894340	-1.772611	-2.565241
H	5.814111	-3.168086	-2.640624

H	-3.163760	1.269031	2.618121
C	-3.128639	-0.795174	3.239182
H	-2.202152	-0.670288	3.817640
H	-3.969926	-0.728565	3.945146
H	-3.124450	-1.807571	2.807562
Si	-2.366171	-1.399160	-1.171278
C	-1.771310	-4.105187	-0.674840
H	-1.436349	-3.818956	0.335763
H	-2.090361	-5.162217	-0.630292
H	-0.897247	-4.055904	-1.344430
C	-2.924032	-3.215833	-1.166174
C	-4.134438	-3.397877	-0.238938
H	-3.889598	-3.143689	0.803816
H	-4.991181	-2.773604	-0.541088
H	-4.474689	-4.449118	-0.254323
C	-3.314451	-3.622039	-2.596197
H	-4.163651	-3.029524	-2.974896
H	-3.618545	-4.683903	-2.625048
H	-2.479642	-3.503519	-3.306617
C	-3.676242	-0.276015	-1.903279
H	-4.687062	-0.549252	-1.563582
H	-3.655876	-0.343292	-3.003640
H	-3.499482	0.777963	-1.635822
H	0.065426	-1.745812	-1.637417
C	-0.763977	-1.212963	-2.128896
H	-0.476541	-0.155488	-2.230386
H	-0.874480	-1.620929	-3.147296
Si	0.332901	2.961186	-1.044198
C	-1.255903	2.854199	-2.032331
H	-2.111969	3.243974	-1.458803
H	-1.478831	1.812111	-2.309008
H	-1.180990	3.433852	-2.967246
C	1.724883	2.113920	-1.968969
H	1.520532	1.038871	-2.098830
H	1.829625	2.552376	-2.975249
H	2.690551	2.214414	-1.449445
C	0.759497	4.764292	-0.626132
C	-0.439392	5.429461	0.067422
H	-1.321709	5.478558	-0.591392
H	-0.733579	4.890038	0.982770
H	-0.191175	6.465779	0.359991
C	1.973828	4.799336	0.313623
H	1.760275	4.299239	1.270728
H	2.257034	5.843124	0.540114
H	2.856763	4.309896	-0.129833
C	1.090696	5.522862	-1.920596
H	1.314694	6.582186	-1.700056
H	1.973071	5.102534	-2.430627
H	0.252126	5.509991	-2.636477

TSReendo_S2_MeOH_wB97XD

SCF Energy: -2019.35286511

Num. Imaginary Frequencies: 1

C	-0.074053	0.823874	-1.395643
C	-1.223492	-0.172079	-1.469816
C	-1.436459	-0.940253	-0.177306
C	-0.224456	-1.798532	0.208032
C	1.008234	-0.959035	0.554911
C	1.306897	0.186283	-1.139709
C	2.186588	-1.662969	0.859499
C	4.185520	-0.346904	-0.467176
C	3.608840	0.913543	-0.310660
C	2.252566	1.097842	-0.631397
C	4.318112	2.104587	0.297689
C	5.478804	-0.860210	-0.047419
C	6.289984	-0.131672	1.000310
C	5.886792	-2.052807	-0.575894
C	7.208410	-2.689693	-0.259789
C	1.693711	-0.832128	-2.205872
C	3.072197	-1.274763	1.908223
O	3.972834	-1.974370	2.388998
O	-2.578803	-1.762295	-0.330297
O	-0.370476	1.778931	-0.403920
H	0.005667	1.311381	-2.388628
H	-2.139590	0.390034	-1.705006
H	-1.076435	-0.892535	-2.288285
H	-1.598176	-0.214721	0.643308
H	0.778300	-0.123353	1.226356
H	2.350406	-2.656186	0.425956
H	3.629166	-1.029954	-1.092855
H	1.831777	2.046049	-0.287940
H	4.325086	2.067155	1.398591
H	5.359414	2.185296	-0.039945
H	3.803416	3.032468	0.009144
H	6.932665	0.651984	0.567898
H	5.633737	0.348865	1.736239
H	6.936141	-0.818350	1.560595
H	7.882729	-2.063881	0.335747
H	7.048832	-3.640208	0.279249
H	2.553164	-0.473615	-2.792802
H	1.959161	-1.819554	-1.801433
H	0.868666	-0.992758	-2.912299
H	2.873159	-0.260981	2.336450
C	-0.565575	-2.688662	1.410159
H	-0.766137	-2.075644	2.304396
H	-1.457945	-3.295670	1.205007
H	0.266189	-3.366990	1.646467
H	0.016460	-2.453929	-0.647939
H	7.726034	-2.951640	-1.197641
Si	-0.886598	3.364370	-0.699564
Si	-4.069374	-1.390128	0.381467
C	-1.209818	4.054874	1.036187

C	0.477084	4.287812	-1.593835
H	1.364346	4.433728	-0.957753
H	0.793053	3.733341	-2.493327
H	0.127750	5.279632	-1.924656
C	-2.426539	3.337295	-1.764150
H	-2.209696	2.892691	-2.749603
H	-3.239276	2.757966	-1.299652
H	-2.793900	4.361955	-1.939582
C	-5.242959	-2.726548	-0.277245
C	-3.905676	-1.446719	2.247690
H	-3.125228	-0.746687	2.588632
H	-4.850356	-1.142051	2.727661
H	-3.645029	-2.452355	2.612878
C	-4.585143	0.337596	-0.130084
H	-3.857305	1.075409	0.245227
H	-4.651004	0.444165	-1.224001
H	-5.566992	0.596976	0.299291
C	5.045986	-2.845304	-1.547718
H	5.509637	-3.818727	-1.758954
H	4.034949	-3.038963	-1.153804
H	4.924298	-2.322992	-2.510462
C	-1.574375	5.543496	0.925883
H	-2.475739	5.705082	0.311527
H	-1.780786	5.965314	1.925945
H	-0.756686	6.136441	0.483824
C	-2.368885	3.286155	1.689258
H	-3.309750	3.402803	1.127173
H	-2.153299	2.207682	1.764929
H	-2.550638	3.658617	2.713506
C	0.054893	3.897178	1.894868
H	-0.110472	4.315538	2.904014
H	0.335724	2.839111	2.017805
H	0.919920	4.424766	1.460395
C	-4.648525	-4.114898	0.005458
H	-4.485211	-4.284067	1.082627
H	-5.331808	-4.906925	-0.350788
H	-3.682862	-4.255457	-0.505559
C	-5.425635	-2.547840	-1.792234
H	-4.463390	-2.588818	-2.328434
H	-6.067301	-3.348875	-2.201614
H	-5.905740	-1.586652	-2.038250
C	-6.604047	-2.597169	0.423917
H	-7.314603	-3.344896	0.027837
H	-6.525661	-2.764951	1.510617
H	-7.057546	-1.603666	0.270187

TSReexo_S2_MeOH_wB97XD
SCF Energy: -2019.35330018
Num. Imaginary Frequencies: 1

C	-0.062698	1.052198	-1.378971
C	-1.042913	-0.114900	-1.413969
C	-1.222003	-0.799686	-0.064847
C	0.069037	-1.393938	0.517503
C	1.151539	-0.347095	0.762096
C	1.388072	0.645522	-1.060167
C	2.394835	-0.794594	1.232362
C	4.095294	-0.612445	-0.787884
C	3.158246	-1.055537	-1.717139
C	1.902116	-0.423241	-1.814409
C	3.355677	-2.296840	-2.561195
C	5.301281	-1.271432	-0.310334
C	5.359138	-2.784096	-0.261951
C	6.322494	-0.531283	0.210005
C	7.562701	-1.189559	0.753057
C	2.261604	1.837571	-0.702469
C	3.219603	-0.011775	2.099312
O	4.259291	-0.396909	2.642037
O	-2.181636	-1.830446	-0.215965
O	-0.513799	1.986760	-0.420658
H	-0.045239	1.522958	-2.382350
H	-2.021361	0.270854	-1.737534
H	-0.744628	-0.866506	-2.159585
H	-1.585985	-0.045939	0.659474
H	0.788428	0.590102	1.204434
H	2.680514	-1.843411	1.110106
H	3.981381	0.410580	-0.458359
H	1.186368	-0.958337	-2.445753
H	4.414051	-2.479290	-2.789760
H	2.954925	-3.200880	-2.074162
H	2.824481	-2.185399	-3.518240
H	4.356834	-3.224058	-0.333164
H	5.970406	-3.217472	-1.070806
H	5.788298	-3.125876	0.691362
H	7.838879	-2.104835	0.211404
H	8.419990	-0.500992	0.721089
H	2.777453	1.740861	0.262091
H	3.030000	2.005224	-1.472755
H	1.647553	2.742534	-0.632634
H	2.853806	1.025838	2.298210
C	-0.235671	-2.121929	1.832120
H	-0.597275	-1.413648	2.595920
H	-1.007365	-2.890086	1.685201
H	0.663915	-2.613454	2.229172
H	0.457449	-2.134232	-0.204308
H	7.408290	-1.464213	1.812219
Si	-3.772298	-1.715719	0.350200
Si	-1.380827	3.403077	-0.747820
C	-4.556398	-3.370690	-0.145215
C	-3.773316	-1.460445	2.207155
H	-3.184635	-0.568509	2.477690
H	-4.801562	-1.295269	2.569360
H	-3.354496	-2.322981	2.748408

C	-4.616225	-0.252552	-0.460102
H	-5.678219	-0.200310	-0.168240
H	-4.139070	0.683844	-0.129495
H	-4.564549	-0.298127	-1.559054
C	-2.018108	3.937980	0.956772
C	-2.767908	3.045932	-1.954680
H	-3.341110	3.965691	-2.158000
H	-2.364846	2.691517	-2.917864
H	-3.468152	2.285512	-1.577066
C	-0.225196	4.671285	-1.501864
H	0.560997	4.987108	-0.797873
H	0.266501	4.260697	-2.399506
H	-0.782985	5.569461	-1.814233
C	6.341386	0.967956	0.310200
H	5.369618	1.453390	0.158634
H	6.719518	1.265839	1.301308
H	7.042012	1.389065	-0.431784
C	-0.843014	4.016738	1.943573
H	-1.195760	4.349512	2.936346
H	-0.355018	3.038082	2.076809
H	-0.072159	4.732586	1.613705
C	-2.683521	5.317972	0.839289
H	-3.523574	5.313808	0.124783
H	-3.088258	5.635522	1.817070
H	-1.970320	6.093017	0.513785
C	-3.044165	2.913682	1.465520
H	-3.937621	2.873013	0.821582
H	-2.619840	1.897193	1.516226
H	-3.385246	3.179647	2.482211
C	-3.696510	-4.527079	0.387695
H	-3.596249	-4.496896	1.485271
H	-4.153172	-5.499116	0.127417
H	-2.682390	-4.511682	-0.041869
C	-4.641193	-3.460165	-1.676654
H	-3.650599	-3.354677	-2.148599
H	-5.052340	-4.438394	-1.984992
H	-5.298015	-2.681852	-2.098337
C	-5.968155	-3.462218	0.454343
H	-6.456785	-4.404813	0.148302
H	-5.949603	-3.446870	1.556465
H	-6.616508	-2.635627	0.118742

TSSiendo_S2_MeOH_wB97XD
SCF Energy: -2019.34990483
Num. Imaginary Frequencies: 1

C	0.687949	0.712606	-0.615661
C	1.378961	0.058287	-1.799805
C	1.253405	-1.456964	-1.764162
C	-0.191642	-1.940709	-1.929032
C	-1.096263	-1.548864	-0.754433
C	-0.825275	0.466366	-0.502133
C	-2.477421	-1.822403	-0.846453
C	-3.639692	0.320891	0.568773
C	-2.535178	0.475822	1.408804
C	-1.251171	0.536806	0.845270
C	-2.605787	0.480821	2.920674
C	-5.026166	0.023344	0.865924
C	-5.427908	-0.485317	2.231333
C	-5.924723	0.122680	-0.161733
C	-7.394199	-0.134640	-0.005668
C	-1.617495	1.130966	-1.621851
C	-3.219728	-2.406142	0.217830
O	-4.373194	-2.854556	0.135153
O	1.760606	-1.947977	-0.537236
O	0.899416	2.115339	-0.674685
H	1.150500	0.297425	0.295760
H	0.980261	0.450796	-2.747962
H	2.443724	0.336029	-1.764350
H	1.829702	-1.875282	-2.610502
H	-0.644341	-1.862081	0.191787
H	-2.993716	-1.751742	-1.808986
H	-3.452381	0.541665	-0.472315
H	-0.438843	0.474325	1.578162
H	-3.457253	1.064862	3.293055
H	-2.688305	-0.535052	3.337904
H	-1.691007	0.928701	3.335193
H	-5.582968	0.327738	2.958191
H	-6.351948	-1.073841	2.189352
H	-4.654149	-1.148043	2.639001
H	-7.727047	-0.257859	1.030997
H	-7.963840	0.697426	-0.451207
H	-2.401161	0.492171	-2.049528
H	-2.101048	2.051784	-1.258818
H	-0.952008	1.419791	-2.446625
H	-2.664300	-2.493986	1.184659
C	-0.732775	-1.655249	-3.327442
H	-1.687228	-2.172059	-3.501246
H	-0.890882	-0.585499	-3.517122
H	-0.021129	-2.024368	-4.082344
H	-0.123210	-3.039598	-1.832076
H	-7.676650	-1.039732	-0.571959
Si	3.272533	-2.674314	-0.330074
Si	1.922898	2.935643	0.397096
C	3.452485	-2.808798	1.554146
C	4.601496	-1.598621	-1.097142
H	4.436905	-1.491818	-2.182205
H	4.623879	-0.590160	-0.655457
H	5.596332	-2.053739	-0.959911
C	3.253514	-4.348081	-1.170551
H	2.477955	-5.005945	-0.746955
H	3.046792	-4.232995	-2.247754
H	4.226578	-4.856867	-1.073989

C	1.258579	2.789236	2.143884
H	1.844306	3.419349	2.833747
H	0.203867	3.099938	2.208373
H	1.332948	1.750931	2.506371
C	1.895692	4.725954	-0.228787
C	3.630394	2.168518	0.320487
H	4.078911	2.250660	-0.682002
H	4.311545	2.648029	1.042647
H	3.572237	1.100365	0.585340
C	-5.517963	0.497770	-1.565485
H	-4.735064	-0.175537	-1.952008
H	-6.375227	0.435921	-2.249483
H	-5.122166	1.524208	-1.624329
C	0.469505	5.285267	-0.110353
H	0.425760	6.318600	-0.499337
H	-0.254579	4.684684	-0.684662
H	0.124430	5.314930	0.936130
C	2.339954	4.762778	-1.699054
H	3.367827	4.385821	-1.828450
H	1.679381	4.158170	-2.340693
H	2.320233	5.798889	-2.082448
C	2.854954	5.577215	0.617343
H	2.574788	5.582274	1.683697
H	3.895631	5.220089	0.546013
H	2.845055	6.626832	0.272335
C	3.461900	-1.400111	2.167926
H	3.529599	-1.458554	3.269225
H	4.321331	-0.804812	1.819249
H	2.543769	-0.840748	1.923248
C	4.769785	-3.524854	1.889835
H	4.899892	-3.600344	2.984436
H	4.796191	-4.550621	1.486553
H	5.646690	-2.986124	1.494010
C	2.273153	-3.606672	2.131094
H	1.307523	-3.120180	1.919024
H	2.228476	-4.630849	1.725907
H	2.366725	-3.692432	3.228724

TSSiexo_S2_MeOH_wB97XD
SCF Energy: -2019.35396495
Num. Imaginary Frequencies: 1

C	-0.614227	0.755694	0.327753
C	-1.127141	0.092684	1.597663
C	-1.031741	-1.426943	1.525394
C	0.403530	-1.963721	1.426145
C	1.127769	-1.510856	0.163088
C	0.880165	0.558789	0.047498
C	2.480146	-1.846975	-0.019102
C	3.888513	0.441578	0.112458
C	3.136857	0.921076	1.181008
C	1.733748	0.986215	1.081617
C	3.732039	1.254062	2.531320
C	5.269667	-0.004089	0.077474
C	5.899860	-0.592716	1.322368
C	5.950282	-0.014626	-1.106038
C	7.369988	-0.507634	-1.183534
C	1.200961	0.801386	-1.418831
C	3.027355	-2.150492	-1.302814
O	4.170236	-2.569397	-1.515947
O	-1.770167	-1.885425	0.406058
O	-0.884163	2.149763	0.354341
H	-1.156422	0.289803	-0.512920
H	-0.596371	0.465851	2.487040
H	-2.185369	0.367883	1.723937
H	-1.460301	-1.838867	2.457960
H	0.508830	-1.616343	-0.736811
H	3.122054	-2.070376	0.836555
H	3.416892	0.524372	-0.856811
H	1.234279	1.264673	2.015639
H	3.719484	0.388491	3.214648
H	4.768669	1.607935	2.455138
H	3.143458	2.049990	3.011696
H	6.594370	0.101983	1.823083
H	5.137178	-0.883281	2.055106
H	6.466118	-1.503138	1.077458
H	7.946579	-0.314869	-0.268521
H	7.376885	-1.598724	-1.358520
H	1.566092	1.829347	-1.573437
H	1.953688	0.121567	-1.835007
H	0.293914	0.670303	-2.025822
H	2.331636	-2.007249	-2.166449
C	1.174325	-1.779952	2.730294
H	2.135710	-2.312881	2.710678
H	1.382059	-0.723092	2.949624
H	0.592875	-2.187555	3.571748
H	0.272617	-3.052410	1.283123
H	7.900983	-0.043438	-2.027831
Si	-3.240854	-2.712588	0.512903
Si	-2.173266	2.859822	-0.486096
C	-3.803677	-2.884555	-1.290663
C	-4.446139	-1.714012	1.543551
H	-4.658689	-0.730977	1.094905
H	-5.401639	-2.252308	1.656522
H	-4.043658	-1.545956	2.556294
C	-2.934428	-4.370502	1.329985
H	-3.862257	-4.961896	1.397913
H	-2.189348	-4.963289	0.775847
H	-2.557541	-4.229491	2.356757
C	-3.774777	2.020101	0.003919
H	-3.712037	0.944031	-0.224906
H	-3.996792	2.130836	1.076834
H	-4.624383	2.428325	-0.567873

C	-1.914836	2.640049	-2.329156
H	-1.955811	1.572904	-2.602716
H	-2.710490	3.152861	-2.894708
H	-0.945187	3.041632	-2.662441
C	-2.105011	4.681011	0.038002
C	5.398368	0.443463	-2.426398
H	5.818072	1.429318	-2.692288
H	5.712706	-0.254861	-3.218141
H	4.305446	0.528701	-2.465601
C	-3.257585	5.448253	-0.627734
H	-4.242903	5.052999	-0.329992
H	-3.231038	6.513674	-0.336136
H	-3.199862	5.410171	-1.728116
C	-2.237462	4.778368	1.565540
H	-1.433878	4.227581	2.080114
H	-2.181374	5.832503	1.891934
H	-3.200029	4.376445	1.922246
C	-0.761856	5.286058	-0.398866
H	-0.640311	5.271134	-1.494367
H	-0.689125	6.340060	-0.075224
H	0.092033	4.744835	0.040098
C	-3.933574	-1.490568	-1.923852
H	-4.686456	-0.872245	-1.408578
H	-2.978151	-0.941310	-1.904937
H	-4.246577	-1.574263	-2.980237
C	-2.772401	-3.708071	-2.077206
H	-3.077790	-3.799028	-3.135180
H	-1.774881	-3.239937	-2.060815
H	-2.669194	-4.730110	-1.677649
C	-5.165743	-3.594787	-1.330463
H	-5.943344	-3.027585	-0.792722
H	-5.509316	-3.711777	-2.374028
H	-5.119533	-4.603501	-0.887541

System I, Toluene, M06-2X

lineal_scis-scis_S1_tol_M062X
SCF Energy: -1979.75637826
Num. Imaginary Frequencies: 0

C	0.670762	0.329307	0.509757
C	-0.310914	-0.107479	1.596397
C	-1.755609	0.108502	1.148230
C	-2.731097	0.246162	2.338962
C	-4.079152	0.633102	1.812271
C	2.070351	-0.220671	0.709233
C	-5.219666	-0.060970	1.922831
C	4.959383	-1.205326	0.088565
C	3.809673	-1.893407	-0.089138
C	2.507777	-1.196786	-0.108050
H	0.289060	-0.056671	-0.453977
H	-0.101190	0.477695	2.504911
H	-1.792649	1.056087	0.573881
H	-4.111313	1.576944	1.249943
H	4.878443	-0.112867	0.133063
H	1.800496	-1.562986	-0.864304
H	-5.287055	-1.016298	2.449595
C	-6.447284	0.434921	1.280810
O	-7.493494	-0.164649	1.251399
C	2.845072	0.378409	1.848552
H	3.325460	1.322125	1.546574
H	2.174374	0.624509	2.685142
H	3.631275	-0.299329	2.206250
C	3.732285	-3.377454	-0.339729
H	3.406991	-3.917948	0.564116
H	2.979877	-3.585365	-1.116387
H	4.695476	-3.795758	-0.658202
C	6.339153	-1.728468	0.158755
C	7.351264	-0.900047	-0.591296
H	7.124018	-0.895672	-1.669044
H	8.381110	-1.251193	-0.459351
H	7.304491	0.148127	-0.255077
C	6.633770	-2.829488	0.876028
C	7.966464	-3.488382	1.051004
H	8.257598	-3.500867	2.113571
H	8.768999	-3.001509	0.484118
H	7.919091	-4.541609	0.730723
H	-6.347193	1.437666	0.793986
H	-0.175383	-1.174785	1.824703
O	-2.151096	-0.976011	0.340080
O	0.693237	1.746005	0.507656
H	-2.361352	1.105555	2.926368
C	-2.746081	-1.000676	3.212923
H	-1.756866	-1.180333	3.655868
H	-3.467718	-0.898960	4.035802
H	-3.016834	-1.883929	2.616874
Si	-2.705860	-1.031668	-1.245395
C	-2.661044	-3.836616	-1.249682
H	-2.096965	-3.783881	-0.304914
H	-3.201221	-4.799265	-1.263560
H	-1.935758	-3.855284	-2.078415
C	-3.648831	-2.670084	-1.381420
C	-4.690281	-2.762478	-0.260213
H	-4.213113	-2.719871	0.730248
H	-5.431926	-1.948927	-0.310707
H	-5.244482	-3.714536	-0.331374
C	-4.355285	-2.743104	-2.741340
H	-5.105450	-1.944592	-2.856156
H	-4.883597	-3.706587	-2.845887
H	-3.647620	-2.666332	-3.582667
C	-3.824775	0.429181	-1.629543
H	-4.818549	0.307172	-1.172534

H	-3.961614	0.520995	-2.718972
H	-3.400440	1.381471	-1.275572
H	-0.508184	-1.808608	-2.129426
C	-1.241581	-1.043693	-2.427894
H	-0.721054	-0.074756	-2.464558
H	-1.571143	-1.273371	-3.453788
Si	0.849318	2.717757	-0.858582
C	-0.845689	2.930463	-1.641726
H	-1.574764	3.303795	-0.905865
H	-1.225044	1.978746	-2.043900
H	-0.813827	3.645969	-2.478938
C	2.025527	1.922366	-2.085564
H	1.684628	0.911882	-2.362381
H	2.078120	2.516126	-3.011861
H	3.044737	1.826011	-1.680492
C	1.500819	4.376830	-0.215319
C	0.403111	5.076652	0.596573
H	-0.459467	5.349518	-0.031530
H	0.038339	4.440145	1.418593
H	0.792000	6.008073	1.043742
C	2.714919	4.128966	0.687450
H	2.438705	3.526896	1.565695
H	3.128228	5.087702	1.046396
H	3.523513	3.602191	0.154564
C	1.910294	5.263400	-1.398240
H	2.243060	6.252529	-1.038468
H	2.743612	4.823905	-1.968915
H	1.075565	5.434687	-2.097584
H	5.806913	-3.301245	1.417568

lineal_scis-strans_S1_tol_M062X
SCF Energy: -1979.75539749
Num. Imaginary Frequencies: 0

C	0.658608	0.240796	0.516367
C	-0.353695	-0.106290	1.607210
C	-1.781496	0.178150	1.144149
C	-2.753805	0.394627	2.325839
C	-4.078858	0.837644	1.784873
C	2.020842	-0.386686	0.743706
C	-5.253964	0.206824	1.911376
C	4.840787	-1.545631	0.179088
C	3.661005	-2.184440	0.001316
C	2.404977	-1.408218	-0.045328
H	0.260840	-0.148894	-0.439234
H	-0.115995	0.491696	2.500329
H	-1.763581	1.113140	0.548735
H	-4.061592	1.766845	1.198144
H	4.789280	-0.452609	0.202017
H	1.680029	-1.748433	-0.796990
H	-5.370528	-0.730042	2.462189
C	-6.454530	0.748437	1.255507
O	-7.530019	0.202520	1.240098
C	2.819820	0.192720	1.876541
H	3.377246	1.085766	1.553132
H	2.156289	0.518187	2.691343
H	3.546468	-0.529761	2.271339
C	3.472821	-3.666171	-0.219262
H	3.140354	-4.169443	0.703576
H	2.677554	-3.824957	-0.963514
H	4.374024	-4.168351	-0.583192
C	6.211820	-2.065152	0.328466
C	6.454326	-3.511134	0.691619
H	6.495634	-4.161829	-0.195653
H	5.654476	-3.889290	1.341930
H	7.402658	-3.630312	1.230255
C	7.222788	-1.181712	0.183710
C	8.691824	-1.443757	0.277919
H	9.196080	-1.125811	-0.648643
H	8.933798	-2.500669	0.441902
H	9.144652	-0.855393	1.092849
H	-6.303640	1.732257	0.743798
H	-0.280557	-1.172597	1.866550
O	-2.230615	-0.901098	0.357128
O	0.766214	1.653162	0.474011
H	-2.342509	1.247626	2.894715
C	-2.836335	-0.828451	3.229261
H	-1.859910	-1.046756	3.682967
H	-3.556312	-0.671091	4.044775
H	-3.147813	-1.711125	2.652477
Si	-2.783981	-0.958821	-1.228780
C	-2.890642	-3.761068	-1.174733
H	-2.326392	-3.718591	-0.229544
H	-3.481665	-4.693469	-1.169986
H	-2.165782	-3.836097	-2.000634
C	-3.814073	-2.546255	-1.334279
C	-4.861159	-2.558386	-0.214710
H	-4.384272	-2.519259	0.776028
H	-5.557878	-1.707504	-0.285446
H	-5.465305	-3.480832	-0.266766
C	-4.520327	-2.610208	-2.694737
H	-5.224636	-1.774006	-2.830011
H	-5.101132	-3.544982	-2.779789
H	-3.807463	-2.591828	-3.534982
C	-3.818535	0.553786	-1.647260
H	-4.818667	0.499560	-1.191063
H	-3.947631	0.629334	-2.738885
H	-3.340416	1.487581	-1.312986
H	-0.630234	-1.872003	-2.093252
C	-1.320551	-1.073705	-2.406504
H	-0.748460	-0.135159	-2.458643
H	-1.660814	-1.302732	-3.429039
Si	0.988980	2.575186	-0.917020

C	-0.688080	2.889554	-1.705615
H	-1.389097	3.325087	-0.976724
H	-1.133795	1.960557	-2.092426
H	-0.607013	3.587255	-2.554521
C	2.104528	1.667260	-2.122085
H	1.695336	0.674919	-2.370450
H	2.195042	2.230039	-3.064626
H	3.115732	1.512940	-1.715021
C	1.756833	4.201171	-0.317805
C	0.711453	4.999020	0.472268
H	-0.128948	5.315680	-0.165233
H	0.301655	4.412129	1.309845
H	1.165386	5.911958	0.895671
C	2.949953	3.892134	0.593929
H	2.630649	3.337778	1.488789
H	3.432269	4.828242	0.925470
H	3.717809	3.292384	0.078110
C	2.228571	5.023595	-1.523637
H	2.629437	5.996648	-1.190387
H	3.029448	4.511233	-2.079870
H	1.408360	5.233463	-2.229607
H	6.947477	-0.144990	-0.041641

lineal_strans-scis_S1_tol_M062X
SCF Energy: -1979.75696301
Num. Imaginary Frequencies: 0

C	0.576182	0.450006	0.694894
C	-0.497026	0.130031	1.733035
C	-1.908170	0.237314	1.161253
C	-2.972495	0.411780	2.270552
C	-4.298452	0.691466	1.631592
C	1.970334	0.128938	1.204935
C	-5.409355	-0.052183	1.720665
C	4.661408	-1.956253	-0.238534
C	4.057125	-1.303389	0.783935
C	2.708980	-0.767601	0.522276
H	0.382161	-0.164651	-0.202369
H	-0.382843	0.835132	2.571539
H	-1.940765	1.138292	0.516964
H	-4.338867	1.592529	1.003795
H	4.075613	-2.069982	-1.159564
H	2.252671	-1.161952	-0.393519
H	-5.464835	-0.972165	2.308131
C	-6.616200	0.334347	0.973340
O	-7.629393	-0.318517	0.926191
C	2.369867	0.896130	2.438691
H	1.851241	1.866064	2.440031
H	2.075751	0.367494	3.360580
H	3.446987	1.088307	2.489117
C	4.661475	-1.187128	2.160153
H	5.173143	-0.225181	2.317741
H	3.880641	-1.271980	2.928105
H	5.402432	-1.980746	2.323870
C	5.991598	-2.592160	-0.278434
C	6.024437	-3.899725	-1.029605
H	5.395001	-4.651071	-0.527251
H	7.034298	-4.312578	-1.133988
H	5.608283	-3.764048	-2.040590
C	7.069903	-2.008691	0.280042
C	8.475575	-2.520610	0.326508
H	9.157382	-1.833628	-0.200206
H	8.589691	-3.518076	-0.114280
H	8.830845	-2.570335	1.368246
H	-6.533660	1.304917	0.422289
H	-0.348337	-0.891669	2.113743
O	-2.196679	-0.921171	0.412312
O	0.465825	1.828015	0.385006
H	-2.685411	1.328770	2.815506
C	-2.993642	-0.767992	3.233562
H	-2.036251	-0.858872	3.764447
H	-3.783542	-0.648898	3.988605
H	-3.169527	-1.705921	2.687275
Si	-2.652526	-1.082417	-1.197638
C	-2.475881	-3.873638	-1.027476
H	-1.995679	-3.739084	-0.045366
H	-2.965467	-4.863070	-1.028489
H	-1.683727	-3.898420	-1.792427
C	-3.504610	-2.770156	-1.306422
C	-4.626600	-2.850421	-0.264828
H	-4.233045	-2.722446	0.754699
H	-5.400363	-2.082144	-0.424526
H	-5.126486	-3.833301	-0.316486
C	-4.094438	-2.956273	-2.710305
H	-4.864981	-2.201378	-2.934241
H	-4.572172	-3.947640	-2.795714
H	-3.323582	-2.896861	-3.495660
C	-3.802576	0.307620	-1.728495
H	-4.823034	0.169799	-1.340718
H	-3.860184	0.344766	-2.828227
H	-3.439967	1.291047	-1.389892
H	-0.358339	-1.760696	-1.929894
C	-1.118044	-1.046445	-2.282967
H	-0.666548	-0.043170	-2.285859
H	-1.363554	-1.295219	-3.327635
Si	0.846192	2.596016	-1.065065
C	-0.762686	2.958368	-1.965685
H	-1.425861	3.591195	-1.354971
H	-1.307494	2.030314	-2.198052
H	-0.581857	3.476781	-2.920321
C	1.960545	1.522790	-2.129431
H	1.476328	0.575167	-2.412377
H	2.203524	2.053059	-3.064619

H	2.904269	1.279345	-1.619586
C	1.714225	4.208858	-0.573294
C	0.901690	4.902077	0.527400
H	-0.113696	5.161701	0.186971
H	0.803399	4.260796	1.416229
H	1.395149	5.840374	0.835582
C	3.113462	3.877348	-0.039492
H	3.071146	3.147259	0.784841
H	3.604642	4.787817	0.346021
H	3.762332	3.460136	-0.825343
C	1.832939	5.138248	-1.787133
H	2.386027	6.054438	-1.516056
H	2.376566	4.664242	-2.620770
H	0.845360	5.450271	-2.161808
H	6.918412	-1.027780	0.741864

lineal_strans-strans_S1_tol_M062X
SCF Energy: -1979.75456278
Num. Imaginary Frequencies: 0

C	0.611901	0.831394	0.707682
C	-0.392746	0.344817	1.751295
C	-1.786671	0.185467	1.146596
C	-2.903020	0.239088	2.214985
C	-4.231344	0.259040	1.522360
C	2.056172	0.657693	1.142155
C	-5.206927	-0.654281	1.617137
C	4.546833	-1.885018	0.135722
C	4.187574	-0.716588	0.723609
C	2.789047	-0.294641	0.530875
H	0.455165	0.227889	-0.204725
H	-0.417777	1.073720	2.576109
H	-1.949578	1.030162	0.447504
H	-4.395132	1.106567	0.842074
H	3.769478	-2.372469	-0.462973
H	2.261713	-0.878625	-0.233046
H	-5.136147	-1.539305	2.254572
C	-6.426043	-0.511651	0.805696
O	-7.315677	-1.324828	0.758360
C	2.495483	1.578236	2.253791
H	3.061451	2.440085	1.868018
H	1.619376	1.989676	2.773303
H	3.123354	1.069207	2.994751
C	5.136850	0.189970	1.469313
H	4.902280	1.239256	1.247546
H	5.072413	0.065066	2.561419
H	6.175067	0.017836	1.169831
C	5.813339	-2.635763	0.156379
C	6.841090	-2.399333	1.239199
H	7.564020	-1.614433	0.967647
H	7.411955	-3.313585	1.445047
H	6.357491	-2.094500	2.176363
C	5.980642	-3.583031	-0.791832
C	7.163748	-4.473564	-0.997050
H	6.882170	-5.533600	-0.884777
H	7.989246	-4.262151	-0.306838
H	7.549586	-4.364435	-2.023198
H	-6.477387	0.430121	0.203314
H	-0.076102	-0.629281	2.151949
O	-1.851077	-1.044407	0.461699
O	0.333671	2.198342	0.456057
H	-2.790099	1.218875	2.712427
C	-2.762253	-0.874907	3.243662
H	-1.819265	-0.778687	3.799037
H	-3.584236	-0.847036	3.972914
H	-2.765847	-1.856660	2.748677
Si	-2.207073	-1.398465	-1.142287
C	-1.553535	-4.097038	-0.749888
H	-1.135677	-3.806993	0.227152
H	-1.864573	-5.154006	-0.680811
H	-0.744985	-4.040882	-1.495750
C	-2.747727	-3.214512	-1.135469
C	-3.872985	-3.412863	-0.113317
H	-3.542110	-3.141025	0.900163
H	-4.763000	-2.807308	-0.349250
H	-4.191740	-4.469596	-0.096172
C	-3.250277	-3.606055	-2.531075
H	-4.132266	-3.016916	-2.828875
H	-3.546221	-4.669333	-2.545923
H	-2.476540	-3.472214	-3.304354
C	-3.570398	-0.286752	-1.806178
H	-4.559767	-0.592922	-1.434148
H	-3.591801	-0.336436	-2.906709
H	-3.415296	0.768430	-1.532955
H	0.190180	-1.737310	-1.750900
C	-0.659167	-1.193783	-2.192765
H	-0.365421	-0.138809	-2.300274
H	-0.822618	-1.588558	-3.208256
Si	0.449313	2.968650	-1.036945
C	-1.197836	2.801924	-1.927119
H	-2.027569	3.129256	-1.281396
H	-1.392266	1.761901	-2.229607
H	-1.220968	3.414387	-2.842731
C	1.817932	2.198681	-2.064873
H	1.682348	1.109681	-2.161138
H	1.816546	2.620371	-3.082547
H	2.811945	2.368529	-1.623656
C	0.803486	4.787448	-0.638109
C	-0.438858	5.422651	-0.000602
H	-1.286220	5.458275	-0.703263
H	-0.762354	4.869278	0.895527
H	-0.223675	6.460556	0.308170
C	1.973945	4.867431	0.348661

H	1.725758	4.368377	1.296835
H	2.218942	5.920947	0.569866
H	2.885184	4.395724	-0.054449
C	1.162669	5.538085	-1.926558
H	1.324586	6.609108	-1.713692
H	2.087878	5.149947	-2.381165
H	0.362533	5.473339	-2.682031
H	5.163712	-3.717809	-1.509984

pp_Reendo_S1_tol_M062X
SCF Energy: -1979.75269421
Num. Imaginary Frequencies: 0

C	0.064301	0.672465	-1.460518
C	-1.091519	-0.339155	-1.396894
C	-1.473025	-0.954632	-0.044431
C	-0.478531	-1.971385	0.547348
C	0.732659	-1.287616	1.128069
C	1.462061	0.075881	-1.547427
C	1.839897	-1.908281	1.561453
C	4.195739	-1.198207	-0.797984
C	3.851661	0.102501	-0.662125
C	2.448195	0.541845	-0.761343
C	4.821764	1.203817	-0.315357
C	5.530672	-1.816188	-0.653388
C	5.871294	-2.805862	-1.738984
C	6.309707	-1.539678	0.408227
C	7.661864	-2.096367	0.727035
C	1.629060	-0.962858	-2.621197
C	2.926232	-1.127100	2.170798
O	3.923468	-1.593315	2.666576
O	-2.716717	-1.598265	-0.242592
O	-0.070483	1.583521	-0.397327
H	-0.073013	1.194832	-2.432177
H	-1.992466	0.201552	-1.726760
H	-0.938200	-1.153928	-2.121112
H	-1.575681	-0.131853	0.691303
H	0.674414	-0.197566	1.246197
H	1.983359	-2.990969	1.486028
H	3.394749	-1.901997	-1.049113
H	2.178043	1.356925	-0.079809
H	4.732638	1.483913	0.748350
H	5.862825	0.911490	-0.498202
H	4.597649	2.106384	-0.904193
H	5.932171	-2.303563	-2.717729
H	6.818197	-3.329795	-1.563391
H	5.075870	-3.564171	-1.822190
H	8.050269	-2.768975	-0.047402
H	8.391004	-1.281705	0.863657
H	2.665915	-1.006937	-2.979191
H	1.356229	-1.970682	-2.264742
H	0.972840	-0.740036	-3.477562
H	2.751830	-0.020825	2.161730
C	-1.144519	-2.815006	1.644811
H	-1.487492	-2.172015	2.470535
H	-2.008091	-3.360437	1.244685
H	-0.427043	-3.536857	2.058161
H	-0.157697	-2.654853	-0.259113
H	7.632679	-2.649203	1.679565
Si	-0.239847	3.249192	-0.619013
Si	-4.187313	-0.984068	0.298799
C	-0.424298	3.925614	1.137615
C	1.277547	3.929425	-1.488579
H	2.168083	3.921822	-0.842347
H	1.510500	3.330483	-2.383772
H	1.106107	4.965445	-1.820833
C	-1.756343	3.573177	-1.677098
H	-1.609166	3.198305	-2.702482
H	-2.655667	3.089541	-1.267039
H	-1.956209	4.653679	-1.754850
C	-5.479233	-2.157114	-0.432684
C	-4.234074	-0.967669	2.176476
H	-3.401236	-0.372236	2.583648
H	-5.166828	-0.502601	2.533110
H	-4.170726	-1.978535	2.606382
C	-4.389994	0.783382	-0.307826
H	-3.588249	1.416285	0.106721
H	-4.354587	0.857427	-1.405061
H	-5.347593	1.208736	0.032441
C	0.739854	3.414218	1.996204
H	0.657936	3.803932	3.025647
H	0.741652	2.314660	2.051908
H	1.717287	3.735380	1.601249
C	-1.748204	3.433609	1.735674
H	-2.618087	3.805673	1.171161
H	-1.795858	2.332578	1.752323
H	-1.854995	3.786064	2.776318
C	-0.407050	5.458848	1.103403
H	-1.221479	5.867424	0.483419
H	-0.533807	5.866842	2.121072
H	0.545270	5.848171	0.709474
C	-5.078898	-3.601817	-0.106929
H	-5.020776	-3.777830	0.979437
H	-5.823774	-4.307235	-0.514870
H	-4.099950	-3.850843	-0.542953
C	-6.858556	-1.854705	0.165286
H	-7.624432	-2.508146	-0.287482
H	-6.880043	-2.028426	1.252811
H	-7.169267	-0.812807	-0.016846
C	-5.523312	-1.973522	-1.954878
H	-4.530299	-2.121631	-2.408117
H	-6.212219	-2.706006	-2.410462
H	-5.879092	-0.969470	-2.235130

H	5.896899	-0.858367	1.158785

pp_Reexo_S1_tol_M062X
SCF Energy: -1979.74960939
Num. Imaginary Frequencies: 0

C	0.218009	0.769698	-1.387350
C	-0.801968	-0.359138	-1.224867
C	-1.240655	-0.755871	0.191913
C	-0.137852	-1.267960	1.141334
C	0.716573	-0.154223	1.674808
C	1.697769	0.420601	-1.234545
C	2.002387	-0.279212	2.033026
C	4.380005	-0.928091	-0.377247
C	3.560156	-1.309420	-1.381295
C	2.164394	-0.822892	-1.448870
C	3.934335	-2.279289	-2.473955
C	5.771409	-1.334207	-0.089882
C	6.615608	-0.208763	0.453229
C	6.189593	-2.606437	-0.231513
C	7.553420	-3.161249	0.041579
C	2.566865	1.616906	-0.970374
C	2.734605	0.873402	2.568792
O	3.926240	0.901233	2.770730
O	-2.211551	-1.769531	0.028546
O	-0.120506	1.825535	-0.501345
H	0.122254	1.132828	-2.432773
H	-1.725665	-0.037531	-1.732924
H	-0.474935	-1.268320	-1.748509
H	-1.690616	0.135566	0.673678
H	0.222346	0.813961	1.832356
H	2.559621	-1.209430	1.884302
H	3.984755	-0.194837	0.332867
H	1.448545	-1.598782	-1.741218
H	5.021969	-2.364714	-2.591240
H	3.536799	-3.287312	-2.267371
H	3.500232	-1.955455	-3.431796
H	6.705039	0.601584	-0.287958
H	6.118670	0.221378	1.337750
H	7.625075	-0.522896	0.742552
H	7.947019	-3.673957	-0.850760
H	8.280533	-2.395036	0.335891
H	2.492768	1.942840	0.079502
H	3.619868	1.418186	-1.200916
H	2.223709	2.466831	-1.579328
H	2.101388	1.772585	2.775261
C	-0.753998	-1.992506	2.348885
H	-1.390976	-1.309599	2.932809
H	-1.365465	-2.841135	2.017264
H	0.040025	-2.362361	3.011946
H	0.500523	-1.983018	0.596920
H	7.513590	-3.917936	0.841772
Si	-3.862700	-1.603478	0.303782
Si	-0.867834	3.259991	-0.981447
C	-4.597578	-3.222371	-0.343525
C	-4.219547	-1.350835	2.130587
H	-3.696300	-0.459473	2.512198
H	-5.297316	-1.180860	2.283760
H	-3.919268	-2.211632	2.746329
C	-4.510384	-0.100457	-0.618442
H	-5.607526	-0.037805	-0.538758
H	-4.103935	0.820902	-0.170853
H	-4.247914	-0.114794	-1.686811
C	-1.362367	4.088715	0.646693
C	-2.350424	2.871421	-2.066111
H	-2.884972	3.797522	-2.331864
H	-2.033575	2.401162	-3.010937
H	-3.066538	2.196497	-1.575785
C	0.312796	4.334141	-1.970128
H	1.183165	4.659099	-1.380690
H	0.683198	3.801351	-2.860274
H	-0.210849	5.234423	-2.329347
C	-0.135438	4.148185	1.565008
H	0.259687	3.140659	1.766113
H	0.680123	4.743306	1.124034
H	-0.397781	4.612266	2.531495
C	-2.466120	3.264799	1.321619
H	-2.728146	3.700182	2.301547
H	-3.386353	3.240869	0.715945
H	-2.144928	2.224722	1.496983
C	-1.874487	5.509081	0.377480
H	-2.194193	5.985845	1.320189
H	-1.094331	6.148108	-0.065119
H	-2.742278	5.514180	-0.302050
C	-3.822325	-4.398571	0.263984
H	-4.235207	-5.356994	-0.096289
H	-2.758535	-4.359838	-0.013860
H	-3.885249	-4.407625	1.364318
C	-6.077015	-3.321394	0.047587
H	-6.210402	-3.353283	1.140523
H	-6.665765	-2.473895	-0.340135
H	-6.521445	-4.243738	-0.365033
C	-4.462875	-3.258381	-1.871101
H	-5.061482	-2.468755	-2.352485
H	-3.415282	-3.131235	-2.186942
H	-4.816581	-4.226848	-2.265655
H	5.447560	-3.340904	-0.560687

pp_Siendo_S1_tol_M062X
SCF Energy: -1979.75220709
Num. Imaginary Frequencies: 0

C	-1.008044	0.553887	0.646699
C	-1.259337	-0.349303	1.854344

C	-0.698893	-1.779117	1.795350
C	0.685100	-2.048773	2.430134
C	1.864267	-1.693561	1.573868
C	0.415216	1.044037	0.467907
C	3.041815	-1.231199	2.023089
C	3.407514	1.387167	-0.343975
C	2.361855	1.221391	-1.185460
C	1.036558	0.793194	-0.701119
C	2.429121	1.422084	-2.679201
C	4.812152	1.729498	-0.640636
C	5.469666	2.547308	0.441074
C	5.452114	1.244942	-1.722174
C	6.879588	1.461700	-2.117413
C	0.955187	1.879012	1.594011
C	4.201991	-1.104342	1.126945
O	5.292793	-0.728201	1.485631
O	-0.699272	-2.253697	0.467374
O	-1.855483	1.683296	0.808231
H	-1.288099	-0.016997	-0.255834
H	-0.935923	0.160841	2.774969
H	-2.356579	-0.424290	1.920377
H	-1.389002	-2.385972	2.414067
H	1.760818	-1.932110	0.508989
H	3.216090	-0.973651	3.071724
H	3.205402	1.249223	0.721867
H	0.456770	0.227172	-1.442078
H	3.273303	2.059372	-2.970025
H	2.532466	0.459993	-3.208942
H	1.497828	1.886138	-3.037915
H	5.499500	1.952840	1.369078
H	6.496883	2.841251	0.197423
H	4.888768	3.458516	0.652378
H	7.392208	2.205883	-1.496358
H	7.445948	0.518515	-2.049891
H	1.555623	1.274455	2.295230
H	1.604280	2.684854	1.222254
H	0.123806	2.328266	2.155289
H	4.016809	-1.406502	0.067530
C	0.775225	-1.543216	3.864768
H	1.621100	-2.003536	4.393500
H	0.911014	-0.452027	3.902597
H	-0.140252	-1.791116	4.422405
H	0.724862	-3.156067	2.458311
H	6.945137	1.791305	-3.166353
Si	-1.745643	-3.450991	-0.093332
Si	-2.798152	2.307103	-0.438892
C	-1.421563	-3.526615	-1.955905
C	-3.512429	-2.953287	0.301626
H	-3.694847	-2.969181	1.387984
H	-3.741776	-1.941050	-0.065334
H	-4.231611	-3.650646	-0.156946
C	-1.339697	-5.068984	0.766065
H	-0.319023	-5.409013	0.532848
H	-1.416371	-4.957933	1.859693
H	-2.041946	-5.864508	0.471915
C	-1.724715	2.744507	-1.916682
H	-2.300801	3.310665	-2.666408
H	-0.854505	3.349474	-1.620489
H	-1.351573	1.833637	-2.410899
C	-3.628621	3.834110	0.311357
C	-4.051425	1.005909	-0.957942
H	-4.709502	0.715166	-0.124640
H	-4.682630	1.366177	-1.785352
H	-3.535272	0.101252	-1.317867
C	-2.574780	4.930352	0.514176
H	-3.024715	5.808323	1.009842
H	-1.741912	4.581598	1.144970
H	-2.152704	5.273269	-0.443731
C	-4.243660	3.460124	1.665582
H	-5.009656	2.674216	1.564656
H	-3.477153	3.093765	2.364226
H	-4.731972	4.339458	2.120874
C	-4.727052	4.344847	-0.629346
H	-4.335017	4.591827	-1.629533
H	-5.533629	3.605425	-0.756030
H	-5.183698	5.263502	-0.221709
C	0.091203	-3.575844	-2.204532
H	0.588016	-2.673035	-1.818208
H	0.560155	-4.449859	-1.724362
H	0.299049	-3.643447	-3.286534
C	-2.004511	-2.273014	-2.621081
H	-1.767280	-2.263210	-3.699092
H	-3.101088	-2.229631	-2.524422
H	-1.585889	-1.351646	-2.182414
C	-2.083555	-4.777994	-2.546343
H	-1.942486	-4.805521	-3.640637
H	-1.648342	-5.702491	-2.135235
H	-3.169226	-4.801869	-2.356569
H	4.885750	0.579269	-2.381042

pp_Siexo_S1_tol_M062X
SCF Energy: -1979.75201400
Num. Imaginary Frequencies: 0

C	0.021904	0.791482	0.464986
C	-0.523369	0.131328	1.740266
C	-1.039200	-1.302494	1.581422
C	0.017602	-2.403185	1.320515
C	0.549100	-2.374341	-0.079362
C	1.529166	0.793747	0.236715
C	1.829876	-2.513206	-0.453098
C	4.506051	-0.038883	0.185384
C	3.892820	0.669116	1.163268

C	2.416562	0.682764	1.241064
C	4.569614	1.431708	2.277007
C	5.929839	-0.203887	-0.157129
C	6.977149	0.728975	0.401953
C	6.228074	-1.193087	-1.028007
C	7.576106	-1.586202	-1.541477
C	1.885045	1.053481	-1.199670
C	2.173352	-2.505430	-1.880918
O	3.296851	-2.564160	-2.322115
O	-2.014240	-1.335961	0.557070
O	-0.389147	2.150743	0.399867
H	-0.422932	0.241657	-0.388059
H	0.191340	0.171169	2.573599
H	-1.388083	0.732756	2.055618
H	-1.501725	-1.565910	2.553047
H	-0.213187	-2.269966	-0.861807
H	2.652350	-2.612917	0.260757
H	3.844787	-0.608367	-0.475503
H	2.025489	0.624213	2.262180
H	5.595830	1.104825	2.467409
H	4.581468	2.514231	2.068221
H	3.998746	1.302291	3.209414
H	6.582847	1.750276	0.491743
H	7.320971	0.418291	1.400978
H	7.859152	0.771099	-0.248960
H	8.397435	-0.996715	-1.116218
H	7.773431	-2.646818	-1.316882
H	2.917004	1.403091	-1.323841
H	1.758880	0.146650	-1.816031
H	1.200421	1.815020	-1.605180
H	1.296318	-2.437650	-2.571985
C	1.088419	-2.464497	2.400910
H	1.665352	-3.397092	2.326977
H	1.793949	-1.626334	2.315589
H	0.631739	-2.433607	3.401554
H	-0.568130	-3.340561	1.367577
H	7.615734	-1.493992	-2.639225
Si	-3.482568	-2.167427	0.654439
Si	-1.763962	2.703458	-0.395684
C	-4.147240	-2.196131	-1.119408
C	-4.625511	-1.279092	1.849088
H	-4.853125	-0.251239	1.531608
H	-5.577165	-1.823297	1.956297
H	-4.166784	-1.226821	2.849843
C	-3.199146	-3.908793	1.303486
H	-4.165999	-4.416962	1.446049
H	-2.591871	-4.524556	0.622570
H	-2.700323	-3.890246	2.285824
C	-3.281626	2.015712	0.468923
H	-3.186426	0.919422	0.496908
H	-3.358228	2.374760	1.506915
H	-4.215876	2.268132	-0.056596
C	-1.751617	2.120056	-2.184105
H	-1.557695	1.037733	-2.253034
H	-2.727300	2.306779	-2.660064
H	-0.982595	2.634224	-2.780725
C	-1.643531	4.588637	-0.278091
C	-2.765748	5.230654	-1.102647
H	-3.763811	4.914991	-0.756958
H	-2.723319	6.330757	-1.020067
H	-2.683860	4.978492	-2.172114
C	-1.770401	5.013131	1.190246
H	-1.011255	4.520351	1.817616
H	-1.631222	6.103959	1.288188
H	-2.762761	4.770391	1.601911
C	-0.279096	5.035767	-0.817614
H	-0.144214	4.759131	-1.875658
H	-0.180893	6.133394	-0.750467
H	0.543580	4.583510	-0.243618
C	-4.609040	-0.796019	-1.541739
H	-5.429120	-0.423397	-0.907377
H	-3.785918	-0.066124	-1.496311
H	-4.978347	-0.815169	-2.582021
C	-3.035274	-2.664623	-2.066414
H	-3.420649	-2.751474	-3.097012
H	-2.199641	-1.948244	-2.079417
H	-2.633388	-3.650739	-1.781405
C	-5.332203	-3.168794	-1.193085
H	-6.138689	-2.892277	-0.494211
H	-5.764751	-3.165842	-2.208396
H	-5.029464	-4.203487	-0.967980
H	5.389567	-1.788555	-1.407236

TS_Reendo_S1_tol_M062X
SCF Energy: -1979.71896455
Num. Imaginary Frequencies: 1

C	0.052773	0.819965	-1.484026
C	-1.201829	-0.047109	-1.506312
C	-1.403272	-0.867712	-0.241681
C	-0.253855	-1.845390	0.032198
C	1.043891	-1.103015	0.343655
C	1.365713	0.028186	-1.391037
C	2.195173	-1.840305	0.652810
C	4.068468	-1.029438	-0.831183
C	3.773573	0.334839	-0.710017
C	2.473049	0.788860	-0.973689
C	4.752273	1.341207	-0.150837
C	5.285384	-1.758292	-0.478288
C	5.493715	-3.018688	-1.283318
C	6.066185	-1.398614	0.564927
C	7.266332	-2.106332	1.102105
C	1.511092	-1.017180	-2.490967

C	3.077036	-1.398689	1.715921
O	3.912375	-2.073458	2.285624
O	-2.615545	-1.582167	-0.365780
O	-0.043823	1.731280	-0.414289
H	0.095104	1.363890	-2.451681
H	-2.069533	0.619769	-1.629618
H	-1.202869	-0.732913	-2.366174
H	-1.447450	-0.172092	0.620841
H	0.884966	-0.212496	0.962960
H	2.296152	-2.883345	0.335282
H	3.410243	-1.606462	-1.470677
H	2.249856	1.801615	-0.626237
H	4.739199	1.365433	0.950967
H	5.782643	1.120241	-0.462074
H	4.492807	2.349886	-0.501111
H	5.511716	-2.798470	-2.361719
H	6.421344	-3.543334	-1.029721
H	4.658364	-3.717038	-1.109871
H	7.601867	-2.943326	0.479094
H	8.107531	-1.405605	1.221182
H	2.430060	-0.843782	-3.067930
H	1.537118	-2.054105	-2.125848
H	0.671799	-0.948588	-3.196389
H	2.917341	-0.327078	2.009302
C	-0.617425	-2.757856	1.209243
H	-0.739617	-2.165877	2.130973
H	-1.557943	-3.288026	1.008520
H	0.173224	-3.497747	1.391292
H	-0.122874	-2.477313	-0.863862
H	7.036918	-2.495933	2.107106
Si	-0.403611	3.370305	-0.578193
Si	-4.029779	-1.144563	0.434864
C	-0.498074	3.993717	1.204737
C	0.962125	4.216519	-1.551587
H	1.904842	4.274612	-0.986542
H	1.167409	3.676208	-2.489759
H	0.667998	5.242166	-1.824512
C	-2.025637	3.571955	-1.501527
H	-1.938019	3.190030	-2.531451
H	-2.853229	3.037251	-1.011445
H	-2.303635	4.635456	-1.574099
C	-5.334905	-2.345179	-0.225900
C	-3.798672	-1.306973	2.291718
H	-2.955561	-0.686807	2.635699
H	-4.696452	-0.955137	2.824344
H	-3.602843	-2.344637	2.601040
C	-4.435330	0.648668	0.042839
H	-3.643985	1.307360	0.436950
H	-4.525084	0.825965	-1.039525
H	-5.379844	0.956008	0.519384
C	0.795238	3.612537	1.937226
H	0.758348	3.958899	2.984611
H	0.945163	2.521980	1.946499
H	1.682552	4.071383	1.471989
C	-1.692193	3.335368	1.907282
H	-2.649213	3.616424	1.439188
H	-1.611192	2.236355	1.891109
H	-1.737931	3.649802	2.964420
C	-0.667046	5.517981	1.211961
H	-1.583008	5.834442	0.687114
H	-0.737751	5.891388	2.248213
H	0.187395	6.026409	0.737327
C	-4.791410	-3.775865	-0.119775
H	-4.561097	-4.051706	0.922054
H	-5.537805	-4.498304	-0.493845
H	-3.872215	-3.897391	-0.711933
C	-6.624133	-2.219377	0.594830
H	-7.403580	-2.887785	0.189472
H	-6.467120	-2.499113	1.648563
H	-7.029843	-1.194553	0.574172
C	-5.624273	-2.018760	-1.696395
H	-4.705549	-2.041645	-2.303630
H	-6.326063	-2.756606	-2.122876
H	-6.083225	-1.023988	-1.811242
H	5.772186	-0.517565	1.136791

TS_Reexo_S1_tol_M062X
SCF Energy: -1979.71797123
Num. Imaginary Frequencies: 1

C	-0.001969	1.133700	-1.374675
C	-0.869945	-0.118587	-1.400418
C	-0.949874	-0.834663	-0.056688
C	0.403312	-1.312785	0.484701
C	1.369616	-0.166115	0.750024
C	1.482860	0.866149	-1.097390
C	2.663948	-0.485785	1.172181
C	4.205614	-0.178444	-0.637991
C	3.385812	-0.677252	-1.655074
C	2.096634	-0.147220	-1.847863
C	3.731682	-1.921198	-2.443637
C	5.492534	-0.728468	-0.173350
C	6.519885	0.321102	0.165923
C	5.670888	-2.051652	0.006624
C	6.888383	-2.753155	0.518269
C	2.237945	2.137314	-0.736357
C	3.384943	0.378925	2.099468
O	4.401024	0.085710	2.692453
O	-1.808798	-1.947300	-0.205348
O	-0.508702	2.011969	-0.388184
H	-0.056123	1.619122	-2.371679
H	-1.891304	0.177625	-1.687697
H	-0.524650	-0.834753	-2.159889

H	-1.360196	-0.121731	0.687144
H	0.918050	0.734573	1.186692
H	3.019318	-1.517652	1.123715
H	4.066181	0.861647	-0.361185
H	1.455228	-0.737685	-2.509165
H	4.815840	-2.033293	-2.574717
H	3.362337	-2.837471	-1.954992
H	3.263764	-1.874619	-3.436945
H	6.676975	1.004233	-0.683277
H	6.156866	0.922321	1.014223
H	7.489848	-0.103713	0.448519
H	7.763225	-2.097504	0.599326
H	6.692641	-3.179395	1.515840
H	2.587300	2.171900	0.304675
H	3.109253	2.274377	-1.391196
H	1.577000	3.002345	-0.870205
H	2.914704	1.384755	2.258527
C	0.187508	-2.117703	1.770785
H	-0.252694	-1.480851	2.555442
H	-0.489972	-2.962329	1.587835
H	1.138965	-2.508966	2.155471
H	0.854855	-1.980664	-0.270717
H	7.152207	-3.597691	-0.137306
Si	-3.381325	-2.010158	0.388332
Si	-1.471928	3.359249	-0.709232
C	-4.062283	-3.649372	-0.267417
C	-3.377471	-1.953038	2.265918
H	-2.863230	-1.049047	2.628978
H	-4.409223	-1.913623	2.650095
H	-2.879927	-2.826414	2.713437
C	-4.342270	-0.523945	-0.243074
H	-5.390370	-0.554100	0.094814
H	-3.899517	0.402433	0.157986
H	-4.338464	-0.462416	-1.341760
C	-2.030226	3.941290	1.001452
C	-2.912976	2.870505	-1.809174
H	-3.568111	3.737361	-1.991237
H	-2.555107	2.525235	-2.792583
H	-3.525813	2.069101	-1.370778
C	-0.465148	4.671241	-1.600889
H	0.326780	5.098501	-0.967383
H	0.010567	4.258198	-2.504784
H	-1.117941	5.495895	-1.928188
C	-0.799492	4.098846	1.903711
H	-0.259024	3.146509	2.014953
H	-0.091097	4.843515	1.506653
H	-1.102553	4.437060	2.909728
C	-2.974362	2.894939	1.606600
H	-3.267160	3.186041	2.630314
H	-3.899458	2.788565	1.017632
H	-2.490971	1.906220	1.668662
C	-2.757566	5.286151	0.880679
H	-3.113497	5.619476	1.870844
H	-2.096572	6.074601	0.487119
H	-3.638337	5.222510	0.221149
C	-3.071369	-4.769919	0.073053
H	-3.447716	-5.739989	-0.296104
H	-2.089522	-4.586846	-0.388320
H	-2.920638	-4.868821	1.160262
C	-5.421286	-3.946730	0.377728
H	-5.337465	-4.072550	1.468826
H	-6.154734	-3.146580	0.185204
H	-5.843084	-4.881947	-0.029796
C	-4.221871	-3.556922	-1.790087
H	-4.978672	-2.809535	-2.076652
H	-3.273188	-3.285353	-2.279406
H	-4.545736	-4.528487	-2.202384
H	4.816741	-2.703656	-0.202674

TS_Siendo_S1_tol_M062X
SCF Energy: -1979.71304874
Num. Imaginary Frequencies: 1

C	-0.620636	0.792864	0.573621
C	-1.320757	0.058574	1.708623
C	-1.022150	-1.432577	1.714648
C	0.455992	-1.761083	1.956299
C	1.352866	-1.271494	0.816390
C	0.910032	0.749331	0.609534
C	2.746174	-1.441712	0.886118
C	3.808929	0.744247	-0.019367
C	2.842610	0.946883	-1.013205
C	1.485975	0.946262	-0.663369
C	3.177589	1.031567	-2.484164
C	5.249489	0.547566	-0.140191
C	6.025957	0.935409	1.095163
C	5.804049	-0.075856	-1.204550
C	7.233598	-0.456057	-1.403249
C	1.495896	1.417303	1.849107
C	3.466082	-1.986419	-0.244930
O	4.593119	-2.445614	-0.228959
O	-1.420857	-1.985968	0.474073
O	-1.022980	2.151480	0.604926
H	-0.936050	0.312393	-0.370761
H	-1.054821	0.513410	2.674571
H	-2.405196	0.202756	1.577942
H	-1.591579	-1.896550	2.543853
H	0.919870	-1.561587	-0.145846
H	3.276021	-1.449494	1.843362
H	3.500576	0.963325	0.996289
H	0.787190	0.908775	-1.507611
H	4.130098	1.553232	-2.651421
H	3.260993	0.036706	-2.950561

H	2.385660	1.575580	-3.017444
H	5.784510	1.962950	1.406061
H	5.754838	0.269288	1.931008
H	7.111011	0.870281	0.958149
H	7.907626	-0.053108	-0.638823
H	7.317399	-1.554760	-1.390452
H	2.202803	0.787348	2.404146
H	2.018919	2.343380	1.567848
H	0.689501	1.702658	2.538015
H	2.873379	-1.978013	-1.198320
C	0.887081	-1.419374	3.379708
H	1.940851	-1.677557	3.553544
H	0.753171	-0.358487	3.624930
H	0.287748	-2.001496	4.095746
H	0.507417	-2.860688	1.862143
H	7.590103	-0.123612	-2.390731
Si	-2.757699	-2.995033	0.294083
Si	-2.088442	2.811678	-0.518972
C	-2.865513	-3.311755	-1.568375
C	-4.288257	-2.128159	0.953897
H	-4.149414	-1.842784	2.009172
H	-4.527201	-1.215129	0.386874
H	-5.164865	-2.793720	0.913094
C	-2.463475	-4.571513	1.269802
H	-1.512901	-5.047136	0.984694
H	-2.424284	-4.363132	2.350857
H	-3.272820	-5.301161	1.109666
C	-1.308379	2.792875	-2.228391
H	-1.915974	3.370747	-2.943168
H	-0.295056	3.222016	-2.214360
H	-1.241224	1.765350	-2.620626
C	-2.394417	4.573017	0.099558
C	-3.656318	1.775943	-0.565211
H	-4.204833	1.799097	0.388829
H	-4.335713	2.118990	-1.361351
H	-3.398608	0.727187	-0.787736
C	-1.096683	5.380194	-0.034652
H	-1.229959	6.393786	0.382152
H	-0.265469	4.901269	0.506548
H	-0.793846	5.494435	-1.087581
C	-2.813013	4.521709	1.574154
H	-3.746907	3.954048	1.715641
H	-2.035516	4.050407	2.193431
H	-2.986319	5.541786	1.959097
C	-3.503743	5.232999	-0.728393
H	-3.252817	5.272728	-1.800819
H	-4.462847	4.700661	-0.625597
H	-3.666427	6.271812	-0.392255
C	-1.652928	-4.138809	-2.014129
H	-0.704377	-3.642029	-1.756310
H	-1.648077	-5.138232	-1.551431
H	-1.668710	-4.282700	-3.108473
C	-2.865826	-1.966969	-2.306452
H	-2.910100	-2.128007	-3.397685
H	-3.736656	-1.350117	-2.031392
H	-1.954335	-1.388936	-2.086650
C	-4.156225	-4.075002	-1.891329
H	-4.212737	-4.291927	-2.972115
H	-4.209231	-5.039977	-1.361549
H	-5.053585	-3.493886	-1.625705
H	5.136483	-0.404161	-2.002746

TS_Siexo_S1_tol_M062X
SCF Energy: -1979.71766251
Num. Imaginary Frequencies: 1

C	-0.489661	0.843267	0.229294
C	-0.898438	0.190505	1.541940
C	-0.696888	-1.319831	1.503015
C	0.767036	-1.756945	1.357355
C	1.403835	-1.284063	0.055415
C	1.005292	0.773544	-0.083690
C	2.768147	-1.508168	-0.173654
C	3.988735	0.731943	-0.113241
C	3.259538	1.253366	0.959171
C	1.857192	1.281156	0.913746
C	3.905576	1.652113	2.269063
C	5.387632	0.328095	-0.158611
C	6.117169	-0.088660	1.096810
C	5.940979	0.194621	-1.387383
C	7.314607	-0.284933	-1.717005
C	1.275776	1.017048	-1.560678
C	3.274720	-1.821695	-1.493257
O	4.412153	-2.172281	-1.749769
O	-1.446691	-1.849900	0.423595
O	-0.897542	2.199938	0.206634
H	-1.003587	0.279742	-0.571136
H	-0.359255	0.633754	2.392681
H	-1.969105	0.392857	1.701713
H	-1.060035	-1.737936	2.461946
H	0.753823	-1.448248	-0.813835
H	3.451805	-1.723500	0.649323
H	3.530487	0.800500	-1.094925
H	1.372001	1.581007	1.848126
H	4.050081	0.795084	2.946350
H	4.882575	2.127596	2.118005
H	3.261952	2.373752	2.791345
H	6.605873	0.753714	1.608977
H	5.421784	-0.548807	1.811525
H	6.888346	-0.834870	0.868737
H	7.984580	-0.310174	-0.849051
H	7.254389	-1.301822	-2.139590
H	1.717732	2.012649	-1.718278

H	1.943933	0.279030	-2.021188
H	0.329220	0.980405	-2.118720
H	2.520994	-1.732641	-2.318693
C	1.572696	-1.471942	2.621866
H	2.571881	-1.926355	2.573386
H	1.701664	-0.395536	2.800492
H	1.063084	-1.900742	3.498112
H	0.709213	-2.855985	1.251954
H	7.773773	0.352806	-2.487209
Si	-2.738003	-2.912278	0.630484
Si	-2.296202	2.713332	-0.579838
C	-3.322422	-3.309312	-1.125282
C	-4.073583	-2.069936	1.647948
H	-4.505047	-1.201468	1.126634
H	-4.891903	-2.768774	1.882366
H	-3.664954	-1.716693	2.608543
C	-2.136254	-4.443169	1.536191
H	-2.939088	-5.191897	1.627182
H	-1.289230	-4.914508	1.015288
H	-1.808353	-4.194885	2.558181
C	-3.723685	1.581178	-0.113419
H	-3.420257	0.532500	-0.267918
H	-4.030997	1.696799	0.937310
H	-4.601976	1.767125	-0.751568
C	-2.045201	2.622576	-2.439215
H	-2.003897	1.576434	-2.782167
H	-2.881219	3.103064	-2.972269
H	-1.113137	3.120061	-2.746732
C	-2.551283	4.491423	0.013381
C	-3.902004	5.018254	-0.486142
H	-4.743678	4.428192	-0.089244
H	-4.050416	6.062894	-0.161546
H	-3.970077	5.005604	-1.586034
C	-2.522492	4.514895	1.546576
H	-1.564827	4.135420	1.932592
H	-2.657890	5.545871	1.917356
H	-3.328109	3.901190	1.981090
C	-1.417251	5.369251	-0.531327
H	-1.436191	5.424707	-1.631355
H	-1.511229	6.400172	-0.147546
H	-0.429900	4.987220	-0.227540
C	-3.533164	-2.000278	-1.896311
H	-4.301491	-1.365575	-1.425908
H	-2.600801	-1.417279	-1.956606
H	-3.867971	-2.212187	-2.926765
C	-2.257166	-4.153837	-1.836073
H	-2.550920	-4.338680	-2.883945
H	-1.278432	-3.648497	-1.848350
H	-2.125191	-5.135094	-1.353798
C	-4.642611	-4.088214	-1.066106
H	-5.447768	-3.494681	-0.604760
H	-4.973946	-4.357952	-2.083867
H	-4.544534	-5.026223	-0.495661
H	5.310743	0.440547	-2.247990

pf_Reendo_S1_tol_M062X
SCF Energy: -1979.81416774
Num. Imaginary Frequencies: 0

C	0.429111	0.637522	-1.752013
C	-1.079807	0.459822	-1.646025
C	-1.467504	-0.438494	-0.475996
C	-0.729832	-1.793210	-0.471323
C	0.791723	-1.522164	-0.536447
C	1.149437	-0.725425	-1.819772
C	1.744005	-2.726134	-0.417027
C	3.226050	-2.243426	-0.261115
C	3.574426	-1.143879	-1.237713
C	2.632410	-0.470486	-1.902470
C	5.040098	-0.855907	-1.403407
C	3.604115	-1.862618	1.177542
C	4.314933	-2.947045	1.943899
C	3.339067	-0.638739	1.661051
C	3.649055	-0.109090	3.028746
C	0.751669	-1.447052	-3.121599
C	1.484580	-3.658603	0.741302
O	1.517141	-4.859441	0.650144
O	-2.860405	-0.661700	-0.505905
O	0.889293	1.351833	-0.624914
H	0.664674	1.191853	-2.680852
H	-1.551280	1.447519	-1.517581
H	-1.487008	0.024164	-2.570088
H	-1.178184	0.077225	0.462604
H	1.019750	-0.853055	0.311079
H	1.684471	-3.350817	-1.321106
H	3.852939	-3.114504	-0.519001
H	2.940147	0.305577	-2.614993
H	5.497429	-0.581548	-0.439598
H	5.574251	-1.747387	-1.770687
H	5.211627	-0.035464	-2.113503
H	5.321984	-3.101000	1.520364
H	4.427138	-2.723936	3.011299
H	3.793042	-3.912166	1.851581
H	4.126955	-0.849941	3.681164
H	4.322007	0.761266	2.962590
H	1.055253	-0.839767	-3.988758
H	1.270961	-2.411577	-3.206727
H	-0.326223	-1.632619	-3.209196
H	1.328366	-3.167661	1.730646
C	-1.194925	-2.588728	0.746888
H	-0.822383	-2.140138	1.682374
H	-2.292774	-2.586053	0.782712
H	-0.883652	-3.640534	0.714246

H	-1.050050	-2.340884	-1.373544
H	2.733493	0.242786	3.529723
Si	1.574670	2.886137	-0.572010
Si	-3.994858	0.141772	0.439843
C	1.000299	3.568988	1.100270
C	3.446148	2.768088	-0.665253
H	3.840380	2.013051	0.032443
H	3.768606	2.486274	-1.679457
H	3.917280	3.735406	-0.428493
C	0.934558	3.912178	-2.009682
H	1.326430	3.544965	-2.971010
H	-0.164696	3.905562	-2.067185
H	1.261567	4.959211	-1.908806
C	-5.624734	-0.746531	0.063515
C	-3.527267	0.005654	2.254955
H	-2.511114	0.391728	2.434266
H	-4.213182	0.604793	2.874518
H	-3.561256	-1.033416	2.616240
C	-4.070123	1.955397	-0.045023
H	-3.152093	2.484594	0.254914
H	-4.192345	2.074567	-1.132244
H	-4.913597	2.462382	0.450498
C	1.513967	2.636190	2.204063
H	1.167869	2.979769	3.194956
H	1.147849	1.607291	2.056695
H	2.615054	2.605142	2.232421
C	-0.532782	3.576046	1.119988
H	-0.951565	4.259990	0.363964
H	-0.929521	2.567083	0.923830
H	-0.908836	3.902640	2.105341
C	1.532593	4.987604	1.328558
H	1.178297	5.689609	0.556859
H	1.190195	5.373995	2.304333
H	2.633786	5.018514	1.333651
C	-5.412714	-2.259753	0.196442
H	-5.086650	-2.541917	1.210834
H	-6.354604	-2.798674	-0.007138
H	-4.653755	-2.618923	-0.514388
C	-6.707050	-0.288556	1.048856
H	-7.672173	-0.767472	0.808312
H	-6.456090	-0.558780	2.086863
H	-6.866022	0.801710	1.013069
C	-6.060406	-0.418684	-1.370306
H	-5.280232	-0.685399	-2.100683
H	-6.972013	-0.983238	-1.633388
H	-6.289398	0.651772	-1.493014
H	2.856700	0.072370	0.977367

pf_Reexo_S1_tol_M062X
SCF Energy: -1979.81828135
Num. Imaginary Frequencies: 0

C	-0.550293	-1.311987	1.156071
C	-0.499153	0.197135	1.326877
C	-0.176589	0.868108	0.001463
C	1.180100	0.392833	-0.525177
C	1.222428	-1.148306	-0.659238
C	0.779391	-1.889791	0.624368
C	2.624885	-1.623892	-1.083155
C	3.711285	-1.488344	0.010381
C	3.165368	-1.625201	1.420446
C	1.858496	-1.775467	1.676589
C	4.190271	-1.718283	2.519486
C	4.581368	-0.254215	-0.233312
C	5.547743	-0.426428	-1.375421
C	4.477015	0.858451	0.506333
C	5.233707	2.142633	0.355234
C	0.543923	-3.390302	0.365317
C	2.606671	-2.989559	-1.735527
O	3.476030	-3.815699	-1.650587
O	-0.150502	2.270134	0.176110
O	-1.588805	-1.638657	0.252672
H	-0.735307	-1.786573	2.141033
H	-1.469256	0.558931	1.702179
H	0.273654	0.475388	2.061452
H	-0.955109	0.580616	-0.733775
H	0.511125	-1.424370	-1.460068
H	2.914965	-0.999160	-1.947961
H	4.382307	-2.354859	-0.134036
H	1.545235	-1.938259	2.715652
H	4.846359	-2.587253	2.346595
H	4.841569	-0.833715	2.554946
H	3.712198	-1.841661	3.500740
H	6.375216	-1.089779	-1.073767
H	5.062499	-0.915998	-2.235139
H	5.979437	0.518393	-1.726297
H	5.779814	2.383693	1.281066
H	5.959390	2.123811	-0.466997
H	-0.150091	-3.544664	-0.473406
H	1.482127	-3.925122	0.168795
H	0.100900	-3.855393	1.260486
H	1.721109	-3.166217	-2.396330
C	1.526152	1.104308	-1.830055
H	0.913433	0.725381	-2.665761
H	1.338580	2.181529	-1.726955
H	2.586100	0.988583	-2.098774
H	1.912741	0.697411	0.237287
H	4.537639	2.978448	0.177570
Si	-1.387193	3.288386	-0.333105
Si	-3.104020	-2.211868	0.708276
C	-0.875768	4.998376	0.297066
C	-1.524895	3.245200	-2.206834
H	-1.654120	2.211197	-2.564603

H	-2.403186	3.817448	-2.545183
H	-0.634998	3.663262	-2.701213
C	-3.017610	2.707612	0.399347
H	-3.843025	3.382711	0.122590
H	-3.270323	1.708459	0.008182
H	-2.978080	2.647831	1.497479
C	-4.070137	-2.306888	-0.916821
C	-3.891905	-1.027725	1.935792
H	-4.908274	-1.359282	2.201908
H	-3.308814	-0.991570	2.870188
H	-3.961348	-0.002698	1.541257
C	-2.935318	-3.896185	1.522019
H	-2.512578	-4.648266	0.839081
H	-2.285105	-3.841588	2.409579
H	-3.917301	-4.259089	1.864867
C	-3.252957	-3.105224	-1.940398
H	-2.285321	-2.621487	-2.142166
H	-3.052319	-4.132456	-1.595847
H	-3.801664	-3.179827	-2.895478
C	-4.302455	-0.887564	-1.450154
H	-4.818932	-0.922541	-2.425270
H	-4.928447	-0.290183	-0.768090
H	-3.350036	-0.353048	-1.598116
C	-5.419084	-2.997449	-0.681389
H	-6.004007	-3.025669	-1.617081
H	-5.292262	-4.037704	-0.342172
H	-6.029042	-2.469124	0.069379
C	0.575336	5.267052	-0.122355
H	0.899633	6.260691	0.233332
H	1.257482	4.513482	0.298965
H	0.695286	5.255556	-1.217835
C	-1.794039	6.072267	-0.298580
H	-1.712115	6.117711	-1.396190
H	-2.852811	5.897618	-0.046113
H	-1.524569	7.068603	0.093127
C	-0.974813	5.022999	1.827537
H	-2.014340	4.903315	2.171832
H	-0.371338	4.222255	2.283382
H	-0.606250	5.986366	2.221245
H	3.750015	0.846417	1.327002

pf_Siendo_S1_tol_M062X
SCF Energy: -1979.81415640
Num. Imaginary Frequencies: 0

C	1.166271	-0.163184	0.722875
C	0.812675	0.880036	1.782338
C	-0.696222	1.099323	1.879796
C	-1.461443	-0.209939	2.134616
C	-1.036250	-1.234414	1.064996
C	0.481081	-1.519051	1.004378
C	-1.833765	-2.548705	1.058362
C	-1.617193	-3.286811	-0.297124
C	-0.158350	-3.272384	-0.709746
C	0.748160	-2.471557	-0.136007
C	0.213285	-4.236756	-1.802375
C	-2.548453	-2.788423	-1.406666
C	-3.860947	-3.523424	-1.493265
C	-2.181943	-1.800087	-2.236904
C	-2.967703	-1.212659	-3.369459
C	1.095262	-2.168309	2.259636
C	-3.291015	-2.254128	1.315483
O	-3.921359	-2.693995	2.242322
O	-1.153903	1.649146	0.657089
O	2.565708	-0.323450	0.647396
H	0.763377	0.197223	-0.244222
H	1.223151	0.572102	2.755659
H	1.294702	1.833806	1.515707
H	-0.906930	1.792645	2.717172
H	-1.275490	-0.736663	0.109335
H	-1.504241	-3.206956	1.875942
H	-1.888090	-4.343905	-0.128880
H	1.794064	-2.534796	-0.456466
H	0.034133	-5.275812	-1.480954
H	-0.398398	-4.069061	-2.702342
H	1.271928	-4.140890	-2.079530
H	-4.275959	-3.729215	-0.494105
H	-4.622663	-2.984299	-2.069615
H	-3.707693	-4.507045	-1.968793
H	-3.991461	-1.601292	-3.434092
H	-3.022887	-0.117035	-3.276070
H	0.479987	-3.007555	2.613907
H	2.088869	-2.565467	2.010108
H	1.232113	-1.466002	3.089989
H	-3.770561	-1.556719	0.584380
C	-1.393874	-0.658773	3.594329
H	-1.838164	-1.656444	3.726619
H	-0.370774	-0.689794	3.989019
H	-1.966358	0.038372	4.224596
H	-2.515674	0.041067	1.926989
H	-2.468602	-1.418170	-4.330273
Si	-1.636023	3.245590	0.443505
Si	3.470199	0.331304	-0.614201
C	-2.237137	3.296644	-1.350698
C	-0.185083	4.398056	0.749138
H	0.200431	4.266017	1.773101
H	0.646169	4.217066	0.050479
H	-0.490150	5.452030	0.652394
C	-3.011109	3.645672	1.658925
H	-3.804364	2.883092	1.633064
H	-2.628936	3.699993	2.690322
H	-3.469410	4.621547	1.432932
C	3.019570	-0.514862	-2.230649

H	3.483183	0.005625	-3.083641
H	3.343845	-1.566351	-2.257948
H	1.928955	-0.496069	-2.388732
C	5.271104	0.013643	-0.129257
C	3.074086	2.161995	-0.769593
H	3.262331	2.708185	0.166965
H	3.672059	2.632179	-1.566322
H	2.012714	2.293271	-1.037146
C	5.433849	-1.467096	0.237084
H	6.479666	-1.679449	0.519950
H	4.789139	-1.741331	1.085384
H	5.181163	-2.129880	-0.606302
C	5.629589	0.879937	1.084609
H	5.592296	1.954411	0.844923
H	4.945372	0.695655	1.927873
H	6.654051	0.654377	1.428698
C	6.193942	0.360306	-1.303978
H	5.994991	-0.275008	-2.181690
H	6.087620	1.411832	-1.617284
H	7.249954	0.208714	-1.020249
C	-3.503561	2.438937	-1.470714
H	-3.324368	1.405267	-1.132492
H	-4.333763	2.850639	-0.875059
H	-3.842598	2.398600	-2.520852
C	-1.144806	2.722817	-2.261874
H	-1.484375	2.716751	-3.312637
H	-0.221139	3.322655	-2.220490
H	-0.890853	1.689010	-1.979983
C	-2.547433	4.740193	-1.764127
H	-2.931062	4.769383	-2.798790
H	-3.313668	5.199873	-1.118970
H	-1.649726	5.377701	-1.728879
H	-1.175467	-1.385991	-2.102184

pf_Siexo_S1_tol_M062X
SCF Energy: -1979.80586693
Num. Imaginary Frequencies: 0

C	0.581622	0.773203	-0.159568
C	0.891501	0.121708	-1.498363
C	0.522839	-1.356409	-1.451255
C	-0.974847	-1.528834	-1.183905
C	-1.367381	-0.834910	0.146606
C	-0.897051	0.639027	0.274351
C	-2.890283	-0.999584	0.418167
C	-3.757119	0.297251	0.351925
C	-3.138609	1.386379	-0.517694
C	-1.806886	1.530846	-0.538931
C	-4.062393	2.358714	-1.195913
C	-5.195265	-0.048426	0.004255
C	-5.438985	-0.686392	-1.341733
C	-6.169480	0.176381	0.898460
C	-7.625424	-0.142614	0.755072
C	-0.946682	1.087542	1.746945
C	-3.113485	-1.646904	1.762895
O	-3.635163	-2.716787	1.927317
O	1.264707	-1.987565	-0.422662
O	0.943548	2.138254	-0.187304
H	1.173696	0.233833	0.604578
H	0.341843	0.638380	-2.300440
H	1.966577	0.230418	-1.710411
H	0.749938	-1.823013	-2.429168
H	-0.814860	-1.394964	0.921515
H	-3.291636	-1.719212	-0.307757
H	-3.792791	0.720261	1.372554
H	-1.350608	2.357299	-1.092610
H	-4.733566	1.866608	-1.915942
H	-4.712427	2.851887	-0.455043
H	-3.492596	3.133973	-1.725855
H	-6.429667	-0.436480	-1.743736
H	-4.688763	-0.355634	-2.073863
H	-5.375123	-1.785632	-1.282686
H	-7.867669	-0.606624	-0.208990
H	-7.945005	-0.836012	1.549040
H	-0.555873	2.111333	1.831082
H	-1.965849	1.090131	2.154114
H	-0.328002	0.425191	2.374859
H	-2.746087	-1.055945	2.641186
C	-1.774529	-1.142509	-2.428787
H	-2.844452	-1.348935	-2.300012
H	-1.673041	-0.081656	-2.691943
H	-1.431940	-1.741453	-3.286926
H	-1.134960	-2.608140	-1.016267
H	-8.240141	0.764800	0.865753
Si	2.547379	-3.037377	-0.716121
Si	2.381858	2.719784	0.467178
C	3.247702	-3.422205	0.999380
C	3.811525	-2.193945	-1.821493
H	4.259778	-1.308757	-1.344246
H	4.625621	-2.886953	-2.086446
H	3.345674	-1.867855	-2.765410
C	1.891234	-4.571317	-1.576771
H	2.671463	-5.341430	-1.682144
H	1.049431	-5.009565	-1.019442
H	1.533389	-4.330215	-2.590283
C	3.818828	1.687724	-0.168024
H	3.679622	0.637952	0.139396
H	3.908122	1.715280	-1.264395
H	4.772994	2.029399	0.263347
C	2.345010	2.575603	2.339828
H	2.163541	1.532815	2.645336
H	3.314203	2.874766	2.769539
H	1.563023	3.201315	2.795390

C	2.462663	4.521431	-0.104892
C	3.688897	5.210034	0.506111
H	4.628540	4.712819	0.215319
H	3.752355	6.257185	0.162427
H	3.642812	5.228413	1.606715
C	2.556653	4.556944	-1.635338
H	1.711714	4.026595	-2.101416
H	2.542287	5.599691	-1.997567
H	3.488825	4.095807	-1.998447
C	1.186221	5.245110	0.342988
H	1.088306	5.263188	1.440155
H	1.198497	6.293383	-0.003234
H	0.285930	4.763171	-0.067592
C	3.541337	-2.103903	1.726430
H	4.294522	-1.501866	1.192502
H	2.630033	-1.494820	1.833548
H	3.937483	-2.302153	2.737641
C	2.215754	-4.227486	1.799105
H	2.582392	-4.409843	2.824274
H	1.255858	-3.693150	1.877474
H	2.019836	-5.209511	1.340476
C	4.542343	-4.233231	0.863664
H	5.325035	-3.669739	0.331270
H	4.941139	-4.488049	1.860899
H	4.381924	-5.180888	0.324375
H	-5.879643	0.632330	1.852809

System I, Toluene, B3LYP-D3

lineal_scis-scis_S1_tol_B3LYPD3
SCF Energy: -1980.62906249
Num. Imaginary Frequencies: 0

C	0.670342	0.317685	0.506206
C	-0.320703	-0.090375	1.602182
C	-1.771732	0.122263	1.157844
C	-2.758814	0.243020	2.355007
C	-4.101677	0.660162	1.831761
C	2.075053	-0.220345	0.728170
C	-5.259852	-0.019037	1.908360
C	4.990151	-1.210149	0.112807
C	3.829713	-1.890013	-0.083441
C	2.529139	-1.194934	-0.091694
H	0.298949	-0.099443	-0.444345
H	-0.106894	0.507686	2.501444
H	-1.813576	1.077869	0.601383
H	-4.108449	1.615762	1.288896
H	4.913098	-0.118042	0.169304
H	1.823266	-1.565846	-0.847704
H	-5.343833	-0.987974	2.407060
C	-6.475870	0.485800	1.260881
O	-7.527886	-0.117802	1.201793
C	2.843182	0.381567	1.873731
H	3.342363	1.316616	1.571904
H	2.172537	0.644641	2.706623
H	3.621100	-0.299856	2.247651
C	3.751239	-3.371803	-0.368830
H	3.425975	-3.935914	0.523428
H	2.998309	-3.570551	-1.151001
H	4.713959	-3.789537	-0.695709
C	6.372531	-1.722903	0.177024
C	7.382693	-0.857785	-0.543016
H	7.160105	-0.814140	-1.623641
H	8.418610	-1.203046	-0.424814
H	7.331347	0.181768	-0.173196
C	6.686618	-2.844810	0.865097
C	8.028215	-3.492777	1.027611
H	8.315449	-3.541592	2.093878
H	8.834917	-2.979898	0.485051
H	7.999740	-4.539201	0.672465
H	-6.369131	1.501076	0.791742
H	-0.185523	-1.153006	1.852751
O	-2.159811	-0.957463	0.328117
O	0.678173	1.743370	0.454320
H	-2.381514	1.093328	2.954745
C	-2.782239	-1.013634	3.224368
H	-1.793908	-1.203982	3.667887
H	-3.503452	-0.913531	4.049996
H	-3.057821	-1.895290	2.627493
Si	-2.715545	-1.058496	-1.258600
C	-2.649974	-3.878211	-1.109111
H	-2.135022	-3.778658	-0.139336
H	-3.176935	-4.850315	-1.107494
H	-1.879030	-3.929197	-1.895917
C	-3.645730	-2.725469	-1.344173
C	-4.739697	-2.777780	-0.261520
H	-4.310747	-2.701838	0.748683
H	-5.481088	-1.969587	-0.368049
H	-5.292205	-3.733646	-0.319441
C	-4.295097	-2.877455	-2.733829
H	-5.039663	-2.087911	-2.931141
H	-4.822423	-3.846222	-2.809048
H	-3.552569	-2.850177	-3.549262
C	-3.843720	0.391553	-1.673909
H	-4.820557	0.303569	-1.174405
H	-4.021164	0.439848	-2.761462
H	-3.395482	1.352891	-1.375687
H	-0.520444	-1.853789	-2.164184
C	-1.250317	-1.078388	-2.446775
H	-0.721188	-0.112968	-2.466440
H	-1.583538	-1.287836	-3.477189
Si	0.852883	2.732692	-0.901006

C	-0.827611	2.952796	-1.724791
H	-1.579441	3.319682	-1.007689
H	-1.195531	2.004245	-2.144967
H	-0.773604	3.676819	-2.555338
C	2.060788	1.964044	-2.121609
H	1.708101	0.973036	-2.452057
H	2.163185	2.593556	-3.021652
H	3.061815	1.827124	-1.682951
C	1.484170	4.394982	-0.202597
C	0.415731	4.994535	0.732460
H	-0.515361	5.240209	0.194959
H	0.159732	4.303113	1.552098
H	0.782921	5.931723	1.190358
C	2.778530	4.158674	0.597981
H	2.602806	3.492980	1.456781
H	3.171314	5.114930	0.990425
H	3.574666	3.709714	-0.019702
C	1.765104	5.372310	-1.360164
H	2.110384	6.346886	-0.968386
H	2.551645	4.998305	-2.037052
H	0.865921	5.569141	-1.968318
H	5.870340	-3.348245	1.395027

lineal_scis-strans_S1_tol_B3LYPD3
SCF Energy: -1980.62830618
Num. Imaginary Frequencies: 0

C	0.664465	0.197393	0.498280
C	-0.352247	-0.122738	1.599907
C	-1.787218	0.172622	1.151459
C	-2.762456	0.377444	2.346868
C	-4.075798	0.876377	1.820180
C	2.034588	-0.413841	0.746131
C	-5.280222	0.287015	1.923240
C	4.881409	-1.561259	0.169256
C	3.695128	-2.207370	-0.004412
C	2.436305	-1.437316	-0.041891
H	0.274375	-0.224935	-0.442485
H	-0.101077	0.478887	2.487019
H	-1.768816	1.118510	0.577714
H	-4.018060	1.816102	1.253290
H	4.815017	-0.469305	0.189037
H	1.711197	-1.789146	-0.788999
H	-5.431424	-0.659592	2.448323
C	-6.462329	0.865355	1.274205
O	-7.559038	0.344897	1.246812
C	2.828644	0.174056	1.881584
H	3.397652	1.060446	1.557135
H	2.167916	0.512447	2.694836
H	3.551903	-0.546833	2.290016
C	3.505759	-3.695289	-0.212729
H	3.249199	-4.203611	0.734143
H	2.658166	-3.873936	-0.895163
H	4.381600	-4.196102	-0.639610
C	6.261555	-2.044428	0.323050
C	6.546829	-3.506222	0.587528
H	6.501467	-4.108469	-0.335191
H	5.814831	-3.932088	1.289723
H	7.544909	-3.656098	1.021139
C	7.250838	-1.115090	0.263340
C	8.729273	-1.311073	0.388663
H	9.243194	-0.991362	-0.536780
H	9.024419	-2.351278	0.585681
H	9.143263	-0.680936	1.197215
H	-6.283554	1.854484	0.772234
H	-0.284198	-1.186393	1.872430
O	-2.244517	-0.894789	0.341049
O	0.753728	1.618503	0.405656
H	-2.328315	1.210064	2.932995
C	-2.867565	-0.860800	3.236467
H	-1.892424	-1.110704	3.679592
H	-3.576291	-0.699003	4.063127
H	-3.204806	-1.731283	2.654919
Si	-2.810684	-0.981412	-1.243092
C	-2.954264	-3.791991	-1.017320
H	-2.446899	-3.703599	-0.042554
H	-3.550037	-4.723353	-0.999390
H	-2.178008	-3.919043	-1.790269
C	-3.860314	-2.577069	-1.297594
C	-4.966993	-2.516837	-0.228452
H	-4.545213	-2.433385	0.784079
H	-5.650134	-1.664403	-0.373479
H	-5.582943	-3.434387	-0.260116
C	-4.503334	-2.720752	-2.690930
H	-5.182679	-1.882832	-2.921541
H	-5.102740	-3.648139	-2.745147
H	-3.751373	-2.774843	-3.496261
C	-3.831686	0.539950	-1.679141
H	-4.806078	0.536238	-1.167388
H	-4.018137	0.578573	-2.765571
H	-3.308966	1.470870	-1.406966
H	-0.682418	-1.948908	-2.144146
C	-1.353309	-1.123798	-2.432136
H	-0.754542	-0.200091	-2.458466
H	-1.701973	-1.315131	-3.460932
Si	1.005114	2.559220	-0.972004
C	-0.651450	2.877071	-1.812789
H	-1.385898	3.291600	-1.103670
H	-1.073132	1.951803	-2.234433
H	-0.545523	3.594133	-2.644391
C	2.162215	1.677916	-2.165073
H	1.750516	0.698520	-2.459727
H	2.298951	2.268278	-3.086802

H	3.154671	1.497395	-1.722878
C	1.746069	4.192367	-0.312562
C	0.709158	4.898963	0.582254
H	-0.191755	5.194395	0.019028
H	0.388536	4.255531	1.418171
H	1.136659	5.821143	1.017777
C	3.005670	3.887975	0.519664
H	2.766662	3.265414	1.395247
H	3.461704	4.825209	0.888955
H	3.776585	3.361657	-0.068268
C	2.118566	5.108253	-1.494347
H	2.527440	6.067392	-1.126361
H	2.887377	4.655629	-2.142953
H	1.247560	5.350371	-2.126727
H	6.944516	-0.075407	0.089841

lineal_strans-scis_S1_tol_B3LYPD3
SCF Energy: -1980.63001957
Num. Imaginary Frequencies: 0

C	0.582290	0.453575	0.718946
C	-0.508684	0.159855	1.753569
C	-1.919689	0.256966	1.166313
C	-3.008926	0.444934	2.264194
C	-4.316618	0.764027	1.602085
C	1.978634	0.154821	1.245976
C	-5.454135	0.047683	1.642666
C	4.671127	-1.958697	-0.197784
C	4.077659	-1.280763	0.825945
C	2.728042	-0.752305	0.576448
H	0.399090	-0.187861	-0.158834
H	-0.403119	0.879086	2.580741
H	-1.946583	1.153083	0.518264
H	-4.311195	1.672995	0.984526
H	4.061577	-2.100010	-1.100815
H	2.267363	-1.159765	-0.331634
H	-5.546282	-0.881975	2.209973
C	-6.629511	0.452863	0.863513
O	-7.652682	-0.194582	0.770377
C	2.377382	0.952801	2.463039
H	1.829886	1.906733	2.471900
H	2.125796	0.426814	3.400717
H	3.448656	1.185365	2.489257
C	4.712709	-1.131138	2.188720
H	5.200874	-0.151672	2.323291
H	3.956451	-1.225811	2.981786
H	5.482054	-1.899238	2.352027
C	6.000551	-2.589810	-0.269659
C	6.013149	-3.910434	-1.008202
H	5.396260	-4.659803	-0.481950
H	7.019858	-4.330397	-1.135954
H	5.570106	-3.792861	-2.013036
C	7.106041	-2.001209	0.244642
C	8.514643	-2.512334	0.252231
H	9.184323	-1.830129	-0.302970
H	8.623289	-3.516724	-0.180610
H	8.907520	-2.549573	1.284677
H	-6.518831	1.432422	0.324667
H	-0.363470	-0.852833	2.159414
O	-2.193956	-0.912886	0.417232
O	0.464019	1.829460	0.358555
H	-2.710403	1.358689	2.812774
C	-3.066715	-0.729739	3.240327
H	-2.116142	-0.838574	3.782731
H	-3.861409	-0.587301	3.988658
H	-3.257537	-1.671698	2.705742
Si	-2.638470	-1.159699	-1.189045
C	-2.458490	-3.953085	-0.827797
H	-2.015269	-3.762179	0.163467
H	-2.938856	-4.948397	-0.791177
H	-1.634292	-4.017623	-1.557680
C	-3.487485	-2.870519	-1.207988
C	-4.647456	-2.898766	-0.195480
H	-4.290900	-2.728976	0.831436
H	-5.415316	-2.137943	-0.409475
H	-5.151666	-3.882486	-0.216038
C	-4.036211	-3.151015	-2.620876
H	-4.800310	-2.414590	-2.921829
H	-4.513973	-4.147316	-2.658068
H	-3.243155	-3.144600	-3.387745
C	-3.792768	0.201400	-1.793065
H	-4.807117	0.092873	-1.380615
H	-3.868667	0.176995	-2.893160
H	-3.419617	1.200653	-1.515364
H	-0.336661	-1.874113	-1.888132
C	-1.098189	-1.178307	-2.274512
H	-0.645329	-0.177284	-2.332190
H	-1.344938	-1.483514	-3.305332
Si	0.848279	2.598276	-1.094202
C	-0.763799	2.926224	-2.012937
H	-1.456103	3.529620	-1.402822
H	-1.274899	1.983258	-2.263389
H	-0.589461	3.465144	-2.959199
C	1.988211	1.531553	-2.145429
H	1.504747	0.585432	-2.437724
H	2.255883	2.061658	-3.075363
H	2.918886	1.280484	-1.614261
C	1.688588	4.243467	-0.599349
C	0.811171	4.967844	0.439540
H	-0.182329	5.225577	0.034915
H	0.654396	4.350244	1.338174
H	1.287319	5.913560	0.758655
C	3.070097	3.949255	0.016197

H	2.997080	3.284726	0.891325
H	3.551845	4.886143	0.352335
H	3.753085	3.474083	-0.707302
C	1.862926	5.139645	-1.840549
H	2.372168	6.082603	-1.568138
H	2.475319	4.656731	-2.621242
H	0.896244	5.413357	-2.294943
H	6.980129	-1.011845	0.697353

lineal_strans-strans_S1_tol_B3LYPD3
SCF Energy: -1980.62928075
Num. Imaginary Frequencies: 0

C	0.561526	0.527633	0.784513
C	-0.570089	0.288119	1.789011
C	-1.954604	0.315920	1.135236
C	-3.096087	0.556936	2.167502
C	-4.376535	0.808474	1.427344
C	1.937923	0.296454	1.391166
C	-5.508411	0.083609	1.474320
C	4.742419	-1.788128	0.163963
C	4.084780	-1.114349	1.154101
C	2.734583	-0.636016	0.816764
H	0.428846	-0.180074	-0.050284
H	-0.513452	1.066538	2.565956
H	-1.967093	1.164334	0.425726
H	-4.352612	1.668283	0.743453
H	4.162005	-1.934018	-0.754950
H	2.322397	-1.108524	-0.082905
H	-5.617179	-0.801258	2.106566
C	-6.653372	0.414770	0.618827
O	-7.667887	-0.247546	0.536321
C	2.269604	1.187110	2.563273
H	3.335666	1.438324	2.621458
H	1.710688	2.130532	2.475859
H	1.980048	0.729336	3.525782
C	4.619997	-0.896319	2.553621
H	5.142851	0.068708	2.663065
H	3.797812	-0.901679	3.282582
H	5.318054	-1.685558	2.852740
C	6.094474	-2.351629	0.066036
C	7.157058	-2.021297	1.091678
H	7.109924	-0.962268	1.384798
H	8.168290	-2.209901	0.706270
H	7.044761	-2.619551	2.011218
C	6.354547	-3.140652	-1.010261
C	7.623608	-3.847045	-1.369363
H	7.456842	-4.938792	-1.422671
H	8.444947	-3.673934	-0.660150
H	7.971859	-3.545436	-2.374488
H	-6.527266	1.350136	0.009412
H	-0.426633	-0.689936	2.272958
O	-2.174932	-0.907809	0.457482
O	0.434066	1.871062	0.317516
H	-2.836852	1.510385	2.666368
C	-3.182151	-0.550968	3.216837
H	-2.254462	-0.610173	3.804668
H	-4.009584	-0.370520	3.920153
H	-3.339355	-1.528812	2.738677
Si	-2.538875	-1.268625	-1.147639
C	-2.371220	-4.023425	-0.560410
H	-1.993443	-3.751569	0.438963
H	-2.848439	-5.017421	-0.476960
H	-1.501624	-4.136357	-1.229129
C	-3.378453	-2.983351	-1.088561
C	-4.600313	-2.943582	-0.152072
H	-4.311033	-2.687240	0.877962
H	-5.358077	-2.211623	-0.475085
H	-5.095696	-3.931598	-0.124257
C	-3.835030	-3.378127	-2.506861
H	-4.579335	-2.672837	-2.913553
H	-4.308055	-4.377330	-2.495374
H	-2.994489	-3.427279	-3.219654
C	-3.669350	0.038748	-1.897465
H	-4.697416	-0.039059	-1.512896
H	-3.707039	-0.072176	-2.994239
H	-3.305544	1.057477	-1.686638
H	-0.208497	-2.024685	-1.684082
C	-0.945748	-1.352230	-2.150655
H	-0.485201	-0.357283	-2.242514
H	-1.139414	-1.717607	-3.173169
Si	0.879388	2.541805	-1.165783
C	-0.683569	2.746892	-2.198384
H	-1.430667	3.366993	-1.676103
H	-1.148044	1.770900	-2.409684
H	-0.468269	3.223295	-3.169443
C	2.108479	1.439266	-2.069056
H	1.668419	0.459805	-2.317241
H	2.415130	1.909151	-3.019125
H	3.012685	1.256320	-1.468935
C	1.639245	4.247072	-0.749760
C	0.681318	5.013800	0.182124
H	-0.295201	5.205106	-0.294372
H	0.493158	4.458410	1.114653
H	1.108006	5.996964	0.454698
C	2.991860	4.048447	-0.039027
H	2.889990	3.450033	0.879838
H	3.424603	5.024440	0.249150
H	3.729329	3.544300	-0.685366
C	1.856662	5.055972	-2.043032
H	2.320697	6.033283	-1.814435
H	2.526898	4.538763	-2.750837
H	0.909556	5.262388	-2.568623

H	5.530467	-3.302498	-1.716928

pp_Reendo_S1_tol_B3LYPD3
SCF Energy: -1980.62511571
Num. Imaginary Frequencies: 0

C	0.074667	0.675436	-1.540201
C	-1.085287	-0.337094	-1.426337
C	-1.443755	-0.917193	-0.045937
C	-0.418819	-1.902130	0.573423
C	0.765959	-1.177351	1.166003
C	1.473308	0.071297	-1.633142
C	1.886650	-1.760636	1.632990
C	4.230427	-1.204930	-0.834077
C	3.868462	0.100070	-0.722271
C	2.468422	0.534824	-0.848382
C	4.827345	1.211734	-0.359862
C	5.558226	-1.825135	-0.648572
C	5.917040	-2.837197	-1.713458
C	6.322016	-1.543429	0.430172
C	7.662102	-2.107926	0.791030
C	1.634382	-0.976904	-2.702206
C	2.952915	-0.960505	2.240412
O	3.967751	-1.406743	2.740135
O	-2.688880	-1.583975	-0.214632
O	-0.045474	1.611914	-0.487561
H	-0.082445	1.177846	-2.519309
H	-1.990344	0.193426	-1.758701
H	-0.947215	-1.173081	-2.128772
H	-1.555035	-0.073721	0.661424
H	0.676782	-0.089239	1.261357
H	2.056768	-2.841124	1.574765
H	3.443097	-1.917950	-1.099071
H	2.200761	1.360507	-0.181607
H	4.721326	1.492568	0.703657
H	5.876454	0.930515	-0.523035
H	4.610437	2.117815	-0.950058
H	6.002752	-2.353794	-2.702826
H	6.858672	-3.366553	-1.513199
H	5.119811	-3.596457	-1.807038
H	8.068755	-2.802033	0.041585
H	8.400312	-1.297455	0.932492
H	2.671684	-1.033898	-3.061636
H	1.355177	-1.983094	-2.342493
H	0.982671	-0.761039	-3.566183
H	2.759800	0.145344	2.226008
C	-1.068967	-2.779371	1.663603
H	-1.455377	-2.159388	2.488400
H	-1.903618	-3.359965	1.249690
H	-0.329766	-3.476042	2.085994
H	-0.061460	-2.578188	-0.225039
H	7.608694	-2.642451	1.756900
Si	-0.297271	3.275310	-0.650089
Si	-4.183252	-1.016088	0.326112
C	-0.512702	3.868818	1.149895
C	1.194385	4.056159	-1.488955
H	2.100448	3.985798	-0.866435
H	1.408589	3.547475	-2.444193
H	1.016971	5.121276	-1.714297
C	-1.833781	3.572176	-1.695631
H	-1.684153	3.207690	-2.726157
H	-2.716935	3.059224	-1.283555
H	-2.065564	4.648579	-1.762832
C	-5.436131	-2.237312	-0.432981
C	-4.235464	-1.022366	2.208529
H	-3.430224	-0.392849	2.623220
H	-5.190861	-0.611090	2.576110
H	-4.118751	-2.035676	2.623934
C	-4.448432	0.752413	-0.267644
H	-3.678771	1.415901	0.159051
H	-4.404383	0.836967	-1.364797
H	-5.428281	1.136458	0.063127
C	0.708259	3.428231	1.980961
H	0.605521	3.765553	3.028699
H	0.815628	2.331987	1.994174
H	1.650415	3.851785	1.594833
C	-1.786599	3.243079	1.750222
H	-2.696359	3.557455	1.212710
H	-1.746312	2.141819	1.730801
H	-1.909246	3.550109	2.805183
C	-0.629059	5.404985	1.176304
H	-1.493143	5.766920	0.593376
H	-0.763170	5.765525	2.212713
H	0.274212	5.895558	0.776241
C	-5.047457	-3.673515	-0.031831
H	-5.059860	-3.817307	1.061758
H	-5.758171	-4.402152	-0.464014
H	-4.039852	-3.933596	-0.392853
C	-6.853876	-1.921293	0.080104
H	-7.590859	-2.613237	-0.367738
H	-6.932179	-2.028462	1.175095
H	-7.172640	-0.897292	-0.179749
C	-5.400066	-2.111181	-1.968189
H	-4.388435	-2.293493	-2.365991
H	-6.080141	-2.847927	-2.434417
H	-5.720714	-1.112392	-2.308948
H	5.903631	-0.854348	1.169945

pp_Reexo_S1_tol_B3LYPD3
SCF Energy: -1980.62285277
Num. Imaginary Frequencies: 0

C	0.217789	0.783200	-1.425931
C	-0.780132	-0.366304	-1.220598

C	-1.205973	-0.742975	0.211531
C	-0.088927	-1.221118	1.175499
C	0.760506	-0.083736	1.670328
C	1.710269	0.467530	-1.284380
C	2.050558	-0.175682	2.042932
C	4.421719	-0.881172	-0.406507
C	3.585180	-1.273992	-1.401771
C	2.193425	-0.780377	-1.467958
C	3.937960	-2.280687	-2.473108
C	5.804138	-1.288489	-0.087790
C	6.628337	-0.163104	0.499014
C	6.245028	-2.560566	-0.225898
C	7.605549	-3.109021	0.084284
C	2.570889	1.682870	-1.072124
C	2.778495	0.996551	2.528993
O	3.975614	1.036488	2.746024
O	-2.170513	-1.777194	0.070231
O	-0.138201	1.860300	-0.557693
H	0.097953	1.116099	-2.478771
H	-1.711639	-0.078476	-1.731980
H	-0.436110	-1.280367	-1.725520
H	-1.666587	0.148997	0.675538
H	0.259461	0.885176	1.778058
H	2.617142	-1.105886	1.936361
H	4.035003	-0.125753	0.281018
H	1.477598	-1.566925	-1.732451
H	5.024047	-2.372318	-2.614681
H	3.548929	-3.285769	-2.226892
H	3.484271	-1.994495	-3.436540
H	6.722914	0.670355	-0.219284
H	6.114545	0.244912	1.387026
H	7.639888	-0.468962	0.797963
H	8.031699	-3.617660	-0.799795
H	8.325830	-2.344058	0.406757
H	2.502270	2.051701	-0.036584
H	3.626920	1.485724	-1.296389
H	2.226249	2.509441	-1.713121
H	2.142446	1.908726	2.683896
C	-0.688802	-1.925125	2.411949
H	-1.336851	-1.241976	2.984519
H	-1.288721	-2.793063	2.107940
H	0.114918	-2.267046	3.081182
H	0.549158	-1.949009	0.647897
H	7.550582	-3.875749	0.879060
Si	-3.835827	-1.661746	0.311549
Si	-0.949123	3.276674	-0.996961
C	-4.500104	-3.328485	-0.335735
C	-4.222647	-1.406306	2.136816
H	-3.750285	-0.482380	2.510676
H	-5.309743	-1.300439	2.292407
H	-3.869625	-2.242103	2.760883
C	-4.527446	-0.192852	-0.642673
H	-5.627010	-0.155782	-0.561144
H	-4.140779	0.749880	-0.222345
H	-4.268341	-0.226073	-1.712330
C	-1.533441	4.020696	0.662428
C	-2.387293	2.866515	-2.141059
H	-2.942639	3.781534	-2.408356
H	-2.024391	2.422679	-3.083594
H	-3.098960	2.159598	-1.689415
C	0.215691	4.446220	-1.901577
H	1.081425	4.731932	-1.283306
H	0.597881	3.983020	-2.826655
H	-0.311547	5.369498	-2.195742
C	-0.322431	4.186878	1.600324
H	0.173826	3.223621	1.797042
H	0.435805	4.869769	1.182417
H	-0.638392	4.606082	2.573266
C	-2.565175	3.085247	1.321318
H	-2.892061	3.492917	2.295532
H	-3.468968	2.963263	0.701479
H	-2.148615	2.082797	1.509132
C	-2.181565	5.396303	0.411028
H	-2.539280	5.833586	1.361228
H	-1.471269	6.115480	-0.029415
H	-3.052852	5.329348	-0.262577
C	-3.759599	-4.477787	0.375186
H	-4.122043	-5.456632	0.010104
H	-2.674544	-4.431930	0.191537
H	-3.916896	-4.460320	1.466935
C	-6.011493	-3.435429	-0.057442
H	-6.237903	-3.405913	1.021623
H	-6.583026	-2.625320	-0.541903
H	-6.409952	-4.390337	-0.447046
C	-4.245150	-3.420662	-1.852568
H	-4.791844	-2.643045	-2.412129
H	-3.174096	-3.316394	-2.091000
H	-4.580108	-4.399223	-2.243585
H	5.526273	-3.307352	-0.578730

pp_Siendo_S1_tol_B3LYPD3
SCF Energy: -1980.62596651
Num. Imaginary Frequencies: 0

C	-0.627865	0.790354	0.674168
C	-1.135535	-0.016216	1.880390
C	-1.097532	-1.551696	1.787974
C	0.231155	-2.298779	2.094766
C	1.215470	-2.294873	0.960820
C	0.877213	0.973607	0.585934
C	2.552273	-2.439104	1.041932
C	3.941905	0.593766	0.012397
C	2.939746	0.639097	-0.905271

C	1.519828	0.555842	-0.528054
C	3.171157	0.732098	-2.397253
C	5.403156	0.635170	-0.192361
C	6.129634	1.530456	0.786783
C	6.012538	-0.130128	-1.124547
C	7.476005	-0.243480	-1.422926
C	1.507368	1.714777	1.734801
C	3.362134	-2.567616	-0.173933
O	4.547597	-2.835450	-0.198710
O	-1.564525	-1.964801	0.514610
O	-1.229783	2.085947	0.767567
H	-0.974355	0.268750	-0.233618
H	-0.648082	0.323669	2.807310
H	-2.197324	0.260777	1.975436
H	-1.789819	-1.899818	2.579877
H	0.760668	-2.256763	-0.034265
H	3.090702	-2.505584	1.992010
H	3.649344	0.529768	1.064128
H	0.885347	0.111060	-1.306076
H	4.178504	1.094848	-2.642079
H	3.048378	-0.254622	-2.879848
H	2.432872	1.405967	-2.863114
H	5.889752	1.238767	1.825151
H	7.222246	1.500642	0.677310
H	5.805520	2.580293	0.675824
H	8.104298	0.439599	-0.833691
H	7.826162	-1.274920	-1.235520
H	1.918333	1.028397	2.495455
H	2.337713	2.353966	1.398426
H	0.758578	2.350160	2.230109
H	2.784876	-2.426371	-1.126513
C	0.818988	-1.931563	3.457960
H	1.584216	-2.657246	3.771641
H	1.290355	-0.937405	3.441127
H	0.036477	-1.924101	4.233629
H	-0.098406	-3.356638	2.146861
H	7.673064	-0.043237	-2.491886
Si	-3.027137	-2.740820	0.182747
Si	-1.940987	2.923956	-0.511854
C	-2.965556	-3.044949	-1.699515
C	-4.448999	-1.615968	0.686479
H	-4.445629	-1.449986	1.777328
H	-4.378663	-0.631306	0.197794
H	-5.426152	-2.057145	0.427109
C	-3.108774	-4.346067	1.162352
H	-2.285639	-5.028684	0.895478
H	-3.042936	-4.147218	2.245725
H	-4.060327	-4.875828	0.987649
C	-0.805555	2.931813	-2.013990
H	-1.224474	3.559525	-2.818971
H	0.197324	3.313204	-1.766480
H	-0.686092	1.914098	-2.420716
C	-2.219342	4.677222	0.188206
C	-3.558892	2.075300	-0.969621
H	-4.254196	2.038290	-0.115530
H	-4.067060	2.587574	-1.803838
H	-3.362425	1.040302	-1.293323
C	-0.852296	5.332060	0.465997
H	-0.985927	6.333011	0.916756
H	-0.246737	4.731472	1.164104
H	-0.263062	5.467000	-0.456470
C	-3.013254	4.576204	1.504810
H	-4.012408	4.133771	1.352672
H	-2.484392	3.958810	2.248065
H	-3.165071	5.579595	1.944343
C	-3.004896	5.531287	-0.824958
H	-2.474019	5.630521	-1.787144
H	-4.003200	5.111906	-1.035382
H	-3.158021	6.553818	-0.432949
C	-1.708050	-3.865971	-2.044472
H	-0.785389	-3.344119	-1.744331
H	-1.708275	-4.853200	-1.552916
H	-1.650592	-4.045173	-3.133889
C	-2.908225	-1.693215	-2.437338
H	-2.833681	-1.851049	-3.529053
H	-3.811135	-1.086744	-2.258681
H	-2.033715	-1.097046	-2.129553
C	-4.223151	-3.818700	-2.140484
H	-4.205488	-3.995264	-3.231633
H	-4.295032	-4.805854	-1.653642
H	-5.151596	-3.266138	-1.917269
H	5.378115	-0.801946	-1.709455

pp_Siexo_S1_tol_B3LYPD3
SCF Energy: -1980.62591506
Num. Imaginary Frequencies: 0

C	-0.012360	0.792785	0.449480
C	-0.533366	0.141521	1.745754
C	-1.018661	-1.312169	1.629986
C	0.061263	-2.410800	1.391716
C	0.580278	-2.426760	-0.013868
C	1.493043	0.801452	0.192750
C	1.854990	-2.595801	-0.413301
C	4.506373	-0.005819	0.194709
C	3.871167	0.757349	1.127159
C	2.395771	0.754201	1.195885
C	4.528432	1.609824	2.191977
C	5.924343	-0.183849	-0.151323
C	6.982101	0.753537	0.387620
C	6.217249	-1.200271	-1.004919
C	7.554763	-1.618920	-1.529559
C	1.831369	0.996272	-1.260568

C	2.187990	-2.628276	-1.838819
O	3.313325	-2.714894	-2.293003
O	-2.007712	-1.385899	0.611705
O	-0.436057	2.159644	0.382800
H	-0.473852	0.236146	-0.386503
H	0.188643	0.220633	2.570401
H	-1.408952	0.727079	2.058934
H	-1.467140	-1.557083	2.612883
H	-0.193955	-2.328182	-0.783568
H	2.687779	-2.687747	0.288501
H	3.850047	-0.624337	-0.422214
H	2.003603	0.748585	2.219239
H	5.544690	1.291769	2.448644
H	4.569686	2.670629	1.885363
H	3.930417	1.583277	3.118559
H	6.629456	1.795936	0.379864
H	7.258269	0.511851	1.427924
H	7.904895	0.714318	-0.207310
H	8.389918	-0.994836	-1.180780
H	7.774694	-2.662225	-1.236279
H	2.865628	1.329782	-1.417492
H	1.690100	0.065446	-1.837163
H	1.151797	1.745527	-1.698060
H	1.303302	-2.563836	-2.526893
C	1.135879	-2.436294	2.478007
H	1.723757	-3.365630	2.428204
H	1.834978	-1.594560	2.378135
H	0.679262	-2.387438	3.479560
H	-0.514773	-3.353042	1.470188
H	7.560559	-1.611480	-2.635120
Si	-3.475867	-2.226727	0.666220
Si	-1.804754	2.746272	-0.407911
C	-4.106256	-2.224900	-1.137815
C	-4.651661	-1.356880	1.849810
H	-4.839114	-0.311300	1.560598
H	-5.622885	-1.877953	1.896591
H	-4.234580	-1.350990	2.871620
C	-3.194445	-3.982588	1.290582
H	-4.156403	-4.512881	1.390578
H	-2.553661	-4.573252	0.616212
H	-2.725943	-3.977280	2.289288
C	-3.345570	2.109343	0.465911
H	-3.289707	1.012465	0.516503
H	-3.416654	2.490756	1.497303
H	-4.272537	2.379276	-0.066140
C	-1.814617	2.155795	-2.198593
H	-1.688133	1.062342	-2.258808
H	-2.771035	2.400287	-2.690209
H	-1.004998	2.616267	-2.787237
C	-1.625084	4.641537	-0.282712
C	-2.793631	5.324845	-1.017678
H	-3.772627	5.045145	-0.592014
H	-2.709688	6.424960	-0.943125
H	-2.811891	5.073339	-2.091782
C	-1.632398	5.053912	1.201935
H	-0.830745	4.549055	1.764948
H	-1.477506	6.144255	1.302456
H	-2.590499	4.816285	1.693858
C	-0.287875	5.067774	-0.918314
H	-0.238125	4.815739	-1.990961
H	-0.150778	6.161989	-0.835583
H	0.567129	4.583133	-0.420689
C	-4.546095	-0.809873	-1.559156
H	-5.368819	-0.425721	-0.933993
H	-3.717685	-0.087849	-1.503735
H	-4.905828	-0.815883	-2.604655
C	-2.979841	-2.701661	-2.075099
H	-3.345263	-2.766071	-3.116401
H	-2.127665	-2.004263	-2.066235
H	-2.600104	-3.700660	-1.801622
C	-5.308438	-3.184729	-1.247133
H	-6.134258	-2.897308	-0.573871
H	-5.713150	-3.177694	-2.275717
H	-5.032840	-4.226598	-1.014350
H	5.377143	-1.807949	-1.362721

TS_Reendo_S1_tol_B3LYPD3
SCF Energy: -1980.59420569
Num. Imaginary Frequencies: 1

C	0.072749	0.795361	-1.524437
C	-1.193966	-0.062128	-1.516648
C	-1.403336	-0.837651	-0.219857
C	-0.250614	-1.807711	0.100458
C	1.068293	-1.060173	0.342845
C	1.383113	-0.012339	-1.396665
C	2.214850	-1.822857	0.674503
C	4.173566	-0.986264	-0.886565
C	3.820590	0.375865	-0.782396
C	2.509488	0.786091	-1.047175
C	4.778346	1.425248	-0.257655
C	5.373371	-1.697067	-0.486097
C	5.577423	-3.017935	-1.200069
C	6.141262	-1.307501	0.568947
C	7.305388	-2.020656	1.173137
C	1.529480	-1.086178	-2.480357
C	3.130759	-1.406406	1.702904
O	4.021721	-2.087178	2.205674
O	-2.623071	-1.559100	-0.327109
O	-0.017494	1.742145	-0.474538
H	0.123006	1.312202	-2.506267
H	-2.056233	0.603887	-1.668594
H	-1.200020	-0.777080	-2.352722

H	-1.456623	-0.110327	0.613099
H	0.928404	-0.169955	0.966862
H	2.311682	-2.856395	0.326863
H	3.526035	-1.588624	-1.513715
H	2.278688	1.813316	-0.756445
H	4.783570	1.462873	0.845407
H	5.812770	1.235513	-0.581854
H	4.485673	2.425474	-0.611874
H	5.438137	-2.911169	-2.288204
H	6.573507	-3.448951	-1.033972
H	4.835998	-3.757211	-0.847324
H	7.634325	-2.903192	0.607901
H	8.167895	-1.339440	1.285066
H	2.397762	-0.877438	-3.123352
H	1.648078	-2.105142	-2.084199
H	0.647868	-1.108545	-3.135995
H	2.968403	-0.348589	2.048665
C	-0.600878	-2.658159	1.334061
H	-0.703169	-2.023048	2.230163
H	-1.550484	-3.189329	1.180367
H	0.184518	-3.399314	1.540748
H	-0.136551	-2.491258	-0.759531
H	7.035709	-2.351664	2.191915
Si	-0.433616	3.374206	-0.582785
Si	-4.068280	-1.134382	0.432175
C	-0.588328	3.909806	1.241081
C	0.930856	4.304383	-1.487472
H	1.873870	4.313271	-0.917437
H	1.136635	3.837231	-2.465703
H	0.641739	5.351443	-1.678796
C	-2.046824	3.571014	-1.532296
H	-1.934423	3.218046	-2.571541
H	-2.872927	3.006636	-1.072537
H	-2.346493	4.631705	-1.580172
C	-5.333750	-2.382393	-0.260497
C	-3.878187	-1.274853	2.300245
H	-3.065092	-0.621322	2.658291
H	-4.800695	-0.958861	2.816098
H	-3.644996	-2.303398	2.617765
C	-4.510948	0.647680	0.009123
H	-3.748495	1.333775	0.412571
H	-4.579962	0.811250	-1.077870
H	-5.476839	0.934548	0.458302
C	0.716577	3.561479	1.983674
H	0.645547	3.853385	3.047619
H	0.929030	2.481285	1.946245
H	1.588678	4.087964	1.560865
C	-1.761873	3.156114	1.896559
H	-2.727900	3.405362	1.427329
H	-1.627554	2.063929	1.835709
H	-1.842682	3.420002	2.967091
C	-0.840017	5.427788	1.319049
H	-1.767631	5.723494	0.799734
H	-0.941156	5.749953	2.371763
H	-0.010945	6.008428	0.880492
C	-4.823005	-3.813475	-0.004197
H	-4.706926	-4.026065	1.071946
H	-5.534985	-4.557140	-0.407929
H	-3.847950	-3.985894	-0.486717
C	-6.696661	-2.187117	0.430466
H	-7.441470	-2.896764	0.025156
H	-6.639804	-2.363054	1.517911
H	-7.100379	-1.171795	0.276373
C	-5.485853	-2.161027	-1.777731
H	-4.520681	-2.260820	-2.300451
H	-6.179194	-2.905527	-2.211141
H	-5.893537	-1.163144	-2.011545
H	5.864359	-0.392604	1.092273

TS_Reexo_S1_tol_B3LYPD3
SCF Energy: -1980.59235685
Num. Imaginary Frequencies: 1

C	-0.031831	1.158434	-1.352137
C	-0.822902	-0.150533	-1.375691
C	-0.894448	-0.841845	-0.014989
C	0.480935	-1.236046	0.557451
C	1.383962	-0.022502	0.789266
C	1.462490	0.979657	-0.996701
C	2.694634	-0.255576	1.264978
C	4.320376	-0.079321	-0.677136
C	3.428470	-0.519893	-1.668489
C	2.147796	0.041094	-1.816342
C	3.726456	-1.735354	-2.529407
C	5.562220	-0.707856	-0.210923
C	6.636574	0.277617	0.192434
C	5.674900	-2.050203	-0.060998
C	6.844798	-2.828253	0.453337
C	2.089262	2.306920	-0.597909
C	3.373455	0.699671	2.117236
O	4.436011	0.516294	2.696862
O	-1.701069	-2.004176	-0.152184
O	-0.648469	2.029128	-0.416253
H	-0.064440	1.607453	-2.366675
H	-1.848824	0.075393	-1.703002
H	-0.409751	-0.860313	-2.107647
H	-1.353350	-0.135008	0.702894
H	0.866794	0.827269	1.253958
H	3.124992	-1.257661	1.235948
H	4.241941	0.963054	-0.388290
H	1.519933	-0.497039	-2.533444
H	4.805711	-1.883871	-2.675273
H	3.324459	-2.664215	-2.089364

H	3.257434	-1.623001	-3.519560
H	6.813643	1.020161	-0.604015
H	6.304778	0.824908	1.090345
H	7.596714	-0.200931	0.427227
H	7.092827	-3.658658	-0.231971
H	7.750076	-2.221817	0.594451
H	1.498768	2.801866	0.182138
H	3.119074	2.232447	-0.241643
H	2.097966	2.970996	-1.480131
H	2.834099	1.679316	2.233375
C	0.300919	-2.017472	1.869719
H	-0.177259	-1.386998	2.638389
H	-0.332802	-2.900563	1.709431
H	1.268199	-2.353092	2.271087
H	0.970886	-1.901763	-0.175018
H	6.601363	-3.295971	1.425398
Si	-3.291745	-2.154849	0.388029
Si	-1.640381	3.351271	-0.758011
C	-3.835078	-3.864429	-0.260995
C	-3.346692	-2.059299	2.267928
H	-2.921993	-1.105029	2.621985
H	-4.386050	-2.108792	2.634417
H	-2.778764	-2.875023	2.742480
C	-4.340412	-0.753680	-0.310324
H	-5.396051	-0.859714	-0.007838
H	-3.986706	0.214771	0.079323
H	-4.304842	-0.715477	-1.410494
C	-2.269276	3.889409	0.960470
C	-3.038734	2.825339	-1.903636
H	-3.720038	3.669185	-2.105870
H	-2.641957	2.488421	-2.876434
H	-3.635477	2.002378	-1.480486
C	-0.625867	4.694363	-1.600363
H	0.187404	5.062237	-0.954819
H	-0.170633	4.312900	-2.530098
H	-1.257426	5.555375	-1.877038
C	-1.063629	4.123546	1.891365
H	-0.465164	3.207307	2.016741
H	-0.392726	4.913021	1.513046
H	-1.404860	4.439883	2.894266
C	-3.158159	2.778105	1.552042
H	-3.496879	3.052342	2.568063
H	-4.061798	2.602728	0.945259
H	-2.614379	1.822883	1.633013
C	-3.085319	5.189966	0.832269
H	-3.470146	5.504314	1.819817
H	-2.478281	6.023305	0.440442
H	-3.958417	5.069985	0.168283
C	-2.829887	-4.928899	0.219730
H	-3.118197	-5.929869	-0.151609
H	-1.812443	-4.715537	-0.144284
H	-2.785983	-4.991196	1.320202
C	-5.241718	-4.203366	0.267622
H	-5.268412	-4.260307	1.368836
H	-5.995159	-3.461264	-0.047480
H	-5.573867	-5.185458	-0.116790
C	-3.852399	-3.840799	-1.801532
H	-4.594868	-3.126958	-2.196276
H	-2.868170	-3.564699	-2.213794
H	-4.114549	-4.837577	-2.202236
H	4.796199	-2.658738	-0.296559

TS_Siendo_S1_tol_B3LYPD3
SCF Energy: -1980.58991061
Num. Imaginary Frequencies: 1

C	-0.661525	0.735386	0.595596
C	-1.349090	0.012264	1.751157
C	-1.019293	-1.477083	1.793952
C	0.473237	-1.766371	2.039502
C	1.355068	-1.248951	0.890253
C	0.876633	0.720788	0.628650
C	2.764595	-1.408134	0.964415
C	3.793525	0.845312	-0.078755
C	2.779391	0.962095	-1.053744
C	1.436468	0.928426	-0.669864
C	3.077948	1.000529	-2.537826
C	5.223611	0.649311	-0.203726
C	6.017740	1.049584	1.023138
C	5.784458	-0.021269	-1.248725
C	7.211084	-0.423033	-1.423166
C	1.450760	1.471578	1.834344
C	3.514590	-1.965657	-0.126857
O	4.691400	-2.322454	-0.098901
O	-1.398504	-2.071435	0.558082
O	-1.094536	2.093378	0.590377
H	-0.970478	0.225092	-0.332833
H	-1.089934	0.492361	2.706778
H	-2.435277	0.135714	1.622505
H	-1.582615	-1.935799	2.630109
H	0.937222	-1.596090	-0.060088
H	3.295861	-1.318983	1.916294
H	3.495916	1.099495	0.932032
H	0.722132	0.863980	-1.497775
H	3.998475	1.563293	-2.755032
H	3.207441	-0.011443	-2.958902
H	2.248922	1.474002	-3.085717
H	5.882519	0.299163	1.822480
H	7.095624	1.130705	0.829342
H	5.678331	2.018780	1.422543
H	7.888841	-0.014824	-0.661300
H	7.279932	-1.524701	-1.383134
H	2.240256	0.923007	2.363745

H	1.868702	2.440126	1.518823
H	0.660194	1.693604	2.563385
H	2.918863	-2.074239	-1.074821
C	0.902484	-1.408388	3.464954
H	1.951281	-1.683920	3.649600
H	0.791811	-0.340452	3.693378
H	0.288324	-1.964785	4.191888
H	0.555109	-2.865212	1.949877
H	7.584964	-0.122621	-2.418387
Si	-2.745575	-3.043480	0.275032
Si	-2.147398	2.776478	-0.535884
C	-2.728295	-3.297523	-1.615973
C	-4.302737	-2.160494	0.862068
H	-4.259780	-1.975865	1.949032
H	-4.440813	-1.188549	0.362074
H	-5.202108	-2.770472	0.672248
C	-2.548573	-4.659616	1.218941
H	-1.630323	-5.191007	0.920183
H	-2.485843	-4.469810	2.304272
H	-3.404538	-5.335553	1.054499
C	-1.364510	2.768583	-2.249427
H	-1.983219	3.331237	-2.969142
H	-0.358997	3.218236	-2.237495
H	-1.272294	1.740363	-2.637387
C	-2.417380	4.547643	0.117859
C	-3.741216	1.773076	-0.595038
H	-4.249296	1.743378	0.382061
H	-4.447838	2.186175	-1.334577
H	-3.522969	0.735930	-0.898766
C	-1.067196	5.290592	0.121385
H	-1.185180	6.308266	0.537710
H	-0.316506	4.763979	0.732676
H	-0.653619	5.401110	-0.895138
C	-2.963943	4.475683	1.556625
H	-3.946122	3.975243	1.601353
H	-2.278181	3.927006	2.221600
H	-3.097089	5.491649	1.972423
C	-3.420270	5.296921	-0.779431
H	-3.065979	5.380796	-1.820813
H	-4.407158	4.804196	-0.800228
H	-3.578785	6.326062	-0.407497
C	-1.392354	-3.943908	-2.030737
H	-0.531168	-3.322108	-1.737757
H	-1.255047	-4.939620	-1.576972
H	-1.351244	-4.077716	-3.127549
C	-2.868991	-1.930830	-2.314283
H	-2.828346	-2.050586	-3.412670
H	-3.827654	-1.440446	-2.077271
H	-2.057395	-1.243313	-2.026184
C	-3.896693	-4.211623	-2.031608
H	-3.898378	-4.364462	-3.126583
H	-3.828915	-5.209194	-1.565689
H	-4.876835	-3.782073	-1.763218
H	5.126778	-0.366341	-2.046599

TS_Siexo_S1_tol_B3LYPD3
SCF Energy: -1980.59514461
Num. Imaginary Frequencies: 1

C	-0.517657	0.724882	0.300889
C	-0.934130	0.079506	1.620139
C	-0.774928	-1.440968	1.582568
C	0.681984	-1.914571	1.417158
C	1.304461	-1.451936	0.095981
C	0.969592	0.569092	-0.060054
C	2.666435	-1.745920	-0.160717
C	4.011675	0.574568	-0.117761
C	3.261629	1.097566	0.953734
C	1.862604	1.123732	0.903346
C	3.904479	1.527686	2.259635
C	5.382231	0.118728	-0.181381
C	6.155405	-0.219508	1.073631
C	5.872711	-0.137514	-1.431202
C	7.198646	-0.699563	-1.816187
C	1.183768	0.794304	-1.553101
C	3.168812	-2.059397	-1.468008
O	4.323424	-2.399100	-1.729622
O	-1.542651	-1.955687	0.500040
O	-0.837324	2.113172	0.313397
H	-1.090997	0.211840	-0.489068
H	-0.370733	0.506974	2.463656
H	-1.994419	0.318689	1.794141
H	-1.143455	-1.851757	2.542618
H	0.637173	-1.655424	-0.750930
H	3.364018	-1.920579	0.659939
H	3.537639	0.629729	-1.091617
H	1.383266	1.473162	1.822674
H	4.141709	0.670091	2.910876
H	4.836926	2.086665	2.098524
H	3.220768	2.181010	2.822645
H	6.523823	0.675250	1.599003
H	5.519703	-0.773155	1.781007
H	7.024546	-0.853895	0.856296
H	7.888389	-0.837148	-0.972292
H	7.047680	-1.679671	-2.302525
H	1.358434	1.863084	-1.756598
H	2.025511	0.234628	-1.975339
H	0.289394	0.487165	-2.115223
H	2.413495	-1.970707	-2.296392
C	1.517885	-1.647378	2.672421
H	2.498888	-2.141338	2.615632
H	1.697700	-0.575591	2.835414
H	1.006275	-2.042506	3.565302

H	0.597440	-3.012457	1.312601
H	7.694581	-0.052324	-2.561385
Si	-2.988392	-2.814582	0.609973
Si	-2.148845	2.827897	-0.469991
C	-3.576986	-2.945049	-1.200525
C	-4.206851	-1.866684	1.689632
H	-4.398397	-0.853043	1.303067
H	-5.174068	-2.393014	1.755810
H	-3.821333	-1.765488	2.718474
C	-2.646327	-4.498070	1.377873
H	-3.566273	-5.098631	1.475627
H	-1.922778	-5.074489	0.778614
H	-2.222325	-4.380978	2.390035
C	-3.759281	2.119145	0.204246
H	-3.832679	1.047388	-0.042873
H	-3.830939	2.222989	1.298769
H	-4.635943	2.616925	-0.243816
C	-2.069484	2.479381	-2.319186
H	-2.144195	1.397433	-2.519155
H	-2.910174	2.963035	-2.844981
H	-1.132119	2.842487	-2.769248
C	-1.941167	4.682190	-0.075839
C	-3.049546	5.500647	-0.764121
H	-4.057226	5.202363	-0.427780
H	-2.936366	6.576249	-0.534051
H	-3.019822	5.399850	-1.862246
C	-2.019792	4.883882	1.449823
H	-1.254853	4.290130	1.975692
H	-1.857535	5.946390	1.709864
H	-3.005098	4.597059	1.854593
C	-0.561238	5.147440	-0.580405
H	-0.467528	5.051827	-1.675393
H	-0.395846	6.212128	-0.331522
H	0.253679	4.564020	-0.122810
C	-3.839560	-1.530602	-1.753192
H	-4.648795	-1.015950	-1.209288
H	-2.938876	-0.898513	-1.694242
H	-4.141731	-1.578403	-2.815586
C	-2.480589	-3.623708	-2.044112
H	-2.792651	-3.690701	-3.102742
H	-1.534431	-3.060299	-2.009602
H	-2.270107	-4.650788	-1.702020
C	-4.872659	-3.775543	-1.271003
H	-5.690054	-3.322145	-0.684822
H	-5.226881	-3.852944	-2.315449
H	-4.726067	-4.804465	-0.901459
H	5.214654	0.086329	-2.276389

pf_Reendo_S1_tol_B3LYPD3
SCF Energy: -1980.67262444
Num. Imaginary Frequencies: 0

C	0.448072	0.609960	-1.791861
C	-1.056691	0.380984	-1.680592
C	-1.414515	-0.491722	-0.478354
C	-0.634732	-1.829539	-0.435025
C	0.886980	-1.519377	-0.521516
C	1.223227	-0.732993	-1.828052
C	1.883699	-2.693871	-0.377676
C	3.360405	-2.156910	-0.240479
C	3.669666	-1.071749	-1.251480
C	2.701172	-0.434580	-1.919656
C	5.128282	-0.748889	-1.438567
C	3.743578	-1.727263	1.189517
C	4.521049	-2.759246	1.968069
C	3.422375	-0.505470	1.654220
C	3.710226	0.075509	3.007006
C	0.852902	-1.503208	-3.120019
C	1.658978	-3.624446	0.791619
O	1.711692	-4.831343	0.712478
O	-2.809326	-0.752327	-0.489882
O	0.883101	1.368975	-0.673581
H	0.662751	1.153123	-2.731929
H	-1.563556	1.354043	-1.588616
H	-1.447155	-0.097822	-2.590872
H	-1.135766	0.061469	0.439043
H	1.098873	-0.829829	0.310089
H	1.844982	-3.332643	-1.272926
H	4.007800	-3.017306	-0.484020
H	2.979379	0.338156	-2.646812
H	5.589311	-0.437964	-0.485733
H	5.688232	-1.635357	-1.786824
H	5.279014	0.059471	-2.170083
H	5.518248	-2.902135	1.512957
H	4.669851	-2.491651	3.022923
H	4.030466	-3.746433	1.938198
H	4.251365	-0.609767	3.674724
H	4.312189	0.997367	2.915847
H	1.115300	-0.901671	-4.005762
H	1.418896	-2.443143	-3.190397
H	-0.214940	-1.749311	-3.194308
H	1.509828	-3.123569	1.778859
C	-1.065174	-2.606957	0.812879
H	-0.703782	-2.120516	1.734267
H	-2.161861	-2.648020	0.862669
H	-0.712082	-3.646824	0.807585
H	-0.946223	-2.415042	-1.316358
H	2.775516	0.371622	3.514184
Si	1.384229	2.972961	-0.579524
Si	-3.993658	0.076490	0.377446
C	0.728317	3.568200	1.114445
C	3.262156	3.043072	-0.662800
H	3.723072	2.375738	0.082515

H	3.615905	2.721781	-1.656457
H	3.639526	4.065044	-0.489405
C	0.644406	3.958388	-2.004064
H	1.040535	3.615753	-2.974775
H	-0.453919	3.874806	-2.040135
H	0.898027	5.027819	-1.910738
C	-5.570873	-0.965533	0.109487
C	-3.497508	0.168303	2.192596
H	-2.544799	0.710546	2.313672
H	-4.255647	0.711065	2.781858
H	-3.372631	-0.832462	2.636256
C	-4.197413	1.823668	-0.298193
H	-3.308423	2.436838	-0.078951
H	-4.345399	1.818718	-1.390156
H	-5.064055	2.330057	0.159904
C	1.323043	2.678506	2.222303
H	0.934808	2.978573	3.213396
H	1.065643	1.618570	2.070807
H	2.421426	2.753277	2.268081
C	-0.806101	3.435012	1.130253
H	-1.287509	4.075831	0.372782
H	-1.118871	2.396558	0.940143
H	-1.215086	3.730671	2.113986
C	1.126210	5.035389	1.359112
H	0.710515	5.712815	0.594034
H	0.747811	5.381823	2.338618
H	2.220663	5.172506	1.368552
C	-5.296234	-2.424599	0.521131
H	-5.009294	-2.510501	1.582808
H	-6.201147	-3.043948	0.377956
H	-4.488792	-2.868256	-0.082014
C	-6.724946	-0.398728	0.958308
H	-7.649746	-0.981629	0.792159
H	-6.505324	-0.440764	2.038468
H	-6.954669	0.650062	0.704077
C	-5.957587	-0.924095	-1.381826
H	-5.138840	-1.288943	-2.023357
H	-6.840026	-1.563020	-1.571696
H	-6.217048	0.095068	-1.714161
H	2.897094	0.167718	0.967325

pf_Reexo_S1_tol_B3LYPD3
SCF Energy: -1980.67548289
Num. Imaginary Frequencies: 0

C	-0.537008	-1.340782	1.191387
C	-0.475757	0.175045	1.326526
C	-0.206959	0.816620	-0.028805
C	1.124910	0.326612	-0.615626
C	1.214357	-1.226286	-0.667662
C	0.791826	-1.935031	0.652402
C	2.637792	-1.680647	-1.078487
C	3.728544	-1.483884	0.012128
C	3.191460	-1.629080	1.427205
C	1.885160	-1.795950	1.691115
C	4.227505	-1.701221	2.520753
C	4.556708	-0.216834	-0.247389
C	5.555959	-0.373689	-1.365993
C	4.389184	0.911113	0.464624
C	5.080615	2.232114	0.303152
C	0.558382	-3.450059	0.433997
C	2.660582	-3.062443	-1.702657
O	3.542502	-3.879750	-1.584407
O	-0.159722	2.229985	0.118650
O	-1.594857	-1.682010	0.304239
H	-0.713815	-1.790454	2.188775
H	-1.426211	0.550986	1.734006
H	0.325159	0.465524	2.025381
H	-1.022346	0.525572	-0.717952
H	0.510556	-1.558717	-1.451512
H	2.912088	-1.073620	-1.960883
H	4.429216	-2.327659	-0.125127
H	1.579092	-1.960860	2.732035
H	4.882849	-2.577188	2.363860
H	4.886243	-0.818892	2.527437
H	3.766606	-1.797818	3.515673
H	6.369428	-1.055336	-1.058244
H	5.095476	-0.836805	-2.255931
H	6.012045	0.573896	-1.682815
H	5.618934	2.511607	1.226903
H	5.804631	2.253416	-0.523957
H	-0.167606	-3.629832	-0.371466
H	1.491912	-3.980010	0.203262
H	0.159353	-3.907262	1.354006
H	1.788817	-3.262324	-2.380651
C	1.370763	0.967659	-1.983998
H	0.670187	0.574396	-2.741399
H	1.229438	2.055187	-1.922561
H	2.395353	0.799473	-2.347678
H	1.894757	0.696085	0.074460
H	4.340823	3.033628	0.124842
Si	-1.382842	3.298489	-0.327222
Si	-3.139694	-2.209201	0.722577
C	-0.774647	4.982665	0.331993
C	-1.580851	3.300251	-2.200654
H	-1.789139	2.281900	-2.569706
H	-2.425190	3.939043	-2.510494
H	-0.674787	3.662363	-2.712294
C	-3.015594	2.766149	0.448481
H	-3.820353	3.484679	0.217789
H	-3.326379	1.788454	0.045042
H	-2.942829	2.677400	1.543907
C	-4.079312	-2.214640	-0.938758

C	-3.911928	-1.030009	1.972131
H	-4.937111	-1.345340	2.230527
H	-3.329999	-1.018043	2.909389
H	-3.960604	0.003134	1.593862
C	-3.033875	-3.926886	1.485654
H	-2.605594	-4.662122	0.785905
H	-2.398920	-3.913046	2.387675
H	-4.029331	-4.288346	1.794223
C	-3.304075	-3.073280	-1.956532
H	-2.290507	-2.677958	-2.128366
H	-3.203442	-4.120522	-1.625274
H	-3.828514	-3.088572	-2.929918
C	-4.186923	-0.772081	-1.470209
H	-4.690101	-0.757730	-2.454672
H	-4.773695	-0.125064	-0.797354
H	-3.193978	-0.312057	-1.600585
C	-5.491474	-2.797322	-0.739205
H	-6.050533	-2.793199	-1.693071
H	-5.462997	-3.841355	-0.384567
H	-6.084306	-2.213346	-0.014628
C	0.641468	5.254437	-0.212415
H	1.023937	6.220023	0.167534
H	1.349081	4.467639	0.094038
H	0.658986	5.309479	-1.314085
C	-1.728815	6.103108	-0.122509
H	-1.772246	6.190467	-1.221268
H	-2.758699	5.946224	0.241478
H	-1.392685	7.081323	0.268441
C	-0.725897	4.935260	1.871339
H	-1.726504	4.791785	2.312745
H	-0.079463	4.118130	2.230935
H	-0.324181	5.882474	2.276744
H	3.646620	0.887894	1.270824

pf_Siendo_S1_tol_B3LYPD3
SCF Energy: -1980.67301692
Num. Imaginary Frequencies: 0

C	1.141090	-0.205341	0.734475
C	0.832781	0.818061	1.833020
C	-0.670963	1.079520	1.967791
C	-1.474646	-0.218011	2.201757
C	-1.093711	-1.229113	1.092466
C	0.421771	-1.559566	0.990347
C	-1.938067	-2.519925	1.037547
C	-1.756166	-3.213026	-0.357612
C	-0.293748	-3.252440	-0.767467
C	0.642968	-2.492734	-0.179843
C	0.038862	-4.206219	-1.885278
C	-2.657172	-2.630069	-1.460132
C	-3.978123	-3.339593	-1.626632
C	-2.253087	-1.594050	-2.218251
C	-2.991718	-0.905794	-3.326939
C	1.039032	-2.267122	2.219968
C	-3.387159	-2.209917	1.328069
O	-4.023084	-2.684967	2.241203
O	-1.144013	1.673315	0.762700
O	2.542896	-0.390812	0.624548
H	0.732369	0.193779	-0.212150
H	1.247451	0.467666	2.790289
H	1.343445	1.762361	1.591225
H	-0.845206	1.758246	2.825058
H	-1.332063	-0.687708	0.164044
H	-1.613705	-3.225362	1.816986
H	-2.079468	-4.260681	-0.224370
H	1.682811	-2.582696	-0.508163
H	-0.185373	-5.248038	-1.593067
H	-0.566294	-3.993446	-2.782726
H	1.101317	-4.153022	-2.167506
H	-4.465051	-3.531594	-0.655587
H	-4.693512	-2.791942	-2.255404
H	-3.817558	-4.332373	-2.085730
H	-4.017501	-1.274313	-3.470310
H	-3.044995	0.180032	-3.140955
H	0.430891	-3.130383	2.527088
H	2.041872	-2.637904	1.964028
H	1.156263	-1.607106	3.088050
H	-3.858189	-1.467226	0.634120
C	-1.418856	-0.702702	3.654872
H	-1.944113	-1.662249	3.775131
H	-0.396284	-0.832339	4.032088
H	-1.919323	0.027027	4.312620
H	-2.521740	0.072289	2.010687
H	-2.455287	-1.027229	-4.285637
Si	-1.488863	3.295015	0.473361
Si	3.468953	0.239077	-0.639267
C	-2.117695	3.293349	-1.329194
C	0.062835	4.341750	0.682358
H	0.459860	4.247948	1.707502
H	0.861482	4.042433	-0.014751
H	-0.153404	5.410344	0.513813
C	-2.801738	3.878901	1.690146
H	-3.675890	3.207597	1.690733
H	-2.401497	3.908986	2.717880
H	-3.152727	4.896302	1.447746
C	3.016170	-0.616944	-2.254914
H	3.536754	-0.150225	-3.108281
H	3.273538	-1.688084	-2.245364
H	1.932826	-0.536321	-2.445417
C	5.268852	-0.111121	-0.116488
C	3.113382	2.080385	-0.822573
H	3.307962	2.636437	0.107914
H	3.728841	2.527023	-1.621635

H	2.057313	2.235176	-1.098899
C	5.439247	-1.622649	0.130384
H	6.471933	-1.847970	0.455383
H	4.755341	-1.984118	0.914670
H	5.249093	-2.216078	-0.779770
C	5.574716	0.654102	1.185393
H	5.508161	1.746558	1.048472
H	4.878485	0.373539	1.992319
H	6.599939	0.431638	1.534983
C	6.235414	0.344287	-1.226150
H	6.062793	-0.194086	-2.173426
H	6.150600	1.424434	-1.434839
H	7.283320	0.152724	-0.929835
C	-3.460810	2.540553	-1.394573
H	-3.368752	1.507517	-1.022149
H	-4.244170	3.042536	-0.802507
H	-3.826531	2.489460	-2.436683
C	-1.085886	2.579196	-2.224273
H	-1.431955	2.556949	-3.274179
H	-0.108560	3.090992	-2.217518
H	-0.921245	1.539140	-1.902118
C	-2.312914	4.740414	-1.819827
H	-2.701183	4.749436	-2.855053
H	-3.035716	5.297139	-1.199048
H	-1.367383	5.308240	-1.822846
H	-1.245601	-1.204114	-2.032512

pf_Siexo_S1_tol_B3LYPD3
SCF Energy: -1980.66308881
Num. Imaginary Frequencies: 0

C	0.595929	0.700142	-0.220321
C	0.883129	0.054552	-1.571721
C	0.497189	-1.424067	-1.538726
C	-1.005675	-1.583429	-1.259333
C	-1.376294	-0.900709	0.092127
C	-0.885250	0.574228	0.241835
C	-2.904576	-1.059550	0.386366
C	-3.760564	0.252355	0.351620
C	-3.139934	1.349918	-0.515401
C	-1.804386	1.487874	-0.540464
C	-4.059778	2.330289	-1.191595
C	-5.221354	-0.063356	0.049357
C	-5.527172	-0.722860	-1.277146
C	-6.164530	0.209041	0.969792
C	-7.637321	-0.059933	0.886914
C	-0.902070	0.995723	1.731673
C	-3.095374	-1.750691	1.717474
O	-3.516311	-2.874211	1.854285
O	1.232986	-2.079627	-0.511649
O	0.973612	2.068408	-0.241859
H	1.195221	0.152478	0.528074
H	0.331420	0.583801	-2.363861
H	1.954637	0.156651	-1.798944
H	0.717588	-1.884404	-2.521020
H	-0.819288	-1.480734	0.846881
H	-3.313912	-1.762223	-0.349175
H	-3.751425	0.666017	1.376411
H	-1.345659	2.317557	-1.085718
H	-4.705185	1.850205	-1.945532
H	-4.742569	2.796874	-0.460400
H	-3.491675	3.130373	-1.690286
H	-6.523217	-0.454152	-1.657899
H	-4.791999	-0.439575	-2.044157
H	-5.496750	-1.823642	-1.195420
H	-7.946284	-0.507478	-0.068541
H	-7.951529	-0.749025	1.691707
H	-0.507713	2.016187	1.832983
H	-1.911625	0.990634	2.162469
H	-0.273403	0.322083	2.337967
H	-2.793519	-1.143763	2.613084
C	-1.824025	-1.175878	-2.491642
H	-2.891557	-1.393060	-2.356486
H	-1.737466	-0.107227	-2.729232
H	-1.488406	-1.749639	-3.371672
H	-1.173320	-2.663219	-1.101299
H	-8.218649	0.868348	1.032796
Si	2.594581	-3.054073	-0.695530
Si	2.415610	2.690911	0.372723
C	3.297186	-3.196414	1.073709
C	3.814820	-2.240046	-1.878528
H	4.129193	-1.242951	-1.531578
H	4.721152	-2.857875	-1.996737
H	3.369750	-2.121491	-2.881080
C	2.069705	-4.721693	-1.391375
H	2.932090	-5.391990	-1.544632
H	1.354808	-5.229600	-0.723556
H	1.575908	-4.591990	-2.369863
C	3.885250	1.855057	-0.459249
H	3.911734	0.784603	-0.197030
H	3.844268	1.937516	-1.557008
H	4.837636	2.296396	-0.119733
C	2.520078	2.366739	2.225160
H	2.454042	1.286443	2.436749
H	3.484173	2.718224	2.630114
H	1.713769	2.868176	2.783337
C	2.316130	4.552984	-0.029593
C	3.546770	5.280192	0.544675
H	4.491648	4.894428	0.125510
H	3.504091	6.359467	0.308164
H	3.606638	5.191357	1.642591
C	2.271678	4.738486	-1.558640
H	1.416951	4.206303	-2.006738

H	2.172129	5.809090	-1.817079
H	3.189780	4.370552	-2.046948
C	1.033143	5.138584	0.591432
H	1.024692	5.045448	1.690529
H	0.945993	6.215569	0.355933
H	0.130644	4.637631	0.206984
C	3.770167	-1.807988	1.546798
H	4.597374	-1.418571	0.930566
H	2.953022	-1.069216	1.519052
H	4.136460	-1.856200	2.588829
C	2.192802	-3.705089	2.020122
H	2.574960	-3.782601	3.054853
H	1.325574	-3.025872	2.033153
H	1.828207	-4.705493	1.732649
C	4.484534	-4.177998	1.088792
H	5.301368	-3.854261	0.421234
H	4.909521	-4.256274	2.106488
H	4.185458	-5.194735	0.783307
H	-5.832955	0.673798	1.907631