

Supporting Information

Strategies for Remote Enantiocontrol in Chiral Gold(III) Complexes Applied to Catalytic Enantioselective γ,δ -Diels-Alder Reactions

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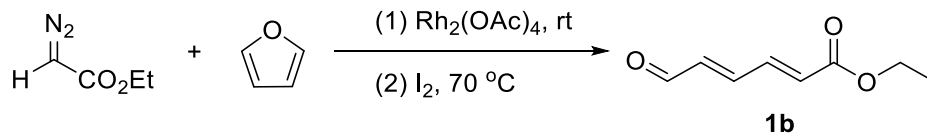
1. General Information

Unless otherwise mentioned, all reactions were performed in oven-dried glassware sealed with rubber septa under a nitrogen atmosphere and were stirred with Teflon-coated magnetic stir bars. Dry tetrahydrofuran (THF), toluene, dimethylformamide (DMF), acetonitrile, triethylamine (TEA) and dichloromethane (DCM) were obtained by passing these previously degassed solvents through activated alumina columns. Dimethyl sulfoxide (DMSO), benzotrifluoride (PhCF₃) and nitromethane (MeNO₂) were distilled from CaH₂ and kept in a sealed tube with 4Å molecular sieves. All other reagents were used as received. Reactions were monitored by thin layer chromatography (TLC) on Silicycle Siliplate™ glass backed TLC plates (250 µm thickness, 60 Å porosity, F-254 indicator) and visualized by UV irradiation and Cerium Ammonium Molybdate stain. Volatile solvents were removed under reduced pressure with a rotary evaporator and dried on high vacuum on a Schlenk line. ¹H-NMR, ¹³C-NMR, and ¹⁹F-NMR spectra were taken with Bruker spectrometers operating at 300, 400, 500, 600 or 700 MHz for ¹H (75, 100, 125, 150 and 175 MHz for ¹³C). Chemical shifts are reported relative to the residual solvent signal. NMR data are reported as follows: chemical shift (multiplicity, coupling constants where applicable, number of hydrogens). Splitting is reported with the following symbols: s = singlet, bs = broad singlet, d = doublet, t = triplet, q = quartets, hept = heptet, dd = doublet of doublets, dt = doublet of triplets, m = multiplet, at = apparent triplet, dq = doublet of quartets. High-resolution mass spectra (HRMS) were performed on a Thermo LTQ-FTICR (7T, ESI) by the QB3 mass spectral facility at the University of California, Berkeley. Elemental Analyses were performed by the Microanalytical Facility at the University of California, Berkeley. Previously reported compounds were synthesized according to literature procedures.

2. Preparation of $\alpha,\beta,\gamma,\delta$ -unsaturated aldehydes

Compound **1a** ((2E,4E)-hepta-2,4-dienal) was purchased from commercial source with an isomer ratio of 86:14 and used as received. Compounds **1b-1p** and **1s** were prepared according to Wenkert et al.¹ Compound **1q** (ethyl (2E,4E)-5-methyl-6-oxohexa-2,4-dienoate) was prepared by the reaction of ethyl diazoacetate with 3-methylfuran according to the following general procedure. Compound **1r** (ethyl (2E,4E)-6-oxohepta-2,4-dienoate) was prepared by the reaction of ethyl diazoacetate with 2-methylfuran according to the following general procedure. Compound **1t** ((1E,3E)-5-oxopenta-1,3-dien-1-yl acetate) was prepared according to Grabowski et al.²

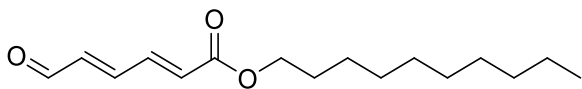
Typical experimental procedures for the preparation of (2E,4E)-6-oxohexa-2,4-dienoate 1b-1s (1b as an example):



(A modified procedure as described in ref. 1 was used). A solution of 20 mmol of ethyl diazoacetate (2.47 mL, 85% purity in DCM from commercial source) in 2 mL of the required furan was slowly (over 10 min) added to a stirring suspension of 0.01 mmol of dirhodium tetraacetate in 8 mL of furan. The reaction mixture was kept stirring at room temperature for over 12 h. The mixture was filtered through a short column of silica gel to remove $\text{Rh}_2(\text{OAc})_4$, washed with DCM or ethyl acetate, and the filtrate was collected in a sealed tube. A small amount of I_2 (ca. 2~5%) was added into the tube, and the mixture was heated to $70\text{ }^\circ\text{C}$ for 6 h. Then cooled down to rt, the mixture was washed with $\text{Na}_2\text{S}_2\text{O}_3$ (aq.), dried over Na_2SO_4 , after the solvent was removed under vacuum, the residue was purified by silica gel column

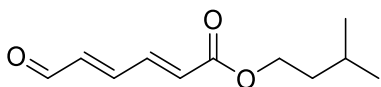
chromatography with petroleum ether (PE)/ethyl acetate (EA) (20:1~5:1) as the eluent to give **1b** as a light yellow oil (1.63 g, 53% yield).

Decyl (2E,4E)-6-oxohexa-2,4-dienoate (1e)



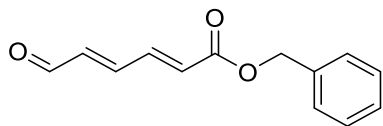
^1H NMR (700 MHz, CDCl_3) δ 9.66 (d, $J = 7.5$ Hz, 1H), 7.40 (dd, $J = 15.1, 11.5$ Hz, 1H), 7.16 (dd, $J = 15.1, 11.6$ Hz, 1H), 6.41 (dd, $J = 15.4, 7.6$ Hz, 1H), 6.30 (d, $J = 15.4$ Hz, 1H), 4.18 (t, $J = 6.5$ Hz, 2H), 1.70 – 1.63 (m, 2H), 1.40 – 1.19 (m, 14H), 0.87 (t, $J = 6.8$ Hz, 3H). ^{13}C NMR (176 MHz, CDCl_3) δ 192.96, 165.55, 147.30, 140.27, 136.97, 130.01, 65.34, 31.89, 29.53, 29.51, 29.30, 29.24, 28.58, 25.91, 22.68, 14.13. HRMS (m/z): calculated for $\text{C}_{16}\text{H}_{26}\text{NaO}_3$ [$\text{M} + \text{Na}$] $^+$, 289.1774; observed, 289.1792.

Isopentyl (2E,4E)-6-oxohexa-2,4-dienoate (1f)



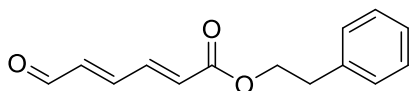
^1H NMR (700 MHz, CDCl_3) δ 9.66 (d, $J = 7.7$ Hz, 1H), 7.40 (dd, $J = 15.3, 11.4$ Hz, 1H), 7.16 (dd, $J = 15.3, 11.4$ Hz, 1H), 6.41 (dd, $J = 15.5, 7.7$ Hz, 1H), 6.30 (d, $J = 15.4$ Hz, 1H), 4.22 (t, $J = 6.9$ Hz, 2H), 1.71 (dt, $J = 13.4, 6.7$ Hz, 1H), 1.57 (q, $J = 6.9$ Hz, 2H), 0.93 (d, $J = 6.8$ Hz, 6H). ^{13}C NMR (176 MHz, CDCl_3) δ 192.96, 165.54, 147.28, 140.28, 136.98, 129.99, 63.82, 37.26, 25.07, 22.46. HRMS (m/z): calculated for $\text{C}_{11}\text{H}_{16}\text{NaO}_3$ [$\text{M} + \text{Na}$] $^+$, 219.0992; observed, 219.1001.

Benzyl (2E,4E)-6-oxohexa-2,4-dienoate (1g)



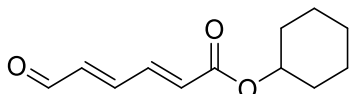
^1H NMR (700 MHz, CDCl_3) δ 9.67 (d, $J = 7.7$ Hz, 1H), 7.45 (dd, $J = 15.3, 11.4$ Hz, 1H), 7.41 – 7.33 (m, 5H), 7.16 (dd, $J = 15.4, 11.4$ Hz, 1H), 6.41 (dd, $J = 15.5, 7.7$ Hz, 1H), 6.35 (d, $J = 15.4$ Hz, 1H), 5.24 (s, 2H). ^{13}C NMR (176 MHz, CDCl_3) δ 192.92, 165.27, 147.07, 140.84, 137.19, 135.46, 129.53, 128.69, 128.54, 128.44, 66.93. HRMS (m/z): calculated for $\text{C}_{13}\text{H}_{12}\text{NaO}_3$ [$\text{M} + \text{Na}$] $^+$, 239.0679; observed, 239.0688.

Phenethyl (2E,4E)-6-oxohexa-2,4-dienoate (1h)



^1H NMR (700 MHz, CDCl_3) δ 9.67 (d, $J = 7.7$ Hz, 1H), 7.39 (dd, $J = 15.4, 11.3$ Hz, 1H), 7.32 (t, $J = 7.4$ Hz, 2H), 7.26 – 7.23 (m, 3H), 7.15 (dd, $J = 15.4, 11.3$ Hz, 1H), 6.41 (dd, $J = 15.4, 7.7$ Hz, 1H), 6.29 (d, $J = 15.4$ Hz, 1H), 4.42 (t, $J = 7.0$ Hz, 2H), 3.01 (t, $J = 7.0$ Hz, 2H). ^{13}C NMR (176 MHz, CDCl_3) δ 192.94, 165.36, 147.16, 140.55, 137.54, 137.10, 129.70, 128.91, 128.60, 126.73, 65.54, 35.06. HRMS (m/z): calculated for $\text{C}_{14}\text{H}_{14}\text{NaO}_3$ [$\text{M} + \text{Na}$] $^+$, 253.0835; observed, 253.0847.

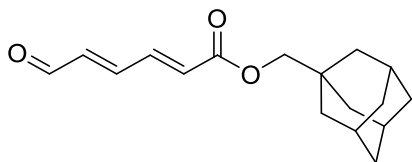
Cyclohexyl (2E,4E)-6-oxohexa-2,4-dienoate (1j)



^1H NMR (700 MHz, CDCl_3) δ 9.66 (d, $J = 7.7$ Hz, 1H), 7.39 (dd, $J = 15.3, 11.3$ Hz, 1H), 7.16 (dd, $J = 15.4, 11.3$ Hz, 1H), 6.41 (dd, $J = 15.4, 7.7$ Hz, 1H), 6.29 (d, $J = 15.4$ Hz, 1H), 4.90 – 4.83 (m, 1H), 1.92 – 1.85 (m,

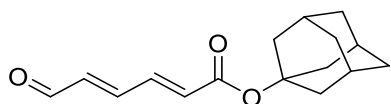
2H), 1.77 – 1.73 (m, 2H), 1.58 – 1.54 (m, 1H), 1.49 – 1.44 (m, 2H), 1.42 – 1.34 (m, 2H), 1.30 – 1.23 (m, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 193.01, 164.90, 147.44, 139.99, 136.85, 130.66, 73.58, 31.60, 25.33, 23.74. HRMS (m/z): calculated for C₁₂H₁₆NaO₃ [M + Na]⁺, 231.0992; observed, 231.0981.

((1*s*,3*s*)-adamantan-1-yl)methyl (2*E*,4*E*)-6-oxohexa-2,4-dienoate (1k)



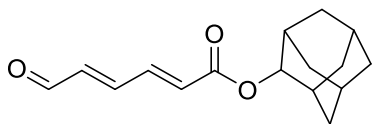
¹H NMR (700 MHz, CDCl₃) δ 9.69 – 9.65 (m, *J* = 7.7 Hz, 1H), 7.41 (dd, *J* = 15.3, 11.4 Hz, 1H), 7.17 (dd, *J* = 15.4, 11.4 Hz, 1H), 6.43 (dd, *J* = 15.5, 7.7 Hz, 1H), 6.34 (d, *J* = 15.4 Hz, 1H), 3.80 (s, 2H), 2.00 (s, 3H), 1.76 – 1.73 (m, 3H), 1.68 – 1.64 (m, 3H), 1.56 (s, 6H). ¹³C NMR (176 MHz, CDCl₃) δ 192.97, 165.68, 147.31, 140.21, 136.97, 130.08, 74.64, 39.28, 36.92, 33.36, 28.00. HRMS (m/z): calculated for C₁₇H₂₂NaO₃ [M + Na]⁺, 297.1461; observed, 297.1475.

(3*s*,5*s*,7*s*)-Adamantan-1-yl (2*E*,4*E*)-6-oxohexa-2,4-dienoate (1l)



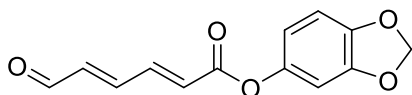
¹H NMR (700 MHz, CDCl₃) δ 9.65 (d, *J* = 7.7 Hz, 1H), 7.30 (dd, *J* = 15.0, 11.6 Hz, 1H), 7.14 (dd, *J* = 15.2, 11.5 Hz, 1H), 6.39 (dd, *J* = 15.4, 7.7 Hz, 1H), 6.22 (d, *J* = 15.3 Hz, 1H), 2.19 (s, 3H), 2.15 (s, 6H), 1.71 – 1.63 (m, 6H). ¹³C NMR (176 MHz, CDCl₃) δ 193.09, 164.37, 147.72, 139.26, 136.56, 132.26, 81.69, 41.30, 36.13, 30.85. HRMS (m/z): calculated for C₁₆H₂₀NaO₃ [M + Na]⁺, 283.1305; observed, 283.1320.

(1*R*,2*S*,5*S*)-Adamantan-2-yl (2*E*,4*E*)-6-oxohexa-2,4-dienoate (1*m*)



^1H NMR (700 MHz, CDCl_3) δ 9.68 (d, $J = 7.7$ Hz, 1H), 7.42 (dd, $J = 15.3, 11.4$ Hz, 1H), 7.17 (dd, $J = 15.4, 11.4$ Hz, 1H), 6.43 (dd, $J = 15.5, 7.7$ Hz, 1H), 6.35 (d, $J = 15.4$ Hz, 1H), 5.04 (s, 1H), 2.05 (t, $J = 15.7$ Hz, 4H), 1.91 – 1.70 (m, 9H), 1.61 – 1.57 (m, 1H). ^{13}C NMR (176 MHz, CDCl_3) δ 193.01, 164.84, 147.47, 139.92, 136.85, 130.84, 77.97, 37.32, 36.31, 31.88, 31.83, 27.19, 26.94. HRMS (m/z): calculated for $\text{C}_{16}\text{H}_{20}\text{NaO}_3$ $[\text{M} + \text{Na}]^+$, 283.1305; observed, 283.1311.

Benzo[*d*][1,3]dioxol-5-yl (2*E*,4*E*)-6-oxohexa-2,4-dienoate (1*s*)

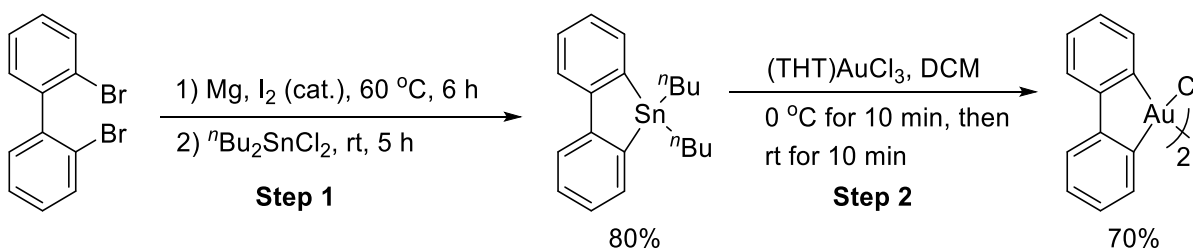


^1H NMR (700 MHz, CDCl_3) δ 9.71 (d, $J = 7.6$ Hz, 1H), 7.58 (dd, $J = 15.4, 11.3$ Hz, 1H), 7.23 (dd, $J = 15.4, 11.3$ Hz, 1H), 6.79 (d, $J = 8.4$ Hz, 1H), 6.66 (d, $J = 2.2$ Hz, 1H), 6.58 (dd, $J = 8.4, 2.3$ Hz, 1H), 6.50 – 6.45 (m, 2H), 6.00 (s, 2H). ^{13}C NMR (176 MHz, CDCl_3) δ 192.83, 164.19, 148.11, 146.62, 145.62, 144.66, 142.12, 137.66, 128.73, 113.79, 108.07, 103.54, 101.83. HRMS (m/z): calculated for $\text{C}_{13}\text{H}_{10}\text{NaO}_5$ $[\text{M} + \text{Na}]^+$, 269.0420; observed, 269.0425.

3. Preparation of Au(III) complexes

IPrAu(III)(biphenyl)Cl was prepared according to reference 3.

3.1. Preparation of (biphenyl)Au(III)Cl dimer:



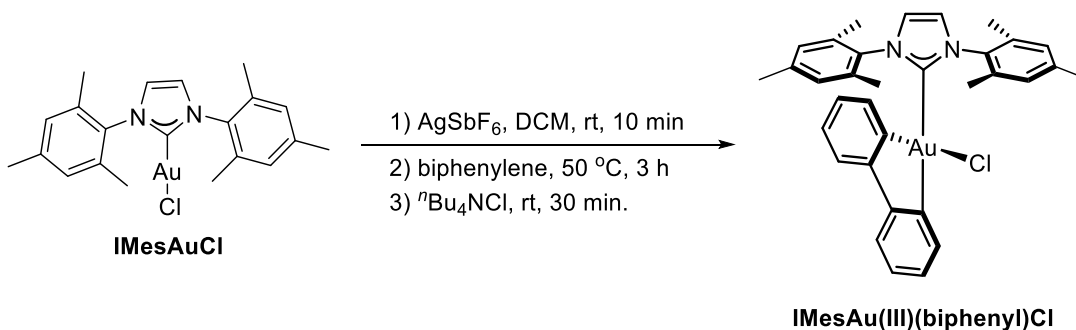
Step 1: (A modified procedure by using Grignard reagent was employed) A 100-mL flask charged with a stir bar, a condenser, and Mg (528 mg, 22 mmol), was added 50 mL THF, and a small piece of I₂ (catalytic amount). 1 mL of 2,2'-Dibromo-1,1'-biphenyl (3.12 g, 10 mmol in 10 mL THF) was added, then the reaction mixture was heated with a heat gun, until the color of I₂ disappeared (the reaction was initiated), stopped heating, and the residue 2,2'-Dibromo-1,1'-biphenyl (in THF) was added. The reaction mixture was heated to 60 °C for 6 h, then cooled down to rt, and dibutyltin(II) chloride (3.03 g, 10 mmol) in 10 mL THF was added, and the reaction was stirred at rt for 5 h. The reaction was quenched with water 40 mL, and extracted with Et₂O, dried over Na₂SO₄. After removing the solvent under vacuum, the residue was purified by column chromatography (the silica gel was neutralized by 5% Et₃N/hexanes) with 2% Et₃N/hexanes as eluent to give 5,5-dibutyl-5H-dibenzo[b,d]stannole as a white solid (3.08 g, 80% yield).

Step 2: 5,5-Dibutyl-5H-dibenzo[b,d]stannole (102 mg, 0.26 mmol) was placed in a 20 mL vial with 5 mL DCM and cooled down to 0 °C, then (THT)AuCl₃ (104 mg, 0.26 mmol) was added portionwise in 10 min.

The cold bath was removed and the reaction was kept stirring for additional 10 min. In a 100-mL flask was charged with a stir bar and 70 mL hexanes, the reaction mixture was passed through a pad of celite into the flask with continuous stirring, a white precipitate was formed, the white solid was collected by filtration (73 mg, 72% yield).

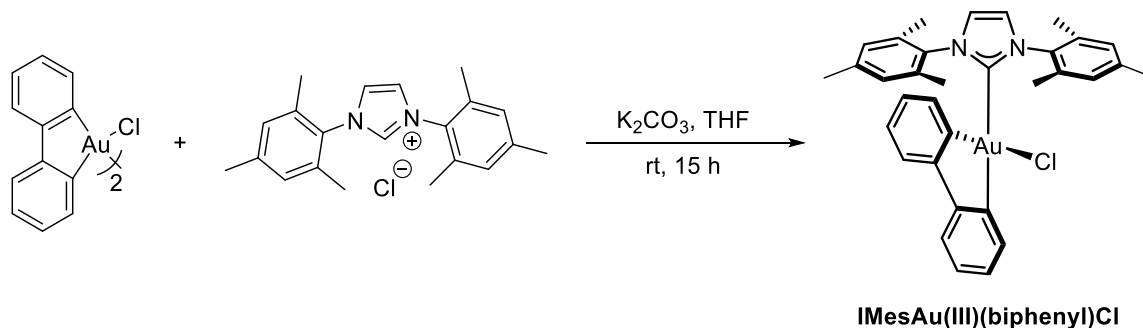
3.2. Preparation of IMesAu(III)(biphenyl)Cl:³ (This compound was prepared via a modified procedure according to IPrAu(III)(biphenyl)Cl).

Method A:



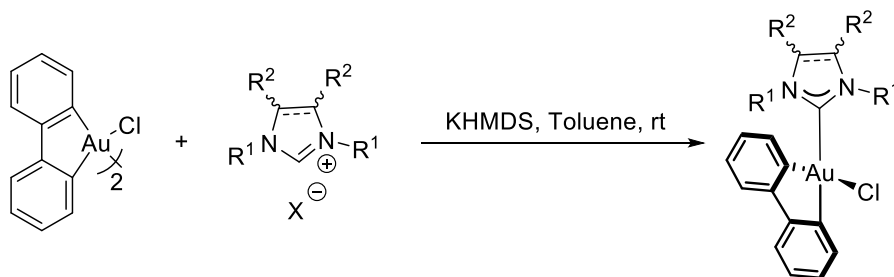
To a mixture of IMesAuCl (43.0 mg, 0.08 mmol) and AgSbF₆ (30.0 mg, 0.09 mmol) was added CH₂Cl₂ (4 mL) at rt and stirred for 10 min. The reaction mixture was then passed through glass fiber to remove AgCl, then biphenylene (27.4 mg, 0.18 mmol) was added, and the reaction mixture was heated to 50 °C and stirred for 3 h. After this time, tetrabutylammonium chloride (27.0 mg, 0.10 mmol) was added and stirred for another 0.5 h. The title complex 3 was purified by flash column chromatography with hexanes/EA (v/v, 5:1) to give a yellow solid (36 mg, 65% yield).

Method B:



A mixture of (biphenyl)Au(III)Cl dimer (112.6 mg, 0.147 mmol), 1,3-dimesityl-1H-imidazol-3-ium chloride (101 mg, 0.294 mmol), and K₂CO₃ (102 mg, 0.735 mmol, 2.5 equiv) was contained in a flask and purged with nitrogen gas. THF (6 mL) was added, and the reaction mixture was kept stirring for 15 h at rt. The mixture was filtered through celite, and product was purified by column chromatography with hexanes/EA = 5:1 as eluent to give a yellow solid (198 mg, 98% yield).

3.3. General procedure for the preparation of (NHC)Au(III)(biphenyl)Cl (For the C₂ symmetric NHC ligand):⁴

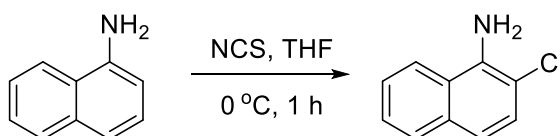


In a glovebox, to the imidazolium salt (1 equiv) in toluene (0.1 M) was added KHMDS (1.2 equiv) in one portion at rt. The reaction mixture was stirred for 2 h and then (biphenyl)Au(III)Cl dimer (0.5 equiv) was added in one portion. The reaction mixture was stirred for 8 h and then the reaction vessel was taken

out from the glovebox. The reaction mixture was then passed through celite and dried under vacuum to give the crude product, which was used as received.

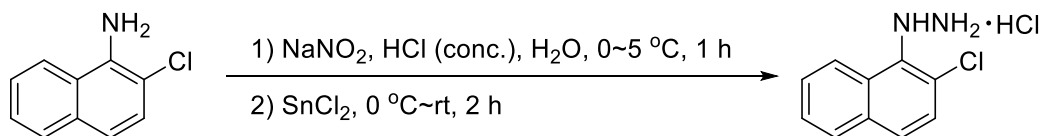
3.4. Path A: General procedure for the synthesis of 1,2,4-triazolo NHC ligand coordinated Au(III) complexes (Take 4y as an example).

3.4.1. Synthesis of 2-chloronaphthalen-1-amine.⁵



To a solution of naphthalen-1-amine (716 mg, 5.0 mmol) in anhydrous THF (50 mL) at 0 °C was added *N*-chlorosuccinimide (NCS, 668 mg, 5.0 mmol, 1.0 equiv.) in one portion. The ice bath was removed and the mixture was stirred for 1 h. The reaction was quenched with water and extracted with ethyl acetate (50 mL × 3). The combined organic phase was dried over sodium sulfate. The solvent was removed under vacuum and the crude product was purified by column chromatography (eluent: hexanes:EA = 5:1) to afford 2-chloronaphthalen-1-amine as a dark red solid (686 mg, 72 %). This unstable amine was used immediately for next step. ¹H NMR (400 MHz, CDCl₃) δ 7.84 (d, *J* = 8.1 Hz, 1H), 7.79 (d, *J* = 7.5 Hz, 1H), 7.53 – 7.44 (m, 2H), 7.36 (d, *J* = 8.8 Hz, 1H), 7.28 – 7.25 (m, 1H), 4.90 (bs, 2H).

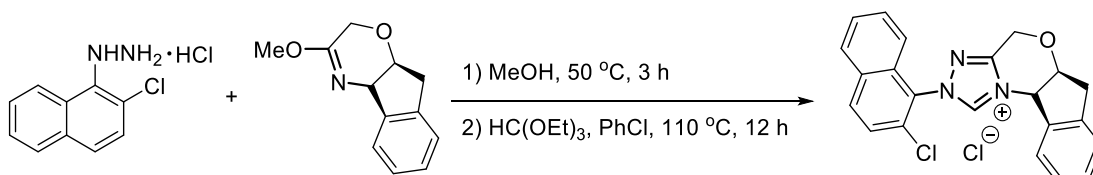
3.4.2. Synthesis of (2-chloronaphthalen-1-yl)hydrazine hydrogen chloride.^{4b}



To a 100 mL-flask charged with a stir bar and 2-chloronaphthalen-1-amine (686 mg, 3.86 mmol), was added 8 mL concentrated HCl (12 M). NaNO₂ (320 mg, 4.63 mmol) in 5 mL water was cooled down to 0

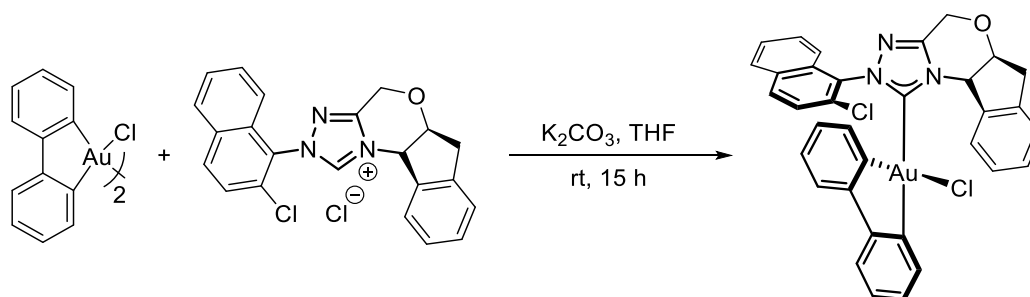
°C, then added dropwise to the reaction mixture. After NaNO₂ was added, the reaction mixture was kept stirring at 0 °C for additional 1 h. SnCl₂ (1.46 g, 7.72 mmol) in 3 mL concentrated HCl (12 M) was cooled down to 0 °C and added slowly (note that when SnCl₂ was added, the reaction foamed), the resulting mixture was slowly warmed up to rt in 1 h. The suspension was filtered to collect the solid, washed with cold brine, then water and Et₂O. The poorly soluble pale yellow solid was used for next step as received.

3.4.3. Synthesis of (5a*S*,10*bS*)-2-(2-chloronaphthalen-1-yl)-2,5a,6,10*b*-tetrahydro-4*H*-indeno[2,1-*b*][1,2,4]triazolo[4,3-*d*][1,4]oxazin-11-ium chloride.



To a flame-dried 10-mL flask was added (4*aS*,9*aS*)-3-methoxy-2,4*a*,9,9*a*-tetrahydroindeno[2,1-*b*][1,4]oxazine (80 mg, 0.4 mmol), (2-chloronaphthalen-1-yl)hydrazine hydrogen chloride (92 mg, 0.4 mmol), and dry MeOH (3 mL). The resulting mixture was heated to 50 °C for 3 h, cooled down and the solvent was removed under reduced pressure. HC(OEt)₃ (1 mL, excess) and PhCl (2 mL) were added, then the reaction mixture was heated to 110 °C for 5 h. Cooled down, and 10 mL of hexanes added. The solid was collected by filtration and washed with Et₂O. The received solid was used directly for next step.

3.4.4. Synthesis of Complex 4y.

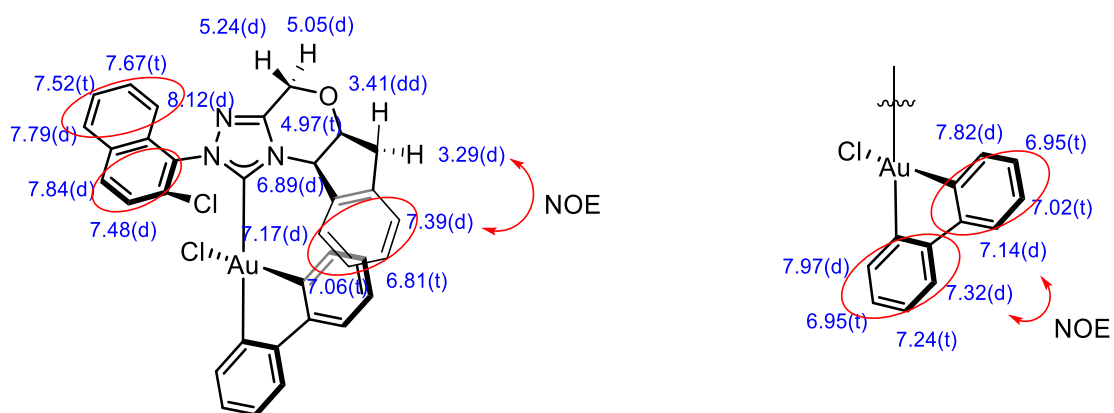


A mixture of (biphenyl)Au(III)Cl dimer (63 mg, 0.15 mmol), (5a*S*,10b*S*)-2-(2-chloronaphthalen-1-yl)-2,5a,6,10b-tetrahydro-4*H*-indeno[2,1-*b*][1,2,4]triazolo[4,3-*d*][1,4] oxazin-11-ium chloride (58 mg, 0.15 mmol), and K₂CO₃ (42 mg, 0.3 mmol, 2.0 equiv) in a 10 mL Schlenk tube was purged with nitrogen gas, then THF (5 mL) was added, and the reaction mixture was kept stirring for 15 h at rt. The resulting mixture was filtered and washed with DCM, after removing the solvent under reduced pressure, the collected solid (112 mg, 98% yield) was composed of four isomers with a ratio of 1.00: 0.15: 1.57: 3.30 (corresponding chemical shifts: 8.44 / 8.39 / 8.18 / 8.12 ppm). The four isomers can be separated by TLC with hexanes/EA = 2:1; however, separation of the isomers by preparative TLC or column chromatography was less successful, because the isomers quickly formed equilibrium in solution. By carefully running a column chromatography with hexanes/EA = 10:1, we successfully obtained one of the major isomers, which was assumed to be the most stable isomer. The product purified by PTLC or column chromatography was dissolved in DCM, then dropwise added to hexanes, the resulting precipitate was collected by filtration, dried and used as catalyst.

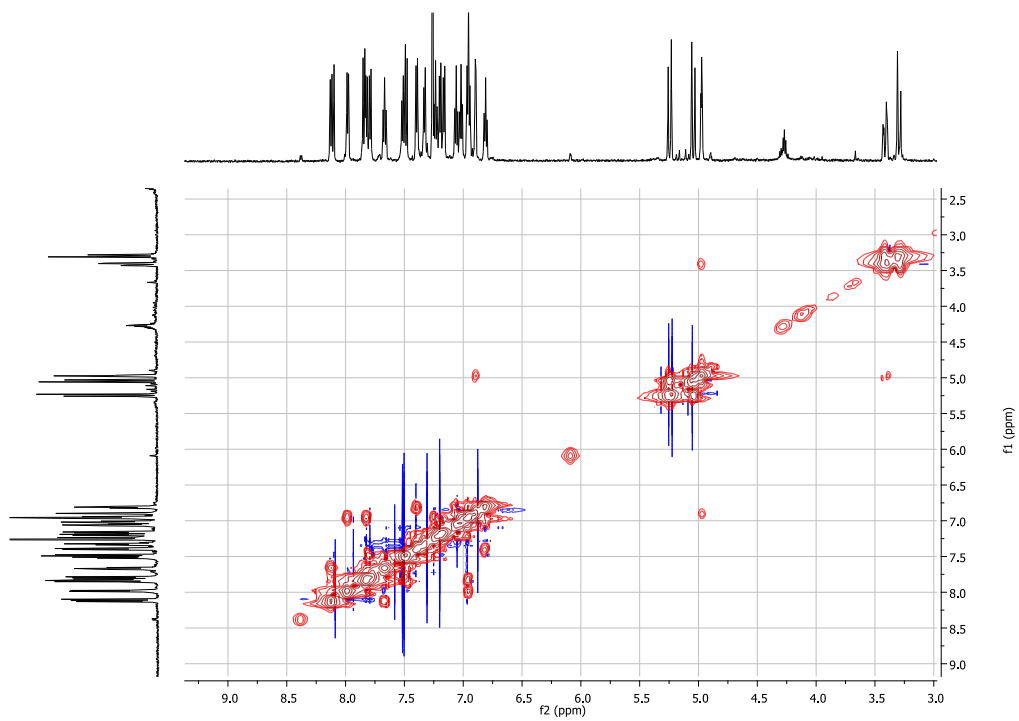
¹H NMR (600 MHz, CD₂Cl₂) δ 8.12 (d, *J* = 8.5 Hz, 1H), 7.90 (dd, *J* = 11.0, 8.9 Hz, 2H), 7.86 (d, *J* = 7.7 Hz, 1H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.52 (d, *J* = 8.9 Hz, 1H), 7.41 (d, *J* = 6.7 Hz, 1H), 7.34 (d, *J* = 7.5 Hz, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 7.22 – 7.20 (m, 1H), 7.16 (d, *J* = 6.3 Hz, 1H), 7.08 (t, *J* = 7.0 Hz, 1H), 7.01 (dd, *J* = 7.4, 6.2 Hz, 1H), 6.93 (dt, *J* = 7.4, 6.9 Hz, 2H), 6.88 (d, *J* = 3.6 Hz,

1H), 6.85 (td, $J = 7.6, 1.5$ Hz, 1H), 5.27 (d, $J = 16.3$ Hz, 1H), 5.08 (d, $J = 16.3$ Hz, 1H), 4.99 (t, $J = 4.1$ Hz, 1H), 3.44 (dd, $J = 16.8, 4.4$ Hz, 1H), 3.28 (d, $J = 16.8$ Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 158.14, 153.18, 152.87, 149.44, 140.18, 137.41, 135.10, 132.93, 132.48, 132.26, 131.77, 130.15, 130.05, 128.92, 128.84, 128.07, 127.67, 127.56, 127.46, 127.20, 126.94, 126.83, 126.57, 125.49, 124.62, 123.92, 121.56, 120.66, 78.50, 62.39, 37.47, 31.60. HRMS (m/z): calculated for $\text{C}_{34}\text{H}_{24}\text{AuCl}_2\text{N}_3\text{NaO}$ [$\text{M} + \text{Na}$] $^+$, 780.0854; observed, 780.0837.

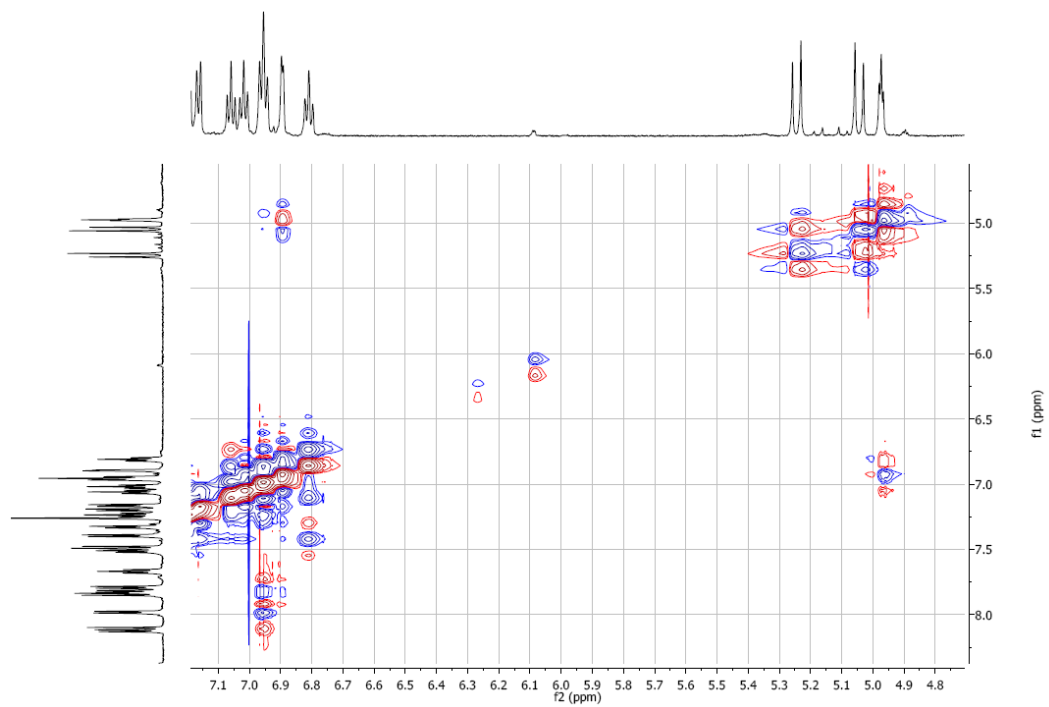
The ^1H - ^1H COSY and 2D-NOESY analysis showed that the structure of the isomer 4y-1 (likely the most stable isomer) is as followed:



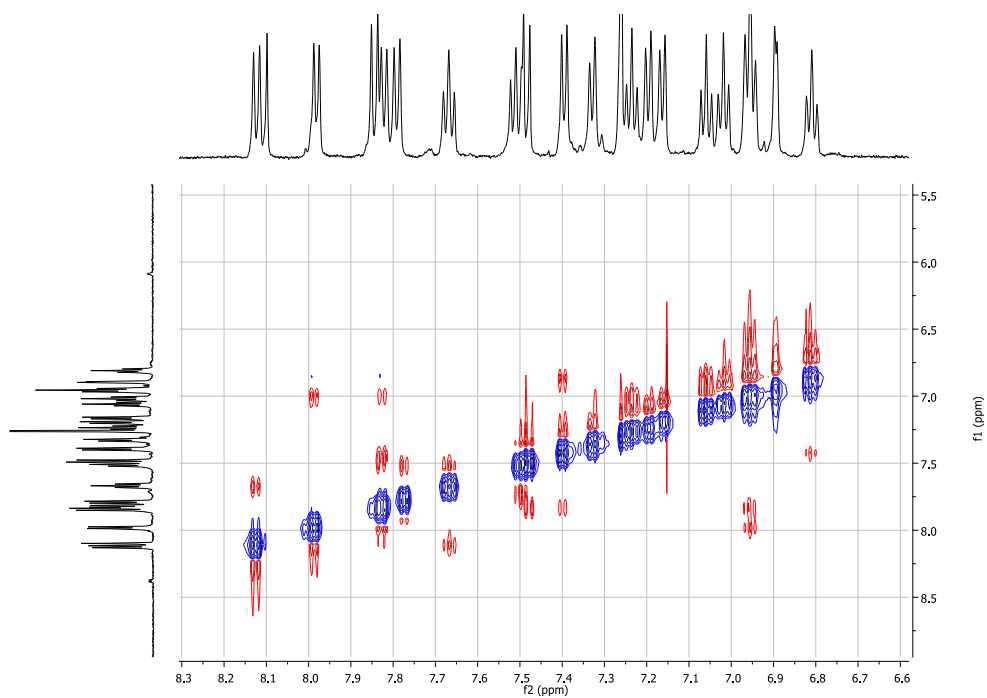
^1H - ^1H COSY spectrum of **4y-1**:



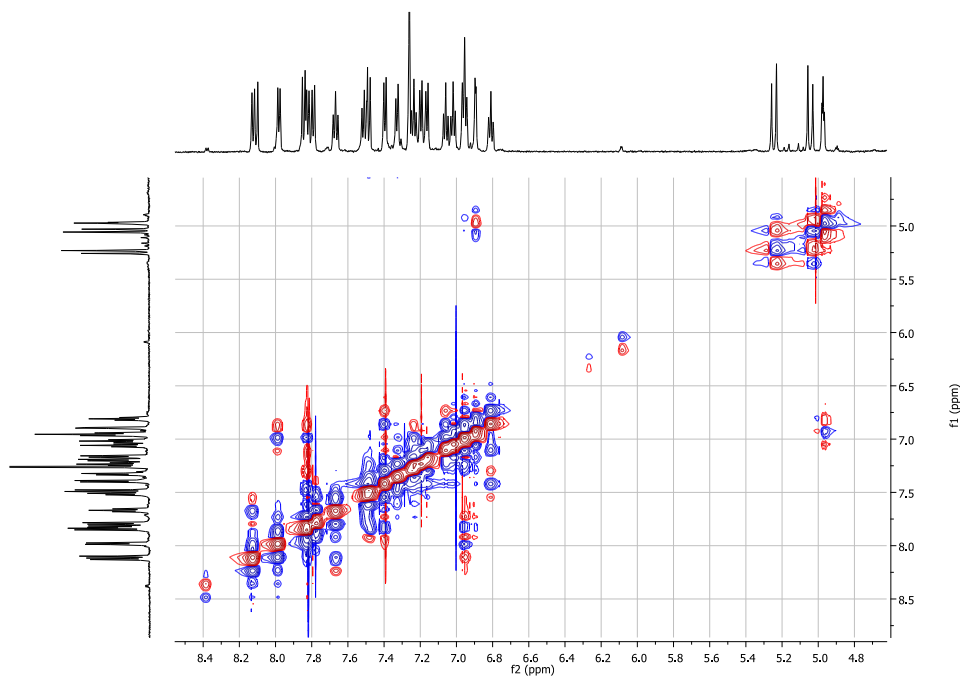
2D-NOESY spectrum of **4y-1**:



2D-NOESY spectrum of **4y-1**:

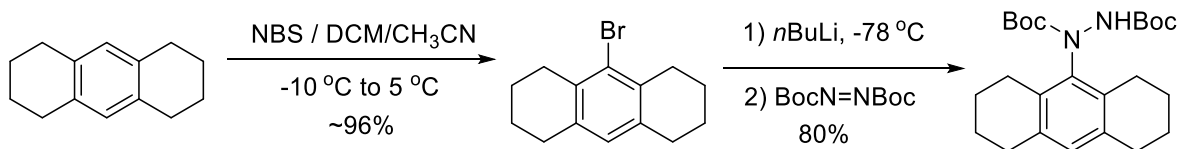


2D-NOESY spectrum of **4y-1**:



3.5. Path B: General procedure for the synthesis of 1,2,4-triazolo NHC ligand coordinated Au(III) complexes (Take 4z as an example).

3.5.1. Synthesis of di-tert-butyl 1-(1,2,3,4,5,6,7,8-octahydroanthracen-9-yl)hydrazine-1,2-dicarboxylate.

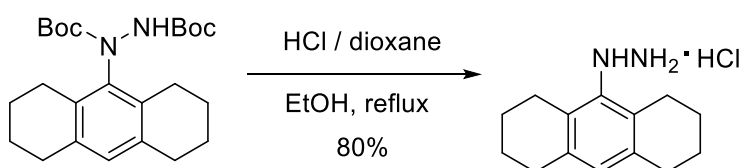


Step 1: 1,2,3,4,5,6,7,8-Octahydroanthracene (2.72 g, 14.6 mmol) was added to a 50-mL flask, 20 mL of DCM and CH₃CN (v/v = 1:1) were added. The solution was cooled down to -10 °C (an ice/EtOH bath), NBS (2.55 g, 14.3 mmol) was added slowly in 30 min. Note: to reduce the dibromonation side reaction, lower NBS loadings were employed. The reaction was kept stirring at -10~5 °C for 7 h, quenched with Na₂S₂O₃ (sat. aq.), the mixture was extracted with Et₂O (30 mL × 3) and dried over MgSO₄. After removing the solvent under reduced pressure, the residue was purified by column chromatography with hexanes as eluent to give product containing some 1,2,3,4,5,6,7,8-octahydroanthracene, which was used in the next step.

Step 2: The product of the first step (3.86 g, 96% purity, 14 mmol) was dissolved in 20 mL of THF and added into a 50-mL flask. The resulting mixture was cooled down to -78 °C, ⁿBuLi (5.6 mL, 2.5 M in hexane) was added slowly. The resulting mixture was kept stirring at -78 °C for additional 1 h, then di-*tert*-butyl (*E*)-diazene-1,2-dicarboxylate (3.22 g, 14 mmol) was dissolved in 7 mL of THF and added slowly. The reaction stirred at -78 °C for an additional 1 h and then the reaction was quenched with water. The material was extracted with EA (50 mL × 3) and dried over MgSO₄. After removing the solvent under reduced pressure, the residue was purified by column chromatography with hexanes/EA = 3:1 to give

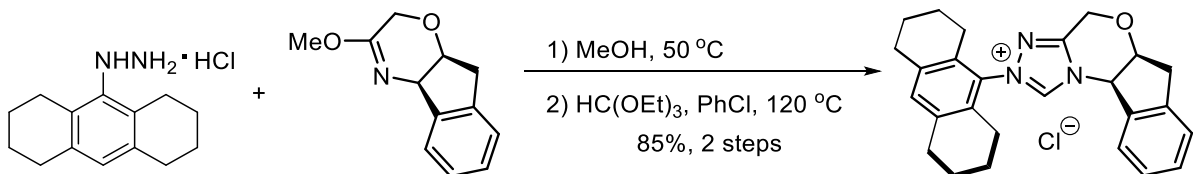
the product di-*tert*-butyl 1-(1,2,3,4,5,6,7,8-octahydroanthracen-9-yl)hydrazine-1,2-dicarboxylate as a white solid (4.66 g, 80% yield). (Note that the 1,2,3,4,5,6,7,8-octahydroanthracene impurity containing in the starting material could be easily removed by column chromatography at this step.) ¹H NMR (500 MHz, CDCl₃) δ 6.80 (s, 1H), 6.54 (s, 1H), 2.92 (s, 2H), 2.71 (d, *J* = 5.8 Hz, 4H), 2.65 – 2.45 (m, 2H), 1.87 – 1.65 (m, 8H), 1.52 (s, 6H), 1.46 (s, 9H), 1.36 (s, 3H).

3.5.2. Synthesis of (1,2,3,4,5,6,7,8-octahydroanthracen-9-yl)hydrazine hydrochloride.



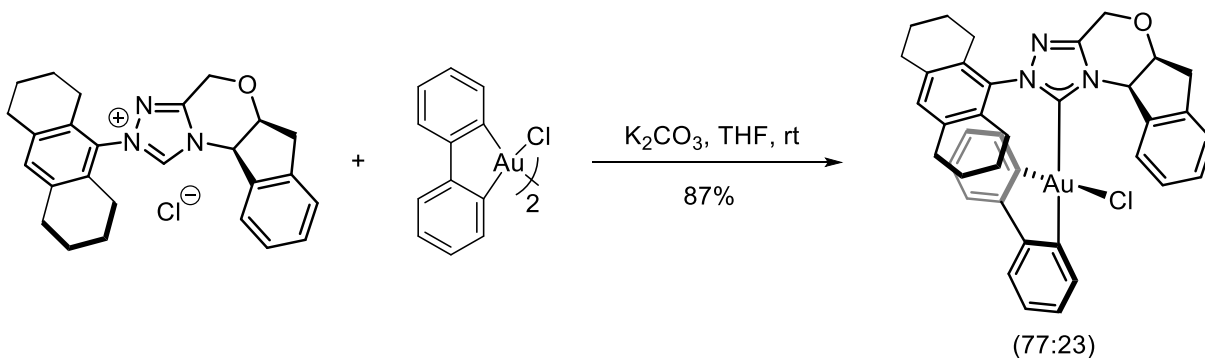
Di-*tert*-butyl 1-(1,2,3,4,5,6,7,8-octahydroanthracen-9-yl)hydrazine-1,2-dicarboxylate (4.66 g, 11.2 mmol) was dissolved in 10 mL of anhydrous EtOH, 20 mL of HCl (1.5 M in 1,4-dioxane) was added at rt. The resulting solution was heated to reflux for 15 min. The solvent was mostly removed and Et₂O (ca. 20 mL) added. The precipitate was collected by filtration and washed by Et₂O to give a white solid, which was poorly soluble in MeOH or DMSO, and used without further purification.

3.5.3. Synthesis of (5a*S*,10*bR*)-2-(1,2,3,4,5,6,7,8-octahydroanthracen-9-yl)-5a,10*b*-dihydro-4*H*,6*H*-indeno[2,1-*b*][1,2,4]triazolo[4,3-*d*][1,4]oxazin-2-ium chloride.



To a flame-dried 10-mL flask was added (4a*S*,9a*S*)-3-methoxy-2,4a,9,9a-tetrahydroindeno[2,1-*b*][1,4]oxazine (72 mg, 0.356 mmol), (1,2,3,4,5,6,7,8-octahydroanthracen-9-yl)hydrazine hydrochloride (90 mg, 0.356 mmol), and dry MeOH (3 mL). The resulting mixture was heated to 50 °C for 16 h, cooled down and the solvent was removed under reduced pressure. HC(OEt)₃ (1 mL, excess) and PhCl (2 mL) were added, then the reaction mixture was heated to 120 °C for 5 h. After cooling, 10 mL of toluene was added, the solid was collected by filtration and washed with toluene to give a brown solid. The received solid was used directly for next step. ¹H NMR (500 MHz, DMSO) δ 11.05 (s, 2H), 7.68 (d, *J* = 5.4 Hz, 1H), 7.38 – 7.23 (m, 4H), 6.98 (s, 1H), 6.70 (s, 1H), 5.02 (s, 1H), 4.74 (t, *J* = 4.3 Hz, 1H), 4.58 (d, *J* = 16.4 Hz, 1H), 4.46 (t, *J* = 13.6 Hz, 1H), 3.43 – 3.24 (m, 1H), 2.98 (d, *J* = 16.9 Hz, 1H), 2.76 – 2.67 (m, 8H), 1.79 – 1.55 (m, 8H).

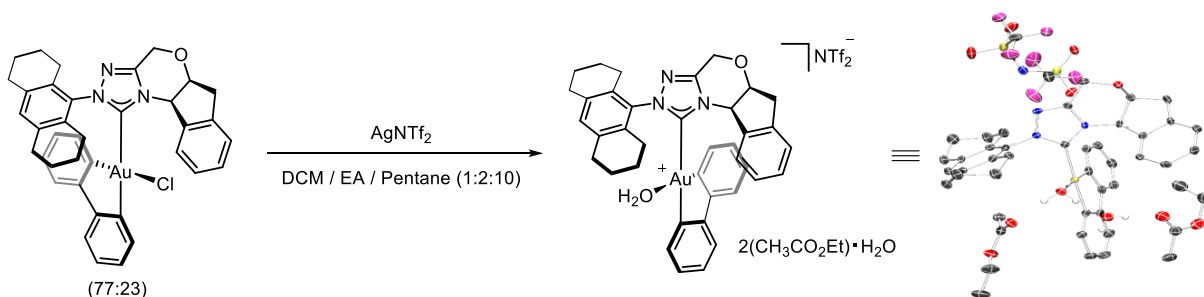
3.5.4. Synthesis of complex 4z.



A mixture of (biphenyl)Au(III)Cl dimer (63 mg, 0.15 mmol), (5a*S*,10b*R*)-2-(1,2,3,4,5,6,7,8-octahydroanthracen-9-yl)-5a,10b-dihydro-4H,6H-indeno[2,1-*b*][1,2,4]triazolo[4,3-*d*][1,4] oxazin-2-ium chloride (65 mg, 0.15 mmol), and K₂CO₃ (42 mg, 0.3 mmol, 2.0 equiv) in a 10 mL Schlenk tube was purged with nitrogen gas, then THF (5 mL) was added, and the reaction mixture was kept stirring for 15 h at rt. This mixture was filtered and washed with DCM. After removing the solvent under reduced pressure, the collected solid (102 mg, 87% yield) was composed of two isomers with a ratio of 77:23

(corresponding chemical shifts: 8.40 / 8.15 ppm). The two isomers cannot be separated by preparative TLC or column chromatography, because the isomers quickly formed equilibrium in solution.

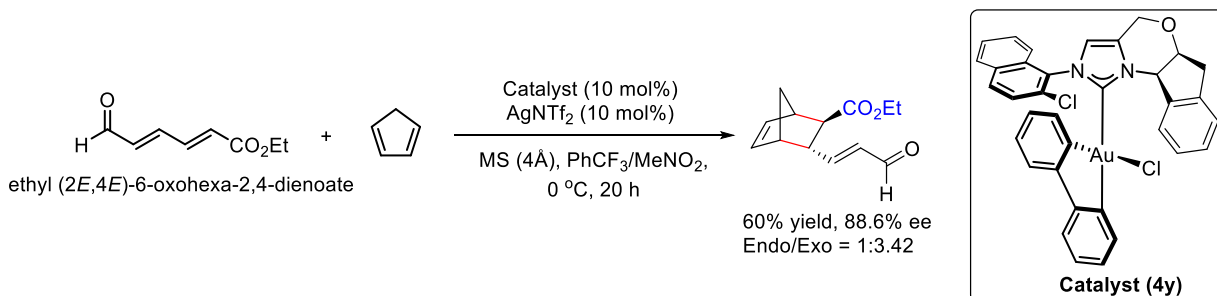
3.5.5. X-ray crystallographic analysis of complex **4z**-NTf₂.



Complex **4z** (10 mg, 0.01279 mmol) and AgNTf₂ (4.96 mg, 0.01279 mmol) was dissolved in 0.5 mL of DCM/EA (1:2, v/v), after stirring at rt for 15 min, the mixture was passed through glass fiber into a 3 mL vial, then pentane (2 mL) was added slowly along the wall of the vial to the top of the solution. The vial was placed in a freezer (the temperature was kept between -20 °C ~ -10 °C) for 53 days, upon which time, needle-like crystals were formed. These were analyzed by X-ray crystallography. (Note that when other silver salts such as AgSbF₆ and AgOTf were used, no crystal was obtained)

4. Characterization of Products

4.1 General procedure for Diels–Alder reaction of 2,4-hexadienal with cyclopentadiene (Take **4y catalyzed ethyl (2*E*,4*E*)-6-oxohexa-2,4-dienoate (**1b**) with cyclopentadiene as an example).**



Au(III) catalyst **4y** (2.3 mg, 0.003 mmol, 10 mol%) and AgNTf₂ (1.2 mg, 0.003 mmol, 10 mol%) were added into a 3 mL vial, then dry PhCF₃ (200 μ L) and MeNO₂ (50 μ L) were added. The resulting mixture was stirred at rt for 15 min, 4 Å MS (ca. 20 mg) were added, and cooled to 0 °C. Ethyl (2*E*,4*E*)-6-oxohexa-2,4-dienoate (4.6 mg, 3.8 μ L, 0.03 mmol) and cyclopentadiene (35 μ L, 0.45 mmol, 15 equiv) were added via a syringe, the vial was capped and wound with parafilm. The mixture was cooled to 0 °C with an ice bath and kept stirring for 24 h. Then the reaction mixture was filtered by glass fiber, and the product was purified by preparative TLC with hexanes/EA = 5:1 as eluent to give product **3b** as a colorless liquid (4 mg, 60% yield).

Note:

(1) Previous reports^{3,4a} employed glass fiber to remove AgCl before adding substrates, we tested the reaction in the presence of AgCl and found almost no influence on the yield and selectivity. Therefore, we continued to use the procedure above without removal of AgCl.

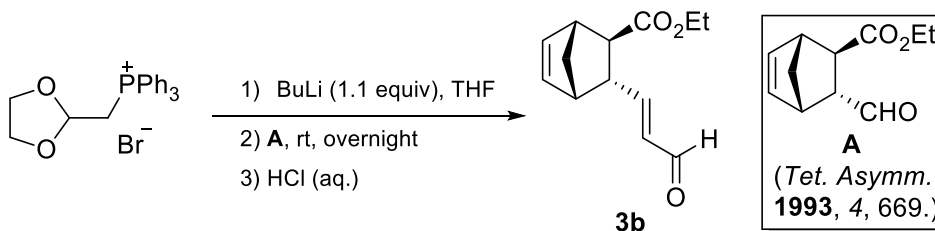
(2) The product yields and ee of Diels-Alder reaction referred to the major diastereomer (isolated or ^1H NMR yields), the minor isomer was often with the same R_f with double bond isomerized side-products of starting material (or unreacted starting material). The ratio of diastereomers and the side-products could be determined by ^1H NMR.

(3) Other solvents, such as toluene was used, the operation was similar with this procedure. For rt temperature reactions, the capped vial was placed on a stir plate at rt.

(4) The purification of product can be performed on column chromatography with same eluent as preparative TLC. Specifically, when the reaction was scaled up to 1 mmol scale with 1 mol% catalyst loading, the product was isolated by column chromatography.

4.2 Determination of Absolute Stereochemistry of **3b**

To determine the absolute configuration of the products, the enantioenriched compound **3b** was synthesized from configurationally well-defined compound **A**, which was reported in literature.⁶ The following HPLC spectra were enantioenriched compound **3b** (synthesized from reported compound **A**) and mixture of enantioenriched compound **3b** and racemic compound **3b** (synthesized from our method). HPLC analysis of the mixture of racemic and enantioenriched compound **3b** showed the configuration of major enantiomer of the product was as drawn in the manuscript (Figure S1 and S2).



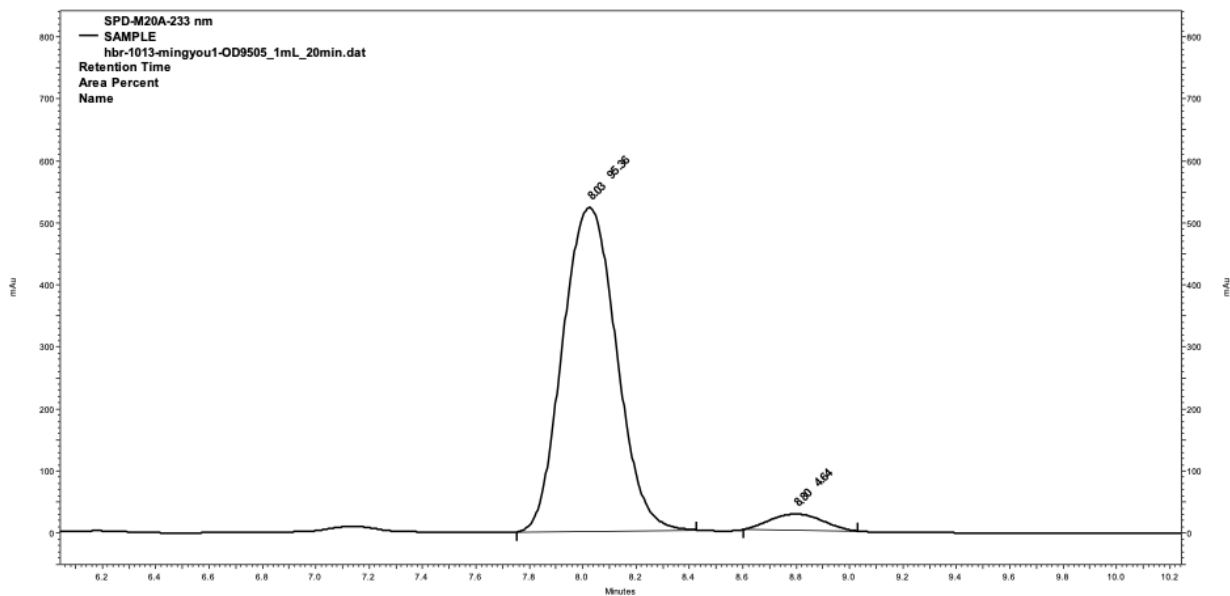


Figure S1. HPLC spectrum of enantioenriched compound **3b** synthesized from configurationally well-defined compound **A**.

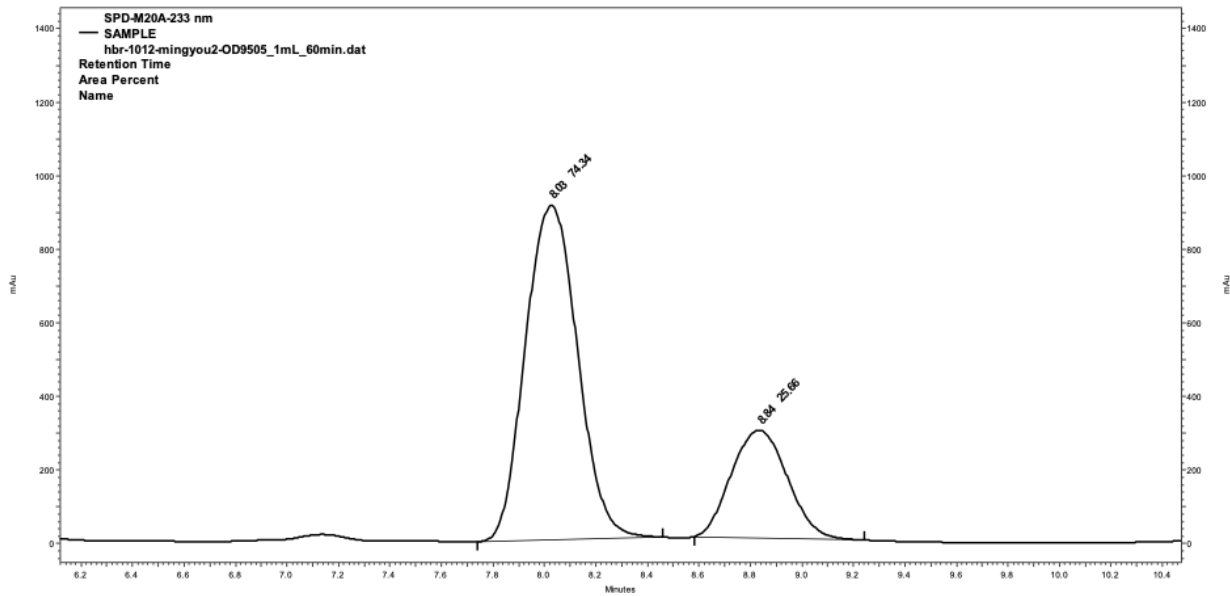
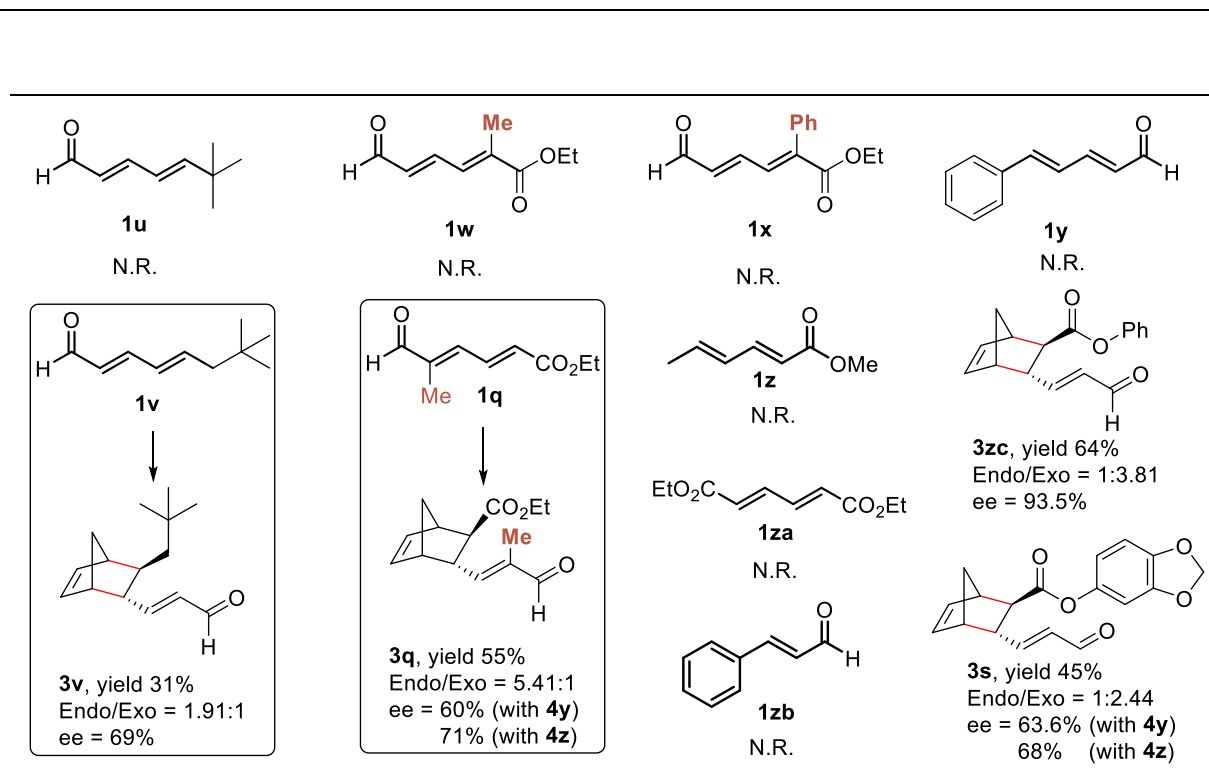


Figure S2. HPLC spectrum of mixed sample of enantioenriched compound **5b** and racemic compound **5b**.



Dienes:

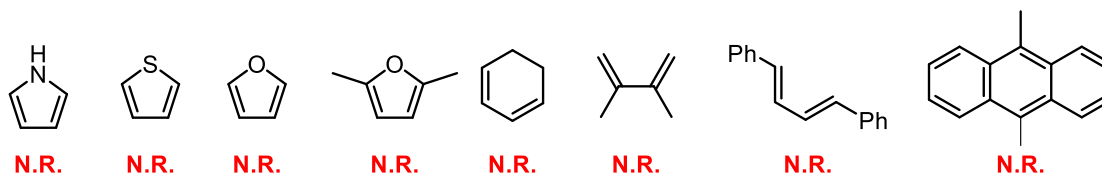
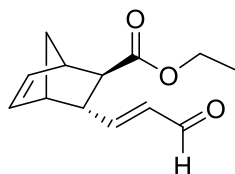


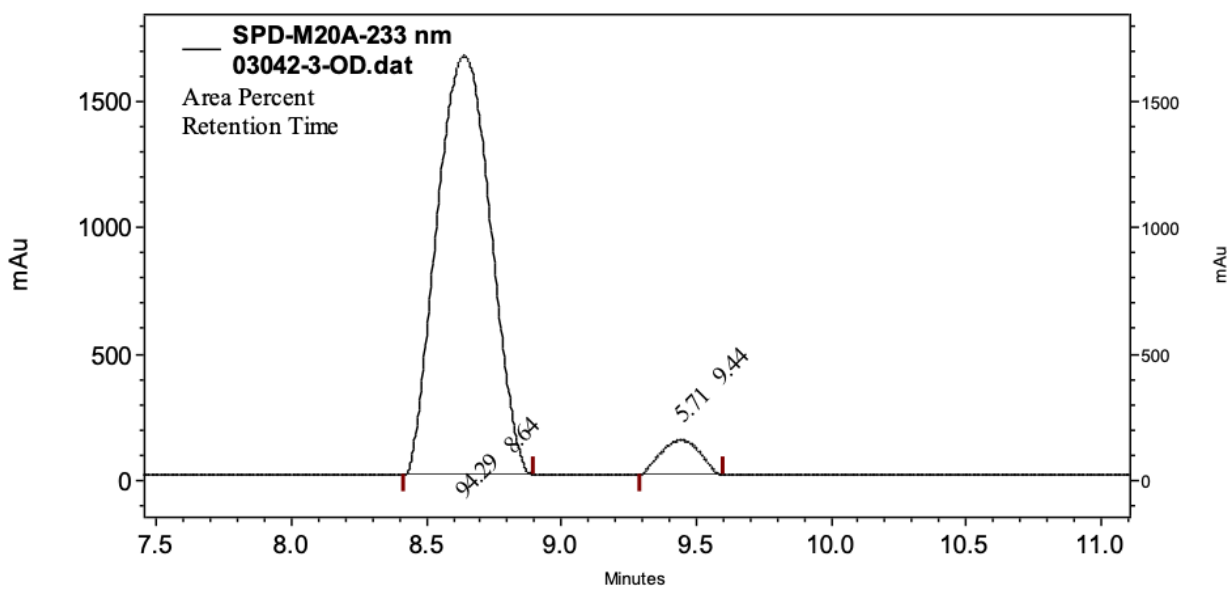
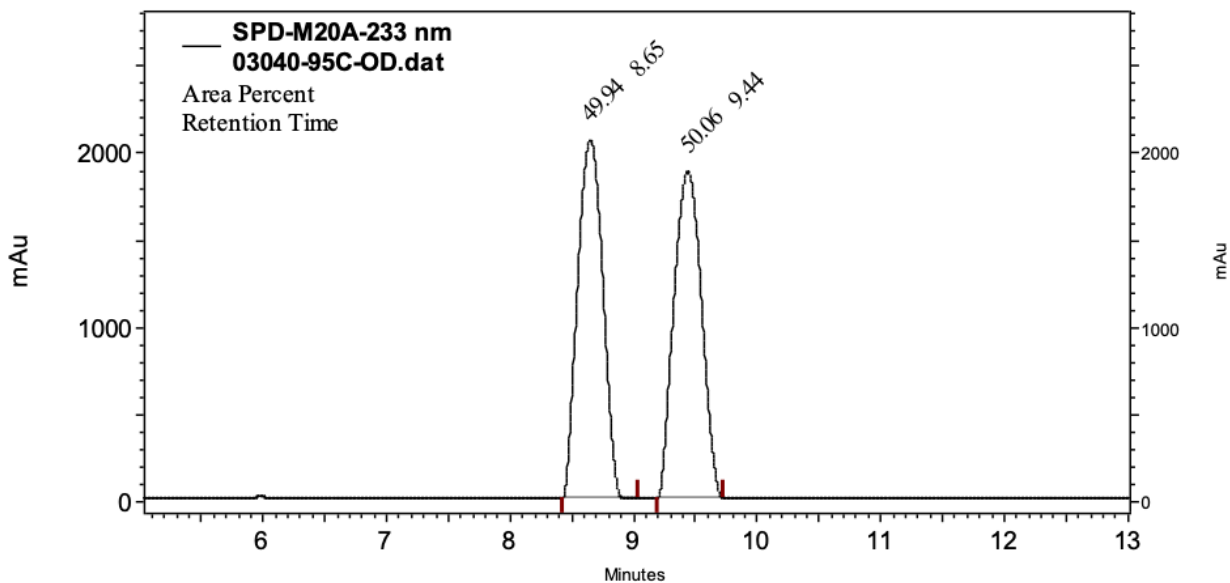
Table S1. Results with other substrates and catalyst.

Ethyl (1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (**3b**):

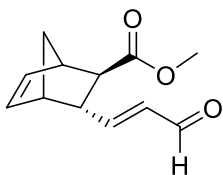


Colorless oil, 4.0 mg, 60% yield. ¹H NMR (600 MHz, CDCl₃/TMS) δ 9.39 (d, *J* = 7.8 Hz, 1H), 6.45 (dd, *J* = 15.6, 8.2 Hz, 1H), 6.28 (dd, *J* = 5.3, 3.3 Hz, 1H), 6.12 – 6.04 (m, 2H), 4.11 (q, *J* = 7.1 Hz, 2H), 3.23 (dt, *J* = 8.1, 4.0 Hz, 1H), 3.09 (s, 1H), 2.98 (s, 1H), 2.06 (d, *J* = 4.7 Hz, 1H), 1.69 (d, *J* = 8.8 Hz, 1H), 1.49 (d, *J* = 8.8

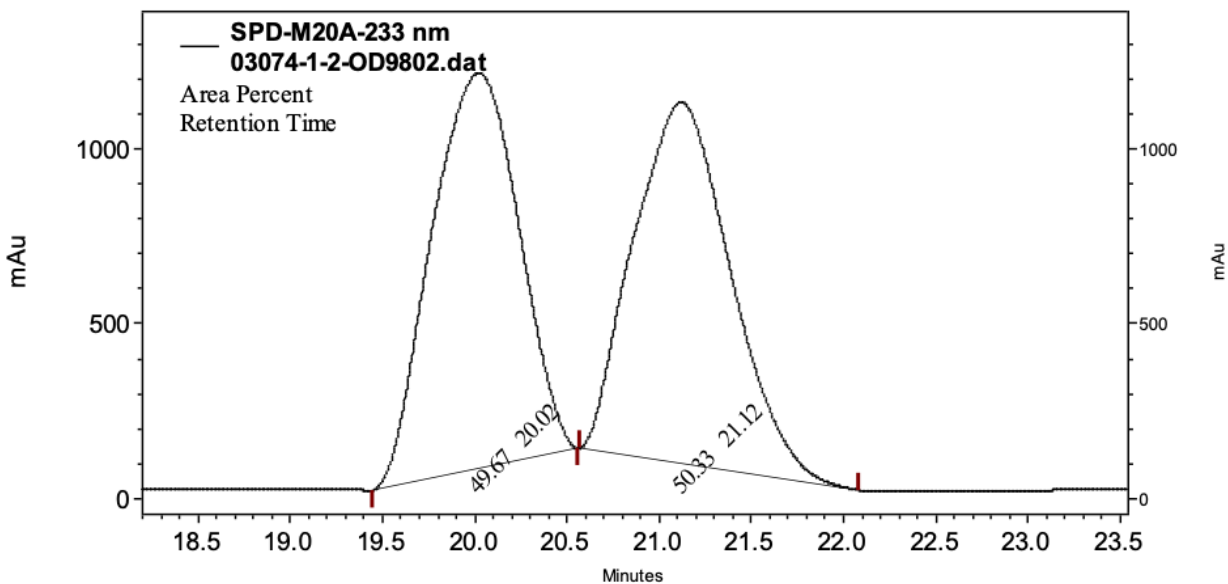
Hz, 1H), 1.22 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 193.69, 174.19, 160.44, 137.76, 134.96, 132.82, 60.80, 50.12, 47.63, 47.50, 47.37, 47.21, 14.17. HRMS (m/z): calculated for $\text{C}_{13}\text{H}_{16}\text{NaO}_3[\text{M} + \text{Na}]^+$, 243.0992; observed, 243.1002. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), $t_r = 8.65$ min (major), 9.44 min (minor); ee = 89%.

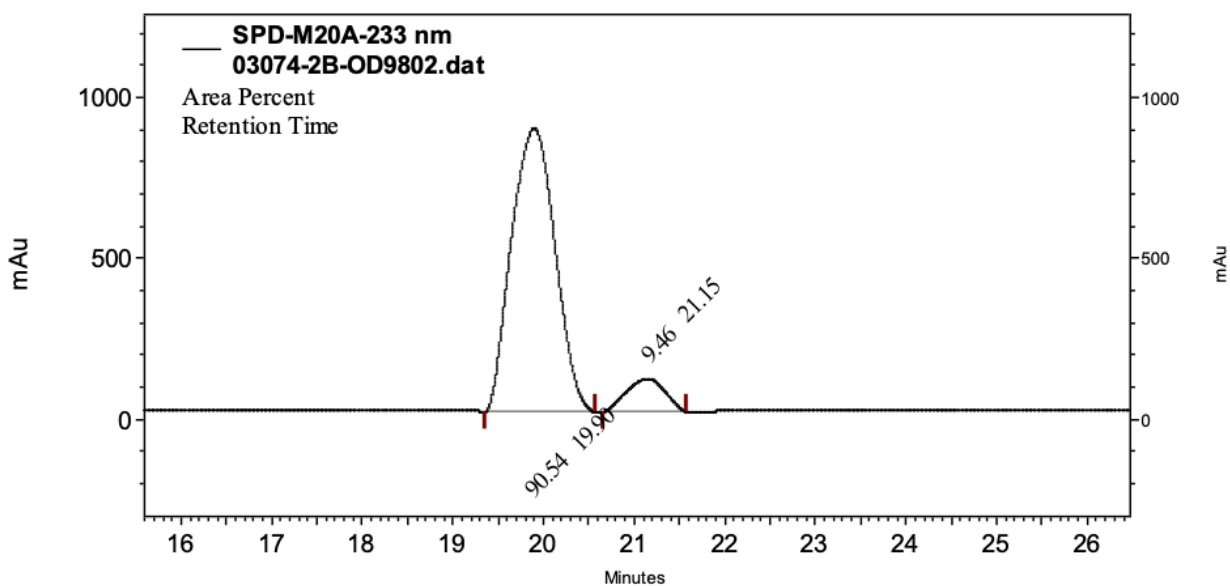


Methyl (1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3)

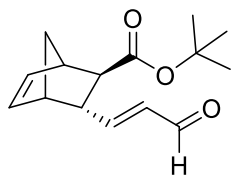


Colorless oil, 4.0 mg, 65% yield. ^1H NMR (700 MHz, CDCl_3) δ 9.44 (d, $J = 7.8$ Hz, 1H), 6.49 (dd, $J = 15.6$, 8.2 Hz, 1H), 6.32 (dd, $J = 5.6$, 3.2 Hz, 1H), 6.17 – 6.10 (m, 2H), 3.71 (s, 3H), 3.28 (dt, $J = 8.2$, 4.1 Hz, 1H), 3.14 (s, 1H), 3.03 (s, 1H), 2.12 (dd, $J = 4.8$, 1.3 Hz, 1H), 1.74 (d, $J = 8.8$ Hz, 1H), 1.60 (s, 0H), 1.55 (dd, $J = 8.8$, 1.5 Hz, 1H). ^{13}C NMR (176 MHz, CDCl_3) δ 193.78, 174.80, 160.32, 137.80, 135.05, 132.96, 52.15, 50.03, 47.76, 47.61, 47.44, 47.31. HRMS (m/z): calculated for $\text{C}_{12}\text{H}_{14}\text{NaO}_3[\text{M} + \text{Na}]^+$, 229.0835; observed, 229.0824. HPLC (Chiralpak OD-H column, 98:2 hexanes/isopropanol, 1 ml/min), $t_r = 19.90$ min (major), 21.15 min (minor); ee = 81%.

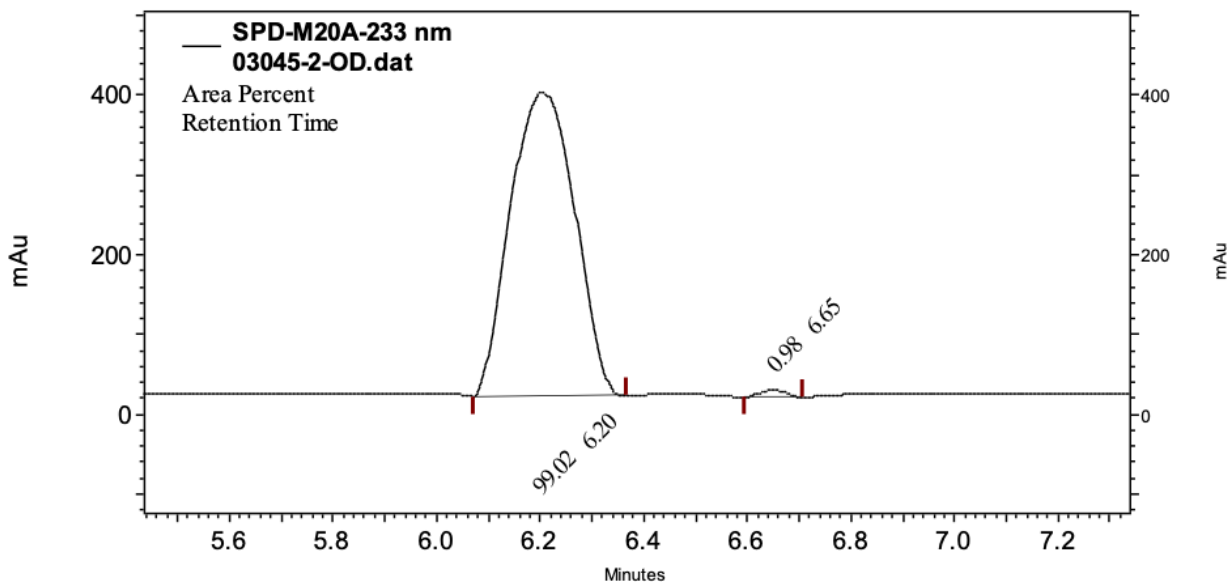
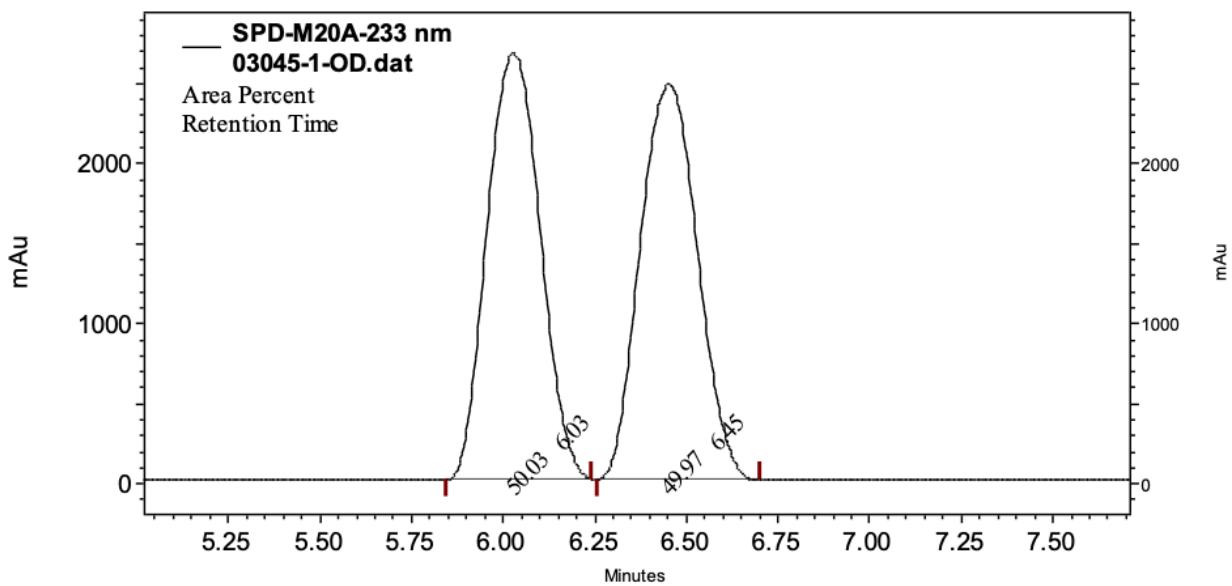




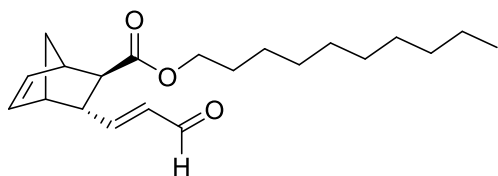
***tert*-Butyl (1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3d):**



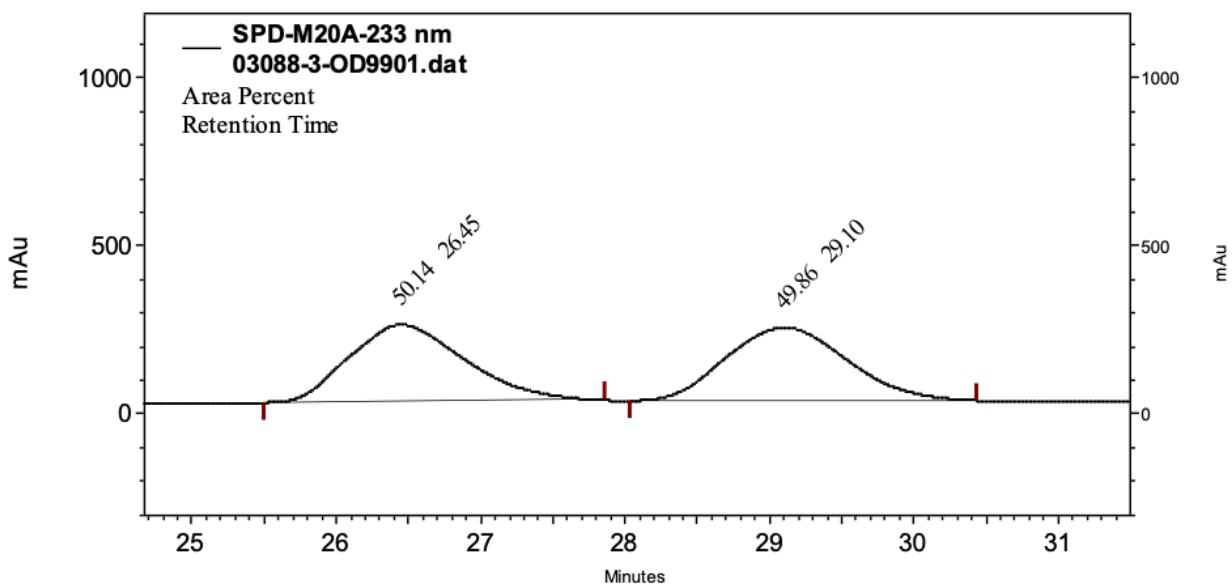
An inseparable mixture with side-product. The product yield was determined by ^1H NMR. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), t_r = 6.20 min (major), 6.65 min (minor); ee = 98%.

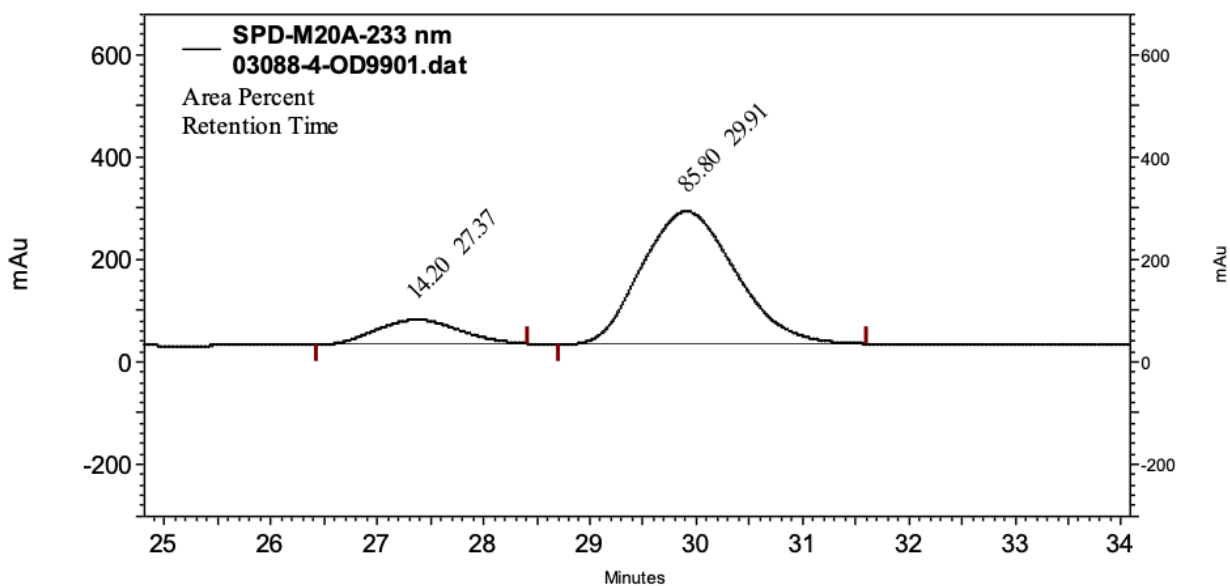


Decyl (1*R*,2*R*S,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3e):

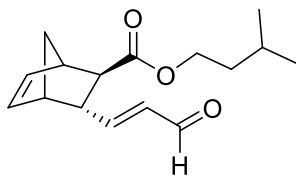


An inseparable mixture with side-product. The product yield was determined by ^1H NMR. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), t_r = 27.37 min (minor), 29.91 min (major); ee = 72%.

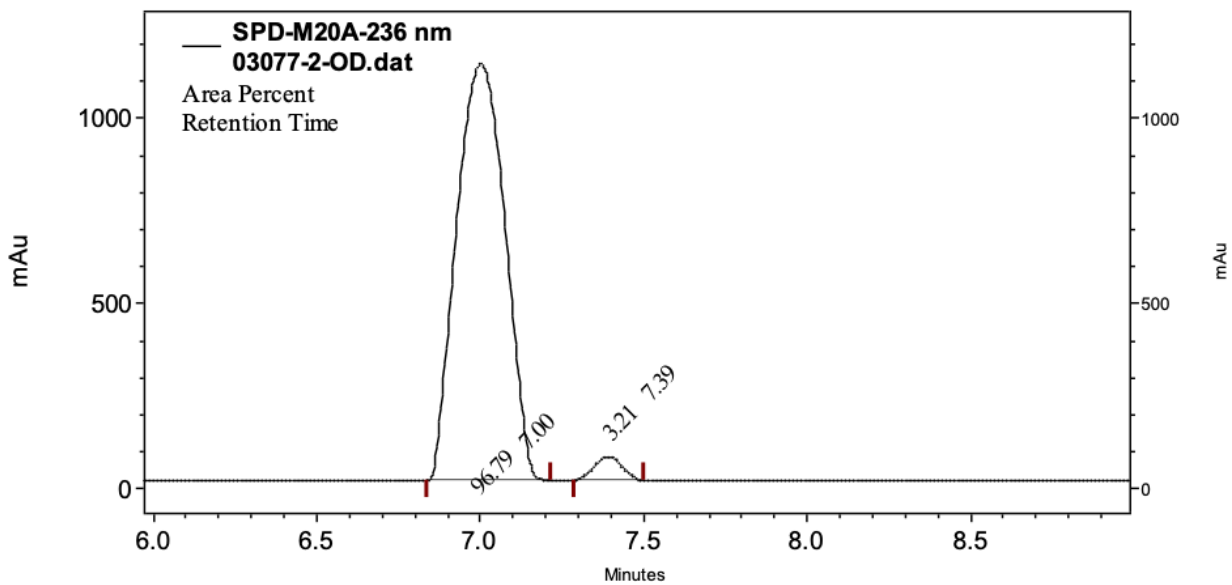
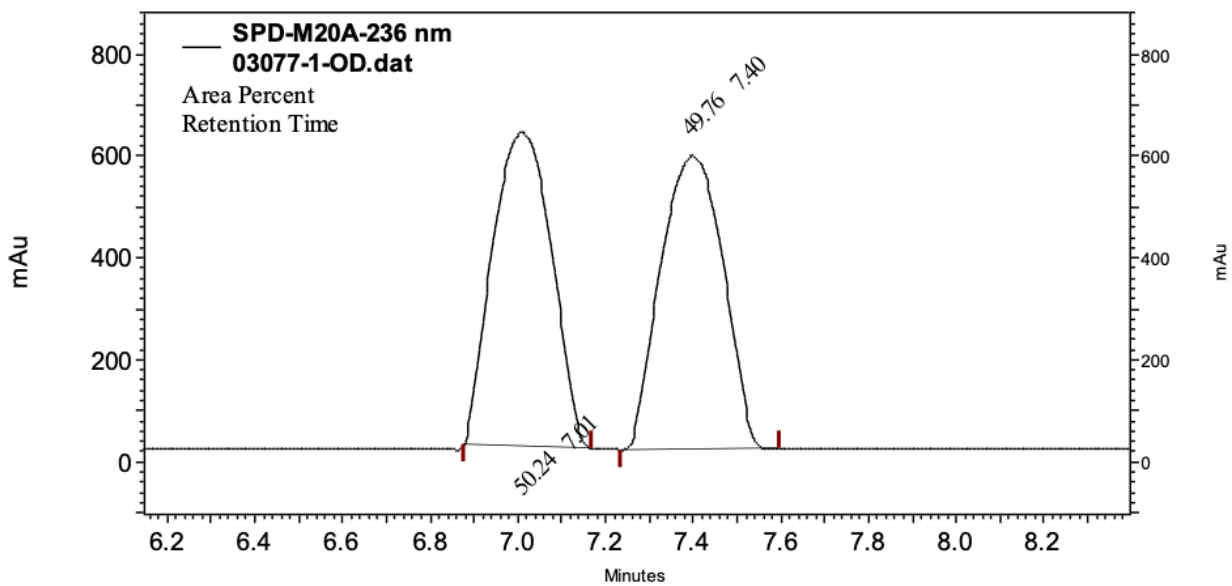




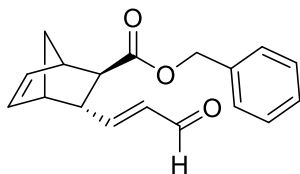
Isopentyl (1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3f):



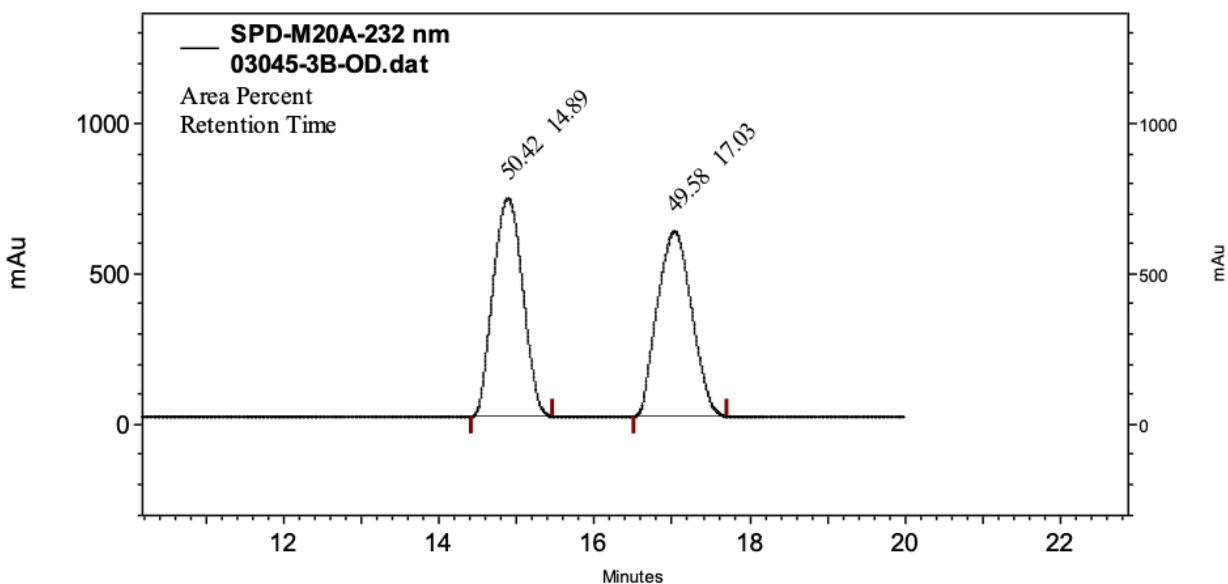
Colorless oil, 4.7 mg, 60% yield. ^1H NMR (500 MHz, CDCl_3) δ 9.44 (d, $J = 7.8$ Hz, 1H), 6.49 (dd, $J = 15.6$, 8.3 Hz, 1H), 6.32 (dd, $J = 5.5$, 3.2 Hz, 1H), 6.17 – 6.07 (m, 2H), 4.12 (t, $J = 6.9$ Hz, 2H), 3.27 (dt, $J = 8.1$, 3.9 Hz, 1H), 3.13 (s, 1H), 3.02 (s, 1H), 2.13 – 2.07 (m, 1H), 1.77 – 1.60 (m, 2H), 1.55-1.50 (m, 3H), 0.91 (d, $J = 6.6$ Hz, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 193.87, 174.41, 160.60, 137.87, 135.03, 132.91, 63.67, 50.25, 47.77, 47.62, 47.43, 47.36, 37.31, 25.12, 22.48. HRMS (m/z): calculated for $\text{C}_{16}\text{H}_{22}\text{NaO}_3[\text{M} + \text{Na}]^+$, 285.1461; observed, 285.1477. HPLC (Chiralpak OD-H column, 98:2 hexanes/isopropanol, 1 ml/min), $t_r = 7.00$ min (major), 7.39 min (minor); ee = 94%.

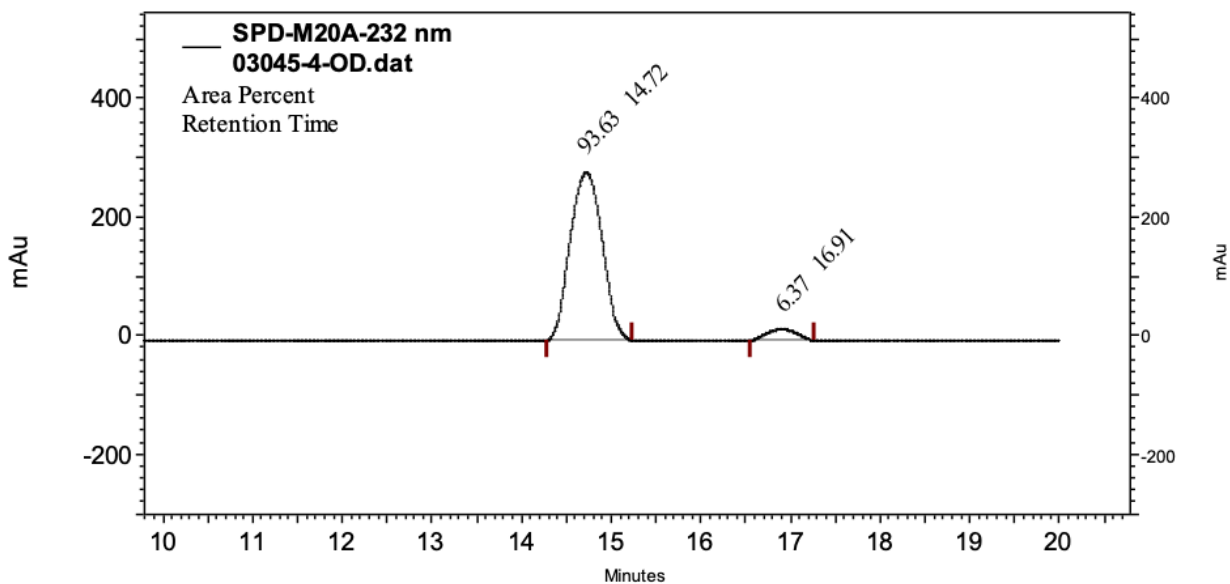


Benzyl (1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3g):

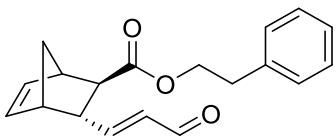


Colorless oil, 6.7 mg, 79% yield. ^1H NMR (700 MHz, CDCl_3) δ 9.44 (d, $J = 7.8$ Hz, 1H), 7.41 – 7.27 (m, 5H), 6.48 (dd, $J = 15.6, 8.3$ Hz, 1H), 6.32 (dd, $J = 5.2, 3.3$ Hz, 1H), 6.13 (ddd, $J = 23.4, 10.5, 5.2$ Hz, 2H), 5.15 (s, 2H), 3.29 (dt, $J = 8.0, 3.9$ Hz, 1H), 3.16 (s, 1H), 3.03 (s, 1H), 2.18 (d, $J = 4.5$ Hz, 1H), 1.74 (d, $J = 8.8$ Hz, 1H), 1.55 (d, $J = 8.8$ Hz, 1H). ^{13}C NMR (176 MHz, CDCl_3) δ 193.76, 174.14, 160.30, 137.81, 135.82, 135.11, 132.99, 128.67, 128.38, 128.16, 66.75, 50.18, 47.76, 47.67, 47.48, 47.38. HRMS (m/z): calculated for $\text{C}_{18}\text{H}_{18}\text{NaO}_3$ [$\text{M} + \text{Na}$] $^+$, 305.1148; observed, 305.1139. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), $t_r = 14.72$ min (major), 16.91 min (minor); ee = 87%.

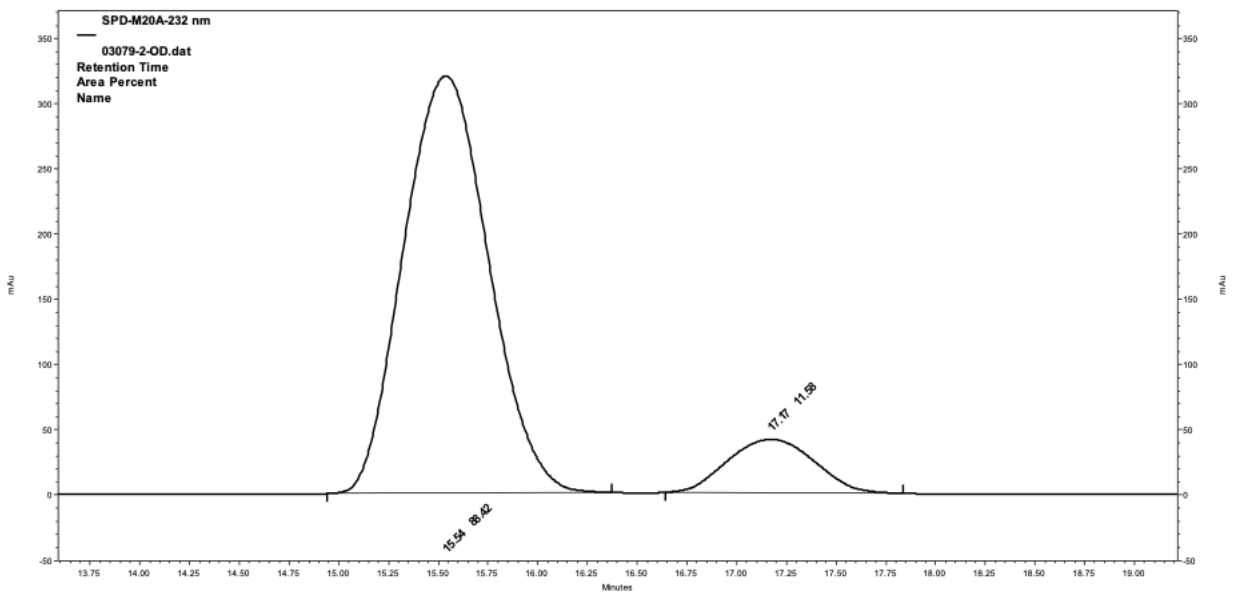
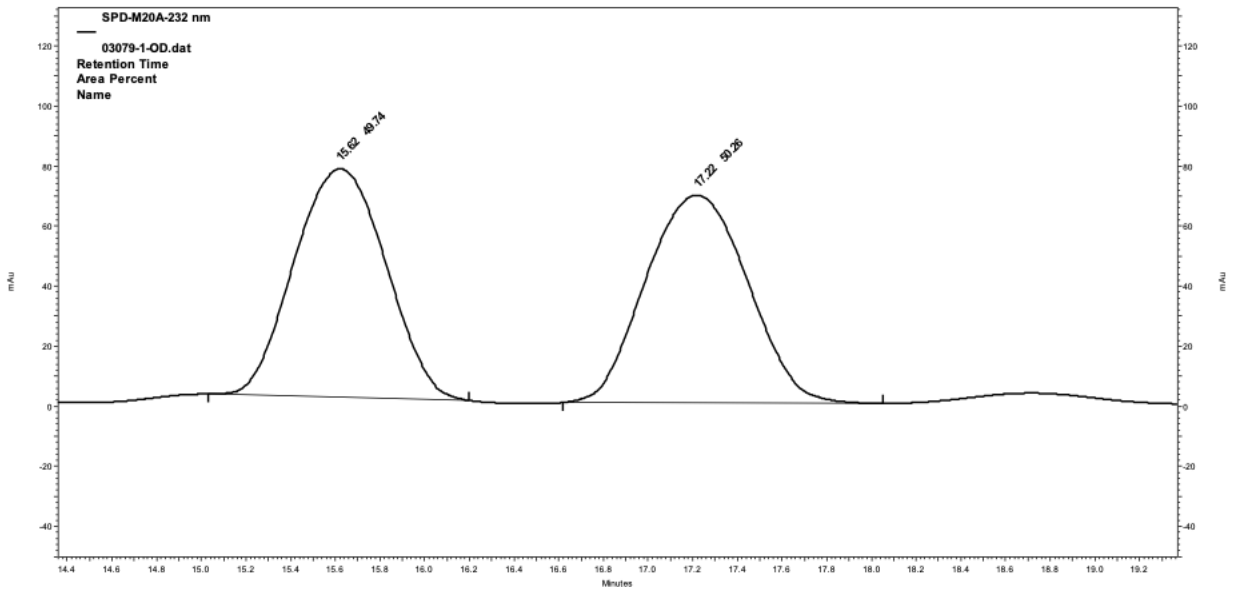




Phenethyl (1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3h):

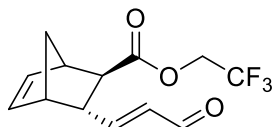


Colorless oil, 7.7 mg, 87% yield. ^1H NMR (700 MHz, CDCl_3) δ 9.43 (d, $J = 7.8$ Hz, 1H), 7.30 (t, $J = 7.4$ Hz, 2H), 7.23 (t, $J = 7.4$ Hz, 1H), 7.20 (d, $J = 7.6$ Hz, 2H), 6.45 (dd, $J = 15.6, 8.2$ Hz, 1H), 6.30 (d, $J = 3.4$ Hz, 1H), 6.15 – 6.11 (m, 1H), 6.06 (dd, $J = 15.6, 7.8$ Hz, 1H), 4.39 – 4.31 (m, 2H), 3.20 – 3.16 (m, 1H), 3.08 (s, 1H), 2.99 (s, 1H), 2.95 (t, $J = 6.9$ Hz, 2H), 2.08 (d, $J = 4.6$ Hz, 1H), 1.66 (d, $J = 8.8$ Hz, 1H), 1.51 (d, $J = 8.8$ Hz, 1H). ^{13}C NMR (176 MHz, CDCl_3) δ 193.80, 174.23, 160.39, 137.78, 137.60, 135.04, 132.91, 128.89, 128.55, 126.68, 65.24, 50.15, 47.79, 47.58, 47.32, 47.29, 35.10. HRMS (m/z): calculated for $\text{C}_{18}\text{H}_{18}\text{NaO}_3$ $[\text{M} + \text{Na}]^+$, 319.1305; observed, 319.1312. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), $t_r = 15.62$ min (major), 17.22 min (minor); ee = 77%.

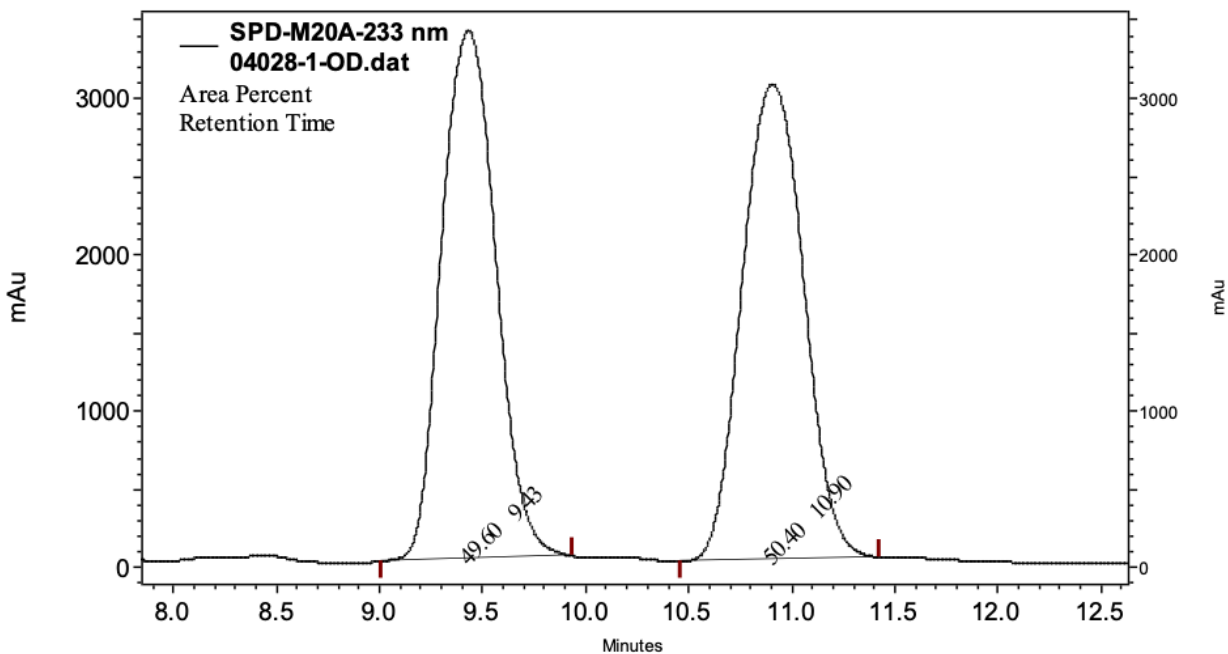


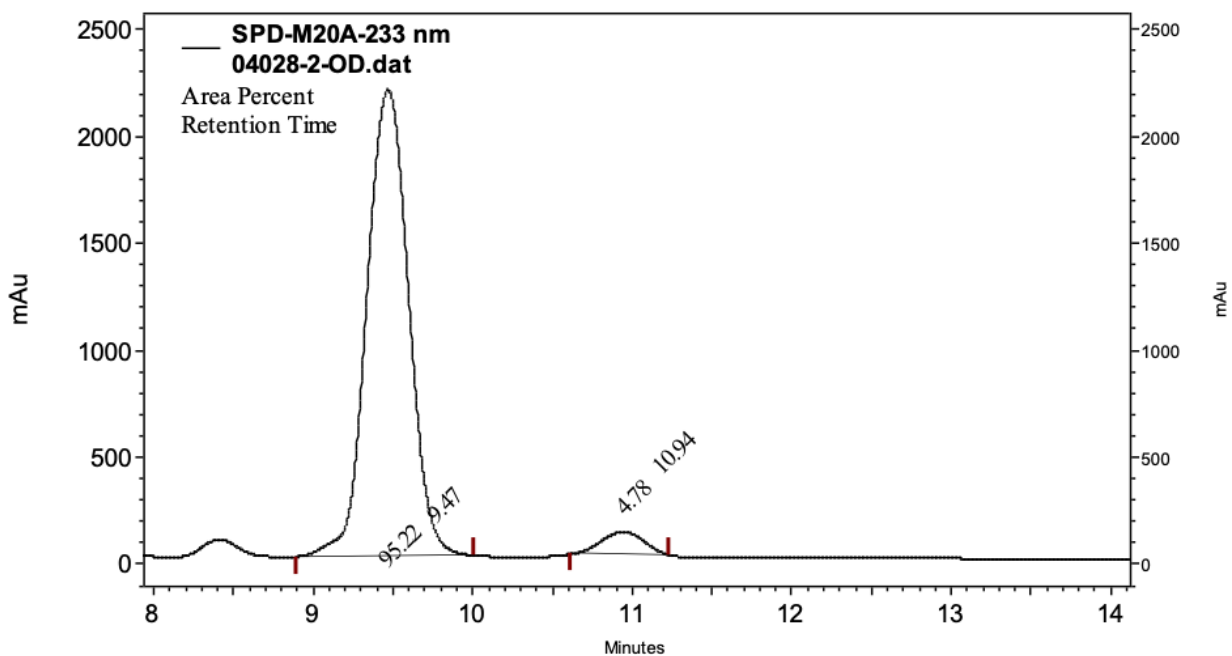
2,2,2-Trifluoroethyl (1R,2R,3R,4S)-3-((E)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate

(3i):

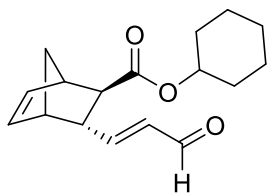


Colorless oil, 5.5 mg, 67% yield. ^1H NMR (700 MHz, CDCl_3) δ 9.44 (d, $J = 7.8$ Hz, 1H), 6.46 (dd, $J = 15.6$, 8.3 Hz, 1H), 6.34 (dd, $J = 5.6$, 3.1 Hz, 1H), 6.17 (dd, $J = 5.6$, 2.8 Hz, 1H), 6.12 (dd, $J = 15.6$, 7.8 Hz, 1H), 4.50 (qd, $J = 8.4$, 2.7 Hz, 2H), 3.31 – 3.26 (m, 1H), 3.18 (s, 1H), 3.05 (s, 1H), 2.23 – 2.18 (m, 1H), 1.70 (d, $J = 9.0$ Hz, 1H), 1.58 (dd, $J = 9.0$, 1.5 Hz, 1H). ^{13}C NMR (176 MHz, CDCl_3) δ 193.56, 172.81, 159.28, 137.56, 135.30, 133.14, 122.88 (q, $J = 277.4$ Hz), 60.50 (q, $J = 36.5$ Hz), 49.75, 47.71, 47.68, 47.43, 47.41. HRMS (m/z): calculated for $\text{C}_{13}\text{H}_{13}\text{F}_3\text{NaO}_3[\text{M} + \text{Na}]^+$, 297.0709; observed, 297.0715. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), $t_r = 9.47$ min (major), 10.94 min (minor); ee = 90%.

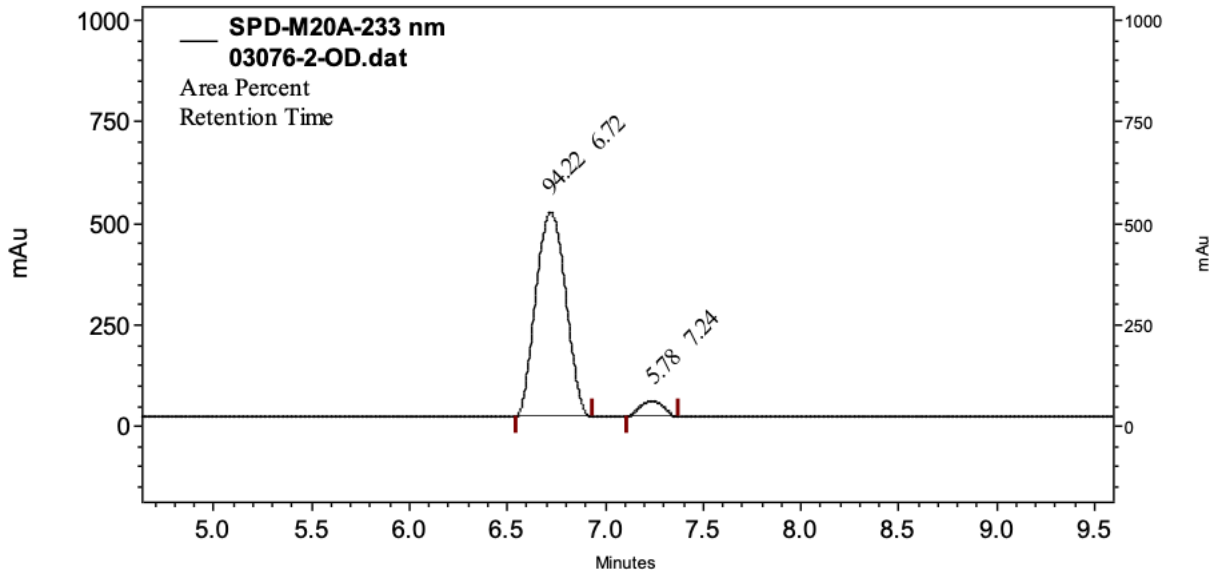
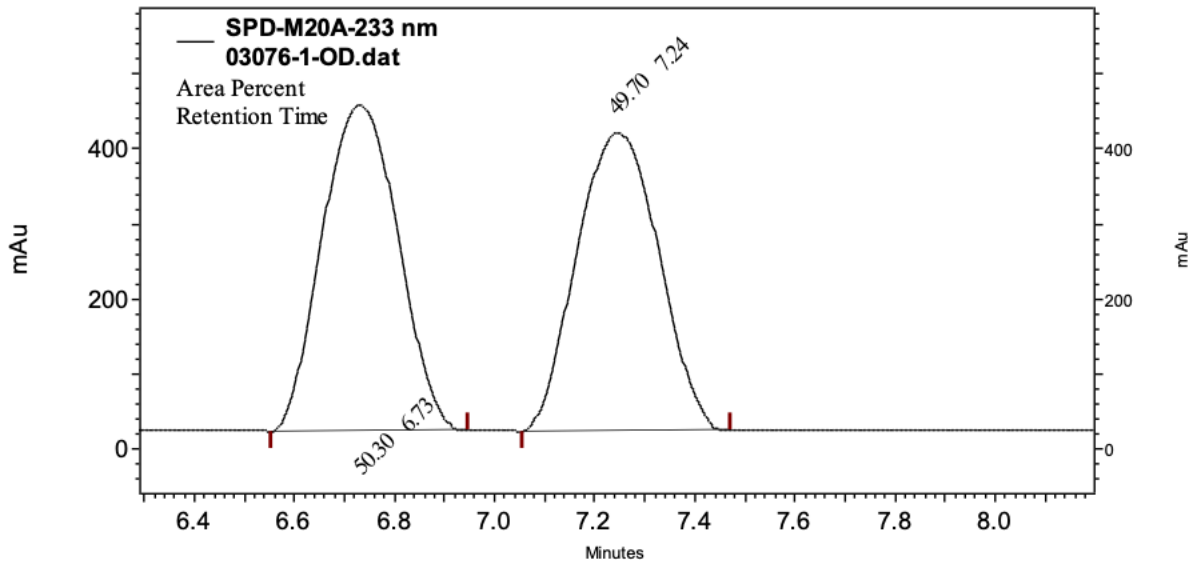




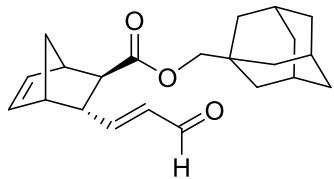
Cyclohexyl (1R,2R,3R,4S)-3-((E)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3j):



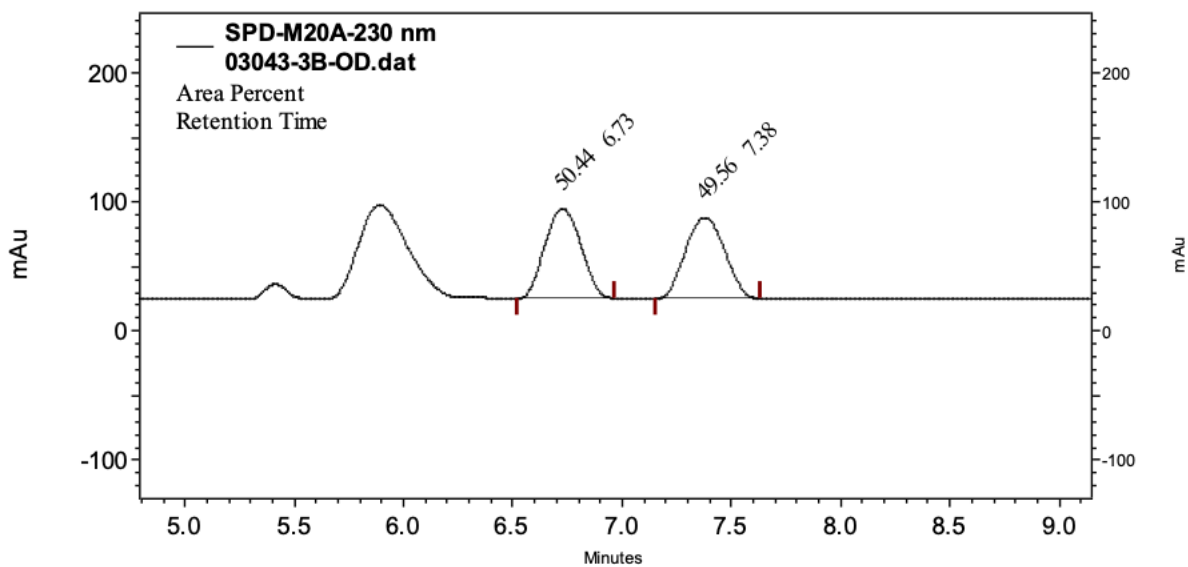
An inseparable mixture with side-product. The product yield was determined by ^1H NMR. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), t_r = 6.72 min (major), 7.24 min (minor); ee = 88%.

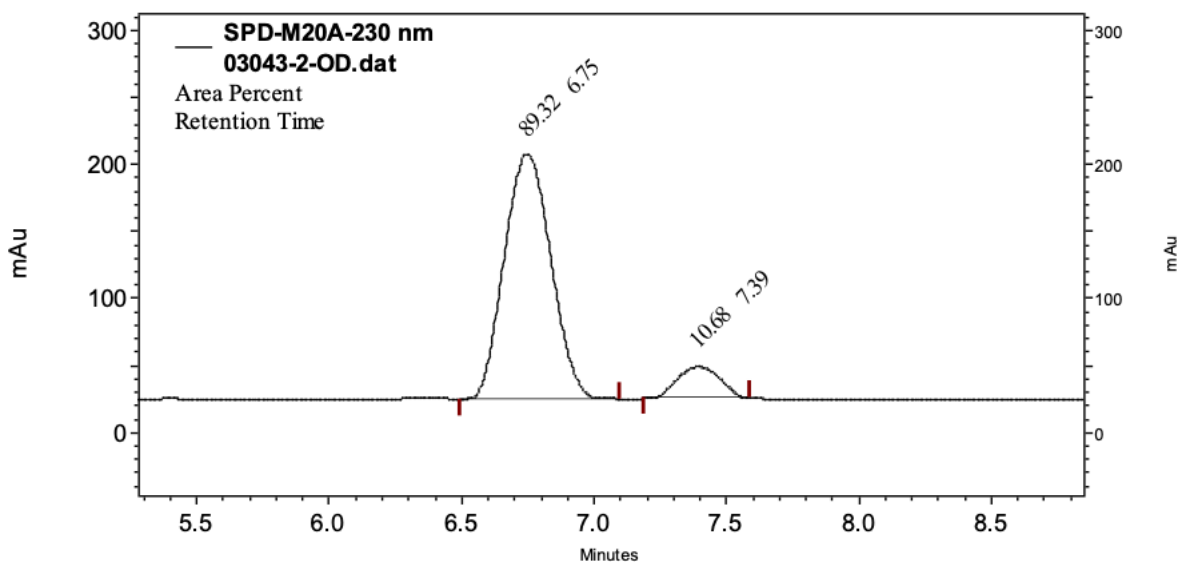


((3*R*,5*R*,7*R*)-adamantan-1-yl)methyl (1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3k**):**

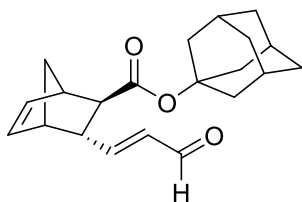


An inseparable mixture with side-product. The product yield was determined by ^1H NMR. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), t_r = 6.75 min (major), 7.39 min (minor); ee = 79%.

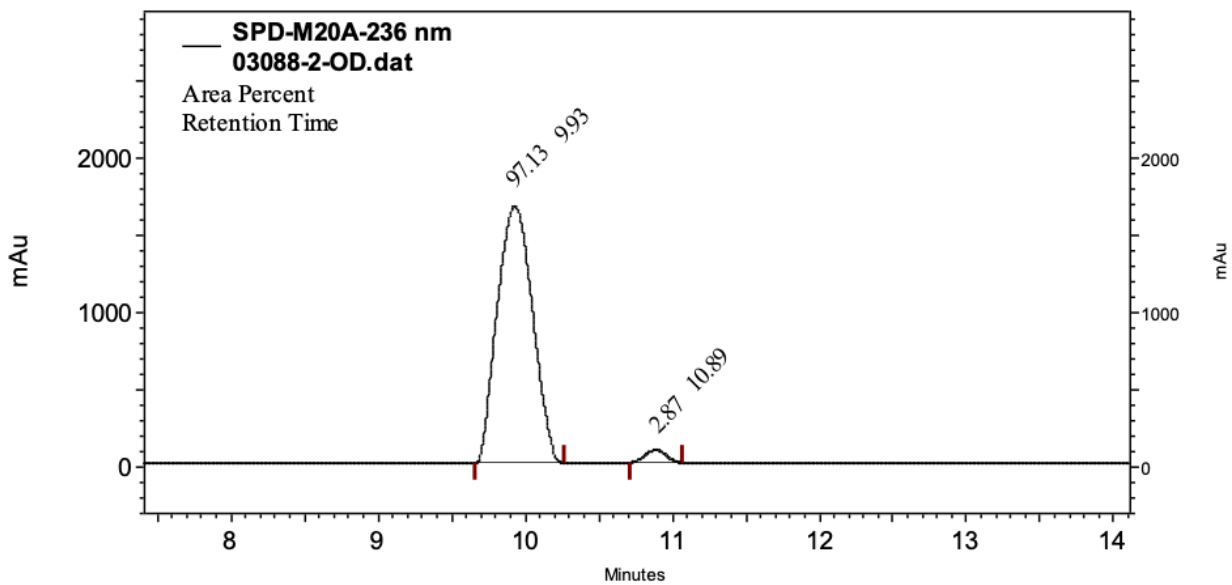
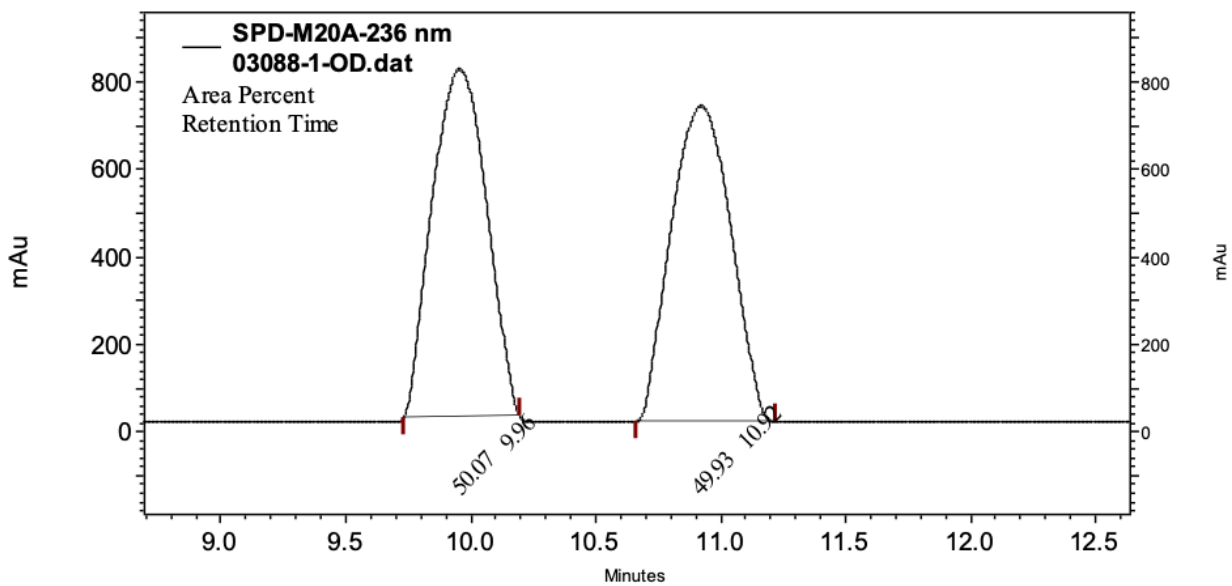




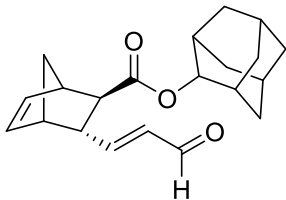
(3*R*,5*R*,7*R*)-adamantan-1-yl (1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (**3l**):



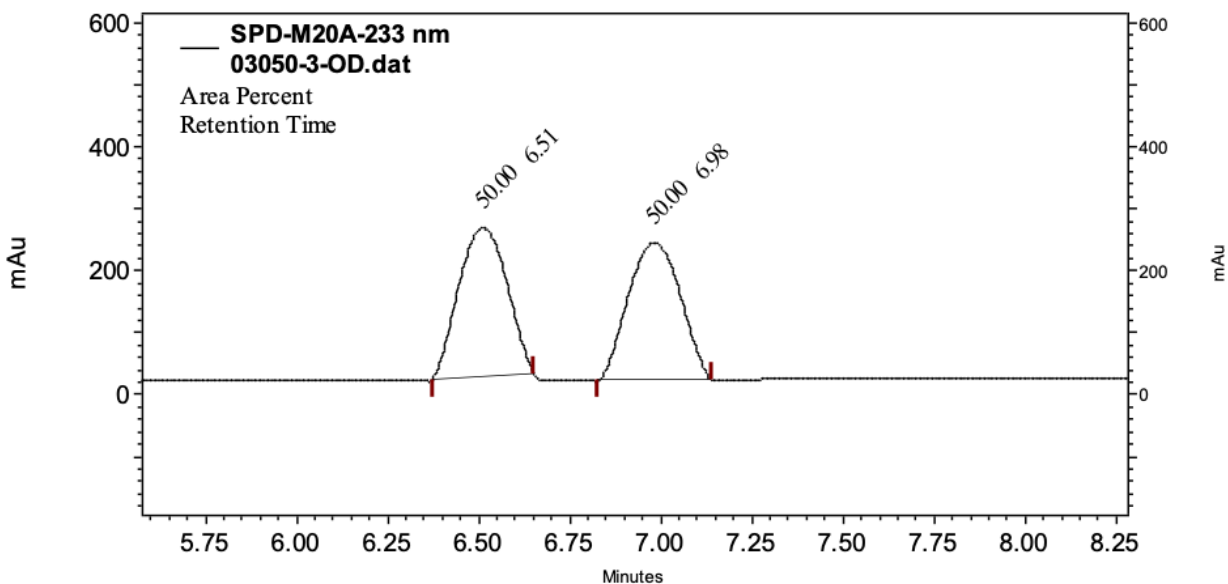
Colorless solid, 3.3 mg, 34% yield. ^1H NMR (700 MHz, CDCl_3) δ 9.44 (d, $J = 7.9$ Hz, 1H), 6.47 (dd, $J = 15.5$, 9.3 Hz, 1H), 6.32 (dd, $J = 5.4$, 3.0 Hz, 1H), 6.07 (dd, $J = 15.5$, 7.9 Hz, 1H), 6.04 – 6.00 (m, 1H), 2.86 (s, 1H), 2.63 (s, 1H), 2.45 – 2.40 (m, 1H), 1.54 – 1.36 (m, 4H), 1.25 (s, 3H), 0.89 – 0.85 (m, 8H). ^{13}C NMR (176 MHz, CDCl_3) δ 194.18, 163.55, 138.84, 133.28, 131.90, 53.18, 50.07, 49.79, 48.19, 46.90, 42.81, 31.16, 30.04. HRMS (m/z): calculated for $\text{C}_{21}\text{H}_{26}\text{NaO}_3[\text{M} + \text{Na}]^+$, 349.1774; observed, 349.1788. HPLC (Chiralpak OD-H column, 98:2 hexanes/isopropanol, 1 ml/min), $t_r = 9.93$ min (major), 10.89 min (minor); ee = 94%.

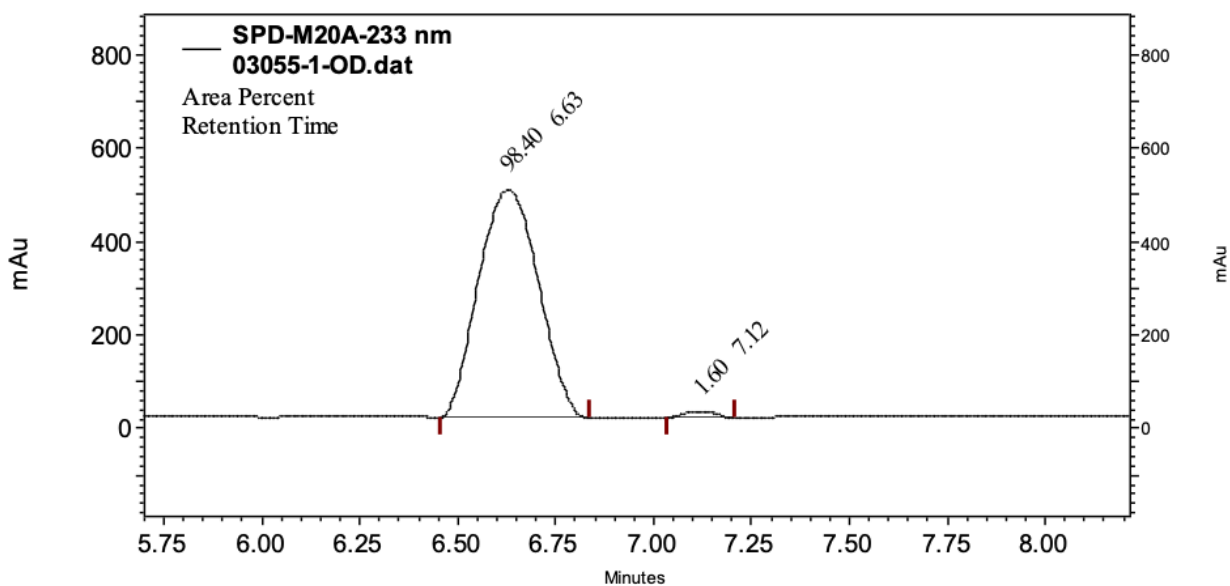


(1*R*,2*S*,5*S*)-adamantan-2-yl (1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3m):



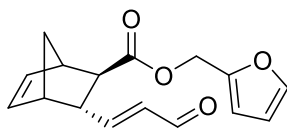
Colorless solid, 3.5 mg, 36% yield. ¹H NMR (499 MHz, CDCl₃) δ 9.46 (d, *J* = 7.8 Hz, 1H), 6.52 (dd, *J* = 15.6, 8.3 Hz, 1H), 6.35 (s, 1H), 6.15 (t, *J* = 11.3 Hz, 2H), 4.95 (s, 1H), 3.29 (s, 1H), 3.18 (s, 1H), 3.03 (s, 1H), 2.16 (s, 1H), 1.97 (d, *J* = 22.4 Hz, 4H), 1.84 (s, 4H), 1.76 (d, *J* = 23.9 Hz, 6H). ¹³C NMR (176 MHz, CDCl₃) δ 193.83, 173.61, 160.71, 137.94, 134.94, 132.88, 77.60, 50.69, 47.93, 47.64, 47.57, 47.31, 37.33, 36.30, 31.88, 27.17, 26.95. HRMS (*m/z*): calculated for C₂₁H₂₆NaO₃[*M* + Na]⁺, 349.1774; observed, 349.1784. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), *tr* = 6.63 min (major), 7.12 min (minor); *ee* = 97%.



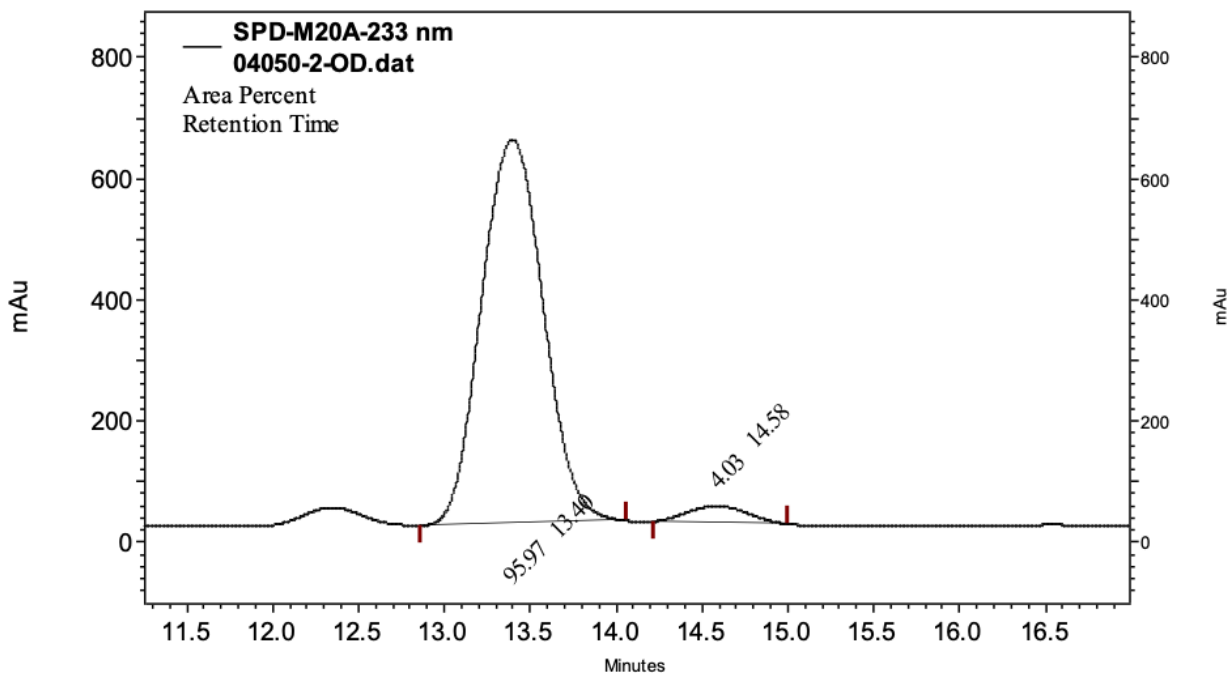
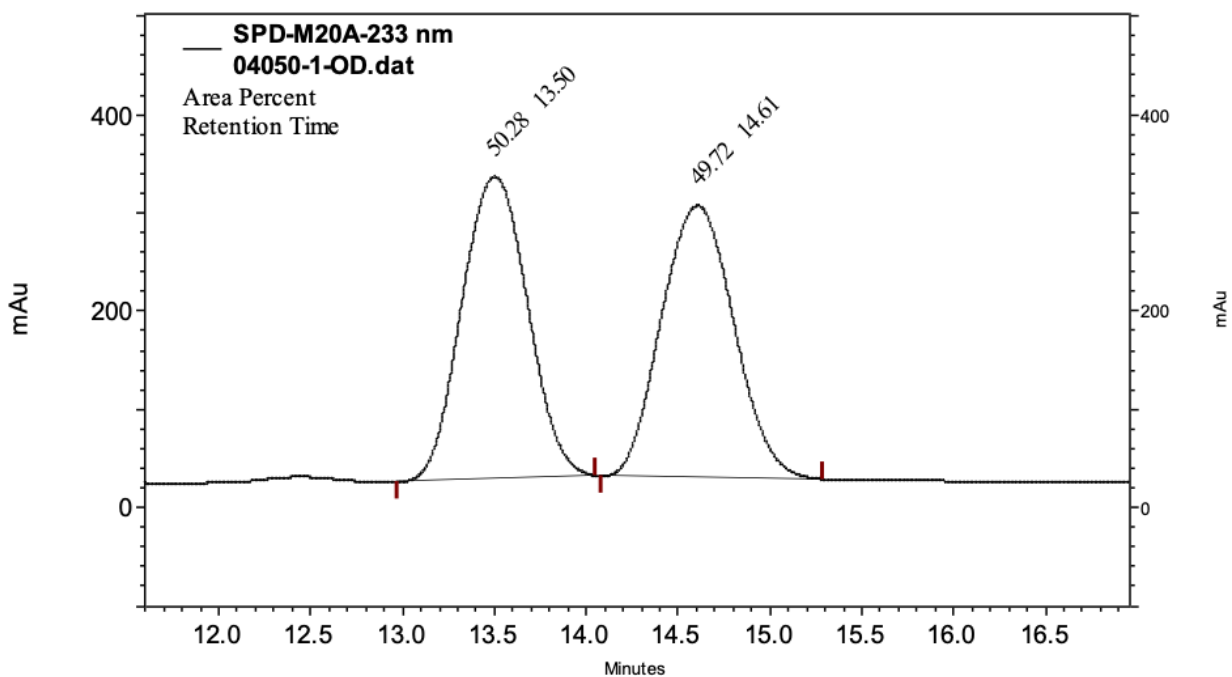


Furan-2-ylmethyl (1R,2R,3R,4S)-3-((E)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate

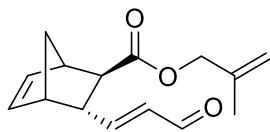
(3n):



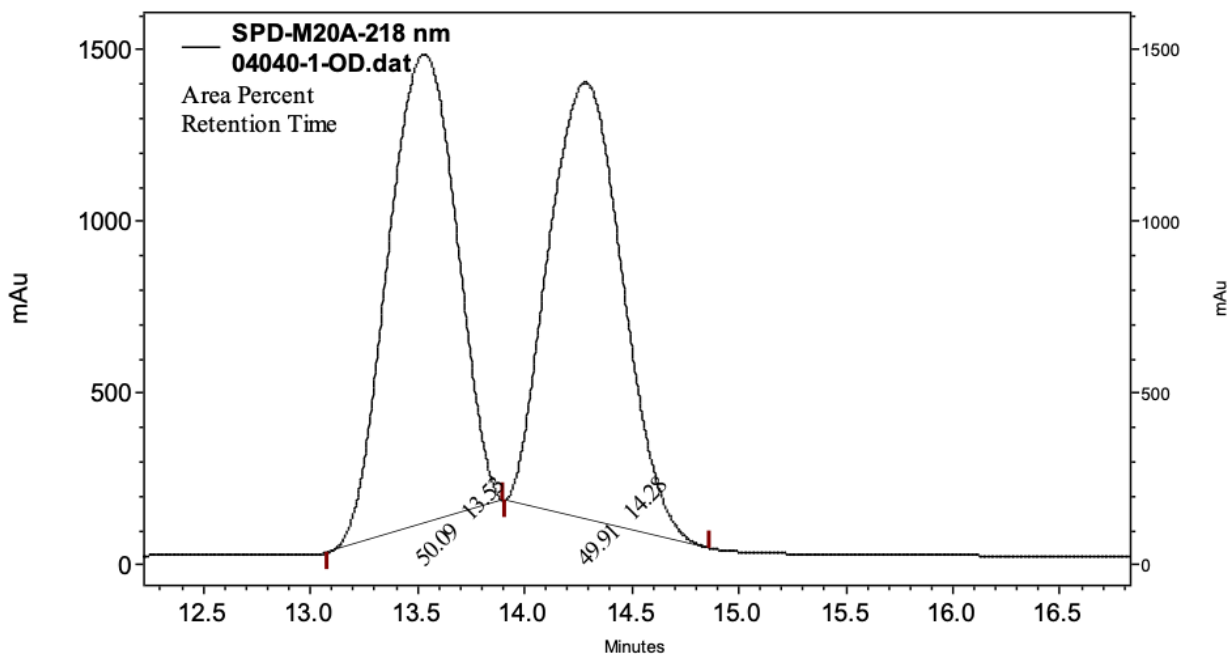
Colorless oil, 5.9 mg, 73% yield. ^1H NMR (500 MHz, CDCl_3) δ 9.43 (d, $J = 7.8$ Hz, 1H), 7.42 (s, 1H), 6.46 (dd, $J = 15.6, 8.3$ Hz, 1H), 6.42 – 6.34 (m, 2H), 6.31 (dd, $J = 5.3, 3.2$ Hz, 1H), 6.12 (ddd, $J = 23.4, 10.5, 5.2$ Hz, 2H), 5.09 (s, 2H), 3.28 (dt, $J = 7.5, 3.7$ Hz, 1H), 3.14 (s, 1H), 3.02 (s, 1H), 2.14 (d, $J = 4.7$ Hz, 1H), 1.74 (d, $J = 8.8$ Hz, 1H), 1.54 (d, $J = 8.9$ Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 193.83, 173.99, 160.25, 149.27, 143.40, 137.80, 135.13, 133.00, 110.73, 110.62, 58.51, 50.06, 47.70, 47.65, 47.51, 47.36. HRMS (m/z): calculated for $\text{C}_{16}\text{H}_{16}\text{NaO}_4[\text{M} + \text{Na}]^+$, 295.0941; observed, 295.0955. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), $t_r = 13.40$ min (major), 14.58 min (minor); ee = 92%.

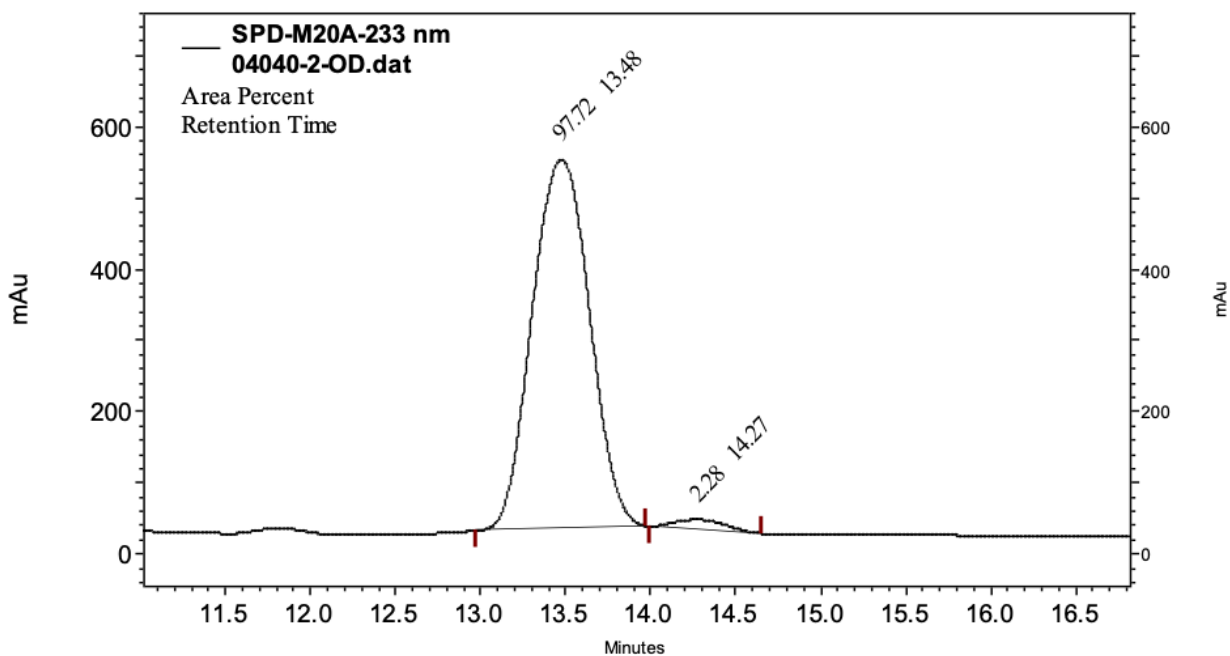


2-Methylallyl (1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3o):

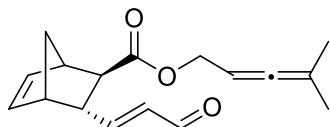


An inseparable mixture with side-product. The product yield was determined by ¹H NMR. HPLC (Chiralpak OD-H column, 98:2 hexanes/isopropanol, 1 ml/min), *t_r* = 13.48 min (major), 14.27 min (minor); ee = 95%.

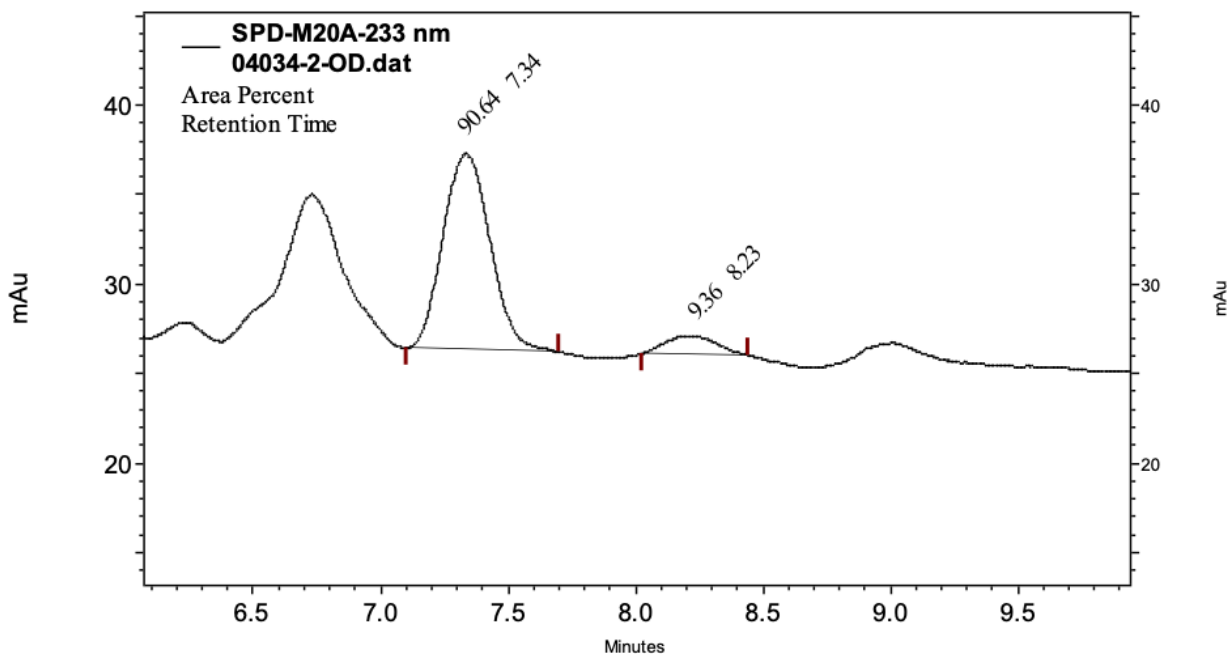
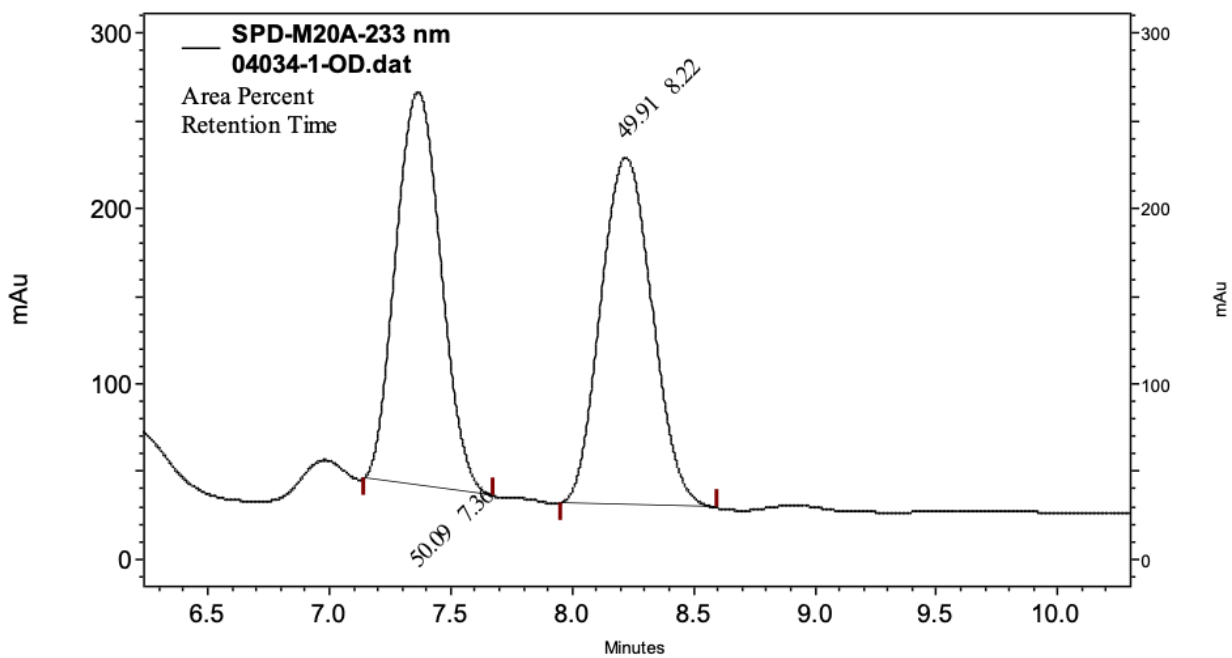




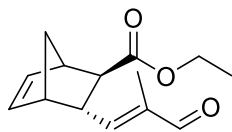
4-Methylpenta-2,3-dien-1-yl (1R,2R,3R,4S)-3-((E)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3p):



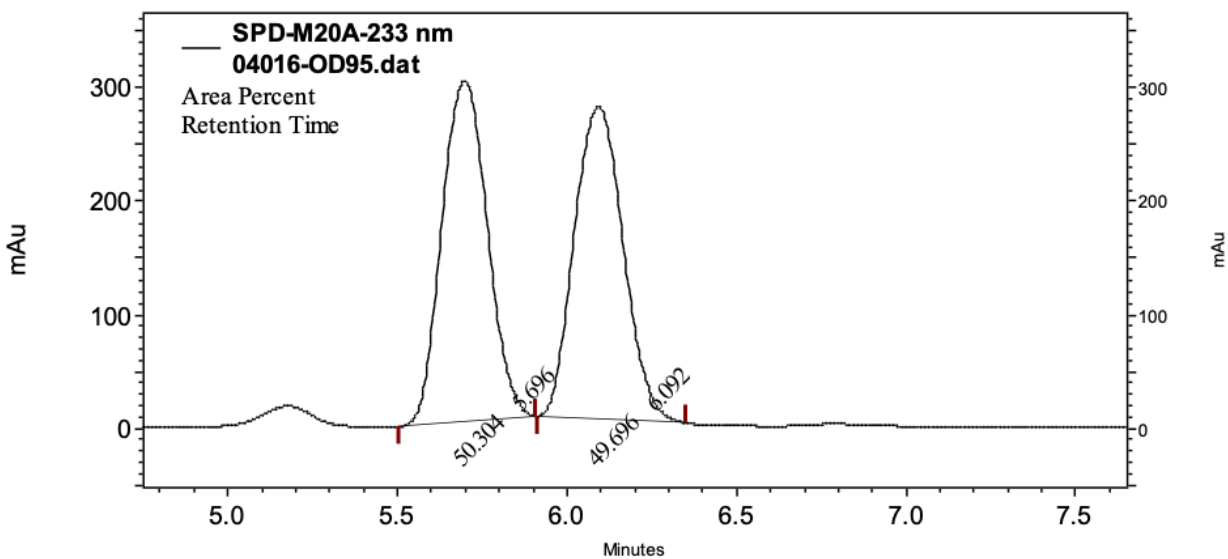
An inseparable mixture with side-product. The product yield was determined by ^1H NMR. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), t_r = 7.34 min (major), 8.23 min (minor); ee = 81%.



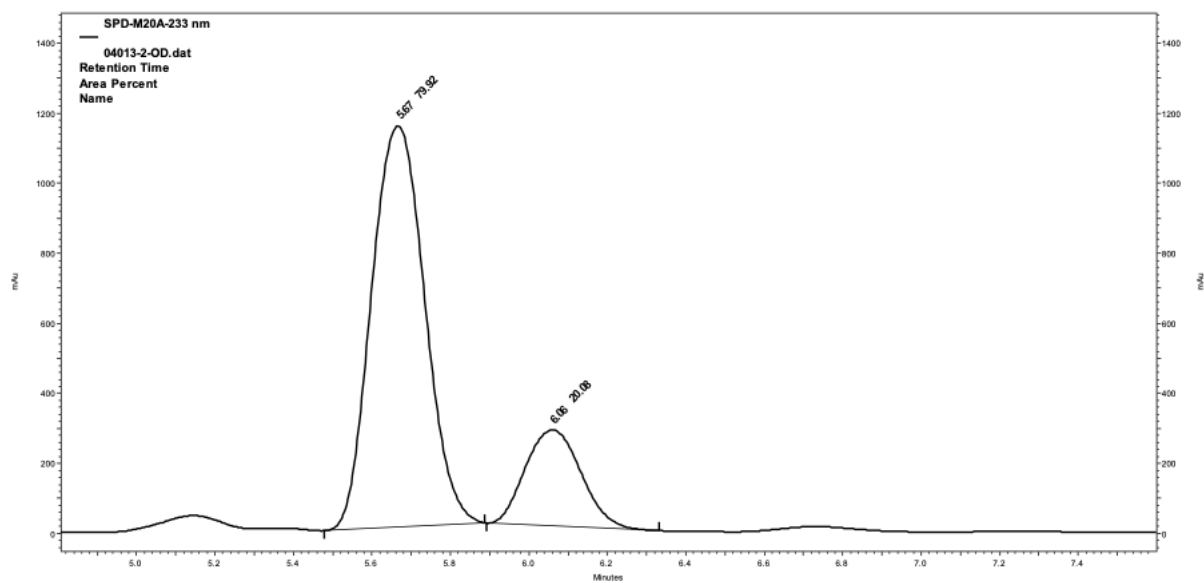
Ethyl (1R,2R,3S,4S)-3-((E)-2-methyl-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3q):



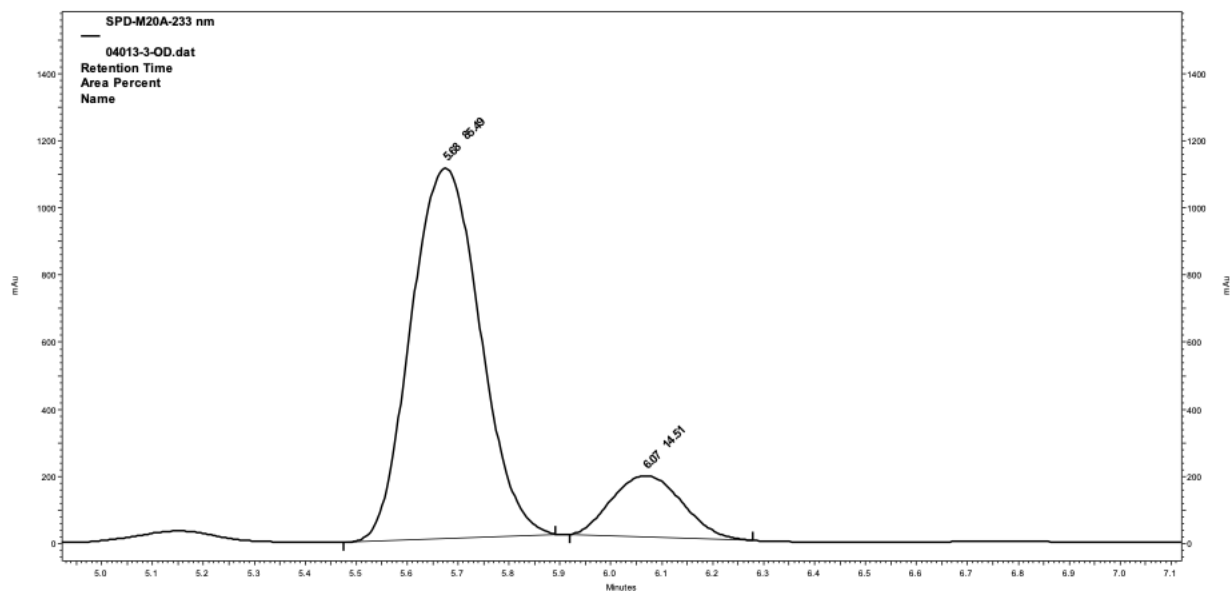
Colorless oil, 3.9 mg, 55% yield. ^1H NMR (700 MHz, CDCl_3) δ 9.33 (s, 1H), 6.40 – 6.35 (m, 1H), 6.21 (s, 2H), 6.02 (d, $J = 10.0$ Hz, 1H), 4.16 (q, $J = 7.3$ Hz, 2H), 3.51 (d, $J = 9.9$ Hz, 1H), 3.15 (s, 1H), 3.08 (s, 1H), 2.98 (s, 1H), 2.60 (s, 1H), 2.04 (d, $J = 4.0$ Hz, 1H), 1.81 (s, 3H), 1.77 (d, $J = 8.7$ Hz, 2H), 1.27 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (176 MHz, CDCl_3) δ 174.53, 157.22, 139.51, 138.03, 135.28, 133.21, 60.87, 47.80, 47.69, 47.36, 45.61, 43.61, 14.27, 14.18. HRMS (m/z): calculated for $\text{C}_{14}\text{H}_{18}\text{NaO}_3[\text{M} + \text{Na}]^+$, 257.1148; observed, 257.1156. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), $t_r = 33.38$ min (major), 48.32 min (minor); ee = 60%.



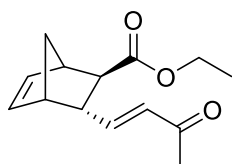
With 4y as catalyst:



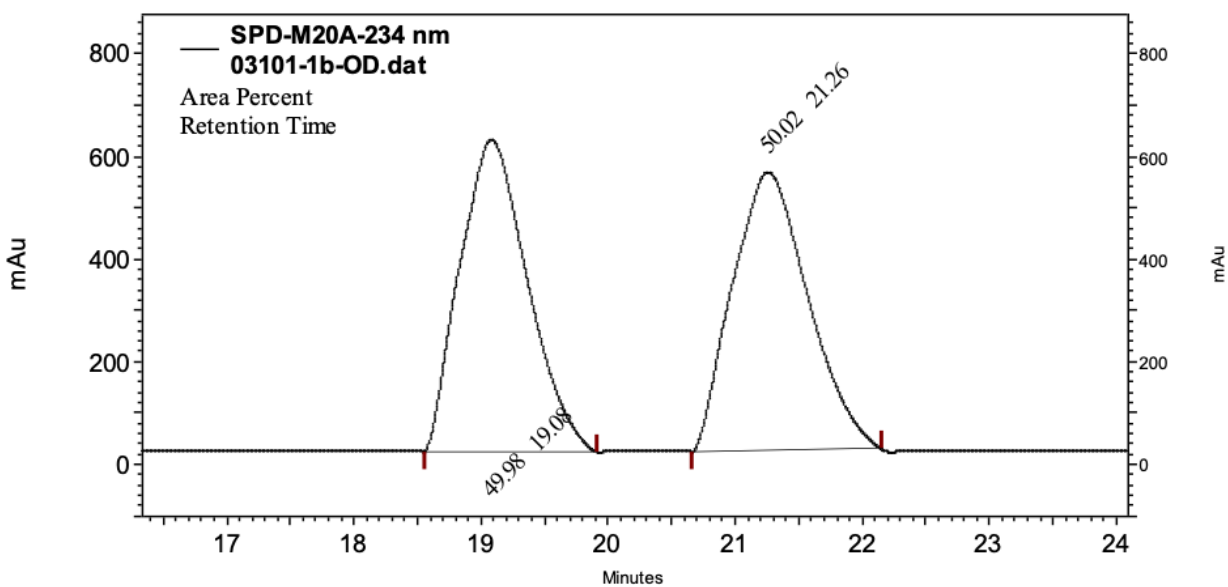
With 4z as catalyst:

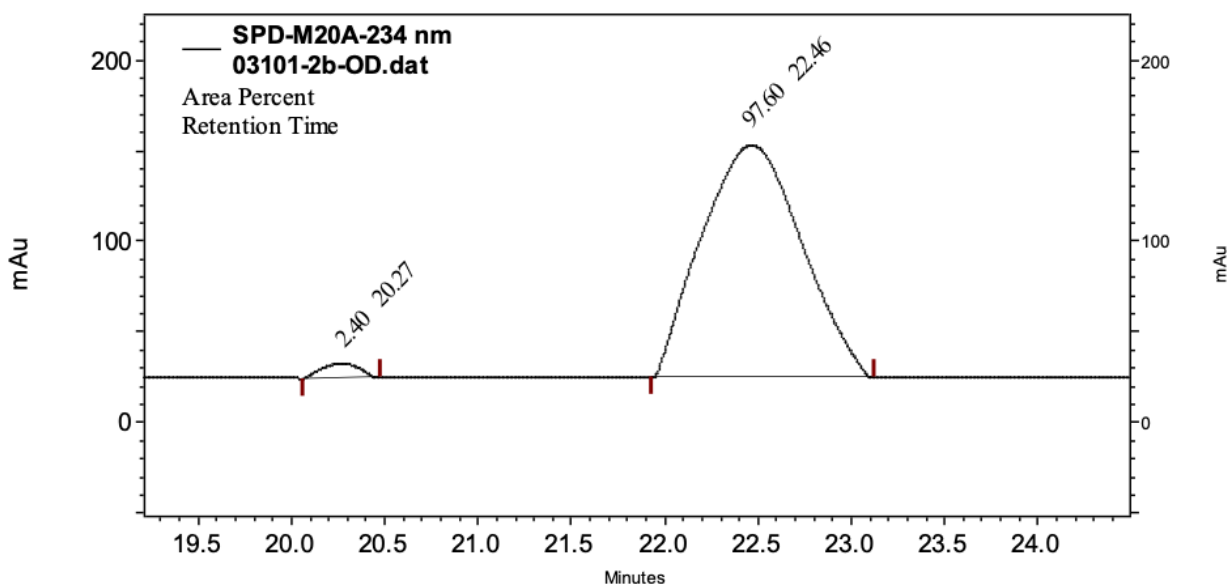


Ethyl (1R,2R,3R,4S)-3-((E)-3-oxobut-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3r):

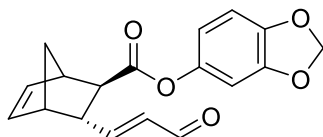


Colorless oil, 1.1 mg, 15% yield. ^1H NMR (700 MHz, CDCl_3) δ 6.42 (dd, $J = 15.9, 8.5$ Hz, 1H), 6.30 (dd, $J = 5.5, 3.2$ Hz, 1H), 6.14 (dd, $J = 5.6, 2.8$ Hz, 2H), 6.11 (d, $J = 15.9$ Hz, 1H), 4.15 (q, $J = 7.1$ Hz, 2H), 3.15 (dt, $J = 8.3, 4.1$ Hz, 1H), 3.10 (s, 1H), 2.97 (s, 1H), 2.20 (s, 3H), 2.12 (s, 0H), 2.06 (dd, $J = 4.7, 1.1$ Hz, 1H), 1.71 (d, $J = 8.8$ Hz, 1H), 1.51 (dd, $J = 8.8, 1.5$ Hz, 1H), 1.26 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 198.49, 174.59, 150.30, 137.64, 135.22, 131.20, 77.30, 77.05, 76.79, 60.84, 50.13, 47.70, 47.64, 47.50, 47.10, 27.21, 14.28. HRMS (m/z): calculated for $\text{C}_{14}\text{H}_{18}\text{NaO}_3[\text{M} + \text{Na}]^+$, 257.1148; observed, 257.1159. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), $t_r = 20.27$ min (minor), 22.46 min (major); ee = 95%.

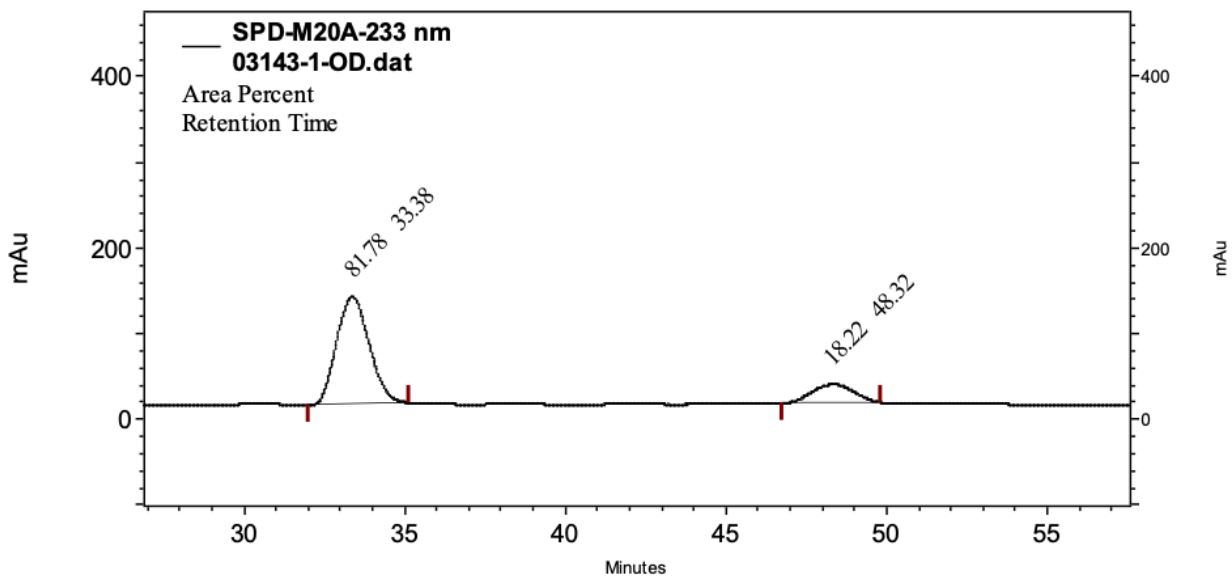
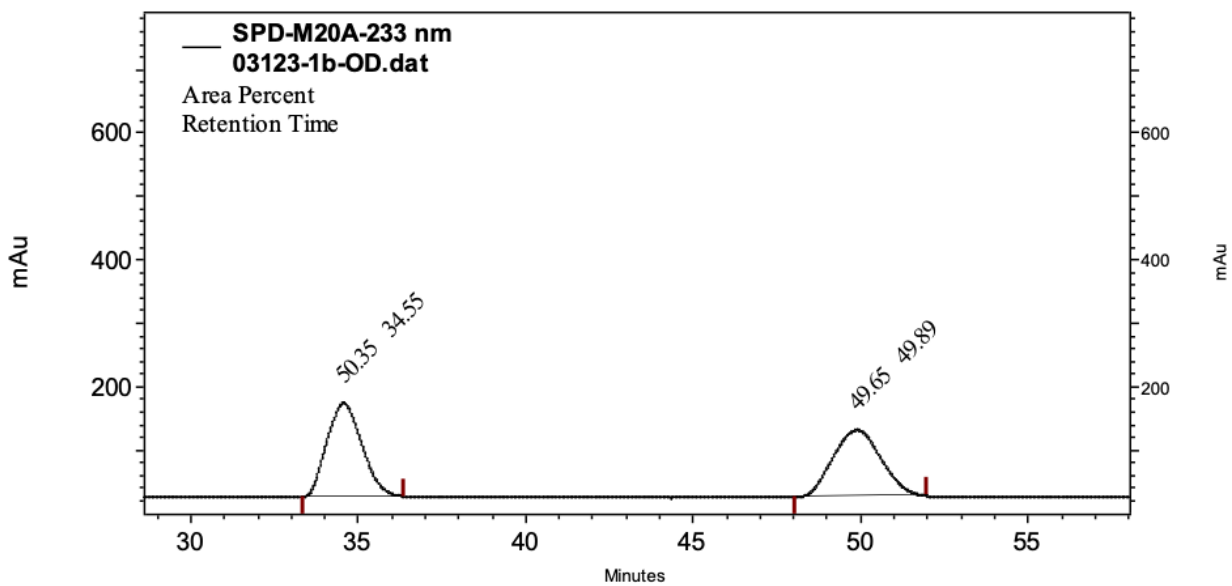




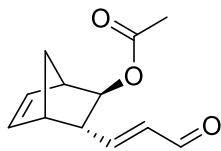
Benzo[d][1,3]dioxol-5-yl (1R,2R,3R,4S)-3-((E)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3s):



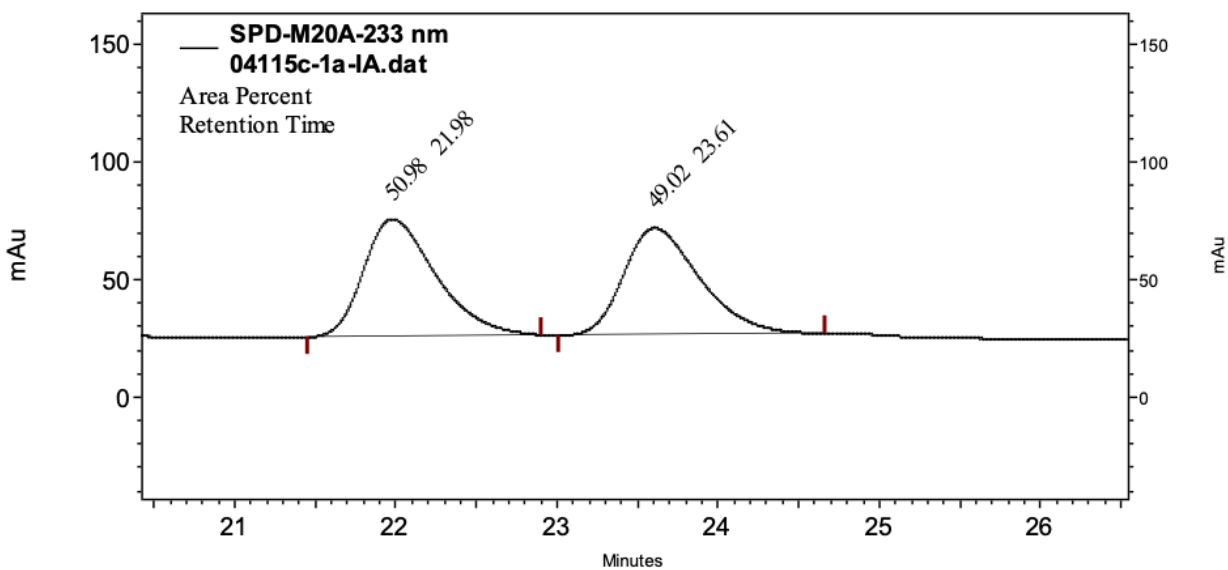
Colorless solid, 4.2 mg, 45% yield. ^1H NMR (700 MHz, CDCl_3) δ 9.48 (d, $J = 7.8$ Hz, 1H), 6.59 (s, 1H), 6.56 – 6.51 (m, 2H), 6.41 – 6.38 (m, 1H), 6.22 – 6.17 (m, 2H), 5.98 (s, 2H), 3.40 (dt, $J = 8.0, 4.0$ Hz, 1H), 3.30 (s, 1H), 3.09 (s, 1H), 2.35 (d, $J = 4.7$ Hz, 1H), 1.80 (d, $J = 8.9$ Hz, 1H), 1.62 (d, $J = 9.0$ Hz, 1H). ^{13}C NMR (176 MHz, CDCl_3) δ 193.67, 173.26, 159.77, 145.47, 144.96, 137.70, 135.34, 133.15, 113.75, 108.01, 103.57, 101.78, 50.23, 47.79, 47.77, 47.65, 47.51. HRMS (m/z): calculated for $\text{C}_{18}\text{H}_{16}\text{NaO}_5[\text{M} + \text{Na}]^+$, 335.0890; observed, 335.0905. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), $t_r = 33.38$ min (major), 48.32 min (minor); ee = 64%.

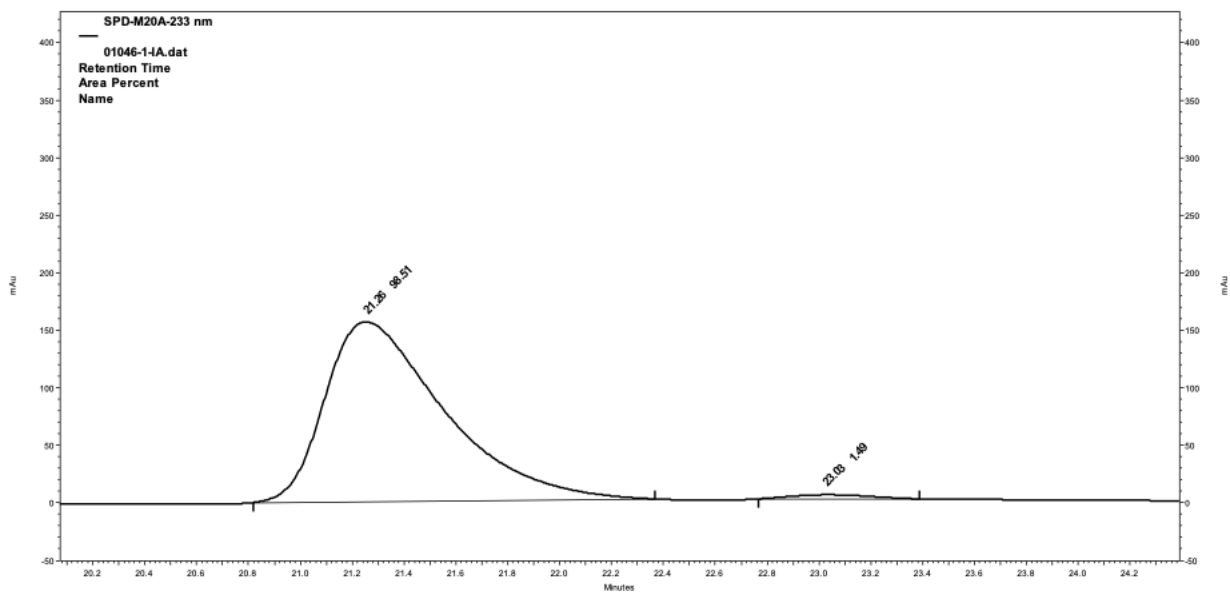


(1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-en-2-yl acetate (3t):

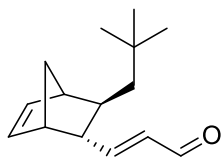


Colorless oil, 3.1 mg, 50% yield. ^1H NMR (700 MHz, CDCl_3) δ 9.46 (d, $J = 7.8$ Hz, 1H), 6.64 (dd, $J = 15.7$, 7.8 Hz, 1H), 6.25 (s, 1H), 6.18 (d, $J = 3.7$ Hz, 1H), 6.13 (dd, $J = 15.7$, 7.8 Hz, 1H), 4.49 (s, 1H), 2.96 (d, $J = 14.4$ Hz, 2H), 2.75 (s, 1H), 2.07 (s, 3H), 1.86 (d, $J = 8.6$ Hz, 1H), 1.75 (d, $J = 8.6$ Hz, 1H). ^{13}C NMR (176 MHz, CDCl_3) δ 193.83, 159.46, 138.07, 134.27, 133.58, 133.12, 79.69, 51.19, 48.20, 47.24, 46.38, 21.25. HRMS (m/z): calculated for $\text{C}_{12}\text{H}_{14}\text{NaO}_3$ [$\text{M} + \text{Na}$] $^+$, 229.0835; observed, 229.0842. HPLC (Chiralpak IA-H column, 99:1 hexanes/isopropanol, 1 ml/min), $t_r = 21.88$ min (major), 23.80 min (minor); ee = 97%.

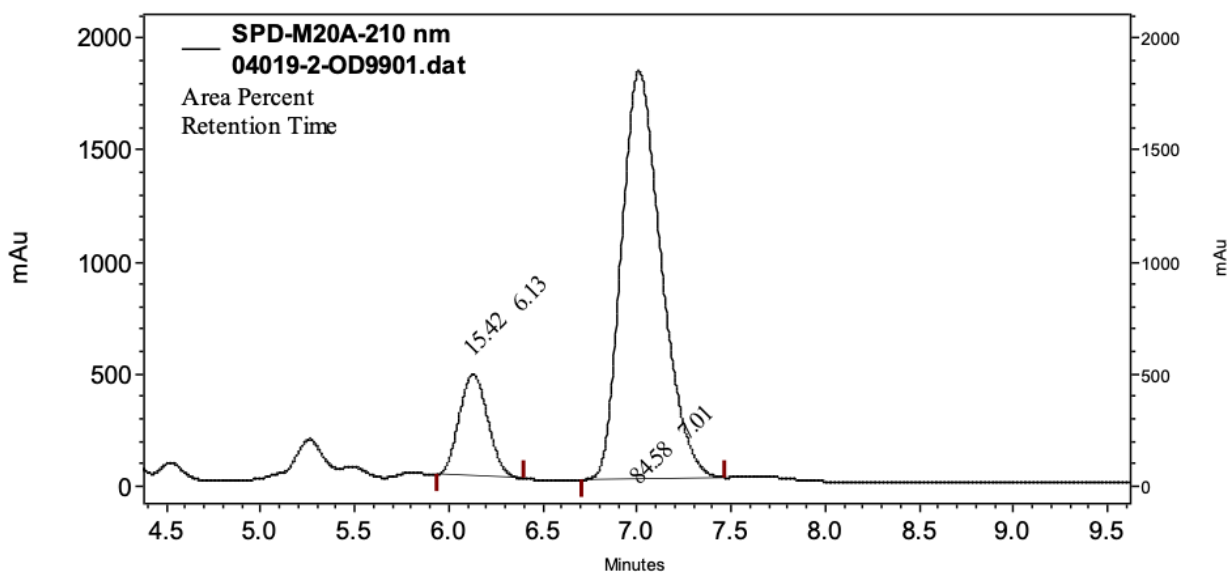
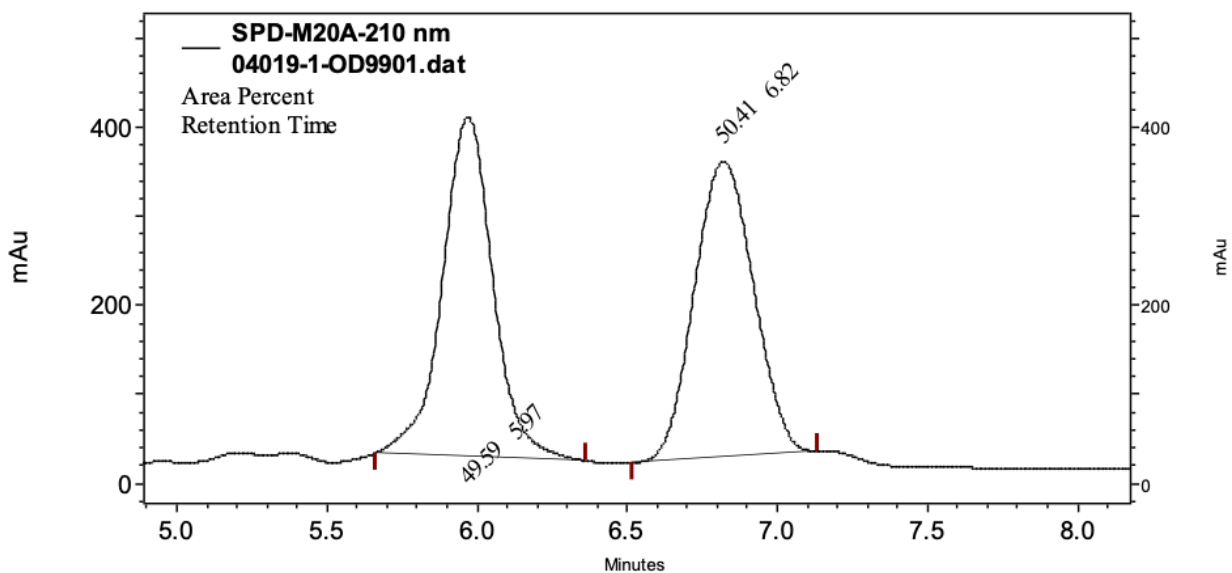




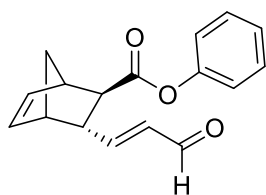
(E)-3-((1S,2R,3R,4R)-3-neopentylbicyclo[2.2.1]hept-5-en-2-yl)acrylaldehyde (3v):



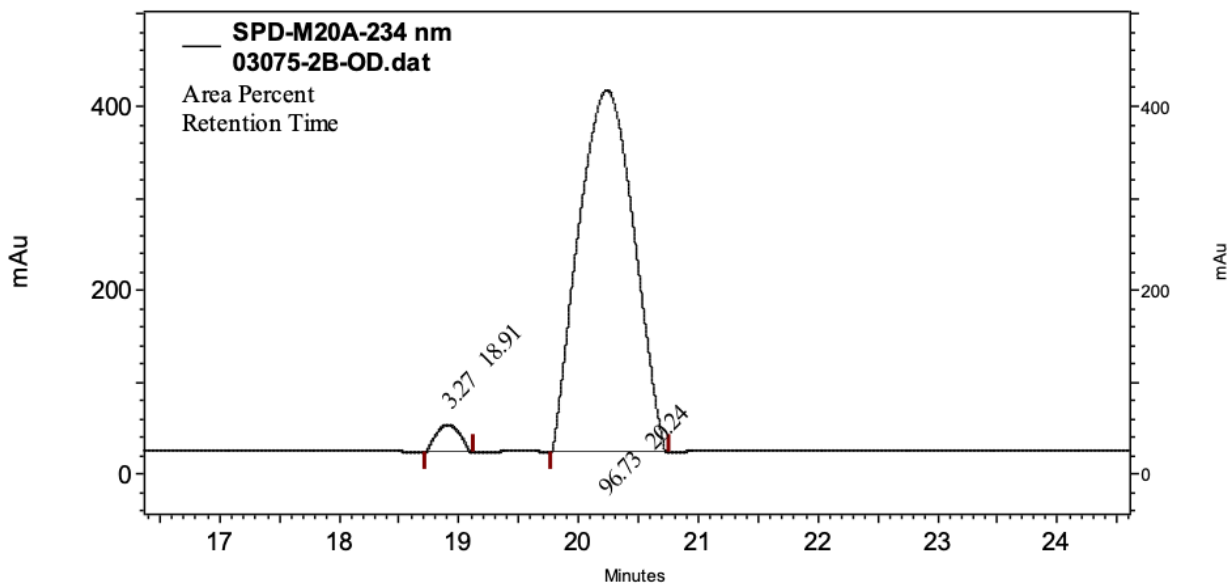
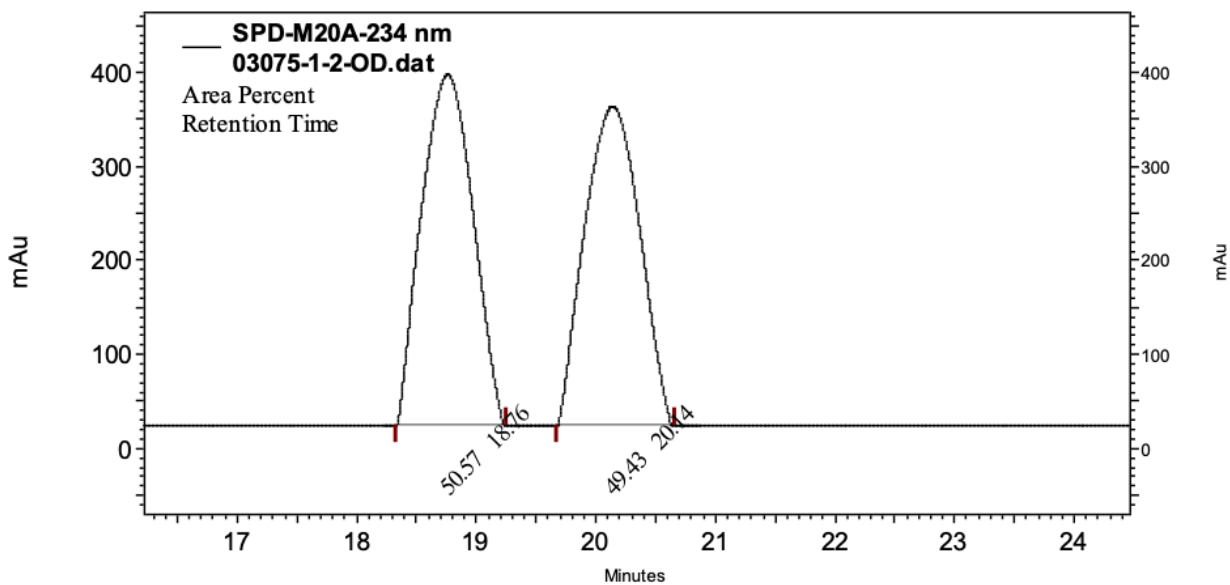
An inseparable mixture with side-product. The product yield was determined by ^1H NMR. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), t_r = 33.38 min (major), 48.32 min (minor); ee = 69%.



Phenyl (1*R*,2*R*,3*R*,4*S*)-3-((*E*)-3-oxoprop-1-en-1-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylate (3zc):



An inseparable mixture with side-product. The product yield was determined by ^1H NMR. HPLC (Chiralpak OD-H column, 95:5 hexanes/isopropanol, 1 ml/min), $t_r = 18.91$ min (minor), 20.24 min (major); ee = 94%.



5. Full list of authors in the Gaussian09 reference

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

6. Computational Methods

Catalyst-substrate structures (**4g-4y**) were optimized in the gas-phase with the M06 density functional,⁷ and the triple- ζ valence quality def2-TZVP basis set of Weigend and Ahlrichs,⁸ as implemented in Gaussian 09 (revision D.01).⁹ All of the optimized geometries were verified by frequency computations as minima (zero imaginary frequencies). Parameters were acquired from these ground state structures. NBO charges were calculated using NBO6,¹⁰ at the same level. Sterimol values were calculated using a modified version of Paton's Python script.¹¹ Multidimensional regression analyses were performed using MATLAB®.¹² Substrate structures, 3b-3s, were optimized with the M06-2X density functional,⁷ and the triple- ζ valence quality def2-TZVP basis set.⁸ NBO charges were calculated at the same level using NBO6.¹⁰ For the substrate calculations with the model catalyst system, transition states were located with the B3LYP density functional^{13,14} and the split-valence polarized 6-31G(d,p) basis set.^{15,16} Single point energy calculations were performed on the resulting structures at the M06-2X/6-31G(d,p) level. These single point calculations were used to correct the gas phase energy. Similarly, parameters were collected from the lowest energy structure determined from this process and NBO charges were calculated at the M06-2X/def2-TZVP level of theory.

Transition states with the full catalyst system were located with the M06 density functional and a mixed basis set of lanl2dz^{17,18} for gold and 6-31G(d) for all other atoms, unless otherwise noted. Single point energy calculations were performed on the resulting structures using the M06 density functional and the def2-TZVP basis set. These single point calculations were used to correct the gas phase energy. Free energies in solution were derived from structures optimized in the gas phase by means of a single point calculation using M06/def2-TZVP with the polarizable continuum model (IEFPCM).¹⁹

Conformational searches were performed with Macromodel version 11.7²⁰ and the OPLS_2005 force field.²¹⁻²³ Other conformers that could not be located using this method were generated by hand.

7. Cartesian Coordinates

7.1 Cartesian coordinates of the transition state structures with the full catalyst system

TS1

M06/lanl2dz-6-31G(d) Energy = -2646.117328

M06/lanl2dz-6-31G(d) Free Energy = -2645.482352

M06/def2-TZVP Derived free energy = -2646.594240

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.625573

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.651607

Number of Imaginary Frequencies = 1 (-372.18)

M06/lanl2dz-6-31G(d) Geometry

C	3.67740	-1.54269	-0.23666
C	4.90564	-2.32652	0.26867
C	2.63767	-2.35270	1.89298
N	2.63915	-1.52485	0.79476
C	1.51707	-0.77260	0.81869
N	0.89270	-1.19244	1.92785
N	1.57327	-2.17108	2.61503
C	5.59175	-2.77683	-1.01730
C	4.43871	-2.94980	-1.96991
C	3.31184	-2.26989	-1.50449
C	2.10734	-2.30701	-2.19200
C	2.05041	-3.03428	-3.38034
C	3.17591	-3.70148	-3.85932
C	4.37850	-3.66688	-3.15547
C	-0.39998	-0.78715	2.37251
C	-0.55798	0.47406	3.00800
C	-1.86770	0.86075	3.41979

C	-2.94649	-0.03363	3.21590
C	-2.76364	-1.25190	2.61493
C	-1.47577	-1.62717	2.17810
C	0.52216	1.35723	3.24011
C	0.30847	2.58115	3.82348
C	-0.98834	2.97247	4.21982
C	-2.05009	2.12504	4.02853
H	3.94954	-0.49376	-0.43781
H	5.54331	-1.71944	0.93588
H	6.16711	-3.69378	-0.84140
H	6.29477	-2.00463	-1.36422
H	1.21173	-1.80964	-1.81471
H	1.11542	-3.08484	-3.93480
H	3.11248	-4.26706	-4.78707
H	5.24981	-4.20782	-3.52241
H	-3.94030	0.26188	3.55383
H	-3.59130	-1.94067	2.45860
Cl	-1.28229	-3.14777	1.36927
H	1.52822	1.06073	2.95322
H	1.14984	3.25272	3.98379
H	-1.14031	3.94441	4.68424
H	-3.05312	2.41127	4.34401
Au	0.96928	0.86167	-0.49089
C	0.50284	2.45376	-1.69731
C	1.30983	3.59028	-1.52041
C	-0.51492	2.44184	-2.63654
C	1.06170	4.72532	-2.28867
C	-0.75092	3.58591	-3.40475
H	-1.11788	1.54793	-2.79187
C	0.03148	4.72065	-3.22527
H	1.67375	5.61893	-2.16860
H	-1.54529	3.58369	-4.14943
H	-0.15576	5.60965	-3.82448
C	2.43124	2.16898	0.09268
C	3.39519	1.88557	1.04789
C	2.36790	3.43154	-0.52541

C	4.31919	2.87079	1.40809
H	3.44764	0.90905	1.53044
C	3.30000	4.39970	-0.15375
C	4.26732	4.12218	0.80710
H	5.07650	2.65228	2.15878
H	3.27102	5.38432	-0.61950
H	4.98616	4.89008	1.08584
O	-0.72234	-0.39442	-1.19564
C	-2.99385	-0.98117	-0.97603
C	-1.87235	-0.17623	-0.73017
C	-5.35933	-1.46094	-0.37722
C	-4.18890	-0.69194	-0.34720
C	-6.47835	-1.18346	0.42260
H	-2.02981	0.70912	-0.07944
H	-4.20216	0.19941	0.29326
H	-2.87779	-1.86678	-1.60115
C	-7.36225	-2.30473	0.88969
H	-6.33780	-0.37727	1.15297
H	-5.36264	-2.36845	-0.98564
H	-7.49915	-3.05808	0.10356
H	-6.89751	-2.80995	1.74809
H	-8.35089	-1.95534	1.21134
C	-7.77001	-0.03276	-0.69900
C	-8.17405	-0.92263	-1.69488
C	-7.24674	-0.88736	-2.76476
C	-6.33023	0.10057	-2.51797
C	-6.77750	0.89677	-1.34346
H	-8.43595	0.29210	0.10007
H	-9.01235	-1.61072	-1.61770
H	-7.24368	-1.56158	-3.61589
H	-5.47684	0.35627	-3.14007
H	-5.98373	1.29380	-0.70289
H	-7.34310	1.76873	-1.71861
C	3.80644	-3.24544	2.14150
H	4.47520	-2.77214	2.88463
H	3.47487	-4.20475	2.55157

O 4.48246 -3.49868 0.94136

TS2

M06/lanl2dz-6-31G(d) Energy = -2646.114718

M06/lanl2dz-6-31G(d) Free Energy = -2645.480221

M06/def2-TZVP Derived free energy = -2646.592129

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.623262

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.648663

Number of Imaginary Frequencies = 1 (-381.61)

M06/lanl2dz-6-31G(d) Geometry

C	-0.97518	3.08190	-0.32308
C	-0.83521	4.39085	-1.12960
C	-1.86175	2.20314	-2.49815
N	-1.42080	2.00233	-1.21111
C	-1.44238	0.67572	-0.95069
N	-1.89685	0.14739	-2.09955
N	-2.15825	1.07831	-3.07543
C	-0.99446	5.48362	-0.07819
C	-1.90938	4.85059	0.93493
C	-1.92972	3.46371	0.77952
C	-2.70586	2.66050	1.60302
C	-3.47190	3.26918	2.59577
C	-3.45020	4.65287	2.75731
C	-2.66776	5.45376	1.92773
C	-2.11598	-1.23832	-2.34668
C	-0.99647	-2.11300	-2.38740
C	-1.24092	-3.51209	-2.49729
C	-2.57335	-3.97626	-2.60714
C	-3.63100	-3.10677	-2.62606
C	-3.39717	-1.72357	-2.49309
C	0.34323	-1.65424	-2.33651
C	1.38516	-2.54842	-2.36977
C	1.14466	-3.93688	-2.44415
C	-0.14281	-4.40452	-2.51112
H	0.00234	2.76738	0.07510

H	0.11741	4.43597	-1.68682
H	-1.39506	6.39668	-0.53546
H	-0.01734	5.73446	0.36153
H	-2.73428	1.57681	1.48018
H	-4.09410	2.65714	3.24568
H	-4.05675	5.11377	3.53458
H	-2.66321	6.53628	2.04882
H	-2.74887	-5.04813	-2.68972
H	-4.65466	-3.45959	-2.72368
Cl	-4.76969	-0.66208	-2.45717
H	0.54424	-0.58425	-2.30962
H	2.40983	-2.17806	-2.36216
H	1.98137	-4.63179	-2.46460
H	-0.34295	-5.47277	-2.58691
Au	-0.60931	-0.31394	0.80084
C	0.19342	-1.26198	2.43677
C	-0.63515	-2.23189	3.02799
C	1.44687	-0.99197	2.96169
C	-0.16839	-2.95189	4.12501
C	1.90242	-1.71541	4.06786
H	2.07409	-0.20820	2.53782
C	1.10042	-2.69652	4.63816
H	-0.79845	-3.70651	4.59526
H	2.88422	-1.50239	4.48816
H	1.45650	-3.25869	5.49938
C	-2.21977	-1.42596	1.38699
C	-3.46260	-1.33326	0.78958
C	-1.96567	-2.32834	2.43409
C	-4.48228	-2.19387	1.20624
H	-3.66527	-0.60338	0.00922
C	-2.99626	-3.17732	2.83444
C	-4.24300	-3.11615	2.21716
H	-5.46051	-2.12901	0.73124
H	-2.82939	-3.88962	3.64206
H	-5.03637	-3.78747	2.54003
O	1.25358	0.81245	0.23321

C	3.48767	0.82175	-0.50987
C	2.32017	0.20118	-0.04467
C	5.82448	0.56313	-1.30128
C	4.61952	0.07476	-0.78597
C	6.89792	-0.25673	-1.68407
H	2.35373	-0.90005	0.08020
H	4.55194	-1.00824	-0.62086
H	3.48248	1.90262	-0.65548
C	7.80338	0.17591	-2.80151
H	6.69859	-1.33368	-1.64609
H	5.89964	1.63710	-1.48974
H	7.99448	1.25574	-2.76162
H	8.76657	-0.34840	-2.79116
H	7.32456	-0.03656	-3.76728
C	8.18770	-0.37692	-0.08476
C	8.66347	0.93077	0.01686
C	7.78840	1.69149	0.83126
C	6.83441	0.85594	1.34802
C	7.19520	-0.55201	1.03193
H	8.80812	-1.19799	-0.44292
H	9.51804	1.32980	-0.52421
H	7.84704	2.76496	0.98347
H	6.00452	1.14586	1.98673
H	7.74380	-0.96720	1.89651
H	6.35538	-1.22839	0.84300
O	-1.91979	4.52351	-2.02998
C	-1.89535	3.58112	-3.06536
H	-1.01725	3.73000	-3.72121
H	-2.79489	3.72300	-3.67298

TS3

M06/lanl2dz-6-31G(d) Energy = -2646.117014

M06/lanl2dz-6-31G(d) Free Energy = -2645.480715

M06/def2-TZVP Derived free energy = -2646.593025

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.623504

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.648284

Number of Imaginary Frequencies = 1 (-393.76)

M06/lanl2dz-6-31G(d) Geometry

C	-0.05937	3.03952	0.23877
C	0.25686	4.43773	-0.33501
C	-1.34766	2.78992	-1.89525
N	-0.81120	2.25677	-0.74813
C	-1.09170	0.93344	-0.71373
N	-1.78848	0.74050	-1.84595
N	-1.95717	1.88191	-2.59613
C	0.43637	5.30715	0.90488
C	-0.47301	4.65738	1.91202
C	-0.79097	3.35608	1.51931
C	-1.61768	2.55510	2.29468
C	-2.12832	3.07727	3.48194
C	-1.80851	4.37367	3.87944
C	-0.97844	5.17348	3.09660
C	-2.33899	-0.49067	-2.30752
C	-3.75286	-0.64770	-2.33190
C	-4.28008	-1.91481	-2.71713
C	-3.39354	-2.95615	-3.07946
C	-2.03691	-2.77060	-3.07866
C	-1.51182	-1.52188	-2.69368
C	-4.65083	0.38488	-1.96713
C	-6.00584	0.16326	-1.97981
C	-6.52988	-1.09223	-2.35608
C	-5.68215	-2.10690	-2.71866
H	0.87103	2.48331	0.42961
H	1.13372	4.42222	-1.00619
H	0.18339	6.35017	0.67819
H	1.48565	5.28620	1.23602
H	-1.87812	1.54021	1.99121
H	-2.78177	2.46587	4.10107
H	-2.21643	4.76805	4.80827
H	-0.74015	6.19087	3.40441
H	-3.80957	-3.91967	-3.37129

H	-1.35408	-3.56368	-3.37184
Cl	0.21861	-1.31569	-2.74185
H	-4.26277	1.36348	-1.69215
H	-6.68415	0.96787	-1.70278
H	-7.60645	-1.24813	-2.36275
H	-6.07282	-3.07922	-3.01693
Au	-0.31844	-0.49977	0.73190
C	0.42696	-1.88326	2.05331
C	-0.52282	-2.77152	2.58558
C	1.76083	-1.97396	2.41610
C	-0.10308	-3.77827	3.45201
C	2.16992	-2.98321	3.29232
H	2.48777	-1.25527	2.03856
C	1.24142	-3.88548	3.79762
H	-0.82425	-4.47945	3.87150
H	3.21651	-3.05672	3.58495
H	1.56207	-4.67242	4.47762
C	-2.06339	-1.36468	1.35773
C	-3.31538	-0.91989	0.97653
C	-1.89926	-2.48493	2.19188
C	-4.44591	-1.62819	1.39370
H	-3.43983	-0.03378	0.35799
C	-3.03954	-3.17674	2.59726
C	-4.30322	-2.75538	2.19278
H	-5.43373	-1.28744	1.08742
H	-2.94327	-4.04925	3.24281
H	-5.18329	-3.30893	2.51444
O	1.70292	0.29126	0.13683
C	3.72209	-0.09946	-1.02479
C	2.49283	-0.48276	-0.46580
C	5.76121	-0.85589	-2.24293
C	4.49717	-1.04818	-1.67459
C	6.45241	0.36014	-2.19602
H	2.22154	-1.55229	-0.56315
H	4.07647	-2.05607	-1.74048
H	4.01215	0.94862	-0.95693

C	7.58170	0.61322	-3.15192
H	5.86947	1.24805	-1.94493
H	6.23904	-1.70548	-2.73227
H	8.21838	1.45170	-2.84873
H	8.21386	-0.27307	-3.28812
H	7.16417	0.86398	-4.13713
C	7.46838	0.35126	-0.36832
C	6.46996	0.35234	0.60384
C	6.14826	-0.98430	0.95865
C	6.98984	-1.83279	0.29868
C	8.04289	-1.04287	-0.39381
H	8.07419	1.23097	-0.57969
H	5.97725	1.23788	0.99830
H	5.33289	-1.27700	1.61429
H	6.97773	-2.91754	0.35052
H	8.95066	-1.04565	0.23628
H	8.34995	-1.42979	-1.37120
O	-0.86701	4.94087	-1.03391
C	-1.14303	4.23248	-2.20959
H	-0.32001	4.33519	-2.94134
H	-2.04549	4.65955	-2.65899

TS4

M06/lanl2dz-6-31G(d) Energy = -2646.117511

M06/lanl2dz-6-31G(d) Free Energy = -2645.482023

M06/def2-TZVP Derived free energy = -2646.592162

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.623131

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.647825

Number of Imaginary Frequencies = 1 (-401.91)

M06/lanl2dz-6-31G(d) Geometry

C	-3.04534	-0.66004	2.27057
C	-3.50405	-1.63401	3.37424
C	-2.80562	-2.83229	1.00584
N	-2.54353	-1.48561	1.14343
C	-1.78739	-1.09351	0.08994

N	-1.62818	-2.22045	-0.61321
N	-2.25261	-3.31373	-0.06699
C	-2.21686	-1.95617	4.16073
C	-1.45079	-0.67009	4.02670
C	-1.94735	0.09266	2.96412
C	-1.46745	1.37237	2.70852
C	-0.42859	1.86377	3.49748
C	0.09360	1.09224	4.53635
C	-0.42234	-0.17250	4.81759
C	-0.90527	-2.34382	-1.83669
C	0.41800	-2.85814	-1.80648
C	1.13129	-2.94111	-3.03664
C	0.49839	-2.52657	-4.23352
C	-0.78538	-2.04910	-4.23665
C	-1.49411	-1.96002	-3.02130
C	1.05302	-3.27848	-0.61440
C	2.33723	-3.76137	-0.64598
C	3.04928	-3.84266	-1.86291
C	2.45669	-3.43847	-3.03207
H	-3.85693	-0.03073	1.88323
H	-4.18252	-1.07526	4.03101
H	-1.66792	-2.79737	3.70832
H	-2.42772	-2.23821	5.19900
H	-1.90935	1.99121	1.92756
H	-0.04164	2.86486	3.31546
H	0.89239	1.49568	5.15634
H	-0.03945	-0.75031	5.65793
H	1.05158	-2.59777	-5.16948
H	-1.27524	-1.73848	-5.15597
Cl	-3.12466	-1.36864	-3.05454
H	0.51648	-3.21535	0.33116
H	2.81413	-4.08413	0.27792
H	4.06637	-4.23002	-1.86798
H	2.99139	-3.50000	-3.97957
Au	-0.85949	0.78136	-0.42955
C	0.02399	2.57016	-0.89894

C	-0.86642	3.64012	-1.08934
C	1.39307	2.75432	-1.01231
C	-0.35634	4.90810	-1.36374
C	1.89192	4.02965	-1.29428
H	2.07537	1.90986	-0.89755
C	1.01909	5.09988	-1.46117
H	-1.02925	5.75222	-1.51326
H	2.96709	4.18377	-1.39083
H	1.41077	6.09187	-1.67816
C	-2.53152	1.91029	-0.74967
C	-3.82249	1.41480	-0.67551
C	-2.27868	3.27143	-1.00163
C	-4.89979	2.28956	-0.84320
H	-4.00846	0.35403	-0.50812
C	-3.36779	4.12699	-1.16366
C	-4.66851	3.63894	-1.08172
H	-5.91756	1.90733	-0.79073
H	-3.20112	5.18566	-1.36109
H	-5.50757	4.31949	-1.21151
O	1.09919	-0.19273	-0.11914
C	3.02283	-0.53906	1.18578
C	1.66239	-0.22380	1.00948
C	5.19981	-1.04974	0.07450
C	3.82141	-0.81308	0.08347
C	6.01548	-0.99772	1.21081
H	1.06661	0.01547	1.91120
H	3.30473	-0.83547	-0.87967
H	3.40858	-0.55825	2.20365
C	7.37312	-1.63722	1.18141
H	5.51652	-1.04341	2.18055
H	5.67071	-1.25956	-0.88788
H	8.01593	-1.31292	2.00704
H	7.25729	-2.72644	1.27208
H	7.89723	-1.44741	0.23592
C	6.54255	1.01962	1.41183
C	5.35640	1.66318	1.75705

C	4.70727	2.13312	0.58566
C	5.50161	1.87373	-0.49461
C	6.82510	1.37765	-0.02566
H	7.33951	0.84725	2.13327
H	4.96070	1.75073	2.76627
H	3.71745	2.58295	0.55977
H	5.26388	2.09555	-1.53187
H	7.27851	0.59490	-0.64273
H	7.53587	2.22359	-0.02900
O	-4.26198	-2.71261	2.89429
C	-3.58008	-3.58546	2.03337
H	-2.89950	-4.25576	2.58655
H	-4.33204	-4.21791	1.54916

Other conformations

Conformer clustering notation: cyclopentadiene approach (top or bottom), aldehyde orientation (towards or away from the aromatic R substituent), aldehyde coordination site (site 1 or 2), orientation of cyclopentadiene with respect to the aldehyde (*endo* or *exo*) and aromatic group orientation (naphthyl substituent towards the aldehyde or away).

Top, away, 1, endo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.116148

M06/lanl2dz-6-31G(d) Free Energy = -2645.478670

M06/def2-TZVP Derived free energy = -2646.589233

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.620268

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.645327

Number of Imaginary Frequencies = -1 (-387.23)

M06/lanl2dz-6-31G(d) Geometry

C	-3.25798	2.45224	-0.29758
C	-3.52674	3.96825	-0.29219
C	-1.81349	3.11191	1.66978
N	-2.17508	2.20809	0.69307
C	-1.36630	1.12848	0.79642

N	-0.56919	1.43636	1.82880
N	-0.82722	2.66433	2.38670
C	-2.45924	4.54664	-1.24243
C	-2.29220	3.42384	-2.22832
C	-2.79320	2.22776	-1.70487
C	-2.83550	1.06608	-2.46636
C	-2.29361	1.09254	-3.74969
C	-1.75784	2.27385	-4.26185
C	-1.77092	3.45078	-3.51514
C	0.55456	0.67817	2.27011
C	0.35481	-0.53298	2.98755
C	1.50325	-1.29439	3.35979
C	2.79158	-0.79732	3.04858
C	2.95500	0.38751	2.38054
C	1.82443	1.12335	1.97283
C	-0.92752	-1.01639	3.33845
C	-1.06549	-2.21421	3.99318
C	0.06767	-2.97761	4.34629
C	1.32473	-2.52121	4.04172
H	-4.12838	1.85695	0.00725
H	-4.51505	4.11926	-0.74449
H	-1.51454	4.75471	-0.71521
H	-2.78194	5.49100	-1.69671
H	-3.30359	0.15886	-2.08209
H	-2.30672	0.19077	-4.35912
H	-1.34844	2.28369	-5.27030
H	-1.38730	4.37780	-3.93950
H	3.66405	-1.37240	3.36008
H	3.94344	0.78381	2.16021
Cl	2.07438	2.58114	1.06269
H	-1.81050	-0.43684	3.08041
H	-2.06131	-2.57600	4.24264
H	-0.06008	-3.92508	4.86515
H	2.20780	-3.09505	4.32126
Au	-1.25978	-0.67316	-0.38251
C	-1.22480	-2.38930	-1.50943

C	-2.26330	-3.29744	-1.24007
C	-0.29054	-2.65098	-2.49870
C	-2.32755	-4.48952	-1.95837
C	-0.36800	-3.84902	-3.21514
H	0.49162	-1.92892	-2.73221
C	-1.37762	-4.76370	-2.93872
H	-3.12319	-5.20900	-1.76547
H	0.36253	-4.06106	-3.99421
H	-1.43418	-5.69581	-3.49781
C	-2.95717	-1.57359	0.31713
C	-3.80396	-1.01057	1.25903
C	-3.21175	-2.84738	-0.22339
C	-4.92388	-1.72529	1.69267
H	-3.61186	-0.02055	1.67387
C	-4.33389	-3.54523	0.22306
C	-5.18144	-2.98961	1.17632
H	-5.59169	-1.28667	2.43193
H	-4.55150	-4.53365	-0.18068
H	-6.05335	-3.54735	1.51238
O	0.62975	0.12400	-1.22990
C	2.96437	0.01122	-1.46027
C	1.73484	-0.38125	-0.90557
C	5.39493	-0.42040	-1.67885
C	4.12985	-0.63980	-1.11206
C	6.52666	-1.19800	-1.39004
H	1.76033	-1.20288	-0.15933
H	4.04910	-1.43428	-0.35896
H	2.96307	0.81113	-2.20161
C	7.57474	-1.41164	-2.44522
H	6.34491	-2.06394	-0.74324
H	5.47119	0.33642	-2.46340
H	7.24109	-2.18802	-3.14725
H	7.74546	-0.49623	-3.02607
H	8.53346	-1.73933	-2.02488
C	7.57578	-0.21588	0.08160
C	8.01285	0.93720	-0.57262

C	6.99996	1.92402	-0.51419
C	5.97557	1.45728	0.26781
C	6.41861	0.20656	0.94595
H	8.25504	-1.01663	0.37297
H	8.94047	1.02537	-1.13278
H	7.01304	2.86950	-1.04811
H	5.03829	1.97246	0.47027
H	6.82968	0.47849	1.93544
H	5.64326	-0.54835	1.11846
O	-3.62841	4.51535	0.99773
C	-2.45954	4.45260	1.76955
H	-1.72867	5.22376	1.46992
H	-2.74192	4.66279	2.80716

M06/lanl2dz-6-31G(d) Energy = -2646.113504

M06/lanl2dz-6-31G(d) Free Energy = -2645.473215

M06/def2-TZVP Derived free energy = -2646.582692

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.613017

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.637306

Number of Imaginary Frequencies = -1 (-382.42)

M06/lanl2dz-6-31G(d) Geometry

C	1.03223	-0.88431	3.51208
C	-0.13686	-0.90497	4.53748
C	0.61650	1.51746	3.31726
N	0.87942	0.32717	2.68036
C	1.04614	0.56507	1.35982
N	0.90145	1.90156	1.28194
N	0.62273	2.51320	2.48438
C	-1.21423	-1.76440	3.87015
C	-0.41704	-2.68905	2.99918
C	0.86550	-2.18139	2.78796
C	1.79597	-2.85547	2.00331
C	1.41204	-4.05153	1.40150
C	0.12771	-4.55811	1.60295
C	-0.79123	-3.88843	2.40845

C	1.09135	2.70026	0.11618
C	2.34380	3.34722	-0.06491
C	2.56398	4.05896	-1.27906
C	1.52449	4.13486	-2.23613
C	0.30613	3.54865	-2.01490
C	0.09332	2.83033	-0.82203
C	3.37681	3.30125	0.90181
C	4.57794	3.92213	0.66354
C	4.80572	4.61186	-0.54717
C	3.81708	4.67980	-1.49487
H	2.01036	-0.78763	4.00529
H	0.24634	-1.40627	5.44295
H	-1.85388	-1.10798	3.25819
H	-1.85888	-2.27173	4.59751
H	2.80170	-2.45709	1.85835
H	2.11582	-4.59101	0.77077
H	-0.15510	-5.49703	1.12998
H	-1.78616	-4.30136	2.57033
H	1.70361	4.68303	-3.16032
H	-0.50007	3.62379	-2.73992
Cl	-1.47347	2.11478	-0.55533
H	3.20614	2.78376	1.84473
H	5.36151	3.88754	1.41802
H	5.76460	5.09593	-0.71944
H	3.97769	5.21674	-2.42911
Au	1.02621	-0.89831	-0.26473
C	0.96199	-2.28803	-1.77183
C	2.08874	-2.31833	-2.61062
C	-0.08179	-3.18102	-1.95075
C	2.12566	-3.22826	-3.66566
C	-0.03084	-4.09257	-3.00920
H	-0.92708	-3.19588	-1.26270
C	1.06341	-4.10527	-3.86694
H	2.98970	-3.26589	-4.32894
H	-0.84770	-4.79725	-3.15704
H	1.09906	-4.81381	-4.69239

C	2.89027	-0.64409	-1.05941
C	3.82909	0.22273	-0.53092
C	3.15024	-1.39490	-2.22059
C	5.05348	0.38450	-1.18487
H	3.62636	0.78813	0.37607
C	4.38078	-1.22551	-2.85312
C	5.32188	-0.33540	-2.34259
H	5.78944	1.07769	-0.77964
H	4.61201	-1.79617	-3.75245
H	6.27607	-0.21059	-2.85106
O	-1.10748	-1.18328	0.38902
C	-3.40284	-0.86902	-0.02915
C	-2.04946	-0.93057	-0.40259
C	-5.74321	-0.44106	-0.74199
C	-4.36172	-0.52597	-0.96147
C	-6.67650	-0.17791	-1.75700
H	-1.82310	-0.73784	-1.47081
H	-4.00792	-0.32679	-1.98133
H	-3.67227	-1.07752	1.00710
C	-8.05982	-0.75821	-1.66769
H	-6.26087	-0.14111	-2.77050
H	-6.11431	-0.67407	0.25919
H	-8.77844	-0.23313	-2.30879
H	-8.04192	-1.80938	-1.98632
H	-8.43379	-0.73457	-0.63614
C	-7.03811	1.83686	-1.74917
C	-7.67641	2.03174	-0.52227
C	-6.70525	2.22236	0.48947
C	-5.46698	2.27520	-0.09550
C	-5.63020	2.34060	-1.57284
H	-7.56561	1.91559	-2.69964
H	-8.74671	1.94209	-0.35286
H	-6.90949	2.26978	1.55495
H	-4.51583	2.38293	0.41986
H	-5.62278	3.40487	-1.87006
H	-4.85270	1.84503	-2.16336

C	0.24123	1.43831	4.75520
H	1.13135	1.30436	5.39560
H	-0.27543	2.34856	5.07187
O	-0.65936	0.36174	4.88015

M06/lanl2dz-6-31G(d) Energy = -2646.114746

M06/lanl2dz-6-31G(d) Free Energy = -2645.476715

M06/def2-TZVP Derived free energy = -2646.586823

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617614

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642135

Number of Imaginary Frequencies = -1 (-374.98)

M06/lanl2dz-6-31G(d) Geometry

C	1.89214	3.15808	-0.43963
C	1.64524	4.55329	-1.04575
C	0.92201	2.46341	-2.66575
N	1.27834	2.17036	-1.36644
C	0.97261	0.87317	-1.12693
N	0.44712	0.46112	-2.28688
N	0.40478	1.42970	-3.25866
C	0.23160	4.93315	-0.56307
C	0.18462	4.26013	0.78009
C	1.15785	3.25852	0.86447
C	1.37741	2.56360	2.04780
C	0.56096	2.83865	3.14256
C	-0.43340	3.81209	3.05188
C	-0.61870	4.54019	1.87760
C	-0.15712	-0.80672	-2.52722
C	0.65548	-1.93853	-2.80144
C	0.00695	-3.19002	-3.02297
C	-1.40583	-3.25597	-2.97748
C	-2.16640	-2.14692	-2.71140
C	-1.52998	-0.91165	-2.47962
C	2.06803	-1.87704	-2.85893
C	2.80135	-3.00956	-3.11051
C	2.16325	-4.25024	-3.32508

C	0.79515	-4.33557	-3.28532
H	2.95685	2.90685	-0.35058
H	2.36723	5.23625	-0.58107
H	-0.54540	4.53447	-1.23513
H	0.08837	6.01930	-0.52023
H	2.18937	1.84061	2.13288
H	0.71730	2.30704	4.07915
H	-1.05317	4.02834	3.92026
H	-1.36907	5.32845	1.82906
H	-1.88931	-4.21576	-3.15722
H	-3.25142	-2.20222	-2.66762
Cl	-2.50619	0.47892	-2.10459
H	2.57243	-0.92584	-2.70132
H	3.88707	-2.94848	-3.14686
H	2.76091	-5.13630	-3.52708
H	0.29198	-5.28696	-3.45508
Au	1.27224	-0.36080	0.61730
C	1.65346	-1.46993	2.30498
C	3.01602	-1.69420	2.56950
C	0.67917	-1.93667	3.17276
C	3.38089	-2.41706	3.70317
C	1.05776	-2.65836	4.30854
H	-0.37616	-1.73996	2.98736
C	2.40190	-2.90054	4.56647
H	4.43199	-2.60421	3.92259
H	0.29606	-3.02930	4.99246
H	2.69303	-3.46539	5.45007
C	3.31746	-0.38572	0.55046
C	4.07041	0.21533	-0.44614
C	3.92943	-1.10468	1.59337
C	5.46388	0.11467	-0.41184
H	3.59542	0.75917	-1.26282
C	5.32133	-1.19120	1.61126
C	6.08254	-0.58560	0.61663
H	6.05792	0.58623	-1.19256
H	5.81918	-1.73978	2.41028

H	7.16747	-0.66383	0.64557
O	-0.93796	-0.53744	0.78938
C	-2.85022	-1.92704	0.75831
C	-1.47781	-1.66218	0.59555
C	-5.08246	-1.16074	1.51496
C	-3.73370	-0.95877	1.20089
C	-5.87723	-0.18610	2.13871
H	-0.83889	-2.51380	0.29370
H	-3.31181	0.03702	1.37526
H	-3.19227	-2.94583	0.57539
C	-6.97335	-0.60521	3.07637
H	-5.34492	0.72569	2.43211
H	-5.50144	-2.15997	1.37014
H	-7.71923	0.18353	3.23461
H	-7.48877	-1.50166	2.70865
H	-6.54424	-0.85266	4.05706
C	-6.90918	0.81372	0.66580
C	-7.78137	-0.16916	0.19742
C	-7.14086	-0.92640	-0.81475
C	-5.92440	-0.35836	-1.08203
C	-5.82344	0.94256	-0.36788
H	-7.24865	1.66235	1.25907
H	-8.76173	-0.38571	0.61481
H	-7.53813	-1.82984	-1.26781
H	-5.18641	-0.71562	-1.79507
H	-4.82341	1.20624	-0.00787
H	-6.13020	1.74072	-1.06808
C	1.07867	3.83452	-3.23008
H	1.54125	3.78178	-4.22189
H	0.08129	4.28898	-3.36152
O	1.90964	4.62414	-2.42315

Top, towards, 1, endo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.117469

M06/lanl2dz-6-31G(d) Free Energy = -2645.479337

M06/def2-TZVP Derived free energy = -2646.588747

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.619903

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.645543

Number of Imaginary Frequencies = 1 (-380.15)

M06/lanl2dz-6-31G(d) Geometry

C	0.35934	-1.79129	2.70294
C	-0.62325	-2.08957	3.85031
C	-0.25252	0.57161	3.33920
N	0.26168	-0.33265	2.43398
C	0.62549	0.34412	1.31680
N	0.31359	1.61332	1.61274
N	-0.23246	1.77880	2.86150
C	-1.98947	-2.22334	3.14545
C	-1.58314	-2.82918	1.83006
C	-0.21998	-2.61522	1.59105
C	0.41293	-3.16350	0.48178
C	-0.35629	-3.87071	-0.44144
C	-1.72286	-4.05039	-0.22892
C	-2.34192	-3.55039	0.91709
C	0.37248	2.72109	0.71559
C	1.62431	3.30870	0.39354
C	1.63890	4.37329	-0.55567
C	0.41765	4.82974	-1.10437
C	-0.78082	4.26186	-0.75791
C	-0.79426	3.19052	0.15387
C	2.84670	2.87677	0.95894
C	4.03189	3.45086	0.57371
C	4.05217	4.49237	-0.37877
C	2.87884	4.94822	-0.92327
H	1.40331	-2.01797	2.95428
H	-0.34923	-3.06990	4.26000
H	-2.46665	-1.23891	2.99665
H	-2.69358	-2.83608	3.72062
H	1.48985	-3.06315	0.34314
H	0.11847	-4.29625	-1.32348

H	-2.30929	-4.61058	-0.95474
H	-3.40113	-3.73624	1.09696
H	0.44105	5.65208	-1.81845
H	-1.71899	4.61433	-1.17851
Cl	-2.32220	2.43979	0.53726
H	2.84588	2.08315	1.70212
H	4.96483	3.09747	1.00924
H	5.00076	4.93543	-0.67383
H	2.88075	5.75944	-1.65040
Au	1.52854	-0.37339	-0.52126
C	2.44492	-1.10684	-2.20318
C	3.78391	-1.49662	-2.03388
C	1.80506	-1.24617	-3.42255
C	4.47323	-2.03829	-3.11685
C	2.51008	-1.78969	-4.50081
H	0.76949	-0.93170	-3.54279
C	3.83462	-2.18289	-4.34564
H	5.51167	-2.35111	-3.00853
H	2.01835	-1.90311	-5.46574
H	4.37754	-2.60720	-5.18812
C	3.39458	-0.74722	0.23691
C	3.75981	-0.51590	1.55425
C	4.30807	-1.28699	-0.68736
C	5.06189	-0.80827	1.96974
H	3.05402	-0.10171	2.27517
C	5.60311	-1.57136	-0.25358
C	5.97757	-1.33068	1.06448
H	5.35237	-0.62410	3.00255
H	6.32944	-1.98382	-0.95333
H	6.99221	-1.55678	1.38641
O	-0.39130	-0.09159	-1.60991
C	-2.71717	-0.41333	-1.81326
C	-1.49889	-0.41381	-1.11381
C	-5.17199	-0.80823	-1.68941
C	-3.88094	-0.73514	-1.14727
C	-6.29013	-1.23448	-0.95552

H	-1.54535	-0.72145	-0.04731
H	-3.77873	-0.98795	-0.08281
H	-2.71914	-0.14484	-2.86975
C	-7.42112	-1.93384	-1.65609
H	-6.06529	-1.62050	0.04597
H	-5.29225	-0.60106	-2.75531
H	-7.62284	-1.47735	-2.63352
H	-7.15616	-2.98494	-1.83478
H	-8.34902	-1.92349	-1.07109
C	-7.19701	0.43140	-0.19123
C	-7.70023	1.05766	-1.33423
C	-6.69866	1.88296	-1.89936
C	-5.61303	1.89086	-1.06279
C	-5.98030	1.22018	0.21427
H	-7.84648	-0.04775	0.54135
H	-8.67139	0.85911	-1.78103
H	-6.76799	2.38575	-2.85940
H	-4.66989	2.40494	-1.23225
H	-5.17549	0.66298	0.70607
H	-6.31392	1.99629	0.92657
C	-0.83136	0.13686	4.64306
H	-0.42838	0.74633	5.45954
H	-1.92230	0.30424	4.62275
O	-0.51826	-1.20004	4.92858

M06/lanl2dz-6-31G(d) Energy = -2646.114915

M06/lanl2dz-6-31G(d) Free Energy = -2645.477824

M06/def2-TZVP Derived free energy = -2646.590214

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.621584

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.647291

Number of Imaginary Frequencies = 1 (-381.36)

M06/lanl2dz-6-31G(d) Geometry

C	-0.60749	3.17936	-0.11457
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C	-0.72619	4.65688	0.31171
C	-1.03769	2.72261	2.30336
N	-0.95323	2.29784	0.99706
C	-1.12881	0.95557	0.96756
N	-1.30967	0.64649	2.25746
N	-1.25964	1.72636	3.10642
C	0.20531	5.38093	-0.65914
C	1.27124	4.35326	-0.93662
C	0.82296	3.08374	-0.57258
C	1.64033	1.97089	-0.67232
C	2.92222	2.13432	-1.19171
C	3.36959	3.39362	-1.58632
C	2.54969	4.51454	-1.45254
C	-1.39901	-0.68120	2.77000
C	-2.63917	-1.36870	2.72744
C	-2.66668	-2.72279	3.17375
C	-1.47733	-3.31392	3.66228
C	-0.29647	-2.61948	3.70757
C	-0.25985	-1.29010	3.24641
C	-3.83456	-0.77519	2.25667
C	-4.99793	-1.50219	2.21288
C	-5.02610	-2.84688	2.64132
C	-3.88482	-3.44021	3.11668
H	-1.30528	2.96057	-0.93878
H	-1.76975	5.01678	0.28906
H	0.58482	6.30552	-0.20752
H	-0.34006	5.65835	-1.57361
H	1.29854	0.99668	-0.32441
H	3.57334	1.26485	-1.28537
H	4.37379	3.50820	-1.99222
H	2.91474	5.50043	-1.73693
H	-1.51190	-4.34660	4.00772
H	0.61608	-3.07389	4.08491
Cl	1.25430	-0.43721	3.26323
H	-3.82980	0.26642	1.93995
H	-5.91083	-1.03550	1.84825

H	-5.95762	-3.40694	2.59886
H	-3.89568	-4.47479	3.45792
Au	-1.27490	-0.43330	-0.69585
C	-1.49077	-1.69754	-2.29788
C	-2.52255	-1.35246	-3.18756
C	-0.70418	-2.81486	-2.52553
C	-2.72667	-2.12672	-4.32715
C	-0.92104	-3.58644	-3.67100
H	0.06678	-3.11148	-1.81576
C	-1.92197	-3.23662	-4.56928
H	-3.52065	-1.87425	-5.02951
H	-0.30682	-4.46645	-3.85439
H	-2.08811	-3.83815	-5.46082
C	-2.94167	0.38745	-1.55235
C	-3.65742	1.44236	-1.00873
C	-3.32121	-0.20141	-2.77242
C	-4.76380	1.94850	-1.69754
H	-3.37953	1.88119	-0.05034
C	-4.42399	0.32213	-3.44589
C	-5.13734	1.39213	-2.91421
H	-5.32995	2.77615	-1.27395
H	-4.73765	-0.11612	-4.39288
H	-5.99697	1.78722	-3.45185
O	0.54498	-1.44199	0.09713
C	2.85674	-1.85843	0.04814
C	1.64427	-1.43964	-0.51691
C	5.29148	-2.21638	-0.23072
C	4.03108	-1.80420	-0.68000
C	6.44254	-2.24694	-1.03370
H	1.67522	-1.08115	-1.56734
H	3.96186	-1.43827	-1.71283
H	2.84750	-2.22032	1.07693
C	7.50356	-3.27847	-0.77363
H	6.27862	-2.01604	-2.09256
H	5.36021	-2.61228	0.78576
H	7.64915	-3.43491	0.30279

H	7.19682	-4.24028	-1.20681
H	8.46930	-3.01094	-1.21939
C	7.45419	-0.48987	-0.72241
C	7.83519	-0.57794	0.61767
C	6.79048	-0.08795	1.43899
C	5.80365	0.42278	0.63740
C	6.29665	0.47037	-0.76618
H	8.17092	-0.56988	-1.53936
H	8.74793	-1.04485	0.97988
H	6.76164	-0.15114	2.52256
H	4.85746	0.84496	0.96864
H	5.54879	0.28991	-1.54611
H	6.70950	1.47916	-0.94997
O	-0.18527	4.82387	1.60848
C	-0.92626	4.17787	2.60965
H	-1.93847	4.61448	2.69825
H	-0.41126	4.33049	3.56330

M06/lanl2dz-6-31G(d) Energy = -2646.117044

M06/lanl2dz-6-31G(d) Free Energy = -2645.479623

M06/def2-TZVP Derived free energy = -2646.589536

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.620424

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.645510

Number of Imaginary Frequencies = 1 (-390.18)

M06/lanl2dz-6-31G(d) Geometry

C	0.72196	-1.91830	2.68996
C	-0.05586	-2.29494	3.96494
C	0.12272	0.40003	3.48593
N	0.52443	-0.45926	2.48520
C	0.72544	0.26731	1.35788
N	0.43463	1.51727	1.74250
N	0.05954	1.62507	3.05883
C	-1.50359	-2.49983	3.47267
C	-1.26956	-3.05696	2.09587
C	0.02262	-2.74766	1.65398

C	0.50818	-3.23504	0.44657
C	-0.34591	-3.98449	-0.36097
C	-1.64617	-4.26473	0.05841
C	-2.11071	-3.82108	1.29673
C	0.38928	2.66601	0.89684
C	1.59357	3.31851	0.52199
C	1.50292	4.43263	-0.36322
C	0.23069	4.86822	-0.80220
C	-0.91923	4.23627	-0.40614
C	-0.83011	3.12007	0.44573
C	2.86695	2.90871	0.98007
C	4.00040	3.55353	0.55254
C	3.91601	4.64534	-0.33774
C	2.69146	5.07911	-0.77781
H	1.80183	-2.09736	2.76943
H	0.33351	-3.26310	4.30449
H	-2.05292	-1.54414	3.42395
H	-2.07643	-3.16334	4.13106
H	1.54095	-3.05734	0.14580
H	0.01361	-4.36712	-1.31420
H	-2.29691	-4.86341	-0.57627
H	-3.11170	-4.08586	1.63679
H	0.17511	5.72763	-1.46935
H	-1.89662	4.57303	-0.74157
Cl	-2.30022	2.30164	0.90118
H	2.94687	2.08036	1.67972
H	4.97303	3.21763	0.90734
H	4.82442	5.14517	-0.66657
H	2.61263	5.92805	-1.45598
Au	1.40193	-0.33835	-0.61018
C	2.12516	-0.94079	-2.43323
C	3.48129	-1.30762	-2.44681
C	1.35132	-1.00985	-3.57868
C	4.04973	-1.75536	-3.63742
C	1.93588	-1.45864	-4.76711
H	0.30355	-0.71410	-3.55654

C	3.27589	-1.82913	-4.79209
H	5.09953	-2.04596	-3.67355
H	1.33822	-1.51401	-5.67558
H	3.72492	-2.17868	-5.71994
C	3.35662	-0.68734	-0.10867
C	3.87235	-0.51216	1.16554
C	4.15836	-1.16832	-1.16027
C	5.21474	-0.81097	1.41355
H	3.25130	-0.13792	1.97977
C	5.49514	-1.46317	-0.89218
C	6.01922	-1.28482	0.38425
H	5.62387	-0.67274	2.41278
H	6.13696	-1.83657	-1.68961
H	7.06451	-1.51960	0.57557
O	-0.66286	-0.10420	-1.41807
C	-2.97319	-0.55046	-1.33630
C	-1.67263	-0.52655	-0.80284
C	-5.38224	-1.11581	-0.89339
C	-4.02003	-1.01409	-0.56187
C	-5.96246	-0.70906	-2.10248
H	-1.55521	-0.91218	0.23168
H	-3.74563	-1.37044	0.43809
H	-3.10509	-0.20908	-2.36343
C	-7.19015	-1.40556	-2.61388
H	-5.27199	-0.37597	-2.88332
H	-6.03379	-1.59680	-0.16249
H	-6.90072	-2.33775	-3.11861
H	-7.86637	-1.67310	-1.79195
H	-7.74723	-0.80061	-3.33971
C	-6.63787	1.23473	-1.80454
C	-7.70778	1.03937	-0.93077
C	-7.23656	1.06152	0.40324
C	-5.90458	1.38711	0.39435
C	-5.50460	1.78133	-0.98003
H	-6.77610	1.49882	-2.85250
H	-8.72605	0.80279	-1.22929

H	-7.82918	0.82435	1.28188
H	-5.26586	1.48098	1.26866
H	-5.53963	2.88380	-1.04771
H	-4.48985	1.48810	-1.27336
O	0.15973	-1.41881	5.03872
C	-0.26624	-0.09814	4.83607
H	-1.35957	0.00016	4.95334
H	0.19716	0.51651	5.61559

Bottom, towards, 1, endo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.116371

M06/lanl2dz-6-31G(d) Free Energy = -2645.477696

M06/def2-TZVP Derived free energy = -2646.587205

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618083

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642749

Number of Imaginary Frequencies = 1 (-375.97)

M06/lanl2dz-6-31G(d) Geometry

C	-2.50661	2.50455	-1.40803
C	-2.90849	3.98932	-1.32981
C	-3.07864	2.62965	1.04815
N	-2.46483	1.99654	-0.01241
C	-1.86510	0.87563	0.45709
N	-2.14682	0.89714	1.76474
N	-2.90255	1.97348	2.15543
C	-1.58244	4.72706	-1.05274
C	-0.59611	3.85664	-1.78113
C	-1.14174	2.59072	-2.02552
C	-0.45592	1.64045	-2.77287
C	0.83061	1.94408	-3.21547
C	1.39413	3.19039	-2.94103
C	0.68038	4.16144	-2.23863
C	-1.68729	-0.04993	2.72813
C	-2.32782	-1.31459	2.81518
C	-1.82210	-2.25959	3.75486

C	-0.73062	-1.89606	4.57897
C	-0.14144	-0.66239	4.48518
C	-0.62215	0.26659	3.54156
C	-3.43339	-1.67449	2.00947
C	-3.99176	-2.92380	2.11153
C	-3.48510	-3.86615	3.03158
C	-2.42727	-3.53580	3.83982
H	-3.22653	1.89142	-1.96516
H	-3.26396	4.27735	-2.32715
H	-1.35700	4.76629	0.02503
H	-1.60460	5.76375	-1.40860
H	-0.91648	0.68456	-3.02320
H	1.38659	1.20875	-3.79460
H	2.39450	3.41898	-3.30465
H	1.11135	5.14718	-2.06750
H	-0.35738	-2.62084	5.30186
H	0.69539	-0.38300	5.12024
Cl	0.16670	1.80906	3.41875
H	-3.84446	-0.95236	1.30710
H	-4.83715	-3.18782	1.47890
H	-3.94121	-4.85115	3.10260
H	-2.03321	-4.25115	4.56106
Au	-0.64414	-0.60964	-0.51528
C	0.51231	-1.97526	-1.51534
C	-0.17900	-2.79778	-2.42082
C	1.88641	-2.07189	-1.36920
C	0.53579	-3.72776	-3.17377
C	2.59125	-3.00826	-2.13017
H	2.40794	-1.42522	-0.66112
C	1.91627	-3.83148	-3.02507
H	0.02260	-4.37740	-3.88252
H	3.67203	-3.09758	-2.01975
H	2.46749	-4.56138	-3.61503
C	-2.09009	-1.53328	-1.62847
C	-3.43276	-1.19390	-1.58846
C	-1.62030	-2.55769	-2.47236

C	-4.34168	-1.88609	-2.39317
H	-3.79351	-0.40151	-0.93210
C	-2.54306	-3.23642	-3.26769
C	-3.89367	-2.90371	-3.22684
H	-5.39789	-1.62445	-2.36364
H	-2.20622	-4.03665	-3.92625
H	-4.60063	-3.44474	-3.85262
O	1.11262	0.15276	0.58583
C	2.88933	1.70137	0.52955
C	1.55692	1.30806	0.32933
C	5.18249	1.08930	1.24902
C	3.82484	0.82416	1.05309
C	6.06610	0.21799	1.90625
H	0.86372	2.06298	-0.08660
H	3.44356	-0.15333	1.36831
H	3.17178	2.71578	0.24852
C	7.25966	0.77670	2.62795
H	5.59453	-0.64139	2.39560
H	5.56699	2.05812	0.91760
H	8.03091	0.01943	2.81429
H	7.71394	1.60248	2.06551
H	6.94873	1.17518	3.60334
C	6.93184	-0.97878	0.48952
C	5.71101	-1.35747	-0.30591
C	5.59462	-0.21864	-1.25437
C	6.79537	0.43977	-1.31128
C	7.64394	-0.07377	-0.30048
H	7.42468	-1.68238	1.15993
H	4.80706	-1.60641	0.26086
H	4.72271	-0.03071	-1.87678
H	7.04619	1.25127	-1.98779
O	-3.99014	4.23496	-0.47109
C	-3.76189	3.94442	0.88254
H	-3.15863	4.72821	1.37252
H	-4.73740	3.93026	1.38077
H	5.97545	-2.25969	-0.88743

H 8.65938 0.26275 -0.10609

Top, away, 2, endo, away

M06/lanl2dz-6-31G(d) Energy = -2646.113520

M06/lanl2dz-6-31G(d) Free Energy = -2645.474132

M06/def2-TZVP Derived free energy = -2646.583704

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.614262

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.638492

Number of Imaginary Frequencies = 1 (-381.56)

M06/lanl2dz-6-31G(d) Geometry

C	0.63319	3.20543	-0.38547
C	0.79822	4.65776	0.10092
C	0.50098	2.79444	2.10057
N	0.70371	2.33235	0.81872
C	0.84285	0.98668	0.86856
N	0.71472	0.71357	2.17737
N	0.49740	1.82087	2.96005
C	2.32299	4.86115	0.18577
C	2.80225	3.98467	-0.93679
C	1.81926	3.05349	-1.28989
C	1.98968	2.20553	-2.37779
C	3.19713	2.24589	-3.07174
C	4.19499	3.14423	-2.69562
C	3.99861	4.03234	-1.63958
C	0.73817	-0.57977	2.77402
C	-0.30945	-1.49335	2.47411
C	-0.22530	-2.81235	3.00702
C	0.86427	-3.15258	3.84366
C	1.83550	-2.23935	4.15497
C	1.77103	-0.94039	3.61140
C	-1.42719	-1.15146	1.67384
C	-2.38873	-2.08890	1.38547
C	-2.29537	-3.40264	1.89158

C	-1.23753	-3.74998	2.69278
H	-0.33357	3.00044	-0.86093
H	0.40553	5.30570	-0.69279
H	2.72488	4.52236	1.15386
H	2.60574	5.91491	0.07714
H	1.18595	1.54538	-2.70817
H	3.35332	1.58424	-3.92124
H	5.12983	3.17053	-3.25235
H	4.76699	4.75958	-1.38066
H	0.91944	-4.16270	4.24754
H	2.66898	-2.49627	4.80375
Cl	3.04677	0.17087	3.99588
H	-1.52948	-0.13631	1.29235
H	-3.23370	-1.80708	0.75555
H	-3.06351	-4.13494	1.65134
H	-1.15692	-4.75624	3.10249
Au	0.94272	-0.39188	-0.81019
C	0.99873	-1.68810	-2.40231
C	2.00733	-2.66540	-2.34537
C	0.13156	-1.63037	-3.48167
C	2.09571	-3.61353	-3.36174
C	0.23409	-2.58260	-4.50071
H	-0.61982	-0.84377	-3.55808
C	1.20455	-3.57489	-4.43107
H	2.86861	-4.38109	-3.33151
H	-0.44438	-2.54084	-5.35119
H	1.28163	-4.31733	-5.22314
C	2.64844	-1.42670	-0.37041
C	3.46559	-1.10433	0.69492
C	2.91402	-2.52217	-1.21000
C	4.56642	-1.91914	0.97397
H	3.26611	-0.23492	1.31702
C	4.01893	-3.31949	-0.91580
C	4.83311	-3.02407	0.17463
H	5.20799	-1.67679	1.82016
H	4.25294	-4.17687	-1.54663

H	5.68997	-3.65823	0.39376
O	-1.03619	0.59481	-1.32799
C	-3.38006	0.35796	-1.41969
C	-2.06248	-0.12684	-1.43770
C	-5.81437	-0.25151	-1.59837
C	-4.43915	-0.52454	-1.56932
C	-6.39694	1.01526	-1.45837
H	-1.93528	-1.22172	-1.55650
H	-4.16358	-1.57492	-1.71434
H	-3.52246	1.43477	-1.32154
C	-7.70293	1.31673	-2.13237
H	-5.70681	1.86271	-1.40734
H	-6.48010	-1.09064	-1.80455
H	-7.51650	1.57272	-3.18470
H	-8.36930	0.44511	-2.12081
H	-8.22757	2.16592	-1.67785
C	-6.86717	1.22872	0.56439
C	-7.92181	0.32803	0.70056
C	-7.41395	-0.94805	1.04777
C	-6.06378	-0.84312	1.25269
C	-5.66763	0.58723	1.20703
H	-7.01284	2.30818	0.54904
H	-8.96377	0.54645	0.47992
H	-8.00057	-1.85948	1.11310
H	-5.39865	-1.65168	1.54512
H	-5.60485	0.96177	2.24463
H	-4.68988	0.78732	0.75058
O	0.03167	4.96864	1.23766
C	0.37141	4.25001	2.39300
H	1.31135	4.61661	2.84093
H	-0.42181	4.41612	3.12999

M06/lanl2dz-6-31G(d) Energy = -2646.114809

M06/lanl2dz-6-31G(d) Free Energy = -2645.476917

M06/def2-TZVP Derived free energy = -2646.586709

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617400

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642040

Number of Imaginary Frequencies = 1 (-373.27)

M06/lanl2dz-6-31G(d) Geometry

C	-1.57697	-1.01121	-2.98200
C	-2.37232	-1.97700	-3.87578
C	-1.33464	-3.11214	-1.61220
N	-1.32358	-1.73808	-1.70716
C	-1.02644	-1.22912	-0.48852
N	-0.85836	-2.32399	0.26961
N	-1.04181	-3.50454	-0.40948
C	-3.82250	-1.83859	-3.36477
C	-3.85675	-0.38574	-2.97186
C	-2.55703	0.10744	-2.81172
C	-2.31536	1.45469	-2.57713
C	-3.40604	2.30608	-2.41184
C	-4.70470	1.81024	-2.51659
C	-4.94049	0.46876	-2.81943
C	-0.56736	-2.35703	1.66462
C	0.71462	-1.94136	2.11941
C	0.96645	-1.94998	3.52239
C	-0.04502	-2.39434	4.40641
C	-1.25862	-2.82356	3.94048
C	-1.51990	-2.80408	2.55579
C	1.75049	-1.53382	1.24405
C	2.96503	-1.13242	1.74492
C	3.21081	-1.12135	3.13347
C	2.22924	-1.52657	4.00132
H	-0.60205	-0.72391	-3.39294
H	-2.32460	-1.58122	-4.89804
H	-4.01184	-2.49425	-2.49894
H	-4.55929	-2.10585	-4.13142
H	-1.29615	1.84355	-2.54175
H	-3.23861	3.36170	-2.20480
H	-5.54767	2.48640	-2.38814
H	-5.95879	0.10377	-2.94679

H	0.15923	-2.39854	5.47633
H	-2.03416	-3.17494	4.61616
Cl	-3.07486	-3.35384	2.01484
H	1.58612	-1.54542	0.16769
H	3.74320	-0.81532	1.05025
H	4.17821	-0.79655	3.51297
H	2.40474	-1.53344	5.07650
Au	-0.82377	0.86334	0.03180
C	-0.68231	2.85821	0.51033
C	-1.68838	3.33912	1.36762
C	0.28630	3.71520	0.01310
C	-1.67295	4.67724	1.75482
C	0.28835	5.05818	0.40222
H	1.03923	3.36310	-0.69223
C	-0.68122	5.53069	1.27850
H	-2.44177	5.06563	2.42272
H	1.04803	5.73395	0.01252
H	-0.67658	6.57552	1.58322
C	-2.52742	1.08242	1.13416
C	-3.46620	0.07783	1.27383
C	-2.70915	2.35266	1.70731
C	-4.60857	0.31925	2.04249
H	-3.33242	-0.89541	0.80589
C	-3.85367	2.57075	2.47294
C	-4.79242	1.55734	2.64513
H	-5.34707	-0.47113	2.16761
H	-4.02178	3.54563	2.93027
H	-5.68024	1.74353	3.24638
O	1.01334	0.74789	-1.26412
C	3.35691	0.76144	-1.49888
C	2.15853	1.00286	-0.80847
C	5.83169	0.96689	-1.51578
C	4.56967	1.09744	-0.92537
C	7.01263	1.46311	-0.93828
H	2.24876	1.44586	0.20426
H	4.53447	1.54998	0.07447

H	3.30692	0.32799	-2.49840
C	8.12298	1.95248	-1.82497
H	6.86903	2.04677	-0.02168
H	5.88358	0.54238	-2.52148
H	9.08680	2.00463	-1.30406
H	8.23792	1.30909	-2.70642
H	7.88856	2.96352	-2.18477
C	7.89932	-0.06824	0.08044
C	8.26869	-0.94445	-0.94241
C	7.18982	-1.81499	-1.23183
C	6.18869	-1.58973	-0.32423
C	6.69288	-0.68052	0.74030
H	8.63066	0.51335	0.64121
H	9.20064	-0.89811	-1.50043
H	7.15238	-2.51410	-2.06176
H	5.22363	-2.09003	-0.29612
H	5.96187	0.01756	1.16341
H	7.05615	-1.30337	1.57793
O	-1.81142	-3.26160	-3.95605
C	-1.76186	-3.97575	-2.75082
H	-2.74006	-4.42379	-2.50302
H	-1.05494	-4.80131	-2.88933

M06/lanl2dz-6-31G(d) Energy = -2646.115389

M06/lanl2dz-6-31G(d) Free Energy = -2645.478944

M06/def2-TZVP Derived free energy = -2646.590418

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.621733

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.647298

Number of Imaginary Frequencies = 1 (-375.46)

M06/lanl2dz-6-31G(d) Geometry

C	1.53866	2.98816	-0.12385
C	1.41366	4.44374	0.37697
C	1.23923	2.45176	2.30821
N	1.31948	2.06067	0.99268
C	1.12765	0.72387	0.92766

N	0.94163	0.38018	2.21314
N	1.00302	1.43976	3.08737
C	2.24796	5.24418	-0.61740
C	3.30381	4.26198	-1.04470
C	2.91497	2.95713	-0.73866
C	3.72737	1.87507	-1.04708
C	4.95030	2.11776	-1.67005
C	5.34037	3.41903	-1.98035
C	4.51913	4.50088	-1.66980
C	0.69316	-0.93529	2.70097
C	-0.53868	-1.56781	2.37919
C	-0.73298	-2.91739	2.79373
C	0.28077	-3.56445	3.53959
C	1.44289	-2.92008	3.86938
C	1.65130	-1.59358	3.44055
C	-1.57291	-0.91944	1.66115
C	-2.72479	-1.59493	1.34007
C	-2.91264	-2.93681	1.73189
C	-1.93668	-3.57852	2.45099
H	0.75267	2.77177	-0.86466
H	0.36058	4.76924	0.44708
H	2.64314	6.14947	-0.14045
H	1.62618	5.56228	-1.46779
H	3.43221	0.85324	-0.80405
H	5.60427	1.28301	-1.91388
H	6.30014	3.59211	-2.46356
H	4.83135	5.51767	-1.90472
H	0.12281	-4.59525	3.85425
H	2.22176	-3.41395	4.44475
Cl	3.16071	-0.83346	3.82829
H	-1.45270	0.12182	1.36535
H	-3.49871	-1.08014	0.77015
H	-3.83123	-3.45755	1.46764
H	-2.06989	-4.61154	2.77036
Au	0.83517	-0.44805	-0.88520
C	0.52121	-1.56716	-2.57770

C	1.29317	-2.73868	-2.66682
C	-0.37160	-1.23265	-3.58302
C	1.11713	-3.59043	-3.75466
C	-0.53431	-2.09107	-4.67465
H	-0.93461	-0.30043	-3.54875
C	0.19925	-3.26871	-4.75095
H	1.70377	-4.50507	-3.83706
H	-1.23159	-1.82955	-5.46888
H	0.06904	-3.93710	-5.59987
C	2.28960	-1.86236	-0.64325
C	3.20911	-1.83190	0.38822
C	2.26692	-2.90053	-1.59064
C	4.12034	-2.88439	0.51429
H	3.24401	-1.00583	1.09584
C	3.18549	-3.93899	-1.44648
C	4.10028	-3.93332	-0.39664
H	4.84260	-2.86959	1.32919
H	3.19550	-4.75782	-2.16549
H	4.81081	-4.75169	-0.29793
O	-0.86821	0.99962	-1.17993
C	-3.20052	1.34841	-1.13874
C	-2.04627	0.56505	-1.28433
C	-5.68462	1.42553	-1.20419
C	-4.45039	0.77203	-1.28521
C	-6.91123	0.80160	-1.48696
H	-2.20095	-0.51131	-1.49918
H	-4.47341	-0.29836	-1.52864
H	-3.09213	2.41209	-0.92372
C	-8.04098	1.60705	-2.06302
H	-6.83303	-0.21996	-1.87624
H	-5.68368	2.49720	-0.99019
H	-9.01454	1.11800	-1.93686
H	-8.09125	2.60379	-1.60664
H	-7.88098	1.74706	-3.14079
C	-7.69533	0.14436	0.29048
C	-7.96351	1.33792	0.96320

C	-6.80651	1.75501	1.66571
C	-5.84833	0.78296	1.54937
C	-6.45396	-0.42356	0.92426
H	-8.48518	-0.49230	-0.10719
H	-8.88391	1.91056	0.87934
H	-6.68982	2.70817	2.17262
H	-4.84122	0.82142	1.95768
H	-5.79825	-1.01041	0.27173
H	-6.77857	-1.10129	1.73470
C	1.36511	3.89477	2.66068
H	0.35784	4.32060	2.82848
H	1.93804	4.01523	3.58576
O	2.03753	4.57763	1.64054

M06/lanl2dz-6-31G(d) Energy = -2646.113570

M06/lanl2dz-6-31G(d) Free Energy = -2645.476042

M06/def2-TZVP Derived free energy = -2646.587495

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618806

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.644433

Number of Imaginary Frequencies = 1 (-385.67)

M06/lanl2dz-6-31G(d) Geometry

C	-0.97985	3.07086	0.08292
C	-0.58184	4.48297	-0.40071
C	-0.53974	2.46749	-2.31169
N	-0.80615	2.10797	-1.01182
C	-0.83208	0.75840	-0.93425
N	-0.58189	0.37606	-2.19854
N	-0.39109	1.42312	-3.06895
C	-1.36651	5.41765	0.51344
C	-2.59854	4.61908	0.83956
C	-2.39436	3.26514	0.56863
C	-3.39560	2.33017	0.79244
C	-4.61876	2.77196	1.29333
C	-4.82508	4.12242	1.56730
C	-3.81518	5.05593	1.34294

C	-0.50714	-0.96619	-2.67009
C	0.54608	-1.80204	-2.20760
C	0.54410	-3.17117	-2.60250
C	-0.46713	-3.63800	-3.47576
C	-1.44430	-2.80102	-3.94378
C	-1.46744	-1.45409	-3.52942
C	1.58576	-1.33690	-1.36551
C	2.54597	-2.20302	-0.90276
C	2.53271	-3.56440	-1.27227
C	1.55601	-4.03220	-2.11423
H	-0.30989	2.73933	0.89163
H	0.51149	4.63773	-0.37413
H	-1.57016	6.36625	0.00156
H	-0.78252	5.64805	1.41717
H	-3.24717	1.27172	0.57438
H	-5.41829	2.05463	1.46694
H	-5.78728	4.45321	1.95365
H	-3.98398	6.11247	1.54752
H	-0.45759	-4.68474	-3.77681
H	-2.21921	-3.15560	-4.61869
Cl	-2.76729	-0.44967	-4.08598
H	1.62183	-0.28457	-1.08688
H	3.32494	-1.82632	-0.23825
H	3.29735	-4.23921	-0.89238
H	1.53941	-5.07801	-2.41891
Au	-0.91986	-0.42600	0.89185
C	-0.99626	-1.55242	2.60814
C	-1.96158	-2.57498	2.60414
C	-0.18687	-1.34996	3.71429
C	-2.06717	-3.41729	3.70813
C	-0.30683	-2.19745	4.82016
H	0.52634	-0.52654	3.74767
C	-1.23555	-3.23095	4.80919
H	-2.80732	-4.21704	3.72191
H	0.32449	-2.03926	5.69286
H	-1.32480	-3.89047	5.67023

C	-2.54739	-1.58754	0.47463
C	-3.31199	-1.43126	-0.66604
C	-2.80996	-2.59702	1.41577
C	-4.35708	-2.32737	-0.90833
H	-3.12116	-0.62713	-1.37373
C	-3.85808	-3.47836	1.15474
C	-4.62042	-3.34799	-0.00310
H	-4.95852	-2.21427	-1.80917
H	-4.08724	-4.27172	1.86555
H	-5.43315	-4.04652	-0.19237
O	0.97072	0.72748	1.35415
C	3.32321	0.66898	1.46165
C	2.04199	0.11033	1.59392
C	5.79583	0.28361	1.69549
C	4.44521	-0.08793	1.76442
C	6.26978	1.53297	1.27330
H	1.98936	-0.94569	1.92645
H	4.25033	-1.10195	2.13044
H	3.39011	1.71013	1.14312
C	7.55421	2.07675	1.82543
H	5.50911	2.29184	1.06662
H	6.52880	-0.44031	2.05381
H	7.36264	2.53300	2.80672
H	8.29604	1.28222	1.97410
H	7.99388	2.85169	1.18579
C	6.68995	1.35068	-0.76696
C	7.82472	0.54246	-0.74283
C	7.43900	-0.81957	-0.79712
C	6.08318	-0.88564	-0.97750
C	5.55018	0.47951	-1.21944
H	6.73212	2.41726	-0.98461
H	8.84331	0.89785	-0.60832
H	8.11095	-1.66572	-0.69008
H	5.49461	-1.79501	-1.06965
H	5.43642	0.61682	-2.30996
H	4.56450	0.68087	-0.78150

C	-0.41016	3.90790	-2.67213
H	0.66111	4.17363	-2.74853
H	-0.87374	4.10170	-3.64501
O	-1.05953	4.69693	-1.71646

Top, towards, 2, endo, away

M06/lanl2dz-6-31G(d) Energy = -2646.115474

M06/lanl2dz-6-31G(d) Free Energy = -2645.475815

M06/def2-TZVP Derived free energy = -2646.586197

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617317

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642539

Number of Imaginary Frequencies = 1 (-376.41)

M06/lanl2dz-6-31G(d) Geometry

C	1.49624	2.11294	-0.78507
C	2.22552	3.27192	-1.49656
C	-0.53453	3.44948	-1.38551
N	0.04921	2.31870	-0.86044
C	-0.92529	1.43319	-0.55157
N	-2.04642	2.07810	-0.92400
N	-1.82595	3.32846	-1.44314
C	3.59172	3.31184	-0.81953
C	3.30159	2.81872	0.57157
C	2.09067	2.12182	0.59895
C	1.62236	1.54314	1.77107
C	2.37744	1.69048	2.93510
C	3.57737	2.39973	2.91534
C	4.05072	2.96464	1.73088
C	-3.36100	1.53377	-0.82503
C	-3.65291	0.33821	-1.54061
C	-4.86705	-0.34189	-1.23464
C	-5.77550	0.23975	-0.31814
C	-5.50638	1.43505	0.29246
C	-4.27457	2.07549	0.05199
C	-2.77508	-0.23096	-2.49916

C	-3.06435	-1.44350	-3.07666
C	-4.24200	-2.14117	-2.73581
C	-5.12886	-1.59148	-1.84523
H	1.69040	1.16392	-1.30379
H	2.27512	3.11820	-2.58909
H	4.01504	4.32258	-0.86523
H	4.28552	2.63363	-1.34249
H	0.67527	1.00076	1.79717
H	2.01744	1.26110	3.86801
H	4.14616	2.52120	3.83543
H	4.98311	3.52919	1.72289
H	-6.70494	-0.28469	-0.09958
H	-6.20434	1.88419	0.99449
Cl	-3.90795	3.50767	0.96147
H	-1.87126	0.30163	-2.79294
H	-2.37790	-1.86593	-3.80809
H	-4.45039	-3.10579	-3.19332
H	-6.05388	-2.10855	-1.59184
Au	-0.91418	-0.69926	-0.02768
C	-1.27647	-2.70943	0.18009
C	-2.25840	-3.04407	1.12833
C	-0.74392	-3.67197	-0.66182
C	-2.66882	-4.37087	1.24086
C	-1.16376	-4.99977	-0.53865
H	-0.02345	-3.40625	-1.43537
C	-2.11668	-5.34444	0.41310
H	-3.42965	-4.65093	1.96936
H	-0.74791	-5.76116	-1.19657
H	-2.44277	-6.37866	0.50575
C	-2.22722	-0.66212	1.54073
C	-2.54683	0.49533	2.22515
C	-2.76197	-1.91148	1.89870
C	-3.46941	0.42742	3.27371
H	-2.09856	1.45281	1.96301
C	-3.68952	-1.95385	2.93838
C	-4.04665	-0.78978	3.61395

H	-3.73583	1.33747	3.80924
H	-4.12848	-2.90639	3.23456
H	-4.77084	-0.83974	4.42482
O	0.81197	-0.85277	-1.48584
C	3.15208	-1.16078	-1.47190
C	1.84401	-1.44746	-1.06425
C	5.56761	-1.67925	-1.25332
C	4.21798	-1.87758	-0.95231
C	6.61024	-2.50140	-0.79778
H	1.72267	-2.24894	-0.30724
H	3.97309	-2.69506	-0.26361
H	3.31874	-0.37256	-2.20936
C	7.86779	-2.62294	-1.60978
H	6.29721	-3.42196	-0.29333
H	5.81919	-0.85789	-1.93011
H	7.70723	-3.32916	-2.43580
H	8.15034	-1.65885	-2.05140
H	8.71455	-2.99598	-1.02134
C	7.30146	-1.70808	0.97212
C	7.79223	-0.46057	0.58457
C	6.74192	0.48923	0.61190
C	5.61910	-0.10962	1.12162
C	5.98410	-1.44940	1.65116
H	7.95471	-2.52926	1.26546
H	8.79958	-0.27033	0.22201
H	6.81044	1.51079	0.24822
H	4.63980	0.34980	1.23663
H	6.18667	-1.34197	2.73199
H	5.21887	-2.22636	1.55791
C	0.31861	4.59097	-1.82380
H	0.40690	4.59167	-2.92568
H	-0.13062	5.54247	-1.52181
O	1.58034	4.49696	-1.21687

M06/lanl2dz-6-31G(d) Energy = -2646.115527

M06/lanl2dz-6-31G(d) Free Energy = -2645.475340

M06/def2-TZVP Derived free energy = -2646.585709

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616976

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642293

Number of Imaginary Frequencies = 1 (-374.05)

M06/lanl2dz-6-31G(d) Geometry

C	1.55208	2.04893	-0.76134
C	2.31921	3.18271	-1.47420
C	-0.44097	3.41530	-1.41816
N	0.11127	2.28129	-0.86675
C	-0.88580	1.42114	-0.55814
N	-1.98761	2.08352	-0.95618
N	-1.73386	3.32062	-1.49175
C	3.67016	3.20993	-0.76524
C	3.33805	2.74670	0.62681
C	2.11745	2.06673	0.63466
C	1.61267	1.51131	1.80286
C	2.34152	1.66421	2.98261
C	3.55060	2.35805	2.98245
C	4.05991	2.90040	1.80246
C	-3.31491	1.56918	-0.86309
C	-3.62684	0.37115	-1.56592
C	-4.85944	-0.27680	-1.26445
C	-5.76373	0.33722	-0.36495
C	-5.47324	1.53390	0.23299
C	-4.22473	2.14280	-0.00263
C	-2.75283	-0.22980	-2.50833
C	-3.06450	-1.44237	-3.07393
C	-4.26170	-2.10822	-2.73744
C	-5.14445	-1.52735	-1.86265
H	1.73764	1.08995	-1.26343
H	2.39150	3.00944	-2.56262
H	4.11315	4.21186	-0.81906
H	4.36394	2.50931	-1.25910
H	0.65750	0.98301	1.81245
H	1.95418	1.25179	3.91222

H	4.09804	2.48562	3.91456
H	4.99965	3.45263	1.80990
H	-6.70761	-0.16257	-0.15053
H	-6.16770	2.00823	0.92168
Cl	-3.83617	3.57851	0.89209
H	-1.83399	0.27762	-2.79961
H	-2.38030	-1.88976	-3.79251
H	-4.48800	-3.07306	-3.18586
H	-6.08425	-2.01899	-1.61316
Au	-0.92891	-0.70592	-0.01381
C	-1.32938	-2.70646	0.20845
C	-2.32466	-3.01549	1.15111
C	-0.80447	-3.68524	-0.61927
C	-2.75776	-4.33429	1.27223
C	-1.24692	-5.00479	-0.48744
H	-0.07273	-3.43803	-1.38835
C	-2.21402	-5.32454	0.45866
H	-3.52952	-4.59497	1.99638
H	-0.83731	-5.77936	-1.13376
H	-2.55799	-6.35233	0.55827
C	-2.25563	-0.63023	1.54197
C	-2.56480	0.53905	2.21102
C	-2.81615	-1.86682	1.90547
C	-3.50062	0.49670	3.24931
H	-2.09979	1.48711	1.94377
C	-3.75682	-1.88355	2.93405
C	-4.10211	-0.70725	3.59445
H	-3.75800	1.41620	3.77306
H	-4.21595	-2.82568	3.23302
H	-4.83642	-0.73719	4.39715
O	0.78977	-0.90659	-1.47099
C	3.12691	-1.21775	-1.46824
C	1.82214	-1.50089	-1.04924
C	5.54575	-1.70572	-1.26236
C	4.20213	-1.92077	-0.94793
C	6.61136	-2.50101	-0.81225

H	1.70387	-2.29549	-0.28438
H	3.97098	-2.73400	-0.24965
H	3.28534	-0.43679	-2.21547
C	7.86173	-2.59777	-1.63902
H	6.32633	-3.42574	-0.29890
H	5.77599	-0.88337	-1.94603
H	7.70936	-3.31500	-2.45703
H	8.11345	-1.63039	-2.09199
H	8.72509	-2.94362	-1.05820
C	7.30563	-1.67867	0.93848
C	7.73904	-0.41119	0.54483
C	6.65241	0.49545	0.59507
C	5.56558	-0.14790	1.12825
C	5.99302	-1.47352	1.64476
H	7.99719	-2.47251	1.21897
H	8.73082	-0.18059	0.16325
H	6.66853	1.51961	0.23126
H	4.57179	0.27284	1.26509
H	6.21227	-1.36238	2.72196
H	5.25608	-2.27879	1.56358
C	0.44360	4.52944	-1.86461
H	0.55386	4.50231	-2.96425
H	0.00798	5.49648	-1.59393
O	1.69126	4.42407	-1.23065

M06/lanl2dz-6-31G(d) Energy = -2646.112370

M06/lanl2dz-6-31G(d) Free Energy = -2645.475786

M06/def2-TZVP Derived free energy = -2646.586019

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616686

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641435

Number of Imaginary Frequencies = 1 (-383.40)

M06/lanl2dz-6-31G(d) Geometry

C	0.36909	2.89240	-0.16883
C	0.25437	4.40368	-0.44399
C	-1.20008	2.82881	-2.14604

N	-0.62301	2.22628	-1.04851
C	-1.13901	0.98233	-0.92799
N	-2.00010	0.90267	-1.95222
N	-2.05130	2.03703	-2.72407
C	-0.92955	4.85784	0.43399
C	-0.81738	3.92059	1.60455
C	-0.02539	2.81495	1.27602
C	0.28805	1.84870	2.22229
C	-0.26064	1.95716	3.49783
C	-1.08185	3.03685	3.81771
C	-1.35123	4.03492	2.88152
C	-2.89842	-0.17630	-2.20936
C	-2.38770	-1.43237	-2.63603
C	-3.31208	-2.50233	-2.82212
C	-4.69300	-2.27036	-2.61880
C	-5.15986	-1.04634	-2.21958
C	-4.24860	0.00444	-1.99855
C	-1.01003	-1.67155	-2.85968
C	-0.57103	-2.92502	-3.20916
C	-1.48170	-3.98879	-3.38106
C	-2.82467	-3.77535	-3.20105
H	1.35722	2.47996	-0.41134
H	1.17083	4.87122	-0.06186
H	-1.89288	4.72847	-0.08519
H	-0.85887	5.91773	0.70588
H	0.94650	1.01485	1.97423
H	-0.05145	1.19312	4.24450
H	-1.50669	3.11031	4.81702
H	-1.96505	4.89319	3.15197
H	-5.39098	-3.09159	-2.77715
H	-6.21898	-0.86825	-2.05209
Cl	-4.87181	1.51751	-1.41123
H	-0.28951	-0.86521	-2.74554
H	0.49317	-3.09373	-3.36538
H	-1.11689	-4.97374	-3.66435
H	-3.54141	-4.58396	-3.34060

Au	-0.62567	-0.67023	0.36701
C	-0.26542	-2.32925	1.51964
C	-1.13200	-2.49182	2.61534
C	0.70798	-3.27670	1.24401
C	-0.97042	-3.59131	3.45546
C	0.85730	-4.37959	2.09016
H	1.34255	-3.18632	0.36210
C	0.02759	-4.52683	3.19551
H	-1.63215	-3.73308	4.30962
H	1.61919	-5.12767	1.87687
H	0.14566	-5.38527	3.85405
C	-2.17055	-0.50763	1.69367
C	-3.07635	0.53599	1.66332
C	-2.16444	-1.46371	2.72388
C	-4.02816	0.63164	2.68170
H	-3.04659	1.29347	0.88111
C	-3.12010	-1.34432	3.73218
C	-4.04607	-0.30492	3.70840
H	-4.74787	1.44836	2.66587
H	-3.14222	-2.06775	4.54708
H	-4.78700	-0.22598	4.50172
O	1.29079	-0.74444	-0.83966
C	3.64200	-0.82449	-0.97281
C	2.41733	-0.82782	-0.28695
C	6.10773	-1.07868	-0.83717
C	4.82805	-0.97537	-0.27865
C	7.25841	-1.38449	-0.09319
H	2.47163	-0.92615	0.81763
H	4.75396	-1.07455	0.81173
H	3.63165	-0.74454	-2.06034
C	8.37844	-2.15212	-0.73606
H	7.07971	-1.63074	0.95966
H	6.19590	-1.01002	-1.92436
H	8.13097	-3.22234	-0.75057
H	8.52997	-1.83637	-1.77608
H	9.32808	-2.04237	-0.19840

C	8.16441	0.38990	0.40285
C	8.57202	0.87954	-0.83888
C	7.51468	1.61626	-1.42655
C	6.48817	1.70479	-0.52411
C	6.95167	1.19060	0.79282
H	8.87002	0.00984	1.14117
H	9.51597	0.64564	-1.32506
H	7.50795	2.00387	-2.44083
H	5.52665	2.18309	-0.68966
H	7.30513	2.04994	1.39081
H	6.19770	0.67815	1.39885
C	-0.89664	4.24243	-2.51053
H	-0.66759	4.31816	-3.57918
H	-1.79027	4.86283	-2.32534
O	0.22242	4.72168	-1.81057

M06/lanl2dz-6-31G(d) Energy = -2646.115474

M06/lanl2dz-6-31G(d) Free Energy = -2645.475815

M06/def2-TZVP Derived free energy = -2646.586197

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617317

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642539

Number of Imaginary Frequencies = 1 (-376.41)

M06/lanl2dz-6-31G(d) Geometry

C	1.49623	2.11295	-0.78506
C	2.22550	3.27193	-1.49654
C	-0.53455	3.44950	-1.38548
N	0.04919	2.31871	-0.86043
C	-0.92530	1.43319	-0.55158
N	-2.04643	2.07810	-0.92401
N	-1.82596	3.32847	-1.44313
C	3.59171	3.31185	-0.81953
C	3.30158	2.81872	0.57157
C	2.09066	2.12182	0.59895
C	1.62236	1.54313	1.77107
C	2.37744	1.69047	2.93510

C	3.57737	2.39971	2.91534
C	4.05071	2.96463	1.73088
C	-3.36102	1.53376	-0.82504
C	-3.65290	0.33820	-1.54062
C	-4.86704	-0.34192	-1.23466
C	-5.77550	0.23972	-0.31816
C	-5.50640	1.43502	0.29243
C	-4.27460	2.07547	0.05197
C	-2.77507	-0.23097	-2.49916
C	-3.06432	-1.44351	-3.07667
C	-4.24197	-2.14119	-2.73583
C	-5.12884	-1.59151	-1.84525
H	1.69038	1.16393	-1.30380
H	2.27509	3.11823	-2.58908
H	4.01503	4.32258	-0.86523
H	4.28550	2.63363	-1.34250
H	0.67526	1.00075	1.79717
H	2.01744	1.26108	3.86801
H	4.14617	2.52118	3.83542
H	4.98310	3.52918	1.72289
H	-6.70493	-0.28473	-0.09960
H	-6.20437	1.88416	0.99446
Cl	-3.90799	3.50766	0.96145
H	-1.87125	0.30163	-2.79295
H	-2.37787	-1.86593	-3.80810
H	-4.45035	-3.10581	-3.19333
H	-6.05385	-2.10859	-1.59186
Au	-0.91418	-0.69926	-0.02768
C	-1.27646	-2.70943	0.18010
C	-2.25839	-3.04407	1.12834
C	-0.74391	-3.67197	-0.66180
C	-2.66879	-4.37087	1.24088
C	-1.16373	-4.99977	-0.53863
H	-0.02344	-3.40625	-1.43536
C	-2.11666	-5.34444	0.41312
H	-3.42962	-4.65093	1.96938

H	-0.74787	-5.76117	-1.19654
H	-2.44273	-6.37867	0.50578
C	-2.22722	-0.66211	1.54072
C	-2.54684	0.49533	2.22514
C	-2.76197	-1.91148	1.89870
C	-3.46942	0.42742	3.27371
H	-2.09857	1.45282	1.96299
C	-3.68952	-1.95385	2.93838
C	-4.04666	-0.78978	3.61395
H	-3.73584	1.33747	3.80923
H	-4.12847	-2.90639	3.23456
H	-4.77084	-0.83974	4.42482
O	0.81198	-0.85276	-1.48583
C	3.15209	-1.16077	-1.47189
C	1.84402	-1.44745	-1.06424
C	5.56762	-1.67924	-1.25332
C	4.21799	-1.87757	-0.95232
C	6.61025	-2.50138	-0.79780
H	1.72268	-2.24894	-0.30723
H	3.97311	-2.69506	-0.26362
H	3.31875	-0.37254	-2.20935
C	7.86780	-2.62291	-1.60980
H	6.29724	-3.42194	-0.29335
H	5.81919	-0.85786	-1.93011
H	7.70724	-3.32913	-2.43582
H	8.15034	-1.65881	-2.05143
H	8.71457	-2.99594	-1.02137
C	7.30148	-1.70806	0.97211
C	7.79224	-0.46056	0.58456
C	6.74192	0.48924	0.61190
C	5.61911	-0.10962	1.12161
C	5.98412	-1.44940	1.65115
H	7.95473	-2.52924	1.26544
H	8.79959	-0.27030	0.22200
H	6.81044	1.51080	0.24822
H	4.63980	0.34979	1.23663

H	6.18669	-1.34197	2.73198
H	5.21890	-2.22637	1.55791
O	1.58032	4.49697	-1.21684
C	0.31859	4.59100	-1.82374
H	0.40686	4.59173	-2.92563
H	-0.13064	5.54248	-1.52172

M06/lanl2dz-6-31G(d) Energy = -2646.115527

M06/lanl2dz-6-31G(d) Free Energy = -2645.475340

M06/def2-TZVP Derived free energy = -2646.585709

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616976

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642293

Number of Imaginary Frequencies = 1 (-374.05)

M06/lanl2dz-6-31G(d) Geometry

C	1.55209	2.04893	-0.76133
C	2.31921	3.18271	-1.47421
C	-0.44097	3.41530	-1.41816
N	0.11127	2.28129	-0.86675
C	-0.88579	1.42114	-0.55814
N	-1.98760	2.08352	-0.95618
N	-1.73386	3.32062	-1.49175
C	3.67017	3.20992	-0.76524
C	3.33806	2.74670	0.62681
C	2.11746	2.06673	0.63467
C	1.61267	1.51132	1.80286
C	2.34153	1.66422	2.98261
C	3.55060	2.35806	2.98244
C	4.05991	2.90040	1.80246
C	-3.31490	1.56919	-0.86309
C	-3.62684	0.37115	-1.56592
C	-4.85944	-0.27680	-1.26445
C	-5.76373	0.33723	-0.36495
C	-5.47323	1.53390	0.23300
C	-4.22473	2.14280	-0.00262
C	-2.75283	-0.22980	-2.50833

C	-3.06450	-1.44237	-3.07393
C	-4.26170	-2.10822	-2.73744
C	-5.14445	-1.52734	-1.86265
H	1.73764	1.08995	-1.26342
H	2.39150	3.00944	-2.56262
H	4.11315	4.21185	-0.81907
H	4.36395	2.50931	-1.25910
H	0.65751	0.98302	1.81245
H	1.95419	1.25180	3.91222
H	4.09805	2.48563	3.91456
H	4.99965	3.45263	1.80989
H	-6.70761	-0.16256	-0.15053
H	-6.16770	2.00823	0.92168
Cl	-3.83617	3.57851	0.89209
H	-1.83399	0.27762	-2.79961
H	-2.38030	-1.88976	-3.79251
H	-4.48800	-3.07306	-3.18586
H	-6.08425	-2.01899	-1.61316
Au	-0.92891	-0.70592	-0.01381
C	-1.32938	-2.70646	0.20845
C	-2.32466	-3.01548	1.15111
C	-0.80447	-3.68524	-0.61927
C	-2.75776	-4.33428	1.27223
C	-1.24693	-5.00479	-0.48744
H	-0.07274	-3.43803	-1.38835
C	-2.21402	-5.32454	0.45866
H	-3.52952	-4.59497	1.99638
H	-0.83732	-5.77936	-1.13376
H	-2.55799	-6.35233	0.55827
C	-2.25563	-0.63023	1.54197
C	-2.56480	0.53905	2.21102
C	-2.81615	-1.86681	1.90547
C	-3.50062	0.49671	3.24931
H	-2.09978	1.48711	1.94377
C	-3.75682	-1.88355	2.93405
C	-4.10210	-0.70725	3.59445

H	-3.75800	1.41620	3.77306
H	-4.21595	-2.82568	3.23302
H	-4.83641	-0.73719	4.39715
O	0.78977	-0.90659	-1.47099
C	3.12691	-1.21775	-1.46825
C	1.82213	-1.50089	-1.04925
C	5.54575	-1.70572	-1.26236
C	4.20213	-1.92078	-0.94793
C	6.61135	-2.50101	-0.81225
H	1.70387	-2.29549	-0.28439
H	3.97097	-2.73400	-0.24966
H	3.28534	-0.43678	-2.21547
C	7.86173	-2.59778	-1.63902
H	6.32632	-3.42574	-0.29890
H	5.77599	-0.88337	-1.94602
H	8.72508	-2.94363	-1.05820
H	7.70935	-3.31499	-2.45703
H	8.11345	-1.63039	-2.09198
C	7.30562	-1.67868	0.93848
C	7.73903	-0.41119	0.54484
C	6.65240	0.49545	0.59507
C	5.56557	-0.14791	1.12825
C	5.99301	-1.47353	1.64476
H	7.99718	-2.47252	1.21898
H	8.73082	-0.18060	0.16326
H	6.66852	1.51960	0.23127
H	4.57178	0.27283	1.26509
H	6.21226	-1.36239	2.72196
H	5.25607	-2.27880	1.56357
O	1.69126	4.42407	-1.23066
C	0.44360	4.52943	-1.86461
H	0.55387	4.50230	-2.96426
H	0.00799	5.49647	-1.59394

Bottom, towards, 2, endo, away

M06/lanl2dz-6-31G(d) Energy = -2646.112867

M06/lanl2dz-6-31G(d) Free Energy = -2645.477862

M06/def2-TZVP Derived free energy = -2646.588130

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618801

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.643371

Number of Imaginary Frequencies = 1 (-383.21)

M06/lanl2dz-6-31G(d) Geometry

C	-0.07489	3.02379	-0.25987
C	-0.31912	4.49407	-0.65576
C	-1.57146	2.66021	-2.26289
N	-0.95772	2.19758	-1.11901
C	-1.30857	0.90434	-0.94410
N	-2.12074	0.65959	-1.98241
N	-2.29460	1.73464	-2.81675
C	-1.55686	4.91099	0.16270
C	-1.40572	4.07196	1.39949
C	-0.51900	3.01310	1.17413
C	-0.16344	2.14711	2.19984
C	-0.75482	2.30830	3.45010
C	-1.66409	3.34204	3.66832
C	-1.98393	4.23961	2.65075
C	-2.83431	-0.55425	-2.21373
C	-2.11823	-1.72788	-2.57479
C	-2.85137	-2.94247	-2.71759
C	-4.25564	-2.92940	-2.54433
C	-4.92397	-1.77981	-2.21625
C	-4.19989	-0.58491	-2.03340
C	-0.71562	-1.74686	-2.76957
C	-0.07010	-2.92647	-3.04818
C	-0.79043	-4.13292	-3.17367
C	-2.15376	-4.13510	-3.02241
H	0.95594	2.68827	-0.43472
H	0.54529	5.07039	-0.30274

H	-2.49173	4.67007	-0.36783
H	-1.57607	5.98961	0.35903
H	0.56703	1.35295	2.03825
H	-0.50590	1.62306	4.25837
H	-2.11698	3.46030	4.65095
H	-2.67099	5.06376	2.83830
H	-4.80618	-3.86109	-2.66932
H	-6.00148	-1.76918	-2.07449
Cl	-5.07025	0.83333	-1.53208
H	-0.14033	-0.82735	-2.69258
H	1.01005	-2.92444	-3.18331
H	-0.26355	-5.05768	-3.39914
H	-2.72373	-5.05767	-3.12755
Au	-0.56532	-0.60445	0.40831
C	0.05618	-2.14981	1.60580
C	-0.79964	-2.45113	2.68001
C	1.19226	-2.90738	1.37045
C	-0.47300	-3.50001	3.53656
C	1.50656	-3.96231	2.23258
H	1.82818	-2.70358	0.50793
C	0.68039	-4.24795	3.31349
H	-1.12224	-3.75027	4.37552
H	2.39448	-4.56584	2.05045
H	0.92693	-5.07001	3.98290
C	-2.13538	-0.67801	1.71060
C	-3.20488	0.19678	1.64896
C	-1.99436	-1.61287	2.74999
C	-4.18690	0.13075	2.64107
H	-3.28954	0.94070	0.85812
C	-2.98385	-1.65582	3.73170
C	-4.07355	-0.79184	3.67416
H	-5.03826	0.80784	2.59814
H	-2.90290	-2.37012	4.55064
H	-4.83964	-0.84087	4.44563
O	1.34713	-0.34230	-0.77674
C	3.60976	0.30905	-0.85125

C	2.43469	-0.08936	-0.19653
C	5.97153	1.04365	-0.64246
C	4.75402	0.58686	-0.12559
C	7.05508	1.44351	0.15587
H	2.49124	-0.18581	0.90832
H	4.68673	0.48086	0.96454
H	3.59393	0.40853	-1.93719
C	7.99076	2.50889	-0.34024
H	6.85436	1.47416	1.23275
H	6.04842	1.17397	-1.72488
H	8.18467	2.39596	-1.41447
H	7.53752	3.49846	-0.19038
H	8.95165	2.50477	0.18839
C	8.30175	-0.17689	0.36913
C	8.77265	-0.36791	-0.93071
C	7.87058	-1.19453	-1.64407
C	6.90065	-1.63117	-0.78084
C	7.27786	-1.25347	0.60747
H	8.93405	0.20902	1.16828
H	9.64249	0.12318	-1.36020
H	7.92093	-1.40780	-2.70755
H	6.04985	-2.25740	-1.03503
H	6.44916	-1.00654	1.27872
H	7.80502	-2.11086	1.06356
O	-0.35719	4.70411	-2.04381
C	-1.41791	4.07301	-2.71249
H	-1.19049	4.10457	-3.78365
H	-2.37155	4.60915	-2.56785

M06/lanl2dz-6-31G(d) Energy = -2646.113291

M06/lanl2dz-6-31G(d) Free Energy = -2645.478507

M06/def2-TZVP Derived free energy = -2646.590395

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.621386

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.646852

Number of Imaginary Frequencies = 1 (-382.93)

M06/lanl2dz-6-31G(d) Geometry

C	-0.07196	3.05451	-0.33957
C	0.15216	4.39610	-1.07410
C	-1.96988	2.83975	-1.96355
N	-1.16037	2.31350	-0.98165
C	-1.52539	1.02968	-0.76851
N	-2.53371	0.84980	-1.63926
N	-2.82266	1.96037	-2.39246
C	0.77675	5.29561	-0.01248
C	0.20023	4.76446	1.27120
C	-0.31618	3.48107	1.08556
C	-0.90257	2.78380	2.13271
C	-0.97218	3.39593	3.38291
C	-0.45497	4.67574	3.57333
C	0.13638	5.36863	2.51885
C	-3.27336	-0.35854	-1.80128
C	-2.58721	-1.53029	-2.22600
C	-3.29971	-2.76438	-2.21579
C	-4.67076	-2.77064	-1.86548
C	-5.32096	-1.61918	-1.50998
C	-4.60730	-0.40524	-1.45827
C	-1.22638	-1.53167	-2.62291
C	-0.59190	-2.70974	-2.93242
C	-1.28651	-3.93656	-2.88761
C	-2.61660	-3.95718	-2.55270
H	0.82605	2.42252	-0.42463
H	0.77179	4.27292	-1.97994
H	0.53192	6.34578	-0.21372
H	1.87320	5.20309	-0.03225
H	-1.31775	1.78530	1.99131
H	-1.44036	2.87110	4.21324
H	-0.52273	5.14306	4.55399
H	0.52820	6.37398	2.66884
H	-5.20952	-3.71734	-1.87721
H	-6.37306	-1.62166	-1.23715
Cl	-5.43756	1.00493	-0.87899

H	-0.67653	-0.59544	-2.68996
H	0.45685	-2.69084	-3.22377
H	-0.76925	-4.86128	-3.13396
H	-3.17148	-4.89469	-2.53542
Au	-0.56200	-0.57246	0.34007
C	0.25685	-2.22450	1.24654
C	-0.55024	-2.82639	2.22783
C	1.47078	-2.78975	0.88953
C	-0.09776	-3.97517	2.87292
C	1.91309	-3.94499	1.54061
H	2.07749	-2.35519	0.09441
C	1.13437	-4.52717	2.53368
H	-0.70909	-4.45358	3.63773
H	2.86581	-4.39369	1.26219
H	1.48017	-5.42615	3.04049
C	-2.08301	-1.05304	1.61911
C	-3.26041	-0.33110	1.70257
C	-1.83704	-2.16802	2.43848
C	-4.23980	-0.73416	2.61482
H	-3.44008	0.54377	1.07980
C	-2.82563	-2.54876	3.34494
C	-4.01929	-1.83766	3.42943
H	-5.17082	-0.17342	2.68136
H	-2.66399	-3.40957	3.99305
H	-4.78182	-2.14984	4.14037
O	1.25206	-0.07136	-0.89585
C	3.57171	0.31437	-1.01327
C	2.36309	0.12236	-0.33164
C	6.01481	0.71357	-0.86820
C	4.74866	0.51002	-0.31112
C	7.16209	1.02036	-0.11931
H	2.40658	0.13699	0.77675
H	4.67380	0.54012	0.78306
H	3.56567	0.29007	-2.10363
C	8.25437	1.84491	-0.73864
H	6.98780	1.21326	0.94519

H	6.09940	0.69532	-1.95791
H	8.40466	1.57574	-1.79188
H	7.97852	2.90781	-0.70715
H	9.21172	1.73916	-0.21426
C	8.12417	-0.74747	0.29328
C	8.51750	-1.18504	-0.97236
C	7.47077	-1.93804	-1.55935
C	6.46964	-2.08858	-0.63687
C	6.94355	-1.59470	0.68324
H	8.83521	-0.37091	1.02813
H	9.44270	-0.90736	-1.47150
H	7.45351	-2.29600	-2.58429
H	5.51850	-2.59004	-0.79602
H	6.18539	-1.12227	1.31603
H	7.33310	-2.45785	1.25246
O	-1.09251	4.96849	-1.42445
C	-1.76618	4.24435	-2.41768
H	-1.20053	4.25023	-3.36790
H	-2.73018	4.73138	-2.59677

Top, away, 1, endo, away

M06/lanl2dz-6-31G(d) Energy = -2646.113238

M06/lanl2dz-6-31G(d) Free Energy = -2645.477637

M06/def2-TZVP Derived free energy = -2646.587000

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617893

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642528

Number of Imaginary Frequencies = 1 (-384.12)

M06/lanl2dz-6-31G(d) Geometry

C	1.62657	-1.13186	3.34886
C	0.56720	-1.29879	4.47473
C	1.15872	1.26602	3.48503
N	1.37539	0.16477	2.68869
C	1.38278	0.55561	1.39596
N	1.19648	1.88613	1.48929

N	1.03801	2.34641	2.77743
C	-0.57181	-2.07751	3.81059
C	0.13694	-2.88010	2.76064
C	1.39322	-2.33473	2.49187
C	2.24678	-2.89901	1.54981
C	1.81254	-4.02478	0.85341
C	0.55247	-4.56632	1.11085
C	-0.29002	-4.00526	2.06866
C	1.19922	2.81887	0.41068
C	0.04713	2.94177	-0.41051
C	0.09210	3.85295	-1.50551
C	1.26245	4.61915	-1.72079
C	2.34665	4.51032	-0.89169
C	2.31036	3.60224	0.18562
C	-1.14084	2.20829	-0.17853
C	-2.21847	2.35480	-1.01685
C	-2.17265	3.24212	-2.11237
C	-1.03935	3.97877	-2.34620
H	2.64910	-1.07440	3.74872
H	1.03837	-1.90985	5.26366
H	-1.26306	-1.35485	3.34741
H	-1.14761	-2.67565	4.52663
H	3.23323	-2.47194	1.36062
H	2.45893	-4.48302	0.10770
H	0.23103	-5.45064	0.56315
H	-1.26583	-4.44530	2.27128
H	1.28784	5.31229	-2.56069
H	3.24204	5.10661	-1.04669
Cl	3.70052	3.50611	1.22173
H	-1.19775	1.53198	0.67283
H	-3.11786	1.76968	-0.82639
H	-3.03745	3.34433	-2.76580
H	-0.99024	4.67545	-3.18229
Au	1.23285	-0.68522	-0.39050
C	1.08119	-1.82423	-2.09652
C	2.13671	-1.66379	-3.01207

C	0.05197	-2.71405	-2.36003
C	2.11220	-2.36880	-4.21353
C	0.04125	-3.42187	-3.56577
H	-0.74018	-2.88903	-1.63225
C	1.06182	-3.23863	-4.49141
H	2.91888	-2.25185	-4.93710
H	-0.76606	-4.12225	-3.77442
H	1.05027	-3.78868	-5.43051
C	3.02604	-0.25041	-1.26254
C	3.98843	0.53665	-0.65734
C	3.20731	-0.78640	-2.54908
C	5.16032	0.83507	-1.35859
H	3.84673	0.93581	0.34517
C	4.38415	-0.47750	-3.22982
C	5.34978	0.33359	-2.64038
H	5.91727	1.46406	-0.89276
H	4.55408	-0.87850	-4.22875
H	6.26112	0.56867	-3.18691
O	-0.82919	-1.11608	0.42439
C	-3.17370	-1.07780	0.24349
C	-1.86760	-0.97943	-0.26871
C	-5.61374	-0.99059	-0.22260
C	-4.26373	-0.88725	-0.58380
C	-6.67111	-0.89702	-1.14319
H	-1.77047	-0.76414	-1.35223
H	-4.04907	-0.66617	-1.63776
H	-3.30290	-1.31041	1.30180
C	-7.93209	-1.68041	-0.90861
H	-6.36463	-0.83119	-2.19349
H	-5.84607	-1.24858	0.81367
H	-7.77835	-2.72548	-1.21026
H	-8.20555	-1.68321	0.15426
H	-8.78178	-1.29439	-1.48491
C	-7.33693	1.03448	-1.13248
C	-7.90034	1.15821	0.13957
C	-6.89689	1.52980	1.06659

C	-5.73402	1.76719	0.38266
C	-6.01956	1.76140	-1.07828
H	-7.94388	1.00572	-2.03722
H	-8.92640	0.90678	0.39667
H	-7.02320	1.57677	2.14400
H	-4.77935	2.04962	0.82013
H	-6.20481	2.80427	-1.39433
H	-5.22408	1.37328	-1.72399
C	0.95155	1.01005	4.93568
H	1.91112	0.82341	5.44974
H	0.46587	1.86357	5.41668
O	0.08133	-0.09528	5.03088

M06/lanl2dz-6-31G(d) Energy = -2646.111998

M06/lanl2dz-6-31G(d) Free Energy = -2645.474258

M06/def2-TZVP Derived free energy = -2646.585241

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616245

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641179

Number of Imaginary Frequencies = 1 (-376.94)

M06/lanl2dz-6-31G(d) Geometry

C	-3.79714	-1.10609	1.32210
C	-4.47878	-2.20713	2.15865
C	-2.74327	-3.13927	0.25668
N	-2.76822	-1.78009	0.48156
C	-1.72788	-1.22291	-0.18577
N	-1.13291	-2.27167	-0.76397
N	-1.74469	-3.47443	-0.50348
C	-3.55291	-2.38904	3.37728
C	-3.01786	-0.99670	3.55827
C	-3.19503	-0.24364	2.39268
C	-2.88429	1.11090	2.35759
C	-2.31083	1.69288	3.48592
C	-2.09283	0.93385	4.63524
C	-2.46320	-0.40897	4.68727
C	0.06110	-2.27338	-1.54216

C	1.26465	-2.69863	-0.91765
C	2.43424	-2.81303	-1.72076
C	2.37023	-2.45823	-3.08995
C	1.20399	-2.02326	-3.66093
C	0.03072	-1.95068	-2.88062
C	1.33939	-3.01582	0.45982
C	2.51837	-3.45720	1.00657
C	3.66979	-3.61278	0.20478
C	3.62750	-3.29133	-1.12911
H	-4.48285	-0.58621	0.64093
H	-5.43479	-1.79646	2.50687
H	-2.74266	-3.10608	3.16872
H	-4.09372	-2.77078	4.25146
H	-3.11344	1.71633	1.48085
H	-2.05188	2.75002	3.47243
H	-1.65468	1.40386	5.51387
H	-2.33259	-0.98160	5.60463
H	3.27117	-2.54402	-3.69675
H	1.15169	-1.75641	-4.71330
Cl	-1.44725	-1.48413	-3.65477
H	0.45574	-2.90242	1.08438
H	2.56312	-3.70242	2.06580
H	4.58947	-3.99305	0.64728
H	4.50755	-3.41490	-1.76161
Au	-1.11335	0.83514	-0.25680
C	-0.69303	2.85227	-0.21451
C	-1.61150	3.65949	-0.90973
C	0.34046	3.43202	0.50617
C	-1.44475	5.04288	-0.91240
C	0.49502	4.82134	0.50215
H	1.02890	2.82449	1.09389
C	-0.38815	5.62009	-0.21431
H	-2.14521	5.67966	-1.45248
H	1.30719	5.27688	1.06664
H	-0.26431	6.70133	-0.21931
C	-2.69761	1.53611	-1.34687

C	-3.68101	0.72291	-1.88639
C	-2.70524	2.92832	-1.54457
C	-4.70924	1.30054	-2.63602
H	-3.65715	-0.35813	-1.75504
C	-3.74155	3.48382	-2.29477
C	-4.73604	2.67539	-2.83581
H	-5.48305	0.66665	-3.06499
H	-3.77314	4.56015	-2.46119
H	-5.53705	3.12445	-3.41963
O	0.73177	0.17987	0.81796
C	3.05968	0.40905	1.12184
C	1.85496	0.58369	0.42045
C	5.44078	1.09023	1.33794
C	4.20609	1.03750	0.67534
C	6.49210	1.93583	0.94995
H	1.91968	1.14150	-0.53634
H	4.12232	1.61308	-0.25532
H	3.04458	-0.15027	2.05778
C	7.41738	2.49587	1.99300
H	6.25874	2.62235	0.12840
H	5.54182	0.53263	2.27235
H	7.64152	1.74857	2.76478
H	8.36413	2.85256	1.56935
H	6.93827	3.34902	2.49265
C	7.77146	0.84850	-0.23627
C	8.28468	-0.09338	0.65645
C	7.41097	-1.20602	0.71919
C	6.41836	-1.03875	-0.21100
C	6.75603	0.12328	-1.07561
H	8.37072	1.66871	-0.63069
H	9.16072	0.05065	1.28384
H	7.49266	-2.02814	1.42432
H	5.57737	-1.70615	-0.38395
H	7.28231	-0.25599	-1.97025
H	5.90712	0.71114	-1.43921
C	-3.73074	-4.05939	0.89076

H	-4.12696	-4.75716	0.14473
H	-3.22092	-4.66409	1.66096
O	-4.81850	-3.35099	1.41922

M06/lanl2dz-6-31G(d) Energy = -2646.112232

M06/lanl2dz-6-31G(d) Free Energy = -2645.475812

M06/def2-TZVP Derived free energy = -2646.585535

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616715

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641731

Number of Imaginary Frequencies = 1 (-390.05)

M06/lanl2dz-6-31G(d) Geometry

C	-2.71433	-1.24338	2.34482
C	-2.89024	-2.30029	3.45342
C	-1.89444	-3.27304	1.09031
N	-2.00527	-1.90512	1.21567
C	-1.41094	-1.33200	0.13943
N	-0.96617	-2.38297	-0.56179
N	-1.25645	-3.59963	0.00696
C	-1.57119	-2.24866	4.24841
C	-1.20166	-0.79821	4.11808
C	-1.87945	-0.21063	3.04394
C	-1.78948	1.15418	2.79707
C	-0.95146	1.92343	3.60096
C	-0.24507	1.33410	4.64883
C	-0.37726	-0.02575	4.92537
C	-0.25453	-2.34154	-1.79560
C	1.14105	-2.61381	-1.78855
C	1.84410	-2.56479	-3.02771
C	1.13702	-2.24230	-4.21206
C	-0.20912	-1.99228	-4.19261
C	-0.91364	-2.05565	-2.97112
C	1.85315	-2.92474	-0.60641
C	3.19722	-3.19853	-0.66025
C	3.89550	-3.15897	-1.88657
C	3.23150	-2.84000	-3.04404

H	-3.66724	-0.86731	1.95153
H	-3.70031	-1.94540	4.10279
H	-0.80322	-2.90042	3.80191
H	-1.70280	-2.58055	5.28514
H	-2.38583	1.62329	2.01472
H	-0.86859	2.99379	3.42254
H	0.39356	1.95068	5.27907
H	0.14152	-0.46998	5.77413
H	1.68219	-2.20524	-5.15459
H	-0.75697	-1.75766	-5.10185
Cl	-2.62454	-1.78618	-2.99768
H	1.32493	-2.96229	0.34363
H	3.72706	-3.46720	0.25293
H	4.95831	-3.39439	-1.91255
H	3.75717	-2.80913	-3.99798
Au	-1.17607	0.75464	-0.38008
C	-1.02797	2.76895	-0.76235
C	-2.25690	3.42487	-0.95290
C	0.16122	3.48044	-0.77621
C	-2.26986	4.80077	-1.17273
C	0.13493	4.86030	-0.99910
H	1.11578	2.98336	-0.60905
C	-1.07511	5.51400	-1.19879
H	-3.21346	5.32495	-1.32299
H	1.06727	5.42262	-1.01469
H	-1.09179	6.58812	-1.37331
C	-3.16080	1.19537	-0.63908
C	-4.17938	0.25656	-0.59356
C	-3.42720	2.55283	-0.89177
C	-5.50166	0.67262	-0.77317
H	-3.96836	-0.80271	-0.44684
C	-4.75391	2.94638	-1.06741
C	-5.78348	2.01363	-1.00384
H	-6.30538	-0.06055	-0.73826
H	-4.98648	3.99260	-1.26371
H	-6.81308	2.33641	-1.14471

O	1.03760	0.52810	-0.19859
C	3.11146	0.73450	-1.31687
C	1.72914	0.47294	-1.25307
C	5.14340	1.63232	-0.20979
C	3.80841	1.20701	-0.22031
C	5.74541	2.25019	0.89700
H	1.22648	0.23135	-2.20815
H	3.23532	1.31286	0.70739
H	3.60441	0.62075	-2.28269
C	6.83732	3.26033	0.68961
H	5.07167	2.46522	1.73377
H	5.71053	1.56553	-1.14182
H	7.44333	3.41670	1.59032
H	7.50355	2.96189	-0.12994
H	6.39724	4.22981	0.41819
C	6.70505	0.76795	1.97239
C	7.72781	0.39148	1.10146
C	7.24055	-0.58166	0.19506
C	5.96104	-0.91394	0.55572
C	5.65713	-0.30780	1.87981
H	6.89295	1.32040	2.89265
H	8.71207	0.85100	1.05452
H	7.77744	-0.95511	-0.67193
H	5.29667	-1.59435	0.02877
H	4.61852	-0.00179	2.03858
H	5.88973	-1.05524	2.66003
O	-3.31942	-3.55172	2.98449
C	-2.41915	-4.20315	2.13047
H	-1.57405	-4.64640	2.68547
H	-2.95892	-5.02849	1.65325

M06/lanl2dz-6-31G(d) Energy = -2646.111462

M06/lanl2dz-6-31G(d) Free Energy = -2645.473323

M06/def2-TZVP Derived free energy = -2646.583308

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.614592

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.639787

Number of Imaginary Frequencies = 1 (-405.20)

M06/lanl2dz-6-31G(d) Geometry

C	-2.78784	-1.74728	1.92205
C	-3.03049	-3.03954	2.72819
C	-1.90979	-3.42708	0.25348
N	-2.03278	-2.12845	0.69804
C	-1.39440	-1.31687	-0.18092
N	-0.91120	-2.17139	-1.09203
N	-1.21913	-3.48752	-0.84550
C	-1.75730	-3.21071	3.57989
C	-1.35949	-1.78186	3.81711
C	-1.97113	-0.93614	2.88552
C	-1.83684	0.44478	2.97147
C	-1.01806	0.97467	3.96587
C	-0.37685	0.13181	4.87301
C	-0.55636	-1.24922	4.81681
C	-0.11962	-1.84385	-2.23145
C	1.27805	-2.10047	-2.18203
C	2.06393	-1.77545	-3.32606
C	1.43380	-1.20606	-4.45929
C	0.08479	-0.97396	-4.48262
C	-0.70225	-1.30959	-3.36025
C	1.91628	-2.64724	-1.04275
C	3.26916	-2.87891	-1.05194
C	4.04788	-2.57100	-2.18862
C	3.45671	-2.02273	-3.29836
H	-3.71647	-1.26483	1.59111
H	-3.87355	-2.83910	3.40092
H	-0.97159	-3.75616	3.03327
H	-1.95175	-3.77535	4.49951
H	-2.38763	1.10470	2.30109
H	-0.90065	2.05337	4.04865
H	0.24792	0.56033	5.65469
H	-0.08867	-1.89761	5.55681
H	2.04192	-0.95677	-5.32822

H	-0.40237	-0.54575	-5.35489
Cl	-2.41127	-1.04779	-3.45256
H	1.32568	-2.89296	-0.16261
H	3.74608	-3.31702	-0.17604
H	5.11652	-2.77922	-2.18575
H	4.04558	-1.78106	-4.18280
Au	-1.19816	0.83722	-0.19740
C	-1.10263	2.88886	-0.12136
C	-2.33888	3.54484	-0.25439
C	0.05875	3.60923	0.10702
C	-2.38589	4.93467	-0.16969
C	-0.00122	5.00326	0.18901
H	1.01615	3.10614	0.23279
C	-1.21799	5.65989	0.04833
H	-3.33497	5.46086	-0.27075
H	0.90928	5.57330	0.36682
H	-1.26204	6.74539	0.11297
C	-3.17681	1.28160	-0.49446
C	-4.16212	0.33099	-0.70820
C	-3.47771	2.65522	-0.46446
C	-5.48665	0.74420	-0.87687
H	-3.92279	-0.73049	-0.76641
C	-4.80602	3.04538	-0.63382
C	-5.80296	2.09659	-0.83504
H	-6.26438	0.00142	-1.04475
H	-5.06594	4.10334	-0.61285
H	-6.83430	2.41792	-0.96609
O	0.99627	0.62911	0.15051
C	3.17941	1.04479	-0.65067
C	1.80903	0.74910	-0.80557
C	4.97818	1.79853	0.94722
C	3.68266	1.38830	0.59354
C	6.09081	1.87674	0.10108
H	1.43281	0.63760	-1.83986
H	2.94382	1.38668	1.39984
H	3.78777	1.06530	-1.55532

C	7.17152	2.88064	0.37693
H	5.91304	1.67512	-0.95998
H	5.11652	2.13362	1.97672
H	6.87207	3.85995	-0.02180
H	7.33514	3.00169	1.45525
H	8.12616	2.61518	-0.09338
C	7.10666	0.06216	0.33460
C	7.54026	0.12188	1.65824
C	6.53069	-0.39104	2.50796
C	5.50926	-0.88055	1.73501
C	5.92866	-0.87091	0.31038
H	7.78251	0.17152	-0.51279
H	8.46576	0.58228	1.99527
H	6.55108	-0.36178	3.59333
H	4.58601	-1.32681	2.09532
H	6.31151	-1.87769	0.05926
H	5.13053	-0.65478	-0.41072
O	-3.43885	-4.12943	1.94305
C	-2.49223	-4.57286	1.00947
H	-1.68193	-5.15039	1.48731
H	-3.00647	-5.25066	0.31944

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M06/lanl2dz-6-31G(d) Energy = -2646.116811

M06/lanl2dz-6-31G(d) Free Energy = -2645.478200

M06/def2-TZVP Derived free energy = -2646.588835

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.620188

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.645402

Number of Imaginary Frequencies = 1 (-385.43)

M06/lanl2dz-6-31G(d) Geometry

C	-3.84505	-1.18455	1.15008
C	-4.59684	-2.34813	1.82582
C	-2.79066	-3.12131	-0.08454
N	-2.80393	-1.79132	0.27467

C	-1.73240	-1.18910	-0.29627
N	-1.12826	-2.18781	-0.95157
N	-1.76745	-3.39872	-0.83626
C	-3.74331	-2.69462	3.06183
C	-3.16290	-1.35465	3.41523
C	-3.25729	-0.47274	2.33347
C	-2.88690	0.86121	2.45930
C	-2.33968	1.29051	3.66617
C	-2.20484	0.40295	4.73324
C	-2.63385	-0.91843	4.62293
C	0.08722	-2.10434	-1.69173
C	1.27672	-2.62058	-1.10650
C	2.48648	-2.53620	-1.85582
C	2.46602	-1.93281	-3.13686
C	1.30688	-1.44325	-3.67725
C	0.10154	-1.54257	-2.94984
C	1.30917	-3.19981	0.18448
C	2.48712	-3.68460	0.69784
C	3.68235	-3.61757	-0.04850
C	3.67972	-3.05118	-1.29784
H	-4.48685	-0.56419	0.51122
H	-5.55964	-1.94883	2.16825
H	-2.95233	-3.42244	2.81977
H	-4.34427	-3.14039	3.86344
H	-3.04940	1.56986	1.64712
H	-2.03528	2.32948	3.77824
H	-1.78765	0.75528	5.67486
H	-2.56817	-1.59283	5.47580
H	3.39548	-1.87448	-3.70317
H	1.28615	-0.99292	-4.66638
Cl	-1.35206	-0.95984	-3.69116
H	0.39372	-3.25617	0.76969
H	2.49761	-4.13080	1.69035
H	4.60570	-4.01197	0.37260
H	4.59541	-2.99350	-1.88772
Au	-1.09185	0.86602	-0.18091

C	-0.59463	2.85096	0.00520
C	-1.49268	3.74806	-0.59993
C	0.49263	3.31833	0.72644
C	-1.26144	5.11811	-0.49630
C	0.71244	4.69529	0.82598
H	1.16705	2.62599	1.22912
C	-0.15783	5.58760	0.21062
H	-1.94524	5.82952	-0.95886
H	1.56454	5.06793	1.39265
H	0.01553	6.65924	0.28909
C	-2.65542	1.70690	-1.19880
C	-3.67015	0.97512	-1.79352
C	-2.62361	3.11121	-1.27149
C	-4.69319	1.64684	-2.46780
H	-3.67374	-0.11391	-1.76309
C	-3.65416	3.76170	-1.95003
C	-4.68176	3.03442	-2.54196
H	-5.49245	1.07782	-2.93907
H	-3.65431	4.84906	-2.01965
H	-5.47823	3.55689	-3.06815
O	0.72045	0.14790	0.89418
C	3.04867	-0.18094	0.90354
C	1.83280	0.19063	0.30864
C	5.48560	-0.54094	0.63126
C	4.22257	-0.12961	0.18125
C	6.62453	-0.58807	-0.18494
H	1.87869	0.54493	-0.74318
H	4.15396	0.22080	-0.85720
H	3.03286	-0.54490	1.93175
C	7.67965	-1.62776	0.06746
H	6.44722	-0.36280	-1.24335
H	5.55663	-0.93746	1.64760
H	7.36285	-2.59102	-0.35791
H	8.64374	-1.37155	-0.38874
H	7.83561	-1.78061	1.14308
C	7.65644	1.16884	0.09520

C	8.07480	1.07105	1.42341
C	7.05130	1.55066	2.27593
C	6.04249	2.06531	1.50417
C	6.49853	2.12936	0.08936
H	8.34954	1.09183	-0.74231
H	8.99803	0.60364	1.75725
H	7.05138	1.47862	3.35940
H	5.10616	2.48265	1.86488
H	5.72691	1.96655	-0.66980
H	6.91139	3.13839	-0.09111
O	-4.92453	-3.39471	0.94819
C	-3.82756	-4.07547	0.40292
H	-4.20046	-4.67950	-0.43166
H	-3.37374	-4.77229	1.12880

M06/lanl2dz-6-31G(d) Energy = -2646.119554

M06/lanl2dz-6-31G(d) Free Energy = -2645.481060

M06/def2-TZVP Derived free energy = -2646.592952

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.624538

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.650402

Number of Imaginary Frequencies = 1 (-381.24)

M06/lanl2dz-6-31G(d) Geometry

C	-3.73115	-1.29378	0.78538
C	-4.92638	-2.26797	0.74135
C	-2.68501	-2.95285	-0.76957
N	-2.70806	-1.71283	-0.17492
C	-1.61192	-1.02468	-0.56850
N	-0.98111	-1.89186	-1.37152
N	-1.62990	-3.09755	-1.51339
C	-5.56792	-2.10521	2.11598
C	-4.39488	-1.77190	2.99859
C	-3.31102	-1.34027	2.23213
C	-2.09858	-1.00486	2.81783
C	-1.98955	-1.09364	4.20526
C	-3.07345	-1.50638	4.97711

C	-4.28367	-1.85271	4.37896
C	0.28179	-1.70222	-2.00293
C	1.41839	-2.34631	-1.44112
C	2.67344	-2.18701	-2.09648
C	2.74898	-1.37840	-3.25679
C	1.64132	-0.75524	-3.76775
C	0.39012	-0.93131	-3.13908
C	1.35295	-3.11987	-0.25796
C	2.48316	-3.72031	0.23991
C	3.72307	-3.58409	-0.41942
C	3.81435	-2.82976	-1.56168
H	-4.05382	-0.28170	0.49291
H	-5.60515	-2.05797	-0.10379
H	-6.09572	-3.02325	2.40153
H	-6.30689	-1.29020	2.09665
H	-1.23456	-0.70204	2.22278
H	-1.04723	-0.84144	4.68766
H	-2.97011	-1.57145	6.05861
H	-5.12233	-2.19349	4.98468
H	3.71375	-1.26075	-3.75051
H	1.69606	-0.14039	-4.66266
Cl	-0.99972	-0.16884	-3.83975
H	0.40159	-3.23048	0.25979
H	2.42069	-4.31412	1.14966
H	4.60736	-4.07411	-0.01465
H	4.76844	-2.71200	-2.07729
Au	-1.04899	1.00594	-0.06934
C	-0.60107	2.94389	0.43870
C	-1.50469	3.90772	-0.03949
C	0.47889	3.31228	1.22426
C	-1.29473	5.24987	0.26820
C	0.67842	4.66242	1.52722
H	1.16302	2.56351	1.62158
C	-0.20303	5.62340	1.04702
H	-1.98285	6.01285	-0.09502
H	1.52378	4.95884	2.14637

H	-0.04474	6.67372	1.28446
C	-2.59885	1.96756	-0.99571
C	-3.56218	1.32533	-1.75664
C	-2.60349	3.36458	-0.83339
C	-4.57621	2.07923	-2.35435
H	-3.53066	0.24856	-1.91828
C	-3.62502	4.09675	-1.43640
C	-4.60677	3.45782	-2.18767
H	-5.33539	1.58061	-2.95416
H	-3.65480	5.17999	-1.32323
H	-5.39659	4.04408	-2.65302
O	0.73505	0.14784	0.96154
C	3.05395	-0.24821	1.01191
C	1.87367	0.24090	0.43282
C	5.47948	-0.68611	0.74242
C	4.25096	-0.15118	0.33196
C	6.62028	-0.71256	-0.07048
H	1.97394	0.74352	-0.55239
H	4.22671	0.34065	-0.64946
H	2.99103	-0.75031	1.97812
C	7.59488	-1.84846	0.05437
H	6.47245	-0.34392	-1.09255
H	5.51070	-1.20919	1.70194
H	7.20010	-2.73190	-0.46945
H	8.57382	-1.61768	-0.38305
H	7.74220	-2.13103	1.10451
C	7.77345	0.93017	0.42434
C	8.16188	0.64221	1.73259
C	7.16221	1.09014	2.63068
C	6.20449	1.76548	1.92057
C	6.68243	1.96105	0.52526
H	8.46937	0.90094	-0.41370
H	9.04401	0.07163	2.01286
H	7.14178	0.89002	3.69778
H	5.29669	2.20613	2.32348
H	5.91200	1.94083	-0.25206

H	7.16316	2.95413	0.46454
C	-3.82033	-3.89437	-0.55215
H	-4.52407	-3.81845	-1.40206
H	-3.46033	-4.92710	-0.50672
O	-4.45813	-3.60244	0.66008

Top, towards, 1, endo, away

M06/lanl2dz-6-31G(d) Energy = -2646.113994

M06/lanl2dz-6-31G(d) Free Energy = -2645.476270

M06/def2-TZVP Derived free energy = -2646.585423

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616502

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641697

Number of Imaginary Frequencies = 1 (-382.04)

M06/lanl2dz-6-31G(d) Geometry

C	-2.79179	-0.93040	2.34281
C	-2.99457	-1.90980	3.51417
C	-2.20275	-3.09545	1.18600
N	-2.18430	-1.71851	1.23616
C	-1.51144	-1.26230	0.14966
N	-1.15308	-2.38625	-0.48321
N	-1.57082	-3.53728	0.14064
C	-1.61469	-1.96336	4.20231
C	-1.11298	-0.56431	3.97487
C	-1.82266	0.05047	2.93594
C	-1.61900	1.38796	2.61702
C	-0.62796	2.09181	3.29930
C	0.11308	1.46953	4.30387
C	-0.13616	0.14494	4.66255
C	-0.32043	-2.49551	-1.63610
C	1.03717	-2.86888	-1.44157
C	1.86209	-3.02738	-2.59214
C	1.31049	-2.79370	-3.87532
C	0.00029	-2.42986	-4.03334
C	-0.82777	-2.29055	-2.89906

C	1.59538	-3.09024	-0.15985
C	2.90810	-3.47092	-0.02952
C	3.72183	-3.65088	-1.16912
C	3.20947	-3.42390	-2.42223
H	-3.72603	-0.49503	1.96627
H	-3.70994	-1.44442	4.20357
H	-0.95340	-2.70722	3.72744
H	-1.69000	-2.23936	5.26071
H	-2.23338	1.88749	1.86772
H	-0.44628	3.13695	3.05585
H	0.87789	2.03380	4.83445
H	0.41316	-0.31837	5.48139
H	1.94833	-2.91594	-4.74992
H	-0.42708	-2.25863	-5.01799
Cl	-2.49281	-1.87932	-3.13854
H	0.97038	-2.98030	0.72593
H	3.32296	-3.64623	0.96179
H	4.75341	-3.97905	-1.05121
H	3.82765	-3.55952	-3.30921
Au	-1.15213	0.78159	-0.45882
C	-0.92844	2.76386	-0.94140
C	-2.12222	3.44646	-1.22931
C	0.28778	3.42515	-0.93418
C	-2.07287	4.80982	-1.51233
C	0.32370	4.79285	-1.22033
H	1.20570	2.88381	-0.70814
C	-0.85150	5.47799	-1.50774
H	-2.98621	5.35930	-1.73992
H	1.27538	5.32236	-1.21908
H	-0.81946	6.54276	-1.73099
C	-3.09944	1.25570	-0.88333
C	-4.14489	0.34672	-0.84091
C	-3.31933	2.60960	-1.19649
C	-5.44599	0.78717	-1.09929
H	-3.97186	-0.70854	-0.62974
C	-4.62542	3.02844	-1.44839

C	-5.68111	2.12381	-1.39718
H	-6.27035	0.07707	-1.06986
H	-4.82244	4.07232	-1.69113
H	-6.69447	2.46616	-1.59728
O	1.01853	0.57520	-0.02157
C	2.74578	0.18322	1.54060
C	1.43527	0.05245	1.04656
C	4.97300	1.26574	1.36918
C	3.66937	1.01150	0.92868
C	5.80781	2.24647	0.81066
H	0.72928	-0.55018	1.65299
H	3.31927	1.55180	0.04273
H	3.00007	-0.34969	2.45702
C	6.84431	2.91622	1.66754
H	5.33193	2.89824	0.07005
H	5.33189	0.72210	2.24743
H	6.37190	3.70172	2.27319
H	7.30784	2.20176	2.36006
H	7.63729	3.39079	1.07701
C	6.94883	1.33714	-0.64455
C	7.72561	0.44520	0.09584
C	7.01147	-0.76443	0.27513
C	5.84584	-0.69712	-0.44302
C	5.87740	0.51351	-1.30568
H	7.36477	2.23072	-1.10923
H	8.68377	0.67923	0.55347
H	7.31984	-1.58523	0.91598
H	5.06219	-1.45042	-0.48598
H	6.26129	0.21400	-2.29767
H	4.91369	1.00171	-1.48048
O	-3.58586	-3.12412	3.13539
C	-2.82336	-3.91582	2.26590
H	-3.49835	-4.66173	1.83124
H	-2.03202	-4.46910	2.80087

Bottom, towards, 1, endo, away

M06/lanl2dz-6-31G(d) Energy = -2646.115711
M06/lanl2dz-6-31G(d) Free Energy = -2645.474883
M06/def2-TZVP Derived free energy = -2646.584312
M06/def2-TZVP Derived free energy in solution (toluene) = -2646.615274
M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.639785
Number of Imaginary Frequencies = 1 (-392.92)

M06/lanl2dz-6-31G(d) Geometry

C	-3.31852	-0.74785	1.98797
C	-3.84219	-1.76084	3.02437
C	-2.91963	-2.88208	0.69871
N	-2.69758	-1.53518	0.89109
C	-1.83945	-1.10840	-0.06668
N	-1.58969	-2.21522	-0.77500
N	-2.24949	-3.33026	-0.32044
C	-2.61359	-2.07814	3.90181
C	-1.87659	-0.76816	3.87135
C	-2.30668	0.01415	2.79333
C	-1.85137	1.31615	2.61907
C	-0.89537	1.81189	3.50408
C	-0.43794	1.02293	4.56046
C	-0.93604	-0.26436	4.76133
C	-0.71164	-2.31279	-1.89472
C	0.58512	-2.85850	-1.70052
C	1.45813	-2.92795	-2.82409
C	1.00588	-2.46025	-4.08170
C	-0.25225	-1.94350	-4.24248
C	-1.12091	-1.87425	-3.13428
C	1.04297	-3.32048	-0.44423
C	2.30966	-3.83196	-0.31228
C	3.17679	-3.90743	-1.42463
C	2.75791	-3.46219	-2.65284
H	-4.11107	-0.13180	1.54469
H	-4.58186	-1.23403	3.64003
H	-2.00554	-2.88878	3.46876

H	-2.89859	-2.40095	4.91009
H	-2.25114	1.94894	1.82686
H	-0.52365	2.82765	3.38030
H	0.29405	1.42907	5.25662
H	-0.60771	-0.85566	5.61529
H	1.67993	-2.51958	-4.93559
H	-0.60296	-1.58842	-5.20804
Cl	-2.71482	-1.23290	-3.37111
H	0.38046	-3.27061	0.41833
H	2.65019	-4.18611	0.65916
H	4.17417	-4.32616	-1.30356
H	3.41457	-3.51903	-3.52065
Au	-0.89123	0.80007	-0.38181
C	-0.00219	2.63483	-0.61136
C	-0.89052	3.69336	-0.86896
C	1.36004	2.86483	-0.49384
C	-0.38974	4.98836	-0.98837
C	1.85014	4.16765	-0.61945
H	2.04893	2.03720	-0.31601
C	0.97682	5.22222	-0.86144
H	-1.06091	5.82334	-1.18836
H	2.91970	4.35762	-0.53080
H	1.36161	6.23567	-0.95864
C	-2.53517	1.90992	-0.87264
C	-3.80723	1.38248	-1.02126
C	-2.28850	3.28867	-1.01100
C	-4.87373	2.24197	-1.29969
H	-3.98492	0.31029	-0.94385
C	-3.36771	4.12831	-1.28515
C	-4.65063	3.60801	-1.42522
H	-5.87573	1.83477	-1.42208
H	-3.20709	5.20020	-1.39831
H	-5.48185	4.27609	-1.64170
O	1.02767	-0.18045	0.09937
C	2.89900	-0.41585	1.50070
C	1.54253	-0.13949	1.25049

C	5.12904	-0.98769	0.48978
C	3.74445	-0.77345	0.45842
C	5.97729	-0.75610	1.58133
H	0.90821	0.14670	2.11135
H	3.25304	-0.91764	-0.50833
H	3.24643	-0.34121	2.53040
C	7.26254	-1.51974	1.71137
H	5.49270	-0.51404	2.53221
H	5.58666	-1.36118	-0.42874
H	7.99140	-1.01372	2.35608
H	7.06206	-2.50418	2.15693
H	7.72459	-1.69108	0.73081
C	6.64238	1.21128	1.37495
C	5.35996	1.88647	0.97037
C	5.36616	1.71008	-0.50324
C	6.63165	1.37548	-0.91367
C	7.43378	1.14075	0.22786
H	7.06408	1.31439	2.37430
H	4.44361	1.55787	1.47543
H	4.52192	1.93881	-1.14998
H	6.96084	1.27399	-1.94352
O	-4.53781	-2.83861	2.45678
C	-3.77297	-3.67445	1.63011
H	-3.13397	-4.35612	2.21812
H	-4.47152	-4.29856	1.06220
H	8.48119	0.84994	0.20710
H	5.46577	2.96401	1.19160

Top, away, 2, endo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.113970

M06/lanl2dz-6-31G(d) Free Energy = -2645.476454

M06/def2-TZVP Derived free energy = -2646.587363

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617844

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641761

Number of Imaginary Frequencies = 1 (-379.89)

M06/lanl2dz-6-31G(d) Geometry

C	0.64396	3.02590	-0.79298
C	-0.08797	4.39974	-0.57558
C	0.42995	2.74048	1.67458
N	0.56119	2.20128	0.42079
C	0.68036	0.86052	0.53289
N	0.61217	0.66243	1.86165
N	0.44416	1.82024	2.59096
C	0.94559	5.49664	-0.91006
C	2.23312	4.77494	-1.17230
C	2.06576	3.39384	-1.11862
C	3.12884	2.52763	-1.35650
C	4.37742	3.06778	-1.64327
C	4.55174	4.45221	-1.69371
C	3.48380	5.31268	-1.46230
C	0.66470	-0.59083	2.53674
C	1.80036	-0.89733	3.33571
C	1.87372	-2.18897	3.93363
C	0.81648	-3.10786	3.73507
C	-0.28482	-2.77809	2.99061
C	-0.35733	-1.50392	2.39638
C	2.86469	0.01388	3.54102
C	3.95039	-0.34653	4.30036
C	4.02838	-1.62783	4.88770
C	3.00921	-2.52733	4.70692
H	0.15362	2.44300	-1.58291
H	-0.94947	4.45184	-1.24879
H	1.01219	6.21881	-0.08330
H	0.62230	6.07580	-1.78591
H	2.99218	1.44469	-1.32398
H	5.22104	2.40822	-1.83611
H	5.53410	4.86253	-1.92004
H	3.62480	6.39194	-1.50803
H	0.88769	-4.09380	4.19285
H	-1.10390	-3.47799	2.84793

Cl	-1.79482	-1.10570	1.48699
H	2.80749	1.01031	3.10744
H	4.75710	0.36699	4.45641
H	4.89615	-1.89567	5.48659
H	3.05553	-3.51833	5.15714
Au	0.71937	-0.54593	-1.13267
C	0.69443	-1.90237	-2.66958
C	1.70304	-2.87992	-2.62033
C	-0.24472	-1.90027	-3.68764
C	1.73307	-3.87481	-3.59447
C	-0.20119	-2.90181	-4.66247
H	-1.00439	-1.12156	-3.74619
C	0.77875	-3.88584	-4.60853
H	2.50519	-4.64342	-3.57265
H	-0.93415	-2.90471	-5.46745
H	0.80974	-4.66448	-5.36827
C	2.42806	-1.58382	-0.70998
C	3.29142	-1.23818	0.31247
C	2.66062	-2.70094	-1.53182
C	4.40325	-2.04602	0.56644
H	3.11896	-0.35367	0.92254
C	3.77672	-3.49168	-1.26389
C	4.63610	-3.17020	-0.21624
H	5.08089	-1.78530	1.37820
H	3.98487	-4.36416	-1.88279
H	5.50102	-3.80019	-0.01769
O	-1.17001	0.51098	-1.72516
C	-3.51016	0.53184	-1.40824
C	-2.26197	-0.09017	-1.53405
C	-5.93734	0.22954	-0.96484
C	-4.62922	-0.23488	-1.13475
C	-7.04029	-0.61807	-0.77013
H	-2.25200	-1.19553	-1.45134
H	-4.47584	-1.31956	-1.06398
H	-3.57496	1.61701	-1.49243
C	-8.39900	-0.19510	-1.25124

H	-6.82870	-1.68769	-0.88063
H	-6.11470	1.30387	-1.05714
H	-9.21028	-0.74787	-0.76217
H	-8.56181	0.87780	-1.08754
H	-8.48134	-0.37821	-2.33125
C	-7.31914	-0.81450	1.25009
C	-7.70114	0.47367	1.63044
C	-6.54723	1.24859	1.90115
C	-5.44588	0.43751	1.82081
C	-5.89049	-0.97621	1.69579
H	-8.01911	-1.64963	1.23571
H	-8.72009	0.85304	1.61763
H	-6.53981	2.31674	2.09617
H	-4.41004	0.74324	1.94596
H	-5.25385	-1.62471	1.08542
H	-5.91014	-1.41881	2.70798
O	-0.66123	4.54853	0.70964
C	0.19520	4.20376	1.77179
H	1.14885	4.76006	1.73226
H	-0.30783	4.45489	2.71017

M06/lanl2dz-6-31G(d) Energy = -2646.113678

M06/lanl2dz-6-31G(d) Free Energy = -2645.473363

M06/def2-TZVP Derived free energy = -2646.582670

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.612880

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.637110

Number of Imaginary Frequencies = 1 (-391.81)

M06/lanl2dz-6-31G(d) Geometry

C	-0.77186	-0.19956	3.41218
C	-1.73883	0.44293	4.44145
C	-0.27909	2.11836	2.78083
N	-0.53040	0.82820	2.37678
C	-0.58102	0.79565	1.02696
N	-0.33578	2.07601	0.69030
N	-0.15466	2.91769	1.76584

C	-3.12443	0.18921	3.83395
C	-2.93311	-1.12984	3.14353
C	-1.57224	-1.37138	2.93112
C	-1.12378	-2.56080	2.36791
C	-2.07173	-3.50711	1.98027
C	-3.43145	-3.25782	2.16109
C	-3.87230	-2.07356	2.75117
C	-0.39675	2.63026	-0.62185
C	-1.55219	3.37558	-0.98455
C	-1.64755	3.86114	-2.32045
C	-0.58771	3.61424	-3.22477
C	0.53329	2.92674	-2.84115
C	0.62510	2.43774	-1.52364
C	-2.61027	3.64149	-0.08180
C	-3.71177	4.35097	-0.49187
C	-3.81347	4.82315	-1.81843
C	-2.80081	4.58209	-2.71100
H	0.20600	-0.46775	3.83443
H	-1.63150	-0.12960	5.37714
H	-3.34888	0.99793	3.11760
H	-3.92197	0.19357	4.58589
H	-0.05840	-2.74381	2.22431
H	-1.74625	-4.44198	1.52817
H	-4.15880	-4.00570	1.85130
H	-4.93522	-1.90108	2.91406
H	-0.67124	3.99122	-4.24339
H	1.35412	2.75040	-3.53133
Cl	2.07959	1.59466	-1.05784
H	-2.53924	3.29327	0.94767
H	-4.51303	4.55624	0.21540
H	-4.69329	5.38435	-2.12556
H	-2.86421	4.94611	-3.73586
Au	-0.72330	-0.98164	-0.22159
C	-0.81070	-2.65993	-1.39787
C	-1.89001	-2.70880	-2.29620
C	0.09897	-3.70208	-1.32384

C	-2.01024	-3.79912	-3.15528
C	-0.03576	-4.79480	-2.18568
H	0.90992	-3.68526	-0.59504
C	-1.07949	-4.83339	-3.10316
H	-2.83692	-3.85410	-3.86332
H	0.67727	-5.61606	-2.13437
H	-1.17923	-5.68213	-3.77710
C	-2.50383	-0.66016	-1.16662
C	-3.33470	0.40232	-0.86683
C	-2.82230	-1.59143	-2.17104
C	-4.50107	0.58498	-1.61478
H	-3.08953	1.10165	-0.07007
C	-3.99196	-1.39310	-2.90306
C	-4.81952	-0.30667	-2.63181
H	-5.15402	1.42782	-1.39336
H	-4.26536	-2.09591	-3.68975
H	-5.72703	-0.16324	-3.21517
O	1.32771	-1.39468	0.65689
C	3.65766	-1.33384	0.25871
C	2.30927	-1.40181	-0.13025
C	6.02887	-1.21996	-0.58948
C	4.63506	-1.31892	-0.72259
C	6.73679	-1.06965	0.61011
H	2.12184	-1.46375	-1.22091
H	4.26894	-1.41312	-1.75072
H	3.88756	-1.29512	1.32392
C	8.13643	-1.60005	0.72315
H	6.15102	-1.12994	1.53275
H	6.61409	-1.30713	-1.50611
H	8.10483	-2.67821	0.93287
H	8.68882	-1.46388	-0.21521
H	8.70272	-1.12508	1.53355
C	7.02076	0.98147	0.86151
C	7.88986	1.29195	-0.18420
C	7.14028	1.59991	-1.34467
C	5.80728	1.60166	-1.02187

C	5.66122	1.47532	0.45011
H	7.33947	0.95079	1.90290
H	8.97315	1.20955	-0.14355
H	7.55714	1.76917	-2.33313
H	4.98061	1.80190	-1.69971
H	5.52666	2.48756	0.87219
H	4.80035	0.88553	0.78624
O	-1.54803	1.81628	4.71411
C	-0.35417	2.39444	4.23866
H	0.53161	1.99305	4.76186
H	-0.40624	3.47006	4.42848

Bottom, away, 2, endo, toward

M06/lanl2dz-6-31G(d) Energy = -2646.116486

M06/lanl2dz-6-31G(d) Free Energy = -2645.479990

M06/def2-TZVP Derived free energy = -2646.591415

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.621836

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.646326

Number of Imaginary Frequencies = 1 (-368.67)

M06/lanl2dz-6-31G(d) Geometry

C	-0.55431	3.14955	-0.19132
C	-0.32228	4.46281	-0.96996
C	-1.45937	2.36325	-2.39337
N	-1.04883	2.11371	-1.10578
C	-1.16424	0.78793	-0.86503
N	-1.64503	0.30830	-2.02398
N	-1.83257	1.27081	-2.98940
C	-0.44169	5.54453	0.09812
C	-1.41067	4.94724	1.08219
C	-1.50547	3.56636	0.90194
C	-2.33865	2.79435	1.69967
C	-3.08697	3.42851	2.68999
C	-2.99244	4.80622	2.87484
C	-2.15240	5.57557	2.07218

C	-1.91912	-1.05887	-2.31783
C	-3.26792	-1.48316	-2.46886
C	-3.51739	-2.87539	-2.63796
C	-2.42789	-3.77659	-2.69119
C	-1.13431	-3.33815	-2.59131
C	-0.88519	-1.96501	-2.40531
C	-4.36637	-0.59078	-2.42479
C	-5.65080	-1.06586	-2.52600
C	-5.90116	-2.44664	-2.68035
C	-4.85376	-3.32964	-2.73972
H	0.39512	2.77014	0.21678
H	0.64328	4.46231	-1.50587
H	-0.78121	6.48641	-0.35004
H	0.53882	5.73222	0.56107
H	-2.42246	1.71514	1.56162
H	-3.74994	2.84067	3.32167
H	-3.58468	5.28748	3.65081
H	-2.08874	6.65388	2.21262
H	-2.63310	-4.83835	-2.82273
H	-0.29428	-4.02517	-2.65053
Cl	0.77532	-1.44306	-2.30443
H	-4.18737	0.47773	-2.32329
H	-6.48576	-0.36855	-2.49545
H	-6.92528	-2.80467	-2.76025
H	-5.03117	-4.39708	-2.86666
Au	-0.46438	-0.27619	0.90112
C	0.21248	-1.33198	2.52670
C	-0.70024	-2.26083	3.05627
C	1.47081	-1.17928	3.08534
C	-0.31408	-3.05804	4.13118
C	1.84524	-1.98048	4.16836
H	2.16358	-0.43061	2.70218
C	0.95792	-2.91975	4.67993
H	-1.00722	-3.78422	4.55540
H	2.83078	-1.86064	4.61587
H	1.25116	-3.54202	5.52341

C	-2.17054	-1.28411	1.40266
C	-3.38576	-1.08025	0.77704
C	-2.01600	-2.23807	2.42386
C	-4.47735	-1.87863	1.12868
H	-3.50997	-0.31550	0.01404
C	-3.11771	-3.02165	2.76337
C	-4.33655	-2.84972	2.11216
H	-5.42921	-1.73478	0.61833
H	-3.02718	-3.77093	3.54947
H	-5.18520	-3.47370	2.38589
O	1.49412	0.73280	0.44265
C	3.65390	0.54828	-0.48932
C	2.47500	0.03542	0.06944
C	5.86644	0.04363	-1.49990
C	4.66417	-0.31264	-0.87880
C	6.79688	-0.89007	-1.98296
H	2.42276	-1.06564	0.18599
H	4.48655	-1.38440	-0.72272
H	3.74890	1.62584	-0.62711
C	7.64814	-0.54818	-3.17250
H	6.47264	-1.93581	-1.93713
H	6.04918	1.10468	-1.68785
H	7.96994	0.50052	-3.14166
H	8.53981	-1.18237	-3.24734
H	7.06784	-0.68732	-4.09484
C	8.19561	-1.19036	-0.50846
C	8.83155	0.05013	-0.44004
C	8.12451	0.89594	0.44916
C	7.12322	0.17133	1.03992
C	7.29090	-1.26488	0.69192
H	8.68052	-2.07315	-0.92453
H	9.67915	0.35305	-1.05001
H	8.32199	1.95280	0.60148
H	6.39002	0.54751	1.74821
H	7.86418	-1.74821	1.50354
H	6.36725	-1.84115	0.57902

O	-1.37644	4.67432	-1.89176
C	-1.38161	3.74732	-2.94077
H	-0.47219	3.84198	-3.56330
H	-2.24651	3.96027	-3.57728

M06/lanl2dz-6-31G(d) Energy = -2646.113547

M06/lanl2dz-6-31G(d) Free Energy = -2645.475886

M06/def2-TZVP Derived free energy = -2646.585819

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.615674

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.639410

Number of Imaginary Frequencies = 1 (-384.83)

M06/lanl2dz-6-31G(d) Geometry

C	0.14458	2.79731	1.37319
C	-0.07972	4.29437	1.65423
C	-1.13145	3.39713	-0.71697
N	-0.67188	2.45595	0.17616
C	-1.01893	1.22933	-0.28206
N	-1.66565	1.49972	-1.42731
N	-1.74665	2.84085	-1.71709
C	-1.38212	4.33582	2.47807
C	-1.29195	3.04426	3.24228
C	-0.38279	2.17390	2.63076
C	-0.04573	0.95780	3.21359
C	-0.69145	0.58114	4.38923
C	-1.63041	1.42692	4.97831
C	-1.92316	2.67112	4.42138
C	-2.21000	0.54459	-2.33532
C	-3.62092	0.46836	-2.50005
C	-4.14450	-0.56420	-3.33117
C	-3.25477	-1.45194	-3.98109
C	-1.89798	-1.33242	-3.83965
C	-1.37675	-0.31903	-3.01262
C	-4.52280	1.35212	-1.85886

C	-5.87742	1.20723	-2.02932
C	-6.39821	0.17900	-2.84407
C	-5.54634	-0.68503	-3.48232
H	1.18174	2.53587	1.13258
H	0.74682	4.62505	2.29580
H	-2.27218	4.35302	1.82879
H	-1.43898	5.22562	3.11625
H	0.72695	0.32306	2.77792
H	-0.44995	-0.37166	4.85631
H	-2.12338	1.12262	5.89971
H	-2.62684	3.34262	4.91169
H	-3.66748	-2.23722	-4.61324
H	-1.21154	-2.00033	-4.35331
Cl	0.35656	-0.17722	-2.89293
H	-4.13476	2.16084	-1.24315
H	-6.55840	1.89866	-1.53680
H	-7.47438	0.08050	-2.96846
H	-5.93296	-1.47940	-4.11986
Au	-0.46249	-0.69866	0.55021
C	0.08969	-2.53434	1.28945
C	-0.94861	-3.47692	1.38678
C	1.38078	-2.86451	1.66884
C	-0.65921	-4.76728	1.82449
C	1.65882	-4.16068	2.11431
H	2.18024	-2.12360	1.63333
C	0.64358	-5.10739	2.17934
H	-1.45059	-5.51237	1.90366
H	2.67182	-4.42556	2.41347
H	0.86258	-6.11692	2.52212
C	-2.29576	-1.58328	0.71945
C	-3.48321	-0.91204	0.50147
C	-2.26965	-2.94624	1.06321
C	-4.68668	-1.61987	0.56319
H	-3.50126	0.15102	0.27472
C	-3.48062	-3.63418	1.12181
C	-4.67990	-2.97669	0.86094

H	-5.62333	-1.09780	0.37118
H	-3.49043	-4.69194	1.38372
H	-5.61681	-3.52877	0.90471
O	1.62891	0.14815	0.38626
C	3.70285	0.19402	-0.73228
C	2.47793	-0.38899	-0.37172
C	5.81694	-0.09309	-2.06760
C	4.56527	-0.49076	-1.57292
C	6.47680	1.10613	-1.77146
H	2.26202	-1.39080	-0.79447
H	4.20956	-1.46580	-1.92221
H	3.91942	1.19465	-0.35649
C	7.41318	1.71217	-2.77502
H	5.92167	1.83197	-1.16959
H	6.29566	-0.76213	-2.78410
H	8.12389	2.41383	-2.32160
H	7.97827	0.93832	-3.30982
H	6.83385	2.27107	-3.52316
C	7.75341	0.68681	-0.16373
C	8.69088	-0.15943	-0.75275
C	8.24177	-1.49958	-0.66112
C	7.08932	-1.52792	0.07987
C	6.84827	-0.18426	0.66321
H	7.97638	1.71892	0.10437
H	9.57981	0.16536	-1.28789
H	8.71907	-2.35409	-1.13157
H	6.50486	-2.41110	0.32263
H	5.79531	0.11234	0.72972
H	7.23601	-0.18170	1.69783
C	-0.97789	4.85837	-0.46371
H	-0.66340	5.36818	-1.38088
H	-1.95677	5.28144	-0.17723
O	-0.00128	5.10692	0.51056

Top, towards, 2, endo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.110778

M06/lanl2dz-6-31G(d) Free Energy = -2645.475430

M06/def2-TZVP Derived free energy = -2646.586242

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617192

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642700

Number of Imaginary Frequencies = 1 (-373.49)

M06/lanl2dz-6-31G(d) Geometry

C	0.50995	2.86755	0.35419
C	1.01877	4.24217	-0.13632
C	-0.84801	2.97442	-1.74449
N	-0.40162	2.29082	-0.63735
C	-0.89822	1.03143	-0.67711
N	-1.61378	1.02482	-1.81488
N	-1.59475	2.22133	-2.49260
C	1.38206	4.98079	1.14716
C	0.44771	4.38664	2.16443
C	-0.08093	3.17830	1.70619
C	-0.96269	2.44105	2.48586
C	-1.31596	2.93574	3.74030
C	-0.78941	4.14118	4.20004
C	0.09706	4.87507	3.41486
C	-2.33700	-0.08174	-2.35111
C	-3.75772	-0.02065	-2.39631
C	-4.46388	-1.17770	-2.83582
C	-3.73832	-2.32399	-3.23802
C	-2.36948	-2.34324	-3.22418
C	-1.66522	-1.20697	-2.77939
C	-4.49683	1.12015	-1.99933
C	-5.86919	1.10505	-2.03065
C	-6.57049	-0.04338	-2.45587
C	-5.87862	-1.15880	-2.85233
H	1.35527	2.16845	0.43554
H	1.85766	4.13931	-0.84785

H	1.26430	6.06240	1.00773
H	2.43454	4.79505	1.40973
H	-1.39010	1.50206	2.13120
H	-2.01144	2.37537	4.36173
H	-1.07978	4.51658	5.17942
H	0.49817	5.82243	3.77305
H	-4.29070	-3.20274	-3.56880
H	-1.80929	-3.21756	-3.54511
Cl	0.07517	-1.27510	-2.79050
H	-3.97100	2.01940	-1.68603
H	-6.42352	1.99235	-1.73057
H	-7.65806	-0.03703	-2.47406
H	-6.40583	-2.05138	-3.18755
Au	-0.48968	-0.68678	0.60894
C	-0.15192	-2.41791	1.66513
C	-1.30152	-3.01698	2.20932
C	1.08939	-3.01857	1.80248
C	-1.17991	-4.21235	2.91352
C	1.19794	-4.21852	2.51164
H	1.98169	-2.57805	1.35961
C	0.06890	-4.80735	3.06753
H	-2.06006	-4.68898	3.34467
H	2.17237	-4.69088	2.62579
H	0.15741	-5.74062	3.62042
C	-2.40096	-1.10491	1.21112
C	-3.48149	-0.28356	0.94458
C	-2.54014	-2.28634	1.96046
C	-4.75122	-0.66019	1.39059
H	-3.36480	0.65044	0.39877
C	-3.81469	-2.64205	2.39923
C	-4.91313	-1.83814	2.10845
H	-5.60626	-0.02247	1.17192
H	-3.95342	-3.55452	2.97834
H	-5.90179	-2.13265	2.45515
O	1.69828	-0.34701	0.21370
C	3.83980	-0.24375	1.21117

C	2.44792	-0.05448	1.18957
C	5.85634	-1.23209	0.16413
C	4.49828	-0.90365	0.18513
C	6.44171	-2.05193	-0.81351
H	1.98717	0.37727	2.10033
H	3.87580	-1.24521	-0.64900
H	4.38628	0.08388	2.09509
C	7.62353	-2.90844	-0.45967
H	5.74057	-2.50390	-1.52382
H	6.47567	-0.90362	1.00328
H	8.19142	-3.22939	-1.34146
H	8.30570	-2.38294	0.22063
H	7.27948	-3.81554	0.05595
C	7.21492	-0.81697	-2.27500
C	8.22372	-0.13979	-1.59047
C	7.68015	1.00734	-0.96004
C	6.36949	1.13334	-1.33526
C	6.07335	0.15322	-2.41400
H	7.42339	-1.57847	-3.02580
H	9.24646	-0.49049	-1.47566
H	8.20970	1.64956	-0.26284
H	5.67445	1.89555	-0.99415
H	5.06352	-0.26948	-2.41163
H	6.19721	0.66442	-3.38586
O	-0.03376	4.95909	-0.74935
C	-0.43629	4.38984	-1.96508
H	-1.27512	4.97648	-2.35317
H	0.37828	4.42878	-2.71201

M06/lanl2dz-6-31G(d) Energy = -2646.109971

M06/lanl2dz-6-31G(d) Free Energy = -2645.473176

M06/def2-TZVP Derived free energy = -2646.584594

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.615405

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.640403

Number of Imaginary Frequencies = 1 (-391.46)

M06/lanl2dz-6-31G(d) Geometry

C	-1.36251	-2.25644	0.24005
C	-1.91462	-3.68813	0.06641
C	0.24534	-3.07000	-1.52717
N	-0.14298	-2.14020	-0.58947
C	0.75394	-1.12755	-0.59352
N	1.64769	-1.51639	-1.51523
N	1.35068	-2.71602	-2.11216
C	-1.20468	-4.52637	1.14406
C	-0.95881	-3.50916	2.21974
C	-1.05923	-2.21013	1.71145
C	-0.89295	-1.10561	2.53930
C	-0.59503	-1.31238	3.88367
C	-0.48443	-2.60757	4.38873
C	-0.67371	-3.71361	3.56362
C	2.80564	-0.77769	-1.90113
C	4.08012	-1.21854	-1.45452
C	5.20748	-0.39257	-1.73030
C	5.02483	0.81347	-2.44795
C	3.79073	1.19382	-2.90473
C	2.67176	0.38182	-2.63319
C	4.27089	-2.42372	-0.73705
C	5.52526	-2.78857	-0.31502
C	6.64339	-1.96942	-0.58178
C	6.48454	-0.79664	-1.27433
H	-2.05752	-1.48489	-0.11454
H	-2.98489	-3.64740	0.30724
H	-0.25364	-4.94038	0.77374
H	-1.81191	-5.38044	1.46723
H	-0.99757	-0.09137	2.15068
H	-0.45539	-0.45915	4.54410
H	-0.25812	-2.75560	5.44300
H	-0.60184	-4.72233	3.96845
H	5.89375	1.43924	-2.64809
H	3.65182	2.10946	-3.47362
Cl	1.12282	0.88724	-3.24103

H	3.41769	-3.06971	-0.53874
H	5.66148	-3.72413	0.22429
H	7.63012	-2.27561	-0.24099
H	7.34005	-0.15785	-1.49135
Au	0.66807	0.90466	0.18641
C	0.75933	2.91235	0.61578
C	1.91436	3.31934	1.30700
C	-0.16215	3.84632	0.17055
C	2.10797	4.67278	1.57295
C	0.04364	5.20259	0.44167
H	-1.03474	3.54591	-0.40897
C	1.17070	5.60910	1.14535
H	2.99665	5.00687	2.10791
H	-0.67743	5.93910	0.09100
H	1.32993	6.66532	1.35428
C	2.41343	0.95328	1.24157
C	3.12568	-0.18630	1.56709
C	2.81680	2.22988	1.66795
C	4.30817	-0.05769	2.30066
H	2.78182	-1.17304	1.26291
C	4.00067	2.33502	2.39646
C	4.74412	1.19880	2.70274
H	4.88139	-0.94758	2.55462
H	4.34287	3.31161	2.73805
H	5.66679	1.29686	3.27154
O	-1.37706	0.88429	-0.76730
C	-3.69456	1.27594	-0.72878
C	-2.39469	1.36058	-0.20354
C	-6.10782	1.90464	-0.41772
C	-4.75576	1.84550	-0.04532
C	-6.65762	1.36208	-1.58631
H	-2.28082	1.88856	0.76649
H	-4.50351	2.34282	0.89699
H	-3.81163	0.79924	-1.70316
C	-7.86404	1.99753	-2.21201
H	-5.94994	0.92897	-2.29974

H	-6.77254	2.47534	0.23216
H	-7.54928	2.85966	-2.81644
H	-8.40530	1.31351	-2.87696
H	-8.56033	2.36905	-1.44973
C	-7.36573	-0.53812	-1.06934
C	-8.44124	-0.22548	-0.24010
C	-7.98759	-0.10099	1.09585
C	-6.66171	-0.44367	1.14494
C	-6.24978	-0.99622	-0.17077
H	-7.49223	-0.91798	-2.08249
H	-9.45164	-0.01083	-0.57897
H	-8.58845	0.24192	1.93289
H	-6.03280	-0.44300	2.03097
H	-5.22778	-0.74964	-0.48289
H	-6.30280	-2.09860	-0.11486
C	-0.55765	-4.30178	-1.77344
H	-0.65506	-4.47222	-2.85093
H	-0.04237	-5.18072	-1.35018
O	-1.85585	-4.15893	-1.25575

M06/lanl2dz-6-31G(d) Energy = -2646.111477

M06/lanl2dz-6-31G(d) Free Energy = -2645.472980

M06/def2-TZVP Derived free energy = -2646.582211

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.612912

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.637682

Number of Imaginary Frequencies = 1 (-388.10)

M06/lanl2dz-6-31G(d) Geometry

C	-1.75958	-1.52861	0.97004
C	-2.63946	-2.79264	1.06801
C	-0.79668	-2.81082	-0.97727
N	-0.76064	-1.75338	-0.09843
C	0.32476	-0.99510	-0.38567
N	0.89559	-1.65528	-1.40387
N	0.21436	-2.78218	-1.79289
C	-1.91564	-3.71861	2.05952

C	-1.20702	-2.73338	2.94360
C	-1.12846	-1.47723	2.33298
C	-0.53095	-0.40374	2.98304
C	0.02191	-0.60619	4.24448
C	-0.04673	-1.86076	4.84959
C	-0.66884	-2.92946	4.20872
C	2.09825	-1.27622	-2.07082
C	3.29168	-1.99011	-1.78021
C	4.50658	-1.52577	-2.36123
C	4.47737	-0.40558	-3.22581
C	3.30732	0.24558	-3.51445
C	2.10567	-0.19727	-2.92686
C	3.32775	-3.11271	-0.91861
C	4.51948	-3.73357	-0.63732
C	5.72675	-3.26754	-1.20065
C	5.71640	-2.18946	-2.04800
H	-2.33850	-0.63733	0.68939
H	-3.59501	-2.48239	1.51326
H	-1.19437	-4.37486	1.54748
H	-2.61298	-4.37574	2.59272
H	-0.49187	0.58474	2.52292
H	0.50127	0.22137	4.76311
H	0.38216	-2.00307	5.83974
H	-0.73483	-3.90214	4.69463
H	5.41243	-0.05988	-3.66513
H	3.28341	1.10342	-4.18143
Cl	0.63972	0.66238	-3.29190
H	2.40068	-3.49055	-0.49038
H	4.53333	-4.60007	0.02122
H	6.66194	-3.77167	-0.96674
H	6.64064	-1.82361	-2.49410
Au	0.83658	1.04766	0.19062
C	1.39992	2.99888	0.48529
C	2.68181	3.17547	1.03440
C	0.63533	4.08817	0.10185
C	3.16692	4.46718	1.22451

C	1.13406	5.37990	0.29629
H	-0.33726	3.95409	-0.37046
C	2.39021	5.56422	0.86133
H	4.15728	4.62562	1.65113
H	0.53779	6.24044	-0.00240
H	2.77661	6.57058	1.01122
C	2.68052	0.75703	1.01507
C	3.19348	-0.49881	1.28165
C	3.38368	1.93087	1.33494
C	4.46967	-0.60450	1.84082
H	2.62273	-1.39925	1.06230
C	4.65142	1.80287	1.90036
C	5.19311	0.54321	2.14181
H	4.88926	-1.59092	2.03262
H	5.22398	2.69395	2.15653
H	6.18734	0.45956	2.57665
O	-1.26480	1.45111	-0.50641
C	-3.49496	2.05850	-0.01611
C	-2.10968	2.02329	0.23408
C	-5.37185	1.46005	-1.57382
C	-4.03091	1.49907	-1.16848
C	-6.46461	1.92921	-0.83316
H	-1.75602	2.53694	1.14886
H	-3.29969	1.06616	-1.85677
H	-4.11267	2.59474	0.70366
C	-7.69756	2.41657	-1.53378
H	-6.23329	2.45441	0.09829
H	-5.57597	1.05786	-2.56737
H	-8.58263	2.40984	-0.88599
H	-7.54167	3.45359	-1.86262
H	-7.91387	1.81867	-2.42812
C	-7.17856	0.27408	0.24583
C	-7.71262	-0.51192	-0.77251
C	-6.71037	-1.37406	-1.28034
C	-5.57651	-1.23096	-0.52411
C	-5.87770	-0.36618	0.64689

H	-7.79594	0.83330	0.94768
H	-8.71508	-0.41043	-1.18107
H	-6.81867	-2.01797	-2.14797
H	-4.63950	-1.76582	-0.67463
H	-6.08400	-1.01337	1.51893
H	-5.06701	0.31045	0.94560
C	-1.89165	-3.82059	-0.93410
H	-2.25650	-4.01832	-1.94755
H	-1.51598	-4.77587	-0.53180
O	-2.98140	-3.33610	-0.18663

Bottom, towards, 2, endo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.113654

M06/lanl2dz-6-31G(d) Free Energy = -2645.477254

M06/def2-TZVP Derived free energy = -2646.589244

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.620131

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.644953

Number of Imaginary Frequencies = 1 (-377.16)

M06/lanl2dz-6-31G(d) Geometry

C	0.62897	2.72117	-0.15304
C	1.00693	4.13964	-0.63397
C	-1.49057	3.21293	-1.38469
N	-0.68507	2.34594	-0.68385
C	-1.28433	1.13140	-0.64894
N	-2.41810	1.33407	-1.34285
N	-2.56401	2.61947	-1.80855
C	1.97529	4.64286	0.43159
C	1.53554	3.91769	1.67352
C	0.73522	2.82122	1.34741
C	0.21350	1.99665	2.33587
C	0.50501	2.28557	3.66802
C	1.30654	3.37712	3.99589
C	1.82750	4.20113	3.00016
C	-3.41681	0.36040	-1.64260

C	-4.71545	0.50791	-1.07918
C	-5.66902	-0.52408	-1.31672
C	-5.30809	-1.63460	-2.11515
C	-4.06392	-1.73419	-2.67750
C	-3.11315	-0.72125	-2.44241
C	-5.09255	1.61407	-0.27939
C	-6.35315	1.68497	0.26052
C	-7.29539	0.65938	0.03402
C	-6.95681	-0.42062	-0.73984
H	1.34263	1.99241	-0.56157
H	1.43425	4.12633	-1.65221
H	1.92147	5.73585	0.50740
H	3.00877	4.38062	0.15824
H	-0.42823	1.14891	2.09110
H	0.09624	1.65644	4.45619
H	1.51951	3.59431	5.04101
H	2.44090	5.06278	3.26124
H	-6.04642	-2.41716	-2.28621
H	-3.78924	-2.57835	-3.30455
Cl	-1.55435	-0.88629	-3.20084
H	-4.38337	2.42111	-0.10938
H	-6.63054	2.54632	0.86530
H	-8.28970	0.73310	0.46926
H	-7.67561	-1.21756	-0.92763
Au	-0.55230	-0.79385	0.09371
C	-0.00655	-2.70946	0.60140
C	-0.90700	-3.38379	1.44442
C	1.10648	-3.35952	0.09349
C	-0.65139	-4.70743	1.79533
C	1.35129	-4.68888	0.45049
H	1.78114	-2.85519	-0.59749
C	0.47857	-5.35409	1.30330
H	-1.33781	-5.24636	2.44794
H	2.22287	-5.20493	0.05068
H	0.67093	-6.38928	1.57892
C	-2.10909	-1.28694	1.32761

C	-3.11480	-0.40321	1.67361
C	-2.05909	-2.58840	1.85651
C	-4.13275	-0.82913	2.53118
H	-3.12991	0.61635	1.29481
C	-3.08176	-2.99272	2.71336
C	-4.11595	-2.12104	3.04120
H	-4.93215	-0.13961	2.79699
H	-3.06856	-3.99762	3.13461
H	-4.90888	-2.45313	3.70853
O	1.35388	-0.31035	-0.99655
C	3.66594	0.10630	-0.88802
C	2.44695	-0.35265	-0.36945
C	6.09146	0.47761	-0.51543
C	4.82304	0.02824	-0.13303
C	7.21019	0.46858	0.33240
H	2.46478	-0.76902	0.65855
H	4.72800	-0.39294	0.87571
H	3.68056	0.51590	-1.89930
C	8.28286	1.50654	0.16459
H	7.00595	0.18427	1.37083
H	6.19625	0.92300	-1.50821
H	8.47025	1.71614	-0.89626
H	7.96365	2.44688	0.63470
H	9.23020	1.21215	0.63230
C	8.23503	-1.28304	-0.01685
C	8.68254	-1.11385	-1.32756
C	7.68521	-1.55971	-2.22952
C	6.66483	-2.12322	-1.51039
C	7.08000	-2.24455	-0.08749
H	8.90748	-1.24760	0.83984
H	9.61006	-0.62415	-1.61436
H	7.71283	-1.43538	-3.30782
H	5.74119	-2.52848	-1.91485
H	6.28617	-2.11656	0.65535
H	7.49040	-3.25934	0.06361
O	-0.12789	4.98183	-0.60970

C	-1.06932	4.62833	-1.58639
H	-0.65249	4.75162	-2.60311
H	-1.92775	5.30099	-1.49191

M06/lanl2dz-6-31G(d) Energy = -2646.111884

M06/lanl2dz-6-31G(d) Free Energy = -2645.476002

M06/def2-TZVP Derived free energy = -2646.588265

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618969

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.644018

Number of Imaginary Frequencies = 1 (-385.62)

M06/lanl2dz-6-31G(d) Geometry

C	0.27077	2.88701	0.18044
C	0.64115	4.30033	-0.32394
C	-1.41260	2.99406	-1.66740
N	-0.74291	2.29122	-0.69374
C	-1.19389	1.01473	-0.69574
N	-2.11577	1.01990	-1.67251
N	-2.26541	2.23939	-2.29064
C	1.14417	5.01406	0.92669
C	0.37522	4.34923	2.03526
C	-0.15599	3.13215	1.60573
C	-0.90824	2.33626	2.45908
C	-1.12955	2.78176	3.76132
C	-0.59804	3.99468	4.19452
C	0.16051	4.78652	3.33453
C	-2.91100	-0.08735	-2.09211
C	-4.30798	-0.06709	-1.82513
C	-5.07392	-1.21645	-2.17593
C	-4.43172	-2.31662	-2.79197
C	-3.08998	-2.29897	-3.06471
C	-2.32555	-1.16853	-2.71417
C	-4.95989	1.02608	-1.20426
C	-6.30615	0.97303	-0.93995
C	-7.06587	-0.16584	-1.28276
C	-6.45966	-1.23523	-1.89011

H	1.15159	2.23109	0.12823
H	1.37652	4.26456	-1.14706
H	0.96810	6.09356	0.84374
H	2.22848	4.86449	1.04078
H	-1.33264	1.38756	2.12740
H	-1.72597	2.17672	4.44130
H	-0.78353	4.33066	5.21297
H	0.56440	5.73971	3.67353
H	-5.02744	-3.18983	-3.05556
H	-2.59708	-3.13754	-3.54977
Cl	-0.62753	-1.17918	-3.09267
H	-4.39122	1.91870	-0.95083
H	-6.79498	1.82251	-0.46664
H	-8.13205	-0.18884	-1.06808
H	-7.03440	-2.11956	-2.16358
Au	-0.40788	-0.73153	0.34920
C	0.28436	-2.47043	1.20163
C	-0.64568	-3.14991	2.00820
C	1.54307	-3.00627	0.97926
C	-0.27498	-4.34486	2.62066
C	1.90324	-4.20793	1.59563
H	2.25307	-2.51652	0.31345
C	0.99974	-4.86676	2.42028
H	-0.98220	-4.88128	3.25280
H	2.89165	-4.63126	1.42220
H	1.28213	-5.80098	2.90189
C	-2.09123	-1.32352	1.34827
C	-3.27407	-0.60682	1.33428
C	-1.95542	-2.51021	2.08929
C	-4.37163	-1.08858	2.05252
H	-3.37093	0.32140	0.77505
C	-3.05979	-2.96853	2.80647
C	-4.26056	-2.26470	2.78326
H	-5.30760	-0.53257	2.03253
H	-2.98573	-3.88666	3.38868
H	-5.11441	-2.63895	3.34468

O	1.55572	-0.12508	-0.56679
C	3.86150	0.30255	-0.39623
C	2.60430	-0.04177	0.12474
C	6.30226	0.63254	0.11350
C	4.96807	0.34311	0.43699
C	6.79423	0.91501	-1.16707
H	2.55263	-0.24930	1.21307
H	4.77264	0.13895	1.49497
H	3.91859	0.52570	-1.46241
C	8.00472	1.78586	-1.33072
H	6.05141	1.01320	-1.96442
H	7.01037	0.67818	0.94212
H	7.70691	2.84185	-1.26660
H	8.73879	1.60341	-0.53591
H	8.49759	1.64528	-2.30041
C	7.44915	-0.91471	-1.96052
C	8.55244	-1.19341	-1.15626
C	8.13372	-1.91807	-0.01336
C	6.79922	-2.20344	-0.13788
C	6.33886	-1.81500	-1.49420
H	7.53979	-0.58643	-2.99526
H	9.56141	-0.82657	-1.32798
H	8.76377	-2.17418	0.83318
H	6.18947	-2.74446	0.58074
H	6.35098	-2.71637	-2.13346
H	5.31807	-1.41967	-1.54715
C	-1.07949	4.42559	-1.91140
H	-0.38252	4.49997	-2.76685
H	-1.98102	4.99351	-2.16275
O	-0.51984	4.98409	-0.75472

M06/lanl2dz-6-31G(d) Energy = -2646.113110

M06/lanl2dz-6-31G(d) Free Energy = -2645.474410

M06/def2-TZVP Derived free energy = -2646.584951

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.615416

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.640081

Number of Imaginary Frequencies = 1 (-376.37)

M06/lanl2dz-6-31G(d) Geometry

C	-0.62077	3.28439	-0.18978
C	-0.75565	4.66120	-0.88011
C	-2.21962	2.58008	-1.98586
N	-1.39428	2.28012	-0.92664
C	-1.38576	0.93844	-0.75431
N	-2.20309	0.50129	-1.72805
N	-2.73171	1.50476	-2.50360
C	-0.51988	5.66547	0.24330
C	-0.97597	4.92909	1.47238
C	-1.06163	3.55800	1.22569
C	-1.44672	2.67304	2.22466
C	-1.75670	3.18322	3.48419
C	-1.67316	4.55190	3.73289
C	-1.28056	5.43420	2.72890
C	-2.51514	-0.86499	-1.99430
C	-3.83340	-1.33724	-1.74337
C	-4.07615	-2.73700	-1.85821
C	-3.01970	-3.59710	-2.23944
C	-1.77285	-3.11015	-2.52892
C	-1.52471	-1.72859	-2.41198
C	-4.89999	-0.48865	-1.35972
C	-6.14403	-1.00967	-1.10199
C	-6.38398	-2.39664	-1.20580
C	-5.36841	-3.23975	-1.57622
H	0.42597	2.94885	-0.22917
H	-0.05417	4.76574	-1.72633
H	-1.07363	6.59111	0.04357
H	0.54692	5.92793	0.30382
H	-1.52021	1.60036	2.03864
H	-2.06916	2.50631	4.27681
H	-1.92243	4.93581	4.72030
H	-1.22450	6.50426	2.92461
H	-3.21673	-4.66579	-2.31513

H	-0.96607	-3.76502	-2.84770
Cl	0.07191	-1.15636	-2.81201
H	-4.73622	0.58442	-1.29106
H	-6.95738	-0.34375	-0.81994
H	-7.37646	-2.79109	-0.99869
H	-5.53871	-4.31215	-1.66565
Au	-0.17715	-0.36411	0.50515
C	0.93952	-1.81876	1.43384
C	0.19026	-2.83099	2.05875
C	2.32100	-1.90672	1.36266
C	0.85128	-3.91925	2.62495
C	2.97215	-3.00460	1.93228
H	2.90256	-1.13261	0.86219
C	2.23907	-4.00307	2.56249
H	0.28698	-4.71291	3.11395
H	4.05897	-3.08194	1.87819
H	2.74846	-4.85619	3.00665
C	-1.67661	-1.44602	1.38009
C	-3.00664	-1.06687	1.35927
C	-1.25325	-2.61157	2.04239
C	-3.95894	-1.88961	1.96742
H	-3.32666	-0.14296	0.88119
C	-2.21935	-3.42090	2.63797
C	-3.56454	-3.06609	2.59179
H	-5.00905	-1.60284	1.93724
H	-1.91937	-4.33161	3.15586
H	-4.30734	-3.70898	3.05998
O	1.63393	0.73672	-0.22439
C	3.73188	1.58908	0.44371
C	2.35692	1.36298	0.60567
C	5.79860	1.12231	-0.85690
C	4.43003	1.01094	-0.60715
C	6.42650	0.54618	-1.97481
H	1.88592	1.75423	1.52898
H	3.83205	0.41840	-1.30826
H	4.24981	2.18585	1.19369

C	7.66642	1.17471	-2.54251
H	5.74584	0.11817	-2.71900
H	6.40210	1.72779	-0.17542
H	8.23568	0.48531	-3.17766
H	7.39015	2.03878	-3.16232
H	8.32767	1.54008	-1.74666
C	7.08064	-1.32137	-1.41730
C	8.06175	-1.02537	-0.46933
C	7.46367	-0.90044	0.80849
C	6.13891	-1.23342	0.70552
C	5.88018	-1.79964	-0.64578
H	7.32343	-1.70555	-2.40767
H	9.10638	-0.82193	-0.69266
H	7.96663	-0.55508	1.70665
H	5.40454	-1.19702	1.50772
H	5.95248	-2.90039	-0.57483
H	4.89744	-1.58243	-1.07657
O	-2.08045	4.84682	-1.33864
C	-2.40258	3.99807	-2.40591
H	-1.77174	4.21077	-3.28880
H	-3.44476	4.18412	-2.68493

M06/lanl2dz-6-31G(d) Energy = -2646.112786

M06/lanl2dz-6-31G(d) Free Energy = -2645.474898

M06/def2-TZVP Derived free energy = -2646.584127

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.614664

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.638867

Number of Imaginary Frequencies = 1(-373.64)

M06/lanl2dz-6-31G(d) Geometry

C	1.49858	-1.51672	-1.36933
C	2.91316	-2.18922	-1.25402
C	1.05233	-2.49901	0.87494
N	0.80515	-1.54142	-0.07566
C	-0.22673	-0.77289	0.34059
N	-0.55001	-1.31993	1.52487

N	0.24314	-2.38747	1.88372
C	2.94664	-3.31720	-2.30738
C	1.57703	-3.34010	-2.91782
C	0.77114	-2.32590	-2.40700
C	-0.53479	-2.14389	-2.85310
C	-1.03281	-3.00923	-3.82046
C	-0.23153	-4.03233	-4.33182
C	1.07610	-4.20193	-3.88912
C	-1.60029	-0.89491	2.39158
C	-2.74466	-1.72683	2.53730
C	-3.82372	-1.24650	3.33398
C	-3.71070	0.01269	3.97006
C	-2.58503	0.78092	3.83877
C	-1.51941	0.31722	3.04213
C	-2.87000	-2.98818	1.90574
C	-4.01786	-3.72757	2.05095
C	-5.09120	-3.24983	2.83296
C	-4.99083	-2.03592	3.46271
H	1.59400	-0.45850	-1.64327
H	3.68096	-1.43241	-1.45689
H	3.22679	-4.27089	-1.83608
H	3.72165	-3.11836	-3.06036
H	-1.15959	-1.34018	-2.45805
H	-2.05026	-2.88457	-4.18550
H	-0.63404	-4.70259	-5.08901
H	1.69788	-4.99786	-4.29730
H	-4.54263	0.36741	4.57730
H	-2.49209	1.74440	4.33312
Cl	-0.10654	1.32050	2.89997
H	-2.04462	-3.37853	1.31371
H	-4.09841	-4.69742	1.56359
H	-5.99265	-3.84953	2.93775
H	-5.80916	-1.65682	4.07390
Au	-0.96346	1.10009	-0.50589
C	-1.68730	2.89931	-1.17821
C	-3.04248	2.89772	-1.55145

C	-0.94141	4.06514	-1.22304
C	-3.62303	4.07796	-2.00929
C	-1.53572	5.24472	-1.68197
H	0.09322	4.08284	-0.88304
C	-2.86713	5.24481	-2.08017
H	-4.67163	4.09746	-2.30542
H	-0.95388	6.16412	-1.71899
H	-3.32649	6.16401	-2.43870
C	-2.90870	0.58461	-0.85705
C	-3.40686	-0.68357	-0.62285
C	-3.71453	1.61385	-1.37395
C	-4.75443	-0.94564	-0.88323
H	-2.77452	-1.47760	-0.23212
C	-5.05270	1.32749	-1.64040
C	-5.56899	0.05834	-1.39189
H	-5.15418	-1.93878	-0.68323
H	-5.70350	2.10428	-2.04086
H	-6.61803	-0.14473	-1.59893
O	1.19406	1.68063	-0.27409
C	3.32448	1.82386	-1.26493
C	1.94122	2.07908	-1.20929
C	5.25468	0.56994	-0.31425
C	3.92999	1.01325	-0.31718
C	5.72176	-0.40864	0.57831
H	1.49113	2.64652	-2.04536
H	3.27251	0.62559	0.47070
H	3.89524	2.23335	-2.09746
C	6.81800	-1.34337	0.15960
H	4.95106	-0.86684	1.20739
H	5.92814	0.93535	-1.09425
H	7.57114	-0.83282	-0.45403
H	7.32311	-1.81138	1.01323
H	6.38534	-2.15405	-0.44534
C	6.54901	0.58083	2.20001
C	7.64703	1.21337	1.61981
C	7.25208	2.47626	1.10951

C	5.95017	2.70445	1.46507
C	5.50687	1.64437	2.40925
H	6.64813	-0.27587	2.86570
H	8.63141	0.76873	1.49358
H	7.87297	3.13050	0.50494
H	5.35405	3.57330	1.20000
H	5.63240	2.02966	3.43728
H	4.46037	1.33521	2.32059
O	3.22740	-2.63558	0.05419
C	2.20997	-3.40345	0.65904
H	1.92523	-4.26869	0.03483
H	2.58931	-3.78295	1.61241

M06/lanl2dz-6-31G(d) Energy = -2646.111884

M06/lanl2dz-6-31G(d) Free Energy = -2645.475998

M06/def2-TZVP Derived free energy = -2646.588261

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618965

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.644014

Number of Imaginary Frequencies = 1 (-385.60)

M06/lanl2dz-6-31G(d) Geometry

C	0.27008	2.88720	0.18054
C	0.64066	4.30032	-0.32419
C	-1.41244	2.99348	-1.66811
N	-0.74308	2.29101	-0.69396
C	-1.19387	1.01445	-0.69580
N	-2.11534	1.01921	-1.67295
N	-2.26489	2.23851	-2.29149
C	1.14305	5.01452	0.92643
C	0.37344	4.35016	2.03483
C	-0.15752	3.13291	1.60548
C	-0.91034	2.33739	2.45868
C	-1.13244	2.78344	3.76059
C	-0.60117	3.99653	4.19362
C	0.15793	4.78800	3.33378
C	-2.91025	-0.08825	-2.09258

C	-4.30732	-0.06818	-1.82603
C	-5.07296	-1.21770	-2.17694
C	-4.43040	-2.31786	-2.79263
C	-3.08857	-2.30005	-3.06491
C	-2.32443	-1.16944	-2.71428
C	-4.95956	1.02496	-1.20547
C	-6.30589	0.97173	-0.94155
C	-7.06534	-0.16727	-1.28451
C	-6.45880	-1.23664	-1.89157
H	1.15096	2.23128	0.12912
H	1.37642	4.26428	-1.14695
H	0.96712	6.09400	0.84296
H	2.22728	4.86489	1.04116
H	-1.33455	1.38859	2.12710
H	-1.72929	2.17869	4.44045
H	-0.78729	4.33293	5.21182
H	0.56162	5.74133	3.67263
H	-5.02592	-3.19118	-3.05631
H	-2.59540	-3.13861	-3.54971
Cl	-0.62628	-1.17988	-3.09219
H	-4.39109	1.91767	-0.95195
H	-6.79498	1.82119	-0.46846
H	-8.13160	-0.19040	-1.07017
H	-7.03334	-2.12106	-2.16514
Au	-0.40776	-0.73141	0.34967
C	0.28461	-2.47002	1.20259
C	-0.64542	-3.14941	2.00926
C	1.54338	-3.00580	0.98043
C	-0.27463	-4.34414	2.62207
C	1.90364	-4.20726	1.59713
H	2.25337	-2.51616	0.31452
C	1.00016	-4.86595	2.42192
H	-0.98184	-4.88049	3.25428
H	2.89210	-4.63054	1.42387
H	1.28262	-5.80001	2.90381
C	-2.09120	-1.32349	1.34852

C	-3.27421	-0.60710	1.33398
C	-1.95528	-2.50991	2.08995
C	-4.37184	-1.08889	2.05211
H	-3.37117	0.32090	0.77440
C	-3.05972	-2.96825	2.80701
C	-4.26065	-2.26473	2.78328
H	-5.30795	-0.53312	2.03166
H	-2.98559	-3.88618	3.38953
H	-5.11455	-2.63900	3.34461
O	1.55584	-0.12458	-0.56612
C	3.86167	0.30286	-0.39570
C	2.60451	-0.04154	0.12532
C	6.30249	0.63262	0.11386
C	4.96832	0.34318	0.43743
C	6.79434	0.91532	-1.16670
H	2.55297	-0.24939	1.21359
H	4.77299	0.13878	1.49537
H	3.91867	0.52630	-1.46183
C	8.00482	1.78619	-1.33034
H	6.05142	1.01366	-1.96396
H	7.01069	0.67808	0.94241
H	8.73896	1.60362	-0.53563
H	8.49760	1.64574	-2.30009
H	7.70701	2.84217	-1.26604
C	7.44917	-0.91428	-1.96053
C	8.55251	-1.19316	-1.15639
C	8.13385	-1.91802	-0.01361
C	6.79932	-2.20332	-0.13809
C	6.33888	-1.81462	-1.49431
H	7.53976	-0.58581	-2.99522
H	9.56148	-0.82631	-1.32812
H	8.76394	-2.17431	0.83284
H	6.18961	-2.74446	0.58047
H	6.35093	-2.71587	-2.13372
H	5.31810	-1.41925	-1.54712
C	-1.07934	4.42495	-1.91245

H	-0.38205	4.49908	-2.76765
H	-1.98080	4.99273	-2.16433
O	-0.52016	4.98389	-0.75575

Top, away, 1, exo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.113121

M06/lanl2dz-6-31G(d) Free Energy = -2645.475339

M06/def2-TZVP Derived free energy = -2646.586116

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617223

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642272

Number of Imaginary Frequencies = 1 (-380.54)

M06/lanl2dz-6-31G(d) Geometry

C	3.51244	-2.20244	-0.32826
C	3.94020	-3.68171	-0.35945
C	2.09535	-3.06951	1.57373
N	2.38462	-2.10103	0.63627
C	1.47294	-1.10940	0.75723
N	0.68875	-1.53040	1.75989
N	1.05683	-2.74513	2.28329
C	2.96653	-4.33706	-1.35913
C	2.71124	-3.20678	-2.31756
C	3.06503	-1.98238	-1.74135
C	3.00612	-0.79785	-2.46512
C	2.51232	-0.83815	-3.76695
C	2.12269	-2.05163	-4.33334
C	2.23713	-3.24524	-3.62221
C	-0.49404	-0.88231	2.22010
C	-0.39163	0.35547	2.91492
C	-1.59535	1.01621	3.30024
C	-2.83875	0.39702	3.02973
C	-2.90778	-0.80744	2.38152
C	-1.72460	-1.44644	1.95920
C	0.84765	0.96361	3.22526
C	0.89009	2.18698	3.84600

C	-0.30044	2.85158	4.20896
C	-1.51595	2.27028	3.95079
H	4.30562	-1.52828	0.02081
H	4.95099	-3.71329	-0.78473
H	2.03438	-4.65712	-0.86629
H	3.39776	-5.22858	-1.82977
H	3.36392	0.13902	-2.03714
H	2.45069	0.07994	-4.34827
H	1.74970	-2.07067	-5.35567
H	1.96852	-4.19233	-4.08838
H	-3.75060	0.89834	3.35664
H	-3.85869	-1.29638	2.18346
Cl	-1.87553	-2.93324	1.07794
H	1.77429	0.45812	2.96680
H	1.85419	2.64462	4.06115
H	-0.24969	3.81971	4.70228
H	-2.44211	2.76498	4.24205
Au	1.17947	0.72552	-0.34406
C	0.94435	2.48489	-1.37672
C	1.90096	3.47447	-1.08743
C	-0.04995	2.71639	-2.31386
C	1.82259	4.70808	-1.73014
C	-0.11607	3.95719	-2.95513
H	-0.77311	1.94106	-2.56623
C	0.81228	4.94792	-2.65734
H	2.55483	5.48745	-1.51959
H	-0.89426	4.14269	-3.69386
H	0.75683	5.91322	-3.15710
C	2.82068	1.74054	0.33099
C	3.75431	1.20648	1.20501
C	2.92852	3.06328	-0.13393
C	4.81455	2.00150	1.64874
H	3.67292	0.17910	1.56107
C	3.99268	3.84190	0.32251
C	4.92558	3.31553	1.21024
H	5.54876	1.58735	2.33747

H	4.09742	4.87071	-0.02078
H	5.74994	3.93603	1.55617
O	-0.65730	-0.24514	-1.10990
C	-2.98318	-0.36934	-1.37651
C	-1.80885	0.18803	-0.84590
C	-5.40230	-0.14841	-1.81851
C	-4.21100	0.23087	-1.18026
C	-6.57307	0.62989	-1.84260
H	-1.91868	1.07556	-0.18864
H	-4.24892	1.11088	-0.52563
H	-2.88264	-1.23771	-2.02907
C	-7.47585	0.53887	-3.04591
H	-6.47494	1.63712	-1.42992
H	-5.36596	-1.04147	-2.44919
H	-6.98538	1.00687	-3.90998
H	-7.68495	-0.50508	-3.31521
H	-8.43115	1.05307	-2.89395
C	-7.82859	-0.13915	-0.42910
C	-7.32080	0.44177	0.73600
C	-6.26886	-0.35578	1.23403
C	-6.17701	-1.49693	0.47469
C	-7.36362	-1.57284	-0.42019
H	-8.79253	0.14757	-0.84638
H	-7.61386	1.41193	1.12934
H	-5.61105	-0.07597	2.05244
H	-5.44354	-2.29215	0.59140
H	-7.20440	-2.04932	-1.39219
H	-8.14158	-2.16355	0.09772
C	2.87120	-4.34051	1.65100
H	3.14380	-4.55506	2.69037
H	2.23237	-5.17212	1.30616
O	4.06197	-4.25818	0.91591

M06/lanl2dz-6-31G(d) Energy = -2646.117087

M06/lanl2dz-6-31G(d) Free Energy = -2645.476048

M06/def2-TZVP Derived free energy = -2646.585037

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.615570

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.640144

Number of Imaginary Frequencies = 1 (-390.86)

M06/lanl2dz-6-31G(d) Geometry

C	-0.83448	-0.16838	3.18439
C	-2.36616	-0.17301	3.45698
C	-1.15364	2.03793	2.17760
N	-0.56552	0.79780	2.10094
C	0.29500	0.78316	1.05816
N	0.20057	2.04122	0.58391
N	-0.70304	2.83529	1.25612
C	-2.89487	-1.37884	2.67989
C	-1.71030	-2.29536	2.60623
C	-0.53182	-1.59634	2.86368
C	0.71113	-2.21792	2.80539
C	0.76221	-3.56542	2.45551
C	-0.41507	-4.26724	2.19406
C	-1.65812	-3.64296	2.27753
C	1.03434	2.61084	-0.42402
C	2.20611	3.30249	-0.01390
C	3.09933	3.76818	-1.02092
C	2.77635	3.56017	-2.38285
C	1.61408	2.93724	-2.75462
C	0.73671	2.46624	-1.75899
C	2.52607	3.52936	1.34636
C	3.68781	4.17676	1.68760
C	4.58314	4.62449	0.69216
C	4.29142	4.42489	-0.63293
H	-0.27160	0.20183	4.05393
H	-2.50191	-0.31719	4.54241
H	-3.15914	-1.03483	1.66577
H	-3.78937	-1.82072	3.13494
H	1.62667	-1.66571	3.02530
H	1.72338	-4.07090	2.38730
H	-0.36020	-5.32144	1.92880

H	-2.57069	-4.20299	2.07733
H	3.46770	3.91819	-3.14477
H	1.35433	2.79498	-3.80036
Cl	-0.75151	1.71271	-2.25768
H	1.83783	3.19830	2.12308
H	3.91855	4.35375	2.73636
H	5.49885	5.13599	0.98057
H	4.97051	4.77323	-1.41033
Au	1.05006	-0.97405	-0.02345
C	1.67038	-2.56314	-1.15735
C	3.04366	-2.58911	-1.45368
C	0.81764	-3.55036	-1.62118
C	3.54232	-3.61131	-2.25810
C	1.33228	-4.57143	-2.42604
H	-0.23915	-3.54386	-1.35486
C	2.68487	-4.59361	-2.74689
H	4.60351	-3.65122	-2.50332
H	0.66986	-5.35058	-2.79974
H	3.08018	-5.38845	-3.37658
C	3.06627	-0.65477	-0.00447
C	3.66689	0.34214	0.74116
C	3.81499	-1.52718	-0.81433
C	5.05000	0.52097	0.64939
H	3.08132	0.99277	1.38704
C	5.19333	-1.33359	-0.89036
C	5.80390	-0.30932	-0.17070
H	5.52648	1.31804	1.21866
H	5.79968	-1.99279	-1.51131
H	6.88058	-0.16876	-0.24456
O	-1.14586	-1.44232	-0.16994
C	-3.19887	-1.12358	-1.27500
C	-1.79826	-1.22494	-1.22223
C	-5.13934	-0.25974	-2.58106
C	-3.79608	-0.61874	-2.41654
C	-6.12608	-0.42404	-1.60116
H	-1.25545	-1.08473	-2.17806

H	-3.13651	-0.44283	-3.27234
H	-3.76619	-1.34068	-0.36930
C	-7.57118	-0.41955	-2.01083
H	-5.89275	-1.09715	-0.77394
H	-5.43521	0.17217	-3.53816
H	-8.25534	-0.31983	-1.16118
H	-7.78912	0.38045	-2.73003
H	-7.80568	-1.37168	-2.50687
C	-6.06835	1.29702	-0.41964
C	-4.86454	1.20829	0.27703
C	-3.84420	1.88506	-0.44328
C	-4.39789	2.48303	-1.53906
C	-5.88063	2.36107	-1.47075
H	-7.02953	1.12657	0.06281
H	-4.71250	0.68528	1.21958
H	-2.78656	1.88001	-0.17931
H	-3.86787	3.05970	-2.29189
H	-6.29148	3.30479	-1.06855
H	-6.38189	2.19535	-2.43039
O	-3.04160	1.00186	3.04666
C	-2.27847	2.18584	3.14148
H	-1.91632	2.35344	4.17107
H	-2.91997	3.02680	2.86082

M06/lanl2dz-6-31G(d) Energy = -2646.117087

M06/lanl2dz-6-31G(d) Free Energy = -2645.476035

M06/def2-TZVP Derived free energy = -2646.585023

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.615556

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.640130

Number of Imaginary Frequencies = 1 (-390.84)

M06/lanl2dz-6-31G(d) Geometry

C	-0.83437	-0.16941	3.18416
C	-2.36607	-0.17446	3.45663
C	-1.15393	2.03713	2.17803
N	-0.56558	0.79712	2.10097

C	0.29476	0.78290	1.05805
N	0.20002	2.04107	0.58411
N	-0.70364	2.83479	1.25668
C	-2.89441	-1.38020	2.67917
C	-1.70964	-2.29646	2.60552
C	-0.53133	-1.59722	2.86317
C	0.71177	-2.21848	2.80484
C	0.76319	-3.56590	2.45472
C	-0.41391	-4.26795	2.19308
C	-1.65711	-3.64400	2.27659
C	1.03355	2.61112	-0.42377
C	2.20514	3.30305	-0.01360
C	3.09813	3.76922	-1.02060
C	2.77509	3.56139	-2.38255
C	1.61299	2.93817	-2.75435
C	0.73585	2.46670	-1.75874
C	2.52516	3.52973	1.34667
C	3.68675	4.17738	1.68794
C	4.58185	4.62558	0.69252
C	4.29007	4.42618	-0.63258
H	-0.27165	0.20075	4.05383
H	-2.50188	-0.31896	4.54201
H	-3.15843	-1.03604	1.66504
H	-3.78895	-1.82235	3.13388
H	1.62717	-1.66609	3.02490
H	1.72448	-4.07114	2.38645
H	-0.35877	-5.32209	1.92763
H	-2.56953	-4.20421	2.07621
H	3.46627	3.91978	-3.14445
H	1.35319	2.79604	-3.80009
Cl	-0.75217	1.71279	-2.25743
H	1.83708	3.19830	2.12338
H	3.91753	4.35422	2.73672
H	5.49744	5.13729	0.98095
H	4.96899	4.77488	-1.40998
Au	1.05026	-0.97393	-0.02382

C	1.67123	-2.56276	-1.15775
C	3.04462	-2.58847	-1.45359
C	0.81883	-3.55007	-1.62199
C	3.54375	-3.61050	-2.25793
C	1.33392	-4.57097	-2.42678
H	-0.23807	-3.54376	-1.35609
C	2.68664	-4.59290	-2.74714
H	4.60503	-3.65021	-2.50278
H	0.67177	-5.35018	-2.80081
H	3.08231	-5.38760	-3.37677
C	3.06640	-0.65420	-0.00427
C	3.66658	0.34288	0.74148
C	3.81555	-1.52644	-0.81392
C	5.04967	0.52205	0.65007
H	3.08071	0.99338	1.38722
C	5.19386	-1.33254	-0.88956
C	5.80399	-0.30810	-0.16977
H	5.52579	1.31930	1.21940
H	5.80052	-1.99159	-1.51036
H	6.88066	-0.16728	-0.24337
O	-1.14554	-1.44276	-0.17065
C	-3.19878	-1.12351	-1.27514
C	-1.79818	-1.22508	-1.22273
C	-5.13966	-0.25995	-2.58076
C	-3.79631	-0.61876	-2.41656
C	-6.12610	-0.42451	-1.60061
H	-1.25561	-1.08488	-2.17870
H	-3.13699	-0.44292	-3.27256
H	-3.76589	-1.34032	-0.36922
C	-7.57134	-0.42030	-2.00980
H	-5.89234	-1.09762	-0.77351
H	-5.43585	0.17195	-3.53777
H	-8.25521	-0.32197	-1.15975
H	-7.78998	0.38047	-2.72793
H	-7.80553	-1.37194	-2.50692
C	-6.06859	1.29660	-0.41916

C	-4.86477	1.20795	0.27749
C	-3.84452	1.88499	-0.44272
C	-4.39830	2.48303	-1.53840
C	-5.88101	2.36075	-1.47018
H	-7.02977	1.12600	0.06325
H	-4.71266	0.68482	1.21996
H	-2.78689	1.88018	-0.17866
H	-3.86841	3.05994	-2.29114
H	-6.29206	3.30436	-1.06790
H	-6.38220	2.19505	-2.42985
C	-2.27877	2.18447	3.14198
H	-1.91669	2.35163	4.17167
H	-2.92039	3.02547	2.86170
O	-3.04171	1.00040	3.04658

Bottom, away, 1, exo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.114604

M06/lanl2dz-6-31G(d) Free Energy = -2645.475219

M06/def2-TZVP Derived free energy = -2646.585497

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616502

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641659

Number of Imaginary Frequencies = 1 (-371.45)

M06/lanl2dz-6-31G(d) Geometry

C	3.87149	-1.41032	-0.89913
C	4.58468	-2.72645	-1.25880
C	2.95075	-2.88696	0.93445
N	2.89404	-1.73803	0.17399
C	1.79938	-1.03757	0.54903
N	1.26254	-1.79342	1.51615
N	1.95996	-2.94817	1.77202
C	3.62684	-3.41476	-2.25262
C	3.01462	-2.23019	-2.94778
C	3.19501	-1.06692	-2.19195
C	2.80825	0.17736	-2.67496

C	2.15829	0.24009	-3.90588
C	1.93850	-0.92249	-4.64378
C	2.38193	-2.16086	-4.18197
C	-0.00048	-1.57308	2.14121
C	-0.14034	-0.54036	3.10712
C	-1.43062	-0.31897	3.67319
C	-2.50699	-1.15263	3.28598
C	-2.34147	-2.15218	2.36296
C	-1.07608	-2.35400	1.77460
C	0.93725	0.27886	3.51767
C	0.73801	1.29096	4.42246
C	-0.53962	1.51947	4.97663
C	-1.59755	0.72484	4.61447
H	4.55107	-0.64209	-0.50887
H	5.50451	-2.45643	-1.79255
H	2.85954	-4.01049	-1.73248
H	4.15527	-4.09894	-2.92705
H	3.03216	1.08899	-2.11981
H	1.83893	1.20359	-4.29869
H	1.43978	-0.85786	-5.60916
H	2.24392	-3.05634	-4.78643
H	-3.48412	-0.99004	3.74130
H	-3.16812	-2.79239	2.06291
Cl	-0.91622	-3.57461	0.55298
H	1.92869	0.10588	3.10645
H	1.57703	1.91925	4.71603
H	-0.67946	2.32113	5.69854
H	-2.58521	0.88235	5.04729
Au	0.98150	0.80627	-0.21089
C	0.25644	2.58180	-0.94688
C	0.96234	3.72644	-0.53742
C	-0.81528	2.68696	-1.81951
C	0.55041	4.97923	-0.98776
C	-1.21578	3.94846	-2.26916
H	-1.33741	1.79683	-2.17004
C	-0.53951	5.08739	-1.84681

H	1.08352	5.87878	-0.68059
H	-2.05375	4.03720	-2.95926
H	-0.85399	6.06841	-2.19807
C	2.36053	2.09188	0.58255
C	3.44663	1.69336	1.34563
C	2.11624	3.45202	0.31652
C	4.30862	2.65884	1.87277
H	3.64032	0.63971	1.54838
C	2.98769	4.40003	0.85223
C	4.07369	4.00641	1.62745
H	5.16250	2.34994	2.47308
H	2.81887	5.45937	0.66031
H	4.74483	4.75836	2.03778
O	-0.66534	-0.42271	-1.05875
C	-2.94890	-1.00024	-1.00937
C	-1.81924	-0.29043	-0.57383
C	-5.37123	-1.45599	-0.65558
C	-4.16514	-0.79383	-0.38963
C	-6.51439	-1.31782	0.15402
H	-1.97799	0.43422	0.25219
H	-4.18526	-0.06119	0.42749
H	-2.83124	-1.73096	-1.81012
C	-7.51089	-2.44688	0.19977
H	-6.34874	-0.82666	1.11680
H	-5.39310	-2.17624	-1.47755
H	-7.78096	-2.78642	-0.80885
H	-7.07120	-3.30597	0.72417
H	-8.43064	-2.17538	0.72940
C	-7.66880	0.13371	-0.67026
C	-6.99063	1.31109	-0.33656
C	-6.00635	1.58068	-1.31131
C	-6.12922	0.66278	-2.32555
C	-7.38054	-0.11448	-2.12953
H	-8.63009	-0.12131	-0.22617
H	-7.12742	1.86885	0.58676
H	-5.24569	2.35347	-1.24262

H	-5.49399	0.59374	-3.20430
H	-8.18197	0.37666	-2.71125
H	-7.35128	-1.15851	-2.45722
C	3.99242	-3.92824	0.69936
H	4.45974	-4.22007	1.64653
H	3.50820	-4.82975	0.28607
O	5.01263	-3.45626	-0.13875

M06/lanl2dz-6-31G(d) Energy = -2646.114604

M06/lanl2dz-6-31G(d) Free Energy = -2645.475220

M06/def2-TZVP Derived free energy = -2646.585498

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616503

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641660

Number of Imaginary Frequencies = 1 (-371.46)

M06/lanl2dz-6-31G(d) Geometry

C	3.87147	-1.41034	-0.89915
C	4.58462	-2.72648	-1.25885
C	2.95073	-2.88700	0.93441
N	2.89402	-1.73806	0.17397
C	1.79937	-1.03759	0.54902
N	1.26253	-1.79345	1.51613
N	1.95994	-2.94821	1.77198
C	3.62673	-3.41476	-2.25266
C	3.01455	-2.23016	-2.94780
C	3.19498	-1.06690	-2.19196
C	2.80826	0.17740	-2.67495
C	2.15828	0.24016	-3.90586
C	1.93845	-0.92241	-4.64377
C	2.38184	-2.16080	-4.18198
C	-0.00049	-1.57310	2.14120
C	-0.14033	-0.54038	3.10712
C	-1.43061	-0.31899	3.67319
C	-2.50699	-1.15264	3.28599
C	-2.34148	-2.15218	2.36295
C	-1.07610	-2.35401	1.77459

C	0.93727	0.27882	3.51768
C	0.73804	1.29091	4.42248
C	-0.53958	1.51943	4.97666
C	-1.59752	0.72481	4.61449
H	4.55108	-0.64214	-0.50888
H	5.50445	-2.45648	-1.79262
H	2.85942	-4.01045	-1.73250
H	4.15513	-4.09896	-2.92710
H	3.03220	1.08901	-2.11979
H	1.83895	1.20368	-4.29866
H	1.43971	-0.85775	-5.60914
H	2.24378	-3.05626	-4.78644
H	-3.48411	-0.99005	3.74131
H	-3.16814	-2.79239	2.06291
Cl	-0.91625	-3.57460	0.55295
H	1.92870	0.10583	3.10644
H	1.57707	1.91918	4.71606
H	-0.67941	2.32107	5.69858
H	-2.58518	0.88232	5.04732
Au	0.98151	0.80627	-0.21089
C	0.25646	2.58181	-0.94685
C	0.96238	3.72644	-0.53738
C	-0.81526	2.68699	-1.81948
C	0.55046	4.97924	-0.98769
C	-1.21575	3.94851	-2.26910
H	-1.33740	1.79688	-2.17002
C	-0.53946	5.08743	-1.84673
H	1.08358	5.87879	-0.68051
H	-2.05372	4.03727	-2.95920
H	-0.85394	6.06846	-2.19798
C	2.36056	2.09185	0.58256
C	3.44666	1.69331	1.34563
C	2.11628	3.45200	0.31655
C	4.30867	2.65877	1.87276
H	3.64035	0.63965	1.54835
C	2.98775	4.39999	0.85226

C	4.07376	4.00635	1.62747
H	5.16256	2.34986	2.47306
H	2.81893	5.45933	0.66036
H	4.74491	4.75829	2.03779
O	-0.66534	-0.42269	-1.05876
C	-2.94890	-1.00021	-1.00939
C	-1.81924	-0.29041	-0.57383
C	-5.37124	-1.45596	-0.65558
C	-4.16514	-0.79380	-0.38963
C	-6.51439	-1.31779	0.15401
H	-1.97799	0.43422	0.25220
H	-4.18525	-0.06119	0.42751
H	-2.83126	-1.73090	-1.81016
C	-7.51089	-2.44685	0.19976
H	-6.34873	-0.82664	1.11679
H	-5.39311	-2.17620	-1.47757
H	-7.78097	-2.78639	-0.80886
H	-7.07121	-3.30593	0.72417
H	-8.43064	-2.17535	0.72939
C	-7.66880	0.13375	-0.67026
C	-6.99063	1.31113	-0.33654
C	-6.00634	1.58072	-1.31128
C	-6.12920	0.66283	-2.32553
C	-7.38053	-0.11443	-2.12953
H	-8.63010	-0.12128	-0.22618
H	-7.12743	1.86887	0.58678
H	-5.24568	2.35350	-1.24257
H	-5.49396	0.59379	-3.20427
H	-8.18196	0.37672	-2.71125
H	-7.35128	-1.15845	-2.45723
O	5.01259	-3.45632	-0.13882
C	3.99238	-3.92828	0.69931
H	4.45972	-4.22011	1.64647
H	3.50815	-4.82979	0.28603

M06/lanl2dz-6-31G(d) Energy = -2646.116403

M06/lanl2dz-6-31G(d) Free Energy = -2645.479329
M06/def2-TZVP Derived free energy = -2646.591439
M06/def2-TZVP Derived free energy in solution (toluene) = -2646.622968
M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.649015
Number of Imaginary Frequencies = 1 (-368.00)

M06/lanl2dz-6-31G(d) Geometry

C	3.87623	-1.06974	-0.50339
C	5.24229	-1.70163	-0.16347
C	3.15907	-2.14558	1.64201
N	2.94603	-1.26212	0.60954
C	1.73037	-0.69752	0.77123
N	1.27154	-1.27134	1.89012
N	2.14270	-2.17644	2.45097
C	5.85389	-1.97845	-1.53316
C	4.64803	-2.25844	-2.38958
C	3.49042	-1.76966	-1.78172
C	2.24058	-1.94375	-2.35915
C	2.16824	-2.60774	-3.58319
C	3.32204	-3.08100	-4.20447
C	4.57133	-2.91323	-3.60971
C	-0.05220	-1.13957	2.40124
C	-0.39081	-0.01810	3.20295
C	-1.73075	0.08176	3.68209
C	-2.65790	-0.93851	3.35934
C	-2.30468	-2.00824	2.57851
C	-0.98723	-2.10189	2.08465
C	0.53530	1.00003	3.53207
C	0.14347	2.07534	4.28995
C	-1.18208	2.17852	4.76425
C	-2.09590	1.19905	4.46947
H	3.98237	0.01772	-0.65036
H	5.85578	-1.05015	0.48391
H	6.56235	-2.81356	-1.47313
H	6.40937	-1.09645	-1.88590
H	1.32521	-1.60413	-1.87022

H	1.19880	-2.76307	-4.05265
H	3.24539	-3.59985	-5.15820
H	5.46862	-3.30530	-4.08680
H	-3.67380	-0.86095	3.74710
H	-3.01874	-2.78698	2.32050
Cl	-0.57522	-3.42821	1.04791
H	1.56274	0.92670	3.18026
H	0.86421	2.85422	4.53040
H	-1.47306	3.03533	5.36810
H	-3.11924	1.26442	4.83829
Au	0.78284	0.87006	-0.36345
C	-0.03794	2.41139	-1.44462
C	0.60952	3.64967	-1.29540
C	-1.12561	2.28065	-2.29349
C	0.13425	4.75693	-1.99449
C	-1.59277	3.39837	-2.99123
H	-1.60698	1.31388	-2.43855
C	-0.96706	4.62965	-2.83666
H	0.62287	5.72569	-1.89148
H	-2.44237	3.30011	-3.66569
H	-1.33056	5.49802	-3.38288
C	2.06273	2.37253	0.16645
C	3.12023	2.21431	1.04814
C	1.76123	3.62633	-0.39615
C	3.90993	3.31911	1.37895
H	3.34285	1.24503	1.49537
C	2.56280	4.71480	-0.05532
C	3.62973	4.56173	0.82506
H	4.74063	3.20047	2.07225
H	2.35234	5.69649	-0.47855
H	4.24383	5.42258	1.08206
O	-0.75560	-0.61311	-0.96193
C	-2.98517	-1.35808	-0.83248
C	-1.92603	-0.50005	-0.50929
C	-5.40768	-1.85815	-0.54324
C	-4.24296	-1.11645	-0.31222

C	-6.61925	-1.61973	0.13435
H	-2.15476	0.33485	0.18526
H	-4.33692	-0.26524	0.37463
H	-2.79281	-2.19920	-1.49950
C	-7.60191	-2.75203	0.28171
H	-6.54438	-0.97348	1.01283
H	-5.35178	-2.70026	-1.23815
H	-7.77599	-3.26108	-0.67551
H	-7.20085	-3.49968	0.97918
H	-8.56851	-2.42127	0.67696
C	-7.71189	-0.35698	-1.01593
C	-7.09092	0.88058	-0.81204
C	-6.02393	1.02854	-1.72407
C	-6.03459	-0.03864	-2.58870
C	-7.28287	-0.81831	-2.38585
H	-8.70690	-0.56974	-0.62727
H	-7.32512	1.57031	-0.00476
H	-5.28791	1.82789	-1.71098
H	-5.31430	-0.22484	-3.38072
H	-8.03532	-0.45202	-3.10804
H	-7.20139	-1.89897	-2.53964
C	4.46484	-2.85940	1.73502
H	5.12650	-2.31810	2.43714
H	4.32262	-3.87330	2.12207
O	5.04825	-2.95599	0.46515

M06/lanl2dz-6-31G(d) Energy = -2646.114604

M06/lanl2dz-6-31G(d) Free Energy = -2645.475219

M06/def2-TZVP Derived free energy = -2646.585497

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616502

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641659

Number of Imaginary Frequencies = 1 (-371.46)

M06/lanl2dz-6-31G(d) Geometry

C	3.87148	-1.41033	-0.89914
C	4.58466	-2.72647	-1.25880

C	2.95078	-2.88693	0.93448
N	2.89405	-1.73802	0.17400
C	1.79939	-1.03755	0.54903
N	1.26257	-1.79339	1.51617
N	1.96000	-2.94813	1.77207
C	3.62678	-3.41481	-2.25258
C	3.01457	-2.23025	-2.94775
C	3.19497	-1.06696	-2.19196
C	2.80822	0.17731	-2.67500
C	2.15823	0.24001	-3.90591
C	1.93843	-0.92259	-4.64377
C	2.38185	-2.16095	-4.18194
C	-0.00045	-1.57304	2.14125
C	-0.14030	-0.54029	3.10714
C	-1.43058	-0.31889	3.67320
C	-2.50695	-1.15257	3.28603
C	-2.34144	-2.15214	2.36302
C	-1.07605	-2.35397	1.77466
C	0.93728	0.27894	3.51766
C	0.73805	1.29106	4.42243
C	-0.53958	1.51958	4.97660
C	-1.59751	0.72494	4.61447
H	4.55108	-0.64211	-0.50892
H	5.50448	-2.45648	-1.79258
H	2.85948	-4.01051	-1.73240
H	4.15519	-4.09902	-2.92700
H	3.03214	1.08895	-2.11987
H	1.83887	1.20350	-4.29874
H	1.43969	-0.85798	-5.60914
H	2.24382	-3.05644	-4.78637
H	-3.48408	-0.98998	3.74134
H	-3.16809	-2.79236	2.06299
Cl	-0.91619	-3.57460	0.55307
H	1.92872	0.10595	3.10644
H	1.57707	1.91937	4.71597
H	-0.67942	2.32126	5.69848

H	-2.58517	0.88245	5.04729
Au	0.98150	0.80627	-0.21091
C	0.25643	2.58178	-0.94692
C	0.96233	3.72643	-0.53749
C	-0.81530	2.68692	-1.81955
C	0.55039	4.97921	-0.98784
C	-1.21580	3.94842	-2.26922
H	-1.33742	1.79679	-2.17006
C	-0.53953	5.08736	-1.84689
H	1.08350	5.87878	-0.68070
H	-2.05377	4.03714	-2.95932
H	-0.85402	6.06837	-2.19817
C	2.36053	2.09189	0.58250
C	3.44663	1.69339	1.34559
C	2.11623	3.45203	0.31646
C	4.30862	2.65888	1.87271
H	3.64032	0.63974	1.54834
C	2.98768	4.40005	0.85216
C	4.07368	4.00644	1.62739
H	5.16250	2.34999	2.47303
H	2.81885	5.45939	0.66023
H	4.74482	4.75840	2.03770
O	-0.66534	-0.42273	-1.05873
C	-2.94890	-1.00027	-1.00931
C	-1.81924	-0.29044	-0.57380
C	-5.37123	-1.45602	-0.65551
C	-4.16514	-0.79384	-0.38958
C	-6.51439	-1.31783	0.15406
H	-1.97799	0.43423	0.25219
H	-4.18526	-0.06118	0.42751
H	-2.83124	-1.73102	-1.81004
C	-7.51089	-2.44688	0.19983
H	-6.34875	-0.82666	1.11684
H	-5.39309	-2.17629	-1.47747
H	-7.78098	-2.78643	-0.80879
H	-7.07121	-3.30597	0.72423

H	-8.43063	-2.17538	0.72947
C	-7.66879	0.13370	-0.67024
C	-6.99062	1.31108	-0.33657
C	-6.00635	1.58066	-1.31133
C	-6.12923	0.66274	-2.32556
C	-7.38054	-0.11453	-2.12951
H	-8.63008	-0.12131	-0.22615
H	-7.12739	1.86885	0.58674
H	-5.24570	2.35344	-1.24266
H	-5.49401	0.59369	-3.20432
H	-8.18199	0.37658	-2.71124
H	-7.35127	-1.15856	-2.45717
O	5.01264	-3.45626	-0.13874
C	3.99244	-3.92821	0.69941
H	4.45979	-4.22002	1.64658
H	3.50822	-4.82974	0.28616

Top, towards, 1, exo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.112886

M06/lanl2dz-6-31G(d) Free Energy = -2645.476071

M06/def2-TZVP Derived free energy = -2646.588627

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.619972

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.645966

Number of Imaginary Frequencies = 1 (-375.11)

M06/lanl2dz-6-31G(d) Geometry

C	1.07593	3.11115	-0.30776
C	1.38859	4.48294	-0.94077
C	1.31936	2.27714	-2.65229
N	1.22678	2.04755	-1.29839
C	1.20181	0.71001	-1.08890
N	1.27644	0.20831	-2.32758
N	1.35133	1.16125	-3.31549
C	0.61706	5.46666	-0.06346
C	-0.56871	4.65824	0.39177

C	-0.32473	3.29672	0.21236
C	-1.28150	2.34440	0.52239
C	-2.49752	2.77120	1.05224
C	-2.74223	4.12882	1.25269
C	-1.78137	5.08233	0.91680
C	1.10209	-1.16412	-2.67141
C	2.20736	-2.05160	-2.63364
C	1.96963	-3.42332	-2.94190
C	0.66126	-3.83966	-3.28410
C	-0.38782	-2.95768	-3.31727
C	-0.15953	-1.60596	-3.00031
C	3.51786	-1.63763	-2.29593
C	4.54265	-2.55011	-2.25726
C	4.31088	-3.90981	-2.55745
C	3.05163	-4.33414	-2.89586
H	1.78147	2.89849	0.51140
H	2.47355	4.68095	-0.99376
H	0.35181	6.36221	-0.63834
H	1.23698	5.78889	0.78644
H	-1.09584	1.28766	0.33120
H	-3.25903	2.03452	1.31183
H	-3.69590	4.45188	1.66646
H	-1.98660	6.14293	1.05553
H	0.49399	-4.88935	-3.52347
H	-1.39229	-3.27893	-3.58122
Cl	-1.50338	-0.50169	-3.00258
H	3.71102	-0.58962	-2.07257
H	5.54630	-2.22163	-1.99509
H	5.13608	-4.61759	-2.52160
H	2.86142	-5.38042	-3.13300
Au	1.23413	-0.40403	0.77261
C	1.34681	-1.35832	2.58838
C	2.45165	-0.99353	3.37796
C	0.42299	-2.28067	3.05110
C	2.59567	-1.54780	4.64747
C	0.57935	-2.83198	4.32617

H	-0.41505	-2.59466	2.43116
C	1.65749	-2.46081	5.12048
H	3.44509	-1.27585	5.27379
H	-0.14416	-3.55815	4.69320
H	1.77655	-2.89144	6.11291
C	3.02734	0.32841	1.43067
C	3.86053	1.13808	0.67446
C	3.38039	-0.06970	2.73247
C	5.06179	1.59323	1.22588
H	3.60118	1.41871	-0.34630
C	4.57967	0.40064	3.26620
C	5.41152	1.22984	2.51995
H	5.71999	2.22767	0.63486
H	4.87593	0.10753	4.27289
H	6.34537	1.58573	2.95067
O	-0.67736	-1.36633	0.17171
C	-2.99354	-1.73324	0.29491
C	-1.79228	-1.14364	0.71063
C	-5.44400	-1.95189	0.63212
C	-4.18602	-1.40412	0.91033
C	-6.59453	-1.65601	1.38559
H	-1.84767	-0.44840	1.57490
H	-4.14357	-0.66098	1.71748
H	-2.95803	-2.45246	-0.52472
C	-7.68952	-2.68571	1.47683
H	-6.41630	-1.10510	2.31282
H	-5.50898	-2.70922	-0.15341
H	-7.94757	-3.08930	0.48891
H	-7.34777	-3.52826	2.09296
H	-8.60190	-2.29229	1.93803
C	-7.59338	-0.18374	0.39260
C	-6.83170	0.95928	0.65469
C	-5.79712	1.06681	-0.30115
C	-5.96127	0.07676	-1.23841
C	-7.27700	-0.58004	-1.02736
H	-8.58621	-0.32245	0.81822

H	-6.95459	1.60430	1.52141
H	-4.98226	1.78603	-0.27759
H	-5.30353	-0.12175	-2.08027
H	-8.01509	-0.07934	-1.68044
H	-7.32356	-1.64723	-1.26617
O	0.82190	4.55579	-2.23536
C	1.41613	3.67774	-3.15386
H	2.47834	3.93660	-3.32082
H	0.89187	3.78067	-4.10909

M06/lanl2dz-6-31G(d) Energy = -2646.111661

M06/lanl2dz-6-31G(d) Free Energy = -2645.473139

M06/def2-TZVP Derived free energy = -2646.583813

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.614862

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.640289

Number of Imaginary Frequencies = 1 (-380.07)

M06/lanl2dz-6-31G(d) Geometry

C	3.46341	-1.65488	0.04781
C	4.58360	-2.55470	0.62425
C	2.34637	-2.21511	2.22666
N	2.39429	-1.50080	1.04897
C	1.34612	-0.64185	1.03107
N	0.72356	-0.89177	2.19413
N	1.33205	-1.86075	2.95419
C	5.24787	-3.15799	-0.60704
C	4.13104	-3.20426	-1.61200
C	3.09296	-2.34945	-1.23839
C	1.98510	-2.17816	-2.05695
C	1.90519	-2.90526	-3.24241
C	2.93078	-3.77593	-3.60536
C	4.05470	-3.92408	-2.79606
C	-0.46784	-0.26716	2.66958
C	-0.43273	1.10651	3.03823
C	-1.64309	1.71721	3.48117
C	-2.81607	0.93320	3.57995

C	-2.81679	-0.39570	3.24391
C	-1.63241	-0.99662	2.77256
C	0.74400	1.88983	2.98748
C	0.71408	3.22109	3.32017
C	-0.48693	3.83139	3.73976
C	-1.63726	3.08949	3.82589
H	3.85191	-0.64324	-0.15146
H	5.27170	-1.98897	1.27682
H	5.67655	-4.13769	-0.36319
H	6.06987	-2.51493	-0.95495
H	1.19176	-1.47765	-1.79534
H	1.03953	-2.78614	-3.89094
H	2.85669	-4.33960	-4.53331
H	4.86014	-4.59712	-3.08691
H	-3.73052	1.40180	3.94401
H	-3.71337	-1.00407	3.34176
Cl	-1.68893	-2.67368	2.32236
H	1.68325	1.43487	2.68375
H	1.62980	3.80701	3.26419
H	-0.49412	4.88654	4.00361
H	-2.56795	3.54344	4.16506
Au	0.75032	0.82727	-0.45173
C	0.25258	2.18691	-1.90214
C	1.21232	3.18027	-2.15192
C	-0.92559	2.13001	-2.62591
C	0.96813	4.12264	-3.14835
C	-1.15745	3.08055	-3.62415
H	-1.65918	1.35077	-2.42079
C	-0.21471	4.06967	-3.88072
H	1.69897	4.90279	-3.36007
H	-2.07879	3.04476	-4.20359
H	-0.39850	4.80782	-4.65916
C	2.39519	2.04683	-0.36750
C	3.43220	1.89269	0.53919
C	2.39110	3.10653	-1.29331
C	4.50241	2.79211	0.52402

H	3.42474	1.08732	1.27457
C	3.47030	3.98945	-1.29741
C	4.51947	3.83186	-0.39722
H	5.31650	2.67413	1.23694
H	3.48961	4.81707	-2.00592
H	5.35327	4.53086	-0.41259
O	-1.20037	-0.20376	-0.68661
C	-2.63101	-2.02185	-1.14312
C	-1.40489	-1.44728	-0.77654
C	-4.98393	-1.71445	-1.86939
C	-3.72202	-1.24415	-1.49260
C	-6.00700	-0.88416	-2.36418
H	-0.57695	-2.14458	-0.54898
H	-3.56706	-0.16023	-1.50319
H	-2.70351	-3.10906	-1.14282
C	-7.06491	-1.48284	-3.25280
H	-5.69390	0.12113	-2.65594
H	-5.16308	-2.79275	-1.82863
H	-7.46941	-2.41379	-2.83385
H	-7.89770	-0.79513	-3.43573
H	-6.62469	-1.72950	-4.22845
C	-7.14267	-0.34376	-0.76201
C	-6.37068	0.66683	-0.17900
C	-5.43800	0.09354	0.71263
C	-5.68647	-1.25470	0.79870
C	-6.97148	-1.55877	0.11579
H	-8.08414	-0.13200	-1.26699
H	-6.40489	1.71701	-0.45865
H	-4.61803	0.61801	1.19835
H	-5.10527	-1.97706	1.36774
H	-7.03645	-2.53678	-0.37094
H	-7.77650	-1.53020	0.87285
C	3.39989	-3.22157	2.53535
H	4.13373	-2.78922	3.24080
H	2.95715	-4.10309	3.01045
O	4.01748	-3.63050	1.34801

M06/lanl2dz-6-31G(d) Energy = -2646.112885
M06/lanl2dz-6-31G(d) Free Energy = -2645.476074
M06/def2-TZVP Derived free energy = -2646.588631
M06/def2-TZVP Derived free energy in solution (toluene) = -2646.619976
M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.645971
Number of Imaginary Frequencies = 1 (-375.04)

M06/lanl2dz-6-31G(d) Geometry

C	1.07522	3.11115	-0.30822
C	1.38772	4.48285	-0.94150
C	1.31844	2.27677	-2.65264
N	1.22605	2.04740	-1.29869
C	1.20133	0.70989	-1.08896
N	1.27593	0.20799	-2.32757
N	1.35054	1.16077	-3.31565
C	0.61628	5.46668	-0.06424
C	-0.56939	4.65828	0.39130
C	-0.32539	3.29674	0.21205
C	-1.28210	2.34444	0.52234
C	-2.49806	2.77128	1.05229
C	-2.74278	4.12892	1.25259
C	-1.78199	5.08241	0.91642
C	1.10193	-1.16454	-2.67115
C	2.20751	-2.05165	-2.63349
C	1.97018	-3.42349	-2.94151
C	0.66188	-3.84033	-3.28335
C	-0.38750	-2.95870	-3.31645
C	-0.15959	-1.60685	-2.99977
C	3.51794	-1.63718	-2.29613
C	4.54306	-2.54930	-2.25758
C	4.31169	-3.90912	-2.55751
C	3.05251	-4.33394	-2.89558
H	1.78087	2.89867	0.51090
H	2.47266	4.68091	-0.99471
H	0.35089	6.36211	-0.63924

H	1.23630	5.78910	0.78551
H	-1.09644	1.28768	0.33127
H	-3.25953	2.03464	1.31215
H	-3.69640	4.45202	1.66643
H	-1.98724	6.14302	1.05503
H	0.49490	-4.89011	-3.52252
H	-1.39192	-3.28033	-3.58014
Cl	-1.50379	-0.50301	-3.00205
H	3.71079	-0.58907	-2.07298
H	5.54665	-2.22044	-1.99569
H	5.13714	-4.61661	-2.52176
H	2.86260	-5.38032	-3.13252
Au	1.23418	-0.40386	0.77270
C	1.34733	-1.35790	2.58857
C	2.45224	-0.99285	3.37792
C	0.42371	-2.28032	3.05154
C	2.59656	-1.54696	4.64746
C	0.58037	-2.83147	4.32664
H	-0.41439	-2.59450	2.43177
C	1.65859	-2.46006	5.12072
H	3.44604	-1.27480	5.27362
H	-0.14298	-3.55770	4.69388
H	1.77789	-2.89056	6.11319
C	3.02735	0.32901	1.43039
C	3.86024	1.13877	0.67396
C	3.38070	-0.06891	2.73217
C	5.06149	1.59424	1.22513
H	3.60066	1.41925	-0.34678
C	4.57998	0.40174	3.26565
C	5.41152	1.23104	2.51918
H	5.71946	2.22876	0.63394
H	4.87647	0.10879	4.27232
H	6.34537	1.58718	2.94971
O	-0.67717	-1.36670	0.17228
C	-2.99334	-1.73367	0.29564
C	-1.79211	-1.14378	0.71105

C	-5.44382	-1.95209	0.63307
C	-4.18580	-1.40424	0.91091
C	-6.59432	-1.65555	1.38636
H	-1.84757	-0.44805	1.57492
H	-4.14330	-0.66065	1.71765
H	-2.95780	-2.45333	-0.52360
C	-7.68942	-2.68508	1.47829
H	-6.41601	-1.10411	2.31326
H	-5.50889	-2.70993	-0.15197
H	-7.94694	-3.08990	0.49074
H	-7.34801	-3.52687	2.09565
H	-8.60203	-2.29108	1.93852
C	-7.59281	-0.18373	0.39255
C	-6.83066	0.95927	0.65346
C	-5.79631	1.06564	-0.30275
C	-5.96109	0.07487	-1.23915
C	-7.27698	-0.58130	-1.02719
H	-8.58560	-0.32169	0.81853
H	-6.95306	1.60506	1.51967
H	-4.98111	1.78449	-0.28000
H	-5.30367	-0.12462	-2.08102
H	-8.01511	-0.08095	-1.68048
H	-7.32391	-1.64868	-1.26507
C	1.41491	3.67729	-3.15449
H	2.47704	3.93626	-3.32176
H	0.89040	3.77997	-4.10961
O	0.82079	4.55544	-2.23601

Bottom, towards, 1, exo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.115731

M06/lanl2dz-6-31G(d) Free Energy = -2645.478412

M06/def2-TZVP Derived free energy = -2646.587557

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618574

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.643442

Number of Imaginary Frequencies = 1 (-374.15)

M06/lanl2dz-6-31G(d) Geometry

C	-2.10976	2.67116	-1.56610
C	-2.42927	4.17745	-1.50620
C	-2.96962	2.80574	0.80350
N	-2.26760	2.14885	-0.18543
C	-1.78517	0.99504	0.33558
N	-2.22186	1.02035	1.60017
N	-2.96024	2.13275	1.91463
C	-1.10797	4.82176	-1.03875
C	-0.09158	3.90684	-1.66248
C	-0.67591	2.68168	-2.00628
C	0.04020	1.70456	-2.68716
C	1.38591	1.93950	-2.96447
C	1.98305	3.14263	-2.58819
C	1.24730	4.14146	-1.95075
C	-1.90018	0.05817	2.60351
C	-2.62571	-1.16061	2.66231
C	-2.22904	-2.12640	3.63320
C	-1.16273	-1.82566	4.51352
C	-0.49467	-0.63072	4.44981
C	-0.86631	0.31620	3.47583
C	-3.70851	-1.45549	1.80147
C	-4.34849	-2.66701	1.88127
C	-3.94807	-3.63231	2.83016
C	-2.91547	-3.36230	3.69133
H	-2.78945	2.10715	-2.21750
H	-2.63194	4.50378	-2.53403
H	-1.02292	4.81744	0.06018
H	-1.01987	5.86625	-1.35981
H	-0.44182	0.78353	-3.01665
H	1.96501	1.18575	-3.49503
H	3.03194	3.31834	-2.82241
H	1.71092	5.09504	-1.70097
H	-0.87588	-2.56793	5.25762
H	0.32083	-0.39738	5.12938

Cl	0.01306	1.81234	3.39191
H	-4.04064	-0.71230	1.07934
H	-5.17552	-2.88285	1.20761
H	-4.46715	-4.58694	2.88048
H	-2.60435	-4.09531	4.43493
Au	-0.61640	-0.61350	-0.50352
C	0.42796	-2.18253	-1.31161
C	-0.28441	-2.96181	-2.23800
C	1.74209	-2.47890	-0.99034
C	0.35657	-4.03380	-2.85735
C	2.37084	-3.56141	-1.61268
H	2.27098	-1.87686	-0.25020
C	1.68068	-4.32845	-2.54545
H	-0.17403	-4.65091	-3.58207
H	3.40199	-3.81235	-1.36193
H	2.17395	-5.16865	-3.03073
C	-2.07942	-1.43024	-1.67865
C	-3.37052	-0.93534	-1.77110
C	-1.67036	-2.54300	-2.43791
C	-4.28542	-1.55235	-2.62869
H	-3.68917	-0.07578	-1.18091
C	-2.59779	-3.14480	-3.28767
C	-3.89593	-2.65307	-3.38196
H	-5.30031	-1.16586	-2.70348
H	-2.30703	-4.01007	-3.88290
H	-4.60751	-3.13351	-4.05050
O	1.18446	0.06335	0.59281
C	2.93711	1.63463	0.76620
C	1.61911	1.24438	0.47784
C	5.24075	0.94786	1.42264
C	3.88935	0.70960	1.15573
C	6.09880	-0.04752	1.92893
H	0.93060	2.03189	0.11771
H	3.53702	-0.31951	1.28386
H	3.19569	2.68548	0.63695
C	7.32067	0.37176	2.70257

H	5.59983	-0.93540	2.32495
H	5.63211	1.95915	1.28137
H	8.00417	-0.46173	2.89774
H	7.87805	1.16220	2.18264
H	7.01345	0.77780	3.67579
C	6.96899	-0.95423	0.33902
C	5.94670	-1.74557	-0.19682
C	5.19189	-0.98528	-1.11757
C	5.79229	0.23995	-1.26794
C	7.11391	0.22495	-0.59064
H	7.82955	-1.39413	0.84140
H	5.70368	-2.75498	0.12838
H	4.26334	-1.30030	-1.58854
H	5.42511	1.05856	-1.88126
H	7.88025	-0.04064	-1.34172
H	7.43223	1.17177	-0.14271
O	-3.59572	4.47730	-0.78874
C	-3.56144	4.15552	0.57697
H	-2.99066	4.90084	1.15735
H	-4.59352	4.18376	0.94303

M06/lanl2dz-6-31G(d) Energy = -2646.115731

M06/lanl2dz-6-31G(d) Free Energy = -2645.478411

M06/def2-TZVP Derived free energy = -2646.587555

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618573

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.643442

Number of Imaginary Frequencies = 1 (-374.12)

M06/lanl2dz-6-31G(d) Geometry

C	-2.10926	2.67132	-1.56656
C	-2.42847	4.17767	-1.50680
C	-2.96913	2.80630	0.80301
N	-2.26721	2.14917	-0.18584
C	-1.78494	0.99536	0.33533
N	-2.22163	1.02091	1.59993
N	-2.95985	2.13346	1.91422

C	-1.10707	4.82176	-1.03937
C	-0.09084	3.90658	-1.66298
C	-0.67541	2.68152	-2.00673
C	0.04052	1.70420	-2.68751
C	1.38630	1.93882	-2.96474
C	1.98368	3.14184	-2.58849
C	1.24812	4.14088	-1.95118
C	-1.90033	0.05872	2.60338
C	-2.62625	-1.15982	2.66221
C	-2.23000	-2.12566	3.63322
C	-1.16374	-1.82515	4.51368
C	-0.49533	-0.63041	4.44998
C	-0.86655	0.31654	3.47587
C	-3.70905	-1.45443	1.80127
C	-4.34940	-2.66574	1.88107
C	-3.94938	-3.63110	2.83007
C	-2.91681	-3.36134	3.69135
H	-2.78907	2.10738	-2.21790
H	-2.63103	4.50396	-2.53467
H	-1.02205	4.81753	0.05957
H	-1.01875	5.86619	-1.36053
H	-0.44169	0.78324	-3.01695
H	1.96527	1.18491	-3.49522
H	3.03263	3.31729	-2.82264
H	1.71193	5.09437	-1.70143
H	-0.87723	-2.56745	5.25789
H	0.32013	-0.39724	5.12967
Cl	0.01326	1.81243	3.39199
H	-4.04090	-0.71116	1.07909
H	-5.17641	-2.88137	1.20729
H	-4.46875	-4.58558	2.88038
H	-2.60602	-4.09438	4.43505
Au	-0.61635	-0.61343	-0.50362
C	0.42779	-2.18278	-1.31138
C	-0.28480	-2.96237	-2.23733
C	1.74195	-2.47911	-0.99023

C	0.35598	-4.03467	-2.85635
C	2.37051	-3.56190	-1.61226
H	2.27101	-1.87681	-0.25042
C	1.68013	-4.32929	-2.54457
H	-0.17481	-4.65205	-3.58071
H	3.40171	-3.81280	-1.36161
H	2.17325	-5.16972	-3.02960
C	-2.07958	-1.43038	-1.67836
C	-3.37063	-0.93535	-1.77091
C	-1.67074	-2.54349	-2.43721
C	-4.28568	-1.55260	-2.62815
H	-3.68912	-0.07549	-1.18105
C	-2.59832	-3.14554	-3.28663
C	-3.89642	-2.65369	-3.38100
H	-5.30052	-1.16599	-2.70302
H	-2.30772	-4.01107	-3.88155
H	-4.60812	-3.13432	-4.04927
O	1.18479	0.06342	0.59218
C	2.93735	1.63472	0.76600
C	1.61935	1.24451	0.47756
C	5.24090	0.94777	1.42264
C	3.88952	0.70963	1.15559
C	6.09872	-0.04765	1.92923
H	0.93080	2.03208	0.11767
H	3.53709	-0.31945	1.28372
H	3.19595	2.68558	0.63688
C	7.32060	0.37159	2.70288
H	5.59956	-0.93533	2.32545
H	5.63244	1.95897	1.28123
H	8.00392	-0.46198	2.89833
H	7.87819	1.16180	2.18281
H	7.01337	0.77793	3.67597
C	6.96882	-0.95501	0.33967
C	5.94639	-1.74620	-0.19613
C	5.19200	-0.98596	-1.11726
C	5.79280	0.23904	-1.26789

C	7.11425	0.22387	-0.59027
H	7.82916	-1.39506	0.84231
H	5.70302	-2.75545	0.12930
H	4.26347	-1.30086	-1.58835
H	5.42600	1.05756	-1.88155
H	7.88072	-0.04210	-1.34109
H	7.43269	1.17074	-0.14252
O	-3.59489	4.47782	-0.78943
C	-3.56076	4.15614	0.57631
H	-2.98992	4.90144	1.15667
H	-4.59286	4.18455	0.94228

Top, away, 2, exo, away

M06/lanl2dz-6-31G(d) Energy = -2646.116389

M06/lanl2dz-6-31G(d) Free Energy = -2645.475916

M06/def2-TZVP Derived free energy = -2646.584848

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616700

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642511

Number of Imaginary Frequencies = 1 (-364.19)

M06/lanl2dz-6-31G(d) Geometry

C	0.86181	2.76491	0.08901
C	2.16322	3.58818	-0.03368
C	1.97652	1.31311	-1.62493
N	0.95731	1.55473	-0.73877
C	0.11954	0.49129	-0.74549
N	0.67777	-0.33172	-1.64672
N	1.83948	0.15696	-2.20276
C	1.72669	5.01758	0.26868
C	0.29248	5.04333	-0.18469
C	-0.20708	3.74717	-0.31495
C	-1.51889	3.51907	-0.70794
C	-2.33231	4.61758	-0.97779
C	-1.83718	5.91378	-0.84871
C	-0.52068	6.13587	-0.45024

C	0.16159	-1.59171	-2.07193
C	0.21542	-2.70120	-1.18455
C	-0.36151	-3.93295	-1.61142
C	-0.94185	-4.01652	-2.89919
C	-0.96141	-2.93837	-3.74368
C	-0.40753	-1.71374	-3.32127
C	0.81047	-2.63647	0.09958
C	0.81285	-3.73667	0.92280
C	0.23146	-4.95309	0.50694
C	-0.33884	-5.04578	-0.73703
H	0.73269	2.41435	1.12459
H	2.95535	3.20955	0.63856
H	2.37602	5.73062	-0.25406
H	1.81255	5.22147	1.34644
H	-1.91581	2.50856	-0.81539
H	-3.36157	4.45986	-1.29344
H	-2.48366	6.76145	-1.06736
H	-0.13422	7.15005	-0.35762
H	-1.37809	-4.96266	-3.21706
H	-1.40576	-3.00148	-4.73369
Cl	-0.50416	-0.35439	-4.39562
H	1.27718	-1.71132	0.43754
H	1.27235	-3.66412	1.90880
H	0.23925	-5.81381	1.17190
H	-0.78541	-5.98011	-1.07541
Au	-1.39506	0.08157	0.76916
C	-2.76829	-0.30408	2.24093
C	-4.03608	-0.70641	1.78682
C	-2.50524	-0.17254	3.59363
C	-5.02336	-1.01662	2.71858
C	-3.50721	-0.48012	4.51973
H	-1.53875	0.18956	3.94434
C	-4.75407	-0.90914	4.08064
H	-6.01261	-1.33180	2.38725
H	-3.30926	-0.37645	5.58521
H	-5.53097	-1.14844	4.80413

C	-3.04844	-0.26880	-0.37525
C	-3.04423	-0.14260	-1.75138
C	-4.18246	-0.69750	0.33433
C	-4.19789	-0.48331	-2.46352
H	-2.16672	0.21719	-2.28572
C	-5.32216	-1.03000	-0.39624
C	-5.32598	-0.92889	-1.78512
H	-4.20301	-0.39237	-3.54883
H	-6.21939	-1.36528	0.12339
H	-6.22363	-1.19386	-2.34050
O	0.47130	0.32196	2.02134
C	2.28422	-0.87655	2.93732
C	0.92057	-0.57405	2.79063
C	4.63169	-0.51408	2.23686
C	3.25446	-0.32001	2.11510
C	5.59993	0.16477	1.47513
H	0.20186	-1.16535	3.38834
H	2.90024	0.34797	1.31777
H	2.57122	-1.58128	3.71797
C	6.95394	0.41949	2.08276
H	5.22109	0.98437	0.85725
H	4.97826	-1.16991	3.04086
H	7.67277	0.81731	1.35835
H	6.85831	1.15778	2.89044
H	7.37532	-0.49350	2.52361
C	6.16792	-1.09817	-0.04430
C	5.14465	-0.92679	-0.97919
C	4.08870	-1.82479	-0.70153
C	4.47599	-2.65151	0.32164
C	5.91907	-2.43534	0.60613
H	7.17542	-0.72274	-0.21506
H	5.12529	-0.16730	-1.75839
H	3.12825	-1.83235	-1.20928
H	3.86505	-3.42849	0.77519
H	6.22419	-2.54640	1.65138
H	6.49185	-3.18719	0.03269

O	2.63504	3.56993	-1.37063
C	3.07570	2.30795	-1.77313
H	3.94380	1.98050	-1.16388
H	3.40111	2.37320	-2.81686

M06/lanl2dz-6-31G(d) Energy = -2646.113925

M06/lanl2dz-6-31G(d) Free Energy = -2645.475209

M06/def2-TZVP Derived free energy = -2646.584820

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.615634

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.640411

Number of Imaginary Frequencies = 1 (-368.28)

M06/lanl2dz-6-31G(d) Geometry

C	1.69097	-0.32943	3.12357
C	2.63135	-0.97040	4.15774
C	1.77497	-2.66726	2.18612
N	1.55149	-1.31797	2.01961
C	1.17335	-1.10430	0.73787
N	1.17018	-2.33756	0.20811
N	1.53747	-3.32370	1.09119
C	4.03941	-0.70695	3.58332
C	3.84032	0.63361	2.92818
C	2.47875	0.87523	2.71245
C	2.02521	2.09715	2.23303
C	2.96664	3.06678	1.89176
C	4.32725	2.81418	2.05967
C	4.77392	1.60597	2.59560
C	0.84572	-2.68079	-1.13681
C	-0.49394	-2.51661	-1.58668
C	-0.79129	-2.82043	-2.94727
C	0.23778	-3.30585	-3.78878
C	1.50972	-3.49429	-3.31979
C	1.81617	-3.17759	-1.98057
C	-1.54329	-2.07976	-0.74229
C	-2.81532	-1.92404	-1.23592
C	-3.10514	-2.19596	-2.58898

C	-2.11172	-2.64192	-3.42310
H	0.68512	-0.12419	3.51030
H	2.52438	-0.39933	5.08848
H	4.32721	-1.47475	2.84644
H	4.81199	-0.70855	4.36117
H	0.95675	2.30196	2.14432
H	2.63355	4.02592	1.49916
H	5.05156	3.58108	1.79207
H	5.83689	1.43788	2.76364
H	0.00094	-3.53927	-4.82614
H	2.29951	-3.87657	-3.96124
Cl	3.44519	-3.42982	-1.44029
H	-1.34383	-1.87137	0.30697
H	-3.60405	-1.58260	-0.56395
H	-4.11541	-2.06003	-2.97234
H	-2.32211	-2.87019	-4.46744
Au	0.73356	0.78433	-0.22013
C	0.39681	2.58616	-1.15429
C	1.39066	2.97127	-2.07307
C	-0.68694	3.41277	-0.90511
C	1.25272	4.17290	-2.76421
C	-0.81296	4.61937	-1.60067
H	-1.44011	3.14562	-0.16364
C	0.14934	4.98955	-2.53235
H	2.01178	4.48597	-3.48089
H	-1.66392	5.27009	-1.40566
H	0.04956	5.92829	-3.07408
C	2.45689	0.94154	-1.29929
C	3.50796	0.05268	-1.17111
C	2.52907	2.05875	-2.14825
C	4.65501	0.24215	-1.94665
H	3.46053	-0.78628	-0.47791
C	3.68139	2.22758	-2.91494
C	4.73182	1.31881	-2.82112
H	5.48029	-0.46321	-1.86270
H	3.76734	3.08316	-3.58425

H	5.62336	1.46296	-3.42837
O	-1.11811	0.77740	1.04365
C	-3.44906	0.83113	1.34406
C	-2.28137	0.84691	0.56659
C	-5.90733	1.09822	1.44521
C	-4.69307	0.98417	0.75779
C	-7.11894	1.49276	0.84779
H	-2.41208	0.93356	-0.53110
H	-4.72833	1.07726	-0.33541
H	-3.34771	0.75653	2.42760
C	-8.12176	2.24246	1.68666
H	-7.03764	1.85280	-0.18090
H	-5.88137	0.98814	2.53305
H	-9.08609	2.36523	1.18183
H	-8.29548	1.74377	2.64948
H	-7.73570	3.24724	1.90482
C	-8.19047	-0.19378	0.47740
C	-7.62052	-0.64287	-0.71766
C	-6.50949	-1.46559	-0.42847
C	-6.43426	-1.64586	0.93005
C	-7.66714	-1.10339	1.55970
H	-9.19818	0.21678	0.51526
H	-7.92340	-0.32355	-1.71184
H	-5.81370	-1.86457	-1.16208
H	-5.67121	-2.21221	1.45778
H	-8.38816	-1.93521	1.66194
H	-7.54748	-0.67062	2.55763
O	2.28138	-2.28720	4.49684
C	2.34297	-3.21792	3.45037
H	3.38019	-3.54218	3.25482
H	1.78240	-4.10451	3.76700

Bottom, away, 2, exo, away

M06/lanl2dz-6-31G(d) Energy = -2646.118713

M06/lanl2dz-6-31G(d) Free Energy = -2645.480058

M06/def2-TZVP Derived free energy = -2646.589952

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.620680

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.645422

Number of Imaginary Frequencies = 1 (-400.85)

M06/lanl2dz-6-31G(d) Geometry

C	3.01175	0.53456	-2.60254
C	4.55953	0.68802	-2.65035
C	2.98723	2.70333	-1.46538
N	2.50426	1.41557	-1.52980
C	1.55711	1.26069	-0.57814
N	1.50255	2.47781	-0.01100
N	2.38649	3.39006	-0.54242
C	5.09270	-0.46107	-1.78707
C	4.00527	-1.49204	-1.87658
C	2.82373	-0.92779	-2.35942
C	1.67638	-1.69058	-2.55493
C	1.71915	-3.04467	-2.23164
C	2.88997	-3.60872	-1.72332
C	4.03842	-2.84065	-1.54307
C	0.57968	2.90439	0.98832
C	-0.69872	3.36381	0.57057
C	-1.62158	3.78618	1.57156
C	-1.22770	3.75557	2.93141
C	0.02124	3.33611	3.30393
C	0.93701	2.91235	2.31818
C	-1.08630	3.42061	-0.79042
C	-2.33826	3.86392	-1.13772
C	-3.25865	4.27257	-0.14877
C	-2.90474	4.23523	1.17696
H	2.53574	0.88599	-3.52930
H	4.85698	0.54578	-3.70358
H	5.21840	-0.10107	-0.75326
H	6.07230	-0.81908	-2.12525
H	0.76278	-1.23987	-2.94757
H	0.83318	-3.66231	-2.36572

H	2.90552	-4.66584	-1.46418
H	4.94825	-3.29112	-1.14813
H	-1.93675	4.08749	3.68917
H	0.32936	3.32532	4.34629
Cl	2.51805	2.41956	2.81923
H	-0.38321	3.11089	-1.56233
H	-2.62431	3.90172	-2.18693
H	-4.24593	4.62293	-0.44341
H	-3.60115	4.56277	1.94869
Au	0.58055	-0.54933	0.09931
C	-0.22224	-2.32782	0.74867
C	0.62298	-3.09775	1.56558
C	-1.46528	-2.80959	0.36839
C	0.18388	-4.33798	2.02560
C	-1.89395	-4.05722	0.83318
H	-2.10345	-2.23552	-0.30416
C	-1.07420	-4.81184	1.66461
H	0.82396	-4.94679	2.66402
H	-2.86987	-4.44164	0.53553
H	-1.41122	-5.78086	2.02797
C	2.14314	-1.24032	1.22670
C	3.34492	-0.56918	1.37179
C	1.93117	-2.49842	1.81730
C	4.37680	-1.16291	2.10378
H	3.50250	0.41779	0.93777
C	2.97414	-3.07462	2.54206
C	4.19020	-2.41295	2.68112
H	5.32386	-0.63797	2.22085
H	2.83774	-4.05365	3.00091
H	4.99475	-2.87654	3.24869
O	-1.24620	-0.05926	-1.09485
C	-3.55481	0.38251	-1.04828
C	-2.25223	0.43432	-0.52304
C	-5.96579	0.85695	-0.68118
C	-4.60974	0.94361	-0.34713
C	-6.43852	0.10664	-1.76509

H	-2.13007	0.92742	0.46429
H	-4.35464	1.48172	0.57045
H	-3.68228	-0.10198	-2.01624
C	-7.82520	0.33958	-2.29014
H	-5.70978	-0.15747	-2.53364
H	-6.69101	1.35322	-0.03509
H	-8.19433	-0.49144	-2.90153
H	-8.54677	0.52670	-1.48516
H	-7.81959	1.23293	-2.93023
C	-6.58077	-1.84742	-1.05974
C	-5.28478	-2.23600	-0.71723
C	-5.04448	-1.94589	0.65265
C	-6.19626	-1.47324	1.21221
C	-7.31278	-1.61027	0.23886
H	-7.08490	-2.23937	-1.94208
H	-4.55482	-2.65908	-1.40485
H	-4.08291	-2.04952	1.15151
H	-6.32172	-1.14655	2.24045
H	-7.87698	-2.52865	0.48181
H	-8.04334	-0.79440	0.24834
O	5.05314	1.92334	-2.17804
C	4.17062	3.01394	-2.31296
H	4.68261	3.90966	-1.95099
H	3.88170	3.18071	-3.36601

M06/lanl2dz-6-31G(d) Energy = -2646.115564

M06/lanl2dz-6-31G(d) Free Energy = -2645.479622

M06/def2-TZVP Derived free energy = -2646.592030

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.623211

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.648638

Number of Imaginary Frequencies = 1 (-394.80)

M06/lanl2dz-6-31G(d) Geometry

C	-0.40726	3.12921	-0.16129
C	-0.19636	4.46873	-0.90166
C	-1.78073	2.58421	-2.18863

N	-1.17360	2.21167	-1.01191
C	-1.37562	0.88834	-0.82432
N	-2.09538	0.53371	-1.90217
N	-2.35449	1.57121	-2.76419
C	-0.00080	5.48109	0.22228
C	-0.81284	4.90259	1.34865
C	-1.07844	3.55168	1.12094
C	-1.81086	2.80083	2.02973
C	-2.28063	3.42568	3.18351
C	-2.01352	4.77329	3.41666
C	-1.27748	5.52164	2.50026
C	-2.57092	-0.77995	-2.18094
C	-1.62406	-1.81321	-2.42060
C	-2.10402	-3.14844	-2.54807
C	-3.49663	-3.39310	-2.48638
C	-4.39152	-2.37113	-2.31572
C	-3.92136	-1.05249	-2.15416
C	-0.23264	-1.57343	-2.54336
C	0.63729	-2.61567	-2.75269
C	0.16750	-3.94291	-2.84187
C	-1.17670	-4.19868	-2.74797
H	0.55964	2.63707	0.02953
H	0.64489	4.42073	-1.61579
H	-0.32905	6.47590	-0.10302
H	1.06431	5.55495	0.48887
H	-2.03014	1.74696	1.85114
H	-2.86331	2.85610	3.90460
H	-2.39063	5.24770	4.32065
H	-1.08109	6.57790	2.68039
H	-3.85381	-4.41709	-2.58784
H	-5.46246	-2.55394	-2.27971
Cl	-5.08801	0.19680	-1.85677
H	0.14282	-0.55208	-2.50398
H	1.70086	-2.41027	-2.87418
H	0.87105	-4.75687	-3.00232
H	-1.55668	-5.21602	-2.83481

Au	-0.46868	-0.39504	0.67968
C	0.38799	-1.67492	2.04047
C	-0.49889	-2.59084	2.63328
C	1.73404	-1.68698	2.36928
C	-0.00374	-3.54438	3.51979
C	2.21920	-2.64137	3.26782
H	2.41640	-0.94894	1.94716
C	1.35320	-3.57187	3.82946
H	-0.67630	-4.26454	3.98514
H	3.27543	-2.65103	3.53453
H	1.73228	-4.31596	4.52745
C	-2.14675	-1.29738	1.42244
C	-3.42950	-0.90916	1.08506
C	-1.90043	-2.38339	2.28036
C	-4.51119	-1.65144	1.56800
H	-3.61567	-0.04031	0.45671
C	-2.99344	-3.11033	2.74907
C	-4.28907	-2.75209	2.38600
H	-5.52394	-1.35766	1.29521
H	-2.83515	-3.95881	3.41419
H	-5.13173	-3.33152	2.75813
O	1.48140	0.45688	-0.06823
C	3.63253	0.09761	-0.97025
C	2.36729	-0.31452	-0.52260
C	5.84231	-0.61879	-1.87759
C	4.53240	-0.84633	-1.44226
C	6.45587	0.63956	-1.86189
H	2.15035	-1.39982	-0.58153
H	4.18278	-1.88311	-1.46123
H	3.85987	1.16315	-0.94784
C	7.67611	0.88367	-2.70060
H	5.80022	1.50633	-1.76121
H	6.42119	-1.47383	-2.22866
H	8.23858	1.77134	-2.39066
H	8.35567	0.02225	-2.69981
H	7.36525	1.04630	-3.74215

C	7.24690	0.84509	0.06488
C	6.14431	0.85378	0.91703
C	5.86081	-0.47046	1.34296
C	6.82091	-1.30889	0.85344
C	7.90034	-0.50540	0.21991
H	7.82112	1.74492	-0.14968
H	5.55973	1.73198	1.18082
H	4.99457	-0.76450	1.92892
H	6.86559	-2.38500	0.99371
H	8.72498	-0.39857	0.94750
H	8.34365	-0.94303	-0.68090
C	-1.67717	3.99309	-2.66310
H	-0.90240	4.06212	-3.44941
H	-2.62636	4.32249	-3.09797
O	-1.37949	4.83631	-1.58500

M06/lanl2dz-6-31G(d) Energy = -2646.115563

M06/lanl2dz-6-31G(d) Free Energy = -2645.479650

M06/def2-TZVP Derived free energy = -2646.592059

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.623239

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.648666

Number of Imaginary Frequencies = 1 (-394.79)

M06/lanl2dz-6-31G(d) Geometry

C	-0.40743	3.12913	-0.16190
C	-0.19655	4.46850	-0.90254
C	-1.78074	2.58360	-2.18920
N	-1.17363	2.21135	-1.01238
C	-1.37560	0.88805	-0.82452
N	-2.09528	0.53314	-1.90231
N	-2.35441	1.57045	-2.76457
C	-0.00114	5.48112	0.22118
C	-0.81323	4.90282	1.34762
C	-1.07873	3.55185	1.12019
C	-1.81115	2.80115	2.02911
C	-2.28105	3.42624	3.18271

C	-2.01404	4.77391	3.41558
C	-1.27799	5.52210	2.49906
C	-2.57072	-0.78060	-2.18085
C	-1.62378	-1.81382	-2.42042
C	-2.10365	-3.14908	-2.54787
C	-3.49624	-3.39385	-2.48608
C	-4.39120	-2.37194	-2.31541
C	-3.92114	-1.05325	-2.15401
C	-0.23238	-1.57394	-2.54313
C	0.63762	-2.61612	-2.75247
C	0.16792	-3.94339	-2.84171
C	-1.17626	-4.19925	-2.74779
H	0.55949	2.63711	0.02912
H	0.64476	4.42040	-1.61660
H	-0.32945	6.47584	-0.10436
H	1.06394	5.55513	0.48784
H	-2.03035	1.74723	1.85076
H	-2.86373	2.85678	3.90390
H	-2.39124	5.24851	4.31944
H	-1.08167	6.57841	2.67897
H	-3.85335	-4.41787	-2.58748
H	-5.46212	-2.55482	-2.27931
Cl	-5.08787	0.19601	-1.85681
H	0.14302	-0.55258	-2.50369
H	1.70118	-2.41065	-2.87391
H	0.87152	-4.75730	-3.00218
H	-1.55618	-5.21662	-2.83464
Au	-0.46866	-0.39494	0.67981
C	0.38799	-1.67439	2.04103
C	-0.49891	-2.59007	2.63416
C	1.73404	-1.68636	2.36985
C	-0.00378	-3.54332	3.52099
C	2.21918	-2.64045	3.26871
H	2.41642	-0.94847	1.94749
C	1.35316	-3.57074	3.83067
H	-0.67635	-4.26331	3.98659

H	3.27541	-2.65003	3.53543
H	1.73223	-4.31461	4.52890
C	-2.14674	-1.29700	1.42287
C	-3.42949	-0.90890	1.08534
C	-1.90045	-2.38270	2.28119
C	-4.51120	-1.65097	1.56856
H	-3.61566	-0.04030	0.45665
C	-2.99347	-3.10944	2.75018
C	-4.28909	-2.75131	2.38699
H	-5.52393	-1.35727	1.29567
H	-2.83519	-3.95767	3.41563
H	-5.13176	-3.33058	2.75936
O	1.48140	0.45666	-0.06849
C	3.63251	0.09725	-0.97044
C	2.36736	-0.31485	-0.52253
C	5.84240	-0.61923	-1.87743
C	4.53252	-0.84678	-1.44204
C	6.45579	0.63921	-1.86216
H	2.15056	-1.40021	-0.58091
H	4.18304	-1.88362	-1.46058
H	3.85971	1.16283	-0.94854
C	7.67602	0.88317	-2.70093
H	5.80004	1.50594	-1.76182
H	6.42141	-1.47432	-2.22816
H	8.23846	1.77093	-2.39120
H	8.35561	0.02177	-2.69996
H	7.36514	1.04556	-3.74251
C	7.24665	0.84557	0.06458
C	6.14401	0.85429	0.91668
C	5.86077	-0.46987	1.34302
C	6.82106	-1.30826	0.85380
C	7.90037	-0.50474	0.22010
H	7.82069	1.74545	-0.15023
H	5.55925	1.73246	1.18019
H	4.99456	-0.76392	1.92902
H	6.86595	-2.38431	0.99442

H	8.72491	-0.39749	0.94773
H	8.34387	-0.94256	-0.68053
O	-1.37965	4.83586	-1.58606
C	-1.67721	3.99238	-2.66398
H	-0.90239	4.06127	-3.45025
H	-2.62638	4.32163	-3.09900

M06/lanl2dz-6-31G(d) Energy = -2646.114897

M06/lanl2dz-6-31G(d) Free Energy = -2645.477070

M06/def2-TZVP Derived free energy = -2646.587338

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617802

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641824

Number of Imaginary Frequencies = 1 (-395.94)

M06/lanl2dz-6-31G(d) Geometry

C	-0.74379	3.23057	-0.16546
C	-1.33492	4.60192	-0.54579
C	-2.18166	2.51928	-2.11392
N	-1.46641	2.21258	-0.97728
C	-1.50286	0.87007	-0.80117
N	-2.24149	0.44460	-1.83879
N	-2.66864	1.45062	-2.66867
C	-2.59555	4.72753	0.33236
C	-2.17011	3.98807	1.56922
C	-1.08106	3.15398	1.29425
C	-0.43712	2.45518	2.30860
C	-0.94519	2.53937	3.60310
C	-2.05727	3.33608	3.87227
C	-2.66621	4.07981	2.86275
C	-2.58985	-0.90660	-2.13018
C	-1.57260	-1.80298	-2.55580
C	-1.92091	-3.16999	-2.75742
C	-3.26104	-3.57876	-2.55905
C	-4.23276	-2.68393	-2.19895
C	-3.89224	-1.33304	-1.98825
C	-0.24137	-1.39293	-2.81338

C	0.69770	-2.30321	-3.23352
C	0.36253	-3.66310	-3.40454
C	-0.92233	-4.08276	-3.17261
H	0.32302	3.12309	-0.39547
H	-0.61098	5.36151	-0.22482
H	-3.46754	4.24642	-0.13891
H	-2.87011	5.77324	0.51477
H	0.46672	1.87888	2.10677
H	-0.45839	1.99585	4.41050
H	-2.43917	3.39883	4.88948
H	-3.50831	4.73203	3.09044
H	-3.51711	-4.62621	-2.71353
H	-5.26606	-2.99260	-2.06239
Cl	-5.15243	-0.23878	-1.51017
H	0.02539	-0.34153	-2.71196
H	1.70832	-1.96543	-3.46117
H	1.11891	-4.37074	-3.73677
H	-1.20050	-5.12615	-3.31688
Au	-0.36373	-0.28085	0.64553
C	0.75627	-1.34767	1.99822
C	0.06457	-2.36350	2.67965
C	2.09093	-1.09419	2.27559
C	0.74968	-3.15762	3.59726
C	2.76467	-1.88653	3.21087
H	2.61268	-0.26917	1.78701
C	2.09751	-2.92263	3.85469
H	0.23099	-3.95225	4.13325
H	3.80982	-1.68243	3.44430
H	2.62379	-3.54106	4.57926
C	-1.82630	-1.41300	1.50929
C	-3.16936	-1.23897	1.24163
C	-1.36636	-2.40702	2.39088
C	-4.09365	-2.11876	1.81220
H	-3.51672	-0.43129	0.60211
C	-2.30425	-3.27413	2.94867
C	-3.65751	-3.13772	2.64991

H	-5.15352	-1.99411	1.59417
H	-1.97898	-4.05827	3.63196
H	-4.37710	-3.82579	3.08940
O	1.42721	0.80891	-0.19732
C	3.56585	0.67790	-1.16828
C	2.30123	0.16640	-0.83806
C	5.78815	0.26121	-2.19358
C	4.46408	-0.08154	-1.90371
C	6.40652	1.40860	-1.68073
H	2.07734	-0.87293	-1.15490
H	4.11092	-1.05295	-2.26151
H	3.79087	1.69381	-0.84535
C	7.68577	1.90536	-2.28704
H	5.75158	2.19965	-1.31170
H	6.38185	-0.42472	-2.79877
H	7.44936	2.48433	-3.19082
H	8.24658	2.56801	-1.61833
H	8.34408	1.08341	-2.59534
C	7.02365	0.87901	0.24348
C	5.87043	0.53875	0.95080
C	5.62454	-0.85501	0.81907
C	6.65737	-1.42270	0.13092
C	7.73351	-0.41632	-0.06834
H	7.56731	1.80292	0.43612
H	5.23071	1.23684	1.48648
H	4.73153	-1.37139	1.16455
H	6.74355	-2.46947	-0.14604
H	8.50816	-0.57377	0.70343
H	8.24868	-0.47260	-1.03323
O	-1.47888	4.79350	-1.92958
C	-2.38829	3.92828	-2.55436
H	-2.23047	4.01178	-3.63512
H	-3.43431	4.21988	-2.35573

M06/lanl2dz-6-31G(d) Energy = -2646.114083

M06/lanl2dz-6-31G(d) Free Energy = -2645.476015

M06/def2-TZVP Derived free energy = -2646.586008

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616610

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641125

Number of Imaginary Frequencies = 1 (-376.34)

M06/lanl2dz-6-31G(d) Geometry

C	-1.73878	-0.38206	3.10201
C	-2.75033	-0.15829	4.23950
C	-2.45010	1.97302	2.54915
N	-1.89622	0.76921	2.17394
C	-1.52703	0.85789	0.87476
N	-1.86913	2.11060	0.54159
N	-2.44098	2.82287	1.56718
C	-4.08432	-0.66404	3.65070
C	-3.61184	-1.78443	2.76423
C	-2.24352	-1.65768	2.50077
C	-1.54415	-2.63939	1.81074
C	-2.25362	-3.72303	1.29681
C	-3.62772	-3.82610	1.50878
C	-4.31243	-2.87330	2.26342
C	-1.69326	2.72859	-0.73061
C	-0.37922	3.06367	-1.15843
C	-0.22371	3.66506	-2.44129
C	-1.37006	3.92289	-3.22994
C	-2.62720	3.62056	-2.77988
C	-2.78837	3.02220	-1.51423
C	0.77087	2.85154	-0.35889
C	2.01389	3.21156	-0.81952
C	2.17183	3.79102	-2.09615
C	1.07367	4.01134	-2.88765
H	-0.69215	-0.39731	3.42889
H	-2.45932	-0.81888	5.06580
H	-4.59233	0.12183	3.06858
H	-4.78633	-0.98459	4.42952
H	-0.46141	-2.57454	1.68886
H	-1.72928	-4.49465	0.73577

H	-4.16943	-4.67922	1.10477
H	-5.37651	-2.99124	2.46414
H	-1.23936	4.38299	-4.20875
H	-3.51025	3.83252	-3.37710
Cl	-4.40267	2.68006	-0.97423
H	0.66577	2.41327	0.63279
H	2.88326	3.05740	-0.18105
H	3.16280	4.07367	-2.44530
H	1.17969	4.46743	-3.87150
Au	-0.51589	-0.64789	-0.29886
C	0.42395	-2.09274	-1.42385
C	-0.32043	-2.56778	-2.51912
C	1.67984	-2.61391	-1.15219
C	0.23487	-3.53150	-3.35821
C	2.22340	-3.58885	-1.99440
H	2.24841	-2.28366	-0.28158
C	1.50675	-4.03435	-3.09854
H	-0.32743	-3.90468	-4.21391
H	3.20667	-4.00594	-1.78022
H	1.93234	-4.78991	-3.75632
C	-2.01575	-1.10502	-1.60194
C	-3.29135	-0.58596	-1.49076
C	-1.66982	-2.01650	-2.61423
C	-4.24980	-0.93502	-2.44632
H	-3.56113	0.09258	-0.68388
C	-2.64083	-2.35052	-3.55716
C	-3.91904	-1.80391	-3.47875
H	-5.25195	-0.51507	-2.37456
H	-2.40309	-3.05204	-4.35654
H	-4.66498	-2.07021	-4.22509
O	1.17948	-0.29163	1.12870
C	3.43378	0.29688	1.49318
C	2.30633	0.06621	0.69289
C	5.84899	0.89626	1.55066
C	4.63311	0.65307	0.90217
C	6.98278	1.41257	0.89591

H	2.43825	0.20723	-0.39888
H	4.62819	0.78095	-0.18814
H	3.34997	0.17082	2.57309
C	8.00308	2.16799	1.70603
H	6.80367	1.82492	-0.10017
H	5.89439	0.74037	2.63182
H	8.91032	2.39489	1.13568
H	7.57518	3.12442	2.03548
H	8.29151	1.61347	2.60884
C	8.11449	-0.17341	0.30618
C	7.41676	-0.65781	-0.80456
C	6.42778	-1.57202	-0.37945
C	6.56703	-1.77289	0.97123
C	7.82627	-1.13296	1.43304
H	9.07942	0.32204	0.20856
H	7.54455	-0.30271	-1.82434
H	5.65409	-2.00186	-1.01010
H	5.93247	-2.39852	1.59316
H	7.80662	-0.71595	2.44507
H	8.62220	-1.89983	1.42420
C	-3.06181	2.16962	3.89500
H	-2.71272	3.10956	4.33692
H	-4.15636	2.25309	3.77802
O	-2.71204	1.13793	4.77800

M06/lanl2dz-6-31G(d) Energy = -2646.115564

M06/lanl2dz-6-31G(d) Free Energy = -2645.479642

M06/def2-TZVP Derived free energy = -2646.592051

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.623231

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.648658

Number of Imaginary Frequencies = 1 (-394.80)

M06/lanl2dz-6-31G(d) Geometry

C	-0.40780	3.12922	-0.16152
C	-0.19715	4.46874	-0.90195
C	-1.78114	2.58385	-2.18884

N	-1.17392	2.21148	-1.01212
C	-1.37566	0.88811	-0.82449
N	-2.09534	0.53329	-1.90232
N	-2.35468	1.57071	-2.76437
C	-0.00179	5.48119	0.22194
C	-0.81375	4.90260	1.34833
C	-1.07909	3.55163	1.12068
C	-1.81138	2.80068	2.02949
C	-2.28130	3.42551	3.18323
C	-2.01445	4.77318	3.41631
C	-1.27854	5.52162	2.49989
C	-2.57067	-0.78046	-2.18101
C	-1.62365	-1.81358	-2.42069
C	-2.10341	-3.14888	-2.54817
C	-3.49597	-3.39378	-2.48636
C	-4.39101	-2.37195	-2.31562
C	-3.92107	-1.05323	-2.15415
C	-0.23227	-1.57358	-2.54348
C	0.63780	-2.61568	-2.75292
C	0.16822	-3.94299	-2.84216
C	-1.17593	-4.19896	-2.74818
H	0.55919	2.63729	0.02937
H	0.64413	4.42087	-1.61606
H	-0.33022	6.47593	-0.10341
H	1.06329	5.55527	0.48855
H	-2.03045	1.74676	1.85097
H	-2.86388	2.85585	3.90435
H	-2.39167	5.24757	4.32027
H	-1.08235	6.57792	2.67997
H	-3.85298	-4.41783	-2.58779
H	-5.46192	-2.55494	-2.27952
Cl	-5.08791	0.19589	-1.85681
H	0.14305	-0.55219	-2.50404
H	1.70134	-2.41011	-2.87443
H	0.87188	-4.75683	-3.00270
H	-1.55577	-5.21636	-2.83504

Au	-0.46859	-0.39506	0.67961
C	0.38814	-1.67478	2.04053
C	-0.49876	-2.59051	2.63361
C	1.73422	-1.68691	2.36920
C	-0.00360	-3.54394	3.52024
C	2.21939	-2.64118	3.26786
H	2.41661	-0.94901	1.94687
C	1.35338	-3.57149	3.82977
H	-0.67616	-4.26397	3.98578
H	3.27566	-2.65088	3.53444
H	1.73247	-4.31550	4.52784
C	-2.14664	-1.29725	1.42260
C	-3.42941	-0.90908	1.08520
C	-1.90031	-2.38305	2.28078
C	-4.51110	-1.65117	1.56843
H	-3.61560	-0.04041	0.45662
C	-2.99332	-3.10981	2.74977
C	-4.28896	-2.75160	2.38672
H	-5.52385	-1.35740	1.29565
H	-2.83501	-3.95812	3.41511
H	-5.13162	-3.33088	2.75909
O	1.48142	0.45686	-0.06843
C	3.63269	0.09777	-0.97016
C	2.36744	-0.31448	-0.52264
C	5.84262	-0.61839	-1.87731
C	4.53272	-0.84608	-1.44205
C	6.45601	0.64005	-1.86165
H	2.15062	-1.39981	-0.58153
H	4.18323	-1.88290	-1.46102
H	3.85990	1.16334	-0.94775
C	7.67626	0.88429	-2.70032
H	5.80024	1.50673	-1.76105
H	6.42165	-1.47337	-2.22828
H	8.23855	1.77209	-2.39043
H	8.35597	0.02299	-2.69940
H	7.36542	1.04676	-3.74189

C	7.24693	0.84580	0.06514
C	6.14429	0.85441	0.91724
C	5.86093	-0.46983	1.34324
C	6.82114	-1.30819	0.85381
C	7.90052	-0.50462	0.22029
H	7.82106	1.74568	-0.14945
H	5.55961	1.73256	1.18095
H	4.99470	-0.76393	1.92919
H	6.86594	-2.38428	0.99416
H	8.72511	-0.39765	0.94790
H	8.34391	-0.94225	-0.68048
O	-1.38034	4.83606	-1.58532
C	-1.67786	3.99274	-2.66337
H	-0.90312	4.06189	-3.44969
H	-2.62712	4.32192	-3.09825

M06/lanl2dz-6-31G(d) Energy = -2646.114897

M06/lanl2dz-6-31G(d) Free Energy = -2645.477065

M06/def2-TZVP Derived free energy = -2646.587333

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617797

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641819

Number of Imaginary Frequencies = 1 (-395.92)

M06/lanl2dz-6-31G(d) Geometry

C	-0.74383	3.23044	-0.16571
C	-1.33483	4.60176	-0.54634
C	-2.18161	2.51894	-2.11417
N	-1.46643	2.21235	-0.97744
C	-1.50292	0.86986	-0.80119
N	-2.24151	0.44430	-1.83880
N	-2.66859	1.45023	-2.66881
C	-2.59554	4.72761	0.33165
C	-2.17029	3.98834	1.56868
C	-1.08126	3.15413	1.29398
C	-0.43748	2.45549	2.30854
C	-0.94568	2.53997	3.60297

C	-2.05775	3.33678	3.87187
C	-2.66654	4.08035	2.86213
C	-2.58983	-0.90693	-2.13012
C	-1.57260	-1.80326	-2.55586
C	-1.92087	-3.17028	-2.75746
C	-3.26096	-3.57911	-2.55898
C	-4.23269	-2.68432	-2.19878
C	-3.89220	-1.33342	-1.98810
C	-0.24142	-1.39315	-2.81361
C	0.69765	-2.30337	-3.23384
C	0.36253	-3.66329	-3.40480
C	-0.92229	-4.08301	-3.17275
H	0.32299	3.12283	-0.39559
H	-0.61087	5.36136	-0.22544
H	-3.46752	4.24648	-0.13964
H	-2.87005	5.77337	0.51385
H	0.46636	1.87912	2.10694
H	-0.45900	1.99657	4.41052
H	-2.43977	3.39975	4.88902
H	-3.50862	4.73267	3.08960
H	-3.51701	-4.62657	-2.71345
H	-5.26597	-2.99302	-2.06214
Cl	-5.15238	-0.23920	-1.50992
H	0.02529	-0.34173	-2.71228
H	1.70822	-1.96555	-3.46162
H	1.11891	-4.37090	-3.73710
H	-1.20043	-5.12641	-3.31699
Au	-0.36372	-0.28079	0.64567
C	0.75644	-1.34727	1.99850
C	0.06490	-2.36305	2.68017
C	2.09108	-1.09356	2.27576
C	0.75015	-3.15687	3.59794
C	2.76497	-1.88559	3.21119
H	2.61271	-0.26859	1.78696
C	2.09795	-2.92163	3.85527
H	0.23159	-3.95145	4.13412

H	3.81010	-1.68131	3.44451
H	2.62434	-3.53982	4.57997
C	-1.82609	-1.41306	1.50961
C	-3.16917	-1.23929	1.24185
C	-1.36602	-2.40685	2.39140
C	-4.09334	-2.11913	1.81253
H	-3.51661	-0.43178	0.60216
C	-2.30380	-3.27401	2.94929
C	-3.65707	-3.13787	2.65044
H	-5.15322	-1.99471	1.59441
H	-1.97844	-4.05797	3.63274
H	-4.37657	-3.82599	3.09001
O	1.42707	0.80914	-0.19729
C	3.56569	0.67822	-1.16831
C	2.30102	0.16675	-0.83824
C	5.78792	0.26162	-2.19379
C	4.46382	-0.08107	-1.90402
C	6.40647	1.40874	-1.68056
H	2.07702	-0.87246	-1.15540
H	4.11053	-1.05232	-2.26214
H	3.79083	1.69401	-0.84507
C	7.68584	1.90543	-2.28667
H	5.75167	2.19982	-1.31134
H	6.38154	-0.42421	-2.79917
H	7.44957	2.48494	-3.19015
H	8.24689	2.56756	-1.61766
H	8.34388	1.08343	-2.59543
C	7.02338	0.87855	0.24352
C	5.87011	0.53818	0.95072
C	5.62418	-0.85555	0.81871
C	6.65705	-1.42315	0.13054
C	7.73320	-0.41675	-0.06856
H	7.56707	1.80237	0.43648
H	5.23042	1.23619	1.48655
H	4.73114	-1.37197	1.16405
H	6.74321	-2.46986	-0.14662

H	8.50794	-0.57435	0.70308
H	8.24823	-0.47288	-1.03354
C	-2.38812	3.92788	-2.55484
H	-2.23024	4.01117	-3.63562
H	-3.43413	4.21960	-2.35632
O	-1.47867	4.79312	-1.93017

M06/lanl2dz-6-31G(d) Energy = -2646.113213

M06/lanl2dz-6-31G(d) Free Energy = -2645.471054

M06/def2-TZVP Derived free energy = -2646.578937

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.610017

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.634542

Number of Imaginary Frequencies = 1 (-365.15)

M06/lanl2dz-6-31G(d) Geometry

C	0.89267	2.83226	-0.17917
C	1.02308	4.36191	-0.06678
C	-1.35159	3.46733	-1.12444
N	-0.52079	2.53843	-0.53456
C	-1.18027	1.35700	-0.47645
N	-2.36515	1.63836	-1.04358
N	-2.49171	2.94129	-1.45416
C	0.55918	4.67610	1.36895
C	1.03205	3.45229	2.10378
C	1.25362	2.39792	1.21047
C	1.78507	1.18751	1.64131
C	2.03747	1.01730	3.00121
C	1.78559	2.05392	3.89962
C	1.29726	3.28221	3.45666
C	-3.44018	0.71609	-1.20695
C	-3.23802	-0.44034	-2.01102
C	-4.25081	-1.44261	-2.00797
C	-5.44437	-1.22208	-1.28056
C	-5.64429	-0.06678	-0.57425
C	-4.62344	0.90256	-0.52450
C	-2.07898	-0.64803	-2.80191

C	-1.92100	-1.81258	-3.51327
C	-2.90214	-2.82548	-3.47258
C	-4.04708	-2.63509	-2.74303
H	1.51281	2.39664	-0.97032
H	2.09355	4.59400	-0.13996
H	-0.53668	4.77424	1.42687
H	0.98274	5.61386	1.74746
H	2.00744	0.39370	0.92509
H	2.43567	0.07012	3.36346
H	1.98879	1.90787	4.95892
H	1.13539	4.09612	4.16207
H	-6.21643	-1.99025	-1.29736
H	-6.56363	0.11044	-0.02188
Cl	-4.87341	2.28597	0.49585
H	-1.32296	0.13246	-2.87027
H	-1.03784	-1.94738	-4.13656
H	-2.75607	-3.74451	-4.03565
H	-4.82606	-3.39635	-2.72082
Au	-0.44103	-0.59749	0.11600
C	0.25667	-2.46491	0.62488
C	-0.57931	-3.19794	1.48651
C	1.45102	-3.00882	0.17651
C	-0.21516	-4.49002	1.85844
C	1.81123	-4.30368	0.56392
H	2.11674	-2.44185	-0.47734
C	0.97571	-5.04148	1.39357
H	-0.85448	-5.07321	2.52088
H	2.74409	-4.73884	0.20715
H	1.25384	-6.05178	1.68769
C	-1.85145	-1.14087	1.49027
C	-2.84299	-0.28700	1.93477
C	-1.75090	-2.46342	1.95458
C	-3.80562	-0.77065	2.82526
H	-2.89018	0.75004	1.61034
C	-2.72143	-2.92606	2.84192
C	-3.74867	-2.08699	3.26511

H	-4.59600	-0.10387	3.16775
H	-2.67132	-3.94843	3.21586
H	-4.50031	-2.46318	3.95648
O	1.23727	-0.09327	-1.28554
C	3.01635	-0.82787	-2.63596
C	1.67236	-0.80360	-2.23838
C	5.34777	-0.11100	-2.07371
C	3.96454	-0.12742	-1.90200
C	6.18706	0.72789	-1.31293
H	0.95987	-1.45912	-2.77273
H	3.57340	0.49051	-1.08548
H	3.30402	-1.44500	-3.48571
C	7.55330	1.06492	-1.84603
H	5.68470	1.55383	-0.80372
H	5.79441	-0.75234	-2.83818
H	8.09201	0.16705	-2.17635
H	7.45178	1.72273	-2.71972
H	8.17411	1.58984	-1.11201
C	6.68955	-0.29626	0.36958
C	5.53047	-0.25281	1.15218
C	4.69876	-1.34970	0.83280
C	5.36365	-2.15625	-0.05647
C	6.77052	-1.69737	-0.18293
H	7.58316	0.26496	0.63947
H	5.26138	0.55777	1.82624
H	3.68374	-1.51040	1.19360
H	4.96677	-3.05502	-0.52176
H	7.38924	-2.29475	0.51137
H	7.21911	-1.81158	-1.17513
O	0.42745	5.06506	-1.12441
C	-0.96063	4.90048	-1.24435
H	-1.50645	5.48511	-0.48308
H	-1.25476	5.29202	-2.22393

Top, towards, 2, exo, away

M06/lanl2dz-6-31G(d) Energy = -2646.116339

M06/lanl2dz-6-31G(d) Free Energy = -2645.476622

M06/def2-TZVP Derived free energy = -2646.587511

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618516

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.643749

Number of Imaginary Frequencies = 1 (-396.46)

M06/lanl2dz-6-31G(d) Geometry

C	-1.77068	-2.05867	-0.45136
C	-2.62339	-3.20141	-1.06268
C	0.08420	-3.23929	-1.66179
N	-0.37205	-2.20269	-0.87472
C	0.65544	-1.34837	-0.65936
N	1.66732	-1.91121	-1.34590
N	1.33371	-3.08328	-1.97257
C	-3.75759	-3.41373	-0.06373
C	-3.18565	-2.92986	1.23800
C	-2.03597	-2.16611	1.02799
C	-1.37691	-1.56082	2.09223
C	-1.88020	-1.74122	3.37922
C	-3.02461	-2.50916	3.59128
C	-3.68568	-3.10780	2.52160
C	2.98940	-1.37901	-1.41770
C	3.17057	-0.08559	-1.98426
C	4.43889	0.54282	-1.82096
C	5.48881	-0.16791	-1.19225
C	5.30880	-1.44241	-0.72606
C	4.03897	-2.04574	-0.82370
C	2.14117	0.62244	-2.65669
C	2.35031	1.90652	-3.09826
C	3.59327	2.54318	-2.90054
C	4.61670	1.86751	-2.28579
H	-2.11019	-1.08399	-0.83827
H	-2.96969	-2.94620	-2.08083

H	-4.05571	-4.46950	-0.05902
H	-4.64568	-2.82668	-0.34710
H	-0.47511	-0.96558	1.93850
H	-1.37094	-1.28208	4.22420
H	-3.40232	-2.64524	4.60288
H	-4.57776	-3.70980	2.68992
H	6.45751	0.31834	-1.08301
H	6.11554	-1.99067	-0.24616
Cl	3.82475	-3.61111	-0.10442
H	1.17964	0.14443	-2.83769
H	1.54846	2.43370	-3.61208
H	3.74123	3.56254	-3.24994
H	5.58887	2.33928	-2.14599
Au	0.87671	0.66287	0.18402
C	1.41171	2.58497	0.67978
C	2.53072	2.69086	1.52423
C	0.84129	3.71625	0.11892
C	3.04195	3.95193	1.82312
C	1.36293	4.97625	0.42642
H	0.00623	3.64264	-0.57737
C	2.45414	5.09037	1.27980
H	3.90839	4.05173	2.47665
H	0.91481	5.86766	-0.00961
H	2.85866	6.07245	1.51728
C	2.39448	0.27727	1.50073
C	2.72960	-1.00038	1.90787
C	3.05402	1.41376	1.99777
C	3.78683	-1.16781	2.80744
H	2.19329	-1.87498	1.54234
C	4.11050	1.22316	2.88753
C	4.47878	-0.06033	3.28135
H	4.06494	-2.17255	3.12147
H	4.64468	2.08507	3.28673
H	5.30437	-0.19315	3.97786
O	-1.00159	1.15751	-0.97349
C	-3.19956	2.00951	-0.81340

C	-1.89592	1.78032	-0.34204
C	-5.44160	2.96126	-0.29279
C	-4.09111	2.71653	-0.02096
C	-6.09999	2.46225	-1.42324
H	-1.65948	2.18570	0.66271
H	-3.70159	3.10256	0.92545
H	-3.45442	1.64701	-1.80915
C	-7.41211	3.05703	-1.84475
H	-5.47032	2.13255	-2.25192
H	-6.01548	3.54262	0.42964
H	-7.98230	2.40454	-2.51533
H	-8.04397	3.31105	-0.98445
H	-7.22026	3.99182	-2.38970
C	-6.66268	0.52751	-0.90839
C	-5.47232	-0.16570	-0.68603
C	-5.11295	-0.07581	0.68539
C	-6.10697	0.57733	1.35730
C	-7.26845	0.78068	0.45009
H	-7.27629	0.35455	-1.79134
H	-4.87799	-0.64518	-1.46248
H	-4.17416	-0.42312	1.11487
H	-6.11077	0.81923	2.41609
H	-8.00869	-0.01643	0.64402
H	-7.80208	1.72813	0.57930
C	-0.83439	-4.34930	-2.03467
H	-1.21850	-4.20199	-3.06084
H	-0.30520	-5.30702	-2.00598
O	-1.88471	-4.40259	-1.10669

M06/lanl2dz-6-31G(d) Energy = -2646.112818

M06/lanl2dz-6-31G(d) Free Energy = -2645.474860

M06/def2-TZVP Derived free energy = -2646.583051

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.613986

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.638847

Number of Imaginary Frequencies = 1 (-375.44)

M06/lanl2dz-6-31G(d) Geometry

C	-1.86242	1.90137	-0.59123
C	-2.86910	3.02968	-0.27557
C	-1.11731	2.41085	1.76909
N	-0.92881	1.79316	0.55259
C	0.20533	1.05936	0.61826
N	0.64311	1.28796	1.86780
N	-0.16438	2.11798	2.60111
C	-2.22223	4.31603	-0.81416
C	-1.39279	3.79471	-1.95132
C	-1.19201	2.41584	-1.83402
C	-0.46898	1.71581	-2.79284
C	0.07969	2.41660	-3.86310
C	-0.11143	3.79366	-3.97539
C	-0.85508	4.49050	-3.02610
C	1.86507	0.78568	2.40670
C	2.01206	-0.61506	2.60003
C	3.30348	-1.10789	2.94746
C	4.36434	-0.19350	3.15112
C	4.18207	1.15593	3.00644
C	2.92143	1.64559	2.61284
C	0.95337	-1.54003	2.41538
C	1.18127	-2.88943	2.53281
C	2.46362	-3.38000	2.85726
C	3.49757	-2.50425	3.07041
H	-2.34087	0.91660	-0.70103
H	-3.77585	2.82218	-0.86022
H	-1.58603	4.79933	-0.05616
H	-2.97229	5.05816	-1.11271
H	-0.33449	0.63594	-2.71923
H	0.65110	1.88486	-4.62094
H	0.31768	4.32769	-4.82100
H	-1.01437	5.56314	-3.12824
H	5.34389	-0.58284	3.42591
H	4.99601	1.86027	3.15725
Cl	2.76263	3.34973	2.31499

H	-0.04768	-1.18394	2.17860
H	0.36102	-3.58779	2.37715
H	2.62631	-4.45192	2.94460
H	4.48967	-2.86883	3.33465
Au	0.98178	-0.57729	-0.60210
C	1.82056	-2.25709	-1.43576
C	3.19087	-2.15282	-1.73421
C	1.15397	-3.46192	-1.58626
C	3.86700	-3.26872	-2.22264
C	1.84309	-4.57479	-2.07735
H	0.10404	-3.56214	-1.31136
C	3.19122	-4.47333	-2.39885
H	4.92806	-3.20570	-2.46347
H	1.32185	-5.52250	-2.20243
H	3.72560	-5.34056	-2.78211
C	2.86887	0.11425	-0.95804
C	3.24233	1.42420	-0.71984
C	3.76496	-0.83508	-1.47675
C	4.56735	1.80108	-0.95722
H	2.52871	2.16042	-0.35304
C	5.08220	-0.43787	-1.70339
C	5.48043	0.86936	-1.43654
H	4.87470	2.82724	-0.76101
H	5.80422	-1.15206	-2.09885
H	6.51249	1.16378	-1.61750
O	-1.13054	-1.34208	-0.38634
C	-3.10318	-2.15280	-1.41942
C	-1.75381	-1.77270	-1.40047
C	-5.22444	-2.59294	-0.23562
C	-3.90418	-2.14031	-0.28625
C	-5.96450	-2.75396	0.95055
H	-1.20569	-1.86804	-2.35649
H	-3.44582	-1.79366	0.64604
H	-3.50797	-2.51428	-2.36468
C	-7.06331	-3.78319	0.98201
H	-5.38953	-2.68153	1.87677

H	-5.68359	-2.91736	-1.17436
H	-7.67136	-3.72238	1.89107
H	-7.72813	-3.69142	0.11284
H	-6.62188	-4.78847	0.94984
C	-7.08154	-1.05942	1.18098
C	-6.15405	-0.19252	1.76386
C	-5.43067	0.48188	0.75395
C	-5.96865	0.14649	-0.46310
C	-7.22874	-0.61492	-0.25146
H	-7.91882	-1.47224	1.74119
H	-5.94952	-0.12567	2.82975
H	-4.57988	1.13818	0.92753
H	-5.61120	0.47841	-1.43510
H	-8.06970	0.10162	-0.28724
H	-7.44849	-1.39095	-0.99113
C	-2.28746	3.29914	2.00954
H	-2.70930	3.10812	3.00184
H	-1.97302	4.35565	1.98923
O	-3.30099	3.04312	1.06678

M06/lanl2dz-6-31G(d) Energy = -2646.112818

M06/lanl2dz-6-31G(d) Free Energy = -2645.474861

M06/def2-TZVP Derived free energy = -2646.583052

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.613987

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.638848

Number of Imaginary Frequencies = 1 (-375.44)

M06/lanl2dz-6-31G(d) Geometry

C	-1.86241	1.90138	-0.59123
C	-2.86910	3.02968	-0.27557
C	-1.11732	2.41085	1.76909
N	-0.92882	1.79316	0.55259
C	0.20533	1.05936	0.61826
N	0.64310	1.28796	1.86780
N	-0.16439	2.11797	2.60112
C	-2.22223	4.31603	-0.81416

C	-1.39279	3.79473	-1.95131
C	-1.19201	2.41585	-1.83401
C	-0.46898	1.71582	-2.79284
C	0.07970	2.41662	-3.86309
C	-0.11142	3.79368	-3.97538
C	-0.85507	4.49051	-3.02609
C	1.86506	0.78567	2.40671
C	2.01205	-0.61508	2.60003
C	3.30346	-1.10791	2.94746
C	4.36433	-0.19352	3.15113
C	4.18206	1.15590	3.00646
C	2.92142	1.64558	2.61285
C	0.95335	-1.54004	2.41537
C	1.18125	-2.88944	2.53278
C	2.46360	-3.38001	2.85723
C	3.49755	-2.50427	3.07039
H	-2.34086	0.91661	-0.70104
H	-3.77585	2.82219	-0.86023
H	-1.58604	4.79934	-0.05615
H	-2.97229	5.05817	-1.11271
H	-0.33448	0.63595	-2.71923
H	0.65112	1.88489	-4.62094
H	0.31770	4.32771	-4.82099
H	-1.01437	5.56316	-3.12823
H	5.34387	-0.58287	3.42592
H	4.99600	1.86024	3.15728
Cl	2.76262	3.34972	2.31501
H	-0.04770	-1.18394	2.17859
H	0.36100	-3.58780	2.37711
H	2.62629	-4.45194	2.94457
H	4.48965	-2.86886	3.33464
Au	0.98178	-0.57728	-0.60210
C	1.82057	-2.25708	-1.43576
C	3.19088	-2.15281	-1.73421
C	1.15398	-3.46191	-1.58628
C	3.86701	-3.26871	-2.22265

C	1.84310	-4.57478	-2.07737
H	0.10404	-3.56214	-1.31137
C	3.19123	-4.47332	-2.39886
H	4.92807	-3.20568	-2.46347
H	1.32186	-5.52249	-2.20245
H	3.72561	-5.34055	-2.78212
C	2.86887	0.11426	-0.95803
C	3.24233	1.42420	-0.71983
C	3.76496	-0.83508	-1.47674
C	4.56736	1.80109	-0.95720
H	2.52871	2.16042	-0.35302
C	5.08220	-0.43786	-1.70338
C	5.48043	0.86937	-1.43652
H	4.87471	2.82724	-0.76099
H	5.80423	-1.15205	-2.09883
H	6.51250	1.16379	-1.61747
O	-1.13054	-1.34208	-0.38635
C	-3.10318	-2.15279	-1.41943
C	-1.75381	-1.77269	-1.40048
C	-5.22444	-2.59294	-0.23564
C	-3.90418	-2.14031	-0.28626
C	-5.96449	-2.75397	0.95054
H	-1.20569	-1.86802	-2.35651
H	-3.44582	-1.79367	0.64603
H	-3.50797	-2.51427	-2.36470
C	-7.06330	-3.78319	0.98200
H	-5.38952	-2.68155	1.87675
H	-5.68359	-2.91735	-1.17438
H	-7.67135	-3.72239	1.89105
H	-7.72813	-3.69142	0.11282
H	-6.62188	-4.78848	0.94981
C	-7.08153	-1.05943	1.18098
C	-6.15404	-0.19253	1.76387
C	-5.43066	0.48187	0.75396
C	-5.96864	0.14648	-0.46310
C	-7.22873	-0.61492	-0.25145

H	-7.91881	-1.47225	1.74119
H	-5.94950	-0.12569	2.82975
H	-4.57987	1.13817	0.92753
H	-5.61120	0.47841	-1.43510
H	-8.06969	0.10162	-0.28723
H	-7.44850	-1.39095	-0.99113
O	-3.30099	3.04312	1.06678
C	-2.28747	3.29913	2.00954
H	-2.70931	3.10811	3.00184
H	-1.97303	4.35564	1.98923

M06/lanl2dz-6-31G(d) Energy = -2646.113423

M06/lanl2dz-6-31G(d) Free Energy = -2645.475871

M06/def2-TZVP Derived free energy = -2646.585567

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617099

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642590

Number of Imaginary Frequencies = 1 (-390.26)

M06/lanl2dz-6-31G(d) Geometry

C	-1.52312	1.96364	-0.81211
C	-2.31651	3.27190	-0.62989
C	-1.15015	2.33423	1.65998
N	-0.84619	1.68590	0.48083
C	0.19462	0.84972	0.71433
N	0.46789	1.05157	2.01069
N	-0.35852	1.96333	2.61912
C	-1.29339	4.38935	-0.90546
C	-0.39008	3.73180	-1.91028
C	-0.55105	2.34162	-1.89268
C	0.12776	1.53133	-2.79415
C	1.02441	2.12040	-3.68149
C	1.21253	3.50150	-3.67716
C	0.49589	4.31802	-2.80378
C	1.58655	0.52612	2.72688
C	1.60211	-0.83769	3.12233
C	2.75727	-1.32062	3.80638

C	3.82162	-0.43188	4.08664
C	3.77685	0.88191	3.70084
C	2.64911	1.35869	3.00542
C	0.53795	-1.73213	2.85542
C	0.63139	-3.05021	3.22896
C	1.77453	-3.53293	3.90073
C	2.81116	-2.68206	4.18730
H	-2.17344	1.10630	-1.04044
H	-3.07981	3.29648	-1.41864
H	-0.73774	4.66926	0.00324
H	-1.77270	5.30405	-1.27430
H	-0.02392	0.45114	-2.81289
H	1.58264	1.49673	-4.37732
H	1.91566	3.94906	-4.37691
H	0.62438	5.39932	-2.82908
H	4.69396	-0.81201	4.61693
H	4.59601	1.56507	3.90942
Cl	2.64470	3.01851	2.48411
H	-0.35293	-1.38110	2.33974
H	-0.18977	-3.72884	3.00626
H	1.82844	-4.57961	4.19208
H	3.69759	-3.04032	4.70965
Au	0.97895	-0.76897	-0.50548
C	1.71510	-2.31447	-1.63127
C	2.96129	-2.07253	-2.23599
C	1.06298	-3.52457	-1.79786
C	3.53994	-3.06961	-3.01737
C	1.65496	-4.51682	-2.58542
H	0.10537	-3.71319	-1.31331
C	2.88567	-4.28707	-3.18956
H	4.50724	-2.90503	-3.49213
H	1.15218	-5.47324	-2.71953
H	3.34446	-5.06311	-3.79929
C	2.74347	0.05798	-1.10885
C	3.12371	1.34085	-0.76211
C	3.51904	-0.75257	-1.95429

C	4.33184	1.84030	-1.25534
H	2.50079	1.96628	-0.12423
C	4.71714	-0.22964	-2.44024
C	5.12019	1.05583	-2.08913
H	4.64648	2.84599	-0.98128
H	5.34414	-0.83172	-3.09752
H	6.06056	1.44715	-2.47293
O	-0.99912	-1.75388	-0.00149
C	-3.30136	-1.88237	-0.52590
C	-1.95548	-1.59317	-0.80092
C	-5.65578	-1.66435	-1.34410
C	-4.26862	-1.51811	-1.44969
C	-6.30236	-2.30733	-0.28048
H	-1.74707	-1.18549	-1.81418
H	-3.90185	-1.04730	-2.36784
H	-3.54083	-2.35508	0.42639
C	-7.69960	-2.82248	-0.47547
H	-5.68004	-2.92750	0.36777
H	-6.26954	-1.27815	-2.15915
H	-8.18964	-3.09333	0.46590
H	-8.33333	-2.09929	-1.00422
H	-7.66152	-3.73032	-1.09350
C	-6.64793	-0.84149	1.15952
C	-5.37812	-0.53553	1.64232
C	-4.84423	0.56209	0.91822
C	-5.78712	1.02151	0.04533
C	-7.07584	0.32064	0.29945
H	-7.36127	-1.42672	1.73710
H	-4.85588	-1.08313	2.42371
H	-3.83777	0.95585	1.02520
H	-5.66396	1.85075	-0.64582
H	-7.71436	0.97760	0.91721
H	-7.66205	0.07648	-0.59306
O	-3.03539	3.32243	0.57867
C	-2.23977	3.34968	1.73768
H	-1.80657	4.34873	1.91185

H -2.89878 3.13119 2.58613

M06/lanl2dz-6-31G(d) Energy = -2646.114793

M06/lanl2dz-6-31G(d) Free Energy = -2645.475946

M06/def2-TZVP Derived free energy = -2646.586391

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617543

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642834

Number of Imaginary Frequencies = 1 (-378.06)

M06/lanl2dz-6-31G(d) Geometry

C	1.44955	2.20976	-0.74704
C	2.13932	3.43913	-1.38260
C	-0.62561	3.48479	-1.34094
N	-0.00612	2.36747	-0.82439
C	-0.95333	1.44119	-0.55004
N	-2.09083	2.04691	-0.93770
N	-1.90898	3.31408	-1.42976
C	3.48690	3.52266	-0.67169
C	3.21728	2.89796	0.66979
C	2.03961	2.14748	0.63760
C	1.59842	1.46182	1.76235
C	2.34579	1.55164	2.93663
C	3.51651	2.30780	2.97425
C	3.96325	2.98167	1.83802
C	-3.38221	1.44341	-0.89072
C	-3.58815	0.23943	-1.62243
C	-4.77726	-0.50266	-1.36707
C	-5.74968	0.03076	-0.48759
C	-5.56578	1.23759	0.13274
C	-4.35679	1.93791	-0.05248
C	-2.64703	-0.28052	-2.54817
C	-2.85069	-1.50376	-3.13954
C	-4.00404	-2.26146	-2.84759
C	-4.95148	-1.76096	-1.99124
H	1.68756	1.30283	-1.32169
H	2.22336	3.33753	-2.47907

H	3.82416	4.56526	-0.62189
H	4.24658	2.95998	-1.23795
H	0.67418	0.88120	1.74858
H	2.00253	1.03874	3.83308
H	4.08189	2.38100	3.90170
H	4.87209	3.58235	1.87343
H	-6.66146	-0.53775	-0.30846
H	-6.31380	1.65128	0.80457
Cl	-4.10020	3.38577	0.86864
H	-1.76030	0.29727	-2.80509
H	-2.11635	-1.88713	-3.84558
H	-4.14582	-3.23357	-3.31468
H	-5.85866	-2.32468	-1.77553
Au	-0.89359	-0.68226	-0.00195
C	-1.19122	-2.69705	0.24414
C	-2.18165	-3.04369	1.17934
C	-0.59917	-3.66060	-0.55554
C	-2.54455	-4.38160	1.31912
C	-0.97112	-4.99979	-0.40439
H	0.13497	-3.38666	-1.31319
C	-1.93532	-5.35499	0.53222
H	-3.31062	-4.67092	2.03854
H	-0.50743	-5.76313	-1.02715
H	-2.22316	-6.39838	0.64655
C	-2.22937	-0.65521	1.54645
C	-2.58484	0.50250	2.21289
C	-2.73428	-1.91289	1.91833
C	-3.51382	0.42486	3.25514
H	-2.15799	1.46723	1.94180
C	-3.67100	-1.96538	2.94925
C	-4.06351	-0.80197	3.60611
H	-3.80683	1.33383	3.77824
H	-4.08664	-2.92497	3.25607
H	-4.79307	-0.85989	4.41165
O	0.83837	-0.82756	-1.44117
C	3.17593	-1.15379	-1.51823

C	1.90301	-1.30445	-0.95658
C	5.59485	-1.72576	-1.33173
C	4.26544	-1.74440	-0.90068
C	6.60154	-2.50861	-0.73610
H	1.84696	-1.88206	-0.01126
H	4.06007	-2.31772	0.01187
H	3.28362	-0.60137	-2.45332
C	7.80665	-2.88609	-1.55519
H	6.24831	-3.29654	-0.06673
H	5.84429	-1.13411	-2.21664
H	7.51185	-3.61568	-2.32150
H	8.22981	-2.01826	-2.07816
H	8.59763	-3.34703	-0.95389
C	7.48563	-1.35563	0.69622
C	6.54181	-1.36720	1.72799
C	5.60594	-0.32805	1.52653
C	6.01090	0.42008	0.44961
C	7.37519	-0.00226	0.04073
H	8.43866	-1.87598	0.77988
H	6.47690	-2.12613	2.50411
H	4.69020	-0.16802	2.09192
H	5.47429	1.27226	0.03921
H	7.58915	0.04414	-1.03186
H	8.10405	0.66510	0.53588
C	0.18488	4.67622	-1.71973
H	0.31174	4.71632	-2.81706
H	-0.31889	5.59588	-1.40543
O	1.42734	4.61751	-1.07003

M06/lanl2dz-6-31G(d) Energy = -2646.114794

M06/lanl2dz-6-31G(d) Free Energy = -2645.475953

M06/def2-TZVP Derived free energy = -2646.586398

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617550

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642842

Number of Imaginary Frequencies = 1 (-378.04)

M06/lanl2dz-6-31G(d) Geometry

C	1.44941	2.20989	-0.74697
C	2.13908	3.43936	-1.38246
C	-0.62584	3.48493	-1.34052
N	-0.00627	2.36757	-0.82416
C	-0.95343	1.44124	-0.54980
N	-2.09099	2.04698	-0.93728
N	-1.90922	3.31420	-1.42923
C	3.48674	3.52283	-0.67170
C	3.21730	2.89795	0.66973
C	2.03963	2.14746	0.63759
C	1.59859	1.46165	1.76231
C	2.34610	1.55133	2.93650
C	3.51682	2.30750	2.97408
C	3.96340	2.98151	1.83788
C	-3.38236	1.44346	-0.89020
C	-3.58837	0.23952	-1.62195
C	-4.77743	-0.50260	-1.36649
C	-5.74974	0.03073	-0.48685
C	-5.56580	1.23754	0.13352
C	-4.35685	1.93789	-0.05181
C	-2.64736	-0.28034	-2.54786
C	-2.85108	-1.50353	-3.13930
C	-4.00437	-2.26127	-2.84725
C	-4.95171	-1.76087	-1.99072
H	1.68738	1.30304	-1.32176
H	2.22300	3.33789	-2.47896
H	3.82397	4.56544	-0.62180
H	4.24637	2.96025	-1.23812
H	0.67435	0.88101	1.74858
H	2.00296	1.03831	3.83293
H	4.08231	2.38058	3.90146
H	4.87225	3.58220	1.87325
H	-6.66148	-0.53781	-0.30762
H	-6.31374	1.65116	0.80548
Cl	-4.10018	3.38570	0.86938

H	-1.76068	0.29749	-2.80484
H	-2.11683	-1.88683	-3.84547
H	-4.14619	-3.23336	-3.31439
H	-5.85884	-2.32463	-1.77492
Au	-0.89357	-0.68226	-0.00192
C	-1.19106	-2.69709	0.24405
C	-2.18137	-3.04387	1.17933
C	-0.59900	-3.66056	-0.55573
C	-2.54414	-4.38181	1.31908
C	-0.97081	-4.99979	-0.40460
H	0.13504	-3.38652	-1.31344
C	-1.93489	-5.35511	0.53207
H	-3.31011	-4.67124	2.03856
H	-0.50711	-5.76305	-1.02744
H	-2.22262	-6.39853	0.64639
C	-2.22920	-0.65542	1.54662
C	-2.58468	0.50222	2.21318
C	-2.73402	-1.91315	1.91844
C	-3.51357	0.42445	3.25551
H	-2.15788	1.46699	1.94215
C	-3.67066	-1.96577	2.94942
C	-4.06317	-0.80244	3.60641
H	-3.80658	1.33336	3.77871
H	-4.08622	-2.92542	3.25620
H	-4.79267	-0.86046	4.41200
O	0.83822	-0.82735	-1.44134
C	3.17577	-1.15358	-1.51877
C	1.90293	-1.30430	-0.95696
C	5.59472	-1.72557	-1.33263
C	4.26536	-1.74426	-0.90143
C	6.60149	-2.50846	-0.73718
H	1.84701	-1.88202	-0.01170
H	4.06011	-2.31770	0.01108
H	3.28334	-0.60105	-2.45381
C	7.80653	-2.88582	-1.55644
H	6.24834	-3.29647	-0.06786

H	5.84406	-1.13381	-2.21750
H	7.51168	-3.61535	-2.32278
H	8.22961	-2.01792	-2.07937
H	8.59759	-3.34678	-0.95525
C	7.48569	-1.35561	0.69517
C	6.54196	-1.36728	1.72703
C	5.60605	-0.32812	1.52574
C	6.01091	0.42010	0.44884
C	7.37517	-0.00219	0.03981
H	8.43873	-1.87595	0.77871
H	6.47713	-2.12627	2.50309
H	4.69036	-0.16816	2.09122
H	5.47424	1.27228	0.03854
H	7.58903	0.04430	-1.03280
H	8.10407	0.66515	0.53494
O	1.42710	4.61768	-1.06968
C	0.18457	4.67644	-1.71925
H	0.31133	4.71667	-2.81658
H	-0.31919	5.59604	-1.40478

M06/lanl2dz-6-31G(d) Energy = -2646.109587

M06/lanl2dz-6-31G(d) Free Energy = -2645.474028

M06/def2-TZVP Derived free energy = -2646.584209

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616515

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.643206

Number of Imaginary Frequencies = 1 (-362.68)

M06/lanl2dz-6-31G(d) Geometry

C	-1.14550	2.61163	-0.12137
C	-2.31101	3.50150	0.36963
C	-1.11918	1.88590	2.27540
N	-0.68300	1.75364	0.97543
C	0.15819	0.69258	0.91056
N	0.17543	0.24260	2.17521
N	-0.61611	0.96368	3.03678
C	-2.27643	4.70271	-0.56856

C	-0.82190	4.80664	-0.93615
C	-0.15418	3.61318	-0.65628
C	1.20203	3.47205	-0.91570
C	1.89005	4.55422	-1.46114
C	1.22608	5.74587	-1.74554
C	-0.13618	5.88006	-1.48591
C	0.91032	-0.87892	2.66267
C	0.52462	-2.18711	2.25934
C	1.29685	-3.28817	2.73175
C	2.39112	-3.04763	3.59630
C	2.72589	-1.77908	3.98873
C	1.97668	-0.68425	3.51392
C	-0.58152	-2.44424	1.41215
C	-0.88930	-3.72977	1.03946
C	-0.12021	-4.81989	1.49771
C	0.94756	-4.59918	2.32977
H	-1.50626	1.93438	-0.91401
H	-3.27448	2.95784	0.36882
H	-2.67627	5.59054	-0.06348
H	-2.90442	4.51523	-1.45303
H	1.73365	2.54702	-0.69200
H	2.95571	4.46539	-1.66222
H	1.77838	6.58235	-2.16932
H	-0.64988	6.81675	-1.69861
H	2.97239	-3.89736	3.95224
H	3.56378	-1.59283	4.65547
Cl	2.44347	0.90971	4.01761
H	-1.18317	-1.61864	1.03611
H	-1.73718	-3.90935	0.37944
H	-0.37674	-5.83173	1.19183
H	1.54842	-5.43122	2.69521
Au	1.04235	-0.32529	-0.80707
C	1.88768	-1.38010	-2.35237
C	3.29026	-1.31503	-2.42116
C	1.16932	-2.14473	-3.25639
C	3.95447	-2.00500	-3.43222

C	1.84742	-2.83475	-4.26570
H	0.08547	-2.23049	-3.18691
C	3.23192	-2.75767	-4.35401
H	5.04103	-1.96295	-3.50414
H	1.28658	-3.43557	-4.97966
H	3.75694	-3.29331	-5.14262
C	3.01657	0.05951	-0.44797
C	3.45720	0.84080	0.60523
C	3.90977	-0.51585	-1.36825
C	4.82935	1.05335	0.76565
H	2.76104	1.29422	1.30902
C	5.27354	-0.28827	-1.19117
C	5.72919	0.48924	-0.13001
H	5.18221	1.66225	1.59640
H	5.99010	-0.72146	-1.88849
H	6.79743	0.65502	-0.00457
O	-1.08573	-0.76641	-1.32547
C	-2.96712	-0.71504	-2.73085
C	-1.61659	-0.47014	-2.43657
C	-5.12455	-1.58366	-1.77392
C	-3.74126	-1.39141	-1.80093
C	-5.74938	-2.40119	-0.80550
H	-0.99695	0.02680	-3.20433
H	-3.18305	-1.82826	-0.96637
H	-3.38416	-0.33906	-3.66335
C	-7.14743	-2.89288	-1.07190
H	-5.09925	-3.13877	-0.32855
H	-5.74554	-1.08366	-2.52204
H	-7.59548	-3.37801	-0.19799
H	-7.80913	-2.07679	-1.39135
H	-7.12770	-3.63263	-1.88312
C	-6.03053	-1.26129	0.81854
C	-4.74665	-1.14082	1.37417
C	-4.07831	-0.05441	0.77505
C	-4.95641	0.59415	-0.06196
C	-6.32710	0.06829	0.16579

H	-6.81271	-1.83680	1.31309
H	-4.29352	-1.85092	2.06258
H	-3.01325	0.16002	0.86823
H	-4.71568	1.42736	-0.71890
H	-6.82682	0.70478	0.91851
H	-6.97870	0.04859	-0.71338
O	-2.04409	3.97854	1.67186
C	-2.07883	2.96643	2.63939
H	-3.09631	2.54235	2.73706
H	-1.80631	3.40935	3.60281

M06/lanl2dz-6-31G(d) Energy = -2646.116339

M06/lanl2dz-6-31G(d) Free Energy = -2645.476622

M06/def2-TZVP Derived free energy = -2646.587511

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618516

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.643749

Number of Imaginary Frequencies = 1 (-396.46)

M06/lanl2dz-6-31G(d) Geometry

C	-1.77068	-2.05866	-0.45136
C	-2.62339	-3.20141	-1.06268
C	0.08420	-3.23929	-1.66179
N	-0.37206	-2.20269	-0.87472
C	0.65543	-1.34836	-0.65936
N	1.66732	-1.91120	-1.34591
N	1.33370	-3.08328	-1.97257
C	-3.75760	-3.41373	-0.06372
C	-3.18565	-2.92986	1.23800
C	-2.03597	-2.16611	1.02799
C	-1.37691	-1.56082	2.09223
C	-1.88020	-1.74122	3.37922
C	-3.02461	-2.50916	3.59128
C	-3.68568	-3.10780	2.52160
C	2.98939	-1.37901	-1.41771
C	3.17056	-0.08558	-1.98427
C	4.43888	0.54282	-1.82097

C	5.48881	-0.16790	-1.19226
C	5.30880	-1.44240	-0.72607
C	4.03896	-2.04573	-0.82371
C	2.14116	0.62244	-2.65670
C	2.35030	1.90652	-3.09826
C	3.59326	2.54319	-2.90055
C	4.61669	1.86751	-2.28580
H	-2.11019	-1.08399	-0.83826
H	-2.96970	-2.94620	-2.08082
H	-4.05571	-4.46949	-0.05902
H	-4.64568	-2.82667	-0.34710
H	-0.47511	-0.96558	1.93850
H	-1.37094	-1.28209	4.22421
H	-3.40232	-2.64524	4.60289
H	-4.57776	-3.70980	2.68992
H	6.45750	0.31835	-1.08302
H	6.11553	-1.99066	-0.24617
Cl	3.82475	-3.61111	-0.10443
H	1.17963	0.14443	-2.83769
H	1.54845	2.43370	-3.61209
H	3.74122	3.56254	-3.24995
H	5.58886	2.33928	-2.14600
Au	0.87672	0.66287	0.18402
C	1.41172	2.58497	0.67979
C	2.53073	2.69085	1.52424
C	0.84130	3.71625	0.11893
C	3.04196	3.95192	1.82313
C	1.36295	4.97624	0.42644
H	0.00624	3.64264	-0.57735
C	2.45416	5.09035	1.27982
H	3.90841	4.05172	2.47666
H	0.91483	5.86766	-0.00959
H	2.85868	6.07243	1.51730
C	2.39449	0.27726	1.50073
C	2.72960	-1.00039	1.90787
C	3.05403	1.41375	1.99777

C	3.78684	-1.16783	2.80743
H	2.19329	-1.87499	1.54233
C	4.11051	1.22314	2.88752
C	4.47879	-0.06036	3.28133
H	4.06494	-2.17258	3.12145
H	4.64470	2.08504	3.28672
H	5.30439	-0.19318	3.97784
O	-1.00159	1.15752	-0.97348
C	-3.19956	2.00952	-0.81339
C	-1.89592	1.78032	-0.34203
C	-5.44160	2.96126	-0.29278
C	-4.09112	2.71653	-0.02095
C	-6.09999	2.46225	-1.42323
H	-1.65949	2.18569	0.66272
H	-3.70159	3.10255	0.92546
H	-3.45442	1.64703	-1.80915
C	-7.41210	3.05705	-1.84475
H	-5.47031	2.13256	-2.25192
H	-6.01549	3.54261	0.42965
H	-7.22025	3.99183	-2.38969
H	-7.98229	2.40455	-2.51533
H	-8.04397	3.31105	-0.98445
C	-6.66268	0.52752	-0.90839
C	-5.47233	-0.16569	-0.68603
C	-5.11296	-0.07581	0.68538
C	-6.10698	0.57733	1.35730
C	-7.26845	0.78068	0.45008
H	-7.27629	0.35456	-1.79135
H	-4.87799	-0.64518	-1.46249
H	-4.17416	-0.42312	1.11486
H	-6.11078	0.81923	2.41608
H	-8.00869	-0.01643	0.64401
H	-7.80208	1.72813	0.57929
C	-0.83439	-4.34930	-2.03467
H	-1.21851	-4.20198	-3.06084
H	-0.30520	-5.30701	-2.00598

O -1.88471 -4.40259 -1.10670

M06/lanl2dz-6-31G(d) Energy = -2646.116339

M06/lanl2dz-6-31G(d) Free Energy = -2645.476622

M06/def2-TZVP Derived free energy = -2646.587511

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618516

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.643749

Number of Imaginary Frequencies = 1 (-396.46)

M06/lanl2dz-6-31G(d) Geometry

C -1.77068 -2.05866 -0.45136
C -2.62339 -3.20141 -1.06268
C 0.08420 -3.23929 -1.66179
N -0.37206 -2.20269 -0.87472
C 0.65543 -1.34836 -0.65936
N 1.66732 -1.91120 -1.34591
N 1.33370 -3.08328 -1.97257
C -3.75760 -3.41373 -0.06372
C -3.18565 -2.92986 1.23800
C -2.03597 -2.16611 1.02799
C -1.37691 -1.56082 2.09223
C -1.88020 -1.74122 3.37922
C -3.02461 -2.50915 3.59128
C -3.68568 -3.10780 2.52160
C 2.98939 -1.37901 -1.41771
C 3.17057 -0.08559 -1.98427
C 4.43888 0.54282 -1.82097
C 5.48881 -0.16790 -1.19225
C 5.30880 -1.44240 -0.72607
C 4.03896 -2.04573 -0.82371
C 2.14116 0.62244 -2.65670
C 2.35030 1.90652 -3.09827
C 3.59326 2.54318 -2.90055
C 4.61669 1.86751 -2.28580
H -2.11019 -1.08399 -0.83826
H -2.96970 -2.94620 -2.08082

H	-4.05571	-4.46950	-0.05902
H	-4.64568	-2.82668	-0.34710
H	-0.47511	-0.96558	1.93850
H	-1.37094	-1.28208	4.22421
H	-3.40232	-2.64524	4.60289
H	-4.57776	-3.70980	2.68992
H	6.45750	0.31836	-1.08302
H	6.11553	-1.99066	-0.24616
Cl	3.82475	-3.61111	-0.10443
H	1.17963	0.14443	-2.83769
H	1.54844	2.43370	-3.61209
H	3.74122	3.56254	-3.24995
H	5.58886	2.33928	-2.14600
Au	0.87672	0.66287	0.18402
C	1.41172	2.58497	0.67979
C	2.53073	2.69085	1.52423
C	0.84130	3.71625	0.11893
C	3.04196	3.95192	1.82313
C	1.36294	4.97624	0.42644
H	0.00623	3.64264	-0.57735
C	2.45416	5.09036	1.27982
H	3.90840	4.05172	2.47666
H	0.91482	5.86765	-0.00959
H	2.85867	6.07244	1.51729
C	2.39449	0.27726	1.50073
C	2.72960	-1.00039	1.90787
C	3.05403	1.41375	1.99777
C	3.78684	-1.16783	2.80743
H	2.19329	-1.87498	1.54234
C	4.11051	1.22314	2.88752
C	4.47879	-0.06035	3.28133
H	4.06494	-2.17257	3.12146
H	4.64470	2.08505	3.28672
H	5.30439	-0.19317	3.97784
O	-1.00158	1.15752	-0.97348
C	-3.19956	2.00951	-0.81339

C	-1.89592	1.78032	-0.34203
C	-5.44160	2.96126	-0.29278
C	-4.09112	2.71653	-0.02096
C	-6.09999	2.46225	-1.42324
H	-1.65949	2.18570	0.66272
H	-3.70159	3.10255	0.92546
H	-3.45441	1.64702	-1.80915
C	-7.41210	3.05704	-1.84475
H	-5.47031	2.13255	-2.25192
H	-6.01548	3.54261	0.42964
H	-7.22025	3.99182	-2.38970
H	-7.98229	2.40455	-2.51534
H	-8.04397	3.31105	-0.98445
C	-6.66268	0.52751	-0.90839
C	-5.47233	-0.16570	-0.68603
C	-5.11296	-0.07581	0.68539
C	-6.10697	0.57734	1.35730
C	-7.26845	0.78068	0.45009
H	-7.27629	0.35455	-1.79134
H	-4.87800	-0.64518	-1.46248
H	-4.17416	-0.42312	1.11487
H	-6.11077	0.81924	2.41608
H	-8.00869	-0.01642	0.64402
H	-7.80208	1.72813	0.57929
O	-1.88471	-4.40259	-1.10669
C	-0.83439	-4.34930	-2.03467
H	-1.21851	-4.20198	-3.06084
H	-0.30520	-5.30702	-2.00598

M06/lanl2dz-6-31G(d) Energy = -2646.114794

M06/lanl2dz-6-31G(d) Free Energy = -2645.475957

M06/def2-TZVP Derived free energy = -2646.586401

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617554

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642845

Number of Imaginary Frequencies = 1 (-378.03)

M06/lanl2dz-6-31G(d) Geometry

C	1.44934	2.20993	-0.74713
C	2.13896	3.43940	-1.38268
C	-0.62596	3.48489	-1.34067
N	-0.00635	2.36757	-0.82427
C	-0.95348	1.44123	-0.54985
N	-2.09106	2.04692	-0.93733
N	-1.90933	3.31413	-1.42934
C	3.48665	3.52292	-0.67197
C	3.21726	2.89808	0.66949
C	2.03961	2.14757	0.63742
C	1.59861	1.46180	1.76218
C	2.34616	1.55154	2.93635
C	3.51687	2.30772	2.97385
C	3.96341	2.98170	1.83761
C	-3.38242	1.44338	-0.89021
C	-3.58840	0.23940	-1.62191
C	-4.77744	-0.50275	-1.36639
C	-5.74974	0.03059	-0.48675
C	-5.56583	1.23743	0.13356
C	-4.35691	1.93782	-0.05183
C	-2.64740	-0.28046	-2.54783
C	-2.85110	-1.50368	-3.13923
C	-4.00437	-2.26144	-2.84712
C	-4.95169	-1.76104	-1.99058
H	1.68732	1.30307	-1.32190
H	2.22284	3.33789	-2.47917
H	3.82385	4.56554	-0.62211
H	4.24627	2.96034	-1.23840
H	0.67439	0.88115	1.74851
H	2.00305	1.03856	3.83281
H	4.08239	2.38085	3.90121
H	4.87224	3.58240	1.87293
H	-6.66146	-0.53797	-0.30748
H	-6.31377	1.65106	0.80551
Cl	-4.10026	3.38568	0.86929

H	-1.76074	0.29739	-2.80484
H	-2.11687	-1.88697	-3.84541
H	-4.14617	-3.23354	-3.31423
H	-5.85881	-2.32482	-1.77474
Au	-0.89355	-0.68225	-0.00187
C	-1.19095	-2.69708	0.24419
C	-2.18126	-3.04387	1.17946
C	-0.59883	-3.66056	-0.55555
C	-2.54396	-4.38182	1.31927
C	-0.97058	-4.99980	-0.40436
H	0.13520	-3.38652	-1.31327
C	-1.93466	-5.35513	0.53232
H	-3.30992	-4.67126	2.03876
H	-0.50684	-5.76307	-1.02716
H	-2.22234	-6.39856	0.64668
C	-2.22919	-0.65540	1.54666
C	-2.58472	0.50225	2.21318
C	-2.73396	-1.91314	1.91852
C	-3.51361	0.42447	3.25550
H	-2.15794	1.46702	1.94212
C	-3.67061	-1.96576	2.94950
C	-4.06317	-0.80242	3.60644
H	-3.80665	1.33339	3.77868
H	-4.08613	-2.92541	3.25630
H	-4.79267	-0.86044	4.41204
O	0.83826	-0.82736	-1.44126
C	3.17579	-1.15369	-1.51872
C	1.90297	-1.30431	-0.95686
C	5.59473	-1.72570	-1.33255
C	4.26538	-1.74434	-0.90134
C	6.60153	-2.50850	-0.73701
H	1.84705	-1.88192	-0.01153
H	4.06013	-2.31769	0.01123
H	3.28336	-0.60125	-2.45381
C	7.80656	-2.88595	-1.55623
H	6.24838	-3.29644	-0.06760

H	5.84407	-1.13403	-2.21748
H	7.51173	-3.61569	-2.32239
H	8.22953	-2.01815	-2.07939
H	8.59768	-3.34672	-0.95498
C	7.48570	-1.35547	0.69517
C	6.54200	-1.36705	1.72706
C	5.60603	-0.32798	1.52567
C	6.01082	0.42014	0.44866
C	7.37510	-0.00212	0.03966
H	8.43877	-1.87574	0.77877
H	6.47722	-2.12596	2.50321
H	4.69035	-0.16799	2.09114
H	5.47408	1.27222	0.03825
H	7.58894	0.04425	-1.03296
H	8.10397	0.66531	0.53470
C	0.18442	4.67641	-1.71945
H	0.31114	4.71662	-2.81679
H	-0.31937	5.59601	-1.40499
O	1.42696	4.61771	-1.06991

M06/lanl2dz-6-31G(d) Energy = -2646.114794

M06/lanl2dz-6-31G(d) Free Energy = -2645.475953

M06/def2-TZVP Derived free energy = -2646.586397

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617550

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642842

Number of Imaginary Frequencies = 1 (-378.05)

M06/lanl2dz-6-31G(d) Geometry

C	1.44942	2.20989	-0.74695
C	2.13909	3.43936	-1.38243
C	-0.62583	3.48494	-1.34049
N	-0.00627	2.36757	-0.82414
C	-0.95343	1.44125	-0.54980
N	-2.09098	2.04699	-0.93727
N	-1.90921	3.31422	-1.42921
C	3.48675	3.52283	-0.67166

C	3.21730	2.89793	0.66977
C	2.03963	2.14745	0.63762
C	1.59858	1.46163	1.76233
C	2.34608	1.55130	2.93653
C	3.51680	2.30747	2.97411
C	3.96340	2.98149	1.83792
C	-3.38236	1.44348	-0.89021
C	-3.58836	0.23954	-1.62197
C	-4.77743	-0.50258	-1.36652
C	-5.74974	0.03075	-0.48688
C	-5.56580	1.23754	0.13350
C	-4.35685	1.93790	-0.05181
C	-2.64734	-0.28031	-2.54788
C	-2.85107	-1.50350	-3.13933
C	-4.00436	-2.26124	-2.84729
C	-4.95170	-1.76084	-1.99077
H	1.68739	1.30305	-1.32175
H	2.22301	3.33790	-2.47892
H	3.82398	4.56543	-0.62175
H	4.24638	2.96024	-1.23808
H	0.67434	0.88100	1.74859
H	2.00293	1.03828	3.83295
H	4.08229	2.38055	3.90150
H	4.87224	3.58218	1.87330
H	-6.66148	-0.53780	-0.30767
H	-6.31375	1.65116	0.80545
Cl	-4.10018	3.38570	0.86939
H	-1.76066	0.29752	-2.80485
H	-2.11681	-1.88680	-3.84551
H	-4.14618	-3.23332	-3.31445
H	-5.85884	-2.32461	-1.77498
Au	-0.89357	-0.68227	-0.00193
C	-1.19107	-2.69709	0.24402
C	-2.18139	-3.04388	1.17929
C	-0.59901	-3.66056	-0.55577
C	-2.54416	-4.38182	1.31902

C	-0.97083	-4.99978	-0.40466
H	0.13504	-3.38651	-1.31347
C	-1.93492	-5.35512	0.53201
H	-3.31014	-4.67125	2.03850
H	-0.50713	-5.76305	-1.02750
H	-2.22265	-6.39853	0.64631
C	-2.22921	-0.65543	1.54660
C	-2.58469	0.50221	2.21317
C	-2.73404	-1.91317	1.91840
C	-3.51358	0.42442	3.25549
H	-2.15788	1.46698	1.94215
C	-3.67068	-1.96579	2.94938
C	-4.06320	-0.80246	3.60638
H	-3.80660	1.33333	3.77870
H	-4.08624	-2.92543	3.25615
H	-4.79269	-0.86049	4.41197
O	0.83823	-0.82734	-1.44134
C	3.17578	-1.15357	-1.51876
C	1.90294	-1.30430	-0.95695
C	5.59473	-1.72555	-1.33260
C	4.26537	-1.74426	-0.90142
C	6.60150	-2.50845	-0.73716
H	1.84701	-1.88202	-0.01170
H	4.06011	-2.31769	0.01109
H	3.28336	-0.60103	-2.45379
C	7.80654	-2.88580	-1.55641
H	6.24834	-3.29647	-0.06785
H	5.84408	-1.13379	-2.21747
H	7.51169	-3.61533	-2.32276
H	8.22962	-2.01791	-2.07933
H	8.59759	-3.34678	-0.95523
C	7.48569	-1.35562	0.69521
C	6.54196	-1.36729	1.72706
C	5.60605	-0.32814	1.52578
C	6.01091	0.42010	0.44889
C	7.37518	-0.00219	0.03986

H	8.43873	-1.87596	0.77875
H	6.47712	-2.12630	2.50312
H	4.69036	-0.16818	2.09125
H	5.47425	1.27228	0.03860
H	7.58904	0.04431	-1.03275
H	8.10407	0.66514	0.53500
C	0.18459	4.67645	-1.71921
H	0.31134	4.71669	-2.81654
H	-0.31917	5.59605	-1.40473
O	1.42711	4.61768	-1.06963

M06/lanl2dz-6-31G(d) Energy = -2646.114794

M06/lanl2dz-6-31G(d) Free Energy = -2645.475952

M06/def2-TZVP Derived free energy = -2646.586396

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617549

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642841

Number of Imaginary Frequencies = 1 (-378.05)

M06/lanl2dz-6-31G(d) Geometry

C	1.44944	2.20990	-0.74686
C	2.13913	3.43939	-1.38230
C	-0.62580	3.48499	-1.34036
N	-0.00624	2.36760	-0.82405
C	-0.95341	1.44127	-0.54974
N	-2.09096	2.04703	-0.93720
N	-1.90918	3.31428	-1.42909
C	3.48678	3.52283	-0.67152
C	3.21732	2.89790	0.66988
C	2.03965	2.14741	0.63770
C	1.59859	1.46156	1.76239
C	2.34608	1.55120	2.93660
C	3.51681	2.30736	2.97422
C	3.96341	2.98142	1.83805
C	-3.38234	1.44352	-0.89016
C	-3.58834	0.23962	-1.62199
C	-4.77741	-0.50250	-1.36659

C	-5.74974	0.03079	-0.48693
C	-5.56579	1.23756	0.13351
C	-4.35683	1.93791	-0.05176
C	-2.64731	-0.28020	-2.54790
C	-2.85103	-1.50336	-3.13940
C	-4.00434	-2.26111	-2.84741
C	-4.95169	-1.76074	-1.99088
H	1.68741	1.30307	-1.32169
H	2.22305	3.33796	-2.47879
H	3.82402	4.56543	-0.62158
H	4.24641	2.96025	-1.23796
H	0.67436	0.88093	1.74863
H	2.00293	1.03815	3.83300
H	4.08229	2.38041	3.90161
H	4.87225	3.58210	1.87345
H	-6.66149	-0.53775	-0.30776
H	-6.31374	1.65115	0.80547
Cl	-4.10016	3.38566	0.86952
H	-1.76062	0.29764	-2.80484
H	-2.11677	-1.88664	-3.84558
H	-4.14616	-3.23317	-3.31461
H	-5.85884	-2.32450	-1.77514
Au	-0.89358	-0.68226	-0.00195
C	-1.19110	-2.69710	0.24390
C	-2.18144	-3.04390	1.17915
C	-0.59907	-3.66053	-0.55594
C	-2.54425	-4.38185	1.31880
C	-0.97092	-4.99976	-0.40490
H	0.13499	-3.38646	-1.31363
C	-1.93503	-5.35511	0.53174
H	-3.31024	-4.67130	2.03826
H	-0.50724	-5.76300	-1.02779
H	-2.22280	-6.39853	0.64598
C	-2.22922	-0.65547	1.54657
C	-2.58468	0.50214	2.21319
C	-2.73406	-1.91322	1.91832

C	-3.51357	0.42433	3.25551
H	-2.15786	1.46691	1.94221
C	-3.67070	-1.96588	2.94930
C	-4.06320	-0.80257	3.60635
H	-3.80657	1.33321	3.77875
H	-4.08629	-2.92552	3.25602
H	-4.79270	-0.86062	4.41193
O	0.83823	-0.82730	-1.44137
C	3.17578	-1.15353	-1.51878
C	1.90293	-1.30427	-0.95699
C	5.59472	-1.72553	-1.33262
C	4.26536	-1.74424	-0.90144
C	6.60149	-2.50846	-0.73720
H	1.84699	-1.88203	-0.01175
H	4.06009	-2.31770	0.01105
H	3.28336	-0.60097	-2.45379
C	7.80652	-2.88579	-1.55646
H	6.24832	-3.29649	-0.06792
H	5.84408	-1.13374	-2.21747
H	7.51168	-3.61528	-2.32283
H	8.22962	-2.01788	-2.07934
H	8.59757	-3.34680	-0.95529
C	7.48568	-1.35569	0.69521
C	6.54194	-1.36739	1.72706
C	5.60604	-0.32821	1.52581
C	6.01092	0.42006	0.44896
C	7.37518	-0.00223	0.03991
H	8.43871	-1.87604	0.77874
H	6.47708	-2.12641	2.50309
H	4.69035	-0.16826	2.09129
H	5.47427	1.27227	0.03870
H	7.58905	0.04431	-1.03269
H	8.10408	0.66508	0.53508
C	0.18463	4.67650	-1.71904
H	0.31139	4.71678	-2.81638
H	-0.31913	5.59610	-1.40454

O 1.42715 4.61771 -1.06947

M06/lanl2dz-6-31G(d) Energy = -2646.121134

M06/lanl2dz-6-31G(d) Free Energy = -2645.481881

M06/def2-TZVP Derived free energy = -2646.592781

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.624417

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.650233

Number of Imaginary Frequencies = 1 (-396.08)

M06/lanl2dz-6-31G(d) Geometry

C -1.76812 -2.06333 -0.44733
C -2.62711 -3.18107 -1.08317
C -1.81105 -4.45195 -1.22217
O -0.65797 -4.24881 -2.04811
C 0.10180 -3.24518 -1.65915
N -0.36163 -2.22741 -0.84490
C 0.66574 -1.35928 -0.64971
N 1.66415 -1.90207 -1.36203
N 1.34351 -3.07626 -1.99860
C -3.77107 -3.41656 -0.08073
C -3.20641 -2.93631 1.22670
C -2.05172 -2.17778 1.02848
C -1.39640 -1.58080 2.10062
C -1.91048 -1.76397 3.38251
C -3.06114 -2.52659 3.58307
C -3.71714 -3.11794 2.50655
C 2.97890 -1.35474 -1.44605
C 3.13893 -0.05715 -2.00879
C 4.40032 0.58754 -1.85346
C 5.46403 -0.11148 -1.23480
C 5.30405 -1.38983 -0.77182
C 4.04186 -2.01003 -0.86337
C 2.09426 0.63894 -2.66994
C 2.28332 1.92612 -3.11129
C 3.52000 2.57819 -2.92307
C 4.55685 1.91531 -2.31695

H	-2.07344	-1.07435	-0.82403
H	-2.98433	-2.88697	-2.07900
H	-2.38141	-5.24241	-1.71718
H	-1.48279	-4.81759	-0.23543
H	-4.08656	-4.47022	-0.05580
H	-4.66558	-2.83633	-0.35665
H	-0.49000	-0.99044	1.95450
H	-1.40534	-1.31154	4.23352
H	-3.44715	-2.66411	4.59131
H	-4.61440	-3.71490	2.66592
H	6.42713	0.38695	-1.13103
H	6.12123	-1.92932	-0.29957
Cl	3.85357	-3.58131	-0.15046
H	1.13841	0.14724	-2.84375
H	1.47130	2.44347	-3.61910
H	3.65238	3.59961	-3.27280
H	5.52395	2.39945	-2.18429
Au	0.88126	0.64869	0.20122
C	1.40844	2.57064	0.70930
C	2.52771	2.67531	1.55362
C	0.83206	3.70438	0.15933
C	3.03172	3.93634	1.86477
C	1.34657	4.96441	0.47856
H	-0.00270	3.63336	-0.53755
C	2.43726	5.07665	1.33276
H	3.89786	4.03485	2.51889
H	0.89358	5.85731	0.05067
H	2.83610	6.05868	1.57984
C	2.40429	0.26094	1.51076
C	2.75041	-1.01815	1.90376
C	3.05918	1.39706	2.01485
C	3.81381	-1.18734	2.79555
H	2.21886	-1.89227	1.53088
C	4.12055	1.20493	2.89849
C	4.49965	-0.07976	3.27797
H	4.10155	-2.19342	3.09638

H	4.65133	2.06650	3.30293
H	5.32996	-0.21357	3.96866
O	-0.99929	1.14895	-0.95283
C	-3.19345	2.01064	-0.80817
C	-1.89289	1.77849	-0.32829
C	-5.43741	2.96465	-0.30616
C	-4.08843	2.72216	-0.02431
C	-6.08677	2.45910	-1.43920
H	-1.65963	2.18667	0.67612
H	-3.70468	3.11183	0.92295
H	-3.44236	1.64548	-1.80439
C	-7.39730	3.04916	-1.87246
H	-5.45005	2.12932	-2.26251
H	-6.01717	3.54871	0.40935
H	-7.20380	3.98231	-2.41955
H	-7.96077	2.39265	-2.54482
H	-8.03632	3.30482	-1.01793
C	-6.64466	0.52707	-0.92319
C	-5.45492	-0.16303	-0.68618
C	-5.11041	-0.06736	0.68863
C	-6.11264	0.58597	1.34807
C	-7.26549	0.78238	0.42832
H	-7.24910	0.34822	-1.81136
H	-4.85043	-0.64240	-1.45471
H	-4.17432	-0.40907	1.12812
H	-6.12758	0.83260	2.40566
H	-8.00563	-0.01604	0.61718
H	-7.80297	1.72882	0.54861

Bottom, toward, 2, exo, away

M06/lanl2dz-6-31G(d) Energy = -2646.112490

M06/lanl2dz-6-31G(d) Free Energy = -2645.475892

M06/def2-TZVP Derived free energy = -2646.586364

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617082

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641563

Number of Imaginary Frequencies = 1 (-367.78)

M06/lanl2dz-6-31G(d) Geometry

C	-0.01775	3.13430	-0.21348
C	-0.20122	4.62340	-0.57400
C	-1.77181	2.88147	-2.01282
N	-1.03459	2.36787	-0.96865
C	-1.39412	1.07831	-0.78787
N	-2.33771	0.88837	-1.72374
N	-2.58439	1.99199	-2.49887
C	-1.26703	5.13909	0.41112
C	-1.03179	4.26664	1.61057
C	-0.29424	3.13087	1.26188
C	0.08564	2.20092	2.22179
C	-0.31808	2.39466	3.53995
C	-1.07170	3.51547	3.88631
C	-1.42330	4.46434	2.92842
C	-3.06893	-0.32110	-1.91173
C	-2.37889	-1.48004	-2.36096
C	-3.09065	-2.71436	-2.38694
C	-4.46071	-2.73198	-2.03255
C	-5.11299	-1.59156	-1.64544
C	-4.40207	-0.37758	-1.56955
C	-1.01637	-1.46622	-2.75073
C	-0.38208	-2.63327	-3.09932
C	-1.07737	-3.86087	-3.09943
C	-2.40674	-3.89497	-2.76248
H	0.96264	2.73682	-0.50443
H	0.74986	5.12508	-0.35528
H	-2.28524	4.99818	0.01501
H	-1.15471	6.21113	0.61242
H	0.69415	1.33503	1.95584
H	-0.03809	1.67162	4.30332
H	-1.37664	3.65853	4.92124
H	-1.99226	5.34915	3.21111
H	-4.99796	-3.67899	-2.06830

H	-6.16460	-1.60324	-1.37109
Cl	-5.23512	1.02597	-0.97561
H	-0.46680	-0.52757	-2.77847
H	0.66678	-2.60544	-3.38916
H	-0.55967	-4.77605	-3.37851
H	-2.96003	-4.83348	-2.77467
Au	-0.50448	-0.56349	0.31798
C	0.19862	-2.29667	1.16630
C	-0.65303	-2.88038	2.12141
C	1.36713	-2.93485	0.78205
C	-0.28544	-4.08507	2.71666
C	1.72372	-4.14643	1.38170
H	2.00091	-2.51548	-0.00006
C	0.90363	-4.71059	2.35176
H	-0.93154	-4.54929	3.46153
H	2.64016	-4.65249	1.08113
H	1.18244	-5.65292	2.81972
C	-2.04514	-0.97381	1.59122
C	-3.14106	-0.14222	1.72729
C	-1.88577	-2.13533	2.36521
C	-4.14177	-0.49175	2.63812
H	-3.23070	0.77486	1.14649
C	-2.89505	-2.46205	3.27016
C	-4.01722	-1.64820	3.39896
H	-5.01545	0.14906	2.74475
H	-2.80669	-3.35888	3.88294
H	-4.79872	-1.91844	4.10656
O	1.33627	-0.01037	-0.86926
C	3.61984	0.57310	-0.93210
C	2.46314	0.08029	-0.31352
C	6.03836	1.10207	-0.70285
C	4.81203	0.62272	-0.23070
C	7.16617	1.28734	0.11937
H	2.57215	-0.25298	0.73984
H	4.79020	0.28132	0.81179
H	3.55951	0.90917	-1.96799

C	8.18235	2.32819	-0.27138
H	6.97704	1.22555	1.19393
H	6.09429	1.42466	-1.74605
H	8.47475	2.23151	-1.32534
H	7.74758	3.32888	-0.14466
H	9.08773	2.28513	0.34360
C	8.30855	-0.38723	-0.04138
C	7.62728	-1.30363	0.76609
C	6.63328	-1.95636	0.00461
C	6.75164	-1.55943	-1.30431
C	8.00483	-0.77714	-1.46562
H	9.27521	0.02375	0.24595
H	7.77071	-1.41771	1.83789
H	5.87438	-2.62552	0.40039
H	6.10968	-1.86526	-2.12581
H	8.79966	-1.47148	-1.79420
H	7.97114	0.03112	-2.20284
C	-1.61594	4.29866	-2.44676
H	-1.56007	4.35179	-3.53941
H	-2.50128	4.88120	-2.13919
O	-0.42635	4.84860	-1.94276

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M06/lanl2dz-6-31G(d) Energy = -2646.114670

M06/lanl2dz-6-31G(d) Free Energy = -2645.478465

M06/def2-TZVP Derived free energy = -2646.588691

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.619770

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.644595

Number of Imaginary Frequencies = 1 (-396.76)

M06/lanl2dz-6-31G(d) Geometry

C	0.42718	-0.10795	3.59688
C	-0.91823	0.13906	4.33802
C	0.29850	2.24095	2.91908
N	0.57339	0.93923	2.56597

C	1.01326	0.91839	1.28854
N	1.00405	2.22155	0.95177
N	0.54612	3.05960	1.94382
C	-1.92768	-0.75034	3.60635
C	-1.07750	-1.86932	3.08268
C	0.26782	-1.49815	3.06969
C	1.25641	-2.36104	2.60920
C	0.87348	-3.61214	2.13144
C	-0.47151	-3.98416	2.13463
C	-1.45391	-3.12209	2.61743
C	1.43883	2.77626	-0.28846
C	0.57813	2.71876	-1.41683
C	1.05650	3.23332	-2.65691
C	2.34794	3.80924	-2.71492
C	3.14318	3.88834	-1.60277
C	2.68035	3.36714	-0.37816
C	-0.73076	2.18200	-1.35837
C	-1.51333	2.13756	-2.48699
C	-1.03435	2.62636	-3.72065
C	0.22354	3.16691	-3.79897
H	1.29128	0.00404	4.26731
H	-0.77771	-0.21734	5.37295
H	-2.36143	-0.17078	2.77436
H	-2.75210	-1.07194	4.25401
H	2.30727	-2.06659	2.61822
H	1.62615	-4.30253	1.75595
H	-0.75351	-4.96917	1.76684
H	-2.49949	-3.42844	2.62944
H	2.70502	4.20152	-3.66638
H	4.13059	4.34086	-1.64284
Cl	3.71711	3.48553	1.00987
H	-1.11275	1.80900	-0.40841
H	-2.51941	1.71974	-2.42487
H	-1.66653	2.58171	-4.60490
H	0.60303	3.55803	-4.74237
Au	1.17051	-0.78465	-0.06244

C	1.29666	-2.36443	-1.37439
C	2.57627	-2.58990	-1.91178
C	0.23601	-3.18965	-1.71234
C	2.75867	-3.62080	-2.83143
C	0.43155	-4.22429	-2.63206
H	-0.74650	-3.06036	-1.25791
C	1.68526	-4.42845	-3.19591
H	3.74260	-3.80641	-3.26172
H	-0.40096	-4.87219	-2.90194
H	1.83408	-5.23111	-3.91572
C	3.18221	-0.80241	-0.39936
C	4.06279	0.03205	0.26360
C	3.61648	-1.71803	-1.37372
C	5.41920	-0.01041	-0.07149
H	3.71805	0.72129	1.03199
C	4.97357	-1.74462	-1.69108
C	5.86642	-0.89054	-1.04935
H	6.11775	0.65194	0.43738
H	5.34167	-2.44438	-2.44099
H	6.92231	-0.92089	-1.31102
O	-1.07038	-0.80634	0.18300
C	-3.25909	-0.91521	-0.66775
C	-1.85981	-0.82686	-0.79236
C	-5.45160	-0.93642	-1.85945
C	-4.05370	-0.87252	-1.80009
C	-6.27184	-1.10327	-0.73736
H	-1.45059	-0.77352	-1.82091
H	-3.52911	-0.77016	-2.75553
H	-3.66921	-1.04198	0.33469
C	-7.67400	-1.61121	-0.91511
H	-5.78523	-1.44618	0.17786
H	-5.92452	-0.87004	-2.84008
H	-8.30211	-1.44764	-0.03259
H	-8.16879	-1.15873	-1.78366
H	-7.64074	-2.69516	-1.09231
C	-6.63938	0.80987	-0.00780

C	-5.40474	1.28640	0.43021
C	-4.76670	1.99547	-0.62072
C	-5.61155	2.05547	-1.69221
C	-6.94646	1.53200	-1.29567
H	-7.42218	0.51169	0.68783
H	-4.97488	1.10883	1.41352
H	-3.75824	2.39955	-0.57983
H	-5.40045	2.52333	-2.65003
H	-7.59551	2.39251	-1.05186
H	-7.47420	0.95974	-2.06575
C	-0.35193	2.45250	4.23975
H	0.38016	2.37745	5.06325
H	-0.82322	3.43788	4.28948
O	-1.36582	1.47812	4.35102

M06/lanl2dz-6-31G(d) Energy = -2646.117592

M06/lanl2dz-6-31G(d) Free Energy = -2645.476165

M06/def2-TZVP Derived free energy = -2646.582986

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.614254

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.638935

Number of Imaginary Frequencies = 1 (-363.85)

M06/lanl2dz-6-31G(d) Geometry

C	0.76564	-0.81418	-3.04762
C	2.29101	-0.97328	-3.30620
C	1.25856	1.54405	-2.61530
N	0.57463	0.41000	-2.24164
C	-0.22151	0.70729	-1.18745
N	0.02176	2.01810	-0.99772
N	0.95169	2.55377	-1.86117
C	2.77741	-1.85571	-2.15513
C	1.56928	-2.67618	-1.81726
C	0.41813	-2.08620	-2.34171
C	-0.83462	-2.66685	-2.17804
C	-0.92558	-3.84696	-1.44282
C	0.21986	-4.42674	-0.89720

C	1.47563	-3.85249	-1.08684
C	-0.63153	2.88015	-0.06703
C	-0.21646	2.88963	1.29073
C	-0.90804	3.74540	2.19753
C	-1.95893	4.56190	1.71638
C	-2.31159	4.56485	0.39312
C	-1.63281	3.71951	-0.50643
C	0.86041	2.10786	1.77346
C	1.22242	2.16999	3.09783
C	0.53002	3.00404	4.00120
C	-0.51423	3.77350	3.55618
H	0.20071	-0.66070	-3.97801
H	2.39774	-1.49913	-4.26952
H	3.04961	-1.18804	-1.32002
H	3.66817	-2.44261	-2.41422
H	-1.72634	-2.21028	-2.61037
H	-1.89613	-4.31531	-1.29135
H	0.13161	-5.34996	-0.32737
H	2.36679	-4.32249	-0.67170
H	-2.48203	5.20953	2.41882
H	-3.10438	5.20633	0.01726
Cl	-2.07495	3.78373	-2.18470
H	1.40096	1.45144	1.09077
H	2.05076	1.55633	3.45251
H	0.82812	3.03547	5.04683
H	-1.05588	4.42602	4.24002
Au	-1.34379	-0.65270	0.11235
C	-2.40749	-1.93405	1.31386
C	-3.80556	-1.82007	1.22005
C	-1.82904	-2.88499	2.13793
C	-4.60886	-2.63887	2.01131
C	-2.64518	-3.70371	2.92393
H	-0.74813	-3.01942	2.16548
C	-4.02759	-3.56977	2.86757
H	-5.69454	-2.56173	1.95519
H	-2.19498	-4.44852	3.57820

H	-4.66110	-4.20482	3.48403
C	-3.24133	-0.21900	-0.50145
C	-3.51830	0.64997	-1.54077
C	-4.26419	-0.86355	0.21647
C	-4.85047	0.92422	-1.86241
H	-2.72040	1.13272	-2.10154
C	-5.58620	-0.57905	-0.12221
C	-5.87580	0.31484	-1.14974
H	-5.07472	1.61944	-2.67003
H	-6.40116	-1.06428	0.41430
H	-6.91322	0.52984	-1.39878
O	0.68989	-1.16063	0.89340
C	2.33376	-1.10464	2.57942
C	1.00667	-1.09403	2.11434
C	4.75343	-1.07289	1.96075
C	3.38835	-1.16992	1.68444
C	5.74983	-1.30886	0.99127
H	0.20520	-0.99980	2.86957
H	3.10841	-1.33566	0.64002
H	2.50827	-1.01678	3.65155
C	7.12264	-1.71864	1.45729
H	5.40854	-1.82966	0.09250
H	5.06407	-0.84838	2.98522
H	7.85214	-1.74877	0.64080
H	7.50307	-1.04387	2.23556
H	7.07610	-2.72523	1.89402
C	6.17583	0.45586	0.11233
C	5.11877	0.64094	-0.78835
C	4.05796	1.30852	-0.13736
C	4.46681	1.66624	1.12357
C	5.92568	1.41282	1.25227
H	7.18569	0.23710	-0.23258
H	5.06928	0.25149	-1.80394
H	3.06892	1.48378	-0.56088
H	3.85819	2.17525	1.86798
H	6.45650	2.35308	1.01537

H	6.26938	1.10082	2.24360
O	3.03829	0.22926	-3.33814
C	2.30419	1.39211	-3.66038
H	2.99397	2.24114	-3.64394
H	1.86022	1.32501	-4.66868

M06/lanl2dz-6-31G(d) Energy = -2646.112179

M06/lanl2dz-6-31G(d) Free Energy = -2645.473170

M06/def2-TZVP Derived free energy = -2646.584842

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616055

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641192

Number of Imaginary Frequencies = 1 (-399.43)

M06/lanl2dz-6-31G(d) Geometry

C	2.73491	-1.92998	-1.12676
C	4.01812	-2.82345	-1.05562
C	2.07344	-2.92524	1.03611
N	2.09850	-1.84829	0.18520
C	1.32172	-0.86942	0.69312
N	0.86280	-1.41199	1.83074
N	1.32531	-2.68914	2.07127
C	3.93409	-3.75098	-2.28421
C	2.51633	-3.64807	-2.76701
C	1.83756	-2.61988	-2.11838
C	0.50392	-2.33671	-2.39322
C	-0.14830	-3.10615	-3.35172
C	0.52696	-4.13349	-4.01334
C	1.86000	-4.41208	-3.72673
C	-0.05714	-0.81603	2.73906
C	-1.39722	-1.29128	2.74787
C	-2.31326	-0.70638	3.66917
C	-1.86823	0.33648	4.51824
C	-0.57322	0.78036	4.48480
C	0.34699	0.18590	3.59501
C	-1.85417	-2.31156	1.87757
C	-3.15015	-2.75868	1.95719

C	-4.05183	-2.20243	2.89052
C	-3.64412	-1.18549	3.71683
H	2.98448	-0.90148	-1.42357
H	4.91427	-2.19379	-1.08193
H	4.23350	-4.77094	-2.00562
H	4.64272	-3.42292	-3.05797
H	-0.02243	-1.53269	-1.87248
H	-1.19144	-2.90513	-3.58959
H	0.00312	-4.72642	-4.76079
H	2.37776	-5.22031	-4.24178
H	-2.57590	0.78101	5.21725
H	-0.22759	1.57248	5.14420
Cl	1.98947	0.73347	3.62308
H	-1.16669	-2.75398	1.15809
H	-3.48484	-3.56192	1.30215
H	-5.06746	-2.58956	2.95610
H	-4.33059	-0.74516	4.43955
Au	1.04146	1.09784	-0.14937
C	0.87739	2.96216	-0.99412
C	2.08083	3.68221	-1.08217
C	-0.30730	3.49728	-1.47206
C	2.07356	4.95141	-1.65596
C	-0.30175	4.77316	-2.04392
H	-1.23954	2.93660	-1.41221
C	0.88340	5.49311	-2.13381
H	2.99599	5.52645	-1.73362
H	-1.22965	5.20013	-2.42115
H	0.88436	6.48558	-2.58039
C	2.99300	1.70669	-0.01192
C	4.00210	0.94452	0.55494
C	3.24390	2.98660	-0.53812
C	5.30280	1.45509	0.59162
H	3.80560	-0.03861	0.98120
C	4.54895	3.47501	-0.49074
C	5.57074	2.71387	0.06834
H	6.09945	0.86332	1.03869

H	4.77138	4.46334	-0.89179
H	6.58325	3.11139	0.09939
O	-1.11424	0.62720	-0.50388
C	-3.34994	1.20040	-0.01940
C	-2.00566	0.95894	0.32492
C	-5.02904	1.50340	-1.83476
C	-3.73578	1.28155	-1.35149
C	-6.15802	1.57545	-1.01124
H	-1.72385	1.08193	1.38782
H	-2.93590	1.16069	-2.08591
H	-4.04113	1.40986	0.79582
C	-7.43541	2.15969	-1.53751
H	-5.98304	1.75950	0.05031
H	-5.16806	1.58169	-2.91398
H	-7.36308	3.25601	-1.51055
H	-7.62037	1.87578	-2.58121
H	-8.31068	1.88082	-0.94018
C	-6.70941	-0.42105	-0.69240
C	-5.63664	-0.98508	-0.00545
C	-4.71948	-1.54659	-0.93310
C	-5.23891	-1.43721	-2.19091
C	-6.63930	-0.94178	-2.10654
H	-7.65666	-0.19079	-0.20709
H	-5.47736	-0.94219	1.07024
H	-3.73759	-1.93728	-0.67442
H	-4.76100	-1.75336	-3.11375
H	-6.93470	-0.24553	-2.89880
H	-7.32412	-1.80505	-2.18703
C	2.95332	-4.07339	0.68969
H	3.21321	-4.64669	1.58444
H	2.45629	-4.75404	-0.02385
O	4.14264	-3.52802	0.16730

M06/lanl2dz-6-31G(d) Energy = -2646.117876

M06/lanl2dz-6-31G(d) Free Energy = -2645.475846

M06/def2-TZVP Derived free energy = -2646.583584

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.614542

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.638898

Number of Imaginary Frequencies = 1 (-408.10)

M06/lanl2dz-6-31G(d) Geometry

C	0.80671	-0.53883	-3.20051
C	2.33634	-0.60535	-3.47488
C	1.16495	1.79716	-2.56744
N	0.55600	0.59510	-2.28928
C	-0.29587	0.76587	-1.25318
N	-0.16631	2.07974	-0.98109
N	0.74920	2.73543	-1.77390
C	2.86498	-1.63911	-2.47706
C	1.67684	-2.52054	-2.23156
C	0.50083	-1.88715	-2.63403
C	-0.74067	-2.49707	-2.48948
C	-0.79499	-3.75828	-1.90010
C	0.37799	-4.39334	-1.49149
C	1.62080	-3.78701	-1.66467
C	-0.96652	2.83503	-0.07179
C	-0.66812	2.81782	1.31514
C	-1.51616	3.54851	2.19733
C	-2.60674	4.27569	1.66415
C	-2.85531	4.30235	0.31751
C	-2.02092	3.57837	-0.55673
C	0.43733	2.11825	1.85322
C	0.67788	2.13117	3.20540
C	-0.16677	2.84280	4.08364
C	-1.23902	3.53770	3.58507
H	0.23752	-0.31658	-4.11485
H	2.46091	-0.96866	-4.50906
H	3.15469	-1.11243	-1.55139
H	3.75153	-2.16869	-2.84782
H	-1.65271	-1.99907	-2.82325
H	-1.75629	-4.24899	-1.76096
H	0.31979	-5.38306	-1.04232

H	2.53188	-4.30148	-1.35960
H	-3.25001	4.83078	2.34571
H	-3.68508	4.86967	-0.09608
Cl	-2.35963	3.64425	-2.25924
H	1.09899	1.57201	1.18150
H	1.53073	1.58168	3.60539
H	0.03768	2.84127	5.15189
H	-1.89512	4.09840	4.24981
Au	-1.19549	-0.76171	0.03645
C	-2.00964	-2.14976	1.30937
C	-3.41036	-2.11230	1.41944
C	-1.26482	-3.07802	2.01734
C	-4.04686	-2.99904	2.28539
C	-1.91604	-3.96515	2.87990
H	-0.18306	-3.13425	1.90019
C	-3.29839	-3.91678	3.01745
H	-5.13172	-2.98439	2.38854
H	-1.33687	-4.69617	3.44169
H	-3.80167	-4.60644	3.69233
C	-3.18066	-0.40939	-0.28102
C	-3.64318	0.49127	-1.22185
C	-4.05545	-1.14223	0.54022
C	-5.01942	0.70703	-1.33547
H	-2.95733	1.03441	-1.86859
C	-5.42429	-0.91309	0.40909
C	-5.90095	0.01130	-0.51701
H	-5.39130	1.42283	-2.06719
H	-6.12775	-1.46685	1.03045
H	-6.97241	0.18035	-0.60506
O	0.95580	-1.21311	0.56356
C	2.76209	-0.99525	2.06446
C	1.39488	-0.96235	1.71640
C	5.10289	-1.37244	1.34141
C	3.72131	-1.51493	1.20512
C	5.68973	-0.54084	2.30375
H	0.67909	-0.66451	2.50440

H	3.34566	-2.05708	0.33445
H	3.02529	-0.64324	3.06120
C	7.15942	-0.64257	2.58424
H	5.08364	-0.28507	3.17472
H	5.75092	-1.85293	0.60658
H	7.33475	-1.48524	3.26762
H	7.73994	-0.84080	1.67445
H	7.56531	0.25293	3.06828
C	5.51818	1.39221	1.53478
C	4.16055	1.66410	1.36044
C	3.77982	1.34691	0.02607
C	4.88680	0.97988	-0.68025
C	6.09952	1.19816	0.15337
H	6.09297	1.84867	2.33957
H	3.49063	2.05789	2.12212
H	2.76243	1.36620	-0.36420
H	4.89517	0.67286	-1.72332
H	6.87088	0.42639	0.05288
H	6.57367	2.14684	-0.15507
C	2.26059	1.77855	-3.57296
H	1.86523	1.78352	-4.60373
H	2.91317	2.64814	-3.45092
O	3.02647	0.62013	-3.31638

Bottom, away, 1, exo, away

M06/lanl2dz-6-31G(d) Energy = -2646.115809

M06/lanl2dz-6-31G(d) Free Energy = -2645.476282

M06/def2-TZVP Derived free energy = -2646.587388

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618557

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.643353

Number of Imaginary Frequencies = 1 (-399.89)

M06/lanl2dz-6-31G(d) Geometry

C	-3.22720	-1.16509	1.87539
C	-3.70674	-2.26807	2.83990

C	-2.41957	-3.19482	0.60760
N	-2.41749	-1.83320	0.82075
C	-1.56181	-1.26827	-0.06644
N	-1.08570	-2.31775	-0.74782
N	-1.60518	-3.52515	-0.34938
C	-2.53886	-2.45116	3.82912
C	-1.96772	-1.06239	3.88312
C	-2.39320	-0.30911	2.78364
C	-2.08144	1.04074	2.67246
C	-1.26606	1.61900	3.64268
C	-0.80623	0.86045	4.71860
C	-1.16840	-0.47835	4.85719
C	-0.10542	-2.28574	-1.78258
C	1.22017	-2.70215	-1.47779
C	2.19074	-2.67153	-2.52169
C	1.80717	-2.22802	-3.81032
C	0.52201	-1.83714	-4.07837
C	-0.44684	-1.87810	-3.05378
C	1.61376	-3.13491	-0.18883
C	2.90945	-3.52083	0.04685
C	3.87144	-3.49879	-0.98643
C	3.51760	-3.08124	-2.24317
H	-4.05068	-0.64029	1.37443
H	-4.56646	-1.86083	3.38634
H	-1.79743	-3.17365	3.45251
H	-2.87935	-2.82762	4.80109
H	-2.48813	1.64561	1.86210
H	-1.00619	2.67322	3.56775
H	-0.18119	1.32812	5.47725
H	-0.84353	-1.05123	5.72495
H	2.55547	-2.20893	-4.60207
H	0.22287	-1.50843	-5.07048
Cl	-2.07482	-1.43027	-3.44642
H	0.88260	-3.15800	0.61647
H	3.20030	-3.85183	1.04235
H	4.89238	-3.81426	-0.77821

H	4.24707	-3.06335	-3.05282
Au	-1.01926	0.79880	-0.35859
C	-0.57802	2.79875	-0.52528
C	-1.66296	3.61856	-0.88139
C	0.66096	3.35215	-0.24427
C	-1.47679	4.99718	-0.96645
C	0.83692	4.73568	-0.33415
H	1.49595	2.71913	0.05632
C	-0.22872	5.55127	-0.69636
H	-2.30576	5.64893	-1.24108
H	1.80989	5.17577	-0.11747
H	-0.09101	6.62861	-0.76550
C	-2.85036	1.50464	-0.94183
C	-3.95265	0.69722	-1.17003
C	-2.91126	2.89852	-1.12311
C	-5.15770	1.28258	-1.56854
H	-3.89420	-0.38523	-1.06250
C	-4.12493	3.46208	-1.51695
C	-5.23997	2.65961	-1.73583
H	-6.02648	0.65356	-1.75323
H	-4.20052	4.53919	-1.66282
H	-6.17849	3.11396	-2.04706
O	1.05963	0.22901	0.19320
C	3.32329	0.01073	-0.44968
C	1.96080	0.27691	-0.68706
C	5.10369	-0.62740	1.16233
C	3.77436	-0.37899	0.80151
C	6.18224	-0.48017	0.28318
H	1.68179	0.55314	-1.72252
H	3.00808	-0.48848	1.57209
H	3.98830	0.06644	-1.31018
C	7.50295	-1.11532	0.60802
H	5.95005	-0.45372	-0.78338
H	5.31221	-0.92233	2.19202
H	8.33620	-0.68143	0.04397
H	7.73802	-1.05391	1.67811

H	7.46094	-2.18302	0.34883
C	6.67524	1.55479	0.35063
C	5.55954	2.23277	-0.13766
C	4.70045	2.57629	0.94024
C	5.29504	2.21404	2.11378
C	6.68905	1.76979	1.84401
H	7.59289	1.45934	-0.22785
H	5.35449	2.43383	-1.18641
H	3.71214	3.01685	0.83546
H	4.87370	2.32963	3.10813
H	7.37141	2.61186	2.05848
H	7.03794	0.93194	2.45674
C	-3.24496	-4.11865	1.43771
H	-3.79385	-4.81165	0.79027
H	-2.58444	-4.72857	2.07792
O	-4.19453	-3.41221	2.18839

M06/lanl2dz-6-31G(d) Energy = -2646.115959

M06/lanl2dz-6-31G(d) Free Energy = -2645.477485

M06/def2-TZVP Derived free energy = -2646.587889

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.619334

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.644655

Number of Imaginary Frequencies = 1 (-376.33)

M06/lanl2dz-6-31G(d) Geometry

C	-3.92190	-1.15960	0.95277
C	-4.71984	-2.32474	1.57056
C	-2.82845	-3.08935	-0.25822
N	-2.84125	-1.76618	0.12637
C	-1.72776	-1.17240	-0.36738
N	-1.10350	-2.16833	-1.00849
N	-1.76815	-3.36969	-0.95563
C	-3.93144	-2.70125	2.84015
C	-3.36133	-1.37200	3.24730
C	-3.39199	-0.47152	2.17697
C	-3.01687	0.85646	2.34402

C	-2.52956	1.26069	3.58482
C	-2.45898	0.35474	4.64264
C	-2.89279	-0.96054	4.48803
C	0.15523	-2.09035	-1.67311
C	1.29740	-2.65239	-1.03730
C	2.55183	-2.56546	-1.70947
C	2.62052	-1.91574	-2.96561
C	1.50490	-1.38698	-3.55822
C	0.25593	-1.48918	-2.90894
C	1.23959	-3.27985	0.22983
C	2.37390	-3.81017	0.79348
C	3.61410	-3.73717	0.12480
C	3.69955	-3.12269	-1.09839
H	-4.52244	-0.52381	0.28923
H	-5.69344	-1.91905	1.87232
H	-3.13316	-3.42871	2.62180
H	-4.57407	-3.15872	3.60178
H	-3.12976	1.57906	1.53585
H	-2.22222	2.29463	3.73035
H	-2.08729	0.68768	5.60999
H	-2.87666	-1.64919	5.33182
H	3.58485	-1.85244	-3.46990
H	1.55286	-0.90335	-4.53071
Cl	-1.14080	-0.86039	-3.71983
H	0.28814	-3.33845	0.75406
H	2.31442	-4.29526	1.76585
H	4.50265	-4.16519	0.58576
H	4.65402	-3.05376	-1.62220
Au	-1.03571	0.85719	-0.15630
C	-0.48600	2.81878	0.11836
C	-1.33706	3.76133	-0.48560
C	0.58826	3.23174	0.89082
C	-1.07495	5.12040	-0.32347
C	0.84078	4.59793	1.04687
H	1.22681	2.50541	1.39230
C	0.01487	5.53477	0.43674

H	-1.72265	5.86592	-0.78417
H	1.68231	4.92689	1.65510
H	0.21263	6.59795	0.56035
C	-2.52110	1.77705	-1.22109
C	-3.52177	1.09872	-1.89808
C	-2.45382	3.18211	-1.22869
C	-4.49635	1.82599	-2.58649
H	-3.55073	0.00981	-1.92144
C	-3.43718	3.88851	-1.92095
C	-4.45239	3.21491	-2.59232
H	-5.28489	1.29871	-3.12032
H	-3.40964	4.97759	-1.93957
H	-5.21242	3.78015	-3.12802
O	0.68564	0.03968	0.98586
C	3.01155	-0.31873	1.09946
C	1.83105	0.09891	0.46781
C	5.46377	-0.67125	0.88187
C	4.21094	-0.24162	0.42201
C	6.60461	-0.72036	0.06199
H	1.94075	0.51120	-0.55786
H	4.17992	0.16151	-0.59891
H	2.95036	-0.73482	2.10568
C	7.68355	-1.72277	0.37682
H	6.41764	-0.58297	-1.00690
H	5.52607	-1.07499	1.89639
H	7.95540	-1.70255	1.44051
H	7.32202	-2.73680	0.15382
H	8.59288	-1.56398	-0.21313
C	7.63611	1.01319	0.36228
C	6.88038	1.95291	-0.34635
C	5.84393	2.44121	0.47788
C	6.00241	1.91936	1.73859
C	7.31897	1.23447	1.81984
H	8.62607	0.70138	0.03213
H	7.00495	2.18601	-1.40107
H	5.02724	3.08087	0.15457

H	5.34370	2.08749	2.58617
H	8.05686	1.95787	2.21224
H	7.36174	0.35685	2.47283
C	-3.90253	-4.03713	0.15617
H	-4.24044	-4.61992	-0.70801
H	-3.49433	-4.75401	0.88988
O	-5.01632	-3.35174	0.65930

M06/lanl2dz-6-31G(d) Energy = -2646.115959

M06/lanl2dz-6-31G(d) Free Energy = -2645.477487

M06/def2-TZVP Derived free energy = -2646.587891

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.619336

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.644657

Number of Imaginary Frequencies = 1 (-376.33)

M06/lanl2dz-6-31G(d) Geometry

C	-3.92191	-1.15959	0.95276
C	-4.71985	-2.32473	1.57056
C	-2.82846	-3.08934	-0.25822
N	-2.84127	-1.76617	0.12637
C	-1.72778	-1.17239	-0.36739
N	-1.10352	-2.16833	-1.00849
N	-1.76817	-3.36969	-0.95563
C	-3.93145	-2.70123	2.84015
C	-3.36134	-1.37198	3.24730
C	-3.39201	-0.47150	2.17696
C	-3.01688	0.85648	2.34400
C	-2.52958	1.26071	3.58480
C	-2.45899	0.35476	4.64262
C	-2.89280	-0.96051	4.48802
C	0.15521	-2.09034	-1.67312
C	1.29738	-2.65240	-1.03731
C	2.55181	-2.56547	-1.70948
C	2.62050	-1.91573	-2.96562
C	1.50488	-1.38697	-3.55822
C	0.25591	-1.48916	-2.90895

C	1.23957	-3.27988	0.22980
C	2.37388	-3.81021	0.79345
C	3.61408	-3.73720	0.12477
C	3.69952	-3.12270	-1.09841
H	-4.52246	-0.52380	0.28922
H	-5.69345	-1.91905	1.87233
H	-3.13316	-3.42870	2.62180
H	-4.57407	-3.15870	3.60178
H	-3.12978	1.57907	1.53583
H	-2.22223	2.29465	3.73033
H	-2.08730	0.68771	5.60998
H	-2.87666	-1.64916	5.33182
H	3.58483	-1.85243	-3.46990
H	1.55284	-0.90332	-4.53070
Cl	-1.14082	-0.86036	-3.71983
H	0.28812	-3.33847	0.75404
H	2.31440	-4.29530	1.76581
H	4.50262	-4.16523	0.58573
H	4.65400	-3.05377	-1.62223
Au	-1.03571	0.85719	-0.15629
C	-0.48596	2.81876	0.11836
C	-1.33700	3.76133	-0.48559
C	0.58832	3.23170	0.89082
C	-1.07485	5.12040	-0.32348
C	0.84087	4.59790	1.04685
H	1.22685	2.50536	1.39230
C	0.01498	5.53475	0.43672
H	-1.72254	5.86593	-0.78418
H	1.68241	4.92684	1.65507
H	0.21276	6.59793	0.56032
C	-2.52108	1.77708	-1.22108
C	-3.52176	1.09876	-1.89807
C	-2.45378	3.18213	-1.22868
C	-4.49634	1.82605	-2.58647
H	-3.55074	0.00986	-1.92143
C	-3.43712	3.88855	-1.92094

C	-4.45235	3.21497	-2.59231
H	-5.28488	1.29879	-3.12030
H	-3.40956	4.97763	-1.93956
H	-5.21237	3.78023	-3.12800
O	0.68563	0.03965	0.98587
C	3.01154	-0.31877	1.09947
C	1.83104	0.09888	0.46783
C	5.46376	-0.67128	0.88187
C	4.21093	-0.24165	0.42202
C	6.60460	-0.72037	0.06198
H	1.94075	0.51119	-0.55784
H	4.17990	0.16150	-0.59889
H	2.95034	-0.73487	2.10569
C	7.68354	-1.72277	0.37678
H	6.41761	-0.58296	-1.00690
H	5.52607	-1.07504	1.89638
H	7.95541	-1.70256	1.44048
H	7.32202	-2.73681	0.15379
H	8.59286	-1.56398	-0.21317
C	7.63608	1.01318	0.36229
C	6.88034	1.95291	-0.34632
C	5.84390	2.44119	0.47794
C	6.00240	1.91931	1.73864
C	7.31896	1.23443	1.81986
H	8.62604	0.70138	0.03212
H	7.00489	2.18603	-1.40103
H	5.02719	3.08085	0.15465
H	5.34369	2.08742	2.58623
H	8.05685	1.95783	2.21225
H	7.36174	0.35680	2.47283
O	-5.01633	-3.35173	0.65931
C	-3.90254	-4.03712	0.15618
H	-4.24046	-4.61992	-0.70800
H	-3.49435	-4.75400	0.88988

M06/lanl2dz-6-31G(d) Energy = -2646.118888

M06/lanl2dz-6-31G(d) Free Energy = -2645.480577
M06/def2-TZVP Derived free energy = -2646.592373
M06/def2-TZVP Derived free energy in solution (toluene) = -2646.624068
M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.649991
Number of Imaginary Frequencies = 1 (-377.56)

M06/lanl2dz-6-31G(d) Geometry

C	-3.77248	-1.23636	0.67888
C	-4.99090	-2.17699	0.57490
C	-2.71241	-2.90347	-0.85857
N	-2.72519	-1.67107	-0.24788
C	-1.59834	-1.00689	-0.59273
N	-0.96111	-1.87975	-1.38454
N	-1.63549	-3.06596	-1.56655
C	-5.68161	-2.01385	1.92514
C	-4.53592	-1.72381	2.85737
C	-3.41138	-1.31158	2.14052
C	-2.21622	-1.01252	2.77896
C	-2.16569	-1.12063	4.16832
C	-3.28949	-1.51620	4.89059
C	-4.48277	-1.82434	4.23973
C	0.32790	-1.71232	-1.96799
C	1.42731	-2.39407	-1.37781
C	2.70973	-2.25111	-1.98242
C	2.84834	-1.41909	-3.11999
C	1.77487	-0.76139	-3.65992
C	0.49677	-0.92246	-3.08371
C	1.29865	-3.18942	-0.21432
C	2.39451	-3.82837	0.31131
C	3.66067	-3.71047	-0.30005
C	3.81363	-2.93442	-1.42069
H	-4.05597	-0.21225	0.38825
H	-5.62906	-1.93837	-0.29400
H	-6.24498	-2.92039	2.17765
H	-6.39684	-1.17851	1.88842
H	-1.32268	-0.72219	2.22293

H	-1.23809	-0.89639	4.69136
H	-3.23143	-1.59680	5.97441
H	-5.35354	-2.15053	4.80703
H	3.83369	-1.31284	-3.57417
H	1.87753	-0.13007	-4.53895
Cl	-0.84779	-0.11679	-3.82369
H	0.32632	-3.28573	0.26584
H	2.28396	-4.43892	1.20523
H	4.51574	-4.23330	0.12560
H	4.78899	-2.83077	-1.89824
Au	-0.99844	1.00122	-0.05233
C	-0.51375	2.92141	0.48855
C	-1.37801	3.91361	-0.00482
C	0.55321	3.25407	1.30716
C	-1.14159	5.24668	0.32224
C	0.78022	4.59557	1.62851
H	1.20555	2.48339	1.71602
C	-0.06230	5.58405	1.13420
H	-1.79908	6.03113	-0.05178
H	1.61563	4.86410	2.27340
H	0.11693	6.62761	1.38619
C	-2.49192	2.01363	-1.01717
C	-3.44558	1.40650	-1.81828
C	-2.46656	3.40833	-0.83706
C	-4.42085	2.19358	-2.43728
H	-3.43681	0.33157	-1.99500
C	-3.45036	4.17398	-1.46119
C	-4.42328	3.57007	-2.25181
H	-5.17130	1.72257	-3.06954
H	-3.45680	5.25607	-1.33441
H	-5.18326	4.18232	-2.73307
O	0.71956	0.07273	1.02270
C	3.02618	-0.38982	1.12835
C	1.87991	0.16131	0.54015
C	5.45738	-0.84443	0.91237
C	4.24901	-0.26765	0.49953

C	6.61322	-0.85590	0.11457
H	2.02679	0.70710	-0.41563
H	4.27303	0.29484	-0.44312
H	2.91873	-0.95476	2.05518
C	7.58972	-1.99120	0.26870
H	6.47140	-0.52121	-0.91701
H	5.45953	-1.40784	1.84986
H	7.82457	-2.18318	1.32409
H	7.14431	-2.91162	-0.13661
H	8.52921	-1.81901	-0.26772
C	7.78729	0.70755	0.73051
C	7.15100	1.80426	0.14371
C	6.12082	2.26245	0.99476
C	6.17195	1.55238	2.16858
C	7.41505	0.73728	2.19061
H	8.76009	0.35329	0.39269
H	7.34735	2.17784	-0.85837
H	5.38390	3.01955	0.74217
H	5.49174	1.65812	3.00905
H	8.19455	1.31808	2.71685
H	7.34550	-0.22767	2.70266
C	-3.87894	-3.81754	-0.69553
H	-4.54732	-3.71435	-1.57072
H	-3.54750	-4.85977	-0.64904
O	-4.55466	-3.52239	0.49494

M06/lanl2dz-6-31G(d) Energy = -2646.115959

M06/lanl2dz-6-31G(d) Free Energy = -2645.477487

M06/def2-TZVP Derived free energy = -2646.587891

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.619336

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.644657

Number of Imaginary Frequencies = 1 (-376.33)

M06/lanl2dz-6-31G(d) Geometry

C	-3.92191	-1.15959	0.95276
C	-4.71985	-2.32473	1.57056

C	-2.82847	-3.08934	-0.25822
N	-2.84127	-1.76617	0.12636
C	-1.72778	-1.17239	-0.36739
N	-1.10352	-2.16833	-1.00849
N	-1.76817	-3.36968	-0.95563
C	-3.93145	-2.70123	2.84015
C	-3.36134	-1.37198	3.24729
C	-3.39201	-0.47150	2.17696
C	-3.01689	0.85648	2.34400
C	-2.52958	1.26071	3.58480
C	-2.45899	0.35476	4.64262
C	-2.89280	-0.96051	4.48802
C	0.15521	-2.09034	-1.67312
C	1.29738	-2.65240	-1.03732
C	2.55181	-2.56546	-1.70948
C	2.62050	-1.91573	-2.96562
C	1.50488	-1.38696	-3.55822
C	0.25591	-1.48916	-2.90895
C	1.23956	-3.27988	0.22980
C	2.37388	-3.81021	0.79345
C	3.61408	-3.73720	0.12477
C	3.69952	-3.12270	-1.09842
H	-4.52247	-0.52380	0.28922
H	-5.69345	-1.91904	1.87232
H	-3.13317	-3.42869	2.62180
H	-4.57408	-3.15870	3.60178
H	-3.12979	1.57907	1.53583
H	-2.22224	2.29466	3.73033
H	-2.08731	0.68772	5.60997
H	-2.87667	-1.64916	5.33182
H	3.58483	-1.85243	-3.46990
H	1.55284	-0.90332	-4.53070
Cl	-1.14082	-0.86036	-3.71983
H	0.28812	-3.33847	0.75404
H	2.31440	-4.29531	1.76581
H	4.50262	-4.16523	0.58572

H	4.65399	-3.05377	-1.62223
Au	-1.03571	0.85719	-0.15629
C	-0.48596	2.81876	0.11836
C	-1.33699	3.76133	-0.48559
C	0.58832	3.23170	0.89082
C	-1.07484	5.12040	-0.32348
C	0.84088	4.59789	1.04685
H	1.22685	2.50536	1.39230
C	0.01500	5.53474	0.43671
H	-1.72253	5.86593	-0.78418
H	1.68243	4.92683	1.65507
H	0.21278	6.59792	0.56032
C	-2.52108	1.77708	-1.22108
C	-3.52176	1.09876	-1.89807
C	-2.45377	3.18214	-1.22868
C	-4.49634	1.82606	-2.58647
H	-3.55074	0.00986	-1.92143
C	-3.43711	3.88855	-1.92094
C	-4.45234	3.21498	-2.59230
H	-5.28488	1.29880	-3.12030
H	-3.40955	4.97764	-1.93955
H	-5.21236	3.78024	-3.12800
O	0.68563	0.03964	0.98587
C	3.01153	-0.31877	1.09947
C	1.83104	0.09887	0.46783
C	5.46376	-0.67128	0.88187
C	4.21093	-0.24165	0.42202
C	6.60460	-0.72037	0.06198
H	1.94075	0.51118	-0.55784
H	4.17990	0.16150	-0.59889
H	2.95034	-0.73488	2.10569
C	7.68354	-1.72278	0.37678
H	6.41761	-0.58297	-1.00690
H	5.52607	-1.07505	1.89638
H	7.95541	-1.70256	1.44047
H	7.32201	-2.73681	0.15379

H	8.59286	-1.56399	-0.21318
C	7.63608	1.01318	0.36229
C	6.88033	1.95291	-0.34631
C	5.84389	2.44118	0.47795
C	6.00240	1.91930	1.73864
C	7.31896	1.23443	1.81986
H	8.62604	0.70138	0.03212
H	7.00488	2.18603	-1.40103
H	5.02719	3.08085	0.15466
H	5.34370	2.08741	2.58624
H	8.05685	1.95782	2.21226
H	7.36175	0.35679	2.47282
O	-5.01634	-3.35173	0.65931
C	-3.90254	-4.03712	0.15617
H	-4.24046	-4.61992	-0.70800
H	-3.49435	-4.75400	0.88988

Top, toward, 1, exo, away

M06/lanl2dz-6-31G(d) Energy = -2646.112313

M06/lanl2dz-6-31G(d) Free Energy = -2645.473743

M06/def2-TZVP Derived free energy = -2646.584174

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.615566

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.640945

Number of Imaginary Frequencies = 1 (-384.24)

M06/lanl2dz-6-31G(d) Geometry

C	-3.46890	-1.32251	0.91661
C	-4.59678	-2.37094	1.04896
C	-2.39966	-3.10083	-0.49148
N	-2.44307	-1.80887	-0.01896
C	-1.39519	-1.12529	-0.54115
N	-0.77027	-2.04964	-1.28747
N	-1.37929	-3.28345	-1.27391
C	-5.19465	-2.09389	2.42396
C	-4.02605	-1.55711	3.20329

C	-3.01756	-1.12323	2.34163
C	-1.85428	-0.54982	2.83559
C	-1.69718	-0.43515	4.21531
C	-2.69779	-0.87779	5.07782
C	-3.87213	-1.43600	4.57717
C	0.45285	-1.87585	-1.99972
C	1.61199	-2.55656	-1.53217
C	2.83765	-2.35297	-2.22940
C	2.86318	-1.48920	-3.35119
C	1.73181	-0.85335	-3.78571
C	0.51216	-1.05770	-3.10695
C	1.60304	-3.41603	-0.40585
C	2.75011	-4.05739	-0.00777
C	3.96000	-3.87274	-0.70936
C	3.99992	-3.03345	-1.79508
H	-3.86810	-0.38747	0.49321
H	-5.32240	-2.30448	0.21943
H	-5.63118	-3.01049	2.83906
H	-6.00005	-1.34837	2.34725
H	-1.07523	-0.18430	2.16535
H	-0.78796	0.00554	4.61968
H	-2.56193	-0.78423	6.15355
H	-4.65281	-1.77951	5.25457
H	3.80592	-1.34521	-3.87927
H	1.74393	-0.20101	-4.65511
Cl	-0.90162	-0.25873	-3.71410
H	0.67215	-3.59369	0.12840
H	2.72217	-4.72614	0.85035
H	4.85477	-4.40793	-0.39576
H	4.92604	-2.88518	-2.35216
Au	-0.90439	0.98560	-0.32603
C	-0.56385	2.98593	-0.02600
C	-1.64518	3.83117	-0.32272
C	0.61874	3.48909	0.48700
C	-1.52039	5.19839	-0.08688
C	0.73155	4.86334	0.71663

H	1.44815	2.82092	0.71323
C	-0.33395	5.70945	0.43244
H	-2.34606	5.87404	-0.30881
H	1.65708	5.27058	1.12108
H	-0.24253	6.77865	0.61422
C	-2.66265	1.75712	-1.04404
C	-3.64252	0.99856	-1.66465
C	-2.80187	3.14872	-0.89436
C	-4.81352	1.62033	-2.10750
H	-3.50704	-0.06927	-1.83458
C	-3.98129	3.74819	-1.33506
C	-4.98309	2.98783	-1.93027
H	-5.58533	1.02988	-2.59797
H	-4.11520	4.82402	-1.22611
H	-5.89612	3.47136	-2.27193
O	1.14253	0.47458	0.39952
C	2.74796	-0.65884	1.70965
C	1.48863	-0.51171	1.10456
C	4.95781	0.34268	2.25994
C	3.70980	0.33229	1.62581
C	5.81201	1.46030	2.24681
H	0.75767	-1.32448	1.27974
H	3.44961	1.21384	1.03034
H	2.93271	-1.56699	2.28348
C	6.80789	1.63362	3.36142
H	5.36265	2.39117	1.89270
H	5.24450	-0.53204	2.85053
H	7.35236	0.70228	3.56642
H	7.53911	2.42271	3.15514
H	6.27999	1.91082	4.28402
C	7.09196	1.19491	0.66458
C	6.28567	1.47683	-0.44258
C	5.57648	0.31452	-0.81563
C	6.00859	-0.73082	-0.03531
C	7.21405	-0.30710	0.72256
H	7.90711	1.84988	0.96905

H	6.14084	2.46457	-0.87352
H	4.76777	0.26856	-1.54150
H	5.60045	-1.73870	-0.04380
H	7.33755	-0.75410	1.71400
H	8.10694	-0.58876	0.13483
C	-3.46837	-4.06762	-0.11387
H	-4.22281	-4.11710	-0.92107
H	-3.04934	-5.07078	0.01550
O	-4.04812	-3.67525	1.09828

M06/lanl2dz-6-31G(d) Energy = -2646.112669

M06/lanl2dz-6-31G(d) Free Energy = -2645.472837

M06/def2-TZVP Derived free energy = -2646.584630

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616379

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642697

Number of Imaginary Frequencies = 1 (-368.92)

M06/lanl2dz-6-31G(d) Geometry

C	1.35656	2.70186	-1.18096
C	1.41126	3.88124	-2.17797
C	0.33237	1.49036	-3.11527
N	0.90114	1.48561	-1.86197
C	0.86750	0.21887	-1.37838
N	0.27103	-0.46545	-2.36575
N	-0.06486	0.30223	-3.45669
C	1.26713	5.11315	-1.28953
C	0.42354	4.61429	-0.14813
C	0.44282	3.21977	-0.09965
C	-0.26119	2.52749	0.87314
C	-0.98917	3.25166	1.81597
C	-1.00929	4.64524	1.77291
C	-0.30329	5.33540	0.78874
C	-0.05141	-1.85334	-2.33012
C	-1.41822	-2.24252	-2.25087
C	-1.70841	-3.62797	-2.08772
C	-0.64523	-4.56138	-2.02517

C	0.65813	-4.16273	-2.13812
C	0.95415	-2.79347	-2.29927
C	-2.49461	-1.32477	-2.31653
C	-3.79318	-1.76769	-2.22886
C	-4.08229	-3.13716	-2.05537
C	-3.05605	-4.04606	-1.98575
H	2.36081	2.49360	-0.77890
H	2.33193	3.86926	-2.78665
H	0.81503	5.93842	-1.85287
H	2.25399	5.45152	-0.94051
H	-0.24621	1.43791	0.90260
H	-1.53506	2.72392	2.59860
H	-1.57743	5.20050	2.51694
H	-0.32747	6.42361	0.75388
H	-0.88196	-5.61655	-1.89424
H	1.47672	-4.87702	-2.10716
Cl	2.62490	-2.34071	-2.44893
H	-2.29061	-0.26706	-2.47107
H	-4.61355	-1.05459	-2.31303
H	-5.11616	-3.47135	-1.99433
H	-3.26116	-5.10883	-1.86093
Au	1.59216	-0.59918	0.51626
C	2.24662	-1.22636	2.35277
C	3.54170	-0.80628	2.69968
C	1.47607	-1.96954	3.23058
C	4.04164	-1.12443	3.96000
C	1.99187	-2.28568	4.49107
H	0.48602	-2.32022	2.94279
C	3.26433	-1.85875	4.85214
H	5.04308	-0.80860	4.25162
H	1.39502	-2.87312	5.18682
H	3.66186	-2.10643	5.83453
C	3.52494	0.06352	0.44113
C	4.11189	0.59861	-0.69353
C	4.25193	-0.10539	1.63309
C	5.44115	1.02893	-0.63705

H	3.56534	0.66136	-1.63440
C	5.57323	0.33837	1.67101
C	6.16004	0.90968	0.54592
H	5.91043	1.44743	-1.52571
H	6.15752	0.22015	2.58299
H	7.19383	1.24652	0.58967
O	-0.42085	-1.52554	0.69199
C	-2.71673	-1.36938	1.16477
C	-1.37563	-1.00744	1.32833
C	-5.08936	-0.85739	1.64697
C	-3.71255	-0.66497	1.81417
C	-6.07503	-0.20725	2.41390
H	-1.16295	-0.20372	2.06644
H	-3.40110	0.11060	2.52528
H	-2.96196	-2.16386	0.45843
C	-7.41697	-0.87144	2.58063
H	-5.71098	0.29494	3.31363
H	-5.40458	-1.60006	0.90709
H	-7.81485	-1.22678	1.62071
H	-7.31292	-1.74763	3.23442
H	-8.15979	-0.20886	3.03802
C	-6.61946	1.45171	1.38703
C	-5.58012	2.34363	1.67823
C	-4.52675	2.15792	0.75794
C	-4.92960	1.24831	-0.18864
C	-6.38464	0.98806	-0.02960
H	-7.62473	1.59430	1.78118
H	-5.54639	2.99522	2.54812
H	-3.54195	2.61561	0.82098
H	-4.31605	0.86601	-1.00050
H	-6.93276	1.68090	-0.69412
H	-6.72152	-0.02256	-0.28202
C	0.28135	2.75572	-3.89992
H	1.14660	2.79819	-4.58724
H	-0.62963	2.79697	-4.50543
O	0.27736	3.85140	-3.02571

Bottom, towards, 1, exo, away

M06/lanl2dz-6-31G(d) Energy = -2646.115312

M06/lanl2dz-6-31G(d) Free Energy = -2645.478520

M06/def2-TZVP Derived free energy = -2646.588861

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.620766

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.646888

Number of Imaginary Frequencies = 1 (-374.34)

M06/lanl2dz-6-31G(d) Geometry

C	0.94570	-0.23501	3.19821
C	0.44926	0.34432	4.53929
C	1.34821	2.21545	2.74877
N	1.21239	0.91753	2.30111
C	1.39697	0.91371	0.95722
N	1.61599	2.20154	0.67191
N	1.59352	3.02929	1.76715
C	-1.06302	0.56013	4.32549
C	-1.39639	-0.56516	3.38807
C	-0.23996	-1.05003	2.76538
C	-0.28029	-2.17337	1.94653
C	-1.51370	-2.77456	1.69812
C	-2.67401	-2.26994	2.28638
C	-2.62272	-1.17230	3.14617
C	1.86392	2.75247	-0.62081
C	0.80175	3.40373	-1.30189
C	1.07211	3.96063	-2.58518
C	2.37376	3.84511	-3.12935
C	3.38196	3.21632	-2.44797
C	3.12253	2.67115	-1.17416
C	-0.50153	3.51580	-0.76482
C	-1.48840	4.15887	-1.46921
C	-1.22372	4.71601	-2.73899
C	0.03086	4.61531	-3.28390
H	1.87907	-0.80443	3.29070

H	0.58457	-0.43945	5.29529
H	-1.27181	1.53942	3.86624
H	-1.62145	0.52837	5.26851
H	0.63381	-2.59356	1.52632
H	-1.56249	-3.65518	1.06008
H	-3.62866	-2.76180	2.10104
H	-3.52649	-0.81346	3.63892
H	2.56856	4.27287	-4.11222
H	4.38296	3.13205	-2.86313
Cl	4.42769	1.91352	-0.31733
H	-0.71894	3.08767	0.21299
H	-2.48657	4.24188	-1.04147
H	-2.01657	5.22744	-3.28087
H	0.24783	5.04026	-4.26340
Au	1.28012	-0.67268	-0.50440
C	1.14107	-2.22889	-1.82921
C	2.10904	-3.23528	-1.67249
C	0.15686	-2.33004	-2.79837
C	2.06707	-4.35253	-2.50399
C	0.12687	-3.45522	-3.62739
H	-0.57909	-1.53695	-2.92509
C	1.07708	-4.45897	-3.47744
H	2.80981	-5.14357	-2.40201
H	-0.63889	-3.54156	-4.39684
H	1.05273	-5.33264	-4.12615
C	2.92283	-1.75175	0.06376
C	3.79676	-1.35652	1.06337
C	3.09117	-2.96842	-0.62361
C	4.86509	-2.19116	1.40407
H	3.68020	-0.39737	1.56858
C	4.16210	-3.78649	-0.26539
C	5.04030	-3.40088	0.74294
H	5.55997	-1.88530	2.18408
H	4.31741	-4.73395	-0.78087
H	5.87341	-4.04848	1.00892
O	-0.55352	0.33693	-1.26495

C	-2.86827	0.71770	-1.02539
C	-1.63799	0.15263	-0.65441
C	-5.29555	0.89454	-0.48879
C	-3.99113	0.42765	-0.27539
C	-6.34218	0.69061	0.42962
H	-1.64850	-0.50197	0.24016
H	-3.84261	-0.21826	0.60028
H	-2.90923	1.36815	-1.90001
C	-7.47918	1.67812	0.46746
H	-6.03258	0.32310	1.41205
H	-5.48304	1.51478	-1.36945
H	-7.87267	1.87824	-0.53797
H	-8.30812	1.34137	1.09955
H	-7.12393	2.63464	0.87384
C	-7.34412	-0.97164	-0.16365
C	-6.49546	-2.01019	0.23641
C	-5.53937	-2.25235	-0.77246
C	-5.84110	-1.46933	-1.86065
C	-7.17598	-0.84927	-1.65751
H	-8.30466	-0.79587	0.31900
H	-6.50748	-2.47968	1.21762
H	-4.67701	-2.90815	-0.68616
H	-5.26920	-1.41171	-2.78265
H	-7.31290	0.14672	-2.09021
H	-7.93137	-1.50543	-2.12747
O	1.20269	1.43248	4.99943
C	1.16262	2.57318	4.18347
H	0.21650	3.12871	4.30474
H	1.96964	3.23675	4.51237

M06/lanl2dz-6-31G(d) Energy = -2646.117956

M06/lanl2dz-6-31G(d) Free Energy = -2645.479615

M06/def2-TZVP Derived free energy = -2646.588656

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.619839

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.644561

Number of Imaginary Frequencies = 1 (-366.91)

M06/lanl2dz-6-31G(d) Geometry

C	-3.49880	-1.18651	1.45788
C	-4.08767	-2.34356	2.28971
C	-2.62234	-3.13772	0.11606
N	-2.59709	-1.80006	0.44873
C	-1.63166	-1.19941	-0.28815
N	-1.12376	-2.20409	-1.01103
N	-1.72410	-3.41785	-0.77977
C	-3.01398	-2.62729	3.35964
C	-2.43835	-1.25658	3.57800
C	-2.74945	-0.41371	2.50508
C	-2.42229	0.93732	2.53265
C	-1.70493	1.42767	3.62294
C	-1.35953	0.58147	4.67723
C	-1.73819	-0.76077	4.67105
C	-0.05897	-2.11752	-1.95588
C	1.24055	-2.53893	-1.56648
C	2.28902	-2.45553	-2.52671
C	2.00245	-1.96319	-3.82325
C	0.73886	-1.57002	-4.17563
C	-0.30401	-1.65554	-3.23001
C	1.53195	-3.03009	-0.27157
C	2.80570	-3.42486	0.05225
C	3.84500	-3.35610	-0.90123
C	3.59094	-2.87656	-2.16198
H	-4.25858	-0.60939	0.91580
H	-4.98363	-1.95426	2.78911
H	-2.24843	-3.32695	2.98798
H	-3.44031	-3.07628	4.26447
H	-2.74265	1.60933	1.73697
H	-1.43366	2.48142	3.65631
H	-0.81411	0.98140	5.53023
H	-1.50418	-1.40314	5.51906
H	2.80968	-1.90751	-4.55299
H	0.51552	-1.20140	-5.17360

Cl	-1.90126	-1.18823	-3.71628
H	0.73671	-3.09376	0.46893
H	3.01727	-3.79623	1.05343
H	4.84526	-3.69443	-0.63368
H	4.38188	-2.82541	-2.91036
Au	-0.90058	0.82602	-0.26680
C	-0.23215	2.76309	-0.18626
C	-1.15078	3.72771	-0.63427
C	1.01092	3.13825	0.29949
C	-0.79722	5.07541	-0.58994
C	1.35342	4.49313	0.33982
H	1.72095	2.38528	0.64700
C	0.45155	5.45383	-0.10500
H	-1.49398	5.83900	-0.93551
H	2.32827	4.79757	0.72095
H	0.72051	6.50800	-0.07446
C	-2.52423	1.77547	-1.06366
C	-3.66538	1.12091	-1.49697
C	-2.41780	3.17810	-1.11566
C	-4.73785	1.86930	-1.98992
H	-3.73159	0.03340	-1.47624
C	-3.49973	3.90599	-1.60988
C	-4.65159	3.25527	-2.04197
H	-5.63653	1.36153	-2.33538
H	-3.44471	4.99303	-1.66158
H	-5.48733	3.83745	-2.42501
O	0.98159	0.01594	0.51323
C	2.56857	-0.31792	2.20410
C	1.26634	-0.08324	1.74256
C	4.96713	-0.60701	1.59765
C	3.61466	-0.43301	1.29774
C	5.95362	-0.83197	0.61721
H	0.46049	0.03700	2.49047
H	3.33656	-0.40746	0.23840
H	2.74332	-0.37826	3.27745
C	7.22357	-1.53617	1.01610

H	5.57010	-1.11919	-0.36598
H	5.26996	-0.59986	2.64910
H	7.98313	-1.51396	0.22705
H	7.65832	-1.10205	1.92640
H	7.00579	-2.59156	1.23252
C	6.69664	0.98791	0.10717
C	5.73830	1.45392	-0.79992
C	4.71076	2.12545	-0.10249
C	5.06048	2.19980	1.22347
C	6.47127	1.75811	1.38441
H	7.69552	0.69471	-0.21293
H	5.73042	1.23522	-1.86497
H	3.77630	2.47518	-0.53560
H	4.45099	2.62066	2.01967
H	7.11679	2.65468	1.34659
H	6.70697	1.24212	2.32034
C	-3.54392	-4.09599	0.79178
H	-4.04985	-4.71988	0.04686
H	-2.95630	-4.77239	1.43642
O	-4.53886	-3.42200	1.51456

Top, away, 2, exo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.115119

M06/lanl2dz-6-31G(d) Free Energy = -2645.475567

M06/def2-TZVP Derived free energy = -2646.585845

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617329

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.643237

Number of Imaginary Frequencies = 1 (-374.53)

M06/lanl2dz-6-31G(d) Geometry

C	1.57310	-1.16128	1.85913
C	2.88868	-0.98519	2.64320
C	1.40505	1.31335	2.19495
N	0.97694	0.15263	1.59850
C	-0.02120	0.45190	0.73390

N	-0.13253	1.78518	0.85046
N	0.74928	2.34307	1.74869
C	3.07151	-2.32575	3.34751
C	1.65454	-2.77937	3.57666
C	0.77654	-2.08792	2.74043
C	-0.58871	-2.33339	2.76916
C	-1.07184	-3.29063	3.65972
C	-0.19849	-3.98565	4.49389
C	1.17206	-3.73538	4.45822
C	-1.01061	2.62596	0.10658
C	-2.09634	3.25962	0.77002
C	-3.01142	4.01585	-0.01770
C	-2.79524	4.13763	-1.41070
C	-1.71790	3.55141	-2.02108
C	-0.81906	2.79322	-1.24753
C	-2.31556	3.15312	2.16470
C	-3.40263	3.75999	2.74394
C	-4.31813	4.49948	1.96403
C	-4.12220	4.62549	0.61286
H	1.77086	-1.60855	0.87243
H	3.72888	-0.69936	1.98087
H	3.65551	-2.19738	4.26707
H	3.62091	-3.02546	2.69970
H	-1.27915	-1.78915	2.12259
H	-2.13973	-3.49432	3.70356
H	-0.59220	-4.72710	5.18647
H	1.84930	-4.27388	5.11984
H	-3.50206	4.71951	-2.00097
H	-1.54133	3.65740	-3.08822
Cl	0.55638	2.07983	-2.05093
H	-1.60706	2.59903	2.77770
H	-3.55624	3.67642	3.81809
H	-5.17252	4.97490	2.44091
H	-4.81611	5.20046	0.00070
Au	-1.00320	-0.94177	-0.63424
C	-1.92633	-2.21325	-1.95469

C	-3.32913	-2.12688	-1.98238
C	-1.25389	-3.09829	-2.78098
C	-4.04080	-2.90623	-2.89093
C	-1.98018	-3.88214	-3.68297
H	-0.17160	-3.20872	-2.72516
C	-3.36438	-3.77483	-3.74336
H	-5.12828	-2.84935	-2.93152
H	-1.45727	-4.58064	-4.33390
H	-3.92640	-4.38339	-4.44915
C	-2.95690	-0.62560	-0.12454
C	-3.34550	0.16227	0.94236
C	-3.89614	-1.24103	-0.97016
C	-4.70675	0.39480	1.15819
H	-2.61513	0.60609	1.61549
C	-5.24894	-0.99931	-0.73664
C	-5.64968	-0.17876	0.31457
H	-5.01373	1.02887	1.98884
H	-5.99988	-1.46285	-1.37584
H	-6.70984	0.00268	0.48075
O	1.10186	-1.30186	-1.31021
C	2.73314	-0.71551	-2.91654
C	1.43213	-1.04426	-2.50339
C	5.08919	-0.22669	-2.30771
C	3.76826	-0.57591	-2.00852
C	6.13516	-0.25072	-1.36595
H	0.64811	-1.07146	-3.28175
H	3.52831	-0.77982	-0.95842
H	2.90555	-0.55022	-3.97951
C	7.54779	-0.42625	-1.85763
H	5.91408	-0.77768	-0.43391
H	5.33090	0.01776	-3.34613
H	8.29078	-0.27048	-1.06788
H	7.67993	-1.44880	-2.23585
H	7.77488	0.25812	-2.68576
C	6.25790	1.61809	-0.58032
C	5.19023	1.63610	0.32360

C	4.01065	2.03552	-0.34174
C	4.33670	2.39514	-1.62753
C	5.81566	2.44416	-1.76107
H	7.29435	1.60670	-0.24620
H	5.25291	1.28400	1.35206
H	3.00027	2.02199	0.06787
H	3.63805	2.71868	-2.39489
H	6.21746	2.16489	-2.73995
H	6.13957	3.48437	-1.57289
O	2.72724	-0.00962	3.65714
C	2.53396	1.28601	3.16811
H	3.44633	1.67281	2.67431
H	2.32173	1.93947	4.02091

M06/lanl2dz-6-31G(d) Energy = -2646.114936

M06/lanl2dz-6-31G(d) Free Energy = -2645.476607

M06/def2-TZVP Derived free energy = -2646.586391

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616693

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641241

Number of Imaginary Frequencies = 1 (-367.41)

M06/lanl2dz-6-31G(d) Geometry

C	-1.06036	-0.63265	3.24803
C	-1.71816	-0.19024	4.56551
C	-0.92654	1.86663	2.94094
N	-0.92218	0.59444	2.41554
C	-0.75578	0.68672	1.07526
N	-0.65692	2.00848	0.86800
N	-0.76028	2.76203	2.01377
C	-3.22260	-0.12825	4.22827
C	-3.34657	-1.23535	3.21638
C	-2.09062	-1.57113	2.69830
C	-1.92627	-2.64927	1.83734
C	-3.05969	-3.34716	1.42420
C	-4.31953	-2.98393	1.89717
C	-4.47100	-1.94318	2.81352

C	-0.45634	2.66004	-0.38411
C	-1.53583	3.37565	-0.97137
C	-1.33560	3.96028	-2.25586
C	-0.07364	3.83934	-2.88378
C	0.96485	3.18247	-2.27852
C	0.76665	2.59446	-1.01484
C	-2.79259	3.53065	-0.33905
C	-3.80591	4.21320	-0.96459
C	-3.61703	4.77311	-2.24592
C	-2.40422	4.65179	-2.87377
H	-0.05754	-1.05730	3.37434
H	-1.55796	-0.99644	5.29226
H	-3.50247	0.84665	3.79667
H	-3.85098	-0.27112	5.11536
H	-0.93323	-2.95907	1.50728
H	-2.95615	-4.18073	0.73187
H	-5.19566	-3.54060	1.56999
H	-5.45463	-1.70124	3.21409
H	0.06778	4.29064	-3.86523
H	1.94003	3.10467	-2.75241
Cl	2.12136	1.79435	-0.25820
H	-2.94424	3.12585	0.65953
H	-4.76532	4.33081	-0.46399
H	-4.43255	5.30773	-2.72796
H	-2.24103	5.08896	-3.85827
Au	-0.64620	-0.93602	-0.35566
C	-0.53421	-2.43713	-1.75266
C	-1.55721	-2.42968	-2.71773
C	0.45393	-3.40804	-1.77796
C	-1.54257	-3.38294	-3.73346
C	0.45508	-4.36388	-2.79875
H	1.22197	-3.44692	-1.00565
C	-0.53295	-4.34089	-3.77602
H	-2.32464	-3.39110	-4.49235
H	1.22993	-5.12837	-2.82387
H	-0.52779	-5.08338	-4.57180

C	-2.39936	-0.62125	-1.34924
C	-3.36283	0.27132	-0.91818
C	-2.59327	-1.42564	-2.48609
C	-4.53044	0.42686	-1.67020
H	-3.22921	0.84600	-0.00294
C	-3.76270	-1.25243	-3.22462
C	-4.71908	-0.32309	-2.82421
H	-5.28606	1.14047	-1.34518
H	-3.94028	-1.86023	-4.11150
H	-5.62701	-0.19802	-3.41106
O	1.22526	-1.45273	0.75685
C	3.57232	-1.29413	0.89739
C	2.35183	-1.31545	0.20979
C	6.04459	-1.13061	0.74927
C	4.75735	-1.14844	0.19924
C	7.22446	-1.18252	-0.01684
H	2.40231	-1.20527	-0.89223
H	4.68659	-1.06944	-0.89313
H	3.56641	-1.39958	1.98269
C	8.46400	-1.76591	0.61033
H	7.08927	-1.44398	-1.06916
H	6.13250	-1.16728	1.83869
H	9.35826	-1.61102	-0.00294
H	8.64957	-1.34133	1.60601
H	8.33605	-2.84938	0.73637
C	7.84203	0.72905	-0.29828
C	6.99352	1.17025	-1.31944
C	5.80243	1.67780	-0.75686
C	5.92974	1.68352	0.61019
C	7.33781	1.37073	0.96991
H	8.90388	0.55613	-0.46759
H	7.17779	1.03803	-2.38294
H	4.91300	1.96675	-1.31067
H	5.16767	1.99323	1.32071
H	7.87857	2.32731	1.09122
H	7.48092	0.81181	1.89983

O	-1.11959	0.94265	5.14147
C	-1.20515	2.11894	4.38469
H	-2.19903	2.59109	4.47768
H	-0.47496	2.82547	4.79494

Bottom, away, 2, exo, toward

M06/lanl2dz-6-31G(d) Energy = -2646.118224

M06/lanl2dz-6-31G(d) Free Energy = -2645.480488

M06/def2-TZVP Derived free energy = -2646.590631

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.621333

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.645687

Number of Imaginary Frequencies = 1 (-400.64)

M06/lanl2dz-6-31G(d) Geometry

C	-3.21985	-0.60917	-2.51547
C	-4.75973	-0.81633	-2.38713
C	-2.98466	-2.76521	-1.36835
N	-2.55670	-1.46335	-1.50904
C	-1.49348	-1.26974	-0.70064
N	-1.31807	-2.47828	-0.14120
N	-2.24000	-3.42235	-0.53245
C	-5.25591	0.36484	-1.54496
C	-4.19733	1.41016	-1.74236
C	-3.04672	0.86048	-2.30816
C	-1.93490	1.64283	-2.60663
C	-1.97926	3.00083	-2.30120
C	-3.11823	3.55141	-1.71169
C	-4.23361	2.76472	-1.43233
C	-0.20139	-2.86689	0.65671
C	-0.24138	-2.70013	2.06572
C	0.91430	-3.06450	2.81843
C	2.03550	-3.60656	2.14435
C	2.03995	-3.77820	0.78397
C	0.90925	-3.39409	0.03411
C	-1.37038	-2.18496	2.74357

C	-1.34309	-2.01333	4.10454
C	-0.19749	-2.36167	4.85213
C	0.90417	-2.88173	4.22152
H	-2.84357	-0.95476	-3.48913
H	-5.17341	-0.76220	-3.40913
H	-5.31819	0.05096	-0.49067
H	-6.25938	0.69405	-1.84032
H	-1.04778	1.20283	-3.06691
H	-1.12065	3.63320	-2.51890
H	-3.13627	4.61287	-1.47170
H	-5.12194	3.20679	-0.98279
H	2.90567	-3.89963	2.73159
H	2.89536	-4.20527	0.26518
Cl	0.96023	-3.56712	-1.69230
H	-2.26146	-1.92262	2.17791
H	-2.21616	-1.60552	4.61049
H	-0.19492	-2.22254	5.93097
H	1.78903	-3.16488	4.79086
Au	-0.53246	0.55857	-0.06358
C	0.27523	2.32606	0.60154
C	-0.53847	3.05659	1.48400
C	1.50017	2.82612	0.18874
C	-0.08812	4.28464	1.96565
C	1.94157	4.05927	0.67936
H	2.11337	2.27572	-0.52602
C	1.15066	4.77996	1.56707
H	-0.70250	4.86759	2.65161
H	2.90449	4.45679	0.35776
H	1.49613	5.73924	1.94796
C	-2.04510	1.18514	1.16174
C	-3.22151	0.48301	1.36363
C	-1.82000	2.42340	1.78923
C	-4.20728	1.01415	2.19978
H	-3.40375	-0.47443	0.87339
C	-2.81921	2.94187	2.61314
C	-4.00488	2.24288	2.81668

H	-5.13300	0.46287	2.35965
H	-2.67100	3.90386	3.10323
H	-4.77267	2.66002	3.46537
O	1.26354	0.08133	-1.28297
C	3.53322	-0.53360	-1.21133
C	2.23161	-0.46252	-0.69059
C	5.91081	-1.09516	-0.77443
C	4.54745	-1.11050	-0.46366
C	6.43380	-0.40881	-1.87769
H	2.07412	-0.89850	0.31865
H	4.25186	-1.58667	0.47652
H	3.69891	-0.11406	-2.20314
C	7.82195	-0.71486	-2.35851
H	5.73370	-0.14906	-2.67346
H	6.60379	-1.59203	-0.09435
H	8.24338	0.08142	-2.98223
H	8.51299	-0.91080	-1.52930
H	7.79321	-1.62486	-2.97406
C	6.62529	1.56815	-1.25160
C	5.33816	2.01576	-0.94948
C	5.06692	1.79671	0.42838
C	6.19154	1.30819	1.02730
C	7.32781	1.36294	0.06870
H	7.15701	1.90335	-2.14110
H	4.63376	2.43449	-1.66576
H	4.10223	1.95568	0.90658
H	6.28903	1.02361	2.07098
H	7.92083	2.27033	0.28215
H	8.02754	0.52207	0.12454
O	-5.14218	-2.03334	-1.78271
C	-4.27011	-3.11386	-2.03175
H	-4.70682	-4.01318	-1.58892
H	-4.13391	-3.28900	-3.11366

M06/lanl2dz-6-31G(d) Energy = -2646.117014

M06/lanl2dz-6-31G(d) Free Energy = -2645.480715

M06/def2-TZVP Derived free energy = -2646.593025

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.623504

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.648284

Number of Imaginary Frequencies = 1 (-393.76)

M06/lanl2dz-6-31G(d) Geometry

C	-0.05937	3.03952	0.23877
C	0.25686	4.43773	-0.33501
C	-1.34766	2.78992	-1.89525
N	-0.81120	2.25677	-0.74813
C	-1.09170	0.93344	-0.71373
N	-1.78848	0.74050	-1.84595
N	-1.95717	1.88191	-2.59613
C	0.43637	5.30715	0.90488
C	-0.47301	4.65738	1.91202
C	-0.79097	3.35608	1.51931
C	-1.61768	2.55510	2.29468
C	-2.12832	3.07727	3.48194
C	-1.80851	4.37367	3.87944
C	-0.97844	5.17348	3.09660
C	-2.33899	-0.49067	-2.30752
C	-3.75286	-0.64770	-2.33190
C	-4.28008	-1.91481	-2.71713
C	-3.39354	-2.95615	-3.07946
C	-2.03691	-2.77060	-3.07866
C	-1.51182	-1.52188	-2.69368
C	-4.65083	0.38488	-1.96713
C	-6.00584	0.16326	-1.97981
C	-6.52988	-1.09223	-2.35608
C	-5.68215	-2.10690	-2.71866
H	0.87103	2.48331	0.42961
H	1.13372	4.42222	-1.00619
H	0.18339	6.35017	0.67819
H	1.48565	5.28620	1.23602
H	-1.87812	1.54021	1.99121
H	-2.78177	2.46587	4.10107

H	-2.21643	4.76805	4.80827
H	-0.74015	6.19087	3.40441
H	-3.80957	-3.91967	-3.37129
H	-1.35408	-3.56368	-3.37184
Cl	0.21861	-1.31569	-2.74185
H	-4.26277	1.36348	-1.69215
H	-6.68415	0.96787	-1.70278
H	-7.60645	-1.24813	-2.36275
H	-6.07282	-3.07922	-3.01693
Au	-0.31844	-0.49977	0.73190
C	0.42696	-1.88326	2.05331
C	-0.52282	-2.77152	2.58558
C	1.76083	-1.97396	2.41610
C	-0.10308	-3.77827	3.45201
C	2.16992	-2.98321	3.29232
H	2.48777	-1.25527	2.03856
C	1.24142	-3.88548	3.79762
H	-0.82425	-4.47945	3.87150
H	3.21651	-3.05672	3.58495
H	1.56207	-4.67242	4.47762
C	-2.06339	-1.36468	1.35773
C	-3.31538	-0.91989	0.97653
C	-1.89926	-2.48493	2.19188
C	-4.44591	-1.62819	1.39370
H	-3.43983	-0.03378	0.35799
C	-3.03954	-3.17674	2.59726
C	-4.30322	-2.75538	2.19278
H	-5.43373	-1.28744	1.08742
H	-2.94327	-4.04925	3.24281
H	-5.18329	-3.30893	2.51444
O	1.70292	0.29126	0.13683
C	3.72209	-0.09946	-1.02479
C	2.49283	-0.48276	-0.46580
C	5.76121	-0.85589	-2.24293
C	4.49717	-1.04818	-1.67459
C	6.45241	0.36014	-2.19602

H	2.22154	-1.55229	-0.56315
H	4.07647	-2.05607	-1.74048
H	4.01215	0.94862	-0.95693
C	7.58170	0.61322	-3.15192
H	5.86947	1.24805	-1.94493
H	6.23904	-1.70548	-2.73227
H	8.21838	1.45170	-2.84873
H	8.21386	-0.27307	-3.28812
H	7.16417	0.86398	-4.13713
C	7.46838	0.35126	-0.36832
C	6.46996	0.35234	0.60384
C	6.14826	-0.98430	0.95865
C	6.98984	-1.83279	0.29868
C	8.04289	-1.04287	-0.39381
H	8.07419	1.23097	-0.57969
H	5.97725	1.23788	0.99830
H	5.33289	-1.27700	1.61429
H	6.97773	-2.91754	0.35052
H	8.95066	-1.04565	0.23628
H	8.34995	-1.42979	-1.37120
C	-1.14303	4.23248	-2.20959
H	-0.32001	4.33519	-2.94134
H	-2.04549	4.65955	-2.65899
O	-0.86701	4.94087	-1.03391

M06/lanl2dz-6-31G(d) Energy = -2646.117014

M06/lanl2dz-6-31G(d) Free Energy = -2645.480715

M06/def2-TZVP Derived free energy = -2646.593025

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.623504

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.648284

Number of Imaginary Frequencies = 1 (-393.76)

M06/lanl2dz-6-31G(d) Geometry

C	-0.05937	3.03952	0.23877
C	0.25686	4.43773	-0.33501
C	-1.34766	2.78992	-1.89525

N	-0.81120	2.25677	-0.74813
C	-1.09170	0.93344	-0.71373
N	-1.78848	0.74050	-1.84595
N	-1.95717	1.88191	-2.59613
C	0.43637	5.30715	0.90488
C	-0.47301	4.65738	1.91202
C	-0.79097	3.35608	1.51931
C	-1.61768	2.55510	2.29468
C	-2.12832	3.07727	3.48194
C	-1.80851	4.37367	3.87944
C	-0.97844	5.17348	3.09660
C	-2.33899	-0.49067	-2.30752
C	-3.75286	-0.64770	-2.33190
C	-4.28008	-1.91481	-2.71713
C	-3.39354	-2.95615	-3.07946
C	-2.03691	-2.77060	-3.07866
C	-1.51182	-1.52188	-2.69368
C	-4.65083	0.38488	-1.96713
C	-6.00584	0.16326	-1.97981
C	-6.52988	-1.09223	-2.35608
C	-5.68215	-2.10690	-2.71866
H	0.87103	2.48331	0.42961
H	1.13372	4.42222	-1.00619
H	0.18339	6.35017	0.67819
H	1.48565	5.28620	1.23602
H	-1.87812	1.54021	1.99121
H	-2.78177	2.46587	4.10107
H	-2.21643	4.76805	4.80827
H	-0.74015	6.19087	3.40441
H	-3.80957	-3.91967	-3.37129
H	-1.35408	-3.56368	-3.37184
Cl	0.21861	-1.31569	-2.74185
H	-4.26277	1.36348	-1.69215
H	-6.68415	0.96787	-1.70278
H	-7.60645	-1.24813	-2.36275
H	-6.07282	-3.07922	-3.01693

Au	-0.31844	-0.49977	0.73190
C	0.42696	-1.88326	2.05331
C	-0.52282	-2.77152	2.58558
C	1.76083	-1.97396	2.41610
C	-0.10308	-3.77827	3.45201
C	2.16992	-2.98321	3.29232
H	2.48777	-1.25527	2.03856
C	1.24142	-3.88548	3.79762
H	-0.82425	-4.47945	3.87150
H	3.21651	-3.05672	3.58495
H	1.56207	-4.67242	4.47762
C	-2.06339	-1.36468	1.35773
C	-3.31538	-0.91989	0.97653
C	-1.89926	-2.48493	2.19188
C	-4.44591	-1.62819	1.39370
H	-3.43983	-0.03378	0.35799
C	-3.03954	-3.17674	2.59726
C	-4.30322	-2.75538	2.19278
H	-5.43373	-1.28744	1.08742
H	-2.94327	-4.04925	3.24281
H	-5.18329	-3.30893	2.51444
O	1.70292	0.29126	0.13683
C	3.72209	-0.09946	-1.02479
C	2.49283	-0.48276	-0.46580
C	5.76121	-0.85589	-2.24293
C	4.49717	-1.04818	-1.67459
C	6.45241	0.36014	-2.19602
H	2.22154	-1.55229	-0.56315
H	4.07647	-2.05607	-1.74048
H	4.01215	0.94862	-0.95693
C	7.58170	0.61322	-3.15192
H	5.86947	1.24805	-1.94493
H	6.23904	-1.70548	-2.73227
H	8.21838	1.45170	-2.84873
H	8.21386	-0.27307	-3.28812
H	7.16417	0.86398	-4.13713

C	7.46838	0.35126	-0.36832
C	6.46996	0.35234	0.60384
C	6.14826	-0.98430	0.95865
C	6.98984	-1.83279	0.29868
C	8.04289	-1.04287	-0.39381
H	8.07419	1.23097	-0.57969
H	5.97725	1.23788	0.99830
H	5.33289	-1.27700	1.61429
H	6.97773	-2.91754	0.35052
H	8.95066	-1.04565	0.23628
H	8.34995	-1.42979	-1.37120
C	-1.14303	4.23248	-2.20959
H	-0.32001	4.33519	-2.94134
H	-2.04549	4.65955	-2.65899
O	-0.86701	4.94087	-1.03391

M06/lanl2dz-6-31G(d) Energy = -2646.116288

M06/lanl2dz-6-31G(d) Free Energy = -2645.476814

M06/def2-TZVP Derived free energy = -2646.586448

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616380

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.639931

Number of Imaginary Frequencies = 1 (-389.34)

M06/lanl2dz-6-31G(d) Geometry

C	-0.21849	3.17171	0.53321
C	-0.64936	4.65040	0.50416
C	-1.86904	3.06347	-1.36805
N	-1.10843	2.43593	-0.40811
C	-1.29160	1.09702	-0.52642
N	-2.16066	0.99590	-1.54640
N	-2.52949	2.20487	-2.08499
C	-1.80927	4.73596	1.51486
C	-1.40484	3.69407	2.51987
C	-0.46776	2.81346	1.96888
C	0.13503	1.82783	2.74238
C	-0.26469	1.68543	4.06932

C	-1.22610	2.53765	4.61100
C	-1.78992	3.55813	3.84721
C	-2.72424	-0.20022	-2.08141
C	-4.11664	-0.43794	-1.90738
C	-4.65320	-1.67044	-2.38058
C	-3.79652	-2.60463	-3.00900
C	-2.46512	-2.34148	-3.19012
C	-1.93283	-1.12158	-2.72944
C	-4.97939	0.47394	-1.25199
C	-6.30813	0.17428	-1.08000
C	-6.84272	-1.04236	-1.55513
C	-6.02882	-1.94357	-2.19199
H	0.80946	3.00695	0.19254
H	0.19428	5.23243	0.89594
H	-2.77528	4.48711	1.04700
H	-1.91465	5.74181	1.93856
H	0.93009	1.20397	2.33331
H	0.19072	0.91702	4.69072
H	-1.52192	2.42024	5.65181
H	-2.50999	4.24541	4.28960
H	-4.21571	-3.54677	-3.36013
H	-1.80782	-3.04961	-3.68777
Cl	-0.24636	-0.80536	-3.03393
H	-4.58681	1.42355	-0.89475
H	-6.95911	0.88677	-0.57729
H	-7.89934	-1.25991	-1.41498
H	-6.42588	-2.88787	-2.56320
Au	-0.17925	-0.46374	0.50673
C	0.92880	-1.92550	1.43250
C	0.20403	-3.05473	1.84890
C	2.29337	-1.83752	1.66166
C	0.87990	-4.11558	2.44878
C	2.95889	-2.90190	2.27820
H	2.84750	-0.93968	1.38352
C	2.25465	-4.04001	2.65514
H	0.33452	-5.00105	2.77465

H	4.02953	-2.83275	2.47213
H	2.77455	-4.86885	3.13190
C	-1.67473	-1.71752	1.11671
C	-3.01614	-1.41178	0.99912
C	-1.23968	-2.93861	1.66179
C	-3.96728	-2.36431	1.37633
H	-3.34545	-0.44671	0.62260
C	-2.20340	-3.87600	2.02986
C	-3.55826	-3.59436	1.87573
H	-5.02607	-2.13112	1.27071
H	-1.89553	-4.83261	2.45142
H	-4.29854	-4.33775	2.16511
O	1.66211	0.71620	-0.04374
C	3.74911	0.77391	-1.13178
C	2.44342	0.29907	-0.93979
C	5.86793	0.57086	-2.41638
C	4.52198	0.28089	-2.17298
C	6.65110	1.35246	-1.55768
H	2.10038	-0.50980	-1.61427
H	4.03488	-0.42058	-2.85621
H	4.11013	1.54462	-0.45116
C	7.95189	1.92260	-2.04198
H	6.12141	1.99196	-0.84930
H	6.34186	0.12438	-3.29130
H	7.74503	2.82309	-2.63716
H	8.61643	2.22359	-1.22435
H	8.49330	1.22511	-2.69307
C	7.29716	0.03541	-0.07099
C	6.14276	-0.41329	0.57144
C	5.67407	-1.59521	-0.06133
C	6.56600	-1.96246	-1.02753
C	7.77754	-1.10526	-0.93468
H	7.98753	0.73352	0.40025
H	5.64673	0.09037	1.39874
H	4.73057	-2.09091	0.15622
H	6.47205	-2.81334	-1.69609

H	8.55101	-1.65527	-0.36889
H	8.23601	-0.83728	-1.89233
O	-0.86976	5.15282	-0.78899
C	-1.92699	4.54882	-1.48263
H	-1.84151	4.84542	-2.53375
H	-2.90853	4.90545	-1.12430

M06/lanl2dz-6-31G(d) Energy = -2646.117014

M06/lanl2dz-6-31G(d) Free Energy = -2645.480715

M06/def2-TZVP Derived free energy = -2646.593025

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.623504

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.648284

Number of Imaginary Frequencies = 1 (-393.76)

M06/lanl2dz-6-31G(d) Geometry

C	-0.05937	3.03952	0.23877
C	0.25686	4.43773	-0.33501
C	-1.34766	2.78992	-1.89525
N	-0.81120	2.25677	-0.74813
C	-1.09170	0.93344	-0.71373
N	-1.78848	0.74050	-1.84595
N	-1.95717	1.88191	-2.59613
C	0.43637	5.30715	0.90488
C	-0.47301	4.65738	1.91202
C	-0.79097	3.35608	1.51931
C	-1.61768	2.55510	2.29468
C	-2.12832	3.07727	3.48194
C	-1.80851	4.37367	3.87944
C	-0.97844	5.17348	3.09660
C	-2.33899	-0.49067	-2.30752
C	-3.75286	-0.64770	-2.33190
C	-4.28008	-1.91481	-2.71713
C	-3.39354	-2.95615	-3.07946
C	-2.03691	-2.77060	-3.07866
C	-1.51182	-1.52188	-2.69368
C	-4.65083	0.38488	-1.96713

C	-6.00584	0.16326	-1.97981
C	-6.52988	-1.09222	-2.35608
C	-5.68215	-2.10690	-2.71866
H	0.87103	2.48331	0.42961
H	1.13372	4.42222	-1.00619
H	0.18339	6.35017	0.67819
H	1.48565	5.28620	1.23602
H	-1.87812	1.54021	1.99121
H	-2.78177	2.46587	4.10107
H	-2.21643	4.76805	4.80827
H	-0.74015	6.19087	3.40441
H	-3.80957	-3.91967	-3.37129
H	-1.35408	-3.56368	-3.37184
Cl	0.21861	-1.31569	-2.74185
H	-4.26277	1.36348	-1.69215
H	-6.68415	0.96787	-1.70278
H	-7.60645	-1.24813	-2.36275
H	-6.07282	-3.07922	-3.01693
Au	-0.31844	-0.49977	0.73190
C	0.42696	-1.88326	2.05331
C	-0.52282	-2.77152	2.58558
C	1.76083	-1.97396	2.41610
C	-0.10308	-3.77827	3.45201
C	2.16992	-2.98321	3.29232
H	2.48777	-1.25527	2.03856
C	1.24142	-3.88548	3.79762
H	-0.82425	-4.47945	3.87150
H	3.21651	-3.05672	3.58495
H	1.56207	-4.67242	4.47762
C	-2.06339	-1.36468	1.35773
C	-3.31538	-0.91989	0.97653
C	-1.89926	-2.48493	2.19188
C	-4.44591	-1.62819	1.39370
H	-3.43983	-0.03378	0.35799
C	-3.03954	-3.17674	2.59726
C	-4.30322	-2.75538	2.19278

H	-5.43373	-1.28744	1.08742
H	-2.94327	-4.04925	3.24281
H	-5.18329	-3.30893	2.51444
O	1.70292	0.29126	0.13683
C	3.72209	-0.09946	-1.02479
C	2.49283	-0.48276	-0.46580
C	5.76121	-0.85589	-2.24293
C	4.49717	-1.04818	-1.67459
C	6.45241	0.36014	-2.19602
H	2.22154	-1.55229	-0.56315
H	4.07647	-2.05607	-1.74048
H	4.01215	0.94862	-0.95693
C	7.58170	0.61322	-3.15192
H	5.86947	1.24805	-1.94493
H	6.23904	-1.70548	-2.73227
H	8.21838	1.45170	-2.84873
H	8.21386	-0.27307	-3.28812
H	7.16417	0.86398	-4.13713
C	7.46838	0.35126	-0.36832
C	6.46996	0.35234	0.60384
C	6.14826	-0.98430	0.95865
C	6.98984	-1.83279	0.29868
C	8.04289	-1.04287	-0.39381
H	8.07419	1.23097	-0.57969
H	5.97725	1.23788	0.99830
H	5.33289	-1.27700	1.61429
H	6.97773	-2.91754	0.35052
H	8.95066	-1.04565	0.23628
H	8.34995	-1.42979	-1.37120
O	-0.86701	4.94087	-1.03391
C	-1.14303	4.23248	-2.20959
H	-0.32001	4.33519	-2.94134
H	-2.04549	4.65955	-2.65899

M06/lanl2dz-6-31G(d) Energy = -2646.116287

M06/lanl2dz-6-31G(d) Free Energy = -2645.476828

M06/def2-TZVP Derived free energy = -2646.586463

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616396

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.639947

Number of Imaginary Frequencies = 1 (-389.33)

M06/lanl2dz-6-31G(d) Geometry

C	-0.21841	3.17138	0.53471
C	-0.64958	4.64998	0.50650
C	-1.86829	3.06411	-1.36719
N	-1.10796	2.43608	-0.40736
C	-1.29124	1.09724	-0.52628
N	-2.16004	0.99664	-1.54652
N	-2.52866	2.20588	-2.08465
C	-1.81000	4.73453	1.51670
C	-1.40576	3.69204	2.52120
C	-0.46815	2.81210	1.97004
C	0.13457	1.82610	2.74309
C	-0.26580	1.68257	4.06972
C	-1.22775	2.53410	4.61153
C	-1.79147	3.55500	3.84824
C	-2.72376	-0.19922	-2.08196
C	-4.11619	-0.43684	-1.90803
C	-4.65287	-1.66915	-2.38159
C	-3.79627	-2.60324	-3.01028
C	-2.46484	-2.34018	-3.19129
C	-1.93243	-1.12048	-2.73022
C	-4.97886	0.47496	-1.25241
C	-6.30764	0.17539	-1.08052
C	-6.84234	-1.04108	-1.55600
C	-6.02852	-1.94219	-2.19310
H	0.80968	3.00702	0.19426
H	0.19374	5.23192	0.89912
H	-2.77571	4.48574	1.04821
H	-1.91586	5.74007	1.94105
H	0.93004	1.20282	2.33394
H	0.18952	0.91382	4.69078

H	-1.52409	2.41580	5.65210
H	-2.51195	4.24175	4.29078
H	-4.21556	-3.54523	-3.36169
H	-1.80760	-3.04823	-3.68913
Cl	-0.24590	-0.80437	-3.03447
H	-4.58619	1.42443	-0.89491
H	-6.95855	0.88780	-0.57762
H	-7.89898	-1.25856	-1.41592
H	-6.42566	-2.88636	-2.56457
Au	-0.17922	-0.46402	0.50644
C	0.92853	-1.92629	1.43176
C	0.20351	-3.05542	1.84800
C	2.29316	-1.83876	1.66071
C	0.87917	-4.11659	2.44755
C	2.95848	-2.90347	2.27691
H	2.84749	-0.94102	1.38271
C	2.25398	-4.04145	2.65371
H	0.33359	-5.00198	2.77328
H	4.02918	-2.83467	2.47067
H	2.77371	-4.87055	3.13021
C	-1.67496	-1.71765	1.11607
C	-3.01630	-1.41159	0.99849
C	-1.24019	-2.93891	1.66099
C	-3.96766	-2.36395	1.37559
H	-3.34538	-0.44641	0.62207
C	-2.20412	-3.87611	2.02899
C	-3.55891	-3.59414	1.87489
H	-5.02640	-2.13053	1.26996
H	-1.89647	-4.83283	2.45045
H	-4.29936	-4.33738	2.16421
O	1.66225	0.71607	-0.04336
C	3.74932	0.77444	-1.13121
C	2.44363	0.29945	-0.93959
C	5.86825	0.57224	-2.41572
C	4.52230	0.28202	-2.17262
C	6.65124	1.35349	-1.55654

H	2.10063	-0.50902	-1.61457
H	4.03533	-0.41913	-2.85625
H	4.11023	1.54483	-0.45018
C	7.95205	1.92396	-2.04038
H	6.12139	1.99261	-0.84793
H	6.34232	0.12626	-3.29082
H	7.74520	2.82464	-2.63529
H	8.61638	2.22474	-1.22250
H	8.49369	1.22677	-2.69160
C	7.29717	0.03585	-0.07033
C	6.14272	-0.41333	0.57168
C	5.67438	-1.59509	-0.06166
C	6.56658	-1.96179	-1.02781
C	7.77792	-1.10436	-0.93443
H	7.98733	0.73385	0.40139
H	5.64646	0.08986	1.39912
H	4.73092	-2.09104	0.15549
H	6.47292	-2.81241	-1.69675
H	8.55148	-1.65442	-0.36882
H	8.23639	-0.83587	-1.89194
O	-0.86943	5.15324	-0.78640
C	-1.92617	4.54953	-1.48107
H	-1.83995	4.84666	-2.53198
H	-2.90797	4.90595	-1.12325

M06/lanl2dz-6-31G(d) Energy = -2646.114488

M06/lanl2dz-6-31G(d) Free Energy = -2645.478540

M06/def2-TZVP Derived free energy = -2646.587736

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.617764

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.641506

Number of Imaginary Frequencies = 1 (-360.03)

M06/lanl2dz-6-31G(d) Geometry

C	-0.52513	3.20651	0.72144
C	-0.98267	4.66301	0.51970
C	-1.46164	3.00192	-1.60770

N	-1.04790	2.42106	-0.43126
C	-1.14248	1.07475	-0.56254
N	-1.61331	0.92206	-1.81172
N	-1.81617	2.10648	-2.47946
C	-2.40985	4.70079	1.09960
C	-2.30199	3.69714	2.21312
C	-1.19988	2.85847	2.01504
C	-0.82862	1.92080	2.97156
C	-1.62139	1.77918	4.10839
C	-2.74316	2.58684	4.29036
C	-3.08168	3.56285	3.35418
C	-1.88614	-0.30631	-2.48181
C	-3.23423	-0.63518	-2.79525
C	-3.49516	-1.90078	-3.39538
C	-2.41627	-2.77115	-3.67871
C	-1.12290	-2.41677	-3.40170
C	-0.86135	-1.16783	-2.80532
C	-4.32367	0.22286	-2.50871
C	-5.60785	-0.16154	-2.80594
C	-5.86822	-1.41385	-3.40294
C	-4.83081	-2.26293	-3.69084
H	0.56283	3.07761	0.72291
H	-0.33700	5.28779	1.14990
H	-3.15874	4.39028	0.35343
H	-2.69427	5.70551	1.43408
H	0.08185	1.33302	2.85377
H	-1.35140	1.04637	4.86614
H	-3.34755	2.47171	5.18809
H	-3.93470	4.21826	3.52515
H	-2.62843	-3.73705	-4.13559
H	-0.29013	-3.07449	-3.63631
Cl	0.80323	-0.73846	-2.51469
H	-4.13638	1.19799	-2.06366
H	-6.43499	0.51008	-2.58448
H	-6.89192	-1.69868	-3.63608
H	-5.01544	-3.23225	-4.15289

Au	-0.42545	-0.43125	0.84186
C	0.31892	-1.85114	2.12286
C	-0.50737	-2.96865	2.32903
C	1.54718	-1.74844	2.75590
C	-0.06127	-4.00117	3.15077
C	1.98133	-2.78791	3.58443
H	2.16839	-0.86218	2.62319
C	1.18287	-3.91034	3.77009
H	-0.68629	-4.87682	3.32459
H	2.94342	-2.71304	4.08923
H	1.52328	-4.71897	4.41430
C	-2.03847	-1.68038	0.96986
C	-3.26173	-1.40191	0.39226
C	-1.81008	-2.87546	1.67574
C	-4.27941	-2.35751	0.45815
H	-3.44647	-0.45469	-0.10787
C	-2.83776	-3.81509	1.73165
C	-4.06026	-3.56214	1.11487
H	-5.24019	-2.14924	-0.01095
H	-2.68626	-4.75190	2.26755
H	-4.85170	-4.30758	1.16351
O	1.47606	0.77934	0.77734
C	3.60311	0.99863	-0.22503
C	2.47499	0.28097	0.19023
C	5.76906	0.93125	-1.44479
C	4.61233	0.34941	-0.91496
C	6.64533	0.25753	-2.31570
H	2.47987	-0.80766	-0.01684
H	4.47299	-0.72257	-1.10523
H	3.65071	2.07098	-0.03240
C	7.47167	1.06806	-3.27912
H	6.26845	-0.68237	-2.72634
H	5.95265	1.98873	-1.23598
H	8.22536	0.46544	-3.79725
H	6.81668	1.50402	-4.04546
H	7.98104	1.89959	-2.77406

C	8.13242	-0.54303	-1.17659
C	7.51720	-1.66535	-0.61516
C	6.86222	-1.29674	0.58100
C	7.15371	0.01615	0.85478
C	8.21045	0.48661	-0.07811
H	8.90867	-0.63165	-1.93514
H	7.46228	-2.64588	-1.08203
H	6.20345	-1.93574	1.16214
H	6.77485	0.59348	1.69354
H	8.14759	1.53688	-0.37988
H	9.18818	0.36041	0.42196
C	-1.53587	4.48193	-1.77355
H	-1.12084	4.77135	-2.74523
H	-2.59487	4.79450	-1.76750
O	-0.79364	5.14436	-0.78656

M06/lanl2dz-6-31G(d) Energy = -2646.116288

M06/lanl2dz-6-31G(d) Free Energy = -2645.476826

M06/def2-TZVP Derived free energy = -2646.586460

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.616393

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.639944

Number of Imaginary Frequencies = 1 (-389.34)

M06/lanl2dz-6-31G(d) Geometry

C	-0.21861	3.17157	0.53391
C	-0.64973	4.65019	0.50532
C	-1.86889	3.06375	-1.36761
N	-1.10834	2.43599	-0.40778
C	-1.29150	1.09710	-0.52640
N	-2.16048	0.99622	-1.54646
N	-2.52929	2.20531	-2.08479
C	-1.80987	4.73514	1.51581
C	-1.40545	3.69294	2.52052
C	-0.46805	2.81276	1.96940
C	0.13479	1.82696	2.74264
C	-0.26524	1.68390	4.06942

C	-1.22699	2.53568	4.61120
C	-1.79084	3.55636	3.84771
C	-2.72411	-0.19980	-2.08165
C	-4.11652	-0.43751	-1.90760
C	-4.65311	-1.66994	-2.38095
C	-3.79648	-2.60404	-3.00956
C	-2.46508	-2.34090	-3.19068
C	-1.93275	-1.12109	-2.72983
C	-4.97922	0.47429	-1.25205
C	-6.30796	0.17463	-1.08003
C	-6.84259	-1.04194	-1.55531
C	-6.02873	-1.94307	-2.19234
H	0.80942	3.00708	0.19332
H	0.19373	5.23222	0.89750
H	-2.77573	4.48628	1.04765
H	-1.91554	5.74082	1.93987
H	0.93012	1.20349	2.33350
H	0.19019	0.91533	4.69061
H	-1.52306	2.41775	5.65188
H	-2.51116	4.24329	4.29021
H	-4.21571	-3.54612	-3.36081
H	-1.80781	-3.04897	-3.68845
Cl	-0.24627	-0.80488	-3.03425
H	-4.58661	1.42384	-0.89470
H	-6.95891	0.88706	-0.57719
H	-7.89920	-1.25950	-1.41513
H	-6.42582	-2.88732	-2.56365
Au	-0.17920	-0.46384	0.50651
C	0.92882	-1.92574	1.43208
C	0.20402	-3.05495	1.84849
C	2.29343	-1.83788	1.66107
C	0.87988	-4.11588	2.44823
C	2.95894	-2.90233	2.27749
H	2.84757	-0.94006	1.38292
C	2.25467	-4.04041	2.65445
H	0.33448	-5.00133	2.77410

H	4.02961	-2.83327	2.47130
H	2.77455	-4.86932	3.13110
C	-1.67471	-1.71763	1.11639
C	-3.01610	-1.41183	0.99882
C	-1.23970	-2.93874	1.66146
C	-3.96728	-2.36432	1.37605
H	-3.34538	-0.44676	0.62230
C	-2.20345	-3.87608	2.02957
C	-3.55830	-3.59438	1.87547
H	-5.02606	-2.13109	1.27042
H	-1.89561	-4.83270	2.45113
H	-4.29860	-4.33773	2.16489
O	1.66216	0.71626	-0.04368
C	3.74926	0.77427	-1.13147
C	2.44352	0.29942	-0.93982
C	5.86819	0.57183	-2.41596
C	4.52222	0.28169	-2.17281
C	6.65121	1.35312	-1.55686
H	2.10048	-0.50913	-1.61467
H	4.03521	-0.41949	-2.85638
H	4.11023	1.54468	-0.45049
C	7.95203	1.92353	-2.04078
H	6.12140	1.99229	-0.84828
H	6.34222	0.12576	-3.29103
H	7.74519	2.82425	-2.63562
H	8.61646	2.22422	-1.22295
H	8.49355	1.22632	-2.69209
C	7.29720	0.03551	-0.07060
C	6.14276	-0.41357	0.57150
C	5.67429	-1.59529	-0.06178
C	6.56639	-1.96209	-1.02800
C	7.77781	-1.10476	-0.93469
H	7.98744	0.73349	0.40103
H	5.64659	0.08969	1.39895
H	4.73081	-2.09117	0.15546
H	6.47261	-2.81270	-1.69691

H	8.55133	-1.65488	-0.36908
H	8.23629	-0.83634	-1.89222
C	-1.92689	4.54913	-1.48183
H	-1.84108	4.84601	-2.53284
H	-2.90859	4.90559	-1.12374
O	-0.86994	5.15305	-0.78768

M06/lanl2dz-6-31G(d) Energy = -2646.114237

M06/lanl2dz-6-31G(d) Free Energy = -2645.473742

M06/def2-TZVP Derived free energy = -2646.582003

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.612629

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.636959

Number of Imaginary Frequencies = 1 (-365.19)

M06/lanl2dz-6-31G(d) Geometry

C	0.76557	2.77095	0.23695
C	0.78468	4.27419	0.57504
C	-1.48016	3.40651	-0.70246
N	-0.60923	2.44757	-0.23447
C	-1.18697	1.23125	-0.40305
N	-2.37199	1.52788	-0.96093
N	-2.57315	2.87341	-1.15690
C	0.23304	4.34678	2.01185
C	0.76271	3.06470	2.59076
C	1.09838	2.16697	1.57023
C	1.72285	0.95801	1.85574
C	1.94821	0.62060	3.18869
C	1.57590	1.49429	4.20975
C	0.99762	2.72883	3.91773
C	-3.37570	0.60748	-1.38559
C	-4.63334	0.60069	-0.71906
C	-5.59405	-0.37623	-1.11057
C	-5.28243	-1.28137	-2.15228
C	-4.07823	-1.23270	-2.80178
C	-3.12255	-0.27263	-2.41528
C	-4.95792	1.49396	0.33075

C	-6.17546	1.41448	0.96095
C	-7.12737	0.44640	0.57550
C	-6.83974	-0.42741	-0.44102
H	1.44919	2.49348	-0.57303
H	1.83889	4.57923	0.59584
H	-0.86848	4.36317	2.02313
H	0.56956	5.24567	2.54184
H	2.04812	0.30038	1.04941
H	2.42396	-0.32850	3.43280
H	1.76059	1.21995	5.24673
H	0.74810	3.42322	4.71894
H	-6.02615	-2.02298	-2.44102
H	-3.84183	-1.91392	-3.61489
Cl	-1.62575	-0.22247	-3.30476
H	-4.24237	2.25788	0.62665
H	-6.41189	2.11115	1.76287
H	-8.08825	0.40023	1.08344
H	-7.56548	-1.17778	-0.75279
Au	-0.28044	-0.71677	-0.07143
C	0.60544	-2.55289	0.21506
C	-0.18042	-3.49246	0.90607
C	1.88349	-2.88589	-0.20805
C	0.32437	-4.77042	1.13676
C	2.38275	-4.16930	0.03600
H	2.51127	-2.16410	-0.73342
C	1.60204	-5.10785	0.69921
H	-0.27367	-5.50888	1.67033
H	3.38541	-4.43455	-0.29926
H	1.99027	-6.10772	0.88362
C	-1.70337	-1.62110	1.08241
C	-2.83004	-0.97069	1.54703
C	-1.46622	-2.97694	1.36774
C	-3.79067	-1.69239	2.26038
H	-2.98514	0.08956	1.36713
C	-2.43276	-3.67892	2.08621
C	-3.59371	-3.04331	2.51762

H	-4.69048	-1.18557	2.60695
H	-2.27870	-4.73297	2.31609
H	-4.34319	-3.60725	3.06948
O	1.42800	0.13435	-1.23888
C	3.25894	-0.23748	-2.66608
C	1.90885	-0.34916	-2.30557
C	5.54676	0.45861	-1.95410
C	4.16395	0.36077	-1.79993
C	6.36442	1.19915	-1.07709
H	1.23848	-0.91264	-2.97838
H	3.73753	0.81196	-0.89627
H	3.58829	-0.67292	-3.60822
C	7.70642	1.67176	-1.56844
H	5.84055	1.91496	-0.43947
H	6.01263	-0.03349	-2.81258
H	8.27077	0.86014	-2.04645
H	7.56364	2.45601	-2.32413
H	8.32237	2.09691	-0.76870
C	6.93705	-0.05714	0.40898
C	5.79970	-0.14543	1.22033
C	4.96849	-1.19104	0.76140
C	5.61359	-1.84647	-0.25818
C	7.01508	-1.36123	-0.34523
H	7.83348	0.46858	0.73493
H	5.54485	0.55001	2.01703
H	3.96600	-1.41631	1.12056
H	5.21170	-2.67000	-0.84384
H	7.65126	-2.04655	0.24421
H	7.44419	-1.32433	-1.35163
O	0.18993	5.08770	-0.40064
C	-1.17878	4.86281	-0.60385
H	-1.78849	5.30594	0.20317
H	-1.45986	5.36770	-1.53430

Top, towards, 2, exo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.109704
M06/lanl2dz-6-31G(d) Free Energy = -2645.473166
M06/def2-TZVP Derived free energy = -2646.583008
M06/def2-TZVP Derived free energy in solution (toluene) = -2646.613677
M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.638488
Number of Imaginary Frequencies = 1 (-375.92)

M06/lanl2dz-6-31G(d) Geometry

C	-1.18182	1.93108	-1.29741
C	-2.59453	2.56678	-1.07482
C	-0.61203	2.71023	0.97360
N	-0.48786	1.77592	-0.02352
C	0.42619	0.85576	0.34959
N	0.81235	1.29265	1.56063
N	0.16799	2.43846	1.97493
C	-2.73402	3.64877	-2.16336
C	-1.34463	3.86249	-2.69135
C	-0.47013	2.89150	-2.21086
C	0.87111	2.87432	-2.57671
C	1.33345	3.86150	-3.44076
C	0.46265	4.83955	-3.92524
C	-0.87962	4.84650	-3.55778
C	1.77596	0.67030	2.40726
C	3.03692	1.30079	2.59042
C	4.02208	0.61800	3.36032
C	3.70780	-0.63708	3.93399
C	2.47646	-1.21175	3.76399
C	1.50318	-0.54766	2.99136
C	3.36439	2.55093	2.01164
C	4.61675	3.08811	2.18239
C	5.59563	2.41153	2.94139
C	5.29980	1.20401	3.52030
H	-1.26941	0.92703	-1.73189
H	-3.36626	1.79114	-1.16307
H	-3.18998	4.55289	-1.73618
H	-3.41269	3.30756	-2.95845

H	1.54719	2.10416	-2.20031
H	2.37845	3.87059	-3.74343
H	0.83921	5.60577	-4.60023
H	-1.55296	5.61256	-3.94038
H	4.46983	-1.14924	4.52021
H	2.23168	-2.17327	4.20765
Cl	-0.04311	-1.31684	2.78292
H	2.61248	3.08951	1.43741
H	4.85459	4.05093	1.73418
H	6.58125	2.85405	3.06902
H	6.04537	0.67244	4.11063
Au	0.81861	-1.04674	-0.62504
C	1.18770	-2.89631	-1.44056
C	2.53283	-3.14193	-1.76882
C	0.22693	-3.87811	-1.62091
C	2.89051	-4.37729	-2.30264
C	0.59791	-5.11448	-2.15829
H	-0.81160	-3.71169	-1.33629
C	1.92238	-5.35802	-2.50022
H	3.92816	-4.58509	-2.56321
H	-0.15475	-5.88793	-2.30209
H	2.20835	-6.32156	-2.91767
C	2.83218	-0.89545	-0.92102
C	3.56168	0.23803	-0.61072
C	3.43738	-2.03209	-1.48380
C	4.94054	0.24554	-0.83688
H	3.08835	1.12023	-0.18464
C	4.81287	-2.00171	-1.70790
C	5.55917	-0.87229	-1.38216
H	5.51889	1.13248	-0.58293
H	5.31018	-2.86873	-2.14182
H	6.63274	-0.86770	-1.56046
O	-1.40414	-1.26691	-0.41664
C	-3.55235	-1.72223	-1.28748
C	-2.16456	-1.53761	-1.38968
C	-5.54399	-1.98849	0.16974

C	-4.19790	-1.69819	-0.05918
C	-6.07926	-2.17016	1.45850
H	-1.71681	-1.64655	-2.39613
H	-3.57266	-1.48671	0.81503
H	-4.10414	-1.95919	-2.19679
C	-7.28693	-3.05316	1.62386
H	-5.34486	-2.25219	2.26311
H	-6.18683	-2.17889	-0.69447
H	-7.70806	-3.00696	2.63391
H	-8.07744	-2.79587	0.90651
H	-7.00326	-4.09730	1.43445
C	-6.88606	-0.38185	2.03876
C	-5.76164	0.37058	2.38315
C	-5.26401	1.03908	1.24007
C	-6.12724	0.81581	0.19801
C	-7.35114	0.14027	0.70360
H	-7.58652	-0.74979	2.78671
H	-5.28425	0.36510	3.36019
H	-4.33921	1.61069	1.19143
H	-6.00967	1.17805	-0.82027
H	-8.11446	0.91580	0.89741
H	-7.81012	-0.58478	0.02354
O	-2.78286	3.08196	0.23443
C	-1.66681	3.74200	0.79901
H	-1.31932	4.57353	0.16273
H	-1.97479	4.15233	1.76480

M06/lanl2dz-6-31G(d) Energy = -2646.115040

M06/lanl2dz-6-31G(d) Free Energy = -2645.475921

M06/def2-TZVP Derived free energy = -2646.587187

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618038

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642416

Number of Imaginary Frequencies = 1 (-389.19)

M06/lanl2dz-6-31G(d) Geometry

C	-1.69721	-1.81300	0.38918
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C	-2.43161	-3.17001	0.39592
C	-0.19431	-3.06221	-1.20314
N	-0.46063	-1.97207	-0.40658
C	0.56448	-1.09478	-0.52428
N	1.40530	-1.72004	-1.36117
N	0.95292	-2.93998	-1.80085
C	-1.84740	-3.93668	1.59640
C	-1.49963	-2.81664	2.53465
C	-1.42552	-1.59821	1.85056
C	-1.15703	-0.41295	2.52604
C	-0.92361	-0.46135	3.89778
C	-0.98039	-1.67734	4.57826
C	-1.27854	-2.86016	3.90494
C	2.66478	-1.21941	-1.80781
C	3.85085	-1.78360	-1.26593
C	5.09797	-1.20311	-1.63521
C	5.11470	-0.11899	-2.54505
C	3.95813	0.38512	-3.07841
C	2.71990	-0.17314	-2.70225
C	3.84221	-2.87022	-0.35878
C	5.01839	-3.34757	0.16447
C	6.25495	-2.76801	-0.19250
C	6.29050	-1.72023	-1.07641
H	-2.27736	-1.01435	-0.09168
H	-3.48945	-2.95909	0.60743
H	-0.94865	-4.50869	1.31715
H	-2.56184	-4.65843	2.01011
H	-1.12901	0.54238	1.99870
H	-0.70256	0.45487	4.44124
H	-0.80165	-1.70047	5.65151
H	-1.34158	-3.80272	4.44723
H	6.07416	0.31528	-2.82356
H	3.97006	1.21294	-3.78252
Cl	1.27027	0.50115	-3.38543
H	2.89617	-3.33650	-0.08915
H	4.99896	-4.18872	0.85489

H	7.17778	-3.16035	0.22936
H	7.23845	-1.26771	-1.36561
Au	0.70907	1.01182	0.02074
C	0.96727	3.02733	0.31743
C	2.07358	3.37820	1.11038
C	0.18167	4.00419	-0.27184
C	2.34726	4.72455	1.33945
C	0.46745	5.35280	-0.03745
H	-0.63981	3.74036	-0.93698
C	1.53963	5.70682	0.77239
H	3.19892	5.01597	1.95387
H	-0.14729	6.12385	-0.49871
H	1.75943	6.75698	0.95514
C	2.38126	0.97982	1.19114
C	2.98230	-0.19294	1.60832
C	2.84636	2.24102	1.60070
C	4.11550	-0.11993	2.42270
H	2.59173	-1.16462	1.31282
C	3.97335	2.29045	2.41945
C	4.60711	1.11761	2.82027
H	4.60294	-1.03861	2.74473
H	4.36013	3.25356	2.75166
H	5.48908	1.17246	3.45552
O	-1.28647	1.10013	-1.03893
C	-3.60141	1.49333	-1.04663
C	-2.29200	1.69036	-0.57245
C	-6.02062	1.98311	-0.76541
C	-4.66643	2.14738	-0.45088
C	-6.47870	1.10703	-1.75799
H	-2.16115	2.40761	0.26467
H	-4.42588	2.84014	0.36066
H	-3.72591	0.82449	-1.89814
C	-7.86347	1.27321	-2.31284
H	-5.74311	0.76684	-2.48931
H	-6.75458	2.55934	-0.20091
H	-7.85755	2.09560	-3.04154

H	-8.22264	0.38097	-2.83760
H	-8.59136	1.53820	-1.53579
C	-6.61901	-0.75236	-0.84235
C	-5.32317	-1.09287	-0.45309
C	-5.09043	-0.63634	0.87301
C	-6.24612	-0.10364	1.36816
C	-7.35781	-0.36705	0.41597
H	-7.11791	-1.24650	-1.67487
H	-4.59272	-1.59608	-1.08603
H	-4.13101	-0.65701	1.38948
H	-6.37585	0.34617	2.34822
H	-7.91326	-1.25621	0.76538
H	-8.09633	0.43639	0.32536
C	-1.15576	-4.19661	-1.30988
H	-1.26230	-4.49591	-2.35784
H	-0.77456	-5.07223	-0.75796
O	-2.42890	-3.81102	-0.85417

M06/lanl2dz-6-31G(d) Energy = -2646.115039

M06/lanl2dz-6-31G(d) Free Energy = -2645.475921

M06/def2-TZVP Derived free energy = -2646.587187

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618037

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642416

Number of Imaginary Frequencies = 1 (-398.19)

M06/lanl2dz-6-31G(d) Geometry

C	-1.69721	-1.81300	0.38917
C	-2.43160	-3.17001	0.39591
C	-0.19431	-3.06221	-1.20315
N	-0.46063	-1.97207	-0.40659
C	0.56448	-1.09478	-0.52429
N	1.40530	-1.72004	-1.36118
N	0.95293	-2.93998	-1.80086
C	-1.84739	-3.93668	1.59638
C	-1.49962	-2.81664	2.53464
C	-1.42552	-1.59821	1.85055

C	-1.15703	-0.41295	2.52603
C	-0.92361	-0.46136	3.89777
C	-0.98038	-1.67735	4.57824
C	-1.27852	-2.86017	3.90493
C	2.66478	-1.21941	-1.80780
C	3.85085	-1.78361	-1.26592
C	5.09798	-1.20311	-1.63519
C	5.11471	-0.11899	-2.54502
C	3.95814	0.38513	-3.07839
C	2.71991	-0.17313	-2.70224
C	3.84220	-2.87023	-0.35877
C	5.01837	-3.34758	0.16448
C	6.25494	-2.76802	-0.19248
C	6.29050	-1.72024	-1.07638
H	-2.27736	-1.01435	-0.09169
H	-3.48945	-2.95910	0.60742
H	-0.94864	-4.50869	1.31713
H	-2.56183	-4.65844	2.01010
H	-1.12902	0.54238	1.99869
H	-0.70256	0.45486	4.44123
H	-0.80163	-1.70047	5.65150
H	-1.34157	-3.80272	4.44722
H	6.07418	0.31529	-2.82352
H	3.97008	1.21294	-3.78250
Cl	1.27029	0.50116	-3.38543
H	2.89616	-3.33651	-0.08915
H	4.99894	-4.18874	0.85490
H	7.17777	-3.16036	0.22939
H	7.23845	-1.26772	-1.36557
Au	0.70907	1.01182	0.02073
C	0.96726	3.02733	0.31742
C	2.07357	3.37820	1.11038
C	0.18167	4.00420	-0.27185
C	2.34724	4.72456	1.33945
C	0.46745	5.35280	-0.03747
H	-0.63981	3.74036	-0.93700

C	1.53962	5.70683	0.77238
H	3.19890	5.01598	1.95388
H	-0.14729	6.12385	-0.49873
H	1.75942	6.75699	0.95513
C	2.38126	0.97983	1.19114
C	2.98229	-0.19293	1.60833
C	2.84635	2.24102	1.60071
C	4.11548	-0.11993	2.42271
H	2.59172	-1.16462	1.31282
C	3.97333	2.29046	2.41946
C	4.60709	1.11762	2.82028
H	4.60293	-1.03861	2.74475
H	4.36011	3.25357	2.75167
H	5.48906	1.17247	3.45554
O	-1.28647	1.10013	-1.03895
C	-3.60141	1.49332	-1.04663
C	-2.29200	1.69036	-0.57246
C	-6.02062	1.98310	-0.76540
C	-4.66643	2.14737	-0.45087
C	-6.47870	1.10702	-1.75798
H	-2.16115	2.40760	0.26466
H	-4.42587	2.84014	0.36065
H	-3.72591	0.82448	-1.89813
C	-7.86348	1.27321	-2.31282
H	-5.74312	0.76682	-2.48930
H	-6.75458	2.55934	-0.20091
H	-7.85756	2.09558	-3.04154
H	-8.22266	0.38095	-2.83755
H	-8.59136	1.53821	-1.53577
C	-6.61902	-0.75237	-0.84233
C	-5.32318	-1.09288	-0.45307
C	-5.09042	-0.63634	0.87302
C	-6.24611	-0.10363	1.36817
C	-7.35781	-0.36704	0.41599
H	-7.11793	-1.24651	-1.67485
H	-4.59273	-1.59610	-1.08602

H	-4.13101	-0.65702	1.38948
H	-6.37583	0.34619	2.34823
H	-7.91326	-1.25620	0.76541
H	-8.09633	0.43640	0.32538
C	-1.15576	-4.19660	-1.30989
H	-1.26231	-4.49590	-2.35786
H	-0.77455	-5.07223	-0.75798
O	-2.42890	-3.81102	-0.85418

Bottom, towards, 2, exo, towards

M06/lanl2dz-6-31G(d) Energy = -2646.114073

M06/lanl2dz-6-31G(d) Free Energy = -2645.476611

M06/def2-TZVP Derived free energy = -2646.587840

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618718

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.643592

Number of Imaginary Frequencies = 1 (-362.24)

M06/lanl2dz-6-31G(d) Geometry

C	0.00479	3.04252	-0.17828
C	0.05245	4.50715	-0.67035
C	-2.20107	3.04860	-1.35911
N	-1.19951	2.38308	-0.69134
C	-1.50937	1.06531	-0.65338
N	-2.68252	1.00962	-1.30583
N	-3.12846	2.23086	-1.75338
C	0.90239	5.21938	0.37667
C	0.64788	4.42598	1.62824
C	0.10336	3.17756	1.32036
C	-0.21213	2.26817	2.32138
C	0.02320	2.62798	3.64749
C	0.56939	3.87187	3.95742
C	0.88668	4.77933	2.94870
C	-3.45319	-0.16019	-1.57346
C	-4.72184	-0.30224	-0.94536
C	-5.44538	-1.51060	-1.16145

C	-4.89655	-2.50687	-2.00328
C	-3.68595	-2.33320	-2.61954
C	-2.96100	-1.14423	-2.40412
C	-5.28038	0.68644	-0.09894
C	-6.49515	0.47855	0.50635
C	-7.21134	-0.71933	0.29673
C	-6.69510	-1.69013	-0.52249
H	0.85664	2.48470	-0.59178
H	0.45121	4.58340	-1.69713
H	0.60944	6.27403	0.44799
H	1.96419	5.19148	0.08905
H	-0.65187	1.29661	2.09267
H	-0.22818	1.93220	4.44554
H	0.74232	4.14002	4.99801
H	1.30140	5.75624	3.19433
H	-5.45891	-3.42620	-2.16234
H	-3.26889	-3.09117	-3.27752
Cl	-1.43588	-0.95967	-3.22148
H	-4.75061	1.62373	0.05722
H	-6.91399	1.24980	1.14991
H	-8.17469	-0.86548	0.78064
H	-7.23834	-2.61830	-0.69727
Au	-0.30882	-0.62472	0.01308
C	0.74670	-2.32063	0.51497
C	0.12298	-3.14717	1.46642
C	1.94883	-2.70396	-0.06219
C	0.74275	-4.33252	1.85749
C	2.55735	-3.90001	0.33117
H	2.41701	-2.09929	-0.83912
C	1.95997	-4.70426	1.29508
H	0.27196	-4.97995	2.59690
H	3.49384	-4.21035	-0.13336
H	2.43464	-5.63482	1.60052
C	-1.59964	-1.44659	1.37053
C	-2.79043	-0.85217	1.74612
C	-1.16910	-2.65755	1.94002

C	-3.60625	-1.48998	2.68422
H	-3.10432	0.10117	1.32791
C	-1.99331	-3.27390	2.88042
C	-3.20680	-2.69713	3.24379
H	-4.55180	-1.03201	2.97007
H	-1.68659	-4.21516	3.33564
H	-3.84128	-3.19435	3.97485
O	1.31559	0.20838	-1.28644
C	3.64330	0.57982	-1.43240
C	2.44396	0.37578	-0.74401
C	6.12410	0.71961	-1.22862
C	4.82692	0.64066	-0.71512
C	7.26473	0.87001	-0.41480
H	2.51431	0.34172	0.36388
H	4.74014	0.62005	0.37847
H	3.63381	0.60537	-2.52233
C	8.51139	1.45815	-1.02081
H	7.06880	1.18978	0.61161
H	6.25189	0.69909	-2.31414
H	8.76578	0.96943	-1.97058
H	8.34734	2.52272	-1.23539
H	9.37711	1.38852	-0.35349
C	7.92560	-0.99348	0.02962
C	7.01460	-1.43477	0.99649
C	5.90035	-2.02656	0.36242
C	6.14696	-2.08355	-0.98771
C	7.56286	-1.71421	-1.24488
H	8.96030	-0.76258	0.28005
H	7.10122	-1.24988	2.06458
H	4.97625	-2.32995	0.85070
H	5.45860	-2.44773	-1.74680
H	8.16047	-2.64323	-1.28096
H	7.75256	-1.18250	-2.18268
O	-1.24036	5.07756	-0.61997
C	-2.10825	4.52107	-1.56906
H	-3.09097	4.98811	-1.44707

H -1.76006 4.72760 -2.59801

M06/lanl2dz-6-31G(d) Energy = -2646.111520

M06/lanl2dz-6-31G(d) Free Energy = -2645.476543

M06/def2-TZVP Derived free energy = -2646.587704

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.618332

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.642955

Number of Imaginary Frequencies = 1 (-368.83)

M06/lanl2dz-6-31G(d) Geometry

C	0.37256	2.93587	0.22322
C	0.32562	4.47297	0.09723
C	-1.35819	3.12452	-1.60255
N	-0.68293	2.38557	-0.65820
C	-1.16459	1.12134	-0.67970
N	-2.11820	1.17353	-1.62160
N	-2.25464	2.40605	-2.21062
C	-0.71904	4.92633	1.13364
C	-0.59360	3.86239	2.18586
C	0.05196	2.73096	1.67610
C	0.32204	1.63605	2.48761
C	-0.09950	1.66302	3.81427
C	-0.76002	2.78253	4.31919
C	-1.00137	3.89295	3.51333
C	-2.97190	0.09553	-2.00132
C	-4.31990	0.10613	-1.55115
C	-5.12619	-1.03629	-1.82202
C	-4.57572	-2.11320	-2.55741
C	-3.28506	-2.08110	-3.01451
C	-2.47591	-0.96305	-2.72980
C	-4.88041	1.18235	-0.82180
C	-6.17463	1.11498	-0.36894
C	-6.97035	-0.02296	-0.62163
C	-6.45511	-1.07275	-1.33772
H	1.32753	2.51122	-0.10994
H	1.30900	4.84787	0.40790

H	-1.73435	4.94122	0.70659
H	-0.51975	5.93994	1.50155
H	0.86189	0.76984	2.10225
H	0.09707	0.81060	4.46113
H	-1.07736	2.79432	5.36017
H	-1.49538	4.77374	3.92171
H	-5.20196	-2.98051	-2.76329
H	-2.86405	-2.90299	-3.58776
Cl	-0.83558	-0.96323	-3.30310
H	-4.28258	2.07202	-0.63201
H	-6.59568	1.95186	0.18518
H	-7.99387	-0.05918	-0.25491
H	-7.06039	-1.95365	-1.54920
Au	-0.39458	-0.72505	0.17593
C	0.22257	-2.59951	0.75171
C	-0.69422	-3.31094	1.54673
C	1.39759	-3.19791	0.32642
C	-0.39225	-4.61409	1.93532
C	1.68887	-4.50768	0.71961
H	2.08689	-2.67120	-0.33325
C	0.79933	-5.20677	1.52638
H	-1.09042	-5.18044	2.55136
H	2.60959	-4.98238	0.38343
H	1.02668	-6.22683	1.83037
C	-1.99706	-1.28724	1.30677
C	-3.06784	-0.44977	1.55873
C	-1.91389	-2.57349	1.86593
C	-4.12144	-0.91498	2.34986
H	-3.10311	0.55917	1.15245
C	-2.97157	-3.01493	2.66014
C	-4.07127	-2.19371	2.89166
H	-4.97888	-0.26895	2.53225
H	-2.93690	-4.00895	3.10544
H	-4.89229	-2.55501	3.50800
O	1.49733	-0.06779	-0.84696
C	3.77715	0.50819	-0.80302

C	2.62377	-0.09885	-0.28686
C	6.19980	0.97718	-0.51650
C	4.98091	0.40880	-0.12898
C	7.35153	0.97019	0.29220
H	2.73395	-0.63712	0.67832
H	4.97931	-0.14748	0.81683
H	3.70251	1.04889	-1.74765
C	8.36970	2.06487	0.11136
H	7.19304	0.67243	1.33176
H	6.23101	1.51841	-1.46613
H	8.61410	2.21976	-0.94788
H	7.96064	3.01065	0.49186
H	9.30003	1.86972	0.65572
C	8.46642	-0.64009	-0.26989
C	7.78908	-1.70603	0.33008
C	6.76395	-2.15769	-0.52969
C	6.85736	-1.47821	-1.71904
C	8.12092	-0.69646	-1.73641
H	9.44579	-0.31274	0.07576
H	7.95671	-2.05992	1.34447
H	5.99985	-2.88625	-0.27326
H	6.18647	-1.58108	-2.56745
H	8.89457	-1.30975	-2.23363
H	8.08603	0.25679	-2.27313
C	-1.05755	4.56886	-1.82102
H	-0.96359	4.77166	-2.89344
H	-1.89359	5.18422	-1.44644
O	0.16181	4.92378	-1.22287

M06/lanl2dz-6-31G(d) Energy = -2646.110578

M06/lanl2dz-6-31G(d) Free Energy = -2645.474224

M06/def2-TZVP Derived free energy = -2646.584209

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.614890

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.639294

Number of Imaginary Frequencies = 1 (-362.46)

M06/lanl2dz-6-31G(d) Geometry

C	-0.94983	2.59743	-0.93881
C	-1.41843	4.05963	-0.76561
C	-0.18556	2.95573	1.44014
N	-0.21296	2.20701	0.28612
C	0.49225	1.07120	0.49654
N	0.92770	1.21159	1.75832
N	0.51435	2.37138	2.36641
C	-0.26826	4.92223	-1.31594
C	0.33503	4.01775	-2.34991
C	-0.05720	2.69141	-2.14442
C	0.35525	1.68468	-3.00972
C	1.19785	2.01116	-4.06863
C	1.60019	3.33160	-4.26587
C	1.16444	4.34451	-3.41509
C	1.72964	0.27482	2.47464
C	3.09868	0.57857	2.70453
C	3.91177	-0.41647	3.31955
C	3.32872	-1.64574	3.70870
C	1.99737	-1.89959	3.51092
C	1.19325	-0.92497	2.88821
C	3.68870	1.80778	2.32456
C	5.02699	2.02988	2.53495
C	5.83781	1.04086	3.13257
C	5.28776	-0.15450	3.51866
H	-1.78416	1.89169	-1.04031
H	-2.29299	4.19044	-1.41476
H	0.46760	5.16725	-0.53386
H	-0.62892	5.87747	-1.71601
H	0.02007	0.65501	-2.87800
H	1.53307	1.23396	-4.75218
H	2.25020	3.57572	-5.10397
H	1.46427	5.37742	-3.58763
H	3.96066	-2.39838	4.17865
H	1.54563	-2.83879	3.81932
Cl	-0.49239	-1.28506	2.64426

H	3.06999	2.58288	1.87595
H	5.46748	2.98148	2.24338
H	6.89650	1.23376	3.29203
H	5.90053	-0.92391	3.98711
Au	0.58518	-0.78147	-0.64056
C	0.69590	-2.64667	-1.49480
C	1.99526	-3.08064	-1.81268
C	-0.39227	-3.48166	-1.68847
C	2.17535	-4.34686	-2.36428
C	-0.19970	-4.75212	-2.23954
H	-1.39552	-3.16940	-1.40015
C	1.07843	-5.17591	-2.58245
H	3.17478	-4.69627	-2.62287
H	-1.05305	-5.40991	-2.39596
H	1.22609	-6.16364	-3.01520
C	2.60128	-0.91023	-0.93278
C	3.47207	0.12363	-0.64131
C	3.04570	-2.11451	-1.50440
C	4.83885	-0.05561	-0.87110
H	3.11201	1.06761	-0.23664
C	4.41266	-2.27158	-1.72891
C	5.30270	-1.25161	-1.40525
H	5.53295	0.74769	-0.62947
H	4.78883	-3.19783	-2.16255
H	6.36761	-1.39107	-1.58164
O	-1.65823	-0.62977	-0.54760
C	-3.76629	-0.55078	-1.61152
C	-2.38376	-0.78583	-1.57211
C	-5.84081	0.11760	-0.42376
C	-4.46616	-0.11875	-0.49367
C	-6.48000	0.68579	0.69538
H	-1.91277	-1.13817	-2.50904
H	-3.87492	0.07911	0.40679
H	-4.28783	-0.73559	-2.55028
C	-7.79303	1.39521	0.49547
H	-5.81787	1.16110	1.42289

H	-6.44670	-0.11516	-1.30440
H	-8.48730	0.79689	-0.10928
H	-8.28537	1.64472	1.44166
H	-7.62106	2.33735	-0.04242
C	-7.08700	-0.85814	1.87698
C	-5.90328	-1.21331	2.53181
C	-5.19651	-2.15823	1.75534
C	-5.97169	-2.50562	0.67727
C	-7.33124	-1.92980	0.84491
H	-7.90844	-0.36939	2.39889
H	-5.53381	-0.75308	3.44512
H	-4.18827	-2.51125	1.95308
H	-5.68584	-3.18377	-0.12203
H	-7.83836	-1.62717	-0.07669
H	-7.97114	-2.69846	1.31575
C	-0.89894	4.26103	1.53252
H	-1.41072	4.33695	2.49791
H	-0.17566	5.09260	1.48288
O	-1.87720	4.35758	0.53055

M06/lanl2dz-6-31G(d) Energy = -2646.115650

M06/lanl2dz-6-31G(d) Free Energy = -2645.479172

M06/def2-TZVP Derived free energy = -2646.590894

M06/def2-TZVP Derived free energy in solution (toluene) = -2646.621557

M06/def2-TZVP Derived free energy in solution (nitromethane) = -2646.646225

Number of Imaginary Frequencies = 1 (-398.04)

M06/lanl2dz-6-31G(d) Geometry

C	0.19398	3.05342	-0.13619
C	0.32772	4.50432	-0.65260
C	-1.90586	3.09158	-1.49661
N	-0.98403	2.41685	-0.73020
C	-1.33790	1.11094	-0.67951
N	-2.45484	1.07085	-1.42518
N	-2.82430	2.28953	-1.94220
C	1.10172	5.21956	0.44993

C	0.72590	4.45778	1.69071
C	0.17646	3.21705	1.36222
C	-0.23853	2.33257	2.34938
C	-0.10235	2.71187	3.68368
C	0.44613	3.94942	4.01498
C	0.86570	4.83041	3.02025
C	-3.22946	-0.09152	-1.71311
C	-4.53372	-0.20219	-1.15705
C	-5.24497	-1.42114	-1.35395
C	-4.65038	-2.45630	-2.11370
C	-3.40834	-2.30939	-2.67210
C	-2.69436	-1.11170	-2.47042
C	-5.13816	0.82716	-0.39523
C	-6.38405	0.64634	0.15267
C	-7.08502	-0.56498	-0.03069
C	-6.52547	-1.57388	-0.77178
H	1.06048	2.46322	-0.46709
H	0.81833	4.54470	-1.64105
H	0.82693	6.28118	0.47597
H	2.18317	5.16459	0.25440
H	-0.67927	1.36607	2.10030
H	-0.43321	2.03718	4.47072
H	0.53956	4.23405	5.06127
H	1.28309	5.80175	3.28267
H	-5.20247	-3.38444	-2.25672
H	-2.95561	-3.09785	-3.26764
Cl	-1.12150	-0.96690	-3.20394
H	-4.61760	1.77311	-0.26047
H	-6.84014	1.44946	0.72839
H	-8.07143	-0.69102	0.41058
H	-7.05720	-2.51218	-0.92659
Au	-0.28910	-0.63520	0.10674
C	0.59492	-2.40857	0.64562
C	-0.16116	-3.21783	1.50973
C	1.80196	-2.85729	0.13195
C	0.33537	-4.46527	1.88414

C	2.28545	-4.11452	0.50762
H	2.36344	-2.25130	-0.57946
C	1.55794	-4.90790	1.38748
H	-0.23694	-5.10574	2.55487
H	3.22899	-4.47683	0.09880
H	1.93661	-5.88538	1.67998
C	-1.73799	-1.38709	1.34238
C	-2.89875	-0.70526	1.65645
C	-1.44133	-2.64042	1.90806
C	-3.81987	-1.29233	2.52837
H	-3.11241	0.27545	1.23578
C	-2.37094	-3.20591	2.77939
C	-3.55464	-2.53838	3.08236
H	-4.74467	-0.76545	2.75996
H	-2.16960	-4.17685	3.23151
H	-4.27116	-2.99471	3.76256
O	1.55866	0.05300	-0.98108
C	3.85964	0.51025	-0.76858
C	2.55151	0.38252	-0.27795
C	6.24312	0.98215	-0.24464
C	4.88391	0.91400	0.07579
C	6.76043	0.56425	-1.47681
H	2.40341	0.58810	0.80417
H	4.60076	1.18126	1.09809
H	4.01999	0.29880	-1.82543
C	8.13759	0.98911	-1.89349
H	6.05271	0.46703	-2.30197
H	6.93775	1.33306	0.51942
H	8.83459	1.01708	-1.04657
H	8.56376	0.34976	-2.67464
H	8.08733	2.00780	-2.30296
C	7.00141	-1.50791	-1.28887
C	5.72727	-2.02773	-1.06506
C	5.47350	-2.08548	0.33182
C	6.60263	-1.71086	1.00127
C	7.72314	-1.55599	0.03579

H	7.52153	-1.63965	-2.23655
H	5.01520	-2.30485	-1.83979
H	4.51737	-2.33927	0.78434
H	6.71268	-1.63468	2.07920
H	8.41212	-0.73219	0.25038
H	8.33193	-2.47777	0.05618
C	-1.74586	4.55318	-1.73921
H	-1.30074	4.71674	-2.73821
H	-2.71873	5.05463	-1.71862
O	-0.94663	5.11131	-0.73201

Major Endo product

B3LYP/lanl2dz-6-31G(d) Energy = -2647.680522

B3LYP/lanl2dz-6-31G(d) Free Energy = -2647.044305

M06/def2-TZVP Derived free energy = -2646.585124

Number of Imaginary Frequencies = 1 (-354.40)

B3LYP/lanl2dz-6-31G(d) Geometry

C	3.44663	-1.86897	0.01328
C	4.75034	-2.50488	0.57766
C	2.93515	-1.46684	2.43773
N	2.68553	-1.23033	1.10234
C	1.65285	-0.35197	1.00176
N	1.32136	-0.11793	2.28548
N	2.11173	-0.79895	3.19344
C	5.10340	-3.58481	-0.45623
C	3.74945	-4.00089	-0.99228
C	2.77613	-3.03954	-0.68906
C	1.44730	-3.21392	-1.06798
C	1.10406	-4.37512	-1.76968
C	2.07301	-5.33179	-2.08503
C	3.40410	-5.15100	-1.69635
C	0.21329	0.64861	2.77747
C	0.31600	2.06953	2.87846
C	-0.80904	2.79371	3.39585
C	-1.96443	2.07858	3.80585

C	-2.02892	0.70874	3.71651
C	-0.92812	-0.01183	3.19816
C	1.47797	2.79389	2.50246
C	1.51675	4.16611	2.61845
C	0.40344	4.88297	3.11735
C	-0.73316	4.20789	3.49963
H	3.69778	-1.07466	-0.69949
H	5.54398	-1.75973	0.73280
H	5.66254	-4.39687	0.01838
H	5.73884	-3.15920	-1.24470
H	0.67904	-2.48824	-0.81835
H	0.07181	-4.53400	-2.06831
H	1.78898	-6.22846	-2.62855
H	4.15212	-5.90394	-1.93006
H	-2.80762	2.63314	4.20912
H	-2.90669	0.16293	4.04345
Cl	-1.05267	-1.75016	3.10635
H	2.34163	2.26273	2.12235
H	2.41393	4.70296	2.32503
H	0.45236	5.96427	3.20233
H	-1.59033	4.74745	3.89359
Au	0.86745	0.55422	-0.80039
C	0.20318	1.42379	-2.54106
C	1.07920	2.38251	-3.09077
C	-0.98966	1.11255	-3.18435
C	0.72423	3.04067	-4.27257
C	-1.33435	1.77570	-4.37127
H	-1.65386	0.35086	-2.79003
C	-0.48249	2.74004	-4.90756
H	1.38637	3.78364	-4.70857
H	-2.26515	1.53024	-4.87587
H	-0.75014	3.25355	-5.82661
C	2.47190	1.75899	-1.19414
C	3.62034	1.82698	-0.41349
C	2.32781	2.56713	-2.34243
C	4.65117	2.71050	-0.76620

H	3.73588	1.21181	0.47208
C	3.36592	3.44442	-2.67728
C	4.51967	3.51658	-1.89481
H	5.54757	2.76276	-0.15454
H	3.27686	4.07498	-3.55726
H	5.31547	4.20249	-2.17025
O	-0.93493	-0.70496	-0.52192
C	-3.22222	-1.07955	-0.09747
C	-2.08767	-0.26248	-0.22824
C	-5.64891	-1.25320	0.42935
C	-4.46034	-0.53672	0.22669
C	-6.84152	-0.67717	0.94617
H	-2.21698	0.81906	-0.07186
H	-4.50013	0.54430	0.38005
H	-3.10290	-2.15036	-0.24160
C	-7.70910	-1.50151	1.88088
H	-6.73681	0.36333	1.26007
H	-5.61492	-2.33314	0.30067
H	-7.82454	-2.52829	1.51996
H	-7.23797	-1.55018	2.87041
H	-8.70474	-1.06508	2.01096
C	-8.04514	-0.24308	-0.57873
C	-8.39157	-1.49728	-1.12714
C	-7.41441	-1.88737	-2.07289
C	-6.52374	-0.84928	-2.24423
C	-7.05454	0.36946	-1.55563
H	-8.78207	0.37023	-0.06661
H	-9.22017	-2.11478	-0.79799
H	-7.35616	-2.85941	-2.54944
H	-5.65116	-0.85672	-2.88707
H	-6.30173	1.03630	-1.13235
H	-7.63278	0.95831	-2.28775
C	4.09187	-2.32724	2.85722
H	4.92951	-1.68132	3.16938
H	3.81252	-2.95527	3.70616
O	4.47380	-3.18424	1.80199

Minor Endo product

B3LYP/lanl2dz-6-31G(d) Energy = -2647.681910

B3LYP/lanl2dz-6-31G(d) Free Energy = -2647.044844

M06/def2-TZVP Derived free energy = -2646.584476

Number of Imaginary Frequencies = 1 (-347.88)

B3LYP/lanl2dz-6-31G(d) Geometry

C	-0.55949	3.03026	-0.43091
C	-0.22566	4.25343	-1.33419
C	-1.45297	2.07222	-2.57200
N	-1.06735	1.91904	-1.25929
C	-1.20196	0.61003	-0.91283
N	-1.68173	0.04368	-2.03923
N	-1.84005	0.93852	-3.08306
C	-0.31140	5.45140	-0.37633
C	-1.34423	5.00663	0.63772
C	-1.52311	3.61781	0.58893
C	-2.42993	2.98263	1.43367
C	-3.16412	3.76012	2.33582
C	-2.98385	5.14511	2.39089
C	-2.07107	5.77760	1.54101
C	-2.01827	-1.33121	-2.26583
C	-3.39438	-1.69408	-2.40180
C	-3.71305	-3.07509	-2.61324
C	-2.66240	-4.02561	-2.69746
C	-1.34582	-3.64626	-2.60025
C	-1.02598	-2.28503	-2.39522
C	-4.45561	-0.75102	-2.34020
C	-5.76504	-1.16113	-2.46910
C	-6.08140	-2.52630	-2.66618
C	-5.07401	-3.46084	-2.73824
H	0.35258	2.65705	0.04640
H	0.75022	4.14814	-1.82995
H	-0.58684	6.35720	-0.92508
H	0.66533	5.63065	0.09332

H	-2.58166	1.90841	1.39974
H	-3.88021	3.28075	2.99692
H	-3.56223	5.73646	3.09496
H	-1.94182	6.85605	1.57897
H	-2.91160	-5.07136	-2.85470
H	-0.54345	-4.36992	-2.68642
Cl	0.66834	-1.84400	-2.35731
H	-4.23172	0.30189	-2.21238
H	-6.56362	-0.42611	-2.42704
H	-7.11877	-2.83062	-2.76668
H	-5.30422	-4.51103	-2.89590
Au	-0.46666	-0.26235	0.94546
C	0.27205	-1.07421	2.68228
C	-0.65888	-1.83072	3.42392
C	1.57495	-0.91745	3.14131
C	-0.24772	-2.46058	4.60282
C	1.97533	-1.54757	4.32891
H	2.28474	-0.29890	2.60241
C	1.06855	-2.32374	5.04909
H	-0.95084	-3.05109	5.18375
H	2.99304	-1.42308	4.68948
H	1.37956	-2.81363	5.96741
C	-2.18627	-1.07440	1.69025
C	-3.43392	-0.92051	1.10399
C	-2.01818	-1.82491	2.87314
C	-4.54877	-1.54423	1.68344
H	-3.56501	-0.33133	0.20547
C	-3.14149	-2.44395	3.43256
C	-4.39811	-2.30777	2.83887
H	-5.52434	-1.43107	1.21950
H	-3.03973	-3.02699	4.34354
H	-5.25998	-2.79426	3.28649
O	1.48430	0.62013	0.28303
C	3.68919	0.44424	-0.54836
C	2.49395	-0.08213	-0.03181
C	5.96636	-0.01591	-1.45530

C	4.74641	-0.39715	-0.88040
C	6.92473	-0.94205	-1.95164
H	2.44222	-1.17100	0.11070
H	4.58951	-1.46633	-0.71984
H	3.76274	1.51856	-0.69908
C	7.70831	-0.58924	-3.20363
H	6.59323	-1.98204	-1.92984
H	6.13126	1.04357	-1.64088
H	8.05075	0.45015	-3.18347
H	8.57853	-1.23912	-3.34076
H	7.06454	-0.70952	-4.08366
C	8.32238	-1.21240	-0.56345
C	8.96838	0.03892	-0.46016
C	8.28064	0.85259	0.47081
C	7.29157	0.10236	1.06989
C	7.46676	-1.33400	0.68716
H	8.83305	-2.07617	-0.98142
H	9.79993	0.36451	-1.07565
H	8.47729	1.90357	0.65003
H	6.58139	0.45563	1.80855
H	8.08032	-1.82686	1.46032
H	6.54633	-1.91229	0.59335
O	-1.24837	4.43989	-2.31249
C	-1.31913	3.39812	-3.26238
H	-0.42274	3.38116	-3.90454
H	-2.18722	3.58969	-3.89741

Major Endo product (optimized with ultrafine grid)

M06/lanl2dz-6-31G(d) Energy = -2646.117300

M06/lanl2dz-6-31G(d) Free Energy = -2645.483204

M06/def2-TZVP Derived free energy = -2646.593843

Number of Imaginary Frequencies = 1 (-378.16)

M06/lanl2dz-6-31G(d) Geometry

C	3.63504	-1.61463	-0.20688
C	4.82792	-2.45093	0.29909

C	2.54752	-2.41724	1.90207
N	2.58586	-1.57711	0.81357
C	1.49038	-0.78668	0.83983
N	0.84300	-1.19814	1.93966
N	1.48453	-2.20832	2.61840
C	5.51265	-2.90632	-0.98547
C	4.36766	-3.01639	-1.95670
C	3.26054	-2.30305	-1.49438
C	2.06880	-2.27434	-2.20502
C	2.00531	-2.97101	-3.41121
C	3.11165	-3.67261	-3.88563
C	4.30117	-3.70313	-3.15987
C	-0.44068	-0.75865	2.37822
C	-0.57478	0.51291	2.99874
C	-1.87719	0.92889	3.40501
C	-2.97345	0.05452	3.21059
C	-2.81436	-1.17284	2.62224
C	-1.53411	-1.57762	2.19097
C	0.52044	1.38011	3.21983
C	0.32830	2.61496	3.78771
C	-0.96080	3.03418	4.17947
C	-2.03745	2.20321	3.99811
H	3.94703	-0.57236	-0.38411
H	5.47948	-1.87836	0.98314
H	6.04907	-3.84829	-0.81825
H	6.25060	-2.15716	-1.30975
H	1.18739	-1.74780	-1.83378
H	1.07990	-2.96999	-3.98374
H	3.04265	-4.21299	-4.82792
H	5.15754	-4.26860	-3.52500
H	-3.96151	0.37400	3.54338
H	-3.65709	-1.84329	2.46550
Cl	-1.37463	-3.10718	1.39106
H	1.52189	1.06554	2.93610
H	1.18203	3.27280	3.93987
H	-1.09559	4.01388	4.63253

H	-3.03536	2.51058	4.30993
Au	0.99546	0.85882	-0.47653
C	0.58412	2.45319	-1.70032
C	1.42703	3.56408	-1.53144
C	-0.42794	2.46744	-2.64611
C	1.22508	4.69796	-2.31452
C	-0.61951	3.61052	-3.42785
H	-1.06150	1.59469	-2.79895
C	0.20124	4.71925	-3.25756
H	1.86898	5.56961	-2.19870
H	-1.40950	3.62732	-4.17701
H	0.05009	5.60692	-3.86888
C	2.48735	2.12961	0.11053
C	3.43069	1.82926	1.08106
C	2.47034	3.38441	-0.52488
C	4.38190	2.78967	1.43704
H	3.44254	0.85916	1.57884
C	3.42809	4.32824	-0.15667
C	4.37653	4.03331	0.81781
H	5.12375	2.55758	2.19907
H	3.43464	5.30662	-0.63627
H	5.11692	4.78153	1.09384
O	-0.71679	-0.36740	-1.18358
C	-2.99202	-0.93186	-0.95630
C	-1.86789	-0.12461	-0.73307
C	-5.36187	-1.37978	-0.35514
C	-4.19180	-0.61008	-0.35221
C	-6.48796	-1.06599	0.42131
H	-2.02094	0.78052	-0.10900
H	-4.20980	0.31224	0.24262
H	-2.87475	-1.84398	-1.54198
C	-7.36831	-2.16749	0.94043
H	-6.35717	-0.22081	1.10813
H	-5.35754	-2.31762	-0.91574
H	-7.49477	-2.95884	0.19077
H	-6.90699	-2.62661	1.82616

H	-8.36149	-1.80883	1.23709
C	-7.78038	0.01164	-0.76572
C	-8.17019	-0.93476	-1.71398
C	-7.23923	-0.94620	-2.78113
C	-6.33415	0.06336	-2.58436
C	-6.79279	0.91494	-1.45384
H	-8.45381	0.37243	0.01135
H	-9.00160	-1.62658	-1.60292
H	-7.22540	-1.66520	-3.59471
H	-5.48188	0.29471	-3.21736
H	-6.00320	1.34708	-0.83085
H	-7.36188	1.76371	-1.87417
C	3.68124	-3.35438	2.14873
H	4.36154	-2.91311	2.90125
H	3.31361	-4.30591	2.54604
O	4.35562	-3.61699	0.94973

Minor Endo product (optimized with ultrafine grid)

M06/lanl2dz-6-31G(d) Energy = -2646.115071

M06/lanl2dz-6-31G(d) Free Energy = -2645.481698

M06/def2-TZVP Derived free energy = -2646.592361

Number of Imaginary Frequencies = 1 (-375.65)

M06/lanl2dz-6-31G(d) Geometry

C	-1.19165	3.02552	-0.49749
C	-1.13468	4.29350	-1.37693
C	-1.99334	1.96476	-2.62385
N	-1.55576	1.86922	-1.32385
C	-1.48818	0.56131	-0.98777
N	-1.89295	-0.06259	-2.10582
N	-2.20526	0.79068	-3.13707
C	-1.38165	5.43120	-0.39219
C	-2.25944	4.79427	0.65055
C	-2.17907	3.40276	0.57799
C	-2.90361	2.59596	1.44423
C	-3.72150	3.20584	2.39382

C	-3.80130	4.59472	2.47167
C	-3.06976	5.39930	1.60033
C	-1.97999	-1.47258	-2.29279
C	-0.78034	-2.23394	-2.32645
C	-0.88595	-3.65108	-2.42921
C	-2.16674	-4.24442	-2.52819
C	-3.30553	-3.48377	-2.53871
C	-3.20846	-2.08316	-2.42044
C	0.50770	-1.64603	-2.27965
C	1.63291	-2.43303	-2.31190
C	1.53037	-3.83806	-2.38567
C	0.29477	-4.43059	-2.44675
H	-0.19693	2.80386	-0.07970
H	-0.18137	4.37340	-1.92911
H	-1.84195	6.28445	-0.90536
H	-0.42954	5.77744	0.03754
H	-2.85279	1.50779	1.38699
H	-4.30398	2.59051	3.07654
H	-4.44768	5.05579	3.21609
H	-3.14377	6.48465	1.65629
H	-2.23699	-5.32859	-2.60731
H	-4.28972	-3.93661	-2.62759
Cl	-4.67688	-1.15823	-2.40510
H	0.60501	-0.56179	-2.24449
H	2.61488	-1.96086	-2.29812
H	2.43110	-4.44778	-2.40839
H	0.20063	-5.51358	-2.51937
Au	-0.60391	-0.26053	0.81827
C	0.24131	-1.05402	2.51542
C	-0.55110	-2.00462	3.18258
C	1.48825	-0.70714	3.01071
C	-0.05225	-2.63319	4.32082
C	1.97610	-1.33740	4.15931
H	2.08673	0.06610	2.52917
C	1.21187	-2.30380	4.80210
H	-0.65313	-3.37476	4.84687

H	2.95307	-1.06313	4.55459
H	1.59403	-2.79516	5.69489
C	-2.17286	-1.37528	1.50089
C	-3.41986	-1.37323	0.90456
C	-1.88268	-2.18553	2.61160
C	-4.40824	-2.23062	1.39615
H	-3.64803	-0.71824	0.06610
C	-2.88284	-3.03233	3.08645
C	-4.13431	-3.05967	2.47694
H	-5.38965	-2.23912	0.92421
H	-2.68688	-3.67167	3.94695
H	-4.90392	-3.72793	2.85837
O	1.21319	0.86220	0.11535
C	3.45282	0.84056	-0.61874
C	2.30681	0.25995	-0.05779
C	5.81955	0.53577	-1.30951
C	4.61674	0.10154	-0.74281
C	6.93062	-0.29880	-1.51057
H	2.38698	-0.80171	0.25109
H	4.57949	-0.93845	-0.39296
H	3.40980	1.87974	-0.94679
C	7.86237	-0.03587	-2.65926
H	6.76353	-1.35905	-1.28923
H	5.86578	1.56165	-1.68359
H	8.02282	1.04044	-2.80085
H	8.83860	-0.51834	-2.52884
H	7.42415	-0.42766	-3.58744
C	8.16826	-0.09054	0.11888
C	8.59577	1.23258	0.00162
C	7.66839	2.08887	0.64441
C	6.72539	1.31988	1.27330
C	7.14545	-0.10615	1.22247
H	8.82750	-0.93669	-0.07305
H	9.45381	1.56381	-0.57833
H	7.68512	3.17390	0.60660
H	5.86507	1.68441	1.82810

H	7.67971	-0.33906	2.16123
H	6.33709	-0.83914	1.13479
O	-2.21576	4.29818	-2.29092
C	-2.11294	3.30276	-3.27041
H	-1.23690	3.47411	-3.92378
H	-3.01098	3.34801	-3.89507

7.2 Cartesian coordinates of the catalyst-substrate structures

Catalyst 4g

C	-2.91041	-1.49163	-0.00155
C	-4.02977	-2.47205	-0.39125
C	-1.51932	-2.95709	-1.45933
N	-1.70050	-1.79239	-0.76280
C	-0.59572	-1.03237	-0.90885
N	0.19096	-1.77742	-1.68789
N	-0.36101	-2.98075	-2.03183
C	-4.96207	-2.43847	0.80839
C	-4.02919	-2.17284	1.95232
C	-2.82173	-1.66349	1.49016
C	-1.79147	-1.36676	2.35937
C	-1.98943	-1.57665	3.71643
C	-3.19753	-2.06991	4.18322
C	-4.22563	-2.37436	3.30374
C	1.50067	-1.44832	-2.13983
C	2.49311	-2.41107	-2.07764
C	3.77288	-2.08268	-2.48664
C	1.75928	-0.17668	-2.62540
H	-3.20418	-0.46636	-0.25851
H	-4.50994	-2.19627	-1.34087
H	-5.51297	-3.37639	0.89461
H	-5.69583	-1.63362	0.69438
H	-0.83557	-0.99458	2.00368
H	-1.19246	-1.35573	4.41590
H	-3.33552	-2.22937	5.24597

H	-5.16252	-2.77742	3.67195
Au	-0.15536	0.88082	-0.01570
C	0.18239	2.70956	0.84811
C	-0.59352	3.75536	0.33291
C	1.06595	2.93275	1.88319
C	-0.45516	5.02758	0.86616
C	1.19422	4.21416	2.41018
H	1.65023	2.12327	2.30668
C	0.43861	5.25386	1.90029
H	-1.04775	5.84992	0.47995
H	1.88524	4.39333	3.22556
H	0.54096	6.24972	2.31436
C	-1.45975	2.00963	-1.09333
C	-2.22029	1.51209	-2.13050
C	-1.48981	3.36607	-0.74641
C	-3.05553	2.37375	-2.83459
H	-2.17288	0.46746	-2.41709
C	-2.33574	4.20481	-1.45880
C	-3.11386	3.71160	-2.49270
H	-3.65383	1.99082	-3.65269
H	-2.38097	5.25899	-1.20822
H	-3.76554	4.38088	-3.04111
O	1.41396	-0.19641	1.14401
C	3.64101	-0.83948	1.47063
C	2.60330	-0.13165	0.81209
C	6.04527	-1.37058	1.61394
C	4.91803	-0.71405	1.04405
C	7.28846	-1.19021	1.14612
H	2.90478	0.50174	-0.04318
H	5.11144	-0.05640	0.19612
H	3.37787	-1.47344	2.31169
C	8.50271	-1.82448	1.68737
H	7.41983	-0.51684	0.29979
H	5.87574	-2.03232	2.46041
H	9.01610	-2.40085	0.91227
H	9.21738	-1.06453	2.01692

H	8.28150	-2.48385	2.52650
C	-2.61503	-3.95725	-1.53753
H	-3.12147	-3.85506	-2.51085
H	-2.21081	-4.96864	-1.48215
O	-3.50897	-3.78211	-0.48023
C	4.05344	-0.80637	-2.94873
C	3.04695	0.14309	-3.02053
H	4.55558	-2.83019	-2.44281
H	3.25544	1.13165	-3.41095
H	5.05580	-0.55699	-3.27583
H	2.25338	-3.40326	-1.71618
H	0.95632	0.54627	-2.71927

Catalyst 4h

C	-3.07101	-1.76119	-0.21806
C	-3.98992	-2.90418	-0.68109
C	-1.26689	-3.24898	-1.07429
N	-1.69770	-2.02216	-0.64428
C	-0.65345	-1.16939	-0.66139
N	0.35484	-1.93028	-1.10184
N	-0.00633	-3.22596	-1.35415
C	-5.17358	-2.80861	0.26695
C	-4.55120	-2.29224	1.53044
C	-3.31052	-1.72401	1.26680
C	-2.53019	-1.21017	2.28267
C	-3.01670	-1.25636	3.58075
C	-4.26166	-1.80495	3.84541
C	-5.03617	-2.33069	2.82197
C	1.71284	-1.54654	-1.26544
C	2.70398	-2.43859	-0.89670
C	4.02318	-2.04346	-1.02686
C	2.01171	-0.29192	-1.76812
H	-3.38141	-0.81903	-0.68664
H	-4.25727	-2.81643	-1.74372
H	-5.65826	-3.78001	0.37720
H	-5.91826	-2.10995	-0.12846

H	-1.54555	-0.79514	2.08954
H	-2.41727	-0.86474	4.39344
H	-4.62704	-1.83591	4.86485
H	-6.00036	-2.77781	3.03692
Au	-0.64614	0.88321	0.03318
C	-0.77383	2.79599	0.75418
C	-1.61774	3.64689	0.03100
C	-0.14539	3.23315	1.90082
C	-1.80503	4.94794	0.47215
C	-0.34099	4.54173	2.33206
H	0.48365	2.57039	2.48509
C	-1.16448	5.39211	1.61759
H	-2.45648	5.62157	-0.07399
H	0.14892	4.88936	3.23400
H	-1.31638	6.40917	1.95821
C	-1.89122	1.69252	-1.35851
C	-2.33189	1.00585	-2.46942
C	-2.21996	3.03714	-1.14612
C	-3.15492	1.65469	-3.38493
H	-2.03994	-0.02242	-2.65126
C	-3.04778	3.66073	-2.06916
C	-3.51536	2.97265	-3.17635
H	-3.50392	1.12356	-4.26240
H	-3.32173	4.70050	-1.92786
H	-4.15745	3.47563	-3.88913
O	0.90099	0.15580	1.46758
C	3.19785	-0.04423	1.90116
C	2.05606	0.58389	1.34516
C	5.65896	-0.08783	2.08943
C	4.42522	0.46542	1.64686
C	6.83994	0.45320	1.75603
H	2.24181	1.50739	0.76597
H	4.48612	1.36938	1.03878
H	3.06106	-0.94700	2.48875
C	8.15776	-0.06274	2.16268
H	6.83025	1.34820	1.13411

H	5.62616	-0.98284	2.70700
H	8.76462	-0.30236	1.28448
H	8.71611	0.70078	2.71220
H	8.07484	-0.95341	2.78519
C	-2.23382	-4.36574	-1.23360
H	-2.49980	-4.45381	-2.29930
H	-1.77846	-5.30903	-0.92994
O	-3.36432	-4.14848	-0.44489
C	4.36062	-0.78705	-1.50091
C	3.34268	0.07775	-1.85987
Cl	3.73651	1.66345	-2.41800
H	1.23090	0.38364	-2.09795
H	2.45160	-3.41927	-0.51681
Cl	5.27758	-3.12828	-0.55494
H	5.39754	-0.48843	-1.58917

Catalyst 4i

C	-3.27325	-1.95051	-0.47186
C	-4.05687	-3.11862	-1.09609
C	-1.29991	-3.16962	-1.38306
N	-1.86096	-2.04290	-0.84188
C	-0.89914	-1.10990	-0.69682
N	0.19453	-1.72655	-1.16161
N	-0.03445	-3.00864	-1.58160
C	-5.28028	-3.24036	-0.20314
C	-4.76568	-2.80123	1.13521
C	-3.58360	-2.08477	0.99438
C	-2.91203	-1.59103	2.09533
C	-3.44891	-1.81605	3.35434
C	-4.63346	-2.52094	3.49809
C	-5.29933	-3.02092	2.38918
C	1.52126	-1.22417	-1.18593
C	2.56267	-2.07216	-0.85469
C	3.85304	-1.57650	-0.82747
C	1.75839	0.09905	-1.50773
H	-3.64562	-0.99640	-0.86479

H	-4.29060	-2.94118	-2.15548
H	-5.66741	-4.26035	-0.21722
H	-6.07688	-2.58017	-0.56167
H	-1.97416	-1.05147	1.99815
H	-2.93535	-1.44204	4.23161
H	-5.03791	-2.69130	4.48863
H	-6.21694	-3.58625	2.50761
Au	-1.09863	0.85535	0.19601
C	-1.38670	2.69108	1.05729
C	-2.13260	3.59389	0.29148
C	-0.93822	3.03258	2.31546
C	-2.40064	4.85358	0.80457
C	-1.21490	4.30014	2.81859
H	-0.39113	2.32416	2.92812
C	-1.93869	5.20399	2.06291
H	-2.97877	5.56668	0.22678
H	-0.86750	4.57324	3.80808
H	-2.15351	6.18897	2.45927
C	-2.20226	1.74936	-1.26388
C	-2.51502	1.13746	-2.45865
C	-2.56545	3.07531	-0.99742
C	-3.22954	1.84969	-3.41708
H	-2.20594	0.12075	-2.67322
C	-3.27792	3.76440	-1.96840
C	-3.61004	3.15449	-3.16657
H	-3.47814	1.37800	-4.36026
H	-3.57183	4.79296	-1.79009
H	-4.16465	3.70759	-3.91478
O	0.33188	0.04870	1.72091
C	2.62333	-0.11664	2.21814
C	1.46469	0.54946	1.74725
C	5.08967	-0.11955	2.34472
C	3.83085	0.47404	2.05183
C	6.24794	0.48441	2.04024
H	1.62087	1.57227	1.35841
H	3.85297	1.47532	1.61677

H	2.52689	-1.12050	2.62184
C	7.58475	-0.09707	2.24432
H	6.20202	1.47591	1.58877
H	5.09781	-1.11012	2.79353
H	8.10531	-0.19232	1.28601
H	8.20602	0.55909	2.86042
H	7.53562	-1.08107	2.71091
C	-2.15033	-4.33967	-1.71948
H	-2.36964	-4.32169	-2.79924
H	-1.61886	-5.26814	-1.50738
O	-3.32141	-4.31757	-0.96261
C	4.10722	-0.24860	-1.12082
C	3.05398	0.58469	-1.44904
C	3.27750	2.04425	-1.74039
H	0.94230	0.74938	-1.80696
H	2.35965	-3.10841	-0.61156
C	4.95682	-2.51426	-0.41758
H	5.11782	0.13529	-1.08779
F	4.51768	2.41979	-1.45331
F	3.04071	2.32839	-3.01260
F	2.45056	2.79543	-1.00519
F	6.13104	-1.90092	-0.33348
F	4.69294	-3.04610	0.77972
F	5.07679	-3.51866	-1.27435

Catalyst 4j

C	-3.60713	-1.74937	-0.56642
C	-4.47339	-2.76967	-1.32483
C	-1.73013	-2.95490	-1.67559
N	-2.21230	-1.88413	-0.97344
C	-1.19266	-1.03001	-0.74755
N	-0.15162	-1.62834	-1.32901
N	-0.46350	-2.82960	-1.90248
C	-5.69691	-2.92269	-0.43644
C	-5.14212	-2.70491	0.93990

C	-3.91365	-2.05830	0.87360
C	-3.19427	-1.77060	2.01562
C	-3.72843	-2.13496	3.24310
C	-4.95909	-2.76858	3.31499
C	-5.67429	-3.05982	2.16303
C	1.18816	-1.14208	-1.37369
C	2.22541	-1.99551	-1.08771
C	3.54546	-1.54885	-1.08596
C	1.41324	0.19426	-1.63631
H	-3.91858	-0.72883	-0.82189
H	-4.70186	-2.44001	-2.34851
H	-6.15859	-3.90106	-0.57916
H	-6.44402	-2.16368	-0.69085
H	-2.22277	-1.28830	1.96992
H	-3.17762	-1.92491	4.15188
H	-5.36112	-3.04929	4.28116
H	-6.62851	-3.57139	2.22312
Au	-1.18871	0.84193	0.32034
C	-1.22382	2.64621	1.29578
C	-1.88328	3.67337	0.60987
C	-0.66423	2.87583	2.53608
C	-1.96178	4.93228	1.18613
C	-0.75208	4.14297	3.10422
H	-0.17327	2.08002	3.08537
C	-1.39594	5.16368	2.42958
H	-2.46902	5.74010	0.66968
H	-0.31900	4.32533	4.08086
H	-1.46359	6.14823	2.87655
C	-2.22305	1.94389	-1.04221
C	-2.63397	1.45446	-2.26411
C	-2.42486	3.28363	-0.68459
C	-3.28968	2.30227	-3.15119
H	-2.44641	0.42702	-2.55512
C	-3.08488	4.10928	-1.58447
C	-3.51790	3.62075	-2.80591
H	-3.61560	1.92358	-4.11264

H	-3.25799	5.14934	-1.33035
H	-4.03028	4.27927	-3.49676
O	0.09484	-0.16282	1.83556
C	2.23660	-0.53879	2.71934
C	1.31213	0.05710	1.82408
C	4.58506	-0.75425	3.44592
C	3.55046	-0.23169	2.61898
C	5.86839	-0.40255	3.28369
H	1.74019	0.76068	1.08563
H	3.85603	0.46415	1.83485
H	1.86411	-1.22920	3.46991
C	7.00010	-0.91315	4.07539
H	6.10094	0.31571	2.49751
H	4.30985	-1.46499	4.22220
H	7.72497	-1.41045	3.42334
H	7.54121	-0.09158	4.55339
H	6.67904	-1.61705	4.84312
C	-2.65674	-4.02255	-2.13179
H	-2.88651	-3.86352	-3.19764
H	-2.18526	-5.00175	-2.04011
O	-3.81920	-4.02099	-1.35861
C	3.76176	-0.20487	-1.44532
C	2.69997	0.70782	-1.63706
C	2.91253	2.22254	-1.76595
H	0.56915	0.83288	-1.85757
H	1.98907	-3.02521	-0.85574
C	4.62055	-2.56760	-0.66450
O	5.03003	0.27870	-1.59313
C	1.58051	2.96776	-1.84280
C	3.63125	2.73524	-0.51386
C	3.71106	2.61039	-3.01080
C	5.93841	-1.95096	-0.19517
C	4.10787	-3.38683	0.52957
C	4.88908	-3.53777	-1.81613
H	1.77864	4.04087	-1.87029
H	1.01123	2.71992	-2.74366

H	0.94731	2.77983	-0.96954
H	3.80529	3.81058	-0.60439
H	3.01294	2.58433	0.37805
H	4.59550	2.24890	-0.36561
H	3.67212	3.69476	-3.13958
H	4.75990	2.33198	-2.93778
H	3.28620	2.15635	-3.91026
H	6.54692	-2.73958	0.25458
H	6.52806	-1.50704	-0.99258
H	5.63279	-4.27902	-1.51214
H	3.98125	-4.07253	-2.10531
H	5.26892	-3.02925	-2.70405
H	4.89928	-4.05962	0.86641
H	3.83661	-2.74053	1.36972
H	3.24810	-4.01189	0.28851
H	5.76908	-1.18457	0.56510
C	5.63569	-0.02463	-2.83600
H	6.56080	0.54887	-2.88961
H	5.87300	-1.08816	-2.92465
H	4.98982	0.25643	-3.67328

Catalyst 4k

C	-2.94630	-1.70748	0.01013
C	-3.99592	-2.67692	-0.56276
C	-1.51213	-2.64598	-1.80140
N	-1.75221	-1.71000	-0.82802
C	-0.70854	-0.85911	-0.79497
N	0.11018	-1.33138	-1.73535
N	-0.37549	-2.43954	-2.37633
C	-4.84957	-3.03133	0.64404
C	-3.88108	-2.93899	1.78562
C	-2.76314	-2.20154	1.41792
C	-1.72507	-1.98413	2.30147
C	-1.82289	-2.51579	3.57878
C	-2.93986	-3.24614	3.95353
C	-3.97656	-3.46492	3.05873

C	1.38069	-0.80198	-2.08400
C	2.52594	-1.55819	-1.82463
C	3.77165	-1.04075	-2.16696
C	1.46637	0.46051	-2.67607
H	-3.34255	-0.68453	0.00681
H	-4.55973	-2.22805	-1.39336
H	-5.29909	-4.01797	0.52069
H	-5.66460	-2.30867	0.75567
H	-0.84005	-1.42563	2.01191
H	-1.01944	-2.36091	4.28865
H	-2.99966	-3.65740	4.95416
H	-4.84176	-4.04904	3.35210
Au	-0.39320	0.93554	0.34030
C	-0.09012	2.70198	1.33951
C	-0.90765	3.76044	0.92480
C	0.83589	2.88543	2.34599
C	-0.76842	5.00278	1.52505
C	0.96449	4.13565	2.94248
H	1.45370	2.06550	2.69552
C	0.16795	5.18771	2.52927
H	-1.39444	5.83333	1.21674
H	1.68728	4.28078	3.73694
H	0.27051	6.15966	2.99676
C	-1.82686	2.07813	-0.54700
C	-2.66451	1.62099	-1.54259
C	-1.85679	3.41269	-0.12322
C	-3.56907	2.50010	-2.12870
H	-2.61207	0.59931	-1.90070
C	-2.76341	4.27408	-0.72734
C	-3.61443	3.82065	-1.72077
H	-4.23018	2.14565	-2.91071
H	-2.80566	5.31242	-0.41734
H	-4.31712	4.50486	-2.18076
O	1.26007	-0.15139	1.35748
C	3.52043	-0.68751	1.62901
C	2.43932	0.01725	1.03396

C	5.94468	-1.13312	1.68983
C	4.78303	-0.46684	1.20258
C	7.17019	-0.87732	1.21133
H	2.70068	0.74312	0.24171
H	4.93379	0.26970	0.41247
H	3.29519	-1.40857	2.40892
C	8.41431	-1.52139	1.66753
H	7.26218	-0.12831	0.42532
H	5.81473	-1.87057	2.47934
H	8.92512	-2.01193	0.83389
H	9.11557	-0.77311	2.04858
H	8.23139	-2.25834	2.44951
C	-2.53314	-3.68232	-2.10021
H	-3.10772	-3.37857	-2.98993
H	-2.05193	-4.63394	-2.32781
O	-3.37164	-3.86620	-0.99780
C	3.84534	0.21742	-2.73707
C	2.71958	0.98078	-2.98510
H	4.67240	-1.61362	-1.99326
H	2.81222	1.95430	-3.44535
H	4.81663	0.61610	-3.00663
O	2.32701	-2.73854	-1.22819
O	0.30688	1.08475	-2.90367
C	0.33105	2.44097	-3.30304
C	3.43627	-3.58411	-1.01934
H	3.04743	-4.49501	-0.57046
H	3.92958	-3.83102	-1.96366
H	4.16369	-3.13020	-0.33760
H	-0.70562	2.77407	-3.31281
H	0.89555	3.05093	-2.58959
H	0.76043	2.55524	-4.30214

Catalyst 4I

C	3.36023	-0.80478	-0.42086
C	4.72471	-1.34341	0.04481
C	2.51269	-1.98800	1.60238

N	2.33536	-1.10403	0.57263
C	1.06658	-0.64806	0.61921
N	0.54121	-1.29393	1.65659
N	1.42362	-2.12737	2.28744
C	5.49095	-1.53567	-1.25444
C	4.40976	-1.87000	-2.23922
C	3.17020	-1.47334	-1.75390
C	2.01341	-1.68842	-2.47577
C	2.11320	-2.31025	-3.71194
C	3.34856	-2.70134	-4.20463
C	4.50603	-2.48471	-3.47184
C	-0.84501	-1.28792	2.02313
C	-1.63712	-2.33165	1.53544
C	-2.98465	-2.30467	1.86734
C	-1.33287	-0.25280	2.81751
H	3.40343	0.28605	-0.52778
H	5.21346	-0.66397	0.75824
H	6.24790	-2.31370	-1.14317
H	6.00672	-0.60954	-1.52876
H	1.04125	-1.39140	-2.09303
H	1.21904	-2.49423	-4.29500
H	3.40910	-3.18932	-5.17011
H	5.46750	-2.80698	-3.85582
Au	0.13980	0.98879	-0.41953
C	-0.68871	2.63692	-1.32517
C	-0.16173	3.86310	-0.90278
C	-1.67594	2.59492	-2.28946
C	-0.66241	5.03993	-1.43912
C	-2.16511	3.78219	-2.82463
H	-2.06503	1.65107	-2.65521
C	-1.66485	4.99715	-2.39406
H	-0.26504	5.99796	-1.12169
H	-2.93617	3.75056	-3.58551
H	-2.04937	5.91953	-2.81239
C	1.28736	2.45123	0.42288
C	2.29185	2.21895	1.33976

C	0.91461	3.75567	0.07162
C	2.95074	3.29669	1.92243
H	2.57749	1.21433	1.63023
C	1.58466	4.81588	0.66697
C	2.59530	4.58898	1.58507
H	3.73972	3.11570	2.64269
H	1.31110	5.83325	0.40961
H	3.10736	5.42781	2.04070
O	-1.36679	-0.38517	-1.30231
C	-3.62075	-0.96197	-1.56739
C	-2.53900	-0.32007	-0.91013
C	-6.04098	-1.43367	-1.63762
C	-4.87355	-0.84790	-1.07184
C	-7.25511	-1.27441	-1.09189
H	-2.79521	0.27646	-0.01511
H	-5.00943	-0.26342	-0.16132
H	-3.41189	-1.53077	-2.46859
C	-8.50732	-1.84428	-1.61828
H	-7.32956	-0.67260	-0.18683
H	-5.92740	-2.02548	-2.54322
H	-8.98670	-2.48087	-0.86891
H	-9.22685	-1.05067	-1.84020
H	-8.34270	-2.43016	-2.52248
C	3.84612	-2.60353	1.82372
H	4.38021	-2.04012	2.60583
H	3.73706	-3.63046	2.17364
O	4.56967	-2.61939	0.62937
C	-3.50570	-1.28570	2.64510
C	-2.69205	-0.27228	3.11264
H	-3.63499	-3.09928	1.51863
H	-3.10986	0.51050	3.73555
H	-4.55919	-1.29013	2.90148
C	-1.05112	-3.48180	0.74808
C	-0.43680	0.80850	3.40497
C	-0.98468	2.21590	3.22294
C	-0.17479	0.50165	4.87470

H	0.52927	0.76865	2.89294
C	-0.81962	-4.66578	1.68197
C	-1.89177	-3.89776	-0.44698
H	-0.07800	-3.16811	0.35142
H	-0.34735	-5.49073	1.14443
H	-0.18225	-4.39108	2.52443
H	-1.77174	-5.02731	2.08071
H	0.50446	1.24137	5.30394
H	-1.10445	0.52726	5.44949
H	0.27039	-0.48858	4.99705
H	-1.40387	-4.72373	-0.96812
H	-2.88412	-4.24753	-0.15141
H	-2.01190	-3.07922	-1.15933
H	-0.22524	2.94924	3.50477
H	-1.26604	2.41340	2.18396
H	-1.86132	2.39456	3.85033

Catalyst 4m

C	-2.97292	-1.58688	0.07080
C	-4.09496	-2.50107	-0.45211
C	-1.66103	-2.60423	-1.78765
N	-1.81814	-1.65023	-0.81901
C	-0.72589	-0.85807	-0.82290
N	0.03870	-1.38137	-1.77933
N	-0.52706	-2.46817	-2.39307
C	-4.90904	-2.81076	0.79376
C	-3.88444	-2.77108	1.88874
C	-2.74695	-2.09423	1.46770
C	-1.65603	-1.93759	2.29928
C	-1.72092	-2.46694	3.57991
C	-2.85776	-3.13415	4.00874
C	-3.94717	-3.29334	3.16529
C	1.37862	-0.99651	-2.12356
C	2.41452	-1.79735	-1.62383
C	3.70927	-1.44170	-1.96450
C	1.59249	0.11395	-2.93323

H	-3.31740	-0.54548	0.08487
H	-4.67150	-2.02339	-1.25766
H	-5.41502	-3.77229	0.69346
H	-5.67902	-2.04632	0.94139
H	-0.75732	-1.42445	1.96938
H	-0.87633	-2.35918	4.24953
H	-2.89183	-3.54345	5.01133
H	-4.82783	-3.82972	3.50065
Au	-0.37300	0.94409	0.28957
C	-0.07901	2.71460	1.28512
C	-0.91251	3.76305	0.87798
C	0.85448	2.90657	2.28284
C	-0.77900	5.00707	1.47633
C	0.97639	4.15822	2.87752
H	1.48338	2.09241	2.62619
C	0.16545	5.20185	2.47090
H	-1.41528	5.83159	1.17314
H	1.70544	4.31104	3.66473
H	0.26355	6.17538	2.93597
C	-1.82753	2.07195	-0.58759
C	-2.66314	1.61333	-1.58457
C	-1.86622	3.40640	-0.16232
C	-3.57221	2.48828	-2.17042
H	-2.61844	0.58888	-1.93737
C	-2.77984	4.26195	-0.76266
C	-3.62742	3.80621	-1.75806
H	-4.23045	2.13145	-2.95369
H	-2.82804	5.29946	-0.45093
H	-4.33389	4.48732	-2.21666
O	1.31057	-0.10429	1.27147
C	3.58995	-0.53933	1.53683
C	2.48432	0.14846	0.97501
C	6.02295	-0.91971	1.57509
C	4.84658	-0.25301	1.13023
C	7.24064	-0.61005	1.10705
H	2.71139	0.94024	0.23765

H	4.97756	0.53266	0.38542
H	3.38856	-1.31471	2.27054
C	8.49932	-1.25863	1.51221
H	7.31247	0.18755	0.36830
H	5.91107	-1.70881	2.31614
H	9.00567	-1.69319	0.64529
H	9.19465	-0.52186	1.92516
H	8.33788	-2.04153	2.25315
C	-2.75022	-3.58078	-2.04696
H	-3.34111	-3.24051	-2.91256
H	-2.33354	-4.55705	-2.29620
O	-3.55218	-3.72083	-0.91202
C	3.95666	-0.33891	-2.76702
C	2.91475	0.42845	-3.23961
H	4.54012	-2.03297	-1.59850
H	3.11574	1.27919	-3.88147
H	4.97642	-0.08706	-3.03527
C	2.10667	-2.98913	-0.75990
C	0.49206	0.96583	-3.49518
H	-0.48546	0.55147	-3.23940
C	0.57518	2.41634	-3.04095
H	0.55504	0.92646	-4.58754
C	3.30193	-3.73757	-0.21062
H	1.46403	-2.66525	0.07087
H	1.48590	-3.67966	-1.34040
H	2.96976	-4.57354	0.40514
H	3.92360	-4.14934	-1.00806
H	3.93562	-3.10048	0.41330
H	-0.28138	2.98817	-3.40317
H	0.58276	2.49364	-1.94866
H	1.48013	2.90045	-3.41203

Catalyst 4n

C	-3.06903	-1.23505	0.24975
C	-4.32668	-2.04401	-0.11074
C	-2.00172	-2.62415	-1.51912

N	-1.98972	-1.54144	-0.68161
C	-0.81175	-0.90085	-0.83284
N	-0.17190	-1.63483	-1.73963
N	-0.89384	-2.71248	-2.18003
C	-5.09586	-2.09861	1.19956
C	-4.00524	-2.09533	2.22991
C	-2.81845	-1.62807	1.67917
C	-1.65905	-1.55891	2.42468
C	-1.70333	-1.95810	3.75272
C	-2.88767	-2.41291	4.31108
C	-4.04673	-2.48723	3.55297
C	1.18167	-1.45562	-2.17371
C	2.15466	-2.25369	-1.57370
C	3.46688	-2.07583	-1.98828
C	1.46127	-0.51603	-3.16010
H	-3.27849	-0.16149	0.16703
H	-4.88528	-1.58940	-0.94161
H	-5.73668	-2.98109	1.23378
H	-5.73947	-1.21809	1.29571
H	-0.72240	-1.21760	1.99279
H	-0.80502	-1.91777	4.35665
H	-2.90507	-2.72487	5.34840
H	-4.96571	-2.86194	3.98993
Au	-0.14119	0.93580	0.06162
C	0.41334	2.72188	0.90944
C	-0.36345	3.82066	0.52414
C	1.43355	2.87468	1.82573
C	-0.09062	5.06922	1.06199
C	1.69961	4.13287	2.35665
H	2.02302	2.02784	2.15943
C	0.94104	5.22314	1.97355
H	-0.68542	5.92955	0.77439
H	2.49911	4.25346	3.07832
H	1.14862	6.20069	2.39173
C	-1.50359	2.16698	-0.82032
C	-2.43160	1.74715	-1.75118

C	-1.41442	3.51092	-0.43472
C	-3.31182	2.67279	-2.30145
H	-2.48301	0.71414	-2.07573
C	-2.30559	4.41578	-0.99482
C	-3.24945	3.99914	-1.91794
H	-4.04188	2.34800	-3.03322
H	-2.25866	5.46091	-0.70959
H	-3.93702	4.71832	-2.34629
O	1.45060	-0.23710	1.06813
C	3.68777	-0.83629	1.38273
C	2.63714	-0.13806	0.73352
C	6.10390	-1.30165	1.54800
C	4.96544	-0.66917	0.97392
C	7.34713	-1.07960	1.09777
H	2.92311	0.52834	-0.10067
H	5.14784	0.00136	0.13333
H	3.43105	-1.49097	2.21032
C	8.57242	-1.68613	1.64552
H	7.46918	-0.39107	0.26237
H	5.94344	-1.97855	2.38429
H	9.11151	-2.23619	0.86875
H	9.26065	-0.91030	1.99393
H	8.36063	-2.36330	2.47282
C	-3.21599	-3.47549	-1.61048
H	-3.80251	-3.17051	-2.49220
H	-2.93734	-4.52085	-1.74666
O	-3.97134	-3.37051	-0.44049
C	3.78297	-1.13907	-2.95663
C	2.79202	-0.36783	-3.53432
H	4.24514	-2.68587	-1.54150
H	3.04160	0.35043	-4.30722
H	4.81167	-1.01931	-3.27650
C	1.79656	-3.26063	-0.53150
C	0.38669	0.29421	-3.80650
H	0.74391	0.72891	-4.73944
H	-0.49394	-0.31197	-4.03034

H	0.05857	1.11922	-3.16616
H	2.69290	-3.71192	-0.10624
H	1.22038	-2.81041	0.28434
H	1.18162	-4.05981	-0.95161

Catalyst 4o

C	-3.01403	-1.43058	0.08628
C	-4.14567	-2.39186	-0.31616
C	-1.64787	-2.87511	-1.42180
N	-1.80975	-1.72847	-0.68593
C	-0.69517	-0.98402	-0.80565
N	0.08250	-1.72235	-1.60007
N	-0.49160	-2.90239	-1.99581
C	-5.06505	-2.38219	0.89423
C	-4.12027	-2.14621	2.03490
C	-2.91487	-1.63248	1.57296
C	-1.87636	-1.35485	2.43869
C	-2.06352	-1.59027	3.79293
C	-3.26922	-2.08936	4.26010
C	-4.30584	-2.37339	3.38389
C	1.38627	-1.38819	-2.03453
C	2.48904	-2.09729	-1.57611
C	3.76704	-1.78190	-1.98467
C	1.59943	-0.34187	-2.92332
H	-3.29748	-0.39733	-0.14842
H	-4.63415	-2.08691	-1.25253
H	-5.61918	-3.31960	0.96405
H	-5.79652	-1.57205	0.80660
H	-0.92247	-0.97831	2.08141
H	-1.26018	-1.38552	4.49002
H	-3.39857	-2.26947	5.32064
H	-5.24102	-2.78007	3.75242
Au	-0.20831	0.92163	0.06899
C	0.18648	2.74600	0.92011
C	-0.58759	3.80437	0.42873
C	1.10150	2.95567	1.93077

C	-0.41389	5.07390	0.95778
C	1.26586	4.23446	2.45396
H	1.68280	2.13794	2.34260
C	0.51304	5.28613	1.96544
H	-1.00455	5.90555	0.58905
H	1.98166	4.40168	3.25031
H	0.64268	6.28012	2.37635
C	-1.52290	2.07389	-0.97170
C	-2.32487	1.58705	-1.98098
C	-1.52326	3.42908	-0.62103
C	-3.17523	2.46034	-2.65128
H	-2.29325	0.54540	-2.27765
C	-2.38385	4.27993	-1.30058
C	-3.20579	3.79803	-2.30518
H	-3.80592	2.08638	-3.44896
H	-2.40736	5.33390	-1.04629
H	-3.86937	4.47598	-2.82806
O	1.36928	-0.20216	1.18196
C	3.60774	-0.79151	1.52905
C	2.56573	-0.05150	0.91296
C	6.02535	-1.24935	1.70436
C	4.89311	-0.56853	1.17448
C	7.27509	-0.97658	1.30224
H	2.87058	0.68983	0.14989
H	5.08862	0.18934	0.41453
H	3.33832	-1.53300	2.27459
C	8.49372	-1.63268	1.80582
H	7.40799	-0.20426	0.54512
H	5.85396	-2.01021	2.46260
H	9.04588	-2.10283	0.98681
H	9.17490	-0.89477	2.23977
H	8.27109	-2.38882	2.55842
C	-2.75937	-3.85609	-1.52094
H	-3.27659	-3.71387	-2.48337
H	-2.36840	-4.87386	-1.50375
O	-3.63680	-3.70282	-0.44638

C	3.94451	-0.72577	-2.86243
C	2.86830	0.00627	-3.33376
F	0.55330	0.32258	-3.37556
F	2.29409	-3.07422	-0.71186
H	4.59863	-2.36236	-1.60507
H	2.99084	0.82604	-4.02931
H	4.94369	-0.47162	-3.19408

Catalyst 4p

C	-3.10964	-1.20072	0.32328
C	-4.36620	-1.99971	-0.06088
C	-2.02259	-2.59780	-1.43012
N	-2.01473	-1.51517	-0.58855
C	-0.83600	-0.87824	-0.72244
N	-0.19089	-1.61884	-1.62313
N	-0.90930	-2.69183	-2.07871
C	-5.16073	-2.04606	1.23476
C	-4.08981	-2.05041	2.28587
C	-2.88883	-1.59489	1.75673
C	-1.74258	-1.53475	2.52226
C	-1.81457	-1.93041	3.84994
C	-3.01324	-2.37290	4.38749
C	-4.15916	-2.43869	3.60875
C	1.15245	-1.44716	-2.03706
C	2.15247	-2.22597	-1.45951
C	3.46959	-2.07941	-1.85531
C	1.48999	-0.51398	-3.01176
H	-3.30888	-0.12586	0.23597
H	-4.90456	-1.54154	-0.90319
H	-5.80945	-2.92311	1.25774
H	-5.79869	-1.16004	1.31729
H	-0.79617	-1.20586	2.10329
H	-0.92692	-1.89796	4.46985
H	-3.05219	-2.68233	5.42501
H	-5.08915	-2.80418	4.02987
Au	-0.18356	0.98507	0.13683

C	0.33516	2.79160	0.96187
C	-0.47275	3.86792	0.57694
C	1.35833	2.97437	1.86918
C	-0.22665	5.12569	1.10592
C	1.59716	4.24177	2.39104
H	1.97029	2.14363	2.20309
C	0.80860	5.31047	2.00778
H	-0.84467	5.96950	0.81842
H	2.39886	4.38624	3.10584
H	0.99524	6.29538	2.41849
C	-1.57371	2.17957	-0.75436
C	-2.47803	1.73179	-1.69456
C	-1.51887	3.52644	-0.37591
C	-3.37853	2.63216	-2.25354
H	-2.48923	0.69979	-2.02635
C	-2.42962	4.40588	-0.94534
C	-3.35634	3.96062	-1.87210
H	-4.09109	2.28663	-2.99311
H	-2.40969	5.45370	-0.66701
H	-4.05955	4.65971	-2.30823
O	1.45828	-0.14481	1.12204
C	3.71124	-0.67594	1.44290
C	2.64163	0.00146	0.80110
C	6.14152	-1.03651	1.65006
C	4.98845	-0.43419	1.07189
C	7.38423	-0.73613	1.24629
H	2.90988	0.68627	-0.02555
H	5.16134	0.28343	0.26865
H	3.46773	-1.37155	2.24024
C	8.62189	-1.30832	1.80337
H	7.49600	-0.00577	0.44551
H	5.99175	-1.75644	2.45167
H	9.20679	-1.79951	1.02031
H	9.26321	-0.51742	2.20338
H	8.42004	-2.02939	2.59528
C	-3.24047	-3.44217	-1.53849

H	-3.80936	-3.13586	-2.43115
H	-2.96491	-4.48931	-1.66667
O	-4.01440	-3.32923	-0.38187
C	3.78714	-1.14575	-2.82562
C	2.80877	-0.35754	-3.40255
Cl	0.26569	0.44643	-3.74587
Cl	1.75234	-3.35921	-0.22636
H	4.23223	-2.69538	-1.39564
H	3.05070	0.36924	-4.16688
H	4.81686	-1.03447	-3.14349

Catalyst 4q

C	3.07339	-1.38019	-0.36767
C	4.23290	-2.28989	0.07302
C	1.81000	-2.61205	1.39302
N	1.92493	-1.56387	0.51605
C	0.80327	-0.82062	0.58905
N	0.06677	-1.47155	1.48916
N	0.67333	-2.58463	2.00566
C	5.05255	-2.45773	-1.19676
C	4.01878	-2.37193	-2.28072
C	2.85696	-1.78126	-1.79999
C	1.75074	-1.61149	-2.60759
C	1.82405	-2.03684	-3.92590
C	2.98528	-2.61495	-4.41458
C	4.09024	-2.78954	-3.59466
C	-1.27218	-1.18221	1.85466
C	-2.31420	-1.87434	1.24205
C	-3.62548	-1.62024	1.60242
C	-1.55844	-0.23631	2.83270
H	3.37775	-0.32886	-0.29507
H	4.79329	-1.86162	0.91665
H	5.59954	-3.40174	-1.17894
H	5.78834	-1.65130	-1.28163
H	0.83258	-1.17172	-2.22952
H	0.96685	-1.91875	-4.57741

H	3.02575	-2.94436	-5.44589
H	4.98976	-3.25848	-3.97778
Au	0.37428	1.07795	-0.33651
C	0.07403	2.90272	-1.22925
C	0.99324	3.89372	-0.86479
C	-0.90768	3.16684	-2.16201
C	0.89862	5.15206	-1.43943
C	-0.99325	4.43418	-2.73013
H	-1.60453	2.39927	-2.47959
C	-0.09512	5.42012	-2.36668
H	1.60360	5.93086	-1.16931
H	-1.76233	4.64260	-3.46467
H	-0.16327	6.40494	-2.81289
C	1.87612	2.14036	0.54327
C	2.71317	1.62949	1.51310
C	1.98044	3.47003	0.11695
C	3.70625	2.44080	2.05163
H	2.59906	0.61842	1.88757
C	2.98008	4.26065	0.66794
C	3.84123	3.74760	1.62208
H	4.36654	2.04395	2.81366
H	3.08283	5.29269	0.35108
H	4.61589	4.37771	2.04195
O	-1.36208	0.11912	-1.33515
C	-3.65951	-0.15979	-1.67165
C	-2.52464	0.38346	-1.01395
C	-6.11719	-0.30201	-1.82973
C	-4.90280	0.17880	-1.26350
C	-7.31857	0.07483	-1.36892
H	-2.72401	1.07912	-0.17712
H	-4.99367	0.87362	-0.42749
H	-3.49139	-0.85059	-2.49223
C	-8.61538	-0.37738	-1.90114
H	-7.34570	0.77485	-0.53442
H	-6.05035	-0.99587	-2.66481
H	-9.20530	-0.86257	-1.11799

H	-9.21092	0.47625	-2.23779
H	-8.49767	-1.07221	-2.73255
C	2.93885	-3.56173	1.56529
H	3.51633	-3.27531	2.45902
H	2.56091	-4.57187	1.72575
O	3.74177	-3.56669	0.42347
C	-3.89514	-0.66822	2.56951
C	-2.87104	0.02867	3.18394
Br	-0.16995	0.68194	3.70800
Br	-1.95808	-3.15498	-0.09036
H	-4.42615	-2.17345	1.12757
H	-3.07963	0.76474	3.94950
H	-4.92126	-0.47458	2.85894

Catalyst 4r

C	3.10318	-1.22089	-0.32324
C	4.25016	-2.19870	-0.01963
C	1.71345	-2.91995	0.84640
N	1.88112	-1.65391	0.34997
C	0.73385	-0.96638	0.52274
N	-0.06750	-1.86338	1.09945
N	0.51922	-3.08246	1.30949
C	5.21107	-1.97498	-1.17567
C	4.29282	-1.62683	-2.31023
C	3.05385	-1.22404	-1.82633
C	2.02563	-0.88526	-2.68169
C	2.25622	-0.94400	-4.04842
C	3.49435	-1.33157	-4.53592
C	4.52152	-1.67746	-3.67010
C	-1.45192	-1.73376	1.40595
C	-2.39024	-2.32136	0.56172
C	-3.73622	-2.23654	0.88117
C	-1.86202	-1.07349	2.55994
H	3.35155	-0.22410	0.06003
H	4.69015	-2.02439	0.97312
H	5.81634	-2.86525	-1.35275

H	5.89289	-1.15021	-0.94379
H	1.04785	-0.59444	-2.30839
H	1.46130	-0.69084	-4.73918
H	3.65714	-1.37726	-5.60607
H	5.48151	-1.99981	-4.05779
Au	0.37573	1.08879	-0.04698
C	0.20448	3.02817	-0.69810
C	1.14615	3.91536	-0.16415
C	-0.69743	3.45542	-1.65100
C	1.15132	5.23602	-0.58642
C	-0.68279	4.78335	-2.06588
H	-1.40645	2.77105	-2.10341
C	0.23574	5.66774	-1.53213
H	1.87552	5.93489	-0.18182
H	-1.38921	5.11947	-2.81592
H	0.24605	6.70028	-1.85943
C	1.85266	1.95833	1.05999
C	2.57075	1.29093	2.02960
C	2.04253	3.32346	0.81740
C	3.54099	1.98020	2.74899
H	2.38160	0.24887	2.26149
C	3.02174	3.98859	1.54318
C	3.77014	3.31984	2.49594
H	4.10703	1.46279	3.51441
H	3.19175	5.04570	1.37083
H	4.52782	3.85362	3.05668
O	-1.39042	0.36372	-1.20662
C	-3.69946	0.32059	-1.59281
C	-2.53171	0.71470	-0.88987
C	-6.15277	0.44207	-1.80685
C	-4.91243	0.75790	-1.18433
C	-7.32033	0.92978	-1.36219
H	-2.68587	1.37758	-0.01721
H	-4.95418	1.40821	-0.30956
H	-3.58506	-0.32493	-2.45791
C	-8.63784	0.66413	-1.96430

H	-7.29922	1.58322	-0.49058
H	-6.13393	-0.20805	-2.67884
H	-9.32022	0.22981	-1.22799
H	-9.10483	1.59923	-2.28782
H	-8.56969	-0.00677	-2.82047
C	2.85327	-3.87252	0.86190
H	3.30388	-3.86787	1.86746
H	2.50171	-4.88526	0.66277
O	3.78916	-3.53036	-0.11487
C	-4.14813	-1.56409	2.01432
C	-3.21475	-0.98324	2.84942
C	-0.88481	-0.41198	3.50406
C	-2.01757	-3.11014	-0.67661
H	-4.46446	-2.70064	0.22790
H	-3.52942	-0.47043	3.74903
H	-5.20207	-1.50402	2.25523
F	-0.56582	0.80510	3.05687
F	-1.40996	-0.26545	4.70943
F	0.24564	-1.09668	3.64181
F	-2.97262	-2.99945	-1.59967
F	-0.88611	-2.70346	-1.24039
F	-1.89163	-4.39779	-0.38922

Catalyst 4s

C	-3.49427	-1.41922	0.00125
C	-4.55689	-2.41776	-0.48894
C	-1.92342	-2.94083	-1.19693
N	-2.19205	-1.74868	-0.57381
C	-1.06829	-1.00633	-0.56598
N	-0.18029	-1.79754	-1.16941
N	-0.68948	-3.00343	-1.57277
C	-5.62751	-2.35030	0.58879
C	-4.84172	-2.03632	1.82767
C	-3.59037	-1.53214	1.49656
C	-2.67294	-1.19254	2.47022
C	-3.03177	-1.35306	3.80045

C	-4.28442	-1.84207	4.13674
C	-5.19740	-2.19089	3.15247
C	1.19831	-1.53266	-1.34599
C	2.12854	-2.10792	-0.48079
C	3.47706	-1.86505	-0.64789
C	1.64003	-0.71611	-2.38016
H	-3.75043	-0.40635	-0.33357
H	-4.91946	-2.17237	-1.49750
H	-6.18008	-3.28976	0.64072
H	-6.34598	-1.55682	0.35879
H	-1.68301	-0.82510	2.21553
H	-2.32626	-1.09820	4.58181
H	-4.54862	-1.96384	5.18038
H	-6.16878	-2.59084	3.42115
Au	-0.75751	1.01641	0.11998
C	-0.55481	2.95381	0.76593
C	-1.31437	3.89324	0.05917
C	0.22019	3.34288	1.83894
C	-1.26674	5.22662	0.43620
C	0.25906	4.68393	2.20758
H	0.78574	2.62022	2.41640
C	-0.47857	5.61897	1.50576
H	-1.84910	5.96749	-0.10081
H	0.86501	4.99132	3.05191
H	-0.44687	6.66188	1.79673
C	-1.99902	1.94947	-1.20055
C	-2.66241	1.29942	-2.21993
C	-2.10272	3.33538	-1.02942
C	-3.47493	2.03175	-3.07902
H	-2.55025	0.23315	-2.38084
C	-2.92016	4.04523	-1.89826
C	-3.60512	3.39766	-2.91178
H	-3.99787	1.52607	-3.88208
H	-3.01847	5.11917	-1.78513
H	-4.23850	3.96647	-3.58158
O	0.72634	0.20107	1.56451

C	2.91852	0.00213	2.36017
C	1.93321	0.44172	1.44214
C	5.30651	-0.09547	2.97239
C	4.22241	0.29076	2.13709
C	6.57787	0.21859	2.67946
H	2.29313	1.02913	0.57617
H	4.47402	0.85795	1.23998
H	2.59560	-0.56529	3.22762
C	7.75120	-0.13947	3.49335
H	6.76410	0.78227	1.76607
H	5.08092	-0.66049	3.87420
H	8.45999	-0.72981	2.90519
H	8.29436	0.76003	3.79806
H	7.47775	-0.70345	4.38509
C	-3.01154	-3.93001	-1.40643
H	-3.38741	-3.83556	-2.43785
H	-2.62893	-4.94398	-1.28610
O	-4.03107	-3.72828	-0.47508
C	3.89649	-1.03671	-1.67625
C	2.99159	-0.45719	-2.54263
Cl	0.51300	-0.02818	-3.47877
Cl	1.60250	-3.10396	0.81619
H	4.19242	-2.32221	0.02597
C	5.37420	-0.77852	-1.81265
H	3.32147	0.17993	-3.35230
F	5.83911	-0.17570	-0.70781
F	6.04917	-1.91057	-1.94831
F	5.65520	0.00161	-2.84106

Catalyst 4t

C	-3.28658	-1.41699	-0.31689
C	-4.35965	-2.35812	-0.89031
C	-1.71441	-3.03295	-1.37254
N	-1.96520	-1.81968	-0.79111
C	-0.80730	-1.12990	-0.72271
N	0.08173	-1.96616	-1.26829

N	-0.46331	-3.15523	-1.66928
C	-5.51610	-2.20760	0.08433
C	-4.82534	-1.93079	1.38659
C	-3.51823	-1.51345	1.16618
C	-2.67248	-1.22598	2.21792
C	-3.15841	-1.34803	3.51140
C	-4.46635	-1.74807	3.73564
C	-5.30836	-2.04563	2.67446
C	1.48205	-1.75903	-1.41500
C	1.96228	-0.52578	-1.75026
C	3.35248	-0.29890	-1.79784
C	2.34665	-2.84283	-1.17623
C	3.88784	0.97725	-2.07271
H	-3.45932	-0.39377	-0.67185
H	-4.61464	-2.11028	-1.93075
H	-6.13392	-3.10698	0.09257
H	-6.15495	-1.37034	-0.21561
H	-1.64236	-0.92635	2.05250
H	-2.50990	-1.13194	4.35157
H	-4.83103	-1.84037	4.75167
H	-6.32485	-2.37668	2.85599
C	5.23910	1.17256	-2.09474
Au	-0.51344	0.84528	0.10901
C	-0.36006	2.72501	0.91055
C	-1.02718	3.72749	0.19712
C	0.29180	3.01404	2.09110
C	-1.01316	5.02644	0.68179
C	0.29708	4.32141	2.56703
H	0.78380	2.23528	2.66360
C	-0.34991	5.31991	1.86250
H	-1.52532	5.81661	0.14329
H	0.80552	4.55340	3.49565
H	-0.34431	6.33617	2.23766
C	-1.57569	1.89397	-1.27648
C	-2.09382	1.33442	-2.42556
C	-1.68300	3.26693	-1.01822

C	-2.76863	2.14549	-3.33257
H	-1.97679	0.27936	-2.64570
C	-2.36587	4.05465	-1.93455
C	-2.90868	3.49687	-3.07999
H	-3.17672	1.71219	-4.23800
H	-2.46613	5.11984	-1.75665
H	-3.43597	4.12648	-3.78639
O	0.86085	-0.11916	1.57490
C	3.07311	-0.70548	2.09264
C	2.07757	0.05384	1.42818
C	5.46855	-1.24436	2.32309
C	4.37423	-0.51735	1.77353
C	6.73444	-1.01527	1.94670
H	2.44689	0.83237	0.73594
H	4.61634	0.23990	1.02550
H	2.76052	-1.45607	2.81184
C	7.91943	-1.71329	2.47515
H	6.90514	-0.25038	1.18941
H	5.25405	-2.00062	3.07508
H	8.47424	-2.20071	1.66799
H	8.61505	-1.00015	2.92721
H	7.65475	-2.46291	3.22081
C	-2.83041	-3.97510	-1.64359
H	-3.11125	-3.89740	-2.70623
H	-2.51299	-5.00250	-1.46216
O	-3.91554	-3.69642	-0.81134
C	4.23609	-1.38020	-1.54495
C	3.69348	-2.65009	-1.25260
C	5.62597	-1.14793	-1.58943
C	6.11663	0.09846	-1.85623
H	7.18687	0.26456	-1.89576
H	5.64183	2.15539	-2.30780
H	6.29790	-1.98132	-1.41123
H	3.20612	1.79952	-2.26572
H	4.37148	-3.47695	-1.07051
H	1.92783	-3.81208	-0.93927

H	1.28394	0.28816	-1.98912
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Catalyst 4u

C	-3.03240	-1.67081	0.07413
C	-4.04907	-2.74865	-0.33834
C	-1.48807	-2.97864	-1.38157
N	-1.79204	-1.84535	-0.67533
C	-0.76580	-0.97856	-0.80094
N	0.10328	-1.63655	-1.56646
N	-0.32434	-2.88433	-1.93701
C	-4.98827	-2.82123	0.85405
C	-4.09023	-2.49063	2.00910
C	-2.93660	-1.85706	1.56318
C	-1.94180	-1.47890	2.44116
C	-2.12014	-1.73635	3.79274
C	-3.27503	-2.35585	4.24412
C	-4.26802	-2.73963	3.35500
C	1.36765	-1.14298	-2.00850
C	2.55262	-1.71434	-1.48861
C	3.78744	-1.18424	-1.95087
C	3.78436	-0.11919	-2.87676
C	2.61576	0.41664	-3.33394
C	1.38856	-0.10752	-2.89766
C	2.56738	-2.74133	-0.52114
C	3.75179	-3.22830	-0.04681
C	4.97452	-2.72120	-0.51791
C	4.98973	-1.72312	-1.44791
H	-3.41973	-0.67425	-0.17244
H	-4.54662	-2.50704	-1.28855
H	-5.45291	-3.80620	0.92087
H	-5.79001	-2.08318	0.74644
H	-1.02890	-1.00545	2.09359
H	-1.35002	-1.45357	4.50001
H	-3.39782	-2.55215	5.30258
H	-5.16108	-3.24067	3.71157
H	4.73746	0.26777	-3.22215

H	2.62453	1.23403	-4.04366
H	1.63184	-3.14580	-0.15410
H	3.74985	-4.01916	0.69353
H	5.90545	-3.12510	-0.13800
H	5.92936	-1.32330	-1.81618
Au	-0.53335	1.00912	-0.01203
C	-0.39966	2.90709	0.75220
C	-1.31463	3.82287	0.22051
C	0.47383	3.28576	1.75035
C	-1.32716	5.12449	0.69825
C	0.45198	4.59504	2.22062
H	1.16592	2.57532	2.18871
C	-0.44318	5.50760	1.69407
H	-2.03128	5.84642	0.29861
H	1.13513	4.89532	3.00659
H	-0.45874	6.52541	2.06474
C	-1.98469	1.92039	-1.10876
C	-2.70031	1.28872	-2.10412
C	-2.18040	3.27635	-0.81502
C	-3.65943	2.00545	-2.81274
H	-2.52372	0.24893	-2.35591
C	-3.14560	3.96961	-1.53214
C	-3.88229	3.33742	-2.51970
H	-4.22466	1.51496	-3.59625
H	-3.31958	5.01920	-1.32177
H	-4.63100	3.89361	-3.07072
O	1.16890	0.22302	1.18410
C	3.46509	-0.00163	1.57484
C	2.33640	0.43855	0.83694
C	5.91825	-0.04472	1.82422
C	4.71095	0.31646	1.15840
C	7.12294	0.32822	1.37243
H	2.54451	1.00494	-0.09050
H	4.81147	0.90777	0.24755
H	3.29346	-0.58266	2.47582
C	8.41079	0.00660	2.01280

H	7.16022	0.92341	0.46017
H	5.83940	-0.63720	2.73335
H	9.06399	-0.53380	1.32158
H	8.94777	0.92229	2.27730
H	8.28044	-0.59335	2.91340
C	-2.48559	-4.07508	-1.48863
H	-2.98850	-4.00246	-2.46642
H	-1.99162	-5.04634	-1.44533
O	-3.40400	-4.00135	-0.44016
H	0.45273	0.29819	-3.26630

Catalyst 4v

C	-3.45509	-1.42845	-0.44170
C	-4.48322	-2.30260	-1.17970
C	-1.82771	-2.59546	-1.92482
N	-2.13849	-1.58701	-1.05127
C	-1.03705	-0.82964	-0.86997
N	-0.12197	-1.42285	-1.63517
N	-0.59180	-2.52560	-2.29775
C	-5.58317	-2.49847	-0.14946
C	-4.83518	-2.47423	1.15048
C	-3.58512	-1.89127	0.98287
C	-2.69988	-1.77911	2.03559
C	-3.08879	-2.25446	3.27958
C	-4.34000	-2.82441	3.45499
C	-5.22186	-2.94037	2.39079
C	1.23274	-0.99992	-1.78582
C	2.27829	-1.81418	-1.24670
C	3.61113	-1.35362	-1.36675
C	1.47735	0.18235	-2.38838
C	2.01591	-3.02444	-0.58373
C	3.03680	-3.77649	-0.06495
C	4.35526	-3.33981	-0.19711
C	4.63034	-2.15621	-0.83164
H	-3.72816	-0.37020	-0.53405
H	-4.82299	-1.83978	-2.11734

H	-6.12248	-3.42906	-0.33341
H	-6.30681	-1.67892	-0.20997
H	-1.71271	-1.34701	1.90356
H	-2.40823	-2.18197	4.11915
H	-4.62774	-3.19307	4.43234
H	-6.19281	-3.40281	2.52963
H	0.99417	-3.37043	-0.48995
H	2.82037	-4.71177	0.43688
H	5.16652	-3.93795	0.20097
H	5.66254	-1.84098	-0.91740
Au	-0.74341	0.94459	0.30896
C	-0.54860	2.66042	1.41733
C	-1.28411	3.75332	0.94235
C	0.20217	2.76909	2.56934
C	-1.23935	4.95429	1.63390
C	0.24022	3.97989	3.25383
H	0.75182	1.92142	2.96362
C	-0.47573	5.06561	2.78449
H	-1.80349	5.81040	1.27980
H	0.82845	4.06687	4.15984
H	-0.44542	6.00626	3.32110
C	-1.93140	2.18697	-0.77900
C	-2.55216	1.81791	-1.95426
C	-2.03844	3.48959	-0.27512
C	-3.32560	2.75003	-2.63878
H	-2.44146	0.82094	-2.36576
C	-2.81928	4.40104	-0.97262
C	-3.46226	4.03238	-2.14214
H	-3.81557	2.46512	-3.56227
H	-2.92169	5.41434	-0.59979
H	-4.06750	4.75630	-2.67419
O	0.68836	-0.25976	1.51310
C	2.87577	-0.82082	2.14191
C	1.90473	-0.04331	1.46097
C	5.26065	-1.22320	2.62796
C	4.18700	-0.52220	2.00663

C	6.53978	-0.86308	2.45912
H	2.28941	0.80522	0.86596
H	4.45754	0.32384	1.37267
H	2.53617	-1.65399	2.74948
C	7.70179	-1.52825	3.07560
H	6.74415	-0.00543	1.81814
H	5.01437	-2.07441	3.25951
H	8.40105	-1.87702	2.31009
H	8.26421	-0.82365	3.69523
H	7.40676	-2.37649	3.69343
C	-2.88200	-3.54348	-2.37017
H	-3.23821	-3.23772	-3.36703
H	-2.47407	-4.55067	-2.46205
O	-3.92873	-3.57411	-1.44691
H	0.65581	0.76906	-2.78810
C	3.88084	-0.07912	-1.99755
C	2.80362	0.68185	-2.50539
C	3.04450	1.92325	-3.11456
C	4.31699	2.41568	-3.22056
C	5.38684	1.67299	-2.71531
C	5.17263	0.45634	-2.11845
H	2.20053	2.48598	-3.49885
H	4.49580	3.37381	-3.69270
H	6.39598	2.05819	-2.79957
H	6.02592	-0.09639	-1.74585

Catalyst 4w

C	-3.50707	-1.58878	-0.52791
C	-4.45778	-2.52925	-1.28781
C	-1.76774	-2.65654	-1.95869
N	-2.16760	-1.66627	-1.10130
C	-1.12204	-0.84188	-0.88786
N	-0.14746	-1.37931	-1.62022
N	-0.52704	-2.51172	-2.29182
C	-5.56955	-2.79090	-0.28506
C	-4.85963	-2.71282	1.03393

C	-3.64365	-2.05456	0.89537
C	-2.79344	-1.88522	1.96940
C	-3.18586	-2.37757	3.20580
C	-4.40516	-3.02006	3.35290
C	-5.24988	-3.19535	2.26684
C	1.18620	-0.88208	-1.72400
C	2.25208	-1.65190	-1.15450
C	3.55742	-1.10414	-1.23466
C	1.38643	0.32078	-2.30523
C	2.06126	-2.87083	-0.50750
C	3.13573	-3.55393	0.03401
C	4.41469	-3.04005	-0.05658
C	4.64942	-1.81740	-0.68136
H	-3.84386	-0.54992	-0.63344
H	-4.80248	-2.09192	-2.23583
H	-6.04342	-3.75502	-0.47661
H	-6.34216	-2.01964	-0.37021
H	-1.82924	-1.39761	1.86096
H	-2.53279	-2.26093	4.06205
H	-4.69590	-3.40015	4.32498
H	-6.19391	-3.71595	2.38356
H	1.06785	-3.29620	-0.43834
H	2.97043	-4.50561	0.52470
H	5.25500	-3.58265	0.36429
C	5.95739	-1.25044	-0.76894
Au	-1.00325	0.94298	0.30467
C	-0.96402	2.66195	1.42328
C	-1.75610	3.70439	0.92716
C	-0.26117	2.81502	2.60010
C	-1.82216	4.89937	1.62739
C	-0.33277	4.02004	3.29202
H	0.33502	2.00606	3.00790
C	-1.10948	5.05503	2.80523
H	-2.43345	5.71588	1.25812
H	0.21732	4.14197	4.21781
H	-1.16591	5.99065	3.34838

C	-2.22521	2.11103	-0.82725
C	-2.77939	1.70549	-2.02340
C	-2.44413	3.39827	-0.31947
C	-3.59560	2.58419	-2.72879
H	-2.58478	0.72049	-2.43253
C	-3.26411	4.25649	-1.03894
C	-3.83920	3.85045	-2.23133
H	-4.03380	2.27125	-3.66903
H	-3.45258	5.25704	-0.66538
H	-4.47684	4.53280	-2.78023
O	0.41255	-0.19058	1.58595
C	2.59439	-0.70046	2.27461
C	1.62511	0.05591	1.56985
C	4.96797	-1.04405	2.84553
C	3.90173	-0.36449	2.18984
C	6.24202	-0.64399	2.73571
H	2.00386	0.91846	0.99116
H	4.17537	0.49341	1.57317
H	2.25841	-1.54869	2.86314
C	7.39777	-1.29543	3.37794
H	6.44768	0.23161	2.12084
H	4.72117	-1.91451	3.45011
H	8.12590	-1.61577	2.62625
H	7.92827	-0.59144	4.02554
H	7.10300	-2.16139	3.97085
C	-2.74870	-3.66801	-2.43086
H	-3.09641	-3.38443	-3.43721
H	-2.27766	-4.64835	-2.51018
O	-3.81602	-3.76302	-1.53560
H	0.54507	0.86659	-2.72148
C	3.77571	0.16029	-1.83741
C	2.68996	0.89074	-2.37886
C	2.92210	2.13341	-2.96351
C	4.20099	2.65556	-3.01634
C	5.26708	1.95224	-2.48642
C	5.08068	0.70602	-1.89190

H	2.08640	2.68611	-3.37860
H	4.36905	3.62168	-3.47637
H	6.26892	2.36564	-2.53323
C	6.16351	-0.04585	-1.34216
H	7.16247	0.37235	-1.40779
H	6.78844	-1.82117	-0.36660

Catalyst 4x

C	-3.02018	-1.65376	0.19946
C	-4.09744	-2.66729	-0.22284
C	-1.65056	-2.80389	-1.53530
N	-1.86508	-1.75158	-0.68584
C	-0.82051	-0.90361	-0.78701
N	-0.02521	-1.49446	-1.67619
N	-0.52383	-2.67773	-2.15686
C	-4.90174	-2.87597	1.05011
C	-3.87638	-2.69138	2.12959
C	-2.76746	-2.01465	1.63688
C	-1.67436	-1.74818	2.43633
C	-1.70926	-2.16277	3.75997
C	-2.81906	-2.82534	4.26091
C	-3.90991	-3.09716	3.44849
C	1.25965	-1.03481	-2.10514
C	2.40123	-1.64175	-1.52549
C	3.67680	-1.19495	-1.95802
C	3.74791	-0.16196	-2.91578
C	2.62002	0.38981	-3.44241
C	1.33426	-0.05201	-3.05994
C	2.33412	-2.65891	-0.54925
C	3.47645	-3.21876	-0.05004
C	4.73885	-2.78885	-0.49105
C	4.83364	-1.79371	-1.42017
H	-3.41284	-0.63289	0.11369
H	-4.69174	-2.30896	-1.07591
H	-5.37505	-3.85903	1.05091
H	-5.69619	-2.12576	1.12154

H	-0.79606	-1.24002	2.04851
H	-0.86204	-1.96863	4.40634
H	-2.82944	-3.14407	5.29629
H	-4.76737	-3.63227	3.84109
H	4.72582	0.17537	-3.24380
H	2.69394	1.16763	-4.19417
C	0.12589	0.54168	-3.70395
H	1.36911	-3.00415	-0.19501
H	3.40742	-4.00726	0.68987
H	5.63458	-3.24707	-0.08874
H	5.80314	-1.44889	-1.76632
Au	-0.53554	1.02439	0.12391
C	-0.31602	2.89300	0.94589
C	-1.21768	3.85248	0.47136
C	0.61490	3.22332	1.90926
C	-1.15426	5.14735	0.96307
C	0.66766	4.52562	2.39637
H	1.29624	2.48201	2.31142
C	-0.21051	5.48149	1.92049
H	-1.84600	5.90223	0.60503
H	1.39609	4.78615	3.15529
H	-0.16668	6.49423	2.30264
C	-2.04735	1.99614	-0.83646
C	-2.88432	1.40409	-1.75991
C	-2.16789	3.35423	-0.51316
C	-3.87396	2.16489	-2.37344
H	-2.78164	0.35838	-2.02795
C	-3.16238	4.09418	-1.13791
C	-4.01004	3.50406	-2.05952
H	-4.53216	1.70287	-3.09953
H	-3.27567	5.14619	-0.89977
H	-4.78050	4.09610	-2.53829
O	1.17860	0.15473	1.21341
C	3.47632	-0.08365	1.57772
C	2.34313	0.43096	0.89987
C	5.93013	-0.18475	1.78277

C	4.72006	0.26314	1.17841
C	7.13553	0.19940	1.34205
H	2.53998	1.12912	0.06537
H	4.81598	0.94097	0.32930
H	3.31101	-0.76324	2.40818
C	8.42614	-0.21506	1.92033
H	7.17147	0.87628	0.48875
H	5.85315	-0.85941	2.63302
H	9.04787	-0.70811	1.16738
H	8.99603	0.65705	2.25394
H	8.29712	-0.89134	2.76544
C	-2.69002	-3.85562	-1.68330
H	-3.28671	-3.64221	-2.58477
H	-2.22654	-4.83329	-1.81927
O	-3.49566	-3.90413	-0.54384
H	0.38049	0.95972	-4.67764
H	-0.66372	-0.19763	-3.85013
H	-0.29471	1.35281	-3.10167

Catalyst 4y

C	-3.03757	-1.62627	0.24645
C	-4.10344	-2.65527	-0.16566
C	-1.59224	-2.91775	-1.31983
N	-1.83352	-1.80326	-0.56026
C	-0.77862	-0.97071	-0.67598
N	0.05000	-1.63647	-1.48030
N	-0.43802	-2.84771	-1.89654
C	-4.99063	-2.75329	1.06481
C	-4.03154	-2.50184	2.19062
C	-2.88129	-1.88016	1.71994
C	-1.83712	-1.56833	2.56620
C	-1.96084	-1.88286	3.91184
C	-3.11112	-2.49179	4.38864
C	-4.15463	-2.80712	3.53106
C	1.33693	-1.21281	-1.91251
C	2.48317	-1.77554	-1.29828

C	3.76024	-1.35313	-1.75227
C	3.84153	-0.38485	-2.77533
C	2.72320	0.13929	-3.34816
C	1.45540	-0.29271	-2.92189
C	2.41019	-2.72920	-0.26106
C	3.55107	-3.24845	0.28269
C	4.81530	-2.83984	-0.17316
C	4.91452	-1.90837	-1.16552
H	-3.40765	-0.61052	0.06046
H	-4.63493	-2.35593	-1.08059
H	-5.48308	-3.72590	1.10981
H	-5.77210	-1.98729	1.02680
H	-0.92885	-1.10055	2.19861
H	-1.15208	-1.65234	4.59452
H	-3.19095	-2.73365	5.44173
H	-5.04486	-3.29907	3.90690
H	4.82203	-0.06850	-3.11552
H	2.78437	0.87065	-4.14356
Cl	0.06533	0.34609	-3.71113
H	1.44290	-3.05401	0.10420
H	3.47955	-3.98833	1.07089
H	5.70932	-3.26643	0.26588
H	5.88541	-1.58220	-1.52479
Au	-0.52078	1.00982	0.13434
C	-0.34693	2.90340	0.90733
C	-1.28419	3.82500	0.42762
C	0.58072	3.27877	1.85724
C	-1.26046	5.12798	0.90079
C	0.59403	4.58901	2.32533
H	1.29009	2.56672	2.26358
C	-0.32028	5.50772	1.84475
H	-1.97974	5.85369	0.53670
H	1.32060	4.88494	3.07299
H	-0.30718	6.52691	2.21168
C	-2.04176	1.92990	-0.86518
C	-2.82785	1.30585	-1.81056

C	-2.21486	3.28377	-0.55204
C	-3.83205	2.02824	-2.44645
H	-2.66426	0.27142	-2.09034
C	-3.22525	3.98392	-1.19681
C	-4.03075	3.35985	-2.13353
H	-4.45006	1.54272	-3.19234
H	-3.38016	5.03246	-0.96703
H	-4.81332	3.92085	-2.62979
O	1.21594	0.20911	1.26811
C	3.51683	0.03648	1.65906
C	2.37612	0.49021	0.94848
C	5.97295	-0.00578	1.87152
C	4.75487	0.38145	1.24169
C	7.17018	0.38967	1.41840
H	2.56814	1.13948	0.07341
H	4.83964	1.00923	0.35361
H	3.36087	-0.58931	2.53245
C	8.46787	0.04222	2.02422
H	7.19294	1.02612	0.53403
H	5.90892	-0.63873	2.75427
H	9.11172	-0.46421	1.29933
H	9.00703	0.94628	2.32208
H	8.35229	-0.59850	2.89837
C	-2.63368	-3.97086	-1.44168
H	-3.17392	-3.82719	-2.39119
H	-2.17429	-4.95930	-1.47069
O	-3.50405	-3.92055	-0.35151

7.3 Cartesian coordinates of the substrates

3b

H	-4.48088	-1.60787	-0.00006
C	-4.59711	-0.50599	-0.00005
C	-3.33662	0.25172	-0.00003
O	-5.68659	0.00203	-0.00007

C	-2.16056	-0.38313	-0.00002
C	-0.87768	0.29124	0.00000
C	0.28755	-0.35584	0.00001
C	1.56213	0.40151	0.00003
O	2.61341	-0.42567	0.00002
O	1.65289	1.60006	0.00005
C	3.90101	0.20752	0.00004
C	4.94472	-0.88128	0.00002
H	-3.40982	1.33371	-0.00002
H	-2.14843	-1.47080	-0.00003
H	-0.86765	1.37700	0.00001
H	0.34994	-1.43694	-0.00001
H	3.97231	0.84764	0.88061
H	3.97232	0.84769	-0.88049
H	5.93991	-0.43679	0.00004
H	4.84702	-1.50979	0.88481
H	4.84703	-1.50974	-0.88482

3c

C	4.07910	-0.35382	-0.00003
C	2.77111	0.31919	-0.00003
O	5.13203	0.22612	-0.00003
C	1.63913	-0.39076	-0.00002
C	0.31558	0.20005	-0.00001
C	-0.80596	-0.51982	-0.00001
C	-2.12528	0.15526	-0.00000
O	-3.12184	-0.73855	0.00003
O	-2.29594	1.34454	0.00002
C	-4.43572	-0.18314	0.00005
H	4.03695	-1.46096	-0.00002
H	2.77354	1.40359	-0.00002
H	1.69725	-1.47693	-0.00002
H	0.23659	1.28298	-0.00001
H	-0.80004	-1.60259	-0.00001
H	-5.11621	-1.02887	0.00009
H	-4.58493	0.43209	0.88652

H	-4.58498	0.43205	-0.88643
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3d

C	5.30497	0.43197	-0.00003
C	4.01699	-0.27733	-0.00003
O	6.37464	-0.11697	-0.00004
C	2.86513	0.40054	-0.00001
C	1.55850	-0.22669	-0.00001
C	0.41680	0.46070	0.00000
C	-0.88609	-0.25472	0.00000
O	-1.89501	0.61763	0.00002
O	-0.99560	-1.45304	-0.00001
C	-3.28211	0.16258	0.00002
C	-3.56814	-0.63688	1.26374
C	-3.56815	-0.63686	-1.26371
C	-4.06705	1.46449	0.00004
H	5.23098	1.53748	-0.00002
H	4.04945	-1.36126	-0.00003
H	2.89318	1.48793	-0.00001
H	1.50972	-1.31136	-0.00002
H	0.39276	1.54323	0.00001
H	-3.28546	-0.05885	2.14491
H	-4.63833	-0.84122	1.31848
H	-3.02896	-1.58102	1.26637
H	-4.63835	-0.84120	-1.31844
H	-3.28549	-0.05881	-2.14487
H	-3.02898	-1.58100	-1.26636
H	-3.82574	2.05266	-0.88570
H	-5.13641	1.25301	0.00004
H	-3.82573	2.05264	0.88578

3e

C	6.86400	3.10481	-0.27058
C	6.14703	1.97707	0.34296
O	7.68178	3.77309	0.30383
C	5.24876	1.27837	-0.35783

C	4.50092	0.15698	0.17509
C	3.60810	-0.52843	-0.53873
C	2.87454	-1.66493	0.06921
O	2.02927	-2.20946	-0.81328
O	3.01815	-2.05110	1.19865
C	1.23572	-3.31199	-0.34589
C	0.01940	-2.83622	0.42479
C	-0.90398	-1.94162	-0.39312
C	-3.05663	-0.58695	-0.40892
C	-2.13944	-1.50771	0.38564
C	-4.29750	-0.16269	0.36645
C	-5.20952	0.76920	-0.42118
C	-6.45265	1.18934	0.35244
C	-7.36556	2.12104	-0.43508
C	-8.60526	2.53085	0.34930
H	6.59910	3.31037	-1.32645
H	6.38073	1.74602	1.37654
H	5.05466	1.55509	-1.39186
H	4.67815	-0.13645	1.20547
H	3.38463	-0.28797	-1.57086
H	1.86213	-3.95863	0.26770
H	0.94324	-3.83954	-1.25343
H	0.35233	-2.31638	1.32644
H	-0.52589	-3.72509	0.75697
H	-1.21310	-2.47032	-1.30162
H	-0.35431	-1.05616	-0.72499
H	-3.36122	-1.08802	-1.33428
H	-2.49776	0.30442	-0.71372
H	-1.82750	-1.00145	1.30544
H	-2.70018	-2.39459	0.70033
H	-3.99234	0.33004	1.29602
H	-4.86043	-1.05397	0.66410
H	-5.51186	0.27812	-1.35266
H	-4.64748	1.66220	-0.71546
H	-6.15150	1.68098	1.28414
H	-7.01535	0.29669	0.64708

H	-7.66392	1.62839	-1.36538
H	-6.80243	3.01235	-0.72743
H	-9.24928	3.19077	-0.23275
H	-9.19209	1.65500	0.63330
H	-8.32957	3.05508	1.26650

3f

C	-5.72519	-0.94361	-0.09904
C	-4.59474	-0.03659	0.15013
O	-6.86544	-0.69058	0.18630
C	-3.35155	-0.38740	-0.19226
C	-2.18802	0.44989	0.02186
C	-0.95221	0.08535	-0.31892
C	0.19091	0.99538	-0.06640
O	1.34324	0.44123	-0.45916
O	0.10625	2.08808	0.42707
C	2.51978	1.23676	-0.25255
C	3.71802	0.42176	-0.68331
C	3.87972	-0.91825	0.03801
C	3.92547	-0.75037	1.55358
C	5.13737	-1.62117	-0.46232
H	-5.45731	-1.90483	-0.58059
H	-4.81782	0.91540	0.61926
H	-3.18672	-1.35597	-0.65921
H	-2.33259	1.42215	0.48328
H	-0.73762	-0.86985	-0.78194
H	2.56675	1.52072	0.79958
H	2.42682	2.15458	-0.83557
H	4.60960	1.03365	-0.50693
H	3.66199	0.24728	-1.76124
H	3.01442	-1.53829	-0.21291
H	4.72349	-0.05908	1.83975
H	2.98574	-0.36646	1.95257
H	4.12309	-1.70651	2.04042
H	6.02665	-1.03766	-0.20875
H	5.24546	-2.60714	-0.00795

H	5.11814	-1.74844	-1.54621
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3g

C	-5.95976	0.63722	-0.51049
C	-4.68184	0.48273	0.20088
O	-6.93312	1.15989	-0.03654
C	-3.63840	-0.10622	-0.39073
C	-2.34932	-0.29073	0.24530
C	-1.31120	-0.86817	-0.35887
C	-0.02074	-1.01416	0.35554
O	0.89819	-1.58901	-0.43054
O	0.17972	-0.67041	1.49007
C	2.21421	-1.74000	0.13436
C	3.01166	-0.47129	0.01254
C	3.63997	-0.15982	-1.18965
C	4.35916	1.01811	-1.32327
C	4.45798	1.89393	-0.25020
C	3.83704	1.58784	0.95253
C	3.11493	0.40992	1.08356
H	-5.97485	0.23136	-1.54130
H	-4.63014	0.86693	1.21367
H	-3.74623	-0.47285	-1.40907
H	-2.22489	0.06349	1.26410
H	-1.36397	-1.23883	-1.37480
H	2.66569	-2.54190	-0.44641
H	2.11818	-2.04683	1.17492
H	3.56411	-0.84745	-2.02449
H	4.84636	1.25075	-2.26134
H	5.02022	2.81339	-0.35127
H	3.91255	2.26903	1.79023
H	2.61243	0.17310	2.01277

3h

C	6.98934	-0.04461	-0.27758
C	5.62458	0.49139	-0.16148
O	7.96795	0.63738	-0.42665

C	4.58186	-0.32821	0.00276
C	3.21074	0.12469	0.12773
C	2.18047	-0.70437	0.29461
C	0.80425	-0.16967	0.42412
O	-0.07920	-1.16173	0.59167
O	0.51202	0.99650	0.39082
C	-1.45022	-0.77171	0.73596
C	-2.09287	-0.48661	-0.61514
C	-3.53362	-0.09438	-0.42698
C	-4.55373	-1.03326	-0.54468
C	-5.87688	-0.67498	-0.32608
C	-6.19533	0.63063	0.01827
C	-5.18461	1.57516	0.14110
C	-3.86406	1.21336	-0.07916
H	7.06655	-1.14803	-0.21726
H	5.51018	1.56856	-0.21440
H	4.75571	-1.40097	0.04900
H	3.01651	1.19215	0.08578
H	2.30407	-1.77898	0.34548
H	-1.50730	0.10653	1.37931
H	-1.93690	-1.61286	1.22693
H	-2.01748	-1.37844	-1.23987
H	-1.54103	0.31900	-1.10148
H	-4.30881	-2.05381	-0.81764
H	-6.65937	-1.41600	-0.42880
H	-7.22658	0.91243	0.18683
H	-5.42631	2.59692	0.40507
H	-3.07500	1.95192	0.01369

3i

C	5.75847	-0.67152	0.00000
C	4.55304	0.17364	0.00003
O	6.87869	-0.23697	0.00005
C	3.33465	-0.37479	-0.00002
C	2.10772	0.39655	-0.00000
C	0.89498	-0.15798	-0.00005

C	-0.30820	0.69884	-0.00003
O	-1.43134	-0.04777	-0.00007
O	-0.32418	1.89804	-0.00000
C	-2.63457	0.69337	-0.00007
C	-3.76620	-0.30636	0.00002
F	-4.93222	0.34660	-0.00001
F	-3.73638	-1.09196	-1.07619
F	-3.73635	-1.09179	1.07635
H	5.56800	-1.76267	-0.00007
H	4.70414	1.24757	0.00010
H	3.24081	-1.45822	-0.00009
H	2.18422	1.47970	0.00006
H	0.74364	-1.22981	-0.00010
H	-2.71048	1.32042	-0.88892
H	-2.71042	1.32051	0.88871

3j

C	-6.18353	0.33468	-0.30968
C	-4.90526	-0.24045	0.13406
O	-7.26009	-0.11157	-0.01407
C	-3.74474	0.31309	-0.23087
C	-2.44697	-0.19282	0.16992
C	-1.29832	0.38100	-0.18738
C	-0.00434	-0.18257	0.27009
O	1.01643	0.57053	-0.15163
O	0.11184	-1.17590	0.93809
C	2.34196	0.15516	0.23072
C	2.84432	-0.93425	-0.70317
C	4.28884	-1.29791	-0.36098
C	5.19221	-0.06747	-0.40225
C	4.66603	1.02705	0.52321
C	3.22191	1.38969	0.18140
H	-6.09556	1.23251	-0.95282
H	-4.95087	-1.12207	0.76392
H	-3.75772	1.19828	-0.86287
H	-2.41215	-1.08005	0.79478

H	-1.26424	1.26939	-0.80575
H	2.28927	-0.23538	1.25065
H	2.19335	-1.80636	-0.63143
H	2.78952	-0.55551	-1.72909
H	4.65071	-2.06262	-1.05004
H	4.32178	-1.73672	0.64178
H	5.23133	0.31622	-1.42727
H	6.21300	-0.33787	-0.12570
H	5.29537	1.91648	0.46457
H	4.71369	0.67451	1.55897
H	3.17153	1.81048	-0.82786
H	2.83279	2.14293	0.86870

3k

C	-7.31378	-1.07696	-0.00002
C	-6.24225	-0.06959	0.00001
O	-8.48646	-0.81173	-0.00010
C	-4.95908	-0.44247	0.00007
C	-3.84424	0.48381	0.00007
C	-2.57132	0.08943	0.00010
C	-1.47400	1.08721	0.00000
O	-0.28166	0.48327	0.00005
O	-1.62437	2.27949	-0.00001
C	0.86358	1.34593	-0.00009
C	2.11915	0.49717	-0.00003
C	2.18080	-0.39279	-1.25118
C	3.47460	-1.21342	-1.25294
C	3.51885	-2.09466	0.00054
C	3.47505	-1.21262	1.25348
C	2.18124	-0.39201	1.25165
C	3.33690	1.43498	-0.00053
C	4.63416	0.61896	-0.00052
C	4.67985	-0.26486	1.25119
C	4.67939	-0.26565	-1.25170
H	-6.96668	-2.12908	-0.00004
H	-6.54248	0.97255	-0.00002

H	-4.71954	-1.50367	0.00009
H	-4.05867	1.54826	0.00002
H	-2.29168	-0.95700	0.00013
H	0.81893	1.98713	0.88431
H	0.81885	1.98686	-0.88468
H	1.31200	-1.05570	-1.27063
H	2.13342	0.23581	-2.14724
H	3.50226	-1.84275	-2.14563
H	4.43109	-2.69833	0.00057
H	2.67088	-2.78601	0.00092
H	3.50304	-1.84138	2.14656
H	2.13417	0.23715	2.14734
H	1.31246	-1.05492	1.27182
H	3.30314	2.08371	0.88136
H	3.30281	2.08318	-0.88279
H	5.48845	1.29995	-0.00090
H	4.66836	0.35803	2.15047
H	5.60932	-0.84131	1.26584
H	5.60885	-0.84211	-1.26634
H	4.66756	0.35668	-2.15137

3l

C	7.01605	0.38504	-0.00033
C	5.71709	-0.30367	-0.00024
O	8.07715	-0.18040	-0.00046
C	4.57657	0.39299	-0.00011
C	3.25884	-0.21064	-0.00002
C	2.13110	0.49912	0.00005
C	0.81231	-0.18737	0.00010
O	-0.17425	0.71071	0.00005
O	0.67582	-1.38273	0.00025
C	-1.56718	0.30427	0.00007
C	-1.92027	-0.49155	-1.25661
C	-3.42989	-0.77465	-1.25341
C	-4.20733	0.54608	-1.25171
C	-3.84152	1.35068	-0.00011

C	-2.33471	1.62554	-0.00010
C	-1.92032	-0.49126	1.25691
C	-3.42994	-0.77434	1.25373
C	-4.20738	0.54639	1.25167
C	-3.78932	-1.58154	0.00025
H	6.95945	1.49164	-0.00026
H	5.73214	-1.38794	-0.00029
H	4.62319	1.47980	-0.00008
H	3.18948	-1.29418	-0.00003
H	2.12961	1.58194	0.00004
H	-1.35933	-1.42565	-1.27403
H	-1.64066	0.09287	-2.13807
H	-3.68302	-1.35072	-2.14599
H	-5.28267	0.34738	-1.26723
H	-3.96884	1.12245	-2.15027
H	-4.37972	2.30109	-0.00023
H	-2.04647	2.20254	-0.88286
H	-2.04652	2.20272	0.88255
H	-1.64074	0.09335	2.13825
H	-1.35941	-1.42536	1.27456
H	-3.68311	-1.35020	2.14644
H	-5.28273	0.34769	1.26720
H	-3.96893	1.12298	2.15011
H	-3.24786	-2.53140	0.00037
H	-4.85836	-1.81209	0.00025

3m

H	6.74196	1.72791	-0.08133
C	6.92394	0.64409	0.06035
O	8.04063	0.21376	0.17581
C	5.71347	-0.19008	0.09243
C	4.50438	0.36110	-0.04808
C	3.26342	-0.38775	-0.03375
C	2.07014	0.18171	-0.19909
C	0.83381	-0.63893	-0.19237
O	-0.23611	0.12309	-0.44048

O	0.79831	-1.82557	-0.00219
C	-2.43688	0.34767	-1.34064
C	-3.78958	-0.36301	-1.47272
C	-4.40166	-0.56932	-0.08234
C	-4.59556	0.79172	0.59698
C	-2.63152	1.70663	-0.65733
C	-3.24361	1.50149	0.73349
C	-1.51801	-0.53272	-0.49880
C	-2.09869	-0.72324	0.90369
C	-2.29670	0.63994	1.57731
C	-3.45302	-1.43066	0.75959
H	5.85129	-1.25678	0.23146
H	4.42967	1.43763	-0.18632
H	3.31111	-1.46262	0.11249
H	1.95599	1.24753	-0.35466
H	-1.98457	0.48332	-2.32590
H	-3.66242	-1.32766	-1.97271
H	-4.45665	0.24028	-2.09425
H	-5.36585	-1.07374	-0.17906
H	-5.04730	0.65447	1.58388
H	-5.28165	1.40731	0.00750
H	-3.28909	2.32928	-1.27042
H	-1.67351	2.22436	-0.57473
H	-3.38518	2.47099	1.21672
H	-1.37182	-1.50555	-0.97343
H	-1.41340	-1.34290	1.48537
H	-1.33493	1.14457	1.69674
H	-2.71275	0.49153	2.57772
H	-3.31746	-2.41008	0.29182
H	-3.87959	-1.60196	1.75161
3n			
C	-5.76743	0.46440	-0.49390
C	-4.47963	0.38826	0.21266
O	-6.77196	0.91552	-0.01158
C	-3.40257	-0.12842	-0.38645

C	-2.10283	-0.23702	0.24541
C	-1.03548	-0.75531	-0.36187
C	0.26182	-0.83226	0.34952
O	1.20036	-1.39244	-0.42673
O	0.45721	-0.45333	1.47346
C	2.51266	-1.48618	0.15615
C	3.25040	-0.20285	0.08183
C	3.37022	0.84765	0.92830
C	4.20817	1.79918	0.26832
C	4.52655	1.24786	-0.92556
O	3.95413	0.03281	-1.05578
H	-5.75848	0.06930	-1.52891
H	-4.44998	0.76592	1.22878
H	-3.49003	-0.49352	-1.40727
H	-1.99619	0.12338	1.26402
H	-1.07052	-1.13101	-1.37672
H	3.02263	-2.24927	-0.42716
H	2.41817	-1.80348	1.19266
H	2.89757	0.92904	1.89250
H	4.52895	2.75908	0.63464
H	5.12860	1.57829	-1.75392

3o

C	-5.35485	-0.65888	-0.18459
C	-4.15053	0.15350	0.04639
O	-6.47657	-0.25393	-0.03341
C	-2.93288	-0.36352	-0.14196
C	-1.70233	0.37393	0.06447
C	-0.49303	-0.15414	-0.12223
C	0.72126	0.66409	0.10847
O	1.83119	-0.04915	-0.11813
O	0.72482	1.81565	0.45200
C	3.06851	0.65565	0.07151
C	4.19280	-0.31976	-0.09790
C	4.16022	-1.52154	0.79778

C	5.16153	-0.08351	-0.97216
H	-5.16309	-1.69847	-0.51618
H	-4.29996	1.17702	0.37227
H	-2.84301	-1.39676	-0.46992
H	-1.77168	1.40828	0.38762
H	-0.35090	-1.17835	-0.44385
H	3.06523	1.08413	1.07760
H	3.12738	1.47385	-0.64642
H	4.12739	-1.21680	1.84716
H	3.26305	-2.11316	0.60801
H	5.03457	-2.15127	0.64407
H	6.00369	-0.75655	-1.07405
H	5.14771	0.79263	-1.60866

3p

C	6.00604	0.33644	-0.45711
C	4.66467	-0.24590	-0.30517
O	6.97361	-0.28777	-0.80369
C	3.63289	0.50784	0.08593
C	2.28349	0.00533	0.25791
C	1.26954	0.77836	0.64868
C	-0.11997	0.29697	0.82860
O	-0.25061	-1.01669	0.59828
O	-1.02341	1.01917	1.15501
C	-1.58619	-1.54496	0.68492
C	-2.35799	-1.25381	-0.56877
C	-3.43085	-0.51331	-0.57242
C	-4.48840	0.24548	-0.53971
C	-5.87120	-0.31773	-0.34822
C	-4.37807	1.73968	-0.69115
H	6.07707	1.41769	-0.22662
H	4.55821	-1.30285	-0.52361
H	3.79816	1.56308	0.29174
H	2.10673	-1.04527	0.05539
H	1.40340	1.83255	0.85891
H	-2.08877	-1.12043	1.55188

H	-1.43921	-2.61502	0.82378
H	-1.97272	-1.67272	-1.49387
H	-6.50516	-0.04975	-1.19691
H	-5.85585	-1.40091	-0.25054
H	-6.32825	0.11100	0.54681
H	-3.34051	2.05665	-0.76459
H	-4.92045	2.06894	-1.58099
H	-4.83314	2.23308	0.17079

3q

H	3.91710	-2.02141	0.00003
C	4.18531	-0.94758	0.00003
O	5.33526	-0.59579	0.00003
C	3.04043	-0.00778	0.00002
C	1.81528	-0.55688	0.00001
C	0.55589	0.15802	0.00000
C	-0.62819	-0.45664	-0.00000
C	-1.87778	0.33891	-0.00001
O	-2.95577	-0.45461	-0.00002
O	-1.93349	1.54024	-0.00001
C	-4.22147	0.22008	-0.00002
C	-5.30098	-0.83327	-0.00002
C	3.38345	1.44476	0.00001
H	1.74743	-1.64238	0.00002
H	0.55799	1.24206	0.00000
H	-0.72386	-1.53527	-0.00000
H	-4.27237	0.86232	-0.88043
H	-4.27237	0.86233	0.88038
H	-5.22462	-1.46472	0.88477
H	-5.22462	-1.46474	-0.88479
H	-6.28064	-0.35546	-0.00002
H	3.99533	1.67818	-0.87291
H	2.50573	2.08452	0.00001
H	3.99533	1.67819	0.87293

3r

C	4.17350	-0.28475	-0.00000
C	2.86243	0.42551	-0.00001
O	4.24146	-1.49003	0.00002
C	1.71192	-0.25093	0.00001
C	0.41102	0.38680	0.00001
C	-0.73709	-0.29102	0.00002
C	-2.02965	0.43312	0.00001
O	-3.06099	-0.42006	0.00002
O	-2.15348	1.62941	-0.00001
C	-4.36322	0.18028	-0.00000
C	-5.37903	-0.93488	-0.00002
C	5.40036	0.58944	-0.00003
H	2.86930	1.51057	-0.00003
H	1.75489	-1.33642	0.00003
H	0.36842	1.47204	-0.00001
H	-0.76966	-1.37318	0.00004
H	-4.45155	0.81858	-0.88049
H	-4.45158	0.81858	0.88049
H	-6.38552	-0.51663	-0.00005
H	-5.26440	-1.56069	-0.88469
H	-5.26444	-1.56069	0.88465
H	5.39037	1.23834	-0.87860
H	5.39039	1.23837	0.87852
H	6.29629	-0.02481	-0.00003

3s

C	7.05482	-0.42866	-0.09362
C	5.75559	0.13638	0.30310
O	8.11225	-0.03038	0.31654
C	4.61751	-0.35536	-0.19507
C	3.30318	0.15091	0.14618
C	2.17457	-0.34170	-0.36429
C	0.86861	0.23216	0.03367
O	-0.13089	-0.40832	-0.61830
O	0.71189	1.12618	0.81273
C	-1.45278	-0.03345	-0.40122

C	-2.33673	-1.07651	-0.11838
C	-3.65268	-0.72338	0.03476
C	-4.08216	0.58899	-0.08748
C	-3.21279	1.61041	-0.37171
C	-1.86321	1.27885	-0.53009
O	-5.44031	0.63377	0.07101
C	-5.79843	-0.64556	0.57324
O	-4.72530	-1.53190	0.27524
H	7.00110	-1.26796	-0.81469
H	5.77007	0.96051	1.00793
H	4.66319	-1.18295	-0.89940
H	3.23772	0.97354	0.85192
H	2.16617	-1.15962	-1.07357
H	-1.98956	-2.09586	-0.03454
H	-3.55690	2.62982	-0.47052
H	-1.13565	2.04906	-0.73676
H	-6.70272	-0.99160	0.07780
H	-5.92741	-0.58816	1.65945

7.4 Cartesian coordinates of the TS with the model catalyst

TS 3b

C	-1.76989	-0.79241	0.17039
C	-0.41417	-0.43678	-0.38820
C	0.69505	-0.74342	0.42912
C	1.99828	-0.81000	-0.03667
C	3.09534	-1.26246	0.73696
C	4.36288	-1.38237	0.24138
O	-2.64425	-1.01093	-0.81325
O	-1.99614	-0.85385	1.36216
C	-4.00375	-1.39507	-0.42222
C	-4.86331	-0.17125	-0.16242
O	4.66638	-1.03669	-1.00974

C	-0.23978	1.97533	1.10032
C	-0.75293	1.67932	-0.29066
C	0.22786	2.11114	-1.19210
C	1.43362	2.39037	-0.49614
C	1.20883	2.23907	0.85310
H	-0.31968	-0.50802	-1.46568
H	0.48793	-0.97704	1.47023
H	2.19408	-0.55548	-1.07635
H	2.93752	-1.56116	1.76800
H	5.16867	-1.76877	0.86214
H	-4.49590	0.39052	0.70023
H	-4.89260	0.48346	-1.03806
H	5.59664	-1.21398	-1.20934
H	-0.46939	1.22675	1.86197
H	-0.70761	2.91343	1.44394
H	-1.80750	1.66010	-0.54000
H	0.10005	2.17412	-2.26743
H	2.37307	2.66877	-0.95766
H	1.94462	2.37050	1.63804
H	-3.93599	-2.03708	0.45777
H	-4.36266	-1.97405	-1.27399
H	-5.88735	-0.48918	0.05579

TS 3c

C	-2.12163	-0.81191	0.13125
C	-0.76431	-0.44415	-0.41079
C	0.33790	-0.74623	0.41812
C	1.64663	-0.80250	-0.03359
C	2.73798	-1.25057	0.75025
C	4.01156	-1.36115	0.26761
O	-2.99365	-1.01228	-0.86062
O	-2.36636	-0.89369	1.31695
C	-4.33153	-1.40019	-0.45664
O	4.32591	-1.00971	-0.97895
C	-0.62979	1.96226	1.08784
C	-1.12063	1.66672	-0.31147

C	-0.13057	2.11109	-1.19730
C	1.06277	2.39648	-0.48343
C	0.82013	2.23738	0.86213
H	-0.65738	-0.51208	-1.48735
H	0.12089	-0.98584	1.45584
H	1.85199	-0.54288	-1.07017
H	2.57115	-1.55374	1.77856
H	4.81305	-1.74471	0.89566
H	5.25934	-1.18037	-1.16955
H	-0.86436	1.21055	1.84488
H	-1.10936	2.89614	1.42675
H	-2.17130	1.64279	-0.57667
H	-0.24421	2.17857	-2.27394
H	2.00633	2.68464	-0.93031
H	1.54385	2.37079	1.65789
H	-4.29720	-2.34813	0.08289
H	-4.89334	-1.50093	-1.38291
H	-4.76769	-0.63277	0.18545

TS 3d

C	1.31324	-0.29474	-0.35822
C	-0.05725	-0.19531	0.27732
C	-1.14647	-0.62300	-0.50989
C	-2.39712	-0.92298	0.00679
C	-3.45209	-1.49410	-0.74795
C	-4.65726	-1.84364	-0.20795
O	2.24304	-0.42828	0.58066
O	1.46544	-0.24169	-1.56371
C	3.69901	-0.59300	0.24648
C	4.19482	0.66389	-0.47000
C	3.88268	-1.86235	-0.58631
C	4.33293	-0.73537	1.62900
O	-4.94449	-1.62894	1.07737
C	-0.70597	2.25190	-1.04220
C	-0.06046	1.96559	0.29512
C	-1.03440	2.17494	1.27709

C	-2.31466	2.29447	0.67031
C	-2.15968	2.26397	-0.69586
H	-0.08837	-0.33525	1.35201
H	-0.96213	-0.75724	-1.57303
H	-2.57260	-0.76891	1.06990
H	-3.30542	-1.69860	-1.80393
H	-5.42709	-2.31295	-0.81755
H	4.01148	1.55622	0.13915
H	5.27625	0.58464	-0.62298
H	3.71983	0.78635	-1.44523
H	3.42311	-1.76994	-1.57203
H	4.95334	-2.04789	-0.72135
H	3.45468	-2.72765	-0.06941
H	4.14550	0.15372	2.23936
H	3.93467	-1.60935	2.15342
H	5.41537	-0.85925	1.52669
H	-5.82760	-1.96525	1.30109
H	-0.41386	1.59060	-1.86192
H	-0.41359	3.26982	-1.35349
H	0.99960	2.09668	0.48057
H	-0.84783	2.19351	2.34610
H	-3.25363	2.38759	1.20353
H	-2.95764	2.32279	-1.42779

TS 3e

H	-7.07419	-1.72730	-1.94451
C	-7.39177	-1.17913	-1.06060
C	-6.50484	-0.47777	-0.29041
O	-8.69402	-1.29087	-0.86650
C	-5.13540	-0.42025	-0.63811
C	-4.17938	0.32124	0.03724
C	-2.85441	0.49267	-0.42084
C	-2.09920	1.66176	0.16514
O	-1.18333	2.10824	-0.69412
C	-0.38156	3.26593	-0.27970
O	-2.32704	2.10156	1.27427

C	0.89003	2.83484	0.43811
C	1.84754	1.99220	-0.41400
C	3.12428	1.59115	0.33547
C	4.08648	0.74460	-0.50666
C	5.36550	0.34738	0.24094
C	6.32784	-0.50027	-0.59989
C	7.60889	-0.89365	0.14580
C	8.57266	-1.74006	-0.69483
C	9.85039	-2.12553	0.05629
C	-2.33697	-1.15755	1.82133
C	-3.31980	-2.23314	1.49724
C	-3.00421	-2.80674	0.28693
C	-1.92660	-2.08504	-0.29119
C	-1.61610	-0.97454	0.50449
H	-6.85550	0.06596	0.58480
H	-4.82770	-0.95956	-1.53392
H	-4.46002	0.85693	0.94010
H	-2.61208	0.25260	-1.44999
H	-1.00562	3.90036	0.35170
H	-0.16352	3.77689	-1.21956
H	0.61788	2.30320	1.35872
H	1.39512	3.75477	0.76083
H	2.11621	2.55545	-1.31823
H	1.33079	1.08886	-0.76713
H	2.85386	1.03814	1.24669
H	3.64150	2.49814	0.67719
H	4.35500	1.29931	-1.41652
H	3.56862	-0.16351	-0.84872
H	5.09682	-0.20456	1.15311
H	5.88276	1.25592	0.57941
H	6.59431	0.05210	-1.51210
H	5.81067	-1.40996	-0.93781
H	7.34364	-1.44612	1.05875
H	8.12593	0.01586	0.48312
H	8.83671	-1.18760	-1.60675
H	8.05620	-2.64962	-1.03086

H	10.51780	-2.72435	-0.57128
H	10.40493	-1.23646	0.37679
H	9.62243	-2.71264	0.95315
H	-1.61417	-1.55955	2.55135
H	-2.74622	-0.24984	2.27053
H	-4.10906	-2.55620	2.16630
H	-3.49348	-3.66502	-0.15721
H	-1.44777	-2.32842	-1.23364
H	-0.67641	-0.44129	0.41667
H	-8.99047	-0.79248	-0.08685

TS 3f

C	-0.73913	-0.46036	-0.87180
C	0.45706	-0.07364	-0.03719
C	1.58071	0.40570	-0.74451
C	2.61444	1.11566	-0.15620
C	3.66791	1.72858	-0.87844
C	4.64346	2.48058	-0.28765
O	-1.86447	-0.36768	-0.16464
O	-0.64853	-0.81948	-2.02849
C	-3.10825	-0.69884	-0.86871
O	4.69531	2.65731	1.03283
C	1.79602	-2.53324	-0.51948
C	0.86521	-2.08535	0.58481
C	1.65698	-1.82301	1.70952
C	3.02711	-1.78762	1.33790
C	3.13177	-2.12430	0.00783
H	0.23306	0.32758	0.94464
H	1.59339	0.23395	-1.81768
H	2.59677	1.26691	0.92134
H	3.70412	1.63240	-1.95853
H	5.41374	2.96238	-0.88637
H	5.42690	3.23956	1.28249
H	1.54792	-2.18233	-1.52372
H	1.76515	-3.63496	-0.56575
H	-0.16445	-2.41498	0.66023

H	1.27629	-1.62687	2.70611
H	3.84814	-1.53052	1.99583
H	4.05062	-2.16974	-0.56529
H	-3.16739	-0.06614	-1.75723
C	-4.26200	-0.48734	0.09493
H	-3.03633	-1.73850	-1.20076
C	-4.48173	0.96223	0.57488
H	-5.16839	-0.84598	-0.41160
H	-4.11508	-1.14387	0.96157
C	-5.55780	0.99224	1.66971
H	-3.53887	1.31163	1.01837
C	-4.85058	1.91051	-0.57580
H	-4.07127	1.96405	-1.34328
H	-5.77928	1.59194	-1.06378
H	-5.00697	2.92730	-0.20265
H	-5.29137	0.34767	2.51426
H	-5.69868	2.00692	2.05463
H	-6.52376	0.64947	1.28068

TS 3g

C	-0.34599	-1.29863	0.11642
C	0.92617	-0.69048	-0.41859
C	2.06561	-0.78268	0.41129
C	3.36063	-0.59232	-0.03886
C	4.51721	-0.82443	0.74694
C	5.78873	-0.69425	0.26619
O	-1.18056	-1.59647	-0.88000
O	-0.55275	-1.45443	1.30339
O	6.03393	-0.29317	-0.98205
C	0.59052	1.68881	1.09272
C	0.16340	1.30113	-0.30550
C	1.04495	1.93315	-1.19271
C	2.15857	2.45249	-0.48155
C	1.95485	2.25033	0.86417
H	1.04561	-0.73175	-1.49525
H	1.89489	-1.06127	1.44786

H	3.51525	-0.30044	-1.07576
H	4.40898	-1.15076	1.77598
H	6.64735	-0.91767	0.89605
H	6.98321	-0.28605	-1.16969
H	0.51498	0.90439	1.84915
H	-0.06815	2.50480	1.43488
H	-0.86446	1.07226	-0.56500
H	0.91834	1.97554	-2.26920
H	3.02493	2.92242	-0.93061
H	2.63895	2.52682	1.65819
C	-2.52340	-2.07784	-0.50211
H	-2.41939	-2.72962	0.36568
H	-2.83113	-2.65951	-1.37130
C	-5.15803	1.24587	0.24310
C	-4.58171	0.56014	1.31385
C	-3.72630	-0.51634	1.07626
C	-3.44709	-0.92061	-0.23662
C	-4.03088	-0.22660	-1.30677
C	-4.88059	0.85272	-1.06857
H	-5.82942	2.07858	0.42929
H	-4.80427	0.85788	2.33396
H	-3.27425	-1.04989	1.90669
H	-3.82953	-0.54317	-2.32711
H	-5.33682	1.37721	-1.90247

TS 3h

C	-0.22574	-1.59227	0.30910
C	0.95869	-0.89903	-0.31188
C	2.13591	-0.85821	0.46278
C	3.38463	-0.54795	-0.05105
C	4.59227	-0.64557	0.68396
C	5.82116	-0.39550	0.14333
O	-1.05317	-2.05094	-0.63517
O	-0.37243	-1.69007	1.51050
O	5.96813	0.00470	-1.12061
C	0.48760	1.51142	1.14519

C	0.03035	1.06204	-0.22256
C	0.83265	1.71939	-1.16125
C	1.93324	2.33900	-0.51027
C	1.79635	2.16502	0.84773
H	1.02583	-0.95693	-1.39193
H	2.04150	-1.12125	1.51306
H	3.46170	-0.26544	-1.09896
H	4.56371	-0.96010	1.72197
H	6.72533	-0.51777	0.73613
H	6.90238	0.10518	-1.35177
H	0.49943	0.74143	1.92020
H	-0.22031	2.28141	1.49519
H	-0.98497	0.74525	-0.43282
H	0.66238	1.71968	-2.23251
H	2.74509	2.85620	-1.00692
H	2.48806	2.51539	1.60514
C	-2.28999	-2.69636	-0.20417
H	-2.30278	-2.72067	0.88560
H	-2.24468	-3.71844	-0.58739
C	-3.48106	-1.94210	-0.79002
H	-4.38289	-2.47892	-0.46715
H	-3.45125	-2.01543	-1.88174
C	-3.73089	2.22878	0.36521
C	-3.65971	1.87332	-0.98258
C	-3.57220	0.52718	-1.34760
C	-3.56042	-0.48401	-0.37708
C	-3.63573	-0.11313	0.97430
C	-3.71914	1.23013	1.34271
H	-3.81276	3.27298	0.65168
H	-3.68390	2.64018	-1.75127
H	-3.52835	0.25668	-2.39958
H	-3.64009	-0.87744	1.74684
H	-3.79143	1.49559	2.39334

TS 3i

C	-0.84609	-0.98531	0.37551
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C	0.43920	-0.53189	-0.25716
C	1.62246	-0.79219	0.47095
C	2.88934	-0.77270	-0.08901
C	4.06436	-1.17260	0.59410
C	5.29681	-1.21083	0.00539
O	-1.78736	-1.18891	-0.57142
O	-0.99969	-1.12558	1.56703
O	5.48677	-0.82856	-1.25704
C	0.60505	1.83990	1.28150
C	-0.03439	1.53243	-0.05406
C	0.81752	2.05073	-1.04261
C	2.06937	2.39202	-0.47159
C	2.00095	2.19521	0.89029
H	0.46089	-0.57570	-1.33999
H	1.50768	-1.06079	1.51789
H	2.99387	-0.49144	-1.13500
H	4.00040	-1.49569	1.62787
H	6.16671	-1.55931	0.55836
H	6.40815	-0.94844	-1.52812
H	0.50131	1.07314	2.05181
H	0.12000	2.74456	1.68586
H	-1.10863	1.46382	-0.18321
H	0.56958	2.13011	-2.09570
H	2.93432	2.74263	-1.02114
H	2.80768	2.35734	1.59587
C	-3.12123	-1.46703	-0.11471
C	-3.94946	-0.19857	-0.25518
F	-4.05696	0.18615	-1.53655
F	-5.17590	-0.39708	0.24188
H	-3.11428	-1.78778	0.92726
H	-3.53240	-2.24387	-0.75951
F	-3.37119	0.82434	0.42674

TS 3j

C	-0.57758	-0.29590	0.48058
C	0.76709	-0.27105	-0.20690

C	1.88236	-0.60050	0.59303
C	3.11947	-0.95360	0.08011
C	4.19835	-1.43035	0.86528
C	5.39170	-1.83046	0.33468
O	-1.55166	-0.52904	-0.39617
O	-0.70309	-0.11073	1.67549
O	5.64168	-1.75905	-0.97328
C	1.39384	2.31107	0.79946
C	0.74828	1.85635	-0.49003
C	1.71529	1.96630	-1.49618
C	2.99410	2.17893	-0.91578
C	2.84433	2.30731	0.44579
H	0.76233	-0.54388	-1.25606
H	1.72694	-0.61086	1.66875
H	3.26676	-0.91978	-0.99763
H	4.08194	-1.51609	1.94057
H	6.18064	-2.22334	0.97272
H	6.51805	-2.11097	-1.18441
H	1.11549	1.74889	1.69403
H	1.08593	3.35359	0.98701
H	-0.31331	1.95252	-0.68630
H	1.52356	1.85595	-2.55809
H	3.92918	2.22490	-1.46040
H	3.64389	2.46363	1.16070
H	-2.88110	-1.00875	1.12637
C	-5.18779	-1.57952	-0.40868
C	-3.70425	-1.52351	-0.81571
C	-2.93581	-0.59369	0.11578
C	-3.52948	0.81321	0.16051
C	-5.01384	0.75586	0.56646
C	-5.81260	-0.17750	-0.35495
H	-5.27623	-2.05712	0.57654
H	-5.73303	-2.21756	-1.11158
H	-3.61326	-1.14716	-1.84281
H	-3.25591	-2.52259	-0.79618
H	-2.96249	1.43312	0.86340

H	-3.43718	1.26282	-0.83739
H	-5.09196	0.40276	1.60346
H	-5.43426	1.76679	0.55115
H	-5.84059	0.24738	-1.36771
H	-6.85163	-0.24151	-0.01502

TS 3k

C	-0.52470	-0.95308	-0.42212
C	-1.75382	-0.37358	0.23526
C	-2.58083	0.42729	-0.58143
C	-3.53432	1.30054	-0.08457
C	-4.26292	2.21909	-0.88026
C	-5.15119	3.11837	-0.36257
O	0.43061	-1.16450	0.48335
O	-0.47198	-1.19351	-1.61150
O	-5.42849	3.16569	0.94096
C	-3.46692	-2.38084	-0.82195
C	-2.70632	-2.28412	0.48113
C	-3.63288	-1.94990	1.47574
C	-4.85766	-1.54850	0.87907
C	-4.76080	-1.71770	-0.48287
H	-1.65325	-0.13602	1.28808
H	-2.41489	0.37092	-1.65410
H	-3.70235	1.33219	0.99010
H	-4.10062	2.24608	-1.95270
H	-5.66244	3.83003	-1.00761
H	-6.05182	3.87773	1.14326
H	-3.66625	-3.44702	-1.02303
H	-2.94754	-2.00043	-1.70456
H	-1.80872	-2.85595	0.68568
H	-3.42930	-1.94994	2.54115
H	-5.71925	-1.16725	1.41327
H	-5.53187	-1.48436	-1.20802
C	1.72475	-1.68160	0.02289
H	4.01767	-1.68764	-1.40593
C	5.45964	0.31120	1.04845

C	5.28355	-0.24117	-0.38072
C	4.13658	-1.27332	-0.39576
C	2.81172	-0.60614	0.05983
C	3.00647	-0.04383	1.48914
C	4.15162	0.99053	1.50282
H	6.28623	1.03177	1.07250
H	5.72510	-0.49988	1.73867
H	2.07431	0.41900	1.83649
H	3.23252	-0.86573	2.18243
C	3.81073	2.14677	0.54061
H	4.27160	1.37986	2.52101
H	2.89194	2.65217	0.86700
H	4.60976	2.89793	0.55901
C	3.63598	1.59537	-0.88935
H	3.38874	2.41486	-1.57506
C	2.48939	0.56247	-0.90242
H	2.33348	0.17745	-1.91830
H	1.55370	1.04977	-0.59721
C	4.94360	0.91455	-1.34302
H	5.76204	1.64461	-1.35643
H	4.83792	0.53602	-2.36781
H	6.20862	-0.73233	-0.70467
H	4.37897	-2.11359	0.26896
H	1.59075	-2.08460	-0.98296
H	1.95390	-2.49158	0.72072

TS 3I

C	0.13095	-0.10537	-0.33367
C	1.50703	-0.11379	0.29888
C	2.55592	-0.62609	-0.49458
C	3.78195	-1.01994	0.01450
C	4.78693	-1.67077	-0.74404
C	5.96551	-2.10536	-0.20859
O	-0.80392	-0.17653	0.60594
O	-0.01712	-0.02880	-1.53882
O	6.27354	-1.90727	1.07421

C	2.30410	2.27371	-1.02659
C	1.67264	2.02836	0.32489
C	2.68253	2.16743	1.28342
C	3.95201	2.20204	0.64625
C	3.76183	2.18709	-0.71591
H	1.52934	-0.26134	1.37251
H	2.35365	-0.74647	-1.55565
H	3.97664	-0.87625	1.07548
H	4.62017	-1.86761	-1.79789
H	6.69473	-2.63176	-0.82096
H	7.12767	-2.30395	1.29643
H	2.07468	3.30941	-1.32908
H	1.94650	1.63653	-1.83880
H	0.63020	2.23477	0.53707
H	2.52303	2.19501	2.35596
H	4.90762	2.22882	1.15532
H	4.54380	2.19209	-1.46642
C	-2.69697	1.08334	-0.41892
C	-2.26047	-0.21421	0.27668
C	-4.47090	-0.37658	1.44959
C	-4.93166	0.91659	0.74579
C	-4.23128	1.03475	-0.62267
H	-2.18890	1.18595	-1.38152
H	-2.42487	1.94340	0.20665
H	-6.01956	0.90249	0.61031
H	-4.70044	1.79084	1.36773
C	-4.58861	-0.18689	-1.49536
H	-4.54697	1.95595	-1.12547
H	-5.67075	-0.21680	-1.66896
H	-4.11013	-0.10348	-2.47911
C	-4.13333	-1.48056	-0.78793
H	-4.38011	-2.34922	-1.40873
C	-4.83510	-1.59780	0.58017
H	-4.53378	-2.52525	1.08320
H	-5.92152	-1.64892	0.44195
H	-4.95222	-0.45908	2.43058

C	-2.59950	-1.43945	-0.58423
H	-2.08879	-1.37786	-1.54852
H	-2.25528	-2.34851	-0.07595
C	-2.93919	-0.33088	1.64724
H	-2.58620	-1.23699	2.15320
H	-2.65480	0.52535	2.27059

TS 3m

C	-0.15379	0.22494	-0.67305
C	-1.44057	0.01495	0.09033
C	-2.52404	-0.51107	-0.64718
C	-3.65009	-1.07066	-0.06737
C	-4.67196	-1.73201	-0.79346
C	-5.74580	-2.33108	-0.19948
O	0.89257	0.20088	0.14885
O	-0.13243	0.41160	-1.87407
O	-5.93137	-2.29789	1.12104
C	-2.58026	2.43711	-0.85544
C	-1.78586	2.10665	0.38825
C	-2.69419	2.04480	1.45229
C	-4.02299	2.02242	0.95228
C	-3.98197	2.17233	-0.41485
H	-1.32698	-0.25093	1.13515
H	-2.42964	-0.50019	-1.72988
H	-3.74029	-1.05674	1.01690
H	-4.60225	-1.80108	-1.87399
H	-6.48859	-2.85842	-0.79449
H	-6.71971	-2.79647	1.37858
H	-2.26149	1.93384	-1.77124
H	-2.47670	3.51794	-1.05007
H	-0.74930	2.39338	0.52202
H	-2.42122	1.97352	2.49965
H	-4.91623	1.90080	1.55260
H	-4.83884	2.18025	-1.07858
H	2.10350	1.07047	-1.29072
C	2.98948	-1.91348	0.27238

C	2.81090	-0.95001	-0.91990
C	2.23436	0.39267	-0.44270
C	3.12758	1.01525	0.63706
C	3.30602	0.04024	1.82093
C	3.92995	-1.27882	1.31854
H	3.40454	-2.86184	-0.08936
H	2.01800	-2.14423	0.72583
H	3.95188	0.50401	2.57606
H	2.34070	-0.15443	2.30268
C	5.30179	-0.98987	0.67361
H	4.05611	-1.96738	2.16232
H	5.98318	-0.55633	1.41620
H	5.76099	-1.92518	0.32991
C	5.12470	-0.02000	-0.51354
H	6.09818	0.18762	-0.97239
C	4.50248	1.29995	-0.01168
H	4.39347	2.00943	-0.84195
H	5.15772	1.77527	0.72756
H	2.67502	1.95395	0.98084
C	4.18701	-0.65527	-1.56128
H	4.61484	-1.59031	-1.94119
H	4.06928	0.01294	-2.42384
H	2.13727	-1.38098	-1.66939

TS 3n

C	-0.61187	-1.17602	0.13883
C	0.68376	-0.62776	-0.40267
C	1.82398	-0.78277	0.41644
C	3.12322	-0.66054	-0.04573
C	4.27330	-0.95361	0.72886
C	5.54523	-0.88908	0.23562
O	-1.46071	-1.44543	-0.85520
O	-0.82566	-1.31855	1.32595
O	5.79836	-0.49970	-1.01450
C	0.49409	1.76366	1.11899
C	0.02560	1.40180	-0.27268

C	0.92507	1.98708	-1.17342
C	2.07610	2.44449	-0.47909
C	1.88310	2.25152	0.86937
H	0.79142	-0.66909	-1.48054
H	1.64873	-1.05419	1.45421
H	3.28341	-0.37637	-1.08395
H	4.15832	-1.27484	1.75876
H	6.39727	-1.15749	0.85680
H	6.74474	-0.54166	-1.21208
H	0.38859	0.98274	1.87542
H	-0.11403	2.61337	1.47230
H	-1.01615	1.22542	-0.51621
H	0.78394	2.03742	-2.24773
H	2.95924	2.86800	-0.94145
H	2.59310	2.49017	1.65281
C	-2.81122	-1.89743	-0.45726
H	-2.70839	-2.57976	0.38597
H	-3.16775	-2.42781	-1.33988
C	-3.68999	-0.76140	-0.10909
C	-4.07284	-0.20058	1.07765
C	-4.94931	0.88155	0.75243
C	-5.03120	0.90401	-0.60805
O	-4.27022	-0.08368	-1.15188
H	-3.76882	-0.53126	2.06021
H	-5.45889	1.54266	1.43787
H	-5.57113	1.52200	-1.30869

TS 3o

C	-1.14470	-0.94191	-0.34787
C	0.15591	-0.51053	0.28217
C	1.32822	-0.76037	-0.46533
C	2.60149	-0.75909	0.07870
C	3.76648	-1.15191	-0.62639
C	5.00536	-1.20822	-0.05434
O	-2.05137	-1.21977	0.59183
O	-1.30447	-0.99858	-1.55012

O	5.21369	-0.85228	1.21382
C	0.29593	1.88950	-1.22438
C	-0.31094	1.56565	0.12181
C	0.56326	2.06523	1.09681
C	1.80189	2.41819	0.49976
C	1.69948	2.24678	-0.86195
H	0.19287	-0.57174	1.36389
H	1.19726	-1.00626	-1.51597
H	2.72088	-0.49727	1.12823
H	3.68767	-1.45454	-1.66532
H	5.86661	-1.54997	-0.62474
H	6.13785	-0.98277	1.46951
H	-0.20182	2.79433	-1.61220
H	0.17574	1.12550	-1.99531
H	-1.38138	1.48551	0.27667
H	0.34370	2.12457	2.15744
H	2.68039	2.75807	1.03437
H	2.48781	2.42265	-1.58475
C	-3.41075	-1.55351	0.12585
H	-3.73860	-2.32935	0.82107
H	-3.33790	-1.95768	-0.88293
C	-4.28211	-0.32577	0.18985
C	-4.66430	0.27818	-0.94089
H	-4.36390	-0.09460	-1.91546
C	-4.68289	0.14365	1.56518
H	-5.30510	1.15515	-0.92683
H	-3.80513	0.30735	2.20162
H	-5.25599	1.07248	1.52232
H	-5.29783	-0.61156	2.07028

TS 3p

C	0.25407	-1.18579	0.25515
C	-0.97531	-0.54503	-0.34119
C	-2.20443	-0.84132	0.28879
C	-3.43956	-0.63349	-0.30082
C	-4.66944	-1.06120	0.25892

C	-5.87266	-0.90346	-0.36744
O	1.22829	-1.26979	-0.64790
O	0.31317	-1.54021	1.41633
O	-5.97912	-0.29000	-1.54705
C	-1.00738	1.52696	1.59678
C	-0.38007	1.42589	0.22407
C	-1.18490	2.16797	-0.65009
C	-2.41459	2.49205	-0.01838
C	-2.36882	2.05455	1.28519
H	-0.94864	-0.39326	-1.41424
H	-2.15195	-1.29756	1.27392
H	-3.47792	-0.16284	-1.28129
H	-4.67431	-1.56664	1.21893
H	-6.78866	-1.27898	0.08399
H	-6.89336	-0.29226	-1.86411
H	-0.45974	2.29660	2.16645
H	-0.97145	0.61961	2.20410
H	0.68513	1.29313	0.06996
H	-0.92697	2.41371	-1.67465
H	-3.24923	2.99375	-0.49242
H	-3.16604	2.14568	2.01388
C	2.51341	-1.83226	-0.18215
C	3.30689	-0.82391	0.59799
H	3.01633	-2.11739	-1.10446
H	2.28136	-2.71587	0.41641
C	4.38747	-0.24700	0.12289
C	5.48132	0.30569	-0.34031
H	2.96357	-0.61208	1.60997
C	6.83788	-0.33719	-0.13984
C	5.45266	1.61746	-1.09558
H	6.06680	2.36547	-0.58050
H	5.87710	1.48904	-2.09833
H	4.43921	2.01120	-1.19626
H	6.76877	-1.27349	0.41652
H	7.30962	-0.54050	-1.10851
H	7.50230	0.34323	0.40562

TS 3q

H	3.85274	-0.66119	-1.96606
C	4.00530	-0.99076	-0.94168
C	2.98010	-0.95852	-0.02440
C	1.72802	-0.50578	-0.52028
C	0.53841	-0.46173	0.18966
C	-0.70783	-0.15262	-0.40412
C	-1.92962	-0.60698	0.35787
O	5.24842	-1.39808	-0.75452
C	-4.20671	-1.26388	0.15128
H	1.69622	-0.21562	-1.57010
H	0.51999	-0.73769	1.23898
H	-0.80118	-0.18414	-1.48415
H	-4.50460	-0.53101	0.90626
H	-3.99628	-2.20741	0.66143
C	0.95121	2.51973	0.77218
C	0.98959	2.76071	-0.58259
C	-0.27982	2.45111	-1.13508
C	-1.10928	1.90060	-0.14667
C	-0.43633	2.15644	1.18456
H	1.77495	2.65448	1.46382
H	1.84387	3.12514	-1.13995
H	-0.55238	2.57296	-2.17795
H	-2.18639	1.85129	-0.26041
H	-0.90541	3.04647	1.63699
H	-0.52487	1.35807	1.92469
H	5.39612	-1.71626	0.15105
C	3.13976	-1.40329	1.40885
H	2.56113	-2.31027	1.61147
H	4.17818	-1.61635	1.67999
H	2.79396	-0.62745	2.09918
O	-1.94204	-0.75472	1.56333
O	-2.96145	-0.79842	-0.46443
C	-5.23117	-1.41509	-0.95226
H	-6.17475	-1.76383	-0.52312

H	-5.41661	-0.46172	-1.45426
H	-4.90389	-2.14536	-1.69679

TS 3r

C	-2.03264	-0.84997	0.15003
C	-0.75131	-0.30404	-0.43316
C	0.41983	-0.55056	0.32216
C	1.70192	-0.49945	-0.20443
C	2.86228	-0.90558	0.49018
C	4.11843	-0.90414	-0.07106
O	-2.90885	-1.13253	-0.81644
O	-2.20927	-0.99135	1.34333
O	4.26217	-0.45113	-1.32396
C	-0.78031	1.98495	1.18009
C	-1.29009	1.70442	-0.21783
C	-0.38793	2.31018	-1.10787
C	0.79817	2.66902	-0.42078
C	0.62848	2.40382	0.92019
H	-0.69349	-0.33061	-1.51562
H	0.28122	-0.85283	1.35685
H	1.82750	-0.17928	-1.23686
H	2.77136	-1.26749	1.50844
C	5.34507	-1.38341	0.63472
H	5.18022	-0.53045	-1.62238
H	-0.91911	1.18313	1.90809
H	-1.33084	2.85661	1.57248
H	-2.34570	1.60791	-0.44668
H	-0.55172	2.42863	-2.17355
H	1.69134	3.07351	-0.88093
H	1.36999	2.55628	1.69588
C	-4.19548	-1.69883	-0.40378
H	-4.02048	-2.35629	0.44956
H	-4.50579	-2.28995	-1.26642
C	-5.19426	-0.60383	-0.07587
H	-6.16284	-1.05656	0.15722
H	-5.33285	0.07109	-0.92524

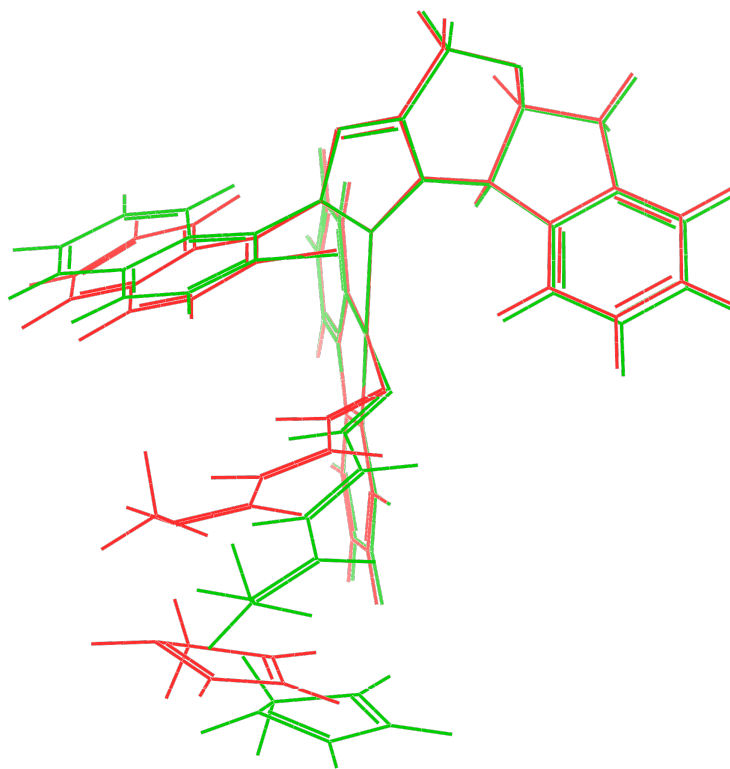
H	-4.87443	-0.02883	0.79707
H	5.12033	-1.72187	1.64603
H	5.79858	-2.21745	0.08426
H	6.09124	-0.58111	0.69285

TS 3s

C	0.09904	-0.11013	-0.25880
C	1.48845	-0.09214	0.31526
C	2.50633	-0.63006	-0.51549
C	3.73871	-1.04352	-0.04830
C	4.70493	-1.71891	-0.83852
C	5.89395	-2.17023	-0.34472
O	-0.79384	-0.15231	0.74309
O	-0.12619	-0.06275	-1.45067
O	6.25313	-1.96956	0.92600
C	2.22024	2.25492	-1.05507
C	1.66331	1.99509	0.32938
C	2.72650	2.16370	1.23213
C	3.95627	2.20385	0.52825
C	3.69220	2.17701	-0.82285
H	1.54710	-0.25405	1.38555
H	2.26241	-0.76048	-1.56646
H	3.97615	-0.89440	1.00328
H	4.49530	-1.92021	-1.88389
H	7.10763	-2.38057	1.11786
H	1.96824	3.29203	-1.33360
H	1.82641	1.62320	-1.85448
H	0.63960	2.23016	0.59867
H	2.62447	2.20196	2.31135
H	4.93830	2.24207	0.98343
H	4.43277	2.17728	-1.61431
H	6.59113	-2.71271	-0.97978
C	-2.86390	-0.19258	-0.63744
C	-2.19026	-0.20366	0.59929
C	-2.85579	-0.26964	1.82415
C	-4.25561	-0.32254	1.87454

H	-2.34886	-0.14628	-1.58357
H	-2.27194	-0.28142	2.73707
H	-4.78790	-0.37283	2.81653
C	-4.92487	-0.31019	0.66495
C	-4.24086	-0.24790	-0.55135
O	-5.13431	-0.24774	-1.58303
C	-6.43974	-0.32881	-0.98760
O	-6.26837	-0.35123	0.43912
H	-7.02562	0.55182	-1.27023
H	-6.93202	-1.25241	-1.31030

Functional dependence on geometry optimization



M06/lanl2dz-6-31G(d) (red) and B3LYP/lanl2dz-6-31G(d) (green) optimized geometry comparison shows that the largest difference is position of the aldehyde relative to the catalyst aromatic substituent. This suggests that the B3LYP method does not capture the important π - π stereocontrolling interaction in the lowest energy TS leading to a reduction in the predicted enantioselectivity with this method.

8. Parameters Collected

The parameters calculated and considered for the systems are reported in Tables S2-S11. Sterimol parameters L, B1 and B5, respectively, represent the length, minimum and maximum widths of the considered substituent and are calculated using the Bondi radii.^{24, 25} IR stretching frequencies, intensities, NBO charges have been found to be useful descriptors of electronic and steric properties, hence these have been calculated.²⁶ Interaction energies have been calculated using the equation $E_{int} = E_{SC} - E_{Cat} - E_{Sub}$. E_{SC} is the energy of the ground state substrate-catalyst complex and this can be dissected into two parts, the catalyst contribution, E_{Cat} and the substrate, E_{Sub} . The difference between these represents, E_{int} , which is the interaction energy calculated upon complex formation, since the energy to distort the aromatic group and substrate in these isolated forms is both small and consistent as shown below. The parameters are defined as shown in Figure S3.

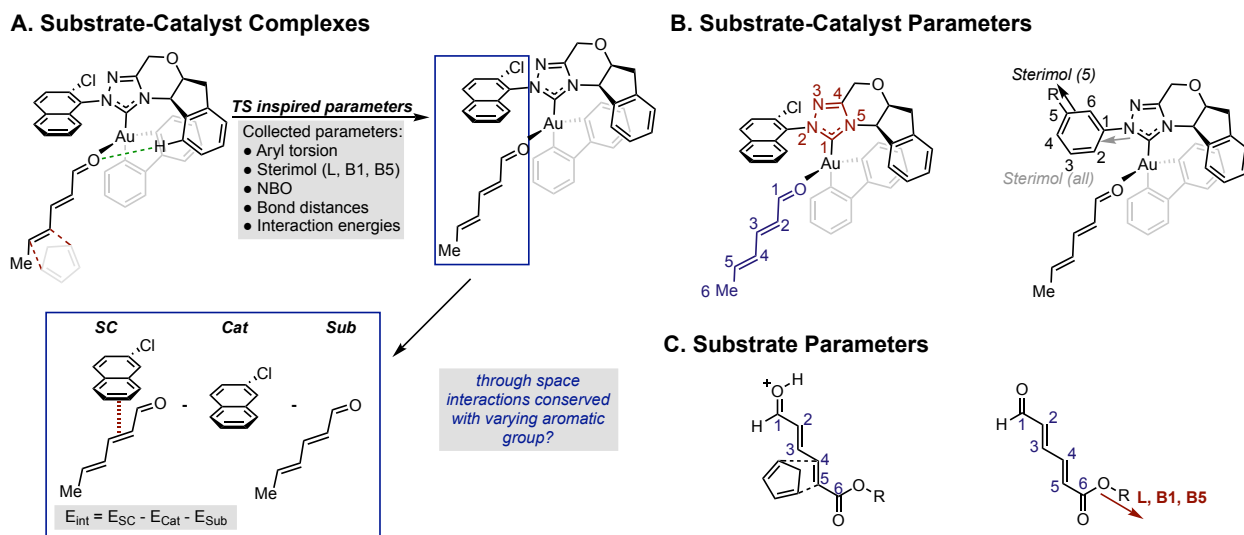


Figure S3. Numbering and definition of parameters collected.

8.1 Select examples of RMSD and Distortion energies

Fragment	RMSD	Distortion Energy
Sub 4g	0.0324	2.23
Cat 4g	0.0244	0.65
Sub 4k	0.0383	2.05
Cat 4k	0.0820	1.25
Sub 4l	0.0300	2.30
Cat 4l	0.2298	1.57
Sub 4o	0.0275	2.14
Cat 4o	0.0188	0.62
Sub 4p	0.0349	2.13
Cat 4p	0.0193	0.63

Distortion energies quoted in kcal mol⁻¹, E_{dis} , are calculated as $E_{dis} = E_g - E_{frag}$. E_g is the ground state of either the aldehyde (sub) or aromatic substituent (cat) and E_{frag} is the distorted aldehyde (sub) or aromatic substituent (cat). Since RMSDs and distortion energies are small and consistent $E_{int} = E_{sc} - E_{cat} - E_{sub}$ accurately reflects the changes in interaction energy on complex formation.

8.2 Catalyst Parameter Tables

Table S2. Interaction energies in kcal mol⁻¹ and aryl torsion as descriptors.

catalyst	interaction energies	aryl torsion
4g	-2.72	134.9
4h	-4.83	139.2
4i	-6.44	138.5
4j	-2.97	133.9
4k	-3.66	113.1
4l	-4.52	94.0
4m	-5.41	99.8
4n	-4.09	97.0
4o	-2.52	110.9
4p	-2.69	97.2
4q	-2.71	95.4
4r	-2.22	100.6
4s	-4.38	99.4
4t	-5.25	139.6
4u	-4.87	110.6
4v	-5.28	111.2
4w	-6.51	111.6
4x	-4.91	99.9
4y	-4.54	102.5

Table S3. NBO charges on the triazole.

catalyst	Au	C1	N2	N3	C4	N5
4g	1.022	0.127	-0.207	-0.250	0.352	-0.369
4h	1.018	0.133	-0.211	-0.250	0.356	-0.370
4i	1.013	0.136	-0.214	-0.252	0.359	-0.369
4j	1.030	0.126	-0.200	-0.249	0.349	-0.370
4k	1.028	0.145	-0.198	-0.232	0.343	-0.373
4l	1.036	0.139	-0.218	-0.253	0.347	-0.380
4m	1.033	0.137	-0.216	-0.251	0.347	-0.378
4n	1.028	0.136	-0.217	-0.251	0.347	-0.376
4o	1.013	0.143	-0.211	-0.237	0.351	-0.368
4p	1.023	0.148	-0.220	-0.239	0.352	-0.373
4q	1.024	0.149	-0.225	-0.240	0.353	-0.374
4r	1.022	0.148	-0.231	-0.245	0.358	-0.374
4s	1.020	0.150	-0.226	-0.240	0.354	-0.374
4t	1.023	0.128	-0.204	-0.252	0.353	-0.370
4u	1.026	0.132	-0.219	-0.247	0.348	-0.373
4v	1.029	0.134	-0.216	-0.247	0.348	-0.374
4w	1.029	0.135	-0.217	-0.247	0.348	-0.374
4x	1.031	0.139	-0.219	-0.248	0.347	-0.376
4y	1.023	0.144	-0.221	-0.244	0.349	-0.375

Table S4. NBO charges on the aromatic substituents.

catalyst	C1	C2	C3	C4	C5	C6
4g	0.121	-0.198	-0.184	-0.197	-0.195	-0.218
4h	0.164	-0.230	-0.005	-0.243	-0.017	-0.255
4i	0.143	-0.156	-0.117	-0.154	-0.128	-0.180
4j	0.113	-0.198	-0.021	0.299	-0.017	-0.234
4k	-0.006	0.346	-0.335	-0.142	-0.329	0.348
4l	0.093	0.034	-0.221	-0.174	-0.217	0.033
4m	0.101	0.019	-0.221	-0.172	-0.208	0.023
4n	0.099	0.014	-0.212	-0.173	-0.205	0.017
4o	-0.027	0.432	-0.291	-0.150	-0.288	0.434
4p	0.066	-0.021	-0.223	-0.161	-0.219	-0.019
4q	0.057	-0.086	-0.225	-0.163	-0.219	-0.083
4r	0.181	-0.129	-0.150	-0.180	-0.154	-0.133
4s	0.084	-0.019	-0.201	-0.100	-0.200	-0.017
4t	0.130	-0.207	-0.149	-0.059	-0.057	-0.193
4u	0.138	-0.062	-0.056	-0.158	-0.203	-0.184
4v	0.135	-0.066	-0.026	-0.028	-0.068	-0.150
4w	0.138	-0.061	-0.012	-0.015	-0.064	-0.149
4x	0.120	-0.049	-0.065	-0.149	-0.200	0.023
4y	0.104	-0.044	-0.063	-0.142	-0.220	-0.020

Table S5. NBO charges on the substrate.

catalyst	O	C1	C2	C3	C4	C5	C6
4g	-0.629	0.418	-0.347	-0.034	-0.284	-0.012	-0.648
4h	-0.634	0.412	-0.353	-0.032	-0.287	-0.01	-0.648
4i	-0.637	0.409	-0.355	-0.034	-0.293	-0.006	-0.649
4j	-0.627	0.419	-0.350	-0.038	-0.289	-0.011	-0.649
4k	-0.620	0.421	-0.349	-0.043	-0.287	-0.017	-0.647
4l	-0.634	0.425	-0.353	-0.034	-0.283	-0.012	-0.647
4m	-0.631	0.423	-0.354	-0.032	-0.288	-0.011	-0.648
4n	-0.635	0.422	-0.353	-0.034	-0.286	-0.01	-0.648
4o	-0.626	0.413	-0.348	-0.037	-0.286	-0.011	-0.648
4p	-0.624	0.417	-0.348	-0.04	-0.285	-0.011	-0.648
4q	-0.624	0.419	-0.348	-0.039	-0.285	-0.012	-0.647
4r	-0.624	0.414	-0.352	-0.038	-0.287	-0.009	-0.648
4s	-0.630	0.412	-0.356	-0.033	-0.291	-0.001	-0.649
4t	-0.630	0.417	-0.35	-0.032	-0.286	-0.015	-0.648
4u	-0.631	0.421	-0.349	-0.032	-0.282	-0.022	-0.645
4v	-0.630	0.421	-0.346	-0.032	-0.28	-0.024	-0.646
4w	-0.632	0.419	-0.347	-0.03	-0.284	-0.02	-0.647
4x	-0.633	0.422	-0.348	-0.029	-0.282	-0.021	-0.645
4y	-0.629	0.421	-0.349	-0.032	-0.282	-0.021	-0.646

Table S6. Sterimol parameters calculated using Bondi radii for the whole aromatic substituent and individual substituents at positions 1-3.

catalyst	L(all)	B1(all)	B5(all)	L(2)	B1(2)	B5(2)	L(3)	B1(3)	B5(3)
4g	6.75	1.70	3.25	2.57	1.09	1.09	2.57	1.09	1.09
4h	6.76	1.70	4.45	2.57	1.09	1.09	3.87	1.75	1.75
4i	7.39	2.43	4.94	2.57	1.09	1.09	3.88	2.07	2.72
4j	8.59	3.17	5.78	2.57	1.09	1.09	4.74	2.82	3.28
4k	6.74	1.90	5.41	4.56	1.52	3.13	2.57	1.09	1.09
4l	6.74	3.01	5.67	4.70	2.00	3.26	2.57	1.09	1.09
4m	6.75	2.01	5.75	4.74	1.70	3.23	2.57	1.09	1.09
4n	6.74	1.93	4.46	3.59	1.70	2.11	2.57	1.09	1.09
4o	6.76	1.70	3.80	3.19	1.47	1.47	2.57	1.09	1.09
4p	6.76	1.74	4.45	3.87	1.75	1.75	2.57	1.09	1.09
4q	6.76	1.84	4.69	4.13	1.85	1.85	2.57	1.09	1.09
4r	6.76	2.41	5.00	3.91	2.07	2.72	2.57	1.09	1.09
4s	8.10	2.32	4.45	3.87	1.75	1.75	2.57	1.09	1.09
4t	8.87	1.70	4.42	2.57	1.09	1.09	2.57	1.09	1.09
4u	6.84	1.70	5.69	6.69	2.24	9.85	7.00	1.97	10.94
4v	8.83	1.70	5.70	6.65	2.18	9.63	6.86	2.21	10.96
4w	8.92	1.70	5.71	6.52	2.30	9.65	6.96	2.24	10.84
4x	6.77	1.76	5.70	7.54	2.33	9.91	7.06	2.02	10.95
4y	6.80	1.70	5.69	7.39	2.33	10.07	6.98	2.02	10.96

Table S7. Sterimol parameters calculated using Bondi radii for the substituents at positions 4-6.

catalyst	L(4)	B1(4)	B5(4)	L(5)	B1(5)	B5(5)	L(6)	B1(6)	B5(6)
4g	2.57	1.09	1.09	2.57	1.09	1.09	2.57	1.09	1.09
4h	2.57	1.09	1.09	3.88	1.75	1.75	2.57	1.09	1.09
4i	2.57	1.09	1.09	3.87	2.07	2.72	2.57	1.09	1.09
4j	4.51	1.40	3.16	4.70	2.82	3.27	2.57	1.09	1.09
4k	2.57	1.09	1.09	2.57	1.09	1.09	4.56	1.39	3.14
4l	2.57	1.09	1.09	2.57	1.09	1.09	4.67	1.97	3.26
4m	2.57	1.09	1.09	2.57	1.09	1.09	4.67	1.70	3.25
4n	2.57	1.09	1.09	2.57	1.09	1.09	3.59	1.70	2.11
4o	2.57	1.09	1.09	2.57	1.09	1.09	3.19	1.47	1.47
4p	2.57	1.09	1.09	2.57	1.09	1.09	3.87	1.75	1.75
4q	2.57	1.09	1.09	2.57	1.09	1.09	4.13	1.85	1.85
4r	2.57	1.09	1.09	2.57	1.09	1.09	3.90	2.08	2.72
4s	3.88	2.07	2.73	2.57	1.09	1.09	3.87	1.75	1.75
4t	4.68	2.78	10.23	5.30	2.03	9.97	2.57	1.09	1.09
4u	2.57	1.09	1.09	2.57	1.09	1.09	2.57	1.09	1.09
4v	4.75	2.93	10.01	4.68	2.10	9.59	2.57	1.09	1.09
4w	4.80	3.00	9.98	4.67	2.26	9.54	2.57	1.09	1.09
4x	2.57	1.09	1.09	2.57	1.09	1.09	3.59	1.70	2.11
4y	2.57	1.09	1.09	2.57	1.09	1.09	3.87	1.75	1.75

8.3 Substrate Parameter Tables

Table S8. NBO charges on the substrate.

substrate	H	C1	O	C2	C3	C4	C5	C6	O(carbonyl)	O(ester)
3b	0.105	0.387	-0.498	-0.271	-0.163	-0.160	-0.270	0.750	-0.591	-0.497
3c	0.105	0.387	-0.497	-0.270	-0.164	-0.158	-0.272	0.746	-0.590	-0.489
3d	0.105	0.387	-0.499	-0.273	-0.161	-0.163	-0.265	0.760	-0.603	-0.516
3e	0.105	0.386	-0.499	-0.270	-0.162	-0.160	-0.269	0.749	-0.597	-0.495
3f	0.105	0.388	-0.499	-0.270	-0.162	-0.159	-0.269	0.752	-0.591	-0.503
3g	0.105	0.387	-0.499	-0.269	-0.162	-0.157	-0.269	0.755	-0.599	-0.488
3h	0.105	0.387	-0.497	-0.270	-0.164	-0.158	-0.271	0.750	-0.598	-0.492
3i	0.107	0.386	-0.492	-0.260	-0.170	-0.144	-0.283	0.751	-0.580	-0.483
3j	0.104	0.388	-0.500	-0.272	-0.161	-0.161	-0.266	0.755	-0.598	-0.498
3k	0.105	0.387	-0.499	-0.272	-0.162	-0.161	-0.268	0.753	-0.590	-0.501
3l	0.104	0.387	-0.500	-0.274	-0.160	-0.165	-0.263	0.761	-0.602	-0.513
3m	0.105	0.387	-0.499	-0.272	-0.161	-0.162	-0.266	0.756	-0.595	-0.509
3n	0.105	0.387	-0.498	-0.269	-0.163	-0.156	-0.270	0.754	-0.597	-0.484
3o	0.105	0.387	-0.498	-0.269	-0.164	-0.158	-0.270	0.751	-0.589	-0.495
3p	0.106	0.387	-0.500	-0.274	-0.160	-0.171	-0.257	0.749	-0.577	-0.502
3q	0.109	0.399	-0.510	-0.079	-0.174	-0.159	-0.274	0.750	-0.595	-0.498
3r	-0.701	0.535	-0.530	-0.287	-0.147	-0.155	-0.275	0.750	-0.596	-0.497
3s	0.105	0.388	-0.497	-0.266	-0.165	-0.153	-0.275	0.754	-0.569	-0.490

Table S9. Sterimol parameters calculated using Bondi radii and polarizability parameters.

substrate	L	B1	B5	polarizability
3b	4.47	1.70	3.24	119.79
3c	3.53	1.70	2.13	106.51
3d	4.55	2.83	3.25	143.81
3e	5.19	1.70	13.40	216.19
3f	4.55	1.70	5.81	156.16
3g	5.06	1.70	6.11	171.38
3h	8.85	1.70	3.78	187.24
3i	5.06	1.70	3.83	120.08
3j	6.54	2.00	3.68	164.35
3k	6.59	1.70	6.47	212.61
3l	6.69	3.17	3.79	200.24
3m	6.59	1.99	5.01	200.20
3n	4.92	1.70	5.48	151.52
3o	4.84	1.70	4.54	144.72
3p	7.00	1.70	6.25	171.19
3q	4.47	1.70	3.24	132.95
3r	4.47	1.70	3.24	130.92
3s	7.69	1.83	3.87	184.66

Table S10. NBO charges from model *exo* TS.

substrate	H	C1	O	H2	C2	C3	C4	C5	C6	O(carbonyl)	O(ester)
3b	0.200	0.295	-0.632	0.511	-0.383	-0.033	-0.285	-0.149	0.750	-0.587	-0.490
3c	0.200	0.296	-0.631	0.512	-0.383	-0.033	-0.284	-0.152	0.746	-0.578	-0.485
3d	0.199	0.293	-0.633	0.511	-0.383	-0.031	-0.287	-0.138	0.761	-0.596	-0.520
3e	0.198	0.318	-0.592	0.500	-0.394	-0.028	-0.299	-0.149	0.753	-0.589	-0.491
3f	0.199	0.293	-0.632	0.511	-0.381	-0.033	-0.285	-0.147	0.752	-0.582	-0.498
3g	0.199	0.291	-0.633	0.510	-0.382	-0.036	-0.285	-0.150	0.755	-0.587	-0.488
3h	0.199	0.291	-0.633	0.510	-0.382	-0.033	-0.285	-0.146	0.757	-0.586	-0.494
3i	0.201	0.295	-0.631	0.512	-0.383	-0.038	-0.281	-0.168	0.760	-0.564	-0.487
3j	0.199	0.292	-0.632	0.511	-0.382	-0.033	-0.286	-0.144	0.755	-0.591	-0.497
3k	0.199	0.292	-0.632	0.510	-0.381	-0.033	-0.285	-0.147	0.756	-0.589	-0.497
3l	0.199	0.290	-0.633	0.510	-0.381	-0.033	-0.287	-0.137	0.762	-0.596	-0.515
3m	0.199	0.290	-0.633	0.510	-0.381	-0.035	-0.285	-0.145	0.756	-0.590	-0.507
3n	0.200	0.292	-0.633	0.511	-0.382	-0.036	-0.285	-0.150	0.753	-0.586	-0.485
3o	0.200	0.292	-0.633	0.511	-0.382	-0.036	-0.284	-0.150	0.756	-0.586	-0.492
3p	0.199	0.291	-0.633	0.510	-0.381	-0.035	-0.286	-0.147	0.751	-0.590	-0.486
3q	0.198	0.320	-0.596	0.499	-0.199	-0.022	-0.311	-0.155	0.755	-0.584	-0.495
3r	-0.690	0.478	-0.636	0.504	-0.378	-0.033	-0.284	-0.169	0.757	-0.590	-0.491
3s	0.199	0.286	-0.635	0.510	-0.380	-0.044	-0.281	-0.158	0.753	-0.579	-0.473

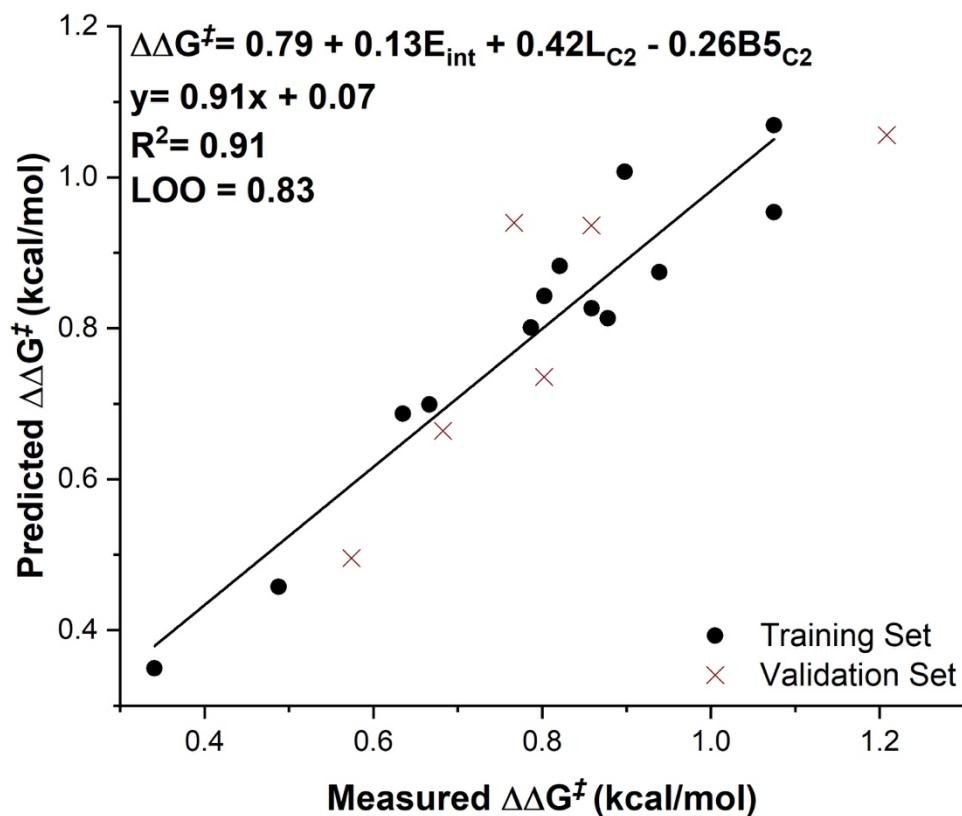
Table S11. Sterimol parameters calculated using Bondi radii from model *exo* TS.

substrate	L	B1	B5
3b	4.59	1.70	3.25
3c	3.55	1.70	2.14
3d	4.59	2.83	3.26
3e	5.48	1.70	13.48
3f	4.80	1.70	5.84
3g	5.08	1.70	6.14
3h	4.55	1.70	7.21
3i	5.12	1.70	3.84
3j	6.58	2.00	3.70
3k	6.81	1.70	6.48
3l	6.74	3.19	3.79
3m	6.66	2.02	5.04
3n	5.01	1.70	5.44
3o	4.65	1.70	4.53
3p	6.78	1.70	6.43
3q	4.50	1.70	3.25
3r	4.59	1.70	3.25
3s	7.90	1.84	3.56

9. Model development

Measured $\Delta\Delta G^\ddagger$ values were calculated using the formula $\Delta\Delta G^\ddagger = -RT\ln(er)$ where R is the gas constant, T is temperature (298.15 K or 273.15 for catalyst 4s) and er is the enantiomeric ratio. Linear regression models were developed using an in-house script implemented in MATLAB® (version R2018b), to obtain the predicted $\Delta\Delta G^\ddagger$.²⁷ A good linear correlation (R^2 close to 1.0 and intercept close to 0.0) between the predicted $\Delta\Delta G^\ddagger$ and the measured $\Delta\Delta G^\ddagger$ indicates that the obtained model adequately approximates the system under study.

Catalyst Model



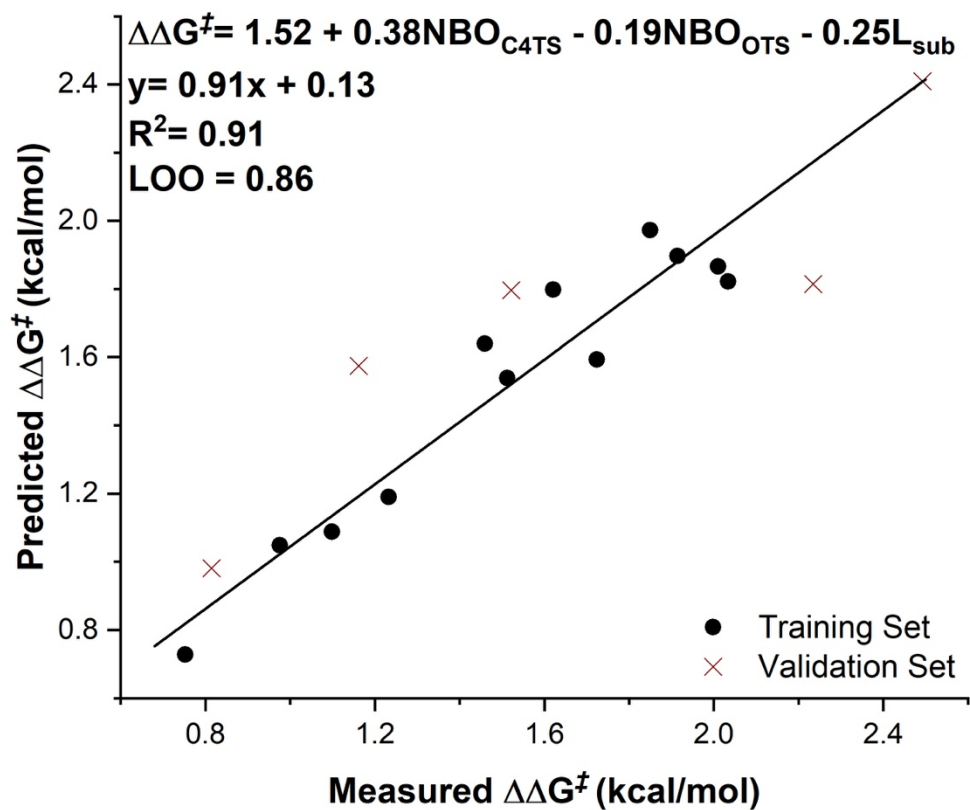
Training Set

measured $\Delta\Delta G^\ddagger$	predicted $\Delta\Delta G^\ddagger$	LOO
0.63	0.69	0.73
0.82	0.88	0.90
0.88	0.81	0.78
0.86	0.83	0.81
1.07	0.95	0.92
0.90	1.01	1.05
0.79	0.80	0.80
0.34	0.35	0.36
0.94	0.87	0.84
0.49	0.46	0.44
0.80	0.84	0.86
0.67	0.70	0.71
1.07	1.07	1.07

Prediction Set

measured $\Delta\Delta G^\ddagger$	predicted $\Delta\Delta G^\ddagger$
0.86	0.94
0.80	0.74
0.77	0.94
0.57	0.50
0.68	0.66
1.21	1.06

Substrate Model



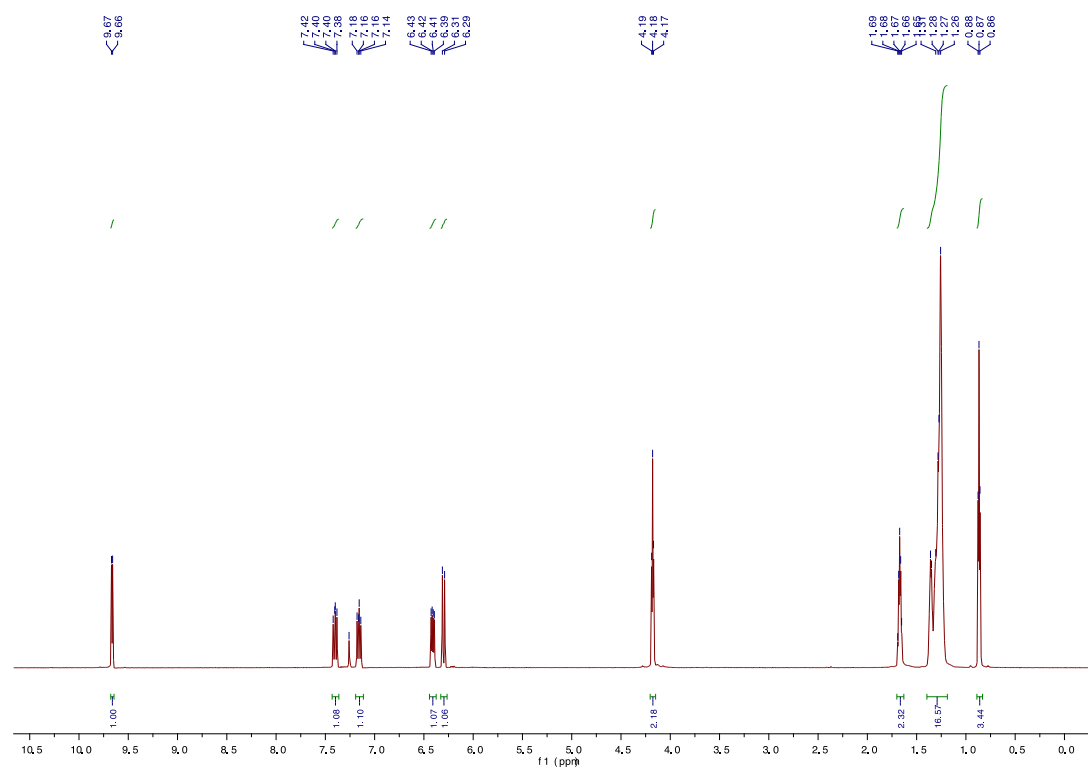
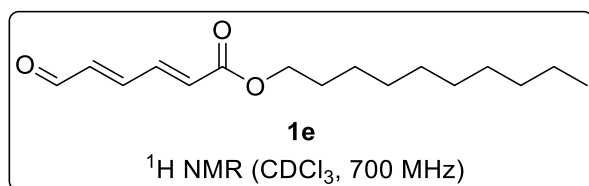
Training Set

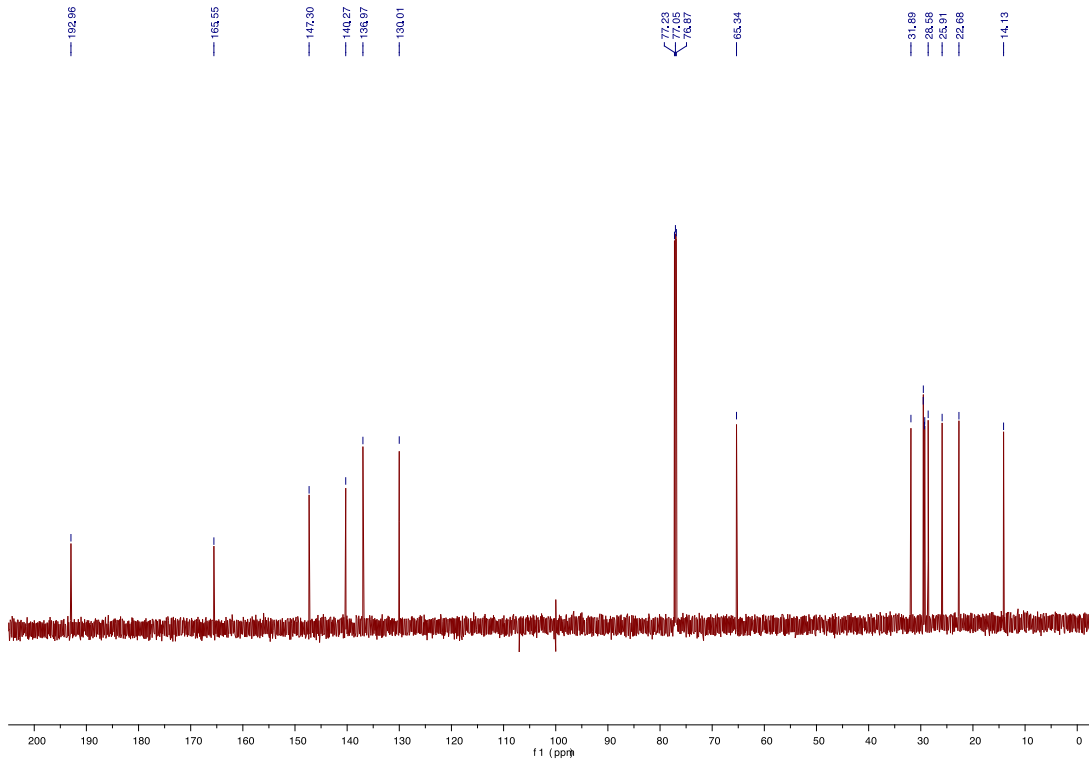
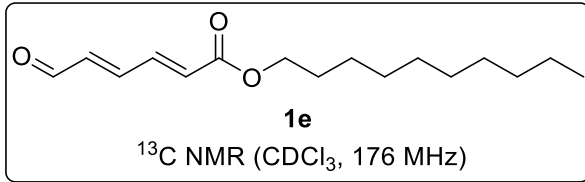
measured $\Delta\Delta G^\ddagger$	predicted $\Delta\Delta G^\ddagger$	LOO
1.85	1.97	2.01
1.46	1.64	1.67
1.10	1.09	1.07
0.98	1.05	1.07
1.51	1.54	1.54
1.91	1.90	1.84
1.62	1.80	1.85
1.23	1.19	1.17
1.72	1.59	1.56
2.03	1.82	1.78
2.01	1.87	1.83
0.75	0.73	0.65

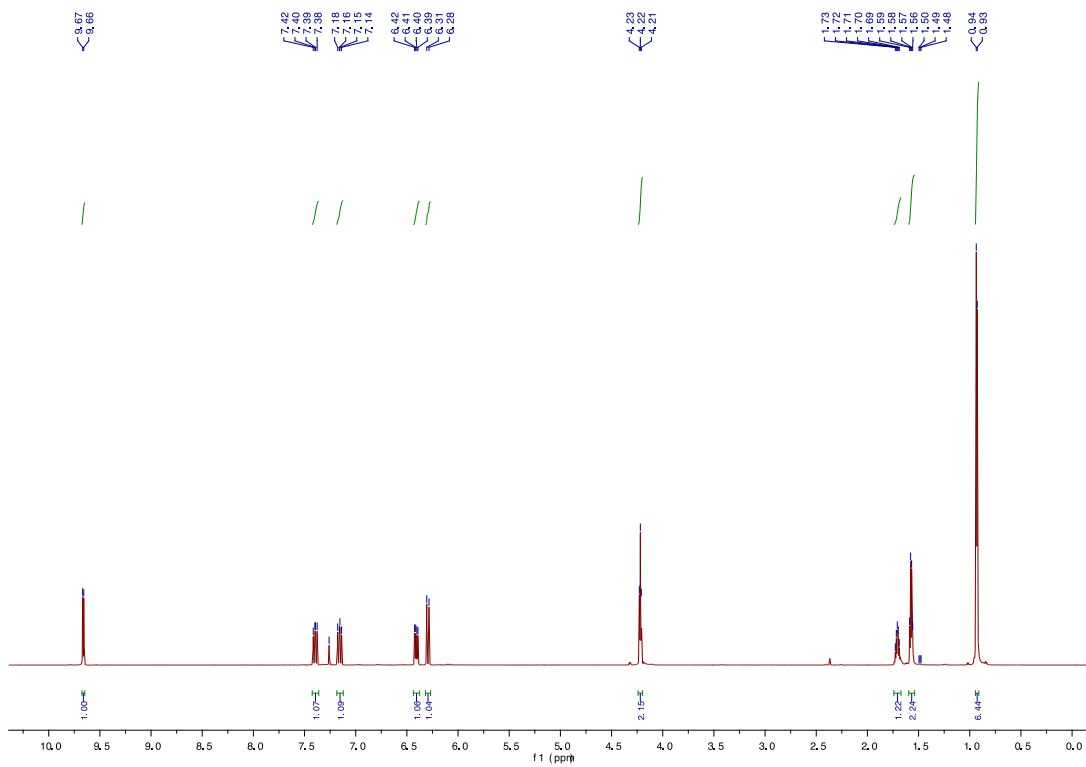
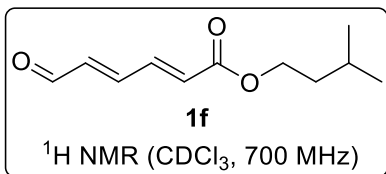
Prediction Set

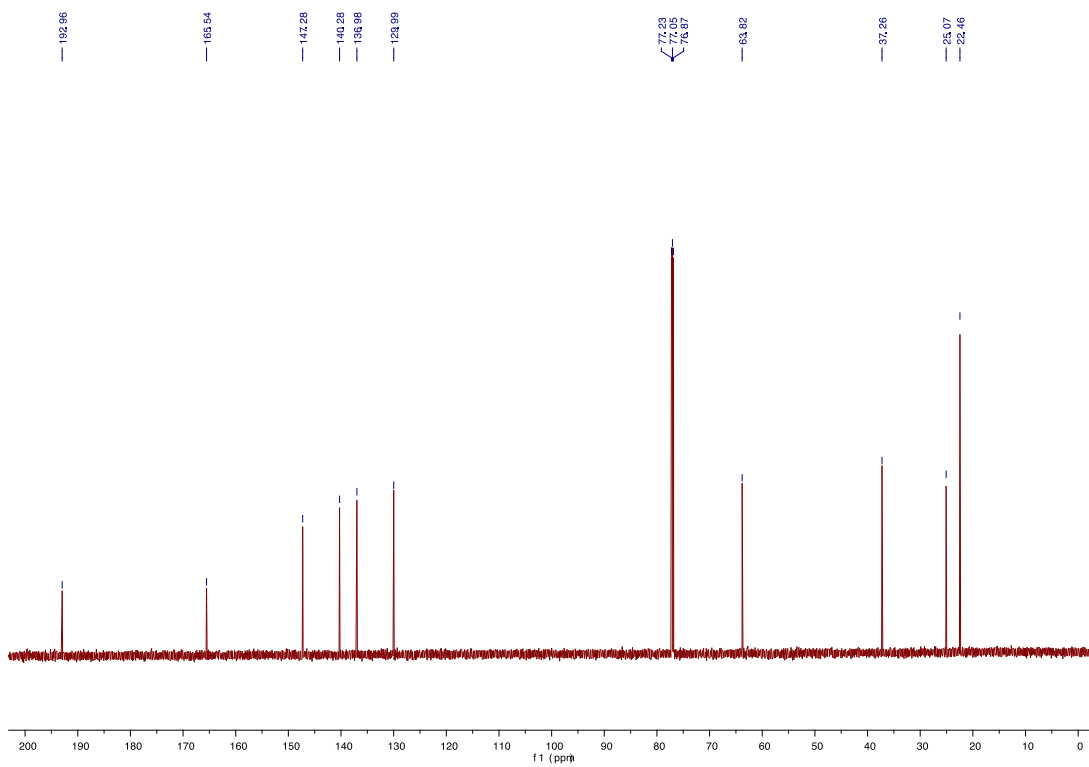
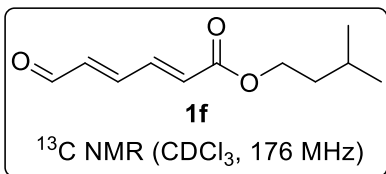
measured $\Delta\Delta G^\ddagger$	predicted $\Delta\Delta G^\ddagger$
1.52	1.80
2.49	2.41
1.16	1.57
2.23	1.81
0.82	0.98

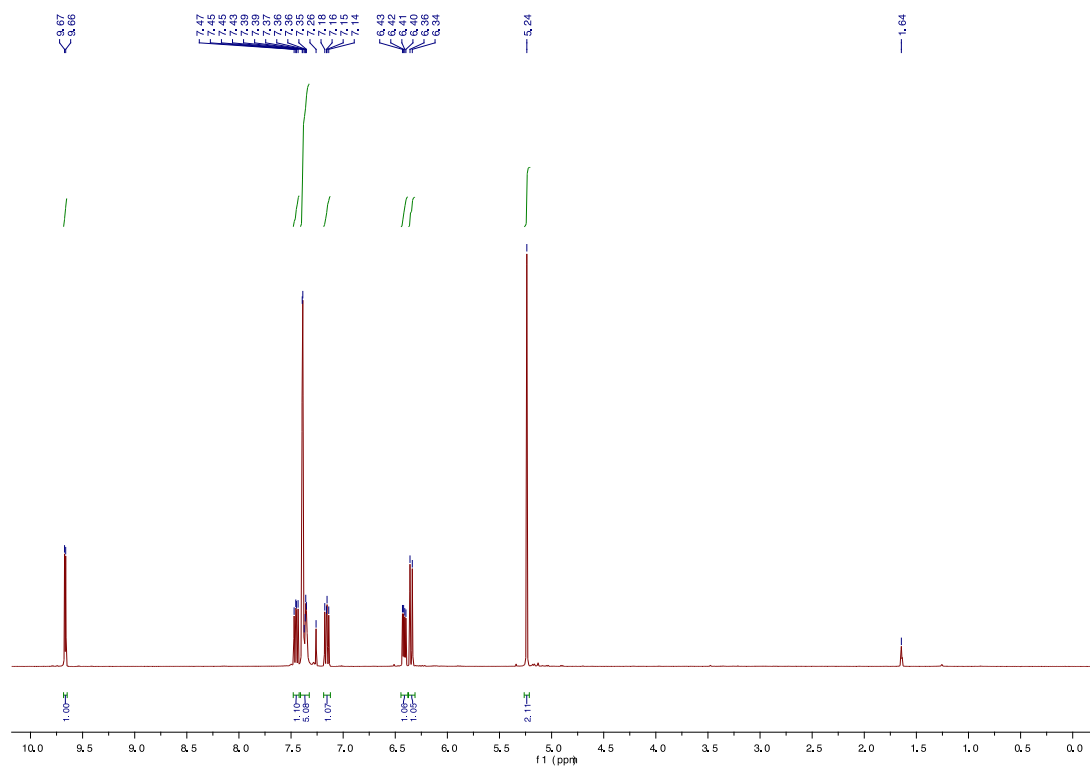
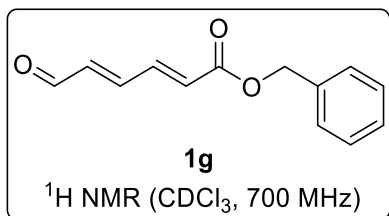
10. ^1H and ^{13}C NMR Spectra of Isolated New Compounds.

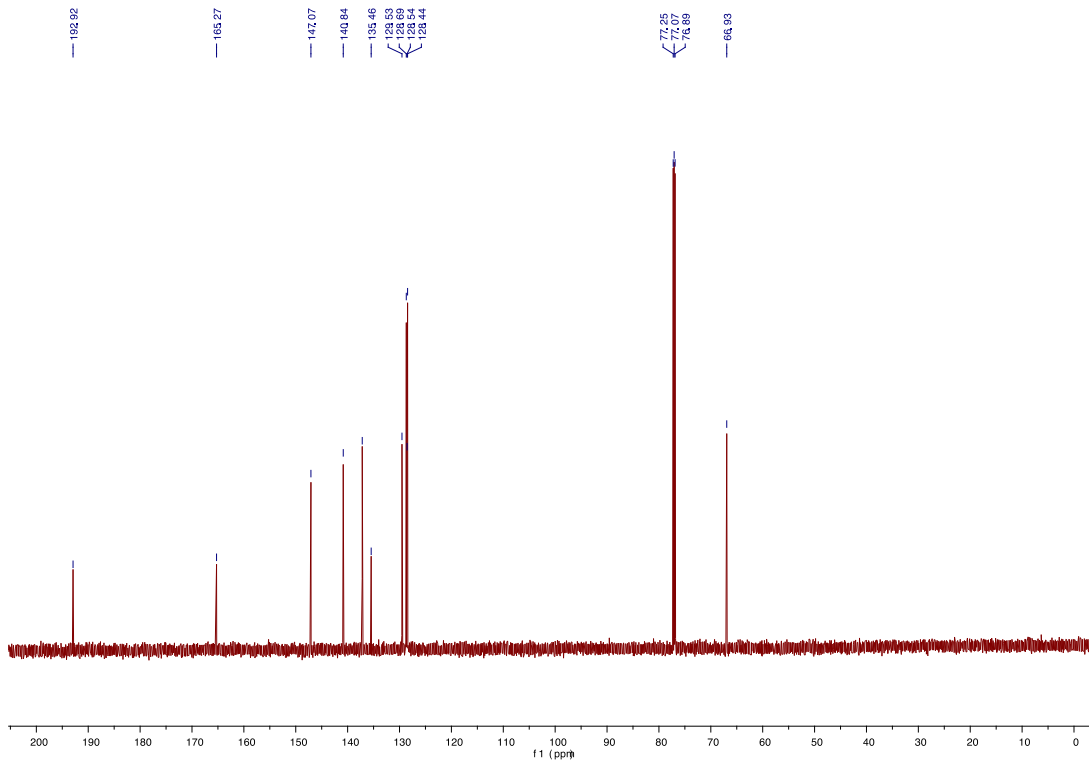
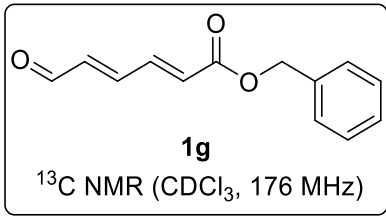


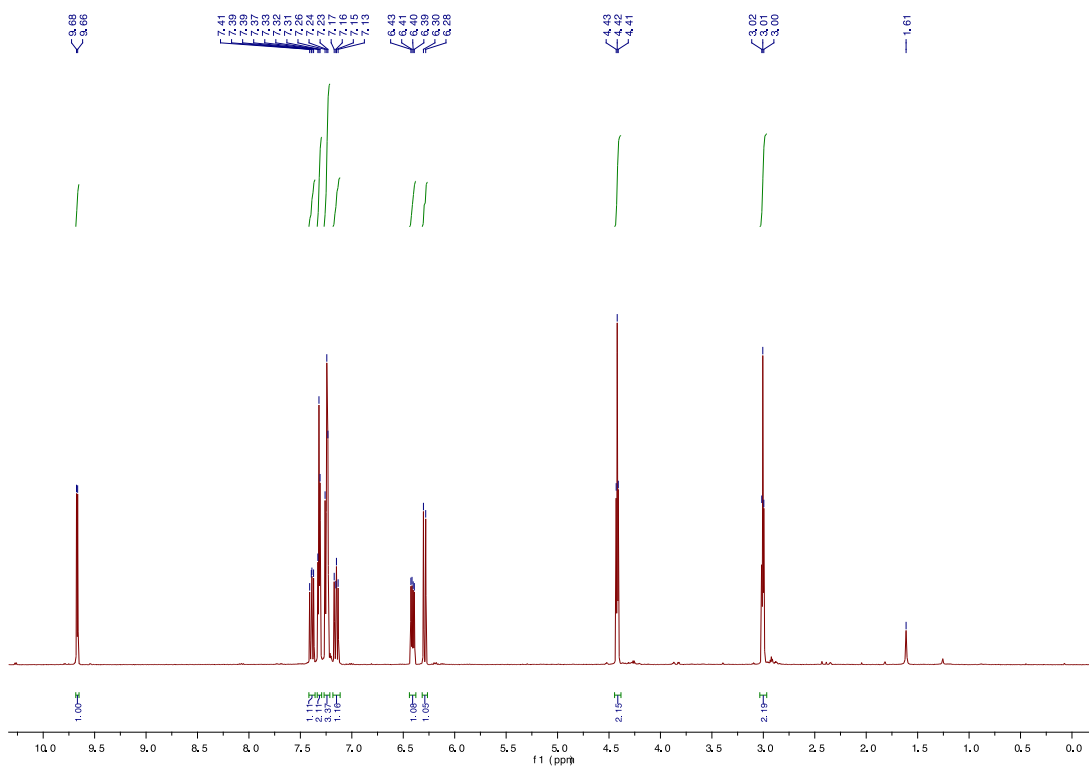
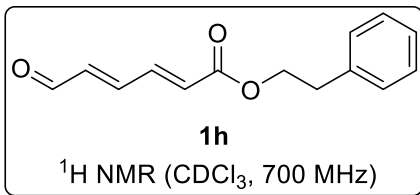


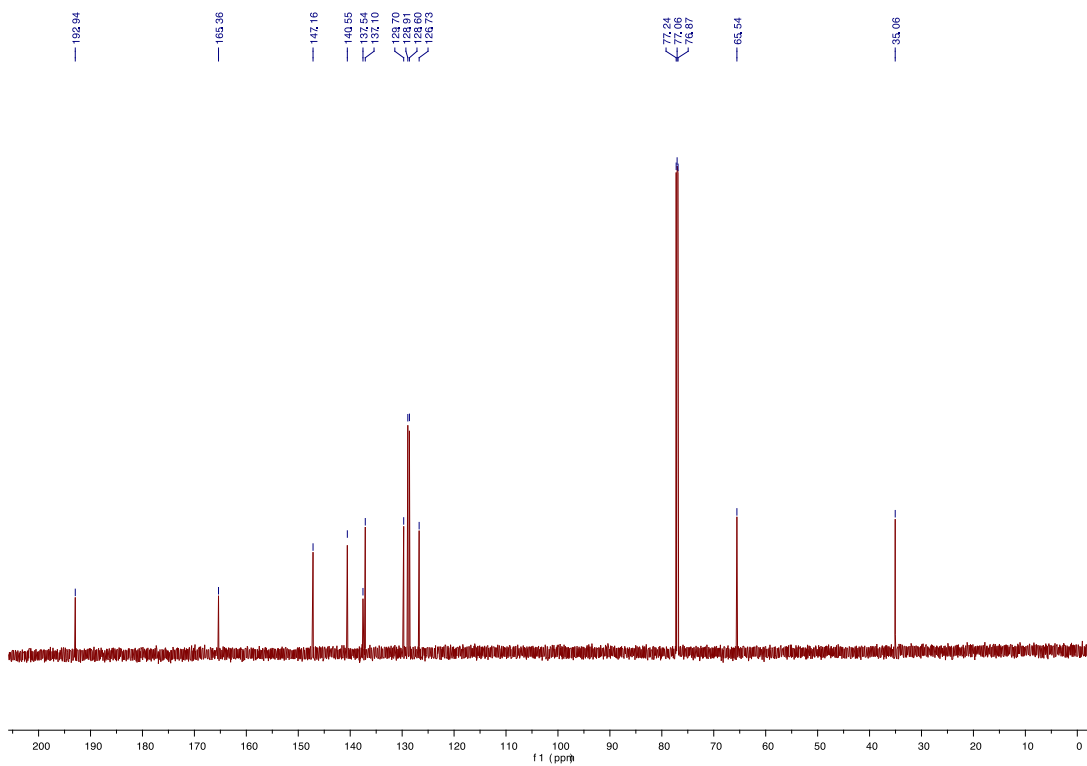
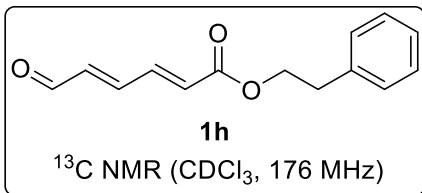


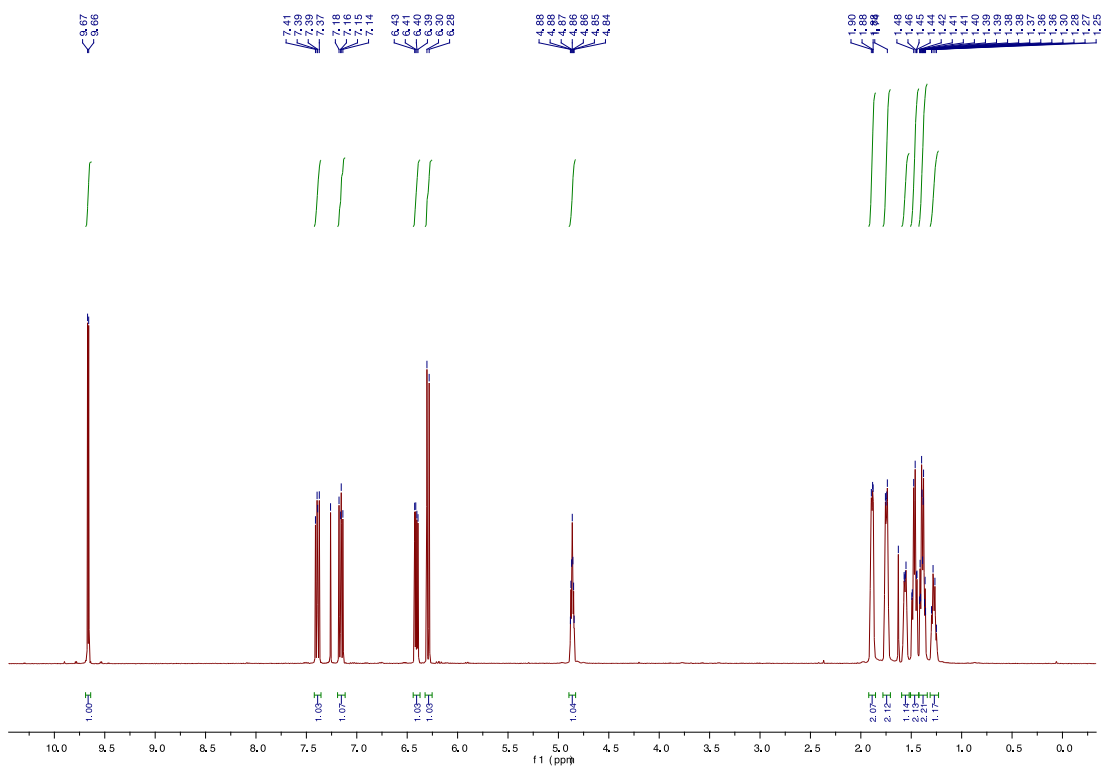
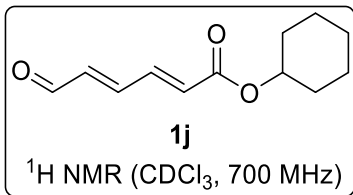


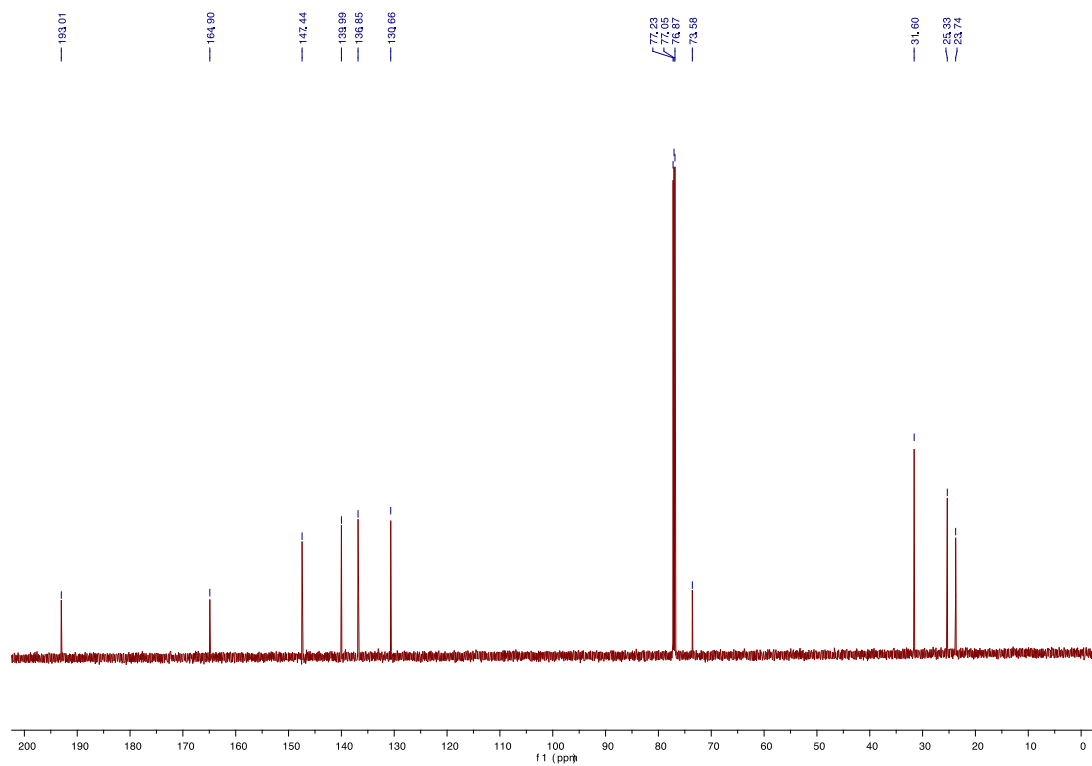
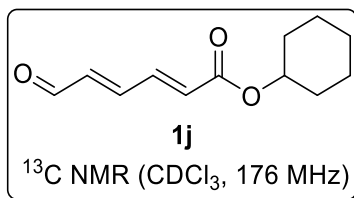


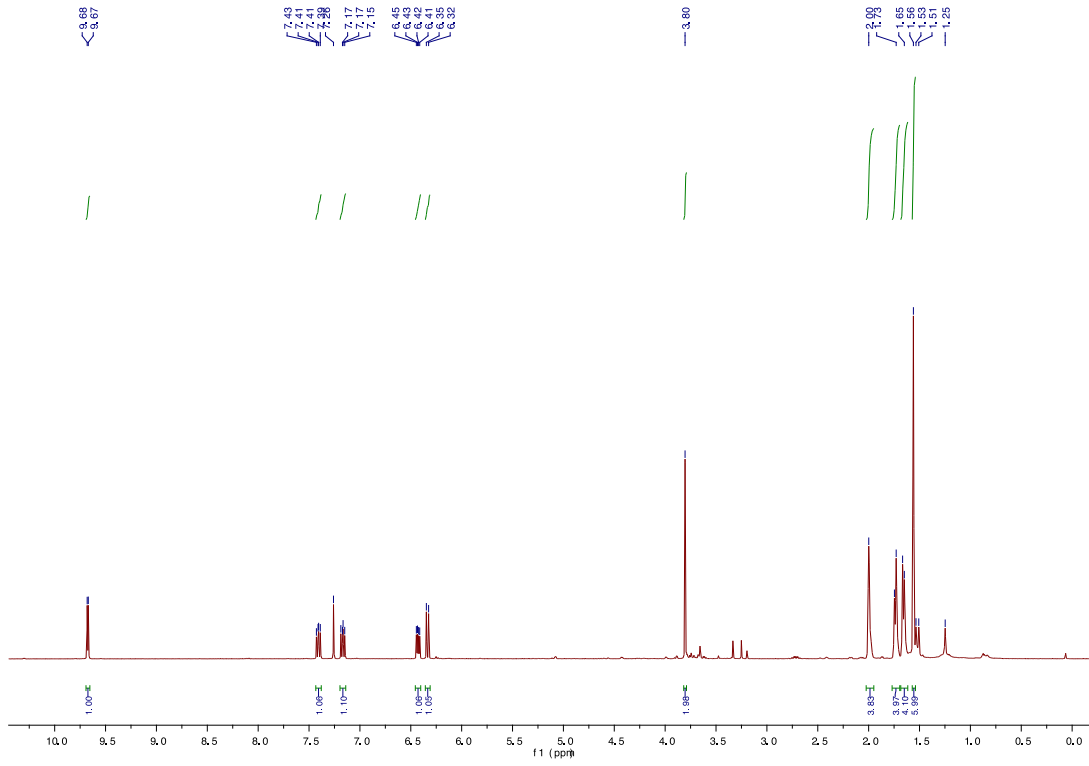
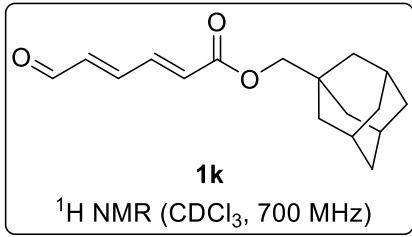


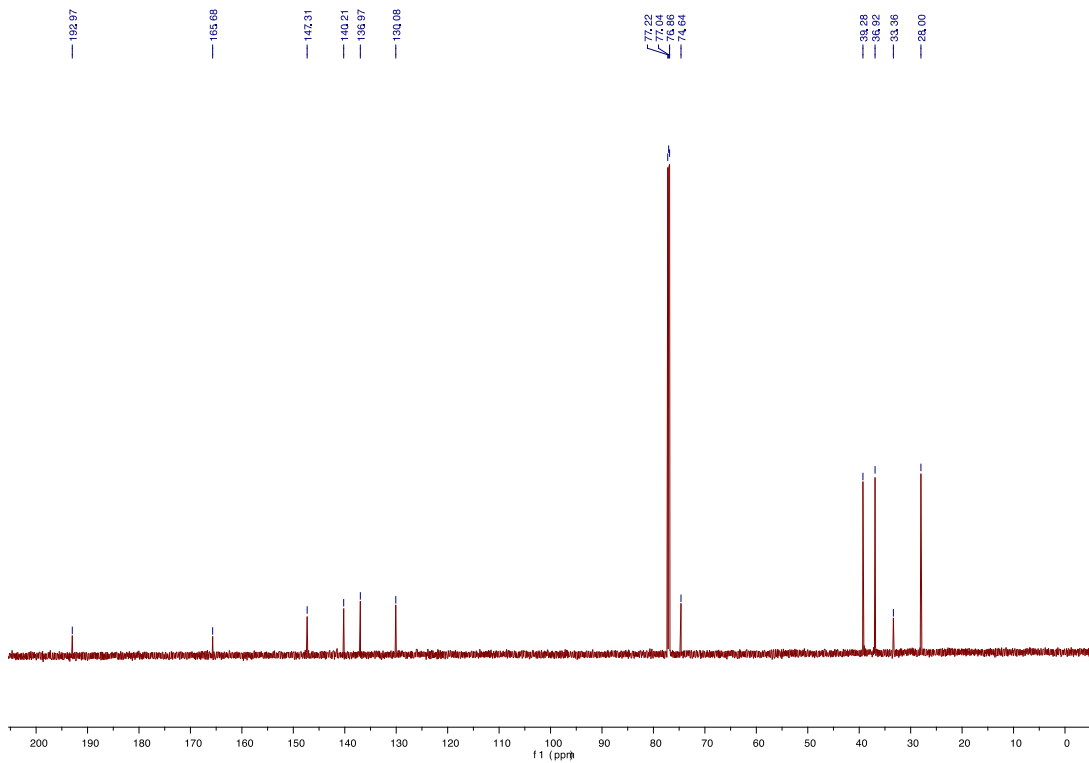
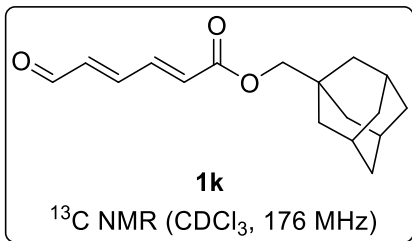


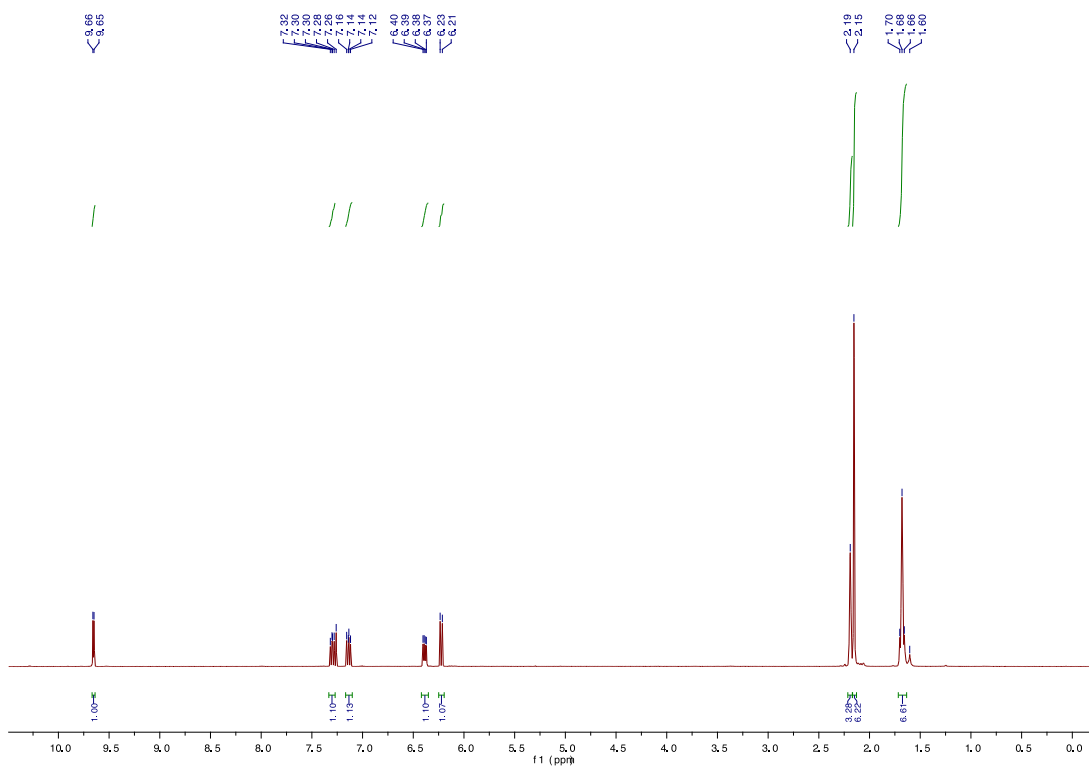
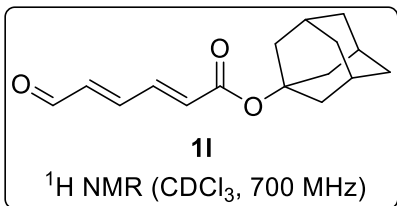


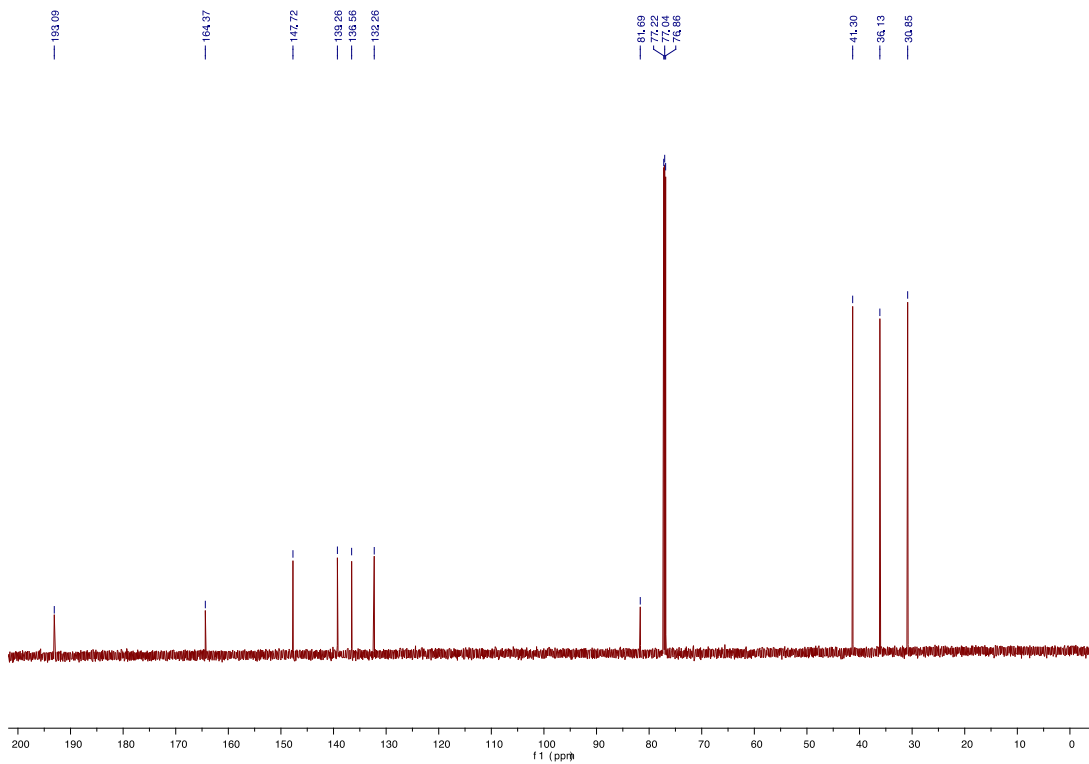
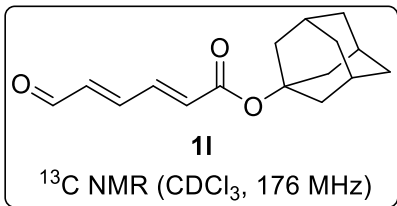


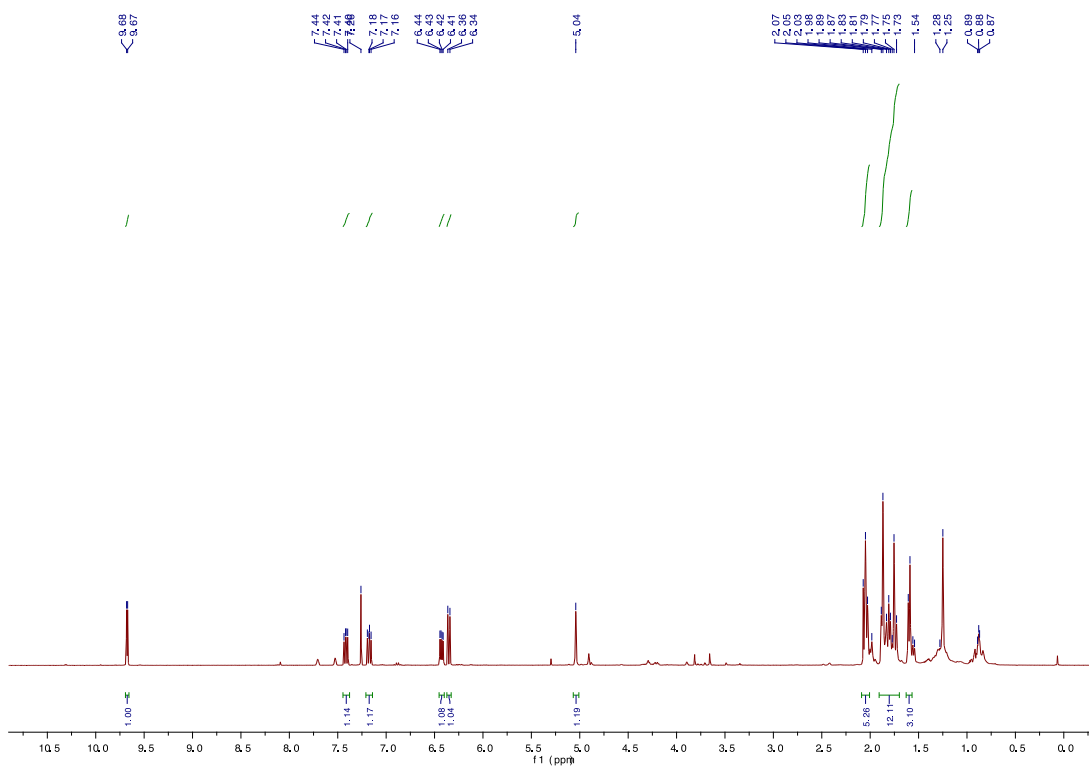
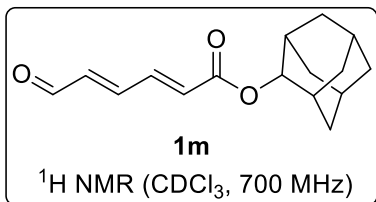


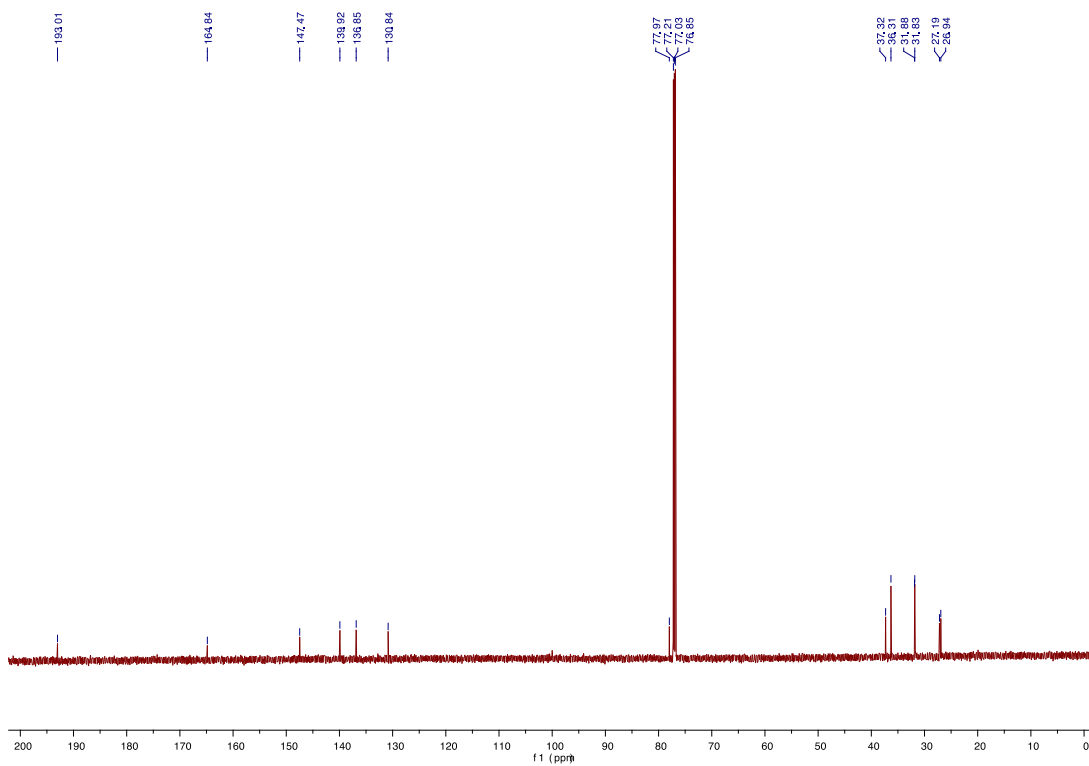
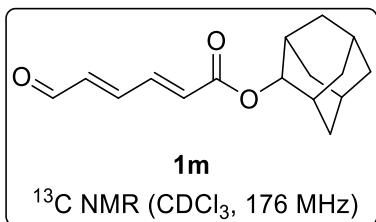


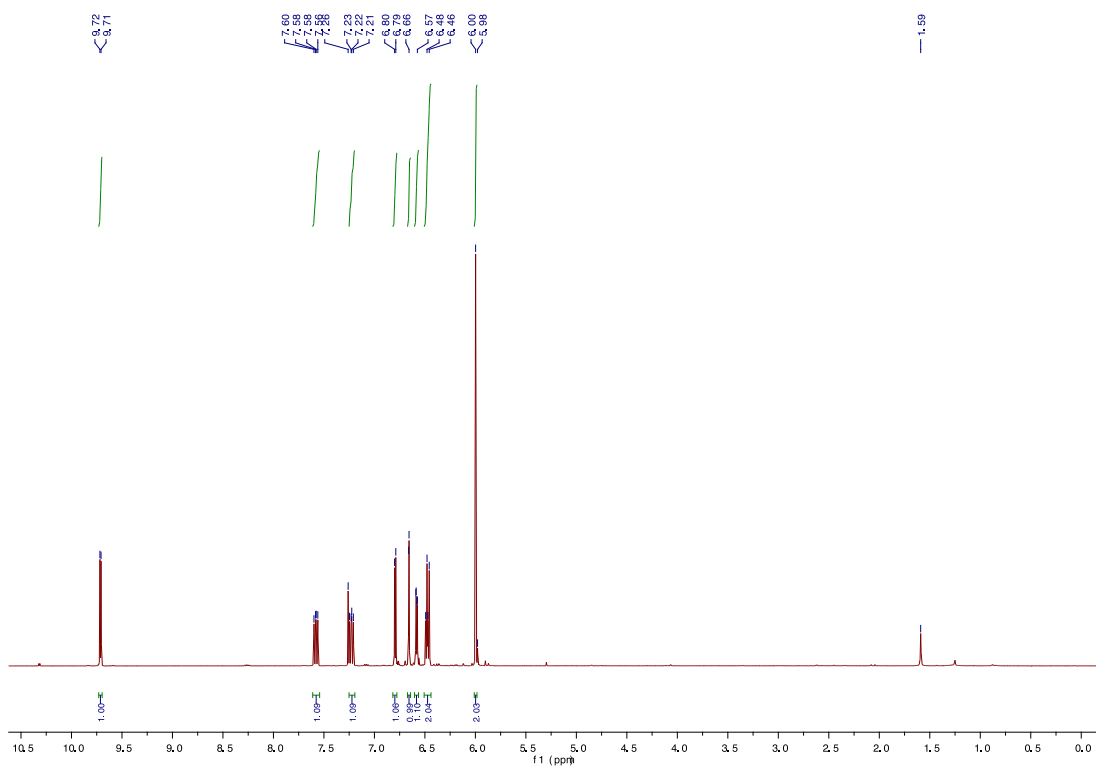
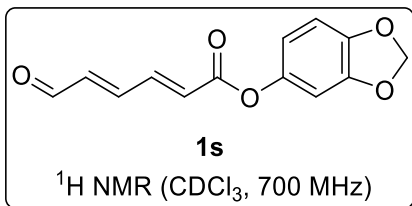


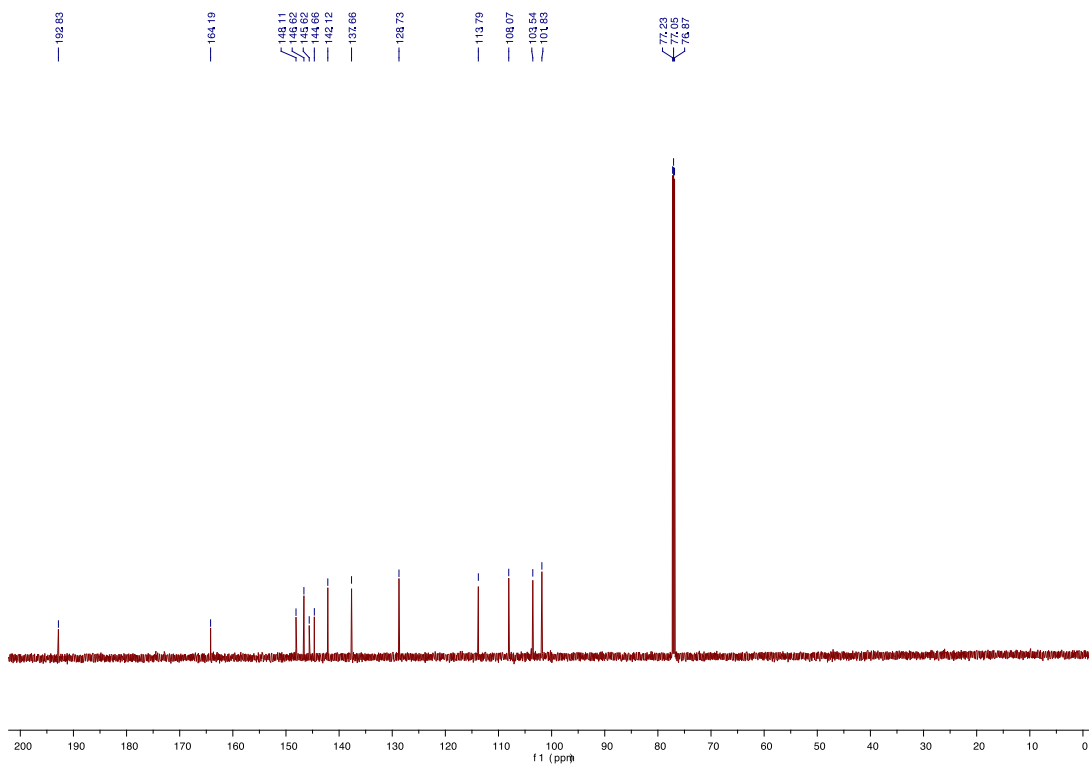
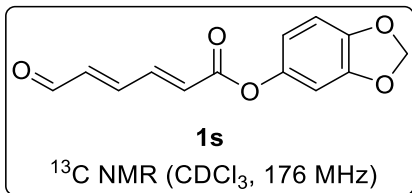


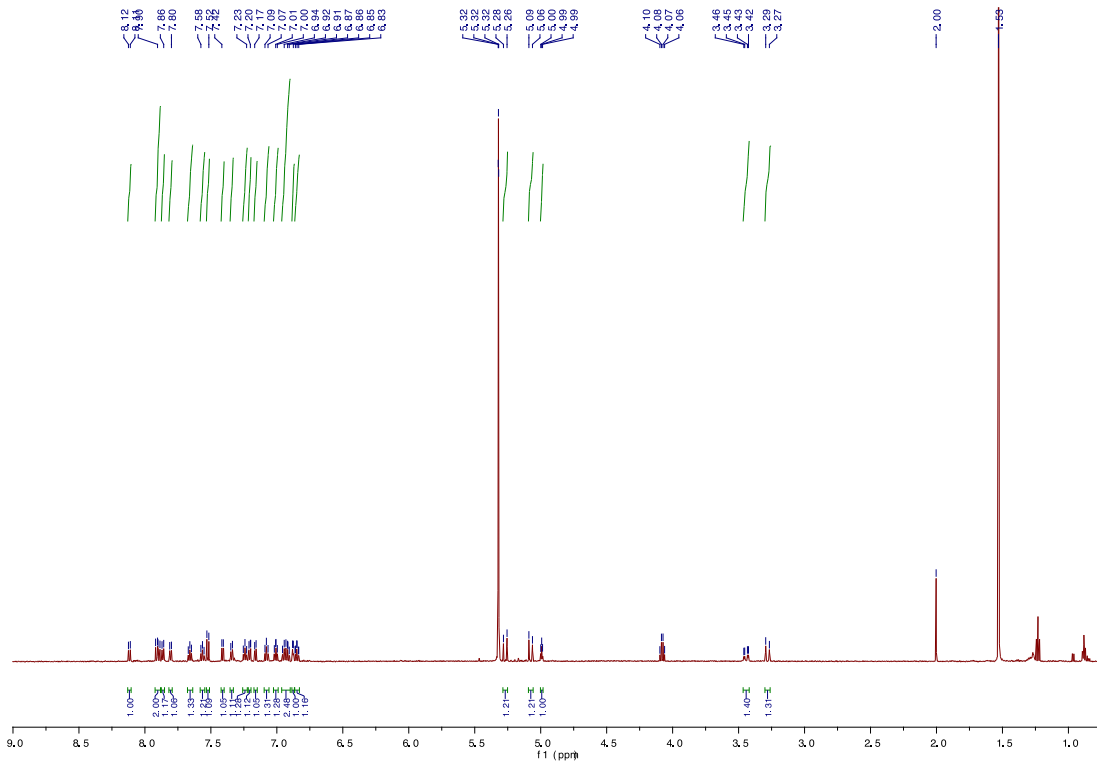
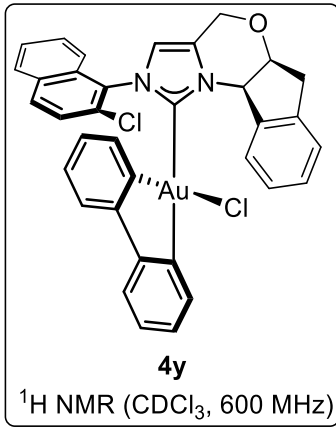


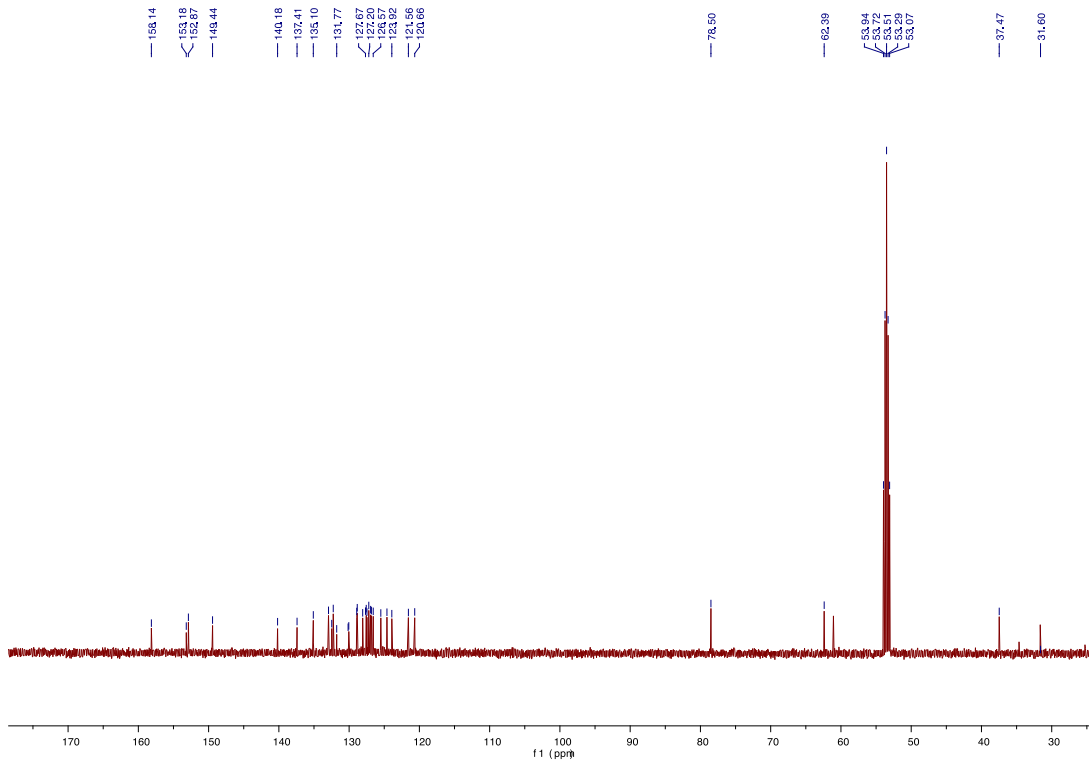
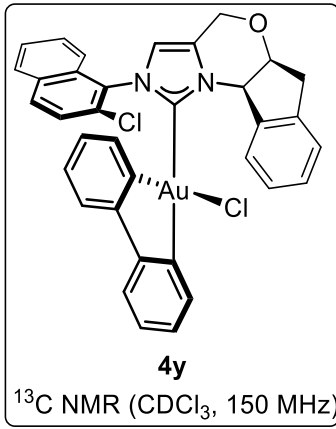


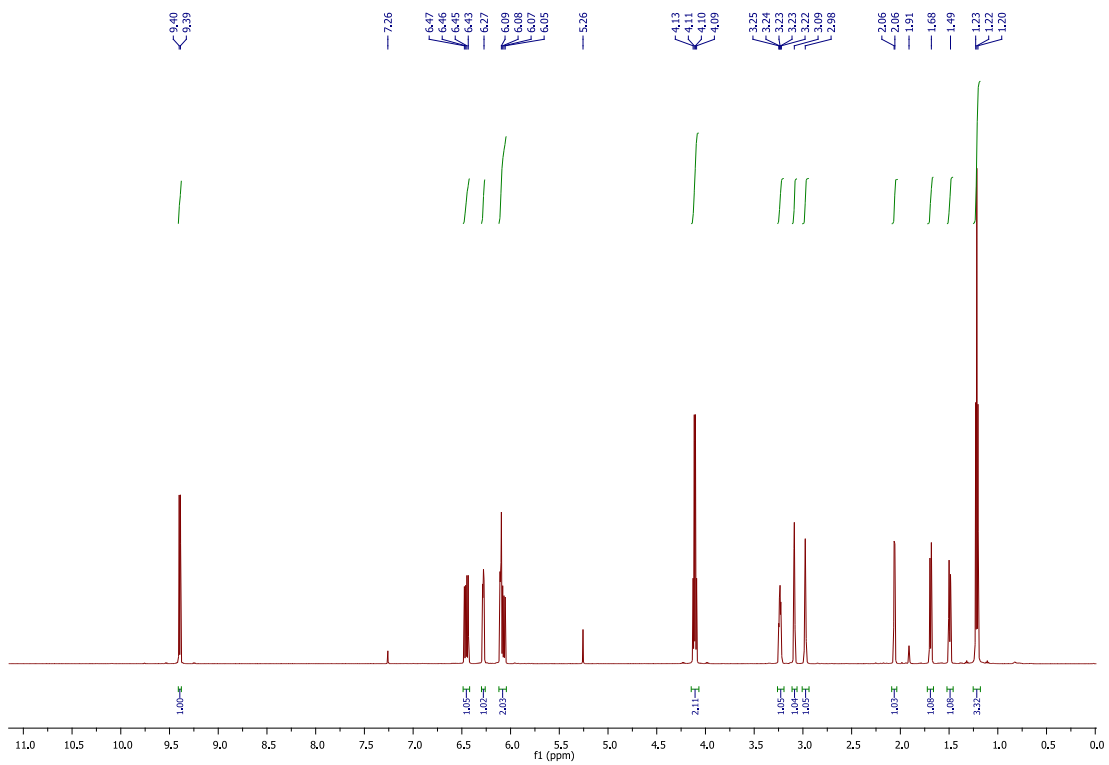
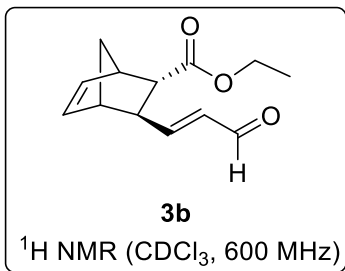


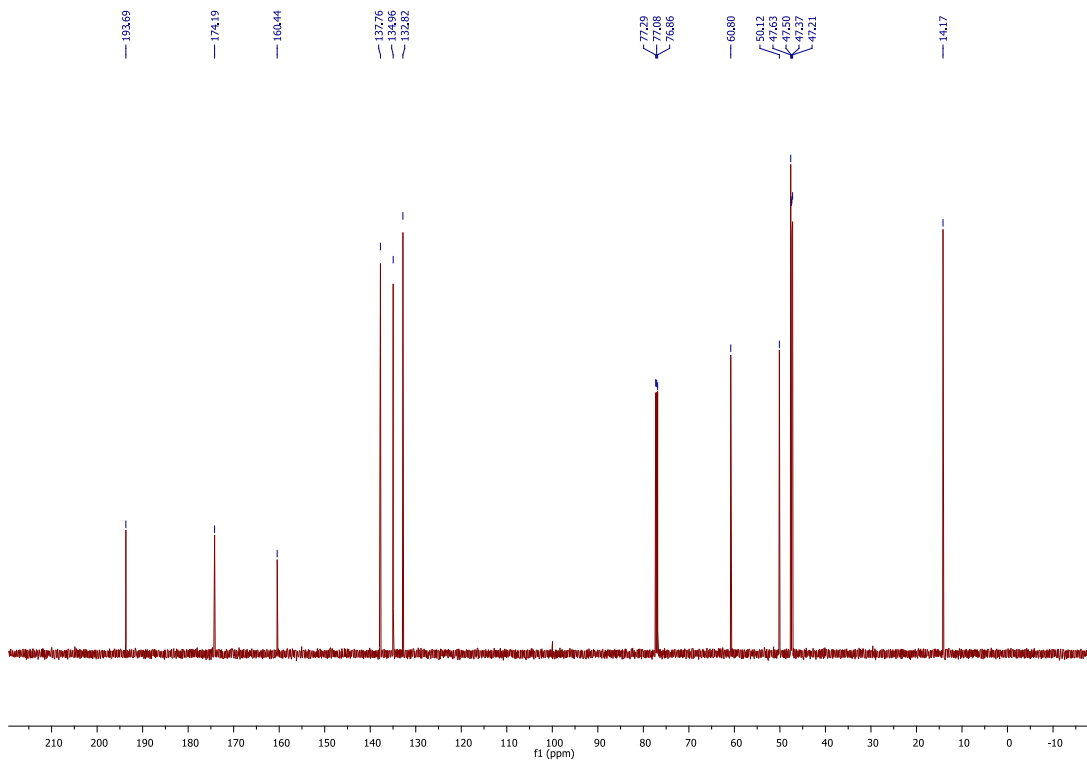
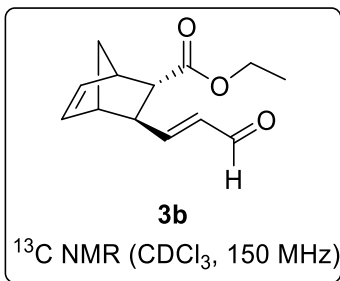


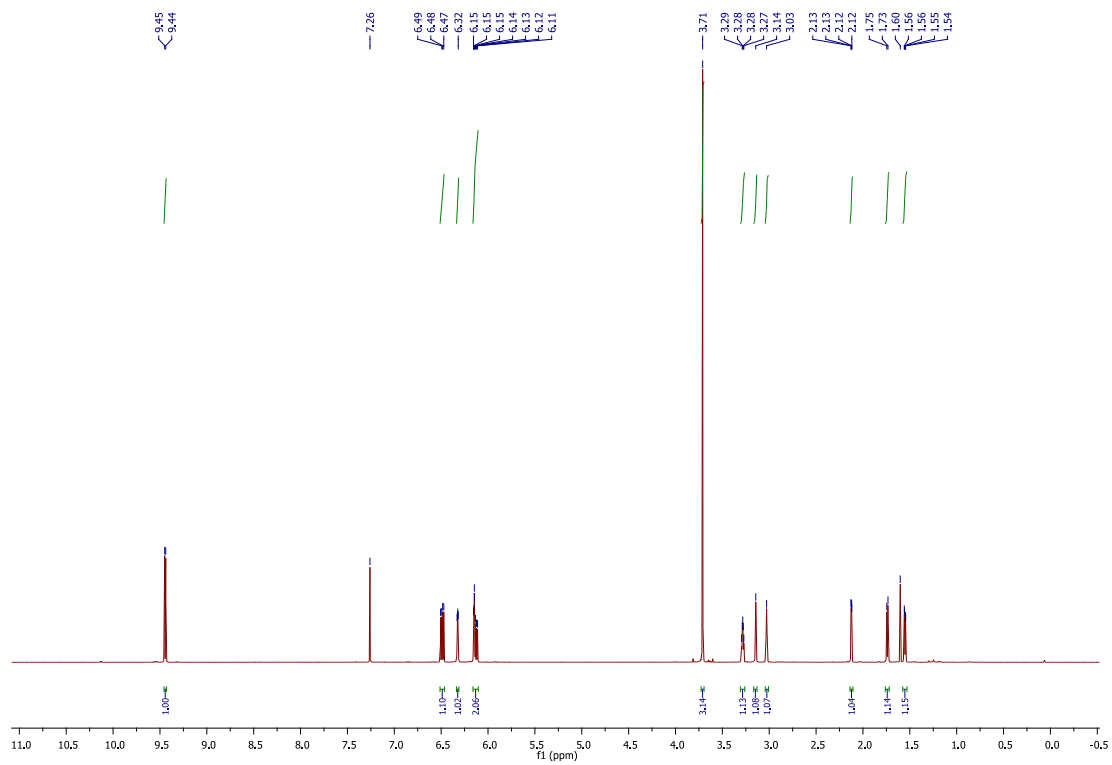
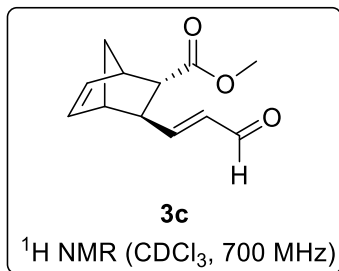


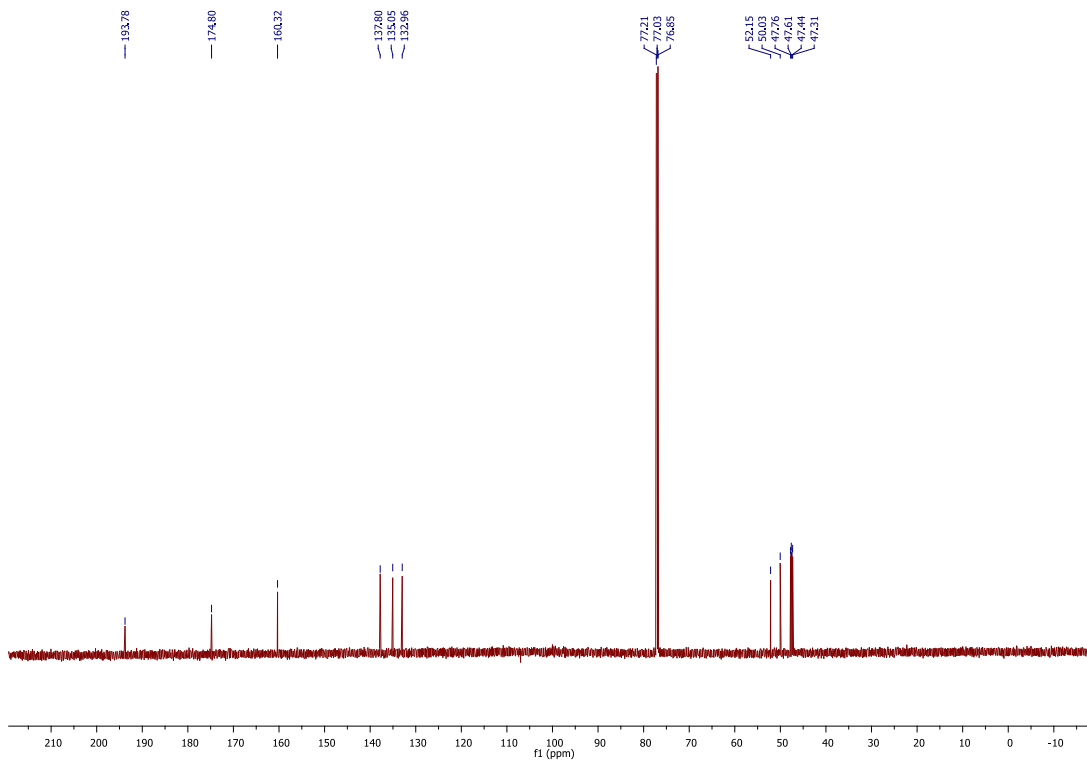
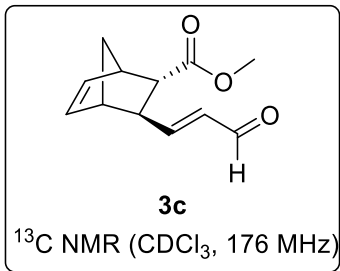


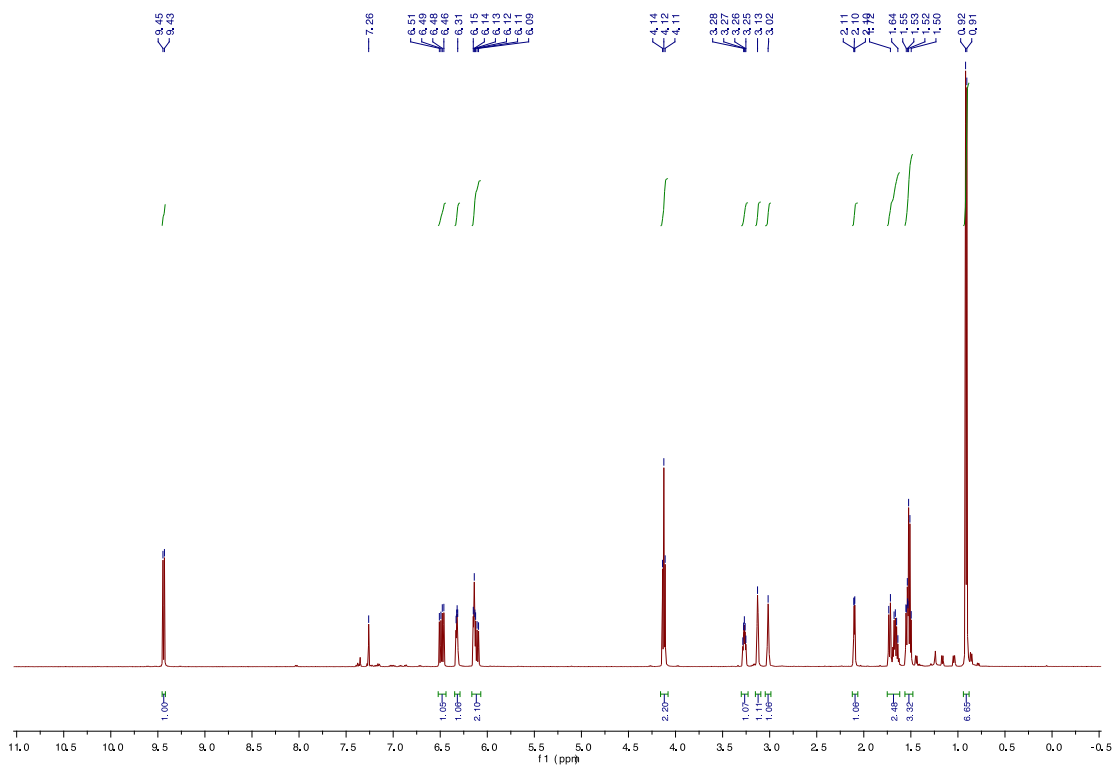
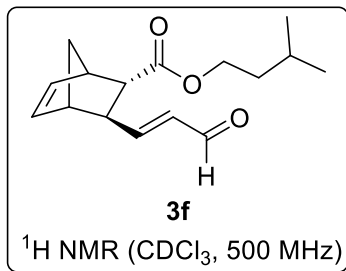


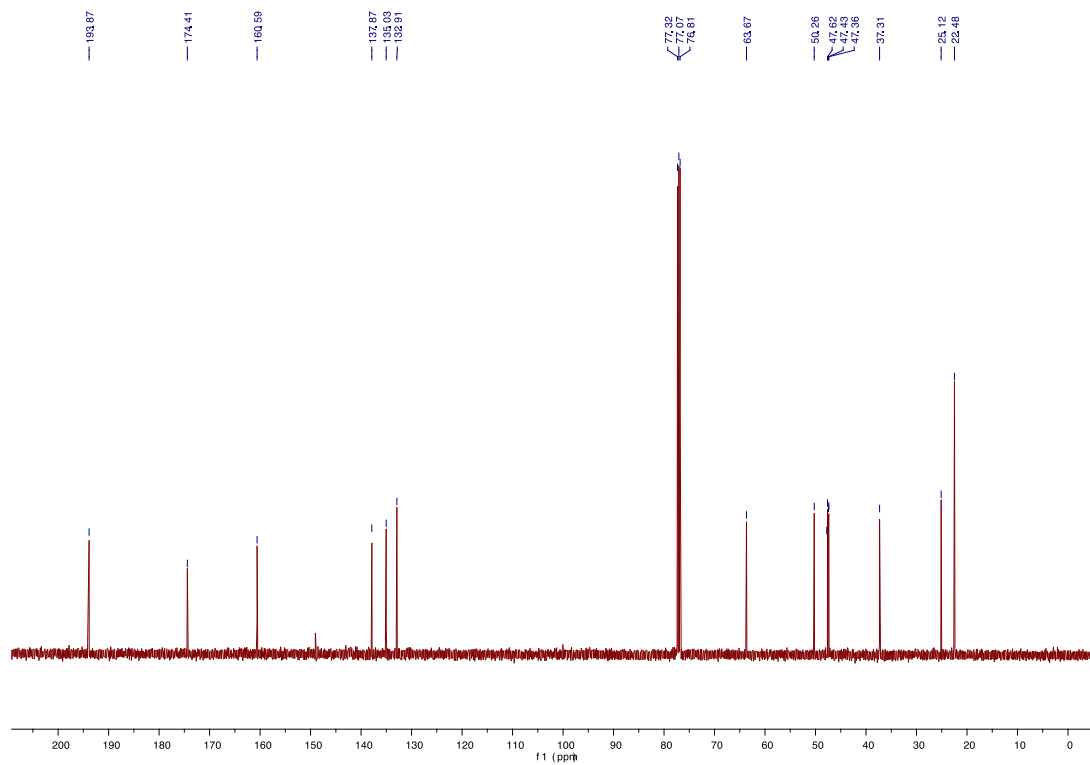
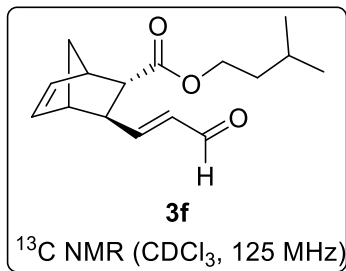


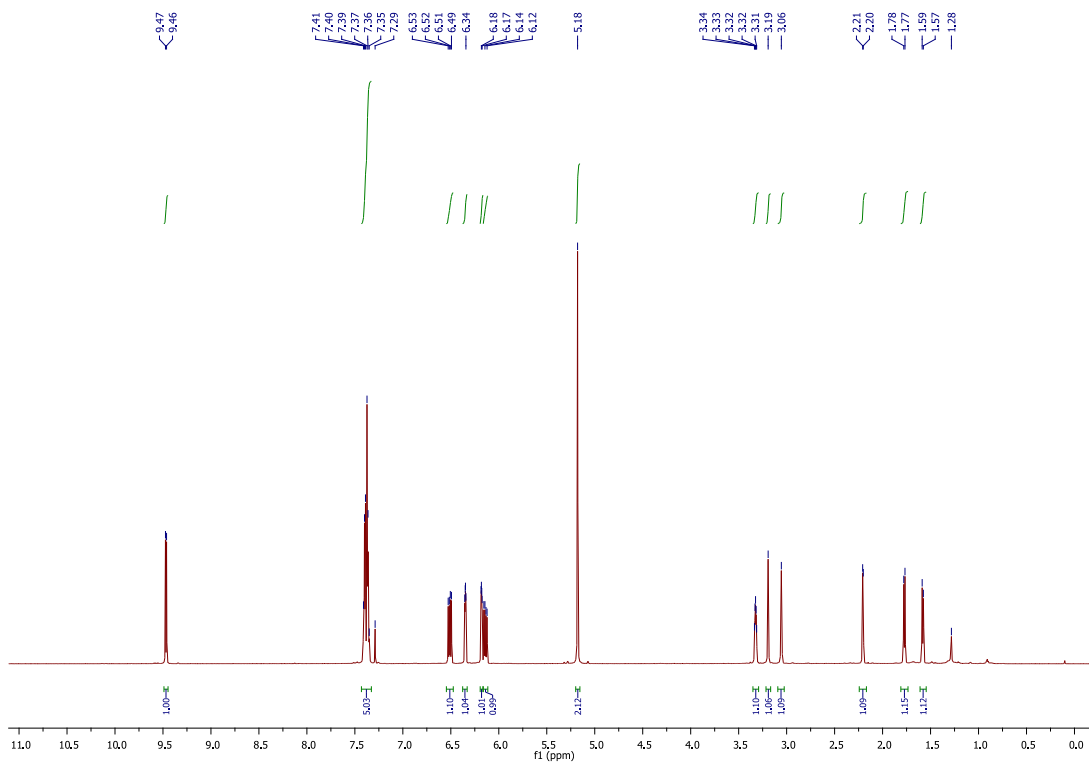
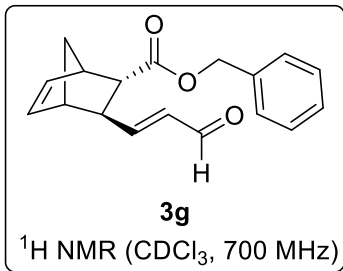


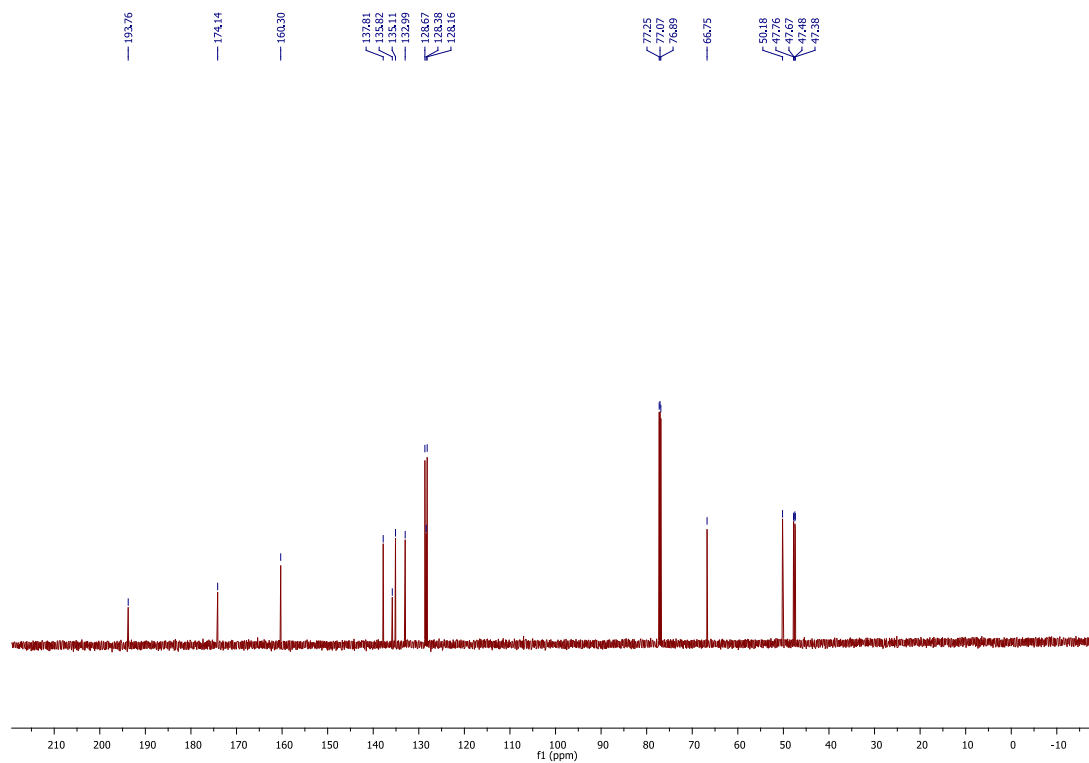
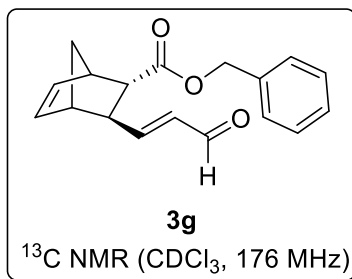


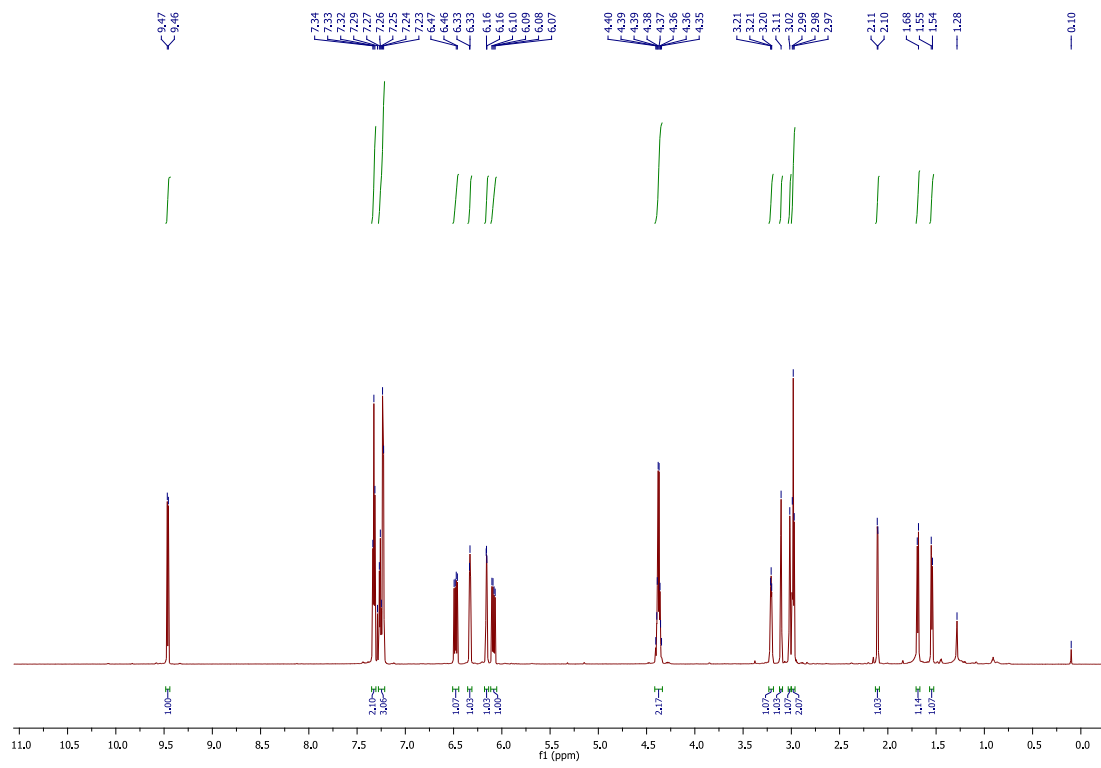
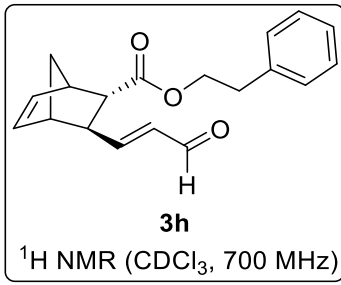


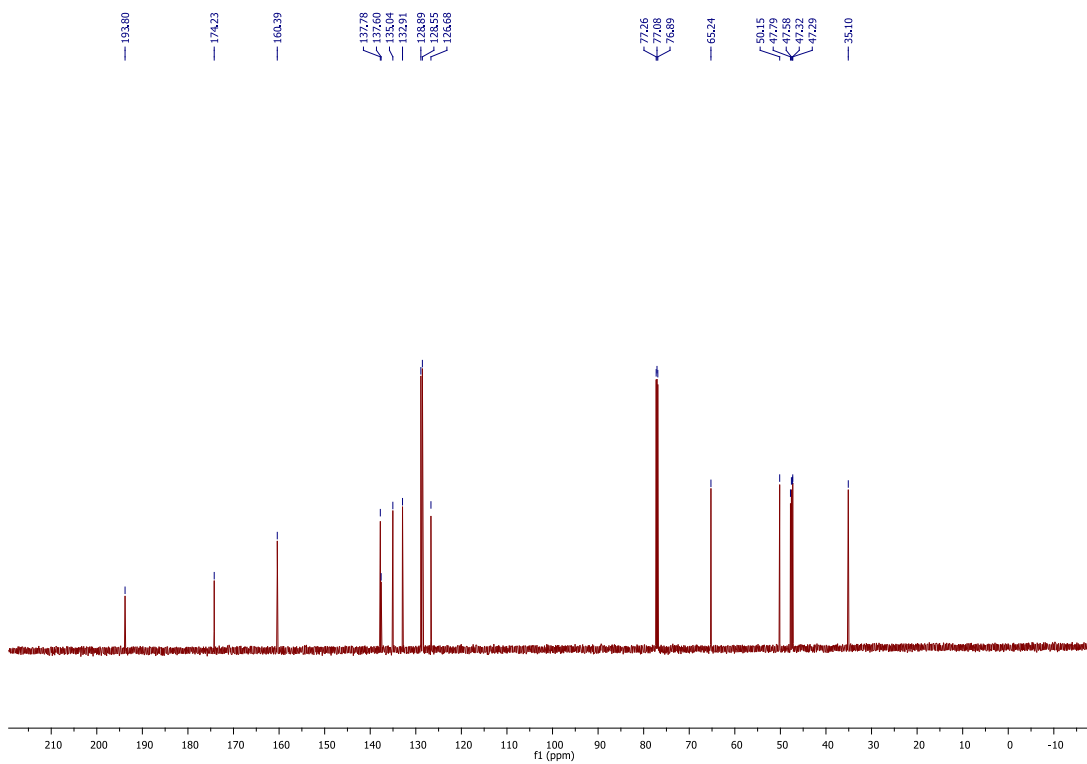
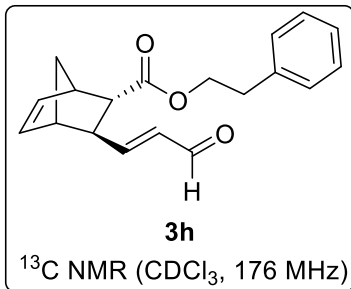


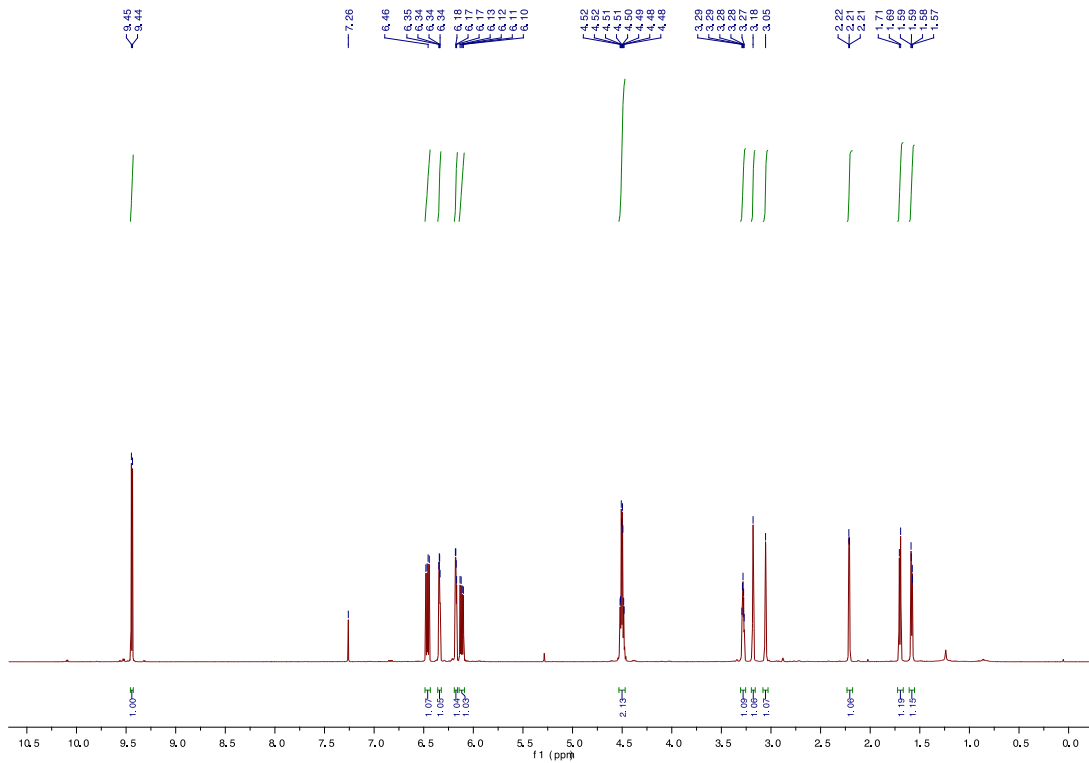
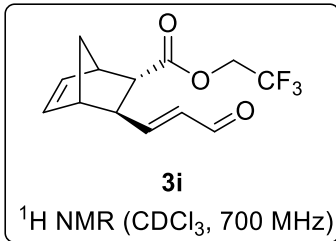


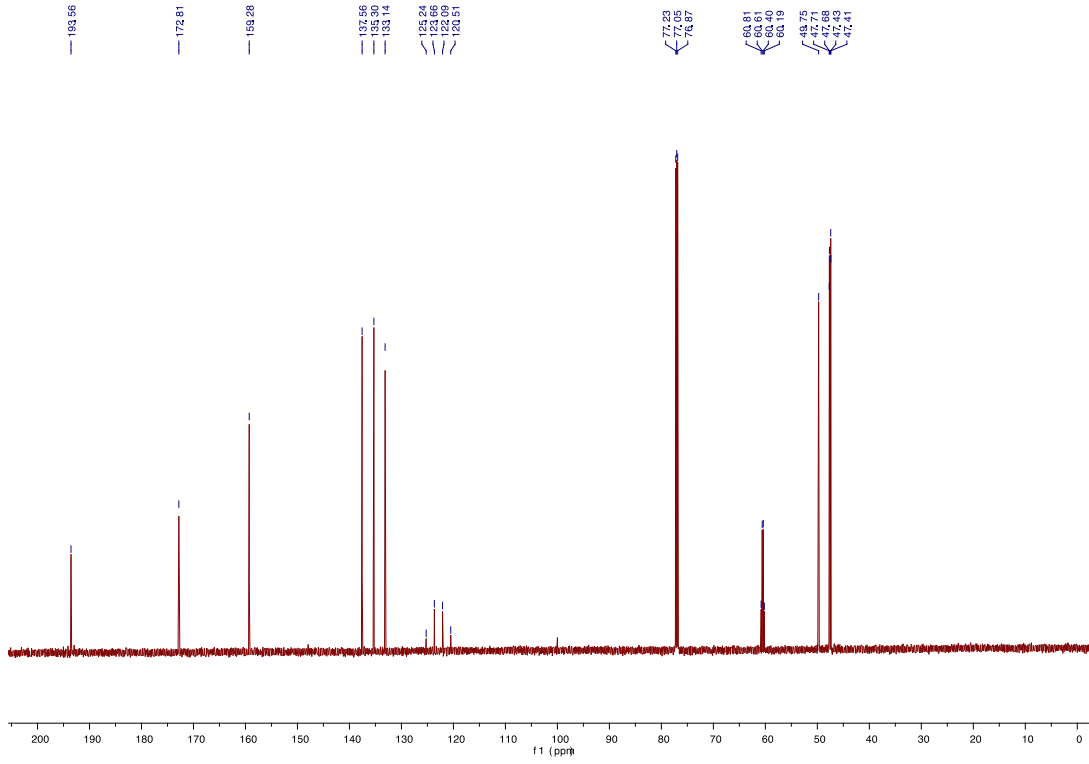
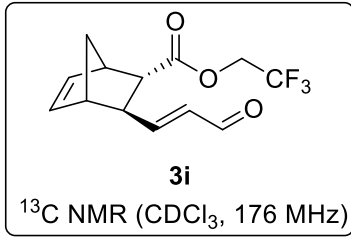


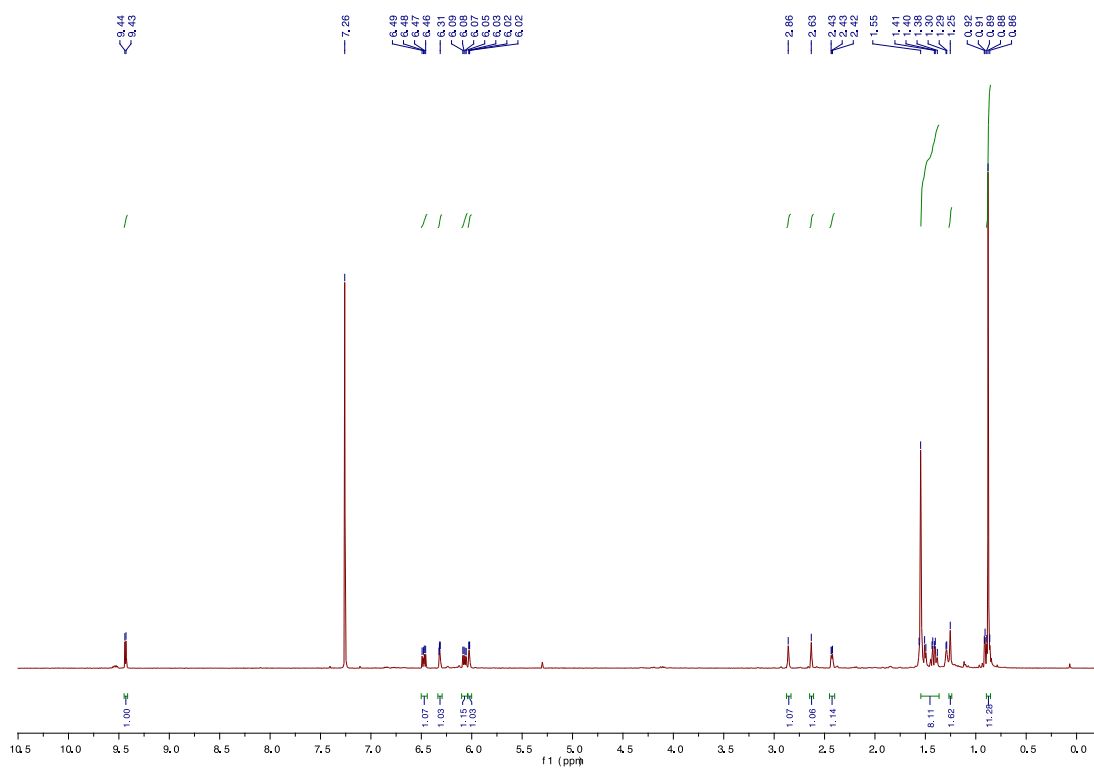
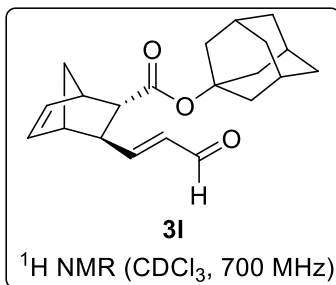


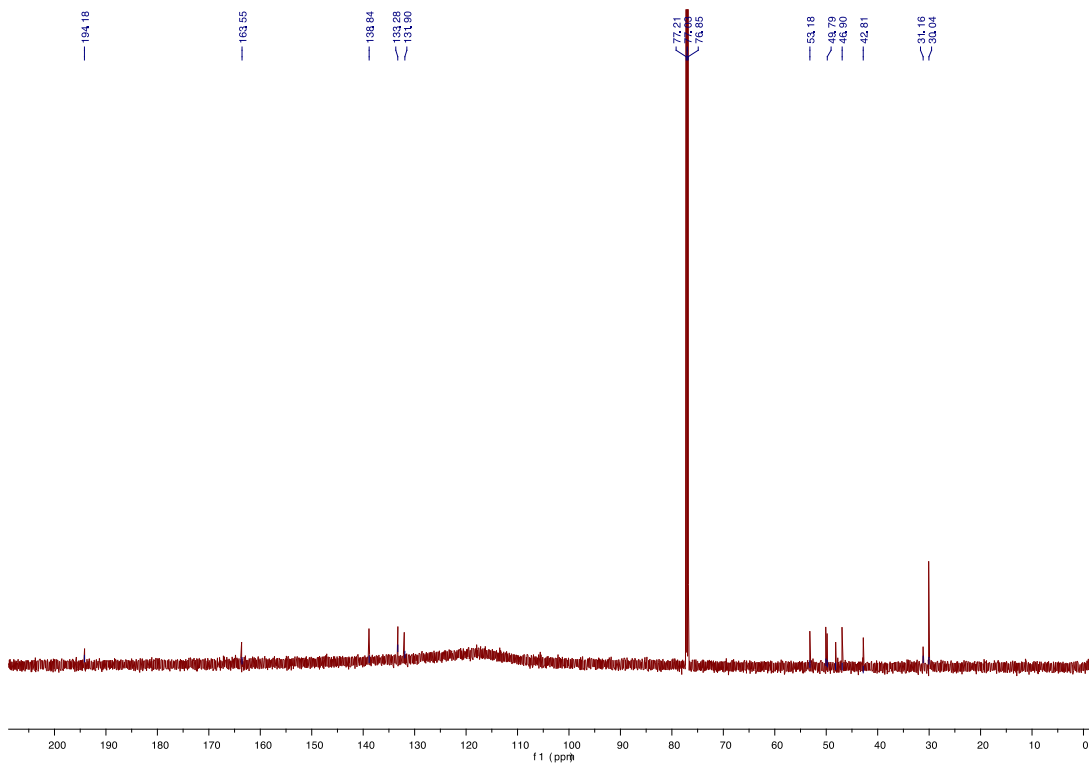
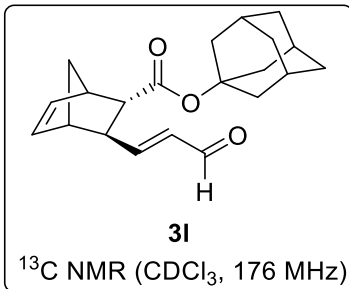


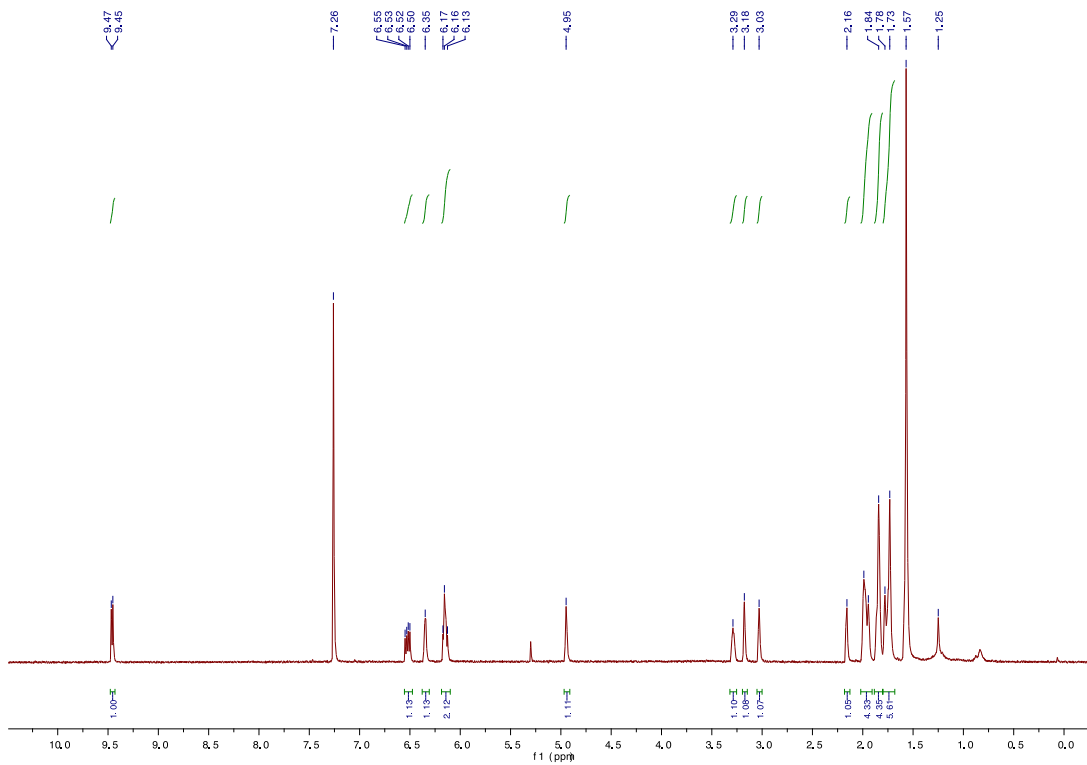
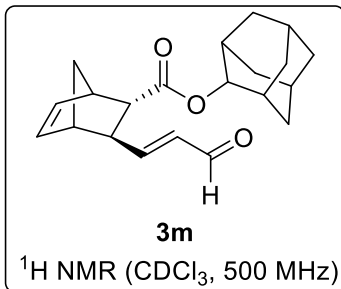


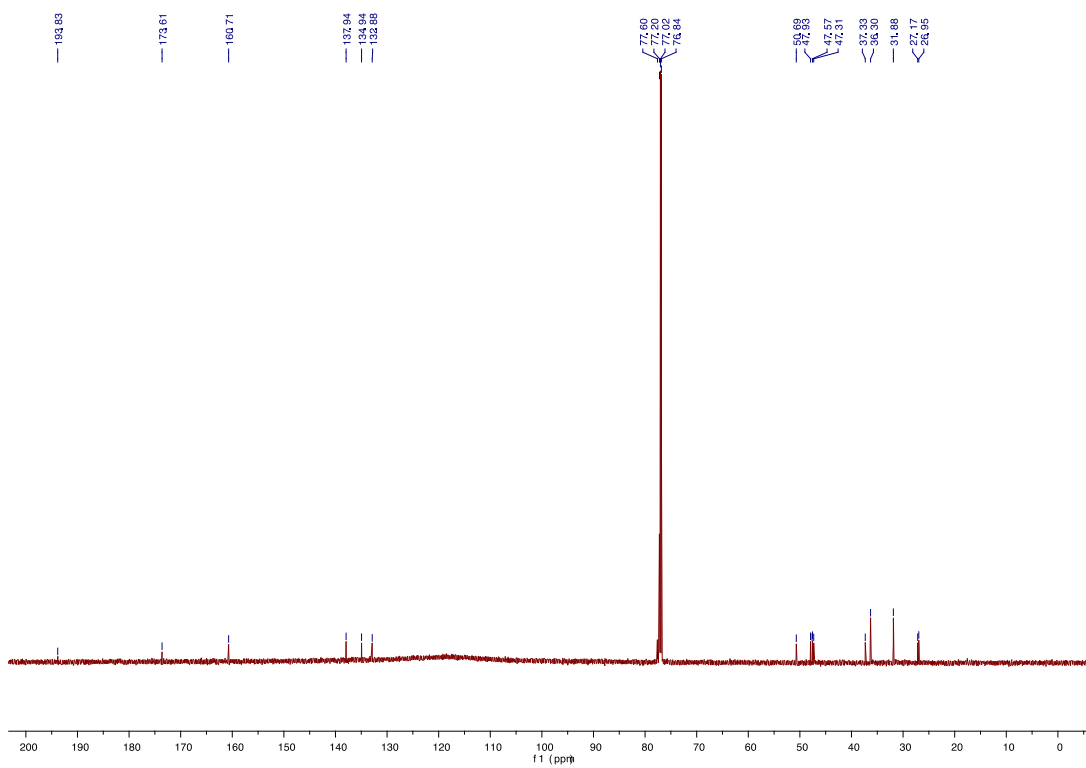
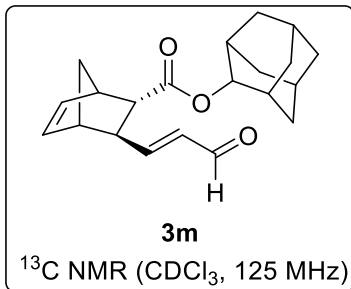


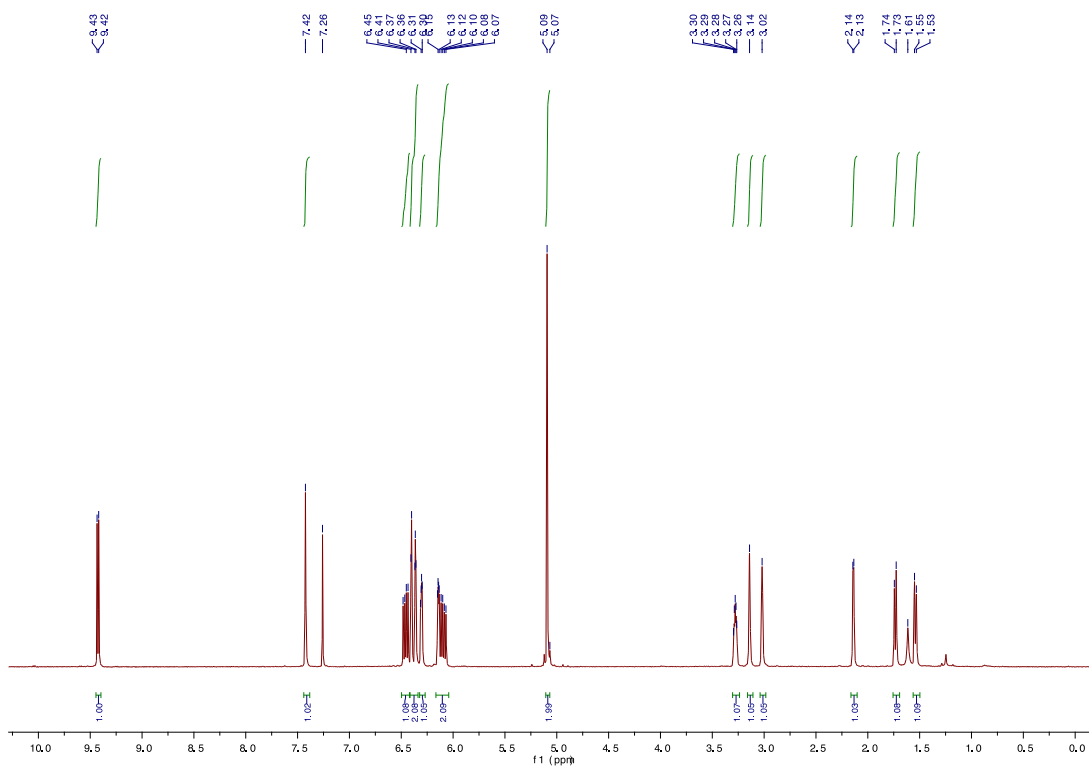
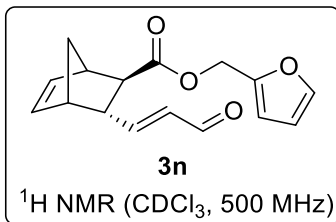


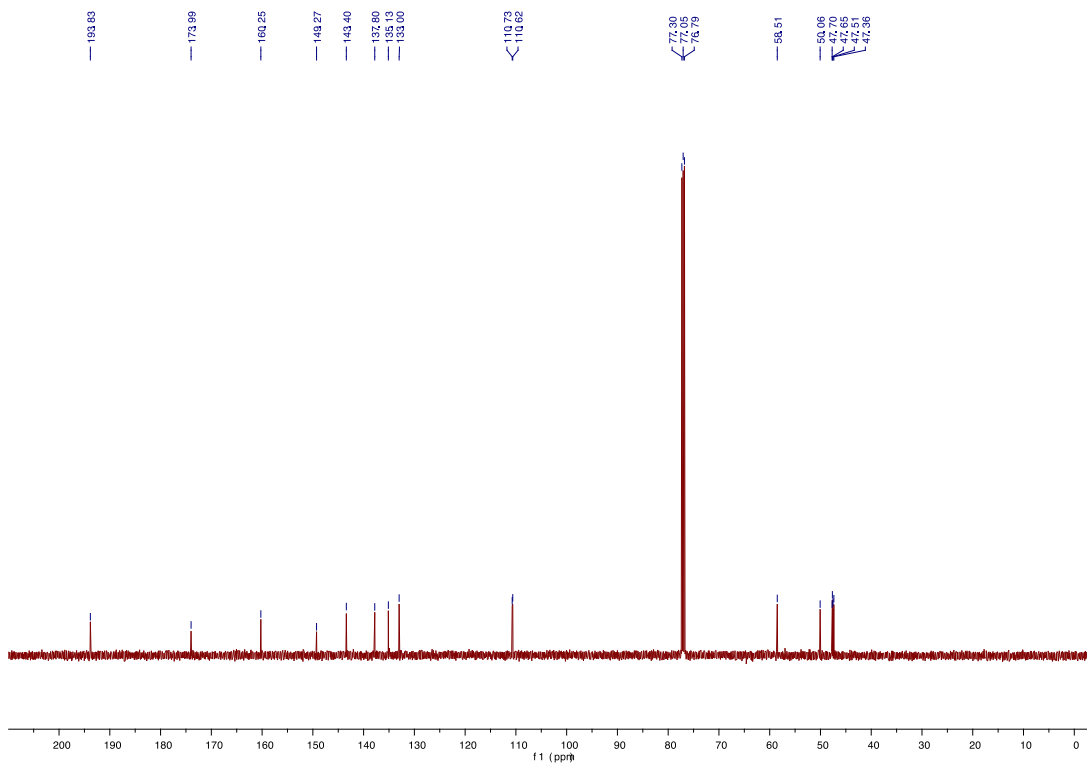
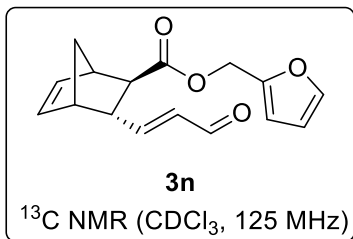


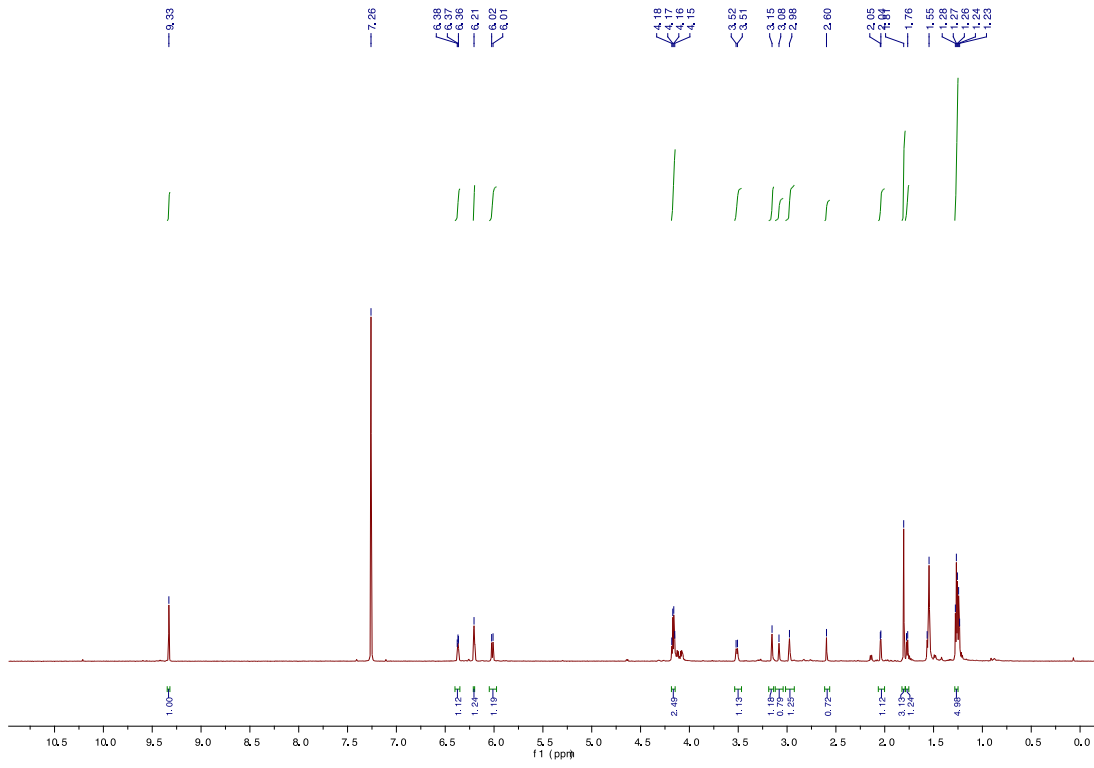
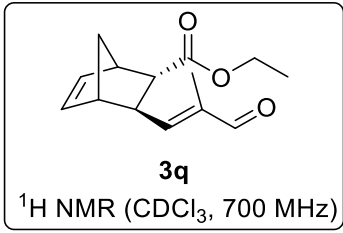


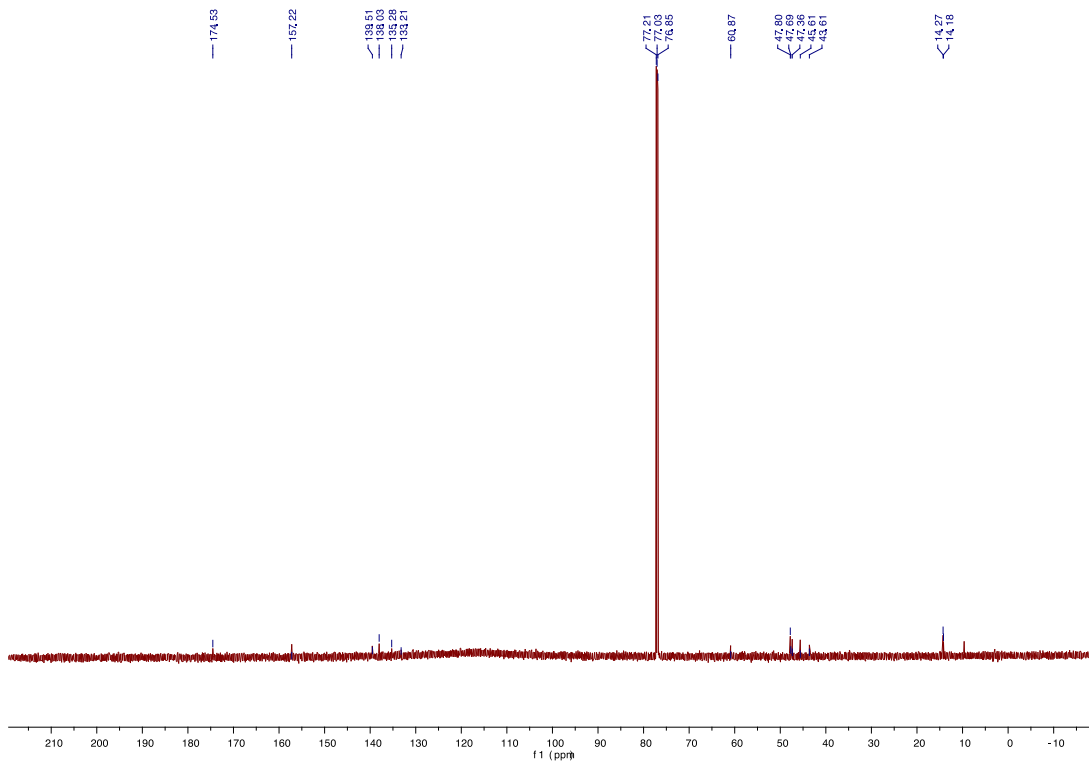
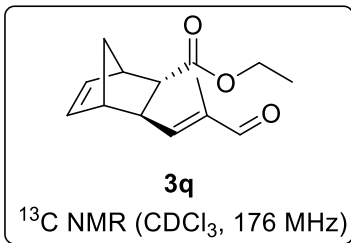


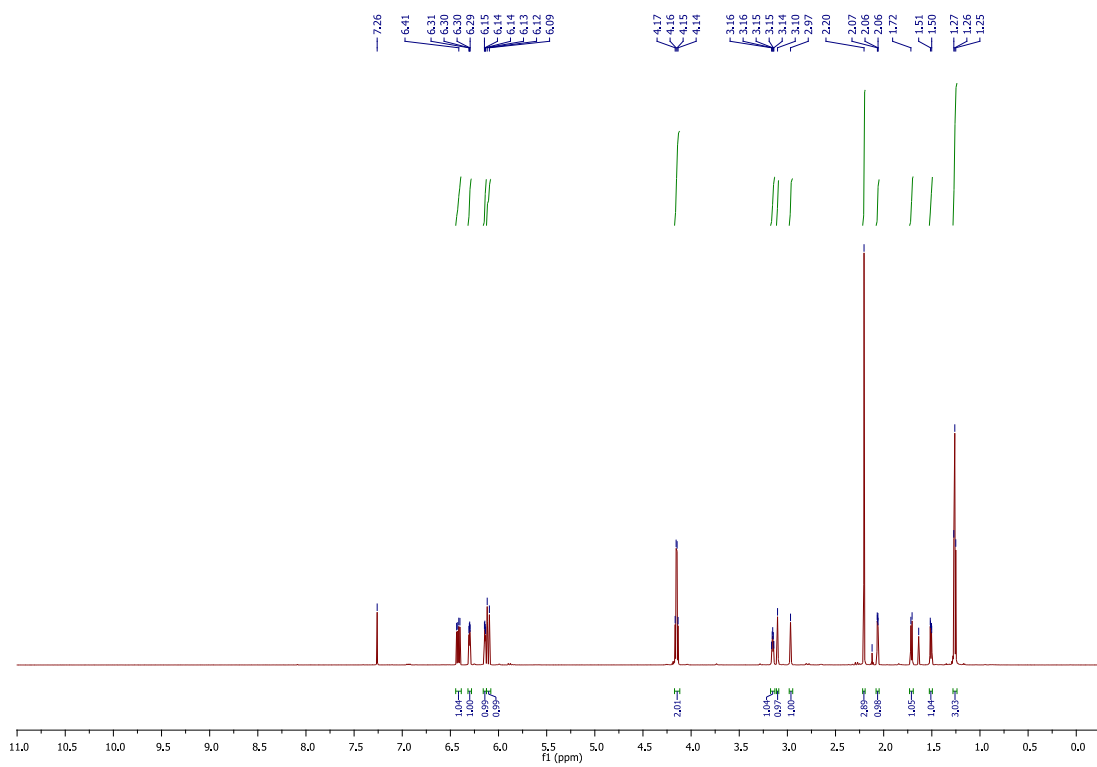
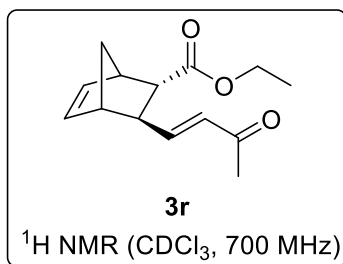


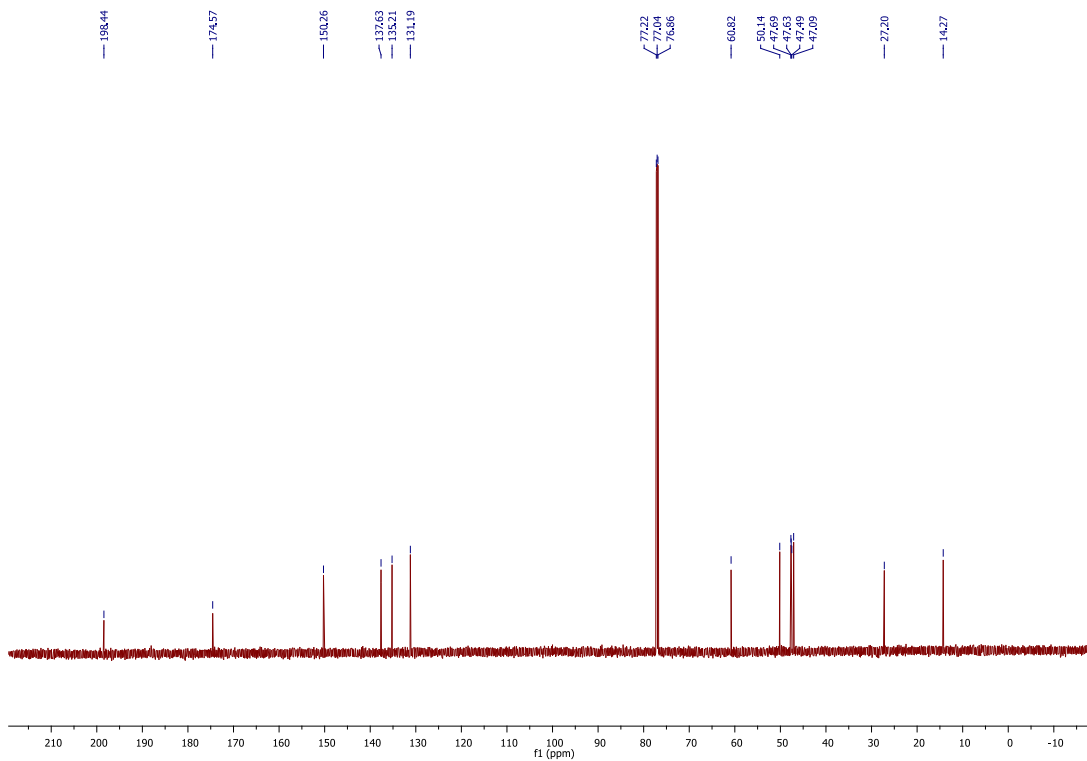
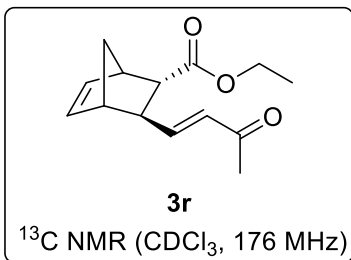


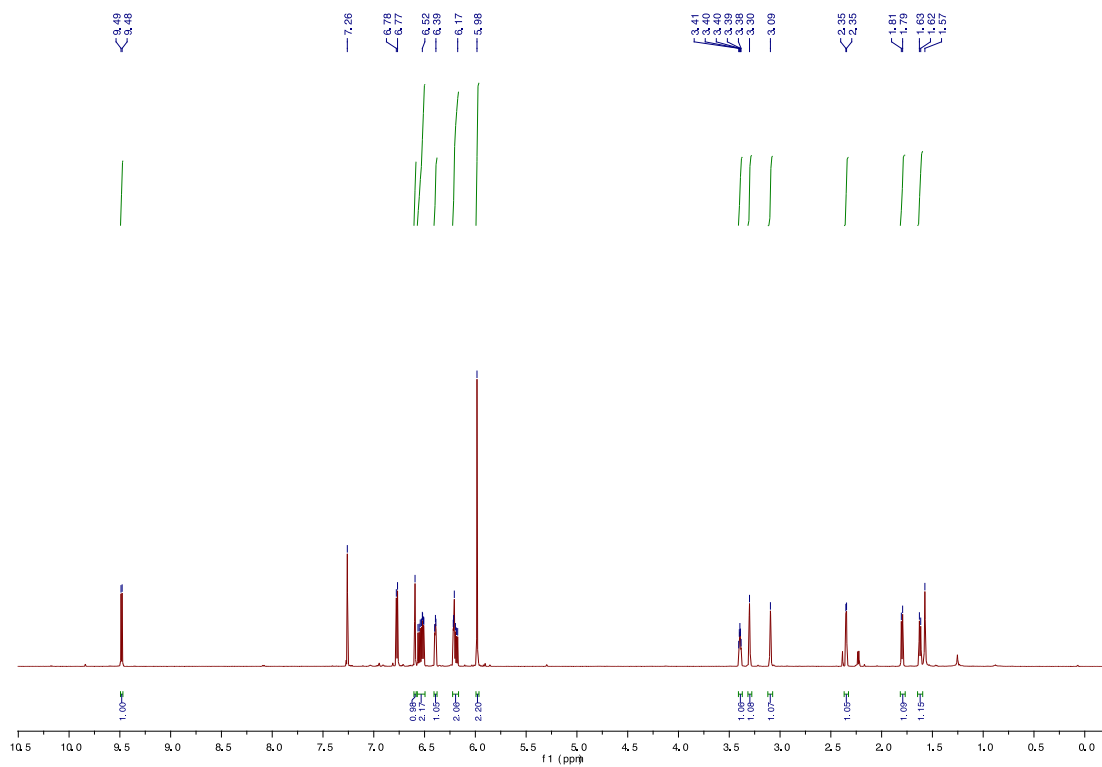
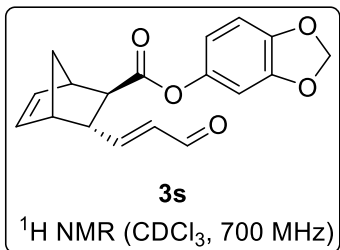


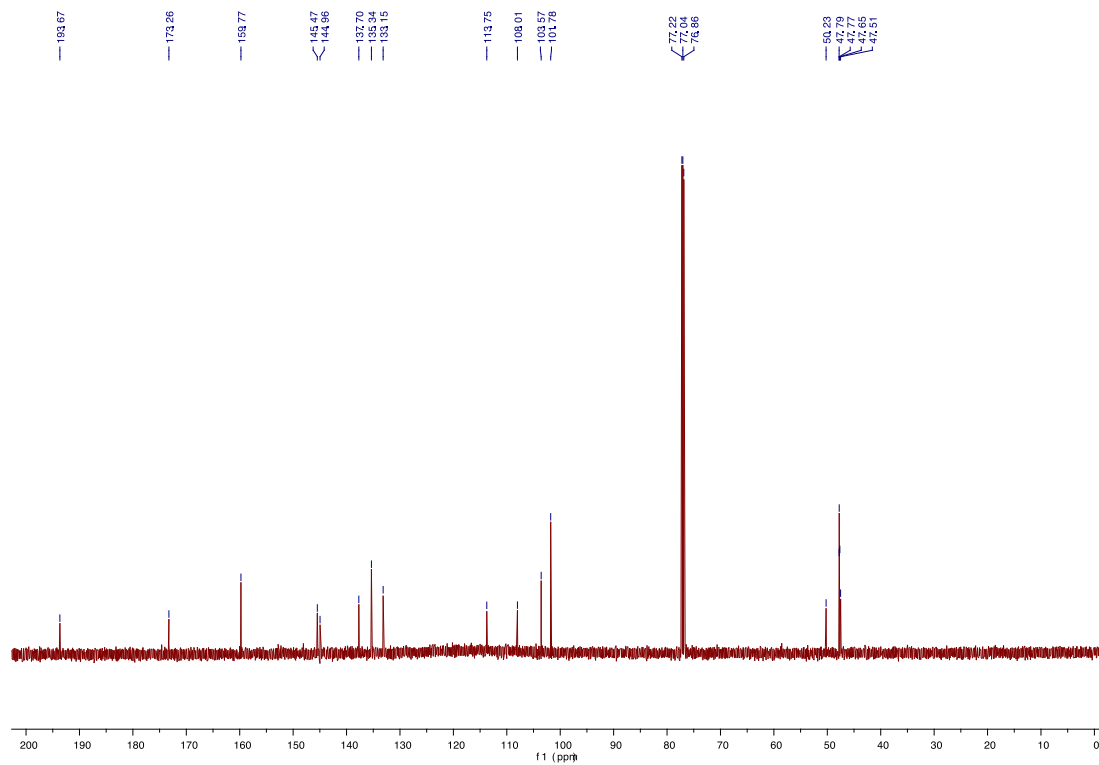
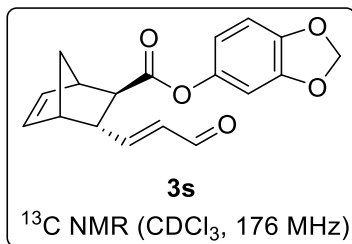


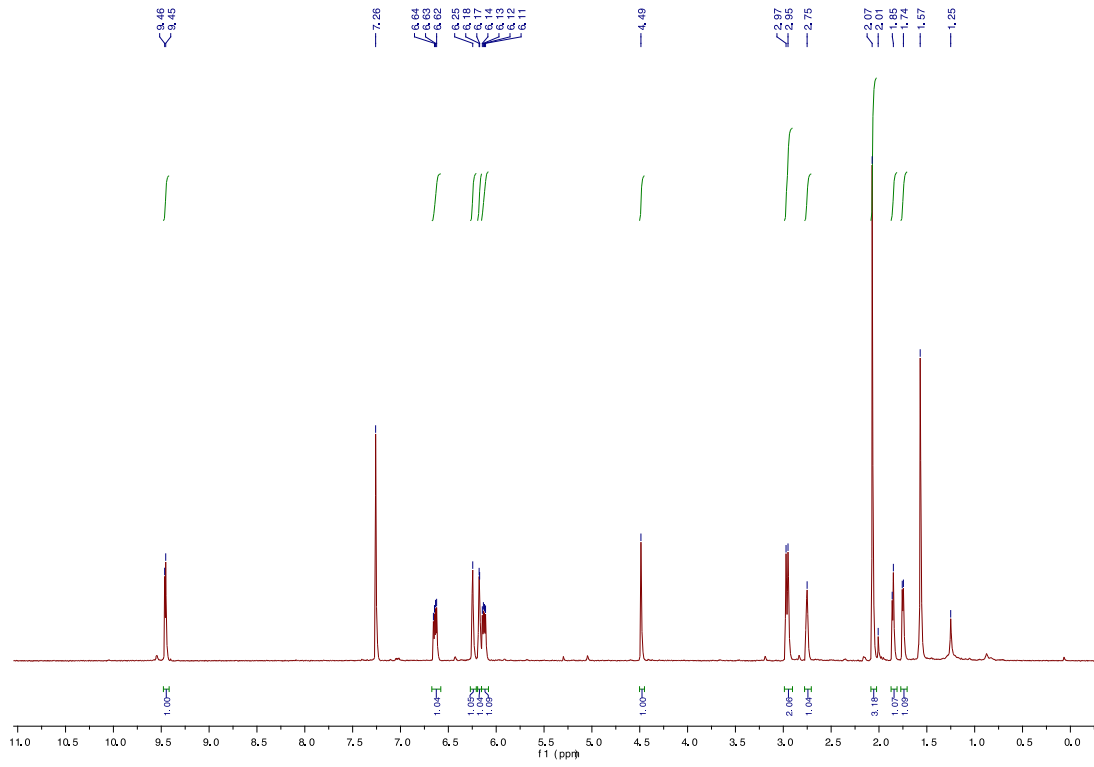
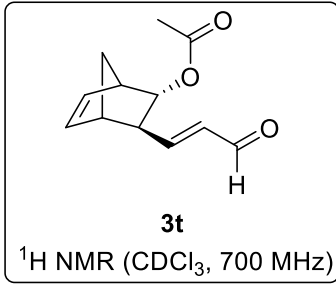


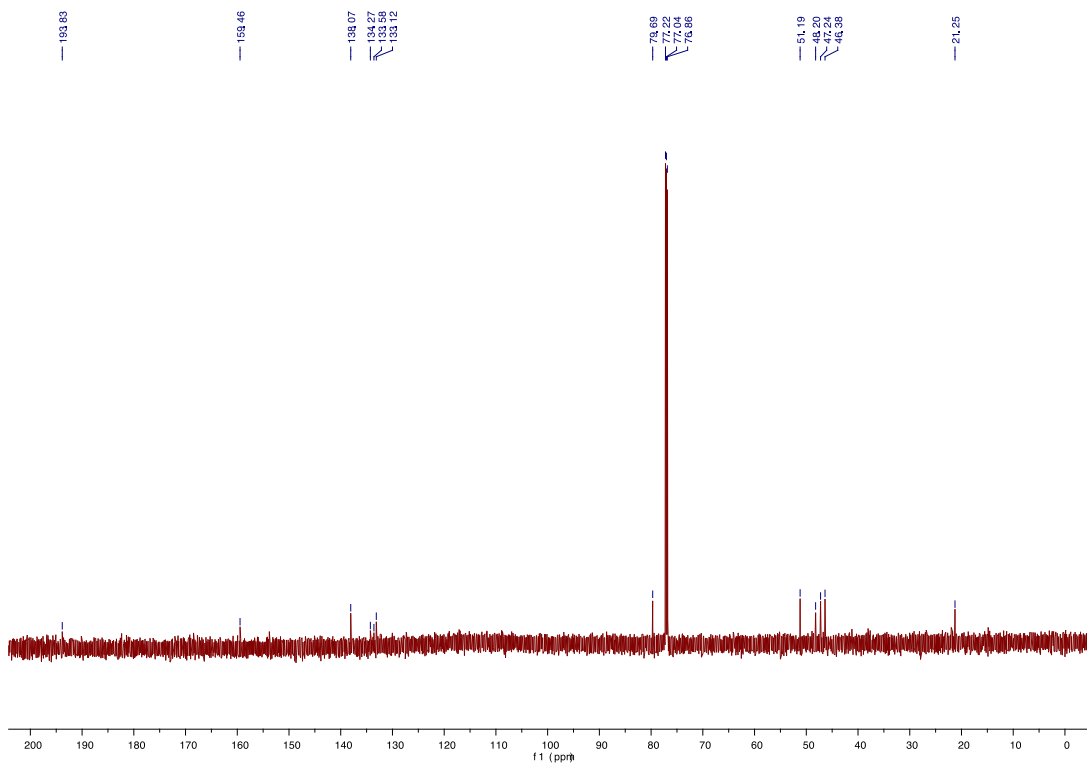
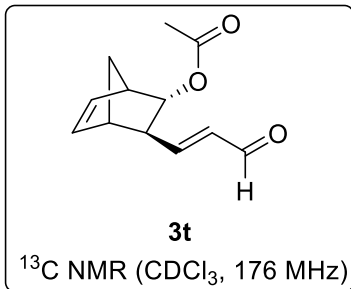












11. Crystal data and structure refinement for 4z-NTf₂.

Identification code	ch_mh_0306
Empirical formula	C ₄₈ H ₅₅ Au F ₆ N ₄ O ₁₁ S ₂
Formula weight	1239.04
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group	P 2 ₁ 2 ₁ 2 ₁
Unit cell dimensions	a = 9.1199(2) Å α = 90° b = 23.4191(6) Å β = 90° c = 23.6083(7) Å γ = 90°
Volume	5042.3(2) Å ³
Z	4
Density	1.632 Mg/m ³
Absorption coefficient	3.086 mm ⁻¹
F(000)	2496
Crystal size	0.3 × 0.1 × 0.05 mm ³
Theta range for data collection	3.316° to 29.698°
Index ranges	-12 ≤ h ≤ 10, -32 ≤ k ≤ 32, -32 ≤ l ≤ 32
Reflections collected	148806
Independent reflections	13136 [R(int) = 0.1034]
Completeness to theta = 25.242°	99.7%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	n/a
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	13136 / 0 / 669

Goodness-of-fit on F^2	1.033
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0309$, $wR_2 = 0.0512$
R indices (all data)	$R_1 = 0.0424$, $wR_2 = 0.0529$
Absolute structure parameter	-0.009(3)
Extinction coefficient	n/a
Largest diff. peak and hole	0.623 and -0.718 \AA^3

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