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SUPPORTING INFORMATION

Synthesis of the Octahydronaphthalene Core of Nahuoic Acid A via a $B(C_6F_5)_3$-Catalyzed Intramolecular Diels-Alder (IMDA) Reaction

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TABLE OF CONTENTS

1. GENERAL METHODS

General. 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) wasperformed on aluminium plates with Merck Kieselgel 60F_{254} and visualized byUV irradiation (254 nm) or by staining with solution of phosphomolibdic acid (in EtOH). 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 Bruker AMX-400 at 400.13 and 100.13, 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 signal in the ^{13}C NMR spectra. Different NOESY and NOE experiments were also performed in selected cases.
Crystallographic data were collected at room temperature using a Bruker Smart 6000 CCD detector and Cu-Kα radiation(λ= 1.54178 Å) generated by a Incoatec microfocus source equipped with Incoatec Quazar MX optics. The software APEX31[1] was used for collecting frames of data, indexing reflections, and the determination of lattice parameters, SAINT2[2] for integration of intensity of reflections, and SADABS3[3] for scaling and empirical absorption correction. The structure was solved by dual-space methods using the program SHELXT.[4]All non-hydrogen atoms were refined with anisotropic thermal parameters by full-matrix least squares calculations on F2 using the program SHELXL-2014.[5] Hydrogen atoms were inserted at calculated positions and constrained with isotropic thermal parameters.

2. EXPERIMENTAL PROCEDURES

[1] APEX3 Version 2016.1 (Bruker AXS Inc.,2016)
[2] SAINT Version 8.37A (Bruker AXS Inc.,2015)
[3] SADABS Version 2014/5 (Sheldrick, Bruker AXS Inc.)
[4] SHELT Version 2014/5 (George M. Sheldrick, *Acta Cryst*. (2015). A71, 3-8)
[5] SHELT Version 2014/7 (George M. Sheldrick, *Acta Cryst*. (2008). A64, 112-122)

(2*E*,4*E*)-5-Iodo-2,4-dimethylpenta-2,4-dien-1-ol (10-2). To a cooled (0 °C) solution of ethyl (2*E*,4*E*)-5-iodo-2,4-dimethylpenta-2,4-dienoate **10.1** (0.07 g, 0.25 mmol) in CH_2Cl_2 (1.2 mL), Dibal-H (0.6 mL, 1M in hexane, 0.6 mmol) was added dropwise. The reaction mixture was stirred at the same temperature for 5.5 h. Diethyl ether (1 mL) and a saturated solution of potassium sodium tartrate tetrahydrate (1 mL) were added and the mixture was stirred at 25 °C for 12 h. The layers were separated and 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 to afford 0.06 g (97%) of a light yellow oil identified as (2*E*,4*E*)-5-iodo-2,4-dimethylpenta-2,4-dien-1-ol **10.2**, which was used without further purification. **MW:** 238.07 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 6.06 (s, 1H, H_5), 5.91 (s, 1H, H_3), 4.06 (d, *J* = 5.8 Hz, 2H, $2H_1$), 1.94 (s, 3H, CH_3), 1.73 (s, 3H, CH_3), 1.44 (t, *J* = 5.8 Hz, 1H, OH) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 144.7 (s), 137.9 (s), 125.9 (d), 80.4 (d), 68.7 (t), 25.5 (q), 15.9 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_7H_{12}IO$ ($[M+H]^+$), 238.9927; found, 238.9939. **IR** (NaCl): ν 3500-3060 (br, O-H), 2911 (w, C-H), 2854 (w, C-H) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 254 nm.

(3*R*,4*E*,6*E*)-3-Hydroxy-7-iodo-*N*-methoxy-*N*,4,6-trimethylhepta-4,6-dienamide (14-1). To a solution of (3*R*,4*E*,6*E*)-3-hydroxy-7-iodo-1-((*S*)-4-isopropyl-2-thioxothiazolidin-3-yl)-4,6-dimethylhepta-4,6-dien-1-one **14** (0.31 g, 0.72 mmol) in CH_2Cl_2 (3.8 mL), MeNHOMe·HCl (0.17 g, 1.79 mmol) and imidazole (0.24 g, 3.58 mmol) were added. The suspension was stirred for 20 h at room temperature. The reaction mixture was quenched with a saturated aqueous solution of NH_4Cl (3.0 mL) at 0 °C. 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 column chromatography (silica gel, 50:50 hexane/EtOAc) to afford 0.23 g (88%) of a yellow oil identified as the title compound. **MW:** 339.17 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 6.06 (s, 1H, H_7), 6.00 (s, 1H, H_5), 4.46 (d, *J* = 9.6 Hz, 1H, H_3), 3.97 (d, *J* = 2.6 Hz, 1H, OH), 3.70 (s, 3H, OMe), 3.21 (s, 3H, NMe), 2.73 (d, *J* = 16.4 Hz, 1H, H_{2A}), 2.59 (dd, *J* = 16.4, 9.6 Hz, 1H, H_{2B}), 1.94 (s, 3H, CH_3), 1.77 (s, 3H, CH_3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 173.5 (s), 144.5 (s), 138.5 (s), 126.3 (d), 80.2 (d), 72.7 (d), 61.5 (q), 37.1 (t), 32.1 (q), 25.3 (q), 14.6 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{11}H_{19}INO_3$ ($[M+H]^+$), 340.0404; found, 340.0409. **IR** (NaCl): ν 3100-3600 (br, O-H), 2936 (w, C-H), 1638 (s, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 245 nm.

(3*R*,4*E*,6*E*)-3-[(*tert*-Butyldimethylsilyl)oxy]-7-iodo-*N*-methoxy-*N*,4,6-trimethylhepta-4,6-dienamide (14-2). To a cooled (0 °C) solution of (3*R*,4*E*,6*E*)-3-hydroxy-7-iodo-*N*-methoxy-*N*,4,6-trimethylhepta-4,6-dienamide **14.1** (0.21 g, 0.61 mmol) in CH_2Cl_2 (5.4 mL), 2,6-lutidine (0.12 mL, 1.03 mmol) and TBDMSOTf (0.21 mL, 0.91 mmol) were added. After stirring for 5.5 h 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 column chromatography (silica gel, 80:20 hexane/EtOAc) to afford 0.26 g (96%) of a yellow oil identified as the title compound. **MW:** 453.44 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 6.02 (s, 1H, H_7), 5.92 (s, 1H, H_5), 4.59 (dd, *J* = 8.9, 3.9 Hz, 1H, H_3), 3.70 (s, 3H, OMe), 3.17 (s, 3H, NMe), 2.96 – 2.77 (m, 1H, H_{2A}), 2.34 (dd, *J* = 14.1, 3.9 Hz, 1H, H_{2B}), 1.91 (s, 3H, CH_3), 1.74 (1, 3H, CH_3) 0.85 (s, 9H, ^{t}Bu), 0.03 (s, 3H, $SiCH_3$), 0.01 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 171.9 (s), 144.5 (s), 140.1 (s), 126.3 (d), 80.0 (d), 75.1 (d), 61.6 (q), 39.3 (t), 32.2 (q), 25.9 (q, 3x), 25.1 (q), 18.3 (s), 13.7 (q), -4.7 (q), -5.0 (q) ppm. **HRMS** (ESI^+): Calcd. for $C_{17}H_{33}INO_3Si$ ($[M+H]^+$), 454.1269; found, 454.1268. **IR** (NaCl): ν 2957 (w, C-H), 2937 (w, C-H), 2854 (w, C-H), 1667 (s, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 246 nm.

(2*S*,3*R*,5*R*,6*E*,8*E*)-5-[(*tert*-Butyldimethylsilyl)oxy]-3-hydroxy-9-iodo-*N*-methoxy-*N*,2,6,8-tetramethylnona-6,8-dienamide (17-1). To a solution of (2*S*,3*R*,5*R*,6*E*,8*E*)-1-[(*R*)-4-benzyl-2-thioxooxazolidin-3-yl]-5-[(*tert*-butyldimethylsilyl)oxy]-3-hydroxy-9-iodo-2,6,8-trimethylnona-6,8-dien-1-one **17** (0.11 g, 0.17 mmol) in CH_2Cl_2 (1.0 mL), MeNHOMe·HCl (0.04 g, 0.42 mmol) and imidazole (0.06 g, 0.84 mmol) were added. The suspension was stirred for 20 h at room temperature. The reaction mixture was quenched with a saturated aqueous solution of NH_4Cl (1.0 mL) at 0 °C. 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 column chromatography (silica gel, 80:20 hexane/EtOAc) to afford 0.08 g (91%) of a yellow oil identified as the title compound. **MW:** 511.16 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 6.01 (s, 1H, H_9), 5.91 (s, 1H, H_7), 4.40 – 4.24 (m, 1H, H_5), 4.09 – 3.96 (m, 1H, H_3), 3.87 (s, 1H, OH), 3.69 (s, 3H, OMe), 3.69 (s, 3H, NCH_3), 2.90 - 2.80 (m, 1H, H_2), 1.91 (s, 3H, CH_3), 1.69 (s, 3H, CH_3), 1.58 – 1.48 (m, 2H, $2H_4$), 1.17 (d, *J* = 7.0 Hz, 3H, C_2CH_3), 0.89 (s, 9H, ^{t}Bu), 0.07 (s, 3H, CH_3), 0.01 (s, 3H, CH_3) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 178.0 (s), 144.6 (s), 140.6 (s), 125.7 (d), 79.7 (d), 74.9 (d), 68.4 (d), 61.7 (q), 40.5 (t), 39.9 (d), 32.1 (q), 26.0 (q, 3x), 25.2 (q), 18.3 (s), 14.3 (q), 11.2 (q), -4.6 (q), -5.0 (q) ppm. **HRMS** (ESI^+): Calcd. for

$C_{20}H_{38}INNaO_4Si$ ([M+Na]$^+$), 534.1507; found, 534.1505. **IR** (NaCl): ν 3500-3400 (br, O-H), 2960 (s, C-H), 2855 (w, C-H), 1637 (s, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 260 nm.

(2*S*,3*R*,5*R*,6*E*,8*E*)-3,5-Bis[(*tert*-butyldimethylsilyl)oxy]-9-iodo-*N*-methoxy-*N*,2,6,8-tetramethylnona-6,8-dienamide (17-2). To a cooled (0 °C) solution of (2*S*,3*R*,5*R*,6*E*,8*E*)-5-[(*tert*-butyldimethylsilyl)oxy]-3-hydroxy-9-iodo-*N*-methoxy-*N*,2,6,8-tetramethylnona-6,8-dienamide **17.1** (0.07 g, 0.141 mmol) in CH_2Cl_2 (1.3 mL), 2,6-lutidine (0.03 mL, 0.24 mmol) and TBDMSOTf (0.06 mL, 0.21 mmol) were added. The reaction was stirred for 5.5 h at the same temperature. The reaction mixture was quenched with a saturated aqueous solution of NH_4Cl (1.0 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 column chromatography (silica gel, 80:20 hexane/EtOAc) to afford 0.08 g (93%) of a yellow oil identified as the title compound. **MW:** 625.78 g/mol. **$[\alpha]_D^{22}$** -14.5 (*c* 0.33, CH_2Cl_2). **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 6.02 (s, 1H, H_9), 5.79 (s, 1H, H_7), 4.07 (t, *J* = 6.1 Hz, 1H, H_5), 3.99 (app. q, *J* = 5.4 Hz, 1H, H_3), 3.64 (s, 3H, OMe), 3.16 (s, 3H, NMe), 3.03 – 2.80 (m, 1H, H_2), 1.92 (s, 3H, CH_3), 1.88 - 1.79 (m, 1H, H_{4A}), 1.72 - 1.69 (m, 1H, H_{4B}), 1.69 (s, 3H, CH_3), 1.12 (d, *J* = 6.9 Hz, 3H, C_2-CH_3), 0.87 (s, 18H, ^{t}Bu), 0.05 (s, 6H, 2x$SiCH_3$), 0.02 (s, 3H, $SiCH_3$), -0.03 (s, 3H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ 175.5 (s), 144.5 (s), 141.1 (s), 126.6 (d), 80.0 (d), 75.7 (d), 70.9 (d), 61.2 (q), 43.0 (t), 41.3 (d), 30.5 (q), 26.1 (q, 3x), 26.0 (q, 3x), 25.1 (q), 18.3 (s), 18.2 (s), 13.1 (q), 12.6 (q), -3.7 (q), -4.1 (q), -4.2 (q), -4.6 (q) ppm. **HRMS** (ESI$^+$): Calcd. for $C_{26}H_{52}INNaO_4Si_2$ ([M+Na]$^+$), 648.2372; found, 648.2366. **IR** (NaCl): ν 2856 (s, C-H), 2953 (s, C-H), 2928 (s, C-H), 1670 (s, C=O) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 246 nm.

(2*E*,4*R*,5*R*,7*R*,8*E*,10*E*)-5,7-Bis[(*tert*-butyldimethylsilyl)oxy]-11-iodo-4,8,10-trimethylundeca-2,8,10-trien-1-ol (20-1). To a cooled (-78 °C) solution of ethyl (2*E*,4*R*,5*R*,7*R*,8*E*,10*E*)-5,7-bis[(*tert*-butyldimethylsilyl)oxy]-11-iodo-4,8,10-trimethylundeca-2,8,10-trienoate **20** (0.18 g, 0.29 mmol) in THF (2.9 mL), Dibal-H (0.72 mL, 1M in THF, 0.72 mmol) was added dropwise. The mixture reaction was stirred for 7 h at -78 °C. Then, a mixture of an aqueous saturated solution of Rochelle's salt and Et_2O (1:1, 20 mL) was added and the reaction was stirred at room temperature until clear solution. 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 column chromatography (silica gel, 90:10 hexane/EtOAc) to afford 0.17 g (100%) of colorless oil identified as the title compound. The major isomer was purified by HPLC (Novapak 6 μm, 5% hexane/tBuOMe, 4 mL/min; t_R = 46.9 min). **MW:** 594.77 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 6.01 (s, 1H, H_{11}), 5.77 (s, 1H, H_9), 5.74 (dd, *J* = 15.4, 6.6 Hz, 1H, H_3), 5.59 (dt, *J* = 15.4, 5.5 Hz, 1H, H_2), 4.10 (br s, 2H, $2H_1$), 4.05 (dd, *J* = 8.2, 3.7 Hz, 1H, H_7), 3.66 (app. dq, *J* = 8.7, 4.4 Hz, 1H, H_5), 2.44 – 2.29 (m, 1H, H_4), 1.91 (s, 3H, CH_3),1.72 – 1.61 (m, 1H, H_{6A}), 1.67 (s, 3H, CH_3),1.39 (ddd, *J* = 14.1, 6.8, 3.8 Hz, 1H, H_{6B}),0.97 (d, *J* = 6.9 Hz, 3H, C_4-CH_3), 0.88 (s, 9H, ^{t}Bu), 0.88 (s, 9H, ^{t}Bu), 0.06 (s, 3H, $SiCH_3$), 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, $CDCl_3$): δ144.5 (s), 141.3 (s), 135.6 (d), 128.7 (d), 126.1 (d), 79.9 (d), 76.0 (d), 73.8 (d), 64.2 (t), 41.6 (t), 41.5 (d), 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 $C_{26}H_{51}INaO_3Si_2$ ([M+Na]$^+$), 617.2314; found, 617.2306. **IR** (NaCl): ν 3500-3200 (br, O-H), 2954 (s, C-H), 2927 (s, C-H), 2856 (s, C-H) cm^{-1}. **UV/Vis** (MeOH): λ_{max} 245 nm.

(*Z*)-*tert*-Butyldimethyl[(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)but-2-en-1-yl)oxy]silane (24). To a cooled (0 °C) solution of (*Z*)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)but-2-en-1-ol (0.10 g, 0.51 mmol) in CH_2Cl_2 (4.6 mL), 2,6-lutidine (0.10 mL, 0.87 mmol) and TBDMSOTf (0.18 mL, 0.77 mmol) were added. The reaction mixture was stirred for 6 h at the same temperature. The reaction mixture was quenched with a saturated aqueous solution of NH_4Cl (2.0 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 column chromatography (silica gel, 90:10 hexane/EtOAc) to afford 0.17 g (100%) of a colorless oil identified as **24**. **MW:** 312.23 g/mol. **^{1}H-NMR** (400.13 MHz, $CDCl_3$): δ 6.37 (s, 1H, CH), 4.30 (s, 2H, CH_2), 1.66 (s, 3H, CH_3), 1.26 (s, 12H, 4xCH_3), 0.90 (s, 9H, $SiCH_3$), 0.07 (s, 1H, $SiCH_3$) ppm. **^{13}C-NMR** (100.16 MHz, $CDCl_3$): δ145.7 (s + d), 83.4 (s, 2x), 60.9 (t), 26.1 (q, 3x), 24.9 (q, 4x), 18.6 (s), 14.3 (q), -5.1 (q, 2x) ppm. **HRMS**(ESI$^+$): Calcd. for $C_{16}H_{34}BO_3Si$ ([M+H]$^+$), 313.2373; found, 313.2364. **IR** (NaCl): ν 2932 (s, C-H) cm^{-1}.

3. COMPUTATIONAL STUDIES

All calculations were carried out with the Gaussian 09 suite of programs.[6] Each geometry was optimized at the ωB97XD[7]/Def2SVP[8] level. 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 or DCM as solvent, was used during the geometry optimization process; thus solvent effects and corrections to the Gibbs energy were taken into account. IRC[10] calculations 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, and these energies are discussed on the manuscript.

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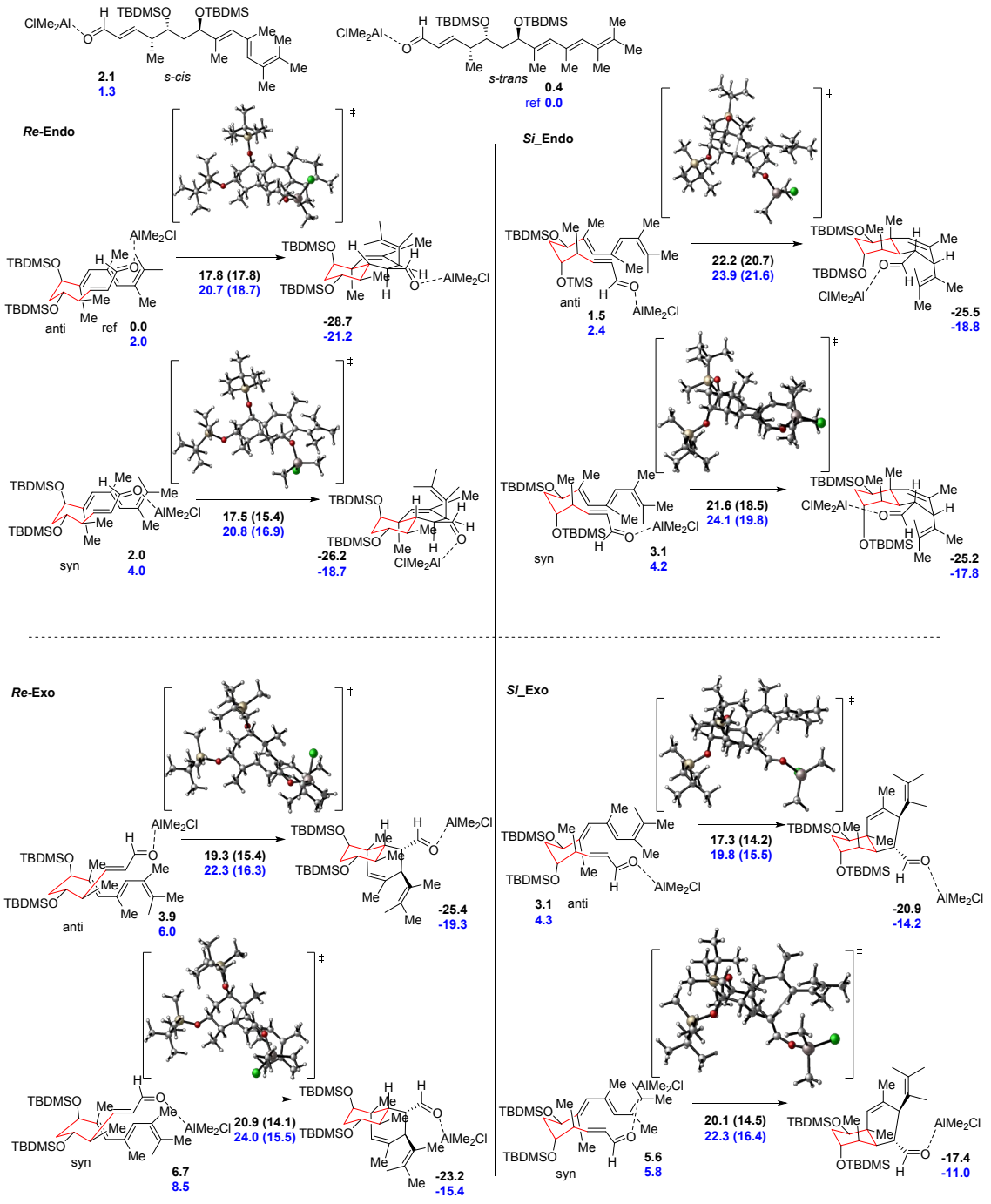

Figure S 1: Schematic representation of all possible diastereofacial orientations to the *s-cis*/*s-cis*trienal conformation for the IMDA reaction with both the synperiplanar and antiperiplanar coordination of the Me_2AlCl catalyst with respect to the carbonyl group in **model system B**. Relative Gibbs energies were calculated at the ωB97XD/Def2SVP(SMD,DCM) in black, and ωB97XD/Def2TZVP(SMD,DCM)//ωB97XD/Def2SVP(SMD,DCM) single point energy correction in blue and are given in kcal/mol, with the TS optimized structure depicted as a CYLView representation.

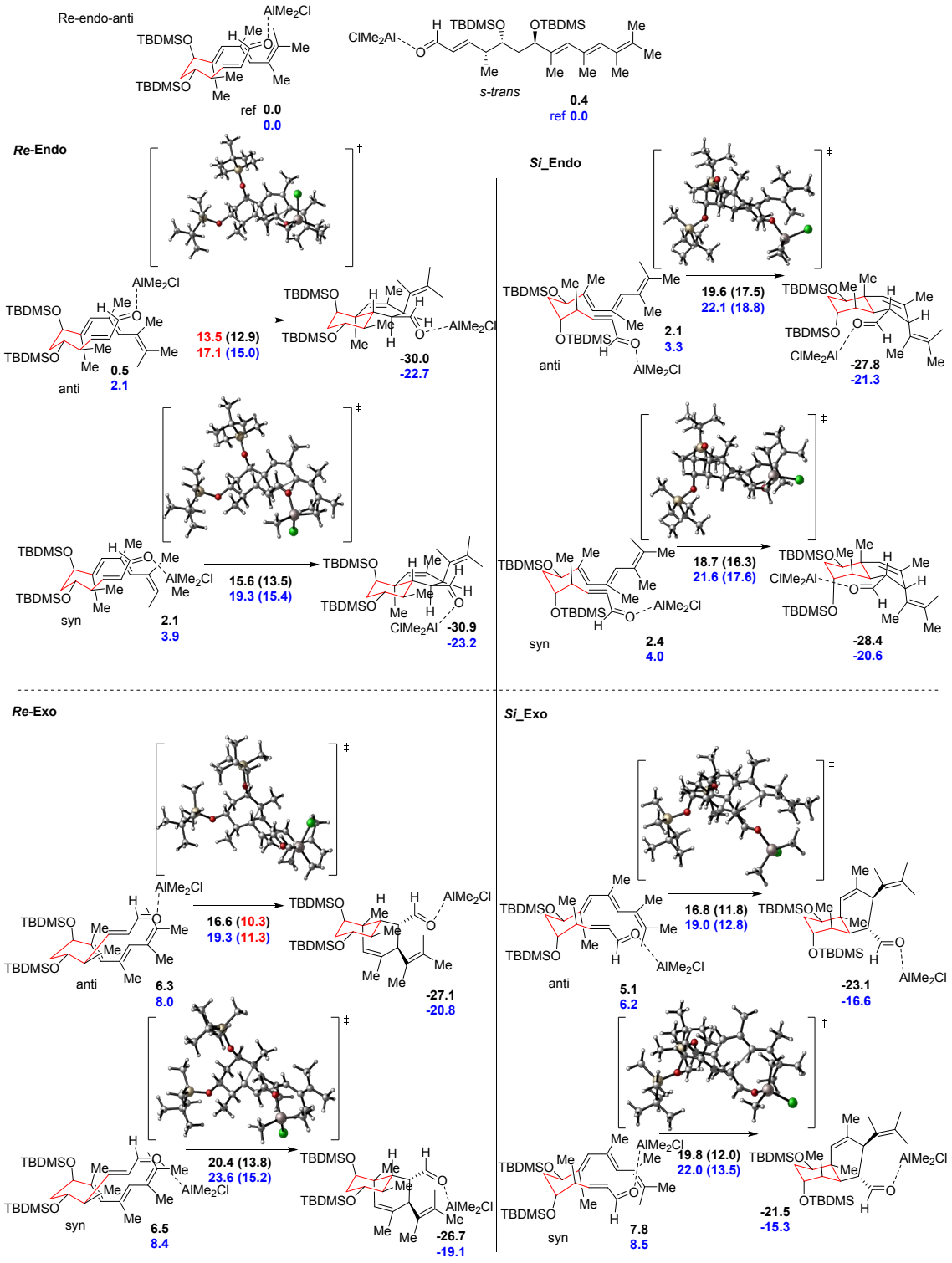

Figure S 2: Schematic representation of all possible diastereofaceorientations to the *s-cis*/*s-cis*trienal conformation for the IMDA reaction with both the synperiplanar and antiperiplanar coordination of the Me_2AlCl catalyst with respect to the carbonyl group in **model system B**. Relative Gibbs energies were calculated at ωB97XD/Def2SVP(SMD,DCM) in black, and ωB97XD/Def2TZVP(SMD,DCM)//ωB97XD/Def2SVP(SMD,DCM) single point energy correction in blue and are given in kcal/mol, with the TS optimized structure depicted as a CYLView representation.

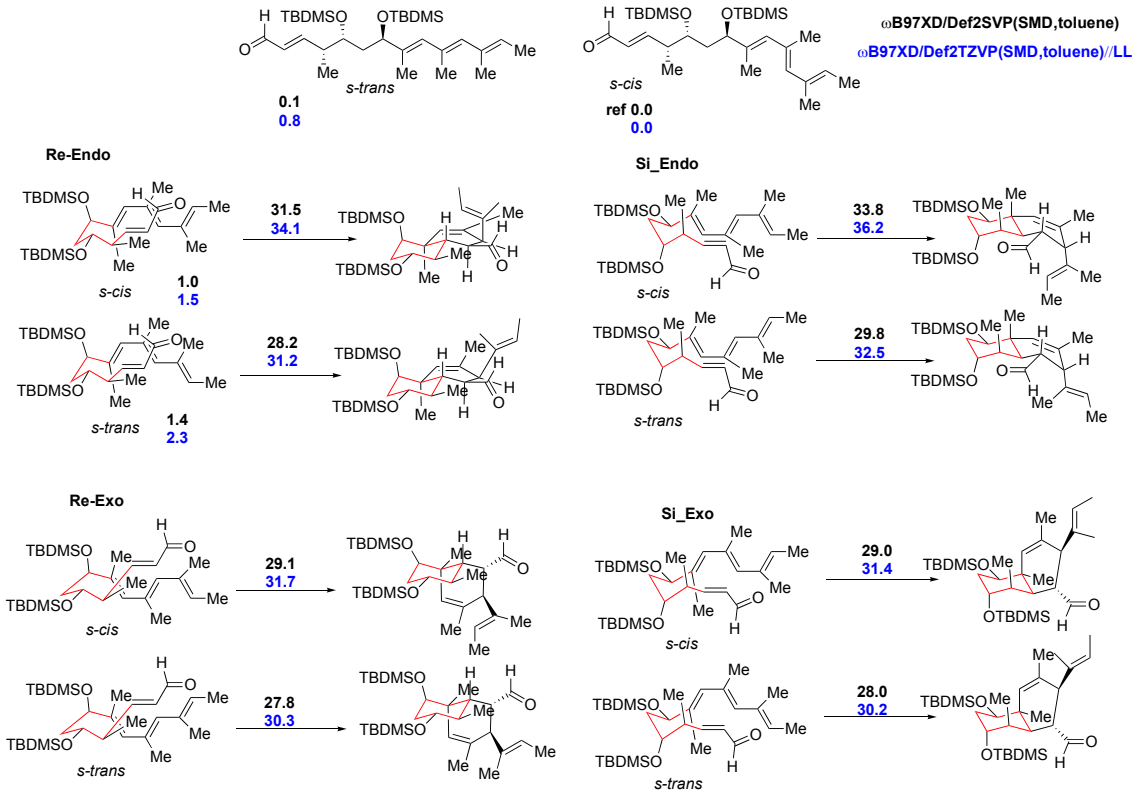

Figure S 3: Schematic representation of all possible diastereofaceorientations to the *s-cis*/*s-cis* trienal conformation of **model system A** for the IMDA reaction. Relative Gibbs energies were calculated at ωB97XD/Def2SVP(SMD,DCM) in black, and ωB97XD/Def2TZVP(SMD,DCM)// ωB97XD/Def2SVP(SMD,DCM) single point energy correction in blue and are given in kcal/mol.

Cartesian Coordinates

AlMe$_2$Cl catalyzed IMDA reaction for model system B

B-scis
SCF Energy: -2801.68075922 H
Num. Imaginary Frequencies: 0

C	-1.784937	0.068866	0.137570
C	-0.967407	-0.711433	-0.899648
C	0.530634	-0.398096	-0.827460
C	1.189274	-0.324025	-2.233296
C	2.559062	0.226280	-2.039703
C	-3.170455	-0.536241	0.300805
C	3.727048	-0.430989	-2.201066
C	-6.068379	-1.547346	-0.414772
C	-5.668753	-0.289860	-0.132520
C	-4.246835	0.110093	-0.178706
C	-6.614297	0.831184	0.212826
C	-7.444990	-2.101741	-0.381944
C	-7.571356	-3.249772	0.593904
C	-8.451398	-1.652935	-1.166117
C	-9.859185	-2.190599	-1.119528
C	-3.194775	-1.863577	1.008459
C	4.914882	0.200949	-1.714969
O	5.993703	-0.400276	-1.588065
O	1.191283	-1.370307	-0.060000
O	-1.825820	1.411417	-0.264365
H	-1.277750	-0.023176	1.117439
H	-1.089837	-1.795991	-0.767718
H	-1.383734	-0.445906	-1.884017
H	0.652098	0.601356	-0.369062
H	2.602469	1.250560	-1.646900
H	3.791072	-1.459553	-2.562007
H	-5.286624	-2.283086	-0.641605
H	-4.056421	1.097230	-0.612798
H	-6.653603	1.571113	-0.604989
H	-7.635651	0.473109	0.396670
H	-6.263624	1.368733	1.108488
H	-7.513941	-2.886225	1.634266
H	-8.498898	-3.825680	0.484413
H	-6.728682	-3.949085	0.463122
H	-2.404511	-1.907842	1.775133
H	-4.163656	-2.047200	1.494376
H	-3.013732	-2.702204	0.315682
H	4.851851	1.259222	-1.397140
C	1.133688	-1.650690	-2.978112
H	1.630407	-1.577193	-3.956935
H	1.621253	-2.447570	-2.398141
H	0.091061	-1.951399	-3.153937
H	0.617364	0.444414	-2.782694

C	7.284614	-0.870561	1.115202
H	7.171523	-1.961221	0.981402
H	6.380159	-0.506662	1.633956
H	8.132613	-0.719516	1.807282
Al	7.574387	0.056699	-0.593251
Cl	7.282386	2.233695	-0.387975
C	9.060286	-0.407085	-1.785082
H	9.003032	0.118402	-2.754500
H	9.082481	-1.490503	-2.000847
H	10.036561	-0.150670	-1.336294
Si	1.981076	-1.268665	1.425226
Si	-1.259978	2.814135	0.476567
C	-0.023817	3.583323	-0.704313
H	0.829449	2.904252	-0.866211
H	-0.479092	3.787498	-1.686683
H	0.375954	4.531339	-0.309967
C	-2.743290	3.971303	0.759478
C	-0.423415	2.388699	2.098556
H	-0.103526	3.311258	2.610070
H	-1.091348	1.840681	2.781635
H	0.477525	1.777197	1.935259
C	0.716765	-1.255155	2.810240
H	0.162125	-0.305554	2.849036
H	-0.011970	-2.071714	2.686052
H	1.210411	-1.386297	3.787369
C	3.046617	0.276689	1.497664
H	3.282980	0.529185	2.544255
H	4.000292	0.134976	0.965821
H	2.539903	1.150295	1.056616
C	3.049727	-2.836388	1.516251
C	-8.270871	-0.571218	-2.199515
H	-7.217002	-0.330696	-2.389062
H	-8.732459	-0.880193	-3.152626
H	-8.782842	0.357422	-1.893166
C	3.943188	-2.759147	2.764974
H	3.356422	-2.665078	3.693635
H	4.554180	-3.674929	2.856343
H	4.641548	-1.907743	2.718930
C	3.935104	-2.939765	0.266565
H	4.590709	-3.826647	0.330820
H	3.331057	-3.034686	-0.648597
H	4.589480	-2.061663	0.148172
C	2.146216	-4.075899	1.603820
H	1.459961	-4.141805	0.743842
H	2.755397	-4.997545	1.613596
H	1.536600	-4.077729	2.521929
C	-3.685238	3.341846	1.797478
H	-4.586764	3.966327	1.932240
H	-4.019464	2.338689	1.489135
H	-3.203578	3.245898	2.784155
C	-2.242456	5.328218	1.280052
H	-3.095889	5.999138	1.485055
H	-1.674129	5.229503	2.219595
H	-1.595469	5.838523	0.548207
C	-3.501639	4.185129	-0.559310
H	-2.863058	4.640956	-1.333614
H	-3.896235	3.240770	-0.965587
H	-4.360914	4.862015	-0.403471

B-strans

SCF Energy: -2801.68154146 H

Num. Imaginary Frequencies: 0

C	-1.639815	-0.402948	-0.090602
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C	0.718148	-0.229061	-1.016760
C	1.501273	0.000033	-2.337409
C	2.827005	0.576033	-1.977047
C	-2.859345	-1.316179	-0.089240
C	4.037719	0.031338	-2.221898
C	-6.480791	-0.576317	-0.307237
C	-5.415881	-1.413008	-0.340780
C	-4.080916	-0.791028	-0.293046
C	-5.568189	-2.905943	-0.490389
C	-7.919638	-0.935837	-0.281563
C	-8.366129	-1.988460	0.718801
C	-8.805019	-0.293440	-1.078840
C	-2.524190	-2.764292	0.173253
C	5.182550	0.632236	-1.609755
O	6.300415	0.092459	-1.604598
O	1.394477	-1.179002	-0.230015
O	-1.957804	0.963817	-0.140017
H	-1.085939	-0.634784	0.839300
H	-0.671623	-1.787480	-1.472405
H	-1.140412	-0.213310	-2.153202
H	0.667086	0.745014	-0.493975
H	2.794519	1.509114	-1.399827
H	4.174371	-0.906189	-2.765123
H	-6.255576	0.496790	-0.284472
H	-4.099245	0.293924	-0.422189
H	-5.397936	-3.441095	0.457200
H	-6.570788	-3.171975	-0.850085
H	-4.841645	-3.297039	-1.217013
H	-7.530173	-2.317338	1.350003
H	-9.142336	-1.593937	1.394170
H	-8.786433	-2.883122	0.231269
H	-1.510867	-2.854693	0.594036
H	-3.218326	-3.226741	0.887053
H	-2.542996	-3.369093	-0.747390
H	5.051583	1.597703	-1.085394
C	1.571774	-1.242962	-3.215048
H	2.165546	-1.055579	-4.121930
H	2.025530	-2.084097	-2.670066
H	0.566994	-1.549613	-3.537042
H	0.952841	0.800744	-2.866457
C	8.012582	-1.071264	0.623905
H	8.008079	-2.030288	0.075172
H	7.177774	-1.104317	1.345493
H	8.946630	-1.044783	1.213583
Al	7.895112	0.460811	-0.599196
Cl	7.265545	2.301838	0.443285
C	9.266747	0.789403	-1.962746
H	9.443244	-0.108402	-2.582218
H	10.236632	1.058740	-1.507665
H	8.992662	1.610686	-2.648074

Si	2.097577	-1.091773	1.299934
Si	-2.061529	2.013455	1.178416
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C	-2.920880	1.156784	2.607093
H	-3.970961	0.919663	2.375697
H	-2.410444	0.211645	2.856477
H	-2.900906	1.789176	3.509682
C	-0.328158	2.512827	1.693800
H	-0.355490	3.247199	2.515418
H	0.241365	1.642901	2.054110
H	0.228677	2.962085	0.856416
C	0.783043	-1.266093	2.630248
H	0.134166	-0.378924	2.694721
H	0.140076	-2.142221	2.451558
H	1.258309	-1.391603	3.617215
C	3.008165	0.534430	1.527034
H	3.196410	0.711681	2.598707
H	3.981699	0.541649	1.013547
H	2.419330	1.388229	1.156157
C	3.292392	-2.567499	1.369122
C	-8.403906	0.752357	-2.085995
H	-7.318331	0.832694	-2.225600
H	-8.851554	0.525987	-3.068463
H	-8.789027	1.744254	-1.791070
C	4.060435	-2.526687	2.700331
H	3.388740	-2.595688	3.571542
H	4.764766	-3.375288	2.763087
H	4.653469	-1.603331	2.806049
C	2.499708	-3.879817	1.269591
H	1.911651	-3.929961	0.338879
H	3.184721	-4.746604	1.277318
H	1.803395	-4.006236	2.114498
C	4.293210	-2.488476	0.207852
H	5.008325	-3.329014	0.256189
H	3.786081	-2.534505	-0.767851
H	4.885092	-1.560173	0.236774
C	-2.234135	4.216056	-0.567892
H	-1.274317	4.612836	-0.199374
H	-2.017625	3.531276	-1.403814
H	-2.805315	5.068981	-0.976386
C	-3.251230	4.494794	1.711452
H	-2.300341	4.831579	2.156223
H	-3.785530	5.396721	1.363081
H	-3.857749	4.046327	2.515314
C	-4.397102	3.081303	-0.012053
H	-4.987334	3.963851	-0.317540
H	-4.286510	2.437302	-0.898235
H	-4.993414	2.531499	0.734339

Reendo-anti-scis

SCF Energy: -2801.68805403 H

Num. Imaginary Frequencies: 0

C	-1.082953	0.336244	-1.953614
C	-2.260940	-0.563475	-1.548387
C	-2.432572	-0.916876	-0.065435
C	-1.318547	-1.802145	0.542683
C	-0.114505	-0.981474	0.895884
C	0.257876	-0.374078	-2.106885
C	1.041296	-1.456513	1.416481
C	3.002365	-1.667447	-1.387777
C	2.742607	-0.347253	-1.540069
C	1.362214	0.161881	-1.555910
C	3.804304	0.717823	-1.591133
C	4.312202	-2.340714	-1.257325
C	4.366181	-3.242460	-0.044823
C	5.326973	-2.203743	-2.143896
C	6.684317	-2.834952	-1.962286
C	0.231731	-1.605038	-2.967648
C	2.075248	-0.512254	1.691928
O	3.176996	-0.815380	2.184842
O	-3.674910	-1.571723	0.051231
O	-1.008564	1.407331	-1.052188
H	-1.330344	0.701078	-2.972735
H	-3.179039	-0.026060	-1.830975
H	-2.256956	-1.496608	-2.132040
H	-2.444024	0.027512	0.512283
H	-0.198040	0.102632	0.753648
H	1.227497	-2.517229	1.603423
H	2.139108	-2.323566	-1.225069
H	1.224186	1.109113	-1.024795
H	4.791944	0.335734	-1.304041
H	3.885539	1.147113	-2.604093
H	3.545510	1.544218	-0.910460
H	3.524561	-3.955754	-0.076785
H	5.289878	-3.828844	0.029752
H	4.249263	-2.661977	0.883672
H	7.469515	-2.111888	-2.237945
H	6.887446	-3.165309	-0.936296
H	1.219802	-1.821732	-3.396420
H	-0.084418	-2.496241	-2.399954
H	-0.488575	-1.484220	-3.793242
H	1.874650	0.550548	1.458805
C	-1.798250	-2.563757	1.788705
H	-2.093078	-1.865796	2.587234
H	-2.664551	-3.188468	1.539427
H	-1.000141	-3.211543	2.178135
H	-1.008698	-2.552959	-0.207276
H	6.810037	-3.702063	-2.634373
Al	4.710280	0.245282	2.617221
C	6.162316	-0.477704	1.511293
Cl	4.022450	2.236962	1.937537
H	6.474994	-1.477965	1.861097
H	7.057111	0.169224	1.554749
H	5.883935	-0.576278	0.448350
C	4.804220	0.153883	4.577512
H	5.637666	0.761601	4.973310
H	3.880980	0.519068	5.061014
H	4.969644	-0.880843	4.928489
Si	-1.181951	3.048578	-1.403114
Si	-5.048329	-0.850714	0.718029
C	-1.008407	3.865454	0.299186
C	0.163247	3.571795	-2.597735
H	1.166449	3.488510	-2.151314
H	0.142403	2.936722	-3.499096

H	0.019292	4.614396	-2.925303
C	-2.863179	3.331531	-2.180844
H	-2.939868	2.794264	-3.140768
H	-3.679458	2.979839	-1.530853
H	-3.028008	4.401196	-2.390004
C	-6.449761	-2.073574	0.347517
C	-4.798959	-0.598758	2.559956
H	-3.904601	0.017526	2.749328
H	-5.659549	-0.067794	2.999038
H	-4.675883	-1.552210	3.096833
C	-5.323560	0.825928	-0.078337
H	-4.470746	1.491317	0.134830
H	-5.441056	0.757764	-1.170884
H	-6.225389	1.308794	0.332677
C	5.203819	-1.440164	-3.436034
H	5.614677	-2.043649	-4.263244
H	4.167364	-1.177480	-3.683374
H	5.794732	-0.508741	-3.408169
C	-6.058601	-3.468217	0.860493
H	-5.866218	-3.471307	1.946057
H	-6.871934	-4.191326	0.669858
H	-5.153368	-3.843240	0.358049
C	-6.685898	-2.136080	-1.169436
H	-5.770700	-2.422522	-1.712313
H	-7.463168	-2.883779	-1.409022
H	-7.027348	-1.168869	-1.572709
C	-7.734173	-1.607111	1.050503
H	-8.570453	-2.290629	0.818382
H	-7.621095	-1.590036	2.146787
H	-8.039943	-0.597501	0.729062
C	-2.157003	3.399764	1.207835
H	-2.167188	2.302896	1.319030
H	-2.051916	3.834598	2.217863
H	-3.141301	3.708294	0.819469
C	0.333940	3.452368	0.923527
H	0.463897	3.921420	1.914862
H	0.394543	2.361302	1.063959
H	1.192578	3.757495	0.304223
C	-1.057025	5.392987	0.142917
H	-2.004111	5.732561	-0.308239
H	-0.968563	5.885162	1.127823
H	-0.232158	5.768350	-0.484706

Reendo-anti-strans

SCF Energy: -2801.68593314 H

Num. Imaginary Frequencies: 0

C	-1.156478	0.566299	-1.916918
C	-2.267187	-0.439520	-1.573044
C	-2.387850	-0.929083	-0.124082
C	-1.240683	-1.835729	0.374956
C	-0.016548	-1.034814	0.702176
C	0.218011	-0.034555	-2.196228
C	1.177483	-1.550454	1.075201
C	3.111161	-1.158269	-1.802823
C	2.726346	0.140389	-1.754168
C	1.310492	0.520924	-1.639682
C	3.680472	1.307972	-1.698583
C	4.480721	-1.692809	-1.951988
C	5.431181	-1.002466	-2.910562
C	4.881661	-2.802052	-1.284272
C	6.288517	-3.329407	-1.421830
C	0.228282	-1.169042	-3.180400
C	2.230788	-0.636627	1.381918
O	3.354347	-0.985868	1.786401
O	-3.607715	-1.629940	-0.034181
O	-1.110162	1.541530	-0.910806
H	-1.465058	1.019667	-2.882529
H	-3.221822	0.062953	-1.790689
H	-2.220571	-1.314992	-2.238530
H	-2.407236	-0.040801	0.536361
H	-0.118515	0.056744	0.683339
H	1.370094	-2.624175	1.142590
H	2.316459	-1.902327	-1.698759
H	1.129244	1.389571	-0.998891
H	4.715083	1.010030	-1.494321
H	3.663355	1.886202	-2.638130
H	3.376301	1.995908	-0.894090
H	4.902941	-0.292611	-3.560664
H	6.227212	-0.445967	-2.386715
H	5.932260	-1.734271	-3.563431
H	7.037003	-2.526072	-1.486140
H	6.554266	-3.966811	-0.565315
H	1.200294	-1.259726	-3.684818
H	0.018837	-2.136081	-2.692608
H	-0.550440	-1.025485	-3.947147
H	2.018685	0.443225	1.270924
C	-1.651963	-2.646963	1.615202
H	-1.905128	-1.980196	2.453869
H	-2.529398	-3.264546	1.387499
H	-0.832831	-3.305380	1.937150
H	-0.978979	-2.554145	-0.423207
H	6.395138	-3.948921	-2.330703
Al	4.875035	0.044380	2.316405
C	6.297120	-0.416558	1.045689
Cl	4.093452	2.095833	2.024917
H	6.009486	-0.226215	-0.001370
H	6.570048	-1.484383	1.121727
H	7.215923	0.163608	1.246337
C	5.070633	-0.381018	4.225045
H	4.158161	-0.152929	4.803801
H	5.296056	-1.451739	4.380226
H	5.896545	0.188713	4.687537
Si	-1.337721	3.203758	-1.092747
Si	-4.989010	-1.012543	0.714778
C	-1.139012	3.856556	0.676624
C	-0.044158	3.890851	-2.261927
H	0.972371	3.817491	-1.845149
H	-0.057233	3.338616	-3.216405
H	-0.244646	4.950331	-2.491008
C	-3.046140	3.511541	-1.798035
H	-3.128967	3.082315	-2.810462
H	-3.834242	3.061127	-1.175022
H	-3.250532	4.591511	-1.882073
C	-6.358385	-2.244091	0.262247

C	-4.714247	-0.909418	2.567478
H	-3.841728	-0.275024	2.794879
H	-5.586576	-0.452893	3.063495
H	-4.543375	-1.898597	3.019833
C	-5.330175	0.716821	0.071570
H	-4.488484	1.384648	0.318657
H	-5.476855	0.738852	-1.019306
H	-6.231730	1.138104	0.545942
C	4.009572	-3.590829	-0.347275
H	4.130627	-4.670744	-0.534278
H	4.310089	-3.413734	0.699286
H	2.943569	-3.346899	-0.428416
C	-2.267852	3.297770	1.557092
H	-3.261029	3.633105	1.216449
H	-2.268954	2.195347	1.564538
H	-2.147671	3.636351	2.601722
C	-1.202402	5.391621	0.664685
H	-2.157806	5.763196	0.258419
H	-1.105956	5.790235	1.690311
H	-0.388631	5.831792	0.065408
C	0.217539	3.400638	1.237955
H	0.363724	3.786579	2.262392
H	0.286185	2.302357	1.286393
H	1.063239	3.762324	0.630971
C	-7.648953	-1.871303	1.008501
H	-8.466508	-2.561305	0.732914
H	-7.525302	-1.931975	2.102121
H	-7.988424	-0.850660	0.765347
C	-5.922169	-3.661959	0.662948
H	-5.721380	-3.743453	1.743903
H	-6.715319	-4.392180	0.421182
H	-5.010283	-3.969784	0.127857
C	-6.607251	-2.196650	-1.253214
H	-5.689700	-2.415197	-1.822917
H	-7.366302	-2.944986	-1.543842
H	-6.978432	-1.211189	-1.578571

Reendo-syn-scis

SCF Energy: -2801.68594026 H

Num. Imaginary Frequencies: 0

C	1.113725	0.930371	1.469222
C	1.727602	-0.477688	1.530172
C	1.928613	-1.218566	0.198480
C	0.765155	-2.144525	-0.216749
C	-0.431331	-1.422960	-0.735523
C	-0.405339	0.972107	1.353688
C	-1.709236	-1.801506	-0.507083
C	-3.426649	1.150906	0.494141
C	-2.415072	1.970827	0.127574
C	-0.992082	1.658564	0.354660
C	-2.635624	3.297087	-0.556004
C	-4.889420	1.371611	0.384565
C	-5.565966	1.240466	1.730538
C	-5.541829	1.590366	-0.780498
C	-7.027153	1.819754	-0.889215
C	-1.128302	0.309645	2.492238
C	-2.756734	-1.194009	-1.269383
O	-3.960481	-1.500233	-1.218569
O	3.085233	-2.018546	0.314667
O	1.765203	1.671065	0.471216
H	1.319066	1.372909	2.466784
H	2.732769	-0.356548	1.957411
H	1.166335	-1.107792	2.237707
H	2.061295	-0.463051	-0.599394
H	-0.243119	-0.618628	-1.458376
H	-1.955305	-2.591544	0.207108
H	-3.168231	0.224121	1.015461
H	-0.310713	2.130253	-0.359770
H	-2.300468	3.258127	-1.606593
H	-3.690209	3.600138	-0.547483
H	-2.043393	4.084528	-0.062804
H	-5.286104	0.278208	2.190511
H	-5.224012	2.032753	2.418003
H	-6.661057	1.280531	1.684783
H	-7.542790	1.902961	0.074590
H	-7.222347	2.747735	-1.453309
H	-2.033245	0.867796	2.774895
H	-1.451336	-0.712951	2.234605
H	-0.481216	0.233439	3.379727
H	-2.465262	-0.420799	-2.001833
C	1.190684	-3.086642	-1.361352
H	1.488675	-2.514316	-2.254236
H	2.044735	-3.696159	-1.041620
H	0.363461	-3.754875	-1.640766
H	0.475613	-2.761720	0.649553
H	-7.502128	1.003747	-1.459738
Al	-5.071760	-2.664837	-0.194704
C	-4.655485	-4.450921	-0.906524
Cl	-4.276646	-2.426882	1.858852
H	-3.581838	-4.699150	-0.831346
H	-4.934205	-4.537797	-1.972528
H	-5.206687	-5.242752	-0.368110
C	-6.873068	-1.906996	-0.360893
H	-6.967081	-0.941157	0.163152
H	-7.146124	-1.737884	-1.418120
H	-7.636227	-2.584507	0.062699
Si	2.333303	3.255350	0.652497
Si	4.587324	-1.599559	-0.329677
C	2.808575	3.785815	-1.107576
C	0.992871	4.348866	1.376768
H	0.144110	4.485441	0.690152
H	0.602169	3.917172	2.312951
H	1.402170	5.343354	1.618949
C	3.795678	3.259266	1.827253
H	3.529689	2.750810	2.769246
H	4.677220	2.751083	1.408517
H	4.084930	4.291755	2.082512
C	5.718917	-3.056531	0.110149
C	4.423581	-1.362876	-2.184195
H	3.640979	-0.621305	-2.414165
H	5.365818	-0.986074	-2.614528
H	4.163448	-2.300732	-2.699427
C	5.141726	0.013379	0.444812
H	4.330464	0.748861	0.334924

H	5.354053	-0.093511	1.520157
H	6.039477	0.420628	-0.047123
C	-4.860821	1.597002	-2.123058
H	-3.803420	1.316343	-2.070837
H	-5.372000	0.896358	-2.804446
H	-4.924092	2.594220	-2.591716
C	1.583804	3.675237	-2.029040
H	1.837112	4.015998	-3.048963
H	1.229324	2.635078	-2.105850
H	0.741365	4.293084	-1.677597
C	3.293932	5.243971	-1.068142
H	4.171205	5.369468	-0.412074
H	3.590731	5.578698	-2.078175
H	2.508404	5.931381	-0.713780
C	3.930280	2.887160	-1.649873
H	4.843184	2.948513	-1.035993
H	3.623806	1.829721	-1.688154
H	4.203501	3.190807	-2.676458
C	7.105880	-2.819016	-0.507717
H	7.792540	-3.643072	-0.243292
H	7.064168	-2.769207	-1.608203
H	7.564908	-1.883584	-0.146565
C	5.122176	-4.359585	-0.443081
H	4.998325	-4.327647	-1.537974
H	5.782754	-5.214774	-0.212810
H	4.136875	-4.571747	0.000948
C	5.846279	-3.165453	1.637450
H	4.863588	-3.295629	2.118420
H	6.470027	-4.035082	1.911814
H	6.319559	-2.272268	2.076415

Reendo-syn-strans

SCF Energy: -2801.68452811 H

Num. Imaginary Frequencies: 0

C	1.113496	1.037889	1.405477
C	1.687883	-0.380146	1.556467
C	1.909500	-1.184390	0.265747
C	0.724917	-2.076473	-0.162978
C	-0.415302	-1.323858	-0.762028
C	-0.398973	1.098083	1.231066
C	-1.715292	-1.660199	-0.602588
C	-3.387296	1.272538	0.248802
C	-2.336097	2.015230	-0.172974
C	-0.933710	1.723312	0.164486
C	-2.491161	3.231012	-1.056105
C	-4.818068	1.457123	-0.105056
C	-5.180854	1.615271	-1.570969
C	-5.767382	1.409102	0.858095
C	-7.237465	1.545716	0.566390
C	-1.177037	0.517730	2.377157
C	-2.702741	-1.041741	-1.433484
O	-3.906427	-1.355894	-1.474543
O	3.028009	-2.022813	0.460683
O	1.814683	1.705278	0.390570
H	1.297186	1.529834	2.383785
H	2.681492	-0.264906	2.011347
H	1.086588	-0.962589	2.271812
H	2.104849	-0.468391	-0.554902
H	-0.160109	-0.542279	-1.488683
H	-2.024152	-2.433796	0.105588
H	-3.182291	0.422074	0.902374
H	-0.212578	2.137519	-0.546510
H	-2.125360	3.029035	-2.077640
H	-3.528344	3.580815	-1.124773
H	-1.883628	4.061401	-0.661933
H	-5.651945	2.588200	-1.786682
H	-4.296075	1.527184	-2.214783
H	-5.886573	0.831969	-1.888730
H	-7.487452	1.456396	-0.498303
H	-7.809779	0.781385	1.117987
H	-2.063275	1.126658	2.609614
H	-1.535616	-0.501911	2.156878
H	-0.558135	0.456839	3.285361
H	-2.361213	-0.262830	-2.136974
C	1.157192	-3.083650	-1.247956
H	1.512551	-2.562871	-2.151384
H	1.972919	-3.711104	-0.868360
H	0.315008	-3.730703	-1.532489
H	0.370044	-2.644504	0.712760
H	-7.608980	2.524823	0.917437
Al	-5.042552	-2.614665	-0.604261
C	-4.424130	-4.352883	-1.290902
Cl	-4.515830	-2.378551	1.530734
H	-3.355326	-4.539682	-1.084115
H	-4.560307	-4.427267	-2.385311
H	-4.988308	-5.190796	-0.843082
C	-6.857141	-1.982259	-0.994837
H	-7.055132	-0.989458	-0.557946
H	-7.035562	-1.905844	-2.082696
H	-7.622061	-2.670761	-0.592859
Si	2.401961	3.289599	0.474113
Si	4.567194	-1.675982	-0.138490
C	2.962413	3.668457	-1.300039
C	1.048926	4.455901	1.044542
H	0.237721	4.551175	0.306980
H	0.604600	4.102641	1.989680
H	1.463569	5.460231	1.230765
C	3.809350	3.363292	1.710940
H	3.474726	2.986536	2.692055
H	4.678139	2.764215	1.399142
H	4.144585	4.403200	1.856483
C	5.634283	-3.147955	0.401089
C	4.484120	-1.509570	-2.006282
H	3.735746	-0.754988	-2.299285
H	5.454550	-1.179751	-2.411850
H	4.215226	-2.459709	-2.493711
C	5.144378	-0.050729	0.593862
H	4.361663	0.704964	0.427652
H	5.317071	-0.122446	1.679230
H	6.070817	0.309311	0.118520
C	-5.454272	1.233311	2.320262
H	-6.050579	1.934040	2.927908
H	-5.723534	0.214445	2.646601
H	-4.395711	1.395369	2.561283

C	1.782634	3.472572	-2.265158
H	2.082807	3.727233	-3.297411
H	1.434085	2.427614	-2.269219
H	0.923323	4.112909	-2.007090
C	3.444697	5.126648	-1.365687
H	4.286630	5.314921	-0.678984
H	3.793400	5.371567	-2.384838
H	2.641419	5.838840	-1.115423
C	4.108562	2.730399	-1.707990
H	4.992577	2.850911	-1.061335
H	3.805025	1.672310	-1.665201
H	4.428064	2.942171	-2.744246
C	7.054028	-2.970560	-0.160025
H	7.702981	-3.805150	0.160615
H	7.063122	-2.954904	-1.262324
H	7.524499	-2.037630	0.192753
C	5.689755	-3.208015	1.935339
H	4.683163	-3.295985	2.374589
H	6.276223	-4.083843	2.266369
H	6.167504	-2.313072	2.365862
C	5.025100	-4.452106	-0.135897
H	4.954444	-4.455279	-1.235961
H	5.647917	-5.317160	0.154782
H	4.013908	-4.620643	0.266737

Reexo-anti-scis

SCF Energy: -2801.68411357 H

Num. Imaginary Frequencies: 0

C	-0.946831	0.495938	-1.964349
C	-2.040170	-0.494786	-1.535946
C	-2.352332	-0.660490	-0.039477
C	-1.283697	-1.307149	0.866451
C	-0.007144	-0.532715	0.936681
C	0.480804	-0.015310	-2.114506
C	1.161692	-1.009036	1.428124
C	3.243578	-1.298007	-1.435892
C	2.153455	-1.931042	-1.920589
C	0.818570	-1.301340	-1.911789
C	2.171399	-3.352814	-2.418257
C	4.634298	-1.804094	-1.346087
C	5.600628	-0.930558	-2.111469
C	4.985671	-2.879128	-0.604383
C	6.386997	-3.424671	-0.514806
C	1.446428	1.069129	-2.507813
C	2.272536	-0.118571	1.449349
O	3.408386	-0.423993	1.859792
O	-3.508474	-1.461880	0.054684
O	-0.894780	1.584071	-1.061074
H	-1.235244	0.868528	-2.967802
H	-2.982951	-0.130195	-1.971105
H	-1.872818	-1.483979	-1.986612
H	-2.544809	0.347646	0.373038
H	-0.047489	0.515967	0.617016
H	1.291816	-2.039608	1.769244
H	3.131294	-0.255452	-1.118316
H	0.011413	-2.009670	-1.696529
H	3.192818	-3.732138	-2.552105
H	1.652115	-4.020217	-1.709070
H	1.637932	-3.432960	-3.379035
H	5.380841	-0.957183	-3.192273
H	5.480926	0.117627	-1.789621
H	6.653847	-1.203485	-1.971423
H	6.777495	-3.323252	0.511853
H	6.381921	-4.504819	-0.740145
H	1.803825	1.637948	-1.634255
H	2.329208	0.666483	-3.023201
H	0.952750	1.793607	-3.174004
H	2.102184	0.907413	1.071049
C	-1.818500	-1.435677	2.305856
H	-2.029287	-0.442380	2.733703
H	-2.746757	-2.019453	2.311223
H	-1.085861	-1.938355	2.952983
H	-1.069545	-2.322062	0.489670
H	7.100092	-2.946577	-1.196954
Al	4.939445	0.723035	1.971088
C	6.510966	-0.408503	1.672868
Cl	4.514711	2.086611	0.273754
H	6.450160	-1.340335	2.263521
H	7.434958	0.109279	1.987566
H	6.638882	-0.694173	0.616251
C	4.681946	1.648311	3.687152
H	5.467549	2.403110	3.870502
H	3.711893	2.174617	3.736569
H	4.713045	0.943017	4.537548
Si	-5.094868	-0.949803	0.307164
Si	-1.594703	3.112168	-1.163437
C	-6.046296	-2.529608	0.764513
C	-5.123987	0.314915	1.692855
H	-4.430150	1.145902	1.483894
H	-6.130916	0.749994	1.800139
H	-4.838099	-0.127793	2.659924
C	-5.786685	-0.187580	-1.260947
H	-6.868257	0.001005	-1.159202
H	-5.304663	0.777087	-1.482138
H	-5.637612	-0.849798	-2.128413
C	-1.089486	3.915668	0.479947
C	-3.452300	2.931995	-1.329252
H	-3.951978	3.914512	-1.319349
H	-3.707111	2.443019	-2.283882
H	-3.873181	2.328705	-0.510000
C	-0.920310	4.032494	-2.648494
H	0.162832	4.212173	-2.565579
H	-1.102917	3.464206	-3.575466
H	-1.421559	5.008092	-2.759510
C	4.006584	-3.641012	0.249828
H	3.844110	-4.659152	-0.144493
H	4.414407	-3.760583	1.267756
H	3.032237	-3.144170	0.328652
C	-1.539215	5.384839	0.490932
H	-1.053789	5.969105	-0.307734
H	-2.630143	5.485093	0.365054
H	-1.275886	5.862005	1.451702
C	-1.756342	3.164311	1.643329
H	-2.856016	3.224239	1.596394

H	-1.477344	2.097859	1.655102
H	-1.446312	3.596922	2.611331
C	0.437457	3.842241	0.636601
H	0.752964	4.316503	1.583015
H	0.793497	2.800409	0.652259
H	0.966043	4.359300	-0.180530
C	-7.463778	-2.146722	1.219952
H	-8.015260	-1.591217	0.443341
H	-8.051442	-3.053171	1.451094
H	-7.449950	-1.525630	2.130463
C	-5.326414	-3.266896	1.903142
H	-5.214309	-2.635975	2.800329
H	-5.897608	-4.163785	2.203176
H	-4.322262	-3.598231	1.596676
C	-6.133036	-3.451956	-0.461651
H	-5.134314	-3.712782	-0.847952
H	-6.643904	-4.395818	-0.199131
H	-6.702160	-2.990554	-1.284808

Reexo-anti-strans

SCF Energy: -2801.68133323 H

Num. Imaginary Frequencies: 0

C	-0.906710	0.358707	-1.937004
C	-2.054048	-0.571010	-1.515027
C	-2.420590	-0.667427	-0.025257
C	-1.405824	-1.314555	0.940720
C	-0.106199	-0.581534	1.027824
C	0.504490	-0.212993	-2.000286
C	1.033714	-1.083898	1.559985
C	3.191874	-1.594343	-1.189437
C	2.078828	-2.195236	-1.662493
C	0.777753	-1.505983	-1.748082
C	2.040326	-3.651510	-2.055133
C	4.503624	-2.247528	-0.929657
C	4.511933	-3.411977	0.044692
C	5.638031	-1.769039	-1.485511
C	6.994194	-2.366780	-1.221516
C	1.534404	0.818334	-2.370281
C	2.167455	-0.224773	1.607474
O	3.276112	-0.552959	2.072304
O	-3.607958	-1.422558	0.060752
O	-0.852077	1.481956	-1.077797
H	-1.136799	0.697876	-2.967140
H	-2.965822	-0.186027	-1.996289
H	-1.912207	-1.582200	-1.923464
H	-2.589204	0.362428	0.341378
H	-0.104865	0.462114	0.689967
H	1.124174	-2.112366	1.919953
H	3.137571	-0.532293	-0.932136
H	-0.069518	-2.172766	-1.556764
H	1.463261	-4.242048	-1.322817
H	1.536765	-3.773585	-3.027579
H	3.042762	-4.091649	-2.136825
H	3.496396	-3.648874	0.389257
H	4.936122	-4.328795	-0.395286
H	5.108511	-3.172999	0.940484
H	7.727703	-1.572725	-1.003786
H	7.006502	-3.077905	-0.385618
H	1.896056	1.374764	-1.490259
H	2.409272	0.364823	-2.856026
H	1.100860	1.561647	-3.056735
H	2.041617	0.796951	1.201331
C	-1.993351	-1.364460	2.364737
H	-2.180748	-0.347342	2.744937
H	-2.942975	-1.912843	2.359446
H	-1.302795	-1.866649	3.056888
H	-1.215805	-2.350795	0.612499
H	7.364104	-2.894292	-2.118546
Al	4.821354	0.569240	2.235029
C	6.364635	-0.632866	2.141774
Cl	4.578250	1.806477	0.413294
H	7.314387	-0.083294	2.269740
H	6.418427	-1.153595	1.171971
H	6.330858	-1.403306	2.932989
C	4.447844	1.626179	3.850750
H	3.494594	2.179548	3.775080
H	4.381506	0.985752	4.749070
H	5.237889	2.372496	4.049045
Si	-5.181713	-0.841634	0.229455
Si	-1.490400	3.027912	-1.270993
C	-6.207598	-2.363101	0.722694
C	-5.212066	0.487365	1.553742
H	-4.477850	1.280616	1.336038
H	-6.204001	0.965445	1.601204
H	-4.981490	0.079481	2.550447
C	-5.788879	-0.131714	-1.397264
H	-6.866372	0.096563	-1.344644
H	-5.266361	0.804760	-1.645783
H	-5.632194	-0.839612	-2.226484
C	-1.030611	3.881416	0.360654
C	-3.344598	2.904188	-1.510796
H	-3.811744	3.901939	-1.547807
H	-3.577430	2.396449	-2.461202
H	-3.816758	2.337883	-0.692943
C	-0.716321	3.862290	-2.758245
H	0.366228	4.015047	-2.626953
H	-0.868589	3.257787	-3.667597
H	-1.181275	4.845597	-2.937587
C	5.658593	-0.603209	-2.436863
H	6.209570	-0.866108	-3.355926
H	4.655442	-0.266531	-2.728765
H	6.186462	0.252726	-1.983853
C	-1.406057	5.369379	0.282455
H	-0.848757	5.892661	-0.511555
H	-2.482010	5.515901	0.090321
H	-1.172482	5.876888	1.235331
C	-1.794039	3.217938	1.518043
H	-2.885013	3.334784	1.412724
H	-1.575356	2.139551	1.587203
H	-1.507978	3.674763	2.482297
C	0.480311	3.743231	0.604542
H	0.769589	4.256055	1.539176
H	0.779974	2.687935	0.698558
H	1.077328	4.185260	-0.209506

C	-7.625001	-1.908839	1.107121
H	-8.127247	-1.370962	0.285988
H	-8.254129	-2.781797	1.357256
H	-7.620237	-1.246474	1.988158
C	-6.285126	-3.338142	-0.462686
H	-5.283745	-3.652042	-0.799530
H	-6.839599	-4.249976	-0.176507
H	-6.807424	-2.895964	-1.326438
C	-5.556511	-3.071646	1.919493
H	-5.453076	-2.404057	2.790803
H	-6.170791	-3.932898	2.238216
H	-4.555052	-3.452131	1.665714

Reexo-syn-scis

SCF Energy: -2801.67906532 H

Num. Imaginary Frequencies: 0

C	-1.195371	1.211738	-1.762139
C	-1.978107	-0.090835	-1.569577
C	-1.979354	-0.754369	-0.182936
C	-0.624087	-1.253533	0.362837
C	0.287604	-0.120372	0.725905
C	0.312090	1.103008	-1.988721
C	1.571890	-0.265398	1.130802
C	3.297105	0.148761	-1.871272
C	2.313728	-0.331771	-2.661044
C	0.890384	-0.043944	-2.392604
C	2.557518	-1.258430	-3.823227
C	4.760355	-0.064178	-1.971564
C	5.508599	1.243520	-2.090948
C	5.343574	-1.281790	-1.882811
C	6.831128	-1.511647	-1.947067
C	1.046370	2.403062	-1.820286
C	2.286570	0.904438	1.526861
O	3.458823	0.938966	1.938128
O	-2.860600	-1.850947	-0.261168
O	-1.437638	2.063551	-0.656714
H	-1.592622	1.686269	-2.682618
H	-3.033815	0.141599	-1.777826
H	-1.685513	-0.839189	-2.320132
H	-2.354872	-0.009554	0.544291
H	-0.142804	0.889556	0.721639
H	2.081879	-1.231406	1.165727
H	3.005754	0.837270	-1.071065
H	0.240095	-0.906571	-2.570281
H	3.622616	-1.324811	-4.080964
H	2.199683	-2.276653	-3.594031
H	2.001489	-0.917416	-4.711368
H	5.255234	1.751450	-3.037055
H	5.203930	1.924258	-1.277804
H	6.599371	1.139677	-2.042368
H	7.202673	-1.861970	-0.968589
H	7.058392	-2.312431	-2.670889
H	1.258560	2.616888	-0.759810
H	2.001694	2.405554	-2.361497
H	0.432320	3.237573	-2.189546
H	1.752192	1.870623	1.463386
C	-0.815625	-2.138214	1.607284
H	-1.291541	-1.573103	2.423821
H	-1.450933	-2.998766	1.363850
H	0.152675	-2.511728	1.969226
H	-0.128271	-1.868061	-0.407519
H	7.412459	-0.627197	-2.233705
Al	4.942484	-0.094484	2.542666
C	4.899106	0.238428	4.480203
Cl	4.427179	-2.197024	2.094403
H	5.052099	1.307732	4.713223
H	5.694252	-0.320600	5.005588
H	3.939508	-0.060807	4.938094
C	6.451586	0.522873	1.451128
H	7.402977	0.100946	1.822763
H	6.351173	0.214541	0.397636
H	6.559976	1.622137	1.468083
Si	-4.404031	-1.922770	0.415081
Si	-2.485442	3.387616	-0.591502
C	-5.045566	-3.636815	-0.083105
C	-4.307777	-1.719573	2.277539
H	-3.789848	-0.782900	2.541553
H	-5.321497	-1.662212	2.707235
H	-3.777087	-2.552111	2.764474
C	-5.460692	-0.534806	-0.271980
H	-6.500475	-0.622246	0.084096
H	-5.077234	0.436288	0.079882
H	-5.475809	-0.523829	-1.372824
C	-2.836576	3.626828	1.260390
C	-4.038983	3.018439	-1.572824
H	-4.754066	3.852624	-1.480347
H	-3.807979	2.904028	-2.644704
H	-4.543770	2.101287	-1.234689
C	-1.649851	4.894640	-1.329628
H	-0.729056	5.165445	-0.789176
H	-1.387415	4.716429	-2.385330
H	-2.328296	5.763109	-1.304110
C	4.567816	-2.553843	-1.663254
H	3.520288	-2.375635	-1.391419
H	4.586359	-3.185826	-2.568153
H	5.033664	-3.140187	-0.855224
C	-6.387236	-3.903449	0.617162
H	-6.792103	-4.885161	0.312621
H	-6.283407	-3.919158	1.714404
H	-7.146451	-3.145174	0.362918
C	-4.024791	-4.705703	0.336838
H	-3.846004	-4.701584	1.424718
H	-4.389259	-5.713706	0.068844
H	-3.055378	-4.556119	-0.163340
C	-5.240582	-3.687009	-1.606341
H	-4.306271	-3.458769	-2.144155
H	-5.568450	-4.693994	-1.921288
H	-6.007479	-2.972066	-1.946424
C	-3.518564	4.988070	1.473468
H	-4.449355	5.082790	0.889405
H	-3.786234	5.120690	2.536847
H	-2.860564	5.826799	1.194950
C	-3.763826	2.510563	1.764805
H	-3.335829	1.510631	1.588468

H	-3.932070	2.608188	2.852144
H	-4.751120	2.543473	1.276414
C	-1.517387	3.587427	2.047253
H	-1.701756	3.786522	3.118023
H	-1.030679	2.602501	1.972974
H	-0.798675	4.344664	1.692477

Reexo-syn-strans

SCF Energy: -2801.67664717 H

Num. Imaginary Frequencies: 0

C	-1.071836	1.400234	-1.558610
C	-1.958921	0.151292	-1.558284
C	-2.084877	-0.665743	-0.263034
C	-0.811405	-1.359187	0.262423
C	0.239704	-0.394524	0.720915
C	0.427612	1.216233	-1.778266
C	1.507503	-0.761442	1.025671
C	3.362907	0.179524	-1.731362
C	2.365602	-0.263666	-2.532698
C	0.955457	0.070336	-2.252589
C	2.551657	-1.155382	-3.737108
C	4.817625	-0.066741	-1.788601
C	5.325369	-1.415939	-2.252270
C	5.654561	0.921957	-1.383868
C	7.153310	0.813453	-1.434798
C	1.223985	2.460713	-1.503965
C	2.418290	0.226335	1.499113
O	3.602507	0.023208	1.826270
O	-3.051131	-1.663050	-0.507690
O	-1.271438	2.114763	-0.350199
H	-1.410035	2.025127	-2.410540
H	-2.982520	0.491463	-1.779196
H	-1.685591	-0.523829	-2.382363
H	-2.429178	0.019049	0.533354
H	-0.062182	0.649268	0.875892
H	1.868645	-1.783662	0.885861
H	3.054681	0.837381	-0.917280
H	0.263917	-0.742083	-2.499310
H	3.576983	-1.141839	-4.124013
H	2.288859	-2.200761	-3.500481
H	1.882459	-0.835781	-4.551267
H	4.541071	-2.178816	-2.170124
H	5.674385	-1.400185	-3.298414
H	6.166203	-1.759781	-1.633244
H	7.554306	1.523507	-2.179775
H	7.597338	1.098023	-0.466601
H	1.488820	2.550736	-0.436886
H	2.157584	2.481879	-2.081752
H	0.636502	3.354545	-1.757792
H	2.048226	1.265173	1.581879
C	-1.139965	-2.295786	1.439575
H	-1.551803	-1.731062	2.290651
H	-1.878942	-3.044550	1.128303
H	-0.236902	-2.820606	1.781672
H	-0.386663	-1.978947	-0.545410
H	7.517775	-0.186765	-1.699322
Al	4.763930	-1.434861	2.244088
C	4.223994	-1.841058	4.092738
Cl	4.187265	-3.082827	0.889223
H	4.413491	-0.990234	4.772075
H	4.778249	-2.705662	4.500117
H	3.148767	-2.083990	4.167928
C	6.566044	-0.774713	1.839070
H	7.332282	-1.356135	2.383157
H	6.803707	-0.851499	0.765431
H	6.696587	0.282307	2.132535
Si	-4.620323	-1.712228	0.105394
Si	-2.219721	3.495870	-0.129783
C	-5.337963	-3.318334	-0.604615
C	-4.591045	-1.720212	1.981423
H	-4.017049	-0.860612	2.365036
H	-5.616170	-1.629697	2.377161
H	-4.145973	-2.638900	2.393288
C	-5.576407	-0.199081	-0.452685
H	-6.646123	-0.302452	-0.206520
H	-5.207038	0.693464	0.077325
H	-5.490512	-0.020244	-1.535610
C	-3.806706	3.342591	-1.115253
H	-4.460787	2.539862	-0.744474
H	-4.372139	4.287897	-1.073856
H	-3.589156	3.140058	-2.177006
C	-1.293731	5.013650	-0.724906
H	-1.865051	5.927303	-0.490924
H	-0.300960	5.105018	-0.257785
H	-1.156922	4.985352	-1.818408
C	-2.536135	3.567074	1.741743
C	5.137947	2.253152	-0.884778
H	4.471487	2.744234	-1.611110
H	4.567098	2.137462	0.052521
H	5.966918	2.944273	-0.675411
C	-3.064433	2.212608	2.238123
H	-3.953477	1.880764	1.676339
H	-2.299298	1.426017	2.150867
H	-3.353659	2.276870	3.302216
C	-3.581698	4.657818	2.026139
H	-4.556118	4.422550	1.567975
H	-3.746549	4.757781	3.113729
H	-3.264780	5.645810	1.652901
C	-1.230714	3.903885	2.479138
H	-1.391814	3.896679	3.572018
H	-0.434335	3.173867	2.259282
H	-0.852613	4.903455	2.210818
C	-5.487039	-3.181721	-2.127806
H	-4.524299	-2.952601	-2.612487
H	-5.863876	-4.123543	-2.565666
H	-6.198977	-2.385817	-2.401225
C	-4.391285	-4.485749	-0.285794
H	-4.248575	-4.616994	0.799588
H	-4.801046	-5.433589	-0.678798
H	-3.399226	-4.335738	-0.739122
C	-6.713909	-3.585675	0.025356
H	-7.160948	-4.501797	-0.400502
H	-6.646479	-3.731835	1.115814
H	-7.423032	-2.761650	-0.159421

Siendo-anti-scis

SCF Energy: -2801.68500605 H

Num. Imaginary Frequencies: 0

C	-1.782888	1.053058	0.702634
C	-2.266094	0.287854	1.942621
C	-1.883427	-1.192963	2.038428
C	-0.431198	-1.554460	2.452132
C	0.533228	-1.540797	1.316984
C	-0.390494	1.639622	0.820141
C	1.884036	-1.495534	1.401792
C	2.698763	1.788738	1.022063
C	1.979409	1.603775	-0.109214
C	0.556428	1.231672	-0.047562
C	2.571416	1.660070	-1.491563
C	4.131167	2.124605	1.154896
C	4.871428	1.155053	2.048211
C	4.707391	3.197675	0.563093
C	6.182989	3.496224	0.640209
C	-0.218086	2.700338	1.870715
C	2.629034	-1.590114	0.188093
O	3.871552	-1.644282	0.142050
O	-2.189595	-1.826365	0.819915
O	-2.690374	2.112649	0.444294
H	-1.781234	0.337114	-0.137408
H	-1.986118	0.814342	2.868051
H	-3.365642	0.310770	1.896913
H	-2.511745	-1.599512	2.853745
H	0.082083	-1.666595	0.326818
H	2.429733	-1.397930	2.343094
H	2.192201	1.572093	1.970146
H	0.234415	0.530366	-0.828894
H	2.263286	2.576154	-2.023256
H	3.669111	1.627745	-1.472386
H	2.206065	0.812061	-2.093604
H	5.017273	0.189825	1.537277
H	5.853095	1.520191	2.375291
H	4.276166	0.950831	2.953944
H	6.789776	2.651478	0.987425
H	6.555026	3.779537	-0.358270
H	-0.015181	2.272178	2.865888
H	0.612113	3.380040	1.633679
H	-1.145678	3.286416	1.951022
H	2.055229	-1.637635	-0.757555
C	0.046099	-0.833571	3.707773
H	0.942620	-1.311237	4.127972
H	0.288452	0.218198	3.497054
H	-0.734304	-0.857732	4.483084
H	-0.496626	-2.635051	2.691557
H	6.377937	4.358739	1.301582
Al	5.012705	-1.941403	-1.373856
C	3.810808	-2.011971	-2.932037
Cl	6.249966	-0.127873	-1.359459
H	3.085275	-2.843799	-2.873054
H	4.397465	-2.175685	-3.854318
H	3.235794	-1.082240	-3.086881
C	6.039160	-3.535182	-0.856864
H	5.388716	-4.420332	-0.734740
H	6.792818	-3.796231	-1.621443
H	6.581449	-3.395487	0.094897
Si	-3.078002	-3.249916	0.617264
Si	-3.727055	2.073915	-0.886575
C	-2.835605	-3.690616	-1.212716
C	-4.870992	-2.915405	1.045784
H	-4.947096	-2.468086	2.050988
H	-5.343689	-2.222425	0.332576
H	-5.455853	-3.849531	1.055998
C	-2.403077	-4.576121	1.758289
H	-1.331563	-4.764489	1.587426
H	-2.537267	-4.290690	2.814878
H	-2.941857	-5.526026	1.606808
C	-2.711301	1.844115	-2.447826
H	-3.331145	1.991025	-3.347611
H	-1.871832	2.556157	-2.488634
H	-2.294593	0.825118	-2.501760
C	-4.627471	3.742233	-0.857353
C	-4.892287	0.619069	-0.679195
H	-5.602642	0.774224	0.148453
H	-5.467761	0.415572	-1.596562
H	-4.297442	-0.278549	-0.448158
C	3.938855	4.230853	-0.216950
H	2.852509	4.152769	-0.080987
H	4.255223	5.241921	0.090860
H	4.153836	4.153434	-1.296648
C	-3.207914	-2.485824	-2.090283
H	-2.582253	-1.608578	-1.860797
H	-3.065914	-2.729078	-3.158455
H	-4.260588	-2.188385	-1.958835
C	-3.740105	-4.882307	-1.565619
H	-3.602870	-5.169682	-2.623260
H	-3.512125	-5.771223	-0.954307
H	-4.807382	-4.644081	-1.427286
C	-1.367754	-4.068446	-1.465799
H	-0.681916	-3.245440	-1.206984
H	-1.062579	-4.954792	-0.886519
H	-1.209749	-4.304295	-2.533289
C	-5.730742	3.739467	-1.927244
H	-5.326496	3.574290	-2.939741
H	-6.486943	2.960051	-1.737227
H	-6.257469	4.710495	-1.940863
C	-5.255622	3.962199	0.527243
H	-5.989144	3.177735	0.776243
H	-4.492904	3.970484	1.321373
H	-5.787223	4.930216	0.560506
C	-3.626357	4.870114	-1.151227
H	-2.798125	4.880782	-0.424394
H	-3.187419	4.777978	-2.158040
H	-4.126530	5.854000	-1.100054

Siendo-anti-strans

SCF Energy: -2801.68412327 H

Num. Imaginary Frequencies: 0

C	2.052636	-0.684658	0.701721
C	2.312851	0.175880	1.939442

C	1.726202	1.592599	1.935483
C	0.247378	1.777210	2.361295
C	-0.734747	1.497677	1.275621
C	0.669975	-1.301505	0.602158
C	-2.032750	1.151959	1.440187
C	-2.316180	-1.941913	0.025004
C	-1.396789	-1.533920	-0.888869
C	-0.080787	-1.018328	-0.483978
C	-1.614054	-1.516942	-2.383277
C	-3.617593	-2.599665	-0.181179
C	-3.808326	-3.498103	-1.387586
C	-4.613930	-2.488718	0.736616
C	-5.938112	-3.183270	0.529158
C	0.316851	-2.275617	1.689822
C	-2.888201	1.125985	0.294811
O	-4.122871	1.001184	0.383065
O	1.905348	2.177128	0.670330
O	3.002815	-1.737869	0.710034
H	2.201946	-0.034422	-0.177139
H	2.022499	-0.360202	2.856577
H	3.407640	0.290233	1.983006
H	2.298050	2.146610	2.704284
H	-0.375243	1.710570	0.263966
H	-2.482491	0.960042	2.417322
H	-2.054673	-1.762930	1.067758
H	0.378140	-0.340028	-1.214696
H	-1.042148	-2.317612	-2.882769
H	-2.666148	-1.614407	-2.669162
H	-1.243432	-0.565579	-2.799049
H	-2.844900	-3.809598	-1.811868
H	-4.351121	-4.414881	-1.113237
H	-4.385964	-3.015974	-2.194142
H	-6.310747	-3.076865	-0.500359
H	-5.856313	-4.265524	0.736764
H	-0.293171	-1.809368	2.480883
H	-0.262541	-3.125651	1.298940
H	1.231922	-2.663501	2.159311
H	-2.424622	1.279173	-0.698353
C	-0.080444	1.155359	3.713036
H	-1.025775	1.547154	4.114928
H	-0.168726	0.061129	3.646078
H	0.709544	1.388823	4.442453
H	0.160053	2.878448	2.465923
H	-6.705426	-2.776330	1.202176
Al	-5.505968	1.227846	-0.916447
C	-4.960192	0.212511	-2.506351
Cl	-7.216080	0.322074	0.121283
H	-3.984188	0.545482	-2.902441
H	-5.691963	0.334761	-3.325404
H	-4.883239	-0.867745	-2.299362
C	-5.667732	3.187326	-1.021778
H	-4.743382	3.649096	-1.415580
H	-6.489411	3.500280	-1.690823
H	-5.863822	3.645671	-0.036107
Si	2.895394	3.495292	0.309700
Si	3.987668	-2.097078	-0.610596
C	2.685443	3.715619	-1.562605
C	4.657802	3.086210	0.796841
H	4.736637	2.950940	1.888305
H	5.009291	2.160763	0.314596
H	5.346023	3.900604	0.516998
C	2.300221	4.985476	1.278195
H	1.269069	5.263740	1.008467
H	2.323781	4.777074	2.360862
H	2.947840	5.859412	1.100171
C	2.942851	-2.279683	-2.158234
H	3.561781	-2.605065	-3.010763
H	2.133124	-3.013358	-2.021241
H	2.482914	-1.317053	-2.435008
C	4.851074	-3.718189	-0.135845
C	5.200315	-0.685745	-0.847677
H	5.850956	-0.554428	0.031415
H	5.840744	-0.844410	-1.730546
H	4.649507	0.255257	-1.007123
C	-4.525166	-1.720021	2.025380
H	-4.798360	-2.378357	2.868063
H	-3.536715	-1.292815	2.230665
H	-5.254745	-0.894719	2.016222
C	5.540138	-3.551654	1.227185
H	4.817377	-3.294695	2.017208
H	6.043131	-4.489975	1.522790
H	6.308612	-2.761445	1.206525
C	3.808126	-4.843236	-0.047947
H	3.324749	-5.032381	-1.020220
H	4.284606	-5.787832	0.270656
H	3.014997	-4.609001	0.680193
C	5.900068	-4.071371	-1.201855
H	6.397273	-5.025831	-0.952107
H	5.451422	-4.190320	-2.202041
H	6.687126	-3.303150	-1.276601
C	1.191390	3.828140	-1.903663
H	1.055183	3.983738	-2.988760
H	0.643051	2.913487	-1.627486
H	0.710596	4.676117	-1.388896
C	3.281937	2.502323	-2.292792
H	4.366905	2.411670	-2.122964
H	2.810613	1.559834	-1.968912
H	3.126889	2.592475	-3.382795
C	3.412737	4.993831	-2.008757
H	4.487806	4.965456	-1.765263
H	3.329328	5.122740	-3.102608
H	2.985888	5.895466	-1.539951

Siendo-syn-scis

SCF Energy: -2801.68526918 H

Num. Imaginary Frequencies: 0

C	-1.905163	-0.539131	-0.715962
C	-2.100585	0.441240	-1.871662
C	-1.631894	1.884794	-1.653144
C	-0.155529	2.218069	-1.987721
C	0.806176	1.875083	-0.904975
C	-0.485556	-0.999535	-0.436019
C	2.093536	1.495484	-1.077835
C	2.381957	-1.550228	0.735900

C	1.233785	-1.368292	1.429508
C	-0.008956	-0.863056	0.818808
C	1.096121	-1.684155	2.897646
C	3.669868	-2.106206	1.204738
C	4.177583	-3.270239	0.372995
C	4.390660	-1.621395	2.241208
C	5.705980	-2.238575	2.643161
C	0.208733	-1.709799	-1.562759
C	2.940122	1.393754	0.071178
O	4.156913	1.143406	0.047940
O	-1.899204	2.288394	-0.334609
O	-2.676582	-1.690715	-1.019707
H	-2.285560	-0.045367	0.194208
H	-1.672488	0.031634	-2.799432
H	-3.190131	0.477170	-2.030301
H	-2.211520	2.495267	-2.371378
H	0.439647	2.051565	0.111820
H	2.520299	1.306129	-2.065693
H	2.362312	-1.330443	-0.335719
H	-0.683187	-0.377125	1.535777
H	1.943917	-2.269632	3.275425
H	1.028691	-0.759754	3.496304
H	0.169142	-2.250653	3.081650
H	5.221703	-3.131967	0.052315
H	4.126903	-4.218125	0.935674
H	3.566104	-3.405969	-0.530850
H	5.764461	-3.313865	2.425231
H	6.533824	-1.741769	2.107518
H	0.951712	-1.061835	-2.056993
H	0.748600	-2.600327	-1.206213
H	-0.518180	-2.030624	-2.322027
H	2.484484	1.594879	1.056830
C	0.259960	1.790866	-3.389633
H	1.186655	2.294534	-3.700670
H	0.427085	0.705397	-3.453780
H	-0.521059	2.057672	-4.117128
H	-0.140963	3.327239	-1.950838
H	5.888567	-2.100945	3.720432
Al	5.409192	0.730325	-1.338540
C	5.766381	2.486954	-2.151327
Cl	7.116609	0.012253	-0.156916
H	6.547433	2.428536	-2.930679
H	6.108590	3.230513	-1.409761
H	4.864394	2.903855	-2.635814
C	4.616438	-0.704279	-2.429368
H	3.854384	-0.328192	-3.135640
H	5.391688	-1.202723	-3.039092
H	4.140285	-1.492063	-1.822085
Si	-3.084134	3.390536	0.145996
Si	-3.787818	-2.375214	0.047891
C	-3.049150	3.302376	2.040893
C	-4.735868	2.867002	-0.567275
H	-4.725506	2.936425	-1.667533
H	-4.988590	1.830603	-0.294879
H	-5.545747	3.521633	-0.205405
C	-2.623368	5.087807	-0.501070
H	-1.661521	5.433506	-0.090021
H	-2.534937	5.068978	-1.600124
H	-3.393046	5.834887	-0.247686
C	-2.951151	-2.788337	1.675271
H	-3.641307	-3.330860	2.342481
H	-2.056253	-3.412213	1.525423
H	-2.641641	-1.869149	2.198253
C	-4.409090	-3.927735	-0.848498
C	-5.161311	-1.135953	0.360179
H	-5.687820	-0.864813	-0.568564
H	-5.903051	-1.530339	1.073754
H	-4.744957	-0.214518	0.798630
C	4.025044	-0.395493	3.028989
H	4.880907	0.300150	3.045084
H	3.157481	0.134796	2.620559
H	3.804401	-0.650851	4.079785
C	-3.933499	4.419787	2.616765
H	-4.975830	4.347426	2.264106
H	-3.957538	4.361963	3.719551
H	-3.557662	5.420906	2.349871
C	-3.581640	1.937003	2.503327
H	-4.636605	1.789413	2.221183
H	-2.998807	1.104670	2.075583
H	-3.521508	1.851157	3.602967
C	-1.606548	3.479894	2.539072
H	-1.576039	3.462203	3.643178
H	-0.950971	2.673387	2.174639
H	-1.170943	4.439463	2.215233
C	-5.542491	-4.571188	-0.034357
H	-5.901151	-5.489782	-0.532442
H	-5.215163	-4.857184	0.978966
H	-6.408562	-3.897360	0.070648
C	-4.932816	-3.539846	-2.239780
H	-4.146633	-3.070488	-2.851430
H	-5.291905	-4.433958	-2.780510
H	-5.776819	-2.833098	-2.179566
C	-3.251412	-4.927202	-0.997450
H	-2.876994	-5.271211	-0.019572
H	-3.582525	-5.821832	-1.554942
H	-2.401996	-4.489460	-1.545954

Siendo-syn-strans

SCF Energy: -2801.68532803 H

Num. Imaginary Frequencies: 0

C	1.885250	0.567053	-0.677312
C	2.067658	-0.372694	-1.867984
C	1.640438	-1.832493	-1.674731
C	0.154884	-2.186278	-1.940285
C	-0.755778	-1.900209	-0.796764
C	0.458915	0.959274	-0.338219
C	-2.064973	-1.569074	-0.890005
C	-2.388544	1.363129	0.918789
C	-1.238728	1.097156	1.584964
C	0.017395	0.724721	0.916035
C	-1.118488	1.162154	3.089413
C	-3.714957	1.693960	1.486475
C	-4.246103	0.879128	2.648874
C	-4.481917	2.666097	0.936835

C	-5.857027	2.966187	1.479656
C	-0.286670	1.705478	-1.407217
C	-2.858301	-1.531030	0.300453
O	-4.091065	-1.365683	0.332938
O	1.985891	-2.274767	-0.386908
O	2.605047	1.753146	-0.970722
H	2.314644	0.059570	0.203019
H	1.595585	0.051175	-2.767733
H	3.151404	-0.376205	-2.065784
H	2.192403	-2.405882	-2.443797
H	-0.329174	-2.089031	0.193568
H	-2.550810	-1.376771	-1.849769
H	-2.354105	1.313214	-0.169918
H	0.732830	0.225212	1.581560
H	-1.950660	1.698913	3.560266
H	-1.068002	0.151044	3.529171
H	-0.185844	1.676400	3.370933
H	-4.348582	1.480340	3.568538
H	-5.242456	0.474862	2.411917
H	-3.595900	0.025738	2.880440
H	-5.859681	3.069548	2.576437
H	-6.262366	3.895399	1.053476
H	-1.064675	1.080670	-1.877059
H	-0.792311	2.593906	-0.997997
H	0.400525	2.040032	-2.196540
H	-2.347997	-1.713846	1.262419
C	-0.343686	-1.721009	-3.302874
H	-1.273682	-2.236117	-3.583970
H	-0.537957	-0.638365	-3.319170
H	0.403403	-1.943425	-4.079297
H	0.164392	-3.295983	-1.941981
H	-6.556960	2.149745	1.231459
Al	-5.424914	-1.060653	-1.001882
C	-5.696836	-2.848609	-1.779089
Cl	-7.127625	-0.467233	0.259658
H	-6.508439	-2.851081	-2.528942
H	-5.961957	-3.602796	-1.017044
H	-4.788141	-3.212127	-2.293234
C	-4.772457	0.409241	-2.139184
H	-4.214256	0.038128	-3.017938
H	-5.604075	1.023826	-2.527157
H	-4.102501	1.092337	-1.590598
Si	3.248555	-3.326729	-0.001780
Si	3.704035	2.461120	0.094543
C	3.302883	-3.302245	1.894401
C	4.833626	-2.693007	-0.774711
H	4.768622	-2.722165	-1.874955
H	5.049013	-1.655770	-0.474578
H	5.692817	-3.318112	-0.480793
C	2.844792	-5.024525	-0.684516
H	1.928160	-5.437147	-0.233737
H	2.692229	-4.973679	-1.775521
H	3.666883	-5.735447	-0.501484
C	2.896621	2.752022	1.762983
H	3.569214	3.322004	2.425371
H	1.951963	3.310147	1.670402
H	2.677926	1.794393	2.262492
C	4.198737	4.085880	-0.750683
C	5.159374	1.298027	0.313553
H	5.668843	1.094792	-0.641672
H	5.900106	1.709226	1.018620
H	4.813300	0.337006	0.727520
C	-4.052599	3.525100	-0.220222
H	-3.081956	3.240883	-0.646242
H	-4.807927	3.493074	-1.023035
H	-3.979982	4.579875	0.097784
C	5.317805	4.764611	0.054540
H	5.010064	4.983364	1.090470
H	6.228093	4.144456	0.099063
H	5.599378	5.725816	-0.411669
C	2.976431	5.014872	-0.817179
H	3.230641	5.951130	-1.345926
H	2.136842	4.546544	-1.355548
H	2.616735	5.293399	0.186740
C	4.696655	3.792014	-2.174081
H	5.584026	3.137720	-2.172883
H	3.919908	3.301177	-2.780925
H	4.981350	4.729410	-2.685019
C	4.263721	-4.395543	2.387974
H	4.340413	-4.372182	3.489626
H	3.919922	-5.403795	2.105164
H	5.282807	-4.263766	1.987773
C	3.795785	-1.929334	2.377791
H	3.784266	-1.881169	3.481320
H	4.828501	-1.724832	2.052351
H	3.157180	-1.111228	2.005622
C	1.895957	-3.562765	2.454245
H	1.188038	-2.776011	2.149509
H	1.488250	-4.530264	2.117938
H	1.918818	-3.582609	3.558508

Siexo-anti-scis

SCF Energy: -2801.68365007 H

Num. Imaginary Frequencies: 0

C	1.589642	-1.032277	0.397504
C	1.982792	-0.479473	1.772027
C	1.746106	1.021135	1.995161
C	0.314198	1.484990	2.356272
C	-0.633596	1.414812	1.208485
C	0.142316	-1.446675	0.171312
C	-1.986347	1.433723	1.282418
C	-2.986665	-1.756283	0.294641
C	-2.083991	-2.182515	1.205908
C	-0.669253	-1.767366	1.195866
C	-2.451000	-3.059238	2.376147
C	-4.431202	-2.086731	0.227249
C	-4.793474	-2.775080	-1.067638
C	-5.311926	-1.753258	1.198210
C	-6.773012	-2.119209	1.180655
C	-0.232819	-1.520876	-1.281314
C	-2.721304	1.430086	0.061532
O	-3.964210	1.474908	-0.000704
O	2.182605	1.722931	0.856030
O	2.398966	-2.157997	0.087612

H	1.795648	-0.222812	-0.327533
H	1.547800	-1.062102	2.597140
H	3.069155	-0.626915	1.848883
H	2.359698	1.293395	2.874903
H	-0.172829	1.434475	0.213558
H	-2.537007	1.440932	2.225746
H	-2.628631	-1.150938	-0.544551
H	-0.230151	-1.742445	2.198129
H	-2.418670	-2.485060	3.318086
H	-3.457035	-3.486356	2.276307
H	-1.727903	-3.883778	2.481326
H	-4.449816	-2.163913	-1.919001
H	-4.281591	-3.749001	-1.147935
H	-5.869742	-2.946029	-1.193524
H	-7.078643	-2.709457	0.308628
H	-7.019977	-2.704497	2.083358
H	-1.027694	-2.253704	-1.475931
H	-0.585627	-0.543331	-1.654419
H	0.644927	-1.796672	-1.883031
H	-2.141915	1.391872	-0.880820
C	-0.209731	0.908759	3.668136
H	-1.090794	1.461591	4.023971
H	-0.493404	-0.148440	3.565851
H	0.562028	0.982871	4.448819
H	0.433008	2.576416	2.506411
H	-7.401193	-1.213869	1.216004
Al	-5.055404	1.580882	-1.572659
C	-5.077580	3.509132	-1.961316
Cl	-3.760792	0.499083	-3.008765
H	-5.575910	4.078450	-1.155564
H	-5.624312	3.734148	-2.894616
H	-4.061644	3.928001	-2.074206
C	-6.725265	0.634319	-1.180600
H	-7.123848	0.914787	-0.189188
H	-7.502687	0.894035	-1.921791
H	-6.612156	-0.461392	-1.195024
Si	3.137330	3.116918	0.816558
Si	3.793944	-2.075084	-0.860336
C	3.150616	3.606046	-1.016341
C	4.848909	2.716606	1.468059
H	5.420872	2.078655	0.776855
H	5.426171	3.639913	1.638981
H	4.779198	2.188769	2.433951
C	2.369618	4.444101	1.896986
H	2.953795	5.376945	1.831406
H	1.333233	4.673723	1.603833
H	2.367357	4.135881	2.955784
C	4.934986	-0.754379	-0.171897
H	4.368691	0.182677	-0.056832
H	5.346451	-1.023677	0.813574
H	5.777033	-0.556431	-0.854733
C	3.343422	-1.607182	-2.620703
H	2.818072	-0.638436	-2.644055
H	4.251478	-1.499395	-3.236545
H	2.695111	-2.357840	-3.099235
C	4.539475	-3.815620	-0.752258
C	-4.923422	-0.964966	2.421095
H	-5.609556	-0.110931	2.549342
H	-5.014049	-1.580176	3.333203
H	-3.899199	-0.577295	2.370086
C	4.146118	4.758487	-1.223501
H	5.176123	4.464197	-0.963525
H	4.153185	5.075832	-2.281469
H	3.887064	5.643965	-0.619565
C	3.573352	2.400154	-1.869433
H	4.582934	2.042219	-1.610634
H	2.878076	1.555127	-1.745071
H	3.584882	2.670391	-2.940455
C	1.744022	4.057951	-1.438827
H	1.727344	4.310971	-2.513906
H	0.994051	3.266880	-1.275644
H	1.414586	4.953153	-0.887048
C	5.845232	-3.861355	-1.561023
H	6.592602	-3.146201	-1.179080
H	6.298026	-4.867674	-1.506771
H	5.679165	-3.635676	-2.627335
C	3.542243	-4.836535	-1.321484
H	3.329440	-4.654603	-2.387485
H	3.948284	-5.860783	-1.238721
H	2.583505	-4.812654	-0.779475
C	4.831365	-4.153369	0.717903
H	3.918166	-4.107488	1.331995
H	5.244368	-5.174378	0.805446
H	5.568524	-3.463687	1.160718

Siexo-anti-strans

SCF Energy: -2801.67965069 H

Num. Imaginary Frequencies: 0

C	-1.876131	0.650845	0.486691
C	-2.314448	-0.057100	1.770692
C	-1.885764	-1.519071	1.944440
C	-0.479018	-1.805090	2.540251
C	0.612556	-1.767328	1.532282
C	-0.367368	0.825522	0.322043
C	1.925950	-1.502968	1.742757
C	2.583591	1.935719	0.444708
C	1.705560	1.839407	1.475596
C	0.285771	1.503653	1.289654
C	2.074037	2.101671	2.919170
C	4.037245	2.190074	0.481989
C	4.847666	1.670514	1.652943
C	4.615176	2.835961	-0.563319
C	6.084588	3.143500	-0.642640
C	0.217644	0.277964	-0.946138
C	2.799758	-1.633800	0.625542
O	4.028842	-1.426940	0.661474
O	-1.995757	-2.199191	0.719177
O	-2.520665	1.911808	0.464494
H	-2.228973	0.030684	-0.355016
H	-2.013844	0.536775	2.647143
H	-3.416215	-0.042288	1.755621
H	-2.583467	-1.945893	2.689977
H	0.308602	-2.080844	0.527827
H	2.333325	-1.183962	2.704805

H	2.164035	1.848921	-0.558085
H	-0.343293	1.832068	2.125198
H	2.282782	1.165159	3.463728
H	2.947737	2.755011	3.024570
H	1.232827	2.586683	3.438083
H	5.061314	2.451256	2.401391
H	4.321105	0.854281	2.163175
H	5.813145	1.265046	1.323375
H	6.670272	2.753861	0.198515
H	6.509580	2.739687	-1.577730
H	0.132219	1.015978	-1.762304
H	1.283583	0.031255	-0.861560
H	-0.328465	-0.621784	-1.270018
H	2.342886	-1.953849	-0.330082
C	-0.192408	-1.060458	3.836987
H	0.672604	-1.493059	4.360337
H	0.020053	0.002261	3.649807
H	-1.055909	-1.123682	4.516088
H	-0.529624	-2.889494	2.772787
H	6.239191	4.235947	-0.681046
Al	5.229008	-1.694791	-0.815139
C	5.301970	-3.655427	-0.967690
Cl	4.022945	-0.820490	-2.450106
H	5.755281	-4.113551	-0.069599
H	5.910711	-3.978709	-1.831178
H	4.302220	-4.108718	-1.092656
C	6.864194	-0.683055	-0.437650
H	7.225504	-0.852016	0.592576
H	7.676412	-1.002249	-1.115759
H	6.739197	0.403258	-0.573656
Si	-3.224509	-3.268338	0.275398
Si	-3.455545	2.457320	-0.826893
C	-2.942579	-3.545338	-1.579825
C	-4.888796	-2.487366	0.638556
H	-4.999946	-1.508968	0.146065
H	-5.708810	-3.137650	0.291722
H	-5.023945	-2.340335	1.722801
C	-3.034426	-4.843211	1.272829
H	-3.851041	-5.552517	1.061317
H	-2.078371	-5.347352	1.059504
H	-3.065379	-4.619329	2.352280
C	-4.917207	1.301776	-1.050634
H	-4.562641	0.285277	-1.287970
H	-5.537993	1.244522	-0.142575
H	-5.559410	1.625593	-1.885965
C	-2.431978	2.458366	-2.398350
H	-2.158592	1.429737	-2.684763
H	-3.000217	2.891713	-3.237857
H	-1.502754	3.037535	-2.278977
C	-3.984930	4.205431	-0.314591
C	3.820343	3.309054	-1.760205
H	2.906554	3.853406	-1.479462
H	4.423837	3.976388	-2.392442
H	3.516557	2.454474	-2.389204
C	-1.469425	-3.903804	-1.828846
H	-0.798022	-3.084291	-1.527442
H	-1.163334	-4.808330	-1.277876
H	-1.296601	-4.099092	-2.902186
C	-3.841478	-4.694316	-2.063503
H	-3.721907	-4.844801	-3.151191
H	-3.590493	-5.648209	-1.571710
H	-4.909620	-4.491750	-1.878249
C	-3.290138	-2.262345	-2.351203
H	-2.693607	-1.402579	-2.004598
H	-3.084913	-2.392094	-3.428769
H	-4.354833	-1.996384	-2.250465
C	-4.719375	4.141133	1.033428
H	-5.635302	3.530338	0.974706
H	-4.080792	3.712542	1.821688
H	-5.020780	5.153399	1.357984
C	-2.736679	5.090845	-0.175156
H	-2.024464	4.677439	0.556713
H	-2.203828	5.203865	-1.133386
H	-3.017229	6.103825	0.165427
C	-4.919539	4.796342	-1.381446
H	-4.433244	4.860222	-2.368852
H	-5.840429	4.201705	-1.498757
H	-5.225204	5.820496	-1.101606

Siexo-syn-scis

SCF Energy: -2801.67906713 H

Num. Imaginary Frequencies: 0

C	-1.521538	1.040629	0.381469
C	-1.814146	0.413797	1.749018
C	-1.673351	-1.110311	1.814460
C	-0.234736	-1.686262	1.804026
C	0.405582	-1.650122	0.460373
C	-0.088845	1.469941	0.087456
C	1.736563	-1.659692	0.215634
C	3.032871	1.803408	0.171982
C	2.110903	2.424607	0.935326
C	0.731971	1.906306	1.059374
C	2.391591	3.659473	1.750206
C	4.433197	2.203890	-0.103849
C	4.680056	2.402857	-1.581670
C	5.388284	2.311503	0.846729
C	6.819633	2.682231	0.547671
C	0.234047	1.480562	-1.379936
C	2.186211	-1.750448	-1.139004
O	3.370542	-1.839504	-1.502297
O	-2.410960	-1.680969	0.759777
O	-2.339558	2.183581	0.177326
H	-1.784442	0.273227	-0.369383
H	-1.232375	0.877889	2.557825
H	-2.867683	0.632045	1.973315
H	-2.096395	-1.413614	2.790727
H	-0.283288	-1.703185	-0.391778
H	2.479787	-1.616623	1.013793
H	2.702185	0.920500	-0.387904
H	0.334480	1.949682	2.080265
H	2.404891	3.421861	2.827774
H	3.357574	4.112707	1.491780
H	1.598754	4.409631	1.599152
H	5.741149	2.487273	-1.844916

H	4.272444	1.549919	-2.148119
H	4.157787	3.304585	-1.945751
H	6.947297	3.231778	-0.393506
H	7.231026	3.305805	1.357587
H	1.099656	2.109905	-1.623937
H	0.444022	0.460839	-1.745612
H	-0.635909	1.849173	-1.945623
H	1.418211	-1.749934	-1.934508
C	0.636465	-1.187325	2.951333
H	1.518900	-1.828099	3.091367
H	0.988459	-0.161068	2.773692
H	0.067558	-1.199885	3.892945
H	-0.393408	-2.772742	1.956493
H	7.445919	1.774314	0.495239
Al	5.097704	-2.149224	-0.713370
C	5.336695	-4.072493	-1.048147
Cl	6.351768	-0.913703	-2.022962
H	5.263226	-4.329060	-2.119647
H	4.577364	-4.674665	-0.516141
H	6.324004	-4.425094	-0.698975
C	5.091525	-1.476293	1.134539
H	4.617627	-2.180592	1.842243
H	6.125635	-1.316533	1.489545
H	4.571550	-0.508532	1.226515
Si	-3.428262	-3.029424	0.834338
Si	-3.799443	2.151973	-0.668921
C	-3.836954	-3.407433	-0.980959
C	-4.942567	-2.600643	1.850534
H	-5.500348	-1.751153	1.427496
H	-5.627516	-3.461845	1.916098
H	-4.650220	-2.333764	2.879806
C	-2.533038	-4.460180	1.653504
H	-3.207584	-5.326686	1.750017
H	-1.647414	-4.782681	1.083337
H	-2.206999	-4.189557	2.671577
C	-4.997511	1.005667	0.207788
H	-4.516550	0.025033	0.344201
H	-5.279798	1.384636	1.202769
H	-5.918170	0.852105	-0.377908
C	-3.506726	1.512102	-2.409942
H	-2.984009	0.541816	-2.392422
H	-4.464524	1.356646	-2.933014
H	-2.901113	2.209881	-3.009492
C	-4.382513	3.956768	-0.664594
C	5.143466	2.013593	2.302462
H	5.936178	1.351108	2.688853
H	5.186073	2.937648	2.905034
H	4.174445	1.532158	2.486242
C	-4.590180	-4.745915	-1.052484
H	-5.518996	-4.731471	-0.458140
H	-4.874453	-4.970668	-2.095858
H	-3.974540	-5.586478	-0.693373
C	-4.715244	-2.295201	-1.573618
H	-5.678362	-2.202284	-1.046198
H	-4.215687	-1.314955	-1.533903
H	-4.940131	-2.508156	-2.634126
C	-2.534201	-3.506659	-1.789895
H	-2.751430	-3.784003	-2.836799
H	-1.996104	-2.545626	-1.806306
H	-1.848664	-4.269345	-1.384833
C	-5.713025	4.062497	-1.425944
H	-6.502712	3.446650	-0.964359
H	-6.073783	5.106764	-1.430823
H	-5.613452	3.746922	-2.477698
C	-4.578792	4.426795	0.784975
H	-3.647897	4.341023	1.367631
H	-4.892462	5.485934	0.808503
H	-5.356213	3.844199	1.305661
C	-3.324002	4.837952	-1.345567
H	-3.173474	4.560707	-2.401639
H	-3.633556	5.898387	-1.326531
H	-2.349215	4.764236	-0.837879

Siexo-syn-strans

SCF Energy: -2801.67676945 H

Num. Imaginary Frequencies: 0

C	-1.847555	-0.863419	-0.413737
C	-1.968123	-0.046123	-1.706173
C	-1.589503	1.443108	-1.632349
C	-0.112557	1.829561	-1.895433
C	0.799600	1.520389	-0.760496
C	-0.501343	-1.473042	-0.048851
C	2.141577	1.358857	-0.835805
C	2.530398	-2.038424	0.393285
C	1.862170	-2.122195	-0.786310
C	0.508212	-1.556456	-0.937179
C	2.402854	-2.711562	-2.068041
C	3.827917	-2.598576	0.805220
C	4.395420	-3.789441	0.058716
C	4.490586	-2.111725	1.889097
C	5.841006	-2.657601	2.288700
C	-0.462109	-2.000995	1.358623
C	2.874594	1.190590	0.378199
O	4.109101	1.103164	0.472630
O	-1.998038	1.960089	-0.391151
O	-2.790545	-1.927202	-0.454219
H	-2.106903	-0.175080	0.412236
H	-1.458299	-0.532509	-2.550738
H	-3.037235	-0.073177	-1.957182
H	-2.148235	1.931658	-2.452812
H	0.330761	1.516751	0.230758
H	2.683285	1.358127	-1.784920
H	2.025084	-1.458762	1.166179
H	0.300979	-1.194731	-1.948020
H	3.493858	-2.793055	-2.085125
H	1.975931	-3.710006	-2.264495
H	2.106934	-2.074457	-2.917199
H	4.930439	-4.466314	0.739386
H	3.598324	-4.376744	-0.415586
H	5.107643	-3.499537	-0.732059
H	6.484946	-2.871720	1.423909
H	6.375098	-1.939845	2.927791
H	0.277999	-2.802177	1.487998
H	-0.216330	-1.200241	2.078056

H	-1.449787	-2.393328	1.637865
H	2.297091	1.159958	1.320317
C	0.391320	1.418887	-3.274976
H	1.316602	1.951294	-3.537491
H	0.595576	0.339948	-3.334945
H	-0.358655	1.666451	-4.040894
H	-0.136256	2.937636	-1.877136
H	5.739187	-3.593969	2.866741
Al	5.607658	1.105017	-0.711766
C	5.673980	2.962670	-1.360110
Cl	7.218822	0.670817	0.717127
H	5.687042	3.693141	-0.531548
H	4.803885	3.209364	-1.995626
H	6.576047	3.153424	-1.968966
C	5.321394	-0.382955	-1.961192
H	4.405419	-0.263320	-2.566269
H	6.163494	-0.481440	-2.669954
H	5.237968	-1.341823	-1.422847
Si	-2.778128	3.424128	-0.071142
Si	-4.313762	-1.855894	0.270228
C	-2.955391	3.425723	1.818004
C	-4.432171	3.463209	-0.951228
H	-5.148244	2.740068	-0.531848
H	-4.880737	4.467827	-0.883892
H	-4.306782	3.231961	-2.022177
C	-1.728477	4.852876	-0.683524
H	-2.181459	5.816030	-0.395816
H	-0.706366	4.823747	-0.274288
H	-1.658026	4.842674	-1.784007
C	-5.183026	-0.278640	-0.257724
H	-4.512359	0.577388	-0.086504
H	-5.456999	-0.284566	-1.324420
H	-6.098624	-0.110228	0.331998
C	-4.134896	-1.836574	2.138593
H	-3.496192	-0.998531	2.461798
H	-5.118016	-1.701253	2.618790
H	-3.693757	-2.768823	2.524864
C	-5.198663	-3.418168	-0.341418
C	3.993167	-1.031183	2.810545
H	2.943045	-0.751278	2.662556
H	4.107622	-1.361903	3.856639
H	4.605457	-0.122490	2.694174
C	-6.611725	-3.470997	0.259722
H	-7.147197	-4.371981	-0.089789
H	-6.590653	-3.510884	1.361297
H	-7.217819	-2.597335	-0.032541
C	-5.290828	-3.384197	-1.874659
H	-4.293758	-3.319488	-2.338287
H	-5.778167	-4.300658	-2.253150
H	-5.883950	-2.526962	-2.232949
C	-4.403830	-4.659175	0.093372
H	-4.338773	-4.743914	1.190380
H	-4.890108	-5.579251	-0.277793
H	-3.376138	-4.640922	-0.302809
C	-3.756848	4.663529	2.250614
H	-4.773899	4.664561	1.825378
H	-3.861779	4.689546	3.349886
H	-3.264988	5.602687	1.947892
C	-3.688959	2.153186	2.268643
H	-4.704713	2.087391	1.846485
H	-3.143483	1.245345	1.966469
H	-3.788509	2.133873	3.368677
C	-1.561637	3.461012	2.463991
H	-1.646693	3.445130	3.565250
H	-0.954268	2.590241	2.167803
H	-1.002074	4.370803	2.192316

prReendo-anti-scis

SCF Energy: -2801.74214114 H

Num. Imaginary Frequencies: 0

C	-1.317715	1.767613	-1.632780
C	-2.336750	0.636463	-1.661251
C	-1.871919	-0.541129	-0.813631
C	-0.483095	-1.051185	-1.239491
C	0.520251	0.126963	-1.204938
C	0.072212	1.296611	-2.115999
C	1.976208	-0.280508	-1.501804
C	2.985820	0.924930	-1.692290
C	2.347728	2.298503	-1.755780
C	1.038292	2.444481	-1.973444
C	3.280624	3.475734	-1.697637
C	4.206656	0.793804	-0.759073
C	5.391938	0.191049	-1.465841
C	4.195857	1.125270	0.551937
C	5.366010	0.932086	1.480914
C	0.019089	0.911364	-3.606134
C	2.534259	-1.084697	-0.375701
O	3.228988	-2.090247	-0.547835
O	-2.817080	-1.583767	-0.893537
O	-1.189428	2.238676	-0.311111
H	-1.650109	2.581353	-2.306564
H	-3.300248	1.005708	-1.279544
H	-2.508881	0.290987	-2.691833
H	-1.776436	-0.189339	0.232757
H	0.499925	0.533822	-0.179494
H	2.015874	-0.912009	-2.400926
H	3.394707	0.777055	-2.704303
H	0.629188	3.452326	-2.105281
H	3.729886	3.590728	-0.699395
H	4.116018	3.352717	-2.407319
H	2.753134	4.408116	-1.945430
H	5.118669	-0.789817	-1.891937
H	5.692481	0.827531	-2.315389
H	6.268794	0.039187	-0.827060
H	5.136104	0.125737	2.197935
H	6.307473	0.682766	0.978569
H	-0.307745	1.774574	-4.207237
H	1.016344	0.620894	-3.969259
H	-0.668329	0.080348	-3.816691
H	2.288224	-0.779344	0.655582
C	-0.081412	-2.246333	-0.376566
H	0.156846	-1.947136	0.657848
H	-0.912707	-2.962661	-0.329180
H	0.774981	-2.793797	-0.793002

H	-0.575198	-1.408391	-2.279756
H	5.530926	1.845400	2.075465
Al	4.049020	-3.243145	0.764065
C	5.973320	-2.975357	0.498583
Cl	3.325345	-2.288911	2.622626
H	6.279107	-3.187084	-0.541585
H	6.563016	-3.647155	1.147928
H	6.286646	-1.943719	0.732325
C	3.174134	-4.968206	0.437494
H	3.555368	-5.752377	1.115707
H	2.081126	-4.918028	0.585608
H	3.349477	-5.324324	-0.593636
Si	-1.913851	3.582474	0.391678
Si	-3.937646	-1.904806	0.324980
C	-1.657310	3.307105	2.252263
C	-1.059055	5.134857	-0.220995
H	0.013252	5.132938	0.031362
H	-1.149847	5.217449	-1.316784
H	-1.513362	6.039734	0.214842
C	-3.731143	3.646504	-0.070102
H	-3.852896	3.761810	-1.159920
H	-4.267561	2.734630	0.236272
H	-4.225323	4.508410	0.407906
C	-4.977049	-3.338395	-0.356090
C	-3.032880	-2.373900	1.900649
H	-2.327528	-1.579055	2.193996
H	-3.742497	-2.503937	2.734161
H	-2.461391	-3.308695	1.789574
C	-4.965203	-0.369267	0.654157
H	-4.325790	0.437418	1.048361
H	-5.460398	0.000119	-0.257455
H	-5.743086	-0.569018	1.409510
C	2.993756	1.690942	1.262358
H	2.114932	1.824076	0.622444
H	2.714552	1.033911	2.104039
H	3.239333	2.670428	1.705636
C	-5.929203	-3.845663	0.738110
H	-5.381977	-4.244768	1.607730
H	-6.603858	-3.052664	1.101640
H	-6.564665	-4.661306	0.348812
C	-5.793050	-2.851426	-1.563542
H	-6.518437	-2.070856	-1.281793
H	-5.144855	-2.438382	-2.353228
H	-6.365477	-3.686609	-2.005839
C	-4.044759	-4.477660	-0.796537
H	-4.632280	-5.329466	-1.184020
H	-3.359369	-4.152150	-1.594447
H	-3.431730	-4.856193	0.037960
C	-2.099813	4.556743	3.028421
H	-1.988894	4.395450	4.115696
H	-1.494494	5.439706	2.765850
H	-3.157568	4.807691	2.842856
C	-0.171051	3.027719	2.522785
H	0.163334	2.115053	2.006976
H	0.475150	3.855964	2.188675
H	0.006150	2.887212	3.604230
C	-2.488170	2.096143	2.704796
H	-2.302974	1.875360	3.771271
H	-3.570066	2.271957	2.590248
H	-2.231503	1.190481	2.130658

prReendo-anti-strans

SCF Energy: -2801.74470688 H

Num. Imaginary Frequencies: 0

C	-1.426350	1.694606	-1.655601
C	-2.369078	0.498125	-1.648705
C	-1.827420	-0.630474	-0.779337
C	-0.398355	-1.051774	-1.175225
C	0.510180	0.201289	-1.148180
C	-0.007584	1.293217	-2.119427
C	2.009849	-0.049506	-1.394167
C	2.883690	1.255535	-1.274942
C	2.162820	2.511850	-1.707732
C	0.876368	2.512517	-2.063987
C	2.998574	3.761369	-1.704988
C	3.496123	1.409632	0.124263
C	2.564881	1.895243	1.213857
C	4.789501	1.094610	0.355686
C	5.400072	1.137682	1.729937
C	-0.047439	0.837971	-3.591758
C	2.608091	-0.962020	-0.383338
O	3.451611	-1.817171	-0.667334
O	-2.693335	-1.739691	-0.849528
O	-1.341910	2.222445	-0.351856
H	-1.807586	2.457460	-2.361777
H	-3.351095	0.815317	-1.266502
H	-2.527652	0.119792	-2.669549
H	-1.768051	-0.256167	0.261672
H	0.420409	0.633717	-0.137776
H	2.171384	-0.495659	-2.386455
H	3.712540	1.113009	-1.981340
H	0.418738	3.452015	-2.396182
H	3.332797	4.014911	-0.685384
H	3.909550	3.629886	-2.312523
H	2.437665	4.619373	-2.102569
H	3.032283	2.664086	1.846544
H	1.656459	2.336534	0.781977
H	2.245111	1.078310	1.883513
H	4.684495	1.376885	2.525636
H	5.849286	0.159156	1.967432
H	-0.422872	1.657038	-4.225472
H	0.961534	0.588131	-3.950650
H	-0.691228	-0.034814	-3.764755
H	2.299016	-0.850577	0.669176
C	0.060941	-2.196187	-0.274693
H	0.219543	-1.865606	0.764844
H	-0.705557	-2.982819	-0.259283
H	0.979885	-2.677239	-0.639116
H	-0.446535	-1.441262	-2.206317
H	6.220330	1.875133	1.765170
Al	4.286426	-3.118009	0.501940
C	6.213967	-2.899166	0.218961
Cl	3.622851	-2.346481	2.459860
H	6.603470	-1.944716	0.611168

H	6.480180	-2.949136	-0.852136
H	6.773283	-3.707921	0.723185
C	3.366440	-4.779765	0.008810
H	2.285409	-4.750103	0.230809
H	3.474526	-5.000391	-1.068486
H	3.782664	-5.645386	0.554691
Si	-2.133531	3.566802	0.275660
Si	-3.824554	-2.122811	0.340401
C	-2.127031	3.277268	2.152422
C	-1.186172	5.109517	-0.210992
H	-0.139898	5.064282	0.131174
H	-1.178411	5.222746	-1.307717
H	-1.647787	6.017326	0.210675
C	-3.877852	3.655930	-0.409686
H	-3.864293	3.766137	-1.506578
H	-4.463356	2.755231	-0.166894
H	-4.412123	4.528693	0.000495
C	-4.606361	-3.745815	-0.256519
C	-2.954170	-2.325800	1.990597
H	-2.396247	-1.412220	2.253841
H	-3.684975	-2.504159	2.796379
H	-2.242511	-3.166171	1.982523
C	-5.086090	-0.740834	0.480559
H	-4.605062	0.181848	0.843436
H	-5.560438	-0.519890	-0.488556
H	-5.880676	-1.001247	1.199193
C	5.737330	0.644682	-0.734073
H	6.763883	0.567572	-0.348829
H	5.465887	-0.345770	-1.134057
H	5.757278	1.344409	-1.584068
C	-3.001172	2.055306	2.474753
H	-2.961443	1.822686	3.553956
H	-4.058815	2.224563	2.215570
H	-2.659988	1.159318	1.930470
C	-2.684471	4.516115	2.869703
H	-2.721483	4.346466	3.960722
H	-2.058042	5.406835	2.698951
H	-3.709330	4.758982	2.542987
C	-0.691569	3.007086	2.627309
H	-0.279195	2.100395	2.159187
H	-0.011760	3.843355	2.395482
H	-0.668720	2.858683	3.721958
C	-5.550801	-4.286935	0.828270
H	-5.013788	-4.524481	1.761110
H	-6.352286	-3.571065	1.075634
H	-6.038688	-5.217116	0.485720
C	-5.399104	-3.489741	-1.547646
H	-6.241450	-2.798213	-1.382971
H	-4.762246	-3.061412	-2.338352
H	-5.821489	-4.434143	-1.935684
C	-3.498795	-4.774017	-0.533813
H	-3.936233	-5.732044	-0.868081
H	-2.813418	-4.425939	-1.322130
H	-2.896706	-4.985987	0.365059

prReendo-syn-scis

SCF Energy: -2801.73858936 H

Num. Imaginary Frequencies: 0

C	-1.093517	1.162466	-1.767324
C	-1.957932	-0.087674	-1.684879
C	-1.640005	-0.885973	-0.428140
C	-0.148153	-1.255109	-0.325536
C	0.708831	0.028819	-0.437926
C	0.410061	0.813847	-1.742943
C	2.225502	-0.209760	-0.328152
C	3.120128	1.078161	-0.542065
C	2.402649	2.243242	-1.193098
C	1.197157	2.099298	-1.749187
C	3.166441	3.535593	-1.267373
C	3.967995	1.441265	0.696517
C	5.418163	1.073024	0.521654
C	3.473117	2.034384	1.805612
C	4.296220	2.362973	3.024843
C	0.786929	0.029574	-3.015633
C	2.644152	-0.759326	0.994983
O	3.496342	-1.638682	1.142286
O	-2.428223	-2.054310	-0.395421
O	-1.381723	1.999036	-0.668911
H	-1.297970	1.688993	-2.719857
H	-3.018849	0.202723	-1.676144
H	-1.804891	-0.727261	-2.566999
H	-1.870024	-0.244430	0.445557
H	0.405015	0.689702	0.390184
H	2.523065	-0.947112	-1.086017
H	3.859424	0.756372	-1.292616
H	0.752723	2.946187	-2.283835
H	3.295565	3.984108	-0.269724
H	4.177867	3.374941	-1.676551
H	2.647943	4.264830	-1.906302
H	5.518188	0.027369	0.189091
H	5.862555	1.686176	-0.281524
H	6.029220	1.207046	1.421330
H	5.276633	1.873999	3.054658
H	4.459213	3.452608	3.090428
H	0.521350	0.616152	-3.909328
H	1.870443	-0.154283	-3.059307
H	0.280755	-0.942667	-3.092998
H	2.171496	-0.359139	1.906473
C	0.085183	-2.050044	0.956762
H	-0.031922	-1.416754	1.851664
H	-0.647194	-2.865796	1.024882
H	1.073194	-2.528981	0.986899
H	0.081988	-1.916071	-1.179146
H	3.747136	2.075375	3.936331
Al	4.441242	-2.981762	0.128588
C	3.062360	-4.360569	-0.106448
Cl	4.926283	-2.012318	-1.795454
H	2.212406	-4.011442	-0.718615
H	2.652652	-4.710578	0.857854
H	3.478195	-5.248443	-0.616135
C	6.049482	-3.276118	1.209550
H	6.620616	-2.345273	1.372389
H	5.801509	-3.685735	2.205194
H	6.735881	-3.995067	0.727804

Si	-2.401045	3.337648	-0.656865
Si	-3.820445	-2.202567	0.544085
C	-2.705712	3.668315	1.187462
C	-1.539971	4.772318	-1.502825
H	-0.593633	5.030093	-1.001400
H	-1.310525	4.518587	-2.551024
H	-2.178639	5.670691	-1.515341
C	-3.991940	2.941519	-1.569406
H	-3.787180	2.701394	-2.625871
H	-4.523529	2.085863	-1.124039
H	-4.672657	3.808720	-1.556781
C	-4.489289	-3.929263	0.131532
C	-3.372276	-2.035146	2.359257
H	-2.865728	-1.074179	2.547177
H	-4.277931	-2.054116	2.987508
H	-2.704389	-2.842435	2.698313
C	-5.030961	-0.840261	0.096971
H	-4.602272	0.143900	0.346942
H	-5.279179	-0.843317	-0.975891
H	-5.969410	-0.943393	0.666366
C	2.033809	2.451077	1.959203
H	1.470964	2.454376	1.019756
H	1.512709	1.786534	2.671502
H	1.979009	3.464175	2.389954
C	-3.499059	4.973272	1.353826
H	-3.714664	5.160749	2.421006
H	-2.940605	5.845031	0.975551
H	-4.467120	4.940384	0.826745
C	-1.357732	3.784780	1.914195
H	-0.731227	4.592844	1.502217
H	-1.513193	4.002316	2.986286
H	-0.784759	2.848372	1.841687
C	-3.501849	2.499040	1.787385
H	-3.638717	2.639991	2.874548
H	-4.505290	2.410489	1.340560
H	-2.982022	1.537770	1.641003
C	-5.683765	-4.246471	1.044686
H	-5.395259	-4.268207	2.108328
H	-6.497861	-3.511067	0.933023
H	-6.104041	-5.238307	0.799351
C	-3.381242	-4.970738	0.352012
H	-2.513626	-4.781394	-0.298982
H	-3.022797	-4.978519	1.394568
H	-3.755128	-5.985756	0.126723
C	-4.939748	-3.966788	-1.337015
H	-5.772632	-3.271021	-1.529602
H	-4.117431	-3.704384	-2.021897
H	-5.288859	-4.979283	-1.608574

prReendo-syn-strans

SCF Energy: -2801.74363436 H

Num. Imaginary Frequencies: 0

C	-1.049007	1.206780	-1.809143
C	-2.045027	0.060371	-1.689414
C	-1.775832	-0.793756	-0.455035
C	-0.317682	-1.288955	-0.366327
C	0.623293	-0.067287	-0.476000
C	0.407114	0.687815	-1.813613
C	2.126088	-0.335117	-0.291491
C	2.982386	0.984197	-0.273291
C	2.477195	2.022068	-1.248797
C	1.330475	1.874721	-1.915327
C	3.349802	3.235731	-1.402002
C	3.146900	1.574635	1.133209
C	1.938691	2.305323	1.682990
C	4.276320	1.417791	1.859120
C	4.403360	1.949363	3.264303
C	0.659327	-0.181898	-3.061063
C	2.484609	-1.001518	0.989656
O	3.342524	-1.879720	1.100294
O	-2.652723	-1.895694	-0.438636
O	-1.211622	2.070820	-0.710559
H	-1.225342	1.745505	-2.759330
H	-3.063881	0.474080	-1.630987
H	-2.007881	-0.580076	-2.583167
H	-1.944399	-0.158499	0.436447
H	0.316740	0.631509	0.317636
H	2.497924	-0.961705	-1.114046
H	3.974144	0.682712	-0.634085
H	1.033122	2.646749	-2.635396
H	3.397078	3.810348	-0.461926
H	4.385737	2.950272	-1.649657
H	2.974890	3.903434	-2.190836
H	2.206159	3.271813	2.136218
H	1.204796	2.509959	0.892112
H	1.423780	1.717421	2.462217
H	3.647512	2.700070	3.525448
H	4.315187	1.121487	3.989743
H	0.476855	0.411510	-3.971049
H	1.706090	-0.517934	-3.099357
H	0.018147	-1.071831	-3.113668
H	1.995203	-0.655909	1.914974
C	-0.144777	-2.108097	0.909205
H	-0.220276	-1.477242	1.810310
H	-0.931532	-2.872297	0.968513
H	0.808935	-2.654860	0.934552
H	-0.145263	-1.963617	-1.221846
H	5.398822	2.395317	3.420498
Al	4.262553	-3.093924	-0.099185
C	2.768386	-4.160669	-0.798387
Cl	5.104944	-1.786406	-1.665172
H	2.009815	-3.540328	-1.307962
H	2.250467	-4.723301	-0.001042
H	3.118961	-4.904935	-1.535837
C	5.659829	-3.856439	1.042532
H	6.338745	-3.085233	1.446683
H	5.231075	-4.399859	1.903539
H	6.286441	-4.577076	0.487418
Si	-1.814459	3.633138	-0.607969
Si	-4.069960	-1.992520	0.467189
C	-2.637030	3.682576	1.104853
C	-0.402155	4.859652	-0.734814
H	0.389881	4.639241	-0.001719
H	0.049796	4.825184	-1.739196

H	-0.751602	5.891109	-0.563157
C	-3.041729	3.927025	-1.994796
H	-2.539467	3.901856	-2.975782
H	-3.842069	3.170343	-2.003961
H	-3.512475	4.918731	-1.894186
C	-4.627359	-3.796967	0.272663
C	-3.702750	-1.559435	2.256597
H	-3.270747	-0.548388	2.337357
H	-4.629362	-1.565202	2.853715
H	-2.996161	-2.268372	2.716097
C	-5.345739	-0.794867	-0.209435
H	-5.034254	0.247072	-0.033001
H	-5.490071	-0.927884	-1.293216
H	-6.321186	-0.934895	0.285134
C	5.506083	0.668682	1.414265
H	5.764698	-0.097948	2.164003
H	5.420928	0.164878	0.444812
H	6.368677	1.354622	1.364085
C	-3.201235	5.083400	1.382820
H	-3.696975	5.112693	2.369767
H	-2.410569	5.851441	1.392332
H	-3.951318	5.383894	0.632633
C	-3.771490	2.647279	1.138464
H	-4.234166	2.605826	2.140948
H	-4.571385	2.886274	0.418667
H	-3.397570	1.637763	0.902823
C	-1.596738	3.321802	2.176709
H	-0.754007	4.032238	2.193145
H	-2.056636	3.334414	3.181372
H	-1.182627	2.314458	2.012325
C	-5.827719	-4.064722	1.194067
H	-5.567771	-3.936547	2.257572
H	-6.677522	-3.397351	0.973979
H	-6.186863	-5.101885	1.067838
C	-5.033067	-4.052726	-1.187266
H	-5.900872	-3.442383	-1.485920
H	-4.209078	-3.829473	-1.884062
H	-5.312307	-5.112064	-1.331110
C	-3.470048	-4.734041	0.650803
H	-2.601053	-4.587555	-0.009197
H	-3.133702	-4.577991	1.689162
H	-3.783858	-5.789883	0.563751

prReexo-anti-scis

SCF Energy: -2801.73443554 H

Num. Imaginary Frequencies: 0

C	-1.192083	0.931007	-1.857658
C	-2.011844	-0.316477	-1.562312
C	-1.734744	-0.791360	-0.146816
C	-0.253113	-1.128947	0.052165
C	0.682579	0.023208	-0.395817
C	0.326532	0.656394	-1.768709
C	2.153425	-0.493543	-0.357936
C	2.877780	-0.713461	-1.734101
C	1.901858	-0.940814	-2.880420
C	0.734830	-0.285351	-2.878365
C	2.354917	-1.773521	-4.044861
C	4.022702	-1.718515	-1.581206
C	5.378061	-1.083527	-1.759513
C	3.824177	-3.019744	-1.287063
C	4.930017	-4.023036	-1.079719
C	1.052894	2.002803	-1.953310
C	2.998895	0.425351	0.434391
O	3.700903	0.035802	1.366090
O	-2.514629	-1.928896	0.149475
O	-1.537190	1.938105	-0.935322
H	-1.396423	1.266978	-2.893265
H	-3.082506	-0.089751	-1.676396
H	-1.765807	-1.120820	-2.273789
H	-1.985355	0.038160	0.541689
H	0.567664	0.824570	0.355549
H	2.176825	-1.452990	0.165471
H	3.366165	0.242434	-1.994641
H	0.068768	-0.378797	-3.743825
H	3.323014	-1.412018	-4.429880
H	2.503182	-2.827375	-3.765298
H	1.622740	-1.733001	-4.864100
H	5.464406	-0.646808	-2.769136
H	5.512171	-0.249789	-1.048642
H	6.218710	-1.773330	-1.622535
H	4.739456	-4.607127	-0.164194
H	4.951563	-4.747693	-1.911947
H	2.144036	1.887407	-2.011056
H	0.729784	2.479368	-2.892198
H	0.821282	2.689983	-1.127326
H	3.012208	1.501274	0.170135
C	-0.009720	-1.516192	1.510616
H	-0.222898	-0.662960	2.176402
H	-0.671136	-2.344358	1.798953
H	1.023105	-1.839067	1.705089
H	-0.051950	-2.004528	-0.589299
H	5.929496	-3.581419	-0.991516
Al	4.977841	0.942895	2.515275
C	6.699412	0.286506	1.841537
Cl	4.571538	3.028935	1.942340
H	6.703340	-0.814878	1.753022
H	7.526130	0.555217	2.523373
H	6.955929	0.696655	0.849448
C	4.324378	0.501099	4.309333
H	4.917545	1.001250	5.095474
H	3.272567	0.802719	4.457468
H	4.384332	-0.584666	4.504612
Si	-3.898564	-1.884429	1.109763
Si	-2.586898	3.227938	-1.192550
C	-4.517374	-3.678059	1.127164
C	-3.458660	-1.273200	2.828768
H	-2.974089	-0.284501	2.775284
H	-4.365693	-1.158757	3.444821
H	-2.773808	-1.958230	3.352384
C	-5.148634	-0.704208	0.358108
H	-6.092982	-0.712020	0.927071
H	-4.757643	0.325679	0.388279
H	-5.377716	-0.954265	-0.689584
C	-2.871339	3.930530	0.547078

C	-4.175625	2.616440	-1.980863
H	-4.880939	3.450540	-2.130344
H	-3.973608	2.177106	-2.971833
H	-4.677765	1.852355	-1.367422
C	-1.774852	4.469140	-2.339786
H	-0.844339	4.876424	-1.914258
H	-1.527931	3.996279	-3.304736
H	-2.452104	5.312596	-2.552406
C	2.455655	-3.636880	-1.136721
H	2.404055	-4.580634	-1.704609
H	2.261602	-3.899325	-0.081976
H	1.634553	-2.997466	-1.481569
C	-3.621656	2.892598	1.396347
H	-4.627195	2.683488	0.996617
H	-3.074565	1.936933	1.447727
H	-3.749791	3.257426	2.431209
C	-1.515846	4.238476	1.201634
H	-1.662084	4.659506	2.212554
H	-0.901198	3.330550	1.303866
H	-0.933961	4.974004	0.622240
C	-3.703086	5.218932	0.453552
H	-3.182149	6.004505	-0.117894
H	-4.680943	5.047283	-0.026380
H	-3.901067	5.624660	1.461829
C	-3.379091	-4.604845	1.581331
H	-3.021355	-4.354223	2.593634
H	-3.722436	-5.654823	1.605973
H	-2.517214	-4.549763	0.898273
C	-5.701213	-3.802256	2.098882
H	-6.537752	-3.139901	1.820489
H	-6.090913	-4.836083	2.102121
H	-5.411805	-3.559252	3.134389
C	-4.967381	-4.077620	-0.286560
H	-4.153319	-3.962611	-1.020213
H	-5.287290	-5.135044	-0.306530
H	-5.820288	-3.471401	-0.632956

prReexo-anti-strans

SCF Energy: -2801.73727475 H

Num. Imaginary Frequencies: 0

C	-1.255001	0.969100	-1.752750
C	-2.130469	-0.257466	-1.542737
C	-1.913331	-0.816731	-0.147706
C	-0.450646	-1.214613	0.082835
C	0.534063	-0.070264	-0.272565
C	0.247134	0.628882	-1.629224
C	1.981735	-0.629643	-0.203750
C	2.738233	-0.860044	-1.567919
C	1.782583	-1.001787	-2.743367
C	0.648673	-0.292062	-2.758351
C	2.236010	-1.825574	-3.914449
C	3.718369	-2.004750	-1.393924
C	3.099762	-3.355899	-1.098929
C	5.050513	-1.803294	-1.440224
C	6.045682	-2.909848	-1.215499
C	1.036134	1.946797	-1.742932
C	2.883148	0.224775	0.595827
O	3.653998	-0.244002	1.432312
O	-2.743703	-1.937937	0.062459
O	-1.591485	1.947436	-0.796246
H	-1.412045	1.359058	-2.777672
H	-3.187814	0.017988	-1.672322
H	-1.897083	-1.033709	-2.288644
H	-2.157095	-0.015626	0.576405
H	0.415209	0.699313	0.510040
H	1.958650	-1.601035	0.300156
H	3.315687	0.050687	-1.791509
H	0.006686	-0.329302	-3.646006
H	2.344858	-2.889477	-3.653604
H	1.524291	-1.748913	-4.749020
H	3.223153	-1.486565	-4.269919
H	2.008226	-3.330855	-1.238109
H	3.491762	-4.145015	-1.758351
H	3.285982	-3.677298	-0.060797
H	6.695721	-2.663098	-0.359016
H	5.584905	-3.885796	-1.018816
H	2.122165	1.784030	-1.777766
H	0.761063	2.472092	-2.671037
H	0.812671	2.613068	-0.897577
H	2.903182	1.315107	0.401597
C	-0.275676	-1.682155	1.527976
H	-0.478285	-0.854185	2.227980
H	-0.980317	-2.494571	1.751401
H	0.735049	-2.058669	1.741662
H	-0.248047	-2.063412	-0.595650
H	6.710219	-3.013899	-2.090216
Al	5.086092	0.548030	2.473921
C	6.611467	-0.612238	2.062569
Cl	5.212599	2.505796	1.470799
H	7.495166	-0.348901	2.670974
H	6.916127	-0.545435	1.004432
H	6.379762	-1.671161	2.275846
C	4.310331	0.661393	4.271361
H	3.376557	1.250596	4.286943
H	4.072249	-0.340162	4.672529
H	5.003773	1.136137	4.988111
Si	-4.161161	-1.883026	0.972491
Si	-2.568925	3.295766	-1.040076
C	-4.900488	-3.621960	0.799655
C	-3.753978	-1.463609	2.755829
H	-3.203323	-0.510336	2.812565
H	-4.676239	-1.343468	3.347744
H	-3.138001	-2.239358	3.236814
C	-5.295991	-0.552514	0.292321
H	-6.250597	-0.528182	0.843370
H	-4.825833	0.437418	0.408808
H	-5.520333	-0.703317	-0.775103
C	-2.850705	3.972248	0.710333
C	-4.170846	2.784825	-1.871927
H	-4.827447	3.657755	-2.021449
H	-3.970591	2.352057	-2.866171
H	-4.725905	2.038370	-1.282900
C	-1.674331	4.521190	-2.142040
H	-0.732010	4.870019	-1.691503

H	-1.435190	4.060672	-3.114851
H	-2.304460	5.402935	-2.343891
C	5.673342	-0.450134	-1.722347
H	6.769919	-0.509445	-1.671820
H	5.415805	-0.078042	-2.727311
H	5.362444	0.323529	-1.001581
C	-3.642908	2.943543	1.532219
H	-4.645897	2.765114	1.111676
H	-3.120792	1.974022	1.581649
H	-3.780935	3.299238	2.569015
C	-1.493749	4.225144	1.385111
H	-1.638121	4.626930	2.404118
H	-0.907040	3.297295	1.472327
H	-0.884839	4.956385	0.828608
C	-3.640590	5.287818	0.632108
H	-3.091837	6.065320	0.075798
H	-4.620359	5.154265	0.144179
H	-3.831768	5.684119	1.645438
C	-6.135493	-3.746755	1.705402
H	-6.910270	-3.003052	1.455141
H	-6.594748	-4.745632	1.596014
H	-5.880533	-3.619634	2.770262
C	-3.851114	-4.665305	1.213319
H	-3.526967	-4.533098	2.258734
H	-4.265516	-5.685824	1.125342
H	-2.955020	-4.611442	0.575627
C	-5.308060	-3.860562	-0.662463
H	-4.453936	-3.738237	-1.347760
H	-5.696526	-4.886631	-0.793378
H	-6.101040	-3.167047	-0.986705

prReexo-syn-scis

SCF Energy: -2801.73552521 H

Num. Imaginary Frequencies: 0

C	1.511534	-1.476997	-1.457264
C	1.928759	-0.021024	-1.593381
C	1.491876	0.756568	-0.365227
C	-0.026391	0.691904	-0.158535
C	-0.578704	-0.757080	-0.195979
C	-0.023259	-1.628234	-1.357723
C	-2.139181	-0.698114	-0.201971
C	-2.858679	-1.084816	-1.548511
C	-1.961863	-0.913896	-2.767834
C	-0.657190	-1.190149	-2.657439
C	-2.606389	-0.591353	-4.085085
C	-4.255866	-0.466323	-1.624922
C	-5.348868	-1.504484	-1.609580
C	-4.464908	0.864358	-1.693246
C	-5.823806	1.513453	-1.694359
C	-0.321594	-3.121696	-1.124446
C	-2.696499	-1.599704	0.834100
O	-3.548182	-1.292259	1.661790
O	1.884684	2.106779	-0.479756
O	2.107050	-2.024119	-0.303417
H	1.829423	-2.035038	-2.359868
H	3.021578	0.041630	-1.705423
H	1.477995	0.429917	-2.491569
H	1.970081	0.289854	0.517142
H	-0.247392	-1.238731	0.741058
H	-2.463040	0.314567	0.055995
H	-3.031338	-2.175440	-1.511511
H	-0.025847	-1.155313	-3.552643
H	-3.424946	-1.296994	-4.304006
H	-3.050951	0.415054	-4.090174
H	-1.874189	-0.649872	-4.903212
H	-5.226470	-2.192380	-2.464089
H	-5.290298	-2.127127	-0.700228
H	-6.361797	-1.089272	-1.661439
H	-5.881281	2.239869	-0.866768
H	-5.978242	2.083067	-2.626526
H	-1.395505	-3.348328	-1.166670
H	0.163771	-3.727625	-1.905642
H	0.065399	-3.453164	-0.150381
H	-2.337565	-2.647064	0.853125
C	-0.385548	1.396004	1.148603
H	0.055230	0.860896	2.007053
H	0.012782	2.419736	1.148630
H	-1.468073	1.470324	1.318744
H	-0.470594	1.250565	-1.000476
H	-6.659688	0.812970	-1.583846
Al	-4.765415	-0.037765	2.481479
C	-4.370316	-0.340993	4.379743
Cl	-4.117330	1.972814	1.862819
H	-4.607330	-1.375487	4.686695
H	-4.962958	0.330420	5.026517
H	-3.307413	-0.163542	4.621624
C	-6.502578	-0.513057	1.707315
H	-7.315313	-0.030008	2.279661
H	-6.604394	-0.181374	0.661131
H	-6.695779	-1.600059	1.734608
Si	3.210441	2.765486	0.323999
Si	3.498308	-2.967498	-0.228724
C	3.268957	4.568464	-0.264780
C	2.957140	2.637017	2.178948
H	2.784379	1.589103	2.474386
H	3.853139	2.984851	2.718899
H	2.097206	3.232027	2.523930
C	4.762111	1.813997	-0.133111
H	5.654752	2.267127	0.328904
H	4.690903	0.779187	0.239233
H	4.921423	1.777289	-1.222118
C	3.937721	-2.982258	1.617800
C	4.854310	-2.202751	-1.275098
H	5.776902	-2.803144	-1.212786
H	4.555652	-2.170981	-2.336018
H	5.095036	-1.175607	-0.960149
C	3.117044	-4.683399	-0.882689
H	2.339339	-5.187901	-0.288058
H	2.762862	-4.626952	-1.925286
H	4.017929	-5.318742	-0.877035
C	-3.347880	1.874178	-1.766686
H	-3.287118	2.440191	-0.822165
H	-2.362346	1.437427	-1.966648
H	-3.555158	2.606888	-2.563952

C	4.343741	5.331732	0.524822
H	4.118343	5.363123	1.603354
H	5.344163	4.883671	0.404272
H	4.410390	6.377272	0.173969
C	3.607255	4.606681	-1.763103
H	4.608670	4.194620	-1.968920
H	2.879015	4.033923	-2.359579
H	3.597925	5.646937	-2.135513
C	1.898227	5.223244	-0.033958
H	1.913584	6.277916	-0.363180
H	1.104549	4.707496	-0.596427
H	1.611626	5.217226	1.030598
C	5.114578	-3.939934	1.859879
H	5.402498	-3.935730	2.926420
H	4.861040	-4.979282	1.594305
H	6.007899	-3.653645	1.280293
C	2.719766	-3.447274	2.430704
H	1.863372	-2.767647	2.298902
H	2.392656	-4.460185	2.143562
H	2.962510	-3.474400	3.508197
C	4.329426	-1.562966	2.057768
H	4.537138	-1.536482	3.142476
H	5.236804	-1.208263	1.542589
H	3.523600	-0.837915	1.857569

prReexo-syn-strans

SCF Energy: -2801.73654080 H

Num. Imaginary Frequencies: 0

C	1.377397	-1.392871	-1.609471
C	1.904057	0.032192	-1.664938
C	1.475467	0.794771	-0.424331
C	-0.051594	0.830384	-0.268420
C	-0.673474	-0.589028	-0.351339
C	-0.165650	-1.430459	-1.552158
C	-2.231268	-0.465050	-0.358589
C	-2.940087	-0.508881	-1.756563
C	-1.991957	-0.428566	-2.942287
C	-0.733544	-0.868097	-2.834350
C	-2.579153	0.008568	-4.254303
C	-4.037335	0.541104	-1.757946
C	-3.553989	1.974824	-1.797540
C	-5.346422	0.254643	-1.609418
C	-6.366013	1.364089	-1.503373
C	-0.589764	-2.905905	-1.429562
C	-2.825989	-1.523690	0.495124
O	-3.405859	-1.334246	1.560336
O	1.972938	2.113767	-0.474125
O	1.895419	-2.039617	-0.470082
H	1.677715	-1.929305	-2.531027
H	3.002265	0.017914	-1.731278
H	1.525533	0.549780	-2.560479
H	1.883538	0.261920	0.456383
H	-0.367196	-1.119625	0.567498
H	-2.493662	0.485387	0.117173
H	-3.407567	-1.501376	-1.864434
H	-0.096191	-0.887807	-3.726047
H	-3.476005	-0.585938	-4.496016
H	-2.897755	1.061951	-4.232900
H	-1.854453	-0.112368	-5.072260
H	-2.461915	2.027589	-1.919181
H	-4.004321	2.542895	-2.627409
H	-3.807682	2.506017	-0.866305
H	-7.382606	0.994375	-1.704042
H	-6.364729	1.786355	-0.483163
H	-1.672093	-3.036783	-1.568249
H	-0.097606	-3.503351	-2.213006
H	-0.303132	-3.325066	-0.454099
H	-2.747802	-2.573726	0.158640
C	-0.398681	1.544717	1.036495
H	-0.032822	0.966771	1.901599
H	0.086525	2.529549	1.061712
H	-1.475224	1.713825	1.174187
H	-0.438520	1.424361	-1.115297
H	-6.165855	2.194404	-2.196456
Al	-3.946084	-0.102912	2.948233
C	-2.381430	-0.130750	4.130574
Cl	-4.204319	1.839072	1.941885
H	-2.195211	-1.141749	4.535173
H	-2.521340	0.540842	4.996329
H	-1.459864	0.193193	3.617463
C	-5.677684	-0.843555	3.493619
H	-6.145749	-0.230589	4.284508
H	-6.396988	-0.890246	2.657075
H	-5.576755	-1.866988	3.897049
Si	3.303539	2.638904	0.416894
Si	3.200091	-3.100959	-0.416465
C	3.570707	4.430325	-0.148106
C	2.925336	2.525115	2.251397
H	2.639709	1.495751	2.523615
H	3.814190	2.786540	2.848863
H	2.103346	3.194005	2.550373
C	4.780811	1.542351	0.046450
H	5.677235	1.892350	0.584456
H	4.577492	0.512974	0.384085
H	5.016928	1.510831	-1.028600
C	3.533879	-3.308259	1.440007
C	4.667928	-2.366860	-1.324847
H	5.529862	-3.053321	-1.287942
H	4.424640	-2.204463	-2.387995
H	4.982910	-1.402114	-0.897888
C	2.719518	-4.715332	-1.241099
H	1.864384	-5.196078	-0.740787
H	2.442792	-4.541612	-2.294184
H	3.561983	-5.426353	-1.237679
C	-5.929254	-1.125290	-1.448678
H	-6.653144	-1.336204	-2.254056
H	-5.190650	-1.936846	-1.443204
H	-6.492917	-1.182039	-0.501934
C	3.964937	-1.956836	2.031179
H	4.120968	-2.042647	3.121461
H	4.910727	-1.598561	1.593226
H	3.201037	-1.179595	1.865913
C	2.251559	-3.782436	2.141068
H	1.433364	-3.054987	2.021410

H	1.900328	-4.751487	1.750064
H	2.428748	-3.910953	3.223976
C	4.649680	-4.343227	1.650643
H	4.870126	-4.459861	2.726852
H	4.367929	-5.336978	1.265546
H	5.589066	-4.045588	1.155946
C	4.678715	5.075769	0.698511
H	4.408975	5.119491	1.766408
H	5.634177	4.531370	0.616105
H	4.864367	6.112695	0.365362
C	3.980060	4.443417	-1.628993
H	4.943143	3.933308	-1.794090
H	3.225679	3.950915	-2.263388
H	4.092952	5.481528	-1.990193
C	2.263448	5.218756	0.026629
H	2.399682	6.267857	-0.292385
H	1.448579	4.788205	-0.575917
H	1.929291	5.237193	1.077025

prSiendo-anti-scis

SCF Energy: -2801.73774737 H

Num. Imaginary Frequencies: 0

C	-1.918944	-0.350596	-0.879651
C	-1.588697	0.734573	-1.904042
C	-0.175144	1.282174	-1.716980
C	0.888497	0.171477	-1.741844
C	0.469946	-0.906146	-0.719455
C	-0.922001	-1.536769	-0.956435
C	1.518870	-2.008975	-0.430758
C	1.166721	-2.739176	0.903321
C	-0.317104	-3.030084	1.001760
C	-1.215652	-2.512602	0.157116
C	-0.712979	-3.987374	2.090932
C	1.835489	-2.113632	2.133236
C	3.263830	-2.591290	2.319144
C	1.297168	-1.238913	3.009690
C	2.101353	-0.749461	4.195766
C	-1.089301	-2.310964	-2.276181
C	2.827434	-1.321025	-0.378496
O	3.697867	-1.465408	-1.237437
O	-0.097637	1.928456	-0.464450
O	-3.245204	-0.791030	-1.041649
H	-1.785075	0.094654	0.124974
H	-1.713246	0.336419	-2.922545
H	-2.306685	1.561038	-1.793076
H	0.045915	1.991506	-2.536726
H	0.380467	-0.345235	0.224580
H	1.551678	-2.732857	-1.257475
H	1.638712	-3.733456	0.818134
H	-2.263789	-2.815546	0.247030
H	-0.181818	-4.948124	1.983970
H	-0.447318	-3.588736	3.083243
H	-1.793928	-4.187013	2.078545
H	3.947058	-1.794912	2.645879
H	3.316136	-3.401558	3.067662
H	3.680197	-3.012456	1.390294
H	2.730905	-1.532167	4.642587
H	2.767350	0.082360	3.905976
H	-0.276325	-3.039043	-2.414440
H	-2.034377	-2.872136	-2.251085
H	-1.121075	-1.664664	-3.161222
H	2.986746	-0.591814	0.439771
C	1.239432	-0.279826	-3.160039
H	1.845067	-1.197916	-3.162748
H	0.353014	-0.466854	-3.780221
H	1.827310	0.503811	-3.662602
H	1.788911	0.659567	-1.332700
H	1.436339	-0.365722	4.983824
Al	5.289686	-0.351029	-1.459745
C	4.552537	1.462752	-1.275988
Cl	6.419286	-0.960253	0.320196
H	3.848650	1.705849	-2.091920
H	5.346687	2.230127	-1.301530
H	4.012533	1.597146	-0.321836
C	6.049723	-1.001890	-3.142350
H	5.356196	-0.836169	-3.986481
H	6.991631	-0.483247	-3.394761
H	6.274020	-2.082474	-3.110642
Si	0.067749	3.581514	-0.198855
Si	-4.464255	-0.313892	0.026354
C	0.181470	3.700200	1.690934
C	-1.431308	4.472521	-0.888780
H	-1.493856	4.329338	-1.980425
H	-2.367533	4.098337	-0.444913
H	-1.373737	5.557607	-0.703109
C	1.618435	4.196677	-1.054296
H	2.520033	3.681621	-0.687349
H	1.555354	4.027711	-2.142147
H	1.754616	5.279466	-0.898627
C	-4.109035	-1.007194	1.733995
H	-4.823316	-0.607148	2.472303
H	-4.171514	-2.106306	1.760134
H	-3.097650	-0.718568	2.065189
C	-6.058058	-1.021890	-0.717769
C	-4.489899	1.559792	0.139042
H	-4.639638	2.034104	-0.843392
H	-5.294580	1.901859	0.810475
H	-3.537417	1.927606	0.555432
C	-0.087855	-0.648965	2.960983
H	-0.622306	-0.831069	2.025373
H	-0.700511	-1.047624	3.788572
H	-0.028213	0.439136	3.118345
C	1.395163	2.886935	2.169593
H	1.447680	2.880986	3.273239
H	1.341338	1.840081	1.831235
H	2.343379	3.309875	1.799484
C	-1.103046	3.119426	2.303482
H	-1.269943	2.078847	1.983146
H	-1.043997	3.124468	3.406852
H	-1.993129	3.705304	2.021255
C	0.341347	5.166395	2.119305
H	-0.514435	5.784889	1.802018
H	0.409645	5.242859	3.219339
H	1.256008	5.620222	1.703419

C	-7.232560	-0.745109	0.233693
H	-8.174319	-1.134795	-0.192657
H	-7.092484	-1.230177	1.213651
H	-7.376979	0.333593	0.410911
C	-6.326710	-0.356971	-2.076589
H	-5.485789	-0.502640	-2.773472
H	-7.228646	-0.788466	-2.546739
H	-6.496739	0.727486	-1.977105
C	-5.900107	-2.537735	-0.913364
H	-5.068547	-2.773632	-1.595698
H	-5.710645	-3.059535	0.039017
H	-6.821030	-2.968988	-1.345424

prSiendo-anti-strans

SCF Energy: -2801.74146602 H

Num. Imaginary Frequencies: 0

C	-2.211893	-0.293008	-0.792746
C	-2.041855	0.777139	-1.872249
C	-0.690251	1.479944	-1.768369
C	0.475438	0.473963	-1.840870
C	0.241947	-0.599465	-0.759550
C	-1.095727	-1.366637	-0.860114
C	1.414608	-1.567307	-0.549335
C	1.259619	-2.386684	0.770676
C	-0.183180	-2.746283	1.060247
C	-1.207883	-2.288285	0.331602
C	-0.381735	-3.673684	2.226664
C	1.941859	-1.695722	1.957488
C	1.174739	-0.576046	2.623911
C	3.197284	-2.001200	2.355229
C	3.847644	-1.243803	3.491227
C	-1.265681	-2.244500	-2.114714
C	2.678469	-0.789432	-0.450090
O	3.702347	-1.094812	-1.059971
O	-0.668749	2.165772	-0.536041
O	-3.479487	-0.894803	-0.892662
H	-2.102089	0.210344	0.186585
H	-2.160720	0.324928	-2.868350
H	-2.839790	1.526468	-1.760583
H	-0.591646	2.197434	-2.604439
H	0.166738	-0.018295	0.173654
H	1.516340	-2.261572	-1.395628
H	1.779043	-3.338735	0.599230
H	-2.220853	-2.630463	0.567799
H	0.195177	-4.604108	2.093415
H	-0.025657	-3.214674	3.164112
H	-1.441111	-3.937532	2.356367
H	1.288046	-0.587973	3.717884
H	1.525896	0.412220	2.277467
H	0.100346	-0.632267	2.401413
H	3.690360	-0.157253	3.417994
H	3.439882	-1.564512	4.465802
H	-0.379056	-2.873448	-2.282870
H	-2.125459	-2.915423	-1.977365
H	-1.452339	-1.666335	-3.028114
H	2.678642	0.115945	0.185944
C	0.760311	0.002550	-3.266885
H	1.513895	-0.799298	-3.287663
H	-0.132266	-0.368454	-3.786354
H	1.159385	0.839738	-3.860220
H	1.369439	1.039876	-1.527793
H	4.931857	-1.424366	3.517514
Al	5.379513	-0.100149	-1.093778
C	5.370351	0.906332	0.593653
Cl	6.799963	-1.762967	-1.058105
H	4.598330	1.695345	0.627140
H	6.341189	1.410206	0.749874
H	5.210318	0.249808	1.466448
C	5.255782	0.796005	-2.835209
H	4.404077	1.499934	-2.867255
H	6.162810	1.381674	-3.068078
H	5.114448	0.077604	-3.661830
Si	0.212428	3.514772	-0.055470
Si	-4.750580	-0.550913	0.162185
C	-0.672701	4.067040	1.531374
C	0.153998	4.809475	-1.409157
H	0.718394	4.476698	-2.295779
H	-0.879902	5.021744	-1.724517
H	0.608072	5.754205	-1.067993
C	1.998507	3.048400	0.293066
H	2.061113	2.211383	1.006217
H	2.520437	2.756808	-0.632461
H	2.551072	3.899008	0.724403
C	-4.253064	-0.988252	1.918946
H	-5.019026	-0.646475	2.634343
H	-4.117130	-2.072313	2.057574
H	-3.306456	-0.492006	2.190061
C	-6.183949	-1.626679	-0.459275
C	-5.146561	1.281346	0.088181
H	-5.381920	1.611142	-0.935848
H	-6.007683	1.524855	0.732090
H	-4.289792	1.875067	0.448204
C	4.073023	-3.065677	1.750798
H	4.455034	-3.732108	2.542062
H	3.582214	-3.687524	0.992484
H	4.958935	-2.608486	1.277371
C	-7.374557	-1.496336	0.503438
H	-8.226967	-2.102127	0.147075
H	-7.125009	-1.848768	1.517724
H	-7.727689	-0.455136	0.587669
C	-6.602002	-1.162441	-1.862961
H	-5.760380	-1.206650	-2.572769
H	-7.407213	-1.806679	-2.259681
H	-6.983236	-0.128293	-1.857442
C	-5.730444	-3.093426	-0.521182
H	-5.419989	-3.472157	0.466502
H	-6.555239	-3.738024	-0.874684
H	-4.882960	-3.225776	-1.211679
C	-2.115241	4.469470	1.189129
H	-2.662166	3.641706	0.710006
H	-2.667158	4.750199	2.104081
H	-2.150375	5.334598	0.506944
C	-0.694015	2.899081	2.530516
H	-1.220206	3.192782	3.456533

H	-1.213915	2.020673	2.116102
H	0.322230	2.584138	2.819166
C	0.062666	5.263203	2.154453
H	-0.459861	5.604592	3.065956
H	1.094167	5.007493	2.446817
H	0.112524	6.123226	1.466279

prSiendo-syn-scis

SCF Energy: -2801.73583913 H

Num. Imaginary Frequencies: 0

C	-1.467116	-0.842306	-0.707400
C	-1.586818	-0.017191	-1.988588
C	-0.618227	1.164743	-2.001925
C	0.838252	0.721042	-1.780604
C	0.884916	-0.137205	-0.499272
C	-0.029087	-1.385721	-0.507016
C	2.284211	-0.523154	0.019752
C	2.183486	-0.918660	1.533288
C	1.016456	-1.859024	1.755461
C	0.069120	-2.071004	0.835479
C	1.018211	-2.575558	3.076506
C	2.313553	0.271992	2.490801
C	3.755068	0.667402	2.759718
C	1.322186	0.963122	3.095695
C	1.669176	2.106275	4.026578
C	0.302370	-2.452415	-1.567681
C	3.220951	0.610485	-0.173565
O	4.320738	0.539820	-0.720612
O	-0.964829	2.061594	-0.967205
O	-2.404888	-1.891103	-0.711811
H	-1.660066	-0.159942	0.142765
H	-1.412015	-0.661413	-2.863530
H	-2.615735	0.363188	-2.073400
H	-0.679713	1.666774	-2.986177
H	0.465738	0.529466	0.271449
H	2.680069	-1.386104	-0.534417
H	3.081865	-1.529148	1.723455
H	-0.712394	-2.809953	1.039943
H	1.945990	-3.157210	3.207504
H	0.973578	-1.859016	3.912707
H	0.163730	-3.261599	3.164581
H	3.940519	1.739967	2.589619
H	4.034001	0.461571	3.807567
H	4.462622	0.098894	2.138573
H	2.439358	1.829161	4.763373
H	2.061040	2.974357	3.468719
H	1.372498	-2.707177	-1.556757
H	-0.256505	-3.372293	-1.344562
H	0.035622	-2.153643	-2.588195
H	2.904527	1.606924	0.186359
C	1.476400	0.149952	-3.046006
H	2.452652	-0.309149	-2.837627
H	0.855259	-0.609856	-3.537510
H	1.642379	0.957407	-3.775714
H	1.376412	1.656477	-1.549865
H	0.783576	2.448446	4.581194
Al	5.534894	-0.858943	-1.338964
C	7.160309	0.169550	-1.711530
Cl	5.679765	-2.029701	0.521967
H	7.996661	-0.489041	-2.006433
H	7.500124	0.752877	-0.837970
H	7.006888	0.882495	-2.541738
C	4.652921	-1.881421	-2.762406
H	4.448591	-1.274353	-3.661715
H	5.326298	-2.698147	-3.081837
H	3.704683	-2.355529	-2.456874
Si	-1.788320	3.519069	-1.143155
Si	-3.811030	-1.833849	0.220733
C	-2.011391	4.112070	0.644917
C	-3.427114	3.226919	-2.006896
H	-3.265265	2.833969	-3.024340
H	-4.056152	2.506202	-1.461134
H	-3.992637	4.168177	-2.105409
C	-0.743936	4.695613	-2.163563
H	0.237502	4.875591	-1.696730
H	-0.567626	4.283489	-3.170991
H	-1.246930	5.668152	-2.290574
C	-3.358762	-1.807718	2.041998
H	-4.256630	-1.654165	2.662975
H	-2.876395	-2.743086	2.365857
H	-2.664825	-0.978443	2.257461
C	-4.766909	-3.400052	-0.258091
C	-4.754069	-0.261829	-0.181873
H	-5.014358	-0.196022	-1.249792
H	-5.686332	-0.199090	0.403063
H	-4.144236	0.619202	0.077805
C	-0.159950	0.726119	2.975999
H	-0.440948	0.015831	2.195139
H	-0.560872	0.357139	3.936509
H	-0.671420	1.679584	2.775659
C	-0.630879	4.224162	1.311970
H	-0.734739	4.499862	2.376914
H	-0.078144	3.273012	1.264684
H	-0.007429	4.997031	0.833235
C	-2.871978	3.087453	1.401200
H	-3.894179	3.031500	0.992742
H	-2.436111	2.077017	1.353799
H	-2.959869	3.363922	2.467305
C	-2.705666	5.481977	0.664276
H	-3.702420	5.446543	0.194340
H	-2.846721	5.829289	1.703523
H	-2.114800	6.251213	0.140347
C	-3.885075	-4.633247	-0.007731
H	-3.599632	-4.728530	1.052720
H	-4.424924	-5.556287	-0.285768
H	-2.958585	-4.596857	-0.601942
C	-6.043389	-3.499096	0.591680
H	-6.620153	-4.400601	0.317504
H	-5.817867	-3.570866	1.668411
H	-6.706864	-2.630737	0.445030
C	-5.141607	-3.334420	-1.746699
H	-4.249945	-3.229039	-2.385123
H	-5.666088	-4.256835	-2.054558
H	-5.813221	-2.488114	-1.964966

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SCF Energy: -2801.74063059 H

Num. Imaginary Frequencies: 0

C	-1.686934	-0.738908	-0.615489
C	-1.850602	0.130783	-1.861547
C	-0.870370	1.303376	-1.873043
C	0.588083	0.830876	-1.747375
C	0.693126	-0.073121	-0.502110
C	-0.248942	-1.300697	-0.489587
C	2.117199	-0.500650	-0.127782
C	2.185501	-1.094813	1.315611
C	0.966510	-1.931060	1.643025
C	-0.098345	-2.008369	0.836818
C	1.044421	-2.680184	2.943890
C	2.458864	-0.022156	2.376357
C	1.282038	0.816388	2.819038
C	3.695910	0.231038	2.858608
C	3.910288	1.349367	3.854500
C	0.018128	-2.354506	-1.581720
C	3.054829	0.655485	-0.162781
O	4.202526	0.619158	-0.603203
O	-1.149828	2.156141	-0.781275
O	-2.630130	-1.783367	-0.621998
H	-1.844214	-0.086099	0.264657
H	-1.717250	-0.484165	-2.764646
H	-2.878977	0.520695	-1.890902
H	-0.976485	1.851569	-2.828514
H	0.336932	0.568294	0.318863
H	2.493560	-1.259730	-0.826788
H	3.037844	-1.787330	1.309749
H	-0.924574	-2.672028	1.111800
H	1.935702	-3.329051	2.971423
H	1.133856	-1.986336	3.796528
H	0.154113	-3.305278	3.103556
H	1.303241	1.020922	3.899726
H	1.270512	1.797441	2.311880
H	0.325492	0.324976	2.593319
H	3.529448	2.312662	3.478229
H	3.388691	1.150877	4.805875
H	1.083379	-2.626261	-1.621807
H	-0.546386	-3.269113	-1.351326
H	-0.289249	-2.029987	-2.583369
H	2.702653	1.624005	0.236789
C	1.145236	0.289057	-3.063608
H	2.129001	-0.183077	-2.925837
H	0.487857	-0.451605	-3.537038
H	1.277659	1.113914	-3.780625
H	1.158447	1.747496	-1.515889
H	4.977174	1.480321	4.084318
Al	5.468172	-0.537338	-1.510759
C	7.185155	-0.017166	-0.718545
Cl	4.877827	-2.580721	-0.925720
H	8.022564	-0.427531	-1.311465
H	7.317111	-0.379375	0.315099
H	7.313271	1.080089	-0.703350
C	5.092623	-0.176626	-3.404344
H	4.938310	0.900065	-3.598089
H	5.945777	-0.493858	-4.030874
H	4.203743	-0.709765	-3.782309
Si	-2.018955	3.596242	-0.830212
Si	-4.008734	-1.776364	0.350776
C	-2.157529	4.096385	0.995470
C	-3.698346	3.315064	-1.616346
H	-3.585780	2.922302	-2.640490
H	-4.309484	2.600015	-1.043718
H	-4.258193	4.261983	-1.689151
C	-1.062432	4.850706	-1.844600
H	-0.037663	4.982874	-1.462816
H	-0.991237	4.525250	-2.895704
H	-1.560357	5.834133	-1.838485
C	-3.510198	-1.851423	2.158942
H	-4.390154	-1.720025	2.809924
H	-3.033000	-2.808945	2.420726
H	-2.799620	-1.043390	2.399544
C	-4.977896	-3.316076	-0.184983
C	-4.962788	-0.187131	0.060429
H	-5.237377	-0.055801	-0.997707
H	-5.887382	-0.164918	0.660326
H	-4.351761	0.677857	0.366690
C	4.955090	-0.494500	2.467776
H	5.455496	-0.894888	3.365453
H	4.812728	-1.321450	1.761992
H	5.664733	0.215109	2.009475
C	-6.199486	-3.494471	0.730064
H	-6.790499	-4.373920	0.417288
H	-5.907436	-3.654610	1.780889
H	-6.872566	-2.621575	0.698228
C	-5.443333	-3.146701	-1.639410
H	-4.594407	-2.974956	-2.320517
H	-5.970021	-4.054331	-1.985134
H	-6.141045	-2.300854	-1.751925
C	-4.071143	-4.552032	-0.079831
H	-3.711460	-4.714446	0.949502
H	-4.621551	-5.461237	-0.381753
H	-3.188538	-4.463090	-0.732152
C	-2.807763	2.950529	1.786380
H	-3.825693	2.727983	1.426460
H	-2.216672	2.023565	1.716517
H	-2.889646	3.215953	2.855690
C	-0.753473	4.369474	1.556147
H	-0.805941	4.610851	2.633019
H	-0.096108	3.492394	1.444404
H	-0.267406	5.220984	1.052721
C	-3.018670	5.362455	1.121470
H	-4.046671	5.199234	0.758569
H	-3.090809	5.677013	2.178030
H	-2.594386	6.209728	0.557616

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SCF Energy: -2801.72698898 H

Num. Imaginary Frequencies: 0

C	2.031555	-0.343559	0.314442
C	2.132628	0.169764	1.741796

C	0.964721	1.101989	2.034146
C	-0.356575	0.324728	1.947117
C	-0.519706	-0.273713	0.526101
C	0.699141	-1.072078	-0.022244
C	-1.858345	-1.094557	0.430952
C	-1.734950	-2.592212	0.016956
C	-0.447742	-3.224406	0.532348
C	0.672027	-2.486917	0.512488
C	-0.437342	-4.685906	0.878941
C	-3.056511	-3.340760	0.226580
C	-3.717398	-3.697765	-1.082865
C	-3.591581	-3.615220	1.433647
C	-4.920089	-4.299301	1.638929
C	0.644388	-1.116126	-1.565599
C	-2.682142	-0.378449	-0.563718
O	-3.623883	0.352618	-0.257392
O	0.996878	2.160282	1.102445
O	3.112453	-1.192942	0.011271
H	2.056092	0.548672	-0.335783
H	2.144292	-0.670233	2.453135
H	3.081267	0.714608	1.859449
H	1.062592	1.498713	3.061560
H	-0.602957	0.611554	-0.128946
H	-2.382235	-1.027696	1.390994
H	-1.604299	-2.586297	-1.076498
H	1.627657	-2.933103	0.802447
H	-1.088084	-4.924607	1.732847
H	-0.803915	-5.286509	0.029370
H	0.582201	-5.021773	1.117407
H	-3.039498	-4.318372	-1.693079
H	-4.659606	-4.246817	-0.973763
H	-3.928391	-2.791876	-1.678690
H	-4.769547	-5.325577	2.016520
H	-5.499709	-3.766755	2.410809
H	1.520662	-1.655054	-1.951864
H	-0.249047	-1.618917	-1.956812
H	0.659640	-0.095415	-1.980618
H	-2.409429	-0.487290	-1.633268
C	-0.471268	-0.644013	3.125139
H	-1.507029	-0.968056	3.281882
H	0.147202	-1.543635	3.001734
H	-0.155014	-0.140725	4.052367
H	-1.168582	1.062325	2.057600
H	-5.542241	-4.358787	0.738354
Al	-4.756472	1.426449	-1.427750
C	-3.697937	3.060674	-1.665731
Cl	-4.684412	0.143530	-3.219022
H	-3.650269	3.665824	-0.743250
H	-4.116209	3.711299	-2.454203
H	-2.660761	2.824269	-1.961795
C	-6.493118	1.395011	-0.524615
H	-6.445427	1.896307	0.458733
H	-7.268991	1.916125	-1.113121
H	-6.854976	0.366416	-0.351519
Si	0.500563	3.752313	1.336245
Si	4.496667	-0.731685	-0.832449
C	1.025185	4.633811	-0.261709
C	1.364450	4.454546	2.845311
H	2.460415	4.430648	2.735783
H	1.059904	5.499304	3.020157
H	1.102115	3.882923	3.750765
C	-1.358210	3.817081	1.585606
H	-1.727662	4.855114	1.543350
H	-1.887841	3.238366	0.812707
H	-1.638007	3.408085	2.570287
C	5.421393	0.582723	0.135872
H	4.830367	1.512046	0.188556
H	5.636432	0.257853	1.165990
H	6.378916	0.830198	-0.351483
C	4.024492	-0.026891	-2.506511
H	3.314624	0.808871	-2.394111
H	4.915569	0.369314	-3.020688
H	3.559766	-0.780394	-3.161265
C	5.495318	-2.337412	-0.996656
C	-2.915329	-3.283138	2.737542
H	-3.465261	-2.486401	3.268010
H	-2.926519	-4.162528	3.403239
H	-1.874827	-2.961770	2.625405
C	0.795078	6.145872	-0.110897
H	-0.258526	6.385899	0.108559
H	1.412561	6.578644	0.693022
H	1.060469	6.670800	-1.045981
C	2.513175	4.366127	-0.533803
H	3.155001	4.725494	0.287434
H	2.712364	3.291491	-0.667045
H	2.836703	4.884826	-1.454044
C	0.187400	4.104867	-1.436164
H	0.508980	4.574338	-2.383216
H	0.293806	3.014239	-1.556691
H	-0.884376	4.326544	-1.309166
C	6.732857	-2.083025	-1.871553
H	7.387050	-1.302620	-1.448629
H	7.338057	-3.003103	-1.959917
H	6.458824	-1.773335	-2.893384
C	4.619298	-3.418189	-1.649112
H	4.278753	-3.121885	-2.654931
H	5.186922	-4.359669	-1.760083
H	3.725124	-3.635828	-1.044480
C	5.938912	-2.811900	0.395793
H	5.078435	-2.971142	1.065376
H	6.485170	-3.769526	0.322045
H	6.612994	-2.087669	0.881624

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SCF Energy: -2801.73238064 H

Num. Imaginary Frequencies: 0

C	-1.818447	-0.685696	-0.320301
C	-2.223163	-0.148716	-1.684297
C	-1.399328	1.088424	-2.024910
C	0.089929	0.735150	-2.094069
C	0.555500	0.143220	-0.736649
C	-0.310797	-1.029494	-0.194593
C	2.067114	-0.208958	-0.794625
C	2.442008	-1.739103	-0.689866

C	1.316310	-2.634942	-1.195047
C	0.046397	-2.293225	-0.941431
C	1.684669	-3.941845	-1.837918
C	3.811138	-1.979662	-1.298656
C	3.940911	-1.713634	-2.783202
C	4.860561	-2.343665	-0.532665
C	6.248548	-2.522987	-1.087823
C	-0.052044	-1.237859	1.312376
C	2.811535	0.437487	0.306238
O	3.885273	1.011266	0.130132
O	-1.591987	2.076195	-1.033957
O	-2.588299	-1.818087	0.011362
H	-2.003403	0.126014	0.406502
H	-2.090011	-0.925864	-2.452888
H	-3.292842	0.108047	-1.665442
H	-1.706647	1.472631	-3.015880
H	0.425157	0.971123	-0.019821
H	2.495292	0.175283	-1.729136
H	2.517630	-1.972957	0.381912
H	-0.768778	-2.963214	-1.230886
H	2.224802	-3.801895	-2.787044
H	2.349499	-4.528024	-1.182066
H	0.787072	-4.543408	-2.041709
H	4.505273	-2.503612	-3.299848
H	2.954347	-1.657660	-3.263190
H	4.454518	-0.758639	-2.986164
H	6.334303	-2.280534	-2.154057
H	6.958395	-1.882548	-0.538345
H	-0.716880	-2.024539	1.695031
H	0.976851	-1.547946	1.537284
H	-0.258037	-0.311987	1.874087
H	2.409781	0.361544	1.335831
C	0.385414	-0.085015	-3.350490
H	1.463127	-0.243496	-3.487221
H	-0.093286	-1.073193	-3.341767
H	0.026267	0.458405	-4.238728
H	0.626900	1.693346	-2.201794
H	6.590725	-3.562158	-0.942607
Al	5.161702	1.779674	1.375133
C	4.984617	3.704169	1.043356
Cl	4.235571	1.148926	3.272291
H	5.280923	3.965391	0.011521
H	5.625366	4.297327	1.719801
H	3.948753	4.059064	1.186224
C	6.810180	0.795447	0.979692
H	7.053447	0.831156	-0.097273
H	7.673706	1.225978	1.517742
H	6.745378	-0.266690	1.270812
Si	-2.622178	3.403330	-1.133603
Si	-3.922935	-1.788611	1.040736
C	-2.724008	4.046261	0.649874
C	-4.299931	2.873573	-1.785588
H	-4.813828	2.179603	-1.102328
H	-4.951528	3.750336	-1.933724
H	-4.197504	2.373772	-2.763052
C	-1.874724	4.662607	-2.304739
H	-2.467746	5.591488	-2.330805
H	-0.844485	4.921271	-2.013099
H	-1.843317	4.262346	-3.331785
C	-5.221027	-0.621286	0.354078
H	-4.835979	0.411582	0.368640
H	-5.499709	-0.868261	-0.682180
H	-6.135429	-0.638677	0.969652
C	-3.413478	-1.168740	2.736923
H	-2.946111	-0.173281	2.661065
H	-4.296320	-1.065372	3.389091
H	-2.698920	-1.842913	3.234000
C	-4.516463	-3.589800	1.087337
C	4.753352	-2.593411	0.959003
H	3.966297	-3.321326	1.210095
H	5.699557	-2.990479	1.353765
H	4.536699	-1.671593	1.524843
C	-1.355825	4.597500	1.080195
H	-1.387590	4.931651	2.132787
H	-0.563593	3.835638	0.999277
H	-1.051572	5.464076	0.471043
C	-3.124091	2.892682	1.583061
H	-4.097140	2.453946	1.306213
H	-2.375134	2.085338	1.567245
H	-3.210997	3.249319	2.625033
C	-3.776484	5.162991	0.731271
H	-3.543471	6.002681	0.055434
H	-4.784912	4.797789	0.476938
H	-3.825654	5.572956	1.755930
C	-5.673688	-3.721391	2.089774
H	-6.528203	-3.077292	1.823719
H	-6.044979	-4.761612	2.115727
H	-5.363236	-3.460051	3.114710
C	-3.355293	-4.498032	1.520855
H	-2.980932	-4.238116	2.524686
H	-3.682893	-5.552675	1.556532
H	-2.507277	-4.434411	0.821279
C	-4.996777	-4.006288	-0.311394
H	-4.201336	-3.892038	-1.065205
H	-5.309055	-5.066153	-0.313714
H	-5.862188	-3.409603	-0.643151

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SCF Energy: -2801.72897401 H

Num. Imaginary Frequencies: 0

C	1.756279	-0.511536	0.243301
C	1.655460	0.096415	1.633162
C	0.504527	1.095924	1.679012
C	-0.820765	0.374121	1.418295
C	-0.779719	-0.284501	0.015331
C	0.453214	-1.188226	-0.270941
C	-2.138521	-1.023301	-0.294448
C	-2.057515	-2.555673	-0.556743
C	-0.921643	-3.220535	0.212639
C	0.237333	-2.557065	0.335690
C	-1.071056	-4.652006	0.642969
C	-3.447932	-3.203790	-0.522148
C	-3.910512	-3.619695	-1.897946
C	-4.191225	-3.356153	0.593091

C	-5.584193	-3.934038	0.617165
C	0.655168	-1.339141	-1.794904
C	-2.677968	-0.327682	-1.488723
O	-3.444144	0.632082	-1.474249
O	0.685200	2.092400	0.695968
O	2.816975	-1.435279	0.181186
H	1.944643	0.328983	-0.448414
H	1.508768	-0.692601	2.386807
H	2.604050	0.600152	1.871267
H	0.451502	1.552981	2.684573
H	-0.680806	0.572080	-0.673472
H	-2.824695	-0.836088	0.539813
H	-1.744773	-2.658988	-1.608347
H	1.097108	-3.039215	0.809775
H	-1.869331	-4.791145	1.386491
H	-1.333317	-5.288194	-0.219324
H	-0.131319	-5.030491	1.070475
H	-4.907653	-4.073709	-1.918187
H	-3.924314	-2.756246	-2.586181
H	-3.203840	-4.348363	-2.330536
H	-6.047608	-4.045469	-0.369923
H	-5.580009	-4.924579	1.104082
H	1.557131	-1.935252	-1.990954
H	-0.182453	-1.838999	-2.298070
H	0.787299	-0.351524	-2.266144
H	-2.318592	-0.665043	-2.480870
C	-1.181000	-0.521159	2.601608
H	-2.234482	-0.820681	2.568224
H	-0.574107	-1.435280	2.653165
H	-1.040284	0.034102	3.542238
H	-1.591566	1.159597	1.363643
H	-6.243048	-3.292396	1.225384
Al	-4.287387	1.845214	-0.213304
C	-2.958993	3.291118	-0.154915
Cl	-6.063063	2.369531	-1.384324
H	-2.875365	3.807247	-1.127262
H	-1.952319	2.922993	0.108506
H	-3.229896	4.055210	0.595603
C	-4.784019	0.792590	1.370431
H	-3.933157	0.587366	2.042431
H	-5.541948	1.327794	1.970222
H	-5.228771	-0.178476	1.088761
Si	1.357346	3.622291	0.907590
Si	4.344795	-1.099299	-0.448230
C	1.854972	4.152136	-0.846207
C	2.833245	3.520833	2.061870
H	3.605876	2.827319	1.695877
H	3.297149	4.514025	2.180049
H	2.522073	3.183629	3.064511
C	0.074931	4.767601	1.653503
H	0.525245	5.729647	1.948013
H	-0.747514	4.972530	0.950907
H	-0.362043	4.314352	2.559043
C	5.118598	0.327313	0.492225
H	4.551671	1.253524	0.305010
H	5.137194	0.149241	1.578712
H	6.153431	0.504505	0.155737
C	4.201787	-0.611874	-2.254457
H	3.499470	0.228926	-2.375003
H	5.178936	-0.278734	-2.641264
H	3.849600	-1.442215	-2.886046
C	5.305384	-2.719565	-0.222434
C	-3.711883	-2.975666	1.968428
H	-4.267277	-2.099523	2.344764
H	-3.907498	-3.797169	2.677778
H	-2.643241	-2.744626	2.010094
C	3.029796	3.286250	-1.326263
H	3.934429	3.444659	-0.717039
H	2.785259	2.211967	-1.290269
H	3.291703	3.530232	-2.371458
C	2.273097	5.630555	-0.836099
H	1.441651	6.290114	-0.538514
H	3.114207	5.819413	-0.148211
H	2.598084	5.947241	-1.843403
C	0.661462	3.961371	-1.794898
H	0.927141	4.283787	-2.817785
H	0.350108	2.906209	-1.846317
H	-0.215034	4.551472	-1.481641
C	6.693675	-2.585139	-0.867441
H	7.280583	-1.765323	-0.421131
H	7.274480	-3.514738	-0.729369
H	6.628571	-2.399102	-1.952049
C	5.461122	-3.017521	1.276785
H	4.484116	-3.089449	1.781019
H	5.985916	-3.978023	1.427897
H	6.048136	-2.239449	1.791601
C	4.535679	-3.866967	-0.894711
H	4.407950	-3.699369	-1.976793
H	5.080360	-4.820570	-0.773133
H	3.533616	-3.995531	-0.456530

prSiexo-syn-strans

SCF Energy: -2801.73363381 H

Num. Imaginary Frequencies: 0

C	1.712237	-0.601156	0.278713
C	1.729339	0.057845	1.649319
C	0.643785	1.126147	1.729491
C	-0.739703	0.492123	1.549408
C	-0.802440	-0.236830	0.182371
C	0.349010	-1.239599	-0.097149
C	-2.210510	-0.901637	-0.025248
C	-2.266239	-2.457327	-0.032934
C	-1.105234	-3.102962	0.710942
C	0.101305	-2.523824	0.661211
C	-1.322595	-4.451672	1.336134
C	-3.657699	-2.905396	0.386594
C	-4.023458	-2.637441	1.832480
C	-4.547665	-3.434039	-0.480115
C	-5.959330	-3.774708	-0.069655
C	0.422634	-1.548106	-1.606168
C	-2.760068	-0.374383	-1.300720
O	-3.415388	0.658280	-1.412112
O	0.843837	2.090667	0.716643
O	2.725491	-1.574060	0.184645

H	1.884086	0.201181	-0.461699
H	1.583161	-0.698990	2.435678
H	2.717147	0.512096	1.816631
H	0.671275	1.604654	2.726163
H	-0.684052	0.572222	-0.558247
H	-2.861788	-0.524322	0.773213
H	-2.122604	-2.765300	-1.078017
H	0.965372	-3.015063	1.118440
H	-2.045576	-4.418922	2.165600
H	-1.728045	-5.161565	0.595723
H	-0.378633	-4.862411	1.722422
H	-4.688039	-1.763561	1.938234
H	-4.534380	-3.493662	2.296644
H	-3.127957	-2.431689	2.433328
H	-6.275884	-3.295762	0.865248
H	-6.666895	-3.470602	-0.858122
H	1.270152	-2.217599	-1.809159
H	-0.481409	-2.044512	-1.985155
H	0.569552	-0.621815	-2.185528
H	-2.535781	-0.925811	-2.234736
C	-1.130647	-0.309421	2.789610
H	-2.175449	-0.642788	2.742158
H	-0.506058	-1.199317	2.944264
H	-1.041633	0.329301	3.682438
H	-1.451821	1.330154	1.475332
H	-6.076479	-4.866104	0.050726
Al	-4.062683	2.119516	-0.301888
C	-2.578538	3.395189	-0.441504
Cl	-5.795285	2.701552	-1.509989
H	-2.377611	3.664894	-1.492920
H	-1.638977	3.000761	-0.017590
H	-2.807992	4.333790	0.094297
C	-4.638862	1.337230	1.407118
H	-3.803729	1.088466	2.084736
H	-5.289655	2.044769	1.951858
H	-5.230096	0.416888	1.254465
Si	1.624964	3.574362	0.888278
Si	4.216942	-1.331873	-0.562374
C	2.135446	4.052932	-0.876811
C	3.112886	3.389069	2.017264
H	3.835562	2.649238	1.639346
H	3.637437	4.353363	2.120179
H	2.802955	3.075670	3.027873
C	0.431262	4.808848	1.638987
H	0.938705	5.753888	1.892439
H	-0.400368	5.036588	0.954294
H	-0.000922	4.403523	2.569205
C	5.139828	0.050808	0.306026
H	4.608214	1.005719	0.167291
H	5.237564	-0.133286	1.387374
H	6.151640	0.175374	-0.113709
C	3.960498	-0.854093	-2.358825
H	3.300720	0.024976	-2.438880
H	4.921319	-0.583890	-2.826997
H	3.511495	-1.669707	-2.946727
C	5.099480	-3.003076	-0.393149
C	-4.276177	-3.745897	-1.931650
H	-3.213444	-3.771844	-2.203155
H	-4.703780	-4.729244	-2.187397
H	-4.776366	-3.011387	-2.586360
C	6.433506	-2.955166	-1.154491
H	7.100231	-2.163704	-0.773781
H	6.972252	-3.913955	-1.049182
H	6.286901	-2.779975	-2.232922
C	5.364736	-3.295324	1.091746
H	4.432129	-3.301741	1.678516
H	5.840924	-4.285057	1.212217
H	6.040343	-2.550425	1.542962
C	4.211897	-4.110966	-0.981203
H	3.998957	-3.945147	-2.050103
H	4.712228	-5.092407	-0.895632
H	3.247009	-4.180143	-0.455148
C	2.663959	5.495775	-0.882125
H	1.888151	6.218194	-0.580232
H	3.525021	5.625184	-0.205359
H	2.999751	5.780199	-1.895485
C	3.235958	3.098457	-1.364279
H	4.159826	3.198024	-0.771847
H	2.914865	2.045355	-1.310271
H	3.497053	3.310643	-2.416598
C	0.920731	3.947831	-1.810965
H	1.200491	4.237388	-2.839972
H	0.525458	2.920552	-1.847438
H	0.098017	4.609236	-1.495174

TSReendo-anti-scis1

SCF Energy: -2801.65911485 H

Num. Imaginary Frequencies: 1

C	-1.197827	1.306446	-1.366064
C	-2.357728	0.351672	-1.604280
C	-2.393143	-0.777210	-0.590938
C	-1.145105	-1.666257	-0.671464
C	0.145927	-0.952065	-0.265808
C	0.200425	0.662355	-1.518642
C	1.336118	-1.720406	-0.401788
C	3.281976	0.391768	-1.648892
C	2.611599	1.248266	-0.798218
C	1.194131	1.325309	-0.786468
C	3.316349	2.070119	0.255110
C	4.721018	0.196881	-1.794655
C	5.177828	-1.243535	-1.887545
C	5.616947	1.208556	-1.943520
C	7.081848	0.890800	-2.088014
C	0.449641	0.093734	-2.904210
C	2.385670	-1.615174	0.489983
O	3.389657	-2.411272	0.511439
O	-3.544930	-1.556495	-0.816154
O	-1.344204	1.880871	-0.095887
H	-1.234118	2.083905	-2.156554
H	-3.289659	0.931113	-1.530722
H	-2.327712	-0.076976	-2.616854
H	-2.415645	-0.334414	0.423849
H	0.044878	-0.408249	0.679469
H	1.388631	-2.501798	-1.166283

H	2.681697	-0.264698	-2.276319
H	0.790781	1.948425	0.015878
H	4.338768	1.712343	0.429118
H	3.366031	3.135282	-0.020459
H	2.767781	2.007436	1.207303
H	4.333590	-1.942593	-1.830747
H	5.731704	-1.436404	-2.820659
H	5.849045	-1.485609	-1.049403
H	7.693844	1.803052	-2.053094
H	7.427536	0.213380	-1.292131
H	1.131901	0.747703	-3.469369
H	0.891178	-0.912009	-2.886743
H	-0.484551	0.020773	-3.475119
H	2.329652	-0.829924	1.266575
C	-1.309509	-2.887775	0.244391
H	-1.355771	-2.579225	1.301530
H	-2.240712	-3.414933	-0.000997
H	-0.470570	-3.587523	0.132363
H	-1.043768	-2.024394	-1.710955
H	7.288207	0.388034	-3.049135
Al	4.727340	-2.592601	1.774925
C	5.973483	-3.945075	1.065999
Cl	5.687485	-0.589636	1.846299
H	5.488757	-4.935630	0.985753
H	6.853973	-4.075512	1.721127
H	6.355810	-3.692163	0.061045
C	3.823989	-2.955547	3.495052
H	4.537351	-3.048551	4.334113
H	3.107444	-2.161438	3.773964
H	3.253409	-3.902118	3.457219
Si	-1.838318	3.467173	0.221483
Si	-4.923290	-1.472229	0.154364
C	-1.923108	3.538371	2.113393
C	-0.557154	4.639479	-0.485311
H	0.411078	4.553000	0.032541
H	-0.388418	4.428158	-1.554549
H	-0.892840	5.686362	-0.407198
C	-3.496897	3.777529	-0.590647
H	-3.415479	3.692834	-1.686896
H	-4.261288	3.062356	-0.249302
H	-3.856560	4.795114	-0.366008
C	-6.178051	-2.603156	-0.708217
C	-4.510191	-2.065369	1.885299
H	-3.691765	-1.465461	2.315914
H	-5.380659	-1.956014	2.552802
H	-4.199532	-3.121656	1.898861
C	-5.506475	0.308659	0.251460
H	-4.729998	0.935357	0.719931
H	-5.731106	0.726067	-0.742375
H	-6.413908	0.393409	0.871705
C	5.262316	2.659516	-2.083031
H	5.614286	3.236345	-1.211147
H	5.782893	3.075832	-2.961527
H	4.187809	2.838467	-2.209913
C	-5.559021	-3.996135	-0.902217
H	-5.275400	-4.459761	0.056924
H	-6.280502	-4.673974	-1.392895
H	-4.657693	-3.953378	-1.533451
C	-6.544625	-2.012411	-2.078414
H	-5.655143	-1.877478	-2.714589
H	-7.239412	-2.683188	-2.615060
H	-7.042613	-1.033630	-1.984371
C	-7.442190	-2.716993	0.158116
H	-8.195487	-3.352641	-0.340851
H	-7.230021	-3.171572	1.139597
H	-7.911661	-1.735427	0.337369
C	-2.234257	4.978134	2.551593
H	-3.194044	5.336896	2.144343
H	-2.303125	5.039387	3.652273
H	-1.449506	5.683924	2.233371
C	-3.027594	2.594529	2.613820
H	-4.022973	2.893027	2.246848
H	-2.847965	1.554663	2.295994
H	-3.069566	2.600480	3.717618
C	-0.573240	3.099989	2.703103
H	-0.600410	3.150138	3.806169
H	-0.326980	2.063326	2.424197
H	0.255282	3.745332	2.367892

TSReendo-anti-strans

SCF Energy: -2801.66614213 H

Num. Imaginary Frequencies: 1

C	-1.249077	1.117961	-1.550917
C	-2.290535	0.007479	-1.595300
C	-2.226159	-0.921683	-0.395647
C	-0.905070	-1.698843	-0.324313
C	0.310765	-0.820270	-0.056983
C	0.213472	0.629717	-1.618090
C	1.568101	-1.454441	-0.124932
C	3.268265	0.532093	-1.615534
C	2.544812	1.542092	-0.992373
C	1.129059	1.508527	-1.024988
C	3.157337	2.647126	-0.158489
C	4.688605	0.257252	-1.692110
C	5.684898	1.204149	-1.069076
C	5.061994	-0.891650	-2.342862
C	6.481263	-1.336555	-2.530248
C	0.520262	-0.161157	-2.877027
C	2.652115	-1.049553	0.645108
O	3.757979	-1.685719	0.712474
O	-3.299723	-1.831603	-0.473974
O	-1.470377	1.892801	-0.402994
H	-1.381361	1.730497	-2.467115
H	-3.281864	0.483426	-1.620971
H	-2.203034	-0.591820	-2.513653
H	-2.299752	-0.310127	0.524764
H	0.169816	-0.104414	0.758721
H	1.681808	-2.355778	-0.735288
H	2.664600	-0.165386	-2.179297
H	0.651951	2.242006	-0.371414
H	3.731921	2.245161	0.688645
H	3.829930	3.287120	-0.745485
H	2.369062	3.291662	0.253789
H	5.551302	2.226098	-1.450265

H	5.572075	1.238102	0.024045
H	6.719862	0.916923	-1.280098
H	7.238294	-0.675508	-2.097192
H	6.612005	-2.340228	-2.093196
H	1.187604	0.411701	-3.539618
H	1.000920	-1.129561	-2.679319
H	-0.396000	-0.372351	-3.443330
H	2.529542	-0.162546	1.291124
C	-0.971733	-2.757187	0.787126
H	-1.070868	-2.279114	1.775300
H	-1.840080	-3.411040	0.633004
H	-0.064574	-3.376804	0.800497
H	-0.762065	-2.219612	-1.287774
H	6.688961	-1.442783	-3.608995
Al	5.123398	-1.547400	1.961565
C	6.846393	-1.812540	1.049055
Cl	4.915543	0.553847	2.681629
H	7.089845	-1.008479	0.335025
H	6.873694	-2.767212	0.492944
H	7.672120	-1.852202	1.783158
C	4.645886	-2.790917	3.418362
H	3.642523	-2.584298	3.832816
H	4.640152	-3.840470	3.070397
H	5.358653	-2.740484	4.261502
Si	-2.156848	3.437864	-0.377550
Si	-4.695011	-1.720194	0.467259
C	-2.295736	3.840495	1.469511
C	-1.015361	4.614329	-1.287421
H	-0.051248	4.739989	-0.770303
H	-0.806867	4.238526	-2.303128
H	-1.476914	5.609518	-1.394199
C	-3.822653	3.398485	-1.233985
H	-3.708098	3.125211	-2.295947
H	-4.509907	2.675275	-0.768651
H	-4.299287	4.391991	-1.201157
C	-5.808290	-3.115044	-0.175763
C	-4.253264	-1.943867	2.276605
H	-3.507514	-1.194590	2.589204
H	-5.141605	-1.805490	2.914537
H	-3.837015	-2.942316	2.482158
C	-5.465322	-0.024712	0.240313
H	-4.769429	0.753995	0.592406
H	-5.708140	0.182234	-0.813537
H	-6.391218	0.071630	0.830871
C	4.064066	-1.843653	-2.958366
H	4.575573	-2.701278	-3.414790
H	3.366368	-2.237172	-2.203857
H	3.464061	-1.362057	-3.746280
C	-3.268846	2.856556	2.137237
H	-4.287335	2.940015	1.724551
H	-2.938579	1.812346	2.014620
H	-3.337322	3.057149	3.221338
C	-0.912479	3.714168	2.126843
H	-0.975965	3.945047	3.205179
H	-0.507482	2.694604	2.028943
H	-0.180801	4.411564	1.687280
C	-2.816701	5.276493	1.637221
H	-3.809237	5.413175	1.176998
H	-2.915925	5.527509	2.708307
H	-2.133829	6.017406	1.189973
C	-7.066519	-3.210230	0.701304
H	-7.740579	-4.000063	0.324018
H	-6.822602	-3.461060	1.746562
H	-7.639975	-2.268350	0.707411
C	-5.041066	-4.445283	-0.122560
H	-4.723787	-4.699012	0.902283
H	-5.678397	-5.273011	-0.482451
H	-4.140271	-4.417192	-0.755343
C	-6.214277	-2.818338	-1.627646
H	-5.334268	-2.700983	-2.280296
H	-6.823632	-3.644915	-2.035285
H	-6.816468	-1.898574	-1.706486

TSReendo-syn-scis

SCF Energy: -2801.66148390 H

Num. Imaginary Frequencies: 1

C	-1.147877	1.196760	-1.401255
C	-2.101347	0.018680	-1.538130
C	-2.094311	-0.884986	-0.318914
C	-0.728905	-1.548139	-0.101916
C	0.383133	-0.569226	0.267022
C	0.346029	0.811146	-1.282756
C	1.683879	-1.121436	0.332963
C	3.414022	1.037914	-0.965146
C	2.515114	1.989824	-0.525402
C	1.114291	1.799302	-0.653709
C	2.936264	3.288700	0.122040
C	4.874783	1.044151	-0.931611
C	5.512741	0.653699	-2.251679
C	5.659773	1.313268	0.145258
C	7.159292	1.292288	-0.006527
C	0.864903	0.040443	-2.486037
C	2.637069	-0.670647	1.232856
O	3.783763	-1.187545	1.450637
O	-3.079578	-1.878592	-0.483884
O	-1.548620	1.972394	-0.303006
H	-1.209341	1.785410	-2.339627
H	-3.114467	0.423620	-1.677472
H	-1.874306	-0.583718	-2.430127
H	-2.309444	-0.267647	0.575051
H	0.108789	0.116937	1.075363
H	1.933722	-1.975676	-0.302929
H	3.013210	0.214388	-1.553293
H	0.517499	2.529806	-0.100962
H	2.777510	3.273739	1.212102
H	3.994982	3.510944	-0.061960
H	2.338118	4.119720	-0.280823
H	4.754596	0.434501	-3.016262
H	6.141987	1.471669	-2.638996
H	6.149644	-0.238602	-2.151331
H	7.500857	2.121518	-0.649361
H	7.664306	1.388810	0.964441
H	1.495972	0.690295	-3.112041
H	1.462047	-0.841381	-2.219222

H	0.036821	-0.314613	-3.112323
H	2.367564	0.184082	1.877386
C	-0.816253	-2.592811	1.020267
H	-1.037636	-2.111295	1.986768
H	-1.618010	-3.310358	0.802148
H	0.128638	-3.143384	1.123769
H	-0.448304	-2.068097	-1.034578
H	7.510796	0.363453	-0.482766
Al	4.707565	-2.673133	0.857787
C	3.784758	-4.247984	1.615151
Cl	4.481898	-2.687556	-1.357065
H	2.724855	-4.308569	1.308857
H	3.799408	-4.235219	2.720736
H	4.261214	-5.195255	1.302968
C	6.584868	-2.357859	1.368301
H	7.019331	-1.473752	0.870473
H	6.682540	-2.195664	2.457692
H	7.231624	-3.218050	1.116609
Si	-2.355192	3.456554	-0.387389
Si	-4.560750	-1.866018	0.323549
C	-2.712204	3.878490	1.425843
C	-1.218669	4.706975	-1.200488
H	-0.340375	4.934267	-0.575967
H	-0.855178	4.326569	-2.169760
H	-1.748821	5.652918	-1.397726
C	-3.913995	3.269712	-1.408509
H	-3.667772	2.997784	-2.448210
H	-4.583558	2.495471	-1.003367
H	-4.472109	4.219844	-1.441606
C	-5.504339	-3.345180	-0.397161
C	-4.272067	-2.042735	2.168841
H	-3.618480	-1.235465	2.538147
H	-5.223503	-1.970671	2.720942
H	-3.800276	-3.004285	2.424440
C	-5.429903	-0.234223	0.004269
H	-4.828718	0.597854	0.405517
H	-5.593055	-0.054458	-1.069704
H	-6.409385	-0.203318	0.509341
C	5.175425	1.603876	1.532608
H	4.091815	1.524373	1.648556
H	5.645369	0.898209	2.235862
H	5.487320	2.617055	1.839954
C	-1.402325	3.837427	2.228611
H	-1.590528	4.096599	3.285771
H	-0.946650	2.835049	2.207991
H	-0.657784	4.554077	1.844695
C	-3.697884	2.853499	2.007661
H	-4.669425	2.874717	1.487927
H	-3.302686	1.826776	1.941993
H	-3.891789	3.066050	3.074178
C	-3.322657	5.286578	1.506632
H	-4.262821	5.363830	0.935793
H	-3.554912	5.546029	2.554876
H	-2.633300	6.057168	1.124237
C	-4.648390	-4.613441	-0.255770
H	-4.409307	-4.835548	0.797248
H	-5.186451	-5.489190	-0.661134
H	-3.697501	-4.522121	-0.803454
C	-6.826198	-3.527990	0.364852
H	-7.402684	-4.369334	-0.059761
H	-6.659627	-3.751626	1.431257
H	-7.466430	-2.632038	0.306023
C	-5.797814	-3.090615	-1.883728
H	-4.873465	-2.911782	-2.456212
H	-6.304148	-3.963882	-2.332846
H	-6.457473	-2.219690	-2.029266

TSReendo-syn-strans

SCF Energy: -2801.66555164 H

Num. Imaginary Frequencies: 1

C	-1.215531	1.301699	-1.380645
C	-2.066808	0.048962	-1.541160
C	-1.986410	-0.892246	-0.351231
C	-0.571279	-1.442789	-0.128124
C	0.433135	-0.377778	0.292992
C	0.302730	1.042163	-1.295914
C	1.776394	-0.786670	0.410723
C	3.319406	1.351673	-0.927164
C	2.398161	2.276612	-0.457973
C	1.012116	2.057805	-0.643786
C	2.772441	3.508012	0.337623
C	4.754692	1.261211	-0.738179
C	5.422552	1.926461	0.444989
C	5.460002	0.532857	-1.656999
C	6.951507	0.395450	-1.623265
C	0.862115	0.297175	-2.494278
C	2.651175	-0.189083	1.313704
O	3.822196	-0.590681	1.615275
O	-2.877448	-1.962305	-0.567469
O	-1.660364	2.004931	-0.250736
H	-1.349755	1.911135	-2.298566
H	-3.111338	0.370592	-1.665715
H	-1.797786	-0.507641	-2.450909
H	-2.267960	-0.329096	0.560137
H	0.060257	0.305949	1.062040
H	2.134841	-1.647597	-0.161431
H	2.918184	0.597948	-1.593667
H	0.373301	2.743522	-0.081181
H	2.874987	3.288825	1.412781
H	3.716355	3.950298	-0.004594
H	1.990415	4.274128	0.236540
H	5.800054	2.933506	0.204102
H	4.727822	2.020703	1.287175
H	6.270009	1.331459	0.807514
H	7.440116	0.941039	-0.808616
H	7.219974	-0.671794	-1.545967
H	1.497958	0.960698	-3.100724
H	1.466277	-0.580515	-2.222517
H	0.055825	-0.063854	-3.145038
H	2.286617	0.687424	1.876999
C	-0.588006	-2.531030	0.955781
H	-0.873390	-2.106658	1.932201
H	-1.314406	-3.311476	0.694115
H	0.401031	-2.996867	1.063729

H	-0.228440	-1.904620	-1.070618
H	7.374467	0.750348	-2.578453
Al	4.848035	-2.123324	1.492670
C	4.056490	-3.373717	2.801419
Cl	4.579176	-2.952383	-0.555504
H	2.983182	-3.557010	2.612240
H	4.138931	-2.986745	3.833901
H	4.555869	-4.359599	2.790260
C	6.712673	-1.545875	1.763967
H	7.100207	-0.933255	0.932138
H	6.819159	-0.946174	2.686613
H	7.392635	-2.411200	1.867490
Si	-2.605552	3.405784	-0.261136
Si	-4.366787	-2.118484	0.207847
C	-2.977154	3.708178	1.573074
C	-1.608213	4.795990	-1.028365
H	-0.742987	5.076595	-0.407321
H	-1.229249	4.496561	-2.019853
H	-2.229221	5.695158	-1.172100
C	-4.154724	3.117886	-1.274278
H	-3.898804	2.907175	-2.325816
H	-4.748474	2.273274	-0.892343
H	-4.794579	4.015635	-1.266621
C	-5.161620	-3.636839	-0.604900
C	-4.098471	-2.359912	2.048776
H	-3.525470	-1.518000	2.470822
H	-5.063206	-2.397414	2.580937
H	-3.549518	-3.288298	2.270496
C	-5.371843	-0.555584	-0.052102
H	-4.855723	0.304825	0.404134
H	-5.528275	-0.336223	-1.119690
H	-6.360322	-0.637185	0.429126
C	4.809474	-0.161432	-2.828009
H	5.543887	-0.769709	-3.372907
H	4.005536	-0.839558	-2.504235
H	4.378772	0.559613	-3.541288
C	-3.724425	5.042228	1.726164
H	-4.675337	5.050634	1.168120
H	-3.966880	5.228570	2.787590
H	-3.121006	5.895072	1.374280
C	-3.846671	2.563077	2.114958
H	-4.824063	2.513012	1.608333
H	-3.352861	1.585301	1.992936
H	-4.042745	2.703185	3.192990
C	-1.658302	3.762422	2.360098
H	-1.855942	3.952532	3.430159
H	-1.104395	2.813334	2.287482
H	-0.995050	4.567275	2.002809
C	-4.198757	-4.830227	-0.505509
H	-3.959379	-5.082329	0.540670
H	-4.649384	-5.728804	-0.964113
H	-3.250260	-4.628348	-1.027157
C	-5.448002	-3.334401	-2.083884
H	-4.532442	-3.045481	-2.624692
H	-5.865076	-4.225312	-2.586895
H	-6.180257	-2.519187	-2.202673
C	-6.476296	-3.973693	0.115908
H	-6.967631	-4.839616	-0.362951
H	-6.310898	-4.235886	1.173694
H	-7.192247	-3.135437	0.085971

TSReexo-anti-scis

SCF Energy: -2801.66034105 H

Num. Imaginary Frequencies: 1

C	-1.043347	0.780061	-1.703657
C	-2.066570	-0.327178	-1.474927
C	-2.126180	-0.785315	-0.022956
C	-0.798061	-1.340040	0.513056
C	0.354245	-0.346678	0.424091
C	0.426654	0.350794	-1.491576
C	1.630765	-0.799630	0.838927
C	3.209921	-0.947743	-1.665948
C	2.071561	-1.498878	-2.211476
C	0.805285	-0.855965	-2.095793
C	2.062615	-2.844485	-2.898810
C	4.569623	-1.490681	-1.584683
C	5.593506	-0.472184	-2.039244
C	4.880698	-2.705905	-1.063511
C	6.288002	-3.227425	-0.954295
C	1.366768	1.538324	-1.427333
C	2.601082	0.050219	1.337844
O	3.761437	-0.332740	1.708966
O	-3.119304	-1.777292	0.100999
O	-1.343263	1.844568	-0.835739
H	-1.112258	1.114483	-2.757923
H	-3.055721	0.064860	-1.754189
H	-1.886314	-1.196269	-2.123720
H	-2.378182	0.095960	0.597242
H	0.092964	0.673748	0.735373
H	1.869459	-1.864132	0.792464
H	3.162334	0.096630	-1.367453
H	-0.018505	-1.480646	-2.452646
H	3.077876	-3.180345	-3.145682
H	1.593726	-3.619434	-2.271692
H	1.482758	-2.787782	-3.832589
H	5.413801	-0.174897	-3.085425
H	5.508199	0.440328	-1.425748
H	6.627038	-0.827999	-1.962970
H	6.621949	-3.198087	0.096709
H	6.315888	-4.285551	-1.261528
H	2.156359	1.448934	-0.673112
H	1.860812	1.682412	-2.401152
H	0.804024	2.444725	-1.181669
H	2.354507	1.123487	1.434289
C	-0.965134	-1.763651	1.977203
H	-1.179750	-0.890801	2.615396
H	-1.798838	-2.472304	2.071362
H	-0.055411	-2.246655	2.360392
H	-0.540590	-2.236767	-0.076405
H	7.020011	-2.680718	-1.559338
Al	5.243024	0.717859	2.093621
C	6.828399	-0.371736	1.676643
Cl	4.990764	2.368139	0.613770
H	6.860035	-1.291574	2.289148

H	7.767526	0.175415	1.876626
H	6.854322	-0.683176	0.618389
C	5.013164	1.419329	3.923467
H	5.818692	2.121147	4.206198
H	4.058053	1.960755	4.049459
H	5.023006	0.606348	4.672836
Si	-4.647011	-1.513243	0.766354
Si	-2.166735	3.270697	-1.215049
C	-5.516213	-3.192676	0.617233
C	-4.477357	-0.957774	2.550102
H	-3.853829	-0.051037	2.615739
H	-5.464471	-0.704863	2.970804
H	-4.021321	-1.730289	3.188401
C	-5.525934	-0.164030	-0.194700
H	-6.555572	-0.024772	0.173907
H	-4.998798	0.794094	-0.059881
H	-5.574459	-0.382980	-1.272716
C	-2.579805	4.008628	0.482110
C	-3.695119	2.877847	-2.226069
H	-4.246725	3.803385	-2.459828
H	-3.417802	2.412049	-3.186210
H	-4.383015	2.196173	-1.703219
C	-1.039088	4.380864	-2.219645
H	-0.166006	4.719485	-1.639875
H	-0.667842	3.848677	-3.111211
H	-1.581134	5.273858	-2.571391
C	3.873745	-3.639999	-0.454950
H	3.802056	-4.570250	-1.043206
H	4.210309	-3.931521	0.553778
H	2.870895	-3.211556	-0.367392
C	-1.299796	4.087851	1.328834
H	-1.518527	4.531561	2.316479
H	-0.864571	3.090690	1.499536
H	-0.526411	4.713287	0.853614
C	-3.606354	3.113681	1.193608
H	-4.565626	3.076711	0.652330
H	-3.240281	2.079446	1.301130
H	-3.817166	3.496637	2.208009
C	-3.163757	5.417981	0.297417
H	-2.441352	6.103806	-0.174437
H	-4.075490	5.411402	-0.322857
H	-3.437472	5.852707	1.275282
C	-4.649227	-4.275809	1.277552
H	-4.478269	-4.072426	2.347504
H	-5.142758	-5.261796	1.206426
H	-3.665096	-4.357946	0.790446
C	-6.881242	-3.126627	1.319843
H	-7.532807	-2.348704	0.888319
H	-7.413053	-4.089784	1.219720
H	-6.780703	-2.919865	2.397880
C	-5.717697	-3.534081	-0.867280
H	-4.761264	-3.552648	-1.414143
H	-6.182630	-4.530510	-0.975437
H	-6.378315	-2.808845	-1.369836

TSReexo-anti-strans

SCF Energy: -2801.66132378 H

Num. Imaginary Frequencies: 1

C	-1.086496	0.878022	-1.676957
C	-2.140574	-0.214940	-1.529873
C	-2.203035	-0.800104	-0.123919
C	-0.903086	-1.479272	0.332811
C	0.300018	-0.548389	0.348361
C	0.370951	0.393436	-1.532455
C	1.557583	-1.114608	0.647261
C	3.121979	-0.928428	-1.835002
C	1.954082	-1.456947	-2.346805
C	0.713611	-0.773366	-2.225170
C	1.895012	-2.835363	-2.967635
C	4.417561	-1.568293	-1.655097
C	4.488035	-3.020168	-1.233031
C	5.531479	-0.801824	-1.827848
C	6.921760	-1.344888	-1.695772
C	1.345585	1.528930	-1.312559
C	2.583420	-0.400771	1.245040
O	3.709246	-0.910758	1.556675
O	-3.250409	-1.741975	-0.072823
O	-1.346272	1.870609	-0.714298
H	-1.165252	1.305178	-2.697038
H	-3.119760	0.232043	-1.757396
H	-1.996593	-1.026885	-2.257257
H	-2.396059	0.033237	0.578383
H	0.105212	0.445057	0.772678
H	1.733851	-2.175813	0.450546
H	3.113372	0.128572	-1.591638
H	-0.130156	-1.346161	-2.619469
H	1.617965	-3.606153	-2.229622
H	1.133675	-2.860720	-3.761483
H	2.853713	-3.127085	-3.415746
H	3.508529	-3.381670	-0.896339
H	4.830107	-3.685256	-2.042214
H	5.179818	-3.142789	-0.386967
H	7.503545	-0.713328	-1.003876
H	6.966026	-2.382792	-1.345605
H	2.131331	1.301910	-0.582154
H	1.845755	1.791060	-2.258797
H	0.814567	2.411325	-0.941817
H	2.406886	0.662988	1.490409
C	-1.082912	-2.058530	1.742031
H	-1.251840	-1.254837	2.477315
H	-1.948428	-2.734053	1.764891
H	-0.193890	-2.622804	2.056890
H	-0.695368	-2.314678	-0.357601
H	7.436626	-1.288089	-2.670626
Al	5.147112	-0.118975	2.428368
C	6.670669	-1.337340	2.172313
Cl	5.378571	1.787002	1.309473
H	7.612299	-0.918039	2.570536
H	6.849463	-1.580237	1.111349
H	6.501773	-2.294535	2.699341
C	4.543991	0.263187	4.269254
H	3.635405	0.891920	4.295154
H	4.305639	-0.667911	4.816073
H	5.313492	0.790516	4.861964

Si	-4.745636	-1.464554	0.657082
Si	-2.107328	3.355574	-0.981532
C	-5.703659	-3.079964	0.390173
C	-4.504460	-1.077296	2.476803
H	-3.824200	-0.219203	2.604073
H	-5.464978	-0.803349	2.943401
H	-4.084157	-1.928918	3.033812
C	-5.578582	0.004304	-0.158296
H	-6.591817	0.159065	0.247691
H	-5.001814	0.920624	0.045775
H	-5.661411	-0.116285	-1.249623
C	-2.465498	3.994591	0.767243
C	-3.664847	3.101550	-1.992739
H	-4.177142	4.064295	-2.154593
H	-3.421559	2.690047	-2.986346
H	-4.375434	2.416742	-1.505731
C	-0.942501	4.478174	-1.928744
H	-0.049608	4.742638	-1.340794
H	-0.603835	3.986431	-2.855871
H	-1.448758	5.413442	-2.218515
C	5.455757	0.653300	-2.221290
H	4.903779	0.804918	-3.161410
H	4.957240	1.245144	-1.436156
H	6.461616	1.076100	-2.350270
C	-1.165506	3.996871	1.586586
H	-1.353381	4.379993	2.605472
H	-0.745908	2.983270	1.683854
H	-0.391498	4.638083	1.134047
C	-3.493629	3.076896	1.446606
H	-4.463299	3.086549	0.922945
H	-3.142450	2.032767	1.487283
H	-3.678795	3.404439	2.485150
C	-3.024718	5.423371	0.682618
H	-3.953643	5.470131	0.090322
H	-3.261355	5.805035	1.691806
H	-2.302088	6.122065	0.230224
C	-7.036545	-3.014370	1.152244
H	-7.623002	-3.935137	0.982709
H	-6.885211	-2.919358	2.239924
H	-7.660593	-2.166052	0.825237
C	-4.869976	-4.260331	0.912171
H	-4.644945	-4.163752	1.987118
H	-5.418263	-5.209990	0.776686
H	-3.912556	-4.346781	0.375256
C	-5.977336	-3.271611	-1.109571
H	-5.044299	-3.282653	-1.695753
H	-6.494305	-4.231517	-1.288658
H	-6.620012	-2.473393	-1.515436

TSReexo-syn-scis

SCF Energy: -2801.65723383 H

Num. Imaginary Frequencies: 1

C	-1.309373	1.299478	-1.587267
C	-2.041178	-0.038981	-1.539185
C	-1.847510	-0.790612	-0.225742
C	-0.380180	-1.087851	0.121618
C	0.451605	0.184712	0.221342
C	0.231459	1.186486	-1.536574
C	1.815273	0.074398	0.590813
C	3.199675	0.477270	-2.003865
C	2.152311	-0.111982	-2.672417
C	0.797221	0.215369	-2.368549
C	2.335930	-1.195515	-3.709066
C	4.627292	0.145144	-2.044360
C	5.483814	1.386083	-2.176315
C	5.116924	-1.111441	-1.871839
C	6.583915	-1.444288	-1.885741
C	0.912641	2.522550	-1.314922
C	2.404820	1.070737	1.356171
O	3.572457	1.066695	1.859171
O	-2.565108	-2.001079	-0.287532
O	-1.746131	2.090200	-0.509393
H	-1.549419	1.797833	-2.547466
H	-3.115438	0.160906	-1.665639
H	-1.753590	-0.692994	-2.375029
H	-2.238993	-0.149182	0.587836
H	-0.081746	1.017682	0.699294
H	2.380592	-0.839127	0.395709
H	2.985574	1.379775	-1.434444
H	0.090791	-0.495060	-2.806831
H	3.380057	-1.271919	-4.036811
H	2.023893	-2.182276	-3.332844
H	1.716058	-0.973690	-4.591308
H	5.263327	1.919210	-3.115635
H	5.258413	2.083310	-1.351895
H	6.559747	1.180988	-2.148913
H	6.756005	-2.320457	-2.532596
H	7.231875	-0.632801	-2.235833
H	1.737037	2.482238	-0.593514
H	1.323904	2.901517	-2.263449
H	0.190630	3.249940	-0.927880
H	1.797631	1.966761	1.581423
C	-0.298309	-1.840010	1.454878
H	-0.671259	-1.214495	2.282439
H	-0.909787	-2.751309	1.409571
H	0.736413	-2.126573	1.688941
H	0.039592	-1.740081	-0.662447
H	6.910793	-1.735704	-0.873313
Al	4.979400	0.018183	2.438783
C	5.074944	0.320044	4.387415
Cl	4.367879	-2.085142	2.059424
H	5.299243	1.376493	4.624534
H	5.870265	-0.286555	4.857961
H	4.131598	0.067024	4.904136
C	6.550444	0.521978	1.361945
H	7.441386	-0.072333	1.635054
H	6.384278	0.379974	0.281989
H	6.818363	1.583962	1.513326
Si	-4.036457	-2.269478	0.493771
Si	-2.902254	3.322259	-0.550763
C	-4.541945	-4.014751	-0.049776
C	-3.805622	-2.143951	2.350947
H	-3.387804	-1.161118	2.624227
H	-4.774845	-2.241161	2.867254

H	-3.130286	-2.920156	2.742822
C	-5.273732	-0.963724	-0.037757
H	-6.258774	-1.144047	0.423313
H	-4.934107	0.030089	0.296593
H	-5.407554	-0.933466	-1.130254
C	-3.271695	3.645083	1.280826
C	-4.412768	2.754314	-1.503271
H	-5.171404	3.553922	-1.527280
H	-4.150143	2.522156	-2.548648
H	-4.877328	1.859472	-1.062012
C	-2.168263	4.819612	-1.407411
H	-1.325043	5.249290	-0.844041
H	-1.801656	4.548166	-2.411374
H	-2.927524	5.608071	-1.537143
C	4.263256	-2.311318	-1.573114
H	4.692062	-2.856502	-0.718700
H	3.226785	-2.060987	-1.321838
H	4.256456	-3.005874	-2.430084
C	-1.958574	3.935379	2.024433
H	-1.261265	3.084808	1.964456
H	-1.442065	4.821748	1.621212
H	-2.156590	4.130026	3.093533
C	-3.941014	2.405325	1.894266
H	-4.127038	2.559653	2.972046
H	-4.913036	2.186892	1.423038
H	-3.307637	1.508818	1.793869
C	-4.212546	4.853743	1.405133
H	-4.453766	5.046688	2.465632
H	-3.757905	5.773041	1.001032
H	-5.167306	4.691184	0.878024
C	-3.402108	-4.995957	0.264966
H	-3.680610	-6.021255	-0.038312
H	-2.478441	-4.727171	-0.270881
H	-3.168373	-5.025718	1.341891
C	-5.810631	-4.438642	0.706616
H	-5.645622	-4.483562	1.795529
H	-6.652464	-3.750440	0.522926
H	-6.134576	-5.444045	0.382967
C	-4.817614	-4.019895	-1.561324
H	-5.665116	-3.367089	-1.826912
H	-3.940070	-3.682245	-2.135875
H	-5.068893	-5.039393	-1.905091

TSReexo-syn-strans

SCF Energy: -2801.66020953 H

Num. Imaginary Frequencies: 1

C	-1.207808	1.415294	-1.495209
C	-2.036467	0.136461	-1.569548
C	-1.942787	-0.725574	-0.314472
C	-0.519923	-1.189565	0.033963
C	0.436223	-0.031448	0.267044
C	0.317643	1.199004	-1.458208
C	1.782101	-0.321606	0.572160
C	3.238654	0.400819	-1.925997
C	2.182294	-0.138522	-2.637276
C	0.843342	0.242572	-2.329320
C	2.316646	-1.210861	-3.699037
C	4.647666	0.060475	-1.896964
C	5.149015	-1.215912	-2.531709
C	5.525382	0.900260	-1.263413
C	7.000961	0.592627	-1.248436
C	1.081731	2.452662	-1.092357
C	2.536433	0.532335	1.364234
O	3.725001	0.332369	1.774847
O	-2.765818	-1.856679	-0.483027
O	-1.593276	2.133924	-0.346982
H	-1.411146	2.016444	-2.404277
H	-3.089050	0.426530	-1.704703
H	-1.773093	-0.471072	-2.447391
H	-2.294031	-0.114008	0.538773
H	-0.003036	0.819705	0.802724
H	2.233234	-1.264188	0.250674
H	2.979388	1.235005	-1.290328
H	0.102687	-0.400279	-2.811738
H	3.196723	-1.055193	-4.334650
H	2.389855	-2.219931	-3.263304
H	1.434128	-1.203851	-4.354718
H	4.423013	-2.028196	-2.414657
H	5.349026	-1.090041	-3.608693
H	6.078172	-1.558358	-2.062302
H	7.390991	0.413903	-2.262896
H	7.575875	1.416291	-0.803846
H	1.770382	2.315865	-0.247436
H	1.679243	2.807247	-1.946441
H	0.386787	3.246533	-0.799066
H	2.069546	1.476352	1.699162
C	-0.546817	-2.059771	1.297428
H	-0.870962	-1.473296	2.172726
H	-1.247133	-2.894945	1.163017
H	0.447626	-2.473543	1.515878
H	-0.142382	-1.809405	-0.796382
H	7.209053	-0.316204	-0.659814
Al	4.773023	-1.099138	2.308587
C	3.848314	-1.811017	3.902977
Cl	4.704230	-2.626609	0.699658
H	3.826786	-1.072292	4.725370
H	4.335783	-2.719048	4.301942
H	2.798595	-2.080884	3.685680
C	6.587187	-0.359826	2.521772
H	7.329954	-1.145342	2.750859
H	6.948176	0.169284	1.623091
H	6.622682	0.363850	3.356979
Si	-4.272780	-2.057938	0.247473
Si	-2.669254	3.433354	-0.262774
C	-4.872960	-3.745898	-0.375489
C	-4.088777	-2.016024	2.113902
H	-3.604412	-1.079245	2.434893
H	-5.077892	-2.054294	2.599260
H	-3.488264	-2.856496	2.494816
C	-5.410062	-0.658341	-0.267425
H	-6.424989	-0.804104	0.137636
H	-5.031914	0.295144	0.134906
H	-5.487769	-0.564899	-1.361789
C	-3.089675	3.552334	1.583105

C	-4.174335	3.095185	-1.327063
H	-4.885640	3.934727	-1.257692
H	-3.887969	2.996434	-2.387232
H	-4.704151	2.177360	-1.030862
C	-1.817940	4.980590	-0.892916
H	-0.970166	5.277911	-0.255564
H	-1.436009	4.823421	-1.915312
H	-2.525015	5.825275	-0.933174
C	5.172741	2.187781	-0.575880
H	4.103087	2.362771	-0.419153
H	5.668995	2.224961	0.406079
H	5.569608	3.036098	-1.160466
C	-1.789834	3.584499	2.402158
H	-2.015821	3.675595	3.479562
H	-1.199429	2.665436	2.261516
H	-1.149347	4.439176	2.128966
C	-3.892542	4.837382	1.839899
H	-4.824814	4.868347	1.251644
H	-4.176336	4.907711	2.905073
H	-3.311466	5.741580	1.595929
C	-3.925148	2.332413	2.001010
H	-4.896704	2.301864	1.481735
H	-3.400770	1.385996	1.790437
H	-4.133891	2.359088	3.085361
C	-3.799153	-4.806538	-0.087753
H	-3.581556	-4.892338	0.989605
H	-4.135744	-5.800380	-0.433866
H	-2.854260	-4.574379	-0.603141
C	-5.126613	-3.672822	-1.889167
H	-4.222795	-3.365003	-2.439303
H	-5.432699	-4.660657	-2.278050
H	-5.930321	-2.960443	-2.137224
C	-6.175800	-4.122718	0.347191
H	-6.556793	-5.090706	-0.024768
H	-6.028694	-4.225935	1.434711
H	-6.971066	-3.376024	0.185699

TSSiendo-anti-scis

SCF Energy: -2801.65519990 H

Num. Imaginary Frequencies: 1

C	-1.952013	0.476550	0.813753
C	-2.593156	-0.417020	1.858907
C	-1.992855	-1.815358	1.829697
C	-0.516234	-1.823734	2.242224
C	0.389620	-1.128277	1.221804
C	-0.432034	0.696852	0.958259
C	1.777407	-1.009036	1.539515
C	2.356447	1.809769	0.242011
C	1.446479	1.358839	-0.695703
C	0.177525	0.869924	-0.299396
C	1.765844	1.240456	-2.166574
C	3.696699	2.345071	0.044946
C	4.726906	1.884827	1.056808
C	4.011020	3.300650	-0.872106
C	5.421551	3.813629	-0.971070
C	-0.057341	1.537344	2.167143
C	2.749097	-1.200382	0.577315
O	4.007429	-1.262400	0.816731
O	-2.089650	-2.350573	0.529183
O	-2.569712	1.743695	0.843776
H	-2.114137	-0.015691	-0.160425
H	-2.498227	0.024504	2.862417
H	-3.669681	-0.470815	1.636005
H	-2.534766	-2.451012	2.554788
H	0.193918	-1.538499	0.227628
H	2.103495	-0.849130	2.570209
H	2.072040	1.724233	1.288547
H	-0.403702	0.449398	-1.127872
H	1.249134	2.011363	-2.759376
H	2.841894	1.332199	-2.356442
H	1.432915	0.262390	-2.546259
H	5.583744	1.393025	0.572187
H	5.126382	2.732598	1.637127
H	4.304739	1.153052	1.757314
H	6.168667	3.015350	-0.858147
H	5.590183	4.314389	-1.935530
H	0.838972	1.175930	2.687545
H	0.126503	2.579577	1.863805
H	-0.878541	1.552314	2.895122
H	2.412966	-1.364267	-0.464277
C	-0.317785	-1.449852	3.707887
H	0.711502	-1.648118	4.037600
H	-0.542186	-0.396443	3.919091
H	-0.982924	-2.062620	4.335559
H	-0.204914	-2.878579	2.133404
H	5.618543	4.558243	-0.179074
Al	5.360428	-1.671886	-0.384089
C	5.132461	-0.530178	-1.982485
Cl	7.181644	-1.098243	0.727474
H	4.212962	-0.776724	-2.544329
H	5.973526	-0.660701	-2.688240
H	5.083517	0.544967	-1.735294
C	5.292121	-3.628344	-0.656604
H	4.332229	-3.941004	-1.109028
H	6.091030	-3.987197	-1.330946
H	5.396625	-4.188982	0.289913
Si	-3.251397	-3.425715	-0.047420
Si	-3.420906	2.415433	-0.450859
C	-3.034476	-5.077298	0.810762
H	-2.037782	-5.505720	0.619821
H	-3.148712	-4.963227	1.901561
H	-3.791555	-5.804666	0.475357
C	-2.886263	-3.522376	-1.907386
C	-4.967398	-2.755246	0.302748
H	-5.144562	-2.687502	1.388901
H	-5.114042	-1.752883	-0.129301
H	-5.740094	-3.422290	-0.113742
C	-2.260599	2.702976	-1.897804
H	-2.760638	3.290643	-2.685434
H	-1.355316	3.249373	-1.588544
H	-1.947463	1.749543	-2.352611
C	-4.106989	4.044444	0.236154
C	-4.774622	1.223814	-0.963759
H	-5.501137	1.055422	-0.153317

H	-5.322487	1.598442	-1.843780
H	-4.339086	0.250047	-1.241165
C	3.022245	4.020983	-1.740646
H	1.977186	3.832063	-1.467804
H	3.203591	5.105873	-1.663059
H	3.163001	3.758298	-2.802403
C	-2.940946	4.985274	0.577605
H	-3.320279	5.929361	1.008190
H	-2.257180	4.535650	1.315332
H	-2.348634	5.247539	-0.314223
C	-4.924469	3.761019	1.505787
H	-5.786983	3.105357	1.302239
H	-4.311853	3.277016	2.282274
H	-5.320867	4.702172	1.927215
C	-5.009467	4.704579	-0.818246
H	-4.465732	4.925056	-1.751667
H	-5.874541	4.071577	-1.075537
H	-5.406822	5.662858	-0.438606
C	-3.139505	-2.148711	-2.547900
H	-2.888606	-2.170238	-3.623524
H	-4.195310	-1.844006	-2.464763
H	-2.524546	-1.362297	-2.079996
C	-1.418630	-3.921794	-2.124407
H	-0.727875	-3.187923	-1.679914
H	-1.188620	-4.905770	-1.684296
H	-1.191833	-3.984307	-3.203810
C	-3.805101	-4.569186	-2.556433
H	-3.633674	-5.577975	-2.146656
H	-4.871874	-4.327317	-2.417722
H	-3.621149	-4.622360	-3.644359

TSSiendo-anti-strans

SCF Energy: -2801.66066952 H

Num. Imaginary Frequencies: 1

C	1.966205	-0.584876	0.687655
C	2.455145	0.220413	1.878889
C	1.796465	1.591367	1.941088
C	0.298467	1.520491	2.263518
C	-0.528893	0.928195	1.129891
C	0.463170	-0.905171	0.661599
C	-1.892601	0.635343	1.354776
C	-2.271509	-1.823140	-0.332474
C	-1.274518	-1.373507	-1.191208
C	-0.041599	-0.944899	-0.649871
C	-1.428996	-1.221597	-2.689075
C	-3.639806	-2.219953	-0.561455
C	-4.300485	-2.037925	-1.907338
C	-4.325820	-2.743134	0.505199
C	-5.713584	-3.295580	0.379665
C	0.034274	-1.878720	1.744449
C	-2.856533	0.850002	0.377148
O	-4.114332	0.757222	0.583931
O	1.954324	2.250982	0.705698
O	2.665625	-1.811975	0.638995
H	2.182536	0.020495	-0.208668
H	2.290627	-0.329495	2.818022
H	3.543731	0.344288	1.769925
H	2.269691	2.170438	2.756305
H	-0.306457	1.424743	0.182614
H	-2.242718	0.326844	2.343357
H	-1.950634	-1.954990	0.691415
H	0.612108	-0.460519	-1.383784
H	-1.916358	-2.092007	-3.145633
H	-2.020274	-0.330520	-2.954114
H	-0.442772	-1.110501	-3.161526
H	-4.062593	-2.855660	-2.607182
H	-5.390008	-1.972230	-1.811603
H	-3.976176	-1.100426	-2.372659
H	-5.994701	-3.559102	-0.646715
H	-5.819689	-4.190861	1.011783
H	-0.897380	-1.594921	2.251009
H	-0.111187	-2.884549	1.319637
H	0.813010	-1.962574	2.513658
H	-2.517141	1.197109	-0.616012
C	0.027610	0.969756	3.660428
H	-1.011818	1.150999	3.968079
H	0.219726	-0.108366	3.738946
H	0.675910	1.477324	4.391117
H	-0.029977	2.576687	2.261008
H	-6.439499	-2.550118	0.748260
Al	-5.484729	1.559857	-0.385121
C	-4.806973	1.939659	-2.204202
Cl	-7.104874	0.052359	-0.428502
H	-3.987176	2.681811	-2.195688
H	-5.608682	2.371472	-2.831156
H	-4.433233	1.050561	-2.741966
C	-6.051342	3.110005	0.698789
H	-5.231136	3.842282	0.817786
H	-6.897007	3.652283	0.237794
H	-6.373258	2.820391	1.715343
Si	3.058467	3.469270	0.339829
Si	3.749443	-2.214418	-0.590681
C	2.934039	3.638513	-1.546668
C	4.774108	2.957503	0.897553
H	4.808877	2.843296	1.993656
H	5.088126	2.003239	0.446578
H	5.517971	3.724063	0.624545
C	2.550654	5.036533	1.233046
H	1.556643	5.384240	0.909575
H	2.507930	4.860237	2.320849
H	3.273113	5.850608	1.059722
C	2.865678	-2.205014	-2.246173
H	3.525273	-2.590971	-3.040995
H	1.955058	-2.824184	-2.226731
H	2.577530	-1.179999	-2.531099
C	4.367141	-3.945222	-0.122729
C	5.126571	-0.942168	-0.626792
H	5.693799	-0.918875	0.317015
H	5.833488	-1.141830	-1.448625
H	4.703717	0.061246	-0.796904
C	-3.763297	-2.807785	1.901658
H	-4.567176	-2.990548	2.627793
H	-3.036943	-3.631280	2.005736
H	-3.254981	-1.877414	2.194023

C	4.950093	-3.912525	1.298397
H	4.198959	-3.590871	2.036599
H	5.304329	-4.916518	1.593622
H	5.809841	-3.226758	1.374714
C	3.192455	-4.934586	-0.171838
H	2.770257	-5.021794	-1.186264
H	3.524084	-5.943377	0.133238
H	2.377890	-4.633428	0.506175
C	5.454978	-4.387511	-1.113947
H	5.814382	-5.401710	-0.863631
H	5.082761	-4.421022	-2.151202
H	6.329699	-3.716929	-1.092981
C	3.766939	4.844614	-2.008044
H	4.828195	4.748364	-1.724390
H	3.730556	4.940862	-3.107904
H	3.390805	5.790221	-1.584698
C	3.468275	2.360126	-2.211227
H	4.537982	2.201263	-1.999571
H	2.921662	1.465225	-1.870699
H	3.356547	2.418083	-3.308748
C	1.465269	3.842680	-1.948837
H	1.377984	3.956253	-3.044254
H	0.841320	2.985255	-1.650909
H	1.032046	4.746845	-1.490766

TSSiendo-syn-scis

SCF Energy: -2801.65834898 H

Num. Imaginary Frequencies: 1

C	1.785677	0.525570	-0.740998
C	2.264230	-0.388894	-1.853545
C	1.786171	-1.817310	-1.640493
C	0.266691	-1.950342	-1.782921
C	-0.509487	-1.259534	-0.663067
C	0.257964	0.658216	-0.580148
C	-1.916525	-1.150264	-0.805469
C	-2.431863	1.528512	0.662828
C	-1.277141	1.321683	1.397769
C	-0.087521	0.883805	0.766023
C	-1.185230	1.547255	2.888506
C	-3.762283	1.939212	1.088540
C	-4.418145	2.960934	0.176013
C	-4.456644	1.439324	2.149376
C	-5.836898	1.951801	2.454606
C	-0.400046	1.423468	-1.717868
C	-2.781615	-1.306638	0.265891
O	-4.058721	-1.316971	0.218250
O	2.154442	-2.258726	-0.353216
O	2.303597	1.821901	-0.949450
H	2.170817	0.099159	0.200827
H	1.937769	-0.015696	-2.836175
H	3.364885	-0.364848	-1.852178
H	2.238105	-2.461288	-2.418025
H	-0.166848	-1.604218	0.316045
H	-2.347273	-0.987043	-1.795551
H	-2.319856	1.512946	-0.419371
H	0.700009	0.604785	1.475814
H	-2.012437	2.168483	3.254750
H	-1.196383	0.601718	3.452832
H	-0.240969	2.057804	3.130575
H	-5.403366	2.621909	-0.179980
H	-4.567970	3.919648	0.699357
H	-3.795050	3.171651	-0.704297
H	-5.928890	3.038737	2.320632
H	-6.562888	1.468037	1.777336
H	-1.360995	1.001190	-2.037826
H	-0.577688	2.468015	-1.419287
H	0.260144	1.446268	-2.594707
H	-2.337122	-1.510630	1.254718
C	-0.211593	-1.666884	-3.204729
H	-1.233177	-2.038777	-3.365736
H	-0.200166	-0.597824	-3.454677
H	0.439431	-2.184940	-3.925488
H	0.063071	-3.017342	-1.576967
H	-6.131250	1.700684	3.483859
Al	-5.248858	-1.105699	-1.189471
C	-5.446906	-2.898522	-1.995391
Cl	-7.108504	-0.518185	-0.139799
H	-6.171482	-2.904058	-2.830152
H	-5.788044	-3.658187	-1.269331
H	-4.485438	-3.257805	-2.408142
C	-4.641785	0.342939	-2.396890
H	-4.015025	-0.050641	-3.218795
H	-5.494232	0.860959	-2.872457
H	-4.048604	1.117873	-1.882909
Si	3.449732	-3.265527	0.031194
Si	3.441377	2.550615	0.062160
C	3.526231	-3.198597	1.926363
C	5.016291	-2.614447	-0.768290
H	4.922520	-2.621937	-1.866900
H	5.245780	-1.584231	-0.454357
H	5.879742	-3.249304	-0.509867
C	3.091295	-4.988946	-0.611556
H	2.174156	-5.406129	-0.166390
H	2.955148	-4.969437	-1.705703
H	3.923139	-5.679120	-0.396029
C	2.717995	2.758074	1.781644
H	3.389609	3.357595	2.418234
H	1.738702	3.261324	1.749936
H	2.587907	1.781093	2.274903
C	3.801784	4.219515	-0.762794
C	4.957942	1.452349	0.161018
H	5.435159	1.317133	-0.822279
H	5.707646	1.869455	0.853081
H	4.677330	0.458069	0.544873
C	-4.025825	0.298863	3.017739
H	-4.835993	-0.447377	3.047386
H	-3.115526	-0.200020	2.677135
H	-3.870539	0.640954	4.054902
C	2.524647	5.073947	-0.764826
H	2.707492	6.040108	-1.268510
H	1.700498	4.572897	-1.297226
H	2.177728	5.298442	0.257037
C	4.262945	3.984916	-2.209511
H	5.192149	3.393498	-2.254445

H	3.498466	3.452702	-2.796839
H	4.463036	4.948425	-2.711634
C	4.907535	4.948068	0.017025
H	4.619995	5.138941	1.064086
H	5.850482	4.377091	0.026587
H	5.122997	5.927770	-0.445683
C	2.167909	-3.614633	2.511504
H	1.360008	-2.944644	2.177076
H	1.891039	-4.642144	2.224508
H	2.196634	-3.579303	3.615348
C	3.853280	-1.765070	2.372816
H	3.859558	-1.694349	3.475249
H	4.844798	-1.439070	2.019104
H	3.108601	-1.043517	1.998475
C	4.618167	-4.155799	2.428988
H	4.689470	-4.115574	3.530610
H	4.407215	-5.202067	2.153583
H	5.612147	-3.896888	2.028208

TSSiendo-syn-strans

SCF Energy: -2801.66258719 H

Num. Imaginary Frequencies: 1

C	1.771535	0.559706	-0.691206
C	2.225914	-0.298143	-1.858407
C	1.806996	-1.750816	-1.682811
C	0.288562	-1.941629	-1.774699
C	-0.465687	-1.332467	-0.596831
C	0.251643	0.630469	-0.459445
C	-1.879608	-1.265331	-0.666877
C	-2.416048	1.351729	0.902070
C	-1.259253	1.035465	1.598376
C	-0.063365	0.734853	0.908385
C	-1.196412	0.956223	3.107594
C	-3.762345	1.550517	1.401358
C	-4.256478	0.808056	2.623645
C	-4.601378	2.406531	0.741786
C	-5.997644	2.637384	1.246452
C	-0.478544	1.416037	-1.533667
C	-2.683294	-1.458365	0.447610
O	-3.959827	-1.527738	0.460717
O	2.238887	-2.227433	-0.428273
O	2.239282	1.878630	-0.880005
H	2.216317	0.115307	0.215125
H	1.842427	0.099814	-2.810374
H	3.323917	-0.234635	-1.906583
H	2.253418	-2.347165	-2.500619
H	-0.062316	-1.695011	0.351627
H	-2.366750	-1.109416	-1.631946
H	-2.294471	1.528972	-0.160707
H	0.751011	0.414985	1.568796
H	-1.896857	1.652574	3.585754
H	-1.422687	-0.056886	3.477983
H	-0.184241	1.210758	3.454492
H	-4.321278	1.459593	3.511071
H	-5.258941	0.398279	2.435665
H	-3.610834	-0.040771	2.873498
H	-6.025562	2.795106	2.335337
H	-6.464059	3.503980	0.758312
H	-1.452595	0.988065	-1.805003
H	-0.646672	2.451293	-1.198658
H	0.127207	1.470050	-2.447343
H	-2.187276	-1.638276	1.416613
C	-0.259368	-1.617273	-3.162311
H	-1.269134	-2.029070	-3.299739
H	-0.307325	-0.538679	-3.362056
H	0.383455	-2.071082	-3.932085
H	0.138643	-3.024736	-1.610152
H	-6.618014	1.749493	1.031962
Al	-5.247642	-1.414229	-0.865060
C	-5.422258	-3.237388	-1.604991
Cl	-7.055251	-0.891313	0.311551
H	-6.198610	-3.297434	-2.389568
H	-5.683522	-3.987101	-0.836756
H	-4.475385	-3.570334	-2.070194
C	-4.784162	0.027635	-2.140764
H	-4.274780	-0.373750	-3.036630
H	-5.675604	0.571894	-2.500879
H	-4.108288	0.777947	-1.697246
Si	3.599935	-3.171920	-0.121412
Si	3.325264	2.651477	0.155073
C	3.703842	-3.210817	1.773365
C	5.110299	-2.376773	-0.897988
H	5.008959	-2.338626	-1.995253
H	5.266656	-1.348942	-0.534803
H	6.018757	-2.959504	-0.673220
C	3.338496	-4.875250	-0.857660
H	2.463168	-5.378027	-0.416697
H	3.172556	-4.803043	-1.945424
H	4.219585	-5.518701	-0.701547
C	2.562456	2.832200	1.860447
H	3.189115	3.473262	2.502453
H	1.556370	3.277840	1.810545
H	2.478500	1.853618	2.360059
C	3.636173	4.332619	-0.666324
C	4.882839	1.614773	0.281920
H	5.382317	1.501062	-0.693034
H	5.602839	2.061594	0.986841
H	4.637845	0.609031	0.660468
C	-4.239143	3.215645	-0.467243
H	-3.275431	2.963501	-0.924492
H	-5.027898	3.117317	-1.229542
H	-4.205143	4.283474	-0.189793
C	2.329106	5.140274	-0.685093
H	2.483130	6.112554	-1.186717
H	1.530647	4.609705	-1.228062
H	1.961092	5.351712	0.332167
C	4.123625	4.114655	-2.107015
H	5.073232	3.555759	-2.140112
H	3.385736	3.556162	-2.703812
H	4.296633	5.084668	-2.606719
C	4.705148	5.100866	0.126477
H	4.399166	5.279992	1.170383
H	5.668230	4.564879	0.146310
H	4.889603	6.088313	-0.333212

C	3.974861	-1.792092	2.297777
H	3.994200	-1.784171	3.402325
H	4.946081	-1.403358	1.951189
H	3.193880	-1.084005	1.975077
C	4.844807	-4.145270	2.204965
H	4.933757	-4.162546	3.305910
H	4.674221	-5.183017	1.874846
H	5.819656	-3.821370	1.804381
C	2.375024	-3.720487	2.351997
H	1.533223	-3.068669	2.069657
H	2.138207	-4.740464	2.007949
H	2.420980	-3.749185	3.455446

TSSiexo-anti-scis

SCF Energy: -2801.66129357 H

Num. Imaginary Frequencies: 1

C	-1.603964	0.781588	0.399593
C	-2.164066	0.283425	1.724518
C	-1.824475	-1.184456	1.959304
C	-0.320772	-1.450504	2.119706
C	0.469147	-1.100384	0.870598
C	-0.070295	0.800780	0.293170
C	1.879862	-1.234111	0.889020
C	2.904894	1.552816	0.578349
C	1.934173	1.905444	1.488918
C	0.570929	1.541697	1.295655
C	2.242161	2.636181	2.774060
C	4.357785	1.736298	0.643613
C	4.895134	2.339127	-0.636644
C	5.132873	1.316708	1.677474
C	6.627997	1.478667	1.717226
C	0.380126	0.832479	-1.156205
C	2.609421	-1.541088	-0.246044
O	3.879032	-1.674975	-0.261714
O	-2.295728	-1.945618	0.869561
O	-2.064668	2.085659	0.121668
H	-1.961485	0.077752	-0.371554
H	-1.819621	0.899509	2.569396
H	-3.258905	0.388070	1.686038
H	-2.309254	-1.507891	2.899388
H	-0.013838	-1.469069	-0.042282
H	2.436938	-1.122759	1.819831
H	2.567654	1.222182	-0.401881
H	-0.072283	1.827279	2.134207
H	2.181853	1.967094	3.647627
H	3.245879	3.079914	2.759547
H	1.510935	3.443390	2.932321
H	4.633779	1.692687	-1.491111
H	4.439478	3.324593	-0.827101
H	5.983519	2.465811	-0.636769
H	7.028608	2.166928	0.964649
H	6.933546	1.846245	2.710561
H	0.502331	1.874298	-1.491082
H	1.324474	0.314325	-1.355827
H	-0.381380	0.359279	-1.791794
H	2.061631	-1.696062	-1.193673
C	0.241752	-0.914455	3.431725
H	1.251454	-1.302232	3.627319
H	0.295811	0.183911	3.447094
H	-0.395701	-1.227868	4.272326
H	-0.245207	-2.552986	2.160566
H	7.118223	0.499940	1.582029
Al	5.002008	-1.817393	-1.734738
C	4.927461	-3.688896	-2.355675
Cl	3.960381	-0.493006	-3.195322
H	5.334741	-4.383444	-1.597841
H	5.515659	-3.845803	-3.278066
H	3.895855	-4.019895	-2.573477
C	6.736237	-1.059681	-1.194597
H	7.167501	-1.609512	-0.337904
H	7.479130	-1.111267	-2.011239
H	6.655971	-0.000584	-0.896306
Si	-3.639846	-2.963114	0.875576
Si	-3.312462	2.451331	-0.956493
C	-3.915785	-3.361429	-0.958171
C	-5.101418	-2.067693	1.637564
H	-5.352055	-1.143754	1.093246
H	-5.995117	-2.713173	1.640366
H	-4.890732	-1.797584	2.685588
C	-3.239417	-4.485159	1.892930
H	-4.099582	-5.172156	1.947044
H	-2.383643	-5.038443	1.474616
H	-2.981879	-4.197314	2.925945
C	-4.897622	1.637190	-0.372131
H	-4.778631	0.541754	-0.378917
H	-5.171796	1.945632	0.648882
H	-5.739157	1.878924	-1.041952
C	-2.892322	1.796338	-2.662415
H	-2.781883	0.699830	-2.644342
H	-3.702557	2.028277	-3.373235
H	-1.958736	2.227440	-3.055684
C	-3.403000	4.345055	-0.915937
C	4.605498	0.567520	2.868400
H	4.738660	1.159465	3.789479
H	3.548901	0.296118	2.784871
H	5.187791	-0.359048	3.002976
C	-3.756263	4.807673	0.506085
H	-3.019508	4.450475	1.243142
H	-3.776015	5.911018	0.559872
H	-4.749023	4.446957	0.821360
C	-4.479894	4.830778	-1.898389
H	-5.477563	4.433425	-1.648386
H	-4.552419	5.932938	-1.876997
H	-4.253128	4.539114	-2.936973
C	-2.037904	4.925247	-1.317633
H	-1.753500	4.637540	-2.343027
H	-2.061725	6.029240	-1.281935
H	-1.238316	4.585316	-0.640542
C	-2.630942	-3.957059	-1.553969
H	-2.775256	-4.191509	-2.623810
H	-1.785224	-3.255568	-1.477672
H	-2.336889	-4.892539	-1.050683
C	-4.270464	-2.066926	-1.706268
H	-5.221200	-1.635087	-1.354059

H	-3.487770	-1.300500	-1.583800
H	-4.379334	-2.260659	-2.788325
C	-5.065282	-4.371253	-1.098350
H	-4.838045	-5.325986	-0.596299
H	-6.008448	-3.986156	-0.676580
H	-5.252268	-4.597690	-2.163252

TSSiexo-anti-strans

SCF Energy: -2801.66210305 H

Num. Imaginary Frequencies: 1

C	-1.686296	0.753032	0.466523
C	-2.303348	0.179834	1.734218
C	-1.967318	-1.298212	1.905425
C	-0.478377	-1.570680	2.165292
C	0.403602	-1.170158	0.997368
C	-0.152002	0.778572	0.428755
C	1.809652	-1.247473	1.126666
C	2.800520	1.534691	0.828197
C	1.814913	1.752903	1.768086
C	0.453785	1.453405	1.496172
C	2.128243	2.231930	3.167405
C	4.246846	1.556397	1.018583
C	4.820514	0.937434	2.277391
C	5.041586	2.085694	0.046927
C	6.535473	2.152018	0.172338
C	0.370426	0.826133	-0.992781
C	2.640033	-1.526535	0.054344
O	3.907451	-1.637376	0.150022
O	-2.349796	-1.997566	0.742103
O	-2.140206	2.071467	0.244728
H	-2.010330	0.093899	-0.356616
H	-2.001811	0.748776	2.627112
H	-3.395866	0.283773	1.649687
H	-2.517855	-1.677684	2.786552
H	0.003417	-1.512901	0.036206
H	2.286206	-1.121136	2.101177
H	2.476030	1.384363	-0.196302
H	-0.218702	1.681772	2.328491
H	2.247869	1.390593	3.869999
H	3.047919	2.830877	3.201205
H	1.306037	2.856640	3.547164
H	5.231295	1.687079	2.972457
H	4.057737	0.363598	2.818037
H	5.628570	0.235067	2.027621
H	6.924840	1.730130	1.106001
H	7.001640	1.618344	-0.672759
H	0.500192	1.871344	-1.315586
H	1.330364	0.317897	-1.140540
H	-0.352206	0.351366	-1.671197
H	2.176808	-1.691424	-0.936561
C	-0.019184	-1.094645	3.539285
H	0.968678	-1.501322	3.797470
H	0.041526	0.001409	3.605127
H	-0.724513	-1.437054	4.311709
H	-0.404594	-2.674425	2.163519
H	6.872218	3.200042	0.100367
Al	5.135924	-1.997059	-1.196113
C	4.752460	-3.825759	-1.836634
Cl	4.564500	-0.524795	-2.757460
H	4.910509	-4.573141	-1.037061
H	5.405571	-4.119801	-2.678423
H	3.710683	-3.945264	-2.185838
C	6.908669	-1.630098	-0.422393
H	7.184311	-2.404166	0.317457
H	7.707327	-1.622526	-1.185991
H	6.951155	-0.658065	0.097619
Si	-3.685054	-3.015205	0.590343
Si	-3.301384	2.508969	-0.900350
C	-3.806564	-3.331688	-1.276222
C	-5.207552	-2.155713	1.269400
H	-5.420087	-1.211615	0.743956
H	-6.095045	-2.803244	1.178654
H	-5.079286	-1.925970	2.340164
C	-3.362942	-4.581351	1.567927
H	-4.214253	-5.278674	1.506114
H	-2.463012	-5.105081	1.208489
H	-3.210011	-4.342000	2.633572
C	-4.922878	1.656582	-0.499207
H	-4.807327	0.566046	-0.607849
H	-5.259602	1.865625	0.528231
H	-5.719980	1.971324	-1.192719
C	-2.747368	1.970516	-2.608944
H	-2.621757	0.876190	-2.650045
H	-3.507125	2.238024	-3.361722
H	-1.794269	2.435437	-2.904908
C	-3.405051	4.395785	-0.739307
C	4.522219	2.739398	-1.201863
H	4.614056	3.835417	-1.108305
H	5.129240	2.436720	-2.067690
H	3.471509	2.517977	-1.424193
C	-4.377602	4.950921	-1.791318
H	-5.393127	4.537281	-1.675678
H	-4.459864	6.048746	-1.699078
H	-4.041999	4.734162	-2.818687
C	-3.904680	4.760028	0.667367
H	-3.246697	4.350378	1.450361
H	-3.933749	5.857044	0.795414
H	-4.923404	4.381853	0.852385
C	-2.008761	4.999046	-0.958114
H	-1.618898	4.779979	-1.965699
H	-2.041648	6.098223	-0.851467
H	-1.281733	4.612383	-0.226686
C	-4.046309	-1.998419	-2.001696
H	-5.001707	-1.534629	-1.707064
H	-3.242175	-1.273660	-1.794414
H	-4.080735	-2.152458	-3.095020
C	-2.494979	-3.954520	-1.778728
H	-2.545531	-4.132733	-2.867793
H	-1.633113	-3.295172	-1.589242
H	-2.287498	-4.924329	-1.297939
C	-4.973550	-4.290277	-1.559610
H	-5.938381	-3.879361	-1.219355
H	-5.063036	-4.478849	-2.644369
H	-4.832816	-5.267456	-1.069061

TSSiexo-syn-scis

SCF Energy: -2801.65670183 H

Num. Imaginary Frequencies: 1

C	1.758956	-0.748073	0.263972
C	2.050473	-0.110560	1.616758
C	1.494844	1.306763	1.711881
C	-0.036314	1.388108	1.614538
C	-0.551496	0.884389	0.280603
C	0.273863	-0.995728	-0.041964
C	-1.942251	0.894609	0.012128
C	-2.634304	-2.097891	-0.018946
C	-1.729652	-2.260927	1.004292
C	-0.413481	-1.709683	0.940904
C	-2.053136	-2.990841	2.285820
C	-4.038198	-2.498920	-0.068346
C	-4.455065	-3.172919	-1.362440
C	-4.949378	-2.236500	0.905493
C	-6.374111	-2.699574	0.779218
C	0.021200	-1.197368	-1.522310
C	-2.400571	1.197035	-1.261782
O	-3.605702	1.404604	-1.617631
O	2.042824	2.080277	0.666941
O	2.430275	-1.983006	0.142128
H	2.123317	-0.039293	-0.500434
H	1.677044	-0.729894	2.446394
H	3.143505	-0.061336	1.733978
H	1.776407	1.724188	2.696577
H	0.071113	1.230812	-0.552974
H	-2.670906	0.786683	0.816931
H	-2.251454	-1.728085	-0.968387
H	0.135671	-1.830081	1.879433
H	-2.208730	-2.293826	3.125049
H	-2.956520	-3.605953	2.188093
H	-1.216418	-3.649967	2.562879
H	-5.350518	-2.703815	-1.797482
H	-3.652179	-3.119843	-2.111688
H	-4.678291	-4.241309	-1.206401
H	-6.477058	-3.633893	0.211317
H	-6.821793	-2.847429	1.773836
H	0.058073	-2.269614	-1.770279
H	-0.946406	-0.813969	-1.865577
H	0.797630	-0.685506	-2.108223
H	-1.648064	1.301746	-2.064569
C	-0.752685	0.869390	2.855310
H	-1.832500	1.071554	2.810782
H	-0.618781	-0.212448	2.998292
H	-0.362291	1.373703	3.752099
H	-0.242514	2.473142	1.556208
H	-6.967139	-1.922076	0.267133
Al	-5.172791	2.061781	-0.870682
C	-5.647091	3.620310	-1.985343
Cl	-6.641419	0.442037	-1.223156
H	-5.731890	3.367299	-3.057487
H	-4.893744	4.425862	-1.903563
H	-6.614995	4.059944	-1.682216
C	-4.913288	2.416198	1.055479
H	-4.052007	3.088462	1.227768
H	-5.799469	2.926876	1.475776
H	-4.746500	1.512445	1.665660
Si	3.216532	3.279260	0.834371
Si	3.861987	-2.211801	-0.724787
C	3.700707	3.691823	-0.952888
C	4.658199	2.608216	1.828840
H	5.124971	1.734960	1.346861
H	5.434450	3.379643	1.961305
H	4.326823	2.302820	2.835185
C	2.461329	4.739734	1.733359
H	3.188260	5.559554	1.853033
H	1.583448	5.134434	1.197825
H	2.133464	4.440539	2.742887
C	5.204998	-1.113681	-0.013118
H	4.924779	-0.055181	-0.136670
H	5.373165	-1.301426	1.058882
H	6.160546	-1.262843	-0.542269
C	3.595922	-1.746400	-2.521881
H	3.330089	-0.680627	-2.614985
H	4.521752	-1.900370	-3.100340
H	2.796873	-2.340808	-2.991341
C	4.231845	-4.058907	-0.507552
C	-4.688902	-1.380127	2.108601
H	-5.506206	-0.647155	2.206972
H	-4.695840	-1.981379	3.033463
H	-3.740334	-0.832214	2.056187
C	2.463770	4.184976	-1.719564
H	2.725495	4.410539	-2.768868
H	1.663175	3.428326	-1.731917
H	2.047085	5.106355	-1.281317
C	4.777239	4.788258	-0.954004
H	5.689291	4.472614	-0.421183
H	5.072853	5.037489	-1.988775
H	4.418748	5.718857	-0.484094
C	4.251167	2.428380	-1.632747
H	5.170907	2.066191	-1.145428
H	3.516750	1.606647	-1.617178
H	4.499852	2.633555	-2.689318
C	4.441010	-4.363564	0.983913
H	3.558699	-4.085392	1.582032
H	4.622283	-5.442680	1.136302
H	5.309869	-3.824569	1.395747
C	3.043793	-4.878584	-1.034900
H	2.872012	-4.709781	-2.110585
H	3.229145	-5.959107	-0.898196
H	2.111814	-4.628805	-0.503586
C	5.501119	-4.426577	-1.291534
H	6.380394	-3.858209	-0.945854
H	5.734949	-5.498851	-1.165143
H	5.386743	-4.242891	-2.372448

TSSiexo-syn-strans

SCF Energy: -2801.65930914 H

Num. Imaginary Frequencies: 1

C	1.778091	-0.732525	0.362945
C	2.144945	-0.011202	1.652917

C	1.621846	1.421165	1.671152
C	0.089626	1.532510	1.686516
C	-0.548785	0.962169	0.437305
C	0.281959	-0.993893	0.149708
C	-1.953794	0.910068	0.323494
C	-2.597217	-2.055903	0.329481
C	-1.681758	-2.166151	1.361022
C	-0.367300	-1.639177	1.205781
C	-1.984655	-2.744554	2.727581
C	-4.016998	-2.340049	0.263581
C	-4.796067	-2.653275	1.521742
C	-4.641848	-2.306988	-0.957313
C	-6.105270	-2.617755	-1.113649
C	-0.052284	-1.247460	-1.304703
C	-2.586645	1.036710	-0.906145
O	-3.841979	1.094356	-1.105731
O	2.106155	2.096684	0.531092
O	2.447848	-1.974125	0.280008
H	2.100510	-0.072035	-0.460664
H	1.799025	-0.561393	2.541253
H	3.243019	0.022993	1.715059
H	1.984682	1.907687	2.595934
H	-0.013827	1.243068	-0.477142
H	-2.578698	0.829635	1.215241
H	-2.174305	-1.734362	-0.611097
H	0.224418	-1.692963	2.124277
H	-2.493413	-2.016307	3.379613
H	-2.613660	-3.640931	2.672008
H	-1.050484	-3.032158	3.230495
H	-5.867530	-2.462259	1.395135
H	-4.681880	-3.706995	1.823466
H	-4.462382	-2.029914	2.359490
H	-6.687593	-1.681095	-1.048462
H	-6.301428	-3.040461	-2.110172
H	-0.154943	-2.326890	-1.499072
H	-0.981382	-0.766825	-1.636374
H	0.749723	-0.861522	-1.948736
H	-1.956370	1.119987	-1.809643
C	-0.531495	1.101378	3.010411
H	-1.591689	1.385803	3.069582
H	-0.467792	0.015616	3.171053
H	-0.013857	1.595166	3.846653
H	-0.098571	2.617864	1.581192
H	-6.492493	-3.318025	-0.363412
Al	-5.309543	1.702984	-0.141731
C	-5.051169	3.661599	-0.101359
Cl	-6.965772	1.134828	-1.495964
H	-4.953097	4.098678	-1.111248
H	-4.133025	3.930330	0.454446
H	-5.887206	4.184994	0.397272
C	-5.546881	0.814933	1.604654
H	-4.613701	0.714683	2.187701
H	-6.240016	1.414308	2.224359
H	-5.989222	-0.190532	1.519896
Si	3.237177	3.347103	0.537935
Si	3.832056	-2.238005	-0.651720
C	3.568163	3.672632	-1.301394
C	4.776312	2.788362	1.452225
H	5.253911	1.922163	0.968011
H	5.518252	3.601911	1.505070
H	4.529847	2.503919	2.488666
C	2.493723	4.830100	1.410153
H	3.192016	5.682898	1.418861
H	1.559104	5.157447	0.927997
H	2.263371	4.583398	2.459986
C	5.165767	-1.020251	-0.146093
H	4.800909	0.008707	-0.295546
H	5.456553	-1.130120	0.910357
H	6.068936	-1.140840	-0.766434
C	3.435764	-1.968501	-2.465090
H	3.163967	-0.916796	-2.653306
H	4.315583	-2.192803	-3.090557
H	2.603513	-2.603583	-2.806135
C	4.299374	-4.037499	-0.278924
C	-3.983699	-1.989407	-2.270288
H	-3.007413	-1.498595	-2.204752
H	-3.852134	-2.920534	-2.848360
H	-4.648417	-1.341240	-2.861058
C	4.537512	-4.199319	1.230360
H	3.643888	-3.924994	1.812742
H	4.787118	-5.248149	1.471716
H	5.373782	-3.574392	1.584371
C	3.151170	-4.959997	-0.717171
H	2.970788	-4.904839	-1.803169
H	3.387777	-6.012224	-0.477416
H	2.208520	-4.705076	-0.207080
C	5.579612	-4.406490	-1.044287
H	5.862871	-5.454370	-0.838931
H	5.451848	-4.311263	-2.135151
H	6.433359	-3.774046	-0.749883
C	4.635021	4.769509	-1.442988
H	5.592863	4.475341	-0.983343
H	4.834309	4.978388	-2.509258
H	4.316892	5.717665	-0.978936
C	4.067514	2.379988	-1.965532
H	5.017295	2.031672	-1.528172
H	3.333281	1.564067	-1.867250
H	4.244090	2.542363	-3.043890
C	2.268961	4.126853	-1.984523
H	2.438332	4.292570	-3.063535
H	1.471174	3.373450	-1.885196
H	1.890771	5.072726	-1.564029

Thermal IMDA reaction Model System A

A-strans

SCF Energy: -2019.38279947 H

Num. Imaginary Frequencies: 0

C	0.340008	-0.338591	0.075117

C	-0.574755	-0.591419	1.277067
C	-1.965329	0.008117	1.078918
C	-2.695670	0.281914	2.415806
C	-3.946913	1.056601	2.132674
C	1.495969	-1.329832	0.028701
C	-5.209607	0.701585	2.407154
C	5.160470	-0.828036	0.201767
C	4.045381	-1.595110	0.225414
C	2.752575	-0.890332	0.216515
C	4.109344	-3.098083	0.326292
C	6.571896	-1.280679	0.146754
C	6.943408	-2.297406	-0.918517
C	7.498509	-0.749482	0.976224
C	8.954920	-1.125809	0.927228
C	1.060076	-2.747925	-0.249311
C	-6.327943	1.560311	1.995413
O	-7.495902	1.282869	2.133679
O	-2.728764	-0.870750	0.291093
O	0.748482	1.003231	0.128452
H	-0.257904	-0.521984	-0.840102
H	-0.695120	-1.668975	1.458977
H	-0.074560	-0.153684	2.155023
H	-1.843267	0.983231	0.568136
H	-3.791192	2.012677	1.612969
H	-5.466101	-0.236820	2.906233
H	5.006569	0.257640	0.213699
H	2.843047	0.187421	0.369933
H	3.886109	-3.593357	-0.631997
H	5.102054	-3.433753	0.653710
H	3.378593	-3.467909	1.059694
H	6.076417	-2.557340	-1.539717
H	7.714617	-1.900149	-1.598309
H	7.339087	-3.232861	-0.490800
H	9.227510	-1.735732	1.806375
H	9.234055	-1.692809	0.030166
H	0.034812	-2.765748	-0.650451
H	1.706791	-3.244081	-0.984591
H	1.055266	-3.369231	0.660555
H	-6.021602	2.526507	1.515869
C	-2.915177	-0.983391	3.235797
H	-3.445766	-0.762360	4.173744
H	-3.502616	-1.721023	2.669769
H	-1.956318	-1.450118	3.502508
H	-2.031294	0.965364	2.976008
H	9.587994	-0.223444	0.968063
Si	-3.514506	-0.701638	-1.183632
Si	0.918896	2.055653	-1.176672
C	1.989982	3.486924	-0.532620
C	1.710507	1.160985	-2.621207
H	2.738608	0.839210	-2.394118
H	1.134124	0.258766	-2.884749
H	1.738866	1.803590	-3.516160
C	-0.780499	2.676407	-1.678910
H	-0.713710	3.407566	-2.500950
H	-1.412991	1.849182	-2.034436
H	-1.298959	3.162231	-0.837418
C	-2.297317	-0.970582	-2.591158
H	-1.567033	-0.150471	-2.671529
H	-1.733861	-1.908238	-2.464750
H	-2.826604	-1.024937	-3.556765
C	-4.289849	0.999999	-1.348759
H	-4.592467	1.180037	-2.393368
H	-5.183831	1.103713	-0.715471
H	-3.584748	1.800699	-1.075294
C	-4.832259	-2.069927	-1.188146
C	7.164813	0.254522	2.047839
H	6.086042	0.380720	2.204598
H	7.607090	-0.052533	3.010558
H	7.597480	1.241662	1.807753
C	-5.700214	-1.939812	-2.449608
H	-5.107997	-2.023709	-3.375742
H	-6.460815	-2.740144	-2.478218
H	-6.239829	-0.979183	-2.481775
C	-4.142241	-3.442904	-1.175110
H	-3.476758	-3.554482	-0.303999
H	-4.892314	-4.252370	-1.125886
H	-3.540733	-3.612526	-2.082912
C	-5.720631	-1.939567	0.057425
H	-6.493801	-2.728262	0.064094
H	-5.132935	-2.037965	0.982222
H	-6.245354	-0.971615	0.099140
C	1.240769	4.226391	0.586851
H	0.312951	4.696457	0.222769
H	0.974330	3.548747	1.413713
H	1.869855	5.031533	1.006622
C	2.274130	4.457185	-1.690741
H	1.349005	4.861217	-2.133908
H	2.865920	5.319206	-1.334924
H	2.851512	3.978085	-2.498221
C	3.320220	2.952160	0.018982
H	3.969191	3.788124	0.335520
H	3.163654	2.307039	0.897170
H	3.879516	2.372878	-0.733674

A-lineal

SCF Energy: -2019.38257185 H

Num. Imaginary Frequencies: 0

C	0.521449	0.078930	-0.110998
C	-0.268628	-0.705926	0.943226
C	-1.752819	-0.338151	0.955608
C	-2.391684	-0.439568	2.359120
C	-3.745133	0.203642	2.321943
C	1.870990	-0.570640	-0.372558
C	-4.923401	-0.338810	2.657323
C	4.724451	-1.765438	0.226087
C	4.387732	-0.483014	-0.018559
C	2.993472	-0.008475	0.104532
C	5.380621	0.585372	-0.394135
C	6.063472	-2.396898	0.121458
C	6.085928	-3.520613	-0.889060
C	7.122684	-2.026938	0.875117
C	8.494668	-2.640097	0.757712
C	1.809117	-1.848889	-1.163208
C	-6.164240	0.432146	2.504118

O	-7.272277	0.006824	2.729378
O	-2.452135	-1.162192	0.057178
O	0.630708	1.406476	0.328614
H	-0.043993	0.035713	-1.061907
H	-0.188983	-1.788410	0.767305
H	0.203679	-0.487031	1.913750
H	-1.837034	0.721294	0.649791
H	-3.752251	1.240391	1.955702
H	-5.021785	-1.364959	3.021931
H	3.910559	-2.455840	0.481103
H	2.868999	0.954784	0.610402
H	5.470934	1.334006	0.411682
H	6.378674	0.174181	-0.592598
H	5.042089	1.127032	-1.291905
H	6.021125	-3.123635	-1.916549
H	6.975963	-4.159152	-0.825004
H	5.204657	-4.168943	-0.751259
H	8.731382	-3.243180	1.651510
H	8.626575	-3.276503	-0.125608
H	1.019471	-1.791753	-1.929953
H	2.764811	-2.064333	-1.661225
H	1.569779	-2.717193	-0.526845
H	-6.016629	1.483521	2.142170
C	-2.383304	-1.860798	2.906362
H	-2.818993	-1.903049	3.915600
H	-2.954193	-2.535416	2.251873
H	-1.356045	-2.247202	2.973416
H	-1.768489	0.203396	3.008134
H	9.258341	-1.845917	0.709178
Si	-3.270689	-0.819893	-1.369297
Si	0.208666	2.856831	-0.412632
C	-1.195731	3.609644	0.577961
H	-2.080208	2.952310	0.571083
H	-0.907461	3.766890	1.629606
H	-1.508190	4.580756	0.162045
C	1.733706	3.993609	-0.376194
C	-0.348268	2.541332	-2.175752
H	-0.463706	3.497801	-2.711572
H	0.376937	1.930874	-2.736772
H	-1.324907	2.034684	-2.210273
C	-2.080765	-0.928583	-2.818516
H	-1.362044	-0.095450	-2.834653
H	-1.506674	-1.867846	-2.780481
H	-2.623864	-0.905537	-3.777507
C	-4.021667	0.898423	-1.272452
H	-4.421557	1.204685	-2.252646
H	-4.845530	0.940652	-0.542869
H	-3.274041	1.653117	-0.979094
C	-4.603458	-2.164548	-1.533179
C	7.040725	-0.966872	1.942544
H	6.008886	-0.674829	2.175185
H	7.515066	-1.327913	2.870740
H	7.593535	-0.059173	1.644121
C	-5.489287	-1.856846	-2.751123
H	-4.911758	-1.811963	-3.689110
H	-6.253749	-2.643635	-2.879103
H	-6.025230	-0.899946	-2.640532
C	-5.473592	-2.204463	-0.269428
H	-6.254043	-2.980339	-0.362744
H	-4.875723	-2.435611	0.624207
H	-5.989274	-1.248195	-0.085916
C	-3.925698	-3.531070	-1.721525
H	-3.247963	-3.767933	-0.885573
H	-4.683026	-4.333628	-1.772069
H	-3.339881	-3.578019	-2.653737
C	2.770329	3.484131	-1.389471
H	3.700414	4.076851	-1.325733
H	3.035787	2.431090	-1.209311
H	2.404186	3.563166	-2.425935
C	1.318647	5.425630	-0.750510
H	2.205739	6.081827	-0.799501
H	0.826205	5.475785	-1.736073
H	0.631212	5.864272	-0.009585
C	2.347657	3.998423	1.031894
H	1.633562	4.352997	1.793191
H	2.685003	2.996253	1.337346
H	3.223755	4.670338	1.068186

A-Reendo-s-cis

SCF Energy: -2019.38317991 H

Num. Imaginary Frequencies: 0

C	-0.031019	0.696342	-1.478934
C	-1.184639	-0.318104	-1.434824
C	-1.600788	-0.904491	-0.078925
C	-0.565985	-1.833778	0.601877
C	0.474778	-1.034641	1.345469
C	1.366919	0.091618	-1.471212
C	1.545164	-1.531284	1.984313
C	3.979831	-1.232664	-0.429611
C	3.670516	0.082731	-0.391033
C	2.291690	0.548097	-0.609714
C	4.653047	1.156094	-0.006357
C	5.278106	-1.882332	-0.145195
C	5.150493	-2.947074	0.919860
C	6.423842	-1.586433	-0.802223
C	7.756405	-2.223656	-0.501362
C	1.607947	-0.954163	-2.523507
C	2.463427	-0.622065	2.676012
O	3.465339	-0.950526	3.269776
O	-2.800542	-1.610099	-0.306563
O	-0.214905	1.628463	-0.447176
H	-0.121176	1.193670	-2.468592
H	-2.076731	0.204027	-1.813529
H	-0.998667	-1.149576	-2.131981
H	-1.781979	-0.060179	0.614233
H	0.322326	0.051384	1.380781
H	1.789469	-2.598418	1.993448
H	3.147068	-1.931166	-0.572145
H	1.974446	1.367487	0.043475
H	5.568729	0.739027	0.433024
H	4.938177	1.769759	-0.877686
H	4.197591	1.841234	0.727599
H	4.394377	-3.690739	0.613459
H	6.081443	-3.492083	1.117273

H	4.794030	-2.508686	1.865983
H	8.538880	-1.448757	-0.441928
H	7.781148	-2.788331	0.438130
H	2.674344	-1.036834	-2.774576
H	1.269910	-1.953238	-2.201031
H	1.051885	-0.714925	-3.445209
H	2.161387	0.456679	2.627079
C	-1.235192	-2.825758	1.563536
H	-1.749294	-2.296301	2.380720
H	-1.973101	-3.442266	1.035236
H	-0.483325	-3.488413	2.015510
H	-0.058016	-2.422653	-0.183210
H	8.056329	-2.905460	-1.316351
Si	-0.450572	3.286242	-0.635626
Si	-4.320086	-1.064391	0.172252
C	-0.714440	3.898226	1.139792
C	1.063823	4.041429	-1.441513
H	1.957480	3.959737	-0.803645
H	1.288788	3.529117	-2.391551
H	0.905138	5.107262	-1.673081
C	-1.949793	3.573368	-1.725123
H	-1.772774	3.192367	-2.744430
H	-2.846490	3.070671	-1.330796
H	-2.174876	4.648521	-1.816596
C	-5.533811	-2.284257	-0.624790
C	-4.439958	-1.069818	2.044887
H	-3.641937	-0.452110	2.488733
H	-5.400718	-0.644092	2.377697
H	-4.354197	-2.084181	2.464274
C	-4.571766	0.697357	-0.428552
H	-3.820917	1.364345	0.025979
H	-4.488280	0.783413	-1.522901
H	-5.563496	1.077248	-0.133125
C	6.491112	-0.607742	-1.945624
H	7.068377	-1.042631	-2.779121
H	5.501490	-0.323768	-2.325220
H	7.019779	0.315194	-1.650468
C	-5.124696	-3.718735	-0.256348
H	-5.124902	-3.883216	0.833706
H	-5.829637	-4.446675	-0.696294
H	-4.117822	-3.958483	-0.631112
C	-5.492286	-2.119775	-2.151799
H	-4.474078	-2.261054	-2.548215
H	-6.145682	-2.864980	-2.639638
H	-5.841947	-1.123746	-2.468618
C	-6.955665	-2.005308	-0.113872
H	-7.679894	-2.686274	-0.595375
H	-7.040696	-2.157524	0.974399
H	-7.283265	-0.975751	-0.334989
C	-2.005045	3.284841	1.704869
H	-1.971358	2.183295	1.688612
H	-2.155181	3.595034	2.754183
H	-2.896185	3.604211	1.140532
C	0.476171	3.463302	2.008575
H	0.347290	3.815164	3.047413
H	0.573960	2.366716	2.039567
H	1.431041	3.874146	1.642150
C	-0.824143	5.430559	1.144512
H	-1.663542	5.788476	0.525647
H	-0.994443	5.803532	2.169987
H	0.095540	5.910869	0.772444

Areendo-strans

SCF Energy: -2019.38060054 H

Num. Imaginary Frequencies: 0

C	-0.080867	0.813782	-1.501802
C	-1.164861	-0.275424	-1.452699
C	-1.515191	-0.912036	-0.100831
C	-0.426100	-1.815242	0.523260
C	0.640763	-0.996800	1.205905
C	1.356547	0.313053	-1.573323
C	1.762367	-1.482329	1.759145
C	4.166205	-0.773664	-0.763212
C	3.719048	0.497810	-0.641729
C	2.288672	0.824004	-0.749947
C	4.601951	1.666359	-0.277499
C	5.562939	-1.254605	-0.727367
C	6.617779	-0.447207	-1.462136
C	5.865252	-2.412636	-0.093358
C	7.265534	-2.954001	-0.001798
C	1.622347	-0.681716	-2.667917
C	2.704967	-0.579217	2.425921
O	3.733811	-0.915766	2.967087
O	-2.689274	-1.665211	-0.310834
O	-0.287859	1.700547	-0.434916
H	-0.242245	1.334178	-2.470541
H	-2.096795	0.195218	-1.801335
H	-0.942187	-1.079184	-2.171223
H	-1.710373	-0.093665	0.619283
H	0.460452	0.082971	1.278323
H	2.020671	-2.545431	1.727004
H	3.400651	-1.547694	-0.872355
H	1.939216	1.594458	-0.055151
H	5.563622	1.354555	0.148216
H	4.799440	2.317074	-1.146331
H	4.096540	2.293920	0.474732
H	6.155838	0.321170	-2.096209
H	7.315767	0.064732	-0.779356
H	7.222202	-1.087108	-2.123460
H	8.027178	-2.293269	-0.433783
H	7.533640	-3.128517	1.054075
H	2.676135	-0.666698	-2.978947
H	1.388820	-1.713608	-2.356155
H	0.996293	-0.468867	-3.550419
H	2.394175	0.497554	2.417399
C	-1.023127	-2.812047	1.527179
H	-1.501817	-2.284979	2.367255
H	-1.776401	-3.446728	1.043936
H	-0.235732	-3.457037	1.942648
H	0.045475	-2.400352	-0.286939
H	7.337000	-3.934093	-0.505541
Si	-0.614171	3.348989	-0.561751
Si	-4.219895	-1.204647	0.218422
C	-0.867162	3.887596	1.238878

C	0.836187	4.213345	-1.375956
H	1.745614	4.174650	-0.756722
H	1.073748	3.736673	-2.341353
H	0.606815	5.271910	-1.580218
C	-2.151115	3.592224	-1.608507
H	-1.975773	3.260941	-2.645322
H	-3.010231	3.026108	-1.216874
H	-2.436438	4.655976	-1.653259
C	-5.391225	-2.472339	-0.567528
C	-4.290309	-1.246538	2.093219
H	-3.514946	-0.594706	2.528147
H	-5.263342	-0.877228	2.456475
H	-4.141262	-2.261326	2.493333
C	-4.577591	0.551265	-0.343667
H	-3.850313	1.247748	0.104747
H	-4.526782	0.660740	-1.437919
H	-5.579470	0.874170	-0.016476
C	4.829783	-3.237987	0.631030
H	5.207266	-4.251102	0.835438
H	4.565969	-2.774724	1.596198
H	3.896398	-3.342411	0.056372
C	-2.110628	3.189381	1.810930
H	-3.030082	3.478995	1.276747
H	-2.019208	2.092367	1.757366
H	-2.252393	3.457396	2.872966
C	-1.055471	5.411167	1.298049
H	-1.925797	5.745111	0.709226
H	-1.221968	5.740565	2.338962
H	-0.170248	5.951067	0.924029
C	0.364214	3.487321	2.066585
H	0.242785	3.801261	3.118415
H	0.517133	2.396660	2.061764
H	1.288240	3.957031	1.691817
C	-6.812915	-2.269424	-0.021727
H	-7.513809	-2.979913	-0.495035
H	-6.865409	-2.437472	1.066283
H	-7.195364	-1.254852	-0.223040
C	-4.904540	-3.889467	-0.227291
H	-4.876281	-4.068326	0.860141
H	-5.580621	-4.645760	-0.664717
H	-3.894213	-4.073463	-0.623754
C	-5.391988	-2.287411	-2.092717
H	-4.377440	-2.376021	-2.512974
H	-6.020883	-3.056309	-2.575978
H	-5.794554	-1.305007	-2.388534

TSReendo-scis

SCF Energy: -2019.33887478 H

Num. Imaginary Frequencies: 1

C	-0.050300	0.783975	-1.436162
C	-1.304509	-0.080209	-1.514024
C	-1.583955	-0.859357	-0.238208
C	-0.440839	-1.811072	0.145449
C	0.839827	-1.031085	0.466627
C	1.246494	-0.022715	-1.223360
C	1.958674	-1.751459	0.943546
C	3.927765	-1.049245	-0.540553
C	3.608033	0.304731	-0.402225
C	2.331555	0.755435	-0.761183
C	4.479876	1.263885	0.376699
C	5.169310	-1.763757	-0.187683
C	4.930159	-3.163351	0.337088
C	6.416813	-1.298547	-0.449606
C	7.658768	-2.062747	-0.058177
C	1.458269	-1.071987	-2.314291
C	2.710475	-1.226077	2.065393
O	3.451691	-1.840329	2.813459
O	-2.780247	-1.584444	-0.408140
O	-0.208951	1.727702	-0.409540
H	0.067217	1.292654	-2.415730
H	-2.160971	0.579178	-1.719953
H	-1.248600	-0.791419	-2.351392
H	-1.687324	-0.132601	0.592156
H	0.619348	-0.129106	1.049789
H	2.066215	-2.816438	0.721293
H	3.250375	-1.662341	-1.123961
H	2.067587	1.754324	-0.405120
H	5.210294	0.728844	0.998348
H	5.038386	1.945899	-0.282878
H	3.862956	1.889276	1.039643
H	4.184654	-3.666728	-0.300925
H	5.834340	-3.783436	0.325091
H	4.523123	-3.146436	1.358836
H	8.489068	-1.362440	0.123565
H	7.529878	-2.664368	0.850567
H	2.417286	-0.915950	-2.827654
H	1.437847	-2.109408	-1.950234
H	0.674155	-0.996693	-3.080835
H	2.528906	-0.132574	2.243579
C	-0.851952	-2.664062	1.350269
H	-1.008632	-2.032836	2.240436
H	-1.787242	-3.200169	1.139452
H	-0.077277	-3.402078	1.599240
H	-0.263776	-2.490653	-0.706599
H	7.986911	-2.735832	-0.870206
Si	-0.593145	3.358880	-0.574255
Si	-4.249113	-1.145650	0.287949
C	-0.812218	3.942242	1.216065
C	0.815317	4.236181	-1.449451
H	1.738233	4.245999	-0.848806
H	1.046804	3.739043	-2.406128
H	0.550989	5.280802	-1.680888
C	-2.157847	3.548664	-1.590520
H	-2.007979	3.167459	-2.614151
H	-3.009441	3.007235	-1.150721
H	-2.441085	4.610332	-1.679242
C	-5.501160	-2.370663	-0.439685
C	-4.134994	-1.275541	2.156422
H	-3.326094	-0.633985	2.542391
H	-5.070421	-0.936711	2.631060
H	-3.935461	-2.304572	2.492767
C	-4.644602	0.635936	-0.155776
H	-3.877777	1.307536	0.264034
H	-4.682956	0.796443	-1.244295

H	-5.613736	0.945717	0.268352
C	6.718083	-0.063392	-1.254186
H	7.157468	0.734179	-0.632100
H	7.475167	-0.312244	-2.017285
H	5.842006	0.341783	-1.774679
C	-5.011222	-3.804511	-0.184778
H	-4.909121	-4.021917	0.891099
H	-5.726970	-4.537121	-0.598874
H	-4.033685	-3.986162	-0.657317
C	-5.623014	-2.135954	-1.953102
H	-4.648633	-2.231252	-2.458096
H	-6.307234	-2.875619	-2.406012
H	-6.025735	-1.136283	-2.184018
C	-6.870694	-2.167038	0.226080
H	-7.617078	-2.857180	-0.206098
H	-6.836661	-2.363262	1.310151
H	-7.255065	-1.143426	0.082726
C	-1.067976	5.456847	1.237351
H	-1.974907	5.732591	0.674228
H	-1.209012	5.811280	2.273801
H	-0.223767	6.024126	0.812179
C	-2.004721	3.206014	1.846243
H	-2.952069	3.440104	1.333858
H	-1.865221	2.113222	1.819312
H	-2.126051	3.498202	2.904376
C	0.461830	3.621168	2.013442
H	0.352779	3.946009	3.063329
H	0.675086	2.540834	2.019225
H	1.347113	4.135655	1.605144

TSReendo-strans

SCF Energy: -2019.34380654 H

Num. Imaginary Frequencies: 1

C	-0.068678	0.854650	-1.441062
C	-1.218713	-0.145363	-1.481175
C	-1.415752	-0.898893	-0.175722
C	-0.192799	-1.737853	0.221028
C	1.025239	-0.869089	0.542364
C	1.313918	0.218492	-1.204672
C	2.215333	-1.517576	0.902366
C	4.130381	-0.409485	-0.477569
C	3.626363	0.892453	-0.410550
C	2.286773	1.130831	-0.754264
C	4.400658	2.069721	0.142539
C	5.410010	-0.954779	-0.037868
C	6.228222	-0.239230	1.013572
C	5.806716	-2.148252	-0.563638
C	7.114251	-2.805735	-0.225686
C	1.665784	-0.839764	-2.244456
C	3.033105	-1.057368	2.001869
O	3.878145	-1.710333	2.589414
O	-2.544846	-1.732459	-0.309364
O	-0.338556	1.815743	-0.453001
H	-0.012886	1.334263	-2.441242
H	-2.141453	0.408640	-1.709910
H	-1.085890	-0.878363	-2.290881
H	-1.575734	-0.156281	0.631121
H	0.770744	0.004432	1.154344
H	2.407717	-2.540883	0.561876
H	3.564113	-1.087549	-1.097709
H	1.899571	2.109081	-0.458490
H	4.404169	2.087446	1.243884
H	5.445999	2.074041	-0.192556
H	3.943374	3.010882	-0.195089
H	6.946419	0.473630	0.576172
H	5.582084	0.315335	1.702597
H	6.791864	-0.947433	1.632513
H	7.792058	-2.179115	0.364833
H	6.935806	-3.740498	0.334480
H	2.568399	-0.553976	-2.804579
H	1.840450	-1.840827	-1.823064
H	0.857183	-0.948291	-2.980329
H	2.801763	-0.006336	2.326273
C	-0.525350	-2.612368	1.436034
H	-0.741380	-1.988126	2.318757
H	-1.405744	-3.236696	1.232416
H	0.317296	-3.269075	1.692621
H	0.047284	-2.408382	-0.623195
H	7.641011	-3.092849	-1.150923
Si	-0.905445	3.382301	-0.700404
Si	-4.043305	-1.414953	0.387484
C	-1.200594	4.032520	1.055723
C	0.397111	4.371840	-1.619859
H	1.301342	4.537876	-1.013797
H	0.704680	3.848541	-2.540419
H	0.006738	5.357670	-1.920646
C	-2.474444	3.341844	-1.726920
H	-2.275320	2.928267	-2.729385
H	-3.262625	2.731228	-1.260670
H	-2.874494	4.358951	-1.870471
C	-5.172043	-2.785935	-0.279208
C	-3.902728	-1.461164	2.258198
H	-3.156465	-0.730664	2.610887
H	-4.862824	-1.195316	2.730109
H	-3.603137	-2.452817	2.630757
C	-4.619955	0.298912	-0.118961
H	-3.926547	1.060503	0.273568
H	-4.673630	0.413745	-1.212594
H	-5.616146	0.523169	0.296293
C	4.965476	-2.928445	-1.546680
H	5.413878	-3.910709	-1.751110
H	3.947221	-3.109875	-1.165269
H	4.864383	-2.408492	-2.513239
C	-2.312236	3.207918	1.722897
H	-3.275740	3.312646	1.198011
H	-2.057449	2.136290	1.754399
H	-2.470955	3.540984	2.763920
C	0.094392	3.893165	1.871473
H	-0.056437	4.261937	2.901584
H	0.421319	2.843800	1.936467
H	0.923094	4.475520	1.436553
C	-1.617239	5.509968	0.994751
H	-2.544355	5.656671	0.416235
H	-1.802990	5.901892	2.010481

H	-0.835529	6.141146	0.541122
C	-6.544461	-2.705871	0.406596
H	-7.223168	-3.479366	0.005030
H	-6.473085	-2.869556	1.494224
H	-7.034026	-1.730868	0.245929
C	-4.530421	-4.152290	0.007521
H	-4.385021	-4.323170	1.086835
H	-5.173820	-4.968157	-0.367905
H	-3.548698	-4.246484	-0.481502
C	-5.342362	-2.611939	-1.796186
H	-4.371473	-2.615735	-2.316737
H	-5.948451	-3.435103	-2.215083
H	-5.855669	-1.669561	-2.047743

TSReexo-scis

SCF Energy: -2019.34348086 H

Num. Imaginary Frequencies: 1

C	-0.249875	1.212535	-1.389153
C	-0.950394	-0.142147	-1.394598
C	-0.952739	-0.839165	-0.038257
C	0.450452	-1.110715	0.526835
C	1.220764	0.183086	0.762867
C	1.253565	1.137085	-1.064219
C	2.515379	0.112783	1.286708
C	4.135686	0.212365	-0.652332
C	3.311254	-0.245682	-1.675140
C	1.987992	0.219039	-1.833878
C	3.723677	-1.379565	-2.590152
C	5.420906	-0.344708	-0.196217
C	6.464329	0.730225	0.009976
C	5.617112	-1.646406	0.129968
C	6.931784	-2.179870	0.641060
C	1.798777	2.509585	-0.716766
C	3.072826	1.211222	2.055629
O	4.152327	1.209296	2.617245
O	-1.657320	-2.053379	-0.167078
O	-0.885634	2.043100	-0.446435
H	-0.335889	1.654588	-2.403352
H	-1.995073	0.014361	-1.703810
H	-0.506171	-0.820891	-2.137475
H	-1.462290	-0.171039	0.684842
H	0.606003	1.013212	1.135135
H	3.043868	-0.836594	1.367941
H	3.980973	1.229446	-0.308196
H	1.401882	-0.393155	-2.527706
H	4.796761	-1.596384	-2.514986
H	3.175008	-2.311134	-2.379149
H	3.506374	-1.107649	-3.634717
H	6.559690	1.368763	-0.882909
H	6.148744	1.376180	0.845835
H	7.459104	0.339290	0.253678
H	6.938097	-2.195858	1.745048
H	7.078009	-3.219809	0.308791
H	1.317972	2.927526	0.176468
H	2.882659	2.544687	-0.581365
H	1.566580	3.187317	-1.555656
H	2.412653	2.116004	2.120593
C	0.350475	-1.915199	1.826287
H	-0.174493	-1.339631	2.606370
H	-0.200974	-2.850157	1.658697
H	1.346784	-2.168722	2.215060
H	1.003704	-1.719573	-0.210230
H	7.803502	-1.600834	0.311853
Si	-3.223729	-2.307644	0.393403
Si	-1.980775	3.284201	-0.747059
C	-3.679578	-4.032772	-0.250441
C	-3.256722	-2.220968	2.267687
H	-2.883575	-1.245146	2.618869
H	-4.286233	-2.328760	2.646756
H	-2.638591	-3.003482	2.734050
C	-4.356654	-0.968366	-0.276761
H	-5.396126	-1.124455	0.055223
H	-4.040205	0.016521	0.103733
H	-4.353489	-0.929215	-1.377004
C	-2.588420	3.762144	0.984912
C	-3.366657	2.662002	-1.847786
H	-4.108548	3.456655	-2.030457
H	-2.976040	2.352876	-2.831430
H	-3.894655	1.801252	-1.409667
C	-1.106819	4.699794	-1.612906
H	-0.300267	5.127586	-0.997670
H	-0.662559	4.360994	-2.563311
H	-1.813676	5.509413	-1.857754
C	4.535415	-2.691972	0.112090
H	4.720940	-3.439084	-0.678653
H	4.539140	-3.243518	1.067536
H	3.530214	-2.283951	-0.042963
C	-1.378952	4.089004	1.874651
H	-1.711102	4.379240	2.887232
H	-0.708754	3.221677	1.980418
H	-0.783546	4.926198	1.475271
C	-3.361271	2.582194	1.594369
H	-4.271086	2.343602	1.019897
H	-2.740466	1.672678	1.639898
H	-3.679465	2.817287	2.625521
C	-3.507983	4.989130	0.891393
H	-2.980876	5.870555	0.491265
H	-4.385285	4.802855	0.249948
H	-3.889274	5.264090	1.890788
C	-2.611686	-5.039990	0.203428
H	-2.537903	-5.098261	1.301775
H	-2.856407	-6.053787	-0.161028
H	-1.616597	-4.774583	-0.185476
C	-5.050213	-4.447463	0.305929
H	-5.847174	-3.742172	0.017079
H	-5.340299	-5.440566	-0.081051
H	-5.046298	-4.516219	1.405992
C	-3.732713	-4.004923	-1.785636
H	-2.777370	-3.667956	-2.218320
H	-3.942474	-5.013505	-2.184571
H	-4.525683	-3.336385	-2.158619

TSReexo-strans

SCF Energy: -2019.34589108 H

Num. Imaginary Frequencies: 1

C	-0.055640	1.044495	-1.419882
C	-1.050859	-0.110390	-1.432233
C	-1.226349	-0.775487	-0.072122
C	0.061683	-1.383690	0.502832
C	1.161488	-0.352519	0.735466
C	1.392426	0.621154	-1.118803
C	2.403298	-0.816515	1.182129
C	4.045807	-0.675412	-0.769913
C	3.128781	-1.112421	-1.725376
C	1.892418	-0.457746	-1.868411
C	3.332463	-2.376594	-2.532575
C	5.236594	-1.339240	-0.256957
C	5.247250	-2.844862	-0.098378
C	6.257320	-0.566916	0.204668
C	7.496849	-1.141221	0.825180
C	2.280484	1.806514	-0.772944
C	3.255596	-0.050770	2.064114
O	4.265409	-0.462539	2.608774
O	-2.201943	-1.786525	-0.197742
O	-0.477406	1.986015	-0.458970
H	-0.049165	1.511406	-2.426736
H	-2.028737	0.281094	-1.751219
H	-0.771011	-0.877383	-2.169023
H	-1.562824	0.000924	0.642822
H	0.817221	0.597200	1.165932
H	2.649731	-1.878021	1.097312
H	3.964759	0.364116	-0.482984
H	1.176677	-0.982266	-2.509176
H	2.881454	-3.259005	-2.049134
H	2.856409	-2.273571	-3.519137
H	4.395783	-2.593560	-2.700473
H	4.251905	-3.272163	-0.269107
H	5.945154	-3.347343	-0.787832
H	5.533100	-3.120389	0.927428
H	7.561153	-0.825714	1.880838
H	7.543391	-2.236194	0.794870
H	2.761176	1.733196	0.212072
H	3.076739	1.934007	-1.522015
H	1.682572	2.724381	-0.750681
H	2.912161	1.003170	2.247510
C	-0.247584	-2.110773	1.816439
H	-0.603906	-1.401293	2.581647
H	-1.024439	-2.872145	1.664559
H	0.648631	-2.605637	2.216040
H	0.433832	-2.129483	-0.221854
H	8.396819	-0.748092	0.323340
Si	-3.785059	-1.676039	0.358495
Si	-1.332496	3.410669	-0.733632
C	-4.578155	-3.321484	-0.154044
C	-3.801583	-1.434154	2.219724
H	-3.221949	-0.540487	2.503098
H	-4.830802	-1.279810	2.583198
H	-3.375606	-2.294393	2.758490
C	-4.631129	-0.198624	-0.432130
H	-5.693158	-0.144491	-0.141722
H	-4.153976	0.732530	-0.086989
H	-4.579705	-0.226088	-1.531538
C	-1.910765	3.932953	0.995743
C	-2.763174	3.095222	-1.905253
H	-3.336106	4.021926	-2.073508
H	-2.396985	2.759315	-2.889438
H	-3.460459	2.332592	-1.527227
C	-0.194292	4.684279	-1.510654
H	0.618688	4.987972	-0.832616
H	0.266041	4.286748	-2.430292
H	-0.753721	5.590892	-1.793521
C	6.223930	0.941107	0.139932
H	6.100290	1.315959	-0.888029
H	5.393600	1.346801	0.741772
H	7.151288	1.373477	0.541218
C	-0.703756	3.963789	1.946092
H	-1.017531	4.272425	2.959095
H	-0.228848	2.974040	2.029452
H	0.067862	4.676955	1.612989
C	-2.942112	2.920197	1.516394
H	-3.856820	2.910491	0.901675
H	-2.534302	1.896369	1.532589
H	-3.246123	3.170211	2.548279
C	-2.549259	5.328678	0.926407
H	-3.411984	5.357849	0.240221
H	-2.916074	5.635952	1.921816
H	-1.830485	6.095322	0.594172
C	-5.994374	-3.417636	0.433511
H	-6.480295	-4.358653	0.119542
H	-5.985863	-3.408460	1.535659
H	-6.641979	-2.591059	0.096712
C	-3.720690	-4.482153	0.373411
H	-3.641158	-4.471583	1.472910
H	-4.165408	-5.452495	0.088413
H	-2.699768	-4.446919	-0.036696
C	-4.649286	-3.396404	-1.686936
H	-3.653655	-3.285854	-2.145272
H	-5.058138	-4.370894	-2.008940
H	-5.302444	-2.614550	-2.107684

TSSiendo-scis

SCF Energy: -2019.33350740 H

Num. Imaginary Frequencies: 1

C	-0.650039	0.761614	0.659052
C	-1.516121	0.162148	1.758306
C	-1.533363	-1.359094	1.719041
C	-0.150016	-1.985616	1.943578
C	0.829355	-1.611600	0.819916
C	0.838130	0.382552	0.721324
C	2.137225	-2.156091	0.834701
C	3.692645	-0.146881	0.144488
C	2.802577	0.216354	-0.868788
C	1.469935	0.496161	-0.541623
C	3.137614	0.066539	-2.335394
C	5.107535	-0.546547	0.067564
C	5.483512	-1.606236	1.081892
C	6.036311	0.070101	-0.706823
C	7.472852	-0.390574	-0.756143

C	1.520804	0.902863	1.985743
C	2.639184	-2.801134	-0.358625
O	3.563238	-3.594357	-0.441222
O	-2.021201	-1.784263	0.464926
O	-0.750065	2.168535	0.714857
H	-1.040226	0.379538	-0.301462
H	-1.183548	0.519876	2.744465
H	-2.541681	0.537404	1.620304
H	-2.190620	-1.722598	2.533132
H	0.321837	-1.766872	-0.137473
H	2.644957	-2.383628	1.775710
H	3.360358	0.000101	1.164869
H	0.788017	0.573847	-1.396201
H	3.351255	1.034846	-2.813614
H	4.014095	-0.579021	-2.480938
H	2.292202	-0.381982	-2.878375
H	5.087998	-2.593001	0.799311
H	6.566704	-1.686733	1.232505
H	5.039465	-1.345996	2.057131
H	7.587235	-1.470802	-0.599847
H	7.911588	-0.148934	-1.736926
H	2.081977	0.138146	2.537527
H	2.216702	1.717908	1.737739
H	0.777832	1.322505	2.676989
H	2.054014	-2.540797	-1.280992
C	0.329208	-1.823917	3.383394
H	1.318168	-2.280313	3.533398
H	0.390680	-0.776205	3.704614
H	-0.368345	-2.334422	4.065448
H	-0.312607	-3.065682	1.784429
H	8.085945	0.131342	0.000083
Si	-3.559919	-2.380147	0.141286
Si	-1.586295	3.103195	-0.407836
C	-3.782184	-4.011109	1.039892
H	-2.974358	-4.718265	0.794386
H	-3.773530	-3.860068	2.131955
H	-4.742919	-4.487479	0.785239
C	-3.587550	-2.581785	-1.745157
C	-4.852888	-1.159107	0.742173
H	-4.743587	-0.977212	1.824197
H	-4.779533	-0.187169	0.229558
H	-5.870654	-1.551065	0.582532
C	-0.786448	2.945295	-2.098760
H	-1.238927	3.650506	-2.815301
H	0.295406	3.146080	-2.059143
H	-0.929247	1.933117	-2.511104
C	-1.466424	4.868707	0.273710
C	-3.356638	2.488669	-0.523640
H	-3.896587	2.584849	0.431200
H	-3.922853	3.036991	-1.294051
H	-3.362154	1.424934	-0.813224
C	5.797411	1.335006	-1.485378
H	4.849701	1.827318	-1.236616
H	6.611467	2.046171	-1.264160
H	5.828277	1.159521	-2.573651
C	0.006867	5.305496	0.280887
H	0.109539	6.314485	0.718830
H	0.631123	4.618957	0.874503
H	0.428734	5.347562	-0.736471
C	-2.014442	4.896792	1.708672
H	-3.078186	4.610364	1.749616
H	-1.457948	4.211707	2.366584
H	-1.933898	5.913260	2.133689
C	-2.284867	5.823693	-0.608464
H	-1.928123	5.835628	-1.651568
H	-3.354799	5.558436	-0.623279
H	-2.211540	6.858481	-0.229044
C	-3.213655	-1.245385	-2.404647
H	-3.216874	-1.342002	-3.504979
H	-3.926071	-0.444289	-2.147822
H	-2.207931	-0.913313	-2.102127
C	-2.569969	-3.656010	-2.159354
H	-1.551830	-3.407914	-1.819649
H	-2.827093	-4.646546	-1.750631
H	-2.538583	-3.755312	-3.259014
C	-4.994078	-3.002181	-2.198704
H	-5.313097	-3.951232	-1.736966
H	-5.752221	-2.239685	-1.956106
H	-5.019362	-3.149676	-3.293002

TSSiendo-strans

SCF Energy: -2019.33972686 H

Num. Imaginary Frequencies: 1

C	0.717011	0.733533	-0.578356
C	1.366946	0.071774	-1.783514
C	1.177887	-1.437415	-1.780120
C	-0.287929	-1.862437	-1.933418
C	-1.149597	-1.455430	-0.731959
C	-0.803968	0.555217	-0.465023
C	-2.535464	-1.695605	-0.767624
C	-3.617668	0.398059	0.532691
C	-2.537681	0.578463	1.403125
C	-1.241616	0.649581	0.876190
C	-2.657480	0.589484	2.912145
C	-5.016308	0.108945	0.803869
C	-5.440613	-0.442590	2.145743
C	-5.906966	0.270899	-0.217342
C	-7.381256	0.025652	-0.073382
C	-1.564178	1.253109	-1.587661
C	-3.232561	-2.345313	0.314242
O	-4.351932	-2.829770	0.256607
O	1.679282	-1.968735	-0.573124
O	0.999103	2.118295	-0.613176
H	1.162877	0.267654	0.318077
H	0.979407	0.507226	-2.717256
H	2.442943	0.303038	-1.752672
H	1.726889	-1.859412	-2.644692
H	-0.666319	-1.783996	0.193585
H	-3.089172	-1.634589	-1.709609
H	-3.415948	0.648641	-0.497644
H	-0.442327	0.600652	1.624573
H	-3.532697	1.156896	3.253851
H	-2.732574	-0.424837	3.334433
H	-1.767680	1.059831	3.354970

H	-5.659193	0.349442	2.880312
H	-6.331555	-1.074709	2.056421
H	-4.656959	-1.082275	2.567522
H	-7.717036	-0.097998	0.962328
H	-7.947291	0.862332	-0.514456
H	-2.333731	0.628225	-2.059954
H	-2.055816	2.163370	-1.211274
H	-0.872065	1.572925	-2.378081
H	-2.632243	-2.418396	1.262055
C	-0.838242	-1.532262	-3.318246
H	-1.834584	-1.971074	-3.469083
H	-0.914932	-0.453486	-3.505863
H	-0.179067	-1.955293	-4.092420
H	-0.259289	-2.964294	-1.858212
H	-7.668336	-0.879364	-0.637422
Si	3.133086	-2.787857	-0.370523
Si	2.062501	2.895449	0.433280
C	3.283260	-2.994877	1.509660
C	4.539158	-1.770937	-1.086740
H	4.386637	-1.600185	-2.165321
H	4.631573	-0.786805	-0.601358
H	5.502557	-2.295087	-0.976376
C	3.038601	-4.431593	-1.268106
H	2.186859	-5.035165	-0.917261
H	2.911728	-4.275140	-2.352138
H	3.957984	-5.023544	-1.130439
C	1.422713	2.796486	2.195551
H	2.032920	3.418023	2.871511
H	0.378079	3.136810	2.268301
H	1.471588	1.763604	2.577169
C	2.118384	4.682055	-0.201083
C	3.735706	2.047189	0.355286
H	4.185814	2.101048	-0.648243
H	4.445111	2.490398	1.072992
H	3.625636	0.983726	0.623834
C	-5.489428	0.701180	-1.602924
H	-6.338295	0.656554	-2.299132
H	-5.104405	1.733549	-1.621718
H	-4.698916	0.049274	-2.009404
C	2.514368	4.680818	-1.685426
H	1.803897	4.098213	-2.291747
H	2.531773	5.711696	-2.082175
H	3.518402	4.254179	-1.844096
C	0.726681	5.314364	-0.044529
H	0.420368	5.379737	1.012187
H	0.719980	6.341782	-0.450574
H	-0.043451	4.738207	-0.581511
C	3.147220	5.489147	0.605156
H	3.178692	6.535865	0.253632
H	2.905161	5.516353	1.680400
H	4.166027	5.080976	0.501343
C	4.596212	-3.716877	1.848751
H	5.479687	-3.151716	1.509053
H	4.694576	-3.848181	2.941009
H	4.645758	-4.720862	1.396184
C	3.271718	-1.609415	2.173914
H	4.130643	-0.993764	1.860659
H	2.351066	-1.054135	1.933013
H	3.324854	-1.705553	3.273003
C	2.093323	-3.816500	2.028876
H	2.145722	-3.921135	3.127266
H	1.131558	-3.338260	1.785328
H	2.077853	-4.833830	1.605597

TSSiexo-scis

SCF Energy: -2019.33972685 H

Num. Imaginary Frequencies: 1

C	0.717018	0.733529	-0.578353
C	1.366950	0.071775	-1.783516
C	1.177888	-1.437414	-1.780131
C	-0.287929	-1.862431	-1.933438
C	-1.149597	-1.455435	-0.731976
C	-0.803961	0.555213	-0.465020
C	-2.535465	-1.695603	-0.767644
C	-3.617659	0.398043	0.532693
C	-2.537672	0.578437	1.403129
C	-1.241607	0.649562	0.876195
C	-2.657473	0.589441	2.912149
C	-5.016301	0.108932	0.803873
C	-5.440602	-0.442639	2.145733
C	-5.906964	0.270929	-0.217326
C	-7.381255	0.025695	-0.073362
C	-1.564172	1.253117	-1.587651
C	-3.232561	-2.345332	0.314212
O	-4.351931	-2.829787	0.256570
O	1.679276	-1.968743	-0.573137
O	0.999109	2.118291	-0.613169
H	1.162885	0.267646	0.318077
H	0.979411	0.507234	-2.717255
H	2.442948	0.303038	-1.752673
H	1.726892	-1.859406	-2.644704
H	-0.666322	-1.784014	0.193564
H	-3.089175	-1.634572	-1.709627
H	-3.415942	0.648641	-0.497638
H	-0.442317	0.600624	1.624576
H	-3.532699	1.156836	3.253859
H	-2.732552	-0.424886	3.334426
H	-1.767680	1.059796	3.354979
H	-5.659205	0.349374	2.880316
H	-6.331528	-1.074777	2.056393
H	-4.656937	-1.082314	2.567507
H	-7.717023	-0.098016	0.962344
H	-7.947283	0.862413	-0.514375
H	-2.333725	0.628237	-2.059951
H	-2.055811	2.163373	-1.211254
H	-0.872059	1.572942	-2.378067
H	-2.632240	-2.418432	1.262022
C	-0.838239	-1.532240	-3.318263
H	-1.834584	-1.971044	-3.469104
H	-0.914921	-0.453462	-3.505871
H	-0.179066	-1.955270	-4.092441
H	-0.259291	-2.964289	-1.858243
H	-7.668358	-0.879279	-0.637456
Si	3.133080	-2.787860	-0.370525

Si	2.062507	2.895447	0.433285
C	3.283246	-2.994867	1.509661
C	4.539154	-1.770944	-1.086742
H	4.386651	-1.600219	-2.165330
H	4.631551	-0.786799	-0.601381
H	5.502555	-2.295081	-0.976347
C	3.038605	-4.431604	-1.268095
H	2.186897	-5.035201	-0.917212
H	2.911681	-4.275157	-2.352122
H	3.958013	-5.023525	-1.130465
C	1.422724	2.796476	2.195557
H	2.032932	3.418009	2.871520
H	0.378090	3.136799	2.268312
H	1.471600	1.763592	2.577170
C	2.118379	4.682054	-0.201076
C	3.735717	2.047197	0.355285
H	4.185826	2.101065	-0.648244
H	4.445119	2.490405	1.072994
H	3.625653	0.983731	0.623827
C	-5.489431	0.701254	-1.602897
H	-4.698936	0.049346	-2.009408
H	-6.338306	0.656670	-2.299097
H	-5.104387	1.733615	-1.621656
C	0.726671	5.314354	-0.044524
H	0.719964	6.341773	-0.450564
H	-0.043455	4.738193	-0.581511
H	0.420354	5.379720	1.012192
C	2.514366	4.680822	-1.685417
H	3.518405	4.254195	-1.844086
H	1.803902	4.098208	-2.291740
H	2.531759	5.711700	-2.082167
C	3.147208	5.489153	0.605166
H	2.905144	5.516360	1.680409
H	4.166017	5.080987	0.501358
H	3.178676	6.535870	0.253640
C	3.271759	-1.609398	2.173901
H	3.324879	-1.705526	3.272992
H	4.130715	-0.993788	1.860648
H	2.351134	-1.054079	1.932985
C	4.596170	-3.716915	1.848758
H	4.694536	-3.848201	2.941019
H	4.645669	-4.720912	1.396211
H	5.479667	-3.151800	1.509042
C	2.093277	-3.816436	2.028888
H	1.131532	-3.338156	1.785343
H	2.077760	-4.833767	1.605615
H	2.145678	-3.921068	3.127278

TSSiexo-strans

SCF Energy: -2019.34515425 H

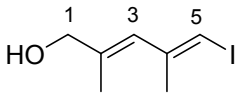
Num. Imaginary Frequencies: 1

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

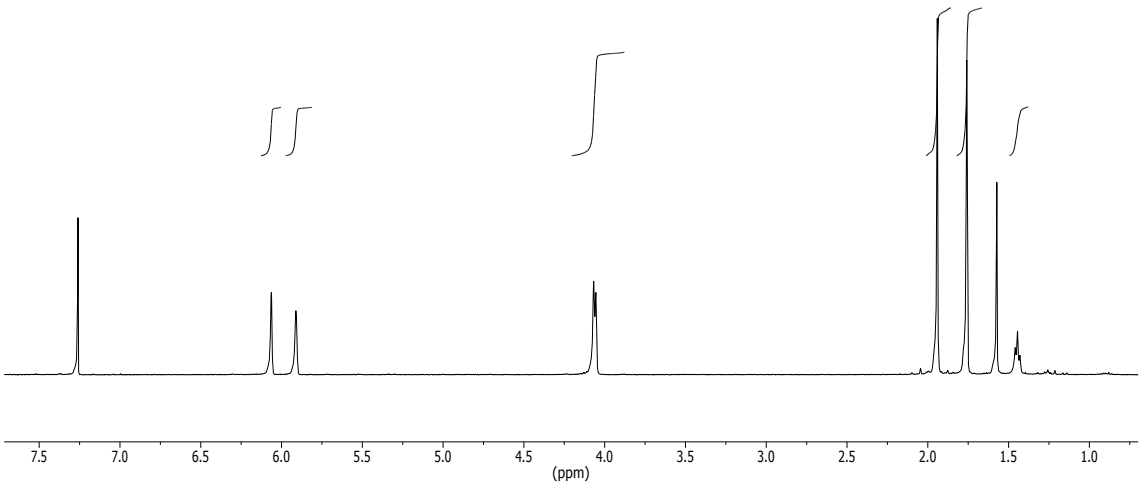
H	-2.876685	3.074122	-2.918272
H	-1.110163	3.002702	-2.690450
C	-2.341035	4.607940	0.014561
C	5.392712	0.546905	-2.443953
H	5.946687	1.439877	-2.781523
H	5.569497	-0.240405	-3.193680
H	4.326028	0.799106	-2.463234
C	-3.534620	5.322775	-0.636634
H	-4.498149	4.884134	-0.328764
H	-3.554056	6.387781	-0.344039
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

4. NMR SPECTRA

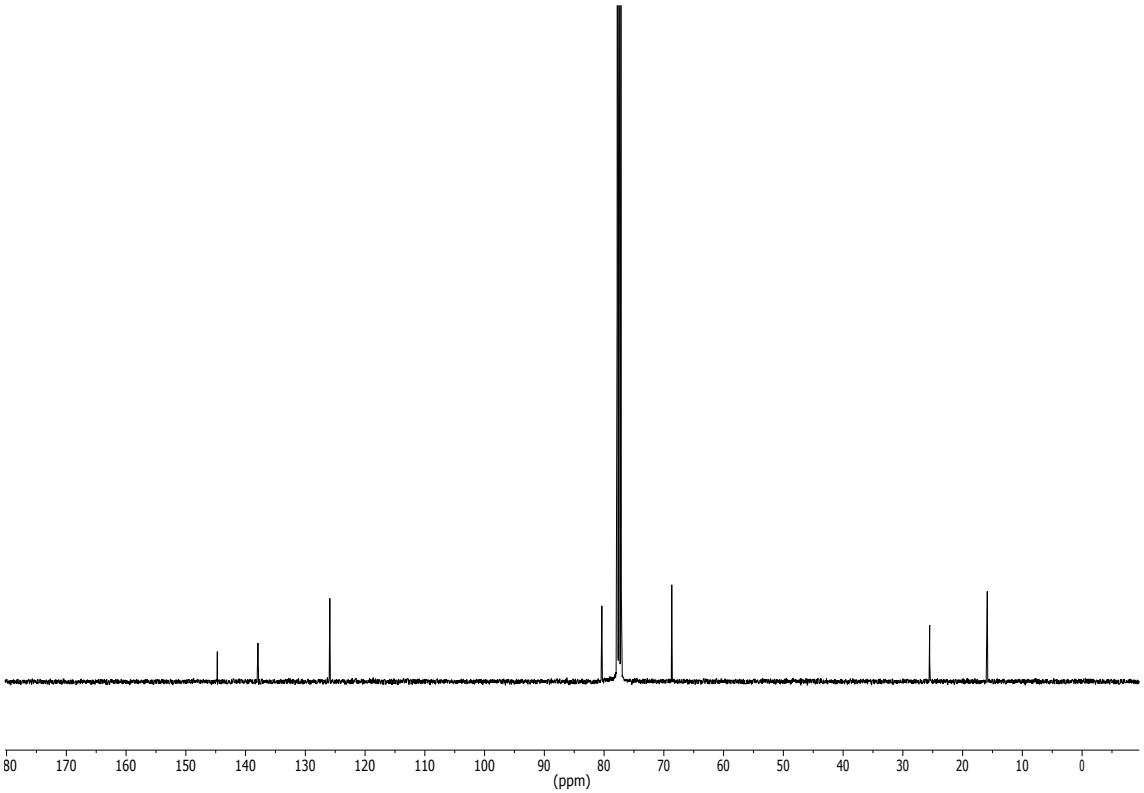
^{1}H-NMR (400.13 MHz, $CDCl_3$)



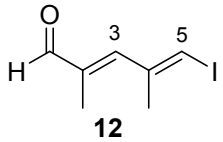
10-2



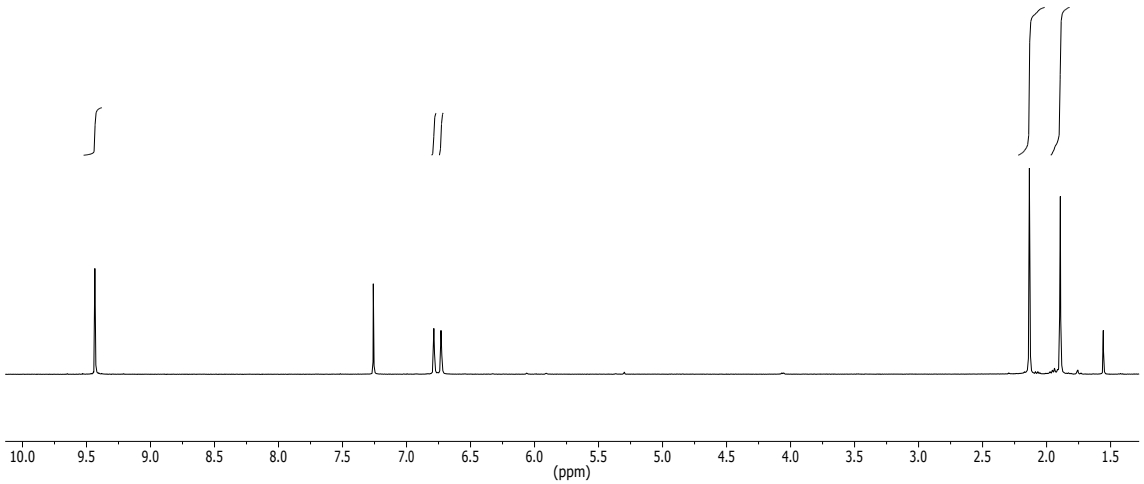
^{13}C-NMR(100.16 MHz, $CDCl_3$)



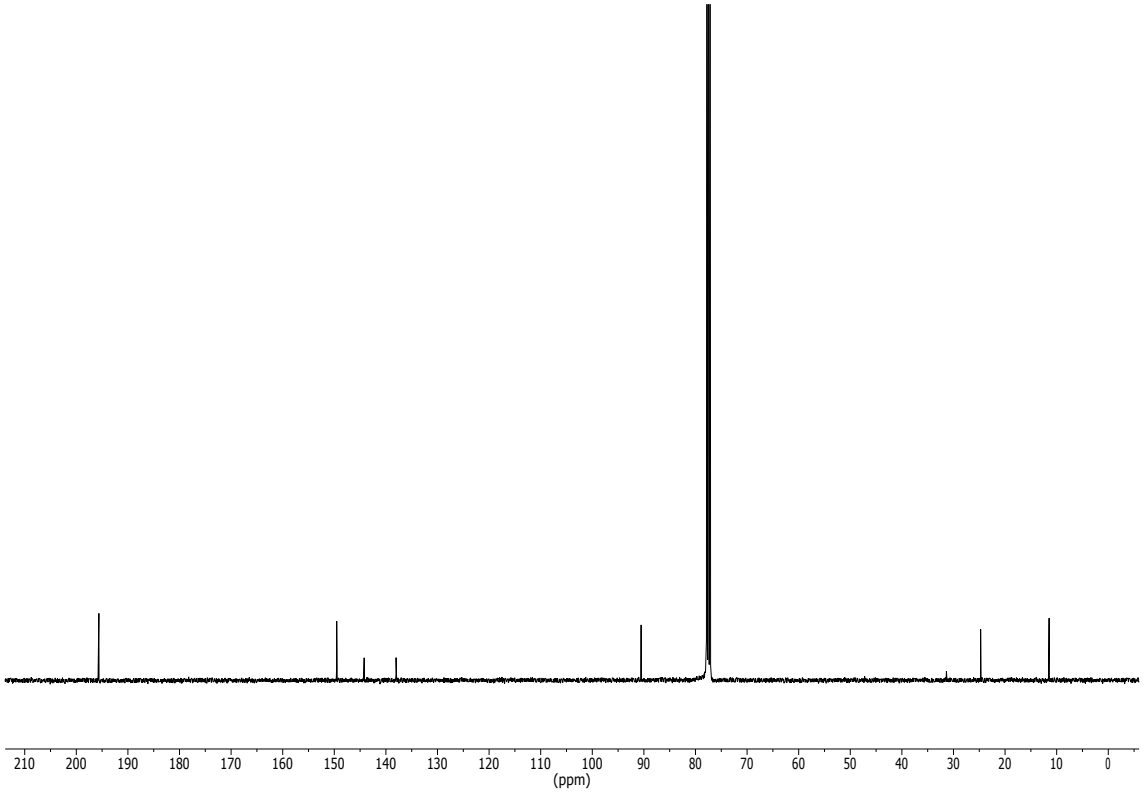
^{1}H-NMR (400.13 MHz, $CDCl_3$)



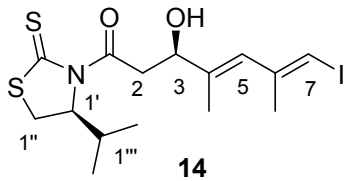
12



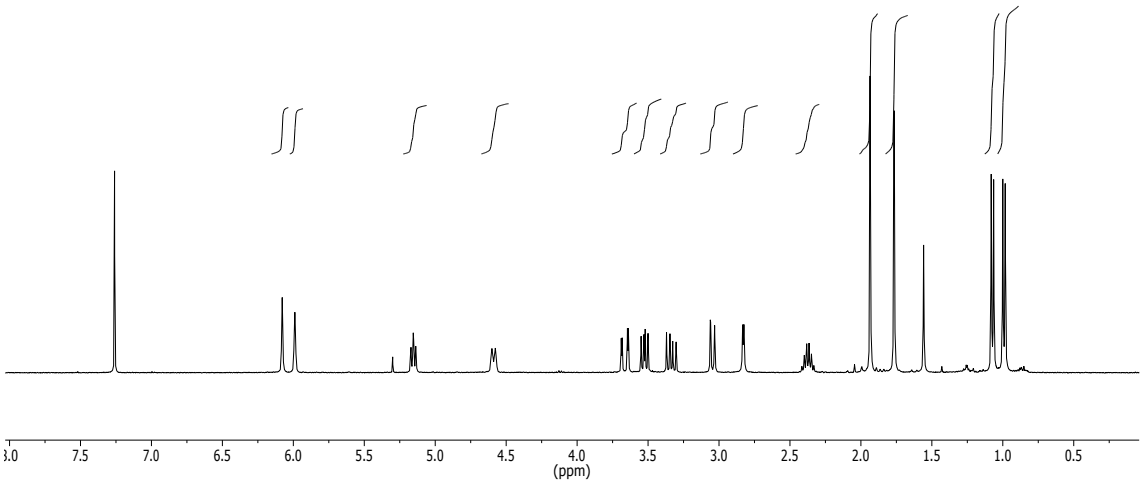
^{13}C-NMR(100.16 MHz, $CDCl_3$)



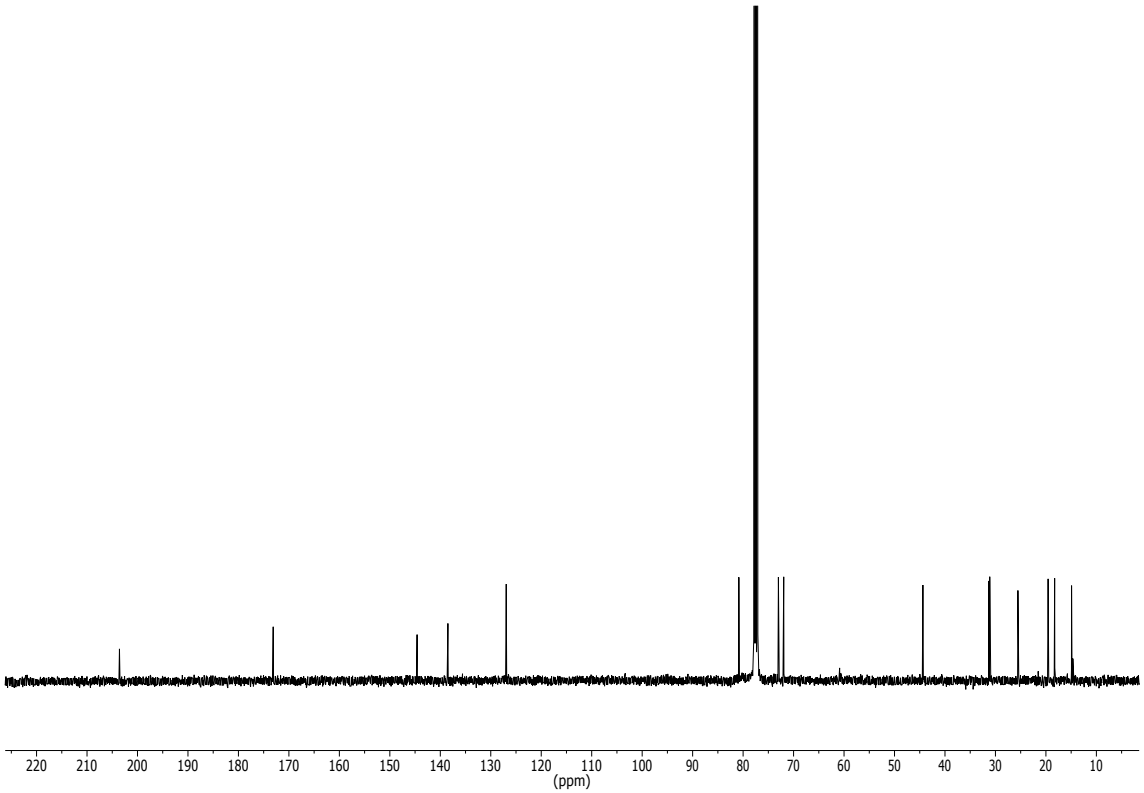
^{1}H-NMR (400.13 MHz, $CDCl_3$)



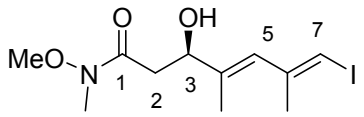
14



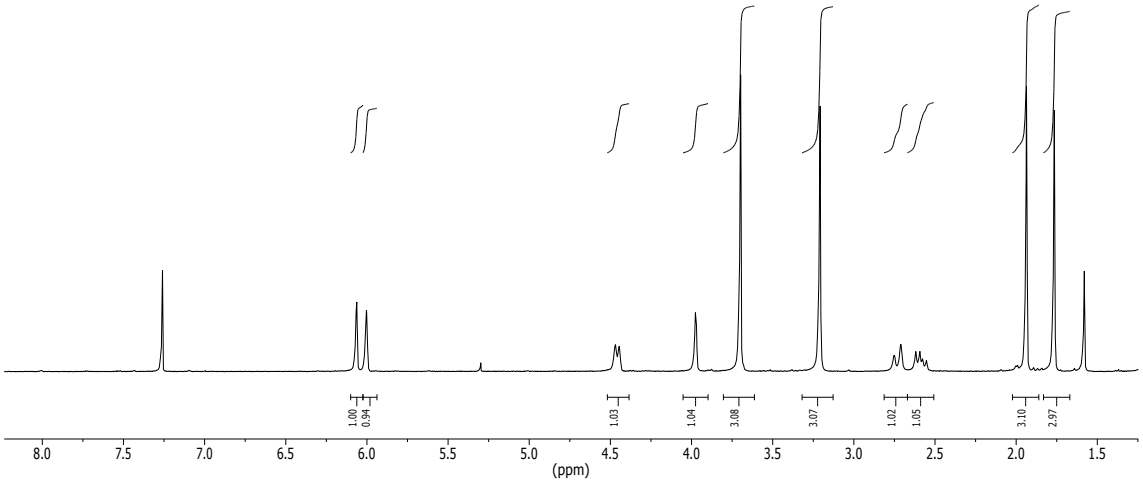
^{13}C-NMR(100.16 MHz, $CDCl_3$)



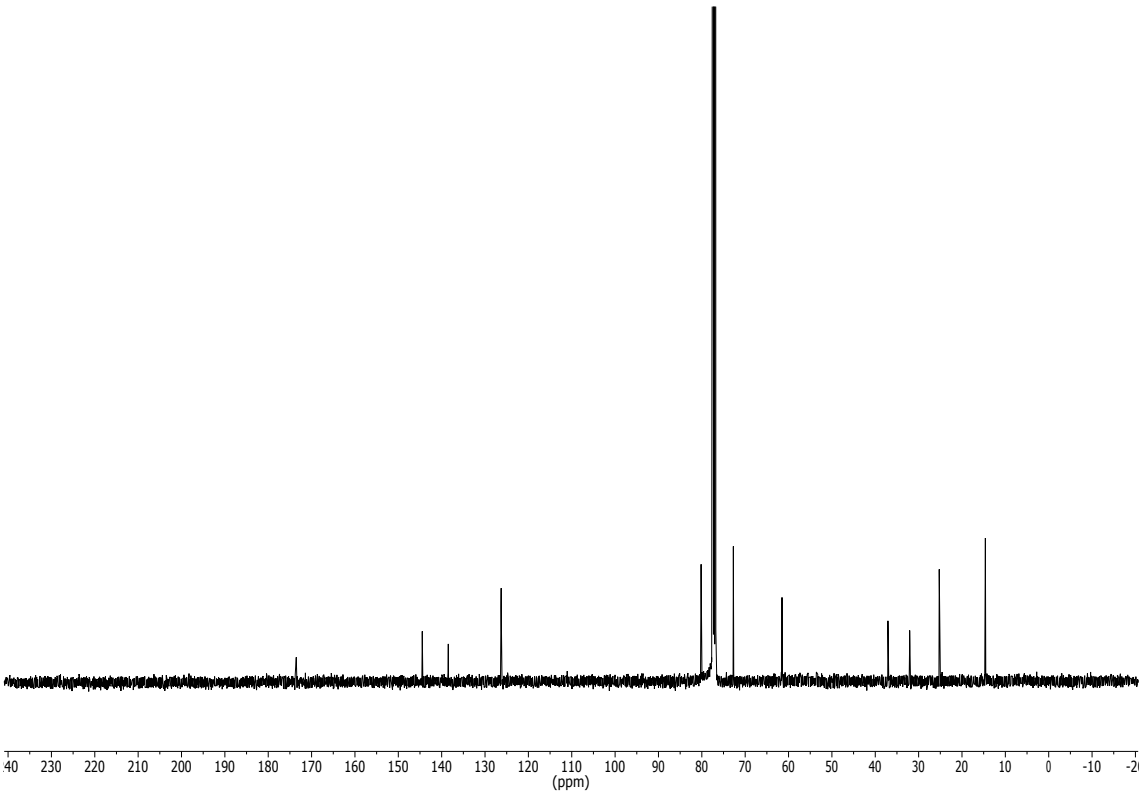
^{1}H-NMR (400.13 MHz, $CDCl_3$)



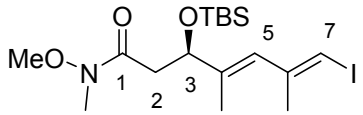
14-1



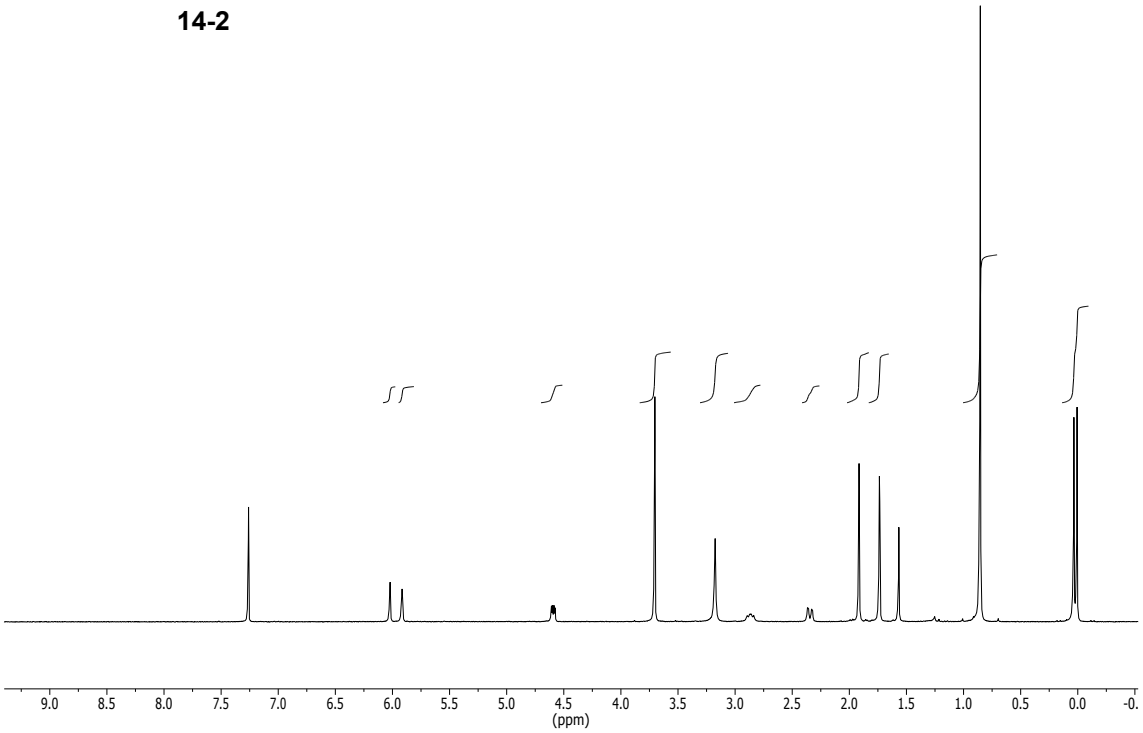
^{13}C-NMR(100.16 MHz, $CDCl_3$)



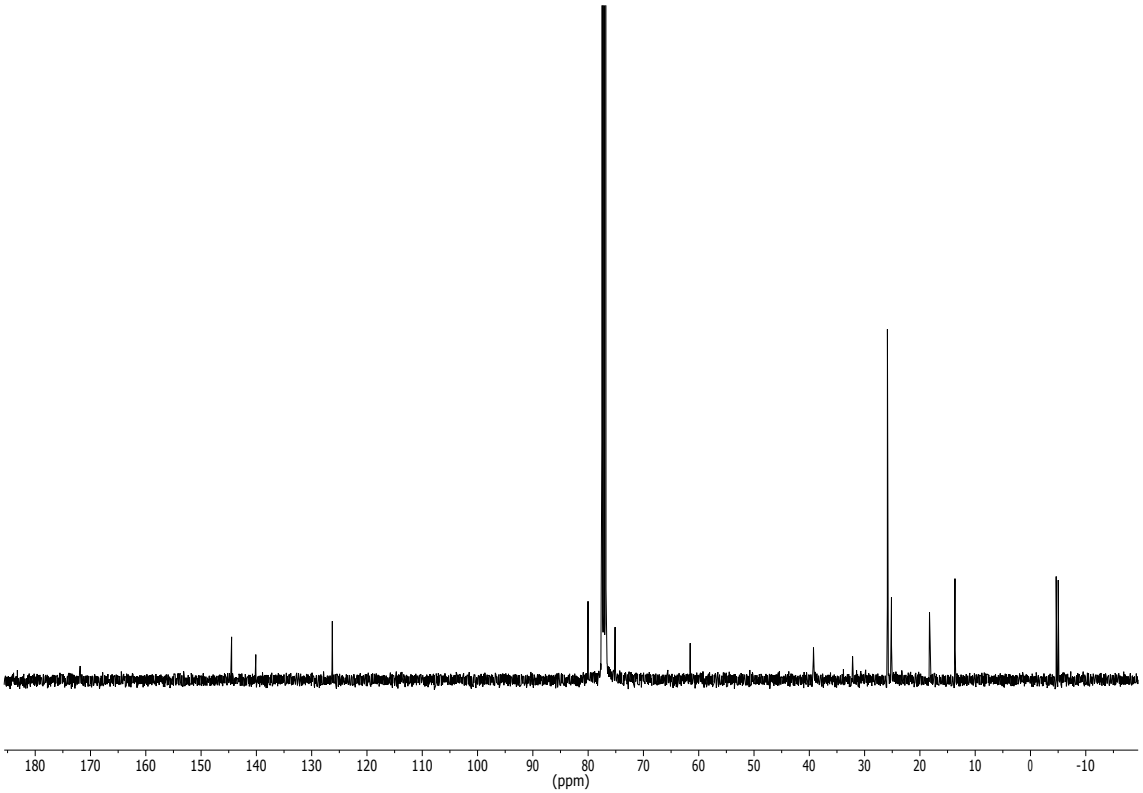
^{1}H-NMR (400.13 MHz, $CDCl_3$)



14-2



^{13}C-NMR (100.16 MHz, $CDCl_3$)



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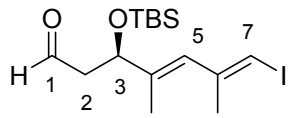

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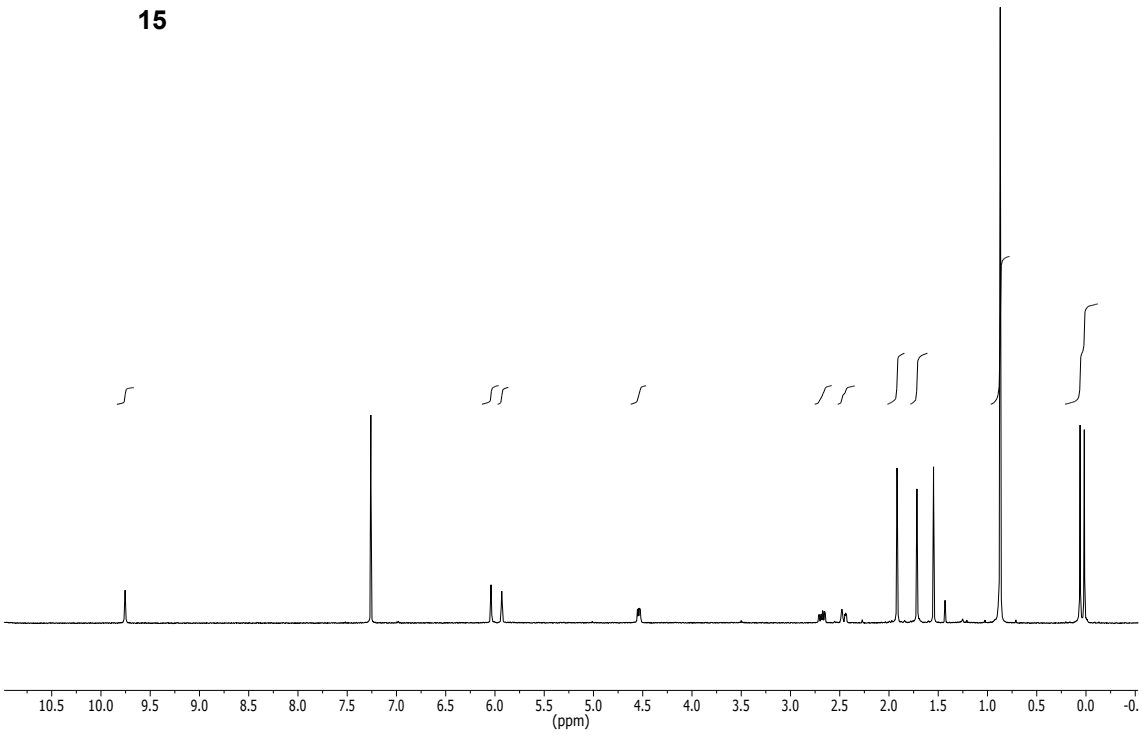
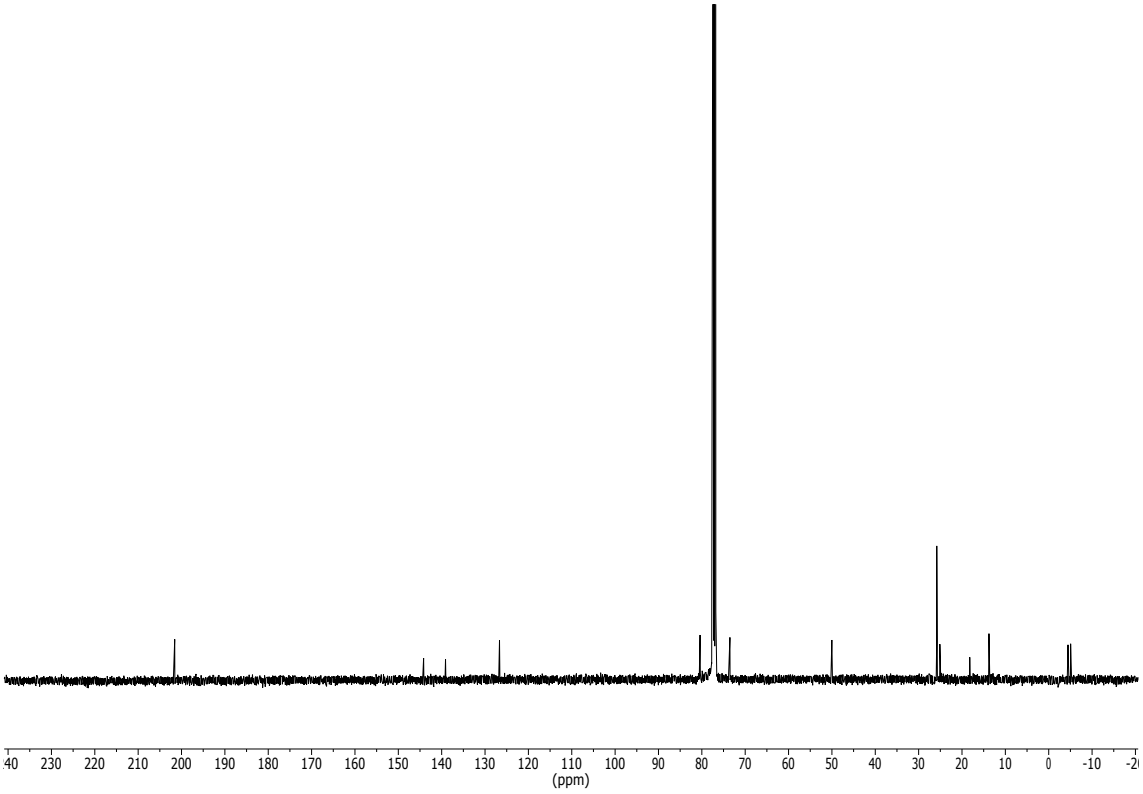
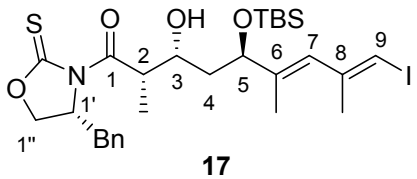


^{13}C-NMR (100.16 MHz, $CDCl_3$)



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



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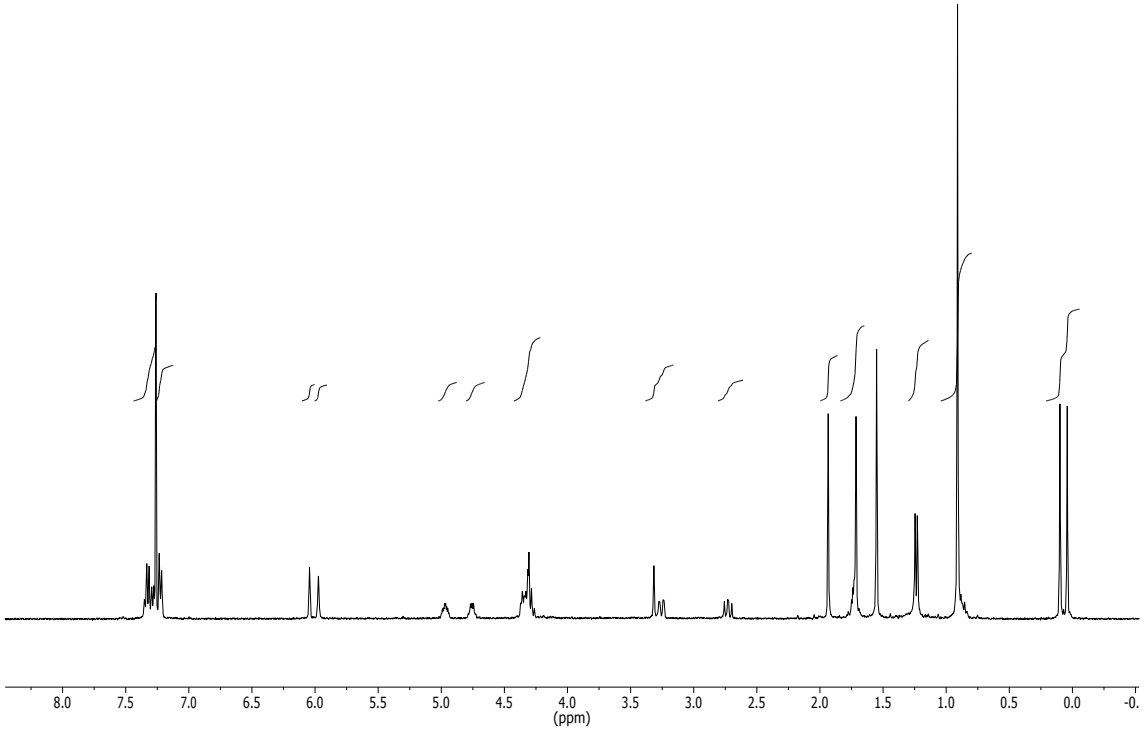
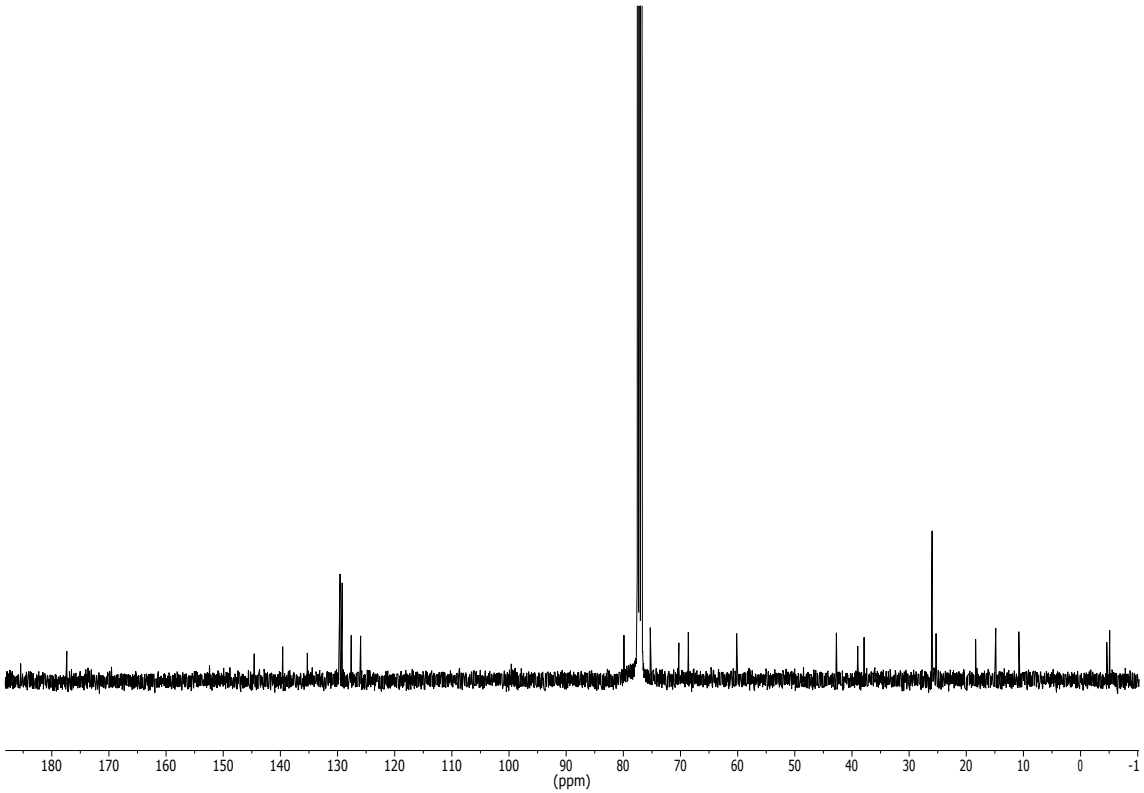
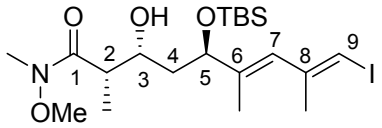


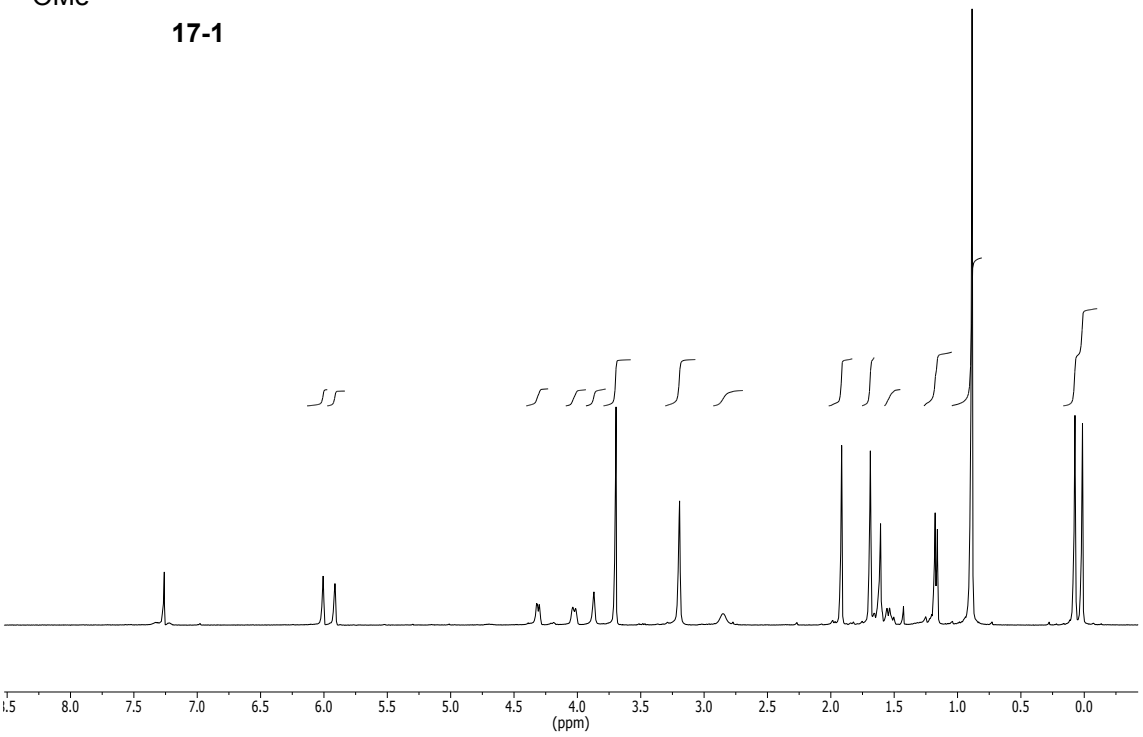
^{13}C-NMR(100.16 MHz, $CDCl_3$)



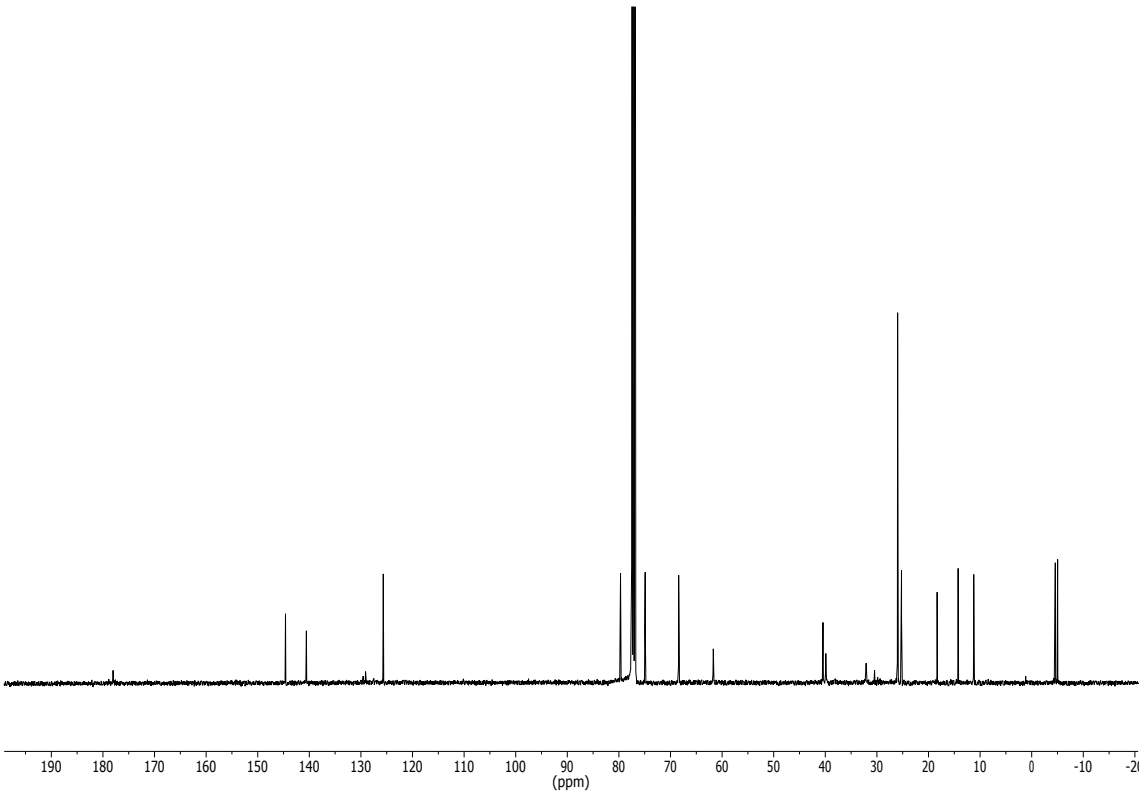
^{1}H-NMR (400.13 MHz, $CDCl_3$)



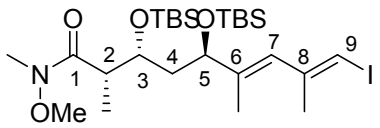
17-1



^{13}C-NMR (100.16 MHz, $CDCl_3$)

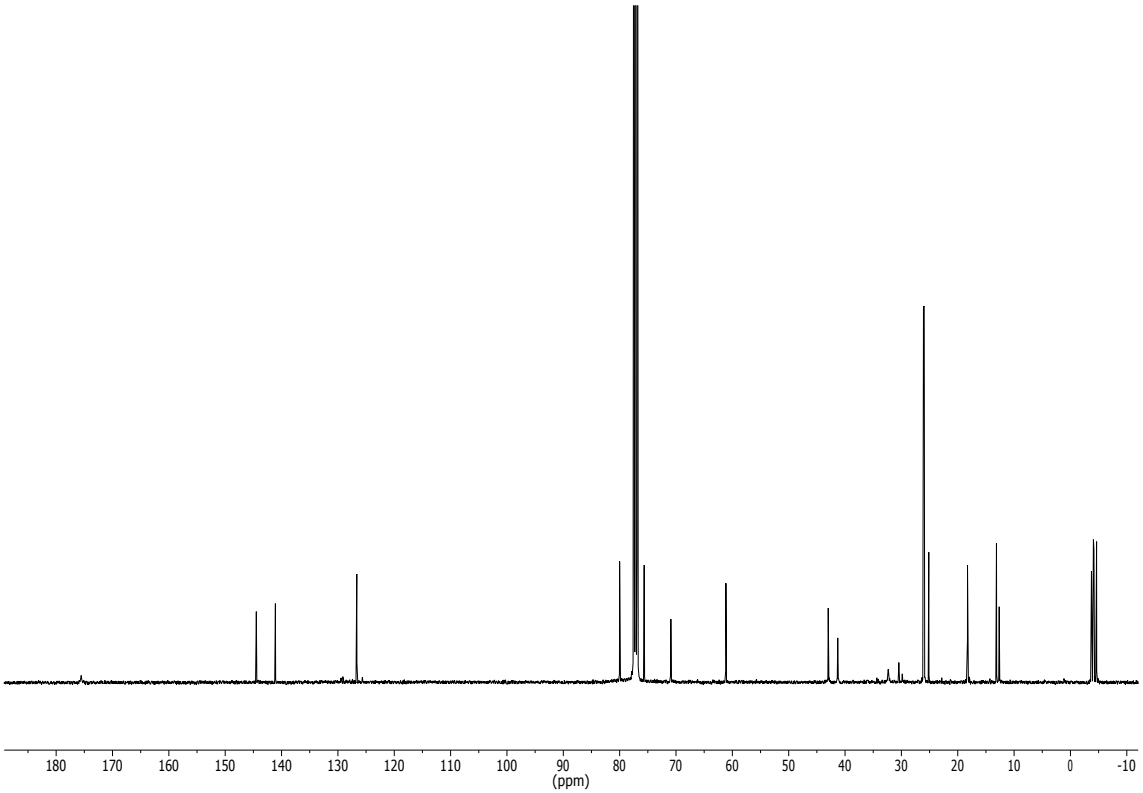


^{1}H-NMR (400.13 MHz, $CDCl_3$)

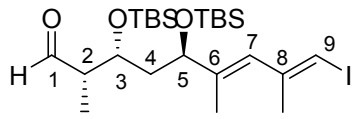


17-2

^{13}C-NMR (100.16 MHz, $CDCl_3$)



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



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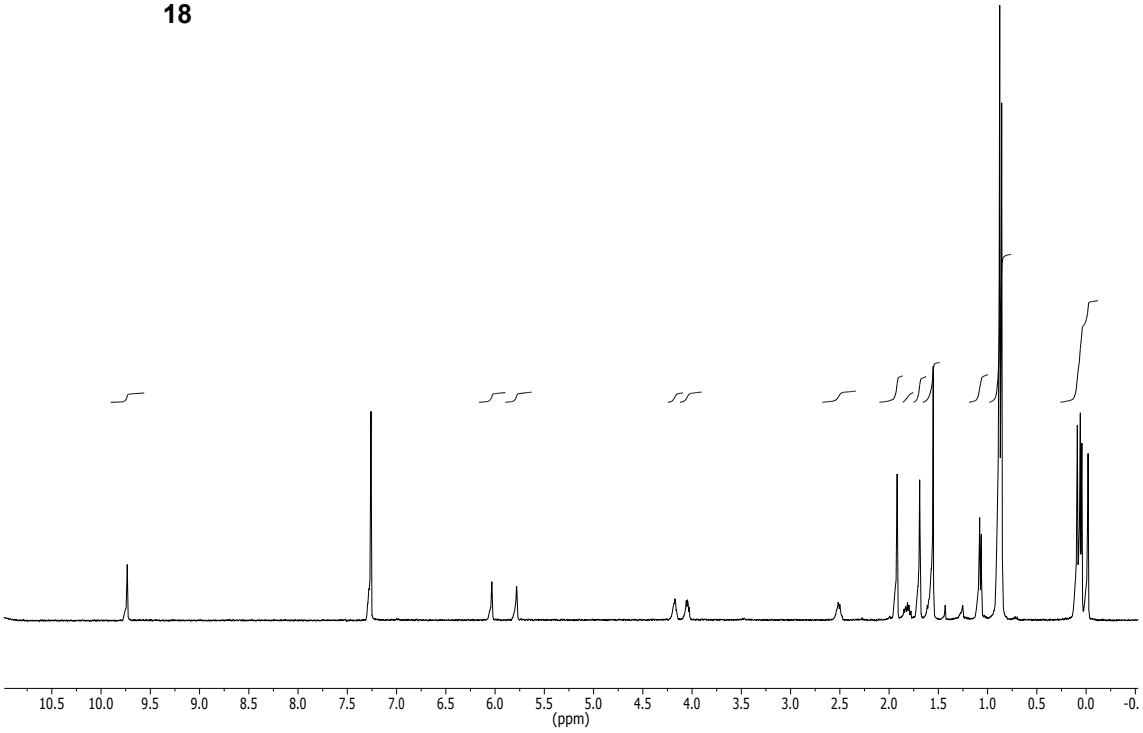
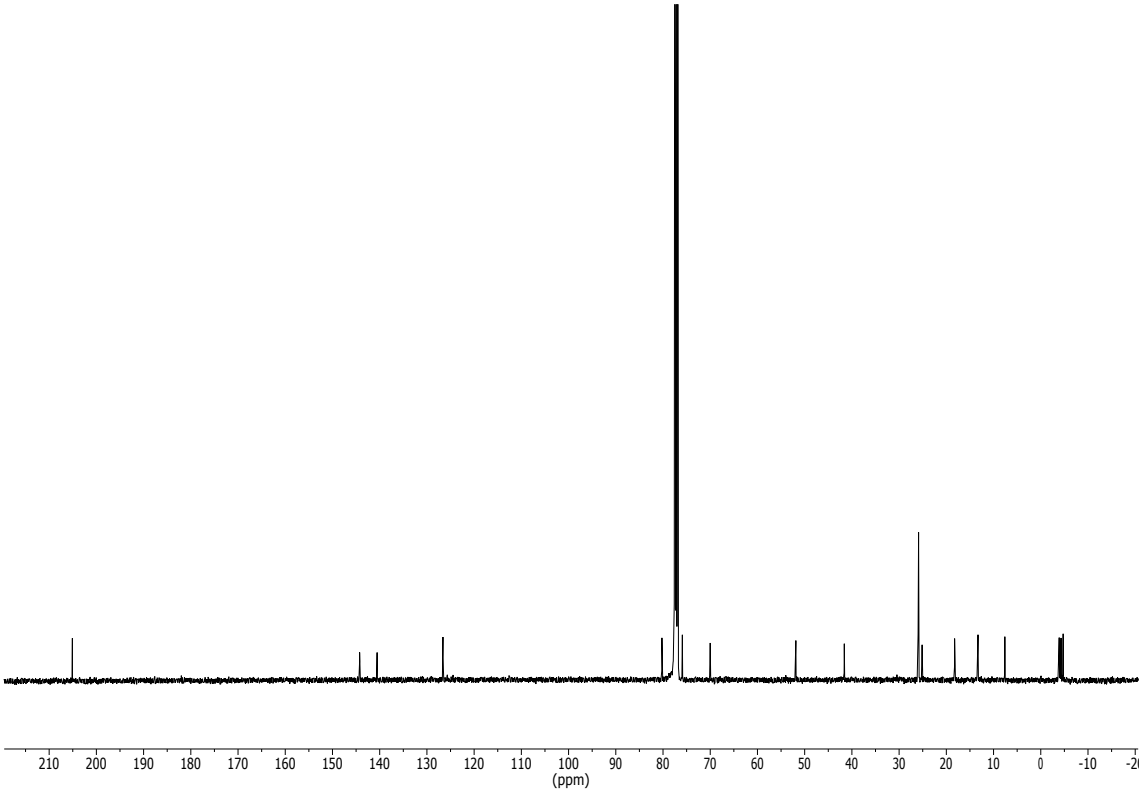
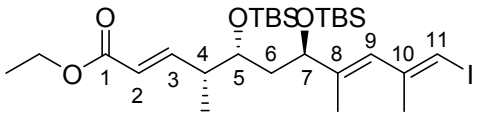


^{13}C-NMR (100.16 MHz, $CDCl_3$)



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



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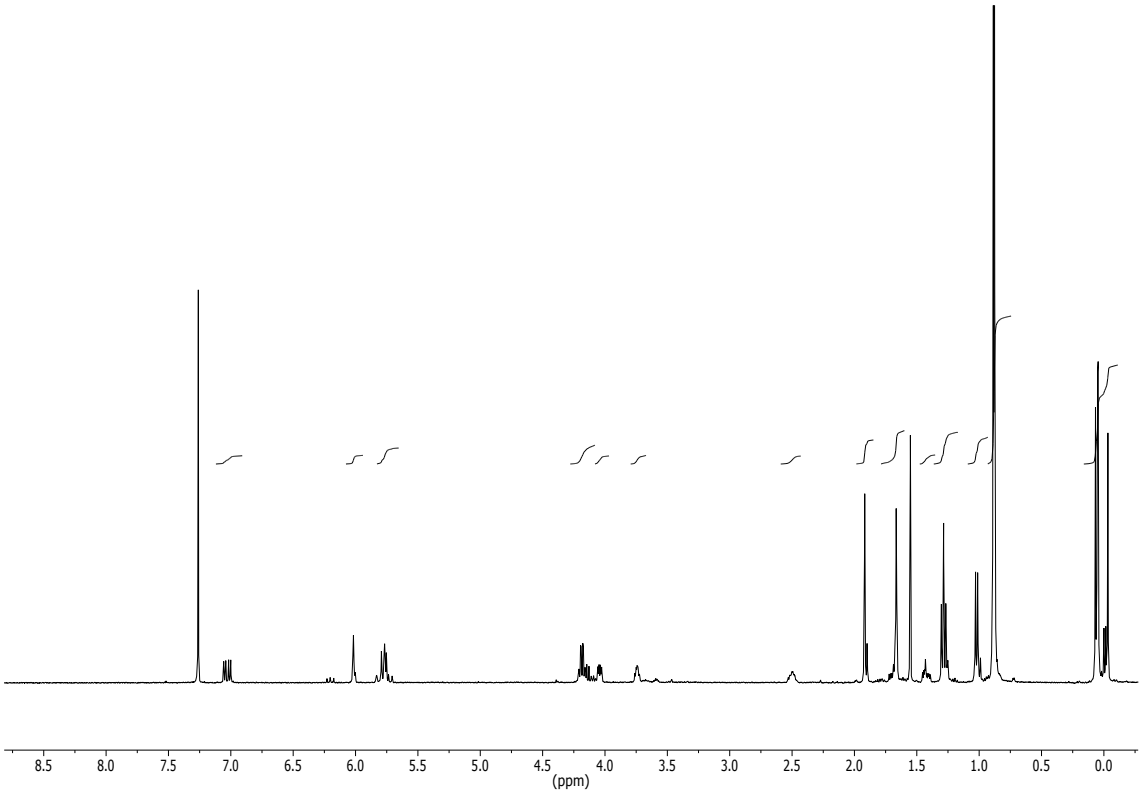
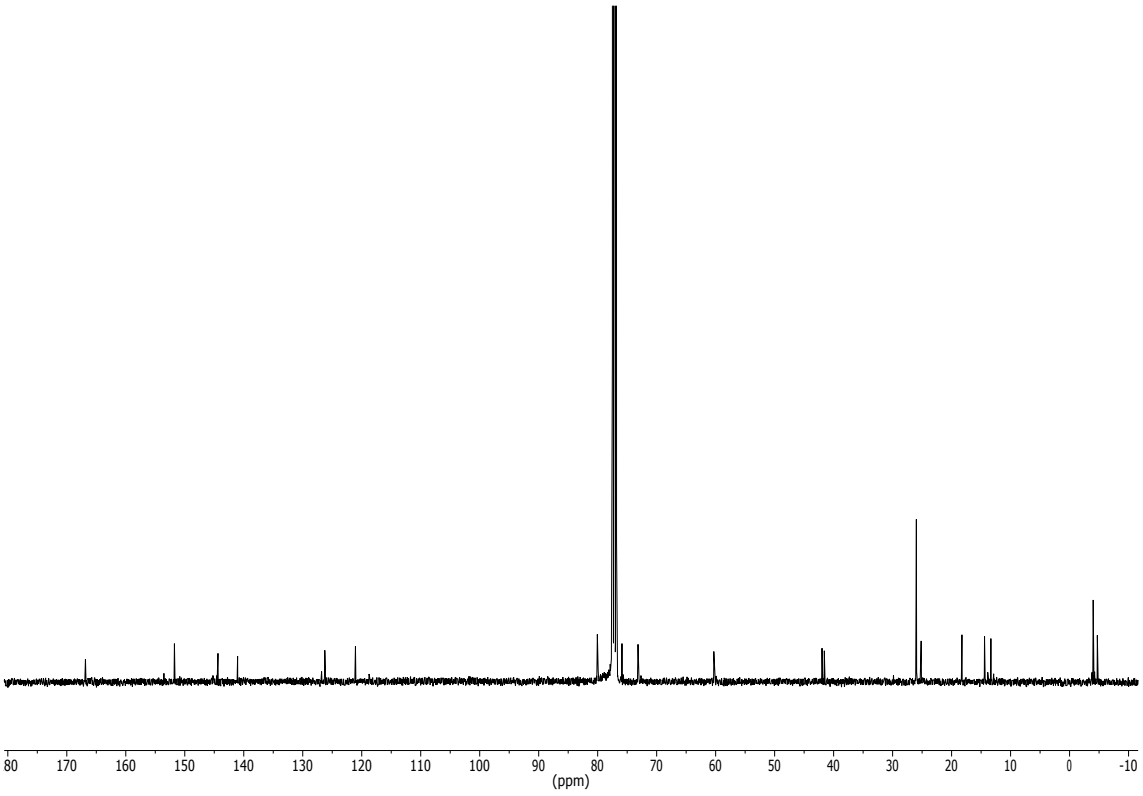
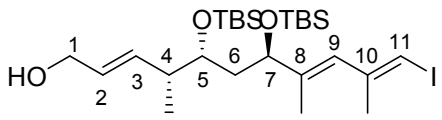


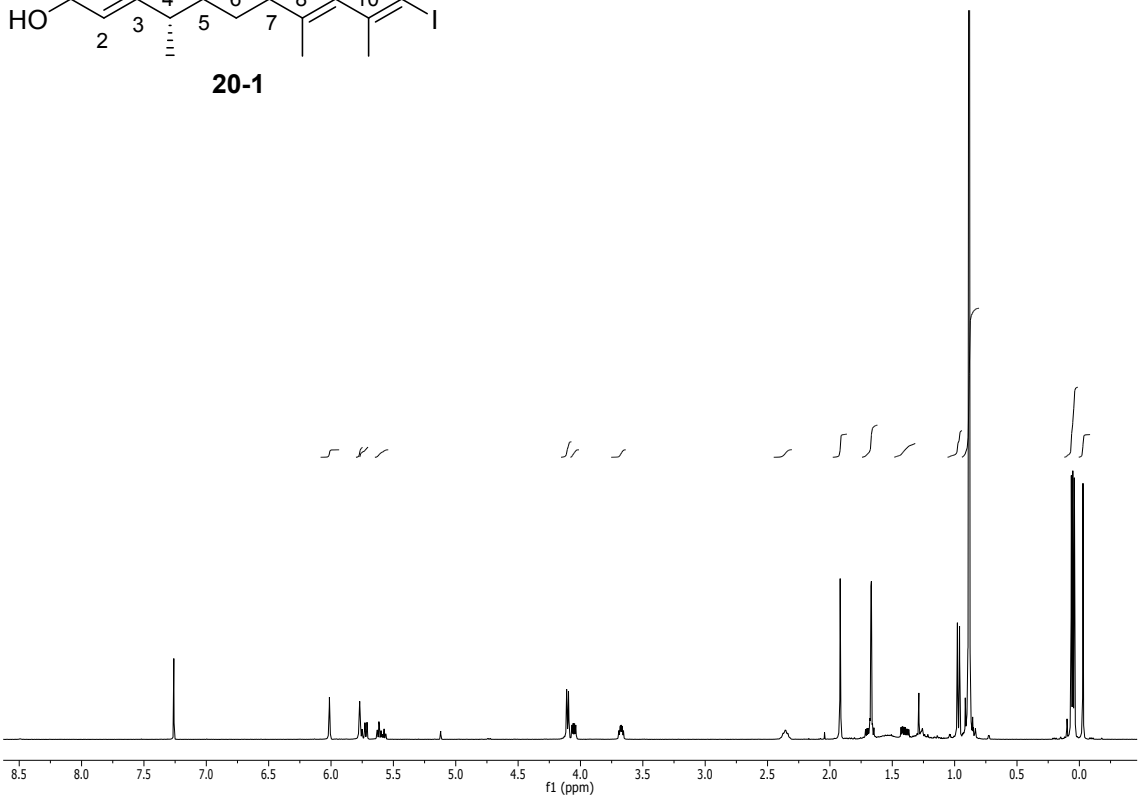
^{13}C-NMR (100.16 MHz, $CDCl_3$)



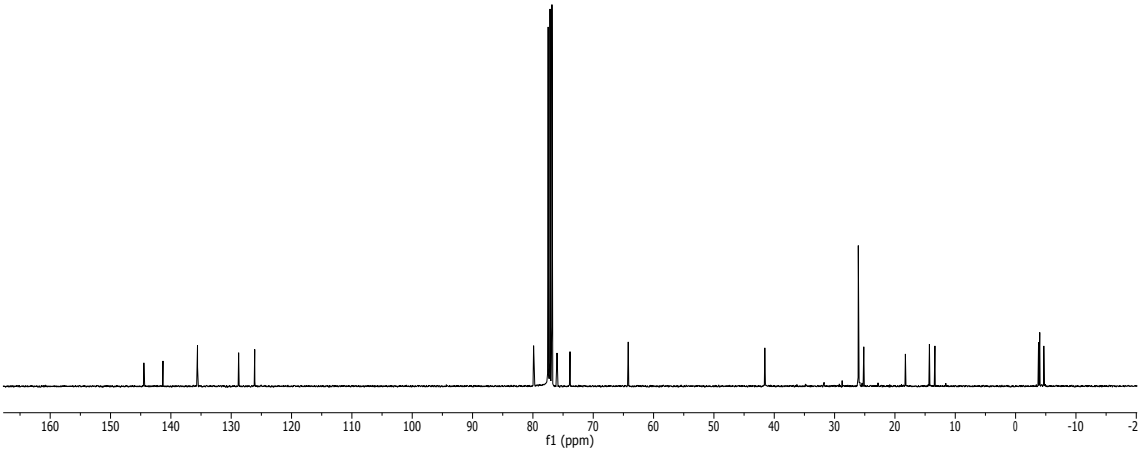
^{1}H-NMR (400.13 MHz, $CDCl_3$)



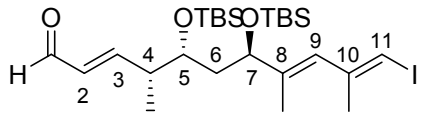
20-1



^{13}C-NMR (100.16 MHz, $CDCl_3$)



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



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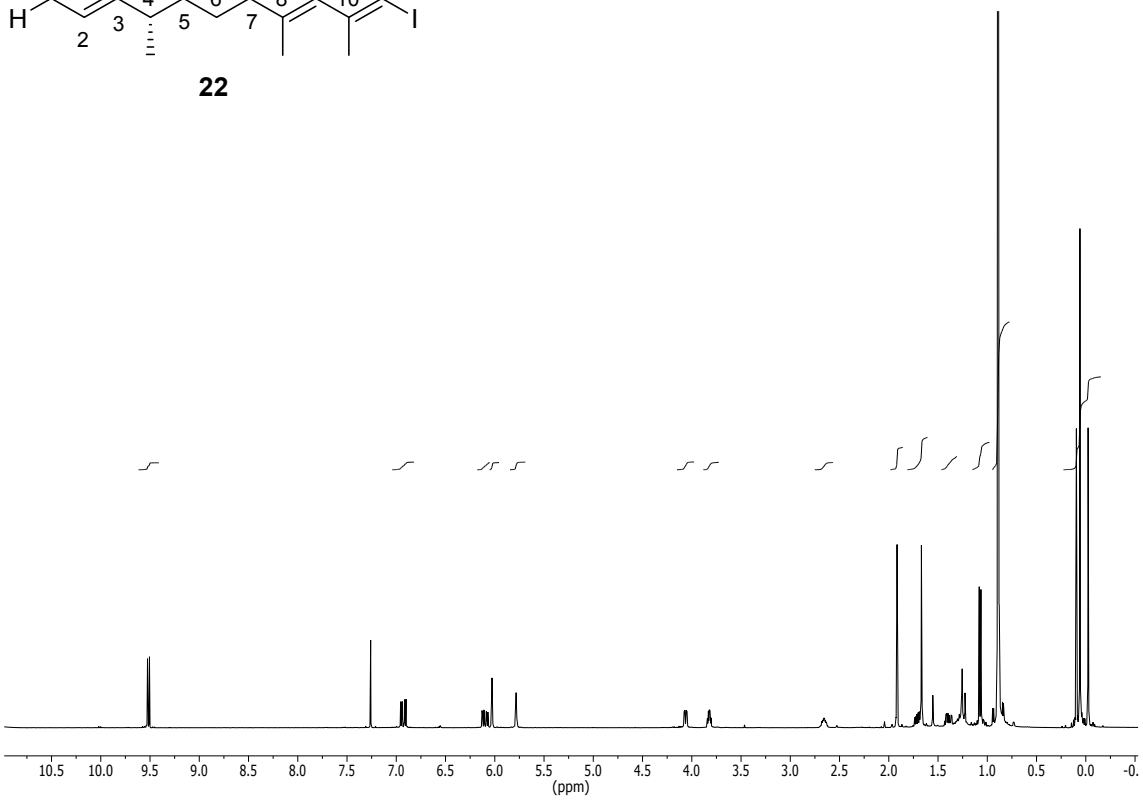
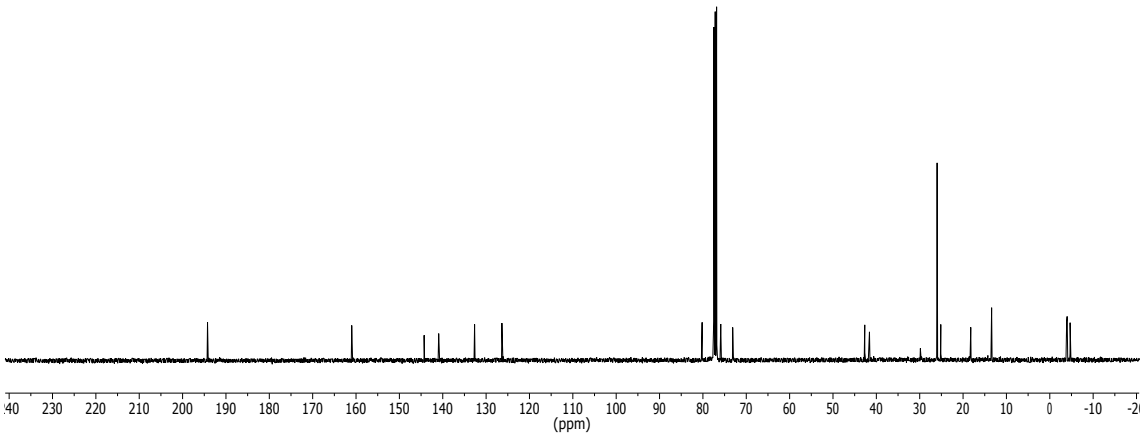
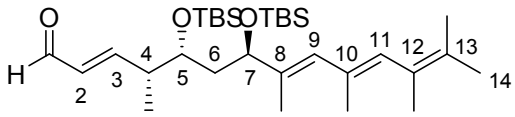


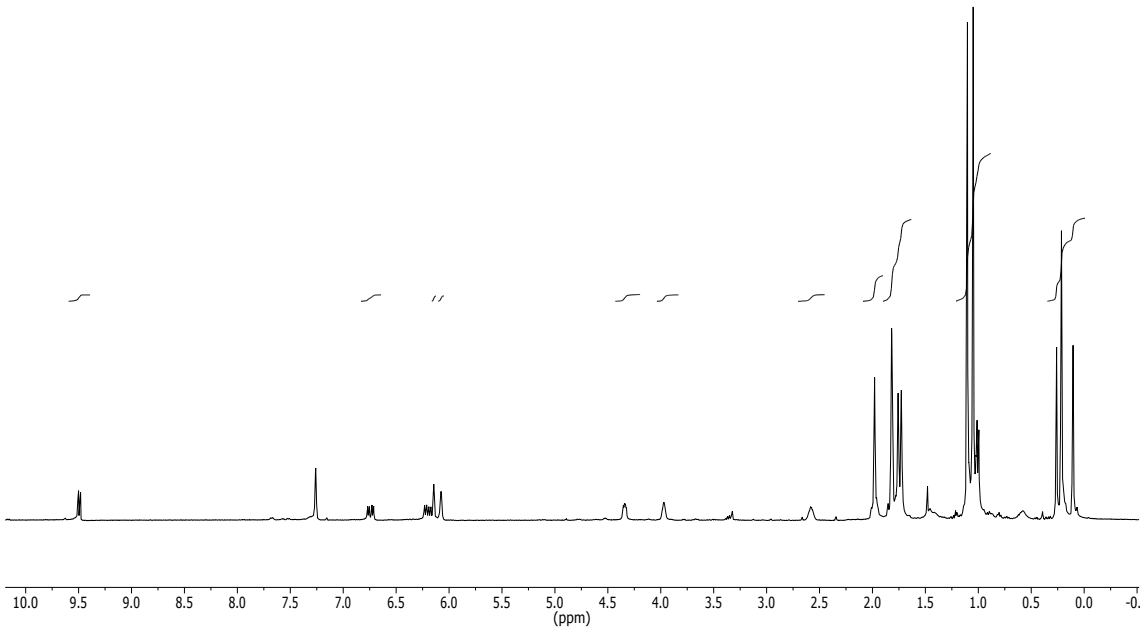
^{13}C-NMR (100.16 MHz, $CDCl_3$)



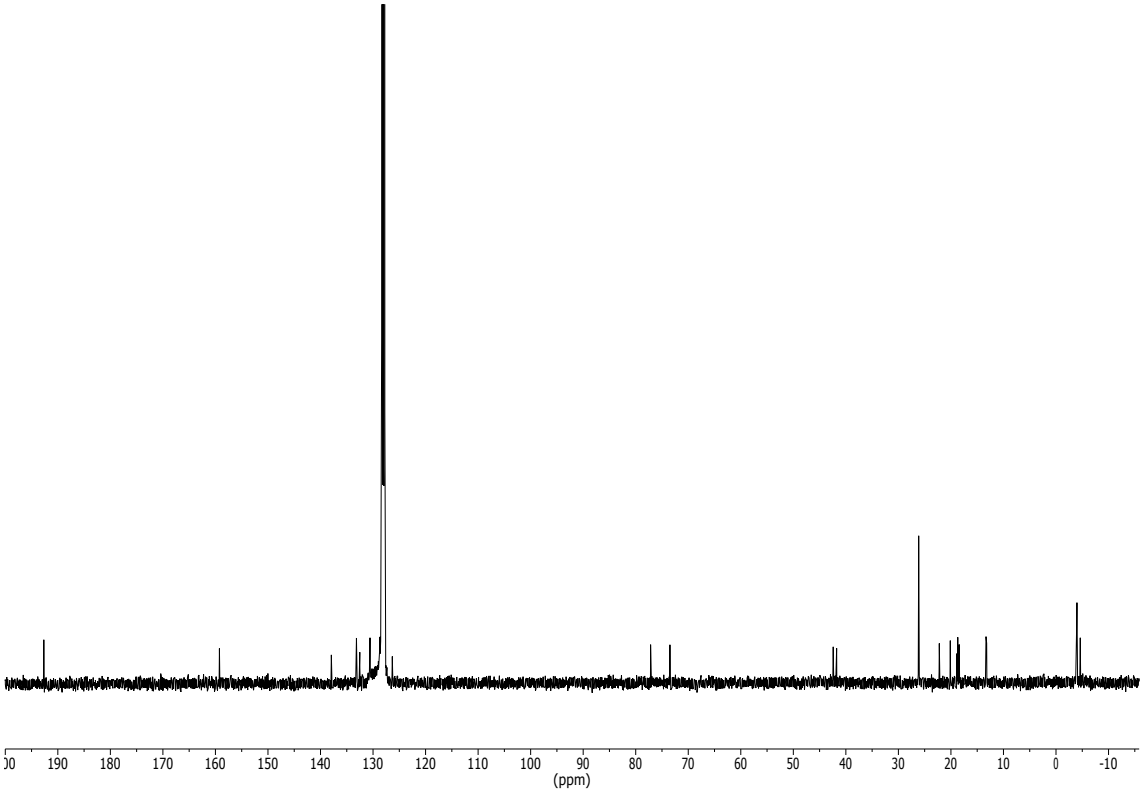
^{1}H-NMR (400.13 MHz, C_6D_6)



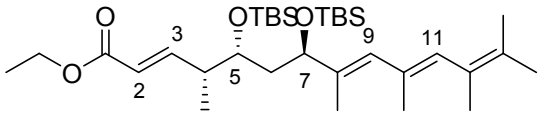
9b



^{13}C-NMR (100.16 MHz, C_6D_6)



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



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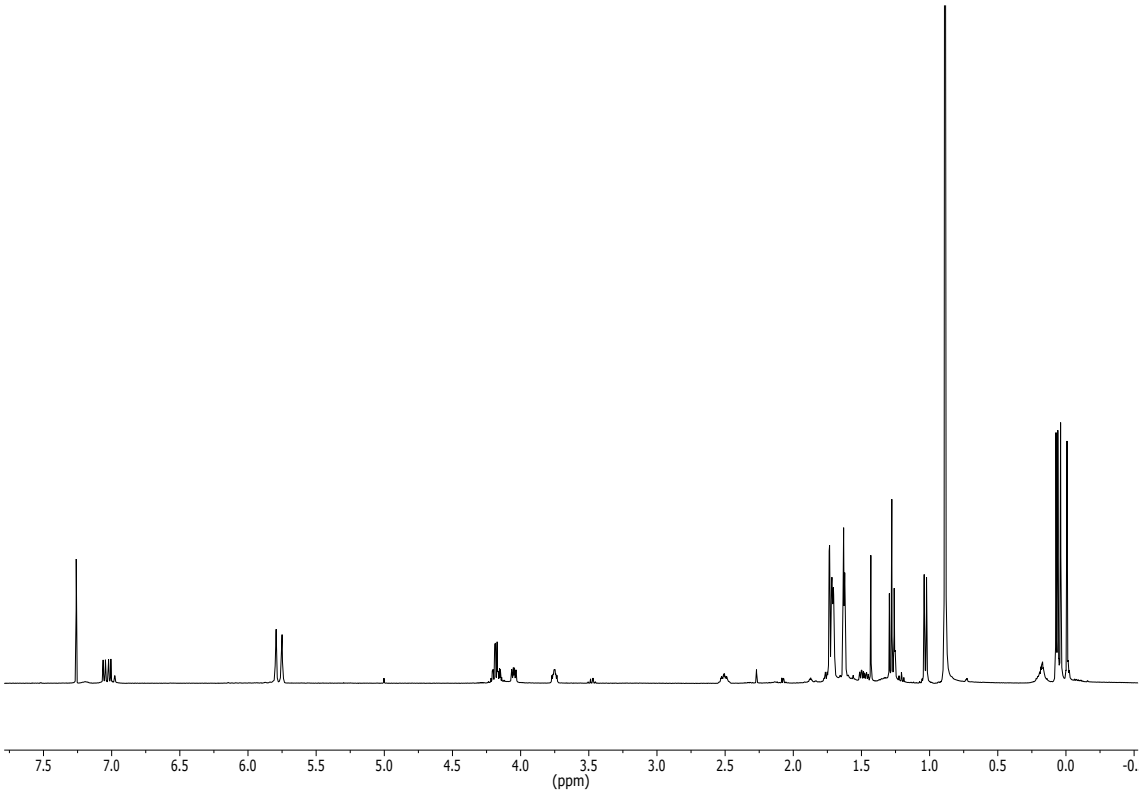
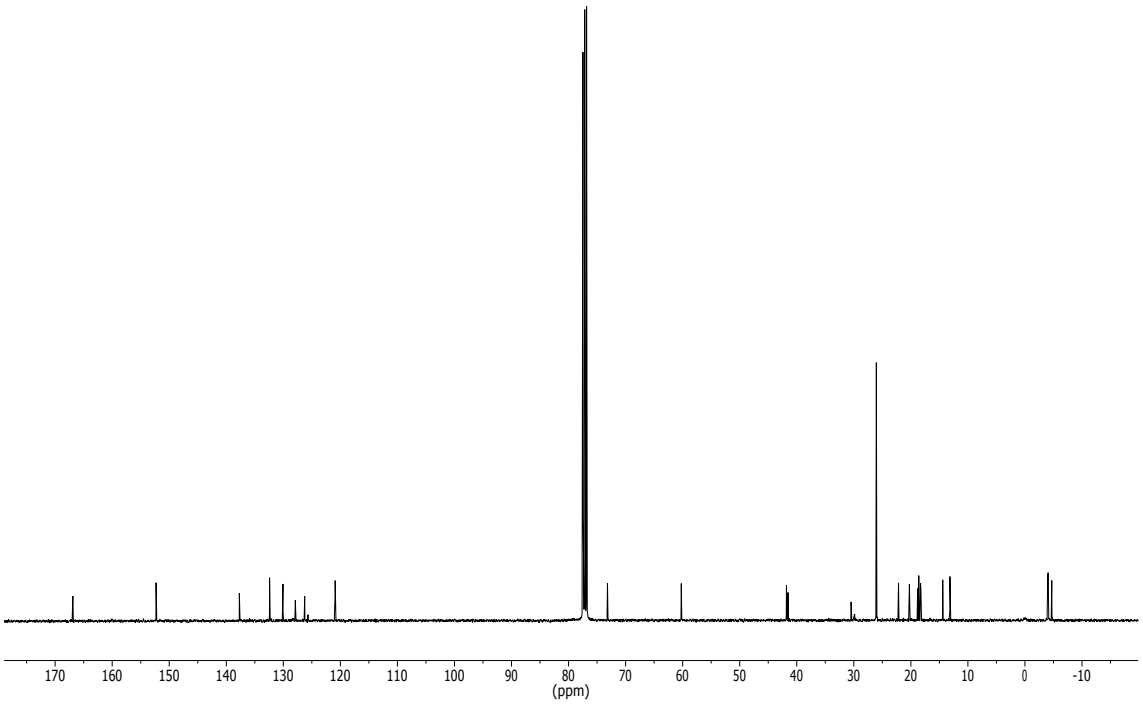
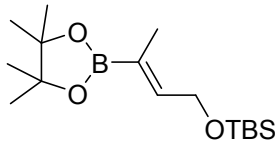


^{13}C-NMR (100.16 MHz, $CDCl_3$)



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



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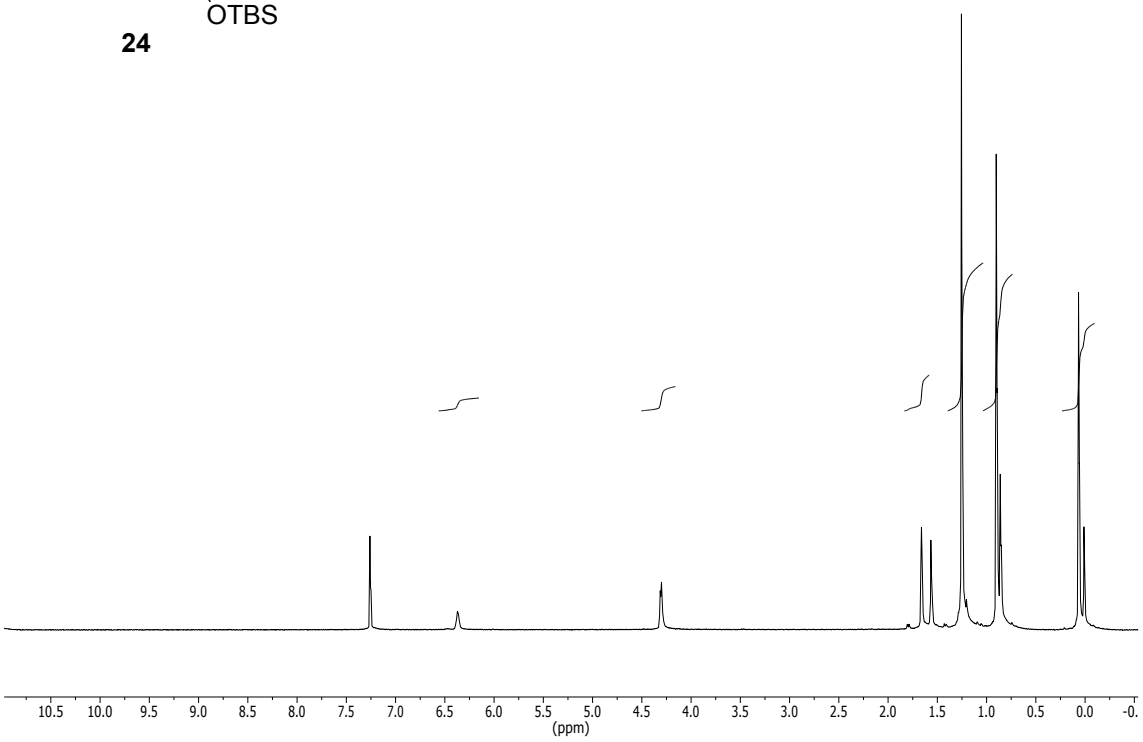
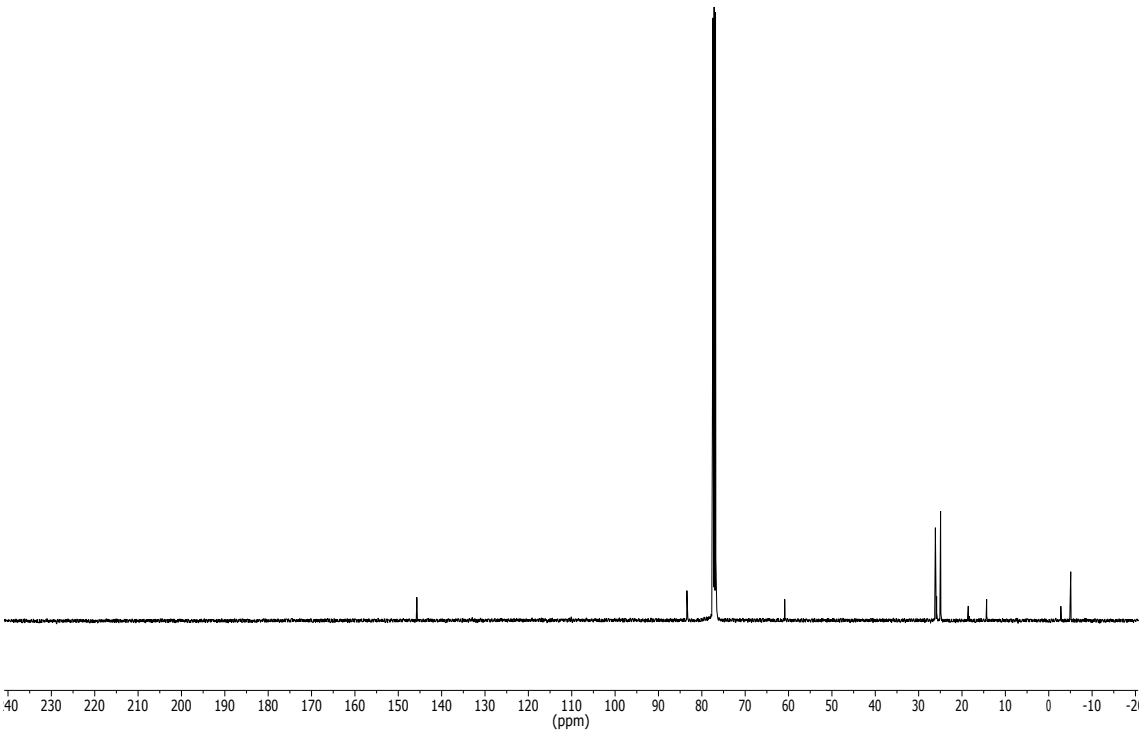
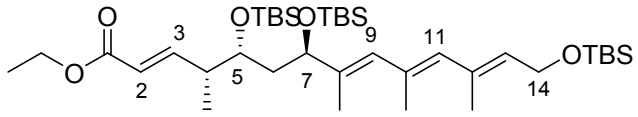


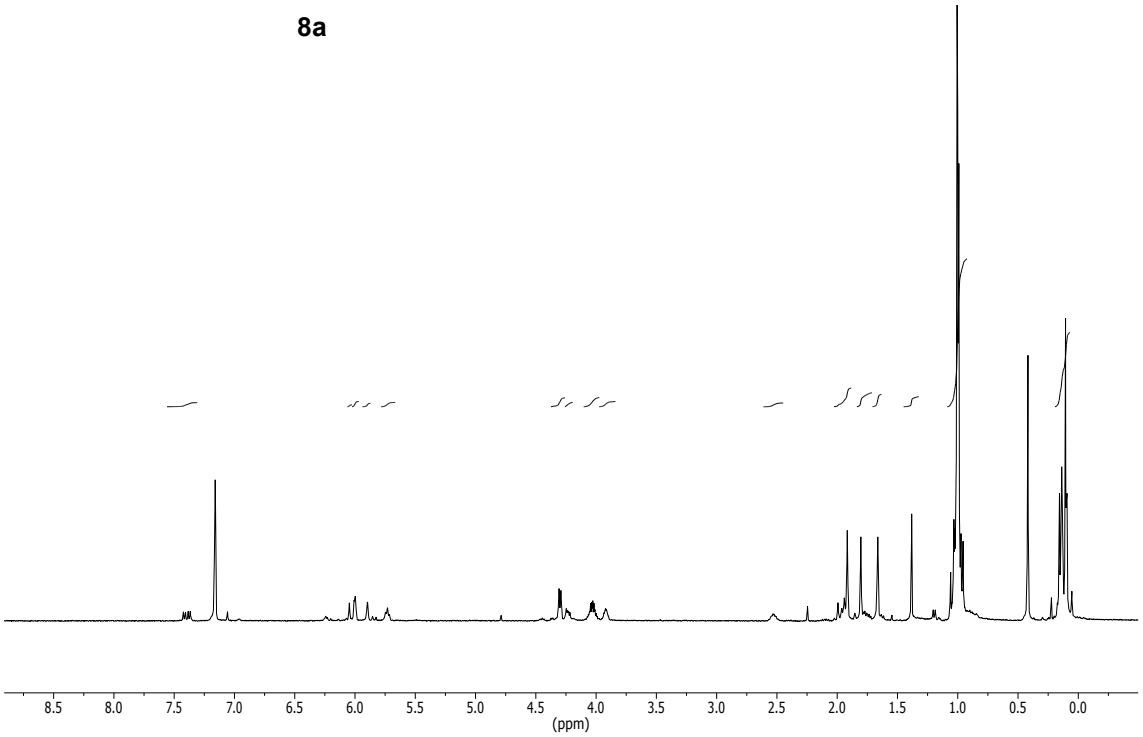
^{13}C-NMR (100.16 MHz, $CDCl_3$)



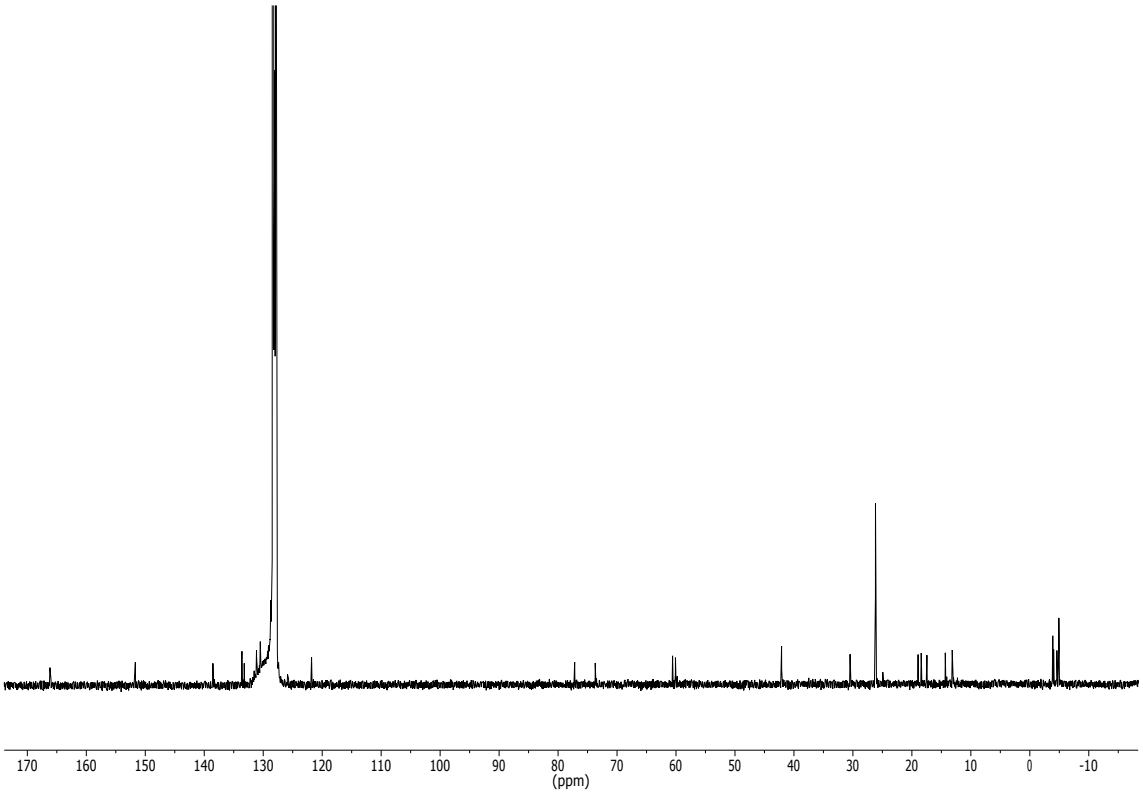
^{1}H-NMR (400.13 MHz, C_6D_6)



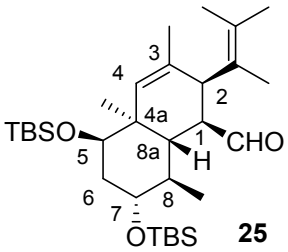
8a



^{13}C-NMR (100.16 MHz, C_6D_6)

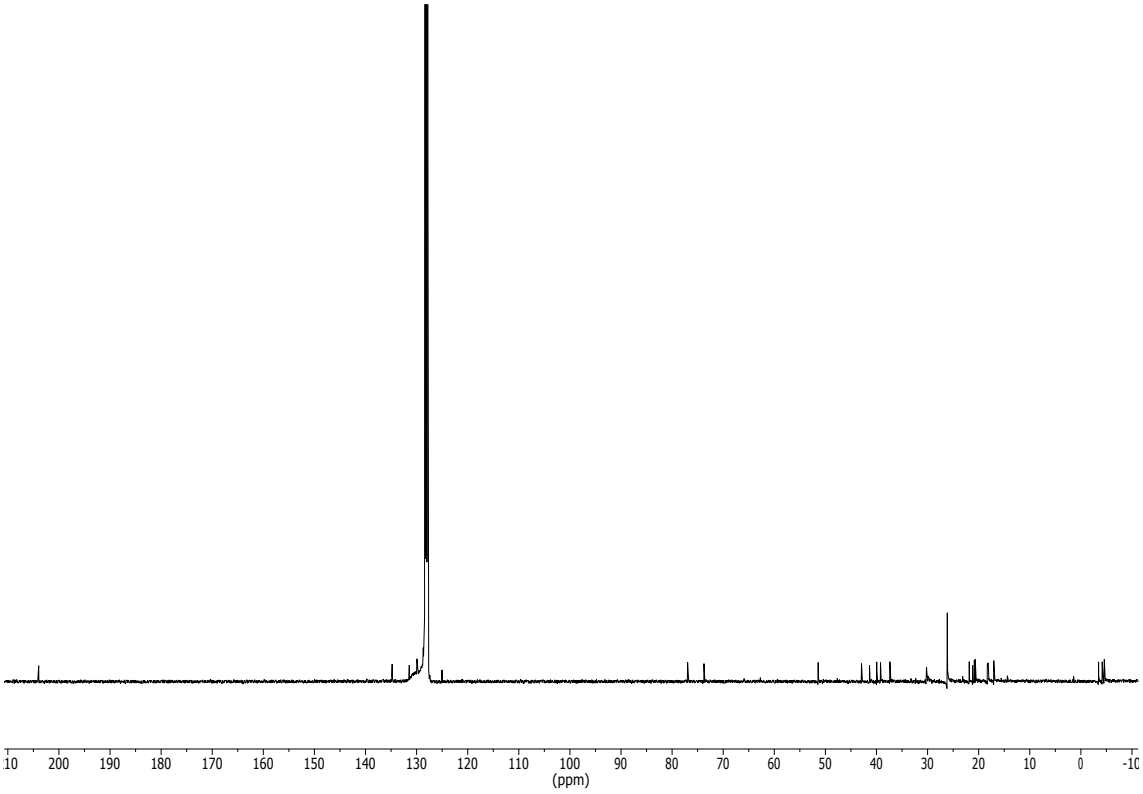


^{1}H-NMR (400.13 MHz, C_6D_6)

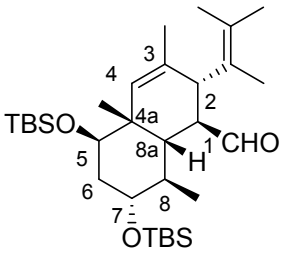


25

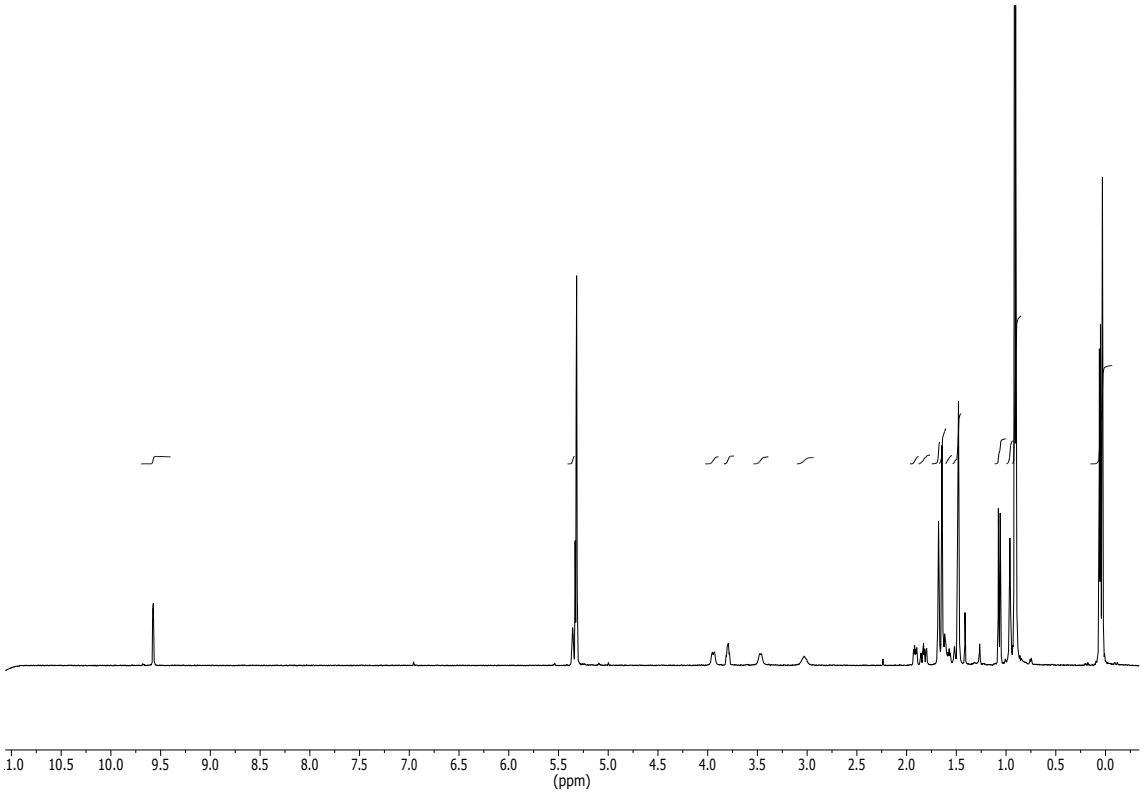
^{13}C-NMR (100.16 MHz, C_6D_6)



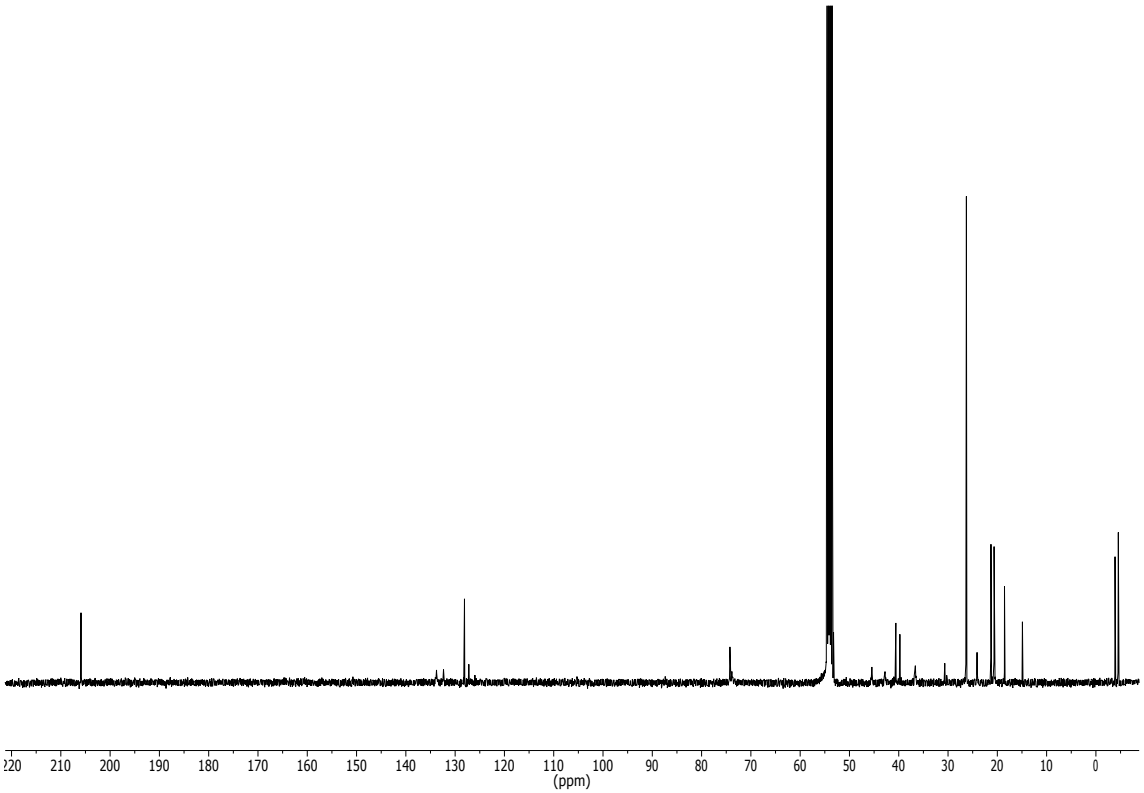
Compound 27. ^{1}H-NMR (400.13 MHz, CD_2Cl_2)



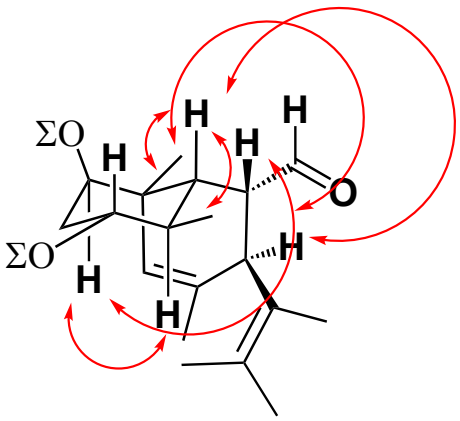
Re-exo
27



^{13}C-NMR (100.16 MHz, CD_2Cl_2)

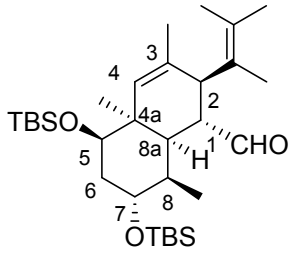


NOE enhancements for compound 27



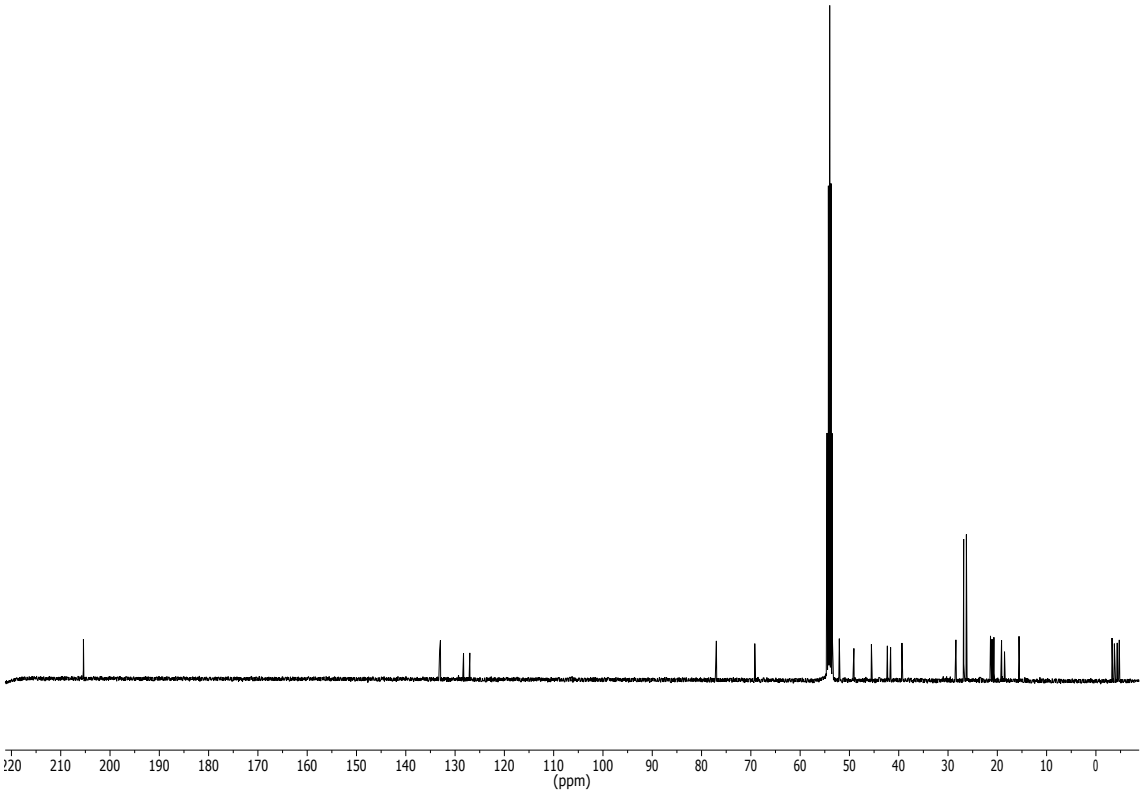
Re-exo

Compound 26.^{1}H-NMR (400.13 MHz, CD_2Cl_2)

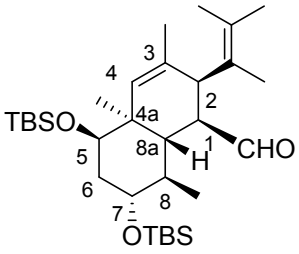


Si-exo
26

^{13}C-NMR (100.16 MHz, CD_2Cl_2)

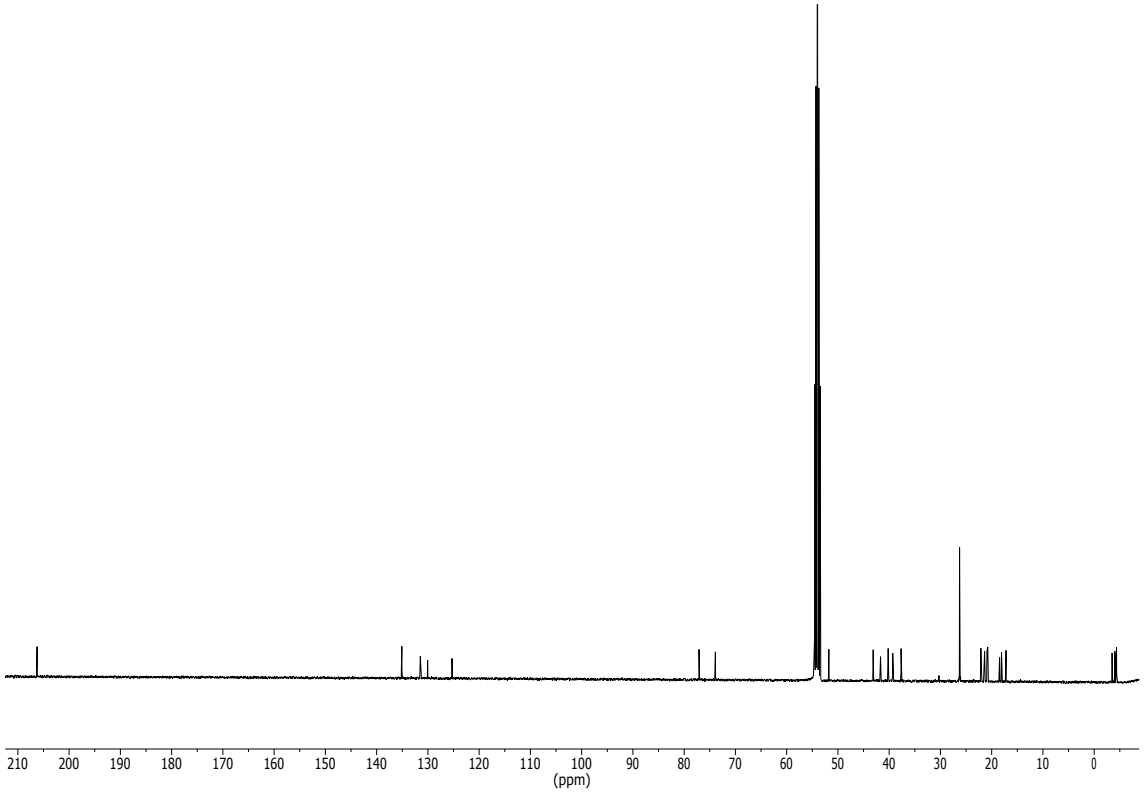


Compound 25.^{1}H-NMR (400.13 MHz, CD_2Cl_2)



Re-endo
25

^{13}C-NMR (100.16 MHz, CD_2Cl_2)



5. SINGLE CRYSTAL X-RAY DATA

Compound 25.

Table 1. Crystal data and structure refinement for compound **25**.

Identification code	ar160769_1_0m	
Empirical formula	C31 H58 O3 Si2	
Formula weight	534.95	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.4726(6) Å	α= 90°.
	b = 20.1154(16) Å	β= 90°.
	c = 23.4601(19) Å	γ = 90°.
Volume	3526.4(5) $Å^3$	
Z	4	
Density (calculated)	1.008 Mg/m^3	
Absorption coefficient	1.098 mm^{-1}	
F(000)	1184	
Crystal size	0.258 x 0.052 x 0.051 mm^3	
Theta range for data collection	2.894 to 65.090°.	
Index ranges	-8<=h<=8, -23<=k<=23, -27<=l<=26	
Reflections collected	35935	
Independent reflections	5895 [R(int) = 0.0941]	
Completeness to theta = 65.090°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6712 and 0.5325	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5895 / 0 / 341	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0701, wR2 = 0.1881	
R indices (all data)	R1 = 0.0863, wR2 = 0.2039	
Absolute structure parameter	0.034(18)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.504 and -0.224 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for compound **25**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4390(5)	3337(2)	4524(2)	70(1)
C(2)	4275(6)	2958(2)	3948(2)	74(1)
C(3)	3268(6)	3337(2)	3490(3)	81(1)
C(4A)	2919(5)	4346(2)	4101(2)	68(1)
C(4)	2694(6)	3947(2)	3569(3)	77(1)
C(5)	3243(5)	5077(2)	3944(2)	71(1)
C(7)	5011(7)	5241(2)	4851(2)	79(1)
C(6)	3508(6)	5501(2)	4468(3)	82(1)
C(8)	4803(6)	4501(2)	5000(2)	73(1)
C(8A)	4566(5)	4097(2)	4452(2)	68(1)
C(9)	5856(7)	2994(2)	4848(3)	81(1)
C(10)	2897(10)	2965(3)	2948(3)	108(2)
C(11)	1135(6)	4297(2)	4430(3)	83(1)
C(12)	6391(8)	4295(3)	5373(3)	96(2)
C(13)	6083(6)	2717(2)	3717(2)	80(1)
C(14)	6589(7)	2075(3)	3753(3)	90(2)
C(15)	5484(10)	1532(3)	4020(3)	113(2)
C(16)	7259(8)	3234(3)	3450(4)	111(2)
C(17)	8376(9)	1848(4)	3533(4)	120(2)
C(51)	7432(7)	5694(3)	2913(4)	102(2)
C(52)	3723(10)	6326(4)	2994(5)	145(4)
C(53)	4139(12)	5003(5)	2392(4)	144(3)
C(71)	5532(16)	6551(4)	6217(4)	148(3)
C(72)	8705(13)	6020(7)	5454(9)	244(9)
C(73)	5894(18)	6946(4)	4969(6)	170(4)
C(511)	7856(11)	5967(5)	2320(5)	152(4)
C(512)	8455(8)	5031(4)	2980(4)	122(2)
C(513)	8028(13)	6151(6)	3399(6)	187(5)
C(711)	5650(30)	6004(7)	6640(6)	224(8)
C(712)	6750(30)	7141(8)	6416(8)	274(10)

C(713)	3630(20)	6777(8)	6187(6)	205(6)
Si(5)	4978(2)	5525(1)	2979(1)	89(1)
Si(7)	6315(3)	6272(1)	5490(1)	120(1)
O(5)	4779(4)	5135(1)	3588(2)	78(1)
O(7)	5063(5)	5625(2)	5358(2)	95(1)
O(9)	5588(6)	2568(2)	5200(2)	105(1)

Table 3. Bond lengths [Å] and angles [°] for compound **25**.

C(1)-C(9)	1.502(7)
C(1)-C(8A)	1.545(5)
C(1)-C(2)	1.554(7)
C(1)-H(1)	0.9800
C(2)-C(3)	1.515(7)
C(2)-C(13)	1.534(7)
C(2)-H(2)	0.9800
C(3)-C(4)	1.314(7)
C(3)-C(10)	1.502(9)
C(4A)-C(4)	1.492(8)
C(4A)-C(5)	1.536(6)
C(4A)-C(11)	1.544(6)
C(4A)-C(8A)	1.563(6)
C(4)-H(4)	0.9300
C(5)-O(5)	1.425(6)
C(5)-C(6)	1.509(8)
C(5)-H(5)	0.9800
C(7)-O(7)	1.419(6)
C(7)-C(6)	1.530(8)
C(7)-C(8)	1.538(6)
C(7)-H(7)	0.9800
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(8)-C(12)	1.531(7)
C(8)-C(8A)	1.532(7)
C(8)-H(8)	0.9800

C(8A)-H(8A)	0.9800
C(9)-O(9)	1.205(6)
C(9)-H(9)	0.9300
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(14)	1.349(7)
C(13)-C(16)	1.498(8)
C(14)-C(17)	1.502(8)
C(14)-C(15)	1.506(9)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(51)-C(511)	1.529(11)
C(51)-C(513)	1.530(13)
C(51)-C(512)	1.544(8)
C(51)-Si(5)	1.871(5)
C(52)-Si(5)	1.866(7)
C(52)-H(52A)	0.9600
C(52)-H(52B)	0.9600
C(52)-H(52C)	0.9600
C(53)-Si(5)	1.841(9)
C(53)-H(53A)	0.9600
C(53)-H(53B)	0.9600
C(53)-H(53C)	0.9600
C(71)-C(711)	1.483(16)

C(71)-C(713)	1.495(16)
C(71)-C(712)	1.565(17)
C(71)-Si(7)	1.889(11)
C(72)-Si(7)	1.858(11)
C(72)-H(72A)	0.9600
C(72)-H(72B)	0.9600
C(72)-H(72C)	0.9600
C(73)-Si(7)	1.853(11)
C(73)-H(73A)	0.9600
C(73)-H(73B)	0.9600
C(73)-H(73C)	0.9600
C(511)-H(51G)	0.9600
C(511)-H(51H)	0.9600
C(511)-H(51I)	0.9600
C(512)-H(51A)	0.9600
C(512)-H(51B)	0.9600
C(512)-H(51C)	0.9600
C(513)-H(51D)	0.9600
C(513)-H(51E)	0.9600
C(513)-H(51F)	0.9600
C(711)-H(71G)	0.9600
C(711)-H(71H)	0.9600
C(711)-H(71I)	0.9600
C(712)-H(71D)	0.9600
C(712)-H(71E)	0.9600
C(712)-H(71F)	0.9600
C(713)-H(71A)	0.9600
C(713)-H(71B)	0.9600
C(713)-H(71C)	0.9600
Si(5)-O(5)	1.637(4)
Si(7)-O(7)	1.631(4)

C(9)-C(1)-C(8A)	116.7(4)
C(9)-C(1)-C(2)	104.8(4)
C(8A)-C(1)-C(2)	113.2(4)
C(9)-C(1)-H(1)	107.2
C(8A)-C(1)-H(1)	107.2
C(2)-C(1)-H(1)	107.2

C(3)-C(2)-C(13)	110.2(4)
C(3)-C(2)-C(1)	113.4(4)
C(13)-C(2)-C(1)	114.4(4)
C(3)-C(2)-H(2)	106.0
C(13)-C(2)-H(2)	106.0
C(1)-C(2)-H(2)	106.0
C(4)-C(3)-C(10)	121.6(5)
C(4)-C(3)-C(2)	122.2(5)
C(10)-C(3)-C(2)	116.1(4)
C(4)-C(4A)-C(5)	109.4(4)
C(4)-C(4A)-C(11)	106.7(4)
C(5)-C(4A)-C(11)	108.4(3)
C(4)-C(4A)-C(8A)	110.9(3)
C(5)-C(4A)-C(8A)	107.9(3)
C(11)-C(4A)-C(8A)	113.4(4)
C(3)-C(4)-C(4A)	125.6(5)
C(3)-C(4)-H(4)	117.2
C(4A)-C(4)-H(4)	117.2
O(5)-C(5)-C(6)	109.0(4)
O(5)-C(5)-C(4A)	110.2(3)
C(6)-C(5)-C(4A)	111.6(4)
O(5)-C(5)-H(5)	108.7
C(6)-C(5)-H(5)	108.7
C(4A)-C(5)-H(5)	108.7
O(7)-C(7)-C(6)	109.0(4)
O(7)-C(7)-C(8)	109.8(4)
C(6)-C(7)-C(8)	113.0(4)
O(7)-C(7)-H(7)	108.3
C(6)-C(7)-H(7)	108.3
C(8)-C(7)-H(7)	108.3
C(5)-C(6)-C(7)	112.4(4)
C(5)-C(6)-H(6A)	109.1
C(7)-C(6)-H(6A)	109.1
C(5)-C(6)-H(6B)	109.1
C(7)-C(6)-H(6B)	109.1
H(6A)-C(6)-H(6B)	107.9
C(12)-C(8)-C(8A)	115.3(4)
C(12)-C(8)-C(7)	108.3(4)

C(8A)-C(8)-C(7)	109.5(4)
C(12)-C(8)-H(8)	107.9
C(8A)-C(8)-H(8)	107.9
C(7)-C(8)-H(8)	107.9
C(8)-C(8A)-C(1)	116.2(4)
C(8)-C(8A)-C(4A)	111.4(3)
C(1)-C(8A)-C(4A)	107.9(3)
C(8)-C(8A)-H(8A)	107.0
C(1)-C(8A)-H(8A)	107.0
C(4A)-C(8A)-H(8A)	107.0
O(9)-C(9)-C(1)	123.5(5)
O(9)-C(9)-H(9)	118.2
C(1)-C(9)-H(9)	118.2
C(3)-C(10)-H(10A)	109.5
C(3)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(3)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(4A)-C(11)-H(11A)	109.5
C(4A)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(4A)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(8)-C(12)-H(12A)	109.5
C(8)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(8)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(16)	121.7(5)
C(14)-C(13)-C(2)	121.8(5)
C(16)-C(13)-C(2)	116.4(4)
C(13)-C(14)-C(17)	121.2(6)
C(13)-C(14)-C(15)	124.5(5)
C(17)-C(14)-C(15)	114.2(6)
C(14)-C(15)-H(15A)	109.5

C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(511)-C(51)-C(513)	113.7(7)
C(511)-C(51)-C(512)	107.5(7)
C(513)-C(51)-C(512)	107.3(8)
C(511)-C(51)-Si(5)	110.1(5)
C(513)-C(51)-Si(5)	109.4(5)
C(512)-C(51)-Si(5)	108.6(4)
Si(5)-C(52)-H(52A)	109.5
Si(5)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
Si(5)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
Si(5)-C(53)-H(53A)	109.5
Si(5)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
Si(5)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(711)-C(71)-C(713)	108.2(13)
C(711)-C(71)-C(712)	109.3(11)
C(713)-C(71)-C(712)	109.5(12)

C(711)-C(71)-Si(7)	111.5(7)
C(713)-C(71)-Si(7)	110.0(8)
C(712)-C(71)-Si(7)	108.4(11)
Si(7)-C(72)-H(72A)	109.5
Si(7)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
Si(7)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
Si(7)-C(73)-H(73A)	109.5
Si(7)-C(73)-H(73B)	109.5
H(73A)-C(73)-H(73B)	109.5
Si(7)-C(73)-H(73C)	109.5
H(73A)-C(73)-H(73C)	109.5
H(73B)-C(73)-H(73C)	109.5
C(51)-C(511)-H(51G)	109.5
C(51)-C(511)-H(51H)	109.5
H(51G)-C(511)-H(51H)	109.5
C(51)-C(511)-H(51I)	109.5
H(51G)-C(511)-H(51I)	109.5
H(51H)-C(511)-H(51I)	109.5
C(51)-C(512)-H(51A)	109.5
C(51)-C(512)-H(51B)	109.5
H(51A)-C(512)-H(51B)	109.5
C(51)-C(512)-H(51C)	109.5
H(51A)-C(512)-H(51C)	109.5
H(51B)-C(512)-H(51C)	109.5
C(51)-C(513)-H(51D)	109.5
C(51)-C(513)-H(51E)	109.5
H(51D)-C(513)-H(51E)	109.5
C(51)-C(513)-H(51F)	109.5
H(51D)-C(513)-H(51F)	109.5
H(51E)-C(513)-H(51F)	109.5
C(71)-C(711)-H(71G)	109.5
C(71)-C(711)-H(71H)	109.5
H(71G)-C(711)-H(71H)	109.5
C(71)-C(711)-H(71I)	109.5
H(71G)-C(711)-H(71I)	109.5

H(71H)-C(711)-H(71I)	109.5
C(71)-C(712)-H(71D)	109.5
C(71)-C(712)-H(71E)	109.5
H(71D)-C(712)-H(71E)	109.5
C(71)-C(712)-H(71F)	109.5
H(71D)-C(712)-H(71F)	109.5
H(71E)-C(712)-H(71F)	109.5
C(71)-C(713)-H(71A)	109.5
C(71)-C(713)-H(71B)	109.5
H(71A)-C(713)-H(71B)	109.5
C(71)-C(713)-H(71C)	109.5
H(71A)-C(713)-H(71C)	109.5
H(71B)-C(713)-H(71C)	109.5
O(5)-Si(5)-C(53)	110.5(3)
O(5)-Si(5)-C(52)	110.6(3)
C(53)-Si(5)-C(52)	109.6(5)
O(5)-Si(5)-C(51)	104.4(3)
C(53)-Si(5)-C(51)	112.0(4)
C(52)-Si(5)-C(51)	109.7(3)
O(7)-Si(7)-C(73)	111.2(4)
O(7)-Si(7)-C(72)	109.0(4)
C(73)-Si(7)-C(72)	109.5(8)
O(7)-Si(7)-C(71)	103.3(4)
C(73)-Si(7)-C(71)	109.0(5)
C(72)-Si(7)-C(71)	114.7(7)
C(5)-O(5)-Si(5)	128.6(3)
C(7)-O(7)-Si(7)	127.5(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **25**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	58(2)	62(2)	89(3)	10(2)	0(2)	2(2)
C(2)	63(2)	63(2)	95(3)	7(2)	-1(2)	-3(2)
C(3)	75(2)	67(2)	101(4)	0(3)	-6(3)	-2(2)
C(4A)	52(2)	62(2)	90(3)	7(2)	-1(2)	1(2)
C(4)	67(2)	73(2)	91(4)	7(2)	-8(2)	-1(2)
C(5)	58(2)	61(2)	93(3)	11(2)	6(2)	5(2)
C(7)	74(2)	70(2)	94(3)	-6(2)	9(3)	-4(2)
C(6)	75(2)	64(2)	106(4)	4(3)	8(3)	6(2)
C(8)	68(2)	68(2)	83(3)	5(2)	4(2)	-1(2)
C(8A)	55(2)	60(2)	91(3)	11(2)	5(2)	3(1)
C(9)	77(3)	74(2)	92(4)	1(3)	0(3)	16(2)
C(10)	122(4)	94(3)	107(5)	-13(4)	-21(4)	-1(3)
C(11)	56(2)	84(3)	109(4)	15(3)	6(2)	1(2)
C(12)	93(3)	90(3)	103(4)	-5(3)	-17(3)	1(3)
C(13)	76(2)	80(3)	86(3)	-3(3)	4(2)	1(2)
C(14)	91(3)	86(3)	94(4)	-14(3)	-10(3)	17(2)
C(15)	143(5)	76(3)	121(5)	4(3)	-5(4)	15(3)
C(16)	86(3)	102(4)	143(6)	-4(4)	30(4)	-11(3)
C(17)	107(4)	134(5)	120(5)	-36(5)	-10(4)	47(4)
C(51)	73(3)	96(3)	138(6)	25(4)	14(3)	-6(2)
C(52)	108(4)	121(5)	206(10)	67(6)	33(6)	43(4)
C(53)	135(6)	182(8)	116(6)	29(6)	-23(5)	-50(6)
C(71)	208(10)	97(4)	140(7)	-20(5)	-43(7)	13(5)
C(72)	99(6)	229(12)	400(20)	-137(15)	2(9)	-33(7)
C(73)	205(10)	106(5)	199(10)	-5(6)	3(8)	-51(6)
C(511)	109(5)	169(7)	179(9)	93(7)	38(5)	-4(5)
C(512)	78(3)	130(5)	159(7)	34(5)	12(4)	26(3)
C(513)	115(6)	171(8)	275(14)	-72(9)	32(7)	-70(6)
C(711)	340(20)	193(12)	138(9)	-12(9)	-35(12)	35(14)
C(712)	390(30)	203(13)	233(15)	-117(12)	-99(17)	-42(14)
C(713)	215(12)	228(13)	172(11)	-41(10)	17(10)	84(11)

Si(5)	68(1)	86(1)	111(1)	28(1)	6(1)	5(1)
Si(7)	111(1)	92(1)	156(2)	-28(1)	-7(1)	-12(1)
O(5)	63(1)	69(2)	103(2)	16(2)	7(2)	2(1)
O(7)	99(2)	78(2)	106(3)	-14(2)	5(2)	-4(2)
O(9)	117(3)	91(2)	106(3)	22(2)	-3(2)	28(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for compound **25**.

	x	y	z	U(eq)
H(1)	3270	3254	4729	83
H(2)	3571	2557	4023	88
H(4)	2097	4149	3267	92
H(5)	2199	5243	3735	85
H(7)	6150	5300	4650	95
H(6A)	2402	5513	4684	98
H(6B)	3786	5952	4352	98
H(8)	3711	4451	5227	88
H(8A)	5630	4177	4217	82
H(9)	7033	3116	4774	97
H(10A)	3962	2952	2720	161
H(10B)	1961	3185	2741	161
H(10C)	2532	2519	3037	161
H(11A)	1252	4516	4791	125
H(11B)	839	3838	4490	125
H(11C)	203	4506	4213	125
H(12A)	6122	3884	5561	143
H(12B)	6613	4634	5653	143
H(12C)	7434	4240	5139	143
H(15A)	5652	1537	4425	170
H(15B)	5851	1109	3870	170
H(15C)	4243	1604	3934	170

H(16A)	6671	3658	3464	166
H(16B)	7489	3117	3060	166
H(16C)	8370	3258	3654	166
H(17A)	8510	1985	3143	181
H(17B)	8449	1373	3556	181
H(17C)	9310	2043	3759	181
H(52A)	2461	6238	3000	217
H(52B)	4015	6582	2662	217
H(52C)	4048	6572	3330	217
H(53A)	4728	4579	2401	216
H(53B)	4380	5218	2034	216
H(53C)	2873	4941	2434	216
H(72A)	8945	5695	5744	366
H(72B)	9451	6403	5514	366
H(72C)	8955	5833	5087	366
H(73A)	6524	6852	4621	255
H(73B)	6307	7361	5123	255
H(73C)	4635	6975	4892	255
H(51G)	7313	5688	2036	228
H(51H)	9128	5974	2265	228
H(51I)	7391	6410	2287	228
H(51A)	8362	4880	3367	184
H(51B)	9691	5097	2885	184
H(51C)	7946	4704	2730	184
H(51D)	7227	6522	3425	281
H(51E)	9219	6308	3325	281
H(51F)	8012	5908	3751	281
H(71G)	4894	5643	6521	337
H(71H)	5254	6163	7005	337
H(71I)	6861	5853	6667	337
H(71D)	7883	6972	6539	411
H(71E)	6177	7370	6726	411
H(71F)	6920	7444	6105	411
H(71A)	3439	7017	5838	308
H(71B)	3374	7062	6505	308
H(71C)	2850	6398	6198	308

Table 6. Torsion angles [°] for compound **25.**

C(9)-C(1)-C(2)-C(3)	-163.4(4)
C(8A)-C(1)-C(2)-C(3)	-35.1(5)
C(9)-C(1)-C(2)-C(13)	-35.8(5)
C(8A)-C(1)-C(2)-C(13)	92.5(4)
C(13)-C(2)-C(3)-C(4)	-124.3(5)
C(1)-C(2)-C(3)-C(4)	5.4(6)
C(13)-C(2)-C(3)-C(10)	58.0(6)
C(1)-C(2)-C(3)-C(10)	-172.3(5)
C(10)-C(3)-C(4)-C(4A)	176.9(5)
C(2)-C(3)-C(4)-C(4A)	-0.6(8)
C(5)-C(4A)-C(4)-C(3)	143.6(5)
C(11)-C(4A)-C(4)-C(3)	-99.3(5)
C(8A)-C(4A)-C(4)-C(3)	24.7(6)
C(4)-C(4A)-C(5)-O(5)	-57.9(5)
C(11)-C(4A)-C(5)-O(5)	-173.9(4)
C(8A)-C(4A)-C(5)-O(5)	63.0(5)
C(4)-C(4A)-C(5)-C(6)	-179.1(3)
C(11)-C(4A)-C(5)-C(6)	64.9(5)
C(8A)-C(4A)-C(5)-C(6)	-58.3(5)
O(5)-C(5)-C(6)-C(7)	-66.8(5)
C(4A)-C(5)-C(6)-C(7)	55.1(5)
O(7)-C(7)-C(6)-C(5)	-174.4(4)
C(8)-C(7)-C(6)-C(5)	-52.0(6)
O(7)-C(7)-C(8)-C(12)	-59.1(5)
C(6)-C(7)-C(8)-C(12)	179.0(4)
O(7)-C(7)-C(8)-C(8A)	174.6(3)
C(6)-C(7)-C(8)-C(8A)	52.7(5)
C(12)-C(8)-C(8A)-C(1)	56.1(5)
C(7)-C(8)-C(8A)-C(1)	178.4(3)
C(12)-C(8)-C(8A)-C(4A)	-179.8(4)
C(7)-C(8)-C(8A)-C(4A)	-57.6(5)
C(9)-C(1)-C(8A)-C(8)	-54.5(6)
C(2)-C(1)-C(8A)-C(8)	-176.4(3)
C(9)-C(1)-C(8A)-C(4A)	179.6(4)
C(2)-C(1)-C(8A)-C(4A)	57.8(5)
C(4)-C(4A)-C(8A)-C(8)	-179.7(4)

C(5)-C(4A)-C(8A)-C(8)	60.4(5)
C(11)-C(4A)-C(8A)-C(8)	-59.7(5)
C(4)-C(4A)-C(8A)-C(1)	-51.0(5)
C(5)-C(4A)-C(8A)-C(1)	-170.9(4)
C(11)-C(4A)-C(8A)-C(1)	69.0(5)
C(8A)-C(1)-C(9)-O(9)	137.0(5)
C(2)-C(1)-C(9)-O(9)	-96.8(6)
C(3)-C(2)-C(13)-C(14)	-127.2(6)
C(1)-C(2)-C(13)-C(14)	103.6(6)
C(3)-C(2)-C(13)-C(16)	52.9(7)
C(1)-C(2)-C(13)-C(16)	-76.3(6)
C(16)-C(13)-C(14)-C(17)	0.9(10)
C(2)-C(13)-C(14)-C(17)	-179.1(6)
C(16)-C(13)-C(14)-C(15)	179.4(6)
C(2)-C(13)-C(14)-C(15)	-0.5(9)
C(511)-C(51)-Si(5)-O(5)	171.7(5)
C(513)-C(51)-Si(5)-O(5)	-62.7(7)
C(512)-C(51)-Si(5)-O(5)	54.2(6)
C(511)-C(51)-Si(5)-C(53)	52.1(7)
C(513)-C(51)-Si(5)-C(53)	177.8(7)
C(512)-C(51)-Si(5)-C(53)	-65.3(7)
C(511)-C(51)-Si(5)-C(52)	-69.8(7)
C(513)-C(51)-Si(5)-C(52)	55.8(8)
C(512)-C(51)-Si(5)-C(52)	172.7(6)
C(711)-C(71)-Si(7)-O(7)	55.3(11)
C(713)-C(71)-Si(7)-O(7)	-64.7(9)
C(712)-C(71)-Si(7)-O(7)	175.6(9)
C(711)-C(71)-Si(7)-C(73)	173.6(11)
C(713)-C(71)-Si(7)-C(73)	53.6(10)
C(712)-C(71)-Si(7)-C(73)	-66.1(10)
C(711)-C(71)-Si(7)-C(72)	-63.3(13)
C(713)-C(71)-Si(7)-C(72)	176.7(9)
C(712)-C(71)-Si(7)-C(72)	57.0(11)
C(6)-C(5)-O(5)-Si(5)	-107.8(4)
C(4A)-C(5)-O(5)-Si(5)	129.5(4)
C(53)-Si(5)-O(5)-C(5)	-82.1(5)
C(52)-Si(5)-O(5)-C(5)	39.4(5)
C(51)-Si(5)-O(5)-C(5)	157.3(4)

C(6)-C(7)-O(7)-Si(7)	-94.7(5)
C(8)-C(7)-O(7)-Si(7)	141.0(4)
C(73)-Si(7)-O(7)-C(7)	59.2(6)
C(72)-Si(7)-O(7)-C(7)	-61.6(8)
C(71)-Si(7)-O(7)-C(7)	176.0(5)

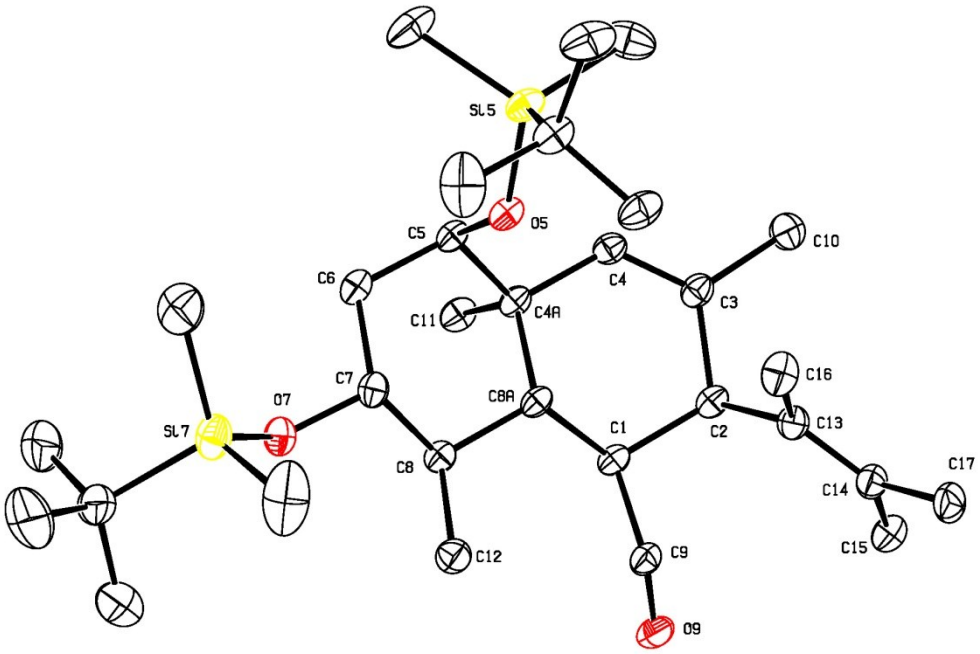


Figure 4 S. Molecular structure of compound **25**. Non-H atoms are present as displacement ellipsoids at the 30% probability level. The H-atoms are omitted for clarity.

Compound 26.

Table 1.1. Crystal data and structure refinement for compound **26**.

Identification code	ar160909_1_0m_a	
Empirical formula	C31 H58 O3 Si2	
Formula weight	534.95	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 8.2887(11) Å	a= 90°.
	b = 17.918(4) Å	b= 104.347(4)°.
	c = 12.294(2) Å	g = 90°.
Volume	1769.0(5) $Å^3$	
Z	2	
Density (calculated)	1.004 Mg/m^3	
Absorption coefficient	1.094 mm^{-1}	
F(000)	592	
Crystal size	0.216 x 0.166 x 0.067 mm^3	
Theta range for data collection	3.711 to 65.082°.	
Index ranges	-8<=h<=9, -21<=k<=21, -14<=l<=14	
Reflections collected	45058	
Independent reflections	5959 [R(int) = 0.0686]	
Completeness to theta = 65.082°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7531 and 0.4574	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5959 / 106 / 381	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0969, wR2 = 0.2401	
R indices (all data)	R1 = 0.1066, wR2 = 0.2533	
Absolute structure parameter	0.02(6)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.555 and -0.271 $e.Å^{-3}$	

Table 2.1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for compound **26**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4262(5)	5419(3)	4471(4)	65(1)
C(2)	4323(6)	5113(3)	3298(4)	72(1)
C(3)	6125(7)	5044(3)	3210(5)	82(1)
C(4A)	7189(6)	5949(3)	4802(4)	74(1)
C(4)	7333(6)	5405(3)	3890(4)	81(1)
C(5)	8143(5)	5630(3)	5957(4)	76(1)
O(5)	7659(4)	4867(2)	6098(3)	80(1)
Si(5)	8927(2)	4150(1)	6460(2)	97(1)
C(51)	7900(11)	3525(5)	7357(7)	121(2)
C(511)	8860(20)	2766(7)	7515(13)	188(6)
C(512)	6122(13)	3361(6)	6747(8)	135(3)
C(513)	7970(30)	3915(9)	8459(9)	198(7)
C(52)	11001(11)	4473(6)	7325(11)	160(4)
C(53)	9200(10)	3649(4)	5206(9)	117(2)
C(6)	7864(7)	6075(3)	6937(5)	86(1)
C(7)	6038(7)	6194(3)	6880(4)	80(1)
O(7)	5856(6)	6650(3)	7800(3)	96(1)
Si(7A)	5967(8)	6374(2)	9096(3)	107(2)
Si(7B)	4822(11)	6466(4)	8800(5)	106(3)
C(72)	4910(30)	5446(8)	9085(12)	237(11)
C(73B)	2620(30)	6710(30)	8550(30)	168(14)
C(73A)	8120(30)	6280(20)	9897(16)	202(14)
C(712)	5830(60)	7876(16)	9680(30)	215(13)
C(711)	4910(50)	6880(20)	10900(20)	214(14)
C(71A)	4940(30)	7115(12)	9718(13)	158(7)
C(713)	3150(50)	7260(40)	9070(30)	290(20)
C(71B)	6050(40)	6940(13)	10059(18)	138(8)
C(715)	6250(90)	7784(18)	9860(50)	182(18)
C(716)	5720(80)	6720(30)	11170(30)	186(16)
C(714)	7970(50)	6710(30)	10200(40)	200(17)

C(8)	5185(6)	6580(3)	5803(4)	74(1)
C(8A)	5338(5)	6131(2)	4754(4)	65(1)
C(9)	2453(7)	5538(4)	4389(6)	95(2)
O(9)	1683(7)	5189(4)	4930(7)	150(3)
C(10)	6405(11)	4545(5)	2291(7)	117(2)
C(11)	8079(9)	6683(4)	4593(7)	103(2)
C(12)	3397(8)	6822(4)	5796(6)	95(2)
C(13)	3333(7)	4391(3)	3033(4)	81(1)
C(14)	1971(8)	4316(5)	2192(6)	106(2)
C(15)	1276(13)	4912(8)	1365(8)	150(4)
C(16)	3955(10)	3758(4)	3820(7)	109(2)
C(17)	976(12)	3606(7)	2021(11)	153(4)

Table 3.1. Bond lengths [Å] and angles [°] compound **26**.

C(1)-C(9)	1.493(7)
C(1)-C(8A)	1.546(6)
C(1)-C(2)	1.555(7)
C(1)-H(1)	0.9800
C(2)-C(13)	1.524(7)
C(2)-C(3)	1.529(7)
C(2)-H(2)	0.9800
C(3)-C(4)	1.307(8)
C(3)-C(10)	1.503(8)
C(4A)-C(4)	1.511(7)
C(4A)-C(5)	1.553(8)
C(4A)-C(8A)	1.556(6)
C(4A)-C(11)	1.561(7)
C(4)-H(4)	0.9300
C(5)-O(5)	1.447(6)
C(5)-C(6)	1.509(8)
C(5)-H(5)	0.9800
O(5)-Si(5)	1.651(4)
Si(5)-C(53)	1.845(9)
Si(5)-C(52)	1.875(8)
Si(5)-C(51)	1.913(9)

C(51)-C(512)	1.508(13)
C(51)-C(513)	1.512(16)
C(51)-C(511)	1.565(15)
C(511)-H(51A)	0.9600
C(511)-H(51B)	0.9600
C(511)-H(51C)	0.9600
C(512)-H(51D)	0.9600
C(512)-H(51E)	0.9600
C(512)-H(51F)	0.9600
C(513)-H(51G)	0.9600
C(513)-H(51H)	0.9600
C(513)-H(51I)	0.9600
C(52)-H(52A)	0.9600
C(52)-H(52B)	0.9600
C(52)-H(52C)	0.9600
C(53)-H(53A)	0.9600
C(53)-H(53B)	0.9600
C(53)-H(53C)	0.9600
C(6)-C(7)	1.513(8)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-O(7)	1.433(6)
C(7)-C(8)	1.507(8)
C(7)-H(7)	0.9800
O(7)-Si(7A)	1.649(5)
O(7)-Si(7B)	1.697(7)
Si(7A)-C(73A)	1.821(18)
Si(7A)-C(71A)	1.842(14)
Si(7A)-C(72)	1.878(12)
Si(7B)-C(73B)	1.83(2)
Si(7B)-C(71B)	1.84(2)
Si(7B)-C(72)	1.860(16)
C(72)-H(72A)	0.9600
C(72)-H(72B)	0.9600
C(72)-H(72C)	0.9600
C(72)-H(72D)	0.9600
C(72)-H(72E)	0.9600
C(72)-H(72F)	0.9600

C(73B)-H(73A)	0.9600
C(73B)-H(73B)	0.9600
C(73B)-H(73C)	0.9600
C(73A)-H(73D)	0.9600
C(73A)-H(73E)	0.9600
C(73A)-H(73F)	0.9600
C(712)-C(71A)	1.56(4)
C(712)-H(71A)	0.9600
C(712)-H(71B)	0.9600
C(712)-H(71C)	0.9600
C(711)-C(71A)	1.53(2)
C(711)-H(71D)	0.9600
C(711)-H(71E)	0.9600
C(711)-H(71F)	0.9600
C(71A)-C(713)	1.52(4)
C(713)-H(71G)	0.9600
C(713)-H(71H)	0.9600
C(713)-H(71I)	0.9600
C(71B)-C(716)	1.51(3)
C(71B)-C(715)	1.55(3)
C(71B)-C(714)	1.61(6)
C(715)-H(71J)	0.9600
C(715)-H(71K)	0.9600
C(715)-H(71L)	0.9600
C(716)-H(71M)	0.9600
C(716)-H(71N)	0.9600
C(716)-H(71O)	0.9600
C(714)-H(71P)	0.9600
C(714)-H(71Q)	0.9600
C(714)-H(71R)	0.9600
C(8)-C(12)	1.542(7)
C(8)-C(8A)	1.551(6)
C(8)-H(8)	0.9800
C(8A)-H(8A)	0.9800
C(9)-O(9)	1.203(9)
C(9)-H(9)	0.9300
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600

C(10)-H(10C)	0.9600
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(14)	1.336(8)
C(13)-C(16)	1.497(9)
C(14)-C(15)	1.488(13)
C(14)-C(17)	1.503(12)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600

C(9)-C(1)-C(8A)	114.2(4)
C(9)-C(1)-C(2)	104.5(4)
C(8A)-C(1)-C(2)	110.5(3)
C(9)-C(1)-H(1)	109.1
C(8A)-C(1)-H(1)	109.1
C(2)-C(1)-H(1)	109.1
C(13)-C(2)-C(3)	113.6(4)
C(13)-C(2)-C(1)	111.0(4)
C(3)-C(2)-C(1)	110.6(4)
C(13)-C(2)-H(2)	107.1
C(3)-C(2)-H(2)	107.1
C(1)-C(2)-H(2)	107.1
C(4)-C(3)-C(10)	122.6(5)
C(4)-C(3)-C(2)	121.4(5)
C(10)-C(3)-C(2)	115.9(5)
C(4)-C(4A)-C(5)	109.0(4)
C(4)-C(4A)-C(8A)	111.5(4)

C(5)-C(4A)-C(8A)	112.7(4)
C(4)-C(4A)-C(11)	107.1(4)
C(5)-C(4A)-C(11)	107.8(5)
C(8A)-C(4A)-C(11)	108.6(4)
C(3)-C(4)-C(4A)	127.2(4)
C(3)-C(4)-H(4)	116.4
C(4A)-C(4)-H(4)	116.4
O(5)-C(5)-C(6)	107.5(4)
O(5)-C(5)-C(4A)	111.3(4)
C(6)-C(5)-C(4A)	113.1(4)
O(5)-C(5)-H(5)	108.3
C(6)-C(5)-H(5)	108.3
C(4A)-C(5)-H(5)	108.3
C(5)-O(5)-Si(5)	126.2(3)
O(5)-Si(5)-C(53)	110.8(3)
O(5)-Si(5)-C(52)	110.2(4)
C(53)-Si(5)-C(52)	109.8(5)
O(5)-Si(5)-C(51)	105.4(3)
C(53)-Si(5)-C(51)	111.2(4)
C(52)-Si(5)-C(51)	109.3(5)
C(512)-C(51)-C(513)	110.6(11)
C(512)-C(51)-C(511)	107.3(9)
C(513)-C(51)-C(511)	112.7(10)
C(512)-C(51)-Si(5)	110.3(5)
C(513)-C(51)-Si(5)	108.8(8)
C(511)-C(51)-Si(5)	107.1(9)
C(51)-C(511)-H(51A)	109.5
C(51)-C(511)-H(51B)	109.5
H(51A)-C(511)-H(51B)	109.5
C(51)-C(511)-H(51C)	109.5
H(51A)-C(511)-H(51C)	109.5
H(51B)-C(511)-H(51C)	109.5
C(51)-C(512)-H(51D)	109.5
C(51)-C(512)-H(51E)	109.5
H(51D)-C(512)-H(51E)	109.5
C(51)-C(512)-H(51F)	109.5
H(51D)-C(512)-H(51F)	109.5
H(51E)-C(512)-H(51F)	109.5

C(51)-C(513)-H(51G)	109.5
C(51)-C(513)-H(51H)	109.5
H(51G)-C(513)-H(51H)	109.5
C(51)-C(513)-H(51I)	109.5
H(51G)-C(513)-H(51I)	109.5
H(51H)-C(513)-H(51I)	109.5
Si(5)-C(52)-H(52A)	109.5
Si(5)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
Si(5)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
Si(5)-C(53)-H(53A)	109.5
Si(5)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
Si(5)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(5)-C(6)-C(7)	112.8(4)
C(5)-C(6)-H(6A)	109.0
C(7)-C(6)-H(6A)	109.0
C(5)-C(6)-H(6B)	109.0
C(7)-C(6)-H(6B)	109.0
H(6A)-C(6)-H(6B)	107.8
O(7)-C(7)-C(8)	108.2(4)
O(7)-C(7)-C(6)	110.1(4)
C(8)-C(7)-C(6)	110.5(4)
O(7)-C(7)-H(7)	109.3
C(8)-C(7)-H(7)	109.3
C(6)-C(7)-H(7)	109.3
C(7)-O(7)-Si(7A)	126.9(4)
C(7)-O(7)-Si(7B)	129.2(4)
O(7)-Si(7A)-C(73A)	111.3(10)
O(7)-Si(7A)-C(71A)	105.4(6)
C(73A)-Si(7A)-C(71A)	109.6(13)
O(7)-Si(7A)-C(72)	110.1(5)
C(73A)-Si(7A)-C(72)	108.1(15)
C(71A)-Si(7A)-C(72)	112.4(11)

O(7)-Si(7B)-C(73B)	119.7(13)
O(7)-Si(7B)-C(71B)	104.2(9)
C(73B)-Si(7B)-C(71B)	110.7(17)
O(7)-Si(7B)-C(72)	108.9(6)
C(73B)-Si(7B)-C(72)	104.9(17)
C(71B)-Si(7B)-C(72)	107.9(11)
Si(7A)-C(72)-H(72A)	109.5
Si(7A)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
Si(7A)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
Si(7B)-C(72)-H(72D)	109.5
Si(7B)-C(72)-H(72E)	109.5
H(72D)-C(72)-H(72E)	109.5
Si(7B)-C(72)-H(72F)	109.5
H(72D)-C(72)-H(72F)	109.5
H(72E)-C(72)-H(72F)	109.5
Si(7B)-C(73B)-H(73A)	109.5
Si(7B)-C(73B)-H(73B)	109.5
H(73A)-C(73B)-H(73B)	109.5
Si(7B)-C(73B)-H(73C)	109.5
H(73A)-C(73B)-H(73C)	109.5
H(73B)-C(73B)-H(73C)	109.5
Si(7A)-C(73A)-H(73D)	109.5
Si(7A)-C(73A)-H(73E)	109.5
H(73D)-C(73A)-H(73E)	109.5
Si(7A)-C(73A)-H(73F)	109.5
H(73D)-C(73A)-H(73F)	109.5
H(73E)-C(73A)-H(73F)	109.5
C(71A)-C(712)-H(71A)	109.5
C(71A)-C(712)-H(71B)	109.5
H(71A)-C(712)-H(71B)	109.5
C(71A)-C(712)-H(71C)	109.5
H(71A)-C(712)-H(71C)	109.5
H(71B)-C(712)-H(71C)	109.5
C(71A)-C(711)-H(71D)	109.5
C(71A)-C(711)-H(71E)	109.5

H(71D)-C(711)-H(71E)	109.5
C(71A)-C(711)-H(71F)	109.5
H(71D)-C(711)-H(71F)	109.5
H(71E)-C(711)-H(71F)	109.5
C(713)-C(71A)-C(711)	107(2)
C(713)-C(71A)-C(712)	104(3)
C(711)-C(71A)-C(712)	113(2)
C(713)-C(71A)-Si(7A)	113(2)
C(711)-C(71A)-Si(7A)	108.4(15)
C(712)-C(71A)-Si(7A)	110.4(17)
C(71A)-C(713)-H(71G)	109.5
C(71A)-C(713)-H(71H)	109.5
H(71G)-C(713)-H(71H)	109.5
C(71A)-C(713)-H(71I)	109.5
H(71G)-C(713)-H(71I)	109.5
H(71H)-C(713)-H(71I)	109.5
C(716)-C(71B)-C(715)	117(4)
C(716)-C(71B)-C(714)	104(4)
C(715)-C(71B)-C(714)	97(4)
C(716)-C(71B)-Si(7B)	117(3)
C(715)-C(71B)-Si(7B)	112(2)
C(714)-C(71B)-Si(7B)	107(2)
C(71B)-C(715)-H(71J)	109.5
C(71B)-C(715)-H(71K)	109.5
H(71J)-C(715)-H(71K)	109.5
C(71B)-C(715)-H(71L)	109.5
H(71J)-C(715)-H(71L)	109.5
H(71K)-C(715)-H(71L)	109.5
C(71B)-C(716)-H(71M)	109.5
C(71B)-C(716)-H(71N)	109.5
H(71M)-C(716)-H(71N)	109.5
C(71B)-C(716)-H(71O)	109.5
H(71M)-C(716)-H(71O)	109.5
H(71N)-C(716)-H(71O)	109.5
C(71B)-C(714)-H(71P)	109.5
C(71B)-C(714)-H(71Q)	109.5
H(71P)-C(714)-H(71Q)	109.5
C(71B)-C(714)-H(71R)	109.5

H(71P)-C(714)-H(71R)	109.5
H(71Q)-C(714)-H(71R)	109.5
C(7)-C(8)-C(12)	112.0(4)
C(7)-C(8)-C(8A)	112.0(4)
C(12)-C(8)-C(8A)	114.6(4)
C(7)-C(8)-H(8)	105.8
C(12)-C(8)-H(8)	105.8
C(8A)-C(8)-H(8)	105.8
C(1)-C(8A)-C(8)	117.0(3)
C(1)-C(8A)-C(4A)	110.1(3)
C(8)-C(8A)-C(4A)	111.1(4)
C(1)-C(8A)-H(8A)	105.9
C(8)-C(8A)-H(8A)	105.9
C(4A)-C(8A)-H(8A)	105.9
O(9)-C(9)-C(1)	123.3(7)
O(9)-C(9)-H(9)	118.3
C(1)-C(9)-H(9)	118.3
C(3)-C(10)-H(10A)	109.5
C(3)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(3)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(4A)-C(11)-H(11A)	109.5
C(4A)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(4A)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(8)-C(12)-H(12A)	109.5
C(8)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(8)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(16)	120.9(6)
C(14)-C(13)-C(2)	123.9(6)
C(16)-C(13)-C(2)	115.1(4)

C(13)-C(14)-C(15)	124.6(8)
C(13)-C(14)-C(17)	121.5(8)
C(15)-C(14)-C(17)	113.9(8)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4.1. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **26**. The anisotropicdisplacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	56(2)	66(2)	75(2)	6(2)	19(2)	3(2)
C(2)	71(2)	64(2)	78(2)	7(2)	12(2)	9(2)
C(3)	76(3)	88(3)	89(3)	3(2)	32(2)	4(2)
C(4A)	64(2)	70(3)	93(3)	-2(2)	28(2)	-10(2)
C(4)	69(2)	88(3)	95(3)	1(2)	37(2)	2(2)
C(5)	53(2)	74(3)	99(3)	-9(2)	14(2)	-6(2)
O(5)	72(2)	68(2)	92(2)	3(2)	9(2)	3(1)
Si(5)	78(1)	80(1)	119(1)	4(1)	-5(1)	10(1)
C(51)	132(6)	109(5)	103(4)	26(4)	-5(4)	6(4)
C(511)	219(14)	127(8)	188(11)	62(8)	-8(9)	32(9)
C(512)	137(6)	128(7)	136(6)	42(5)	27(5)	-17(5)
C(513)	300(20)	185(14)	109(6)	11(7)	53(8)	-40(13)
C(52)	92(5)	144(8)	202(10)	-6(8)	-43(6)	6(5)
C(53)	98(4)	83(4)	170(7)	-5(4)	34(4)	14(3)
C(6)	79(3)	84(3)	89(3)	-10(2)	10(2)	-3(2)
C(7)	86(3)	72(3)	83(3)	-5(2)	22(2)	3(2)
O(7)	108(3)	92(3)	87(2)	-16(2)	24(2)	6(2)
Si(7A)	132(5)	104(2)	83(2)	-4(1)	26(2)	9(2)
Si(7B)	85(5)	145(5)	89(3)	-21(3)	19(3)	-6(3)
C(72)	400(30)	181(13)	167(10)	-49(9)	148(14)	-147(16)
C(73B)	74(13)	250(40)	190(30)	-40(30)	40(15)	13(16)
C(73A)	175(18)	300(40)	106(10)	-7(15)	-12(10)	120(20)
C(712)	370(30)	120(12)	190(30)	-8(14)	130(30)	78(16)
C(711)	350(40)	210(20)	116(11)	9(14)	130(17)	90(20)
C(71A)	209(16)	179(14)	100(9)	3(9)	62(9)	78(13)
C(713)	208(18)	480(60)	179(19)	-30(30)	63(16)	150(30)
C(71B)	166(19)	100(13)	133(15)	-11(12)	8(16)	24(14)
C(715)	260(40)	110(17)	160(30)	-26(18)	10(30)	-40(20)
C(716)	300(50)	120(20)	130(20)	-14(17)	40(30)	10(30)
C(714)	125(17)	240(40)	190(30)	-80(30)	-51(17)	0(20)

C(8)	72(3)	62(2)	91(3)	-1(2)	23(2)	2(2)
C(8A)	65(2)	56(2)	77(2)	9(2)	21(2)	4(2)
C(9)	66(3)	94(4)	126(4)	-24(3)	23(3)	-5(2)
O(9)	101(3)	142(5)	234(7)	-27(5)	92(4)	-32(4)
C(10)	116(5)	135(6)	107(4)	-30(4)	40(4)	9(4)
C(11)	95(4)	93(4)	135(5)	2(3)	52(4)	-27(3)
C(12)	91(4)	91(4)	105(4)	-12(3)	27(3)	25(3)
C(13)	76(3)	77(3)	86(3)	-9(2)	10(2)	1(2)
C(14)	85(4)	110(5)	112(4)	-23(4)	7(3)	0(3)
C(15)	122(6)	182(10)	116(6)	7(6)	-29(5)	11(6)
C(16)	114(5)	69(3)	132(5)	5(3)	8(4)	-6(3)
C(17)	103(5)	161(9)	179(9)	-67(8)	7(5)	-32(6)

Table 5.1. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **26**.

	x	y	z	U(eq)
H(1)	4691	5037	5041	78
H(2)	3778	5483	2741	87
H(4)	8401	5319	3804	97
H(5)	9337	5637	5990	92
H(51A)	10004	2850	7902	282
H(51B)	8360	2432	7946	282
H(51C)	8813	2549	6793	282
H(51D)	6101	3114	6051	202
H(51E)	5624	3044	7204	202
H(51F)	5508	3819	6599	202
H(51G)	9109	4015	8835	297
H(51H)	7365	4376	8318	297
H(51I)	7481	3600	8923	297
H(52A)	11728	4052	7530	240
H(52B)	11480	4818	6896	240

H(52C)	10857	4715	7991	240
H(53A)	9941	3234	5434	175
H(53B)	8140	3470	4780	175
H(53C)	9662	3982	4751	175
H(6A)	8403	6557	6953	103
H(6B)	8380	5816	7628	103
H(7)	5506	5709	6919	96
H(72A)	4986	5290	9843	355
H(72B)	3765	5488	8687	355
H(72C)	5454	5083	8721	355
H(72D)	4332	5336	9651	355
H(72E)	4403	5181	8409	355
H(72F)	6056	5293	9344	355
H(73A)	2221	6570	9193	252
H(73B)	2483	7237	8430	252
H(73C)	1993	6447	7902	252
H(73D)	8147	6116	10646	303
H(73E)	8673	5914	9542	303
H(73F)	8678	6748	9925	303
H(71A)	6985	7832	10075	323
H(71B)	5754	8013	8915	323
H(71C)	5312	8253	10033	323
H(71D)	6027	6782	11334	320
H(71E)	4433	7270	11256	320
H(71F)	4255	6433	10871	320
H(71G)	3129	7412	8321	432
H(71H)	2508	6813	9054	432
H(71I)	2686	7650	9439	432
H(71J)	6458	7859	9135	273
H(71K)	5253	8041	9901	273
H(71L)	7174	7976	10428	273
H(71M)	5622	6186	11199	279
H(71N)	6630	6883	11770	279
H(71O)	4709	6948	11243	279
H(71P)	8293	6835	9520	300
H(71Q)	8656	6982	10815	300
H(71R)	8099	6186	10334	300
H(8)	5807	7044	5788	89

H(8A)	4960	6467	4113	78
H(9)	1892	5900	3896	114
H(10A)	5362	4334	1890	176
H(10B)	6873	4830	1784	176
H(10C)	7158	4151	2614	176
H(11A)	8013	7043	5159	155
H(11B)	9227	6579	4626	155
H(11C)	7546	6879	3866	155
H(12A)	2874	7037	5080	143
H(12B)	3432	7184	6377	143
H(12C)	2771	6394	5925	143
H(15A)	296	4729	841	226
H(15B)	991	5339	1752	226
H(15C)	2091	5053	968	226
H(16A)	4939	3911	4368	164
H(16B)	3112	3616	4192	164
H(16C)	4214	3340	3404	164
H(17A)	48	3658	1379	229
H(17B)	1669	3201	1900	229
H(17C)	574	3506	2675	229

Table 6.1. Torsion angles [°] for compound **26**.

C(9)-C(1)-C(2)-C(13)	-59.3(5)
C(8A)-C(1)-C(2)-C(13)	177.4(4)
C(9)-C(1)-C(2)-C(3)	173.7(5)
C(8A)-C(1)-C(2)-C(3)	50.4(5)
C(13)-C(2)-C(3)-C(4)	-144.4(5)
C(1)-C(2)-C(3)-C(4)	-18.9(7)
C(13)-C(2)-C(3)-C(10)	36.1(7)
C(1)-C(2)-C(3)-C(10)	161.6(5)
C(10)-C(3)-C(4)-C(4A)	176.8(6)
C(2)-C(3)-C(4)-C(4A)	-2.6(9)
C(5)-C(4A)-C(4)-C(3)	117.1(6)
C(8A)-C(4A)-C(4)-C(3)	-8.0(8)
C(11)-C(4A)-C(4)-C(3)	-126.6(6)

C(4)-C(4A)-C(5)-O(5)	-50.3(5)
C(8A)-C(4A)-C(5)-O(5)	74.0(5)
C(11)-C(4A)-C(5)-O(5)	-166.2(4)
C(4)-C(4A)-C(5)-C(6)	-171.5(4)
C(8A)-C(4A)-C(5)-C(6)	-47.1(5)
C(11)-C(4A)-C(5)-C(6)	72.6(5)
C(6)-C(5)-O(5)-Si(5)	-107.5(4)
C(4A)-C(5)-O(5)-Si(5)	128.1(4)
C(5)-O(5)-Si(5)-C(53)	-94.1(5)
C(5)-O(5)-Si(5)-C(52)	27.6(7)
C(5)-O(5)-Si(5)-C(51)	145.4(4)
O(5)-C(5)-C(6)-C(7)	-71.3(6)
C(4A)-C(5)-C(6)-C(7)	52.0(6)
C(5)-C(6)-C(7)-O(7)	-177.1(4)
C(5)-C(6)-C(7)-C(8)	-57.5(6)
C(6)-C(7)-O(7)-Si(7A)	-81.7(7)
C(8)-C(7)-O(7)-Si(7B)	115.6(6)
C(6)-C(7)-O(7)-Si(7B)	-123.5(7)
C(7)-O(7)-Si(7A)-C(73A)	80.2(14)
C(7)-O(7)-Si(7A)-C(71A)	-161.1(10)
C(7)-O(7)-Si(7A)-C(72)	-39.7(10)
C(7)-O(7)-Si(7B)-C(73B)	-88.9(19)
C(7)-O(7)-Si(7B)-C(71B)	146.7(10)
C(7)-O(7)-Si(7B)-C(72)	31.7(10)
O(7)-Si(7A)-C(71A)-C(713)	58(3)
C(73A)-Si(7A)-C(71A)-C(713)	178(3)
C(72)-Si(7A)-C(71A)-C(713)	-62(3)
O(7)-Si(7A)-C(71A)-C(711)	177(2)
C(73A)-Si(7A)-C(71A)-C(711)	-63(3)
C(72)-Si(7A)-C(71A)-C(711)	57(2)
O(7)-Si(7A)-C(71A)-C(712)	-59(2)
C(73A)-Si(7A)-C(71A)-C(712)	61(3)
C(72)-Si(7A)-C(71A)-C(712)	-179(2)
O(7)-Si(7B)-C(71B)-C(716)	-164(3)
C(73B)-Si(7B)-C(71B)-C(716)	66(3)
C(72)-Si(7B)-C(71B)-C(716)	-49(3)
O(7)-Si(7B)-C(71B)-C(715)	57(4)
C(73B)-Si(7B)-C(71B)-C(715)	-73(4)

C(72)-Si(7B)-C(71B)-C(715)	173(4)
O(7)-Si(7B)-C(71B)-C(714)	-49(3)
C(73B)-Si(7B)-C(71B)-C(714)	-179(3)
C(72)-Si(7B)-C(71B)-C(714)	67(3)
O(7)-C(7)-C(8)-C(12)	-50.4(6)
C(6)-C(7)-C(8)-C(12)	-171.0(5)
O(7)-C(7)-C(8)-C(8A)	179.2(4)
C(6)-C(7)-C(8)-C(8A)	58.5(5)
C(9)-C(1)-C(8A)-C(8)	52.7(6)
C(2)-C(1)-C(8A)-C(8)	170.2(4)
C(9)-C(1)-C(8A)-C(4A)	-179.2(4)
C(2)-C(1)-C(8A)-C(4A)	-61.7(5)
C(7)-C(8)-C(8A)-C(1)	73.6(5)
C(12)-C(8)-C(8A)-C(1)	-55.5(6)
C(7)-C(8)-C(8A)-C(4A)	-54.0(5)
C(12)-C(8)-C(8A)-C(4A)	176.9(5)
C(4)-C(4A)-C(8A)-C(1)	39.2(5)
C(5)-C(4A)-C(8A)-C(1)	-83.7(5)
C(11)-C(4A)-C(8A)-C(1)	156.9(4)
C(4)-C(4A)-C(8A)-C(8)	170.5(4)
C(5)-C(4A)-C(8A)-C(8)	47.5(5)
C(11)-C(4A)-C(8A)-C(8)	-71.8(5)
C(8A)-C(1)-C(9)-O(9)	-124.7(7)
C(2)-C(1)-C(9)-O(9)	114.5(7)
C(3)-C(2)-C(13)-C(14)	-118.8(6)
C(1)-C(2)-C(13)-C(14)	115.9(6)
C(3)-C(2)-C(13)-C(16)	63.5(7)
C(1)-C(2)-C(13)-C(16)	-61.8(6)
C(16)-C(13)-C(14)-C(15)	-179.4(9)
C(2)-C(13)-C(14)-C(15)	3.1(11)
C(16)-C(13)-C(14)-C(17)	2.0(11)
C(2)-C(13)-C(14)-C(17)	-175.5(7)

Symmetry transformations used to generate equivalent atoms:

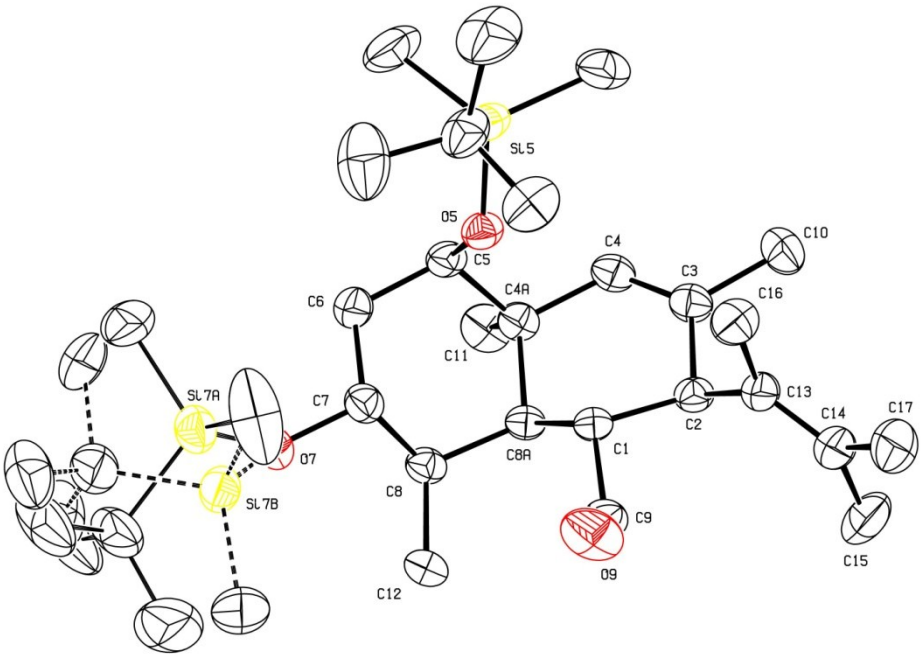


Figure 5 S. Molecular structure of compound **26**. Non-H atoms are present as displacement ellipsoids at the 30% probability level. The H-atoms are omitted for clarity.