Supporting information

DIASTEREO–/ENANTIOSELECTIVE DIELS–ALDER SYNTHESIS OF 14β-HYDROXYSTEROID SCAFFOLDS: A COMBINED EXPERIMENTAL AND DFT STUDY

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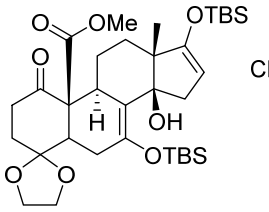
I General remarks

Reactions were carried out under argon with magnetic stirring and degassed solvents. Et_2O and THF were distilled over alumina on a dry solvent station GT S100. Thin layer chromatography (TLC) was carried out on silica gel plates (Merck 60F254) and the spotswerevisualized under UV lamp (254 or 365 nm) and sprayed with phosphomolybdic acidsolution (25 g phosphomolybdic acid, 10 g cerium sulfate, 60 mL H_2SO_4, 940 mLH_2O)followed by heating on a hot plate. For column chromatography, silica gel (Merck Si60 40-60µm) was used. IR spectra were recorded on Bruker Alpha (ATR) spectrophotomer. ^{1}H NMRspectra were recorded at 500 MHz (Bruker AC-500) and ^{13}C NMR spectra at 125 MHz(Bruker AC-500) using the signal of the residual non deuterated solvent as internalreference.Significant ^{1}H NMR data are tabulated in the following order: chemical shift(δ) expressed inppm, multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet), coupling constantsin hertz, number of protons. High-resolution mass spectra (HRMS) were performed on aAgilent 6520 Accurate Mass Q-TOF. High Pressure reactions have been done with a LV30/16 chamber and a U 101 press coming from the High Pressure Research Control ofthe Polish Academy of Sciences (Warsaw, Poland).

II Experimental procedures and spectral tabulations

Compound (±)-33.

Methyl (9S,10S,13S,14R)-7,17-bis((tert-butyldimethylsilyl)oxy)-14-hydroxy-13-methyl-1-oxo-2,3,5,6,9,11,12,13,14,15-decahydrospiro[cyclopenta[a]phenanthrene-4,2'-[1,3]dioxolane]-10(1H)-carboxylate



Chemical Formula: $C_{34}H_{56}O_8Si_2$
Molecular Weight: 648,98
White solid

A solution of diene **(±)-13** (100 mg, 0.23 mmol) and β-ketoester **31** (58 mg, 0.27 mmol) in toluene (1.5 mL) was submitted to high pressure (9 kbar) at 25 °C for 48 h. Solvent was removed under reduced pressure and the crude material was purified by chromatography on silica gel (petroleum ether / ethyl acetate 90/10 to 80/20) to afford **(±)-33** (116 mg, 0.18 mmol, 78%).

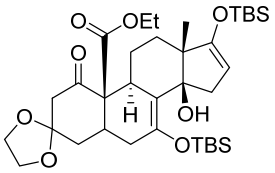
^{1}H NMR (500 MHz, $CDCl_3$): 0.07 (s, 3H, SiC**H**$_3$); 0.14 (s, 3H, SiC**H**$_3$); 0.17 (s, 3H, SiC**H**$_3$); 0.18 (s, 3H, SiC**H**$_3$); 0.87 (s, 9H, Si((CH$_3$)$_2$(C(C**H**$_3$)$_3$)); 0.91 (s, 9H, Si((CH$_3$)$_2$(C(C**H**$_3$)$_3$)); 1.02 (m, 1H); 1.03 (s, 3H, C**H**$_3$); 1.33 (m, 1H); 1.63 (m, 2H); 1.82 (m, 1H); 2.02 (m, 1H); 2.22 (m, 2H); 2.53 (m, 2H); 2.66 (m, 2H); 3.00 (t, J = 7.4 Hz, 1H); 3.32 (m, 1H); 3.67 (s, 3H, OC**H**$_3$); 4.00 (m, 4H,OC**H**$_2$C**H**$_2$O, 4H); 4.38 (t, J = 2.4 Hz, 1H, C**H**=C(OTBS)); 5.24 (s, 1H, CO**H**) ppm.

^{13}C NMR (125 MHz, $CDCl_3$): -5.45 (**C**H$_3$, Si**C**H$_3$); -4.28 (**C**H$_3$, Si**C**H$_3$); -3.2 (**C**H$_3$, Si**C**H$_3$); -2.5 (**C**H$_3$, Si**C**H$_3$); 17.7 (C**H**$_3$); 18.0 (Cq, Si((CH$_3$)$_2$(**C**(CH$_3$)$_3$)); 18.4 (Cq, Si((CH$_3$)$_2$(**C**(CH$_3$)$_3$)); 23.2 (**C**H$_2$); 25.6 (**C**H$_3$, Si((CH$_3$)$_2$(C(**C**H$_3$)$_3$)); 26.1 (**C**H$_3$, Si((CH$_3$)$_2$(C(**C**H$_3$)$_3$)); 29.5 (**C**H$_2$); 32.5 (**C**H$_2$); 33.2 (**C**H$_2$); 35.2 (**C**H); 36.6 (**C**H$_2$); 41.8 (**C**H); 42.6 (**C**H$_2$); 50.8 (Cq); 52.1 (CH$_3$, O**C**H$_3$); 62.3 (Cq); 64.0 (CH$_2$, O**C**H$_2$); 64.9 (CH$_2$, O**C**H$_2$); 81.5 (Cq, **C**OH); 94.6 (=**C**H, **C**H=C(OTBS)); 108.3 (Cq, **C**(OCH$_2$)$_2$); 119.3 (=C); 141.4 (=C); 159.9 (=C); 170.6 (COO); 205.6 (CO) ppm.

IR (ATR) : ν (OH) : 3502 cm^{-1}, ν (CO) : 1720, 1646 cm^{-1}, ν (C=C) : 836 cm^{-1}.
HRMS (ESI) m/z : $C_{34}H_{56}O_8Si_2$ $[M + K]^+$ calc. 687.3151, found. 687.3145.

Compound (±)-34

Ethyl-7,17-bis((*tert*-Butyldimethylsilyl)oxy)-14-hydroxy-13-methyl-1-oxo-1,2,5,6,9,11,12,13,14,15-decahydrospiro[cyclopenta[a]phenanthrene-3,2-[1,3]dioxolane]-10(4*H*)-carboxylate (±)-34

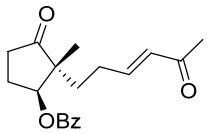


Chemical Formula: $C_{35}H_{58}O_8Si_2$
Molecular Weight: 663,01
White solid

A solution of diene **(±)-13** (100 mg, 0.23 mmol) and β-ketoester **32** (62 mg, 0.27 mmol) in toluene (1.5 mL) was submitted to high pressure (9 kbar) at 25 °C for 48 h. Solvent was removed under reduced pressure and the crude material was purified by silica gel chromatography (petroleum ether / ethyl acetate 90/10) to afford **(±)-34** (129 mg, 0.19 mmol, 85%) as a white solid: mp = 139-140 °C; IR (ATR, cm^{-1}): 3492, 1720 , 840; ^1H NMR (500 MHz, $CDCl_3$) δ 0.10 (s, 3H); 0.14 (s, 3H); 0.15 (s, 3H); 0.16 (s, 3H); 0.87 (s, 9H); 0.91 (s, 9H); 1.02 (s, 3H); 1.10 (m, 1H) 1.21 (t, J = 7.1 Hz, 3H); 1.44 (m, 2H); 1.53 (m, 1H); 1.83 (dd, J = 14.4 Hz, 4.3 Hz, 1H); 2.03 (dd, J = 17.4 Hz, 7.8 Hz, 1H); 2.34 (dd, J = 14.2 Hz, 4.7 Hz, 1H); 2.55 (m, 4H); 2.75 (m, 2H); 3.17 (t, J = 9.3 Hz, 1H); 3.88 (m, 4H); 4.00 (m, 1H); 4.19 (m, 1H); 4.41 (t, J = 2.2 Hz, 1H); 5.63 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ -5.1, -4.6, -3.5, -2.9, 14.0, 18.0, 18.3, 19.3, 23.6, 25.6, 26.0, 30.8, 31.7, 32.1, 33.6, 36.2, 43.0, 50.0, 51.6, 61.3, 62.4, 64.0, 64.8, 81.9, 94.6, 110.4, 119.0, 140.9, 159.1, 170.0, 200.7. IR (ATR, cm^{-1}): 3492, 1720 , 840. HRMS (ESI) *m/z*: calcd for $C_{35}H_{58}O_8Si_2$ $[M + Na]^+$ 685.3568; found, 685.3562.

*Compound (+)-**44***

(1*S*,2*R*)-2-Methyl-3-oxo-2-((*E*)-5'-oxohex-3'-en-1'-yl)cyclopentyl benzoate (+)-44



Chemical Formula: $C_{19}H_{22}O_4$
Molecular Weight: 314,38
Colorless oil

To a solution of aldehyde **(+)-43** (0.44 g, 1.6 mmol) in CH_2Cl_2 (20 mL) was added 1-(triphenylphosphoranylidene)-2-propanone (0.77 g, 2.4 mmol). The reaction mixture was stirred for 20 h at room temperature and the solvent was evaporated under reduced pressure. The crude material was purified by silica gel chromatography (petroleum ether / ethyl acetate, 90/10 to 60/40) to afford compound **(+)-44** (0.43 g, 1.3 mmol, 86 %).

^1H NMR (500 MHz, $CDCl_3$): 0.86 (m, 1H); 1.05 (s, 3H, CH_3); 1.64 (m, 2H); 2.08 (m, 1H); 2.19 (s, 3H, C(O)C**H**$_3$); 2.31 (m, 2H); 2.45 (m, 1H); 2.55 (m, 1H); 5.48 (t, J = 5.5 Hz, 1H, C**H**OCOPh); 6.06 (dt, J = 16.0 Hz, 1.6 Hz, 1H, CH=C**H**-CO); 6.71 (dt, J = 16.0 Hz, 6.7 Hz,

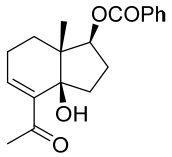
1H, C**H**=CH-CO); 7.43 (m, 2H); 7.55 (m, 2H); 7.99 (m, 2H) ppm.

^{13}C NMR (125 MHz, $CDCl_3$): 16.2 (CH_3); 25.3 (CH_2); 26.9 (CH_2); 27.0(CH_3, C(O)**C**H_3); 33.4 (CH_2); 35.0 (CH_2); 52.2 (Cq); 77.4 (CH, **C**HOCOPh); 128.5 (2 =CH); 129.6 (2 =CH); 129.7 (=C); 131.6 (=CH); 133.4 (=CH); 146.9 (=CH); 165.8 (COO); 198.5 (CO, =CH-**C**O); 218.3 (CO) ppm.

IR (ATR) : ν (COO) : 1741 $cm^{-1;}$ ν (CO) : 1717, 1674 cm^{-1}
HRMS (ESI) m/z : $C_{19}H_{22}O_4$ [M + Na], calc. 337.1416 found. 337.1421.
$[\alpha]^{20}_D$: +57.2 (*c* = 1, $CHCl_3$)

*Compound (+)-**45***

(1*S*,3a*R*,7a*R*)-4-Acetyl-3a-hydroxy-7a-methyl-2,3,3a,6,7,7a-hexahydro-1*H*-inden-1-yl benzoate (-)-45



Chemical Formula: $C_{19}H_{22}O_4$
Molecular Weight: 314,38
Colorless oil

A solution of α,β unsaturated ketone **(+)-44** (94 mg, 0.3 mmol) and *n*-Bu_3P (0.07 mL, 0.3 mmol) in toluene (1.5 mL) was submitted to high pressure (9 kbar) at 25 °C for 48 h. Solvent was removed under reduced pressure and the crude material was purified by silica gel chromatography (petroleum ether / ethyl acetate 80/20) to afford **(-)-45** (54 mg, 0.17 mmol, 57 %).

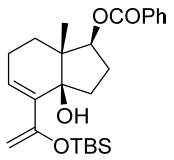
^{1}H NMR (500 MHz, $CDCl_3$): 1.07 (s, 3H); 1.51 (m, 1H); 1.61 (m, 1H); 1.86 (m, 1H); 2.05 (m, 1H); 2.33 (s, 3H, C(O)C**H**$_3$); 2.35 (m, 4H); 4.18 (s, 1H, CO**H**); 5.09 (dd, *J* = 7,7 Hz, 5,2 Hz, 1H, **H**CO_2Ph); 6.9 (t, *J* = 3,9 Hz, 1H, **H**C=C-C(O)); 7.41 (m, 2H); 7.52 (m, 1H); 8.07 (m, 2H) ppm.
^{13}C NMR (125 MHz, $CDCl_3$): 14.0 (CH_3); 23.5 (CH_2); 26.5 (CH_3, C(O)**C**H_3); 28.9 (CH_2); 30.7 (CH_2); 38.5 (CH_2); 47.5 (Cq); 79.9 (**C**OH); 80.5 (CH, H**C**O_2Ph); 128.4 (2 =CH); 129.7 (2 =CH); 130.6 (Cq); 132.9 (=CH); 141.7 (=CH); 142.6 (Cq); 166.5 (COO); 202.2 (CO) ppm.

IR (ATR) : ν (OH) : 3499 cm^{-1}; ν (CO) : 1711, 1651 cm^{-1}

HRMS (ESI) m/z : $C_{19}H_{22}O_4$ [M + Na]$^+$ calc. 337,1416, found. 337,1410.
[α]$^{20}_D$: -63 (*c* = 1, $CHCl_3$)

*Compound (+)-**46***

(1*S*,3a*R*,7a*R*)-4-(1-((*tert*-Butyldimethylsilyl)oxy)vinyl)-3a-hydroxy-7a-methyl-2,3,3a,6,7,7a-hexahydro-1*H*-inden-1-yl benzoate (+)-46



Chemical Formula: $C_{25}H_{36}O_4Si$
Molecular Weight: 428,64
Colorless oi

To a solution of compound **(-)-45** (0.3 g, 0.95 mmol) in CH_2Cl_2 (14 mL) was added Et_3N (0.4 mL, 2.8 mmol) and the reaction mixture was stirred for 0.2 h at room temperature. TBSOTf (0.26 mL, 1.1 mmol) was added and the reaction mixture was stirred 1h at room temperature. Then, the reaction mixture was quenched with addition of water, the layers were separated and the aqueous layer was washed with CH_2Cl_2 (3x 50mL). The combined organic layers were washed with an aqueous sat. solution of $NaHCO_3$ and were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude material was purified by silica gel chromatography (petroleum ether / ethyl acetate / Et_3N, 79/20/1) to afford compound **(+)-46** (0.405 g, 0.94 mmol, 99%)

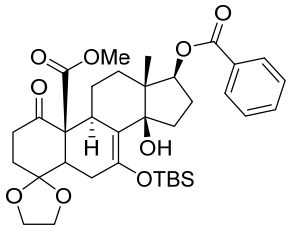
^{1}H NMR (500 MHz, $CDCl_3$): 0.21 (s, 3H, SiC**H**$_3$); 0.22 (s, 3H, SiC**H**$_3$); 0.94 (s, 9H, Si((CH$_3$)$_2$(C(C**H**$_3$)$_3$)); 1.18 (s, 3H); 1.53 (m, 2H); 1.88 (m, 1H); 2.18 (m, 5H); 2.91 (s, 1H, COH); 4.26(d, *J* = 1.4 Hz, 1H, **H**$_2$C=C(OTBS)); 4.55 (d, *J* = 1.4 Hz, 1H, **H**$_2$C=C(OTBS)); 5.15 (m, 1H, **H**CO$_2$Ph); 6.09 (t, *J* = 4.0 Hz, 1H, **H**C=C-COH); 7.41 (m, 2H); 7.54 (m, 1H); 8.03 (m, 2H) ppm.

^{13}C NMR (125 MHz, $CDCl_3$): -4.1 (CH$_3$); -4.2 (CH$_3$); 15.9 (CH$_3$); 18.7 (Si((CH$_3$)$_2$(**C**(CH$_3$)$_3$)); 22.6 (CH$_2$); 26.4 (3 CH$_3$ Si((CH$_3$)$_2$(C(**C**H$_3$)$_3$)); 28.2 (CH$_2$); 29.1 (CH$_2$); 36.7 (CH$_2$); 47.8 (Cq); 78.8 (CH, H**C**O$_2$Ph); 79.4 (COH); 93.5 (=CH$_2$); 128.1 (=CH); 128.8 (2 =CH); 130.0 (2 =CH); 131.1 (Cq); 133.3 (=CH); 139.7 (Cq); 157.7 (Cq); 166.7 (COO) ppm.

IR (ATR) : ν (OH) : 3546 cm^{-1}; ν (CO) : 1716 cm^{-1}; ν (C=C) : 839 cm^{-1}
HRMS (ESI) m/z : $C_{25}H_{36}O_4Si$ [M + K]$^+$ calc. 467.2020, found. 467.2014
[α]$^{20}_D$: +8,8 (*c* = 1, $CHCl_3$)

Compound (+)-48

Methyl (9*S*,10*S*,13*R*,14*R*,17*S*)-17-(benzoyloxy)-7-((*tert*-Butyldimethylsilyl)oxy)-14-hydroxy-13-methyl-1-oxo-2,3,5,6,9,11,12,13,14,15,16,17-dodecahydrospiro[cyclopenta[a]phenanthrene-4,2'-[1,3]dioxolane]-10(1*H*)-carboxylate (+)-48



Chemical Formula: $C_{35}H_{48}O_9Si$
Molecular Weight: 640,85
Colorless oil

A solution of diene **(+)-46** (100 mg, 0.23 mmol) and β-ketoester **31** (59 mg, 0.28 mmol) in toluene (1.5 mL) was submitted to high pressure (9 kbar) at 25 °C for 48 h. Solvent was removed under reduced pressure and the crude material was purified by silica gel chromatography (petroleum ether / ethyl acetate 80/20) to afford **(+)-48** (133 mg, 0.20 mmol, 89 %).

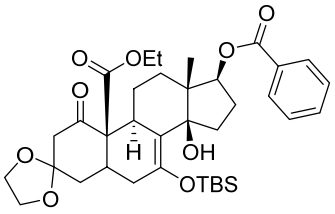
^{1}H NMR (500 MHz, $CDCl_3$): 0.20 (s, 6H, Si-C**H**$_3$); 0.94 (s, 9H, Si-C(C**H**$_3$)$_3$); 1.07 (s, 3H, C**H**$_3$); 1.08 (m, 1H); 1.29 (td, *J* = 13.6 Hz, 3.9 Hz, 1H); 1.59 (dt, *J* = 13.9 Hz, 2.8 Hz, 1H); 1.75 (qd, *J* = 12.9 Hz, 3.8 Hz, 1H); 1.87 (m, 1H); 2.02 (m, 3H); 2.25 (m, 3H); 2.36 (m, 1H); 2.53 (m, 1H); 2.71 (m, 1H); 3.03 (t, *J* = 7.5 Hz, 1H); 3.17 (m, 1H); 3.71 (s, 3H, OC**H**$_3$); 4.00 (m, 4H,OC**H**$_2$C**H**$_2$O, 4H); 4.98 (dd, *J* = 7.9 Hz, 3.3 Hz, 1H, C**H**CO$_2$Ph); 5.40 (s, 1H, OH); 7.38 (m, 2H); 7.49 (m, 1H); 8.06 (m, 2H) ppm.

^{13}C NMR (500 MHz, $CDCl_3$): -2.98 (**C**H$_3$, Si-**C**H$_3$); -2.77 (**C**H$_3$, Si-**C**H$_3$); 14.4 (C**H**$_3$); 18.4 (Cq, Si-**C**(CH$_3$)$_3$); 25.0 (**C**H$_2$); 26.0 (**C**H$_3$, Si-C(**C**H$_3$)$_3$); 29.6 (**C**H$_2$); 29.9 (**C**H$_2$); 32.4 (**C**H$_2$); 35.8 (**C**H$_2$); 36.4 (**C**H); 36.5 (**C**H$_2$); 37.1 (**C**H$_2$); 41.9 (**C**H); 50.6 (Cq); 52.2 (**C**H$_3$, O**C**H$_3$); 62.5 (Cq); 64.0 (CH$_2$, O**C**H$_2$); 65.0 (CH$_2$, O**C**H$_2$); 82.0 (**C**H, **C**HCO$_2$Ph); 85.3 (Cq, **C**OH); 108.2 (Cq, **C**(OCH$_2$)$_2$); 116.2 (=C); 128.2 (2 =CH); 129.8 (2 =CH); 131.1 (=C); 132.5 (=CH); 142.4 (=C); 166.6 (COO); 170.8 (COO) : 205.3 (CO) ppm.

IR (ATR) : ν (OH) = 3495 cm^{-1}, ν (CO) = 1711 cm^{-1}, ν (Ar) = 835 cm^{-1}, ν (C=C) = 713 cm^{-1}
HRMS (ESI) m/z : $C_{35}H_{48}O_9Si$ $[M + K]^+$ calc. 679.2705, found. 679.2699.
$[\alpha]^{20}_D$: +18 (*c* = 1, $CHCl_3$)

*Compound (+)-**49***

Ethyl (9*S*,10*R*,13*R*,14*R*,17*S*)-17-(benzoyloxy)-7-((*tert*-Butyldimethylsilyl)oxy)-14-hydroxy-13-methyl-1-oxo-1,2,5,6,9,11,12,13,14,15,16,17-dodecahydrospiro[cyclopenta[a]phenanthrene-3,2-[1,3]dioxolane]-10(4*H*)-carboxylate (+)-49



Chemical Formula: $C_{36}H_{50}O_9Si$
Molecular Weight: 654,87
White solid

A solution of diene **(+)-46** (100 mg, 0.23 mmol) and β-ketoester **32** (63 mg, 0.28 mmol) in toluene (1.5 mL) was submitted to high pressure (9 kbar) at 25 °C for 48 h. Solvent was removed under reduced pressure and the crude material was purified by silica gel chromatography (petroleum ether / ethyl acetate 85/15) to afford **(+)-49** (130 mg, 0.20 mmol, 85 %).

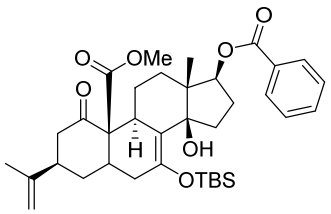
^{1}H NMR (500 MHz, $CDCl_3$): 0.17 (s, 3H, Si-C**H**$_3$); 0.19 (s, 3H, Si-C**H**$_3$); 0.93 (s, 9H, Si-C(C**H**$_3$)$_3$); 1.05 (s, 3H, C**H**$_3$); 1.05 (m, 1H); 1.24 (t, J = 7.1 Hz, 3H, OCH$_2$C**H**$_3$); 1.30 (td, J = 13.5 Hz, 4.3 Hz, 1H); 1.62 (dt, J = 13.8 Hz, 2.8 Hz, 1H); 1.71 (q, J = 12.0 Hz, 1H); 1.86 (dd, J = 15.0 Hz, 5.1 Hz, 1H); 2.02 (m, 3H); 2.38 (m, 4H); 2.65 (q, J = 15.8 Hz, 2H); 2.86 (m, 2H); 3.92 (m, 4H,OC**H**$_2$C**H**$_2$O, 4H); 4.16 (m, 2H, OC**H**$_2$CH$_3$); 4.99 (dd, J = 8.2 Hz, 3.2 Hz, 1H, C**H**CO$_2$Ph); 5.62 (s, 1H, OH); 7.40 (m, 2H); 7.49 (m, 1H); 8.07 (m, 2H) ppm.

^{13}C NMR (500 MHz, $CDCl_3$): -3.2 (**C**H$_3$, Si-**C**H$_3$); -3.0 (**C**H$_3$, Si-**C**H$_3$); 14.0 (CH$_3$, OCH$_2$**C**H$_3$); 14.4 (C**H**$_3$); 18.4 (Cq, Si-**C**(CH$_3$)$_3$); 25.4 (**C**H$_2$); 26.0 (**C**H$_3$, Si-C(**C**H$_3$)$_3$); 29.7 (**C**H$_2$); 31.4 (**C**H); 32.9 (**C**H$_2$); 35.9 (**C**H$_2$); 36.3 (**C**H); 36.5 (**C**H$_2$); 36.9 (**C**H$_2$); 49.8 (**C**H$_2$); 51.3 (Cq); 61.5 (**C**H$_2$, O**C**H$_2$CH$_3$); 62.9 (Cq); 64.1 (CH$_2$, O**C**H$_2$); 64.8 (CH$_2$, O**C**H$_2$); 82.3 (**C**H, **C**HCO$_2$Ph); 85.7 (Cq, **C**OH); 110.0 (Cq, **C**(OCH$_2$)$_2$); 115.1 (=C); 128.2 (2 =CH); 129.8 (2 =CH); 131.0 (=C); 132.6 (=CH); 142.9 (=C); 166.6 (COO); 170.0 (COO) ; 201.0 (CO) ppm.

IR (ATR) : ν (OH) = 3495 cm^{-1}, ν (CO) = 1713 cm^{-1}, ν (Ar) = 838 cm^{-1}, ν (C=C) = 714 cm^{-1}
HRMS (ESI) m/z : $C_{36}H_{50}O_9Si$ [M + K]$^+$ calc. 693.2861, found. 693.2856
[α]$^{20}_D$: +49.8 (c = 1, $CHCl_3$)
mp : 74-75 °C

Compound (+)-50

Methyl (3*R*,9*S*,10*R*,13*R*,14*R*,17*S*)-17-(benzoyloxy)-7-((*tert*-Butyldimethylsilyl)oxy)-14-hydroxy-13-methyl-1-oxo-3-(prop-1'-en-2'-yl)-1,2,3,4,5,6,9,11,12,13,14,15,16,17-tetradecahydro-10*H*-cyclopenta[a]phenanthrene-10-carboxylate (+)-50



Chemical Formula: $C_{36}H_{50}O_7Si$
Molecular Weight: 622,87
White solid

A solution of diene **(+)-46** (100 mg, 0.23 mmol) and β-cetoester **(+)-47** (54 mg, 0.28 mmol) in toluene (1.5 mL) was submitted to high pressure (9 kbar) at 25 °C for 48 h. Solvent was removed under reduced pressure and the crude material was purified by silica gel chromatography (petroleum ether / ethyl acetate 90/10) to afford **(+)-50** (117 mg, 0.19 mmol, 81 %).

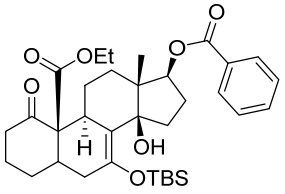
^{1}H NMR (500 MHz, $CDCl_3$): 0.18 (s, 3H, Si-C**H**$_3$); 0.20 (s, 3H, Si-C**H**$_3$); 0.94 (s, 9H, Si-C(C**H**$_3$)$_3$); 0.998 (m, 1H); 1.00 (s, 3H, C**H**$_3$); 1.39 (m, 2H); 1.60 (dt, J = 13.1 Hz, 2.9 Hz, 1H); 1.66 (m, 1H); 1.69 (s, 3H, C**H**$_3$); 2.03 (m, 4H); 2.18 (m, 2H); 2.44 (m, 3H); 2.58 (m, 1H); 2.90 (m, 1H); 2.97 (dd, J = 12.2 Hz, 2.6 Hz, 1H); 3.76 (s, 3H, OC**H**$_3$); 4.71 (s, 1H, =CH); 4.77 (s, 1H, =CH); 5.00 (dd, J = 6.4 Hz, 2.0 Hz, 1H, C**H**CO_2Ph); 5.77 (s, 1H, OH); 7.36 (m, 2H); 7.49 (m, 1H); 8.07 (m, 2H) ppm.

^{13}C NMR (500 MHz, $CDCl_3$): 3.0 (**C**H_3, Si-**C**H_3); -2.9 (**C**H_3, Si-**C**H_3); 14.2 (C**H**$_3$); 18.4 (Cq, Si-**C**$(CH_3)_3$) 20.5 (C**H**$_3$); 25.9 (**C**H_2); 26.0 (**C**H_3, Si-C(**C**H_3)$_3$); 26.9 (**C**H_2); 29.8 (**C**H_2); 30.9 (**C**H_2); 32.8 (**C**H_2); 33.5 (**C**H); 35.9 (**C**H_2); 36.6 (**C**H_2); 36.9 (**C**H); 41.5 (**C**H_2); 44.8 (**C**H_2); 52.1 (Cq); 52.5 (**C**H_3, O**C**H_3); 62.9 (Cq); 82.1 (**C**H, **C**HCO_2Ph); 86.7 (Cq, **C**OH); 110.0 (=CH_2); 115.4 (=C); 128.2 (2 =CH); 129.8 (2 =CH); 131.1 (=C); 132.6 (=CH); 141.7 (=C) 146.5 (=C); 166.6 (COO); 170.9 (COO) : 204.1 (CO) ppm.

IR (ATR) : ν (OH) = 3487 cm^{-1}, ν (CO) = 1714 cm^{-1}, ν (Ar) = 834 cm^{-1}, ν (C=C) = 712 cm^{-1}
HRMS (ESI) m/z : $C_{36}H_{50}O_7Si$ $[M + K]^+$ calc. 661.2963, found. 661.2957.
$[\alpha]^{20}_D$: 107.6 (c = 1, $CHCl_3$)
mp : 180-181 °C

*Compound (+)-**51***

Ethyl (9*S*,10*R*,13*R*,14*R*,17*S*)-17-(benzoyloxy)-7-((*tert*-Butyldimethylsilyl)oxy)-14-hydroxy-13-methyl-1-oxo-1,2,3,4,5,6,9,11,12,13,14,15,16,17-tetradecahydro-10*H*-cyclopenta[a]phenanthrene-10-carboxylate (+)-51



Chemical Formula: $C_{34}H_{48}O_7Si$
Molecular Weight: 596,84
White solid

A solution of diene **(+)-46** (110 mg, 0.25 mmol) and β-ketoester **28** (51 mg, 0.30 mmol) in toluene (1.5 mL) was submitted to high pressure (9 kbar) at 25 °C for 48 h. Solvent was removed under reduced pressure and the crude material was purified by silica gel chromatography (petroleum ether / ethyl acetate 85/15) to afford **(+)-51** (107 mg, 0.17 mmol, 70 %).

^{1}H NMR (500 MHz, $CDCl_3$): 0.18 (s, 3H, SiC**H**$_3$); 0.20 (s, 3H, SiC**H**$_3$); 0.94 (s, 9H, Si((CH$_3$)$_2$(C(C**H**$_3$)$_3$); 1.04 (s, 3H); 1.25 (m, 5H); 1.53 (m, 3H); 1.92 (m, 2H); 2.04 (m, 4H); 2.18 (m, 1H); 3.35 (m, 4H); 2.84 (m, 1H); 2.94 (m, 1H); 4.20 (m, 2H, OC**H**$_2$CH$_3$); 5.00 (m, 1H, C**H**COOPh); 5.71 (s, 1H, O**H**); 7.38 (m, 2H); 7.49 (m, 1H); 8.08 (m, 2H) ppm.

^{13}C NMR (125 MHz, $CDCl_3$): -3.0 (2 CH$_3$ Si**C**H$_3$); 14;1 (CH$_3$, OCH$_2$**C**H$_3$); 14.3 (CH$_3$); 18.4 (Cq, Si((CH$_3$)$_2$(**C**(CH$_3$)$_3$)); 22.9 (CH$_2$); 25.7 (CH$_2$); 25.9 (3 CH$_3$, Si((CH$_3$)$_2$(C(**C**H$_3$)$_3$); 26.1 (CH$_2$); 29.8 (CH$_2$); 32.7 (CH$_2$); 35.0 (CH); 35.9 (CH$_2$); 36.8 (CH$_2$); 36.8 (CH); 39.6 (CH$_2$); 51.9 (Cq); 61.4 (CH$_2$, O**C**H$_2$CH$_3$); 63.6 (Cq); 82.2 (CH, H**C**OOPh); 86.4 (Cq, **C**OH); 115.6 (=C); 128.2 (2 =CH); 129.8 (2 =CH); 131.1 (=C); 132.5 (=C); 141.9 (=C); 166.6 (COO); 170.5 (COO); 205.2 (CO) ppm.

IR (ATR) : ν (OH) : 3465 cm$^{-1;}$ ν (CO) : 1742, 1708, 1667 cm$^{-1;}$ ν (Ar) : 714 cm^{-1}
HRMS (ESI) m/z : $C_{34}H_{48}O_7Si$ [M + Na] calc. : 619.3067 found : 619.3062.
$[\alpha]^{20}_D$: +87.2 (*c* = 1, $CHCl_3$)
mp. : 159-160 °C

Cartesian coordinates of structure of (rac)-17 (X-ray crystallographic analysis)

C	-0.480074	15.747840	19.272703
C	-1.163457	16.495601	18.138132
H	-0.843408	17.432244	18.123497
H	-2.140657	16.509401	18.299418
C	-0.886038	15.847024	16.781311
H	-1.394968	15.000078	16.719737
H	-1.211334	16.449028	16.065496
C	0.590910	15.556199	16.552204
H	1.073607	16.409354	16.409682
H	0.692565	15.008703	15.733928
C	1.217236	14.810680	17.741790
H	2.198370	14.724088	17.568566
C	1.036881	15.550852	19.089918
C	1.710427	14.727193	20.209272
H	2.689593	14.767211	20.009827
C	1.559584	15.359038	21.598198
H	1.916360	16.281709	21.578728
H	0.599436	15.408889	21.832285
C	2.293467	14.560219	22.655859
H	2.219357	15.022502	23.527341
H	3.252959	14.505020	22.419013
C	1.714362	13.142318	22.778804
C	2.698119	12.350570	23.629576
C	3.682533	11.626096	22.740456
H	3.607767	10.646330	22.857745
H	4.610544	11.903811	22.944865
C	3.291653	12.038356	21.311980
H	3.418230	11.284557	20.681093
H	3.834031	12.807680	21.006644
C	1.804211	12.422500	21.414405
C	1.361521	13.230635	20.205498
C	0.889973	12.676067	19.078864
C	0.626982	13.399506	17.812549
H	-0.352841	13.461432	17.683753

H	0.994251	12.866327	17.062366
C	1.718952	16.935461	19.011399
H	1.527448	17.440868	19.828828
H	1.375293	17.425344	18.236262
H	2.687626	16.816440	18.921257
C	0.315458	13.149218	23.381876
H	-0.008526	12.228100	23.467974
H	-0.289225	13.654625	22.800278
H	0.343659	13.570103	24.268429
C	0.255777	8.613143	18.454146
H	1.124763	8.535003	18.009161
H	-0.366614	7.957148	18.074132
H	0.363990	8.443581	19.413925
C	-0.563365	10.725677	16.376878
H	-1.031634	11.579522	16.267291
H	-1.066393	10.016727	15.925162
H	0.332510	10.791225	15.984872
C	-2.088845	10.485910	19.022731
C	-3.148024	9.833883	18.108128
H	-2.898806	8.902415	17.932464
H	-3.195901	10.323766	17.261217
H	-4.022257	9.859757	18.550457
C	-2.467920	11.972809	19.241355
H	-3.329692	12.026282	19.705296
H	-2.536127	12.424743	18.375180
H	-1.778634	12.410943	19.785050
C	-2.088190	9.742461	20.367095
H	-2.986032	9.775235	20.759477
H	-1.450715	10.170246	20.976904
H	-1.827166	8.809269	20.223792
O	-1.113614	15.331957	20.209548
O	2.692217	12.302272	24.835954
O	1.065082	11.219010	21.606197
O	0.689942	11.290940	18.994583
Si	-0.417310	10.322731	18.200494
H	0.911615	10.884371	20.835745

Cartesian coordinates of structure of (rac)-18a (X-ray crystallographic analysis)

C	1.611540	11.332989	11.831420
C	1.085774	12.660046	11.326393
H	0.919555	12.598953	10.353166
H	1.766345	13.362965	11.476920
C	-0.211162	13.045980	12.039422
H	-0.469408	13.964040	11.773257
H	-0.934536	12.431719	11.757008
C	-0.059211	12.983764	13.545459
H	-0.936676	13.159248	13.969615
H	0.567856	13.691352	13.840336
C	0.462988	11.623382	14.011982
H	0.619933	11.680954	14.998024
C	1.809861	11.220435	13.343008
C	2.221485	9.814086	13.854330
H	2.286403	9.887683	14.849779
C	3.590474	9.326618	13.373442
H	3.567645	9.201059	12.392396
H	4.273898	10.011637	13.578723
C	3.970709	8.019255	14.040488
H	4.014939	8.155934	15.019320
H	4.871002	7.747530	13.730362
C	2.959127	6.877978	13.729571
C	3.216659	5.771817	14.742472
C	2.479018	6.079303	16.036381
H	3.154595	6.449625	16.673507
C	1.527360	7.232717	15.676953
H	1.836257	8.078304	16.088863
H	0.611372	7.039899	15.998066
C	1.548049	7.343476	14.123912
C	1.171380	8.724128	13.571735
H	1.125724	8.627870	12.576990
C	-0.220436	9.149980	14.026566
C	-0.618506	10.563471	13.776335
H	-1.391104	10.774764	14.356471

H	-0.925262	10.636866	12.837357
C	2.914897	12.233332	13.750436
H	3.701049	12.106113	13.178883
H	3.163869	12.085052	14.686614
H	2.576752	13.147041	13.642473
C	3.096810	6.398718	12.287932
H	3.960008	5.950060	12.173544
H	3.045447	7.167510	11.681589
H	2.372723	5.771199	12.082507
C	1.856945	4.834098	16.719761
H	2.585312	4.154426	16.809850
C	1.356148	5.143561	18.135803
H	0.646328	5.842262	18.051684
C	0.696979	3.899262	18.734044
C	-0.355266	3.264079	17.915518
H	-1.131431	3.874656	17.841240
H	-0.660596	2.430836	18.355870
C	0.179773	2.939639	16.517557
H	0.885313	2.248305	16.581766
H	-0.552161	2.580895	15.955301
C	0.752623	4.197132	15.871004
H	0.024255	4.854824	15.738408
H	1.119303	3.966646	14.981421
C	2.428367	5.704399	19.039400
H	2.098783	5.727166	19.961941
H	2.656651	6.612305	18.751411
H	3.225220	5.135645	18.991526
C	2.265002	9.886553	19.732857
H	1.665044	10.659925	19.687966
H	2.753672	9.899192	20.580712
H	1.739949	9.061827	19.669698
C	3.227360	9.945108	18.607472
C	4.975157	11.159014	17.643319
H	4.578514	11.321179	16.751810
H	5.482375	10.309478	17.606991
C	5.863323	12.245453	17.989468

H	5.353965	13.081188	18.039814
H	6.560302	12.328166	17.306287
H	6.279227	12.063623	18.858845
O	1.836970	10.415462	11.060507
O	3.940033	4.813500	14.564779
O	1.037264	3.469928	19.826123
O	0.651322	6.359692	13.567576
O	-1.010155	8.350682	14.519341
O	3.430675	9.065145	17.813289
O	3.931473	11.060598	18.629354
H	-0.164079	6.601695	13.808180

Cartesian coordinates of structure of (rac)-29a (X-ray crystallographic analysis)

C	0.887485	11.947927	8.063209
H	0.277934	11.868960	7.273893
C	0.036360	12.407608	9.247466
H	0.607267	12.495526	10.051346
H	-0.660569	11.729723	9.436732
C	-0.626969	13.753632	8.941819
H	-1.151712	14.047024	9.728386
H	-1.250703	13.645226	8.180420
C	0.412713	14.826354	8.598177
H	-0.057110	15.640293	8.285394
H	0.911852	15.063454	9.420001
C	1.389289	14.393525	7.543910
C	1.995604	12.985044	7.688719
C	3.062318	13.046905	8.830597
H	2.562322	13.223537	9.678463
C	4.093434	14.178106	8.688074
H	4.583054	14.072883	7.833761
H	3.625515	15.049531	8.667549
C	5.084477	14.160602	9.847019
H	4.597332	14.301629	10.696849
H	5.730008	14.904326	9.737703
C	5.858029	12.813384	9.915892

C	6.563524	12.797273	11.265208
C	5.628162	12.210488	12.306928
H	5.397819	12.889368	12.990666
H	6.049822	11.435336	12.756901
C	4.376888	11.773085	11.534987
H	3.657877	12.449777	11.617364
H	4.040512	10.904246	11.870677
C	4.850708	11.650159	10.072537
C	3.750871	11.663287	9.001230
H	4.207082	11.471140	8.132675
C	2.722134	10.552772	9.195695
C	1.529874	10.569282	8.280230
H	0.843320	9.957435	8.648376
H	1.805619	10.210050	7.400380
C	2.624096	12.612883	6.335651
C	2.136665	11.809883	4.156904
H	3.000163	11.329914	4.224754
H	2.265352	12.606916	3.582750
C	1.102217	10.921352	3.574291
H	1.044156	10.096672	4.101536
H	1.343982	10.701358	2.650604
H	0.236053	11.377652	3.584733
C	6.819756	12.681905	8.740275
H	7.309091	13.523891	8.622193
H	6.313478	12.481602	7.925640
H	7.454721	11.956480	8.917232
O	1.744035	15.134465	6.648698
O	7.691536	13.182561	11.471508
O	5.621023	10.434023	9.938889
O	2.883945	9.652506	10.002191
O	3.796082	12.657638	6.064188
O	1.683118	12.213273	5.477946
H	5.101801	9.784383	10.066753

Cartesian coordinates of structure of (+)-33a (X-ray crystallographic analysis)

C	2.750984	0.155125	0.921022
H	2.419201	-0.531049	1.553263
H	3.591125	-0.168713	0.509618
C	1.747763	0.444994	-0.103955
H	2.181893	0.655602	-0.967289
H	1.143807	-0.328367	-0.231028
C	1.725832	2.124308	1.503876
C	0.876468	1.938724	2.753992
H	0.822146	0.973778	2.966391
H	-0.041613	2.261203	2.571599
C	1.436225	2.686382	3.965987
H	0.782782	2.634862	4.708113
H	2.268493	2.240822	4.263694
C	1.732580	4.131423	3.673180
C	2.585768	4.389021	2.416284
C	4.043699	3.902472	2.704800
H	3.993763	2.911143	2.825068
C	4.672287	4.465678	3.984975
H	4.725934	5.452025	3.922490
H	4.103982	4.237067	4.763276
C	6.071960	3.887073	4.185760
H	6.012576	2.902085	4.265895
H	6.455703	4.240463	5.027011
C	7.001176	4.251334	3.003955
C	8.260038	3.391352	3.139878
C	8.086611	2.116042	2.338130
H	8.171975	1.321394	2.922303
H	8.766934	2.058521	1.620191
C	6.673217	2.199832	1.740393
H	6.013701	1.741477	2.319551
H	6.644650	1.796960	0.836262
C	6.400593	3.719492	1.681669
C	4.941762	4.150446	1.469371
H	4.964368	5.141774	1.340979

C	4.337805	3.574671	0.191500
C	2.867614	3.810756	-0.024393
H	2.553039	3.201012	-0.738256
H	2.741987	4.738676	-0.346598
C	1.989009	3.603884	1.212564
H	1.102193	4.019665	1.008367
C	2.529758	5.899170	2.115174
C	1.206789	7.638156	1.232044
H	1.436225	8.200117	2.001222
H	0.282296	7.817399	0.961483
H	1.810746	7.841177	0.487043
C	7.329922	5.738043	3.014833
H	7.560145	6.014778	3.926835
H	6.551301	6.246899	2.705663
H	8.089873	5.909474	2.420164
O	2.958264	1.404165	1.586794
O	1.023128	1.572878	0.382133
O	1.372905	5.040886	4.384537
O	3.424672	6.683288	2.294629
O	1.341864	6.238973	1.597059
O	9.241327	3.705225	3.775639
O	7.209693	4.288926	0.633998
O	5.022402	3.051549	-0.672740
H	6.939318	3.906435	-0.080914

Cartesian coordinates of structure of (-)-36 (X-ray crystallographic analysis)

C	5.683005	8.501852	0.296976
C	5.867297	7.224095	-0.472737
H	6.552383	7.369988	-1.171435
H	5.015948	7.001918	-0.927135
C	6.287964	6.035018	0.385683
H	6.605467	5.321763	-0.238462
C	7.488867	6.437416	1.258733
H	7.736259	5.678390	1.843241
H	8.264095	6.638615	0.674306

C	7.177373	7.658914	2.121024
H	6.396135	7.424340	2.698027
C	6.778741	8.890900	1.285442
C	7.998675	9.386746	0.436976
H	8.189978	8.660141	-0.221858
C	7.635098	10.613012	-0.384508
H	6.893924	10.385113	-1.000705
H	7.318597	11.330081	0.218970
C	8.818974	11.121254	-1.191359
H	8.539532	11.902211	-1.732223
H	9.125460	10.412766	-1.810130
C	9.977811	11.528420	-0.260753
C	11.184723	11.701012	-1.172031
C	11.993004	10.436605	-1.216217
H	12.901443	10.588219	-0.854848
H	12.070126	10.102862	-2.146060
C	11.216774	9.437284	-0.340974
H	11.836756	8.849898	0.159104
H	10.614820	8.875643	-0.891795
C	10.403485	10.339343	0.627218
C	9.261676	9.540268	1.274293
C	9.412916	8.843223	2.395688
C	8.343221	8.015541	3.050069
H	7.988659	8.512341	3.829953
H	8.749865	7.178324	3.387375
C	5.160177	5.437142	1.207789
C	5.393547	4.017306	1.658154
H	4.636347	3.719799	2.204980
H	6.216851	3.973443	2.187429
H	5.478681	3.435641	0.874014
C	4.031388	6.061717	1.489817
H	3.352312	5.616409	1.984200
H	3.898177	6.956147	1.199682
C	6.267932	10.001786	2.215482
H	5.857281	10.713134	1.680471
H	7.018121	10.369856	2.727452

H	5.601877	9.631809	2.832548
C	9.651293	12.804269	0.490983
H	10.438541	13.095102	0.997622
H	8.909117	12.638352	1.108937
H	9.396890	13.503222	-0.145994
C	10.711974	7.360452	5.552646
H	10.762053	8.166202	6.108079
H	11.202752	6.632894	5.988039
H	9.774488	7.100133	5.438689
C	11.474182	6.188540	2.824522
H	10.574757	5.799491	2.799928
H	12.103178	5.534404	3.194089
H	11.750620	6.430741	1.916007
C	13.203923	8.420800	4.093823
C	13.152842	9.757677	4.826571
H	12.681094	9.646112	5.677819
H	12.679091	10.414673	4.273486
H	14.065288	10.072349	4.997213
C	13.890010	8.621046	2.727558
H	13.371188	9.257063	2.193271
H	13.939088	7.762851	2.258104
H	14.794443	8.970998	2.864938
C	14.046257	7.430062	4.913835
H	14.956700	7.780014	5.013370
H	14.076305	6.567099	4.451539
H	13.642618	7.312775	5.799566
O	4.699447	9.201757	0.117345
O	11.443133	12.711775	-1.791779
O	11.293896	10.924822	1.579631
H	11.330955	10.439465	2.263546
O	10.601799	8.908064	3.126409
Si	11.462764	7.706305	3.893062

Cartesian coordinates of structure of (+)-36 (X-ray crystallographic analysis)

C	4.348522	1.963112	12.112784

C	4.161770	3.235941	12.889298
H	5.009184	3.454277	13.353145
H	3.469982	3.088160	13.582450
C	3.749107	4.433450	12.029566
H	3.434841	5.148522	12.654326
C	2.544252	4.033962	11.160433
H	1.772141	3.832789	11.746501
H	2.295249	4.794799	10.579671
C	2.847474	2.817386	10.294693
H	3.629625	3.051929	9.717397
C	3.245076	1.573160	11.123766
C	2.027168	1.086910	11.970482
H	1.841420	1.812470	12.633417
C	2.385613	-0.154456	12.788851
H	2.688835	-0.872388	12.178680
H	3.132623	0.061973	13.400482
C	1.199835	-0.652146	13.600075
H	0.898621	0.061020	14.216394
H	1.475947	-1.432052	14.143376
C	0.036146	-1.056400	12.674713
C	-1.169713	-1.228971	13.588342
C	-1.961905	0.048625	13.634010
H	-2.033193	0.383279	14.562151
H	-2.874583	-0.092483	13.275640
C	-1.185778	1.037332	12.760000
H	-0.579334	1.593182	13.310335
H	-1.803266	1.631319	12.264823
C	-0.382541	0.140154	11.788480
C	0.757051	0.934361	11.142092
C	0.611464	1.637039	10.016567
C	1.681777	2.460803	9.360839
H	1.277146	3.297914	9.021606
H	2.037209	1.961206	8.583186
C	4.881671	5.024576	11.208977
C	4.642708	6.444233	10.753713
H	4.586481	7.033453	11.535007

H	3.803325	6.489045	10.250310
H	5.383693	6.732169	10.178898
C	6.014234	4.408660	10.945075
H	6.697989	4.856772	10.460492
H	6.148776	3.515296	11.239102
C	3.757139	0.469088	10.194581
H	4.426838	0.841879	9.582748
H	3.009125	0.104877	9.676904
H	4.163778	-0.245032	10.727429
C	0.369489	-2.335904	11.910568
H	0.596403	-3.046209	12.545993
H	1.131560	-2.172867	11.316460
H	-0.406639	-2.609538	11.377117
C	-1.456870	4.293295	9.585940
H	-1.608481	4.031102	10.518598
H	-2.175767	4.892049	9.293251
H	-0.596403	4.755709	9.512046
C	-0.685763	3.113902	6.847161
H	0.210850	3.492414	6.965950
H	-1.247025	3.751747	6.358635
H	-0.622508	2.278698	6.338195
C	-3.174793	2.056549	8.302169
C	-3.871601	1.859188	9.668376
H	-3.892685	2.711555	10.150475
H	-3.375602	1.198462	10.196180
H	-4.787290	1.541696	9.525962
C	-3.112542	0.713166	7.569344
H	-4.022207	0.394720	7.391918
H	-2.639636	0.059113	8.125669
H	-2.634616	0.826624	6.720031
C	-4.020199	3.040488	7.476421
H	-3.635650	3.126297	6.578847
H	-4.024215	3.915737	7.915215
H	-4.937897	2.703927	7.406215
O	5.322045	1.260434	12.289906
O	-1.431769	-2.239607	14.201306

O	-1.274134	-0.439531	10.834360
H	-1.337389	0.066740	10.167414
O	-0.574314	1.569346	9.285003
Si	-1.438798	2.771430	8.507542

Cartesian coordinates of structure of (+)-37a (X-ray crystallographic analysis)

C	4.752352	2.360134	8.369786
C	4.806762	2.541990	6.868639
H	4.047250	3.113538	6.589912
H	4.690488	1.658689	6.436612
C	6.096963	3.165497	6.362948
H	6.108889	4.116745	6.665567
C	7.314120	2.464052	6.990085
H	8.130278	2.975647	6.763121
H	7.404307	1.562764	6.593894
C	7.227659	2.326161	8.525077
H	7.996860	1.756611	8.817740
C	5.927023	1.616722	8.984977
C	5.898700	1.572757	10.545850
H	6.712622	1.059163	10.820596
C	4.696450	0.791374	11.117241
H	3.854950	1.217038	10.814623
H	4.712103	-0.135893	10.770823
C	4.735209	0.765395	12.642279
H	5.548385	0.283776	12.936933
H	3.949610	0.265790	12.976751
C	4.735209	2.174281	13.263442
C	5.081051	2.024399	14.716807
C	6.584422	1.788586	14.830289
H	6.728274	0.797370	14.834270
C	7.138962	2.324162	13.490406
H	7.529526	1.584747	12.958833
H	7.842573	3.001627	13.653661
C	5.943421	2.959660	12.733860
C	6.028391	2.953665	11.208823

H	5.239065	3.481248	10.894260
C	7.239585	3.683088	10.687205
C	7.396108	3.699075	9.190041
H	8.295000	4.052796	8.969050
H	6.728274	4.322582	8.807786
C	6.213238	3.167496	4.845875
C	7.460208	3.741042	4.282447
H	7.418469	3.717061	3.302920
H	8.228664	3.215458	4.589048
H	7.557849	4.668309	4.583075
C	5.257699	2.709858	4.039556
H	5.372483	2.747828	3.095865
H	4.461665	2.344147	4.405884
C	5.901681	0.165869	8.453404
H	5.024404	-0.233815	8.632586
H	6.596348	-0.359716	8.903350
H	6.067149	0.167867	7.487813
C	3.377181	2.863736	13.058379
H	2.660900	2.274202	13.372942
H	3.248981	3.053586	12.104733
H	3.356311	3.703072	13.564070
C	7.163559	2.334155	16.140307
H	6.638832	1.912488	16.880926
C	7.040576	3.836966	16.323471
H	6.108889	4.114747	16.136326
H	7.632384	4.294605	15.676425
C	7.420705	4.258633	17.748963
H	7.381946	5.255845	17.788781
C	8.889044	3.836966	18.003799
H	9.488305	4.386532	17.440372
H	9.118612	4.010829	18.951472
C	9.112649	2.400102	17.703172
C	8.644569	1.900497	16.343380
H	9.183457	2.390110	15.658507
C	6.459203	3.719060	18.800163
C	5.008007	4.060789	18.559263

H	4.669618	3.537203	17.802717
H	4.927509	5.016034	18.356190
H	4.485516	3.852954	19.361600
C	6.798337	3.019613	19.861318
H	6.131249	2.731840	20.474518
H	7.709900	2.801785	20.016609
C	8.933020	0.435656	16.152253
H	9.863962	0.251801	16.397135
H	8.787676	0.193847	15.214534
H	8.334504	-0.091927	16.723644
C	2.344126	1.213041	1.976974
H	2.767485	0.955245	2.823110
H	2.043004	0.407678	1.505128
H	1.574179	1.790584	2.160137
O	3.785633	2.759818	8.998913
O	4.302160	2.048380	15.646562
O	5.770500	4.308594	13.195751
H	6.427153	4.772227	12.954851
O	8.046799	4.248641	11.411896
O	9.644829	1.638704	18.505508
O	3.260161	1.896501	1.190564
H	3.207986	1.622717	0.398182

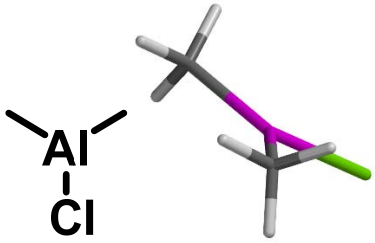
Cartesian coordinates of structure of (+)-51a (X-ray crystallographic analysis)

C	9.898382	5.227688	-3.814111
C	10.985269	6.247763	-3.602887
H	10.653037	6.958240	-2.999688
H	11.213439	6.665594	-4.470087
C	12.244054	5.618876	-2.998314
H	12.671101	5.034547	-3.673842
H	12.886166	6.336327	-2.767082
C	11.940343	4.800233	-1.751068
H	11.611964	5.401455	-1.036889
H	12.772852	4.371369	-1.429684
C	10.891998	3.724699	-2.029283

H	11.268939	3.104401	-2.717557
C	9.575399	4.325585	-2.606685
C	8.881642	5.204228	-1.527908
H	9.556128	5.889443	-1.251121
C	7.663711	5.984698	-2.032033
H	7.925798	6.549122	-2.801411
H	6.966870	5.351984	-2.337636
C	7.104080	6.862893	-0.920601
H	6.323988	7.362004	-1.269150
H	7.792442	7.523967	-0.659108
C	6.670867	6.073462	0.331765
C	6.455031	7.117860	1.452168
H	6.212216	8.000384	1.050307
C	7.780108	7.237601	2.212516
H	7.662940	6.962603	3.155878
H	8.105404	8.172597	2.193783
C	8.776036	6.311112	1.505521
H	9.398106	5.896411	2.154238
H	9.300209	6.805183	0.826085
C	7.880318	5.249323	0.845781
C	8.540159	4.396854	-0.253378
H	7.854880	3.723350	-0.528512
C	9.732651	3.599338	0.254621
C	10.572098	2.894156	-0.782765
H	10.098801	2.072524	-1.065938
H	11.424649	2.618144	-0.362234
C	8.661952	3.184636	-3.083803
C	8.516262	1.260225	-4.463493
H	8.815349	1.064005	-5.386534
H	7.561189	1.521062	-4.498334
C	8.666577	0.059170	-3.631838
H	9.609316	-0.207352	-3.612255
H	8.129300	-0.667886	-4.009789
H	8.362094	0.252052	-2.720727
C	5.433665	5.228175	0.022574
H	5.173892	4.725103	0.822111

H	5.638709	4.604106	-0.703995
H	4.696740	5.814047	-0.248302
C	4.861701	7.566800	3.166533
C	3.760938	6.975958	3.980066
C	3.308454	5.683746	3.765972
H	3.688479	5.158051	3.071687
C	2.305588	5.156002	4.559302
H	2.001106	4.268470	4.409089
C	1.746728	5.911305	5.563839
H	1.065304	5.545978	6.115385
C	2.181483	7.198022	5.764893
H	1.785270	7.727557	6.448289
C	3.186661	7.732089	4.988302
H	3.485748	8.620313	5.144040
O	9.285563	5.137044	-4.853817
O	7.519949	3.018931	-2.748642
O	9.304371	2.363671	-3.917309
O	5.386721	6.665686	2.332260
O	5.234017	8.714650	3.243836
O	7.376110	4.371899	1.873248
O	9.960435	3.466003	1.439598
H	8.070716	3.952531	2.153669

All calculations were performed with the program package *Spartan '10* 1.1.0 of Wavefunction Inc.
(http://www.wavefun.com). All structures were optimized and subjected to frequency analysis with the
B3LYP/6-31G* method, followed by single point calculations to provide the thermodynamic properties.

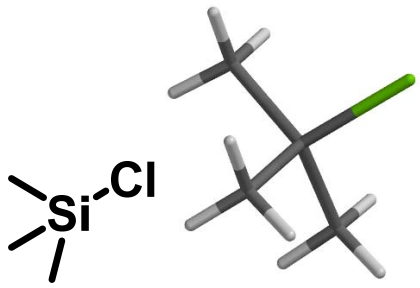


E(B3LYP/6-31G*) = –782.545814 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
Al	-0.383974	0.232600	0.000000
C	-1.246382	0.182596	1.756374
H	-0.865430	-0.649503	2.361898
H	-2.335166	0.077053	1.685377
H	-1.034356	1.100152	2.320449
C	-1.246382	0.182596	-1.756374
H	-0.865430	-0.649503	-2.361898
H	-1.034356	1.100152	-2.320449
H	-2.335166	0.077053	-1.685377
Cl	1.750784	0.372595	0.000000

Requested basis set is 6-31G(d)
There are 30 shells and 80 basis functions



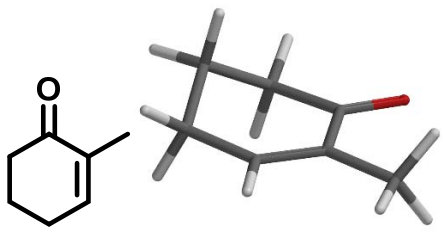
E(B3LYP/6-31G*) = –347.986508 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
Si	0.000000	0.000000	0.353172
C	1.797571	0.000000	0.907491
H	2.325599	-0.885710	0.537733
H	1.865318	0.000000	2.002892
H	2.325599	0.885710	0.537733
C	-0.898785	-1.556742	0.907491
H	-0.395753	-2.456883	0.537733
H	-1.929847	-1.571173	0.537733
H	-0.932659	-1.615413	2.002892
C	-0.898785	1.556742	0.907491
H	-1.929847	1.571173	0.537733
H	-0.395753	2.456883	0.537733
H	-0.932659	1.615413	2.002892
Cl	0.000000	0.000000	-1.757857

Requested basis set is 6-31G(d)

There are 40 shells and 101 basis functions



16

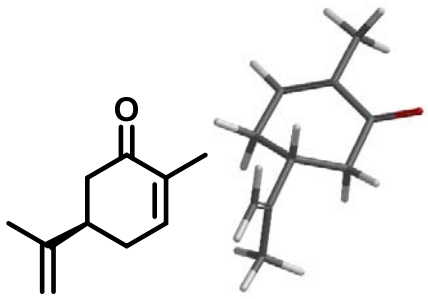
E(B3LYP/6-31G*) = –347.986508 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
H	1.090799	2.314272	-0.161212
C	0.966962	1.301897	0.235770
C	-0.790070	-0.567144	0.007506
C	1.675899	-1.115351	0.129829
C	0.212875	-1.464873	0.077814
C	1.945036	0.302164	-0.390715
C	-0.488522	0.892076	0.037185
H	2.031153	-1.211690	1.169440
H	1.819455	0.310407	-1.481634
H	1.141413	1.362590	1.321696
H	2.250442	-1.853592	-0.444721
H	-0.036987	-2.526233	0.101891
H	2.980997	0.597771	-0.187652
O	-1.380982	1.724218	-0.048841
C	-2.243462	-0.951371	-0.075739
H	-2.807752	-0.533978	0.766076
H	-2.365990	-2.038807	-0.078716
H	-2.702435	-0.543528	-0.983537

Requested basis set is 6-31G(d)

There are 52 shells and 140 basis functions



35

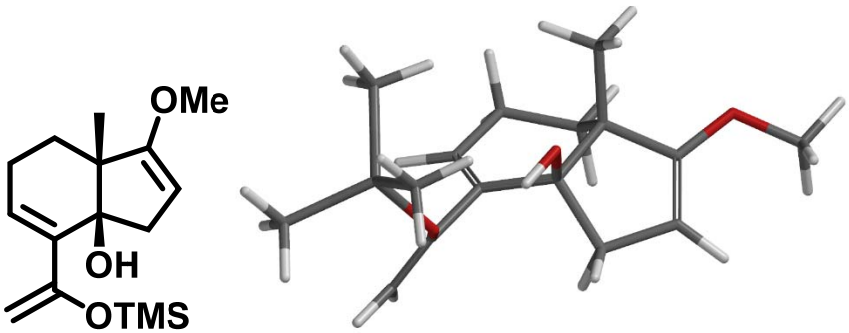
E(B3LYP/6-31G*) = –464.695238 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	1.977538	0.464700	0.079777
C	1.148389	1.509692	0.268093
H	1.578077	2.484839	0.500288
C	1.418221	-0.864271	-0.291631
C	-0.083064	-0.943960	-0.546468
H	-0.393644	-1.986741	-0.427094
H	-0.245161	-0.677557	-1.602125
C	-0.352243	1.442731	0.185092
H	-0.795307	2.102410	0.942340
H	-0.674638	1.850631	-0.786114
C	-0.886121	0.005500	0.364836
H	-0.673485	-0.282803	1.403222
C	3.474802	0.554020	0.204427
H	3.793519	1.573612	0.442282
H	3.963492	0.237603	-0.724094
H	3.840910	-0.119996	0.987443
O	2.140827	-1.841513	-0.428890
C	-2.390108	-0.096194	0.165461
C	-3.191741	-0.386179	1.196248
H	-4.270453	-0.458686	1.079929
H	-2.800035	-0.565401	2.194875
C	-2.949488	0.138193	-1.218923
H	-2.673616	1.125553	-1.612246
H	-4.041654	0.073718	-1.216686
H	-2.573673	-0.601457	-1.937867

Requested basis set is 6-31G(d)

There are 72 shells and 193 basis functions



52-A

E(B3LYP/6-31G*) = –1140.53418 au

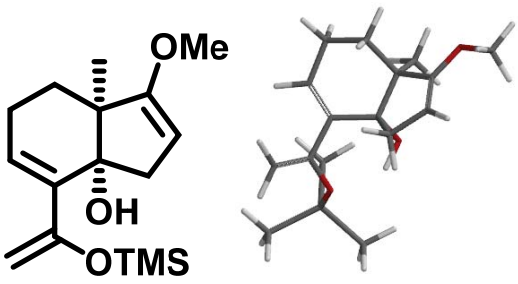
Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	0.185461	0.875633	-0.759278
C	1.946263	0.848747	-2.529739
C	-0.097853	2.189515	-0.738997
C	1.468337	0.411590	-1.356309
H	1.388723	1.565092	-3.120831
H	2.885862	0.478787	-2.926693
H	0.660855	2.890947	-1.083445
C	-1.414740	2.761210	-0.294939
H	-1.690795	3.595272	-0.954843
H	-1.314662	3.204512	0.707369
C	-2.511192	1.692726	-0.317791
H	-3.438401	2.072847	0.127272
C	-2.085166	0.396599	0.419834
C	-0.774720	-0.188027	-0.214401
O	2.135057	-0.588538	-0.658071
H	-2.738107	1.450422	-1.363937
C	-1.968271	0.653747	1.931886
H	-1.177595	1.379014	2.148504
H	-1.729486	-0.266797	2.466103
H	-2.916485	1.045982	2.314469
C	-3.081645	-0.702301	0.092757
C	-2.660814	-1.551492	-0.855634

H	-3.226884	-2.375453	-1.274950
C	-1.272620	-1.183093	-1.313577
H	-0.588105	-2.039106	-1.373476
H	-1.276913	-0.714974	-2.309462
O	-0.126024	-0.937911	0.824193
H	0.694902	-1.272340	0.422661
O	-4.270402	-0.642537	0.745681
C	-5.219875	-1.639013	0.397332
H	-5.492018	-1.568625	-0.664405
H	-6.100887	-1.459434	1.016574
H	-4.824160	-2.643312	0.597486
Si	3.444024	-0.354451	0.407896
C	4.958352	0.197144	-0.567082
H	4.775111	1.143996	-1.087305
H	5.240910	-0.550705	-1.316936
H	5.817441	0.344748	0.099279
C	3.698239	-2.060432	1.154616
H	4.565230	-2.068254	1.826360
H	3.872911	-2.812395	0.376533
H	2.826304	-2.377536	1.738805
C	2.987738	0.907215	1.727622
H	3.768838	0.962459	2.496504
H	2.046491	0.627808	2.213727
H	2.862548	1.912285	1.309440

Requested basis set is 6-31G(d)

There are 133 shells and 356 basis functions



52-B

E(B3LYP/6-31G*) = –1140.53418 au

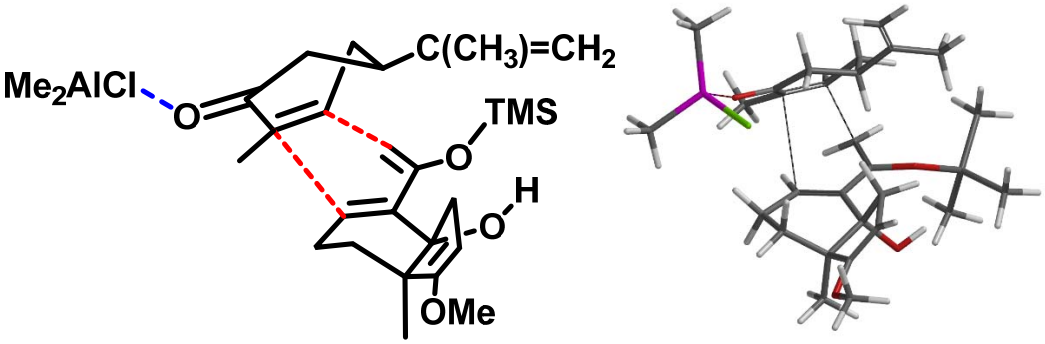
Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	0.185461	0.875633	-0.759278
C	1.946263	0.848747	-2.529739
C	-0.097853	2.189515	-0.738997
C	1.468337	0.411590	-1.356309
H	1.388723	1.565092	-3.120831
H	2.885862	0.478787	-2.926693
H	0.660855	2.890947	-1.083445
C	-1.414740	2.761210	-0.294939
H	-1.690795	3.595272	-0.954843
H	-1.314662	3.204512	0.707369
C	-2.511192	1.692726	-0.317791
H	-3.438401	2.072847	0.127272
C	-2.085166	0.396599	0.419834
C	-0.774720	-0.188027	-0.214401
O	2.135057	-0.588538	-0.658071
H	-2.738107	1.450422	-1.363937
C	-1.968271	0.653747	1.931886
H	-1.177595	1.379014	2.148504
H	-1.729486	-0.266797	2.466103
H	-2.916485	1.045982	2.314469
C	-3.081645	-0.702301	0.092757
C	-2.660814	-1.551492	-0.855634
H	-3.226884	-2.375453	-1.274950
C	-1.272620	-1.183093	-1.313577
H	-0.588105	-2.039106	-1.373476
H	-1.276913	-0.714974	-2.309462
O	-0.126024	-0.937911	0.824193
H	0.694902	-1.272340	0.422661
O	-4.270402	-0.642537	0.745681
C	-5.219875	-1.639013	0.397332

H	-5.492018	-1.568625	-0.664405
H	-6.100887	-1.459434	1.016574
H	-4.824160	-2.643312	0.597486
Si	3.444024	-0.354451	0.407896
C	4.958352	0.197144	-0.567082
H	4.775111	1.143996	-1.087305
H	5.240910	-0.550705	-1.316936
H	5.817441	0.344748	0.099279
C	3.698239	-2.060432	1.154616
H	4.565230	-2.068254	1.826360
H	3.872911	-2.812395	0.376533
H	2.826304	-2.377536	1.738805
C	2.987738	0.907215	1.727622
H	3.768838	0.962459	2.496504
H	2.046491	0.627808	2.213727
H	2.862548	1.912285	1.309440

Requested basis set is 6-31G(d)

There are 133 shells and 356 basis functions



53-TS

E(B3LYP/6-31G*) = –2387.79105 au

v*ts* = 369*i* cm^{-1}

Cartesian Coordinates (Angstroms)

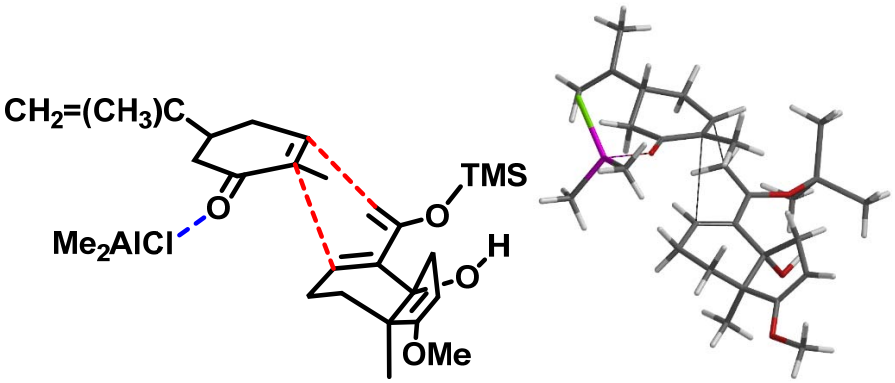
Atom	X	Y	Z
C	-1.847912	-0.564877	-1.062503
C	0.119065	0.515414	-1.970944
C	-0.201078	-2.931632	-1.182956
C	1.041651	-2.369812	-1.566625
C	-1.701788	-1.730768	-1.836053
C	-0.939403	0.560310	-1.107721
H	0.186683	-0.290530	-2.689947
H	-1.295566	-1.618480	-2.834808
C	-1.198058	1.793472	-0.223302
C	-0.316277	3.030110	-0.613609
H	-2.521631	-2.440662	-1.781362
O	-2.796983	-0.528696	-0.095416
C	1.182182	1.556201	-2.075989
H	1.093410	2.038888	-3.062573
H	2.159878	1.052070	-2.091005
C	1.128824	2.569862	-0.934122
H	1.741084	3.446164	-1.171921
H	1.578203	2.115053	-0.045089
C	-0.901633	3.862919	-1.764439
H	-0.264828	4.733770	-1.949624
H	-1.906926	4.211704	-1.522898
H	-0.962152	3.279231	-2.689598
C	-0.279887	3.777815	0.709784
C	-0.582426	3.007054	1.763424
H	-0.541995	3.290664	2.807982
C	-0.915587	1.610248	1.300325
H	-0.077169	0.919536	1.472258
H	-1.785896	1.171905	1.806560
O	0.127466	5.067282	0.651648
O	-2.563132	2.205171	-0.403929
H	-3.088935	1.617877	0.157586
Si	-4.464305	-0.951734	-0.170713
C	-5.216980	0.096156	1.195039
C	-5.117573	-0.467041	-1.864522

C	-4.692706	-2.778894	0.215266
C	1.904838	-1.821901	-0.590619
C	1.598594	-1.941496	0.885571
H	1.987855	-1.053945	1.393623
H	2.210357	-2.784155	1.242258
C	-0.466156	-3.243436	0.278273
H	-0.002860	-4.218093	0.497691
H	-1.540347	-3.368328	0.446426
C	0.123065	-2.179319	1.225555
H	-0.419166	-1.247084	1.020339
H	-0.573064	-3.701116	-1.861080
C	1.501415	-2.445362	-3.002617
H	2.145688	-1.602139	-3.263628
H	0.651954	-2.472039	-3.697182
H	2.087099	-3.357512	-3.182253
C	-0.129322	-2.497840	2.694854
C	0.843037	-2.605860	3.606471
H	0.609605	-2.806232	4.649049
H	1.895005	-2.488244	3.371068
C	-1.580148	-2.638435	3.100683
H	-2.166168	-1.771594	2.766172
H	-1.680542	-2.718944	4.186976
H	-2.047543	-3.528806	2.658879
H	-5.760130	-3.006954	0.328984
H	-4.301116	-3.436611	-0.568341
H	-4.197799	-3.042695	1.156844
H	-6.212415	-0.528652	-1.884873
H	-4.833167	0.565987	-2.095616
H	-4.732167	-1.109054	-2.663712
O	3.032942	-1.327475	-0.945887
Al	4.615249	-0.646958	-0.149753
Cl	3.860761	0.830564	1.343508
C	5.493690	-2.182454	0.740062
H	6.396838	-1.857288	1.274626
H	5.812908	-2.943087	0.013222
H	4.860596	-2.690357	1.480510

C	5.503398	0.274570	-1.655769
H	4.890484	1.085731	-2.071617
H	5.728870	-0.415300	-2.481576
H	6.455996	0.728089	-1.349979
H	-5.164574	1.169155	0.973728
H	-6.275979	-0.153573	1.332676
H	-4.711157	-0.075525	2.152139
C	0.307829	5.724097	1.899772
H	0.647368	6.735823	1.670175
H	1.062444	5.207063	2.506033
H	-0.636215	5.768583	2.458940

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



54-TS

E(B3LYP/6-31G*) = –2387.78548 au

v*ts* = 362*i* cm^{-1}

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.415986	-1.494419	-0.354648
C	-0.444673	0.590698	-1.116791
C	1.175070	-1.939069	0.811996
C	1.338578	-0.557028	1.092685
C	-0.240924	-2.231614	-0.586085

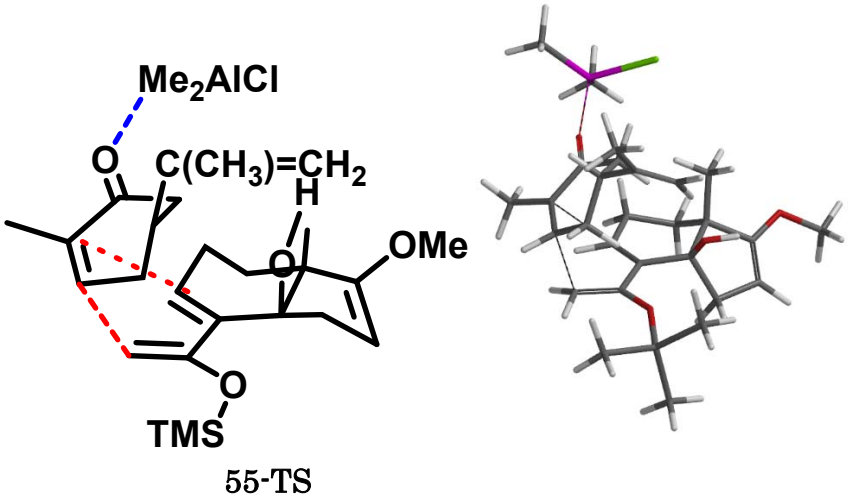
C	-1.520051	-0.072776	-0.596603
H	0.405558	0.033698	-1.493604
H	0.617551	-2.475833	1.579011
H	0.372993	-1.914812	-1.419641
C	2.335035	-2.748720	0.213119
C	2.341829	0.182626	0.425942
C	3.267975	-0.536059	-0.532469
H	4.165850	0.067484	-0.678808
H	2.772674	-0.634810	-1.511446
C	3.630247	-1.922425	0.020158
C	-2.850194	0.652070	-0.308900
C	-2.876326	2.127349	-0.840132
H	2.527581	-3.601754	0.874452
H	2.061821	-3.179062	-0.758191
H	-0.317218	-3.311721	-0.510450
O	-2.471305	-2.065562	0.271693
C	-0.360883	2.068441	-1.290371
H	-0.325078	2.297913	-2.366747
H	0.611220	2.401787	-0.898703
C	-1.503938	2.801205	-0.590195
H	-1.551445	3.845533	-0.916513
H	-1.304198	2.820246	0.487955
C	-3.284775	2.241256	-2.317669
H	-3.289121	3.293461	-2.619976
H	-4.281857	1.828366	-2.477942
H	-2.591573	1.698065	-2.968460
C	-3.889391	2.754623	0.103439
C	-4.082823	2.046339	1.224756
H	-4.708711	2.322336	2.065162
C	-3.248189	0.789030	1.195000
H	-2.360166	0.872566	1.836848
H	-3.789371	-0.104282	1.530713
O	-4.391179	3.952789	-0.277015
C	-5.279029	4.577700	0.640963
H	-5.583240	5.520717	0.183620
H	-4.778417	4.773385	1.598252

H	-6.161851	3.950166	0.819778
O	-3.891466	-0.041894	-1.009546
H	-4.030451	-0.865009	-0.517559
Si	-3.050668	-3.687208	0.306392
C	-4.789132	-3.482229	0.980720
H	-5.269160	-4.459771	1.110785
H	-5.423058	-2.894102	0.306795
H	-4.783610	-2.984542	1.957125
C	-3.066186	-4.356319	-1.450520
H	-2.064592	-4.437916	-1.885079
H	-3.661982	-3.710455	-2.105935
H	-3.518174	-5.355600	-1.469725
C	-2.004031	-4.728263	1.474196
H	-2.020506	-4.316060	2.489700
H	-0.957936	-4.804875	1.158906
H	-2.405713	-5.748119	1.525028
C	0.495315	0.092089	2.158363
H	0.394681	1.166510	1.992222
H	0.947647	-0.044191	3.151041
H	-0.502984	-0.357835	2.195648
H	4.068469	-1.757551	1.015716
C	4.652709	-2.692587	-0.801245
C	5.043140	-2.324150	-2.025781
H	5.778827	-2.904239	-2.577147
H	4.675074	-1.431071	-2.520956
C	5.229256	-3.922551	-0.136694
H	5.714561	-3.661221	0.813296
H	5.973459	-4.406433	-0.775853
H	4.456765	-4.667198	0.097915
O	2.482810	1.433870	0.651210
Al	3.755468	2.805093	0.273703
C	3.264670	4.244436	1.532594
H	3.302426	3.906408	2.576585
H	2.251755	4.633545	1.354256
H	3.951000	5.098457	1.451325
C	3.659418	3.129900	-1.682472

H	3.845721	2.232046	-2.288316
H	4.414242	3.868929	-1.985312
H	2.686149	3.534990	-1.996865
Cl	5.663618	1.826212	0.833683

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



55-TS

E(B3LYP/6-31G*) = –2387.78548 au

v*ts* = 362*i* cm^{-1}

Cartesian Coordinates (Angstroms)

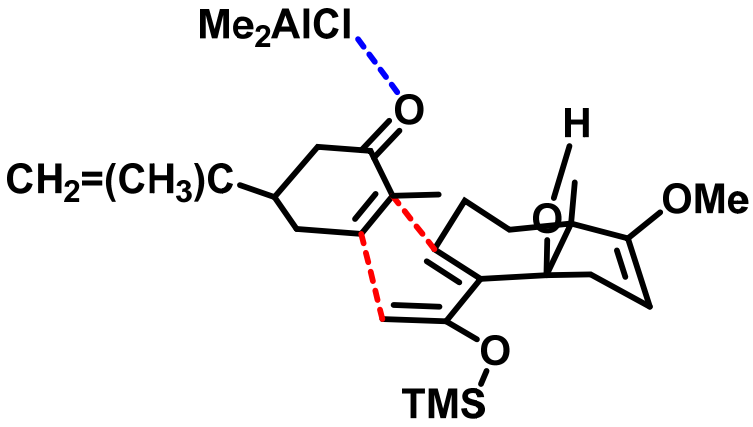
Atom	X	Y	Z
C	1.020005	0.689673	-1.216536
C	1.646816	-1.547828	-2.187695
C	-1.099651	-2.003825	-1.676278
C	0.127995	-2.655995	-1.395798
C	-0.016159	0.815047	-2.091944
C	1.909976	-0.456932	-1.340596
H	1.146594	-1.360532	-3.129460
H	2.433105	-2.291815	-2.262754
H	-0.116996	0.097109	-2.894808
C	-0.995973	1.941839	-2.109741

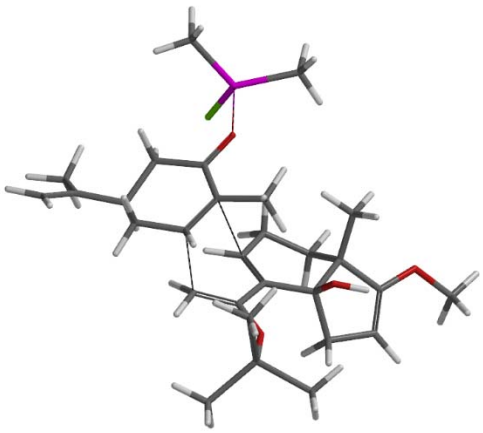
H	-1.945754	1.585594	-1.678816
H	-1.235773	2.192175	-3.151408
C	-0.458529	3.173000	-1.376024
H	-1.243213	3.928965	-1.264231
H	0.336972	3.626546	-1.981735
C	0.099988	2.807209	0.020470
C	1.240730	1.715172	-0.100868
C	-1.055438	2.410762	0.955867
H	-1.591739	1.529239	0.600926
H	-1.772852	3.233999	1.018220
H	-0.713792	2.195601	1.970912
C	0.897926	3.981773	0.568257
C	2.227232	3.851385	0.420246
H	2.979319	4.582540	0.692859
C	2.550345	2.550801	-0.272790
H	2.788761	2.702040	-1.336430
H	3.393093	2.009322	0.167824
O	0.177387	5.000859	1.087672
C	0.916604	6.120183	1.560159
H	1.601594	5.824144	2.365411
H	0.184685	6.833085	1.942802
H	1.494953	6.579246	0.747848
O	1.318796	0.974910	1.128149
H	1.462450	1.634800	1.827657
O	2.919069	-0.505383	-0.472456
H	0.384785	-3.438091	-2.110643
C	0.528266	-2.970412	0.046171
H	1.302190	-2.285029	0.401022
H	0.961690	-3.977639	0.087992
C	-0.656983	-2.845850	1.028715
H	-1.387337	-3.628236	0.780759
C	-1.823444	-1.371122	-0.638510
C	-1.334091	-1.484304	0.789513
H	-2.171417	-1.322062	1.472099
C	-1.679734	-2.049802	-3.069992
H	-0.895005	-2.162351	-3.829077

H	-2.260355	-1.151240	-3.293881
H	-2.361152	-2.903242	-3.188172
Si	4.385599	-1.295654	-0.113872
C	4.430169	-3.095241	-0.671312
H	4.492323	-3.212211	-1.758980
H	3.560950	-3.657197	-0.312932
H	5.323235	-3.570758	-0.245050
C	5.733831	-0.302555	-0.970435
H	5.585697	-0.279956	-2.056660
H	6.720639	-0.741894	-0.779281
H	5.753461	0.733128	-0.613621
C	4.479305	-1.195512	1.755841
H	4.429283	-0.157359	2.101391
H	5.410187	-1.636132	2.132744
H	3.639796	-1.734212	2.210703
H	-0.611470	-0.679066	0.977546
C	-0.200702	-3.069147	2.466878
C	0.470752	-2.141664	3.159335
H	0.798916	-2.329971	4.178798
H	0.704771	-1.163790	2.746242
C	-0.533022	-4.418640	3.054390
H	-0.110321	-4.542853	4.056186
H	-0.155940	-5.233928	2.420682
H	-1.620769	-4.556719	3.123240
O	-2.910257	-0.746319	-0.902386
Al	-4.608302	-0.236871	-0.243600
Cl	-4.290572	0.396335	1.860556
C	-5.681883	-1.899042	-0.320491
H	-5.215502	-2.725944	0.232791
H	-5.838701	-2.247116	-1.351420
H	-6.676652	-1.748510	0.120637
C	-5.078075	1.319047	-1.373392
H	-6.097641	1.669587	-1.161609
H	-5.040521	1.081643	-2.446377
H	-4.414783	2.179198	-1.206853

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions





56-TS

E(B3LYP/6-31G*) = –2387.78622 au

v*ts* = 360*i* cm^{-1}

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	1.312396	0.109356	0.759156
C	0.364063	2.448575	0.703585
C	-1.237745	1.045864	-1.281460
C	-1.068943	2.360690	-0.790227
C	0.177006	-0.395484	1.313170

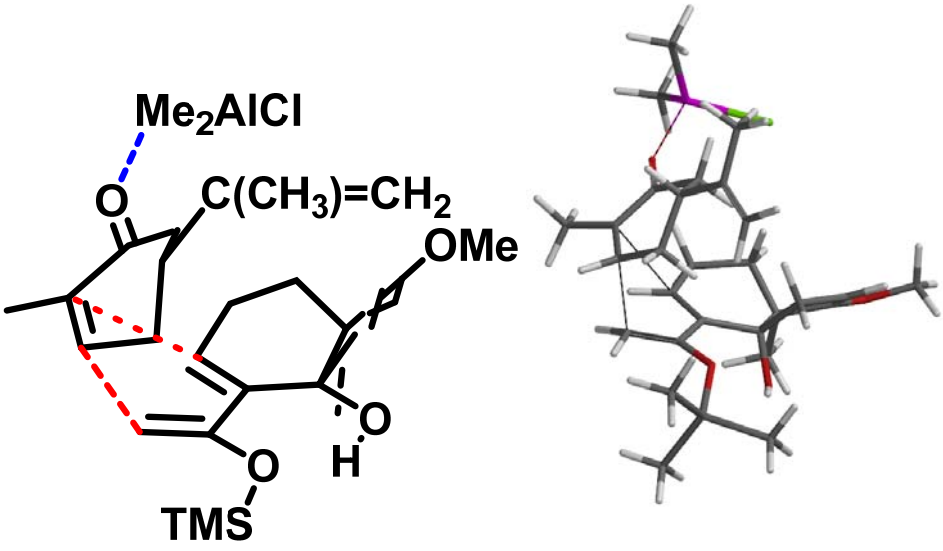
C	1.430774	1.550183	0.545027
H	-0.362845	2.216748	1.468706
H	-0.479984	3.012672	-1.433196
H	0.619086	3.503555	0.664095
H	-0.611071	0.283173	1.618575
C	-0.070634	-1.835410	1.626370
H	-0.815432	-2.230338	0.920149
H	-0.568106	-1.906054	2.602468
C	1.220226	-2.655598	1.619060
H	0.996375	-3.727361	1.652251
H	1.798508	-2.423212	2.522698
C	2.081853	-2.347053	0.372316
C	2.455366	-0.813564	0.329413
C	1.379929	-2.853776	-0.898511
H	0.427309	-2.343575	-1.064215
H	1.182335	-3.926034	-0.805145
H	1.991375	-2.701073	-1.790938
C	3.462440	-2.957362	0.565585
C	4.375013	-2.081272	1.021928
H	5.402266	-2.302674	1.287653
C	3.742265	-0.721193	1.209405
H	3.492086	-0.530627	2.264034
H	4.365773	0.112905	0.873396
C	-2.353018	0.279717	-0.881988
C	-2.227477	3.060587	-0.103449
H	-2.885169	3.446527	-0.896815
H	-1.878441	3.934591	0.458003
C	-3.022847	2.114783	0.804433
H	-2.348279	1.775988	1.607846
C	-3.433591	0.857257	0.009957
H	-4.283595	1.098070	-0.646874
H	-3.780825	0.060658	0.674685
O	3.573238	-4.280019	0.308597
O	2.797312	-0.453470	-1.019129
H	3.539298	-1.032661	-1.263954
O	2.628022	1.969540	0.136340

C	-0.264481	0.513174	-2.298320
H	-0.173981	1.208212	-3.144402
H	-0.594676	-0.453031	-2.683732
H	0.741561	0.380160	-1.880247
Si	3.328429	3.352971	-0.572206
C	2.400243	3.781618	-2.152257
C	5.079186	2.788344	-0.933100
C	3.320064	4.778427	0.660070
C	-4.218008	2.743886	1.507403
C	-4.653967	3.981883	1.251132
H	-5.508444	4.395555	1.780479
H	-4.191789	4.628879	0.512452
C	-4.890375	1.876484	2.546324
H	-5.342931	0.981417	2.101924
H	-5.678084	2.424270	3.072123
H	-4.167957	1.518358	3.292817
H	3.900157	5.620960	0.262765
H	2.313800	5.149850	0.882015
H	3.783297	4.477911	1.607098
H	2.981992	4.491572	-2.753344
H	1.426998	4.243474	-1.952813
H	2.235717	2.885274	-2.760393
H	5.067464	1.889764	-1.559426
H	5.615611	2.545564	-0.008925
H	5.649746	3.564223	-1.457317
O	-2.530605	-0.901130	-1.351989
Al	-3.752874	-2.331180	-1.161797
Cl	-3.784522	-2.620513	1.057723
C	-5.514092	-1.700764	-1.813805
H	-5.470873	-1.381113	-2.865073
H	-5.918943	-0.859197	-1.235976
H	-6.261695	-2.504258	-1.759521
C	-2.843054	-3.842267	-2.050899
H	-1.832168	-4.013185	-1.656495
H	-2.741332	-3.679775	-3.133552
H	-3.396392	-4.782282	-1.920904

C	4.841283	-4.872531	0.562949
H	5.620864	-4.408576	-0.055474
H	4.745021	-5.928432	0.304375
H	5.115619	-4.771094	1.620918

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



57-TS

E(B3LYP/6-31G*) = –2387.78994 au

v*ts* = 371*i* cm^{-1}

Cartesian Coordinates (Angstroms)

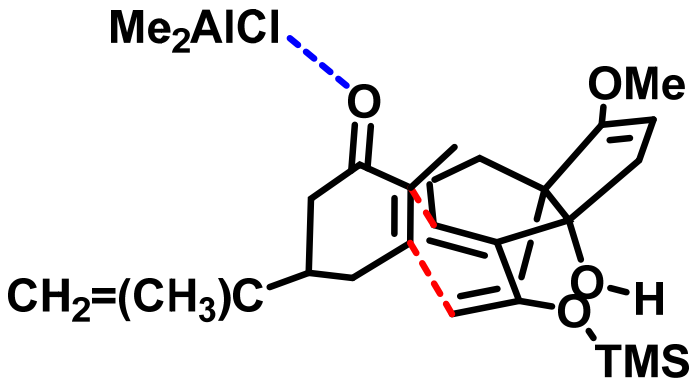
Atom	X	Y	Z
C	1.130493	0.681904	-1.086343
C	1.842114	-1.592399	-1.900891
C	-0.937897	-2.114201	-1.688345
C	0.265593	-2.715030	-1.241927
C	0.106416	0.718864	-1.989876
C	2.012951	-0.463042	-1.083991
H	1.447144	-1.444549	-2.898735

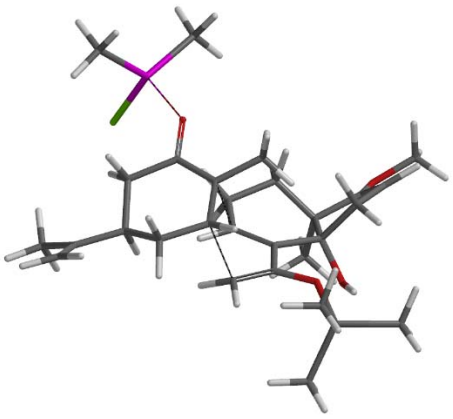
H	2.626836	-2.341211	-1.858829
H	0.057606	-0.023039	-2.777268
C	-0.934757	1.783520	-2.048721
H	-1.916364	1.301373	-2.165112
H	-0.785284	2.362738	-2.974377
C	-0.926080	2.674674	-0.806827
H	-1.538350	3.568152	-0.968674
C	0.505249	3.105341	-0.398451
C	1.382897	1.841682	-0.104231
O	2.938768	-0.492051	-0.093805
H	-1.396864	2.127304	0.017030
C	1.119570	4.045630	-1.448514
H	1.239623	3.542185	-2.414179
H	2.103289	4.397369	-1.133116
H	0.468493	4.913864	-1.592475
C	0.427351	3.727894	0.985981
C	0.727613	2.872199	1.972957
H	0.666238	3.063043	3.037431
C	1.094938	1.527465	1.397500
H	1.972453	1.069319	1.870658
H	0.272685	0.804461	1.507008
O	2.748442	2.259312	-0.244932
H	3.273606	1.565843	0.181221
O	0.001544	5.011660	1.035691
C	-0.196752	5.552141	2.335953
H	-0.959935	4.982980	2.881768
H	-0.532451	6.581028	2.194908
H	0.739297	5.542445	2.909554
H	0.627749	-3.511600	-1.891657
C	-1.841943	-1.544983	-0.760505
C	-1.616428	-1.731456	0.726289
H	-2.594105	-1.747689	1.211447
H	-1.091989	-0.857708	1.135377
C	0.504879	-2.957077	0.246445
H	1.073319	-3.885185	0.375863
H	1.119320	-2.158213	0.673901

C	-0.814309	-3.016091	1.030668
H	-1.405292	-3.857218	0.635321
C	-1.319103	-2.177831	-3.148726
H	-1.866694	-3.103253	-3.374019
H	-0.435764	-2.167580	-3.799976
H	-1.971164	-1.347269	-3.428107
Si	4.526840	-1.160289	-0.054031
C	4.458784	-3.010566	0.284617
H	5.469398	-3.387230	0.486974
H	4.057633	-3.589286	-0.554738
H	3.844739	-3.227352	1.166189
C	5.309042	-0.257656	1.393882
H	6.328217	-0.622357	1.569860
H	4.738523	-0.412836	2.316843
H	5.374353	0.822394	1.217040
C	5.380703	-0.754916	-1.677610
H	6.429462	-1.074551	-1.642792
H	5.367444	0.324486	-1.866995
H	4.910925	-1.250700	-2.533589
C	-0.660771	-3.246448	2.527611
C	0.516151	-3.234140	3.163152
H	0.575139	-3.408212	4.234406
H	1.460577	-3.051758	2.659986
C	-1.945548	-3.508400	3.280600
H	-2.612015	-2.637490	3.262208
H	-1.748415	-3.754394	4.328183
H	-2.503617	-4.341275	2.832168
O	-2.903169	-0.958589	-1.172925
Al	-4.525266	-0.305782	-0.424442
Cl	-3.826896	1.038398	1.201926
C	-5.462544	-1.890960	0.312684
H	-5.707220	-2.623562	-0.469885
H	-6.413797	-1.595914	0.776832
H	-4.894662	-2.425449	1.086609
C	-5.322530	0.706576	-1.920159
H	-5.531346	0.056673	-2.782217

H	-4.674181	1.518044	-2.278862
H	-6.275807	1.170808	-1.633316

Requested basis set is 6-31G(d)
There are 235 shells and 629 basis functions





58-TS

E(B3LYP/6-31G*) = –2387.79215 au
ν*ts* = 363*i* cm^{-1}

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	1.351502	0.067187	0.610962
C	0.410976	2.402159	0.472084
C	-1.279589	0.926464	-1.356428
C	-1.044232	2.264287	-0.952014

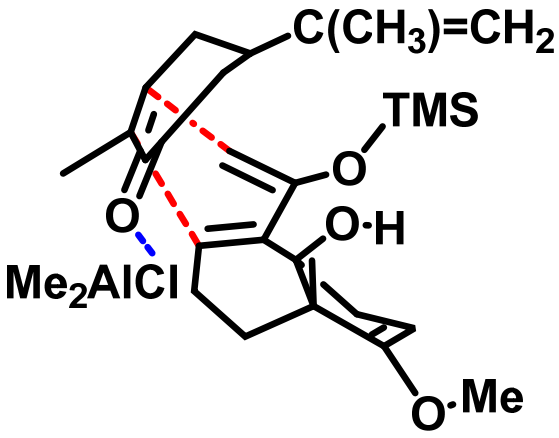
C	0.179194	-0.411264	1.119852
C	1.453063	1.477952	0.288992
H	-0.249526	2.228390	1.310684
H	-0.454206	2.849030	-1.658205
H	0.663067	3.449565	0.341087
H	-0.614507	0.279750	1.379765
C	-0.093449	-1.845614	1.425264
H	-1.102751	-2.102715	1.077750
H	-0.142946	-1.960777	2.520016
C	0.950008	-2.774038	0.808066
H	0.851565	-3.786692	1.213969
C	2.397849	-2.271698	1.039141
C	2.577335	-0.845742	0.410070
C	-2.423694	0.236333	-0.906043
C	-2.172398	3.044012	-0.297160
H	-2.836165	3.385564	-1.104937
H	-1.793321	3.947581	0.193923
C	-2.969344	2.186485	0.691514
H	-2.279845	1.877967	1.493628
C	-3.447415	0.896578	-0.007561
H	-4.318315	1.121847	-0.641935
H	-3.787233	0.148535	0.715332
O	2.591257	1.850340	-0.339137
H	0.762499	-2.849134	-0.269940
C	2.769746	-2.337690	2.529069
H	2.142867	-1.670296	3.129488
H	3.809460	-2.046200	2.685276
H	2.632252	-3.360278	2.894499
C	3.329742	-3.090529	0.160141
C	3.622879	-2.496079	-1.004707
H	4.210048	-2.912930	-1.814191
C	2.964789	-1.140060	-1.074808
H	3.626040	-0.355610	-1.462643
H	2.078588	-1.148340	-1.724262
O	3.696927	-0.251871	1.081739
H	3.938790	0.518219	0.546061

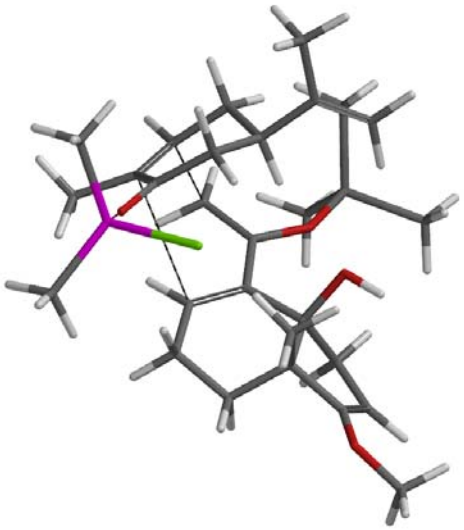
O	3.675462	-4.311168	0.633647
C	4.484670	-5.105553	-0.223325
H	3.961777	-5.325408	-1.163347
H	4.684548	-6.034540	0.313451
H	5.430382	-4.595987	-0.449510
C	-0.372428	0.295596	-2.379760
H	-0.655258	0.603228	-3.397178
H	-0.423660	-0.794618	-2.344275
H	0.666157	0.610015	-2.226861
C	-4.125179	2.901495	1.378994
C	-4.581560	4.099913	0.999072
H	-5.414260	4.569459	1.516445
H	-4.165217	4.659687	0.166939
C	-4.743191	2.163129	2.544013
H	-5.520549	2.763473	3.025283
H	-3.986352	1.914865	3.300767
H	-5.194755	1.212987	2.232960
Si	3.407229	3.358609	-0.487619
C	2.555565	4.426501	-1.781039
H	3.157770	5.321726	-1.981025
H	1.560225	4.765606	-1.473516
H	2.450117	3.883588	-2.727479
C	5.109493	2.830593	-1.073112
H	5.613527	2.194180	-0.335900
H	5.750073	3.704542	-1.242722
H	5.053704	2.273207	-2.015119
C	3.488326	4.182313	1.201222
H	4.143779	5.060979	1.155237
H	3.905950	3.497728	1.948598
H	2.511664	4.518110	1.564358
O	-2.666317	-0.948286	-1.331918
Al	-3.953932	-2.310724	-1.070995
Cl	-4.008505	-2.472231	1.159756
C	-3.103664	-3.911505	-1.854150
H	-2.129125	-4.130480	-1.396926
H	-2.935450	-3.803336	-2.935078

H	-3.724575	-4.806986	-1.716072
C	-5.673078	-1.638315	-1.789999
H	-5.591342	-1.363616	-2.851601
H	-6.065703	-0.761357	-1.258279
H	-6.449444	-2.413294	-1.725533

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions





59-TS

E(B3LYP/6-31G*) = –2387.78994 au

v*ts* = 354*i* cm^{-1}

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.836818	-0.733794	-1.179643
C	-0.008879	0.654495	-1.980335
C	0.201509	-2.816349	-1.169150
C	1.360560	-2.090531	-1.535514
C	-1.447211	-1.863803	-1.923334
C	-1.072846	0.509739	-1.143153
H	0.206637	-0.126758	-2.696259

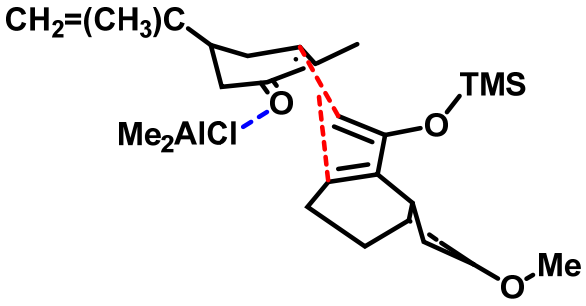
H	-0.983328	-1.699878	-2.888192
H	-2.157870	-2.685674	-1.931403
C	0.867857	1.862750	-2.063489
H	1.132269	2.043397	-3.113585
H	1.823157	1.635976	-1.564461
C	0.195305	3.098327	-1.460140
H	0.910577	3.923340	-1.373588
C	-1.455974	1.616546	-0.156766
C	-0.405295	2.793380	-0.066309
H	-0.600810	3.434432	-2.136780
C	0.721268	2.540767	0.948974
H	1.396657	3.400651	0.978450
H	1.315704	1.662396	0.688189
H	0.338941	2.384425	1.960248
C	-1.316054	3.940904	0.345385
C	-2.619442	3.703518	0.115803
H	-3.437492	4.394387	0.283585
C	-2.798379	2.336649	-0.502010
H	-2.952332	2.397924	-1.590169
H	-3.638079	1.768701	-0.090287
O	-1.579773	1.001902	1.133423
H	-1.818837	1.715112	1.749315
O	-0.705233	5.041373	0.838562
C	-1.549985	6.135631	1.172430
H	-0.897661	6.923539	1.552046
H	-2.273430	5.848291	1.946574
H	-2.093503	6.494997	0.289039
O	-2.892104	-0.786750	-0.365513
Si	-4.315398	-1.715629	-0.190857
C	-5.137396	-1.923884	-1.872801
H	-4.550279	-2.540562	-2.561779
H	-5.309647	-0.954097	-2.353905
H	-6.114376	-2.408187	-1.750026
C	-5.358505	-0.663163	0.958047
H	-4.804838	-0.430782	1.874364
H	-6.280354	-1.184738	1.242099

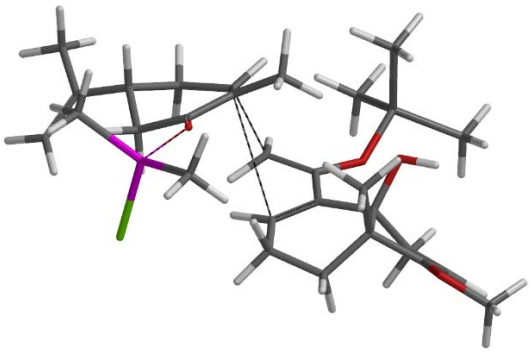
H	-5.641315	0.285138	0.487663
C	-3.925793	-3.372707	0.609073
H	-3.323286	-3.237561	1.514643
H	-3.387885	-4.054868	-0.058198
H	-4.858874	-3.871149	0.901521
H	-0.045258	-3.643026	-1.837275
C	2.147090	-1.445889	-0.552780
C	1.847760	-1.607877	0.922041
H	2.145898	-0.695453	1.447457
H	2.530810	-2.393112	1.281205
C	-0.059838	-3.121690	0.291474
H	0.498962	-4.039989	0.529629
H	-1.116079	-3.352585	0.455641
C	0.384444	-1.977888	1.222383
H	-0.226286	-1.102025	0.986916
C	1.840537	-2.106189	-2.967266
H	2.440738	-1.222530	-3.196672
H	1.003627	-2.160786	-3.677017
H	2.473916	-2.982940	-3.162454
C	0.134831	-2.306202	2.688634
C	-0.806613	-1.644601	3.372511
H	-1.012841	-1.867692	4.417129
H	-1.383458	-0.847045	2.912226
C	0.963149	-3.389603	3.339280
H	0.901439	-4.341499	2.794948
H	0.632811	-3.569555	4.366664
H	2.025944	-3.117806	3.375830
O	3.196738	-0.801920	-0.906548
Al	4.832062	-0.135520	-0.222394
Cl	4.255928	1.072044	1.554133
C	5.468567	1.036254	-1.683348
H	4.765489	1.853598	-1.895825
H	5.612420	0.482498	-2.622517
H	6.430713	1.506939	-1.439742
C	5.860439	-1.745084	0.304515
H	6.802313	-1.468481	0.797956

H	6.125858	-2.363724	-0.565064
H	5.318475	-2.392502	1.008255

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions





60-TS

E(B3LYP/6-31G*) = –2387.78720 au

v*ts* = 344*i* cm^{-1}

Cartesian Coordinates (Angstroms)

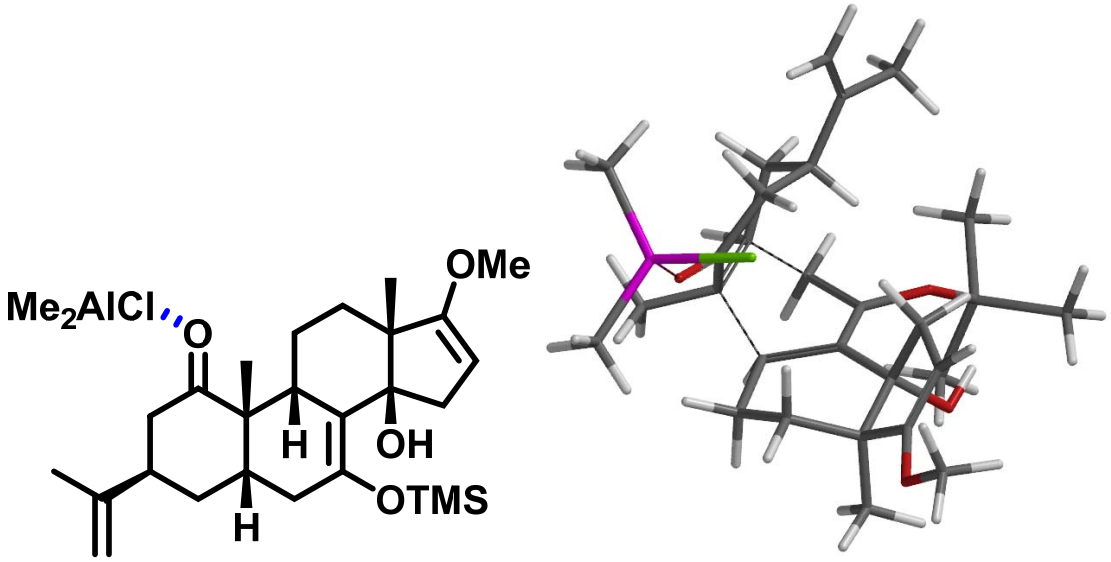
Atom	X	Y	Z
C	-1.117949	1.589846	0.777242
C	-0.323420	-0.676850	1.177952
C	1.414038	2.083949	-0.614260
C	1.423868	0.776801	-1.162093
C	0.136610	2.182866	0.989510
C	-1.328736	0.146993	0.771882
H	0.597303	-0.250174	1.557413
H	0.838624	2.803141	-1.194835
H	0.830208	1.653317	1.628274
C	2.679241	2.676440	0.017773
C	2.372742	-0.163519	-0.702931
C	3.455892	0.293476	0.252380
H	4.301351	-0.393911	0.182295
H	3.088076	0.213631	1.286103

C	3.898539	1.727142	-0.066807
H	2.899258	3.621904	-0.492750
H	2.519694	2.936280	1.071027
H	0.127704	3.255283	1.159100
C	-0.392278	-2.166332	1.211372
H	0.148363	-2.535130	2.090413
H	0.186731	-2.554725	0.360288
C	-1.835338	-2.671254	1.197616
H	-1.864415	-3.757235	1.055432
C	-2.666325	-0.417943	0.291134
C	-2.670533	-1.984337	0.089959
H	-2.292528	-2.466425	2.174063
C	-2.181884	-2.432499	-1.297971
H	-2.211044	-3.524463	-1.364040
H	-1.156307	-2.103321	-1.482310
H	-2.805492	-2.031001	-2.100468
C	-4.144373	-2.286832	0.317756
C	-4.800117	-1.303327	0.958888
H	-5.835671	-1.322335	1.278457
C	-3.853944	-0.167123	1.273206
H	-3.514603	-0.199376	2.319504
H	-4.275255	0.828790	1.107672
O	-2.960483	0.217608	-0.966156
H	-3.832955	-0.119138	-1.232850
O	-4.579466	-3.496582	-0.102048
C	-5.939031	-3.807846	0.178441
H	-6.117093	-4.804297	-0.228925
H	-6.611834	-3.084814	-0.301270
H	-6.125377	-3.808599	1.260122
O	-2.192642	2.345941	0.539288
Si	-2.620400	3.743997	-0.337595
C	-1.756609	5.265599	0.366297
H	-0.677679	5.270697	0.176346
H	-1.912006	5.350746	1.448089
H	-2.170342	6.170691	-0.096694
C	-4.471611	3.872058	-0.056886

H	-4.880510	4.765867	-0.543232
H	-4.701901	3.939837	1.012368
H	-4.997002	2.999600	-0.459800
C	-2.187285	3.491314	-2.147780
H	-2.587526	2.537620	-2.505568
H	-1.104573	3.483779	-2.315073
H	-2.610782	4.298066	-2.758977
C	0.411957	0.407735	-2.214016
H	0.498560	-0.646799	-2.481373
H	0.564521	1.002985	-3.125370
H	-0.616659	0.591612	-1.879911
H	4.235602	1.729705	-1.115330
C	5.059878	2.234841	0.775556
C	5.533482	1.584483	1.843661
H	6.370756	1.981615	2.412084
H	5.130804	0.637689	2.188691
C	5.678518	3.537076	0.318583
H	6.004827	3.472105	-0.728678
H	6.548688	3.798988	0.927804
H	4.969177	4.373739	0.375166
O	2.348259	-1.380415	-1.110051
Al	3.299167	-2.974417	-0.713596
Cl	3.269827	-2.979614	1.520358
C	5.144083	-2.787411	-1.411358
H	5.721985	-1.968503	-0.961773
H	5.153147	-2.628600	-2.499422
H	5.714684	-3.707844	-1.223500
C	2.134377	-4.392478	-1.449853
H	2.546504	-5.392312	-1.256507
H	2.024831	-4.299332	-2.539942
H	1.121429	-4.384098	-1.024892

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



[**53**+Me_2AlCl]

E(B3LYP/6-31G*) = –2387.82629 au

Cartesian Coordinates (Angstroms)

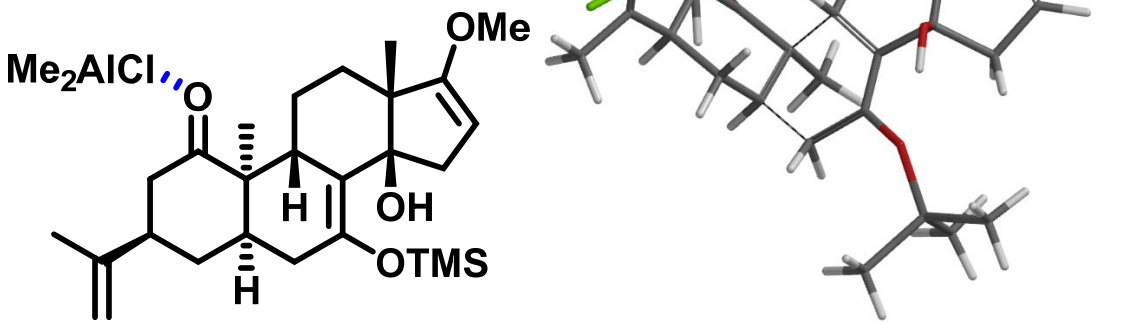
Atom	X	Y	Z
C	-1.965837	-0.650377	-0.685571
C	0.035123	-0.045264	-1.887850
C	-0.337489	-2.534737	-1.208526
C	0.758217	-1.448125	-1.541209
C	-1.778977	-1.976645	-1.372030
C	-1.054023	0.320397	-0.876985
H	-0.479024	-0.325657	-2.818163
H	-1.989398	-1.872977	-2.447432
C	-1.157891	1.676938	-0.167762
C	-0.234257	2.797318	-0.743907
H	-2.488290	-2.713211	-0.984160
O	-3.030541	-0.513811	0.182817
C	0.977494	1.125797	-2.259440
H	0.576960	1.599604	-3.162496
H	1.968453	0.754112	-2.530809
C	1.121450	2.182488	-1.165704
H	1.777019	2.987907	-1.517672
H	1.619008	1.756569	-0.286290

C	-0.879291	3.588467	-1.893748
H	-0.166385	4.317741	-2.292284
H	-1.764408	4.122624	-1.544490
H	-1.195906	2.929622	-2.708986
C	-0.002374	3.652782	0.492203
C	-0.278892	3.019048	1.639804
H	-0.127754	3.400300	2.642510
C	-0.767075	1.624042	1.348835
H	0.018018	0.878392	1.542092
H	-1.634840	1.318644	1.947535
O	0.507930	4.888257	0.271862
O	-2.500584	2.177209	-0.264124
H	-3.037148	1.546091	0.240287
Si	-4.678083	-0.782726	-0.174171
C	-5.591269	0.382064	0.984345
C	-4.984091	-0.349491	-1.978506
C	-5.143589	-2.566414	0.225257
C	1.745370	-1.228556	-0.406844
C	1.487120	-1.614770	1.024870
H	1.700533	-0.740365	1.653635
H	2.295633	-2.325029	1.253555
C	-0.145003	-3.240232	0.151637
H	0.699899	-3.941731	0.084690
H	-1.030716	-3.852674	0.349613
C	0.134632	-2.265677	1.312497
H	-0.639453	-1.488677	1.294639
H	-0.238019	-3.320606	-1.966806
C	1.545707	-1.916384	-2.787842
H	2.330107	-1.216079	-3.077064
H	0.856009	-2.036461	-3.630203
H	2.018769	-2.886992	-2.600516
C	0.043794	-2.923881	2.682708
C	1.070412	-3.028442	3.533814
H	0.939576	-3.490825	4.508679
H	2.067736	-2.658612	3.319322
C	-1.330097	-3.429408	3.064445

H	-2.086855	-2.642925	2.938480
H	-1.353769	-3.762680	4.105932
H	-1.646826	-4.274699	2.439498
H	-6.233452	-2.691936	0.201758
H	-4.716273	-3.286250	-0.481711
H	-4.801620	-2.839182	1.230415
H	-6.056852	-0.349068	-2.205865
H	-4.590873	0.649915	-2.197264
H	-4.500868	-1.057316	-2.661499
O	2.850870	-0.730790	-0.697453
Al	4.556425	-0.261017	0.174717
Cl	3.863738	0.980603	1.855230
C	5.250403	-2.024613	0.743923
H	6.294334	-1.928830	1.073258
H	5.248170	-2.757463	-0.075243
H	4.703358	-2.469436	1.585319
C	5.445949	0.784849	-1.234560
H	4.879614	1.683502	-1.512026
H	5.593990	0.196105	-2.150808
H	6.438855	1.125545	-0.911686
H	-5.382502	1.434274	0.758265
H	-6.675529	0.238668	0.900430
H	-5.314775	0.201073	2.029636
C	0.832682	5.640194	1.433673
H	1.237664	6.591540	1.083835
H	1.582666	5.115896	2.039522
H	-0.061476	5.820744	2.045024

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



[**54**+Me_2AlCl]

E(B3LYP/6-31G*) = –2387.83798 au

Cartesian Coordinates (Angstroms)

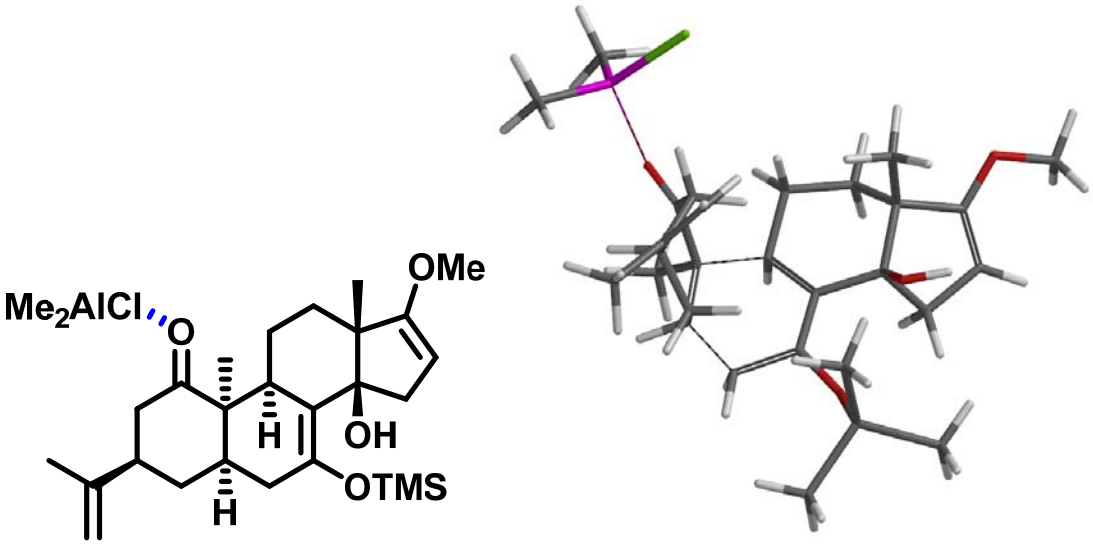
Atom	X	Y	Z
C	-1.368068	-1.611134	0.308450
C	-0.080077	0.459167	-0.203107
C	1.181232	-1.658668	0.481998
C	1.037374	-0.116935	0.739349
C	-0.151275	-2.356039	0.797890
C	-1.386699	-0.326182	-0.093420
H	0.255396	0.287930	-1.233135
H	1.933308	-2.033432	1.190859
H	-0.146891	-3.351529	0.336818
C	1.694255	-1.988403	-0.931540
C	2.373120	0.500968	0.360034
C	2.931076	0.223116	-1.007498
H	3.902629	0.704150	-1.124018
H	2.241793	0.652325	-1.745205
C	3.046437	-1.306281	-1.232813
C	-2.664891	0.260164	-0.721312
C	-2.531416	1.760867	-1.151919
H	1.810814	-3.076247	-1.013027
H	0.960013	-1.702236	-1.694882

H	-0.239153	-2.527961	1.880875
O	-2.514320	-2.376232	0.205783
C	-0.221657	2.004524	-0.057809
H	0.350640	2.478504	-0.864728
H	0.234854	2.352934	0.873434
C	-1.671449	2.494210	-0.097364
H	-1.697493	3.572995	-0.291186
H	-2.133548	2.345544	0.886980
C	-1.995973	1.973492	-2.576752
H	-1.966034	3.044158	-2.803243
H	-2.640690	1.480860	-3.306407
H	-0.986339	1.569743	-2.703105
C	-3.964524	2.247697	-1.003521
C	-4.717014	1.454704	-0.230146
H	-5.746866	1.625102	0.061794
C	-3.916002	0.262678	0.223846
H	-3.620281	0.338875	1.281720
H	-4.461004	-0.679778	0.115326
O	-4.261573	3.426140	-1.604740
C	-5.589979	3.896043	-1.423512
H	-5.667970	4.830949	-1.981438
H	-5.799804	4.078864	-0.361223
H	-6.316190	3.169673	-1.810954
O	-2.981920	-0.480042	-1.908295
H	-3.101359	-1.398235	-1.611466
Si	-3.207571	-3.507566	1.270291
C	-4.961721	-3.715050	0.629347
H	-5.488829	-4.495041	1.192252
H	-4.964230	-4.011048	-0.426128
H	-5.542001	-2.789888	0.718702
C	-2.306756	-5.161657	1.176936
H	-1.286469	-5.114322	1.571461
H	-2.253950	-5.522221	0.142761
H	-2.849593	-5.916715	1.759784
C	-3.186513	-2.822612	3.026326
H	-3.634522	-1.823217	3.064708

H	-2.170644	-2.752790	3.432263
H	-3.762223	-3.471639	3.697842
C	0.721766	0.131490	2.224841
H	0.795878	1.187203	2.491941
H	1.426983	-0.408320	2.865088
H	-0.291129	-0.209267	2.449770
H	3.776985	-1.670157	-0.495655
C	3.573650	-1.679634	-2.612931
C	3.384876	-0.930855	-3.703740
H	3.753422	-1.249837	-4.675000
H	2.867670	0.024088	-3.685533
C	4.325157	-2.988156	-2.671308
H	5.242240	-2.933106	-2.069849
H	4.604053	-3.245679	-3.697137
H	3.730395	-3.816669	-2.263622
O	2.992095	1.172653	1.201352
Al	4.778400	2.006512	1.405325
C	4.793799	2.407923	3.331094
H	4.585883	1.519952	3.941693
H	4.049370	3.170456	3.599849
H	5.771817	2.790846	3.651959
C	4.816091	3.440900	0.047251
H	4.782756	3.078830	-0.988635
H	5.741299	4.026178	0.141142
H	3.985440	4.149850	0.173153
Cl	6.019559	0.264167	0.876590

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



[**55**+Me_2AlCl]

E(B3LYP/6-31G*) = –2387.83219 au

Cartesian Coordinates (Angstroms)

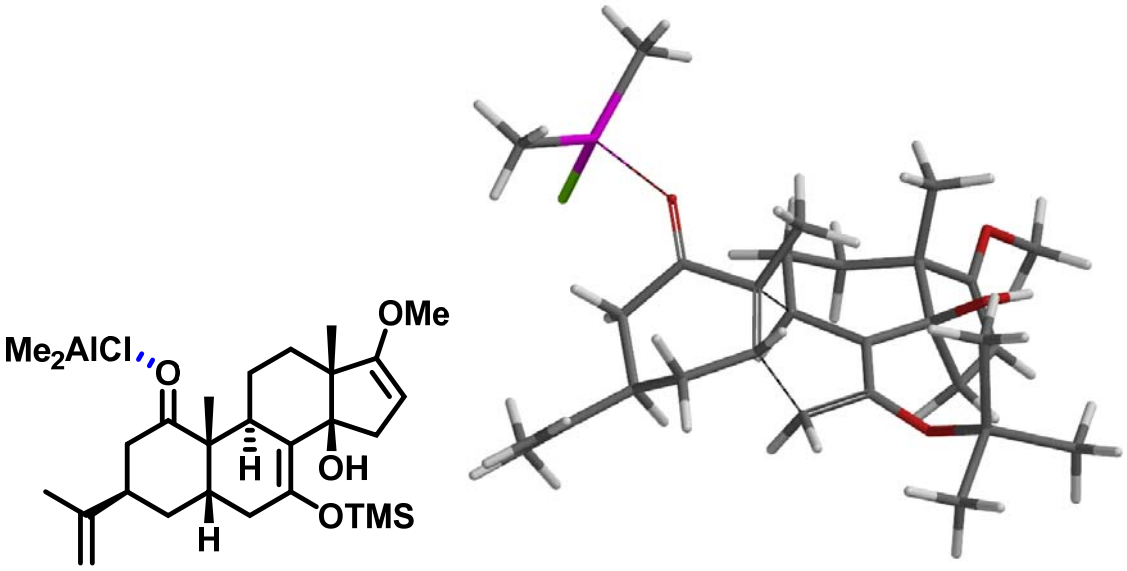
Atom	X	Y	Z
C	1.144158	0.563056	-0.907180
C	1.450052	-1.639094	-2.016113
C	-0.950975	-0.908663	-1.637190
C	0.076446	-2.088467	-1.484394
C	-0.249615	0.536428	-1.543780
C	1.969429	-0.457120	-1.230350
H	1.371695	-1.371878	-3.080694
H	2.166092	-2.465291	-1.957235
H	-0.088133	0.786336	-2.604648
C	-1.213041	1.624589	-1.025932
H	-1.636611	1.362940	-0.050498
H	-2.065465	1.702065	-1.710207
C	-0.505491	2.972143	-0.912973
H	-1.219501	3.758818	-0.643238
H	-0.085191	3.250959	-1.889215
C	0.619720	2.921085	0.145794
C	1.687735	1.825687	-0.240709

C	0.034174	2.735531	1.558412
H	-0.377936	1.733083	1.699688
H	-0.763487	3.463805	1.734598
H	0.794633	2.880540	2.329330
C	1.456931	4.187647	0.046450
C	2.593130	4.026034	-0.652432
H	3.314079	4.799327	-0.892831
C	2.690982	2.606441	-1.156287
H	2.398188	2.532317	-2.214312
H	3.686626	2.162106	-1.076045
O	0.936254	5.294129	0.627469
C	1.686881	6.492629	0.477671
H	2.683236	6.388004	0.926752
H	1.128496	7.273947	0.995820
H	1.798375	6.754462	-0.582462
O	2.384719	1.417153	0.950794
H	2.819356	2.220445	1.286690
O	3.305291	-0.445868	-0.985965
H	-0.298821	-2.895012	-2.128106
C	0.259613	-2.685097	-0.070627
H	0.952667	-2.063837	0.505990
H	0.733127	-3.667942	-0.183479
C	-1.034185	-2.803352	0.754820
H	-1.740067	-3.456581	0.217680
C	-2.027180	-0.998792	-0.570184
C	-1.651178	-1.384842	0.824254
H	-2.520505	-1.330306	1.479856
C	-1.607656	-1.012613	-3.029969
H	-0.829248	-1.060482	-3.798669
H	-2.245553	-0.150912	-3.242203
H	-2.225694	-1.912215	-3.112035
Si	4.368289	-1.199775	0.093139
C	4.977142	-2.805893	-0.692828
H	5.420572	-2.623904	-1.678712
H	4.167618	-3.535131	-0.819639
H	5.744374	-3.276500	-0.064811

C	5.793989	0.015253	0.248433
H	6.202325	0.269466	-0.736649
H	6.610978	-0.398764	0.851876
H	5.457419	0.943005	0.723733
C	3.578798	-1.550862	1.764998
H	3.025893	-0.672492	2.110779
H	4.359005	-1.782231	2.501902
H	2.891318	-2.403239	1.741187
H	-0.884117	-0.689841	1.191859
C	-0.782274	-3.435713	2.115276
C	-0.706064	-2.732872	3.249568
H	-0.504265	-3.222200	4.198783
H	-0.849117	-1.657276	3.291016
C	-0.614630	-4.937505	2.104300
H	-0.399297	-5.321335	3.105738
H	0.200460	-5.256633	1.441084
H	-1.527081	-5.429875	1.741368
O	-3.210255	-0.798158	-0.896000
Al	-5.012793	-0.720283	-0.097630
Cl	-4.624420	0.441363	1.733787
C	-5.398790	-2.625126	0.254726
H	-4.638693	-3.111821	0.880666
H	-5.480157	-3.208010	-0.673593
H	-6.355330	-2.738269	0.782455
C	-5.991496	0.312384	-1.458279
H	-7.051485	0.421935	-1.192188
H	-5.958276	-0.172268	-2.444004
H	-5.591086	1.327310	-1.578965

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



[**56**+Me_2AlCl]

E(B3LYP/6-31G*) = –2387.83421 au

Cartesian Coordinates (Angstroms)

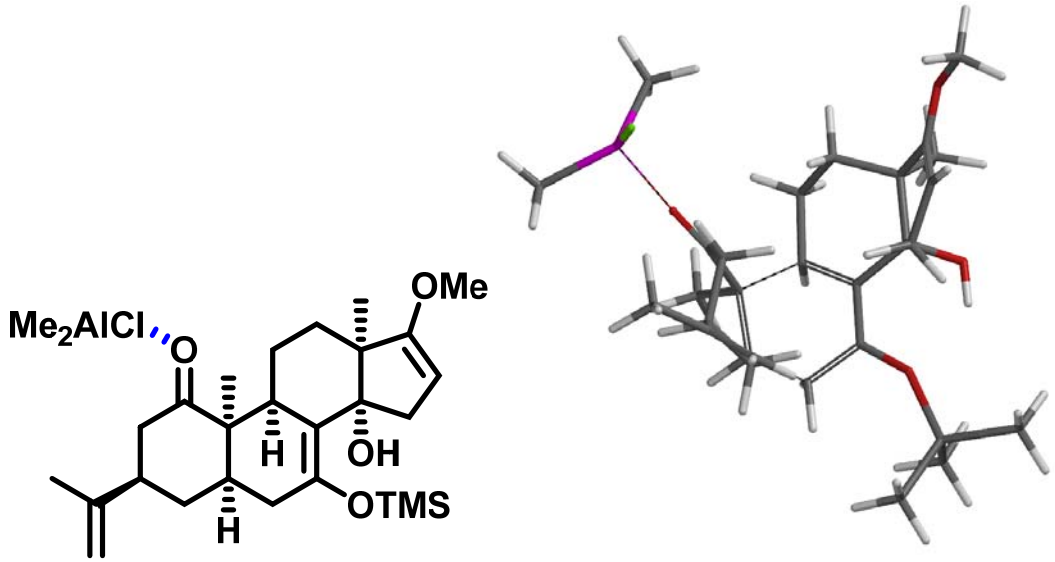
Atom	X	Y	Z
C	1.370248	0.282395	0.283331
C	0.221623	2.451551	0.562745
C	-0.996819	0.506550	-0.667058
C	-0.930389	2.058079	-0.393785
C	-0.056352	-0.270025	0.381051
C	1.469330	1.622303	0.390336
H	-0.116218	2.357640	1.606484
H	-0.699836	2.520258	-1.360264
H	0.455885	3.511429	0.422357
H	-0.433351	0.001761	1.378968
C	-0.179167	-1.805546	0.277286
H	-0.313654	-2.118567	-0.761079
H	-1.080529	-2.136559	0.805246
C	1.045689	-2.515938	0.851592
H	0.899767	-3.601907	0.817718
H	1.175617	-2.250627	1.910002
C	2.324696	-2.145623	0.065154

C	2.606480	-0.604393	0.211067
C	2.227939	-2.614293	-1.398871
H	1.526023	-2.002601	-1.970136
H	1.899370	-3.657964	-1.441305
H	3.194104	-2.552095	-1.906499
C	3.539987	-2.734252	0.763092
C	4.195175	-1.852328	1.535906
H	5.058675	-2.059055	2.157919
C	3.496691	-0.514941	1.497683
H	2.878325	-0.355739	2.393233
H	4.165756	0.346863	1.424264
C	-2.390862	-0.041536	-0.444470
C	-2.261093	2.670412	0.087900
H	-2.974507	2.719713	-0.747028
H	-2.080983	3.703432	0.407307
C	-2.884927	1.855624	1.227617
H	-2.114527	1.693797	1.994345
C	-3.282654	0.475853	0.653220
H	-4.293977	0.522650	0.230097
H	-3.337255	-0.309061	1.420606
O	3.777848	-4.048591	0.538285
O	3.385738	-0.154519	-0.916881
H	4.216813	-0.659663	-0.880433
O	2.654778	2.286016	0.476852
C	-0.542862	0.226050	-2.112928
H	-1.157542	0.795416	-2.819398
H	-0.629636	-0.827062	-2.384148
H	0.497653	0.537202	-2.230327
Si	3.467287	3.267962	-0.640700
C	2.952992	2.846437	-2.400796
C	5.292545	2.931719	-0.343696
C	3.067211	5.070296	-0.243043
C	-4.073479	2.496438	1.929689
C	-4.700571	3.579191	1.458083
H	-5.555236	4.005061	1.977490
H	-4.397119	4.080035	0.544274

C	-4.516175	1.817742	3.204565
H	-4.824258	0.778427	3.028935
H	-5.359810	2.341346	3.663288
H	-3.698415	1.782230	3.937970
H	3.678147	5.749731	-0.850708
H	2.015732	5.308574	-0.442863
H	3.267772	5.294503	0.811021
H	3.549293	3.417592	-3.123302
H	1.898165	3.078080	-2.590826
H	3.108682	1.779086	-2.584918
H	5.522875	1.887179	-0.577029
H	5.560188	3.112766	0.703855
H	5.928526	3.571486	-0.967361
O	-2.790207	-0.973373	-1.169439
Al	-4.338150	-2.196927	-1.233284
Cl	-4.371650	-2.862288	0.873991
C	-5.865005	-1.032538	-1.706308
H	-5.665603	-0.435236	-2.607252
H	-6.170653	-0.338520	-0.913128
H	-6.746473	-1.649360	-1.930492
C	-3.695309	-3.591686	-2.462796
H	-2.748477	-4.037916	-2.132101
H	-3.535737	-3.202443	-3.478090
H	-4.418812	-4.413626	-2.547715
C	4.894119	-4.609132	1.217242
H	5.822309	-4.097684	0.930228
H	4.943170	-5.657615	0.918617
H	4.768390	-4.537726	2.305353

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



[**57**+Me_2AlCl]

E(B3LYP/6-31G*) = –2387.83039 au

Cartesian Coordinates (Angstroms)

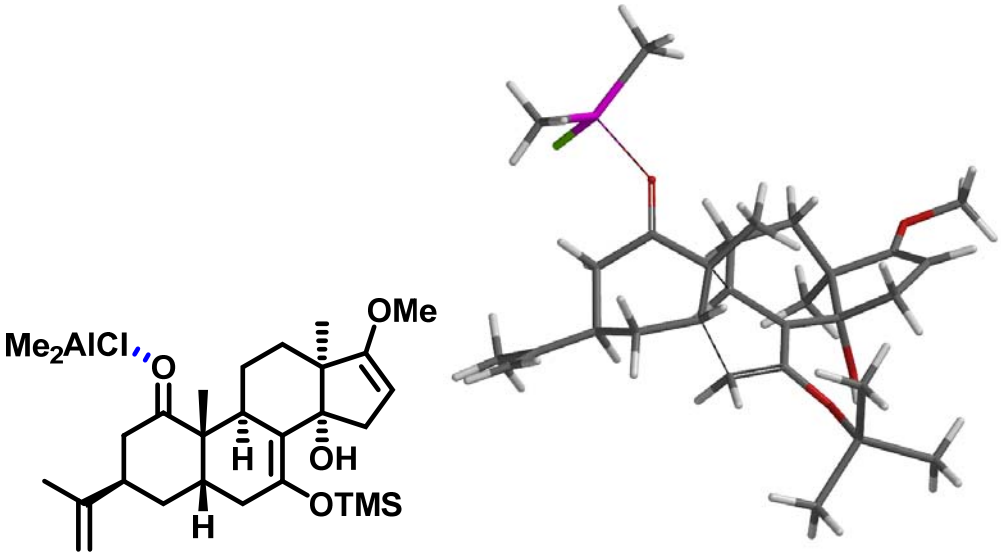
Atom	X	Y	Z
C	1.211006	0.428258	-0.826150
C	1.774802	-1.890957	-1.450134
C	-0.701295	-1.271591	-1.469024
C	0.359908	-2.327258	-0.984043
C	0.009424	0.163700	-1.725010
C	2.116303	-0.570189	-0.803859
H	1.801664	-1.815719	-2.546874
H	2.496785	-2.662983	-1.168972
H	0.415423	-0.006573	-2.730639
C	-0.968234	1.352398	-1.856757
H	-1.979760	0.996904	-2.073438
H	-0.672605	1.947931	-2.726712
C	-0.985300	2.257094	-0.625127
H	-1.711099	3.066550	-0.764472
C	0.406015	2.874786	-0.336567
C	1.461983	1.742506	-0.072378
O	3.288526	-0.447967	-0.093418

H	-1.324321	1.698421	0.257916
C	0.820276	3.846059	-1.457334
H	0.983655	3.327762	-2.406974
H	1.750439	4.354086	-1.199322
H	0.037486	4.598071	-1.599148
C	0.356765	3.569852	1.013597
C	0.906835	2.862264	2.009140
H	0.941646	3.143114	3.055359
C	1.451284	1.560897	1.487837
H	2.466822	1.340646	1.838000
H	0.831932	0.705185	1.796803
O	2.733907	2.284205	-0.454436
H	3.377905	1.594925	-0.223813
O	-0.276087	4.768467	1.038752
C	-0.387126	5.387291	2.313053
H	-0.953927	4.753572	3.007677
H	-0.917456	6.328185	2.155324
H	0.605072	5.586990	2.738222
H	0.106478	-3.261924	-1.500109
C	-1.843179	-1.114175	-0.488239
C	-1.595494	-1.272435	0.977889
H	-2.528654	-1.131635	1.524064
H	-0.876280	-0.511162	1.305877
C	0.417188	-2.648778	0.528580
H	0.916001	-3.618524	0.651121
H	1.048372	-1.906818	1.030196
C	-0.946522	-2.667813	1.218150
H	-1.584813	-3.420426	0.728072
C	-1.266250	-1.731096	-2.831489
H	-1.866664	-2.640811	-2.728181
H	-0.437675	-1.945550	-3.515259
H	-1.897640	-0.965213	-3.287636
Si	4.823689	-1.155231	-0.290108
C	4.878065	-2.858365	0.515435
H	5.908084	-3.237014	0.524285
H	4.262685	-3.602016	-0.003297

H	4.536453	-2.808787	1.555898
C	5.959872	0.024835	0.630538
H	6.997755	-0.328537	0.601644
H	5.669626	0.112979	1.683851
H	5.941447	1.030353	0.193748
C	5.257478	-1.234679	-2.121151
H	6.290271	-1.579796	-2.255135
H	5.176054	-0.244843	-2.584766
H	4.606783	-1.919593	-2.675837
C	-0.933160	-3.000463	2.705107
C	0.169603	-2.929581	3.457610
H	0.138225	-3.164275	4.518310
H	1.138145	-2.641422	3.061314
C	-2.262195	-3.425975	3.283186
H	-3.043982	-2.674083	3.118330
H	-2.188294	-3.606906	4.359350
H	-2.615353	-4.351156	2.806761
O	-2.985837	-0.900387	-0.933163
Al	-4.892196	-0.618833	-0.566076
Cl	-5.042752	-0.422631	1.625541
C	-5.634809	-2.327919	-1.214284
H	-5.435203	-2.486391	-2.282994
H	-6.725238	-2.352851	-1.085977
H	-5.235387	-3.196495	-0.674214
C	-5.193897	1.096791	-1.487545
H	-4.980558	1.035105	-2.563543
H	-4.576072	1.905207	-1.075192
H	-6.239130	1.418066	-1.386310

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



[**58**+Me_2AlCl]

E(B3LYP/6-31G*) = –2387.83096 au

Cartesian Coordinates (Angstroms)

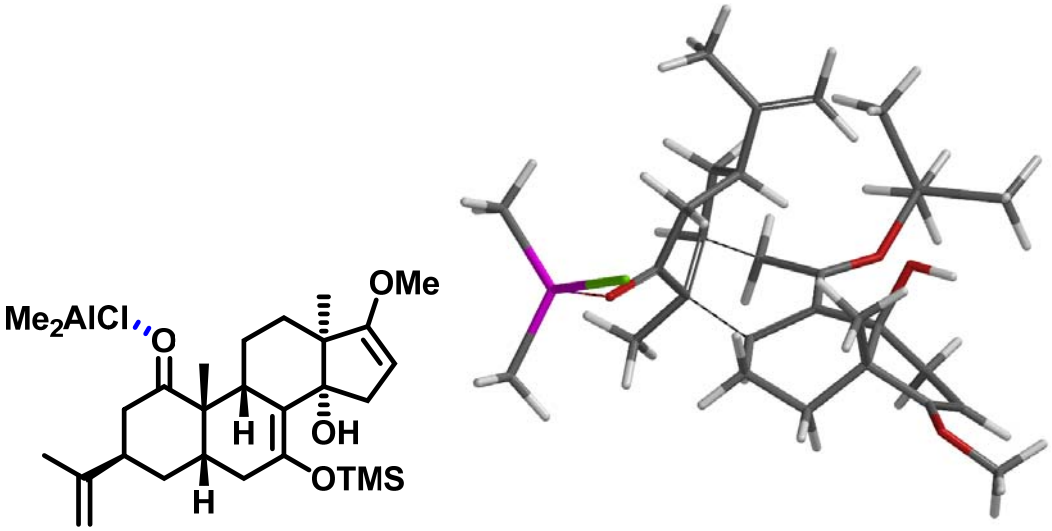
Atom	X	Y	Z
C	1.406388	0.180504	0.400265
C	0.344545	2.408315	0.245413
C	-0.913955	0.310999	-0.668545
C	-0.832250	1.888596	-0.622416
C	-0.041589	-0.303759	0.533351
C	1.550743	1.509786	0.252834
H	0.001646	2.533362	1.283959
H	-0.633540	2.206582	-1.652175
H	0.605756	3.412614	-0.100617
H	-0.453475	0.156479	1.441705
C	-0.198047	-1.839125	0.702131
H	-1.097220	-2.196445	0.192867
H	-0.358371	-2.055385	1.763462
C	1.003078	-2.645882	0.212033
H	0.831262	-3.712029	0.401631
C	2.318939	-2.215957	0.898852
C	2.637301	-0.731333	0.523516

C	-2.343474	-0.134819	-0.440735
C	-2.141894	2.579303	-0.177240
H	-2.877605	2.556639	-0.993650
H	-1.931870	3.636350	0.022920
C	-2.746444	1.903827	1.060062
H	-1.956727	1.808197	1.818651
C	-3.188041	0.481352	0.641536
H	-4.217080	0.502083	0.265947
H	-3.203105	-0.229895	1.479182
O	2.800183	2.090453	0.236937
H	1.113134	-2.538956	-0.874561
C	2.270412	-2.465720	2.415364
H	1.548075	-1.806665	2.906894
H	3.244713	-2.273788	2.866932
H	1.987334	-3.504553	2.614813
C	3.470642	-2.946478	0.229716
C	4.088562	-2.222039	-0.713228
H	4.901059	-2.553424	-1.349520
C	3.464337	-0.853224	-0.804708
H	4.200240	-0.042379	-0.856899
H	2.820007	-0.754999	-1.691823
O	3.498889	-0.238854	1.554821
H	3.674182	0.690091	1.327485
O	3.677824	-4.225704	0.628080
C	4.737304	-4.914203	-0.020867
H	4.548166	-5.000336	-1.099189
H	4.780729	-5.909069	0.426170
H	5.691994	-4.394901	0.134181
C	-0.416484	-0.206720	-2.029266
H	-1.041638	0.182958	-2.840058
H	-0.445246	-1.296799	-2.089807
H	0.609956	0.128284	-2.196004
C	-3.899547	2.639999	1.726186
C	-4.485945	3.717006	1.193832
H	-5.312362	4.211688	1.697817
H	-4.181054	4.148841	0.245581

C	-4.357800	2.064059	3.045677
H	-5.146964	2.675057	3.492997
H	-3.526901	2.002076	3.762038
H	-4.750103	1.044868	2.930890
Si	3.440298	3.434344	-0.584905
C	2.792153	3.472473	-2.355125
H	3.270461	4.284092	-2.917475
H	1.709139	3.634221	-2.406854
H	3.016288	2.533758	-2.874614
C	5.293882	3.139133	-0.548124
H	5.665626	3.065475	0.480392
H	5.829117	3.963424	-1.034941
H	5.563234	2.212714	-1.067838
C	3.028590	5.027306	0.335778
H	3.574699	5.869181	-0.108776
H	3.332821	4.956621	1.386749
H	1.962990	5.280402	0.313746
O	-2.811662	-1.047317	-1.147070
Al	-4.470700	-2.122284	-1.241682
Cl	-4.668640	-2.711868	0.872816
C	-3.907707	-3.606646	-2.403143
H	-3.015412	-4.120982	-2.023399
H	-3.679723	-3.268726	-3.423745
H	-4.696747	-4.365842	-2.488345
C	-5.840631	-0.821713	-1.828212
H	-5.549241	-0.307524	-2.754940
H	-6.083923	-0.049019	-1.087514
H	-6.781879	-1.345887	-2.044728

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



[**59**+Me_2AlCl]

E(B3LYP/6-31G*) = –2387.82873 au

Cartesian Coordinates (Angstroms)

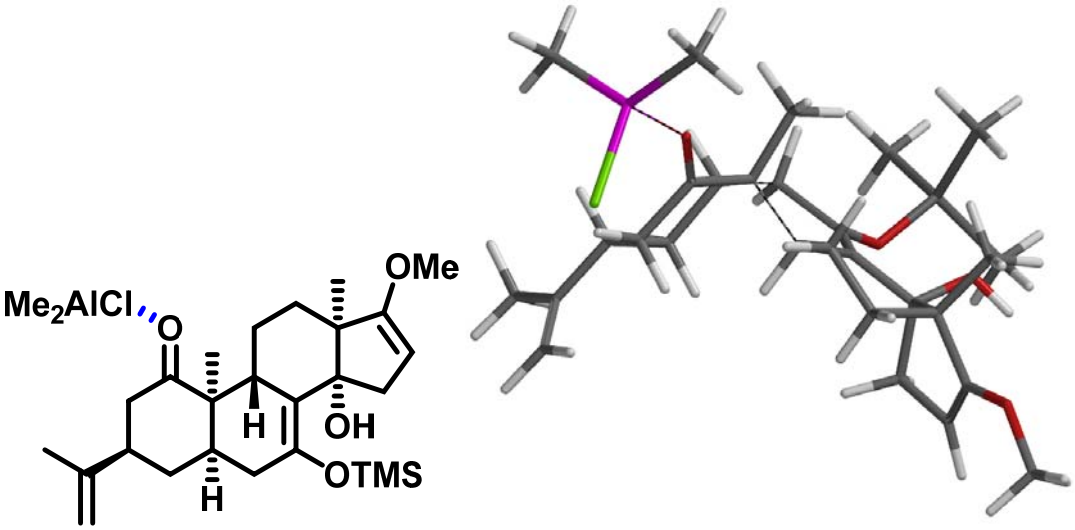
Atom	X	Y	Z
C	-1.884347	-0.697130	-1.156485
C	0.264402	0.405813	-1.571981
C	0.104200	-2.233233	-1.452206
C	1.054305	-1.002334	-1.674352
C	-1.321708	-1.873020	-1.914552
C	-1.102055	0.368254	-0.880937
H	0.046046	0.615814	-2.630959
H	-1.311583	-1.646161	-2.992323
H	-1.976247	-2.742861	-1.794561
C	1.178420	1.562733	-1.120335
H	1.980553	1.694760	-1.854745
H	1.674053	1.339917	-0.170830
C	0.386171	2.857329	-0.959726
H	1.061241	3.693389	-0.743773
C	-1.672283	1.571685	-0.133738
C	-0.648003	2.731780	0.183284
H	-0.127004	3.101960	-1.900505

C	0.056190	2.577754	1.544720
H	0.814085	3.358021	1.664625
H	0.542815	1.604484	1.645853
H	-0.650068	2.670177	2.373534
C	-1.563000	3.945850	0.166698
C	-2.747333	3.720007	-0.424358
H	-3.530743	4.450648	-0.590965
C	-2.815778	2.297092	-0.921051
H	-2.643933	2.237088	-2.005978
H	-3.768313	1.796351	-0.729017
O	-2.209378	1.065993	1.105743
H	-2.661637	1.818815	1.524309
O	-1.054664	5.081410	0.701914
C	-1.880918	6.235891	0.623468
H	-1.320466	7.049108	1.087556
H	-2.824057	6.079867	1.163721
H	-2.104604	6.486737	-0.421489
O	-3.209678	-0.722557	-0.875761
Si	-4.348274	-1.678565	-0.079946
C	-5.342811	-2.582066	-1.403226
H	-4.719318	-3.284182	-1.969304
H	-5.779230	-1.873523	-2.116912
H	-6.165856	-3.154705	-0.957561
C	-5.444919	-0.467624	0.849949
H	-4.860193	0.063518	1.607963
H	-6.277630	-0.977908	1.348888
H	-5.871212	0.279269	0.169869
C	-3.570527	-2.918114	1.107810
H	-2.804589	-2.467702	1.748835
H	-3.120719	-3.771401	0.587155
H	-4.353478	-3.319884	1.764428
H	0.464806	-3.021319	-2.124427
C	2.176447	-1.009911	-0.652393
C	1.924623	-1.335328	0.793981
H	2.205737	-0.455368	1.388686
H	2.672298	-2.095269	1.059528

C	0.120326	-2.831202	-0.015587
H	0.841538	-3.659267	0.010528
H	-0.857889	-3.270574	0.203278
C	0.497841	-1.823006	1.088822
H	-0.181259	-0.969875	1.025952
C	1.656479	-1.085558	-3.092346
H	2.225457	-0.187523	-3.345510
H	0.850383	-1.199064	-3.824846
H	2.329384	-1.943426	-3.188457
C	0.365539	-2.382225	2.498861
C	-0.390094	-1.737776	3.396393
H	-0.500460	-2.101598	4.415230
H	-0.916499	-0.820340	3.142593
C	1.100494	-3.654881	2.848871
H	0.782349	-4.495027	2.217670
H	0.923185	-3.934481	3.891400
H	2.185690	-3.554015	2.714210
O	3.330056	-0.743497	-1.035709
Al	5.151277	-0.565260	-0.299822
Cl	4.782844	0.725781	1.448212
C	6.067985	0.381405	-1.760859
H	5.554273	1.310880	-2.039243
H	6.143979	-0.233560	-2.668331
H	7.091384	0.660043	-1.476221
C	5.628292	-2.419565	0.194896
H	6.673864	-2.455126	0.531454
H	5.549551	-3.112061	-0.654935
H	5.029223	-2.836375	1.015406

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



[**60**+Me_2AlCl]

E(B3LYP/6-31G*) = –2387.84223 au

Cartesian Coordinates (Angstroms)

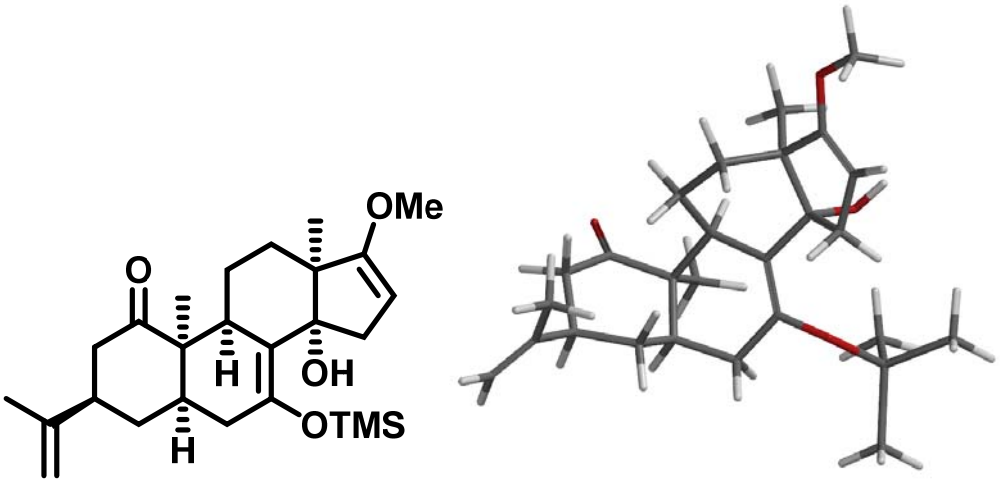
Atom	X	Y	Z
C	-1.012056	1.896545	-0.270884
C	0.015125	-0.362664	-0.023614
C	1.533531	1.627403	-0.531769
C	1.189570	0.155442	-0.932466
C	0.293605	2.509741	-0.725433
C	-1.196565	0.579761	-0.030393
H	0.390786	-0.364243	1.010747
H	2.310894	1.977912	-1.226832
H	0.425817	3.452612	-0.179864
C	2.115530	1.752063	0.888090
C	2.429441	-0.677361	-0.644040
C	3.067289	-0.585536	0.714206
H	3.958887	-1.212615	0.744616
H	2.358084	-0.991281	1.447995
C	3.378561	0.885328	1.079088
H	2.361811	2.806229	1.056897
H	1.366144	1.487275	1.644763

H	0.194046	2.794789	-1.783317
C	-0.332679	-1.832692	-0.315011
H	0.560395	-2.453922	-0.167569
H	-0.631982	-1.968114	-1.358878
C	-1.445851	-2.304792	0.616365
H	-1.633676	-3.377091	0.489380
C	-2.536165	0.038153	0.475777
C	-2.755932	-1.526720	0.357367
H	-1.128539	-2.165943	1.659319
C	-3.368182	-1.948877	-0.992284
H	-3.448145	-3.039563	-1.042527
H	-2.759052	-1.604721	-1.832987
H	-4.368650	-1.533279	-1.130050
C	-3.714842	-1.759320	1.515871
C	-3.733232	-0.755953	2.410876
H	-4.299164	-0.732921	3.335272
C	-2.761136	0.323584	1.995645
H	-1.817520	0.254511	2.558112
H	-3.128425	1.347895	2.119919
O	-3.589341	0.679354	-0.262312
H	-4.413963	0.415085	0.180867
O	-4.375222	-2.940852	1.514464
C	-5.222398	-3.188684	2.630087
H	-5.670750	-4.169725	2.465136
H	-6.010309	-2.427421	2.698822
H	-4.647191	-3.194506	3.564731
O	-1.984567	2.834880	-0.084902
Si	-2.932092	3.687978	-1.199358
C	-2.071162	5.328824	-1.571907
H	-1.108311	5.177113	-2.074147
H	-1.882826	5.895475	-0.652378
H	-2.689430	5.955562	-2.227131
C	-4.560347	4.018490	-0.320498
H	-5.223268	4.644975	-0.929558
H	-4.391184	4.537302	0.630391
H	-5.076099	3.077728	-0.105144

C	-3.156002	2.701877	-2.787157
H	-3.597794	1.726750	-2.563227
H	-2.202154	2.535713	-3.302550
H	-3.814348	3.236636	-3.483144
C	0.827520	0.078482	-2.426431
H	0.782689	-0.953473	-2.778036
H	1.579301	0.593217	-3.034338
H	-0.144437	0.544600	-2.604371
H	4.126595	1.246284	0.353803
C	3.997205	1.041813	2.461383
C	4.092529	0.045014	3.347638
H	4.548386	0.207375	4.320725
H	3.747759	-0.965206	3.151271
C	4.534366	2.418812	2.781167
H	5.238667	2.758141	2.009453
H	5.057523	2.423788	3.741666
H	3.736796	3.170941	2.833075
O	2.910190	-1.382980	-1.544763
Al	4.389366	-2.620522	-1.967310
Cl	4.618259	-3.733935	-0.081605
C	5.873795	-1.369264	-2.323870
H	6.095960	-0.703268	-1.479300
H	5.676127	-0.733822	-3.198429
H	6.799448	-1.920873	-2.537084
C	3.565558	-3.712344	-3.382801
H	4.263282	-4.472805	-3.758625
H	3.257546	-3.106885	-4.246465
H	2.676947	-4.249677	-3.026663

Requested basis set is 6-31G(d)

There are 235 shells and 629 basis functions



57

E(B3LYP/6-31G*) = –1605.25035 au

Cartesian Coordinates (Angstroms)

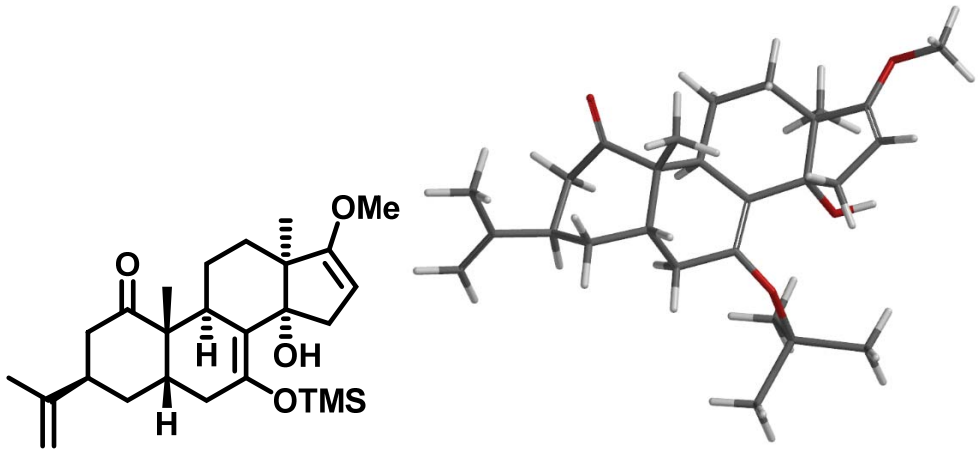
Atom	X	Y	Z
C	0.496469	0.143675	0.238885
C	-0.900063	2.212338	-0.122051
C	-1.810632	0.411998	1.416875
C	-2.149238	1.410908	0.274882
C	-0.597920	-0.533685	1.051042
C	0.359021	1.393416	-0.237556
C	-0.945426	-1.929958	0.461013
H	-1.700818	-1.844891	-0.323603
H	-1.386609	-2.542958	1.255700
C	0.277119	-2.641162	-0.161545
H	0.179414	-3.727782	-0.052096
C	1.637996	-2.185069	0.417128
C	1.804113	-0.634356	0.115582
O	1.371244	2.033988	-0.908557
H	0.290738	-2.443897	-1.239980
C	1.802829	-2.612671	1.886817
H	0.958345	-2.308856	2.508825
H	2.707048	-2.186014	2.329281

H	1.881364	-3.702962	1.938635
C	2.753238	-2.767976	-0.441604
C	3.205155	-1.920924	-1.378967
H	3.953886	-2.136655	-2.132902
C	2.453535	-0.616034	-1.307652
H	3.088491	0.264347	-1.420081
H	1.686467	-0.542657	-2.091092
O	2.727045	-0.042121	1.053610
H	3.573028	-0.505346	0.921530
O	3.101580	-4.054267	-0.189084
C	4.088570	-4.613335	-1.044558
H	3.752511	-4.603618	-2.089587
H	4.238723	-5.642464	-0.713350
H	5.033259	-4.058627	-0.968507
C	-3.054131	-0.447708	1.753794
C	-4.047798	-0.826869	0.651902
H	-5.008493	-1.020332	1.139888
H	-3.709866	-1.795994	0.263521
C	-2.843600	0.756428	-0.930816
H	-3.006477	1.514946	-1.707423
H	-2.197654	-0.007947	-1.377792
C	-4.209839	0.179454	-0.511903
H	-4.796692	1.024602	-0.125603
C	-1.424172	1.193823	2.692813
H	-2.154023	1.983167	2.910161
H	-0.437840	1.655626	2.590521
H	-1.403866	0.517209	3.549520
O	-3.240636	-0.863365	2.883857
Si	2.334402	3.318116	-0.363220
C	1.720263	4.902999	-1.183487
H	2.375602	5.749553	-0.942275
H	0.707108	5.162812	-0.855158
H	1.700660	4.797990	-2.274747
C	4.086739	2.943070	-0.938477
H	4.756779	3.788909	-0.740697
H	4.121266	2.735609	-2.014316

H	4.479852	2.068034	-0.409960
C	2.261495	3.444591	1.513846
H	3.004857	4.164427	1.878715
H	2.480175	2.468530	1.959700
H	1.280658	3.775033	1.873939
C	-5.006028	-0.415130	-1.665696
C	-6.239661	0.024828	-1.936645
H	-6.831034	-0.389844	-2.749406
H	-6.705591	0.817187	-1.355235
C	-4.365310	-1.506700	-2.491987
H	-3.485554	-1.136382	-3.034028
H	-5.067840	-1.905317	-3.229936
H	-4.021688	-2.344961	-1.872035
H	-0.142017	-0.745935	2.025872
H	-0.726521	3.018097	0.606255
H	-1.066544	2.714544	-1.084218
H	-2.872944	2.129612	0.688637

Requested basis set is 6-31G(d)

There are 205 shells and 549 basis functions



58

E(B3LYP/6-31G*) = –1605.24833 au

Cartesian Coordinates (Angstroms)

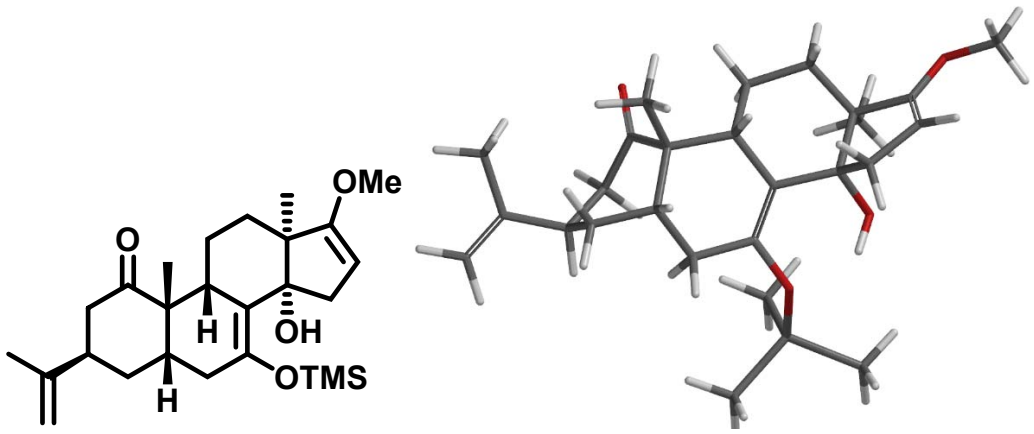
Atom	X	Y	Z
C	0.623106	0.069594	0.088723
C	-1.455469	1.360553	-0.228463
C	-1.543056	-1.218526	-0.487296
C	-2.071294	0.171843	-0.999301
C	-0.362981	-1.005680	0.564305
C	0.050674	1.241425	-0.254931
C	0.284131	-2.338943	1.017032
H	-0.407510	-3.166756	0.833622
H	0.428001	-2.309776	2.102681
C	1.628624	-2.629534	0.350350
H	2.035467	-3.577202	0.724650
C	2.650900	-1.501076	0.616286
C	2.127842	-0.144986	0.007284
C	-2.672354	-1.949888	0.262190
C	-3.609782	0.208137	-1.071649
H	-3.930345	-0.592070	-1.751942
H	-3.943482	1.148837	-1.526885
C	-4.308384	0.027227	0.294859
H	-4.212596	0.967063	0.849446

C	-3.583550	-1.088533	1.122733
H	-4.292786	-1.743040	1.634821
H	-2.970199	-0.606152	1.893926
O	-2.833992	-3.156498	0.180878
O	0.735000	2.317168	-0.746576
H	1.496882	-2.755465	-0.730813
C	2.980259	-1.404417	2.118076
H	2.136593	-1.003142	2.685869
H	3.832213	-0.745792	2.302400
H	3.230473	-2.394057	2.514458
C	3.894894	-1.734311	-0.224680
C	3.930599	-1.001368	-1.350479
H	4.694468	-1.042764	-2.118885
C	2.682087	-0.158060	-1.455640
H	2.853602	0.869330	-1.791906
H	1.956049	-0.599427	-2.153098
O	2.756810	0.947852	0.711629
H	3.710722	0.849136	0.546720
O	4.767515	-2.660789	0.242214
C	5.901936	-2.920021	-0.573518
H	5.598746	-3.294961	-1.559744
H	6.489750	-3.679039	-0.054250
H	6.504785	-2.011901	-0.706919
C	-1.101163	-2.068664	-1.688254
H	-1.910913	-2.130200	-2.424978
H	-0.856707	-3.092052	-1.398283
H	-0.235017	-1.615683	-2.181453
C	-5.797154	-0.254009	0.154968
C	-6.697942	0.579109	0.687464
H	-7.766400	0.392768	0.609754
H	-6.401265	1.479070	1.221430
C	-6.217115	-1.503857	-0.585136
H	-7.292406	-1.677464	-0.482777
H	-5.689820	-2.392649	-0.215853
H	-5.994425	-1.433136	-1.657962
Si	1.117848	3.753412	0.068982

C	0.992815	3.494960	1.928594
H	1.299799	4.396571	2.472941
H	1.637419	2.663881	2.229886
H	-0.033463	3.258545	2.234020
C	-0.095550	5.088116	-0.494458
H	-0.102276	5.181058	-1.587018
H	0.181507	6.065929	-0.079901
H	-1.120657	4.871391	-0.170751
C	2.854398	4.222985	-0.479038
H	3.159232	5.188295	-0.056755
H	2.911926	4.303396	-1.571036
H	3.572042	3.462347	-0.157090
H	-1.755501	2.299551	-0.704524
H	-1.821761	1.392173	0.808649
H	-1.707507	0.281756	-2.028006
H	-0.855983	-0.590474	1.454523

Requested basis set is 6-31G(d)

There are 205 shells and 549 basis functions



59

E(B3LYP/6-31G*) = –1605.24899 au

Cartesian Coordinates (Angstroms)

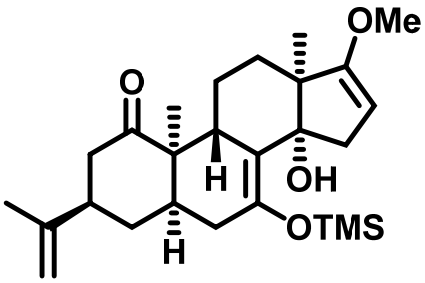
Atom	X	Y	Z
C	0.028278	1.048786	0.741965
C	-0.100019	-1.437664	0.499977
C	2.064333	-0.347776	1.438095
C	1.470453	-1.547058	0.641863
C	1.493892	1.030629	1.061902
C	-0.720555	-0.039314	0.488288
C	-0.665767	-2.267802	-0.673347
H	-0.198620	-3.255804	-0.696843
H	-0.410972	-1.789576	-1.626100
C	-2.179417	-2.408262	-0.537663
H	-2.577827	-3.058374	-1.325843
C	-2.257401	0.008404	0.368020
C	-2.917699	-1.045190	-0.596483
H	-2.402972	-2.908038	0.414512
C	-3.015918	-0.556249	-2.050557
H	-3.544993	-1.299934	-2.655117
H	-2.021061	-0.406776	-2.485140
H	-3.555135	0.389721	-2.110548
C	-4.277863	-1.209380	0.067028
C	-4.297908	-0.824488	1.351485

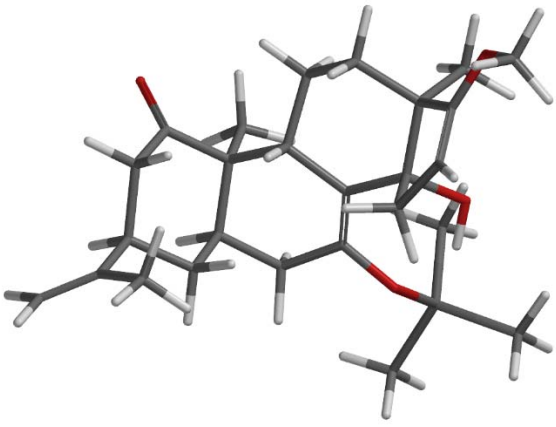
H	-5.133973	-0.906325	2.036341
C	-2.949219	-0.277922	1.747093
H	-2.376633	-0.996556	2.354214
H	-2.996462	0.653448	2.325891
O	-2.726795	1.275274	-0.093614
H	-2.267433	1.933210	0.454460
O	-5.249164	-1.777977	-0.690526
C	-6.500635	-1.973443	-0.049020
H	-7.165249	-2.418439	-0.792048
H	-6.915755	-1.017380	0.296131
H	-6.400334	-2.648985	0.811088
O	-0.509105	2.331988	0.821033
Si	-0.212054	3.635122	-0.237658
C	-0.005433	2.991788	-1.993405
H	-0.875659	2.392004	-2.280652
H	0.886852	2.364186	-2.102838
H	0.087107	3.822924	-2.703319
C	1.311788	4.592053	0.328382
H	1.215320	4.901184	1.375700
H	1.437510	5.499750	-0.275294
H	2.232613	4.005452	0.236204
C	-1.746210	4.707818	-0.072147
H	-1.914155	5.004841	0.969720
H	-2.640170	4.178811	-0.421848
H	-1.648560	5.624880	-0.666083
C	2.207139	-1.706219	-0.711442
C	3.090137	-0.562233	-1.177776
H	2.429895	0.276599	-1.432473
H	3.584851	-0.869951	-2.102539
C	3.601768	-0.338283	1.339980
H	3.983089	-1.294500	1.711732
H	4.017811	0.427571	2.005528
C	4.124384	-0.086041	-0.105631
H	4.238587	0.995414	-0.235379
O	2.141063	-2.740251	-1.353827
C	1.741960	-2.861779	1.422373

H	1.287090	-3.711661	0.909446
H	1.319840	-2.789458	2.431001
H	2.810253	-3.079129	1.515483
C	5.503377	-0.693797	-0.328210
C	6.570125	0.095938	-0.492858
H	7.566185	-0.312068	-0.646319
H	6.488903	1.180509	-0.479633
C	5.626620	-2.199946	-0.357692
H	5.338186	-2.653458	0.600060
H	6.656575	-2.504124	-0.566761
H	4.977661	-2.647415	-1.120556
H	1.790861	-0.514724	2.488692
H	-0.483450	-1.926255	1.411157
H	1.650834	1.712278	1.908762
H	2.048899	1.486738	0.230582

Requested basis set is 6-31G(d)

There are 205 shells and 549 basis functions





60

E(B3LYP/6-31G*) = –1605.26336 au

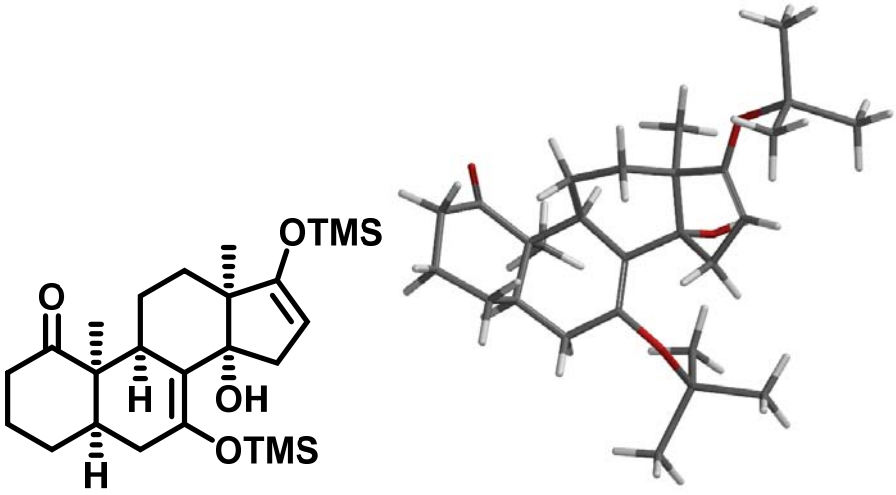
Cartesian Coordinates (Angstroms)

Atom	X	Y	Z

C	0.228603	1.426238	-0.186471
C	-0.632011	-0.662719	0.871351
C	-2.233271	1.284292	0.449200
C	-1.791338	0.205507	1.479710
C	-1.040061	2.187579	0.108745
C	0.443240	0.134727	0.132372
H	-1.082963	-1.335892	0.125911
H	-2.996747	1.909250	0.935826
H	-1.275722	2.792817	-0.776248
C	-2.883130	0.685222	-0.811920
C	-2.995102	-0.727677	1.746060
C	-3.758715	-1.261519	0.536369
H	-4.647370	-1.780181	0.906612
H	-3.131159	-2.006751	0.028937
C	-4.137221	-0.140388	-0.465123
H	-3.162520	1.501212	-1.491244
H	-2.159029	0.064890	-1.354815
O	-3.339154	-1.029432	2.874846
H	-0.862403	2.906407	0.922418
C	0.006161	-1.586748	1.925737
H	-0.781461	-2.132954	2.458943
H	0.534033	-0.988099	2.675364
C	0.968222	-2.566344	1.259471
H	1.378910	-3.270000	1.993307
C	1.653233	-0.671158	-0.374300
C	2.149773	-1.849250	0.548386
H	0.411527	-3.171581	0.531252
C	3.192394	-1.402314	1.585929
H	3.548596	-2.271012	2.148892
H	2.759076	-0.687378	2.294058
H	4.045351	-0.922562	1.105209
C	2.720353	-2.795711	-0.498456
C	2.253953	-2.573523	-1.736027
H	2.474924	-3.156042	-2.622898
C	1.325596	-1.385530	-1.731330
H	0.267752	-1.688460	-1.791022

H	1.496508	-0.683837	-2.557808
O	2.804489	0.147740	-0.579091
H	2.487341	0.911472	-1.089857
O	3.553246	-3.762685	-0.038694
C	4.047657	-4.671797	-1.011026
H	4.699448	-5.369266	-0.481404
H	4.619986	-4.143121	-1.784571
H	3.226540	-5.222592	-1.489234
O	1.149096	2.177524	-0.910507
Si	1.981170	3.563542	-0.361707
C	0.940149	5.102735	-0.678847
H	0.020945	5.116774	-0.083089
H	0.655848	5.168366	-1.735581
H	1.508371	6.008308	-0.431280
C	3.530392	3.612472	-1.423806
H	4.122349	4.508832	-1.201673
H	3.279094	3.638729	-2.490625
H	4.170794	2.739983	-1.250210
C	2.393047	3.363358	1.462094
H	2.925943	2.420869	1.627911
H	1.494323	3.356594	2.089834
H	3.033381	4.183124	1.810117
C	-1.374248	0.871891	2.803069
H	-1.278867	0.131555	3.598461
H	-2.136338	1.589870	3.126513
H	-0.420730	1.399014	2.704075
H	-4.838409	0.529045	0.052879
C	-4.859679	-0.686972	-1.688330
C	-6.158694	-0.433140	-1.879392
H	-6.697570	-0.819999	-2.740954
H	-6.733536	0.169498	-1.180067
C	-4.067854	-1.516865	-2.672327
H	-3.267766	-0.929127	-3.140198
H	-4.710977	-1.900822	-3.469709
H	-3.583979	-2.375898	-2.189379

Requested basis set is 6-31G(d)
There are 205 shells and 549 basis functions



62-DA

E(B3LYP/6-31G*) = –1857.95276 au

Cartesian Coordinates (Angstroms)

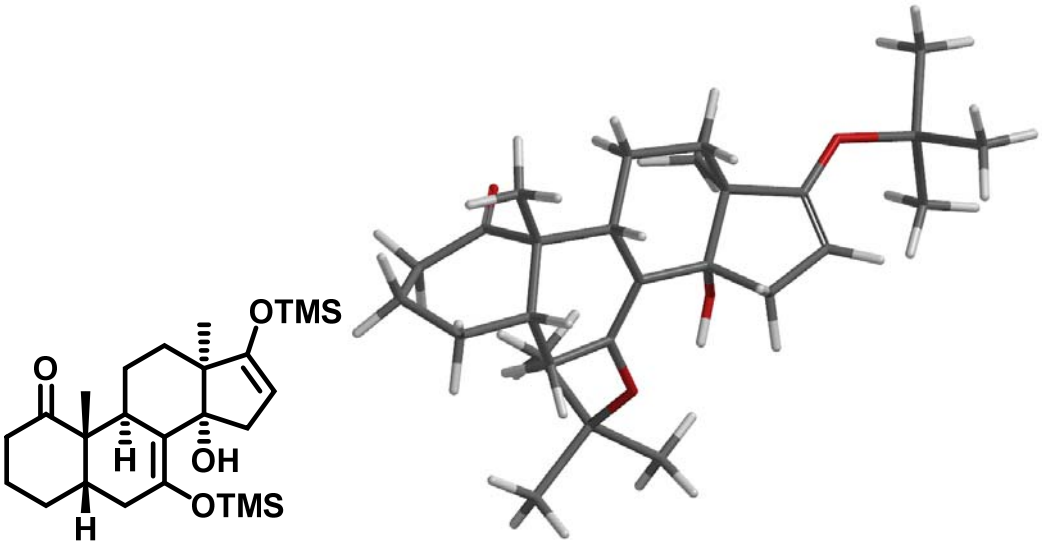
Atom	X	Y	Z
C	-0.941931	0.065537	0.078025
C	-3.326222	0.462163	-0.640105
C	-2.786055	-1.699428	0.582977
C	-3.573550	-1.053831	-0.594001
C	-1.245334	-1.353517	0.537390
C	-1.897154	0.875210	-0.409663
C	-0.305183	-2.372101	-0.169459
H	-0.724813	-2.699221	-1.124107
H	-0.225360	-3.266779	0.459736
C	1.093550	-1.784756	-0.461861
H	1.849131	-2.579537	-0.448989
C	1.513885	-0.654064	0.506337
C	0.484770	0.542076	0.336965
O	-1.636347	2.178194	-0.759147

H	1.100180	-1.373682	-1.478647
C	1.714032	-1.183361	1.938076
H	0.855298	-1.750950	2.303515
H	1.893949	-0.370381	2.646708
H	2.585553	-1.844646	1.955225
C	2.801715	-0.020533	-0.012165
C	2.590040	1.101920	-0.714523
H	3.350868	1.688900	-1.218893
C	1.117896	1.406118	-0.802867
H	0.874356	2.459858	-0.652507
H	0.704574	1.134833	-1.784150
O	0.432292	1.332022	1.544273
H	1.334973	1.668266	1.684723
O	3.962177	-0.677093	0.249333
C	-2.967972	-3.239806	0.576242
C	-3.128502	-3.982546	-0.753080
H	-3.652451	-4.918575	-0.532931
H	-2.114932	-4.270995	-1.062038
C	-3.333161	-1.741397	-1.948228
H	-3.897037	-1.208249	-2.724829
H	-2.277224	-1.675796	-2.238899
C	-3.807238	-3.197477	-1.886469
H	-4.894234	-3.199720	-1.724898
C	-3.340397	-1.169383	1.924897
H	-4.431834	-1.267310	1.968375
H	-3.080826	-0.116482	2.065611
H	-2.923461	-1.744979	2.753874
O	-2.944179	-3.875648	1.615295
Si	-2.199506	3.586786	-0.004885
C	-3.780020	4.161973	-0.863653
H	-4.121988	5.118274	-0.447720
H	-4.596601	3.440086	-0.747215
H	-3.614649	4.308035	-1.937747
C	-0.849151	4.870307	-0.270846
H	-1.182816	5.862427	0.057749
H	-0.578496	4.945899	-1.330542

H	0.057195	4.618256	0.290970
C	-2.494639	3.261029	1.825063
H	-2.640170	4.200027	2.373338
H	-1.629473	2.739239	2.247880
H	-3.382067	2.640049	1.994500
H	-0.947385	-1.380688	1.592211
H	-3.958894	0.964822	0.106710
H	-3.644199	0.864310	-1.611435
H	-4.643125	-1.195607	-0.372786
Si	5.543383	-0.301676	-0.240808
C	6.051100	1.367614	0.472557
H	7.064388	1.635871	0.148736
H	6.047934	1.340409	1.568373
H	5.375969	2.170631	0.158192
C	5.656349	-0.308461	-2.122782
H	6.677998	-0.077388	-2.449228
H	4.986412	0.425535	-2.582836
H	5.395126	-1.294411	-2.524727
C	6.576176	-1.686674	0.495912
H	7.639420	-1.555260	0.260738
H	6.266234	-2.663093	0.106460
H	6.476383	-1.714634	1.586942
H	-3.637753	-3.708333	-2.842213

Requested basis set is 6-31G(d)

There are 210 shells and 557 basis functions



63-DA

E(B3LYP/6-31G*) = –1857.95013 au

Cartesian Coordinates (Angstroms)

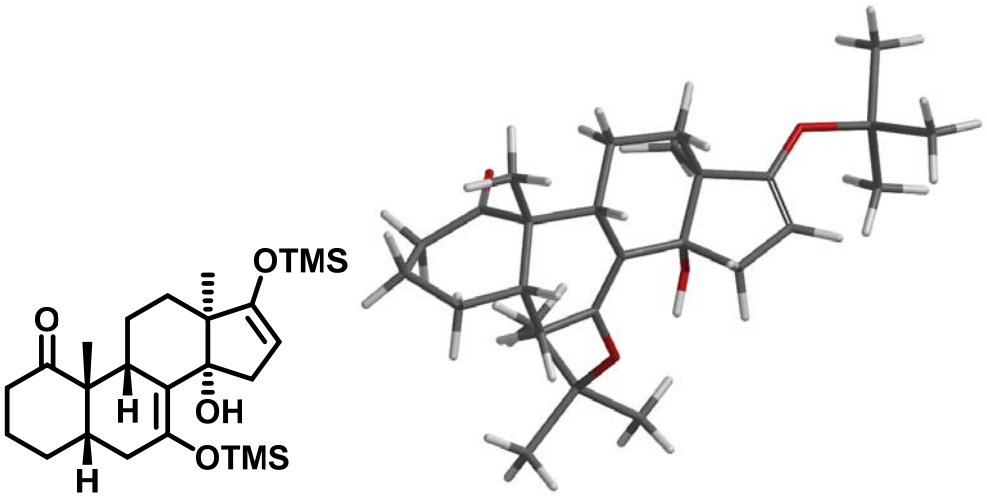
Atom	X	Y	Z
C	1.744329	-0.654912	-0.722752
C	1.061813	1.724821	-0.494671
C	3.405095	1.219263	-1.282249
C	2.575559	2.053872	-0.270378
C	3.164983	-0.283930	-1.055074
C	0.751384	0.220918	-0.481630
C	0.097944	2.530697	0.403439
H	0.264451	3.600982	0.236879
H	0.317011	2.336246	1.453928
C	-1.354968	2.203566	0.069385
H	-2.035011	2.841565	0.647024
C	-0.718005	-0.232084	-0.398188
C	-1.706898	0.723630	0.350271
H	-1.542576	2.431683	-0.989431
C	-1.773708	0.460941	1.862568
H	-2.494484	1.142486	2.326512
H	-0.799009	0.616961	2.335012

H	-2.081996	-0.566231	2.063987
C	-3.014325	0.401013	-0.368346
C	-2.824921	-0.159238	-1.570746
H	-3.598619	-0.399582	-2.292628
C	-1.353437	-0.360196	-1.827074
H	-0.950123	0.395709	-2.519434
H	-1.097670	-1.339043	-2.252676
O	-0.853077	-1.497486	0.256805
H	-0.269645	-2.094647	-0.238612
O	-4.168488	0.791071	0.236075
O	1.524223	-2.029035	-0.797321
Si	2.199891	-3.210115	0.230679
C	2.294126	-2.520834	1.977185
H	1.301332	-2.181077	2.292418
H	2.967128	-1.659177	2.051258
H	2.642602	-3.280512	2.687413
C	3.885314	-3.757725	-0.415623
H	3.822807	-4.053167	-1.469567
H	4.243352	-4.626629	0.151076
H	4.645553	-2.973951	-0.331665
C	0.985022	-4.641418	0.114527
H	0.830478	-4.944972	-0.927508
H	0.008611	-4.373512	0.534993
H	1.353425	-5.516044	0.664216
C	3.095411	1.743393	1.151077
C	4.589841	1.424701	1.295619
H	4.655129	0.335780	1.433085
H	4.919164	1.855452	2.247437
C	4.921769	1.532728	-1.267957
H	5.134293	2.364305	-1.948711
H	5.449681	0.666952	-1.686875
C	5.490471	1.873685	0.135853
H	6.484375	1.428358	0.259124
O	2.395237	1.748138	2.146317
C	2.797430	3.571368	-0.514058
H	2.310854	4.174032	0.257015

H	2.371593	3.853395	-1.484851
H	3.854731	3.846458	-0.523871
H	3.017215	1.463989	-2.280524
H	0.859306	2.078501	-1.522039
H	3.447045	-0.834126	-1.963507
H	3.839749	-0.665370	-0.275082
H	5.644576	2.955481	0.217326
Si	-5.719452	0.128201	0.081851
C	-6.695622	0.947862	1.463468
H	-6.725065	2.035898	1.334357
H	-6.244670	0.739846	2.440318
H	-7.730656	0.585306	1.486537
C	-6.472374	0.576205	-1.590122
H	-5.982739	0.059556	-2.423126
H	-6.395897	1.654291	-1.775195
H	-7.536867	0.310284	-1.616822
C	-5.617960	-1.737951	0.306467
H	-4.886342	-2.174894	-0.381589
H	-6.587737	-2.216046	0.121902
H	-5.304297	-1.991508	1.325523

Requested basis set is 6-31G(d)

There are 210 shells and 557 basis functions



64-DA

E(B3LYP/6-31G*) = –1857.95240 au

Cartesian Coordinates (Angstroms)

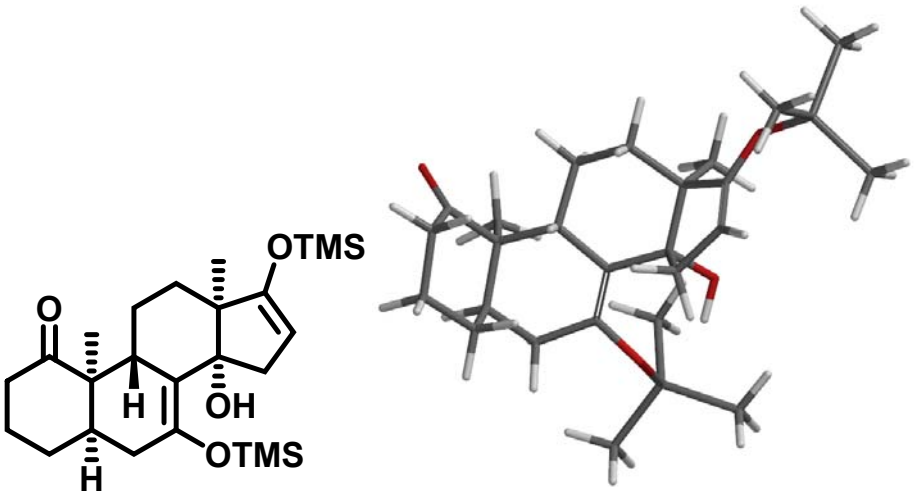
Atom	X	Y	Z
C	1.744329	-0.654912	-0.722752
C	1.061813	1.724821	-0.494671
C	3.405095	1.219263	-1.282249
C	2.575559	2.053872	-0.270378
C	3.164983	-0.283930	-1.055074
C	0.751384	0.220918	-0.481630
C	0.097944	2.530697	0.403439
H	0.264451	3.600982	0.236879
H	0.317011	2.336246	1.453928
C	-1.354968	2.203566	0.069385
H	-2.035011	2.841565	0.647024
C	-0.718005	-0.232084	-0.398188
C	-1.706898	0.723630	0.350271
H	-1.542576	2.431683	-0.989431
C	-1.773708	0.460941	1.862568
H	-2.494484	1.142486	2.326512
H	-0.799009	0.616961	2.335012
H	-2.081996	-0.566231	2.063987

C	-3.014325	0.401013	-0.368346
C	-2.824921	-0.159238	-1.570746
H	-3.598619	-0.399582	-2.292628
C	-1.353437	-0.360196	-1.827074
H	-0.950123	0.395709	-2.519434
H	-1.097670	-1.339043	-2.252676
O	-0.853077	-1.497486	0.256805
H	-0.269645	-2.094647	-0.238612
O	-4.168488	0.791071	0.236075
O	1.524223	-2.029035	-0.797321
Si	2.199891	-3.210115	0.230679
C	2.294126	-2.520834	1.977185
H	1.301332	-2.181077	2.292418
H	2.967128	-1.659177	2.051258
H	2.642602	-3.280512	2.687413
C	3.885314	-3.757725	-0.415623
H	3.822807	-4.053167	-1.469567
H	4.243352	-4.626629	0.151076
H	4.645553	-2.973951	-0.331665
C	0.985022	-4.641418	0.114527
H	0.830478	-4.944972	-0.927508
H	0.008611	-4.373512	0.534993
H	1.353425	-5.516044	0.664216
C	3.095411	1.743393	1.151077
C	4.589841	1.424701	1.295619
H	4.655129	0.335780	1.433085
H	4.919164	1.855452	2.247437
C	4.921769	1.532728	-1.267957
H	5.134293	2.364305	-1.948711
H	5.449681	0.666952	-1.686875
C	5.490471	1.873685	0.135853
H	6.484375	1.428358	0.259124
O	2.395237	1.748138	2.146317
C	2.797430	3.571368	-0.514058
H	2.310854	4.174032	0.257015
H	2.371593	3.853395	-1.484851

H	3.854731	3.846458	-0.523871
H	3.017215	1.463989	-2.280524
H	0.859306	2.078501	-1.522039
H	3.447045	-0.834126	-1.963507
H	3.839749	-0.665370	-0.275082
H	5.644576	2.955481	0.217326
Si	-5.719452	0.128201	0.081851
C	-6.695622	0.947862	1.463468
H	-6.725065	2.035898	1.334357
H	-6.244670	0.739846	2.440318
H	-7.730656	0.585306	1.486537
C	-6.472374	0.576205	-1.590122
H	-5.982739	0.059556	-2.423126
H	-6.395897	1.654291	-1.775195
H	-7.536867	0.310284	-1.616822
C	-5.617960	-1.737951	0.306467
H	-4.886342	-2.174894	-0.381589
H	-6.587737	-2.216046	0.121902
H	-5.304297	-1.991508	1.325523

Requested basis set is 6-31G(d)

There are 210 shells and 557 basis functions



65-DA

E(B3LYP/6-31G*) = –1857.96549 au

Cartesian Coordinates (Angstroms)

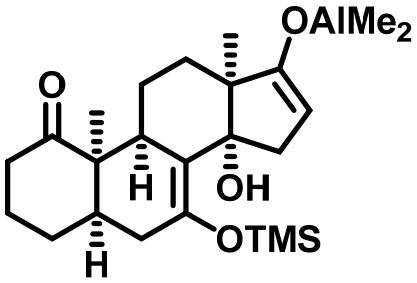
Atom	X	Y	Z
C	2.021190	-0.786493	-0.400674
C	1.145853	1.449815	0.271950
C	3.579765	1.228096	-0.475484
C	2.628559	1.857334	0.586808
C	3.447863	-0.299985	-0.436650
C	0.953505	-0.024202	-0.093480
H	0.822456	2.030243	-0.606400
H	4.608973	1.479955	-0.177759
H	3.924835	-0.735845	-1.324042
C	3.378105	1.802063	-1.890346
C	2.735388	3.396444	0.489591
C	2.645011	4.019944	-0.901268
H	2.870988	5.085337	-0.800236
H	1.607366	3.937434	-1.255089
C	3.576521	3.321629	-1.908355
H	4.096473	1.327066	-2.571205
H	2.380652	1.549282	-2.273922
O	2.894196	4.095859	1.474097
H	3.999911	-0.701453	0.425988
C	0.186074	1.861691	1.407247
H	0.344609	2.918305	1.655701
H	0.407990	1.290187	2.314377
C	-1.261906	1.633575	0.983728
H	-1.953869	1.990947	1.755717
C	-0.500356	-0.504058	-0.261268
C	-1.567517	0.138056	0.700185
H	-1.467510	2.231614	0.085494
C	-1.725008	-0.630725	2.021867
H	-2.511813	-0.168644	2.626737
H	-0.795352	-0.620146	2.602179

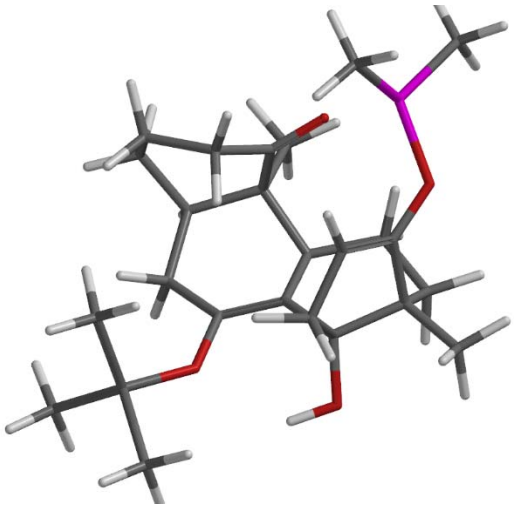
H	-1.990053	-1.672482	1.837415
C	-2.816155	0.070187	-0.172621
C	-2.539016	-0.063262	-1.477071
H	-3.260745	-0.068975	-2.287044
C	-1.050962	-0.163061	-1.690282
H	-0.627226	0.777190	-2.079738
H	-0.751740	-0.953091	-2.391153
O	-0.628785	-1.913739	-0.068757
H	0.071194	-2.310063	-0.614165
O	-4.007544	0.230055	0.459532
O	1.900325	-2.117626	-0.793523
Si	2.490105	-3.465807	0.072229
C	4.285456	-3.805576	-0.393403
H	4.962168	-3.015362	-0.050117
H	4.401461	-3.897509	-1.479675
H	4.623409	-4.747866	0.056321
C	1.401164	-4.884670	-0.506341
H	1.730348	-5.832357	-0.062883
H	1.443948	-4.997381	-1.596100
H	0.352997	-4.731836	-0.225036
C	2.304594	-3.144571	1.916132
H	1.272225	-2.859658	2.145282
H	2.959549	-2.335253	2.259580
H	2.551168	-4.041115	2.497930
C	3.048703	1.412431	1.999932
H	2.583703	2.040817	2.760401
H	4.133318	1.509016	2.124695
H	2.770374	0.371159	2.186927
H	4.620206	3.555421	-1.655513
H	3.403366	3.722375	-2.914440
Si	-5.584534	0.171308	-0.156813
C	-6.659981	0.388427	1.368839
H	-7.726064	0.366735	1.111341
H	-6.455574	1.345513	1.862220
H	-6.475811	-0.408752	2.098021
C	-5.895597	-1.499027	-0.970404

H	-5.191212	-1.696875	-1.785018
H	-6.910698	-1.549443	-1.383551
H	-5.792075	-2.310232	-0.240292
C	-5.857368	1.593298	-1.364733
H	-5.183268	1.542615	-2.226469
H	-5.691049	2.557998	-0.871058
H	-6.886461	1.587574	-1.745436

Requested basis set is 6-31G(d)

There are 210 shells and 557 basis functions





62-Int-I

E(B3LYP/6-31G*) = –1770.98600 au

Cartesian Coordinates (Angstroms)

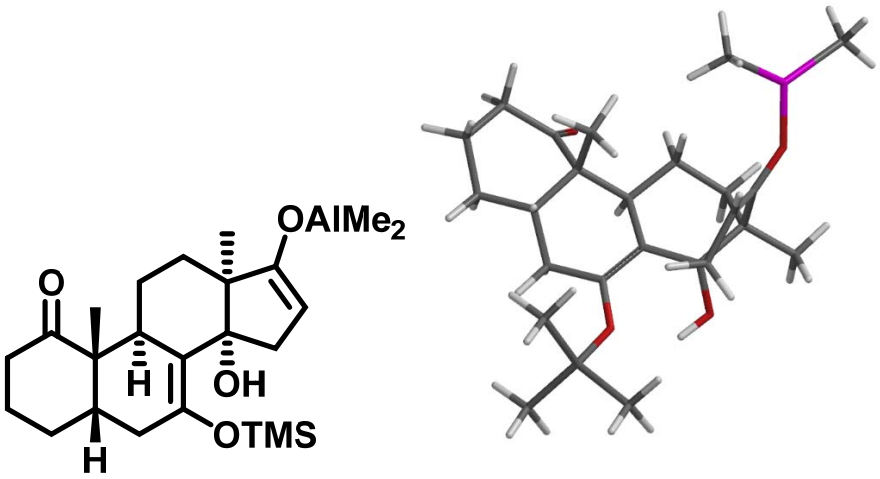
Atom	X	Y	Z
C	0.254868	0.639158	-1.838588
C	-0.483993	-0.463113	-1.067050
C	1.699109	0.314534	-2.280260
H	2.418555	0.749831	-1.589671
H	1.878996	0.785293	-3.253625
C	0.099959	-1.866585	-0.780985
C	1.632483	-1.905369	-1.056604

C	1.985971	-1.179310	-2.358239
H	1.415864	-1.650165	-3.170602
H	3.048699	-1.322355	-2.586135
C	2.145924	-1.254473	0.245982
C	0.034490	-2.165435	0.750365
H	0.053388	-3.255605	0.902306
H	-0.886554	-1.800039	1.213557
C	1.273336	-1.473559	1.252849
H	1.443978	-1.212040	2.291990
C	2.158267	-3.355081	-1.146177
H	3.252067	-3.337946	-1.210440
H	1.761425	-3.854364	-2.035587
H	1.882569	-3.951033	-0.271361
O	-0.557568	-2.845765	-1.584813
H	-1.506585	-2.728728	-1.411821
H	-0.320512	0.801750	-2.763937
Al	3.621220	0.961805	1.111249
C	3.405563	1.025568	3.076487
H	2.466860	0.601023	3.454510
H	3.470986	2.055903	3.455249
H	4.215960	0.466519	3.566002
C	5.109185	1.928237	0.257380
H	6.085188	1.525217	0.560749
H	5.116341	2.995540	0.518995
H	5.067862	1.862229	-0.837798
O	3.314145	-0.604128	0.281709
C	-1.761615	-0.179366	-0.752422
C	0.128389	2.038062	-1.106412
C	-2.374741	1.191147	-0.912391
H	-3.012780	1.192153	-1.808487
H	-3.066568	1.352816	-0.075798
C	-1.386871	2.403254	-0.995501
H	-1.623027	2.920983	-1.931928
C	-1.600034	3.424108	0.139477
H	-2.642797	3.763322	0.150301
C	0.793657	1.931509	0.262962

C	-0.067356	1.843792	1.490883
H	0.563218	1.876797	2.381883
H	-0.507866	0.839598	1.436667
C	-1.202776	2.899074	1.534769
H	-0.888210	3.742675	2.158255
H	-2.064287	2.453873	2.043488
C	0.851503	3.125898	-1.935581
H	0.645937	4.128154	-1.543702
H	0.495871	3.092207	-2.970901
H	1.932301	2.981620	-1.932833
O	2.033715	1.898895	0.331223
O	-2.616244	-1.185650	-0.354057
Si	-3.967144	-1.327023	0.657015
C	-5.477664	-0.496628	-0.108550
H	-6.373632	-0.736365	0.478262
H	-5.648780	-0.855984	-1.129940
H	-5.393418	0.594790	-0.146561
C	-3.597718	-0.598304	2.357140
H	-4.467788	-0.709583	3.016448
H	-3.358967	0.470705	2.311677
H	-2.753650	-1.110079	2.833148
C	-4.238164	-3.181696	0.765880
H	-5.081696	-3.418186	1.425667
H	-3.350909	-3.689810	1.159779
H	-4.457785	-3.608826	-0.219548
H	-1.000330	4.314440	-0.089480

Requested basis set is 6-31G(d)

There are 200 shells and 536 basis functions



63-Int-I

E(B3LYP/6-31G*) = –1770.97034 au

Cartesian Coordinates (Angstroms)

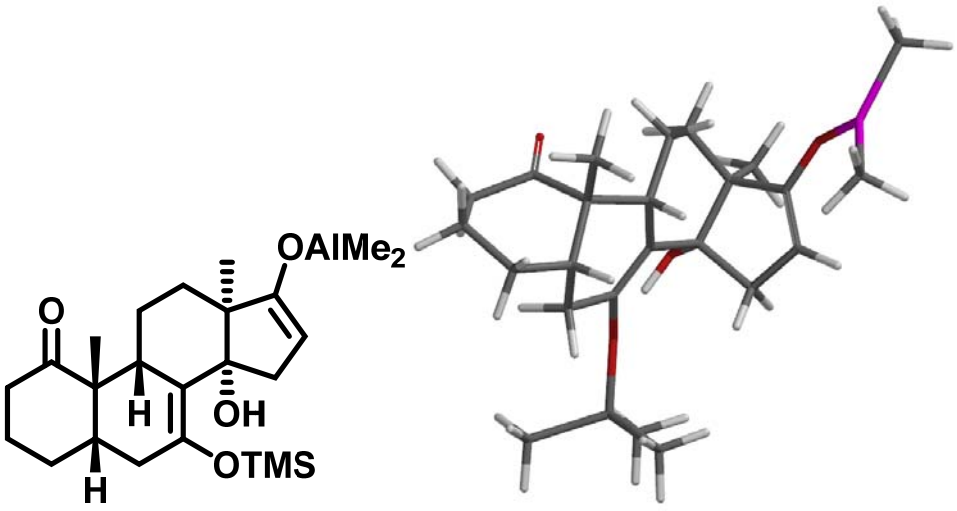
Atom	X	Y	Z
C	-0.139922	1.034424	1.093511
C	0.543743	-0.287775	0.731729
C	-1.657827	0.888715	1.295740
H	-2.178767	0.849283	0.332576
H	-2.025404	1.768888	1.829088
C	-0.131629	-1.677977	0.797268
C	-1.639049	-1.643280	1.241532
C	-1.989386	-0.389912	2.058997
H	-1.444652	-0.419991	3.012480
H	-3.058334	-0.415238	2.303507
C	-2.361998	-1.682669	-0.102029
C	-0.169839	-2.327672	-0.632897
H	0.034169	-3.404590	-0.536191
H	0.600829	-1.912761	-1.292442
C	-1.571995	-2.066051	-1.114974
H	-1.906240	-2.243820	-2.133710
C	-2.032524	-2.901965	2.044995
H	-3.116112	-2.897837	2.208964
H	-1.526532	-2.917961	3.013835

H	-1.768321	-3.820294	1.512764
O	0.571098	-2.493665	1.738376
H	1.506692	-2.445411	1.477514
H	0.249659	1.335128	2.078741
Al	-4.840910	-0.608065	-1.106106
C	-4.254994	0.362312	-2.709759
H	-3.234158	0.750525	-2.617530
H	-4.919931	1.204244	-2.938838
H	-4.265321	-0.297356	-3.588718
C	-6.686733	-0.726052	-0.464304
H	-7.375065	-1.052611	-1.254850
H	-7.048967	0.253147	-0.122304
H	-6.780994	-1.423931	0.374708
O	-3.692587	-1.446727	-0.120585
C	1.869323	-0.205261	0.518031
C	0.252421	2.214281	0.128354
C	2.559637	1.128882	0.565632
H	2.640630	1.474054	1.609273
H	3.585880	1.056699	0.189391
C	1.786304	2.168398	-0.263443
C	-0.025812	3.564930	0.818552
O	2.638451	-1.342759	0.355065
Si	3.943247	-1.727323	-0.655202
C	5.563943	-1.278426	0.197714
H	6.419729	-1.655516	-0.376577
H	5.611936	-1.728700	1.196209
H	5.696057	-0.197001	0.315044
C	3.775998	-0.846076	-2.314608
H	4.542339	-1.206442	-3.012118
H	3.893701	0.240112	-2.229985
H	2.797177	-1.045178	-2.766140
C	3.825685	-3.589716	-0.875796
H	4.659225	-3.967249	-1.480866
H	2.892072	-3.870486	-1.376123
H	3.854935	-4.109591	0.088725
H	1.828513	1.824449	-1.305507

C	2.487648	3.540695	-0.205833
H	3.451340	3.470051	-0.726211
H	2.719378	3.791552	0.840643
C	0.350339	4.831840	0.046069
H	0.472208	5.617326	0.798314
H	-0.506707	5.126059	-0.575172
C	1.626968	4.658651	-0.803736
H	2.184449	5.601467	-0.835341
O	-0.504285	3.656406	1.935021
C	-0.581204	2.167399	-1.180600
H	-0.186447	2.851797	-1.937296
H	-1.631866	2.424994	-1.015278
H	-0.543751	1.154410	-1.595855
H	1.378450	4.412642	-1.843495

Requested basis set is 6-31G(d)

There are 200 shells and 536 basis functions



64-Int-I

E(B3LYP/6-31G*) = –1770.96526 au

Cartesian Coordinates (Angstroms)

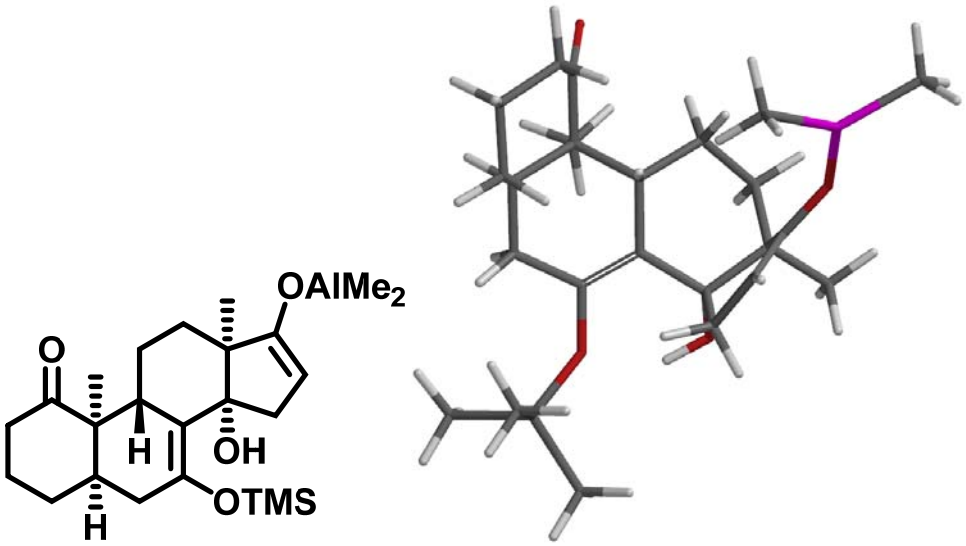
Atom	X	Y	Z

C	-0.410356	1.163995	-0.029071
C	0.354733	-0.126714	0.290251
C	-1.662832	1.406556	0.875089
H	-1.586779	2.369773	1.378129
C	-0.376306	-1.387561	0.827907
C	-1.810986	-1.080730	1.376506
C	-1.883585	0.339483	1.941322
H	-1.119521	0.436069	2.722418
H	-2.857417	0.501682	2.420079
C	-2.673136	-1.310601	0.141038
C	-0.641522	-2.371928	-0.368724
H	-0.570189	-3.406219	0.001341
H	0.101577	-2.262819	-1.167740
C	-2.043210	-2.026663	-0.803059
H	-2.497502	-2.384642	-1.723133
C	-2.234200	-2.089200	2.466927
H	-3.291828	-1.933832	2.708320
H	-1.638562	-1.951068	3.373093
H	-2.105280	-3.123427	2.134215
O	0.360399	-1.985410	1.887675
H	1.284792	-2.013473	1.587757
Al	-5.065011	-0.249467	-1.007077
C	-4.455975	0.063651	-2.846699
H	-3.364370	0.010730	-2.928380
H	-4.781717	1.039698	-3.228424
H	-4.868540	-0.692567	-3.529069
C	-6.860891	0.111213	-0.316291
H	-7.631391	-0.415771	-0.894544
H	-7.105080	1.180404	-0.376285
H	-6.961772	-0.193615	0.731117
O	-3.960734	-0.894042	0.161928
C	1.658666	-0.210266	-0.032188
C	0.517731	2.415884	-0.134574
C	2.484894	0.878227	-0.657383
H	3.283579	1.164004	0.042173
H	3.012227	0.470970	-1.532591

C	1.677026	2.106074	-1.118855
O	2.375591	-1.365036	0.257379
Si	3.560359	-2.268350	-0.547121
C	5.249451	-1.452184	-0.352715
H	6.036464	-2.088141	-0.777121
H	5.486567	-1.293442	0.705754
H	5.298991	-0.482212	-0.858853
C	3.121285	-2.476302	-2.369900
H	3.824179	-3.168473	-2.850929
H	3.158971	-1.533845	-2.928275
H	2.114422	-2.893385	-2.485196
C	3.527588	-3.924167	0.340628
H	4.289429	-4.603210	-0.061248
H	2.552151	-4.411302	0.232472
H	3.722758	-3.803804	1.412589
H	1.202695	1.833662	-2.071861
C	2.614574	3.311404	-1.380415
H	2.209417	3.921067	-2.195362
H	3.571997	2.921996	-1.748506
C	2.482437	3.550175	1.190322
H	3.222633	2.780169	1.451571
H	2.500402	4.267455	2.017653
C	2.849484	4.216867	-0.142423
H	3.894797	4.544219	-0.107069
C	-0.310756	3.606047	-0.689911
H	0.280695	4.519636	-0.788796
H	-1.164019	3.838845	-0.048614
H	-0.695047	3.350597	-1.685414
H	2.259842	5.135465	-0.243750
H	-0.798980	1.032812	-1.051043
C	1.119215	2.852147	1.222030
O	0.565650	2.670316	2.290162
H	-2.550795	1.455120	0.231937

Requested basis set is 6-31G(d)

There are 200 shells and 536 basis functions



65-Int-I

E(B3LYP/6-31G*) = –1770.97683 au

Cartesian Coordinates (Angstroms)

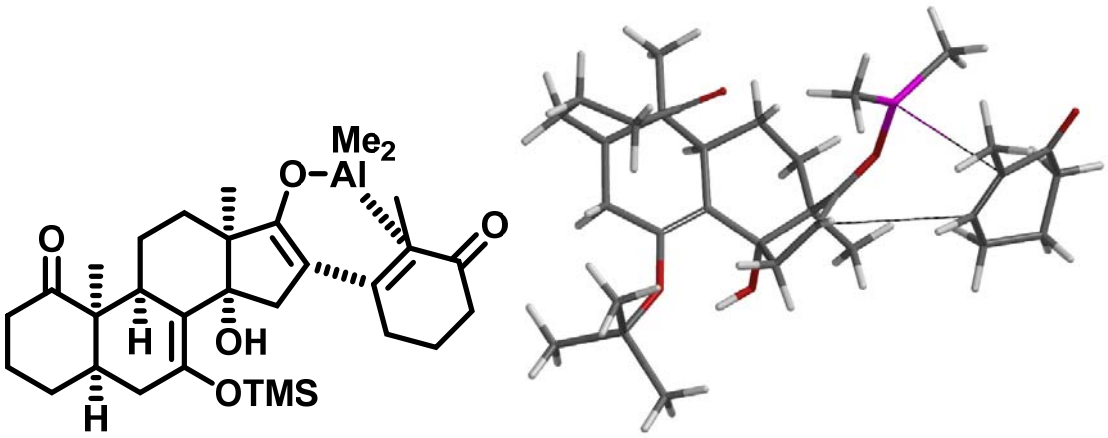
Atom	X	Y	Z
C	-0.450194	0.951125	0.563894
C	0.613818	-0.150402	0.543164
C	-1.705925	0.628894	1.434299
H	-1.854939	1.404064	2.190254
C	0.204910	-1.645653	0.619883
C	-1.259907	-1.855358	1.139672
C	-1.661793	-0.738809	2.109036
H	-0.934465	-0.736427	2.932140
H	-2.640856	-0.959686	2.551279
C	-2.052102	-1.878467	-0.164598
C	0.170686	-2.246443	-0.830009
H	0.479830	-3.301823	-0.783558
H	0.866659	-1.736058	-1.506262
C	-1.274244	-2.104006	-1.235152

H	-1.635397	-2.256734	-2.248854
C	-1.427944	-3.222363	1.838212
H	-2.489694	-3.388121	2.053395
H	-0.866006	-3.248960	2.775338
H	-1.072296	-4.043966	1.209556
O	1.067227	-2.358856	1.498570
H	1.971907	-2.095102	1.257844
Al	-4.654750	-1.072139	-1.058860
C	-4.174676	0.121730	-2.540969
H	-3.105031	0.359890	-2.545409
H	-4.735830	1.064193	-2.499798
H	-4.408870	-0.338087	-3.510981
C	-6.468433	-1.549055	-0.498676
H	-6.883228	-2.339877	-1.138960
H	-7.158480	-0.698535	-0.562271
H	-6.486513	-1.925927	0.530125
O	-3.400697	-1.799772	-0.108234
C	1.903007	0.180234	0.330933
C	0.151867	2.356543	0.935798
C	2.449606	1.578800	0.214857
H	3.056188	1.791090	1.107435
H	3.149482	1.624589	-0.630525
C	1.374789	2.657863	0.019281
O	2.877092	-0.810751	0.301659
Si	4.274988	-1.046195	-0.629334
C	5.666583	0.096884	-0.065904
H	6.612064	-0.201199	-0.536668
H	5.805694	0.035345	1.019820
H	5.488068	1.147064	-0.321650
C	3.884585	-0.794911	-2.456282
H	4.766196	-1.014572	-3.071267
H	3.572310	0.230949	-2.683343
H	3.079437	-1.466282	-2.775769
C	4.736569	-2.832565	-0.274747
H	5.646340	-3.117666	-0.817200
H	3.937253	-3.519289	-0.574987

H	4.926135	-2.989146	0.793717
H	-0.815282	1.021120	-0.468394
H	-2.592571	0.673431	0.790204
C	-0.930678	3.423898	0.675675
O	-1.477747	4.024401	1.583635
H	1.800764	3.615089	0.355433
C	0.585211	2.412739	2.411795
H	-0.273448	2.387209	3.084625
H	1.118668	3.347366	2.617983
H	1.241064	1.572985	2.655166
C	0.995627	2.841242	-1.461758
H	0.614995	1.900091	-1.879684
H	1.902549	3.084514	-2.031740
C	-0.038547	3.959690	-1.638617
H	-0.323235	4.063215	-2.692608
H	0.412288	4.916595	-1.340653
C	-1.291417	3.708740	-0.778975
H	-1.837073	2.843903	-1.182232
H	-1.975202	4.562538	-0.791417

Requested basis set is 6-31G(d)

There are 200 shells and 536 basis functions



62-Complex-Int-I

E(B3LYP/6-31G*) = –2118.96158 au

Cartesian Coordinates (Angstroms)

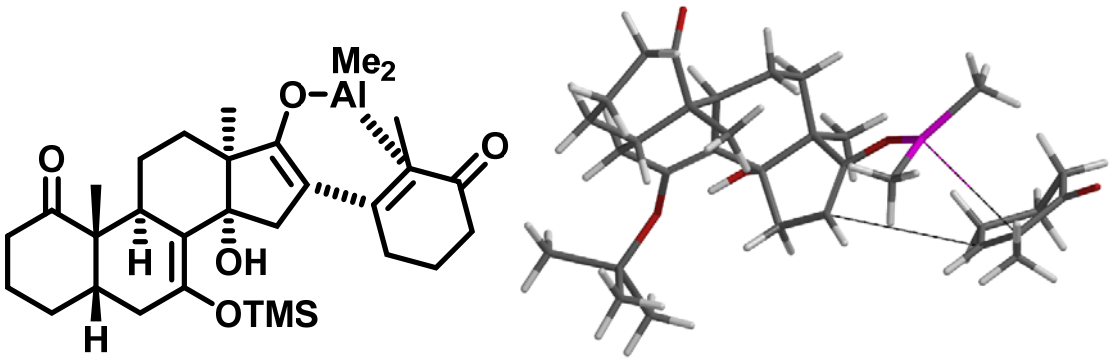
Atom	X	Y	Z
C	1.892479	-1.412337	-1.559044
C	2.006960	0.048928	-1.110168
C	0.452239	-1.844427	-1.875024
H	-0.097595	-2.037350	-0.951643
H	0.476823	-2.784248	-2.437917
C	0.895590	1.107265	-1.335273
C	-0.451067	0.522352	-1.895108
C	-0.260542	-0.773410	-2.693965
H	0.308363	-0.551832	-3.608536
H	-1.244010	-1.138947	-3.011736
C	-1.252122	0.300234	-0.612676
C	0.477267	1.745546	0.038857
H	0.289392	2.819597	-0.112880
H	1.268946	1.663014	0.789385
C	-0.765966	0.994138	0.425839
H	-1.203398	1.028728	1.419291
C	-1.194996	1.552009	-2.774396
H	-2.179920	1.151126	-3.041400
H	-0.636451	1.756862	-3.691637
H	-1.340676	2.502445	-2.252007
O	1.368538	2.083955	-2.267534
H	2.206933	2.406717	-1.895841
C	-4.655020	1.503355	1.149129
C	-6.079531	2.150539	-0.820681
C	-6.717251	0.230366	0.713646
C	-6.708982	0.757384	-0.715743
C	-5.594034	0.644869	1.606047
C	-4.673007	2.151149	-0.208801
H	-6.707169	2.873896	-0.282715
H	-3.968304	1.614397	-0.861516
H	-7.736040	0.727824	-1.092643
H	-4.283751	3.173751	-0.125918

C	-5.598046	0.074445	3.000427
H	-4.748427	0.443156	3.582855
H	-5.566299	-1.020605	2.984580
H	-6.523990	0.345856	3.519899
H	-3.823140	1.766686	1.803405
H	2.427777	-1.488654	-2.522311
O	-7.582294	-0.538363	1.111136
H	-6.126155	0.043194	-1.317527
H	-6.042946	2.476675	-1.866367
Al	-3.126363	-1.569062	0.446968
C	-2.376093	-1.832667	2.238555
H	-1.308919	-2.079095	2.169221
H	-2.878076	-2.652994	2.766525
H	-2.459051	-0.938888	2.870055
C	-4.590768	-2.590193	-0.363051
H	-5.530663	-2.497603	0.195163
H	-4.343469	-3.660903	-0.381685
H	-4.782980	-2.283553	-1.397896
O	-2.364404	-0.465671	-0.674912
C	3.204449	0.456376	-0.650976
C	2.674938	-2.368563	-0.598548
C	4.398673	-0.428592	-0.422236
H	5.215093	-0.103084	-1.083608
H	4.770629	-0.237673	0.593833
C	4.172423	-1.952346	-0.623097
H	4.524322	-2.192804	-1.634503
C	5.040775	-2.756275	0.373973
H	6.009871	-2.251548	0.470299
C	2.104767	-2.337550	0.837140
C	3.095625	-2.115762	1.968876
H	2.597197	-2.372452	2.908385
H	3.320668	-1.041502	2.007234
C	4.385742	-2.936670	1.773638
H	4.138136	-3.994088	1.926661
H	5.095804	-2.680932	2.567766
C	2.545801	-3.833192	-1.086322

H	3.175430	-4.514102	-0.503548
H	2.853746	-3.910192	-2.136272
H	1.515278	-4.182516	-0.997763
O	0.927588	-2.555793	1.067389
O	3.433811	1.804875	-0.435313
Si	4.384059	2.716146	0.629067
C	6.183631	2.712860	0.066733
H	6.786495	3.371494	0.704714
H	6.274256	3.076459	-0.963536
H	6.627429	1.712506	0.110517
C	4.233718	2.079676	2.400332
H	4.672223	2.808516	3.094188
H	4.750951	1.127186	2.562971
H	3.183401	1.947569	2.685063
C	3.653893	4.442906	0.503392
H	4.221404	5.155508	1.114208
H	2.615503	4.453072	0.853403
H	3.662996	4.809798	-0.529367
H	5.264658	-3.741361	-0.047889

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



63-Complex-Int-I

E(B3LYP/6-31G*) = –2118.96197 au

Cartesian Coordinates (Angstroms)

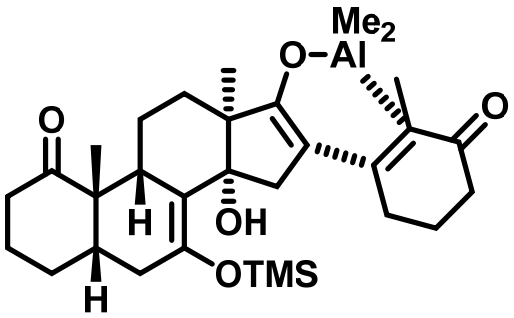
Atom	X	Y	Z
C	1.981578	-1.207533	-1.172849
C	1.958762	0.304327	-0.922514
C	0.618277	-1.778230	-1.604385
H	-0.017573	-1.985953	-0.736648
H	0.788296	-2.733459	-2.107228
C	0.762975	1.236671	-1.219764
C	-0.497975	0.493092	-1.787918
C	-0.130400	-0.809913	-2.516059
H	0.479635	-0.562527	-3.395889
H	-1.047623	-1.282481	-2.887972
C	-1.314312	0.251024	-0.520184
C	0.248027	1.883935	0.114087
H	-0.075315	2.915301	-0.095456
H	1.035548	1.943870	0.873568
C	-0.908766	1.006280	0.513254
H	-1.388255	1.044868	1.487655
C	-1.313975	1.396574	-2.737003
H	-2.250160	0.890207	-2.999689
H	-0.753700	1.602247	-3.652691
H	-1.556391	2.356842	-2.271410
O	1.155111	2.218863	-2.180733
H	1.977600	2.606081	-1.835385
C	-4.804005	1.304967	1.103938
C	-6.223128	1.890987	-0.888974
C	-6.808541	-0.049713	0.640840
C	-6.800079	0.474705	-0.789388
C	-5.714114	0.409290	1.548936
C	-4.827183	1.947863	-0.256250
H	-6.886171	2.591072	-0.363050
H	-4.091545	1.439903	-0.897824
H	-7.819495	0.403869	-1.180996
H	-4.479633	2.985006	-0.170401
C	-5.722165	-0.151678	2.947433

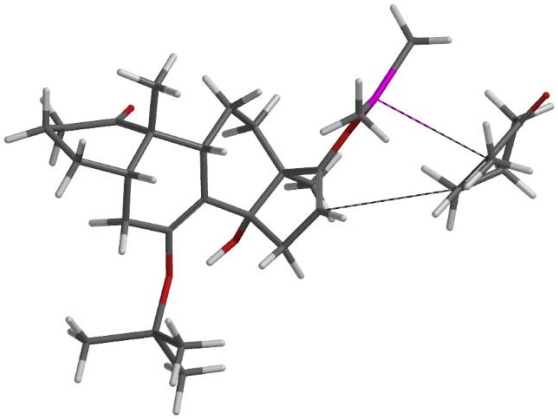
H	-4.886670	0.237548	3.536913
H	-5.671052	-1.245972	2.940439
H	-6.658737	0.106245	3.454678
H	-3.996232	1.607361	1.771445
H	2.644728	-1.372872	-2.035413
O	-7.647763	-0.850864	1.028758
H	-6.180913	-0.217782	-1.380408
H	-6.183141	2.215237	-1.934987
Al	-3.189753	-1.695187	0.473121
C	-2.500875	-1.975919	2.291839
H	-1.458349	-2.320423	2.260170
H	-3.080728	-2.733555	2.832702
H	-2.507533	-1.061400	2.897331
C	-4.582337	-2.757226	-0.401642
H	-5.549241	-2.698550	0.112675
H	-4.296925	-3.818633	-0.409150
H	-4.735739	-2.456211	-1.444289
O	-2.369709	-0.589964	-0.593803
C	3.142168	0.836715	-0.568156
C	2.651831	-2.002055	0.009875
C	4.326018	-0.059034	-0.336196
H	4.712181	-0.436061	-1.297083
H	5.152413	0.486655	0.131343
C	3.928870	-1.243361	0.563465
C	3.100521	-3.394560	-0.473364
O	3.315018	2.206480	-0.487841
Si	4.220310	3.205444	0.539812
C	5.997896	3.338930	-0.076841
H	6.553111	4.076952	0.515928
H	6.021430	3.669382	-1.121880
H	6.541795	2.389786	-0.015480
C	4.159420	2.550330	2.308098
H	4.662697	3.247148	2.990042
H	4.652309	1.576936	2.411335
H	3.124013	2.440889	2.651495
C	3.374006	4.878491	0.412334

H	3.900218	5.629969	1.013601
H	2.338458	4.829031	0.766808
H	3.357054	5.236607	-0.623607
H	3.636108	-0.812745	1.530415
C	5.139907	-2.162051	0.814486
H	5.880213	-1.620706	1.417466
H	5.629875	-2.390725	-0.144100
C	3.818541	-4.281981	0.547559
H	4.379475	-5.019606	-0.034644
H	3.061331	-4.841415	1.113443
C	4.741991	-3.478618	1.489875
H	5.630948	-4.072057	1.732247
O	2.926458	-3.792636	-1.611257
C	1.652847	-2.202855	1.181394
H	2.157882	-2.533378	2.093808
H	0.882498	-2.943213	0.944183
H	1.150043	-1.253453	1.398037
H	4.244378	-3.268198	2.444568

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions





64-DA-Complex-Int-I

E(B3LYP/6-31G*) = –2118.95666 au

Cartesian Coordinates (Angstroms)

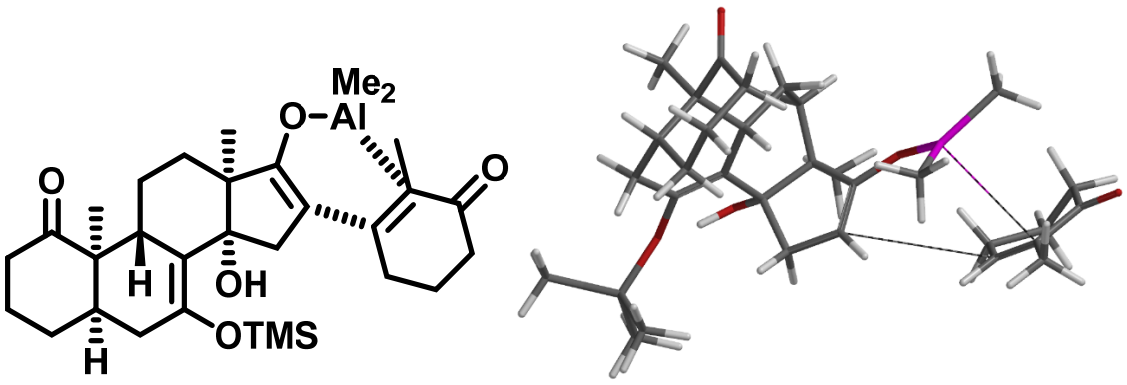
Atom	X	Y	Z
C	-1.545207	-1.379990	0.013997
C	-1.852263	0.080409	0.368004
C	-0.530873	-2.074279	0.981618
H	-0.985310	-2.949973	1.443990
C	-0.759395	0.997151	0.983243
C	0.446407	0.194504	1.578981
C	-0.019434	-1.168935	2.096406
H	-0.820388	-0.997965	2.825669
H	0.799796	-1.670659	2.626207
C	1.395769	0.124550	0.387305
C	-0.106723	1.843258	-0.168925
H	0.176652	2.828039	0.233313
H	-0.804011	2.021578	-0.996028
C	1.099522	1.028052	-0.561693
H	1.677247	1.200613	-1.465821
C	1.139483	0.967379	2.721445
H	2.048546	0.430294	3.015802
H	0.479575	1.047812	3.588876
H	1.418869	1.980095	2.415144
O	-1.292519	1.799336	2.028790
H	-2.138792	2.144248	1.696597
C	4.975843	1.410774	-0.597452
C	6.307154	1.660460	1.520234
C	7.051260	0.104781	-0.350706
C	6.996996	0.341281	1.154005
C	5.954847	0.685136	-1.182711
C	4.921048	1.742032	0.869392
H	6.920544	2.500383	1.167165
H	4.222852	1.046670	1.359443
H	8.019042	0.277562	1.540440
H	4.486929	2.740891	1.000435
C	6.036414	0.433512	-2.666211
H	5.167996	0.847716	-3.188129
H	6.109070	-0.637255	-2.886145

H	6.942296	0.889755	-3.082252
H	4.168266	1.800567	-1.217756
O	7.934175	-0.569954	-0.862593
H	6.440713	-0.502205	1.590979
H	6.226154	1.760450	2.608552
Al	3.359884	-1.672586	-0.689072
C	2.799358	-1.754571	-2.569266
H	1.727558	-1.556123	-2.689274
H	3.011221	-2.740659	-3.002041
H	3.332191	-1.018882	-3.185168
C	4.748889	-2.779433	0.134312
H	5.724171	-2.666376	-0.355017
H	4.483231	-3.843274	0.059894
H	4.876078	-2.552190	1.198911
O	2.447312	-0.723091	0.449654
C	-3.030260	0.614027	-0.002633
C	-2.829400	-2.236261	-0.236269
C	-4.132719	-0.104008	-0.728891
H	-5.020579	-0.152453	-0.081976
H	-4.445755	0.502404	-1.591222
C	-3.741674	-1.497066	-1.252032
O	-3.329358	1.933609	0.316915
Si	-4.114991	3.204706	-0.479071
C	-5.984542	2.963836	-0.426446
H	-6.495928	3.856832	-0.808127
H	-6.326644	2.801946	0.602377
H	-6.317569	2.111417	-1.028181
C	-3.511143	3.364634	-2.259660
H	-4.016596	4.204947	-2.752489
H	-3.711084	2.468239	-2.857852
H	-2.433072	3.558092	-2.297662
C	-3.634564	4.717569	0.526538
H	-4.082085	5.625613	0.104399
H	-2.547972	4.857620	0.546476
H	-3.978028	4.630213	1.563952
H	-3.131461	-1.341730	-2.152964

C	-5.000018	-2.301998	-1.664646
H	-4.756315	-2.954306	-2.510534
H	-5.748797	-1.594782	-2.043767
C	-5.153927	-2.747094	0.878430
H	-5.645245	-1.811534	1.181729
H	-5.447934	-3.486788	1.630960
C	-5.609616	-3.163726	-0.526738
H	-6.704170	-3.131645	-0.574669
C	-2.400027	-3.602156	-0.834368
H	-3.245529	-4.268003	-1.024468
H	-1.710474	-4.129226	-0.171332
H	-1.889621	-3.435222	-1.791186
H	-5.343062	-4.215677	-0.679721
H	-1.045199	-1.344562	-0.965993
C	-3.649701	-2.503207	1.046552
O	-3.167546	-2.519326	2.163468
H	0.322008	-2.431401	0.392313

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



65-DA-Comlex-Int-I

E(B3LYP/6-31G*) = –2118.96810 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z

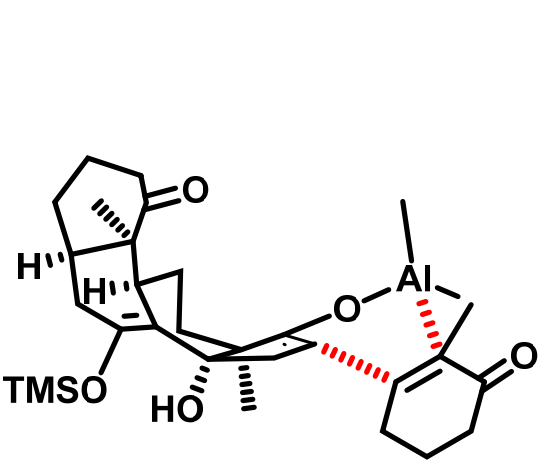
C	1.584501	-1.368104	-0.605710
C	2.025998	0.095852	-0.677533
C	0.524173	-1.783011	-1.672045
H	0.913255	-2.580170	-2.309882
C	1.006271	1.201934	-1.060585
C	-0.285528	0.633490	-1.741215
C	0.031517	-0.631569	-2.546675
H	0.794105	-0.365114	-3.290791
H	-0.856221	-0.953024	-3.103986
C	-1.196165	0.406414	-0.537779
C	0.467075	1.867249	0.255320
H	0.259012	2.930548	0.059936
H	1.202902	1.826028	1.066813
C	-0.791927	1.089700	0.545732
H	-1.319664	1.131474	1.494496
C	-0.945695	1.675191	-2.671084
H	-1.916957	1.294355	-3.008117
H	-0.320542	1.867081	-3.547158
H	-1.107118	2.629841	-2.160904
O	1.585056	2.135449	-1.964165
H	2.457800	2.356432	-1.595801
C	-4.632751	1.697292	0.934698
C	-6.029082	2.352992	-1.052893
C	-6.740548	0.491206	0.522969
C	-6.715894	0.990319	-0.916167
C	-5.605963	0.887839	1.410021
C	-4.623974	2.312822	-0.438395
H	-6.626845	3.114087	-0.533505
H	-3.937766	1.735861	-1.076561
H	-7.745095	0.997623	-1.288274
H	-4.196136	3.321377	-0.377705
C	-5.638377	0.357149	2.819896
H	-4.769938	0.696770	3.392384
H	-5.668794	-0.737903	2.835686
H	-6.547249	0.693578	3.331557
H	-3.793303	1.946072	1.584608

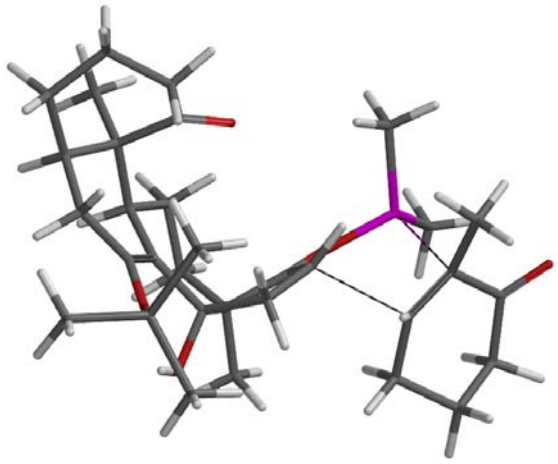
O	-7.627127	-0.244964	0.933739
H	-6.169424	0.239057	-1.506511
H	-5.978617	2.652544	-2.105809
Al	-3.214802	-1.423093	0.322838
C	-2.539488	-1.812308	2.127580
H	-1.492404	-2.143360	2.094047
H	-3.119076	-2.605501	2.614757
H	-2.565676	-0.934505	2.784937
C	-4.682513	-2.349742	-0.581619
H	-5.641033	-2.239248	-0.060087
H	-4.474252	-3.427860	-0.627674
H	-4.815878	-2.001673	-1.612234
O	-2.314266	-0.336878	-0.704328
C	3.260404	0.443229	-0.262625
C	2.802300	-2.362010	-0.587112
C	4.332944	-0.508039	0.199940
H	5.124547	-0.545640	-0.562507
H	4.812545	-0.104939	1.102147
C	3.813090	-1.918975	0.512552
O	3.652241	1.774253	-0.315030
Si	4.620307	2.769270	0.657663
C	6.443906	2.449384	0.303704
H	7.073506	3.175723	0.832941
H	6.650350	2.550644	-0.768171
H	6.761271	1.448162	0.613802
C	4.214616	2.514607	2.482156
H	4.728444	3.268616	3.091765
H	4.517312	1.530437	2.857025
H	3.138226	2.624120	2.658022
C	4.145404	4.505598	0.118307
H	4.727342	5.257969	0.664394
H	3.083608	4.699359	0.307387
H	4.328305	4.657464	-0.951650
H	1.080072	-1.462845	0.364097
H	-0.336840	-2.219872	-1.151637
C	2.268982	-3.764302	-0.227229

O	2.225834	-4.667246	-1.043695
H	4.670168	-2.607137	0.460618
C	3.517273	-2.419922	-1.949279
H	2.912870	-2.930577	-2.699995
H	4.451579	-2.986306	-1.863767
H	3.749655	-1.415667	-2.312924
C	3.247198	-2.034853	1.939778
H	2.409488	-1.339649	2.080998
H	4.022990	-1.727672	2.654158
C	2.809222	-3.472249	2.243133
H	2.384318	-3.546793	3.251291
H	3.693027	-4.125066	2.226888
C	1.792568	-3.984294	1.206472
H	0.839991	-3.451060	1.341667
H	1.586124	-5.051792	1.326927

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions





62-TS2

E(B3LYP/6-31G*) = –2118.92834 au

$\nu ts = 265i\ cm^{-1}$

Cartesian Coordinates (Angstroms)

Atom X Y Z

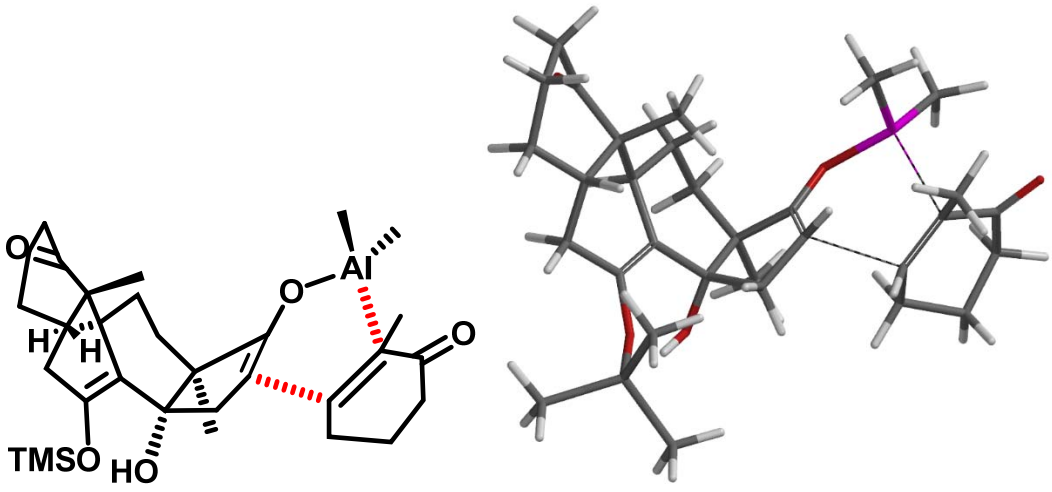
C	1.849631	-1.522701	-1.485765
C	1.770077	-0.040617	-1.105249
C	0.488243	-2.140393	-1.840632
H	-0.086016	-2.365315	-0.938891
H	0.652561	-3.090344	-2.361245
C	0.517692	0.841377	-1.331563
C	-0.695357	0.106149	-2.025498
C	-0.291114	-1.194484	-2.748886
H	0.312598	-0.932965	-3.629508
H	-1.202164	-1.681683	-3.113640
C	-1.593482	-0.252400	-0.840232
C	-0.054243	1.291706	0.068511
H	-0.365637	2.344409	-0.015869
H	0.701601	1.239750	0.856719
C	-1.221954	0.377375	0.329231
H	-1.417264	-0.040589	1.307150
C	-1.425198	1.014409	-3.037733
H	-2.358923	0.532072	-3.347509
H	-0.799111	1.166966	-3.920700
H	-1.650396	2.000626	-2.628434
O	0.859585	1.960102	-2.150310
H	1.638246	2.359960	-1.726132
C	-3.229521	1.458445	0.739065
C	-5.086915	2.631279	-0.428948
C	-5.562238	0.622415	1.063220
C	-6.013512	1.446699	-0.145087
C	-4.094018	0.525069	1.369928
C	-3.637475	2.123254	-0.548308
H	-5.163907	3.373569	0.376913
H	-3.609326	1.402388	-1.371829
H	-7.041599	1.760057	0.059014
H	-2.946100	2.934041	-0.797820
C	-3.805613	0.203371	2.838212
H	-2.757829	-0.071586	2.998246
H	-4.433246	-0.615185	3.191663

H	-4.022052	1.074436	3.472104
H	-2.546864	2.020173	1.372860
H	2.430789	-1.577819	-2.422739
O	-6.391791	0.107580	1.801599
H	-6.049683	0.783928	-1.020821
H	-5.379277	3.136533	-1.356887
Al	-3.822796	-1.564225	0.264573
C	-2.965590	-2.723924	1.613735
H	-2.928146	-3.742019	1.199946
H	-3.524314	-2.788358	2.554565
H	-1.933003	-2.443114	1.851195
C	-5.465691	-2.134796	-0.664145
H	-6.348606	-2.109196	-0.015356
H	-5.343787	-3.174270	-1.001032
H	-5.694010	-1.541530	-1.559026
O	-2.614221	-1.043049	-1.009271
C	2.885181	0.524518	-0.606983
C	2.702703	-2.315111	-0.447117
C	4.168912	-0.200309	-0.302369
H	4.979728	0.222724	-0.913079
H	4.446703	0.037379	0.734345
C	4.146319	-1.739917	-0.496586
H	4.509232	-1.939867	-1.512809
C	5.120293	-2.426121	0.495958
H	5.959120	-1.743625	0.680199
C	2.132247	-2.197456	0.983824
C	3.140065	-2.115345	2.128607
H	2.651488	-2.506689	3.026764
H	3.314920	-1.046599	2.319517
C	4.465029	-2.837502	1.842799
H	4.269602	-3.916145	1.841925
H	5.160453	-2.663987	2.671610
C	2.726210	-3.819726	-0.812304
H	3.416324	-4.387333	-0.182021
H	3.048064	-3.945319	-1.853360
H	1.734833	-4.266473	-0.704092

O	0.937404	-2.196385	1.217948
O	2.915651	1.889533	-0.369579
Si	3.746692	2.913208	0.697104
C	5.552717	3.080265	0.183733
H	6.040992	3.873184	0.764388
H	5.631085	3.351750	-0.875587
H	6.125191	2.159011	0.337260
C	3.596906	2.300941	2.476061
H	3.962122	3.069517	3.169174
H	4.179514	1.392023	2.664371
H	2.552315	2.093124	2.736033
C	2.860518	4.557996	0.495450
H	3.313214	5.325838	1.134764
H	1.802813	4.474880	0.770227
H	2.911586	4.916467	-0.539226
H	5.560851	-3.313828	0.029074

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



63-TS2

E(B3LYP/6-31G*) = –2118.93025 au

v*ts* = 271*i* cm^{-1}

Cartesian Coordinates (Angstroms)

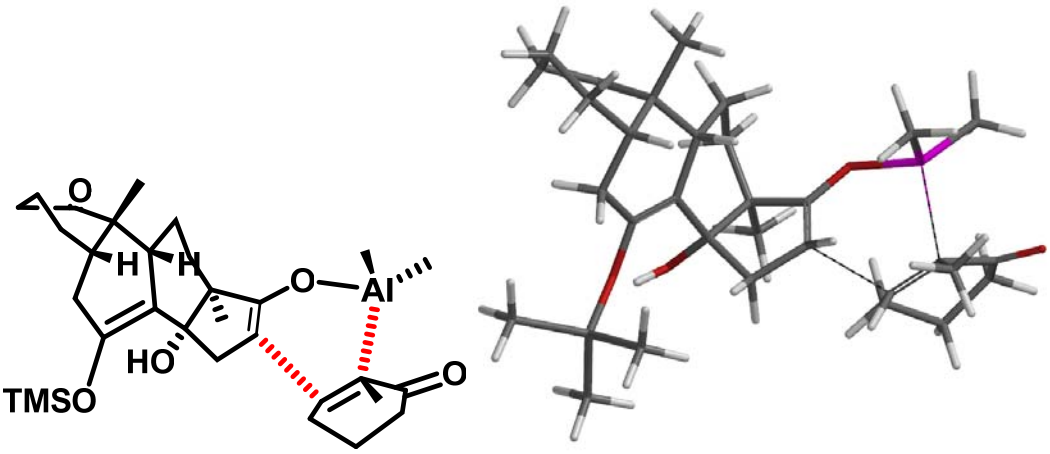
Atom	X	Y	Z
C	1.905722	-1.312321	-1.138082
C	1.702166	0.188230	-0.899329
C	0.630016	-2.035062	-1.607632
H	-0.015324	-2.297200	-0.762823
H	0.919886	-2.975243	-2.082531
C	0.413120	0.973797	-1.232790
C	-0.710401	0.111328	-1.922126
C	-0.165286	-1.171730	-2.581229
H	0.465647	-0.882003	-3.432577
H	-1.010787	-1.740337	-2.984103
C	-1.611131	-0.257895	-0.742691
C	-0.252657	1.485057	0.100121
H	-0.661224	2.489857	-0.086433
H	0.475204	1.578797	0.911637
C	-1.340378	0.483338	0.394998
H	-1.533499	0.115904	1.394133
C	-1.481601	0.909758	-2.995916
H	-2.372012	0.346088	-3.295675
H	-0.846783	1.053782	-3.873733
H	-1.782842	1.900157	-2.650676
O	0.720828	2.052886	-2.114307
H	1.479003	2.511002	-1.711888
C	-3.428806	1.407002	0.681935
C	-5.317692	2.367783	-0.624536
C	-5.705563	0.400459	0.936576
C	-6.145439	1.111138	-0.344727
C	-4.250524	0.435558	1.320358
C	-3.825633	1.986549	-0.650254
H	-5.505931	3.125877	0.147188
H	-3.693193	1.242677	-1.441709
H	-7.212522	1.324901	-0.235189
H	-3.193856	2.845078	-0.898073

C	-4.012094	0.217901	2.816934
H	-2.966185	-0.023065	3.029180
H	-4.633503	-0.593506	3.197647
H	-4.271290	1.121185	3.386180
H	-2.835440	2.055310	1.323825
H	2.611756	-1.405527	-1.976983
O	-6.532436	-0.133011	1.663638
H	-6.040129	0.408145	-1.182615
H	-5.602134	2.811661	-1.585558
Al	-3.758415	-1.677250	0.392019
C	-2.838942	-2.649158	1.850902
H	-2.557312	-3.643980	1.476606
H	-3.483647	-2.811444	2.722838
H	-1.919357	-2.170127	2.207117
C	-5.303166	-2.491576	-0.517371
H	-6.192261	-2.526254	0.122633
H	-5.055243	-3.528745	-0.785001
H	-5.586440	-1.987438	-1.450048
O	-2.549928	-1.147039	-0.880942
C	2.801339	0.849748	-0.493231
C	2.618922	-2.025379	0.068079
C	4.074096	0.094247	-0.230156
H	4.524073	-0.228482	-1.182376
H	4.819385	0.728570	0.260304
C	3.795107	-1.135745	0.653320
C	3.233336	-3.357749	-0.405341
O	2.805739	2.228047	-0.380049
Si	3.566668	3.307134	0.687142
C	5.340438	3.630823	0.138184
H	5.769643	4.462507	0.711275
H	5.370417	3.910325	-0.921418
H	5.998690	2.765167	0.272883
C	3.498440	2.635413	2.448019
H	3.884728	3.379812	3.155451
H	4.094475	1.724526	2.572942
H	2.467215	2.405556	2.740986

C	2.549536	4.878869	0.525574
H	2.948815	5.671230	1.170253
H	1.504787	4.709923	0.809613
H	2.559131	5.254053	-0.504499
H	3.440037	-0.749076	1.618293
C	5.093580	-1.922541	0.922408
H	5.763509	-1.309926	1.539251
H	5.619570	-2.094551	-0.029058
C	3.996540	-4.171129	0.639560
H	4.631700	-4.865532	0.081392
H	3.275791	-4.783052	1.198230
C	4.825963	-3.276186	1.590205
H	5.769311	-3.774710	1.839223
O	3.160839	-3.751162	-1.555668
C	1.621623	-2.322596	1.218272
H	2.139479	-2.633515	2.130563
H	0.903234	-3.106766	0.963216
H	1.056404	-1.412931	1.451655
H	4.300941	-3.119657	2.540628

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



64-TS2

E(B3LYP/6-31G*) = –2118.92517 au

$\nu ts = 273i\ cm^{-1}$

Cartesian Coordinates (Angstroms)

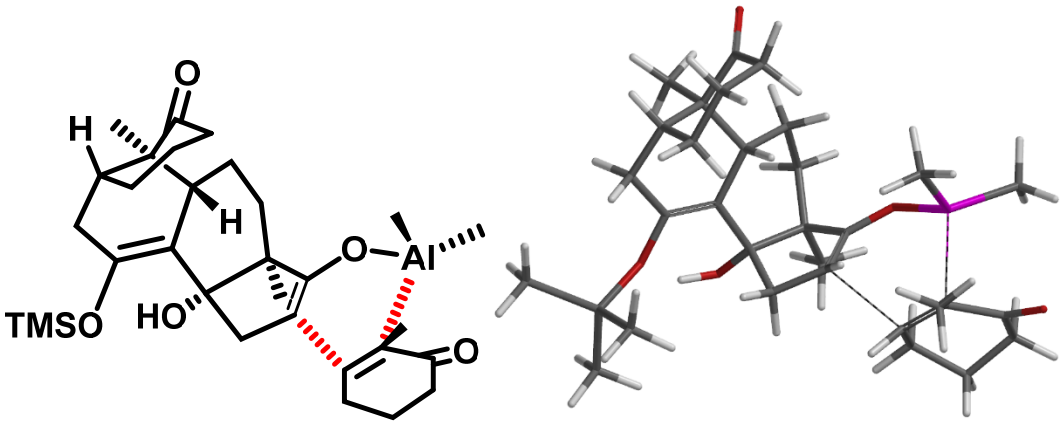
Atom	X	Y	Z
C	-1.364072	-1.502214	0.121364
C	-1.557709	-0.015429	0.444035
C	-0.504595	-2.286527	1.165888
H	-1.097705	-3.076529	1.625361
C	-0.430064	0.804464	1.127317
C	0.664406	-0.099187	1.791941
C	0.053420	-1.417135	2.288513
H	-0.751359	-1.158163	2.987096
H	0.804763	-1.985090	2.849601
C	1.637786	-0.315162	0.632297
C	0.366521	1.583087	0.017747
H	0.768212	2.504291	0.466715
H	-0.271445	1.880663	-0.819813
C	1.464565	0.619911	-0.378120
H	1.702860	0.414974	-1.413737
C	1.341319	0.609996	2.984209
H	2.211388	0.029839	3.311051
H	0.634347	0.680566	3.814245
H	1.661821	1.625685	2.741756
O	-0.947868	1.657736	2.136770
H	-1.748037	2.063725	1.760445
C	3.604378	1.464638	-0.391255
C	5.472177	2.055618	1.147630
C	5.838794	0.393721	-0.741314
C	6.257567	0.834257	0.662093
C	4.405954	0.573943	-1.161742
C	3.963826	1.760657	1.041358
H	5.731494	2.936456	0.545015
H	3.756938	0.887392	1.668628
H	7.335335	1.017613	0.624811

H	3.363916	2.591716	1.423666
C	4.236053	0.647918	-2.681843
H	3.179101	0.657052	-2.968015
H	4.717334	-0.192283	-3.183698
H	4.695818	1.564436	-3.075661
H	3.081170	2.256370	-0.923967
O	6.668329	-0.045290	-1.526745
H	6.097556	-0.007035	1.350963
H	5.728935	2.293275	2.186632
Al	3.790751	-1.624143	-0.613034
C	2.922177	-2.301085	-2.257055
H	2.448986	-3.266665	-2.026985
H	3.653870	-2.491467	-3.052378
H	2.143218	-1.654662	-2.678941
C	5.242074	-2.658843	0.228014
H	6.194979	-2.555273	-0.303324
H	4.980151	-3.726508	0.215656
H	5.415832	-2.392070	1.278355
O	2.539766	-1.249694	0.679450
C	-2.652185	0.623539	-0.008078
C	-2.697188	-2.235557	-0.235254
C	-3.768226	-0.003169	-0.795884
H	-4.685826	0.003928	-0.189429
H	-3.998095	0.631007	-1.664011
C	-3.453189	-1.417378	-1.314527
O	-2.841104	1.968121	0.286545
Si	-3.495824	3.286176	-0.557160
C	-5.377984	3.187595	-0.601702
H	-5.793538	4.103554	-1.040619
H	-5.785995	3.093666	0.411498
H	-5.747589	2.342356	-1.191756
C	-2.777626	3.372931	-2.299744
H	-3.176406	4.244465	-2.834274
H	-3.012475	2.486499	-2.899772
H	-1.686821	3.476300	-2.269177
C	-2.959912	4.771711	0.461016

H	-3.296967	5.704359	-0.007735
H	-1.869766	4.821706	0.559473
H	-3.384689	4.736375	1.471004
H	-2.760764	-1.303551	-2.160234
C	-4.738141	-2.106690	-1.838976
H	-4.485048	-2.759849	-2.681312
H	-5.395084	-1.331434	-2.252900
C	-5.138874	-2.580137	0.673928
H	-5.615323	-1.635800	0.973201
H	-5.521167	-3.328971	1.376707
C	-5.504554	-2.936330	-0.774111
H	-6.585394	-2.817541	-0.911263
C	-2.343453	-3.640773	-0.789926
H	-3.222640	-4.212448	-1.095112
H	-1.804152	-4.237372	-0.050230
H	-1.697229	-3.532236	-1.669561
H	-5.307935	-4.002677	-0.930231
H	-0.788089	-1.527564	-0.817080
C	-3.644766	-2.400316	0.972724
O	-3.273212	-2.368565	2.130764
H	0.325088	-2.772462	0.641471

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



65-TS2

E(B3LYP/6-31G*) = –2118.93586 au

$\nu ts = 265i\ cm^{-1}$

Cartesian Coordinates (Angstroms)

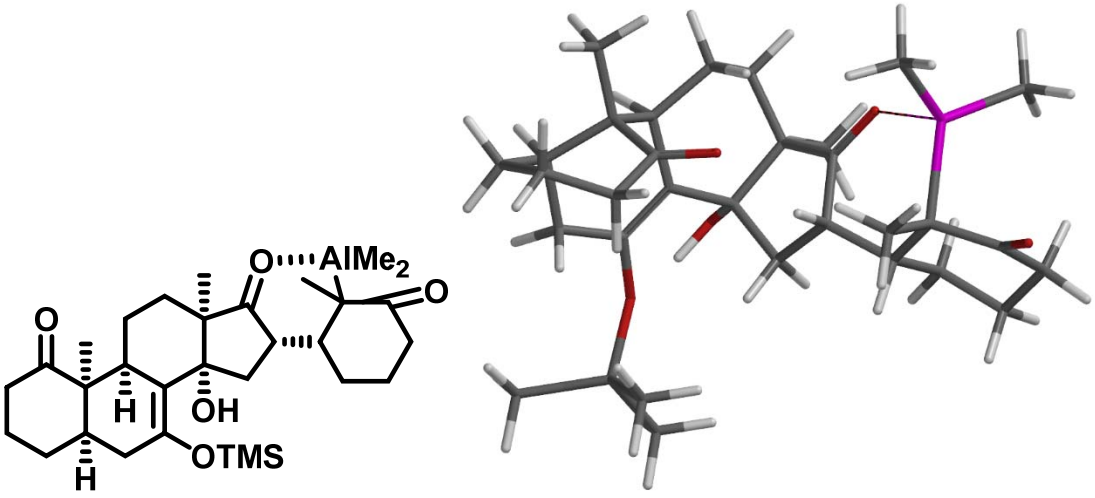
Atom	X	Y	Z
C	1.441445	-1.451928	-0.682975
C	1.762629	0.044626	-0.721054
C	0.540212	-1.956058	-1.854705
H	1.087551	-2.660253	-2.485821
C	0.686752	1.060606	-1.184054
C	-0.502001	0.382420	-1.949697
C	-0.021056	-0.844171	-2.739728
H	0.749458	-0.488151	-3.436637
H	-0.842897	-1.241535	-3.346354
C	-1.436724	0.005136	-0.800509
C	-0.011672	1.669448	0.087892
H	-0.369744	2.678201	-0.165228
H	0.678867	1.771934	0.929969
C	-1.154064	0.714701	0.357412
H	-1.360451	0.327520	1.346011
C	-1.176534	1.362907	-2.933985
H	-2.106101	0.923846	-3.313341
H	-0.509355	1.550838	-3.778856
H	-1.401132	2.329962	-2.478128
O	1.237343	2.047353	-2.043557
H	2.082770	2.313792	-1.641711
C	-3.230583	1.665671	0.678719
C	-5.099033	2.696560	-0.605046
C	-5.523475	0.685982	0.886573
C	-5.945390	1.441756	-0.374393
C	-4.069393	0.682735	1.277273
C	-3.611588	2.297278	-0.634026
H	-5.283151	3.429701	0.191353
H	-3.483581	1.579394	-1.450068
H	-7.010282	1.666056	-0.265375

H	-2.967571	3.155699	-0.847597
C	-3.847695	0.413966	2.768758
H	-2.792929	0.225016	2.990491
H	-4.427535	-0.446015	3.106692
H	-4.168354	1.276295	3.368915
H	-2.631305	2.280802	1.346914
O	-6.360910	0.148354	1.597909
H	-5.842385	0.766446	-1.234965
H	-5.370543	3.177204	-1.551970
Al	-3.610883	-1.401170	0.288131
C	-2.682272	-2.434002	1.702108
H	-2.249511	-3.333111	1.239181
H	-3.371630	-2.782747	2.481018
H	-1.865221	-1.905850	2.206374
C	-5.167354	-2.173929	-0.636599
H	-6.058626	-2.206204	0.000482
H	-4.936524	-3.209765	-0.923967
H	-5.439852	-1.646799	-1.559874
O	-2.400972	-0.848956	-0.975344
C	2.927096	0.494626	-0.213546
C	2.724935	-2.343686	-0.529029
C	4.021923	-0.362793	0.363102
H	4.883476	-0.345900	-0.319690
H	4.380282	0.091501	1.297134
C	3.584319	-1.806292	0.655432
O	3.221589	1.849515	-0.268994
Si	3.980909	2.951316	0.776596
C	5.843652	2.671206	0.834356
H	6.326793	3.495447	1.374541
H	6.266189	2.648285	-0.176790
H	6.124427	1.739416	1.336469
C	3.219257	2.831950	2.496890
H	3.689434	3.551102	3.179073
H	3.339527	1.835030	2.935818
H	2.146819	3.056347	2.466010
C	3.615325	4.612345	-0.023692

H	4.031714	5.435188	0.570044
H	2.537898	4.784260	-0.125495
H	4.057903	4.671925	-1.025090
H	0.841804	-1.594904	0.225334
H	-0.291062	-2.527650	-1.428231
C	2.274703	-3.782341	-0.192700
O	2.395607	-4.695944	-0.988685
H	4.493822	-2.423106	0.703961
C	3.572368	-2.358119	-1.815492
H	3.119141	-2.981271	-2.587257
H	4.562493	-2.782239	-1.612466
H	3.702786	-1.347277	-2.211641
C	2.883655	-1.944127	2.020100
H	1.981669	-1.318735	2.052038
H	3.551269	-1.561952	2.804139
C	2.530064	-3.407597	2.311285
H	2.006887	-3.498612	3.270543
H	3.460356	-3.984976	2.406025
C	1.672085	-4.020152	1.188289
H	0.667758	-3.572765	1.214414
H	1.546633	-5.099541	1.313167

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



62-Int-II

E(B3LYP/6-31G*) = –2118.97164 au

Cartesian Coordinates (Angstroms)

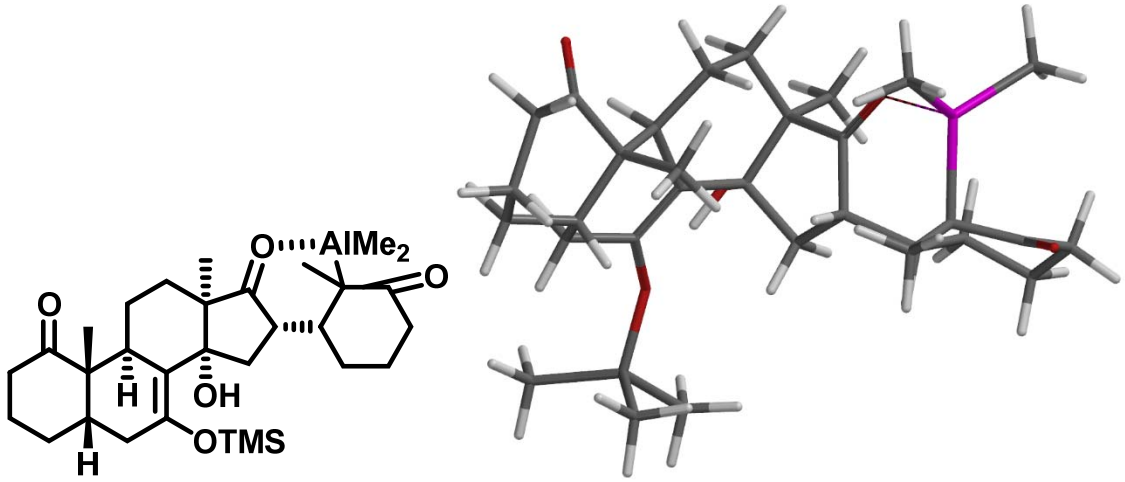
Atom	X	Y	Z
C	1.820325	-1.641033	-1.406789
C	1.694340	-0.127554	-1.189731
C	0.518900	-2.323548	-1.861961
H	-0.154577	-2.482417	-1.016114
H	0.757520	-3.312882	-2.265833
C	0.533332	0.715496	-1.763795
C	-0.624608	-0.135828	-2.387278
C	-0.179594	-1.496006	-2.939393
H	0.491835	-1.320804	-3.790745
H	-1.057013	-2.031183	-3.318309
C	-1.598820	-0.306967	-1.234455
C	-0.202474	1.526732	-0.649753
H	-0.651203	2.402801	-1.130585
H	0.476008	1.885297	0.123257
C	-1.280917	0.589727	-0.077663
H	-0.789452	-0.087041	0.639093
C	-1.381669	0.660038	-3.483453
H	-2.245077	0.076566	-3.817087
H	-0.709655	0.836996	-4.325442
H	-1.734094	1.632898	-3.129738
O	1.038584	1.575596	-2.788938
H	1.779557	2.051731	-2.375945
C	-2.507043	1.222426	0.647918
C	-4.490851	2.777839	0.469054
C	-4.687382	0.643820	1.873896
C	-5.422100	1.720542	1.067512
C	-3.352931	0.153123	1.401752
C	-3.341336	2.113398	-0.292783
H	-4.072328	3.401338	1.272512

H	-3.751124	1.518562	-1.121921
H	-6.174997	2.158348	1.729802
H	-2.703751	2.884072	-0.743697
C	-2.567114	-0.427315	2.598708
H	-1.655048	-0.955362	2.302981
H	-3.189045	-1.128823	3.157198
H	-2.276914	0.372869	3.298735
H	-2.063134	1.895963	1.403879
H	2.510725	-1.773074	-2.257576
O	-5.255109	0.156237	2.850402
H	-5.967175	1.211459	0.260083
H	-5.049890	3.453010	-0.191146
Al	-3.867438	-1.447124	0.151852
C	-3.289982	-3.208394	0.853623
H	-3.422529	-3.999531	0.102547
H	-3.890233	-3.500129	1.726723
H	-2.239368	-3.229752	1.170758
C	-5.567346	-1.361617	-0.867439
H	-6.443885	-1.414031	-0.206957
H	-5.641626	-2.218921	-1.551552
H	-5.686383	-0.458099	-1.481455
O	-2.544690	-1.110286	-1.284094
C	2.738389	0.504138	-0.619863
C	2.544064	-2.321315	-0.203608
C	3.946299	-0.172759	-0.025916
H	4.851469	0.225902	-0.504737
H	4.021305	0.141280	1.025230
C	3.975042	-1.719066	-0.117456
H	4.464050	-1.973108	-1.066306
C	4.829898	-2.318606	1.030176
H	5.618961	-1.599510	1.283710
C	1.807144	-2.085527	1.129791
C	2.658565	-1.983158	2.392776
H	2.059190	-2.361308	3.227393
H	2.791475	-0.908081	2.585569
C	4.020269	-2.686424	2.303344

H	3.847738	-3.768298	2.330440
H	4.605766	-2.460352	3.201492
C	2.631578	-3.851360	-0.433124
H	3.262036	-4.346576	0.309390
H	3.066311	-4.051377	-1.420097
H	1.643556	-4.316908	-0.393980
O	0.594336	-1.979476	1.199430
O	2.780774	1.885712	-0.606250
Si	3.386846	3.044292	0.481612
C	5.269886	3.094874	0.428467
H	5.636863	3.966191	0.985644
H	5.634673	3.185469	-0.601514
H	5.729101	2.204845	0.871686
C	2.771798	2.678589	2.226042
H	3.099917	3.465024	2.917222
H	3.153202	1.726933	2.613696
H	1.677131	2.640791	2.266273
C	2.676099	4.660182	-0.158296
H	3.000884	5.499994	0.467790
H	1.580599	4.646002	-0.154771
H	3.007051	4.864009	-1.183138
H	5.351467	-3.212410	0.672036

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



63-Int-II

E(B3LYP/6-31G*) = –2118.97080 au

Cartesian Coordinates (Angstroms)

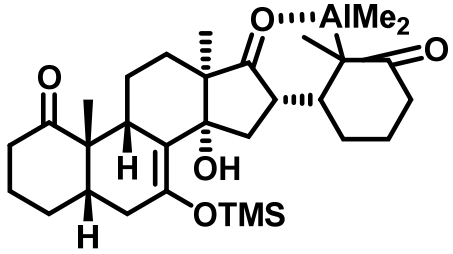
Atom	X	Y	Z
C	1.848811	-1.375988	-1.058961
C	1.596831	0.130704	-0.924222
C	0.638303	-2.147322	-1.617732
H	-0.110563	-2.331779	-0.839569
H	0.979187	-3.125584	-1.964072
C	0.406746	0.880694	-1.563367
C	-0.636663	-0.061875	-2.255235
C	-0.035069	-1.383671	-2.756553
H	0.686376	-1.153864	-3.551384
H	-0.830618	-1.991542	-3.200492
C	-1.672521	-0.295174	-1.171066
C	-0.444070	1.634389	-0.493870
H	-0.924771	2.481018	-0.994234
H	0.168514	2.029896	0.318262
C	-1.487632	0.622341	0.005939
H	-0.995259	-0.019018	0.754667
C	-1.379414	0.659829	-3.411910
H	-2.144112	-0.009186	-3.818027

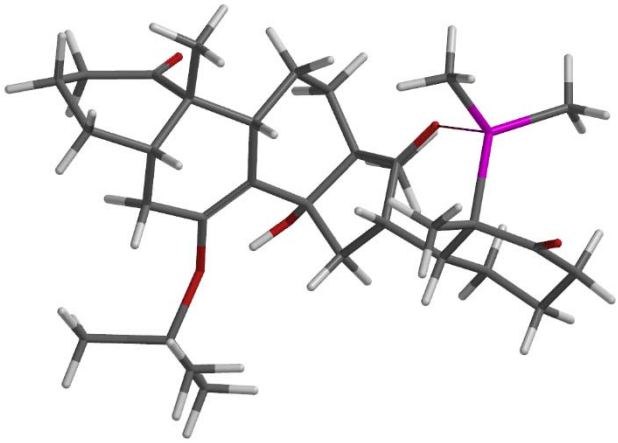
H	-0.660391	0.915715	-4.192017
H	-1.862479	1.586397	-3.088890
O	0.891877	1.776533	-2.564861
H	1.593374	2.293302	-2.131567
C	-2.795511	1.158790	0.658923
C	-4.853277	2.594120	0.391767
C	-5.000531	0.415360	1.748173
C	-5.751457	1.483133	0.943493
C	-3.610725	0.024798	1.345808
C	-3.634378	2.001443	-0.319980
H	-4.509453	3.238162	1.214114
H	-3.973887	1.384795	-1.165072
H	-6.539915	1.873979	1.594029
H	-3.024740	2.809490	-0.742162
C	-2.857892	-0.529551	2.575385
H	-1.924987	-1.042935	2.314941
H	-3.484673	-1.243449	3.111757
H	-2.604644	0.277734	3.281126
H	-2.447183	1.851443	1.447015
H	2.633646	-1.496659	-1.821278
O	-5.597842	-0.153227	2.661225
H	-6.258348	0.971766	0.112871
H	-5.419739	3.238712	-0.291951
Al	-3.965901	-1.582638	0.057587
C	-3.342829	-3.322330	0.776916
H	-3.401839	-4.108727	0.012196
H	-3.972411	-3.649967	1.615580
H	-2.309302	-3.310572	1.149288
C	-5.600634	-1.554095	-1.062853
H	-6.515769	-1.581549	-0.455824
H	-5.633758	-2.436034	-1.717630
H	-5.677647	-0.674128	-1.715996
O	-2.560955	-1.157116	-1.273066
C	2.625971	0.842247	-0.425939
C	2.449289	-2.023190	0.241377
C	3.868012	0.134621	0.039170

H	4.445950	-0.204892	-0.835708
H	4.526617	0.809457	0.594988
C	3.519519	-1.073014	0.925312
C	3.158267	-3.345740	-0.120591
O	2.610778	2.220439	-0.451439
Si	3.301595	3.413591	0.547855
C	5.119188	3.661936	0.117028
H	5.509944	4.548940	0.631703
H	5.245345	3.824792	-0.959828
H	5.750453	2.813199	0.402080
C	3.071962	2.931338	2.354775
H	3.381656	3.752711	3.012595
H	3.659062	2.049349	2.635576
H	2.019349	2.714305	2.571468
C	2.324759	4.961123	0.125417
H	2.726152	5.831546	0.658612
H	1.268966	4.859449	0.400811
H	2.370705	5.180908	-0.947442
H	3.043575	-0.668371	1.828922
C	4.804799	-1.800578	1.367928
H	5.370864	-1.145806	2.042639
H	5.447971	-1.970259	0.490777
C	3.840570	-4.099330	1.020943
H	4.564897	-4.769738	0.549273
H	3.094893	-4.738828	1.512051
C	4.519031	-3.150010	2.035398
H	5.450153	-3.600073	2.397318
O	3.212928	-3.776609	-1.258337
C	1.353430	-2.335858	1.291214
H	1.789421	-2.660307	2.240135
H	0.659858	-3.115867	0.963449
H	0.773586	-1.428924	1.497582
H	3.890303	-2.999669	2.921731

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions





64-Int-II

E(B3LYP/6-31G*) = –2118.96665 au

Cartesian Coordinates (Angstroms)

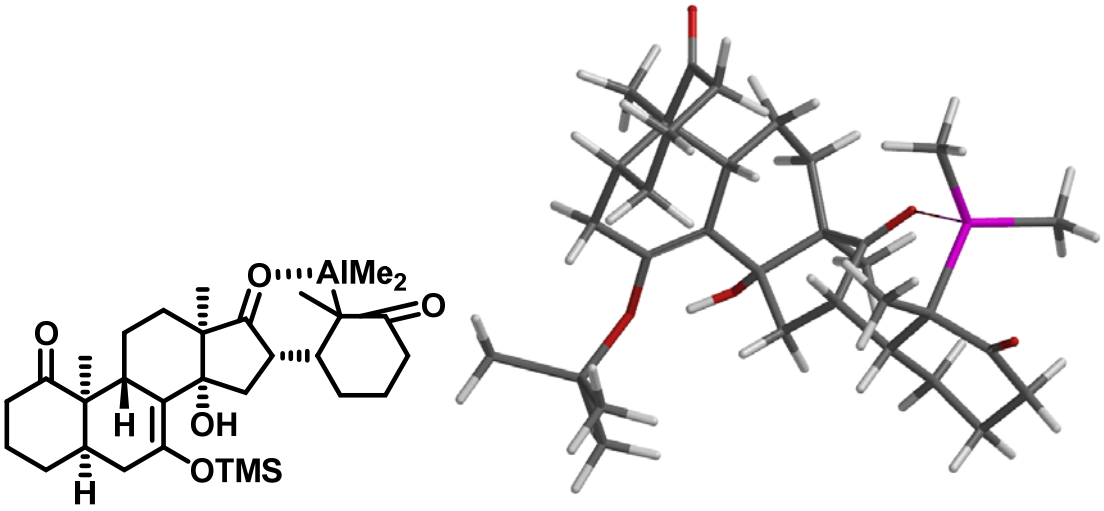
Atom	X	Y	Z
C	-1.328385	-1.536393	0.033597
C	-1.462965	-0.069799	0.470508
C	-0.576218	-2.458034	1.053239
H	-1.219451	-3.279242	1.365839
C	-0.401002	0.610558	1.374134
C	0.588051	-0.414366	2.008666
C	-0.101309	-1.746434	2.316978
H	-0.956648	-1.524019	2.965070
H	0.576696	-2.402649	2.874522
C	1.692243	-0.517120	0.981117
C	0.541293	1.525611	0.528186
H	0.981188	2.265695	1.204621
H	0.007755	2.066391	-0.256511
C	1.623524	0.588528	-0.041279
H	1.215449	0.105319	-0.943140
C	1.245577	0.153077	3.296703
H	2.001641	-0.551930	3.655266
H	0.470561	0.278386	4.054928

H	1.719818	1.126118	3.140166
O	-1.015898	1.315241	2.442977
H	-1.739980	1.824377	2.037881
C	3.001788	1.199344	-0.443133
C	5.052772	2.452647	0.325514
C	5.295270	0.604498	-1.436059
C	5.976981	1.429446	-0.339253
C	3.863118	0.193327	-1.263276
C	3.747261	1.787444	0.768620
H	4.817762	3.259513	-0.383809
H	3.972047	0.994349	1.495883
H	6.857239	1.897364	-0.790897
H	3.113332	2.519892	1.283583
C	3.238695	-0.073372	-2.649610
H	2.270254	-0.583963	-2.595767
H	3.903062	-0.696759	-3.250068
H	3.086263	0.867316	-3.202297
H	2.748085	2.049613	-1.102034
O	5.969384	0.233800	-2.395533
H	6.348635	0.723974	0.417734
H	5.554083	2.924521	1.179836
Al	4.027397	-1.656770	-0.292913
C	3.339792	-3.166859	-1.380496
H	3.295998	-4.091264	-0.788462
H	3.999941	-3.370105	-2.234705
H	2.335926	-3.000451	-1.794133
C	5.583679	-2.004001	0.882009
H	6.525945	-2.010268	0.316827
H	5.489909	-2.997655	1.342442
H	5.712924	-1.288216	1.705073
O	2.557669	-1.408816	1.008819
C	-2.474611	0.676296	-0.011050
C	-2.677584	-2.153105	-0.455709
C	-3.555639	0.191395	-0.934731
H	-4.517410	0.241254	-0.404298
H	-3.657969	0.895058	-1.772468

C	-3.313085	-1.212960	-1.516543
O	-2.615504	1.991252	0.404266
Si	-3.159886	3.413746	-0.355191
C	-5.039174	3.416187	-0.498364
H	-5.385512	4.390411	-0.865730
H	-5.505982	3.248459	0.479294
H	-5.414730	2.651734	-1.187028
C	-2.345762	3.596892	-2.046030
H	-2.594644	4.572783	-2.481604
H	-2.669947	2.829541	-2.758454
H	-1.253741	3.541448	-1.967772
C	-2.602316	4.771557	0.817144
H	-2.935700	5.753737	0.460738
H	-1.511093	4.802995	0.910644
H	-3.019744	4.626274	1.820403
H	-2.566869	-1.105932	-2.315818
C	-4.613806	-1.772798	-2.147162
H	-4.363066	-2.387500	-3.018186
H	-5.192084	-0.926439	-2.537862
C	-5.180618	-2.370708	0.306634
H	-5.582689	-1.401782	0.635531
H	-5.670296	-3.116040	0.942864
C	-5.491133	-2.609786	-1.177578
H	-6.552084	-2.406410	-1.360918
C	-2.380700	-3.530988	-1.104859
H	-3.278837	-4.016171	-1.492909
H	-1.916898	-4.219645	-0.395079
H	-1.688031	-3.395205	-1.944602
H	-5.358056	-3.676196	-1.392784
H	-0.704506	-1.529698	-0.874977
C	-3.696996	-2.352148	0.686973
O	-3.378948	-2.471791	1.855476
H	0.286887	-2.907822	0.550159

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



65-Int-II

E(B3LYP/6-31G*) = –2118.97623 au

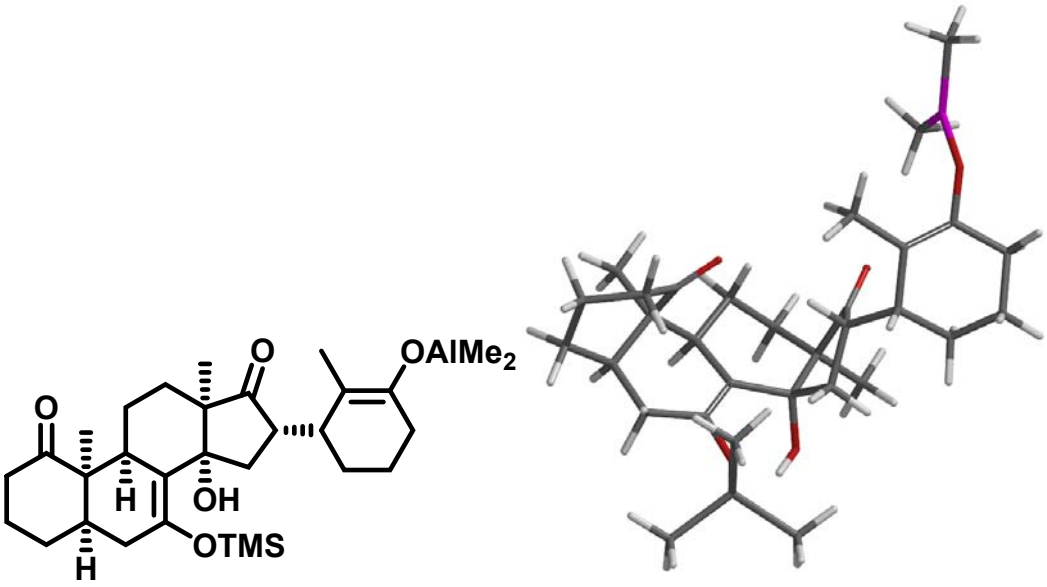
Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.398716	-1.512323	0.660638
C	-1.690916	-0.014554	0.785434
C	-0.732695	-2.157303	1.916916
H	-1.441848	-2.804239	2.436786
C	-0.690420	0.915527	1.516481
C	0.405511	0.109378	2.281033
C	-0.172304	-1.151557	2.928966
H	-0.968545	-0.806228	3.600104
H	0.584653	-1.639061	3.552639
C	1.452363	-0.130655	1.216696
C	0.144821	1.738546	0.487705
H	0.547609	2.614983	1.004721
H	-0.460452	2.092947	-0.348618
C	1.268147	0.786545	0.031983
H	0.852504	0.132723	-0.750058
C	1.097840	0.979691	3.367447

H	1.891075	0.395907	3.843587
H	0.355074	1.265876	4.113995
H	1.539235	1.896458	2.967065
O	-1.351504	1.738228	2.467644
H	-2.121147	2.110792	2.002277
C	2.578082	1.386371	-0.560076
C	4.576261	2.882939	-0.197327
C	4.852498	0.721213	-1.561491
C	5.531656	1.802472	-0.712707
C	3.455254	0.289192	-1.233291
C	3.346441	2.248778	0.457519
H	4.251162	3.522010	-1.030881
H	3.670025	1.641384	1.315525
H	6.338986	2.221519	-1.320993
H	2.691397	3.034021	0.855477
C	2.772226	-0.255145	-2.507942
H	1.850162	-0.810568	-2.299202
H	3.446373	-0.929745	-3.037385
H	2.515106	0.562265	-3.200415
H	2.233064	2.074716	-1.353109
O	5.510240	0.176856	-2.447105
H	6.012218	1.298354	0.137575
H	5.092083	3.539217	0.514354
Al	3.795837	-1.351796	0.022384
C	3.209417	-3.077444	-0.759150
H	3.270382	-3.887004	-0.019320
H	3.847452	-3.372244	-1.603300
H	2.178300	-3.065060	-1.139694
C	5.393545	-1.315542	1.191993
H	6.328701	-1.301993	0.616197
H	5.429903	-2.209779	1.829499
H	5.419882	-0.447555	1.864740
O	2.348599	-0.983340	1.328402
C	-2.756237	0.531579	0.166398
C	-2.650602	-2.338897	0.187121
C	-3.766609	-0.227769	-0.651005

H	-4.711216	-0.277028	-0.090767
H	-3.993700	0.338321	-1.563994
C	-3.298422	-1.637589	-1.043898
O	-3.015369	1.879961	0.335510
Si	-3.681417	3.091196	-0.660196
C	-5.549301	2.884479	-0.793978
H	-5.988530	3.745864	-1.312847
H	-6.005721	2.831504	0.201232
H	-5.841420	1.983966	-1.344643
C	-2.856451	3.054205	-2.355035
H	-3.248813	3.859807	-2.987844
H	-3.025928	2.110155	-2.883994
H	-1.773427	3.200331	-2.270513
C	-3.270269	4.675228	0.261923
H	-3.628122	5.551712	-0.291740
H	-2.190219	4.790488	0.406326
H	-3.744587	4.693463	1.250057
H	-0.652936	-1.602540	-0.141994
H	0.072571	-2.817543	1.575688
C	-2.162111	-3.742137	-0.245516
O	-2.417930	-4.737425	0.406590
H	-4.196395	-2.217010	-1.304427
C	-3.702161	-2.485034	1.304087
H	-3.408543	-3.240084	2.034045
H	-4.657222	-2.816263	0.880645
H	-3.867432	-1.536444	1.822984
C	-2.398973	-1.643298	-2.293025
H	-1.493940	-1.043491	-2.125513
H	-2.935656	-1.158787	-3.119787
C	-2.015801	-3.073100	-2.694474
H	-1.348723	-3.064852	-3.564235
H	-2.920946	-3.616063	-2.999513
C	-1.347127	-3.830985	-1.531743
H	-0.349005	-3.407665	-1.346944
H	-1.206758	-4.890883	-1.761638

Requested basis set is 6-31G(d)
There are 252 shells and 676 basis functions



62-Int-III

E(B3LYP/6-31G*) = –2118.97823 au

Cartesian Coordinates (Angstroms)

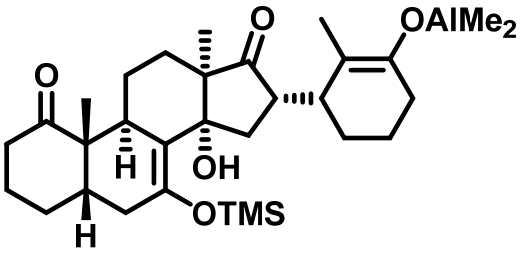
Atom	X	Y	Z
C	-2.307925	2.559138	2.143276
C	-4.465522	3.174549	0.854087
C	-2.321258	2.565829	-0.476190
C	-3.826564	2.269988	-0.230053
C	-1.529265	2.413213	0.838474
C	-3.522347	3.496710	2.044132
H	-3.151535	4.524212	1.951219
H	-2.624053	1.546725	2.434013
H	-4.798909	4.113657	0.399709
C	-1.828047	1.586478	-1.588162
C	-1.956045	0.127706	-1.132090
C	-4.081401	0.774836	0.090449
H	-4.183037	0.638184	1.176235

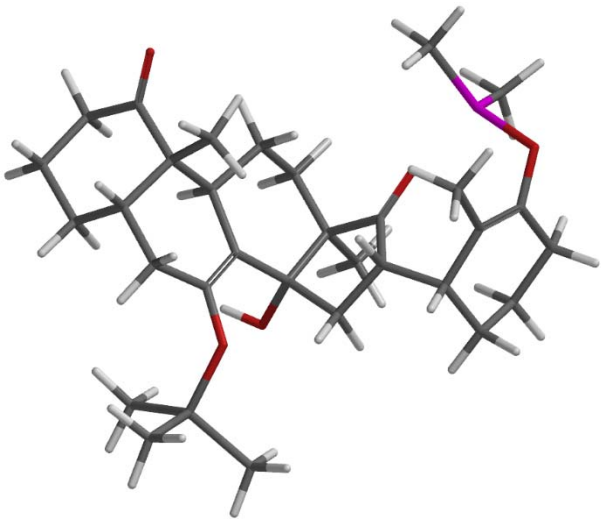
H	-5.059058	0.485014	-0.320675
C	-3.041451	-0.195361	-0.403896
C	-0.466497	1.919248	-2.222266
H	0.305298	2.037385	-1.457536
H	-0.542700	2.877385	-2.747827
C	-1.016092	-0.998119	-1.627692
C	0.182957	-0.508583	-2.503942
C	-0.059659	0.829172	-3.213580
H	-0.836744	0.698744	-3.980014
H	0.864170	1.118346	-3.726534
C	1.360187	-0.364391	-1.511648
C	-0.304495	-1.715949	-0.439892
H	-0.052213	-2.725256	-0.783343
H	-0.949287	-1.813119	0.434726
C	0.965049	-0.902225	-0.140959
H	0.653727	-0.003477	0.411204
O	2.431359	0.121282	-1.820469
O	-0.325972	2.219972	0.861131
C	0.606785	-1.579385	-3.534952
H	1.527986	-1.248459	-4.025246
H	-0.178720	-1.713646	-4.282085
H	0.793285	-2.553341	-3.071894
O	-1.782514	-1.923860	-2.408653
H	-2.522630	-2.187620	-1.835182
O	-3.323312	-1.523764	-0.133168
C	2.066688	-1.618858	0.689280
C	3.858934	-3.416193	0.659203
C	4.470223	-1.012768	1.079529
C	4.975042	-2.369482	0.658140
C	3.169943	-0.667091	1.144454
C	2.620441	-2.857566	-0.042720
H	3.605937	-3.678810	1.695999
H	2.891770	-2.581293	-1.070687
H	5.785927	-2.656300	1.340821
H	1.845282	-3.630093	-0.110994
C	2.746479	0.669100	1.705141

H	2.513172	1.401766	0.920522
H	3.526628	1.090796	2.347090
H	1.837691	0.577226	2.314276
H	1.544092	-1.974147	1.596473
H	-4.330699	2.484875	-1.180901
H	-5.376927	2.683730	1.216665
H	-1.603027	2.887986	2.913721
C	-2.145381	4.033874	-0.938513
H	-2.579712	4.743661	-0.228651
H	-2.642935	4.182795	-1.904538
H	-1.088291	4.284356	-1.052775
H	-2.551956	1.718994	-2.411470
O	5.475537	-0.158978	1.452404
H	5.431753	-2.298821	-0.342246
H	4.196740	-4.338477	0.170473
H	-4.077371	3.468960	2.988393
Si	-3.985737	-2.351112	1.191557
C	-5.861864	-2.168772	1.211808
H	-6.293330	-2.453434	0.244922
H	-6.181749	-1.145035	1.433675
H	-6.300076	-2.824531	1.974865
C	-3.235874	-1.737108	2.811541
H	-3.529366	-2.402307	3.633538
H	-3.571770	-0.727902	3.076046
H	-2.140673	-1.729526	2.769640
C	-3.506616	-4.140064	0.875447
H	-3.882362	-4.488043	-0.093624
H	-3.919814	-4.799906	1.647844
H	-2.417895	-4.263399	0.875709
Al	6.112381	1.249509	0.666802
C	7.343850	2.289992	1.785756
H	7.790014	1.682782	2.581862
H	6.818213	3.123047	2.273452
H	8.157833	2.734333	1.199129
C	5.638486	1.658380	-1.190237
H	5.558319	2.740679	-1.356858

H	4.690878	1.194500	-1.483957
H	6.414125	1.293768	-1.878943

Requested basis set is 6-31G(d)
There are 252 shells and 676 basis functions





63-Int-III

E(B3LYP/6-31G*) = –2118.97752 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
H	-3.311157	3.452037	-1.832667
C	-3.751112	3.833321	-0.899677
C	-4.715786	1.596311	-0.197462
C	-2.385382	2.271827	0.710151
C	-3.727422	1.522442	0.982410
C	-2.722875	3.700320	0.220186
C	-5.034435	3.043503	-0.584728
H	-5.714482	3.074572	-1.444331
H	-3.948312	4.899379	-1.042977
H	-5.642017	1.079606	0.086361
C	-1.597936	1.528005	-0.422064

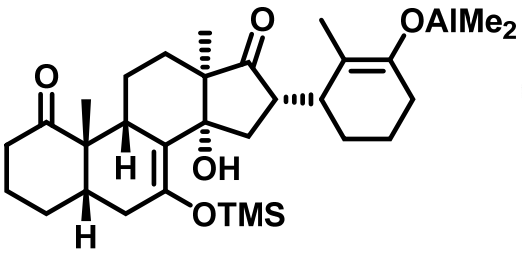
C	-1.471130	0.009777	-0.202863
C	-3.442226	0.074143	1.393061
H	-3.121838	0.020203	2.443183
H	-4.371685	-0.508332	1.347654
C	-2.392215	-0.624404	0.561242
C	-0.248612	2.201336	-0.725144
H	0.414985	2.153855	0.146156
H	-0.405211	3.266458	-0.929619
C	-0.446328	-0.800436	-1.032897
C	0.746167	0.062272	-1.619727
C	0.418882	1.529702	-1.918992
H	-0.242505	1.575235	-2.796427
H	1.342404	2.050482	-2.191978
C	1.832196	-0.040320	-0.542801
C	0.323028	-1.873427	-0.221679
H	0.682212	-2.622217	-0.936333
H	-0.309077	-2.383024	0.499121
C	1.494288	-1.141185	0.446236
H	1.066441	-0.550672	1.276510
O	2.775672	0.758675	-0.521948
O	-2.209410	4.686637	0.714894
C	1.329184	-0.599667	-2.895638
H	2.222591	-0.051617	-3.210681
H	0.587098	-0.564882	-3.697021
H	1.596319	-1.648106	-2.745378
O	-1.141950	-1.499032	-2.087829
H	-1.816535	-0.896697	-2.437985
C	-1.557826	2.368923	2.004501
H	-0.732072	3.073635	1.894562
H	-1.150799	1.394686	2.291820
H	-2.178733	2.737916	2.828112
H	-4.317019	1.052231	-1.065013
H	-4.212745	2.022982	1.833337
O	-2.393204	-1.979369	0.739419
C	2.623379	-2.012630	1.126759
C	4.181512	-2.561641	-0.825731

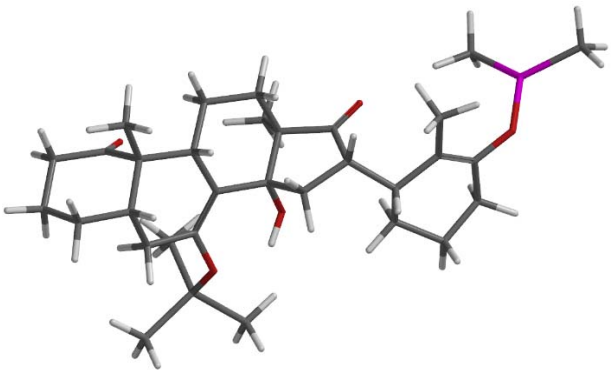
C	4.728547	-0.744563	0.877939
C	5.265082	-1.674129	-0.199107
C	3.658633	-1.045238	1.650547
C	3.224638	-3.112040	0.235785
H	4.638774	-3.387287	-1.385676
H	5.762543	-1.074798	-0.968993
H	2.433539	-3.709766	-0.233668
H	3.619441	-1.975116	-1.565156
H	6.050344	-2.299933	0.251335
H	3.774967	-3.795711	0.895927
C	3.279748	-0.213794	2.850938
H	2.453724	0.492391	2.668143
H	4.131800	0.374882	3.198001
H	2.952185	-0.864166	3.675151
H	2.105159	-2.514576	1.957719
H	-2.183405	1.653570	-1.347886
O	5.376745	0.440779	0.986622
H	-5.560235	3.532473	0.246980
Si	-3.474328	-3.174647	0.208789
C	-4.480985	-2.537377	-1.251029
H	-3.824625	-2.285623	-2.090282
H	-5.068498	-1.648450	-0.994476
H	-5.181673	-3.308150	-1.594791
C	-2.402969	-4.635841	-0.285234
H	-1.757936	-4.953592	0.542313
H	-1.761915	-4.370607	-1.132615
H	-3.016537	-5.497171	-0.576558
C	-4.606583	-3.640788	1.642090
H	-5.276896	-2.819654	1.921473
H	-4.025809	-3.914480	2.530643
H	-5.231673	-4.502533	1.376265
Al	4.477516	1.710643	0.068622
C	5.260882	2.058828	-1.711498
H	5.348708	1.147121	-2.318598
H	4.669750	2.779067	-2.293838
H	6.274623	2.474763	-1.628096

C	3.727207	3.177077	1.156249
H	3.025273	2.826536	1.923472
H	3.198635	3.920576	0.544462
H	4.524615	3.715847	1.687000

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions





64-Int-III

E(B3LYP/6-31G*) = –2118.97753 au

Cartesian Coordinates (Angstroms)

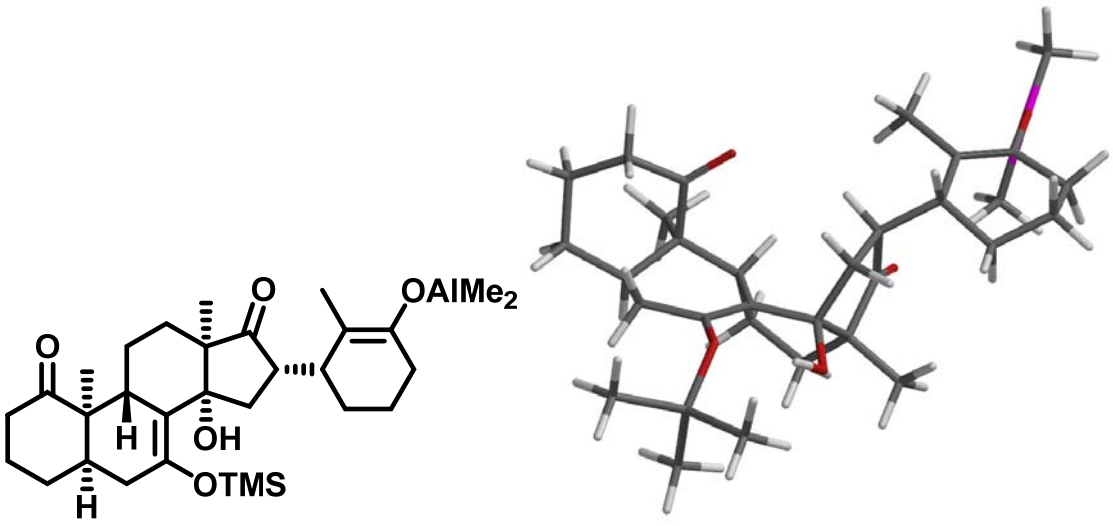
Atom	X	Y	Z
H	6.309666	-3.092618	-0.634778
C	6.119620	-2.027234	-0.815124
C	6.036995	-1.247689	1.630853
C	3.862171	-2.030661	0.464211
C	4.517773	-1.026088	1.467854
C	4.608668	-1.798444	-0.866357
C	6.794113	-1.183595	0.292589
H	6.853590	-0.144047	-0.052045
H	6.524230	-1.782547	-1.801308
H	6.220591	-2.212317	2.117120
C	2.323039	-1.765946	0.406453
C	1.912249	-0.290895	0.323564
C	4.226301	0.419414	1.036118

H	4.440210	1.096087	1.874190
H	4.909157	0.726001	0.230606
C	2.808874	0.671494	0.599505
C	1.605729	-2.616057	-0.668876
H	1.824805	-3.676562	-0.502674
H	1.989276	-2.359111	-1.657348
C	0.417861	-0.009347	0.108115
C	-0.307409	-0.948761	-0.893188
C	0.091345	-2.421432	-0.617956
H	-0.404225	-3.060777	-1.358144
H	-0.277618	-2.744445	0.366034
C	-1.775453	-0.813934	-0.458822
C	-0.382828	-0.196276	1.444282
H	-0.309267	0.725079	2.030852
H	0.055128	-0.994307	2.053619
C	-1.840886	-0.543849	1.052627
H	-2.093759	-1.512671	1.501172
O	-2.726949	-0.973249	-1.196709
O	4.075497	-1.394604	-1.884600
C	-0.108366	-0.589246	-2.368103
H	-0.703352	-1.262137	-2.993696
H	-0.435345	0.433674	-2.559751
H	0.943697	-0.671871	-2.658402
O	0.151938	1.305674	-0.383319
H	0.690454	1.907556	0.159281
C	4.086718	-3.487607	0.948967
H	3.698507	-4.215985	0.231459
H	3.566012	-3.644240	1.901276
H	5.138594	-3.725792	1.112268
H	6.437536	-0.486905	2.313783
H	4.032807	-1.190493	2.440676
O	2.492536	2.027150	0.586340
C	-2.942841	0.458029	1.515957
C	-4.000203	2.732051	1.139829
C	-5.357254	0.633872	0.854722
C	-5.251546	2.101456	0.524551

C	-4.348090	-0.113189	1.341268
C	-2.784992	1.845255	0.865801
H	-4.143233	2.843861	2.223893
H	-5.245401	2.233098	-0.569865
H	-2.664255	1.729419	-0.217597
H	-3.841263	3.739160	0.734644
H	-6.162998	2.596474	0.885444
H	-1.868041	2.323235	1.226766
C	-4.584212	-1.540501	1.772870
H	-4.233320	-2.266777	1.025183
H	-4.054491	-1.762477	2.710145
H	-5.647800	-1.724527	1.946539
H	-2.767470	0.572452	2.601429
H	1.946222	-2.140194	1.375755
O	-6.616346	0.124461	0.665659
H	7.830341	-1.514574	0.429250
Si	3.091997	3.159518	-0.546880
C	4.746234	3.847170	0.046062
H	5.544125	3.096496	0.035636
H	4.667567	4.240013	1.066764
H	5.065067	4.673711	-0.601892
C	3.237453	2.342358	-2.231445
H	3.872039	1.449131	-2.208912
H	3.656848	3.038663	-2.968074
H	2.249408	2.025027	-2.581769
C	1.802938	4.529523	-0.533705
H	1.638983	4.910522	0.481144
H	0.841197	4.178719	-0.924872
H	2.126147	5.373191	-1.155749
Al	-7.289135	-0.717976	-0.692480
C	-6.229547	-0.962690	-2.323184
H	-6.406809	-0.144541	-3.035736
H	-6.492711	-1.893555	-2.841714
H	-5.154961	-0.979220	-2.108582
C	-9.140317	-1.307843	-0.419958
H	-9.274037	-2.367049	-0.675773

H	-9.465877	-1.167934	0.616958
H	-9.833402	-0.744959	-1.060495

Requested basis set is 6-31G(d)
There are 252 shells and 676 basis functions



65-Int-III

E(B3LYP/6-31G*) = –2118.98074 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	2.657834	3.510074	-1.901744
C	4.153175	3.672752	0.208735
C	1.877464	2.457144	0.371375
C	3.403642	2.374791	0.605290
C	1.584174	2.763365	-1.116014
C	3.573894	4.393498	-1.039423
H	3.000045	5.271033	-0.720157
H	3.246374	2.744181	-2.427372
H	4.150374	4.372519	1.052025
C	1.179291	1.129972	0.760253
C	1.858261	-0.107996	0.202161
C	4.021642	1.152147	-0.108625

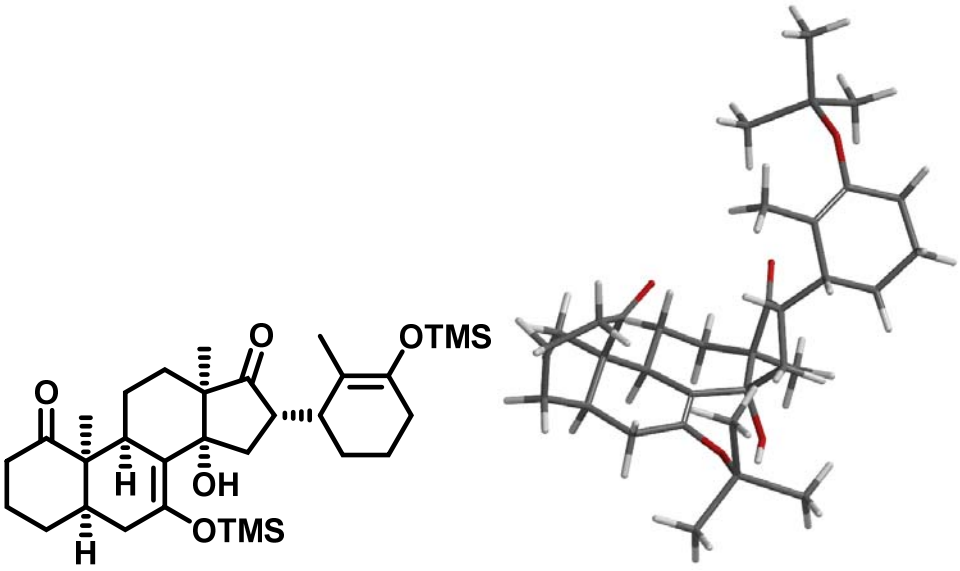
H	4.322088	1.400830	-1.136693
H	4.963485	0.905720	0.401977
C	3.149568	-0.075182	-0.164457
C	0.912247	0.919798	2.271601
H	0.095384	1.576577	2.587832
H	1.795420	1.198782	2.860307
C	0.954020	-1.347671	0.161669
C	-0.039688	-1.314708	1.372787
C	0.545140	-0.551785	2.576827
H	1.439755	-1.102892	2.892179
H	-0.166189	-0.592018	3.408394
C	-1.314589	-0.657468	0.809855
C	0.022219	-1.354872	-1.099197
H	-0.158652	-2.407394	-1.340409
H	0.510250	-0.896260	-1.964707
C	-1.289434	-0.636787	-0.724286
H	-1.193421	0.418474	-1.002734
O	-2.202846	-0.207634	1.509653
O	0.529616	2.455655	-1.643178
C	-0.435506	-2.740681	1.821369
H	-1.216699	-2.671107	2.585645
H	0.434787	-3.255684	2.235783
H	-0.811623	-3.347615	0.993376
O	1.704942	-2.557850	0.227713
H	2.427217	-2.447350	-0.414106
O	3.779764	-1.176841	-0.734572
C	-2.577064	-1.166654	-1.429281
C	-4.275885	-3.043055	-1.578399
C	-5.007353	-0.695885	-1.031412
C	-5.381342	-2.156634	-1.001191
C	-3.766033	-0.224764	-1.259026
C	-2.920440	-2.609750	-1.017314
H	-4.266581	-2.952164	-2.673329
H	-5.608959	-2.455209	0.035501
H	-2.959512	-2.673878	0.078333
H	-4.470623	-4.098071	-1.348809

H	-6.317762	-2.279204	-1.561924
H	-2.134990	-3.297819	-1.351938
C	-3.514929	1.257194	-1.395187
H	-3.075328	1.685361	-0.483249
H	-4.444799	1.791462	-1.607261
H	-2.815076	1.470407	-2.214174
H	-2.313439	-1.178939	-2.502291
H	0.198747	1.207400	0.284344
H	3.543469	2.217633	1.682692
H	5.207193	3.419082	0.039609
H	2.155773	4.089201	-2.683864
C	1.248461	3.629748	1.169226
H	1.604036	4.605934	0.827190
H	1.488349	3.543121	2.233878
H	0.159186	3.617886	1.059179
O	-6.083154	0.136004	-0.854461
H	4.386947	4.783136	-1.661924
Si	5.167581	-1.994710	-0.177413
C	4.939272	-3.754772	-0.797760
H	4.076579	-4.238697	-0.325313
H	5.824197	-4.363688	-0.575648
H	4.786974	-3.776954	-1.883219
C	5.217267	-1.936632	1.703475
H	4.262623	-2.285557	2.112969
H	5.399882	-0.927232	2.089457
H	6.010586	-2.587177	2.091662
C	6.713346	-1.240451	-0.949314
H	6.911795	-0.226802	-0.584268
H	6.618874	-1.191932	-2.040435
H	7.594271	-1.853086	-0.719691
Al	-6.675341	0.910653	0.578479
C	-8.233580	2.062044	0.271608
H	-9.162643	1.543981	0.548163
H	-8.325559	2.347579	-0.782505
H	-8.197527	2.980276	0.871219
C	-5.822929	0.535871	2.303318

H	-6.286178	-0.333591	2.791159
H	-5.918196	1.376955	3.001680
H	-4.757036	0.309664	2.182275

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



62-DAM

E(B3LYP/6-31G*) = –2205.95925 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	-2.534117	2.737414	2.071851
C	-4.727561	3.150377	0.764489
C	-2.564855	2.542828	-0.541352
C	-4.057721	2.208856	-0.269280
C	-1.768129	2.473403	0.775912
C	-3.786983	3.610856	1.909746
H	-3.463178	4.642047	1.726139
H	-2.799888	1.750574	2.478682
H	-5.124139	4.034925	0.254461
C	-2.042059	1.538458	-1.614960

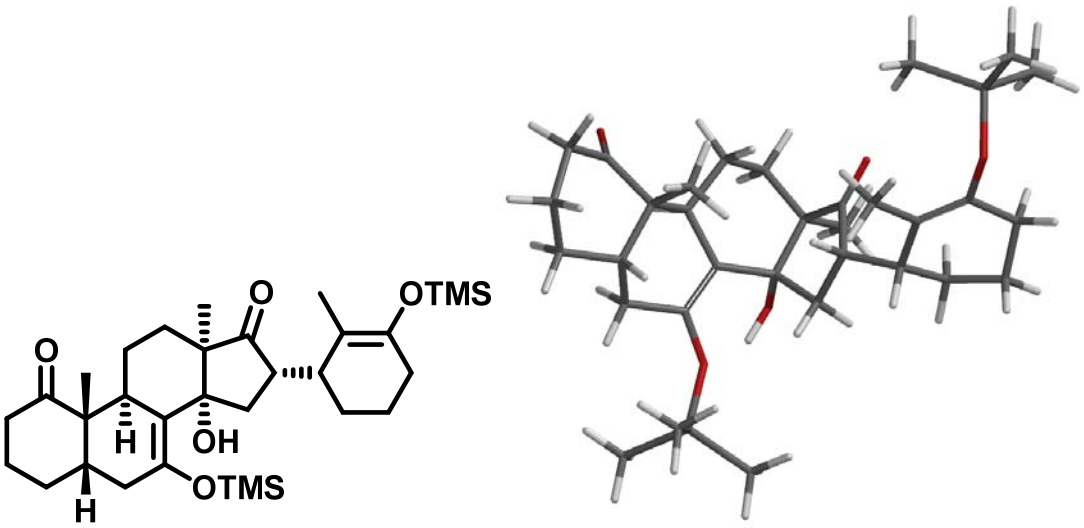
C	-2.151609	0.087560	-1.126530
C	-4.255022	0.728793	0.137420
H	-4.282892	0.635875	1.233580
H	-5.250616	0.404061	-0.197038
C	-3.225680	-0.238332	-0.382268
C	-0.678099	1.879472	-2.239913
H	0.082918	2.016131	-1.467988
H	-0.759127	2.829166	-2.779942
C	-1.208330	-1.036996	-1.617690
C	-0.000954	-0.542942	-2.479173
C	-0.245668	0.781974	-3.211009
H	-1.009546	0.631201	-3.986546
H	0.683792	1.073947	-3.711983
C	1.155199	-0.373481	-1.465828
C	-0.504492	-1.758264	-0.425856
H	-0.239792	-2.763061	-0.773267
H	-1.157207	-1.867427	0.440968
C	0.753578	-0.937148	-0.106659
H	0.435420	-0.052405	0.463596
O	2.219324	0.142115	-1.751654
O	-0.572517	2.241589	0.813784
C	0.452594	-1.621212	-3.489948
H	1.382268	-1.289651	-3.963690
H	-0.315522	-1.764666	-4.253283
H	0.633091	-2.590523	-3.015148
O	-1.968105	-1.961117	-2.407478
H	-2.709540	-2.228878	-1.837630
O	-3.495624	-1.567287	-0.103186
C	1.863819	-1.663819	0.704897
C	3.736159	-3.378821	0.566892
C	4.242585	-0.972939	1.069604
C	4.797221	-2.275993	0.550096
C	2.933348	-0.700198	1.207040
C	2.445939	-2.863760	-0.071996
H	3.539840	-3.682078	1.604776
H	2.666190	-2.559743	-1.104062

H	5.655292	-2.548369	1.178343
H	1.701655	-3.667103	-0.128123
C	2.455026	0.538692	1.923166
H	2.107719	1.322788	1.239386
H	3.250847	0.960034	2.542254
H	1.605885	0.301056	2.579387
H	1.347269	-2.062157	1.597270
H	-4.574332	2.344343	-1.228681
H	-5.602750	2.634805	1.179128
H	-1.828440	3.172013	2.787548
C	-2.441677	3.994651	-1.070494
H	-2.918558	4.719119	-0.404935
H	-2.925346	4.076890	-2.051538
H	-1.394657	4.287265	-1.181040
H	-2.757462	1.634169	-2.450916
O	5.214642	-0.091274	1.508753
H	5.194628	-2.147586	-0.468290
H	4.098568	-4.268872	0.037661
H	-4.332591	3.639793	2.859540
Si	-4.185926	-2.386800	1.211966
Si	5.988149	1.080799	0.571562
C	4.743578	2.320610	-0.104258
H	5.226948	3.023320	-0.794872
H	4.277955	2.903254	0.698625
H	3.949538	1.800059	-0.651840
C	6.914522	0.284453	-0.870020
H	7.500806	1.039472	-1.409649
H	6.224233	-0.167071	-1.592294
H	7.605977	-0.494704	-0.529219
C	7.203447	1.876286	1.769198
H	7.770788	2.680922	1.285196
H	7.922315	1.139740	2.146598
H	6.682856	2.305792	2.632746
C	-6.059539	-2.175024	1.224535
H	-6.492068	-2.439850	0.252444
H	-6.367231	-1.150997	1.461434

H	-6.508790	-2.836662	1.976075
C	-3.435829	-1.790846	2.837991
H	-2.340804	-1.830673	2.812644
H	-3.770852	-2.431981	3.663144
H	-3.730512	-0.764143	3.084030
C	-3.737327	-4.181926	0.885328
H	-2.651309	-4.326578	0.895763
H	-4.109011	-4.511356	-0.091720
H	-4.171711	-4.842302	1.645532

Requested basis set is 6-31G(d)

There are 262 shells and 697 basis functions



63-DAM

E(B3LYP/6-31G*) = –2205.95896 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
H	-3.894766	5.487491	0.075406
C	-3.291496	4.733246	0.589305
C	-4.674144	2.743686	1.268061

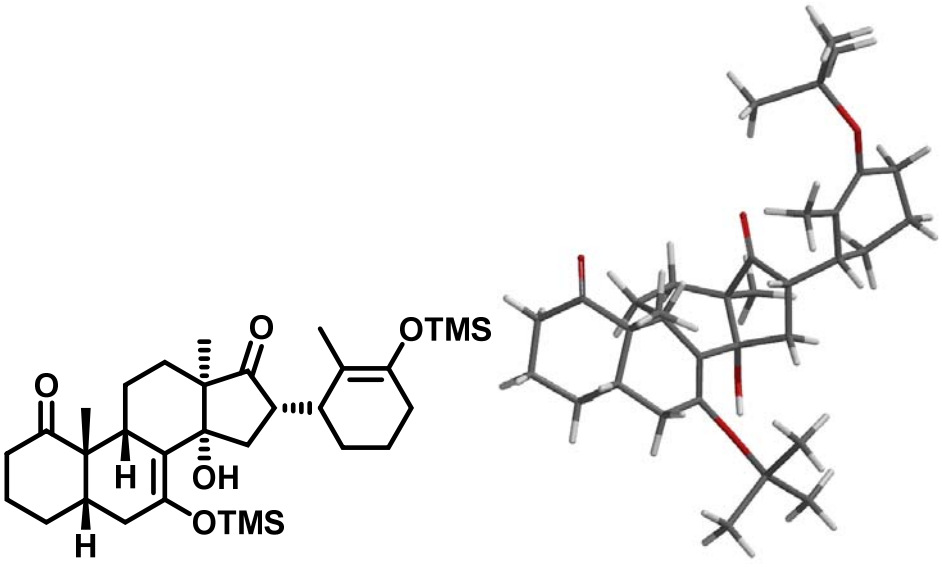
C	-2.404807	2.340956	0.019752
C	-3.588996	1.720285	0.873521
C	-2.867783	3.724882	-0.480617
C	-4.071549	4.069109	1.747447
H	-4.857986	4.744615	2.102269
H	-2.393250	5.245976	0.958997
H	-5.315782	2.303692	2.042366
C	-2.032562	1.428219	-1.205000
C	-2.065780	-0.069377	-0.876296
C	-4.222098	0.504663	0.176607
H	-4.963185	0.056906	0.846671
H	-4.776929	0.840643	-0.714175
C	-3.171192	-0.489731	-0.232644
C	-0.737872	1.865008	-1.914680
H	0.085726	1.985931	-1.202249
H	-0.905139	2.842875	-2.373211
C	-1.089034	-1.112623	-1.465418
C	0.059512	-0.498678	-2.323916
C	-0.302723	0.846960	-2.967388
H	-1.100911	0.686676	-3.704389
H	0.575044	1.222529	-3.504930
C	1.228041	-0.331300	-1.331162
C	-0.326016	-1.886083	-0.347524
H	-0.029388	-2.852830	-0.768655
H	-0.954866	-2.081613	0.524223
C	0.908404	-1.035569	-0.009472
H	0.578426	-0.223290	0.655177
O	2.246778	0.281768	-1.589345
O	-2.929902	4.019674	-1.660453
C	0.545784	-1.483849	-3.412976
H	1.438792	-1.067737	-3.890607
H	-0.236922	-1.624524	-4.161546
H	0.796988	-2.468818	-3.007284
O	-1.822323	-2.012564	-2.304673
H	-2.551919	-2.342333	-1.752387
C	-1.197832	2.558951	0.968114

H	-1.501233	3.069637	1.886551
H	-0.401247	3.150294	0.507461
H	-0.777741	1.589622	1.258001
H	-5.325090	2.940361	0.402262
H	-3.138801	1.346927	1.803256
O	-3.415300	-1.836143	-0.054485
C	2.089113	-1.765137	0.692467
C	4.026078	-3.373323	0.349267
C	4.450404	-0.989628	1.012925
C	5.040531	-2.227858	0.385214
C	3.136692	-0.788731	1.218668
C	2.693865	-2.866258	-0.202918
H	3.880369	-3.766974	1.364798
H	5.400034	-2.008344	-0.631632
H	2.864228	-2.463920	-1.210467
H	4.404369	-4.201398	-0.262423
H	5.928245	-2.507052	0.967316
H	1.983326	-3.694837	-0.304971
C	2.639843	0.384013	2.027962
H	2.246764	1.194919	1.399991
H	3.442615	0.800732	2.640747
H	1.827609	0.073985	2.701173
H	1.635593	-2.258634	1.571151
H	-2.832717	1.606763	-1.939601
O	5.397110	-0.092809	1.472316
H	-3.417282	3.880365	2.606921
Si	6.103645	1.158127	0.582896
Si	-4.338897	-2.741315	1.044147
C	-6.145461	-2.747560	0.508684
H	-6.591703	-1.747165	0.527640
H	-6.742034	-3.388922	1.169632
H	-6.247033	-3.137832	-0.510786
C	-4.143783	-2.070267	2.796624
H	-4.597124	-1.081482	2.928591
H	-3.086423	-1.995000	3.076171
H	-4.625822	-2.747990	3.512534

C	-3.604617	-4.466197	0.918704
H	-2.558953	-4.472699	1.246708
H	-3.634191	-4.840455	-0.110978
H	-4.157328	-5.175938	1.546179
C	7.331289	1.922916	1.786973
H	6.827554	2.280043	2.692404
H	7.851815	2.775786	1.333896
H	8.088870	1.192067	2.092420
C	4.795264	2.392543	0.026648
H	4.334441	2.902500	0.880334
H	4.004935	1.881017	-0.534720
H	5.232855	3.158490	-0.626121
C	7.005774	0.485258	-0.934515
H	7.579329	1.286143	-1.418988
H	6.305882	0.091208	-1.680456
H	7.707490	-0.314325	-0.670653

Requested basis set is 6-31G(d)

There are 262 shells and 697 basis functions



64-DAM

E(B3LYP/6-31G*) = –2205.96105 au

Cartesian Coordinates (Angstroms)

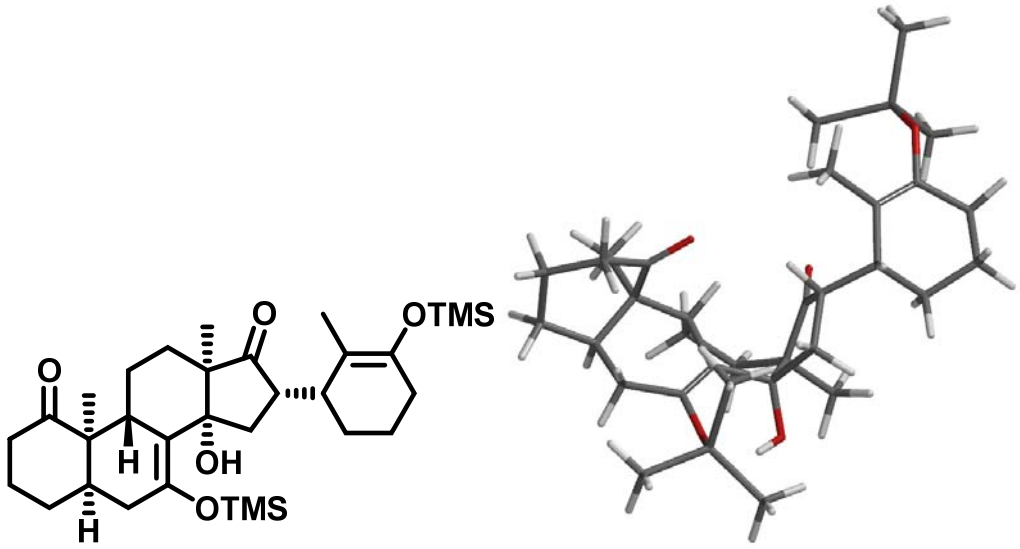
Atom	X	Y	Z
H	-3.084370	4.321238	-1.505804
C	-3.373934	4.489603	-0.459895
C	-4.808906	2.419195	-0.225067
C	-2.393751	2.319204	0.730122
C	-3.886341	1.899456	0.890098
C	-2.296502	3.832741	0.404917
C	-4.795060	3.949596	-0.249665
H	-5.457227	4.335462	-1.034029
H	-3.307863	5.568565	-0.288375
H	-5.830568	2.065511	-0.034633
C	-1.632276	1.495391	-0.385912
C	-2.067572	0.040207	-0.481624
C	-4.012607	0.381597	1.097076
H	-3.781069	0.123624	2.141566
H	-5.056648	0.082420	0.941433
C	-3.141200	-0.427743	0.177952
C	-1.597696	2.080941	-1.818742
H	-1.267226	3.123804	-1.785106
H	-2.607211	2.073994	-2.242737
C	-1.260371	-0.884201	-1.421769
C	-0.202927	-0.091159	-2.241917
C	-0.640550	1.295555	-2.747557
H	-1.113392	1.176812	-3.728073
H	0.278881	1.869986	-2.909643
C	1.008658	-0.020053	-1.288716
C	-0.383343	-1.870751	-0.591687
H	-0.118409	-2.711137	-1.241478
H	-0.923035	-2.273094	0.268627
C	0.861856	-1.067464	-0.175346
H	0.596054	-0.485738	0.717499
O	1.936064	0.755021	-1.420602
O	-1.354284	4.494501	0.801514
C	0.284476	-0.912498	-3.465527

H	1.047741	-0.336941	-4.000216
H	-0.558604	-1.106257	-4.131974
H	0.721962	-1.875925	-3.188149
O	-2.121454	-1.562239	-2.331701
H	-2.837293	-1.931150	-1.785008
C	-1.653212	2.073973	2.064502
H	-2.190205	2.528017	2.905549
H	-0.657679	2.521479	2.028896
H	-1.549759	1.001944	2.261978
H	-4.517250	2.008478	-1.199928
H	-4.243123	2.376608	1.815738
O	-3.540156	-1.743725	-0.011838
C	2.135656	-1.892548	0.173818
C	4.067002	-3.248987	-0.746552
C	4.495671	-1.163882	0.592487
C	5.072709	-2.150750	-0.393097
C	3.189972	-1.063016	0.902079
C	2.708291	-2.619293	-1.056269
H	3.966453	-3.942069	0.100149
H	5.399107	-1.628345	-1.305141
H	2.835267	-1.897332	-1.873185
H	4.426175	-3.837056	-1.599809
H	5.981380	-2.577247	0.051806
H	2.003226	-3.383116	-1.405289
C	2.718601	-0.181468	2.031976
H	2.261117	0.750596	1.673865
H	3.550489	0.086414	2.686505
H	1.963129	-0.700779	2.638823
H	1.779497	-2.661239	0.883687
H	-0.585545	1.522171	-0.050994
O	5.450699	-0.409644	1.246282
H	-5.193107	4.323030	0.704339
Si	6.085482	1.072063	0.736368
Si	-4.067957	-2.944695	1.067443
C	-4.065245	-4.500094	0.014070
H	-4.750060	-4.403099	-0.836688

H	-4.385455	-5.371058	0.598731
H	-3.067276	-4.714028	-0.384845
C	-5.812609	-2.593936	1.692518
H	-6.504241	-2.406716	0.862966
H	-5.854198	-1.732812	2.368016
H	-6.189668	-3.464134	2.245133
C	-2.870159	-3.081511	2.515782
H	-2.754090	-2.128271	3.044330
H	-1.876388	-3.403955	2.185627
H	-3.233451	-3.817447	3.243998
C	4.703206	2.313297	0.434069
H	3.937799	1.893169	-0.229018
H	5.091554	3.226447	-0.034747
H	4.210678	2.604936	1.368865
C	7.099316	0.854477	-0.843376
H	6.472065	0.580231	-1.699658
H	7.866429	0.080211	-0.724886
H	7.608852	1.792159	-1.100167
C	7.207765	1.590746	2.154901
H	7.996053	0.848364	2.324157
H	6.642542	1.696815	3.087848
H	7.692141	2.552251	1.944954

Requested basis set is 6-31G(d)

There are 262 shells and 697 basis functions



65-DAM

E(B3LYP/6-31G*) = –1605.26336 au

Cartesian Coordinates (Angstroms)

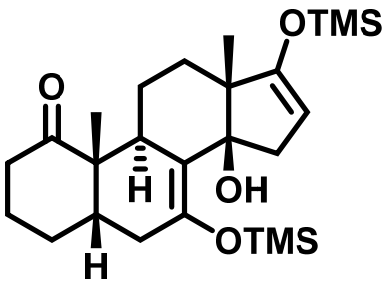
Atom	X	Y	Z
C	-3.057940	3.070458	1.857198
C	-4.405259	3.551779	-0.309775
C	-2.096215	2.405509	-0.493074
C	-3.600419	2.344255	-0.850496
C	-1.936443	2.421380	1.044644
C	-3.937166	4.064151	1.080291
H	-3.373286	4.995450	0.955857
H	-3.667514	2.243813	2.249222
H	-4.354956	4.378456	-1.026733
C	-1.333762	1.191549	-1.085433
C	-2.031070	-0.140179	-0.862167
C	-4.222848	1.015619	-0.372499
H	-4.557359	1.101660	0.671869
H	-5.139708	0.823083	-0.947187
C	-3.324948	-0.184432	-0.507507
C	-0.926267	1.325427	-2.573393
H	-0.123522	2.064673	-2.656365

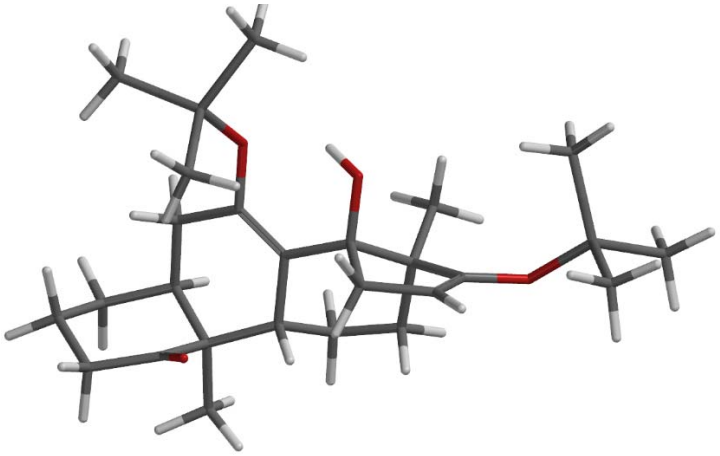
H	-1.768916	1.698846	-3.169311
C	-1.167385	-1.392537	-1.107550
C	-0.009756	-1.048721	-2.100454
C	-0.452127	-0.024892	-3.158324
H	-1.269325	-0.498575	-3.715444
H	0.365233	0.143558	-3.867134
C	1.132151	-0.563798	-1.190707
C	-0.408598	-1.846125	0.181027
H	-0.182453	-2.910254	0.054045
H	-1.027049	-1.743137	1.077924
C	0.877864	-0.999274	0.262415
H	0.635909	-0.078060	0.805527
O	2.087738	0.078360	-1.585633
O	-0.956660	1.964621	1.606383
C	0.508032	-2.317558	-2.819194
H	1.394417	-2.058798	-3.408149
H	-0.266799	-2.708093	-3.483256
H	0.780040	-3.116733	-2.123465
O	-1.924871	-2.459884	-1.665835
H	-2.811938	-2.413797	-1.267423
O	-3.975405	-1.399358	-0.313647
C	2.088767	-1.654216	0.994677
C	3.976442	-3.339020	0.818822
C	4.473061	-0.892739	1.102459
C	5.017752	-2.228260	0.659814
C	3.172971	-0.632374	1.329940
C	2.641587	-2.874844	0.234406
H	3.849960	-3.575825	1.884218
H	5.362328	-2.177619	-0.384022
H	2.800554	-2.606456	-0.818342
H	4.317216	-4.257438	0.325229
H	5.912142	-2.438805	1.261450
H	1.909053	-3.690808	0.250855
C	2.730483	0.651816	1.985942
H	2.285646	1.361211	1.276620
H	3.573321	1.148116	2.472009

H	1.965297	0.450140	2.748092
H	1.672398	-2.013892	1.952588
H	-0.401555	1.168301	-0.514184
H	-3.665565	2.351297	-1.946343
H	-5.462908	3.263690	-0.266252
H	-2.601074	3.538474	2.735987
C	-1.441128	3.723019	-0.987876
H	-1.835391	4.606234	-0.477893
H	-1.611646	3.857608	-2.060444
H	-0.361019	3.696632	-0.810941
O	5.455915	0.044246	1.372823
H	-4.804283	4.330116	1.695597
Si	6.089971	1.146136	0.260038
Si	-4.773089	-1.997495	1.063571
C	-3.806510	-1.534549	2.612781
H	-3.628828	-0.454963	2.681080
H	-2.829065	-2.029033	2.633400
H	-4.353439	-1.837090	3.514338
C	-6.531781	-1.320554	1.149439
H	-6.557258	-0.245579	1.359592
H	-7.092880	-1.825802	1.945812
H	-7.066504	-1.491882	0.208146
C	-4.804339	-3.854239	0.784517
H	-5.302370	-4.370061	1.614312
H	-3.789881	-4.259713	0.697840
H	-5.344449	-4.106330	-0.135557
C	7.406943	2.070517	1.236909
H	6.972137	2.585076	2.101391
H	7.902087	2.824199	0.612518
H	8.176255	1.384306	1.609461
C	4.750249	2.300377	-0.384085
H	4.377369	2.968975	0.400120
H	3.904169	1.723016	-0.775047
H	5.141169	2.922343	-1.199334
C	6.871188	0.243218	-1.204857
H	7.382109	0.958925	-1.861952

H	6.111330	-0.268460	-1.806863
H	7.609567	-0.500426	-0.884060

Requested basis set is 6-31G(d)
There are 262 shells and 697 basis functions





66-DA

E(B3LYP/6-31G*) = –1857.96031 au

Cartesian Coordinates (Angstroms)

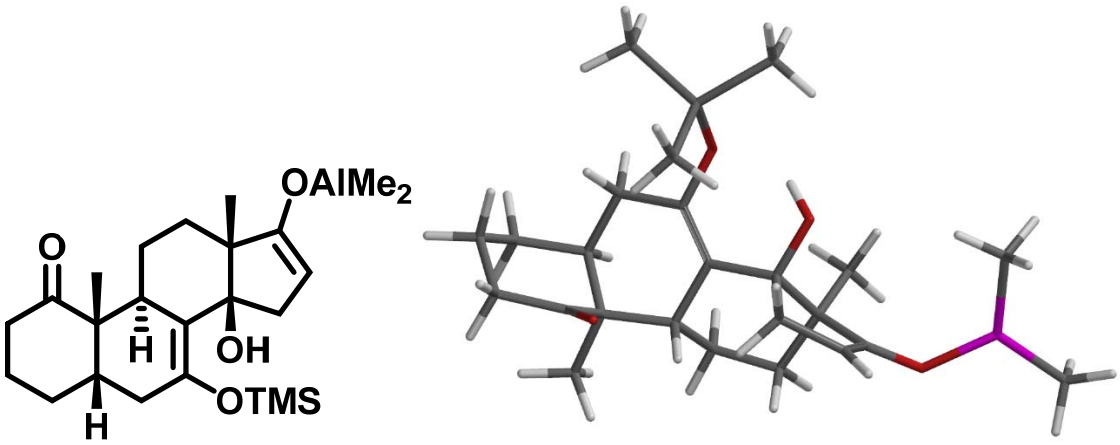
Atom	X	Y	Z
C	0.750258	-0.218180	0.148447
C	3.045480	0.154710	1.148164
C	2.555042	-2.074461	0.018402
C	3.290904	-1.363977	1.187895
C	1.046665	-1.707540	-0.003595
C	1.675845	0.588350	0.697608
H	3.783967	0.644058	0.496199
H	2.853439	-1.750565	2.118540
H	3.223059	0.578751	2.145478
H	0.703850	-2.010090	-1.001037
C	0.147485	-2.454810	1.010163
H	0.361503	-2.112862	2.031162
H	0.330614	-3.534384	0.988649

C	-1.321622	-2.215647	0.640085
H	-1.983893	-2.734500	1.344317
H	-1.495059	-2.678971	-0.339561
C	-1.743933	-0.718009	0.571310
C	-0.684347	0.175758	-0.208765
C	-2.036451	-0.186767	1.980135
H	-1.150934	-0.262296	2.622628
H	-2.839591	-0.770841	2.441287
H	-2.343594	0.860546	1.946433
C	-2.930621	-0.610766	-0.379321
C	-2.569828	-0.277005	-1.625207
H	-3.233503	-0.235185	-2.482082
C	-1.086197	-0.011711	-1.704843
H	-0.542144	-0.832426	-2.191480
H	-0.834502	0.904558	-2.249444
C	3.233114	-1.634770	-1.301876
C	4.802768	-1.671821	1.198447
H	4.957511	-2.739459	1.393818
H	5.276329	-1.139210	2.033746
C	5.496800	-1.275838	-0.116769
H	5.573000	-0.184026	-0.181219
C	4.754120	-1.792995	-1.368139
H	4.967296	-2.862673	-1.502849
H	5.096818	-1.289450	-2.276902
O	2.608502	-1.215118	-2.258962
O	-4.163611	-0.960684	0.089809
O	-0.978351	1.549679	0.058527
H	-0.344942	1.856385	0.728921
O	1.460088	1.941983	0.949207
C	2.720085	-3.614404	0.119681
H	3.742733	-3.943607	-0.077205
H	2.067156	-4.119609	-0.600906
H	2.458142	-3.968503	1.121769
Si	2.048501	3.237671	0.006108
C	2.107842	2.734010	-1.804752
H	2.603990	3.504844	-2.407451

H	1.093456	2.598382	-2.194974
H	2.641628	1.789284	-1.958607
C	3.757767	3.740152	0.630647
H	3.741076	3.931951	1.709787
H	4.087195	4.661804	0.134282
H	4.517713	2.974399	0.438403
C	0.821951	4.625775	0.318175
H	0.753413	4.861000	1.386900
H	-0.177692	4.345652	-0.031580
H	1.120250	5.542716	-0.204733
Si	-5.603340	-0.088943	-0.089338
C	-6.217138	-0.125586	-1.873783
H	-7.225746	0.303098	-1.936254
H	-6.267510	-1.151052	-2.258216
H	-5.571717	0.454379	-2.542638
C	-6.818308	-0.994301	1.025156
H	-6.481218	-0.991470	2.067929
H	-6.933345	-2.039456	0.715210
H	-7.809588	-0.525572	0.992553
C	-5.317007	1.686498	0.472595
H	-5.113436	1.731362	1.548777
H	-6.190059	2.318399	0.267677
H	-4.454391	2.121237	-0.045169
H	6.528895	-1.646589	-0.122750

Requested basis set is 6-31G(d)

There are 210 shells and 557 basis functions



66-Int-I

E(B3LYP/6-31G*) = –1770.97860 au

Cartesian Coordinates (Angstroms)

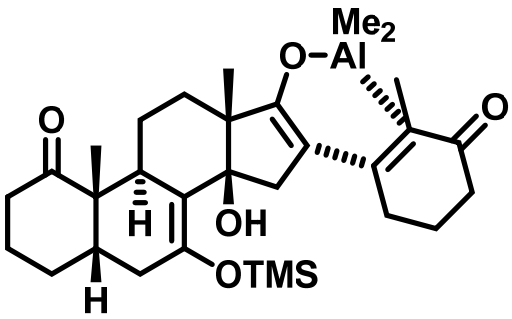
Atom	X	Y	Z
C	0.475548	-0.310530	0.046254
C	2.728041	0.048096	1.144818
C	2.287251	-2.158368	-0.059050
C	2.986807	-1.469843	1.145727
C	0.778993	-1.796156	-0.120304
C	1.378819	0.488133	0.642030
H	3.493856	0.568917	0.551850
H	2.530459	-1.885732	2.054282
H	2.850829	0.436848	2.164777
H	0.468370	-2.082090	-1.132824
C	-0.151716	-2.562048	0.850109
H	0.031808	-2.241896	1.884101
H	0.031121	-3.641231	0.811526
C	-1.609908	-2.312393	0.441397
H	-2.292332	-2.842505	1.117825
H	-1.758092	-2.757000	-0.550536
C	-2.026927	-0.813155	0.384648
C	-0.945335	0.085826	-0.355698
C	-2.348409	-0.301752	1.794589
H	-1.478410	-0.383885	2.456970

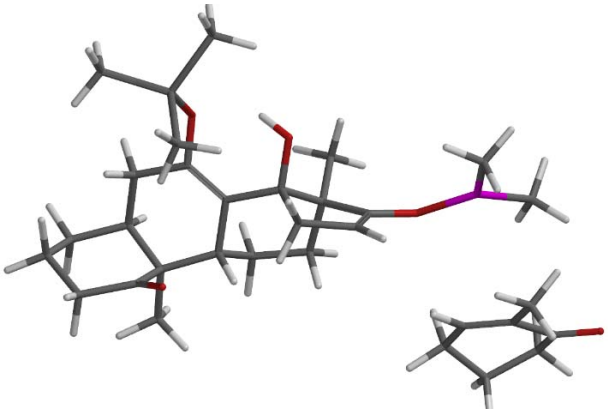
H	-3.156853	-0.895587	2.235968
H	-2.651984	0.748005	1.771969
C	-3.193127	-0.678179	-0.593745
C	-2.789931	-0.343572	-1.826724
H	-3.437404	-0.271371	-2.695480
C	-1.302204	-0.093862	-1.864551
H	-0.746104	-0.914545	-2.337402
H	-1.028304	0.823490	-2.396746
C	3.000088	-1.695027	-1.352873
C	4.501540	-1.762748	1.187484
H	4.663292	-2.832769	1.363918
H	4.948196	-1.243427	2.045700
C	5.223902	-1.332333	-0.101046
H	5.282178	-0.238344	-0.146085
C	4.523110	-1.841875	-1.378354
H	4.748836	-2.908413	-1.517484
H	4.887364	-1.325787	-2.271569
O	2.400247	-1.266663	-2.321855
O	-4.452482	-0.971581	-0.179784
O	-1.249603	1.458380	-0.085517
H	-0.638814	1.759336	0.608378
O	1.150779	1.837431	0.906694
C	2.454887	-3.699608	0.018304
H	3.485823	-4.021200	-0.145750
H	1.831884	-4.192394	-0.736600
H	2.156181	-4.074705	1.002369
Si	1.764009	3.151510	0.005469
C	1.871750	2.684987	-1.812790
H	2.382710	3.468460	-2.386099
H	0.868398	2.555829	-2.232781
H	2.411438	1.744290	-1.970506
C	3.455119	3.644076	0.684714
H	3.413989	3.799771	1.769026
H	3.786965	4.584288	0.226306
H	4.225826	2.891483	0.483355
C	0.525750	4.530358	0.312814

H	0.426873	4.744282	1.383616
H	-0.462952	4.254404	-0.070217
H	0.834884	5.458240	-0.183719
H	6.262091	-1.685283	-0.084659
Al	-5.727035	0.161133	0.160413
C	-5.382757	2.074088	-0.089293
H	-4.312559	2.263795	-0.228467
H	-5.730812	2.665865	0.767396
H	-5.905493	2.464369	-0.973207
C	-7.382882	-0.667597	0.802879
H	-7.525806	-1.670364	0.383573
H	-8.268567	-0.067396	0.560876
H	-7.364653	-0.779221	1.896002

Requested basis set is 6-31G(d)

There are 200 shells and 536 basis functions





66-Complex-Int-I

E(B3LYP/6-31G*) = –2118.96940 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	2.024208	-0.053127	-0.363898
C	4.470368	0.113829	-0.990373
C	3.299349	2.193369	-0.102708
C	4.353935	1.643203	-1.103803

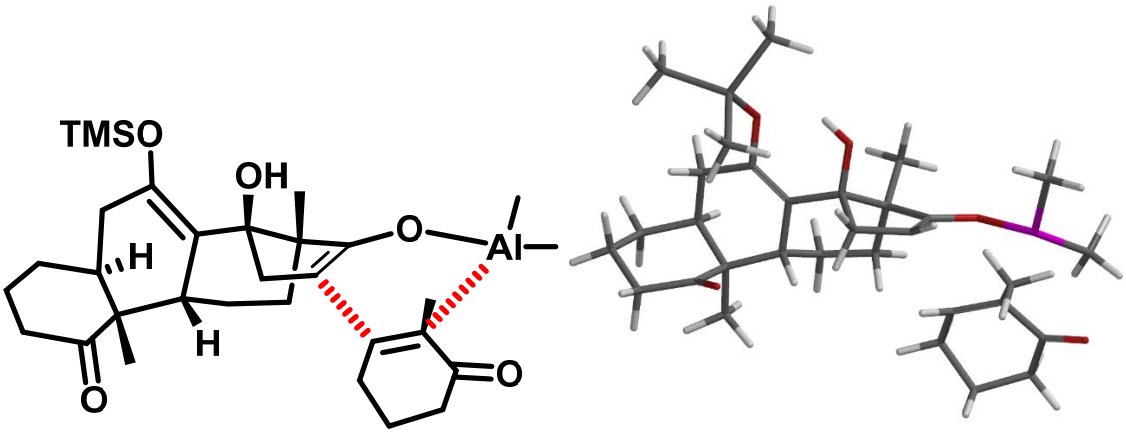
C	1.933477	1.467166	-0.256248
C	3.187915	-0.626032	-0.718871
H	5.186313	-0.158691	-0.201053
H	3.988337	1.878667	-2.112611
H	4.901854	-0.289581	-1.916488
H	1.397853	1.693734	0.674410
C	1.021515	1.954263	-1.407164
H	1.433337	1.646659	-2.377176
H	0.942547	3.046303	-1.423544
C	-0.385263	1.380283	-1.201179
H	-1.054670	1.712096	-2.005167
H	-0.785192	1.809078	-0.272885
C	-0.448489	-0.172268	-1.108263
C	0.689820	-0.776563	-0.176528
C	-0.435314	-0.781688	-2.516095
H	0.478339	-0.508710	-3.059090
H	-1.291599	-0.414002	-3.091230
H	-0.488222	-1.871585	-2.470023
C	0.076053	-0.681298	1.255906
H	0.365131	0.240769	1.778304
H	0.460839	-1.515360	1.852572
C	3.852203	1.986887	1.329014
C	5.733692	2.309221	-0.922583
H	5.660961	3.374410	-1.170955
H	6.441351	1.877514	-1.642455
C	6.290870	2.143395	0.502245
H	6.608036	1.105510	0.657953
C	5.263898	2.515356	1.593899
H	5.194276	3.609161	1.671917
H	5.572321	2.151385	2.578513
O	3.203856	1.469776	2.220545
O	-2.893963	-0.515688	-0.913205
O	0.766770	-2.181972	-0.434540
H	1.550869	-2.332029	-0.988656
O	3.342133	-1.996561	-0.911439
C	3.107840	3.722282	-0.292793

H	3.988057	4.297306	0.002339
H	2.263203	4.081191	0.306125
H	2.905196	3.958811	-1.341901
Si	4.030119	-3.098418	0.196829
C	3.604311	-2.585665	1.954583
H	4.167847	-3.180050	2.684097
H	2.536065	-2.734807	2.143030
H	3.823232	-1.527469	2.137868
C	5.901056	-3.159040	-0.055073
H	6.151753	-3.336483	-1.107314
H	6.336854	-3.977518	0.532100
H	6.398035	-2.233132	0.256331
C	3.274268	-4.752282	-0.276392
H	3.503314	-5.007606	-1.317888
H	2.184820	-4.730512	-0.164339
H	3.663953	-5.559109	0.356306
H	7.194869	2.752000	0.625159
C	-1.406515	-0.767949	0.994995
H	-2.137357	-0.988226	1.767591
C	-1.688236	-0.545222	-0.298528
Al	-4.320638	-1.508496	-0.766267
C	-4.287894	-3.077368	0.408228
H	-4.773717	-2.877577	1.371864
H	-3.258933	-3.389123	0.621716
H	-4.817332	-3.926029	-0.043194
C	-5.754883	-1.024928	-2.010873
H	-5.537616	-0.094763	-2.548316
H	-6.722962	-0.909104	-1.506945
H	-5.890406	-1.811255	-2.766543
C	-5.903755	0.740124	1.529854
C	-6.719027	2.357952	-0.305135
C	-4.314877	2.389780	0.453737
C	-5.543284	3.244663	0.119109
C	-4.660089	1.243134	1.365204
H	-6.472529	1.839281	-1.244167
H	-3.860039	1.982356	-0.462233

H	-5.828689	3.824838	1.006895
H	-7.633203	2.930814	-0.489845
H	-3.533620	3.000073	0.924560
H	-5.304893	3.967383	-0.669763
C	-7.038644	1.281342	0.725105
O	-8.171194	0.838963	0.860669
H	-3.834869	0.807572	1.928216
C	-6.239654	-0.350828	2.513900
H	-6.948204	0.016619	3.265468
H	-5.343706	-0.711048	3.028912
H	-6.732114	-1.196254	2.020848

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



66-TS2

E(B3LYP/6-31G*) = –2118.93653 au

v*ts* = 255*i* cm–1

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	1.753669	-0.018912	-0.420481
C	4.242878	0.137162	-0.845192
C	2.967652	2.268530	-0.282888
C	4.117366	1.645323	-1.123104

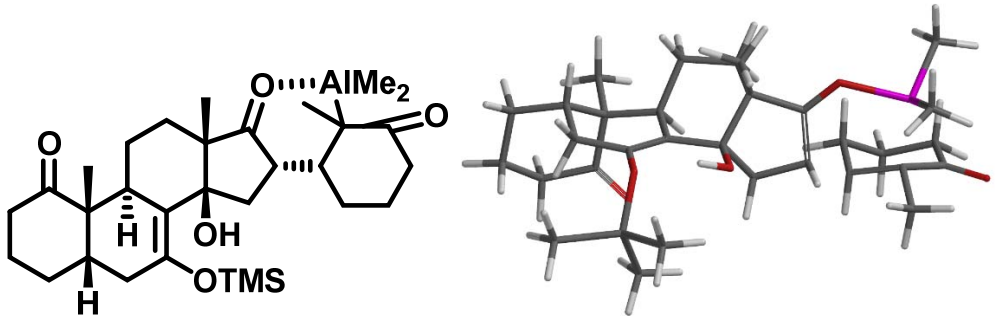
C	1.635108	1.498621	-0.493689
C	2.950038	-0.601062	-0.615184
H	4.886982	-0.037009	0.028564
H	3.844295	1.772978	-2.180057
H	4.762031	-0.347260	-1.682973
H	0.998364	1.819183	0.340554
C	0.855779	1.824603	-1.788473
H	1.375421	1.410504	-2.661864
H	0.773125	2.904603	-1.946013
C	-0.562995	1.259206	-1.657269
H	-1.157402	1.487286	-2.550443
H	-1.035193	1.793872	-0.828485
C	-0.626923	-0.271419	-1.394836
C	0.414493	-0.744858	-0.285755
C	-0.463994	-1.031938	-2.718733
H	0.491974	-0.781814	-3.193872
H	-1.271692	-0.759723	-3.404811
H	-0.496096	-2.110830	-2.557019
C	-0.354946	-0.508461	1.054289
H	-0.194756	0.501406	1.454932
H	0.018221	-1.211671	1.803728
C	3.384964	2.212562	1.206668
C	5.464681	2.359127	-0.882361
H	5.400451	3.392962	-1.242568
H	6.244125	1.875405	-1.485618
C	5.885739	2.348184	0.598416
H	6.204750	1.339362	0.886192
C	4.755485	2.799719	1.548556
H	4.661975	3.894012	1.510631
H	4.974900	2.539827	2.588343
O	2.663508	1.761815	2.077855
O	-3.046234	-0.730549	-1.385525
O	0.523217	-2.167409	-0.362902
H	1.357623	-2.374892	-0.817434
O	3.128209	-1.979419	-0.665394
C	2.769922	3.765088	-0.641577

H	3.603319	4.390658	-0.315822
H	1.861946	4.157366	-0.169139
H	2.674109	3.897917	-1.724005
Si	3.775492	-2.968464	0.567640
C	3.195517	-2.344079	2.242725
H	3.654222	-2.919363	3.056305
H	2.108254	-2.447803	2.323409
H	3.437850	-1.286649	2.399115
C	5.659557	-2.971641	0.452400
H	5.992619	-3.211628	-0.564080
H	6.079140	-3.730075	1.125608
H	6.101466	-2.007849	0.730879
C	3.102967	-4.676290	0.174239
H	3.409937	-5.005360	-0.825400
H	2.007984	-4.683312	0.212388
H	3.469077	-5.417391	0.895117
H	6.763796	2.989224	0.741186
C	-1.798217	-0.762276	0.667845
H	-2.432301	-1.410248	1.256755
C	-1.943499	-0.634658	-0.703092
Al	-4.723659	-1.125078	-0.759552
C	-4.846755	-3.008223	-0.178301
H	-4.093919	-3.324841	0.552586
H	-4.719441	-3.645279	-1.065190
H	-5.832878	-3.243963	0.240890
C	-6.019690	-0.412115	-2.067123
H	-5.697786	0.524364	-2.540640
H	-7.012226	-0.242773	-1.634038
H	-6.144971	-1.144571	-2.877866
C	-4.682406	0.100364	1.277413
C	-5.665330	2.319264	0.308558
C	-3.197417	2.052655	0.631791
C	-4.399323	2.993560	0.842121
C	-3.428120	0.759912	1.369761
H	-5.604192	2.222031	-0.784187
H	-3.113538	1.867143	-0.444994

H	-4.514728	3.225744	1.909219
H	-6.569118	2.895701	0.526758
H	-2.264606	2.521226	0.961504
H	-4.218843	3.944261	0.326250
C	-5.881520	0.925354	0.901470
O	-7.015467	0.518312	1.118492
H	-2.853384	0.622285	2.282368
C	-4.985703	-0.954185	2.343818
H	-5.123226	-0.479949	3.325351
H	-4.173035	-1.681229	2.437503
H	-5.903674	-1.496029	2.115302

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



66-Int-II

E(B3LYP/6-31G*) = –2118.98285 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	1.703927	0.094951	-0.424521
C	4.203710	0.028405	-0.779419
C	3.054781	2.298844	-0.564944
C	4.185530	1.490167	-1.263477
C	1.674927	1.595488	-0.696557
C	2.862017	-0.584350	-0.486344
H	4.821494	-0.071405	0.124626

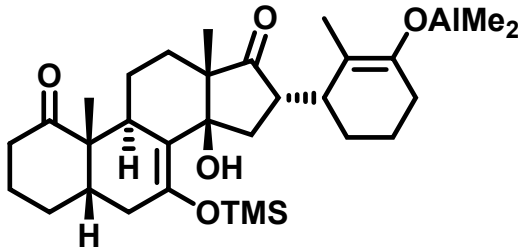
H	3.956339	1.485353	-2.338145
H	4.700122	-0.599150	-1.531593
H	1.065105	2.056758	0.088882
C	0.911367	1.819912	-2.023701
H	1.436318	1.333483	-2.855915
H	0.842419	2.884614	-2.267985
C	-0.524475	1.286338	-1.898682
H	-1.072195	1.417389	-2.839142
H	-1.046071	1.902716	-1.155150
C	-0.590181	-0.222674	-1.503227
C	0.325001	-0.530673	-0.251741
C	-0.312988	-1.114275	-2.718660
H	0.683048	-0.912422	-3.126646
H	-1.053113	-0.925487	-3.501840
H	-0.364070	-2.169978	-2.443233
C	-0.518429	-0.000541	0.938977
H	-0.447463	1.084142	1.039167
H	-0.161342	-0.442247	1.871669
C	3.427034	2.435064	0.932712
C	5.573772	2.137121	-1.067789
H	5.604518	3.107722	-1.576700
H	6.332441	1.515112	-1.560656
C	5.943499	2.312590	0.415715
H	6.167831	1.336027	0.861310
C	4.821136	2.982195	1.237389
H	4.807120	4.060446	1.027613
H	4.988935	2.873020	2.312774
O	2.655712	2.150832	1.830952
O	-2.976867	-0.627302	-1.620272
O	0.332631	-1.947781	-0.065539
H	1.170469	-2.287296	-0.428308
O	2.942205	-1.961283	-0.322344
C	2.966701	3.736245	-1.142350
H	3.846067	4.340262	-0.909760
H	2.093704	4.260502	-0.737041
H	2.873661	3.715841	-2.233262

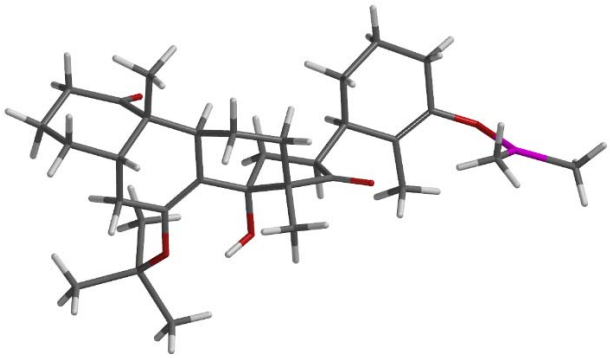
Si	3.509919	-2.779944	1.073345
C	3.030853	-1.797528	2.602252
H	3.468667	-2.243573	3.503592
H	1.942761	-1.783900	2.726391
H	3.364378	-0.754854	2.546709
C	5.379371	-2.999182	0.949293
H	5.657987	-3.456951	-0.007203
H	5.738221	-3.659462	1.749006
H	5.922574	-2.051676	1.039121
C	2.657853	-4.451396	0.995076
H	2.881049	-4.966497	0.053611
H	1.570348	-4.346192	1.076804
H	2.994815	-5.098919	1.813588
H	6.865100	2.899426	0.505280
C	-1.955465	-0.443614	0.590922
H	-2.026031	-1.508497	0.854733
C	-1.968693	-0.454598	-0.916017
Al	-4.831747	-0.911156	-0.971701
C	-5.128359	-2.838501	-1.321892
H	-4.332719	-3.490097	-0.937332
H	-5.218102	-3.037342	-2.398407
H	-6.064217	-3.178102	-0.857384
C	-5.824923	0.404132	-2.073959
H	-5.400674	1.417529	-2.061830
H	-6.873232	0.494601	-1.757836
H	-5.842558	0.083276	-3.125100
C	-4.491611	-0.478665	1.047155
C	-5.708411	1.826541	1.287596
C	-3.225335	1.773175	0.880933
C	-4.363178	2.474605	1.627539
C	-3.151451	0.284213	1.269029
H	-5.978846	2.062800	0.248843
H	-3.391798	1.876524	-0.201488
H	-4.178205	2.406833	2.709163
H	-6.520364	2.205765	1.915770
H	-2.274477	2.272671	1.107257

H	-4.381412	3.543996	1.381988
C	-5.715888	0.299198	1.422102
O	-6.764502	-0.250177	1.756603
H	-2.919741	0.251246	2.348798
C	-4.483142	-1.828566	1.798369
H	-4.207446	-1.689276	2.856083
H	-3.785347	-2.557099	1.370121
H	-5.478269	-2.276198	1.779641

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions





66-Int-III

E(B3LYP/6-31G*) = –2118.98285 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.941853	0.120605	0.423321
C	-4.415175	0.055483	0.939909
C	-3.394797	2.251170	0.157081

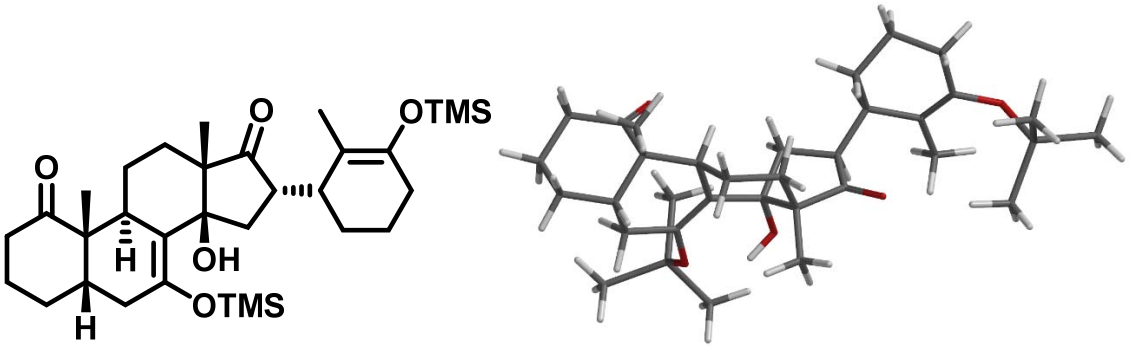
C	-4.430558	1.585247	1.106591
C	-1.976885	1.643156	0.346277
C	-3.062119	-0.563841	0.710809
H	-5.068023	-0.245839	0.108034
H	-4.116779	1.815161	2.134174
H	-4.853742	-0.412742	1.831442
H	-1.433890	1.932341	-0.560592
C	-1.154705	2.191272	1.538439
H	-1.604916	1.876565	2.488794
H	-1.138080	3.285786	1.539157
C	0.294910	1.699169	1.437086
H	0.889125	2.063342	2.283464
H	0.741021	2.152378	0.541609
C	0.430231	0.150116	1.380864
C	-0.538481	-0.474522	0.308543
C	0.290249	-0.451197	2.782067
H	-0.661281	-0.168763	3.245683
H	1.108013	-0.092520	3.414727
H	0.344515	-1.541883	2.744281
C	0.199253	-0.204458	-1.031062
H	0.064011	0.827467	-1.362527
H	-0.202013	-0.856123	-1.811442
C	-3.881103	2.019740	-1.295051
C	-5.854502	2.142202	0.897037
H	-5.878523	3.203045	1.173327
H	-6.546221	1.635592	1.582853
C	-6.352017	1.966511	-0.549032
H	-6.588942	0.911918	-0.732439
C	-5.322678	2.432583	-1.602410
H	-5.341180	3.529264	-1.670967
H	-5.566202	2.053102	-2.599095
O	-3.164191	1.563906	-2.167110
O	2.853215	-0.096629	1.412359
O	-0.492262	-1.899126	0.446968
H	-1.282058	-2.170631	0.945832
O	-3.091389	-1.947645	0.862458

C	-3.341570	3.784708	0.377265
H	-4.257631	4.286311	0.059283
H	-2.513094	4.225571	-0.188623
H	-3.195010	4.020929	1.435685
Si	-3.673830	-3.073026	-0.283953
C	-3.207146	-2.513808	-2.016739
H	-3.709251	-3.126467	-2.775455
H	-2.125851	-2.604236	-2.166269
H	-3.475530	-1.466307	-2.195582
C	-5.544619	-3.254070	-0.107905
H	-5.825943	-3.450967	0.933071
H	-5.899197	-4.099364	-0.711674
H	-6.090775	-2.363992	-0.441087
C	-2.830816	-4.679456	0.204237
H	-3.074150	-4.958711	1.236207
H	-1.741361	-4.591218	0.126414
H	-3.148151	-5.503872	-0.445972
H	-7.293921	2.510107	-0.690303
C	1.817109	-0.143008	0.777469
C	4.139914	-0.466518	-1.410679
C	5.213410	1.781557	-1.854527
C	2.718176	1.620446	-1.703601
C	3.890045	2.182797	-2.509828
H	5.410466	2.414049	-0.973232
H	2.784257	1.996528	-0.673238
H	3.851203	1.783794	-3.532919
H	6.056634	1.948298	-2.538433
H	1.769109	1.979016	-2.120090
H	3.817099	3.274384	-2.591721
C	5.225537	0.329549	-1.446043
C	4.270008	-1.941774	-1.119941
H	3.634217	-2.534379	-1.792453
H	3.967587	-2.186595	-0.092273
H	5.300742	-2.277413	-1.260933
C	1.677639	-0.506217	-0.707924
H	1.778809	-1.599270	-0.715041

C	2.740236	0.080773	-1.680019
H	2.427686	-0.271846	-2.679887
O	6.481475	-0.137265	-1.150182
Al	7.287632	-0.224807	0.383272
C	9.051209	-1.080085	0.309141
H	9.249534	-1.522199	-0.673541
H	9.152939	-1.872556	1.062165
H	9.851772	-0.355346	0.512532
C	6.431521	0.554461	1.964994
H	6.585115	1.642382	2.000150
H	6.831497	0.144994	2.900743
H	5.348563	0.383281	1.946863

Requested basis set is 6-31G(d)

There are 252 shells and 676 basis functions



66-DAM

E(B3LYP/6-31G*) = –2205.95925 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C	-2.172878	0.075384	0.454813
C	-4.648194	0.004654	0.966222
C	-3.639936	2.182010	0.105513
C	-4.686796	1.540902	1.059919
C	-2.220556	1.594473	0.337769

C	-3.288052	-0.608830	0.761473
H	-5.300196	-0.346387	0.153279
H	-4.400781	1.823983	2.082579
H	-5.077378	-0.426427	1.880920
H	-1.664963	1.868189	-0.566165
C	-1.423872	2.176397	1.531128
H	-1.885303	1.875049	2.480276
H	-1.419320	3.270857	1.509985
C	0.032453	1.697827	1.459992
H	0.610379	2.083766	2.307993
H	0.486498	2.140854	0.563447
C	0.187461	0.148931	1.434297
C	-0.763871	-0.509451	0.365642
C	0.042390	-0.426331	2.845977
H	-0.917001	-0.147146	3.295057
H	0.849561	-0.043804	3.478214
H	0.111553	-1.516692	2.831084
C	-0.014877	-0.260632	-0.971774
H	-0.154144	0.763539	-1.324559
H	-0.403559	-0.930906	-1.742773
C	-4.093834	1.902296	-1.348958
C	-6.114202	2.066650	0.794278
H	-6.158733	3.137912	1.023703
H	-6.814331	1.579125	1.485278
C	-6.574020	1.824171	-0.654031
H	-6.776471	0.757293	-0.805669
C	-5.533880	2.283987	-1.697980
H	-5.570729	3.378389	-1.791945
H	-5.748895	1.876022	-2.689840
O	-3.352318	1.432600	-2.192661
O	2.613541	-0.055964	1.490008
O	-0.706341	-1.930345	0.533700
H	-1.491711	-2.196826	1.042421
O	-3.304081	-1.986954	0.957970
C	-3.602332	3.722638	0.276145
H	-4.517127	4.206853	-0.071520

H	-2.768445	4.151382	-0.291151
H	-3.474494	3.995708	1.328309
Si	-3.887504	-3.155437	-0.143687
C	-3.443895	-2.644427	-1.897290
H	-3.916774	-3.307396	-2.632141
H	-2.359309	-2.692958	-2.041770
H	-3.757035	-1.617459	-2.116874
C	-5.753573	-3.352509	0.061673
H	-6.019389	-3.506453	1.113923
H	-6.103089	-4.228677	-0.499480
H	-6.316187	-2.485468	-0.303280
C	-3.018150	-4.735032	0.383851
H	-3.251881	-4.990198	1.424227
H	-1.930617	-4.631720	0.297480
H	-3.325488	-5.581341	-0.242501
H	-7.527288	2.335355	-0.834267
C	1.583059	-0.140800	0.849981
C	3.929406	-0.504707	-1.302556
C	4.991092	1.760619	-1.679489
C	2.496285	1.575326	-1.646198
C	3.698184	2.137718	-2.406360
H	5.125545	2.397096	-0.791547
H	2.513754	1.970247	-0.621147
H	3.713679	1.723546	-3.424050
H	5.867041	1.943091	-2.316006
H	1.561608	1.914772	-2.108651
H	3.618249	3.227156	-2.507181
C	5.004516	0.303290	-1.286363
C	4.058722	-1.991054	-1.080266
H	3.432597	-2.544728	-1.793902
H	3.741422	-2.288041	-0.072316
H	5.092825	-2.315871	-1.216254
C	1.462263	-0.543267	-0.626831
H	1.574348	-1.635161	-0.609880
C	2.531861	0.036249	-1.595883
H	2.238884	-0.337279	-2.593570

O	6.269138	-0.177837	-0.995533
Si	7.019440	-0.162658	0.518635
C	6.031616	-1.164126	1.767794
H	6.466270	-1.071313	2.771470
H	6.014365	-2.228810	1.508099
H	4.994910	-0.811221	1.811679
C	8.710761	-0.920227	0.189291
H	9.287366	-0.311363	-0.516597
H	8.616658	-1.925710	-0.236947
H	9.293264	-1.002932	1.115061
C	7.212100	1.606909	1.151643
H	7.718347	2.247572	0.420302
H	7.808561	1.618403	2.073231
H	6.242717	2.061654	1.386871

Requested basis set is 6-31G(d)

There are 262 shells and 697 basis functions
