CHEMISTRY
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Supporting Information

Highly Diastereoselective Construction of Fused Carbocycles from Cyclopropane-1,1-dicarboxylates and Cyclic Enol Silyl Ethers: Scope, Mechanism, and Origin of Diastereoselectivity

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Contents

1. General Information

All reactions were carried out under dry nitrogen atmosphere. All solvents and reagents were obtained from commercial sources and were purified according to standard procedures. All glassware was oven dried before use. Chemical shifts of ^{1}H NMR are reported in parts per million (ppm) down field from TMS, using residual $CDCl_3$ (7.26 ppm) or TMS (0.00 ppm) as an internal standard. Chemical shifts of ^{13}C NMR are reported in parts per million (ppm) down field from TMS, using the middle resonance of $CDCl_3$ (77.0 ppm) as an internal standard.

2. Optimization Studies

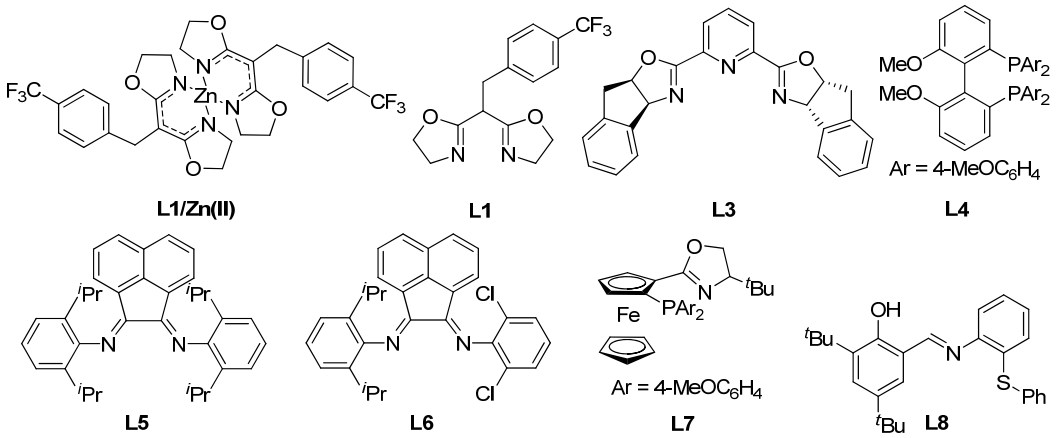
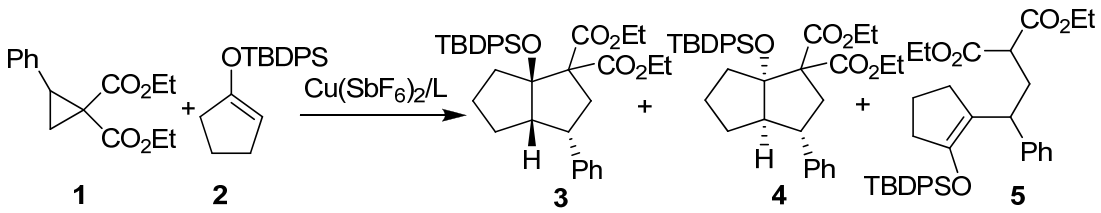


Figure S1. Ligands screened.

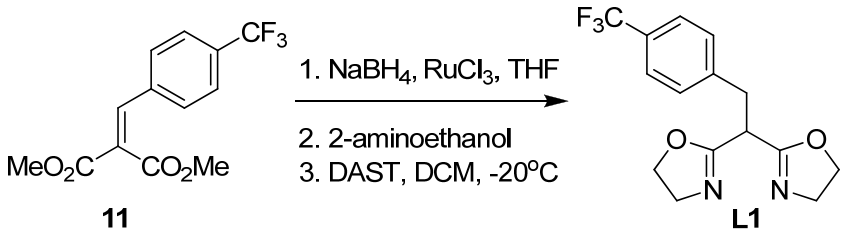
Table S1. Effect of Ligands.



Entry[a]	Ligand	T (°C)	Time	Conv (%)[b]	**3/4/5**[b]
1	**L1/**Zn	80	10 min	99 (93[c])	62/4/34
2	**L1**	80	10 min	100 (95[c])	62/4/34
3	**L3**	80	7 h	0	-
4	**L4**	80	7 h	0	-
5	**L5**	25	5 min	100	54/3/43
6	**L6**	80	7 h	0	-
7	**L7**	25	7 h	54	62/6/32
8	**L8**	80	7 h	0	-

[a] Reaction conditions: **1**:**2**:$CuBr_2$:$AgSbF_6$:Ligand = 0.2 mmol:0.4 mmol:0.02 mmol: 0.04 mmol:0.02 mmol, DCE; [b] Determined by ^{1}H NMR; [c] Total isolated yield.

3. Preparation of L1

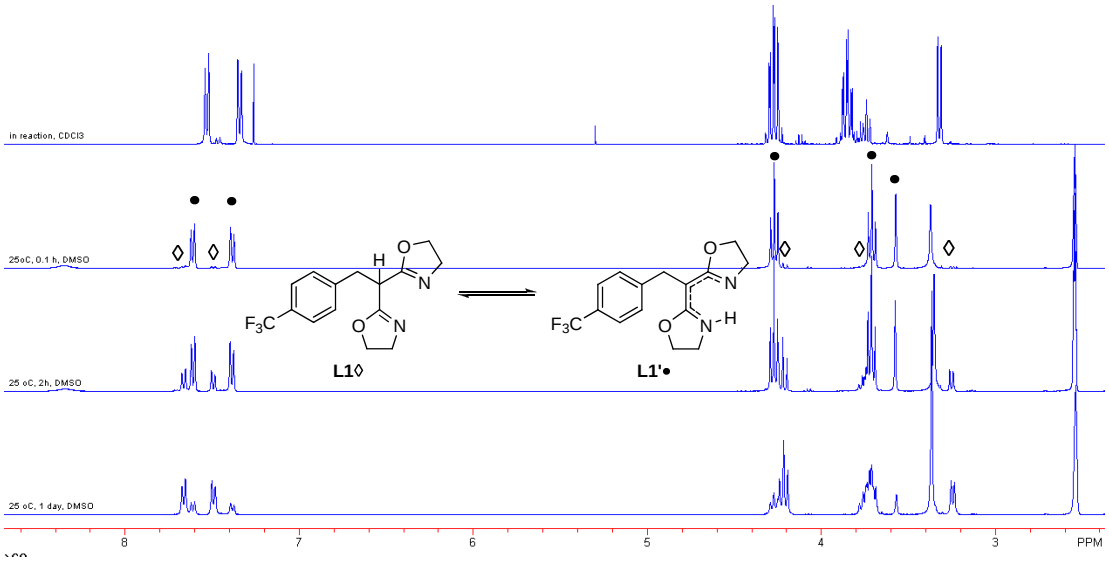


11 **L1**

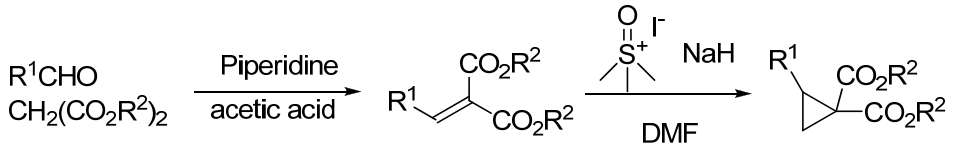
To a stirred solution of **11** (10 mmol) in a mixture of THF (30 mL) and water (10 mL) at 0 °C was added $RuCl_3 \cdot H_2O$ (310 mg, 1 mmol). Then $NaBH_4$ (760 mg, 20 mmol) was added slowly, and a black powder began to separate after a few minutes. The mixture was stirred for another 1 h at room temperature, then water was added and the mixture was extracted with dichloromethane (3×100 mL). The combined organic phase was washed with a saturated aqueous solution of $NaHCO_3$ (3×50 mL), dried (Na_2SO_4), filtered through Celite and concentrated under reduced pressure to give a colorless oil.[1] The colorless oil was then heated with 2-aminoethanol (2 equiv.) at 140 °C without further purification, giving a white solid. Then to a suspension of this white solid in dry CH_2Cl_2 (50 mL) at −20 °C was slowly added (diethylamino)sulfur trifluoride (DAST, 22 mmol). After stirring for 6 h at −20 °C, saturated $NaHCO_3$ (20 mL) was added slowly. Water (100 mL) was then added to the orange solution, and the aqueous layer was extracted with CH_2Cl_2 (3×55 mL). The combined organic layers were dried over $MgSO_4$, concentrated under vacuum, and the resulting off-white solid was recrystallized from EtOAc:hexanes to yield **L1** 1.6 g (5.1 mmol, 51%). White solid, **^{1}H NMR** (400 MHz, DMSO): δ 7.66 (d, *J* = 7.6 Hz, 1.43H), 7.61 (d, *J* = 7.6 Hz, 0.57H), 7.49 (d, *J* = 7.6 Hz, 1.43H), 7.38 (d, *J* = 7.6 Hz, 0.57H), 4.29-4.19 (m, 4H), 3.78-3.68 (m, 4.71H), 3.57 (s, 0.57H), 3.24 (d, *J* = 8.0 Hz, 1.43H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 166.1, 164.5, 142.1, 129.0, 128.8, 128.5, 128.1, 125.3, 125.1(4), 125.1(0), 125.0(6), 125.0(3), 124.5, 67.6, 67.1, 54.1, 48.3, 40.6(6), 40.6(3), 35.3, 30.2; **IR** (KBr, cm^{-1}): 2931, 2858, 1602, 1574, 1461, 1428, 1320, 1299, 1166, 1149, 1113; **LRMS-ESI**: $[M+H]^+$ 313.0; **HRMS-MALDI**: $[M+H]^+$ Calculated for $C_{15}H_{16}O_2N_2F_3$: 313.1158; Found: 313.1158; **Elemental Analysis**: Calculated for $C_{15}H_{15}O_2N_2F_3$: C, 57.69; H, 4.84; N, 8.97; Found: C, 57.57; H, 5.05; N, 8.85.

A mixture of the equilibrious tautomers (**L1** and **L1'**) was obtained.

CCDC 805797 (**L1'**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

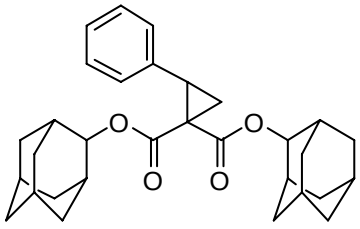


4. Preparation of Cyclopropanes



To a round-bottom flask equipped with a magnetic stirrer, Dean-stark trap and condenser was charged with piperidinium acetate (5 mol %), dimethylmalonate (1 equiv.) and aldehyde (1 equiv.) and benzene. The solution is stirred at reflux. After 18 h, the cooled mixture was washed with water and brine, dired over $MgSO_4$, and concentrated *in vacuo*. The alkylidene malonate is used for the next step without purification.

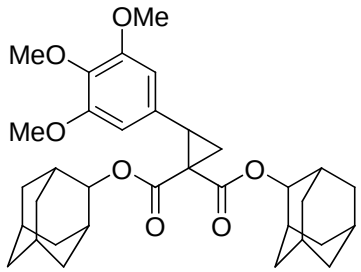
To a flask charged with a magnetic stirrer, trimethylsulfoxonium iodide (1.01 g, 4.60 mmol) was added to a solution of NaH (60% dispersion in oil) (0.218 g, 5.44 mmol) in DMF (6 mL). After gas evolution had subsided and the mixture became clear, a solution of malonate (4.18 mmol) in DMF (6 mL) was added via cannula. The reaction was monitored by TLC until it was completed. The mixture was then diluted with water, and extracted with ethyl ether. The combined extracts were washed with water, brine, and dried over $MgSO_4$. After filtration and concentration *in vacuo*, the residue was purified by flash column chromatography on silica gel (1:50 EtOAc/hexanes) to afford the cyclopropane product.



1h

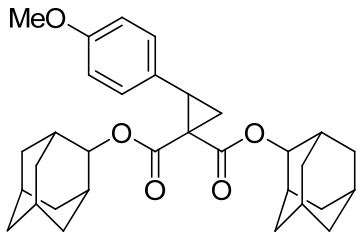
White solid, 3.8 g (81%); **m.p.**: 134 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.25-7.16 (m, 5H), 5.00 (m, 1H), 4.71 (m, 1H), 3,22 (t, *J* = 8.8 Hz, 1H), 2.16 (dd, *J* = 8.0 Hz, 5.2 Hz, 1H), 2.06-1.97 (m, 4H), 1.88-1.53 (m, 21H) 1.42-1.39 (m, 2H) 1.23-1.14 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.3, 166.1, 134.9, 128.3, 128.1, 127.1, 78.6, 78.0, 38.3, 37.1, 37.1, 36.2(8), 36.2(2), 36.2(0), 36.1, 31.9, 31.7(2), 31.6(9), 31.6(7), 31.6(4), 31.4, 31.3, 27.1, 27.0, 26.9, 26.8, 18.8; **IR** (thin film, cm^{-1}):

2908, 2855, 1719, 1452, 1324, 1276, 1212, 1143; **LRMS-EI** (*m/z*): 474 (M^+); **Elemental Analysis**: Calculated for $C_{31}H_{38}O_4$: C, 78.45; H, 8.07; Found: C, 78.31; H, 8.04.



1l

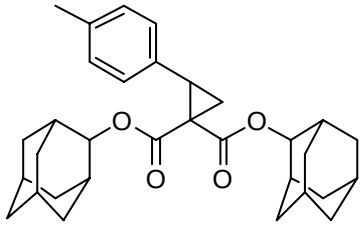
White solid, 2.2 g (67%); **m.p.**: 118 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 6.39 (s, 2H), 4.98 (m, 1H), 4.72 (m, 1H), 3.79 (s, 6H), 3.75 (s, 3H), 3.13 (t, *J* = 8.0 Hz, 1H), 2.09 (dd, *J* = 8.0 Hz, 4.8 Hz, 1H), 2.03-1.94 (m, 4H), 1.85-1.50 (m, 21H) 1.39-1.36 (m, 2H) 1.27-1.18 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.3, 166.0, 152.8, 137.1, 130.5, 105.3, 78.6, 77.9, 60.6, 55.9, 38.3, 37.1, 37.0, 36.2, 36.1(5), 36.1(3), 35.9, 32.1, 31.6(9), 31.6(7), 31.6(1), 31.5(8), 31.5(2), 31.1, 27.0, 26.9, 26.7, 26.6, 18.9; **IR** (thin film, cm^{-1}): 2906, 2854, 1714, 1588, 1451, 1267, 1205, 1128, 1099; **LRMS-EI** (*m/z*): 564 (M^+); **Elemental Analysis**: Calculated for $C_{34}H_{44}O_7$: C, 72.31; H, 7.85; Found: C, 72.61; H, 7.80.



1m

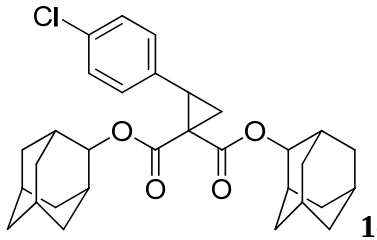
White solid, 5.4 g (93%); **m.p.**: 136 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.14-7.11 (m, 2H), 6.79-6.76 (m, 2H), 4.99 (m, 1H), 4.71 (m, 1H), 3.76 (s, 3H), 3.17 (t, *J* = 8.8 Hz, 1H), 2.11 (dd, *J* = 8.0 Hz, 5.2 Hz, 1H), 2.05-1.96 (m, 4H), 1.89-1.52 (m, 21H), 1.48-1.40 (m, 2H), 1.31 (m, 1H), 1.22-1.19 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.44, 166.31, 158.86, 129.49, 126.87, 113.56, 78.53, 78.03, 55.31, 38.18, 37.24, 37.19, 36.32, 36.24, 36.23, 36.13, 31.74, 31.69, 31.52, 31.49, 31.38, 27.10, 27.06, 26.90, 26.82, 19.02; **IR** (thin film, cm^{-1}): 2906, 2854, 1716, 1516, 1451, 1347,

1315, 1275, 1251, 1211, 1176, 1138, 1099, 1040; **LRMS-EI** (*m/z*): 504 (M^+); **Elemental Analysis**: Calculated for $C_{32}H_{40}O_5$: C, 76.16; H, 7.99; Found: C, 76.28; H, 8.09.



1n

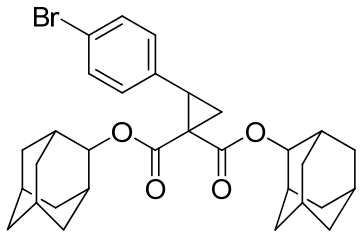
White solid, 1.7 g (66%); **m.p.**: 125 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.09 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 4.99 (m, 1H), 4.71 (m, 1H), 3.18 (t, *J* = 8.4 Hz, 1H), 2.28 (s, 3H), 2.13 (dd, *J* = 8.0 Hz, 5.2 Hz, 1H), 2.05-1.96 (m, 4H), 1.87-1.51 (m, 21H), 1.42-1.39 (m, 2H), 1.28-1.25 (m, 1H), 1.17-1.14 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.4, 166.3, 136.8, 131.7, 128.7, 128.2, 78.5, 78.0, 38.2, 37.2(5), 37.2(1), 36.3, 36.2(4), 36.2(2), 36.1, 31.7(7), 31.7(3), 31.7(0), 31.6(9), 31.6(7), 31.4, 31.3, 27.1, 27.0, 26.9, 26.8, 21.0, 18.9; **IR** (thin film, cm^{-1}): 2908, 2855, 1719, 1323, 1276, 1211, 1141; **LRMS-EI** (*m/z*): 488 (M^+); **Elemental Analysis**: Calculated for $C_{32}H_{40}O_4$: C, 78.65; H, 8.25; Found: C, 78.78; H, 8.53.



1o

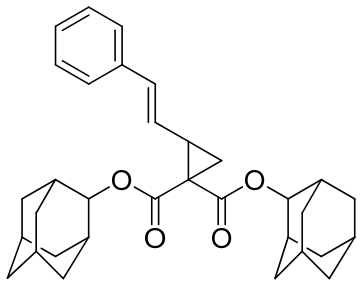
White solid, 4.6 g (81%); **m.p.**: 138 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.18 (d, *J* = 8.4 Hz, 1H), 7.1 (d, *J* = 8.4 Hz, 2H), 4.98 (m, 1H), 4.71 (m, 1H), 3.15 (t, *J* = 8.8 Hz, 1H), 2.09 (dd, *J* = 8.0 Hz, 4.8 Hz, 1H), 2.03-1.94 (m, 4H), 1.85-1.50 (m, 21H), 1.42-1.34 (m, 2H), 1.27 (m, 1H), 1.21-1.17 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 168.9, 165.8, 133.4, 132.9, 129.5, 128.1, 78.6, 78.1, 38.2, 37.0, 36.9, 36.1, 36.0(8), 36.0(6), 35.9, 31.6, 31.5(9), 31.5(4), 31.5(2), 31.4, 31.1, 31.0, 26.9, 26.8, 26.7, 26.6, 18.8; **IR** (thin film, cm^{-1}): 2909, 2856, 1720, 1497, 1451, 1324, 1275, 1212, 1142, 1100; **LRMS-EI** (*m/z*): 508 (M^+); **Elemental Analysis**: Calculated for $C_{31}H_{37}ClO_4$: C,

73.14; H, 7.33; Found: C, 73.09; H, 7.45.



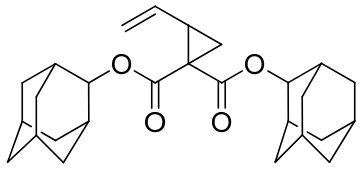
1p

White solid, 2.5 g (70%); **m.p.**: 127 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.33 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 4.98 (m, 1H), 4.71 (m, 1H), 3.13 (t, *J* = 8.4 Hz, 1H), 2.09 (dd, *J* = 12.0 Hz, 4.8 Hz, 1H), 2.03-1.94 (m, 4H), 1.85-1.59 (m, 17H), 1.55-1.50 (m, 2H), 1.42-1.33 (m, 2H), 1.27-1.18 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 168.9, 165.8, 133.9, 131.0, 129.9, 121.0, 78.6, 76.6, 38.2, 37.1, 37.0, 36.2, 36.1, 36.0, 35.9, 31.6, 31.5(9), 31.5(5), 31.5(3), 31.4, 31.1, 31.0, 26.9, 26.8, 26.7, 26.6, 18.7; **IR** (thin film, cm^{-1}): 2905, 2854, 1716, 1451, 1347, 1315, 1276, 1210, 1139, 1099, 1041, 1011; **LRMS-EI** (*m/z*): 552 (M^+); **Elemental Analysis**: Calculated for $C_{31}H_{37}BrO_4$: C, 67.27; H, 6.74; Found: C, 67.53; H, 7.05.



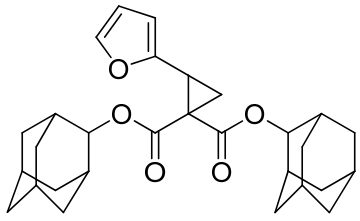
1q

White solid, 2.1 g (70%); **m.p.**: 112 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.27-7.26 (m, 5H), 7.23-7.18 (m, 1H), 6.64 (d, *J* = 15.6 Hz, 1H), 5.82 (dd, *J* = 15.6 Hz, 8.8 Hz, 1H), 5.01 (m, 1H), 4.98 (m, 1H), 4.75 (dd, J = 16.4 Hz, 8.8 Hz, 1H), 2.06-1.97 (m, 6H), 1.89-1.65 (m, 20H), 1.57-1.49 (m, 3H), 1.26-1.23 (m, 1H), 1.17-1.14 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.1, 167.1, 136.6, 133.2, 128.4, 127.3, 125.9, 125.1, 78.5, 78.4, 37.2, 37.1, 36.9, 36.3(9), 36.1(9), 36.13, 31.8, 31.7, 31.6, 31.2, 30.9, 27.1, 27.0, 26.9, 21.1; **IR** (thin film, cm^{-1}): 2907, 2855, 1717, 1451, 1347, 1314, 1278, 1199, 1140, 1100, 1041; **LRMS-EI** (*m/z*): 500 (M^+); **Elemental Analysis**: Calculated for $C_{29}H_{36}O_5$: C, 79.16; H, 8.05; Found: C, 79.41; H, 8.26.



1r

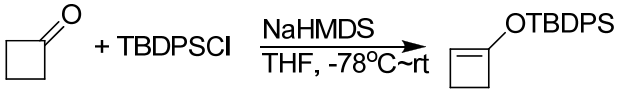
White solid, 5.6 g (88%); **m.p.**: 126 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 5.48-5.39 (m, 1H), 5.28 (d, *J* = 16.8 Hz, 2H), 5.08 (d, *J* = 10.0 Hz, 1H), 4.98 (m, 1H), 4.94 (m, 1H), 2.57 (dd, *J* = 16.0 Hz, 8.0 Hz, 1H), 2.06-1.96 (m, 8H), 1.81-1.65 (m, 17H), 1.54-1.40 (m, 5H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.1, 166.8, 133.3, 118.0, 78.4, 78.3, 37.2(8), 37.2(0), 36.5, 36.3, 36.2, 36.1, 31.8, 31.7(6), 31.7(0), 31.6(5), 31.6(1), 31.5, 30.7, 27.1, 27.0, 26.9, 26.8, 20.3; **IR** (thin film, cm^{-1}): 2910, 2856, 1778, 1721, 1556, 1452, 1358, 1325, 1262, 1203, 1100, 1019; **LRMS-EI** (*m/z*): 424 (M^+); **Elemental Analysis**: Calculated for $C_{27}H_{36}O_4$: C, 76.38; H, 8.55; Found: C, 76.12; H, 8.53.



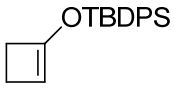
1s

White solid, 2.4 g (60%); **m.p.**: 136 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.24-7.22 (m, 1H), 6.24 (dd, *J* = 4.2 Hz, 3.0 Hz, 1H), 6.10 (d, *J* = 4.2 Hz, 1H), 4.98 (m, 1H), 4.84 (m, 1H), 3.10 (t, *J* = 13.2 Hz, 1H), 2.06-1.90 (m, 7H), 1.86-1.66 (m, 18H), 1.55-1.46 (m, 4H), 1.33-1.30 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 168.8, 166.0, 150.0, 141.9, 110.4, 107.4, 78.8, 78.2, 37.7, 37.24, 37.19, 36.3, 36.2, 31.68, 31.65, 31.62, 31.5, 31.3, 27.1, 26.8, 25.1, 18.7; **IR** (thin film, cm^{-1}): 2908, 2856, 1720, 1357, 1323, 1276, 1200, 1143, 983, 748; **LRMS-EI** (*m/z*): 464 (M^+); **Elemental Analysis:** calculated for $C_{29}H_{36}O_5$ (464.3 g/mol): C, 74.97; H, 7.81; Found: C, 74.94; H, 7.96.

5. Preparation of Enol Silyl Ethers

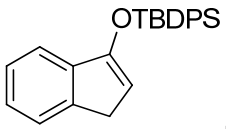


To a stirred solution of sodium hexamethyldisilazide (2M) (12 mmol, 6 mL) in dry THF (20 mL) at -78 °C was added cyclobutanone (10 mmol) dropwise. The resulting pale-yellow solution was stirred for 20 min at −78 °C, and then *tert*-butylchlorodiphenylsilane (12 mmol, 1.2 equiv) was added dropwise by syringe. The reaction mixture was stirred for 5 min at −78 °C, and then the reaction flask was removed from the cooling bath and was allowed to warm to room temperature. The reaction mixture was by TLC until it was completed, and then was concentrated by rotary evaporation. The pale-yellow oily residue was dissolved in pentane (20 mL), then the pentane solution was filtered through a pad of Celite and the filtrate was concentrated. The residue was purified by flash-column chromatography (hexanes) to provide *tert*-butyl(cyclobutenyloxy)diphenylsilane **2e** as a colorless oil.



2e

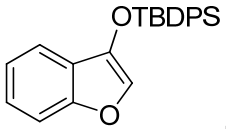
Colorless oil, 1.5 g (71%); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.75-7.72 (m, 4H), 7.45-7.38 (m, 6H), 4.32 (t, *J* = 1.2 Hz, 1H), 2.44-2.42 (m, 2H), 1.89-1.87 (m, 2H), 1.09 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 147.8, 135.4, 133.0, 129.8, 127.6, 104.0, 34.2, 26.5, 19.6, 19.1; **IR** (thin film, cm^{-1}): 2956, 2930, 2857, 1626, 1427, 1290, 1278, 1223, 1112; **LRMS-EI** (*m/z*): 308 (M^+); **HRMS-EI** (*m/z*): Calculated for $C_{20}H_{24}OSi$, 308.1596; Found: 308.1594.



2f

Yellow oil, 4.8 g (52%); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.82-7.75 (m, 4H), 7.60-7.58 (m, 1H), 7.44-7.35 (m, 8H), 7.25-7.21 (m, 1H), 4.89 (t, *J* = 2.4 Hz, 1H), 3.84 (t, *J* = 2.4 Hz, 2H), 1.14 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 153.0, 142.6, 141.7, 135.4,

132.5, 129.8, 127.7, 126.0, 125.1, 123.7, 118.1, 106.8, 34.0, 26.5, 19.4; **IR** (thin film, cm^{-1}): 3071, 2957, 2931, 2857, 1601, 1575, 1427, 1363, 1275, 1260, 1246, 1112, 1080; **LRMS-EI** (*m/z*): 370 (M^+); **HRMS-EI** (*m/z*): Calculated for $C_{25}H_{26}OSi$, 370.1753; Found: 370.1754.



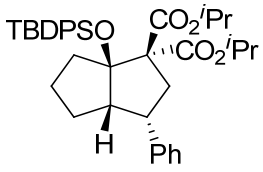
2g

Yellow oil, 2.6 g (70%); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.75-7.72 (m, 4H), 7.66-7.63(m, 1H), 7.45-7.29 (m, 7H), 7.27-7.19 (m, 2H), 6.66 (s, 1H), 1.16 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 153.1, 138.9, 135.4, 132.0, 130.1, 129.5, 127.8, 124.4, 123.7, 122.0, 118.6, 111.5, 26.5, 19.5; **IR** (thin film, cm^{-1}): 2958, 2931, 2858, 1583, 1472, 1452, 1428, 1360, 1275, 1260, 1199, 1113, 1087; **LRMS-EI** (*m/z*): 372 (M^+); **HRMS-EI** (*m/z*): Calculated for $C_{24}H_{24}O_2Si$, 372.1546; Found: 372.1552.

6. Cycloadditions of Cyclopropanes with Enol Silyl Ethers

To an oven-dried Schlenk reaction tube containing a magnetic stirring bar were added **L1** (12.5 mg, 0.04 mmol), $CuBr_2$ (8.9 mg, 0.04 mmol), and $AgSbF_6$ (27.4 mg, 0.08 mmol) under nitrogen atmosphere. Then the Schlenk reaction tube was charged with DCM (1.0 mL) under nitrogen atmosphere. The resulting mixture was stirred rapidly for 24 h under nitrogen atmosphere yielding active catalyst [Cu(**L1**)$(SbF_6)_2$] as a clear green solution.

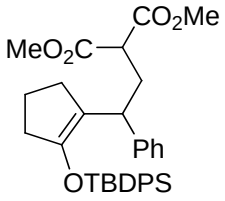
To an oven-dried Schlenk reaction tube containing a magnetic stirring bar were added cyclopropane 1,1-diester **1** (0.20 mmol) and enol silyl ether **2** (0.4 mmol). Then the Schlenk reaction tube was charged with 4Å molecular sieves and DCM (0.5 mL) under nitrogen atmosphere. And the above solution of catalyst [Cu(**L1**)$(SbF_6)_2$] in DCM (0.5 mL) was added to the mixture under nitrogen atmosphere. The resulting solution was stirred until the cyclopropane **1** was completely consumed (monitoring by TLC, hexane/ethyl acetate = 40/1, v/v). Then the mixture was passed through a short silica gel column and eluted with DCM (50 mL). The combined elution was concentrated under reduced pressure, and the residue was purified by flash chromatography on silica gel (hexane/ethyl acetate, v/v, 250/1) to give the product.



3b

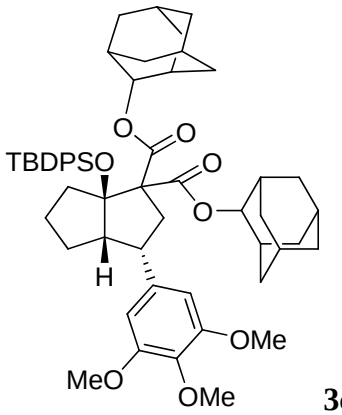
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91-7.85 (m, 4H), 7.43-7.34 (m, 6H), 7.24-7.19 (m, 2H), 7.13-7.09 (m, 1H), 7.04-7.01 (m, 2H), 5.22 (heptet, *J* = 6.4 Hz, 1H), 5.05 (heptet, *J* = 6.4 Hz, 1H), 4.23-4.15 (m, 1H), 2.90 (dd, *J* = 17.6 Hz, 8.4 Hz, 1H), 2.44 (t, *J* = 13.6 Hz, 1H), 2.22 (dd, *J* = 13.6 Hz, 4.8 Hz, 1H), 1.94 (dd, *J* = 13.6 Hz, 4.8 Hz, 1H), 1.47-1.41 (m, 1H), 1.37 (d, *J* = 6.4 Hz, 3H), 1.34 (d, *J* = 6.4 Hz, 3H), 1.29 (d, *J* = 6.4 Hz, 3H), 1.21 (d, *J* = 6.4 Hz, 3H), 1.05 (s, 9H), 1.02-0.95 (m, 1H), 0.89-0.70 (m, 2H), 0.62-0.52 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.8, 168.9, 141.5, 136.4, 136.3, 135.3, 135.1, 129.3, 127.9, 127.7, 127.1(8), 127.1(4), 125.6, 96.0, 68.5, 68.4,

54.7, 41.4, 41.2, 35.5, 29.1, 27.2, 24.6, 21.8, 21.7, 21.6, 21.5, 19.7; **IR** (thin film, cm^{-1}): 2978, 2932, 2857, 1722, 1469, 1273, 1189, 1108, 1061; **LRMS-MALDI**: $[M+Na]^+$ 635.3; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{38}H_{48}O_5SiNa$, 635.3163; Found: 635.3170.



5a

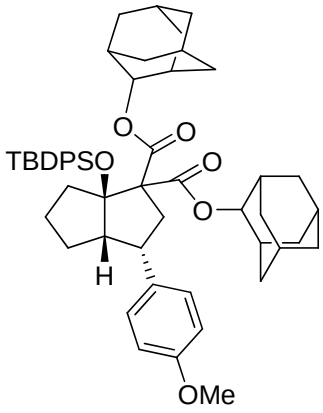
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76-7.74 (m, 2H), 7.68-7.66 (m, 2H), 7.44-7.38 (m, 4H), 7.34-7.27 (m, 6H), 7.22-7.17 (m, 1H), 4.12 (dd, *J* = 9.6 Hz, 6.8 Hz, 1H), 3.72 (s, 3H), 3.66 (s, 3H), 3.44 (t, *J* = 6.8 Hz, 1H), 2.57-2.50 (m, 1H), 2.46-2.38 (m, 1H), 2.26-2.18 (m, 1H), 2.03-1.97 (m, 1H), 1.89-1.74 (m, 2H), 1.58-1.42 (m, 2H), 1.08 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.1, 169.7, 148.8, 143.0, 135.2, 135.1, 133.7, 133.6, 129.8, 129.7, 128.2, 127.7, 127.6, 126.0, 116.3, 52.5, 52.4, 50.1, 40.0, 33.3, 31.4, 27.1, 26.4, 19.8, 19.1; **IR** (thin film, cm^{-1}): 2952, 2856, 1736, 1671, 1430, 1340, 1234, 1149, 1111, 1024; **LRMS-ESI**: $[M+Na]^+$ 579.3; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{34}H_{40}O_5SiNa$, 579.2537; Found: 539.2555.



3c

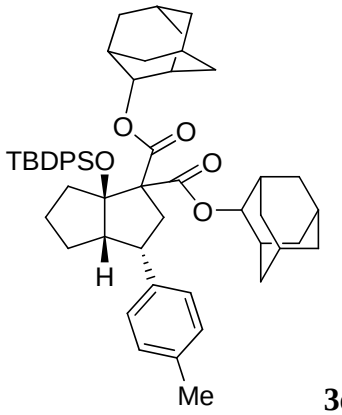
Colorless oil, 160 mg (94%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 6.8 Hz, 2H), 7.85 (d, *J* = 6.8 Hz, 2H),7.41-7.34 (m, 6H), 6.11 (s, 2H), 5.14 (m, 1H), 4.85 (m, 1H), 4.02-3.96 (m, 1H), 3.78 (s, 9H), 2.71 (dd, *J* = 16.8 Hz, 8.0 Hz, 1H), 2.41 (t, *J* = 12.8 Hz, 1H), 2.30 (dd, *J* = 13.2 Hz, 6.0 Hz, 1H), 2.17-2.1.99 (m, 8H), 1.92-1.72 (m, 17H), 1.62-1.49 (m, 5H), 1.18-1.08 (m, 2H), 1.03 (s, 9H), 0.96-0.88 (m, 1H),

0.69-0.61 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.4, 168.7, 152.7, 137.4, 136.5, 136.3, 135.9, 135.6, 135.3, 129.3, 129.1, 127.1, 126.9, 104.6, 96.3, 78.4, 77.8, 68.8, 60.8, 55.9, 53.9, 41.6, 41.3, 37.3, 37.2, 36.4(5), 36.4(1), 36.3, 36.2, 36.0, 32.0, 31.9, 31.7, 31.6, 31.3, 28.8, 27.3, 27.2, 27.1, 27.0, 26.9, 25.3, 24.8, 19.7; **IR** (thin film, cm^{-1}): 2928, 2855, 1719, 1588, 1509, 1452, 1261, 1130, 1108; **LRMS-ESI**: $[M+Na]^+$ 909.7; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{55}H_{70}O_8SiNa$, 909.4732; Found: 909.4764.



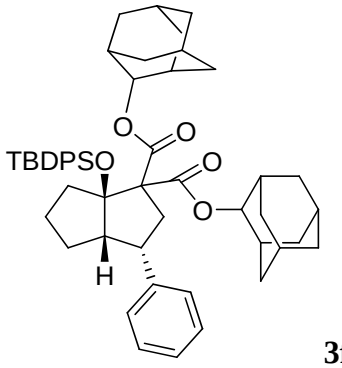
3d

Colorless oil, 140 mg (85%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 18.4 Hz, 6.8 Hz, 2.0 Hz, 4H), 7.43-7.34 (m, 6H), 6.91 (d, *J* = 8.4 Hz, 2H), 6.77 (d, *J* = 8.4 Hz, 2H), 5.12 (m, 1H), 4.93 (m, 1H), 4.11 (dd, *J* = 19.6 Hz, 9.6 Hz, 1H), 3.75 (m, 1H), 2.81 (dd, *J* = 16.8 Hz, 8.4 Hz, 1H), 2.46-2.37 (m, 2H), 2.11-2.02 (m, 8H), 1.94-1.72 (m, 17H), 1.64-1.51 (m, 5H), 1.03 (s, 9H), 0.94-0.84 (m, 3H), 0.66-0.61 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.1, 168.9, 157.6, 136.4, 136.3, 135.3, 135.2, 133.7, 129.3, 129.2, 128.6, 127.1, 127.0, 113.3, 96.5, 78.0, 77.8, 69.0, 55.0, 54.6, 41.3, 40.6, 37.3, 37.2, 36.5, 36.4, 36.30 36.2, 36.0, 32.0, 31.9, 31.8, 31.7, 31.6, 31.5(7), 31.5(1), 31.4, 28.6, 27.2, 27.1, 26.9, 26.8, 24.6, 22.5, 19.6, 14.0; **IR** (thin film, cm^{-1}): 2908, 2855, 1720, 1512, 1451, 1259, 1213 1178, 1099, 1040, 1018; **LRMS-ESI**: $[M+Na]^+$ 849.5; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{53}H_{66}O_6SiNa$, 849.4520; Found: 849.4517.



3e

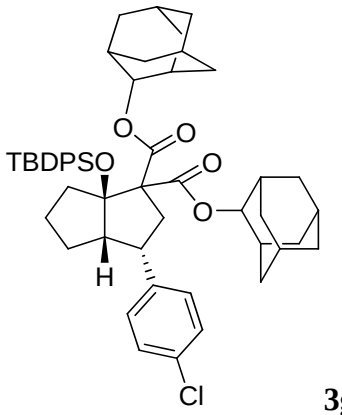
Colorless oil, 117 mg (72%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94-7.88 (m, 4H), 7.45-7.37 (m, 6H), 7.06 (d, *J* = 8.0 Hz, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 5.15 (m, 1H), 4.96 (m, 1H), 4.19-4,12 (m, 1H), 2.85 (dd, *J* = 17.2 Hz, 8.4 Hz, 1H), 2.52-239 (m, 2H), 2.29 (s, 3H), 2.14-2.05 (m, 8H), 1.98-1.74 (m, 17H), 1.69-1.53 (m, 5H), 1.09-1.06 (m, 10H), 0.96-0.88 (m, 2H), 0.73-0.63 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.2, 168.9, 138.6, 136.4, 136.3, 135.4, 135.2, 135.1, 129.3, 129.2, 128.6, 127.6, 127.2, 127.1, 96.6, 78.0, 77.9, 69.1, 54.5, 41.2, 41.0, 37.3, 37.2, 36.4, 36.3, 36.2, 36.1, 32.0, 31.9(8), 31.9(0), 31.7(6), 31.7(1), 31.5, 31.4, 28.6, 27.2, 27.1(9), 27.1(2), 27.0, 26.9, 24.6, 20.9, 19.6; **IR** (thin film, cm^{-1}): 2909, 2855, 1721, 1451, 1261, 1107; **LRMS-ESI**: $[M+Na]^+$ 833.3; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{53}H_{66}O_5SiNa$, 833.4571; Found: 833.4572.



3f

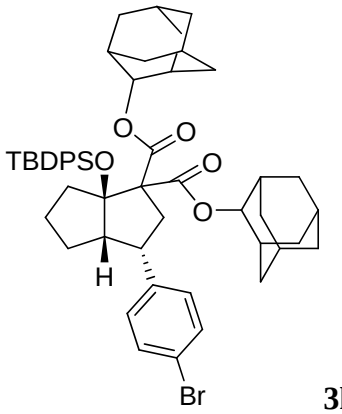
Colorless oil, 127 mg (80%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.92-7.85 (m, 4H), 7.42-7.34 (m, 6H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.11 (t, *J* = 7.2 Hz, 1H), 7.00 (d, *J* = 7.6 Hz, 2H), 5.13 (m, 1H), 4.94 (m, 1H), 4.22-4.15 (m, 1H), 2.86 (dd, *J* = 16.8 Hz, 8.0 Hz, 1H), 2.52-2.39 (m, 2H), 2.15-2.03 (m, 8H), 1.95 -1.71 (m, 17H), 1.66-1.51 (m, 5H), 1.08-1.00 (m, 10H), 0.97-0.83 (m, 2H), 0.69-0.59 (m, 1H); **^{13}C NMR** (100 MHz,

$CDCl_3$) δ 170.1, 168.9, 141.7, 136.4, 136.3, 135.3, 135.2, 129.3, 129.2, 127.9, 127.7, 127.1(3), 127.1(0), 125.7, 96.5, 78.0, 77.9, 69.0, 54.5, 41.3, 37.3, 37.2, 36.4, 36.3, 36.2, 36.1, 32.0, 31.9(8), 31.9(0), 31.7, 31.6, 31.5, 31.4, 28.7, 27.2, 27.1(8), 27.1(1), 26.9, 26.8, 24.6, 19.6; **IR** (thin film, cm^{-1}): 2928, 2856, 1721, 1452, 1275, 1261, 1108; **LRMS-ESI**: $[M+Na]^+$ 819.4; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{52}H_{64}O_5SiNa$, 819.4415; Found: 819.4444.



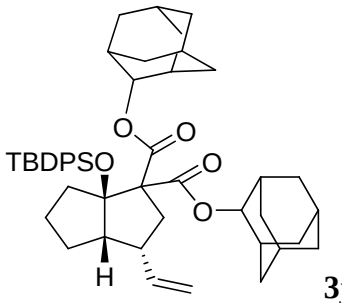
3g

Colorless oil, 127 mg (77%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90-7.84 (m, 4H), 7.43-7.34 (m, 6H), 7.19-7.17 (m, 2H), 6.92-6.89 (m, 2H), 5.12 (m, 1H), 4.92 (m, 1H), 4.15 (dd, *J* = 18.8 Hz, 9.2 Hz, 1H), 2.80 (dd, *J* = 17.2 Hz, 8.0 Hz, 1H), 2.43-2.37 (m, 2H), 2.10-2.01 (m, 8H), 1.92-1.71 (m, 17H), 1.63-1.50 (m, 5H), 1.02 (s, 9H), 1.07-1.00 (m, 1H), 0.93-0.81 (m, 2H), 0.62-0.52 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.0, 168.8, 140.2, 136.4, 136.3, 135.3, 135.1, 131.3, 129.4, 129.3, 128.9, 128.0, 127.2, 127.1, 96.4, 78.1, 78.0, 69.1, 54.4, 41.4, 40.8, 37.2(7), 37.2(1), 36.4, 36.3, 36.2, 36.1, 36.0(8), 32.0(7), 32.0(0), 31.9, 31.8, 31.7, 31.6, 31.5, 31.4, 28.7, 27.2, 27.1, 27.0, 26.9, 26.8, 24.6, 19.6; **IR** (thin film, cm^{-1}): 2927, 2855, 1735, 1469, 1266, 1233, 1188, 1174, 1108, 1066, 1042, 1016; **LRMS-ESI**: $[M+Na]^+$ 853.3; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{52}H_{63}O_5SiClNa$, 853.4025; Found: 853.4017.



3h

Colorless oil, 137 mg (78%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 18.4 Hz, 8.4 Hz, 4H), 7.45-7.34 (m, 8H), 6.87 (d, *J* = 7.2 Hz, 2H), 5.14 (m, 1H), 4.95 (m, 1H), 4.15 (dd, *J* = 18.8 Hz, 9.2 Hz, 1H), 2.82 (dd, *J* = 16.8 Hz, 8.0 Hz, 1H), 2.47-2.40 (m, 2H), 2.18-2.04 (m, 8H), 1.95-1.73 (m, 17H), 1.66-1.53 (m, 5H), 1.05 (s, 9H), 0.94-0.85 (m, 3H), 0.65-0.55 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.0, 168.9, 140.8, 136.4, 136.3, 135.3, 135.1, 130.9, 129.4, 129.3, 127.2, 127.1, 119.4, 96.5, 78.2, 78.0, 69.1, 54.4, 41.4, 40.9, 37.3, 37.2, 36.4, 36.3, 36.2, 36.0, 32.0, 31.9(9), 31.9(1), 31.8, 31.7, 31.5, 31.4, 28.8, 27.2, 27.1(9), 27.1(1), 26.9, 26.8, 24.6, 19.6; **IR** (thin film, cm^{-1}): 2907, 2855, 1721, 1488, 1264, 1233, 1187, 1100, 1071, 1041; **LRMS-ESI**: $[M+Na]^+$ 897; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{52}H_{63}O_5SiBrNa$, 897.3520; Found: 897.3553.



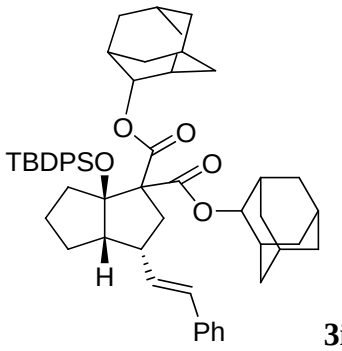
3j

Colorless oil, 105 mg (70%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.2 Hz, 2H), 7.81 (d, *J* = 7.2 Hz, 2H), 7.42-7.33 (m, 6H), 5.67-5.59 (m, 1H), 5.08 (m, 1H), 4.97-4.93 (m, 3H), 3.45-3.41(m, 1H), 2.74-2.69 (m, 1H), 2.32 (dd, *J* = 13.6 Hz, 6.8 Hz, 1H), 2.07-1.95 (m, 10H), 1.83-1.74 (m, 16H), 1.64-1.55 (m, 5H), 1.16-1.04 (m, 3H), 1.01 (s, 9H), 0.90-0.85 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.8, 169.30,

139.4, 136.5, 136.3, 135.2, 135.0, 129.3, 129.2, 127.1, 127.0, 114.6, 97.1, 78.0, 77.7, 69.2, 54.2, 40.7, 40.5, 38.0, 37.3, 37.2, 36.4, 36.2, 36.1, 32.0, 31.9(4), 31.9(2), 31.8, 31.7(8), 31.7(6), 31.5(4), 31.5(1), 27.4, 27.1(8), 27.1(4), 27.0, 26.9(9), 26.9(0), 24.9, 19.6; **IR** (thin film, cm^{-1}): 2908, 2855, 1728, 1451, 1260, 1194; **LRMS-ESI**: $[M+Na]^+$ 769.5; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{48}H_{62}O_5SiNa$, 769.4258; Found: 769.4270.

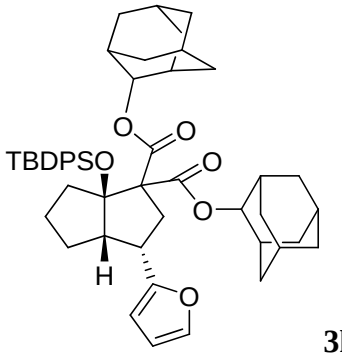
To an oven-dried Schlenk reaction tube containing a magnetic stirring bar were added **L1** (6.2 mg, 0.02 mmol), $CuBr_2$ (4.5 mg, 0.02 mmol), and $AgSbF_6$ (13.7 mg, 0.04 mmol) under nitrogen atmosphere. Then the Schlenk reaction tube was charged with DCM (1.0 mL) under nitrogen atmosphere. The resulting mixture was stirred rapidly for 24 h under nitrogen atmosphere yielding active catalyst [Cu(**L1**)$(SbF_6)_2$] as a clear green solution.

To an oven-dried Schlenk reaction tube containing a magnetic stirring bar were added cyclopropane 1,1-diester **1** (0.20 mmol) and enol silyl ether **2** (0.40 mmol). Then the Schlenk reaction tube was charged with 4Å molecular sieves and DCM (0.5 mL) under nitrogen atmosphere. And the above solution of catalyst [Cu(**L1**)$(SbF_6)_2$] in DCM (0.5 mL) was added to the mixture under nitrogen atmosphere. The resulting solution was stirred until the cyclopropane **1** was completely consumed (monitoring by TLC, hexane/ethyl acetate = 40/1, v/v). Then the mixture was passed through a short silica gel column and eluted with DCM (50 mL). The combined elution was concentrated under reduced pressure, and the residue was purified by flash chromatography on silica gel (hexane/ethyl acetate, v/v, 250/1) to give the product.



3i

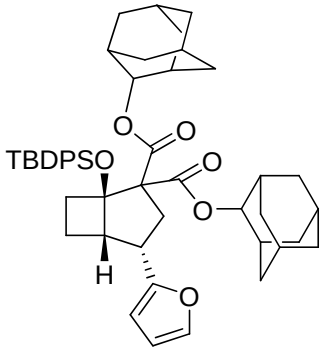
Colorless oil, 106 mg (65%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.91-7.88 (m, 2H), 7.82-7.80 (m, 2H), 7.41-7.32 (m, 6H), 7.29-7.23 (m, 3H), 7.18-7.14 (m, 1H), 6.32 (d, *J* = 15.6 Hz, 1H), 6.01 (dd, *J* = 15.6 Hz, 8.0 Hz, 1H), 5.09 (m, 1H), 4.99 (m, 1H), 3.64-3.55 (m, 1H), 2.81-2.75 (m, 1H), 2.41 (dd, *J* = 14.4 Hz, 7.2 Hz, 1H), 2.14-1.96 (m, 10H), 1.83-1.73 (m, 17H), 1.58-1.55 (m, 4H), 1.25-1.07 (m, 3H), 1.02 (s, 9H), 0.95-0.83 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.8, 169.3, 137.5, 136.5, 136.4, 135.2, 135.1, 131.5, 130.2, 129.4, 129.3, 128.4, 127.2, 127.1, 126.9, 125.9, 97.2, 78.1, 77.8, 69.4, 54.9, 40.5, 40.2, 38.8, 37.3, 36.4, 36.3, 36.2, 32.0, 31.(9), 31.9(3), 31.8, 31.7, 31.5, 27.6, 27.2, 27.1, 27.0, 26.9, 25.1, 19.6; **IR** (thin film, cm^{-1}): 2907, 2855, 1727, 1451, 1260, 1100; **LRMS-ESI**: $[M+Na]^+$ 845.6; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{54}H_{66}O_5SiNa$, 845.4571; Found: 845.4604.



3k

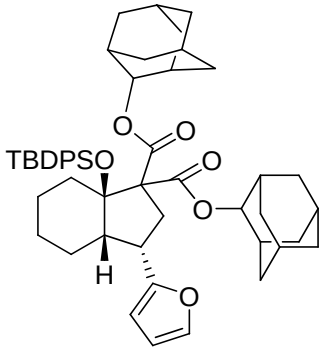
Colorless oil; 111 mg (71%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.91-7.88 (m, 2H), 7.83-7.81 (m, 2H), 7.42-7.33 (m, 6H), 7.25 (dd, *J* = 2.0 Hz, 0.8 Hz, 1H), 6.22 (dd, *J* = 3.2 Hz, 2.0 Hz, 1H), 5.95-5.94 (m, 1H), 5.12 (m, 1H), 4.98 (m, 1H), 4.11 (dd, J = 3.6 Hz, 2.8 Hz, 1H), 2.96-2.89 (m, 1H), 2.48-2.38 (m, 2H), 2.09-1.74 (m, 24H), 1.59-1.55 (m, 6H), 1.15-1.07 (m, 1H), 1.02 (s, 9H), 0.96-0.84 (m, 2H), 0.77-0.68 (m, 1H); **^{13}C**

NMR (100 MHz, $CDCl_3$) δ 169.6, 169.2, 156.6, 141.1, 136.5, 136.4, 135.1, 135.0, 129.3, 129.2, 127.2, 127.1, 109.6, 105.6, 96.9, 78.2, 77.8, 68.9, 54.2, 40.4, 37.3, 37.2, 36.8, 36.4, 36.3, 36.2, 32.0, 31.9(9), 31.9(5), 31.8, 31.7(9), 31.7(6), 31.6, 31.5, 27.9, 27.2, 27.1, 26.9(9), 26.9(9), 24.8, 19.6; **IR** (thin film, cm^{-1}): 2908, 2855, 1727, 1451, 1260, 1100; **LRMS-ESI**: $[M+Na]^+$ 809.4; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{50}H_{62}O_6SiNa$, 809.4207; Found: 809.4223.



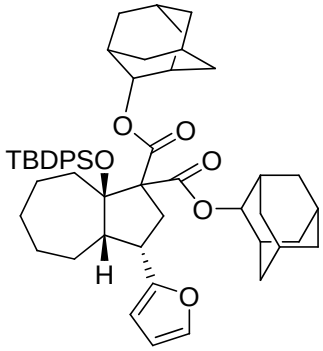
3l

Colorless oil, 143 mg (92%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ7.89-7.876 (m, 2H), 7.83-7.82 (m, 2H), 7.45-7.35 (m, 6H), 7.24-7.23 (m, 1H), 6.13 (dd, *J* = 3.2 Hz, 1.6 Hz, 1H), 5.95 (d, *J* = 3.2 Hz, 1H), 5.09 (m, 1H), 5.00 (m, 1H), 4.33-4.27 (m, 1H), 2.97-2.92 (m, 1H), 2.62 (dd, *J* = 13.6 Hz, 6.4 Hz, 1H), 2.51 (t, *J* = 13.2 Hz, 1H), 2.13-1.74 (m, 25H), 1.59-1.52 (m, 4H), 1.06 (s, 9H), 0.99-0.94 (m, 1H), 0.90-0.75 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.7, 169.3, 155.8, 140.9, 136.4, 136.3, 134.8, 134.7, 129.6, 129.5, 127.4, 109.6, 105.2, 87.5, 78.4, 77.9, 69.2, 49.3, 38.4, 37.3, 37.2, 36.4, 36.3(7), 36.3(1), 36.2, 36.1, 32.9, 32.0(8), 32.0(4), 31.9, 31.8, 31.7, 31.6, 31.5, 27.2, 27.1, 27.0, 26.9, 19.2, 12.9; **IR** (thin film, cm^{-1}): 2908, 2856, 1723, 1451, 1264, 1126, 1100; **LRMS-ESI**: $[M+Na]^+$ 795.6; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{49}H_{60}O_6SiNa$, 795.4051; Found: 795.4058.



3m

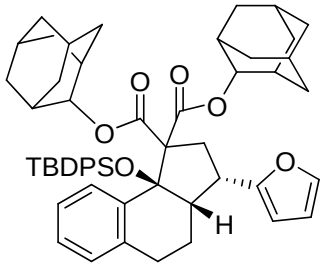
Colorless oil, 50 mg (31%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.93-7.11 (m, 2H), 7.84-7.82 (m, 2H), 7.45-7.37 (m, 6H), 7.26-7.25 (m, 1H), 6.25 (dd, *J* = 2.8 Hz, 2.0 Hz, 1H), 6.10 (d, *J* = 2.8 Hz, 1H), 5.03 (m, 1H), 4.97 (m, 1H), 3.90 (dd, *J* = 17.2 Hz, 9.6 Hz, 1H), 3.15-3.06 (m, 3H), 2.19-1.67 (m, 28H), 1.56 (dd, *J* = 24.8 Hz, 12 Hz, 4H), 1.41-1.37 (m, 1H), 1.17-1.14 (m, 1H), 1.01 (s, 9H), 0.94-0.84 (m, 2H), 0.52-0.49 (m, 1H), 0.37-0.28 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.7, 167.5, 156.6, 140.8, 136.7, 136.2, 135.3, 135.2, 129.8, 129.2, 127.7, 127.0, 109.7, 105.5, 90.5, 78.7, 77.6, 68.7, 51.4, 37.8, 37.3, 37.2, 36.4, 36.3, 36.2, 36.1, 35.9, 34.2, 31.9(5), 31.9(1), 31.8(8), 31.8(5), 31.8(2), 31.6, 27.3, 27.2, 27.1, 26.9, 24.4, 24.0, 23.4, 19.3, ; **IR** (thin film, cm^{-1}): 2907, 2855, 1722, 1451, 1261, 1235, 1211, 1168, 1100, 1077; **LRMS-ESI**: $[M+Na]^+$ 823.6; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{51}H_{64}O_6SiNa$, 823.4364; Found: 823.4396.



3n

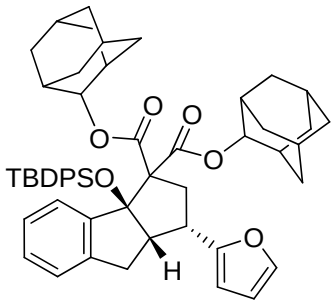
Colorless oil, 98 mg (60%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94-7.79 (m, 4H), 7.47-7.34 (m, 6H), 7.24 (dd, *J* = 2.0 Hz, 0.8 Hz, 1H), 6.23 (dd, *J* = 2.8 Hz, 2.0 Hz, 1H), 5.93 (d, *J* = 2.8 Hz, 1H), 5.13 (m, 1H), 4.96 (m, 1H), 3.90 (dd, *J* = 18.0 Hz, 9.6 Hz, 1H), 3.38 (dd, *J* = 14.4 Hz, 9.6 Hz, 1H), 2.77-2.64 (m, 1H), 2.54 (dd, *J* = 14.4 Hz,

9.6 Hz, 1H), 2.17-1.15 (m, 35H), 0.99 (s, 9H), 0.51-0.46 (m, 1H), 0.26-0.17 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.1, 167.9, 156.5, 140.9, 136.4, 136.3, 135.2, 134.9, 129.8, 129.2, 127.5, 126.9, 109.7, 106.0, 96.6, 78.3, 77.6, 70.2, 56.0, 39.2, 37.3, 37.2, 37.1, 36.4, 36.2, 35.5, 32.1, 32.0, 31.8, 31.7, 31.6, 31.5, 31.4, 31.0, 30.7, 27.2, 27.1, 27.0, 26.9, 24.7, 24.2, 19.9; **IR** (thin film, cm^{-1}): 2929, 2909, 2855, 1730, 1267, 1243, 1102, 1065; **LRMS-ESI**: $[M+Na]^+$ 837.6; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{52}H_{66}O_6SiNa$, 837.4520; Found: 837.4548.



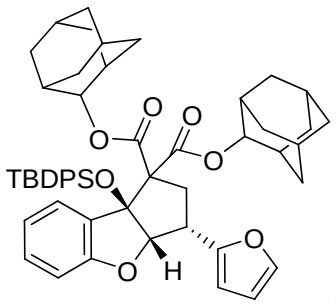
3o

Colorless oil, 97 mg (57%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.25-8.23 (m, 1H), 7.42-7.34 (m, 5H), 7.31-7.22 (m, 4H), 7.18-7.14 (m, 2H), 6.98-6.90 (m, 2H), 6.56 (d, *J* = 6.8 Hz, 1H), 6.27 (dd, *J* = 7.2 Hz, 1.6 Hz, 1H), 5.86 (d, *J* = 7.2 Hz, 1H), 5.26 (m, 1H), 4.59 (m, 1H), 4.28-4.21 (m, 1H), 3.28 (dd, *J* = 13.2 Hz, 6.8 Hz, 1H), 2.54-2.37 (m, 3H), 2.23-2.16 (m, 3H), 2.09-2.06 (m, 1H), 1.93-1.86 (m, 6H), 1.77-1.52 (m, 18H), 1.48-1.45 (m, 1H), 1.40-1.36 (m, 2H), 0.95 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.1, 167.7, 155.0, 141.2, 139.5, 138.3, 136.6, 136.4, 133.9, 133.7, 129.7, 129.2, 128.8, 127.3, 127.0, 126.9, 126.7, 125.4, 109.8, 105.8, 89.2, 78.1, 78.0, 72.7, 53.5, 39.9, 38.0, 37.3, 37.2, 36.4, 36.2(2), 36.2(0), 36.1, 32.1,32.0, 31.9, 31.7, 31.6, 31.5, 31.3, 31.2, 28.3(4), 27.3(3), 27.2, 27.0, 26.9, 26.8, 21.2, 19.4; **IR** (thin film, cm^{-1}): 2909, 2855, 1728, 1452, 1260, 1101, 1042; **LRMS-ESI**: $[M+Na]^+$ 871.7; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{53}H_{64}O_6SiNa$, 871.4364; Found: 871.4381.



3p

Colorless oil, 146 mg (87%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50-7.42 (m, 5H), 7.31-7.23 (m, 3H), 7.20-7.14 (m, 4H), 6.97 (td, *J* = 7.2 Hz, 1.2 Hz, 1H), 6.90 (t, *J* = 7.2 Hz, 1H), 6.55 (d, *J* = 7.2 Hz, 1H), 6.20 (dd, *J* = 6.4 Hz, 3.2 Hz, 1H), 5.82 (d, *J* = 6.4 Hz, 1H), 5.10 (m, 1H), 4.90 (m, 1H), 3.89-3.82 (m, 1H), 3.35-3.29 (m, 1H), 2.60 (dd, *J* = 14.0 Hz, 7.2 Hz, 1H), 2.33 (dd, *J* = 14.0 Hz, 11.2 Hz, 1H), 2.23 (m, 1H), 2.15-2.12 (m, 1H), 2.01-1.53 (m, 26H), 1.47-1.44 (m, 1H), 1.34-1.30 (m, 1H), 1.00 (s, 9H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.4, 156.4, 145.0, 142.3, 141.0, 136.2, 136.1, 134.4, 134.3, 129.0, 128.8, 128.5, 126.9, 126.7, 126.2, 125.8, 123.8, 109.7, 105.9, 97.6, 77.9, 77.6, 69.6, 54.2, 37.5, 37.3, 37.2(9), 37.2(3), 36.2(8), 36.2(7), 36.1, 32.8, 31.8(6), 31.8(3), 31.7(9), 31.7(4), 31.7(3), 31.6, 31.4, 27.2, 27.0, 26.9(7), 26.9(2), 26.8, 19.3; **IR** (thin film, cm^{-1}): 2907, 2855, 1728, 1451, 1259, 1100, 1080; **LRMS-ESI**: $[M+Na]^+$ 857.5; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{54}H_{62}O_6SiNa$, 857.4207; Found: 857.4227.

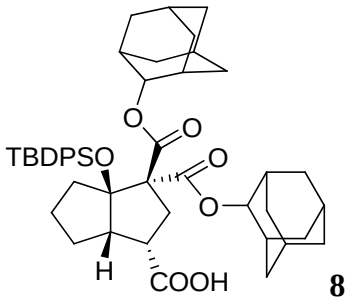


3q

Colorless oil, 132 mg (79%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54-7.52 (m, 2H), 7.47-7.46 (m, 2H), 7.31-7.12 (m, 8H), 6.83 (t, *J* = 3.2 Hz, 1H), 6.50 (t, *J* = 3.2 Hz, 1H), 6.23 (dd, *J* = 2.8 Hz, 2.0 Hz, 1H), 6.07 (d, *J* = 8.0 Hz, 1H), 5.94 (d, *J* = 2.8 Hz, 1H), 5.20 (d, *J* = 7.6 Hz, 1H), 5.09-5.08 (m, 2H), 4.22-4.16 (m, 1H), 2.38-2.27 (m, 2H), 2.22 (m, 1H), 2.14-2.11 (m, 1H), 2.06-2.01 (m, 2H), 1.95-1.47 (m, 24H), 1.03 (s,

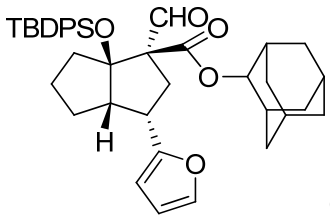
9H), 1.33-1.30 (m, 1H), 0.89-0.83 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.1, 167.3, 161.3, 152.9, 141.4, 136.1, 133.7, 133.5, 130.6, 129.0, 128.9, 127.0, 126.7, 126.6, 125.5, 119.9, 109.9, 106.8, 92.6, 91.5, 78.7, 77.8, 68.7, 39.4, 37.2(7), 37.2(2), 36.3, 36.2, 36.1, 36.0, 31.9, 31.8, 31.7, 31.6, 27.1, 27.0, 26.8(9), 26.8(3), 19.4; **IR** (thin film, cm^{-1}): 2926, 2855, 1729, 1475, 1262, 1100, 1082; **LRMS-ESI**: $[M+Na]^+$ 859.7; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{50}H_{60}O_7SiNa$, 859.4000; Found: 859.4004.

7. Chemical Transformations of 3k



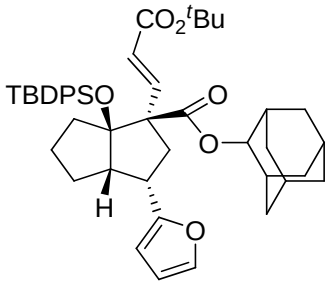
8

A flask is charged with a magnetic stirrer, 3 mL of carbon tetrachloride, 4.5 mL of acetonitrile, 4.5 mL of water, and 64.2 mg (0.3 mmol) of sodium metaperiodate. To this biphasic solution 2 mg (0.01 mol) of ruthenium trichloride hydrate was added, and the entire mixture was stirred vigorously for 2 h at room temperature. Then 77.8 mg (0.1 mmol) of **3k** in 0.5 mL acetonitrile was added, and TLC indicated complete consumption of the starting material after 12 hours. Then 10 mL of CH_2C1_2 was added, and the phases were separated. The upper aqueous phase was extracted 3 times with CH_2C1_2. The combined organic extracts were dried ($MgSO_4$) and concentrated. The resulting residue was diluted with 20 mL of diethyl ether, filtered through a Celite pad, and concentrated. The crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate as eluent) to yield **8** as a colorless oil, 45.4 mg (60%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87-7.77 (m, 4H), 7.40-7.35 (m, 6H), 5.06 (m, 1H), 4.96 (m, 1H), 3.77-3.70 (m, 1H), 2.92-2.85 (m, 1H), 2.46-2.33 (m, 2H), 2.04-1.53 (m, 30H), 1.19-1.14 (m, 1H), 0.98 (s, 9H), 1.04-0.92 (m, 1H), 0.92-0.82 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 179.5, 169.2, 169.0, 136.4, 136.2, 134.8, 134.7, 129.5, 129.4, 127.3, 127.1, 96.6, 78.3, 77.9, 68.8, 52.5, 43.1, 40.0, 37.3, 37.2, 36.4, 36.2, 36.1, 34.2, 31.9, 31.8, 31.7(8), 31.7(3), 31.5, 31.4, 29.1, 27.1, 27.0, 26.9, 26.8, 24.8, 19.5; **IR** (thin film, cm^{-1}): 2908, 2856, 1725, 1451, 1258, 1100, 1066, 1041; **LRMS-MALDI**: $[M+Na]^+$ 787.4; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{47}H_{60}O_7SiNa$, 787.4000; Found: 787.4017.



9

Cycloadduct **3k** (156 mg, 0.2 mmol) was dissolved in dichloromethane (40 mL) and then cooled to -78 °C. DIBAL-H (2.4 mL of 1.0 M solution in hexane, 2.4 mmol) was added dropwise and the reaction stirred for 15 minutes, after which multiply eluted TLC showed complete consumption of the starting material. Methanol (5 mL) was then added slowly to quench the excess DIBAL-H, and the mixture stirred at -78 °C for 20 minutes, after which it was removed from the dry ice bath and allowed to warm to room temperature. The reaction was then poured into 5% HCl (20 mL) and the organic layers were separated. The aqueous layer was extracted 3 times with DCM, and the combined organic layer was washed with 5% HCl. The organic layer was dried with $MgSO_4$, and the solvent removed under reduced pressure. The residual material was purified by flash column chromatography on silica gel (hexanes/ethyl acetate as eluent) to yield aldehyde **9**, 122 mg (96%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.24 (s, 1H), 7.80-7.75 (m, 4H), 7.47-7.36 (m, 6H), 7.28-7.27 (m, 1H), 6.24 (dd, *J* = 3.2 Hz, 2.0 Hz, 1H), 6.01 (d, *J* = 3.2 Hz, 1H), 5.12-5.11 (m, 1H), 4.27 (dt, *J* = 12.0 Hz, 8.0 Hz, 1H), 2.85-2.79 (m, 1H), 2.37-2.26 (m, 2H), 2.11-2.03 (m, 3H), 1.89-1.58 (m, 13H), 1.04 (s, 9H), 1.02-0.92 (m, 1H), 0.91-0.84 (m, 1H), 0.82-0.74 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.6, 169.4, 156.3, 141.0, 136.2, 136.0, 134.5, 134.1, 129.9, 129.7, 127.6, 127.4, 109.7, 105.6, 97.5, 78.6, 71.6, 56.0, 38.3, 38.2, 37.2, 36.3, 36.1, 32.0, 31.8, 31.5(7), 31.5(2), 27.0(5), 27.0(2), 26.8, 26.3, 24.3, 19.3; **IR** (thin film, cm^{-1}): 2929, 2856, 1713, 1470, 1428, 1260, 1177, 1158; **LRMS-ESI**: $[M+Na]^+$ 659.4; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{40}H_{48}O_5SiNa$, 659.3163; Found: 659.3176.

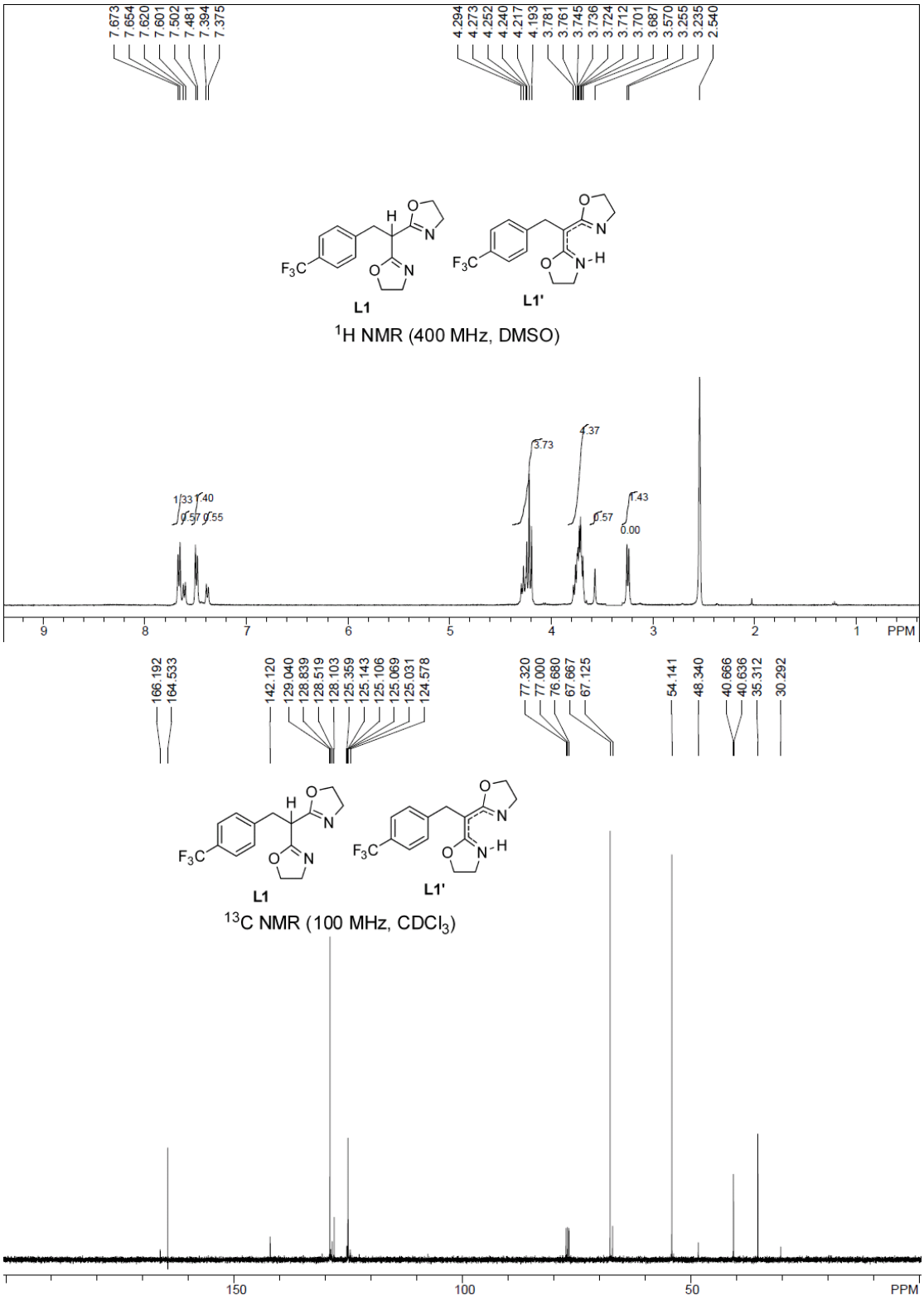


10

Tert-butyl 2-(diethoxyphosphoryl)acetate (35 mg, 0.14 mmol) was dissolved in THF (2 mL) and cooled in an ice bath. NaH (7.2 mg, 0.18 mmol) was added and the slurry was stirred for 10 minutes. Aldehyde **9** (45.2 mg, 0.07 mmol) in THF (2 mL) was then added slowly via cannula, and TLC indicated complete consumption of the starting material after 24 hours. The THF was removed under reduced pressure. To the resulting residue was added water (50 mL), 5% HCl (10 mL), and ethyl acetate (50mL). The layers were separated, and the aqueous washed 3 times with ethyl acetate. The combined organics were washed with water, brine, and dried with $MgSO_4$. The solvent was removed under reduced pressure and the residual material purified by column chromatography on silica gel (hexanes/ethyl acetate as eluent) to yield **10** (40.2 mg, 77%) as a pale yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80-7.77 (m, 4H), 7.67 (d, *J* = 16.4 Hz, 1H), 7.43-7.34 (m, 6H), 7.28 (dd, *J* = 1.6 Hz, 0.8 Hz, 1H), 6.25 (dd, *J* = 3.2 Hz, 1.6 Hz, 1H), 6.01 (d, *J* = 3.2 Hz, 1H), 4.98 (m, 1H), 4.44-4.37 (m, 1H), 2.88-2.82 (m, 1H), 2.43 (dd, *J* = 12.8 Hz, 6.4 Hz, 1H), 2.23-2.19 (m, 1H), 2.07-2.00 (m, 3H), 1.95-1.61 (m, 13H), 1.53 (s, 9H), 1.52-1.48 (m, 1H), 1.04 (s, 9H), 0.99-0.92 (m, 1H), 0.90-0.75 (m, 2H), 0.74-0.63 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.6, 165.5, 156.7, 147.9, 140.9, 136.2, 136.0, 134.8, 134.4, 129.7, 129.4, 127.5, 127.2, 121.0, 109.7, 105.4, 98.2, 80.2, 77.9(8), 77.9(6), 63.8, 55.6, 39.0, 38.4, 37.3, 36.2, 36.0, 35.5, 31.8, 31.7, 31.4, 28.0, 27.2, 27.1, 27.0, 26.8, 24.6, 19.3; **IR** (thin film, cm^{-1}): 2930, 2856, 1712, 1647, 1471, 1428, 1244, 1169; **LRMS-MALDI**: $[M+Na]^+$ 757.4; **HRMS-MALDI**: $[M+Na]^+$ Calculated for $C_{46}H_{58}O_6SiNa$, 757.3894; Found: 757.3900.

8. ^{1}H and ^{13}C NMR Spectra

L1



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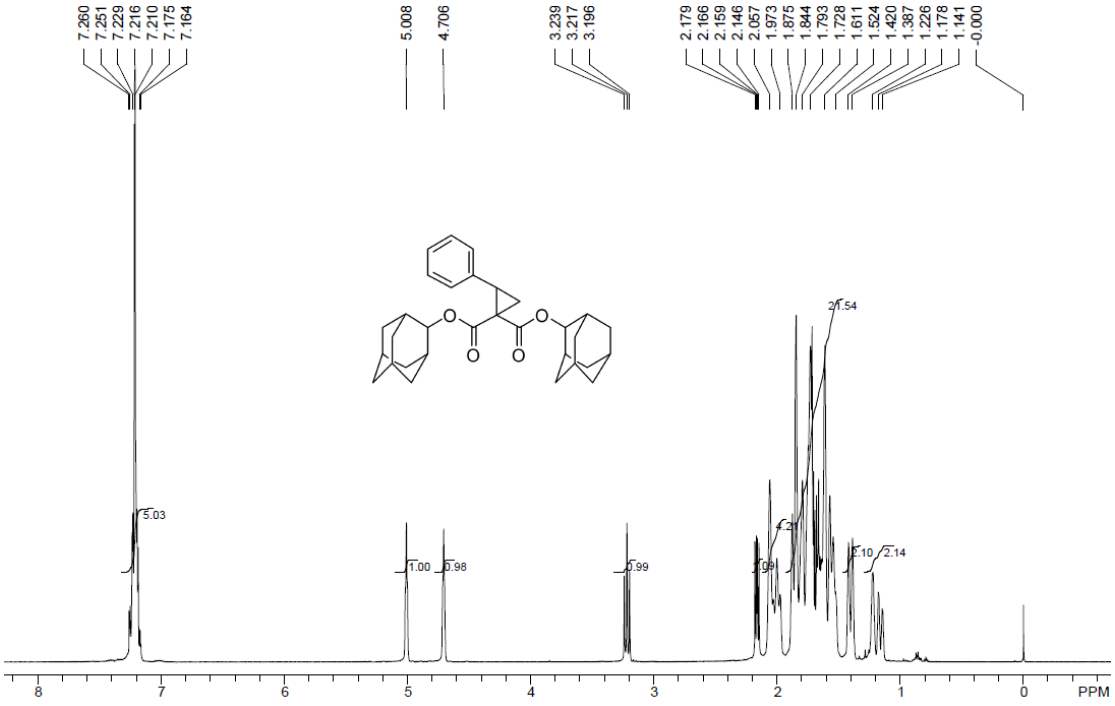
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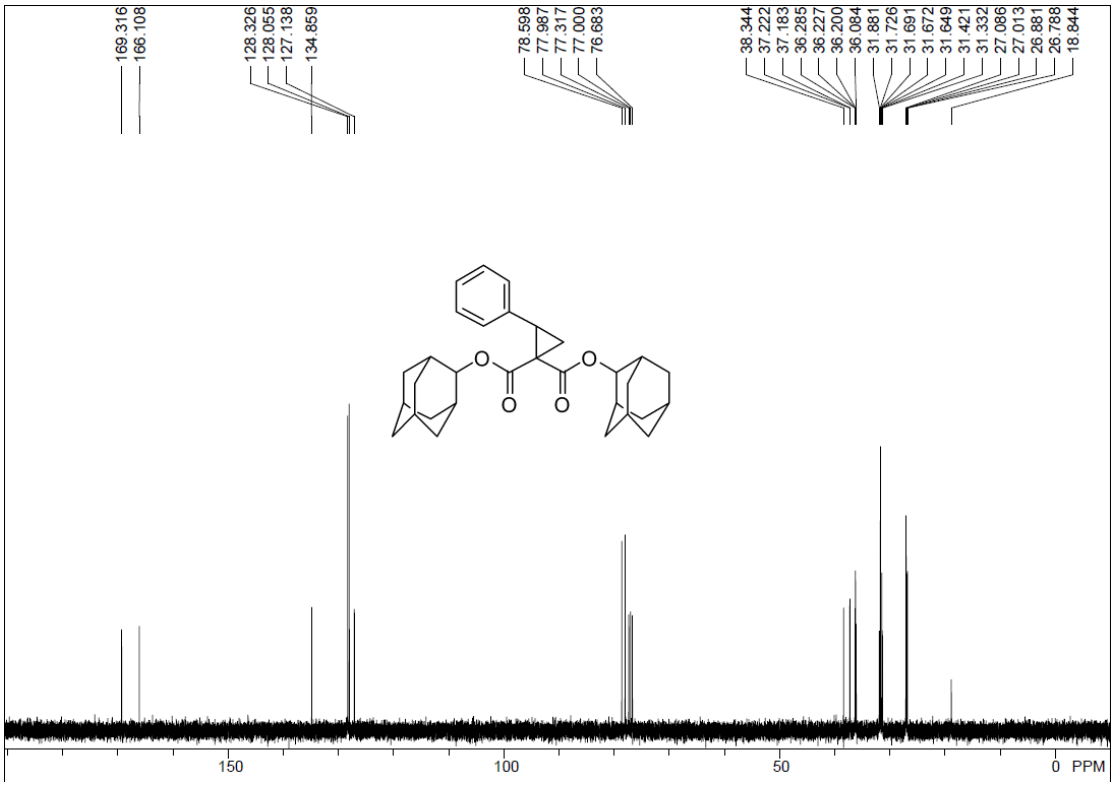
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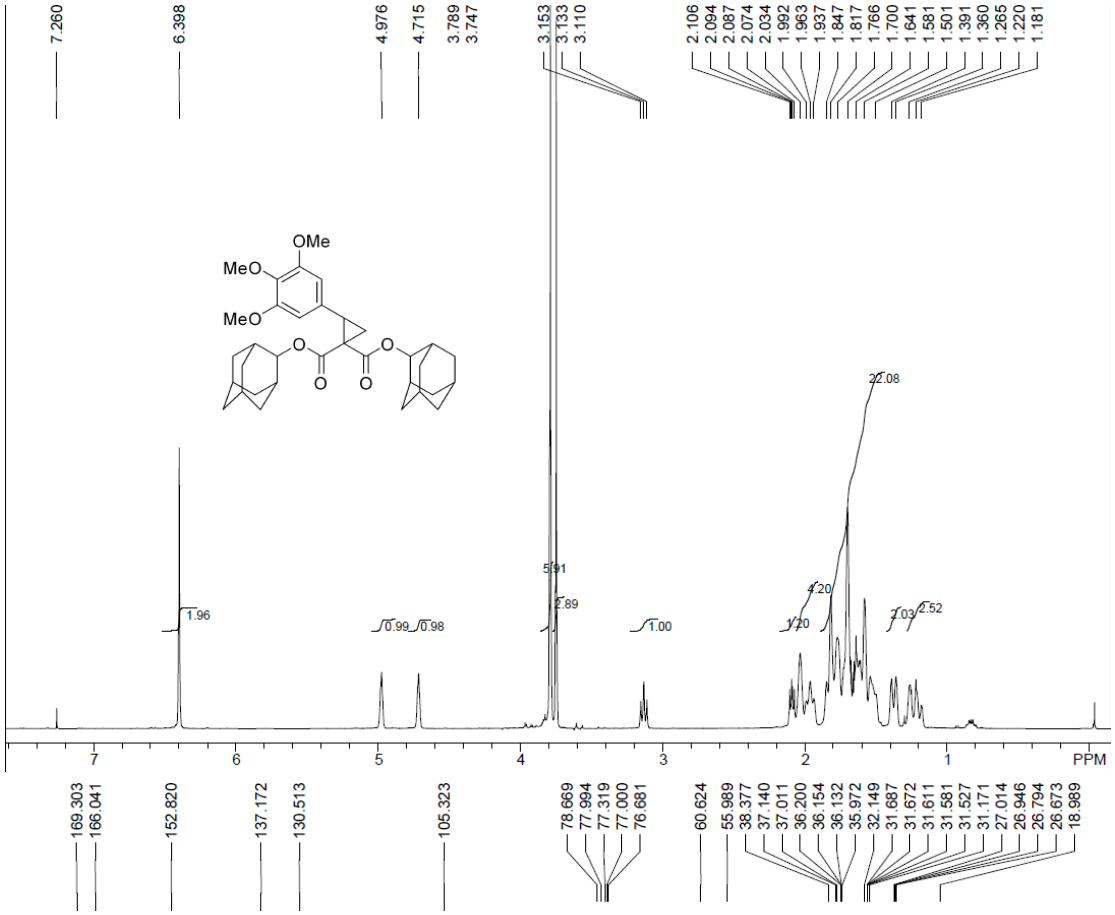
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1.220
1.181
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MeO
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5
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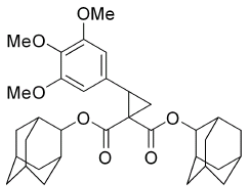
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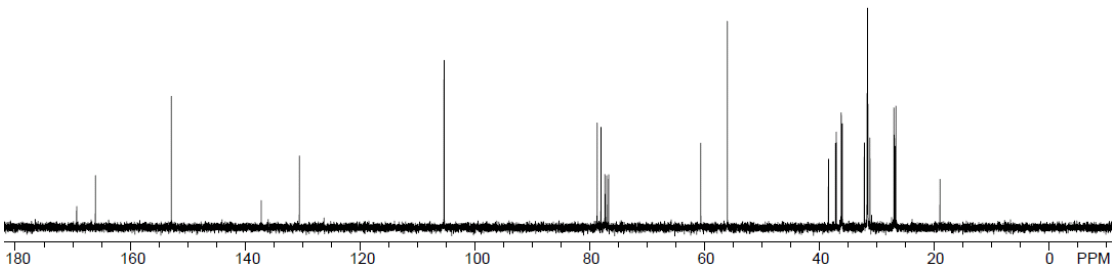
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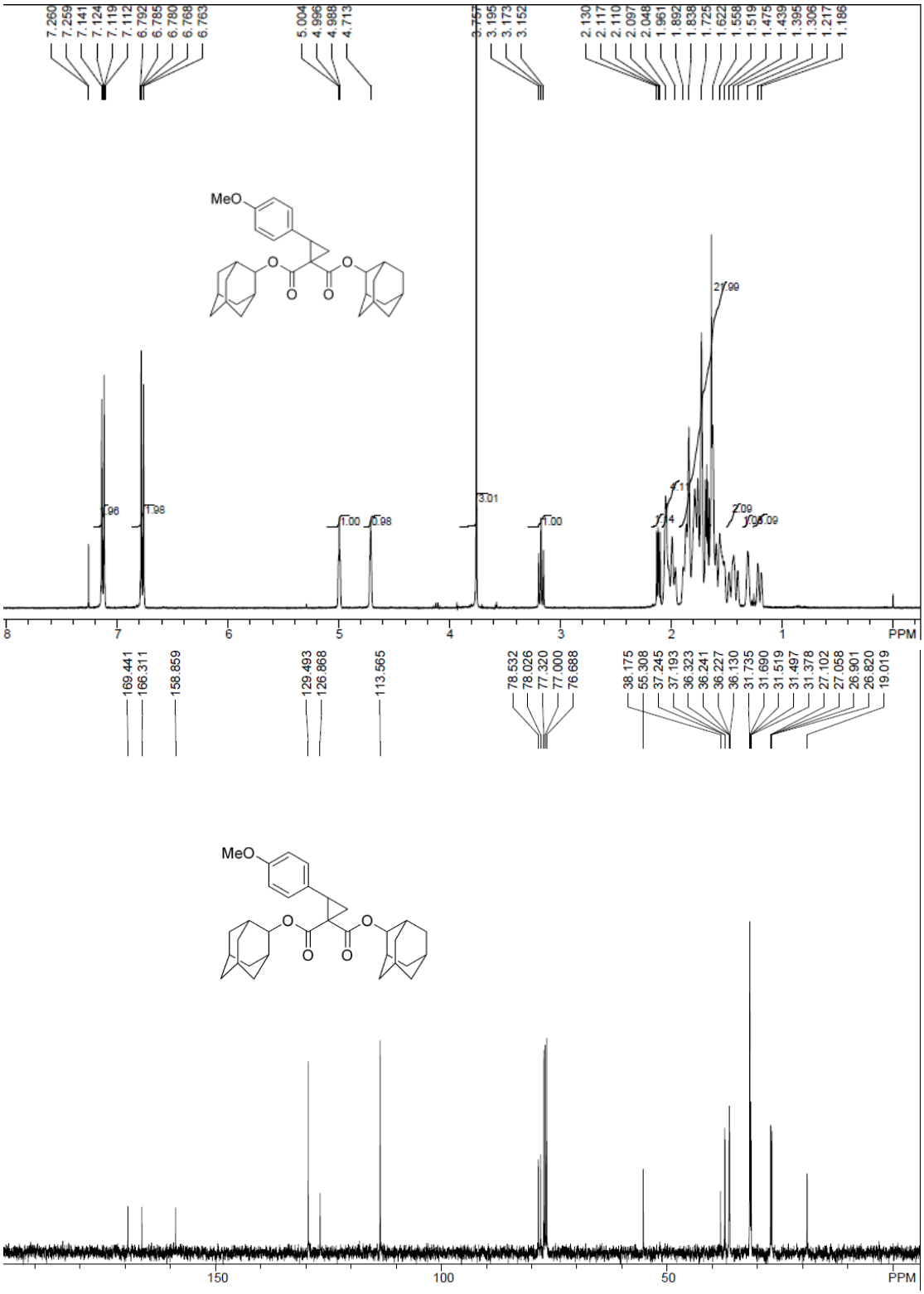
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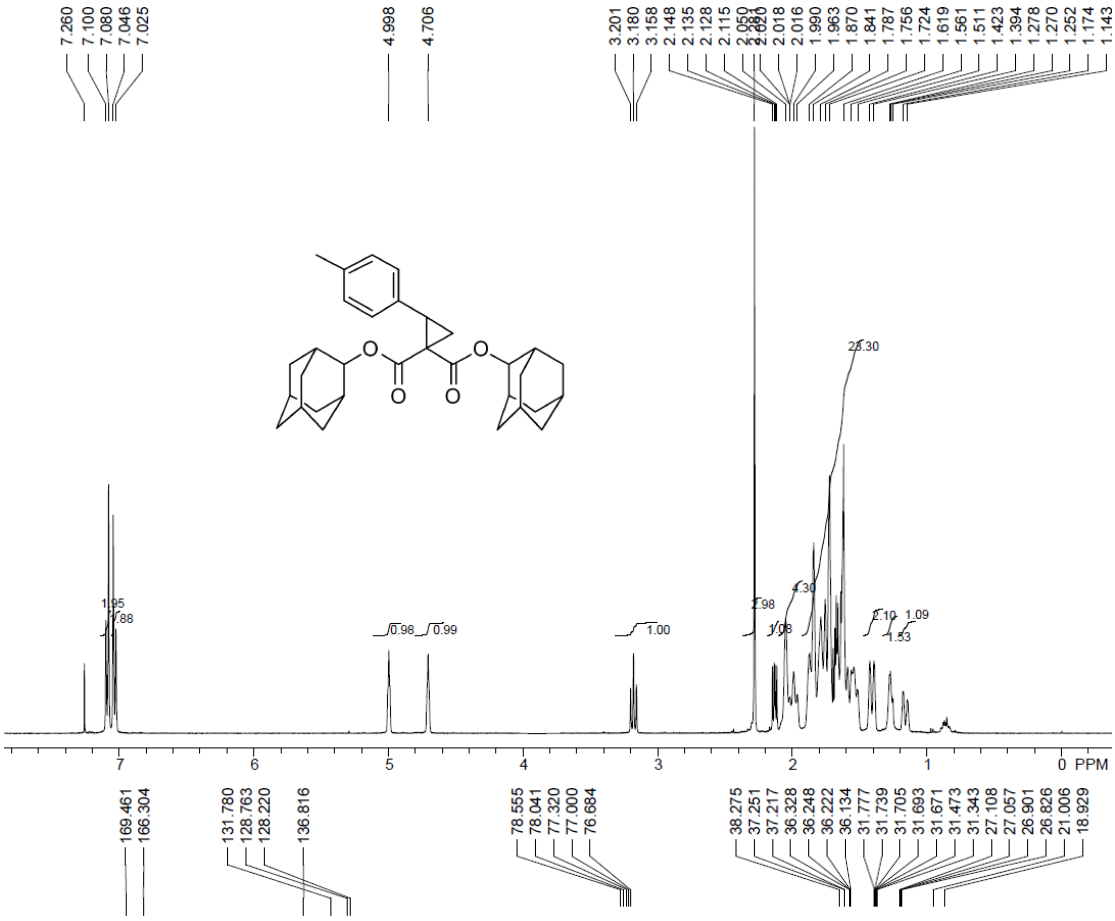
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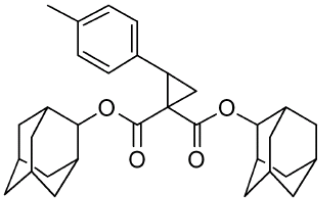
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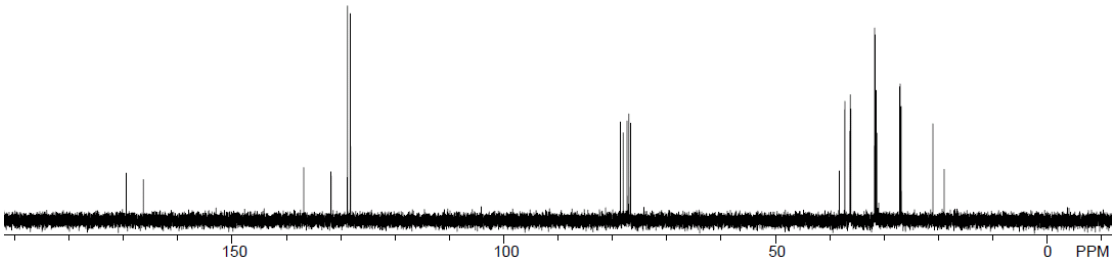
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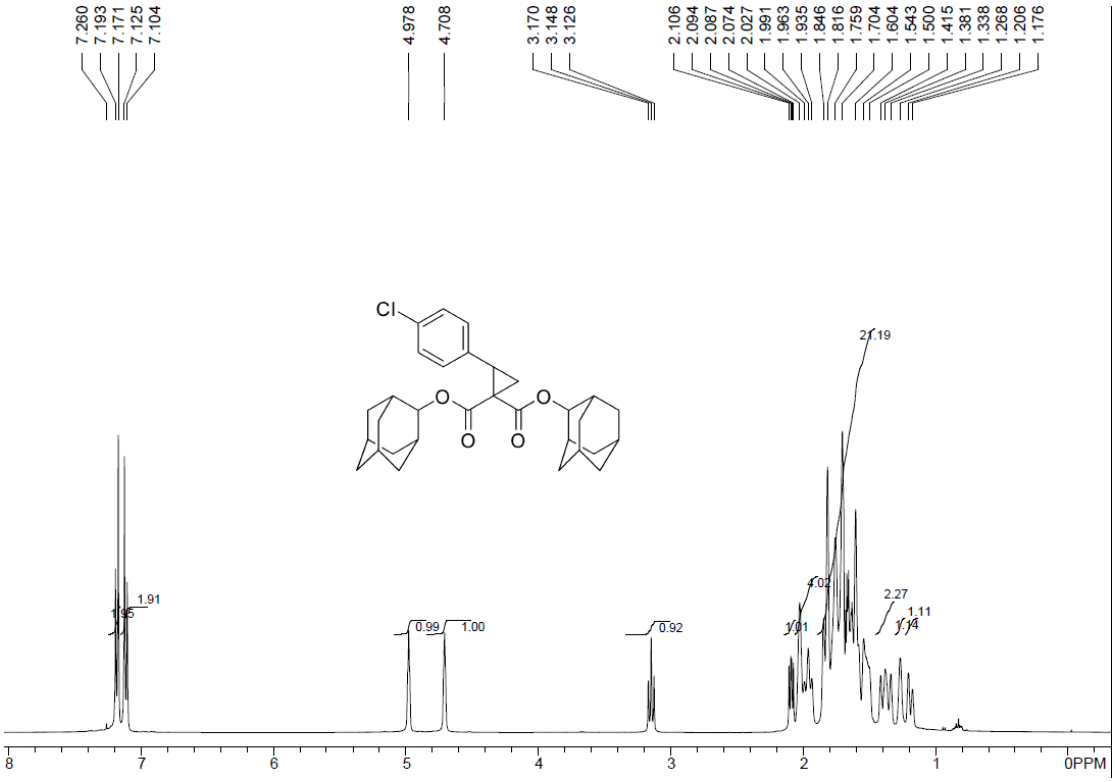
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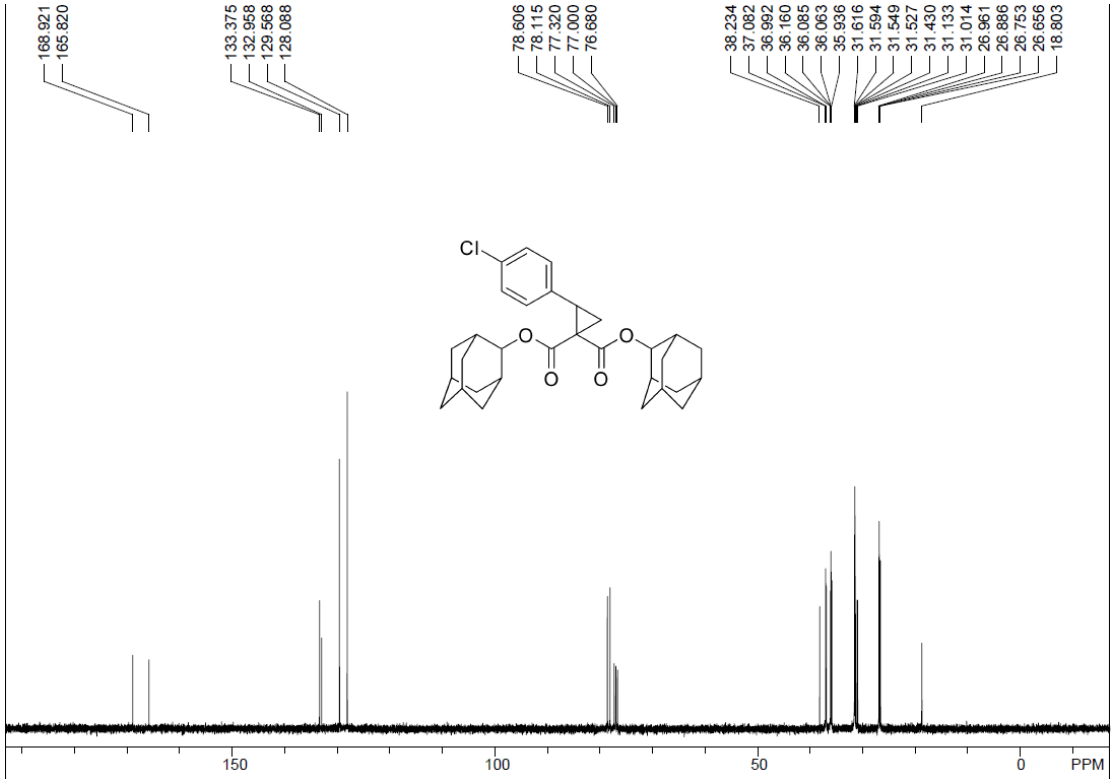
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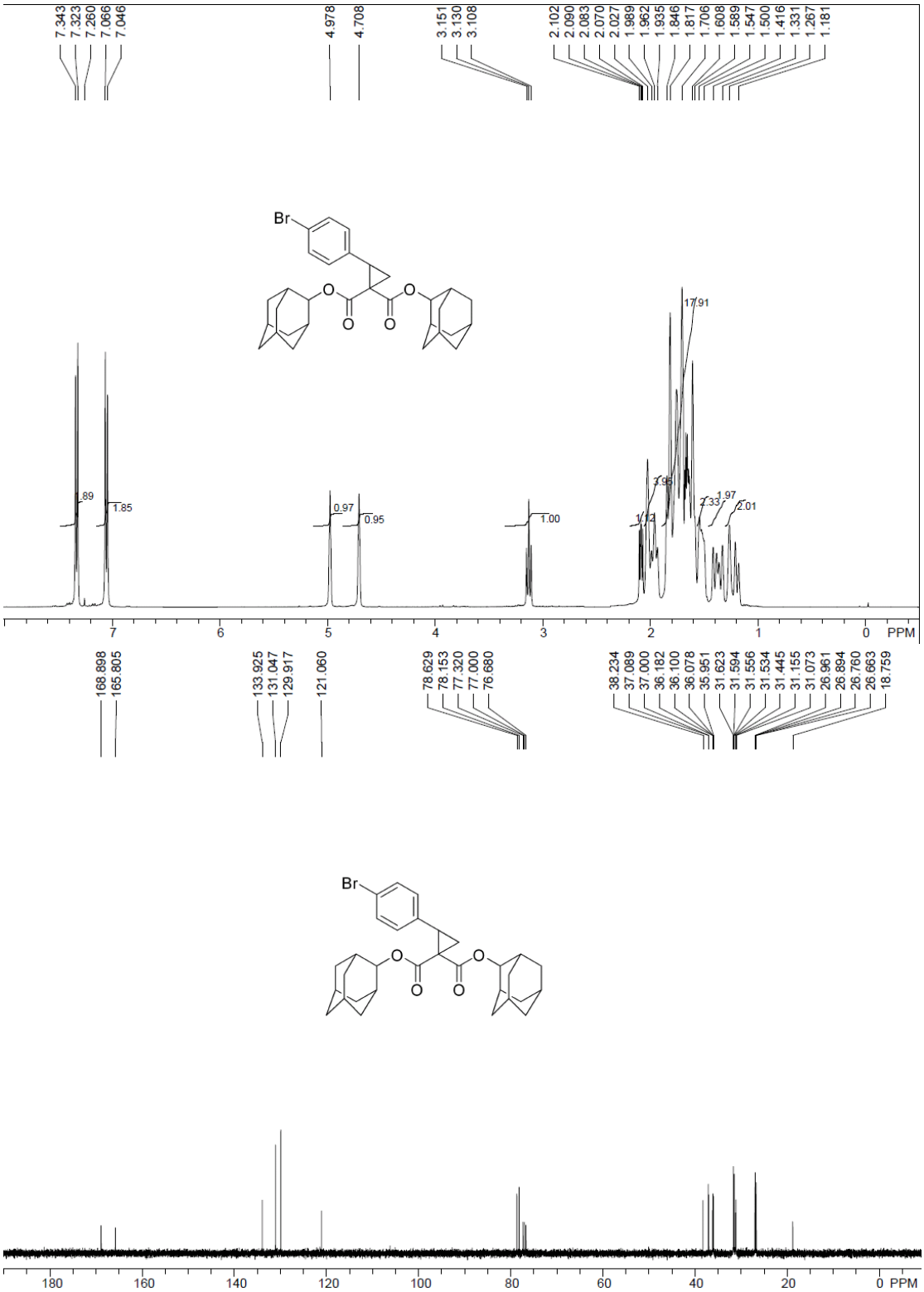
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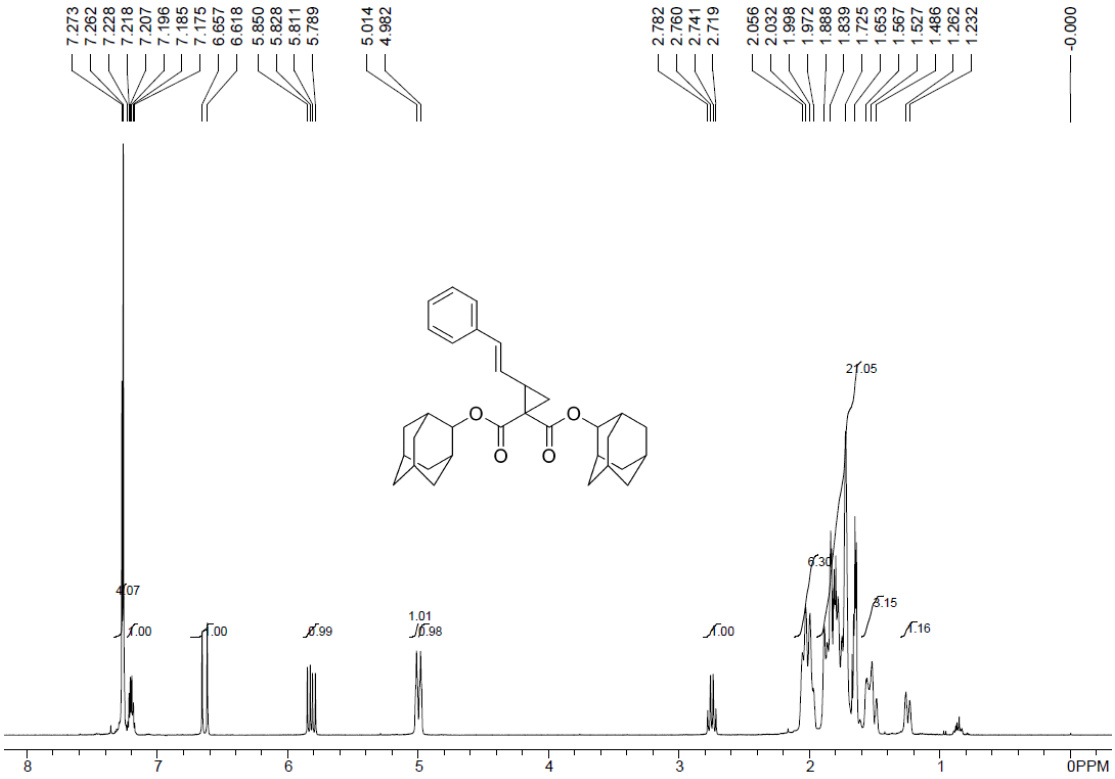
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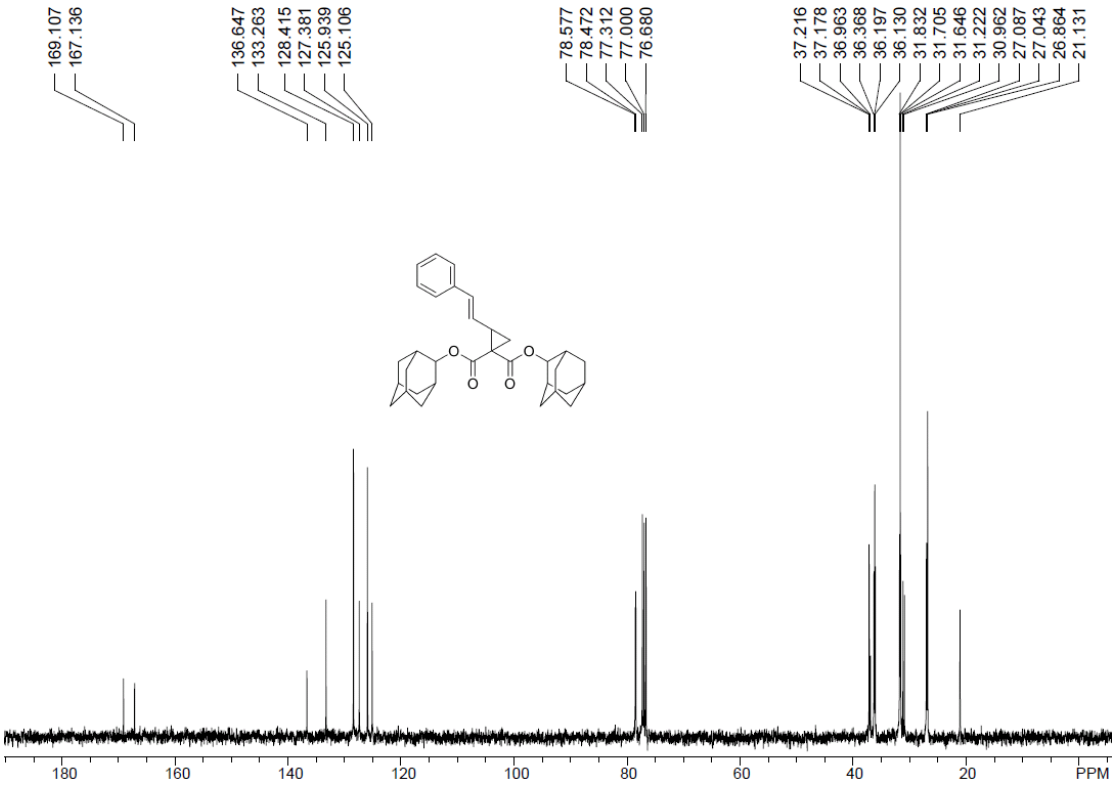
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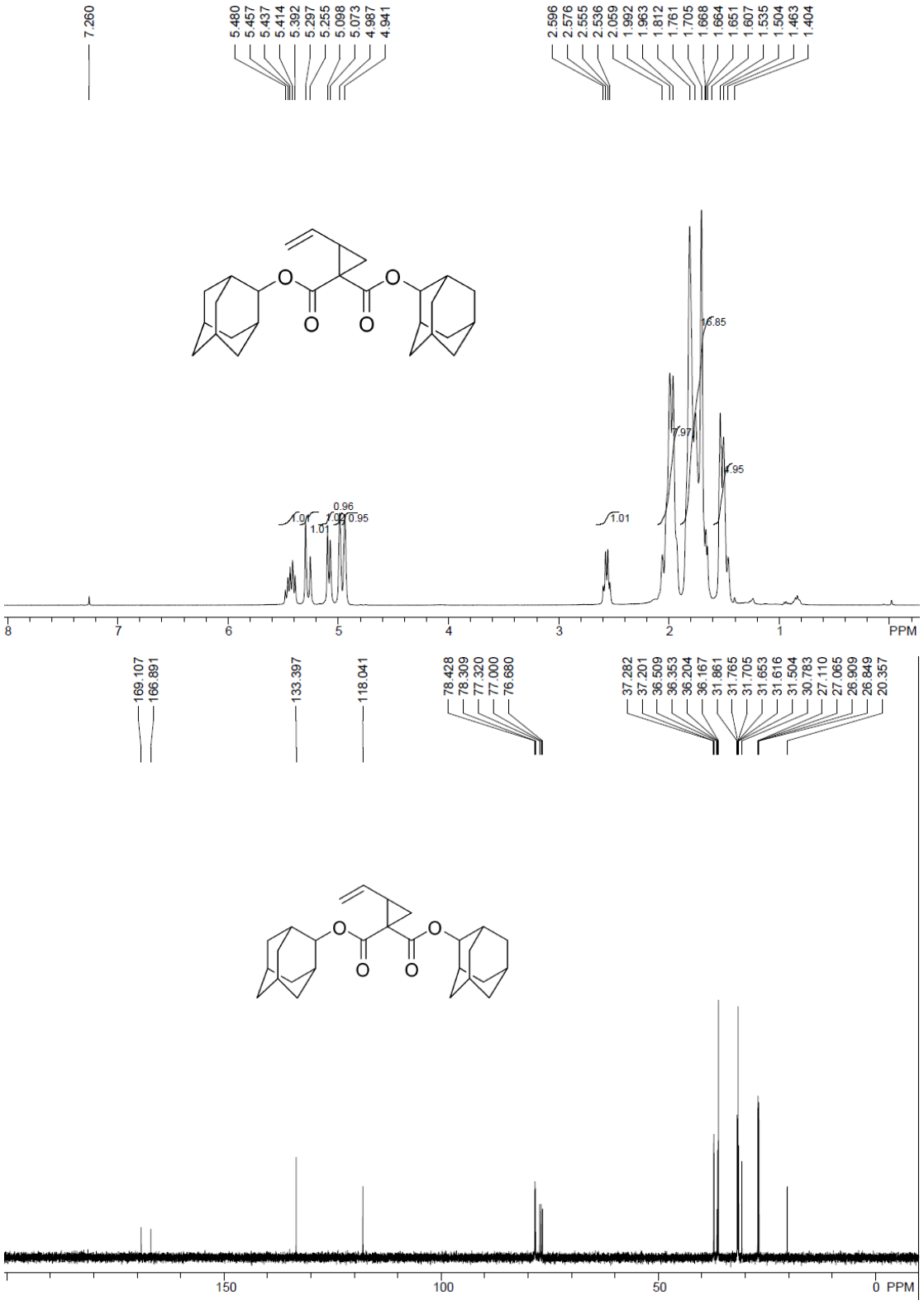
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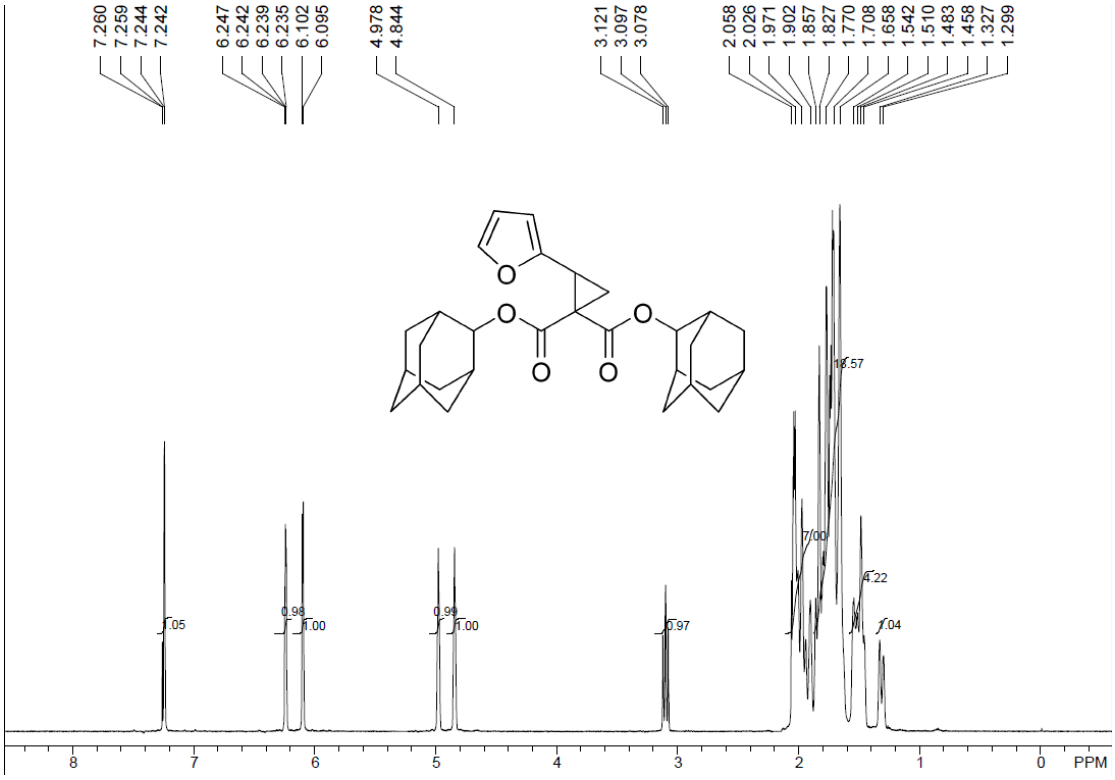
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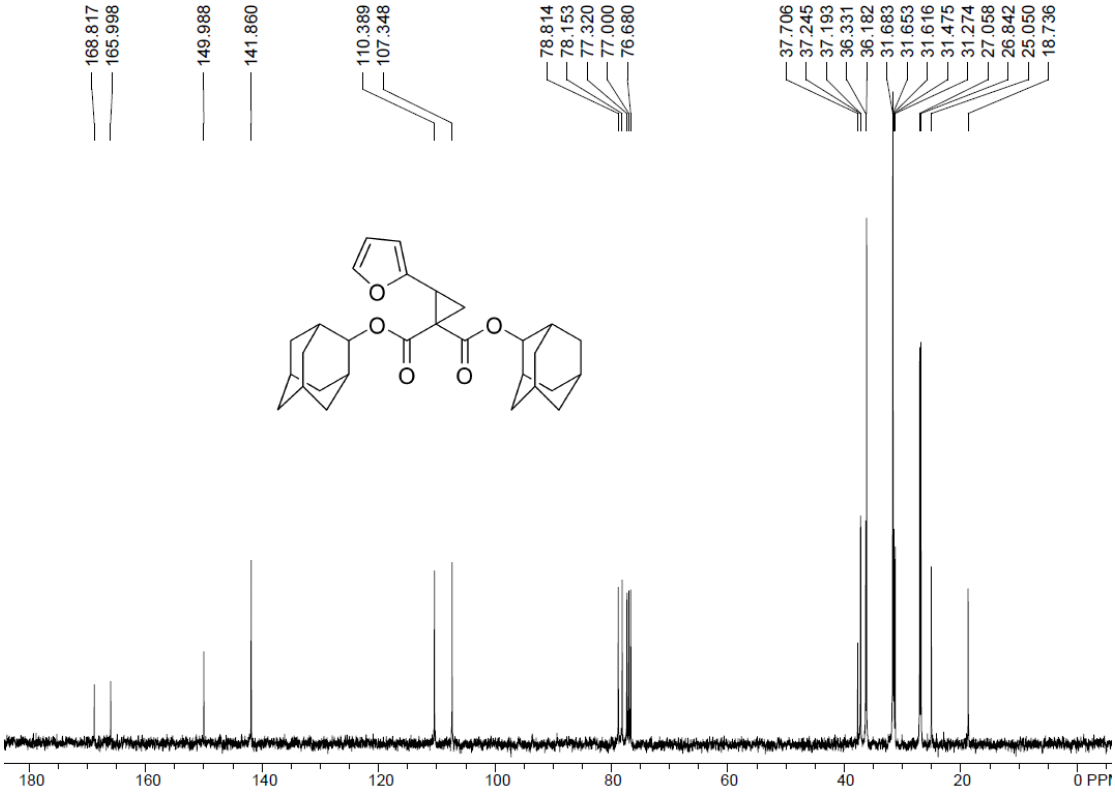
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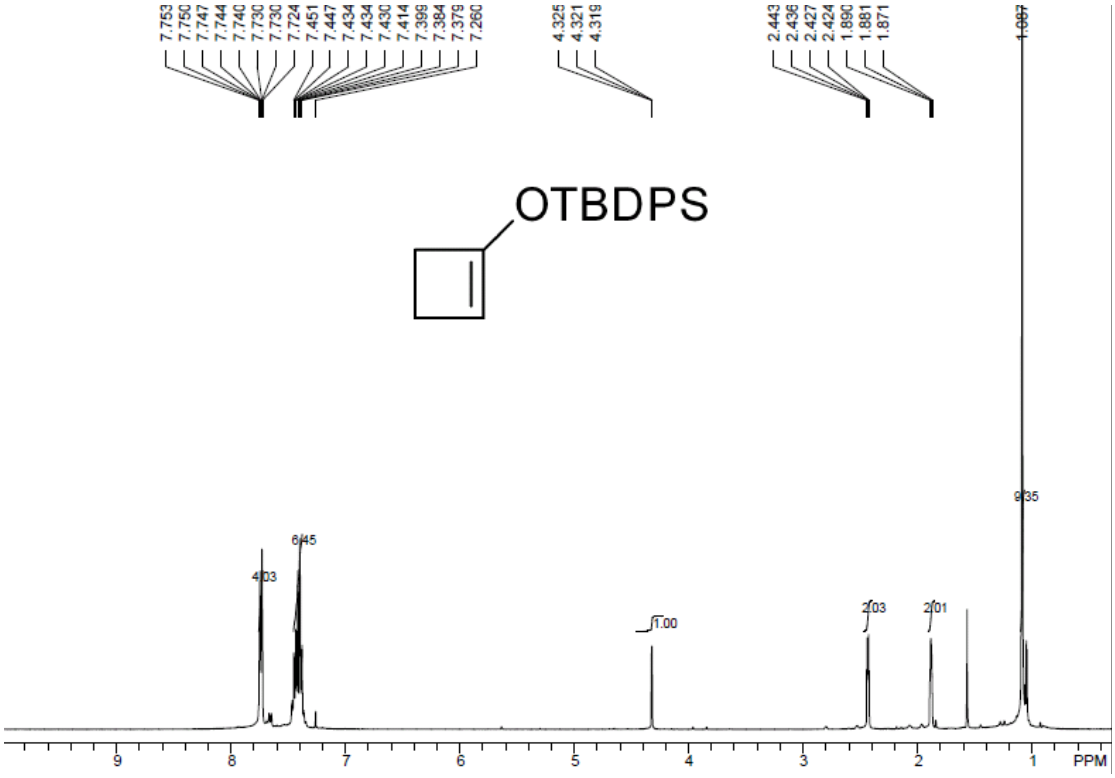
2e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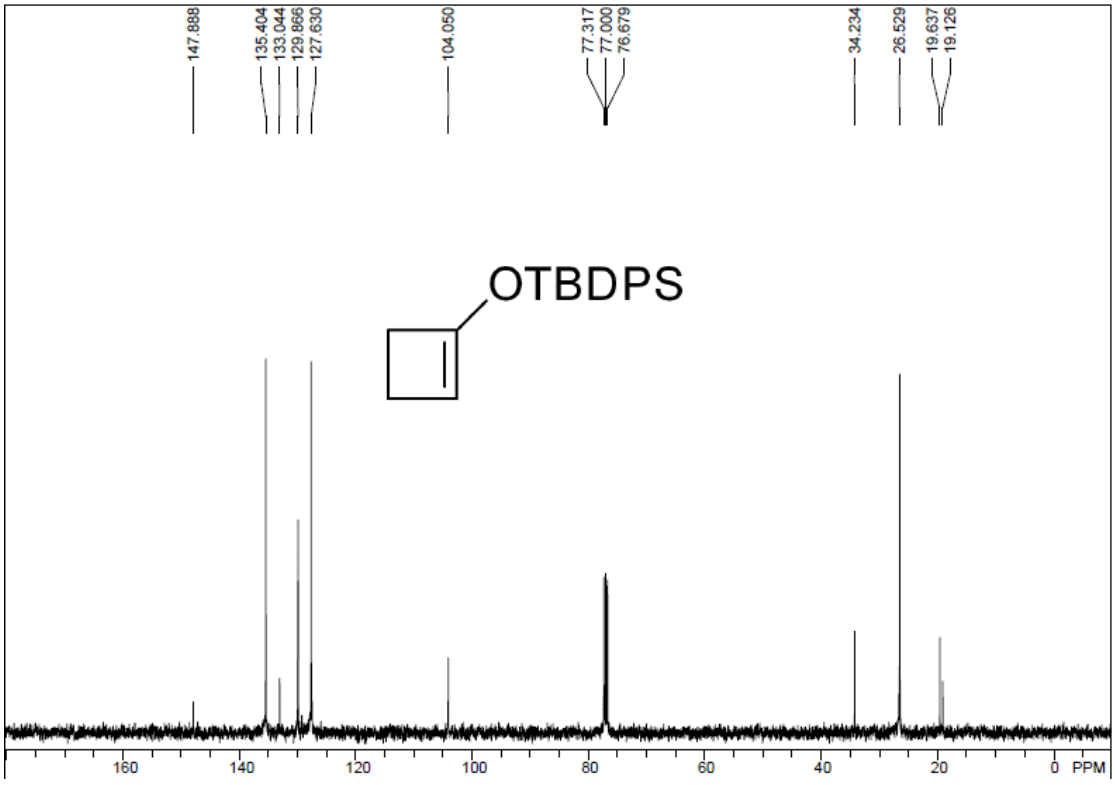
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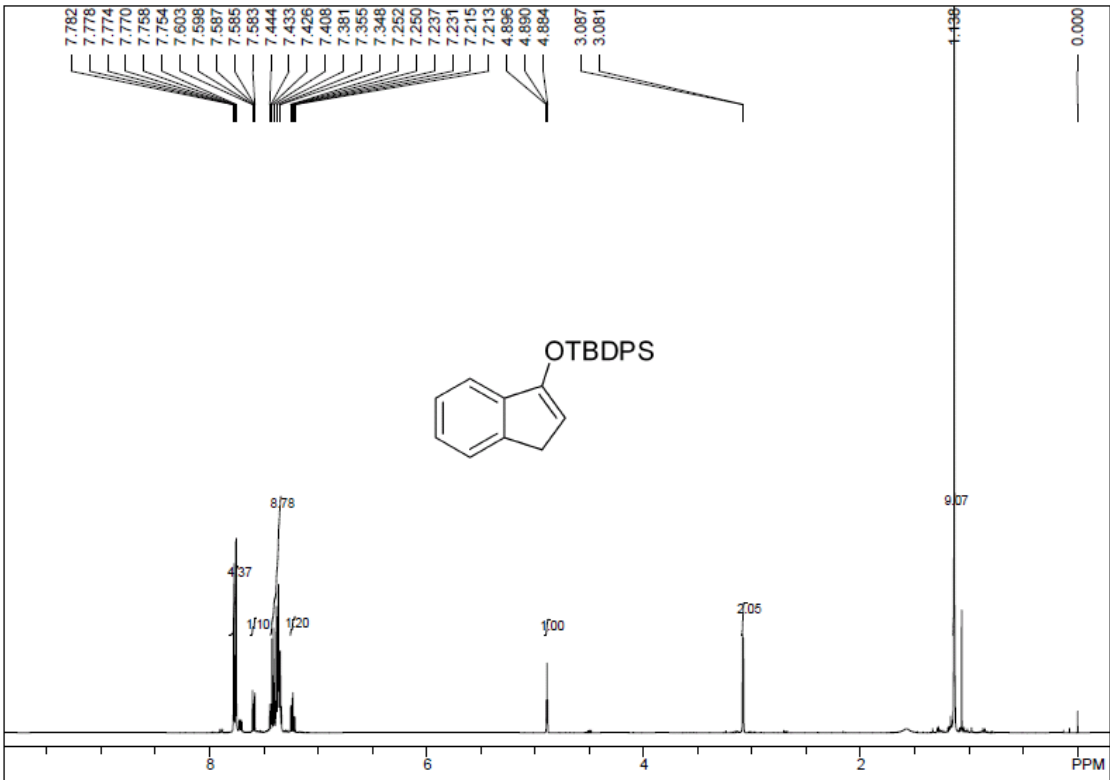
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8
6
4
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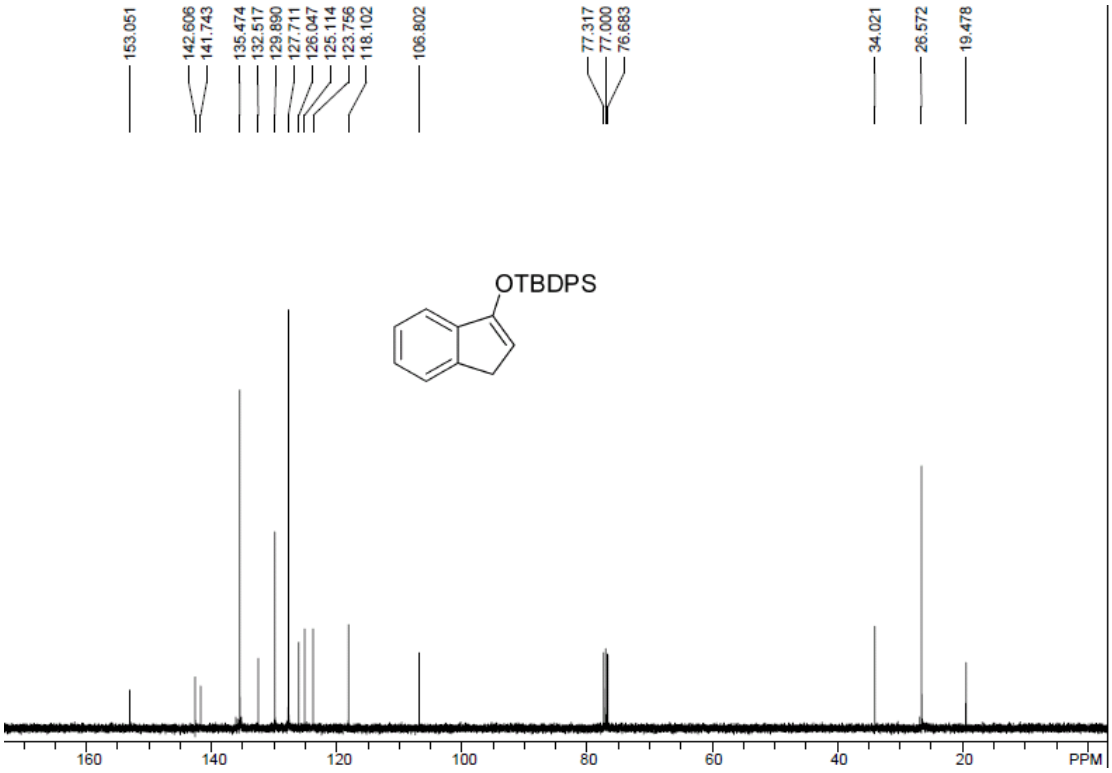
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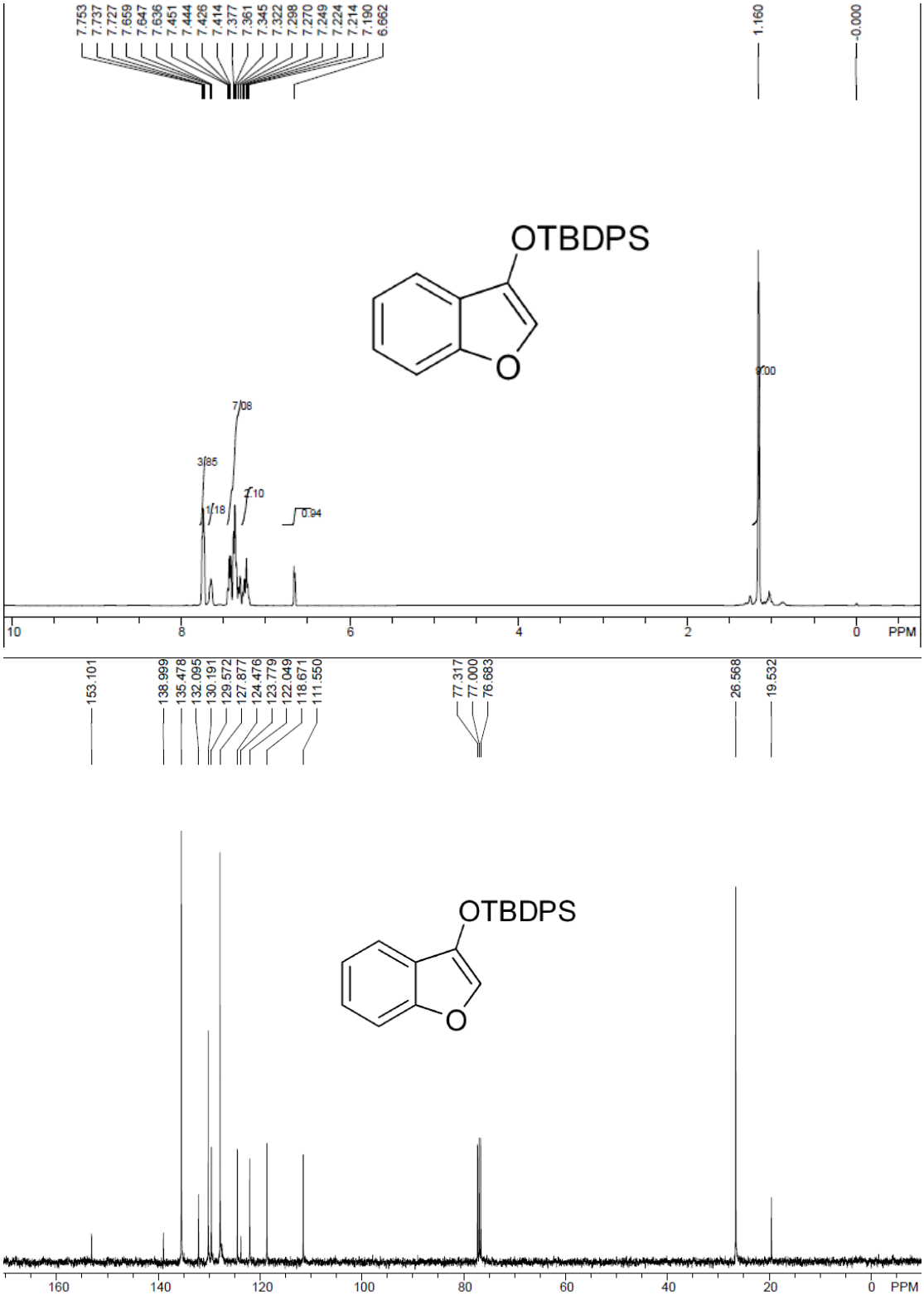
20
PPM

2g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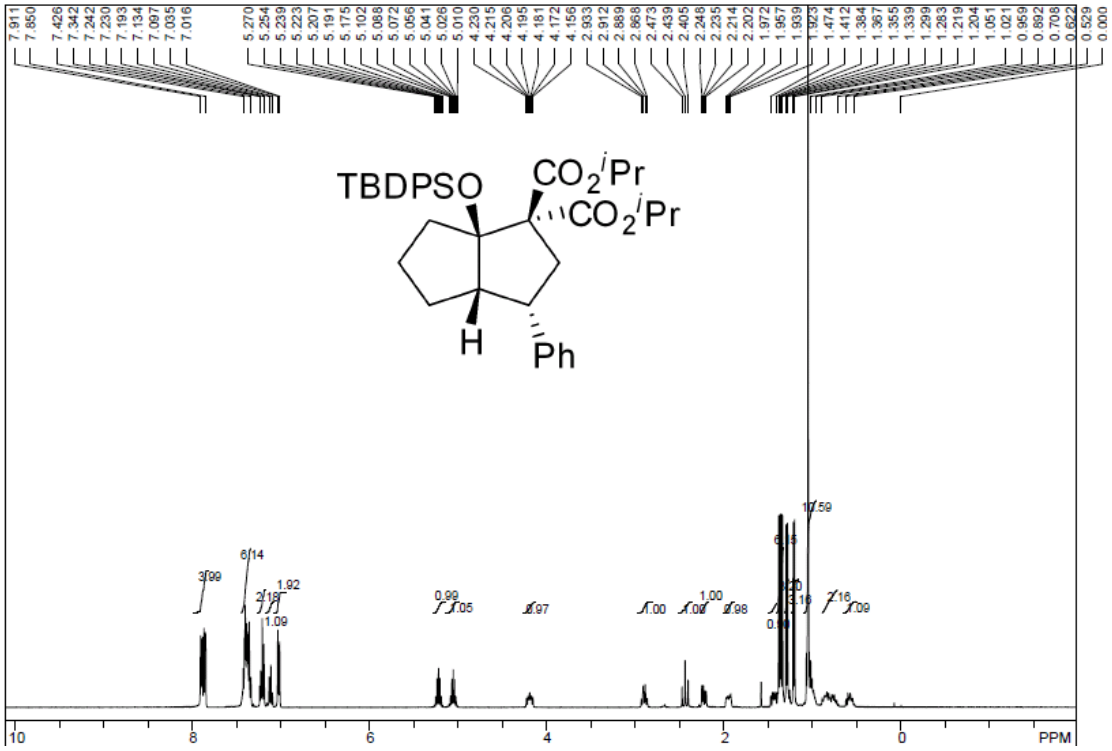

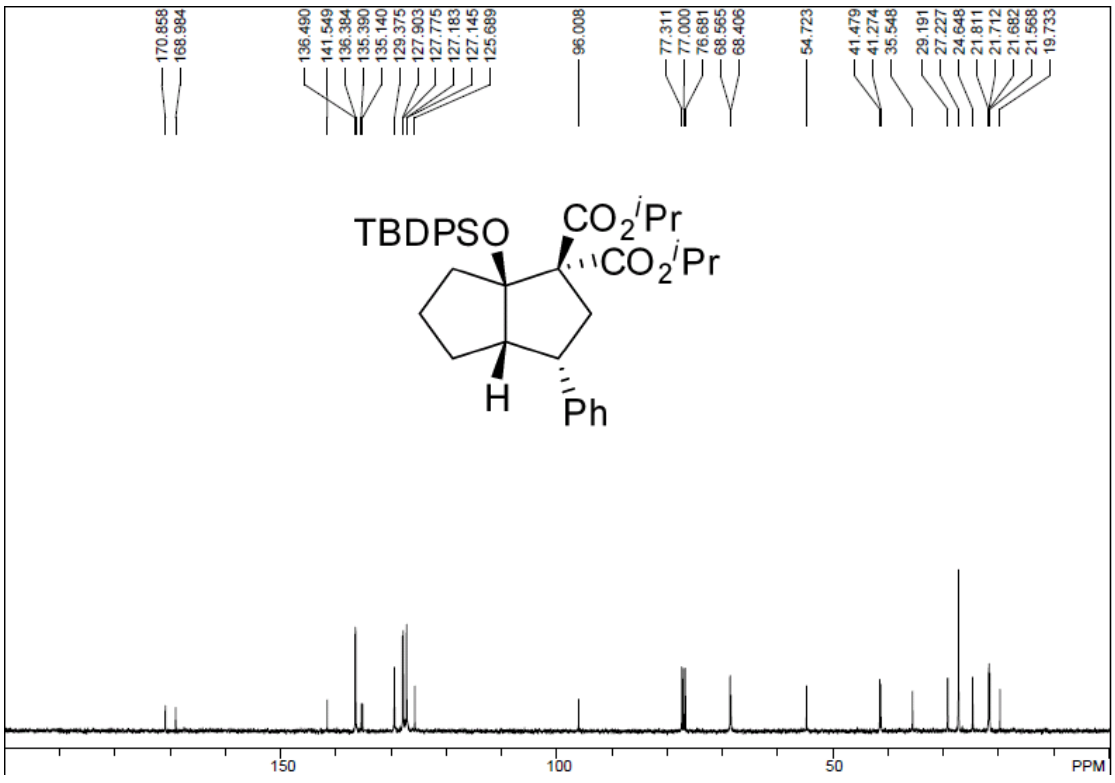

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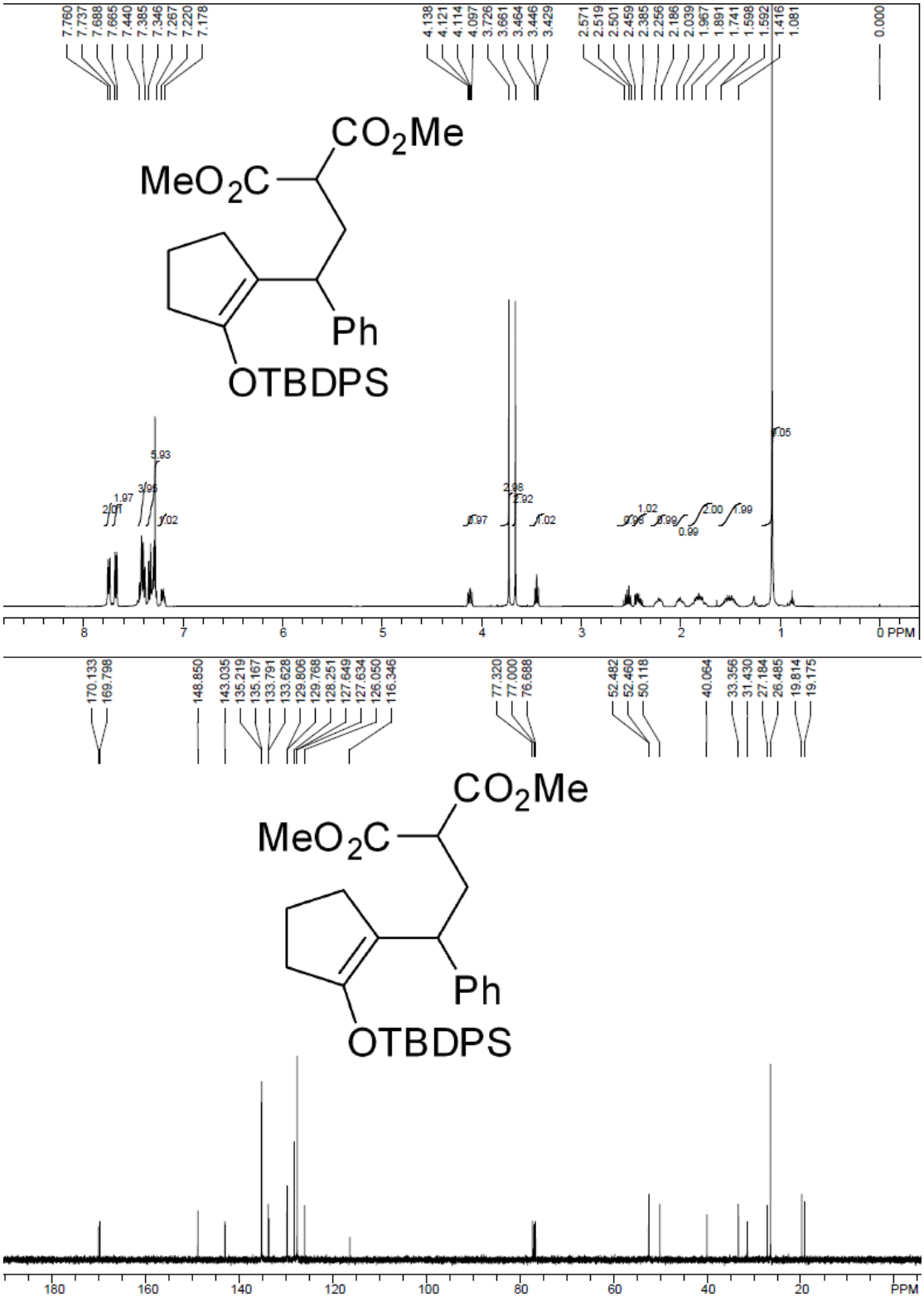
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MeO2C
Ph
OTBDPS
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1.02
0.96
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2.00
1.99
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8
7
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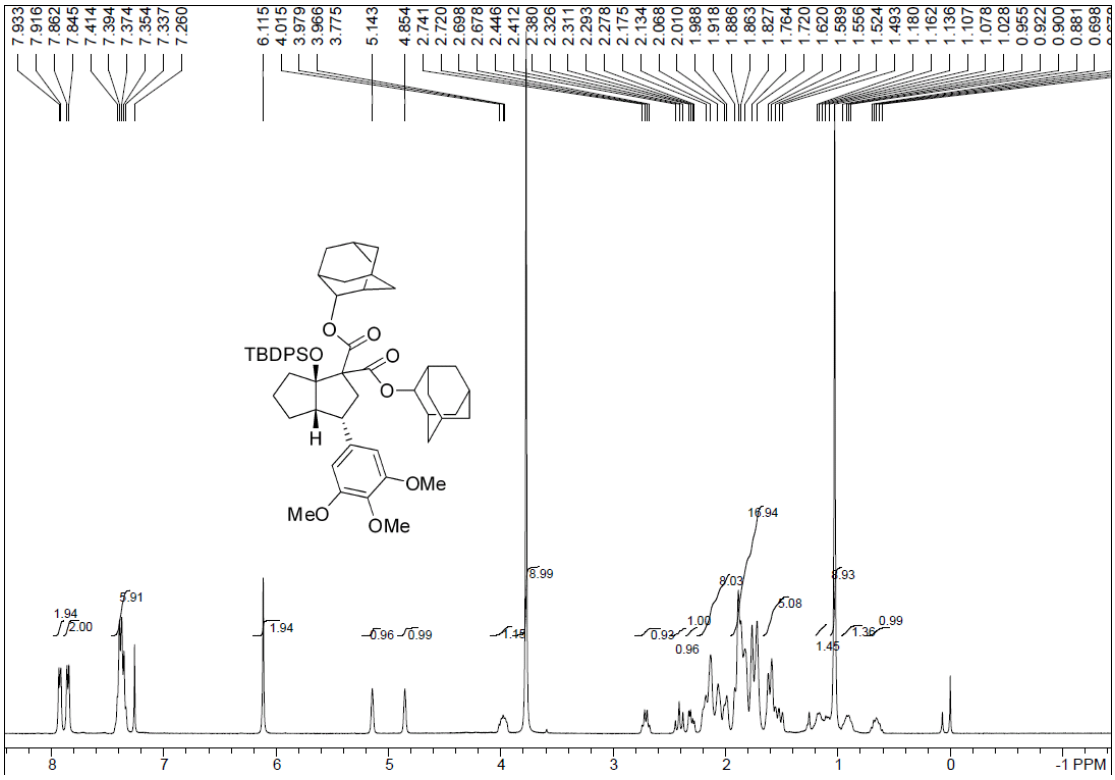

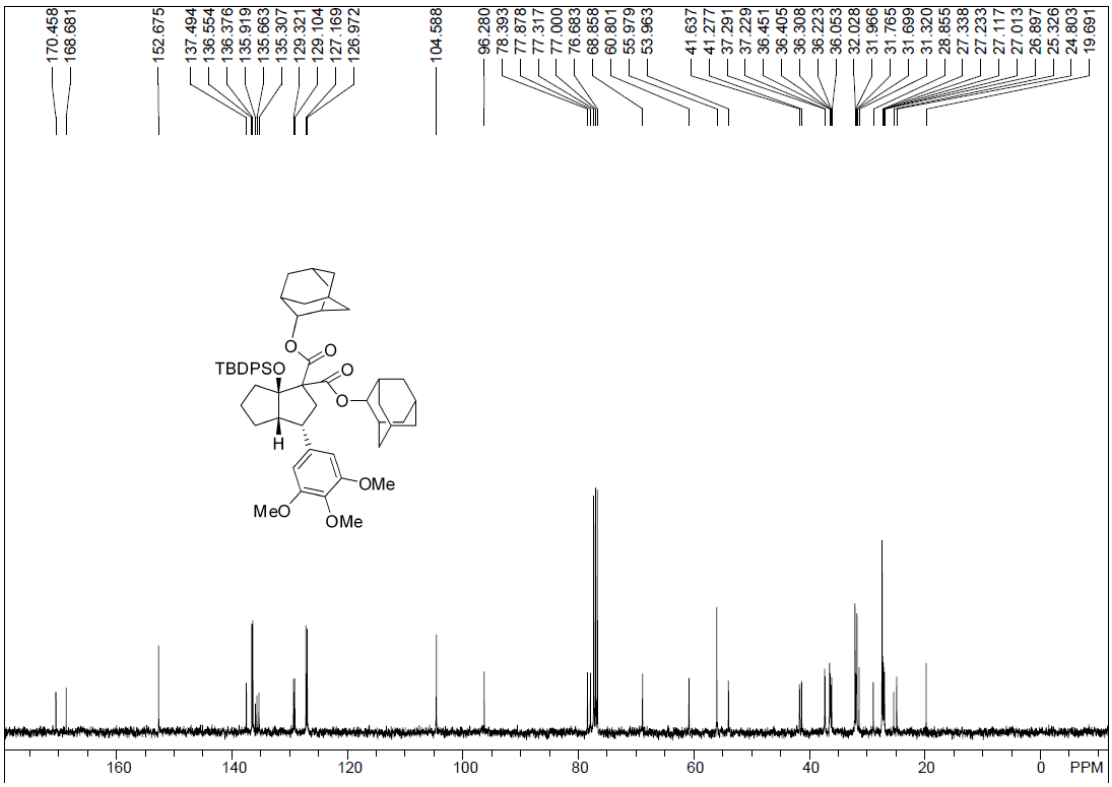

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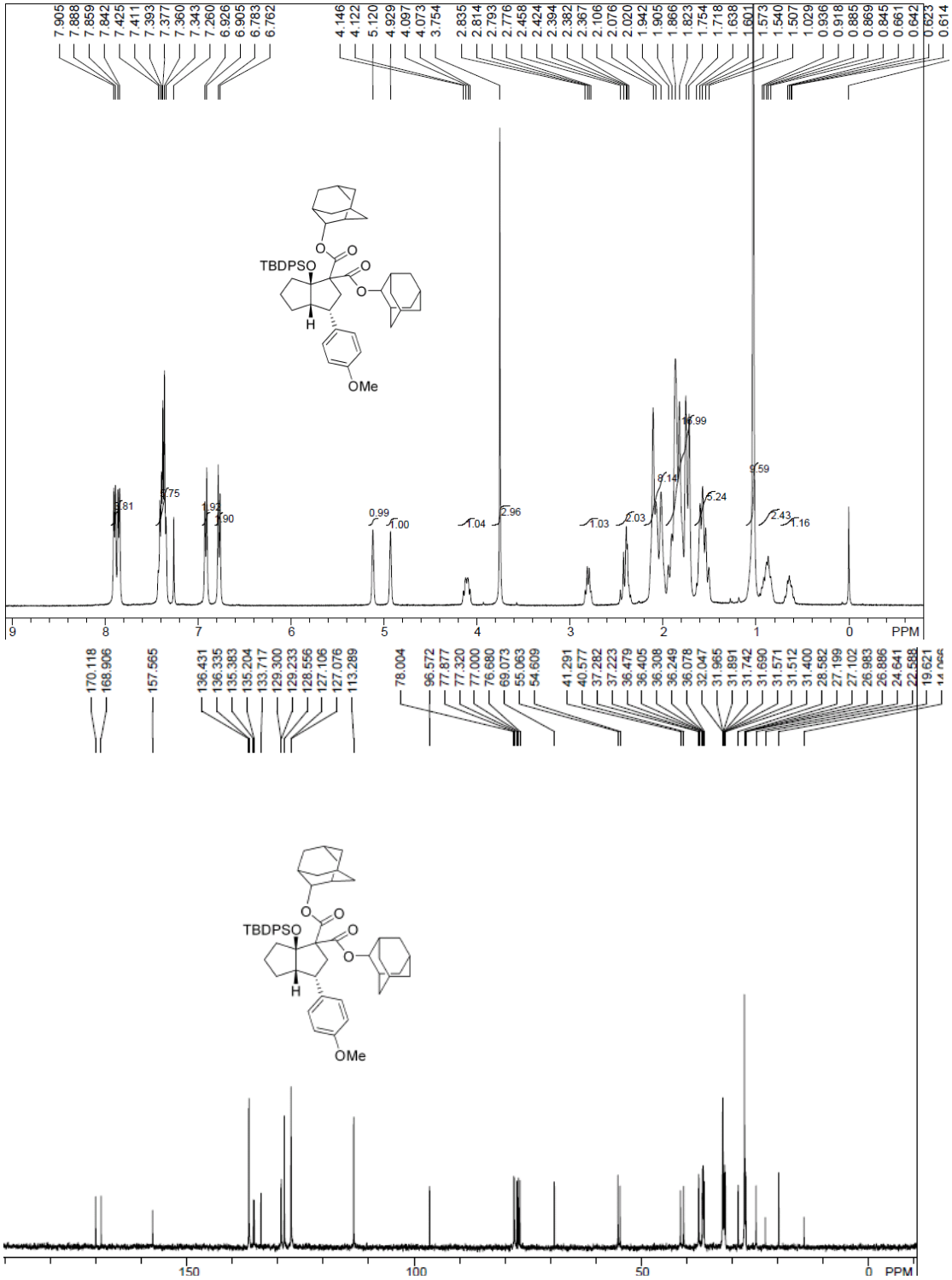
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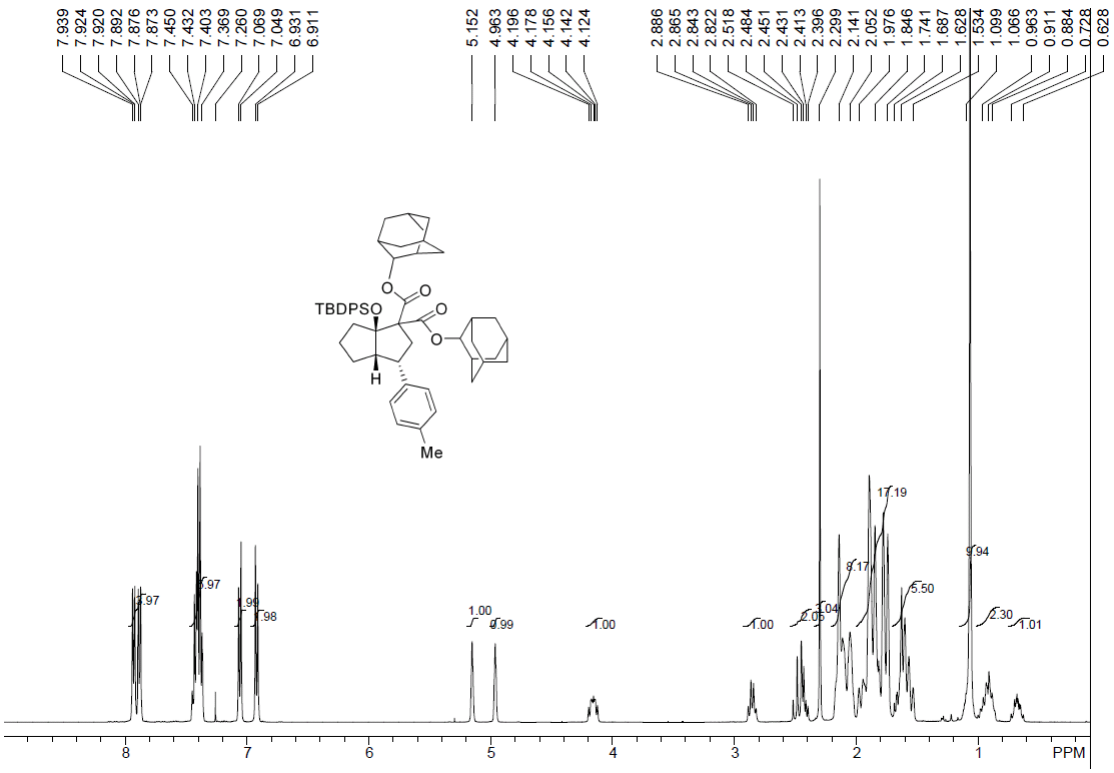
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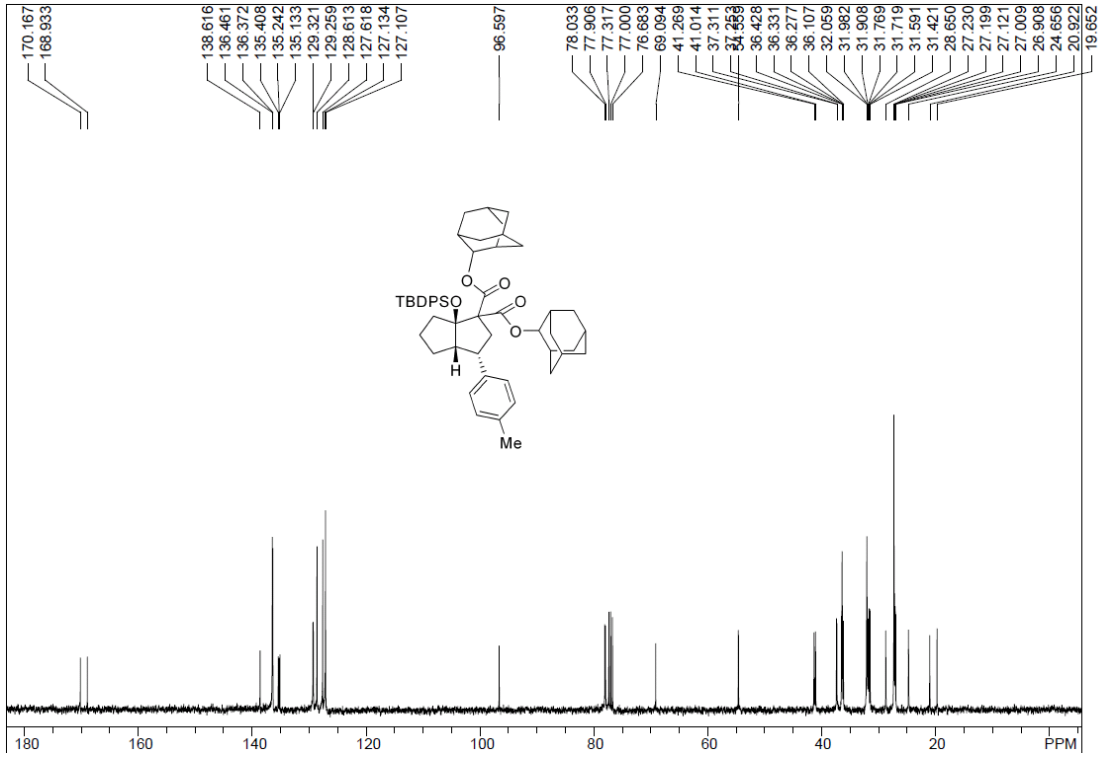
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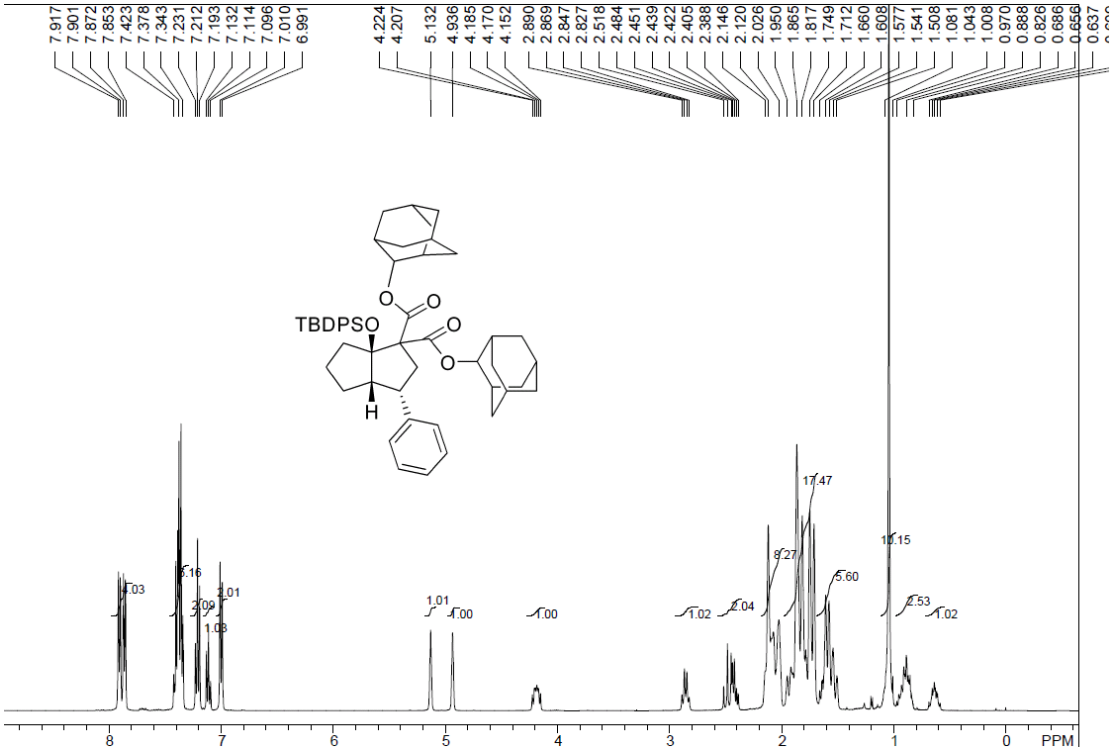
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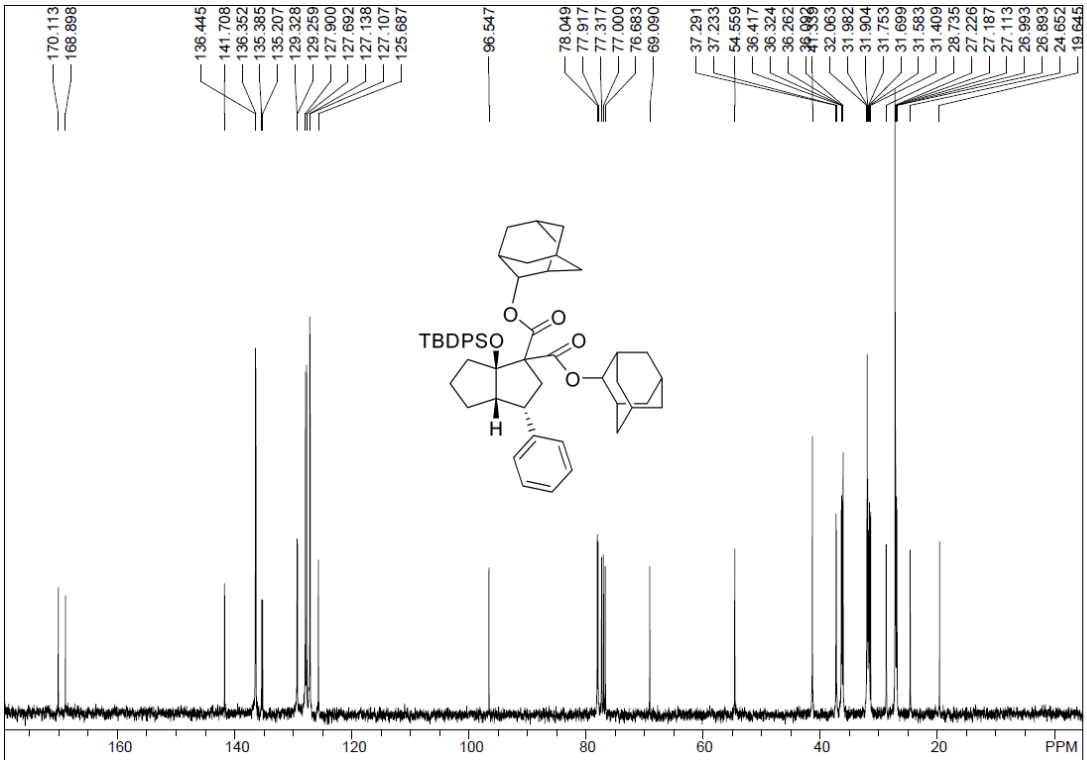
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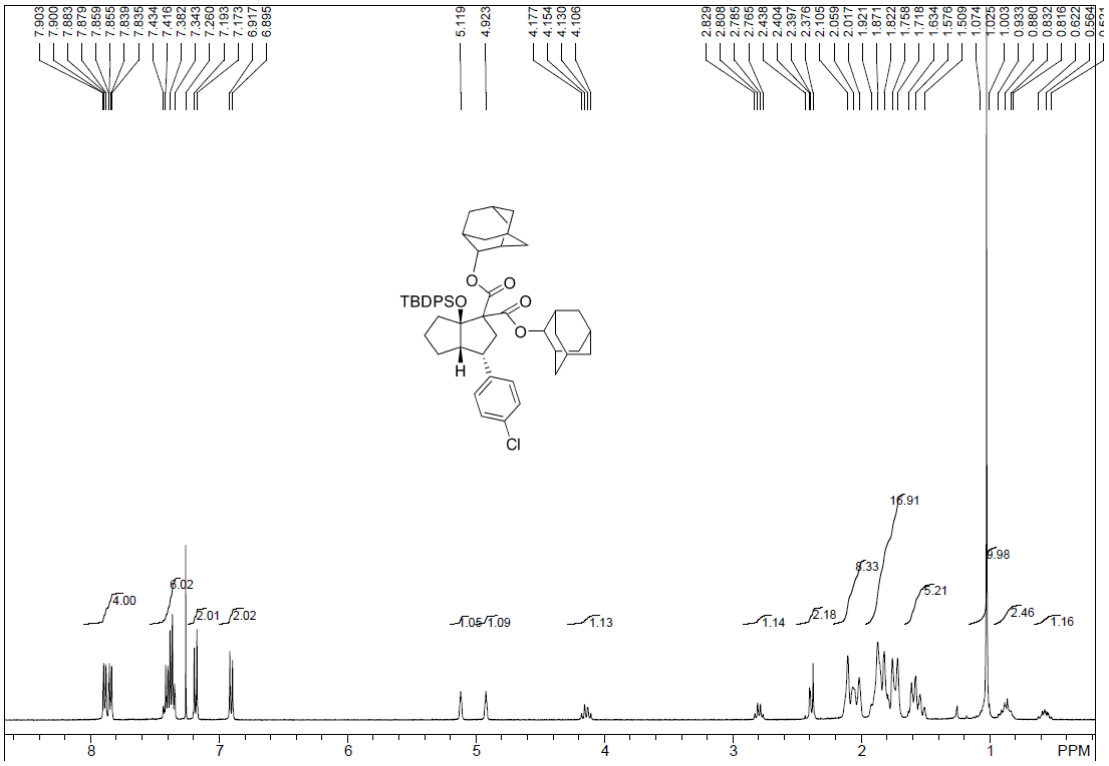
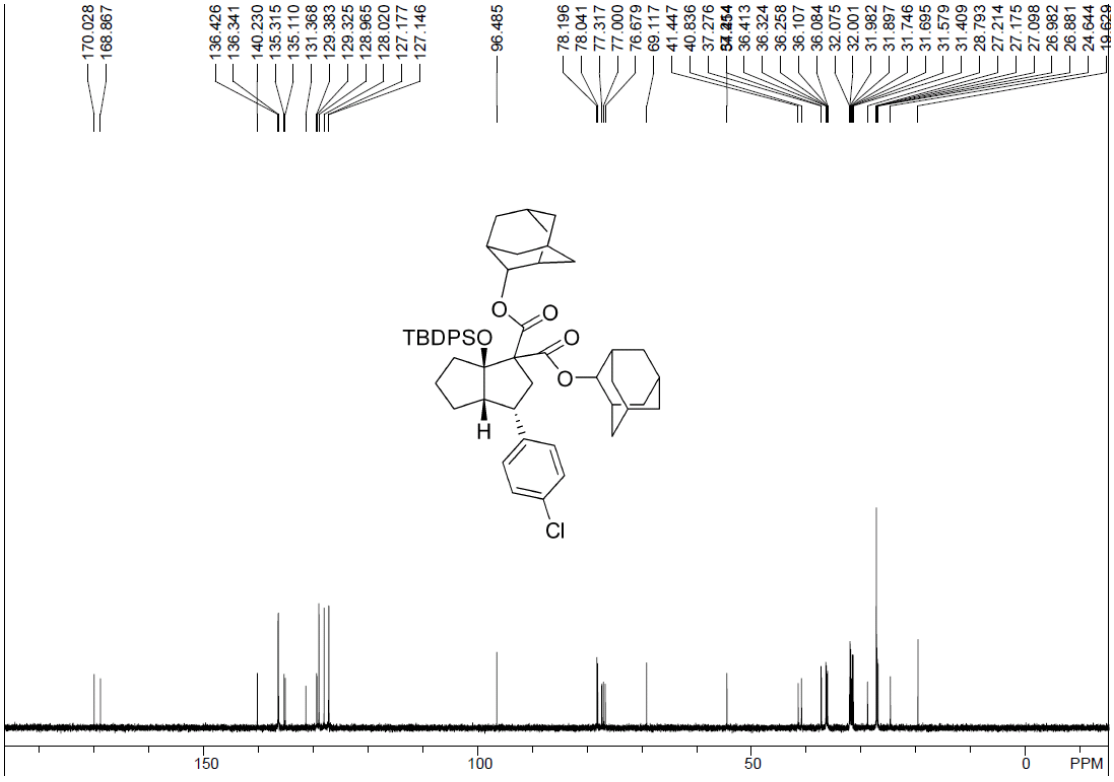
3g





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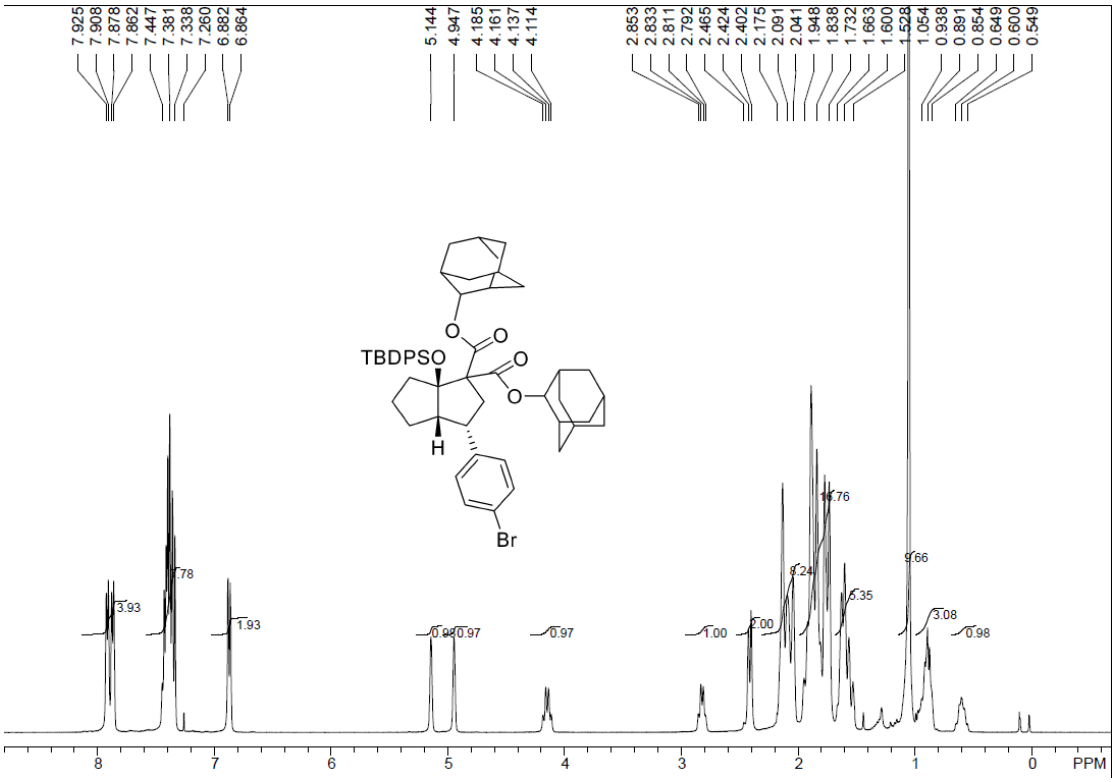
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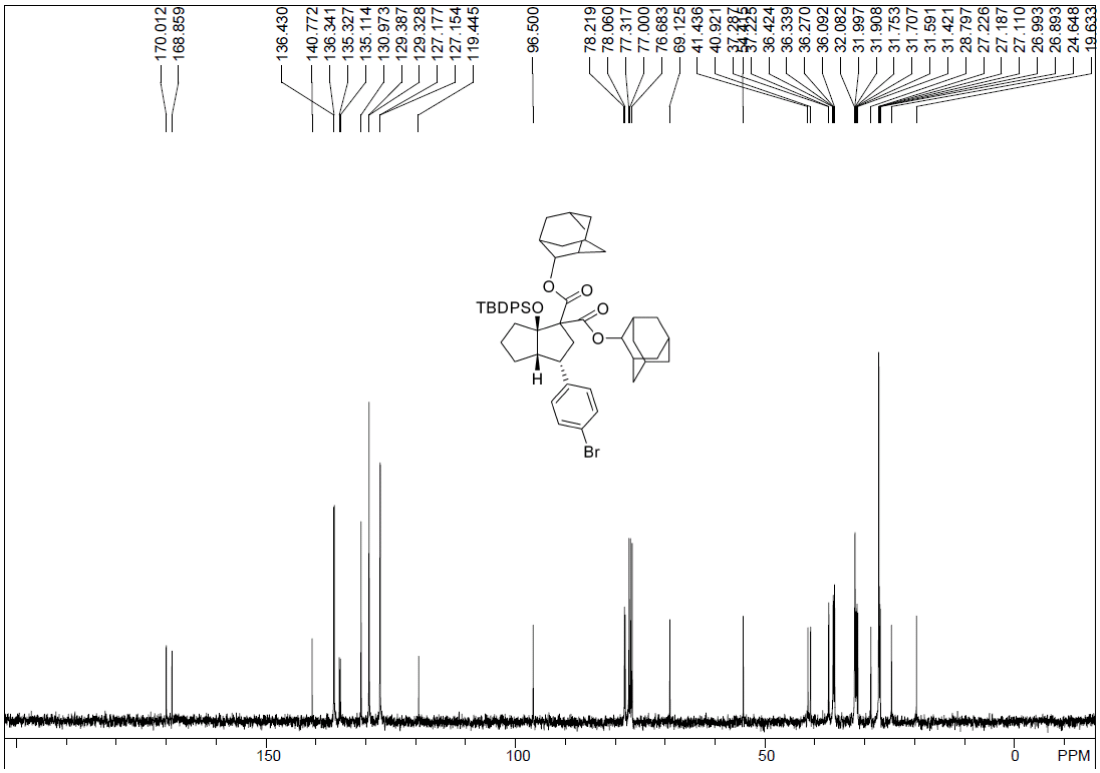
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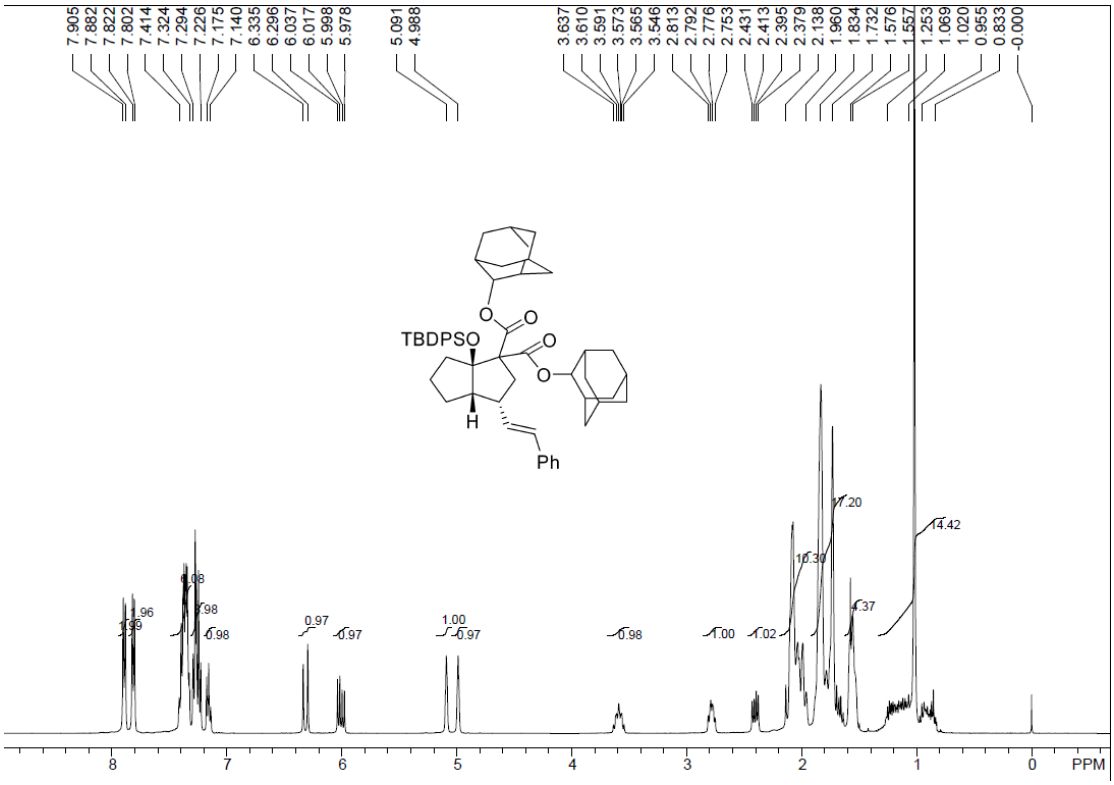
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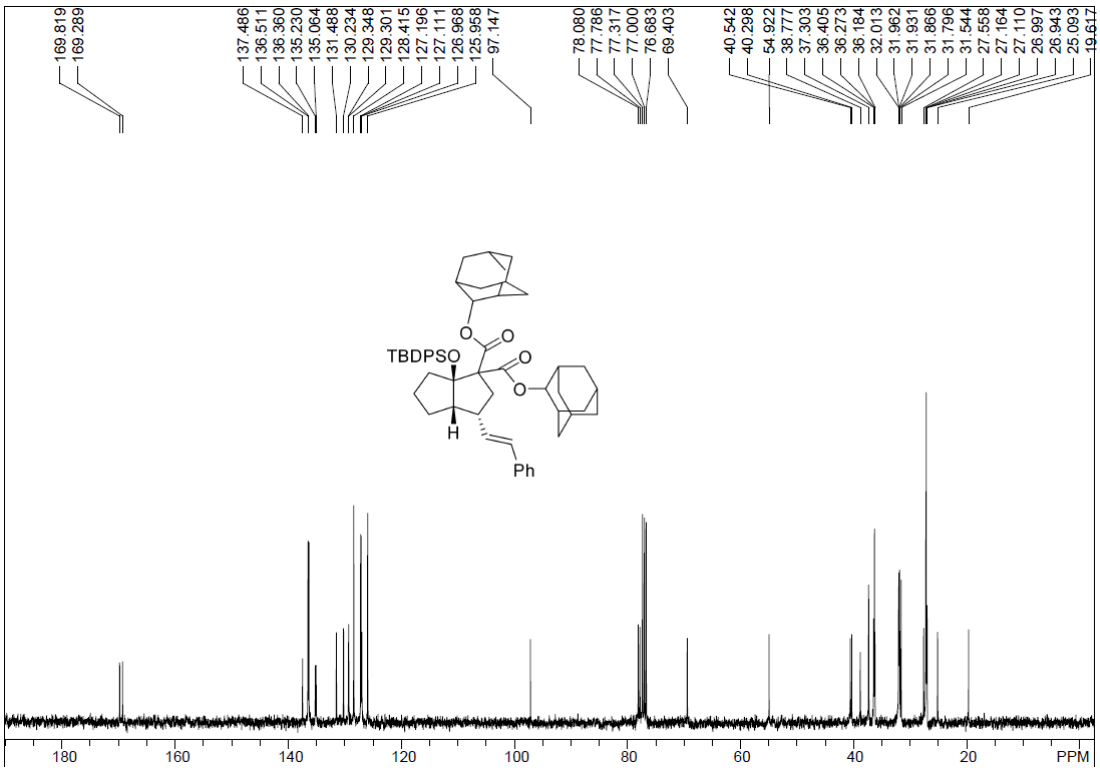
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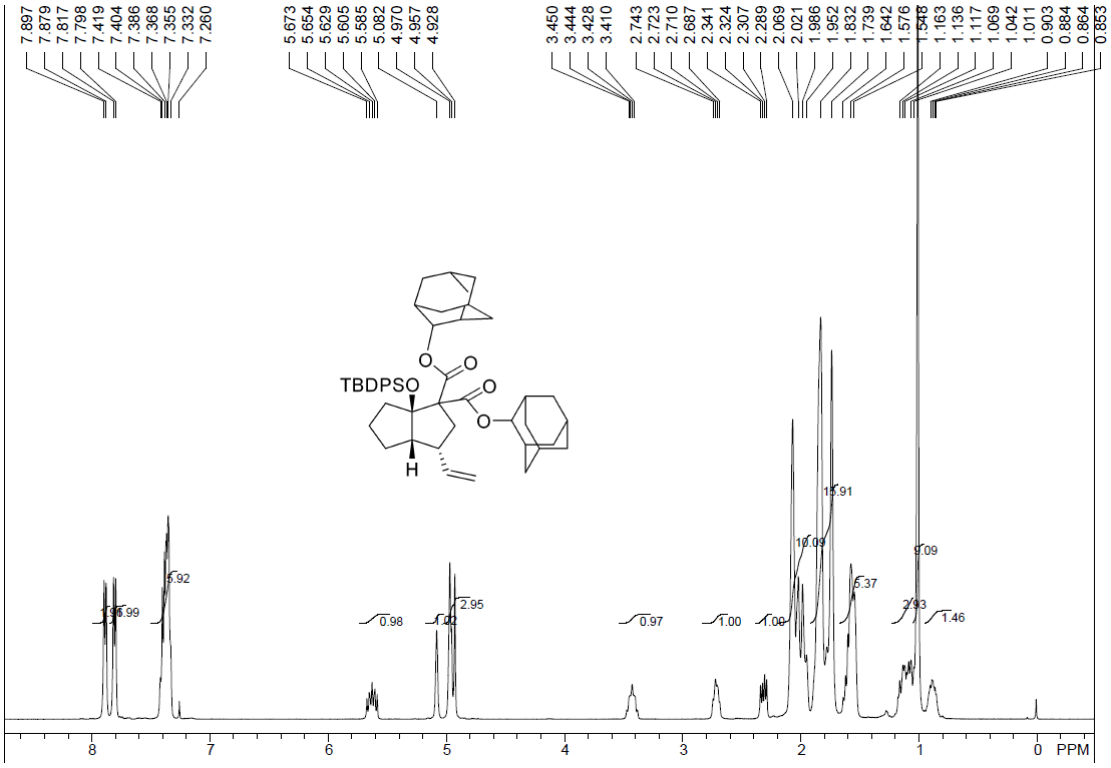
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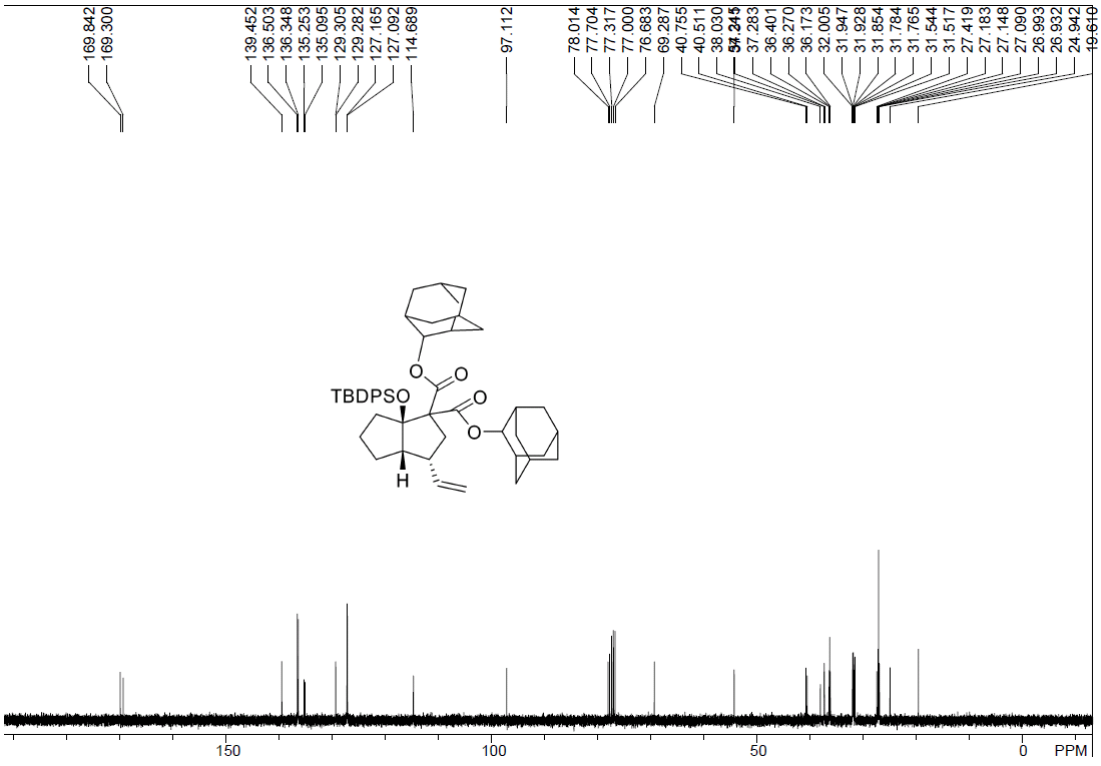
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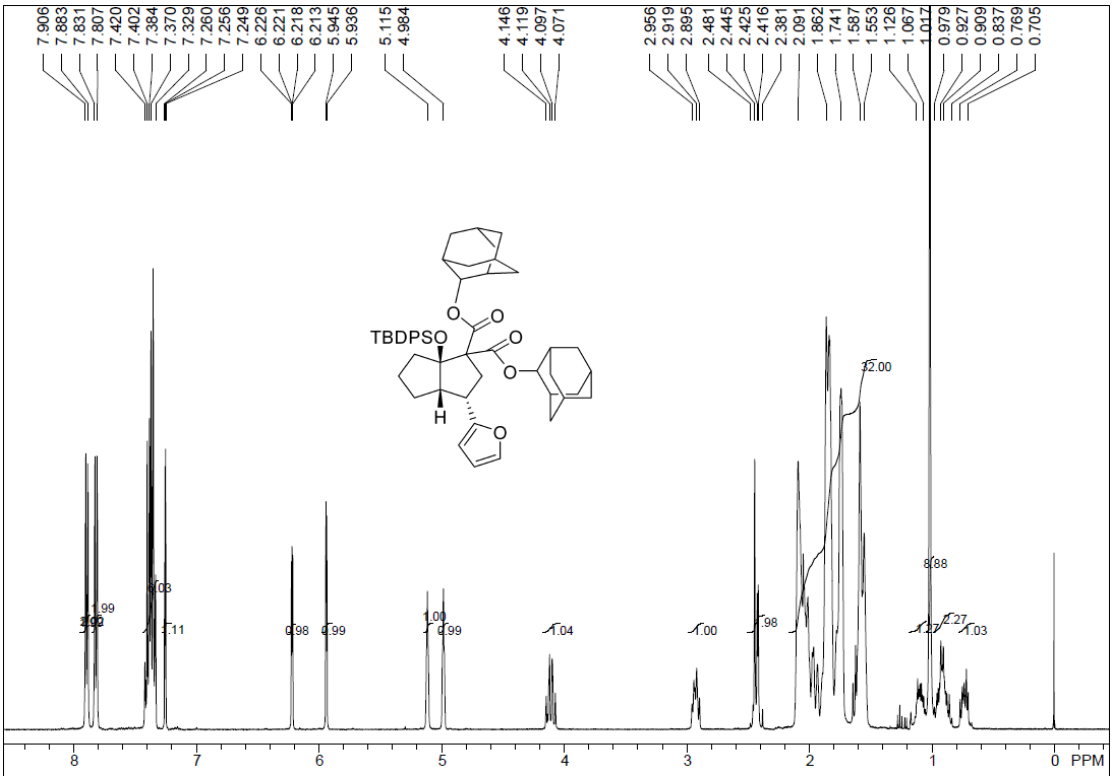
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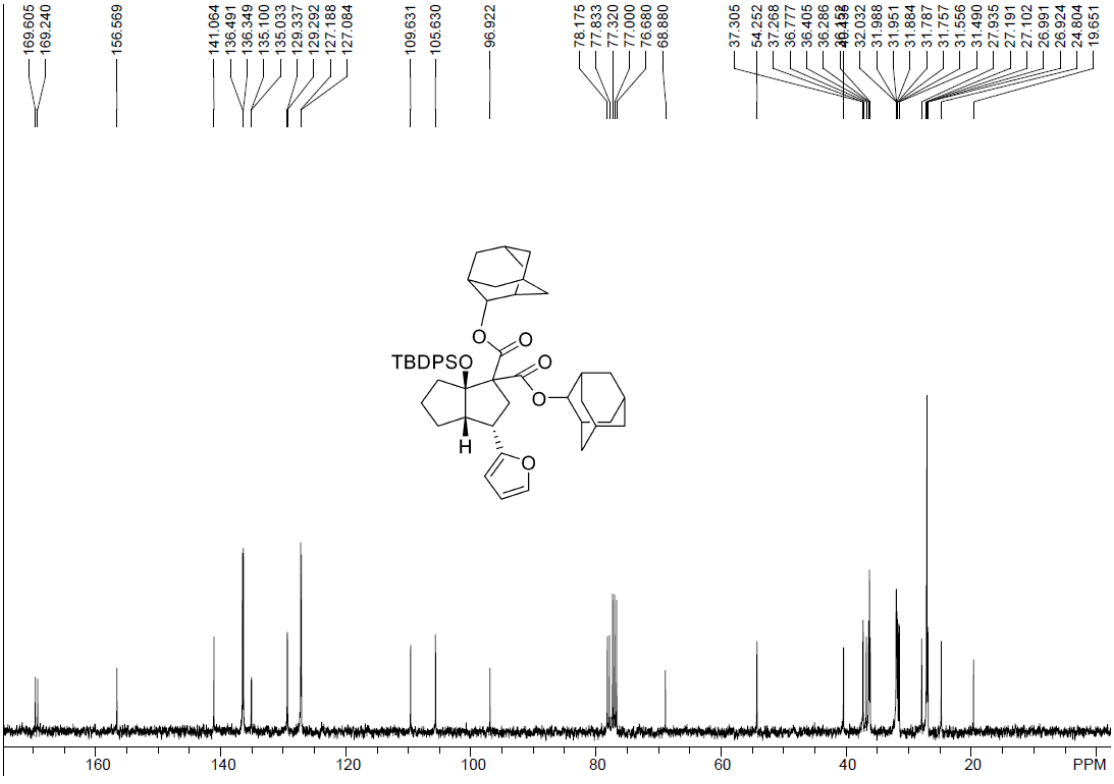
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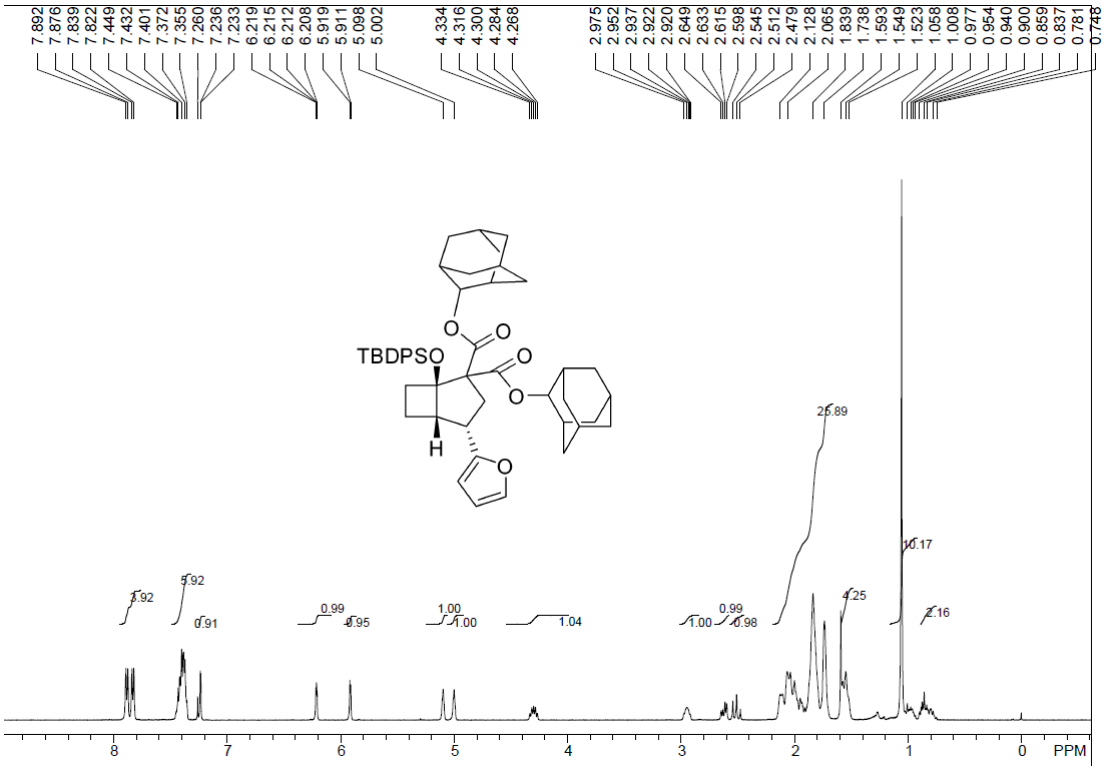
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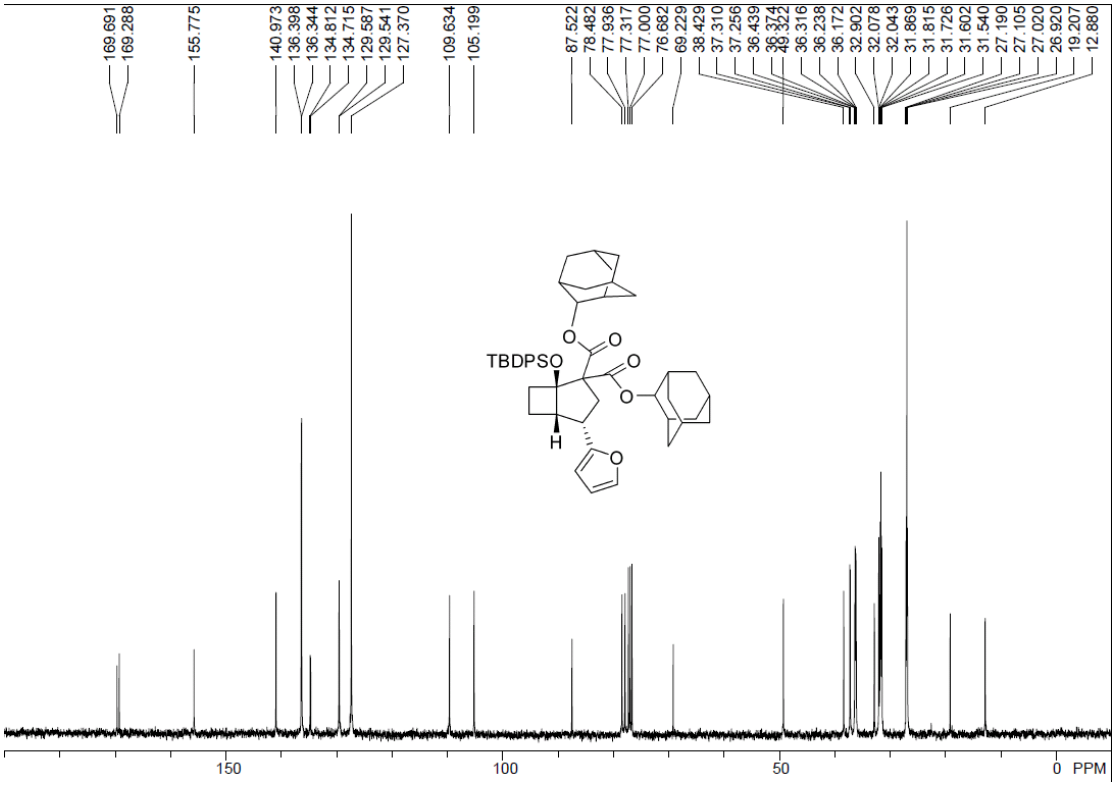
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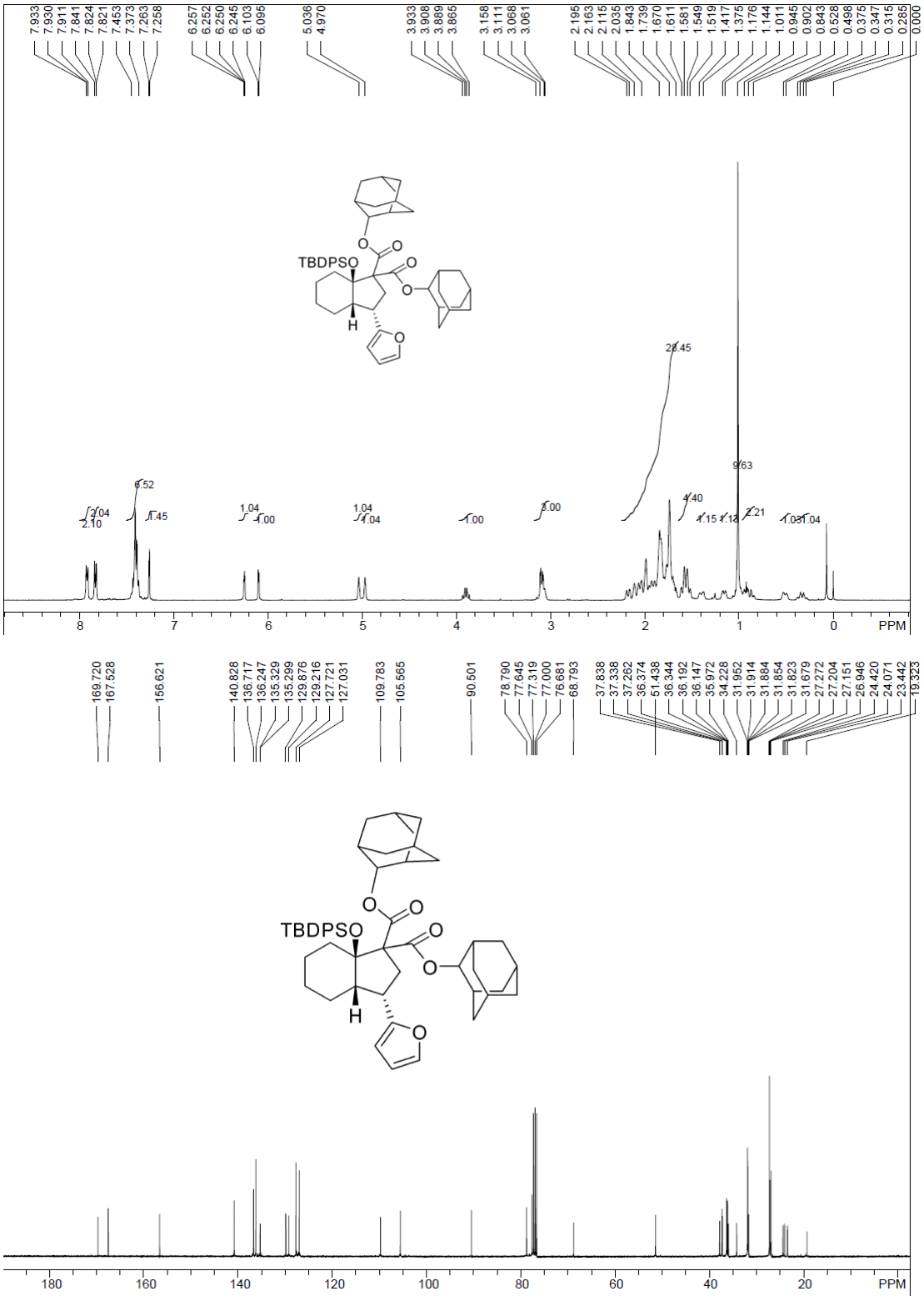
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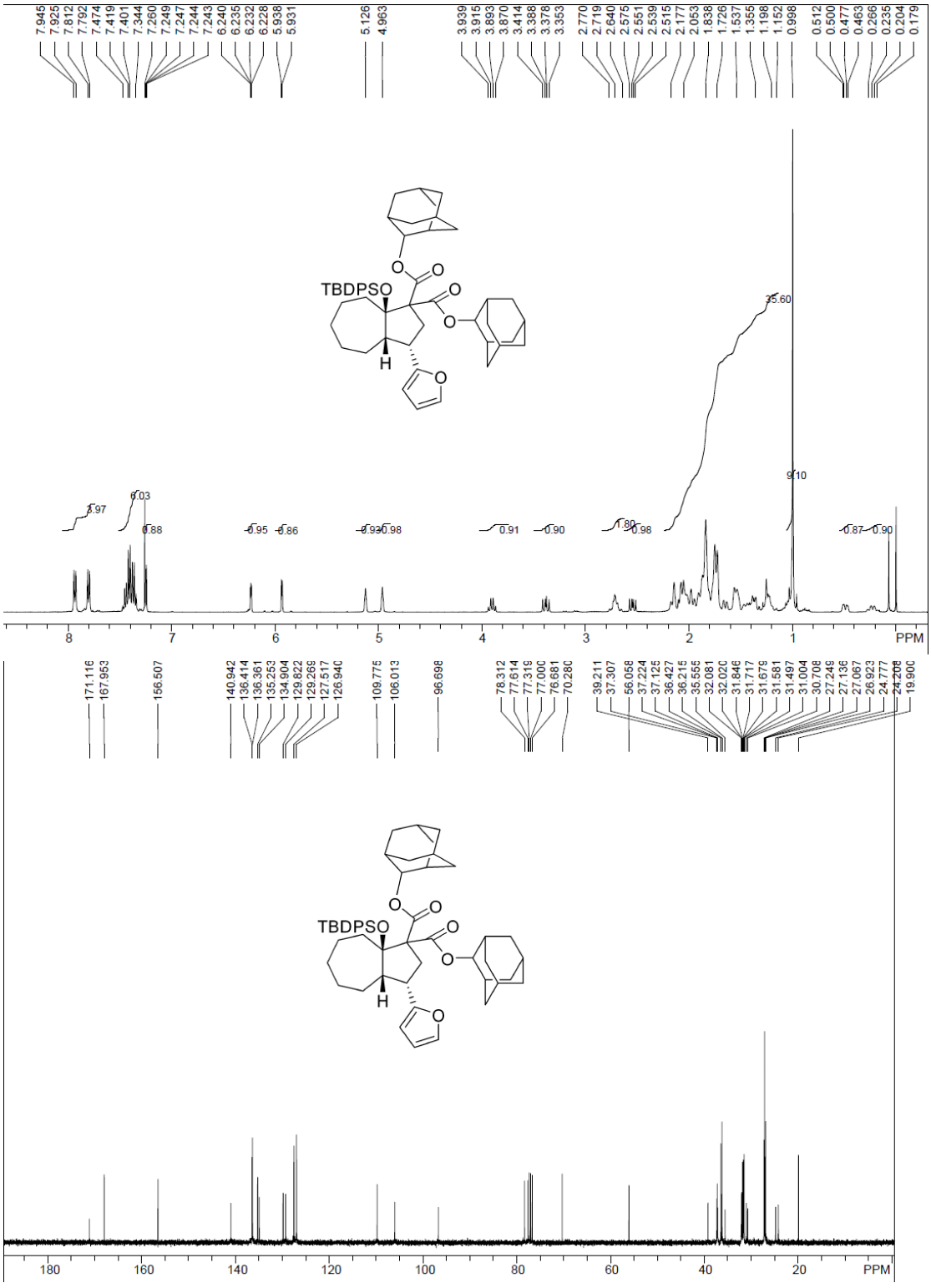

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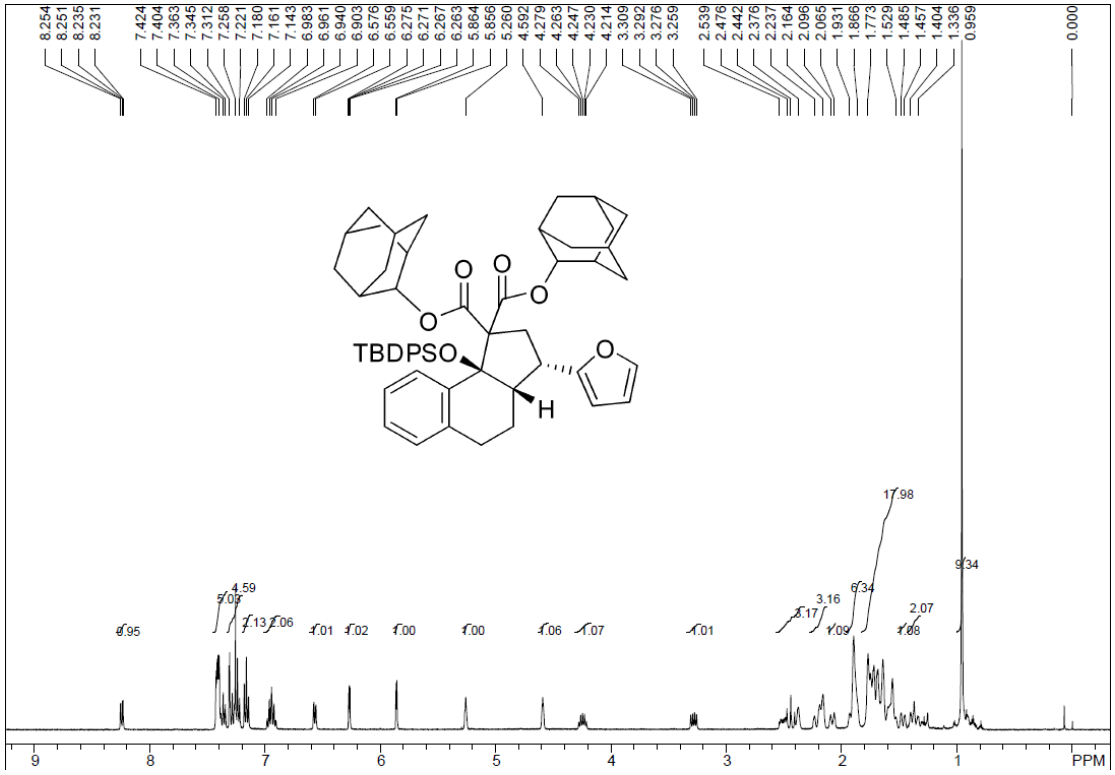
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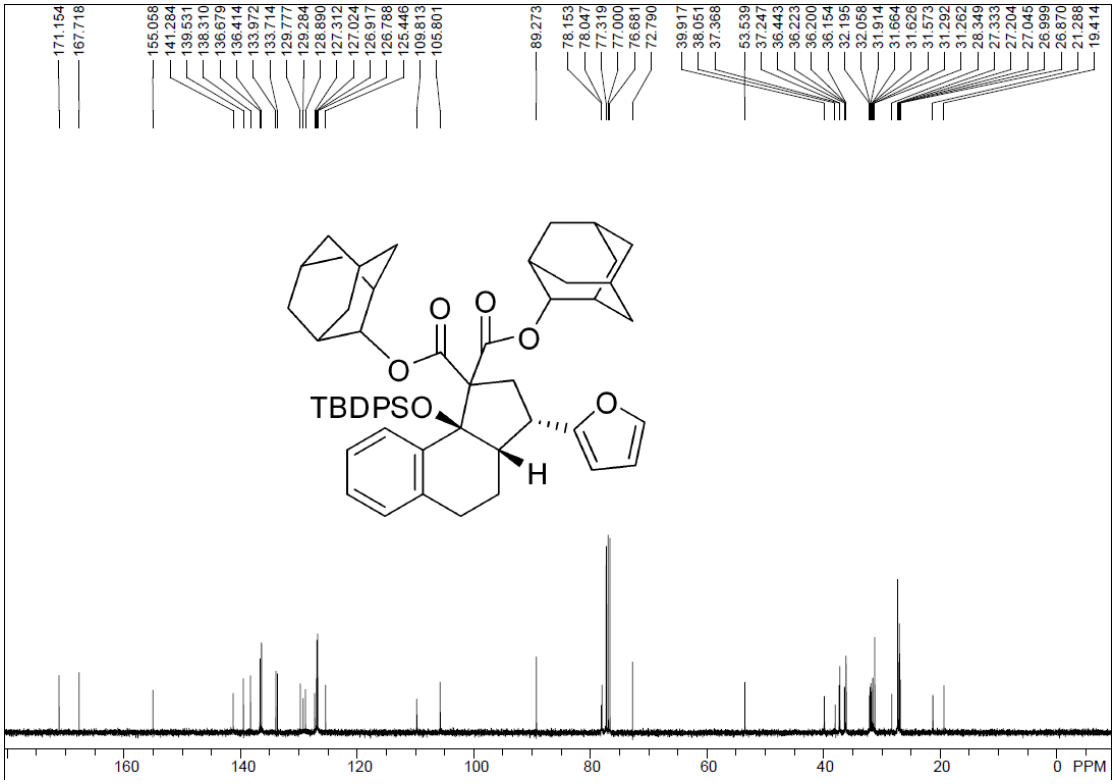
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PPM

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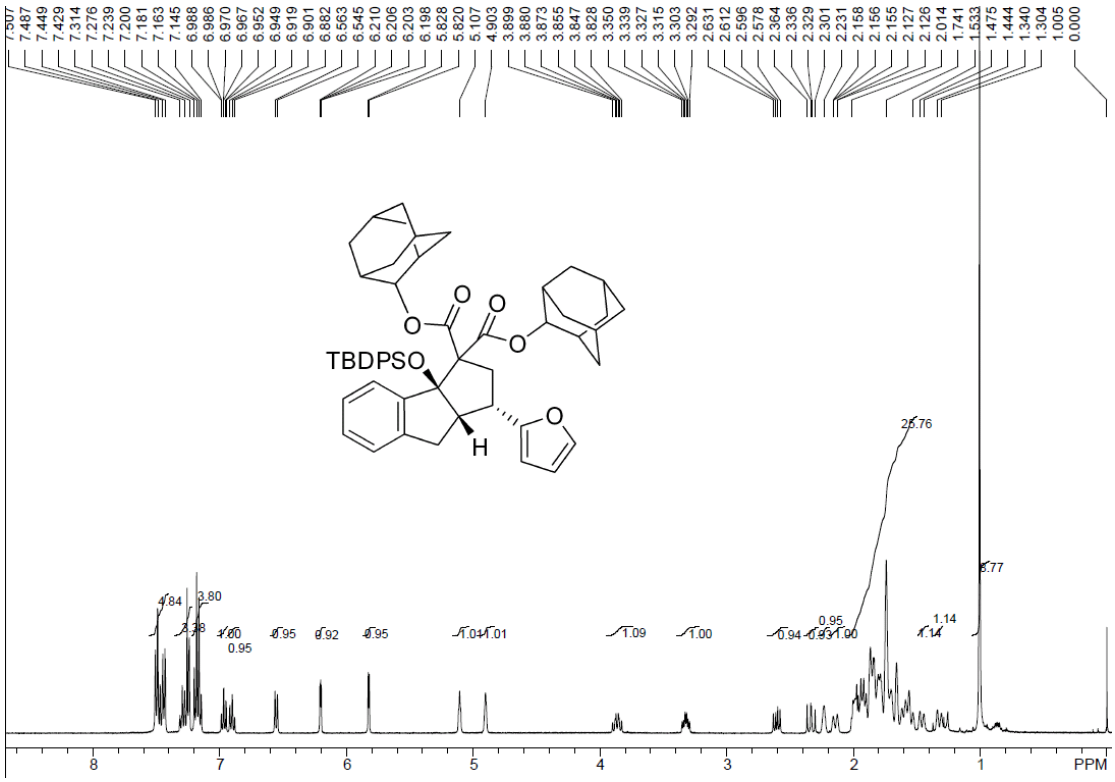

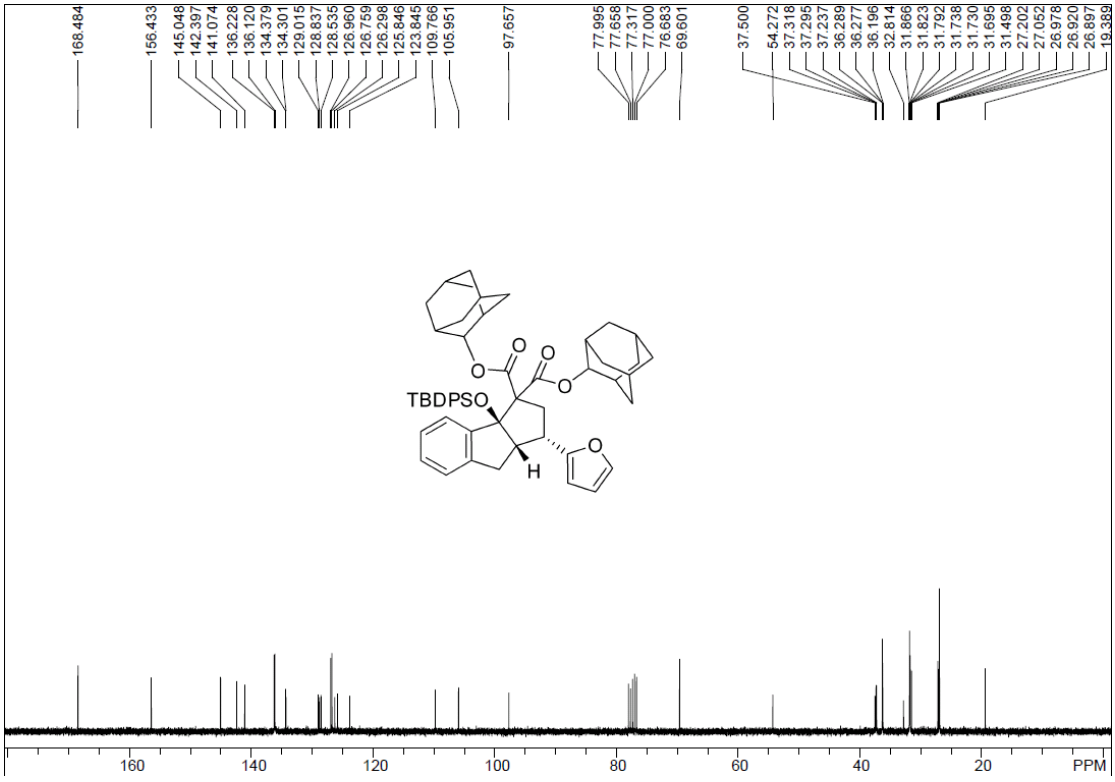

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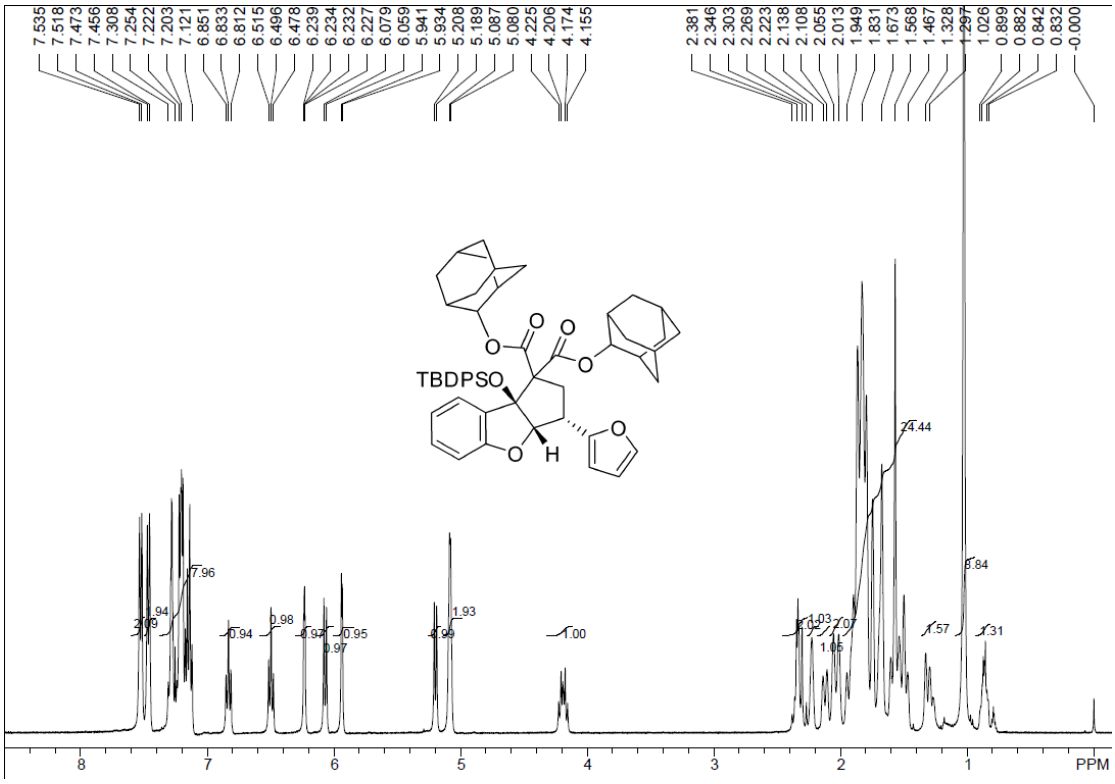
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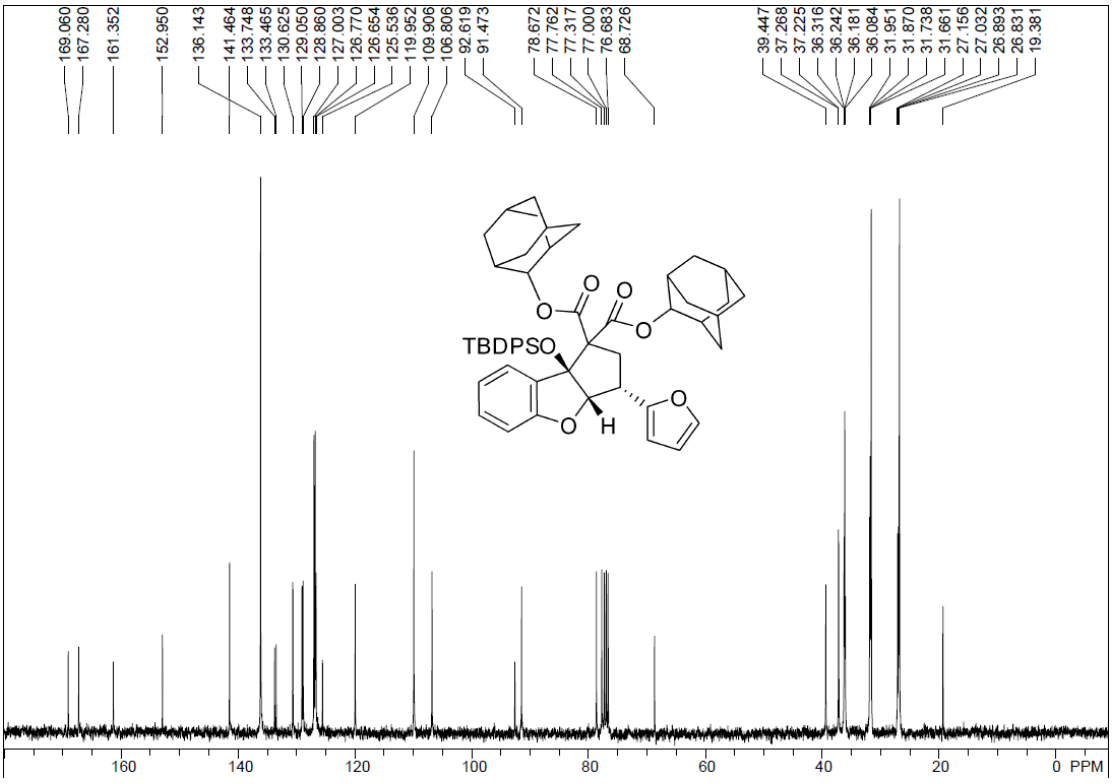
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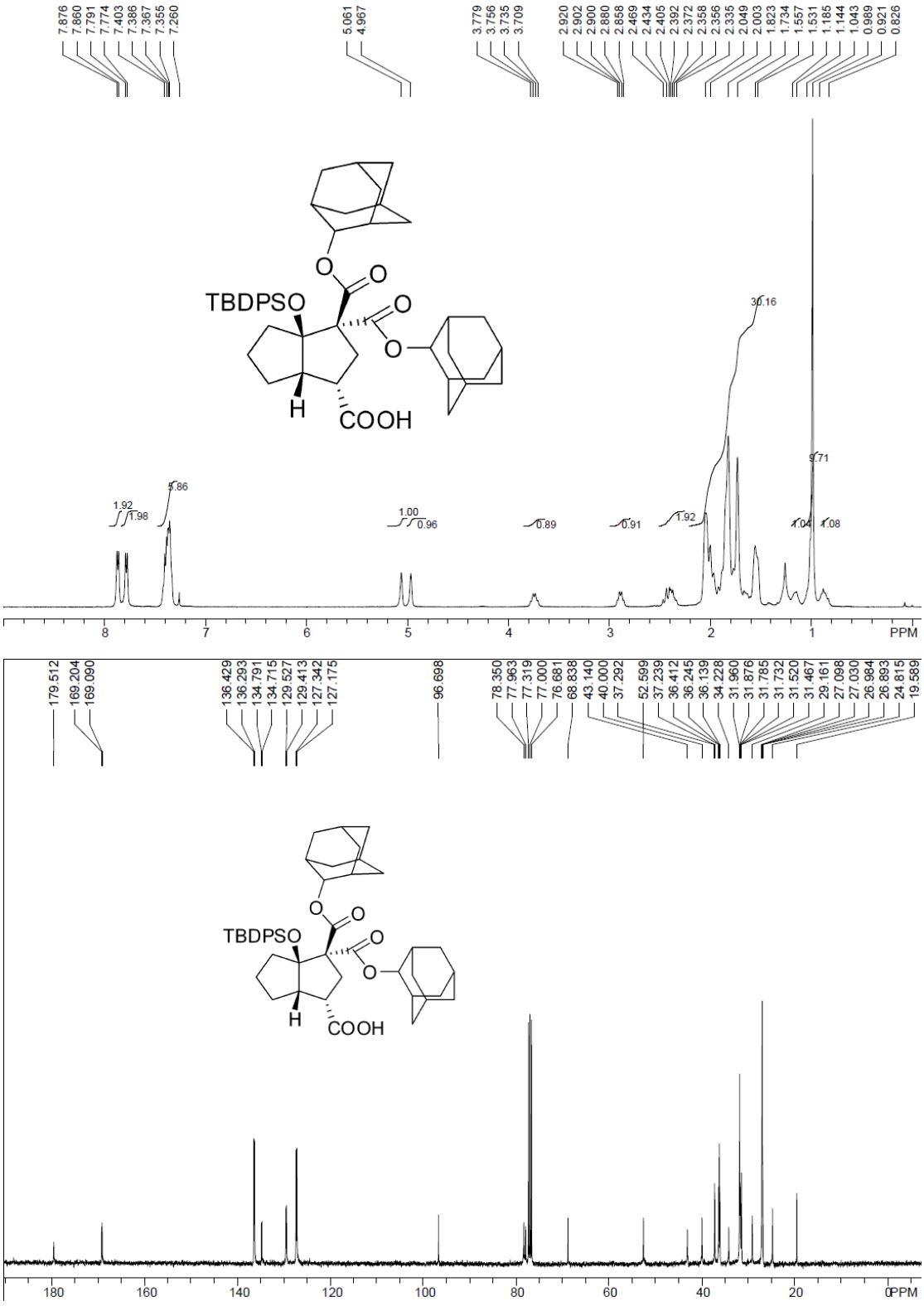
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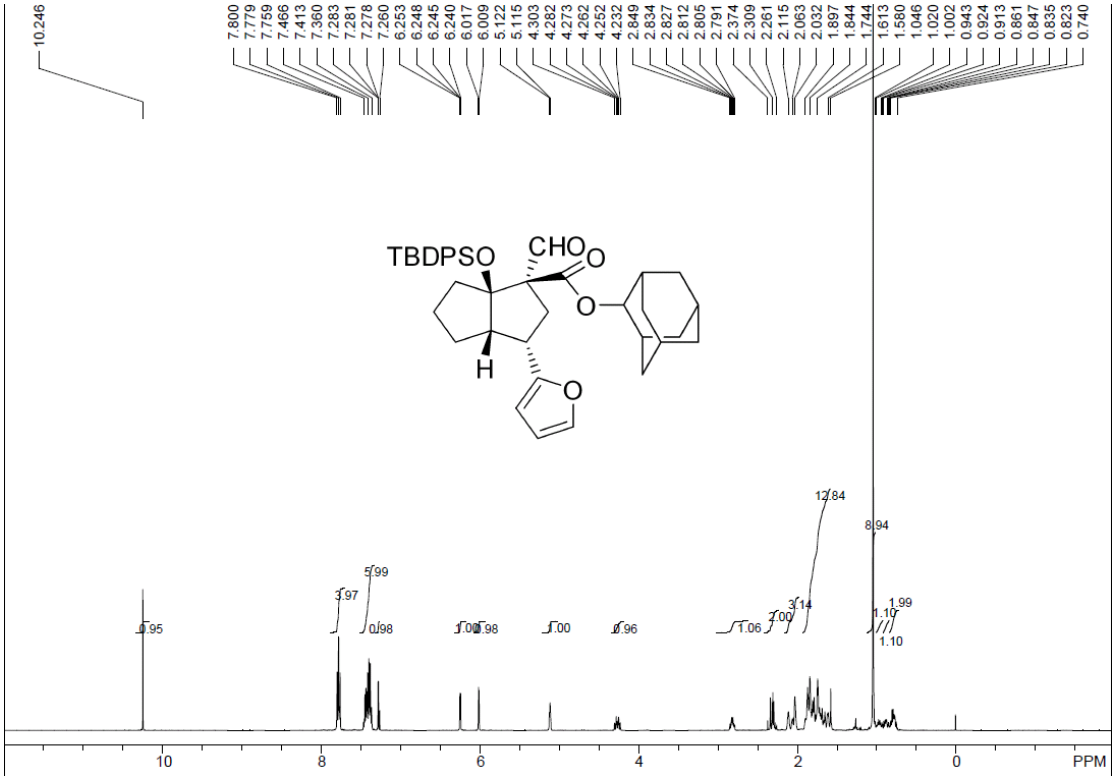
9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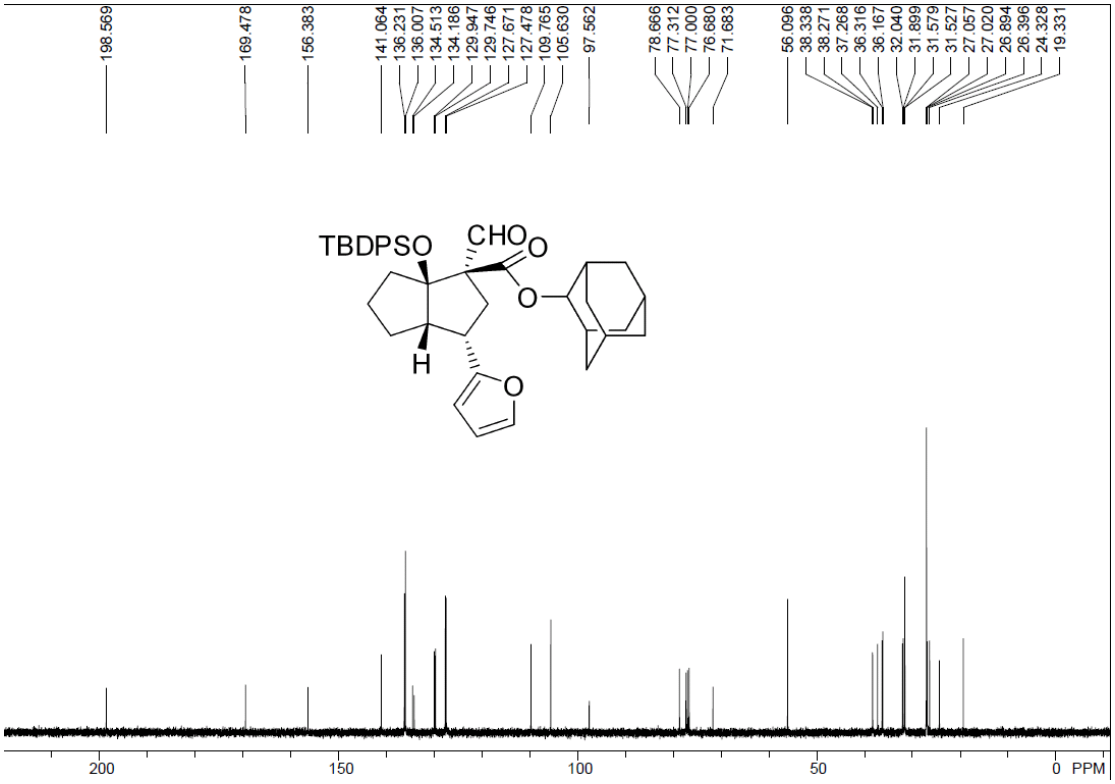
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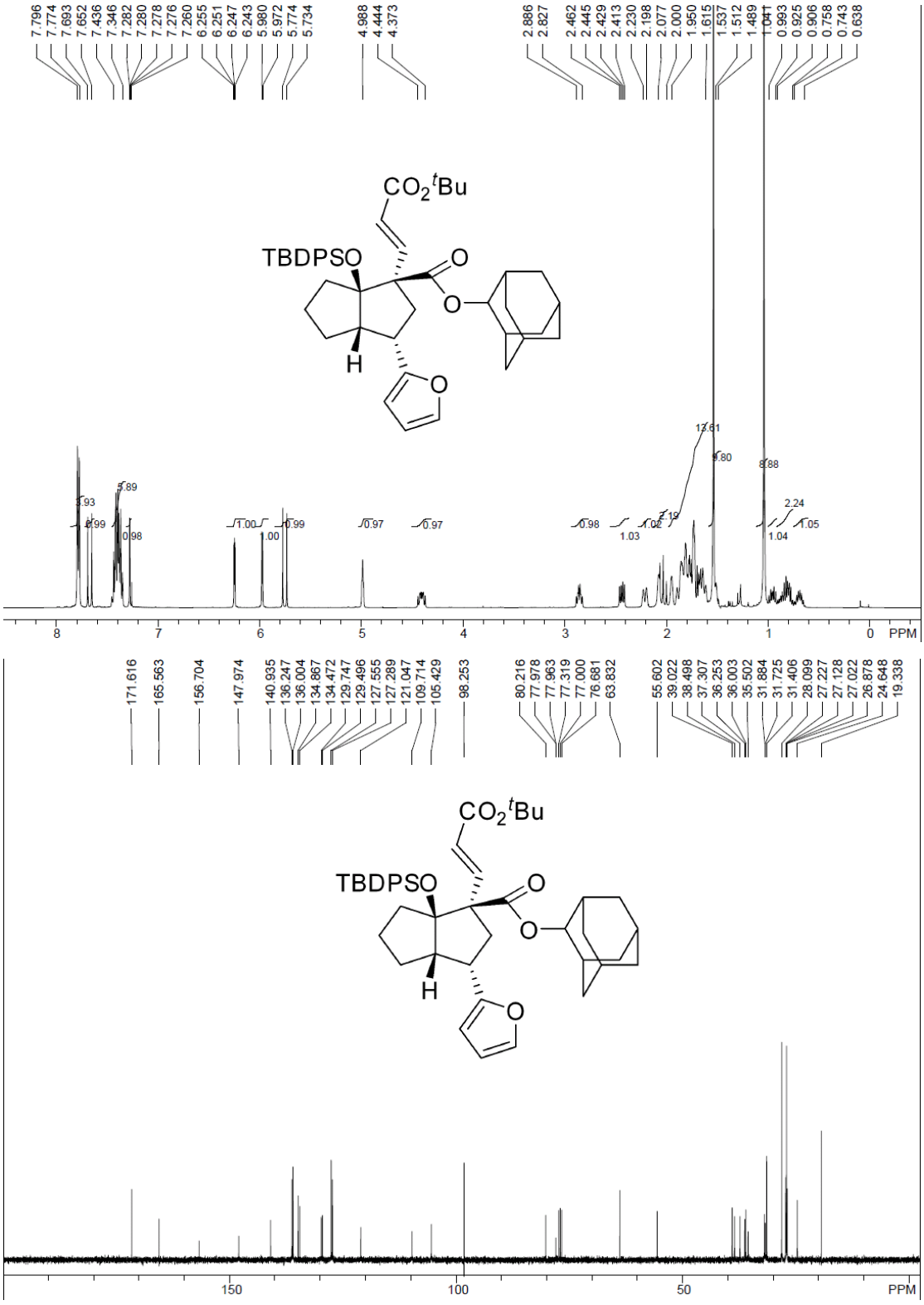
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CO2tBu
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O
O
H
O
150
100
50
PPM

9. DFT Studies

9.1. Computational details

All DFT calculations were performed with the Gaussian 03 software package.[2] Geometry optimization of all the minima and transition states involved was carried out at the (U)B3LYP level of theory.[3] For all mono-radical species, UB3LYP method was used, and the <S2> values are given in Table S2. For even electron species (enol silyl ethers, cyclopropanes, and [3+2] products), B3LYP method was used because these species should not be diradical. The LANL2DZ basis set[4] was used for copper and the 6-31G(d) basis set[5] for the other atoms. The keyword "5D" in Gaussian 03 program was used to specify that five (instead of six) d-type orbitals were used for all elements in the calculations. The vibrational frequencies were computed at the same level to check whether each optimized structure was an energy minimum or a transition state and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K. To improve the calculation accuracy, single-point energies and solvent effects were computed at the (U)B3LYP/6-311G(d,p)-LANL2DZ level (the LANL2DZ basis set[4] for copper and the 6-311G(d,p) basis set[5] for the other atoms), based on the gas-phase-optimized structures. Solvation energies in dichloromethane (DCM) were evaluated by a self-consistent reaction field (SCRF) using the CPCM model,[6] where the simple united atom topological model (UA0) was used to define the atom radii. In the paper and the Supporting Information, all discussed energies are Gibbs free energies in dichloromethane (ΔG_{DCM}) unless specified. The Gibbs free energies in gas phase (ΔG_{gas}) and the enthalpies in dichloromethane (ΔH_{DCM}) are also given for reference (Figure S2). The DFT-calculated structures of complexes **C (A)** and **C (B)** and transition states **TS1-cis (B)** and **TS1-trans (B)** are given in Figure S3. The catalytic circle of [3+2] reactions of cyclopropane 1,1-diesters and cyclic enol silyl ethers is given in Figure S4. DFT-calculated overall free energy surface of Reaction **A** and IRC plot are provided in Figures S5 and S6.

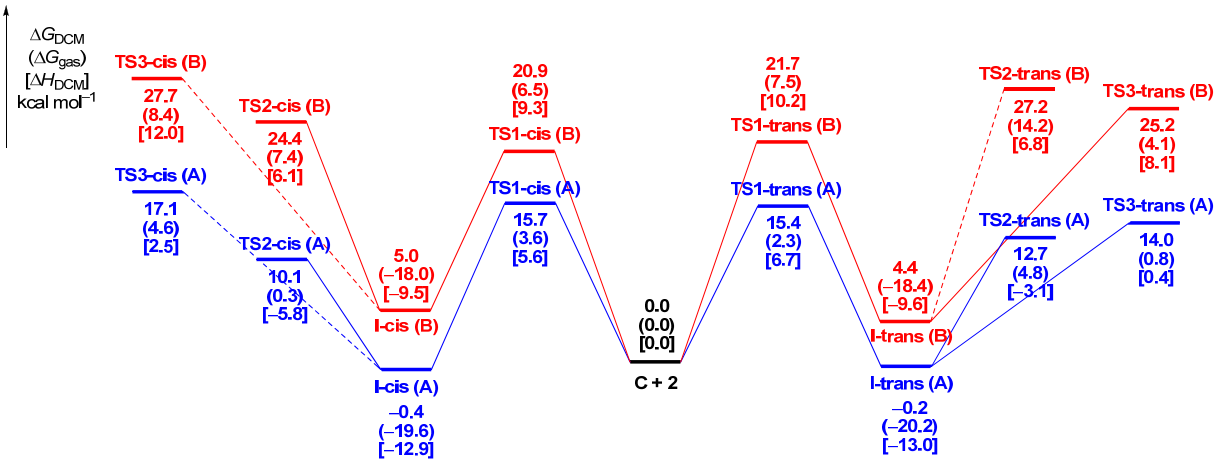


Figure S2. DFT-calculated energy surfaces (Reaction **A**: blue line; Reaction **B**: red line).

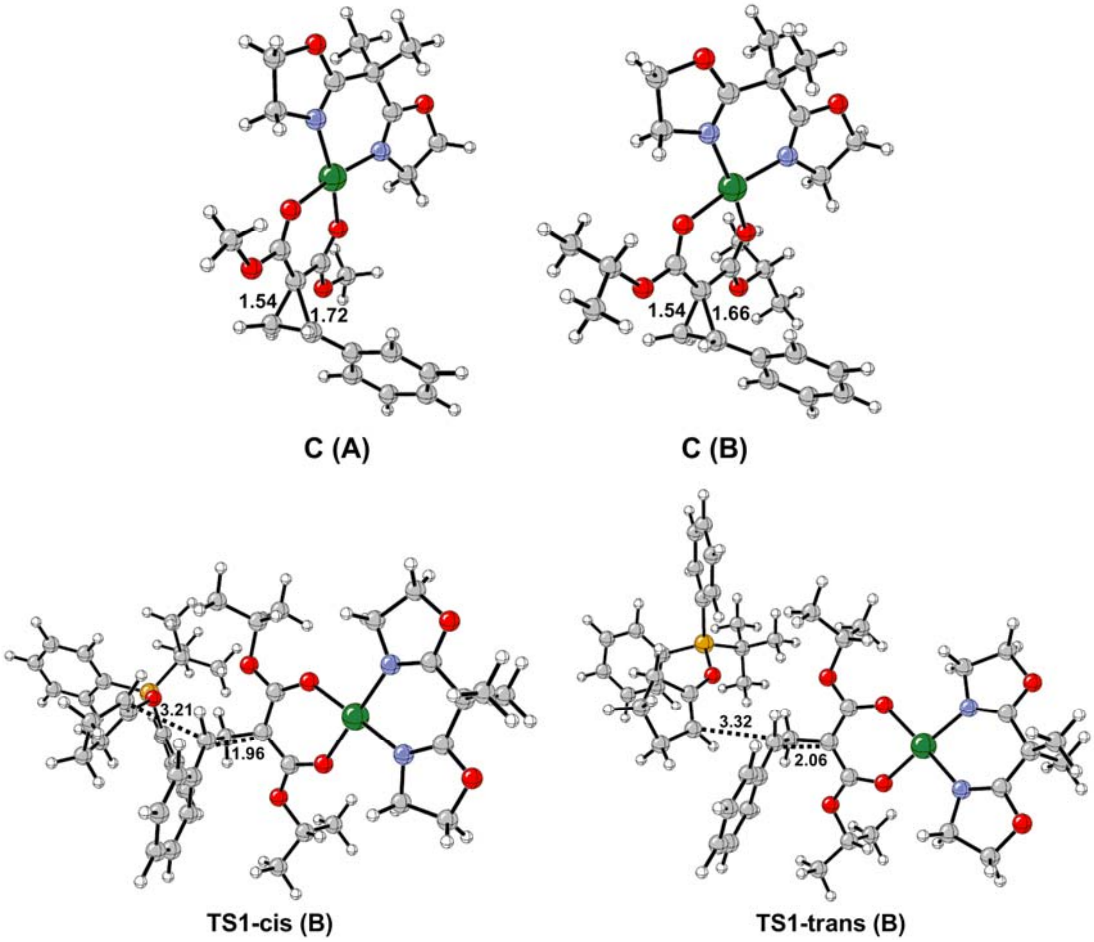


Figure S3. DFT-calculated structures of complexes **C (A)** and **C (B)** and transition states **TS1-cis (B)** and **TS1-trans (B)** (C gray; H white; O red; N blue; Si yellow; Cu green; distances are given in Å).

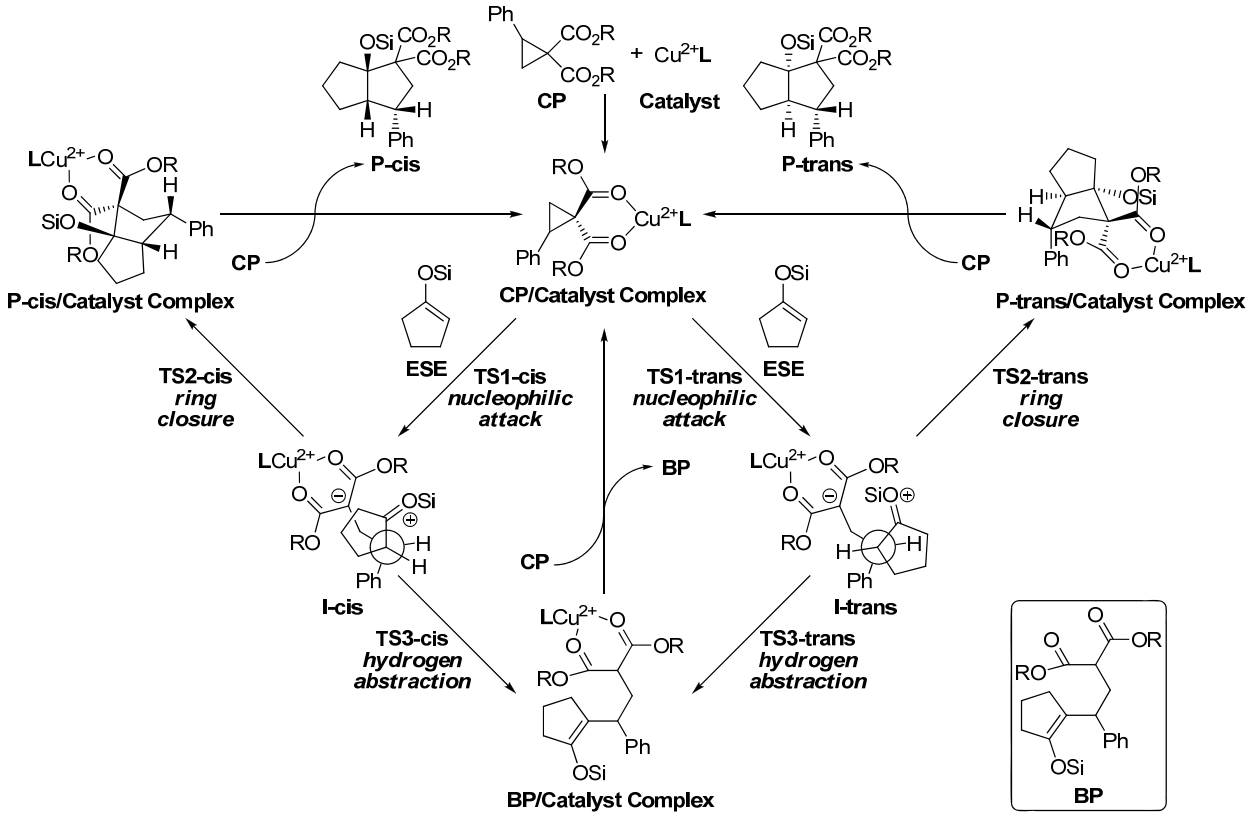


Figure S4. Catalytic circle of [3+2] reactions of cyclopropane 1,1-diesters and cyclic enol silyl ethers.

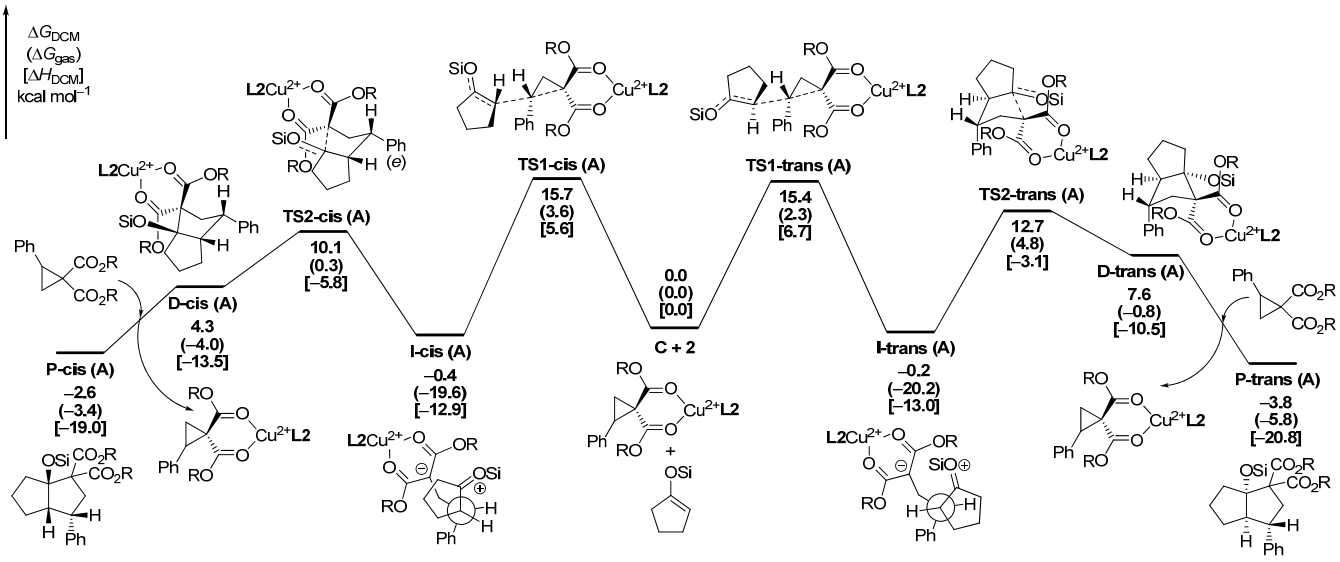
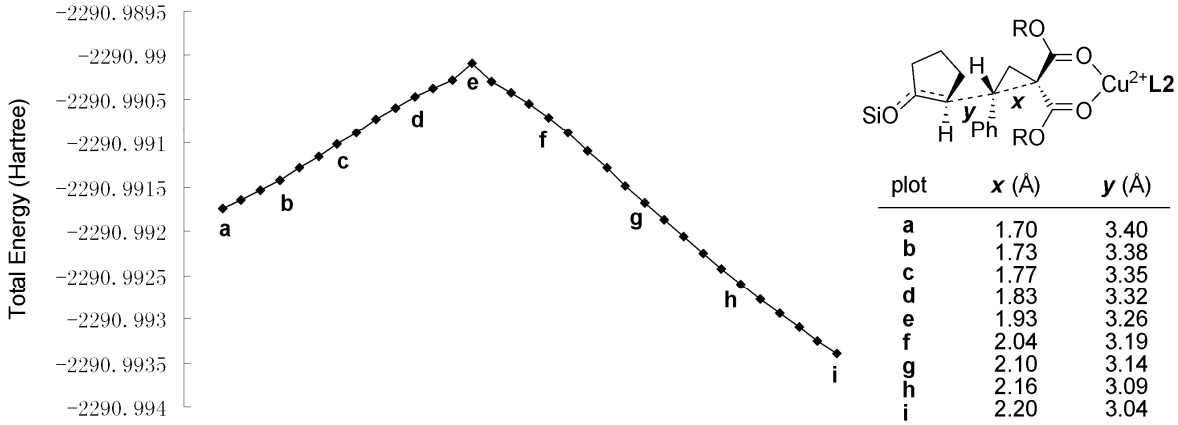


Figure S5. DFT-calculated overall free energy surface of Reaction **A** (**D** is **P/Catalyst Complex** shown in Figure S4, R = Me, and Si = TMS).



plot	*x* (Å)	*y* (Å)
a	1.70	3.40
b	1.73	3.38
c	1.77	3.35
d	1.83	3.32
e	1.93	3.26
f	2.04	3.19
g	2.10	3.14
h	2.16	3.09
i	2.20	3.04

Figure S6. IRC plot (R = Me and Si = TMS).

9.2. Coordinates of all stationary points

$Cu^{2+}L2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000016	-1.314940	0.000089
2	6	0	0.000015	-2.218541	-1.280896
3	1	0	0.000114	-1.622352	-2.198956
4	1	0	0.884277	-2.858339	-1.272438
5	1	0	-0.884331	-2.858226	-1.272559
6	6	0	-0.000132	-2.218154	1.281376
7	1	0	-0.884508	-2.857801	1.273144
8	1	0	0.884103	-2.857990	1.273180
9	1	0	-0.000088	-1.621680	2.199249
10	6	0	1.309842	-0.522145	0.000026
11	8	0	2.374763	-1.282987	0.000139
12	6	0	3.586814	-0.451685	0.000022
13	1	0	4.152917	-0.727822	-0.893109
14	1	0	4.152654	-0.727221	0.893508
15	6	0	3.020723	0.976291	-0.000493
16	1	0	3.309341	1.557956	-0.884787
17	1	0	3.309588	1.558745	0.883190
18	7	0	1.559445	0.778925	-0.000202
19	6	0	-1.309843	-0.522110	-0.000024
20	8	0	-2.374764	-1.282949	-0.000275
21	6	0	-3.586802	-0.451628	-0.000516
22	1	0	-4.153190	-0.727777	0.892425
23	1	0	-4.152355	-0.727153	-0.894192
24	6	0	-3.020696	0.976343	0.000212
25	1	0	-3.309419	1.557942	0.884515
26	1	0	-3.309435	1.558879	-0.883460
27	7	0	-1.559424	0.778966	0.000223
28	29	0	0.000026	1.912224	0.000085

1 (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	-5.109911	-0.816293	-0.852885
2	6	0	-4.058971	-0.859147	-0.579403
3	6	0	-3.687685	-1.015358	0.757057
4	6	0	-3.072704	-0.755663	-1.563601
5	6	0	-2.336988	-1.068753	1.106607
6	1	0	-4.448446	-1.096720	1.529053
7	6	0	-1.723658	-0.811385	-1.213270
8	1	0	-3.353384	-0.628027	-2.605690
9	6	0	-1.340540	-0.968340	0.127466
10	1	0	-2.051213	-1.196165	2.147388
11	1	0	-0.958747	-0.713763	-1.978503
12	6	0	0.111267	-1.087955	0.489139
13	6	0	1.068341	0.115026	0.343596
14	1	0	0.578217	-2.022438	0.186878
15	6	0	0.465159	1.403242	-0.157262
16	6	0	2.475027	-0.106775	-0.130687
17	8	0	0.492730	1.751286	-1.316303
18	8	0	3.204799	0.757063	-0.562699
19	8	0	2.865907	-1.394956	0.035472
20	6	0	4.226299	-1.669951	-0.334608
21	1	0	4.374877	-2.731281	-0.132869
22	1	0	4.385520	-1.452719	-1.393910
23	1	0	4.916098	-1.063863	0.258719
24	8	0	-0.152038	2.099517	0.819945
25	6	0	-0.833316	3.286908	0.381470
26	1	0	-1.290971	3.708062	1.277077
27	1	0	-0.123489	3.992130	-0.058191
28	1	0	-1.595141	3.036493	-0.361216
29	6	0	0.686681	-0.449314	1.708633
30	1	0	1.464669	-0.978709	2.249084
31	1	0	0.047256	0.184797	2.312921

C (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.112134	-3.906974	0.098155
2	6	0	1.041633	-2.835929	-0.201220
3	7	0	1.795051	-1.561730	-0.073963
4	6	0	3.039671	-1.842705	0.154644

5	8	0	3.342607	-3.127245	0.247617
6	29	0	0.960263	0.225197	-0.244712
7	7	0	2.709300	1.105378	0.052188
8	6	0	2.895119	2.579561	0.074870
9	6	0	4.422076	2.738272	0.237458
10	8	0	4.895940	1.359220	0.374205
11	6	0	3.863355	0.544275	0.235921
12	6	0	4.225029	-0.920616	0.324233
13	6	0	5.259000	-1.242739	-0.799433
14	6	0	4.865191	-1.185076	1.722116
15	1	0	4.920731	3.163957	-0.634606
16	1	0	4.724965	3.273981	1.137459
17	1	0	2.520839	3.016040	-0.853781
18	1	0	2.331844	3.003628	0.908916
19	1	0	5.169801	-2.231027	1.789951
20	1	0	5.747046	-0.553132	1.842543
21	1	0	4.162370	-0.968580	2.533252
22	1	0	6.141449	-0.613105	-0.671577
23	1	0	5.560298	-2.289435	-0.726906
24	1	0	4.838906	-1.064096	-1.794629
25	1	0	0.630881	-2.914150	-1.210160
26	1	0	0.214357	-2.853028	0.511777
27	1	0	2.276713	-4.617378	-0.712292
28	1	0	1.955743	-4.441956	1.036185
29	1	0	-6.350301	-2.987095	1.960685
30	6	0	-5.799752	-2.128382	1.588411
31	6	0	-5.996769	-1.688887	0.276283
32	6	0	-4.913352	-1.448667	2.430555
33	6	0	-5.302634	-0.579517	-0.202621
34	1	0	-6.706540	-2.199305	-0.367486
35	6	0	-4.225013	-0.335226	1.958021
36	1	0	-4.776648	-1.775672	3.456691
37	6	0	-4.403862	0.108009	0.632952
38	1	0	-5.490442	-0.228394	-1.212093
39	1	0	-3.557815	0.209420	2.622629
40	6	0	-3.707393	1.335174	0.206027
41	6	0	-2.250466	1.288926	-0.699761
42	1	0	-3.527823	2.055418	1.000086
43	6	0	-1.820321	-0.026092	-1.183919
44	6	0	-1.219323	2.207270	-0.207914
45	8	0	-0.702685	-0.556231	-0.961311
46	8	0	-0.001979	1.938703	-0.051682
47	8	0	-1.678403	3.401849	0.087814
48	6	0	-0.774129	4.411706	0.616711
49	1	0	-1.406755	5.276946	0.803555

50	1	0	-0.320795	4.053106	1.542383
51	1	0	-0.010930	4.643940	-0.127432
52	8	0	-2.730273	-0.662485	-1.876467
53	6	0	-2.459138	-2.009181	-2.355509
54	1	0	-3.353872	-2.290914	-2.906349
55	1	0	-1.587073	-1.996512	-3.010848
56	1	0	-2.302025	-2.675014	-1.505780
57	6	0	-3.602661	1.866119	-1.152688
58	1	0	-3.606877	2.943747	-1.280934
59	1	0	-4.068149	1.315948	-1.963341

2 (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.426748	0.452286	0.184492
2	6	0	-2.997332	-1.019002	-0.080816
3	6	0	-1.489374	-0.960246	-0.002657
4	6	0	-1.050719	0.308427	-0.032994
5	6	0	-2.178675	1.310245	-0.128305
6	8	0	0.213955	0.804714	-0.028682
7	14	0	1.700480	-0.009490	0.008670
8	6	0	2.967188	1.379440	-0.010682
9	6	0	1.842711	-1.022791	1.593482
10	6	0	1.877830	-1.101927	-1.518999
11	1	0	-4.303565	0.748277	-0.399960
12	1	0	-3.688027	0.566144	1.242550
13	1	0	-3.440114	-1.710477	0.648275
14	1	0	-3.332527	-1.363572	-1.072105
15	1	0	-0.864999	-1.847348	0.021653
16	1	0	-2.041546	2.146320	0.568050
17	1	0	-2.209476	1.745631	-1.138324
18	1	0	3.990285	0.984324	0.012387
19	1	0	2.865497	1.993791	-0.912558
20	1	0	2.842813	2.037349	0.856976
21	1	0	2.808062	-1.542622	1.637700
22	1	0	1.053077	-1.777736	1.671836
23	1	0	1.771759	-0.377424	2.476948
24	1	0	1.822223	-0.503441	-2.435910
25	1	0	2.845864	-1.618625	-1.517220
26	1	0	1.093030	-1.864039	-1.573358

I-cis (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.892482	3.211782	0.180612
2	6	0	-4.432710	2.731810	0.037885
3	7	0	-4.557230	1.253775	0.015365
4	6	0	-5.810317	0.952823	0.102033
5	8	0	-6.662560	1.968847	0.194362
6	29	0	-2.971029	0.029922	-0.141547
7	7	0	-4.218332	-1.542622	-0.071672
8	6	0	-3.745980	-2.946756	-0.130281
9	6	0	-5.052289	-3.766875	-0.075562
10	8	0	-6.092970	-2.746852	0.034230
11	6	0	-5.507084	-1.553281	0.018692
12	6	0	-6.481484	-0.401442	0.110502
13	6	0	-7.448962	-0.476962	-1.109798
14	6	0	-7.290510	-0.544148	1.435056
15	1	0	-5.256651	-4.341341	-0.980527
16	1	0	-5.138805	-4.413201	0.799085
17	1	0	-3.180570	-3.103652	-1.051032
18	1	0	-3.081411	-3.141855	0.713931
19	1	0	-8.024189	0.261261	1.502326
20	1	0	-7.815130	-1.501360	1.441373
21	1	0	-6.634465	-0.496349	2.310451
22	1	0	-7.971750	-1.435280	-1.102404
23	1	0	-8.184233	0.327087	-1.041903
24	1	0	-6.906331	-0.378692	-2.055759
25	1	0	-3.958768	3.069896	-0.885569
26	1	0	-3.798988	3.032994	0.874438
27	1	0	-6.252414	3.806319	-0.660280
28	1	0	-6.101861	3.731962	1.116680
29	6	0	-0.538209	1.556039	-0.471700
30	6	0	-0.215406	-0.842898	-0.362142
31	8	0	-1.803974	1.561494	-0.291441
32	8	0	-1.444790	-1.161825	-0.199408
33	8	0	0.677302	-1.856528	-0.377027
34	6	0	0.175870	-3.202145	-0.317452
35	1	0	1.059355	-3.838559	-0.370089
36	1	0	-0.359398	-3.378554	0.618887
37	1	0	-0.481379	-3.408567	-1.165661

38	8	0	0.068241	2.738277	-0.629204
39	6	0	-0.729092	3.935860	-0.648992
40	1	0	-0.017498	4.745681	-0.805318
41	1	0	-1.449114	3.903554	-1.470301
42	1	0	-1.250271	4.067510	0.302352
43	6	0	0.331003	0.441285	-0.525598
44	1	0	2.224120	-0.250016	-1.254094
45	6	0	1.799657	0.669578	-0.845127
46	6	0	2.653479	1.178821	0.351059
47	1	0	1.864229	1.424034	-1.634218
48	6	0	2.994876	0.034190	1.375577
49	6	0	3.883909	1.982402	-0.062190
50	1	0	2.014136	1.856685	0.927492
51	6	0	3.198750	0.478421	2.845589
52	6	0	4.217312	-0.789489	1.093130
53	1	0	2.166227	-0.694707	1.333530
54	6	0	4.290645	3.082589	0.709763
55	6	0	4.628777	1.672878	-1.212454
56	6	0	4.093886	-0.606485	3.472787
57	1	0	2.246518	0.602381	3.367373
58	1	0	3.717389	1.442862	2.866521
59	6	0	5.053309	-0.969990	2.321327
60	8	0	4.461965	-1.272065	-0.044929
61	6	0	5.419259	3.829999	0.366745
62	1	0	3.703225	3.378509	1.576018
63	6	0	5.753684	2.423984	-1.563468
64	1	0	4.314407	0.859067	-1.859396
65	1	0	4.627862	-0.262759	4.361117
66	1	0	3.505259	-1.485888	3.757925
67	1	0	5.535604	-1.949790	2.379125
68	1	0	5.856406	-0.215823	2.246448
69	14	0	5.846334	-2.252600	-0.748582
70	6	0	6.158793	3.499261	-0.769677
71	1	0	5.708911	4.679915	0.977827
72	1	0	6.302551	2.181279	-2.469462
73	6	0	7.406247	-1.323324	-0.306754
74	6	0	5.406753	-2.202254	-2.558741
75	6	0	5.668858	-3.947959	0.023461
76	1	0	7.029713	4.085892	-1.046097
77	1	0	4.405688	-2.606186	-2.744902
78	1	0	6.118825	-2.809894	-3.130797
79	1	0	5.448728	-1.184461	-2.960536
80	1	0	5.888672	-3.965095	1.096034
81	1	0	4.667955	-4.364798	-0.133899
82	1	0	6.381281	-4.629747	-0.458801

83	1	0	8.232003	-1.715492	-0.914494
84	1	0	7.315648	-0.255127	-0.534524
85	1	0	7.699647	-1.436170	0.741921

I-trans (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.623799	-3.483787	-1.915193
2	6	0	3.332720	-2.782397	-1.442965
3	7	0	3.834893	-1.617787	-0.675039
4	6	0	5.125557	-1.632813	-0.716596
5	8	0	5.688897	-2.630693	-1.392381
6	29	0	2.614335	-0.309308	0.241965
7	7	0	4.232384	0.711595	0.861647
8	6	0	4.138012	1.945544	1.678604
9	6	0	5.612273	2.356519	1.877697
10	8	0	6.357976	1.310441	1.179644
11	6	0	5.481441	0.459300	0.653843
12	6	0	6.125227	-0.678032	-0.105379
13	6	0	6.997243	-0.077715	-1.249175
14	6	0	7.028154	-1.477856	0.882255
15	1	0	5.877515	3.307581	1.413058
16	1	0	5.941856	2.349904	2.917699
17	1	0	3.552344	2.694586	1.141698
18	1	0	3.624820	1.721600	2.615592
19	1	0	7.536334	-2.280387	0.344210
20	1	0	7.777995	-0.811058	1.312285
21	1	0	6.439172	-1.915758	1.694872
22	1	0	7.751204	0.586216	-0.822298
23	1	0	7.500024	-0.883965	-1.786612
24	1	0	6.387821	0.491853	-1.958507
25	1	0	2.708687	-2.431637	-2.267416
26	1	0	2.717190	-3.409425	-0.794723
27	1	0	4.741777	-3.521846	-2.999109
28	1	0	4.770446	-4.479348	-1.493058
29	6	0	-0.160003	-0.949997	-0.247304
30	6	0	0.196921	0.903898	1.270470
31	8	0	1.069806	-1.239016	-0.455550
32	8	0	1.476350	0.885546	1.239511
33	8	0	-0.379399	1.805586	2.076145
34	6	0	0.459169	2.709285	2.814072

35	1	0	-0.228157	3.320344	3.398493
36	1	0	1.130123	2.159919	3.478842
37	1	0	1.036452	3.339293	2.132822
38	8	0	-1.079659	-1.715782	-0.868887
39	6	0	-0.615891	-2.790871	-1.701475
40	1	0	-1.518678	-3.254003	-2.099988
41	1	0	0.001780	-2.411080	-2.519155
42	1	0	-0.049090	-3.519229	-1.115998
43	6	0	-0.692158	0.069589	0.560009
44	1	0	-2.663533	-0.713322	0.876048
45	6	0	-2.194720	0.253840	0.675912
46	6	0	-2.867678	0.878959	-0.583358
47	1	0	-2.397937	0.887811	1.542409
48	6	0	-4.386405	1.201122	-0.361717
49	6	0	-2.158467	2.138902	-1.068535
50	1	0	-2.812528	0.140484	-1.391435
51	6	0	-5.080692	2.026504	-1.478136
52	6	0	-5.336063	0.054896	-0.155045
53	6	0	-1.570380	2.167165	-2.339685
54	6	0	-2.088032	3.293923	-0.274057
55	6	0	-6.583703	1.752568	-1.292993
56	1	0	-4.742332	1.668749	-2.458444
57	1	0	-4.827462	3.085119	-1.416483
58	6	0	-6.622219	0.265263	-0.894736
59	8	0	-5.066579	-0.938178	0.574357
60	6	0	-0.924151	3.314390	-2.808286
61	1	0	-1.623174	1.285040	-2.974354
62	6	0	-1.447320	4.442627	-0.739438
63	1	0	-2.532254	3.302607	0.718470
64	1	0	-6.563932	-0.372438	-1.793985
65	1	0	-7.498434	-0.066310	-0.329193
66	14	0	-5.988037	-2.418798	1.149269
67	6	0	-0.862504	4.456480	-2.009204
68	1	0	-0.482047	3.317646	-3.800591
69	1	0	-1.412389	5.331158	-0.115125
70	6	0	-7.278491	-1.734131	2.315128
71	6	0	-4.607684	-3.351982	1.983184
72	6	0	-6.656931	-3.253220	-0.385282
73	1	0	-0.373355	5.354502	-2.375005
74	1	0	-3.799666	-3.589334	1.282503
75	1	0	-4.985201	-4.299658	2.386398
76	1	0	-4.183961	-2.783677	2.818212
77	1	0	-7.478812	-2.704047	-0.855249
78	1	0	-5.877585	-3.429182	-1.135367
79	1	0	-7.052552	-4.236853	-0.100270

80	1	0	-7.789817	-2.571041	2.808160
81	1	0	-6.828910	-1.121131	3.104027
82	1	0	-8.049950	-1.141768	1.811554
83	1	0	-7.171442	1.955582	-2.190530
84	1	0	-6.993671	2.365278	-0.482247
85	1	0	-4.474105	1.766616	0.586377

D-cis (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.870272	3.219925	1.555338
2	6	0	2.538720	2.665597	1.004171
3	7	0	2.936959	1.374414	0.390161
4	6	0	4.206398	1.203983	0.579762
5	8	0	4.835640	2.166655	1.237210
6	29	0	1.677562	0.207531	-0.589599
7	7	0	3.114087	-1.163876	-0.837849
8	6	0	2.902446	-2.472983	-1.506024
9	6	0	4.320504	-3.082350	-1.547073
10	8	0	5.144720	-2.076431	-0.875597
11	6	0	4.369222	-1.057381	-0.536425
12	6	0	5.107466	0.068063	0.151896
13	6	0	5.818106	-0.506078	1.415273
14	6	0	6.170963	0.635253	-0.839534
15	1	0	4.425397	-4.011719	-0.986214
16	1	0	4.722320	-3.208413	-2.553418
17	1	0	2.200267	-3.072118	-0.920752
18	1	0	2.477433	-2.316976	-2.499239
19	1	0	6.742094	1.424667	-0.346986
20	1	0	6.855474	-0.162926	-1.133247
21	1	0	5.701639	1.046985	-1.739170
22	1	0	6.503171	-1.301416	1.116232
23	1	0	6.389541	0.285621	1.902941
24	1	0	5.095844	-0.912184	2.130626
25	1	0	1.800928	2.481406	1.789319
26	1	0	2.088363	3.308902	0.246061
27	1	0	3.885071	3.356288	2.637139
28	1	0	4.212922	4.130624	1.061894
29	6	0	-1.517637	0.525053	-1.012393
30	6	0	-0.660054	1.701629	-1.463106
31	6	0	-0.855046	-0.713569	-1.620229

32	8	0	0.560010	1.779052	-1.221155
33	8	0	0.369941	-0.939523	-1.573865
34	8	0	-1.667227	-1.525853	-2.236642
35	6	0	-1.138608	-2.722450	-2.879963
36	1	0	-2.004516	-3.189459	-3.344135
37	1	0	-0.398339	-2.436897	-3.628853
38	1	0	-0.699040	-3.376352	-2.125590
39	8	0	-1.300511	2.637911	-2.104894
40	6	0	-0.570325	3.818918	-2.558133
41	1	0	-1.304348	4.399787	-3.112096
42	1	0	-0.205424	4.373212	-1.692095
43	1	0	0.257528	3.512865	-3.199043
44	6	0	-0.739704	-3.169219	1.288603
45	14	0	-0.202955	-1.586322	2.162210
46	8	0	-0.358300	-0.255388	1.065132
47	6	0	-1.111742	-1.348602	3.788428
48	6	0	1.645625	-1.627963	2.514720
49	6	0	-1.501089	0.469405	0.613086
50	1	0	-0.749616	-0.470702	4.334890
51	1	0	-0.904089	-2.223199	4.419168
52	1	0	-2.199287	-1.271301	3.702012
53	1	0	1.861643	-2.434497	3.226134
54	1	0	1.984741	-0.691745	2.973754
55	1	0	2.249106	-1.811866	1.619581
56	6	0	-2.922613	-0.100996	0.996585
57	6	0	-1.477400	1.894800	1.230022
58	6	0	-3.543669	0.937549	1.968547
59	6	0	-3.699512	-0.332457	-0.341285
60	1	0	-2.809272	-1.058272	1.509000
61	6	0	-2.372318	1.793339	2.470870
62	1	0	-0.452935	2.215374	1.434825
63	1	0	-1.927700	2.619776	0.539644
64	6	0	-3.021933	0.631498	-1.332828
65	1	0	-4.262065	1.567669	1.433598
66	1	0	-4.101756	0.454827	2.775411
67	6	0	-5.214753	-0.253384	-0.247729
68	1	0	-3.464846	-1.350411	-0.668694
69	1	0	-1.838920	1.298093	3.288044
70	1	0	-2.688878	2.774586	2.836358
71	1	0	-3.252819	0.410173	-2.376873
72	1	0	-3.333733	1.662020	-1.146325
73	6	0	-5.909842	-1.367927	0.247763
74	6	0	-5.952801	0.877282	-0.622723
75	6	0	-7.297249	-1.350539	0.379504
76	1	0	-5.358338	-2.263235	0.529706

77	6	0	-7.344791	0.895870	-0.498094
78	1	0	-5.457027	1.754742	-1.029004
79	6	0	-8.020422	-0.214907	0.006150
80	1	0	-7.814485	-2.224475	0.764570
81	1	0	-7.898910	1.779770	-0.800200
82	1	0	-9.101947	-0.200195	0.100875
83	1	0	-0.144193	-3.351485	0.385194
84	1	0	-1.797385	-3.166388	1.001665
85	1	0	-0.592318	-4.030371	1.951952

D-trans (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.080673	4.070552	-0.373432
2	6	0	1.877285	3.136544	-0.624522
3	7	0	2.465421	1.780124	-0.479892
4	6	0	3.719587	1.907182	-0.182625
5	8	0	4.177771	3.145151	-0.080715
6	29	0	1.442765	0.100837	-0.790802
7	7	0	3.048756	-0.980467	-0.371606
8	6	0	3.079690	-2.463670	-0.448784
9	6	0	4.513368	-2.809095	0.004659
10	8	0	5.153432	-1.498906	0.134109
11	6	0	4.238770	-0.563616	-0.071380
12	6	0	4.764362	0.845989	0.077000
13	6	0	5.298964	1.025646	1.531246
14	6	0	5.930192	1.043181	-0.941082
15	1	0	4.565968	-3.289678	0.983100
16	1	0	5.090352	-3.381416	-0.721927
17	1	0	2.317011	-2.887213	0.207921
18	1	0	2.867919	-2.776018	-1.473855
19	1	0	6.347335	2.045103	-0.825008
20	1	0	6.714309	0.309937	-0.743903
21	1	0	5.585977	0.922343	-1.973534
22	1	0	6.086030	0.293744	1.722519
23	1	0	5.716106	2.028214	1.643502
24	1	0	4.502941	0.890067	2.270589
25	1	0	1.079012	3.264911	0.109696
26	1	0	1.451730	3.249837	-1.623484
27	1	0	2.969168	4.722734	0.493418
28	1	0	3.379258	4.656930	-1.243545

29	6	0	-1.685875	-0.847382	-1.079946
30	6	0	-1.354249	0.641849	-1.248098
31	6	0	-0.647389	-1.587513	-1.915092
32	8	0	-0.203749	1.123627	-1.197556
33	8	0	0.581962	-1.426624	-1.772730
34	8	0	-1.128878	-2.431165	-2.784085
35	6	0	-0.210394	-3.203883	-3.615545
36	1	0	-0.855540	-3.777856	-4.276951
37	1	0	0.429835	-2.524685	-4.179986
38	1	0	0.385211	-3.862391	-2.981562
39	8	0	-2.385658	1.385153	-1.500536
40	6	0	-2.240158	2.826197	-1.650669
41	1	0	-3.261183	3.199798	-1.668301
42	1	0	-1.689608	3.229869	-0.800763
43	1	0	-1.721164	3.035298	-2.587932
44	1	0	-7.318953	1.992240	-1.561020
45	6	0	-6.481751	1.846546	-0.884616
46	6	0	-5.774714	0.645111	-0.907583
47	6	0	-6.129253	2.849846	0.022618
48	6	0	-4.695328	0.416085	-0.038845
49	1	0	-6.077726	-0.135109	-1.603072
50	6	0	-5.065809	2.634574	0.899262
51	1	0	-6.689220	3.779606	0.056692
52	6	0	-3.995415	-0.941702	-0.125688
53	6	0	-4.355397	1.429775	0.865827
54	1	0	-4.794101	3.398596	1.622776
55	6	0	-3.023401	-1.323418	1.018437
56	6	0	-3.156898	-1.182228	-1.417471
57	1	0	-4.805600	-1.679087	-0.144684
58	1	0	-3.532531	1.296434	1.562571
59	6	0	-3.258564	-2.755907	1.573499
60	6	0	-1.543100	-1.318382	0.468449
61	1	0	-3.084015	-0.609066	1.837385
62	1	0	-3.204343	-2.243797	-1.673202
63	1	0	-3.525283	-0.628117	-2.282321
64	6	0	-1.862429	-3.353628	1.792703
65	1	0	-3.872087	-2.745183	2.479067
66	1	0	-3.798358	-3.360320	0.833717
67	6	0	-1.072595	-2.794427	0.600522
68	8	0	-0.654346	-0.421874	1.117995
69	1	0	-1.863704	-4.447269	1.814876
70	1	0	-1.433310	-3.014976	2.741662
71	14	0	-0.180644	-0.182746	2.758192
72	6	0	0.561841	1.546921	2.734128
73	6	0	1.149674	-1.442325	3.206793

74	6	0	-1.603958	-0.225240	3.984797
75	1	0	0.775455	-2.470944	3.242044
76	1	0	1.554542	-1.214586	4.200800
77	1	0	1.987857	-1.409501	2.499188
78	1	0	-1.191800	-0.026778	4.983014
79	1	0	-2.125111	-1.185368	4.044037
80	1	0	-2.347553	0.555503	3.788793
81	1	0	0.014327	-2.859155	0.703287
82	1	0	-1.360263	-3.367877	-0.289965
83	1	0	0.884624	1.826799	3.744375
84	1	0	-0.172738	2.293374	2.410000
85	1	0	1.438197	1.617242	2.079798

P-cis (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.568443	1.182455	0.021709
2	6	0	1.267918	2.348933	0.735012
3	6	0	1.310790	0.967405	-1.311977
4	8	0	2.043439	2.285396	1.660113
5	8	0	0.835253	0.468071	-2.310757
6	8	0	2.576267	1.419317	-1.254230
7	6	0	3.351799	1.263406	-2.453280
8	1	0	4.317495	1.719649	-2.235078
9	1	0	3.474183	0.204064	-2.693339
10	1	0	2.865089	1.766374	-3.292869
11	8	0	0.899647	3.520334	0.160637
12	6	0	1.540709	4.690329	0.691172
13	1	0	1.132980	5.529154	0.125962
14	1	0	1.321161	4.800708	1.756491
15	1	0	2.624000	4.625550	0.557482
16	6	0	1.330016	-2.912504	-1.706090
17	14	0	2.092705	-2.484696	-0.028434
18	8	0	1.685478	-0.945555	0.493960
19	6	0	1.623980	-3.824961	1.221173
20	6	0	3.968286	-2.401037	-0.185412
21	6	0	0.541850	-0.180753	0.836853
22	1	0	2.049262	-3.624173	2.211466
23	1	0	2.013050	-4.795395	0.885612
24	1	0	0.539381	-3.933720	1.337120
25	1	0	4.385295	-3.364524	-0.503824

26	1	0	4.430130	-2.131964	0.771256
27	1	0	4.271095	-1.645807	-0.919945
28	6	0	-0.847344	-0.852820	0.483137
29	6	0	0.493737	-0.000622	2.378583
30	6	0	-1.563961	-1.080772	1.836314
31	6	0	-1.560880	0.097086	-0.527266
32	1	0	-0.667966	-1.821212	0.008708
33	6	0	-0.432652	-1.117903	2.871910
34	1	0	1.500764	-0.004965	2.796218
35	1	0	0.041391	0.964987	2.633503
36	6	0	-0.932486	1.472776	-0.245158
37	1	0	-2.233035	-0.240314	2.059745
38	1	0	-2.187185	-1.981049	1.825421
39	6	0	-3.078002	0.019601	-0.535651
40	1	0	-1.221855	-0.193773	-1.524305
41	1	0	0.082961	-2.084936	2.851642
42	1	0	-0.783148	-0.955642	3.897393
43	1	0	-1.081525	2.182944	-1.061817
44	1	0	-1.354873	1.926575	0.659320
45	6	0	-3.691991	-1.026069	-1.245049
46	6	0	-3.907748	0.929943	0.133305
47	6	0	-5.078268	-1.168028	-1.275043
48	1	0	-3.068030	-1.735711	-1.784786
49	6	0	-5.298753	0.795918	0.102514
50	1	0	-3.474647	1.762682	0.679886
51	6	0	-5.890399	-0.254489	-0.598376
52	1	0	-5.525224	-1.987111	-1.832839
53	1	0	-5.918836	1.518502	0.627171
54	1	0	-6.971935	-0.357747	-0.623255
55	1	0	1.390340	-2.065230	-2.397299
56	1	0	0.274859	-3.200861	-1.630197
57	1	0	1.866023	-3.759174	-2.154844

P-trans (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.317918	1.039581	-0.268123
2	6	0	0.694201	1.356761	1.187405
3	6	0	1.228028	1.932497	-1.120053
4	8	0	1.763248	1.815890	1.529443
5	8	0	2.131894	1.574621	-1.842301

6	8	0	0.869732	3.226020	-0.974909
7	6	0	1.692688	4.177179	-1.668769
8	1	0	1.260338	5.153345	-1.447232
9	1	0	2.722623	4.121492	-1.306831
10	1	0	1.680143	3.985003	-2.744919
11	8	0	-0.285472	1.048128	2.060940
12	6	0	0.048463	1.234105	3.447682
13	1	0	-0.852229	0.970275	4.002459
14	1	0	0.877853	0.579539	3.726898
15	1	0	0.330192	2.272707	3.636658
16	1	0	-6.436944	-0.976607	-1.396756
17	6	0	-5.650503	-0.684543	-0.705470
18	6	0	-4.335454	-0.565183	-1.161663
19	6	0	-5.952178	-0.427370	0.631694
20	6	0	-3.298609	-0.190028	-0.297164
21	1	0	-4.110551	-0.764206	-2.207373
22	6	0	-4.928780	-0.051149	1.506034
23	1	0	-6.973927	-0.517555	0.990794
24	6	0	-1.873793	-0.085068	-0.807173
25	6	0	-3.617438	0.065299	1.046589
26	1	0	-5.153557	0.151957	2.550202
27	6	0	-0.892909	-1.109837	-0.187887
28	6	0	-1.196313	1.300038	-0.583195
29	1	0	-1.908388	-0.269760	-1.888017
30	1	0	-2.829314	0.358237	1.735154
31	6	0	-0.887066	-2.488440	-0.862268
32	6	0	0.507338	-0.517287	-0.481764
33	1	0	-1.051302	-1.172181	0.891952
34	1	0	-1.307198	1.935257	-1.465763
35	1	0	-1.662911	1.836446	0.244032
36	6	0	0.045169	-2.337104	-2.098664
37	1	0	-0.480561	-3.232194	-0.169117
38	1	0	-1.897301	-2.818286	-1.128897
39	6	0	0.760771	-0.967174	-1.944782
40	8	0	1.431268	-1.063817	0.438589
41	1	0	-0.518273	-2.370823	-3.037249
42	1	0	0.766279	-3.158754	-2.141511
43	14	0	3.055227	-1.510878	0.487652
44	6	0	3.328783	-1.887240	2.314680
45	6	0	4.236424	-0.159525	-0.079824
46	6	0	3.347809	-3.087150	-0.518953
47	1	0	4.093402	0.105781	-1.131396
48	1	0	5.273952	-0.493385	0.054386
49	1	0	4.089657	0.752513	0.508290
50	1	0	4.356679	-3.473467	-0.323461

51	1	0	3.267793	-2.919829	-1.599093
52	1	0	2.635317	-3.874869	-0.246400
53	1	0	1.826259	-1.000400	-2.173829
54	1	0	0.332875	-0.234381	-2.635579
55	1	0	4.346523	-2.255574	2.494507
56	1	0	2.628078	-2.649443	2.674869
57	1	0	3.188658	-0.985469	2.922008

TS1-cis (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.970781	2.535526	0.066001
2	6	0	-4.456291	2.382541	-0.190583
3	7	0	-4.240517	0.916568	-0.093297
4	6	0	-5.370950	0.357380	0.200183
5	8	0	-6.412979	1.165639	0.328874
6	29	0	-2.479111	0.042619	-0.408858
7	7	0	-3.276819	-1.735762	-0.003025
8	6	0	-2.503255	-3.003217	-0.028811
9	6	0	-3.550622	-4.065018	0.368818
10	8	0	-4.784493	-3.291569	0.512342
11	6	0	-4.505840	-2.014573	0.293527
12	6	0	-5.702067	-1.100255	0.423842
13	6	0	-6.764227	-1.531218	-0.634724
14	6	0	-6.292640	-1.257235	1.858485
15	1	0	-3.731974	-4.823485	-0.393549
16	1	0	-3.357420	-4.543987	1.329887
17	1	0	-2.095491	-3.159572	-1.029376
18	1	0	-1.671095	-2.942411	0.676157
19	1	0	-7.182200	-0.632267	1.955937
20	1	0	-6.573660	-2.298820	2.024363
21	1	0	-5.568304	-0.961192	2.624362
22	1	0	-7.042473	-2.573388	-0.466842
23	1	0	-7.654447	-0.908000	-0.531082
24	1	0	-6.378061	-1.428742	-1.654151
25	1	0	-4.156029	2.734826	-1.179634
26	1	0	-3.843440	2.890764	0.556984
27	1	0	-6.534568	2.895904	-0.795753
28	1	0	-6.218959	3.129425	0.946348
29	6	0	-0.421995	2.075752	-0.938747
30	6	0	0.287275	-0.282819	-1.335375

31	8	0	-1.601061	1.794031	-0.588639
32	8	0	-0.809344	-0.808736	-0.998849
33	8	0	1.264660	-1.034946	-1.792841
34	6	0	1.096921	-2.473512	-1.850852
35	1	0	2.052815	-2.846561	-2.210457
36	1	0	0.888010	-2.861282	-0.853039
37	1	0	0.292261	-2.722684	-2.545142
38	8	0	-0.053457	3.336810	-1.037186
39	6	0	-0.995728	4.382013	-0.689532
40	1	0	-0.435087	5.308380	-0.797389
41	1	0	-1.840367	4.362303	-1.380325
42	1	0	-1.333788	4.253362	0.340050
43	6	0	0.623281	1.126444	-1.255534
44	1	0	2.432330	0.914419	-2.490727
45	6	0	1.976190	1.604198	-1.786409
46	6	0	2.259055	1.371731	-0.371022
47	1	0	1.964829	2.630692	-2.140204
48	6	0	5.542561	0.221803	-0.392166
49	6	0	2.405358	2.368224	0.676916
50	1	0	2.531670	0.352550	-0.106275
51	6	0	6.475045	0.624056	-1.509672
52	6	0	4.853058	-0.886285	-0.710654
53	1	0	5.497473	0.728652	0.566725
54	6	0	2.448718	1.927177	2.018711
55	6	0	2.599581	3.739244	0.402527
56	6	0	5.984715	-0.229411	-2.715065
57	1	0	7.517118	0.391195	-1.247348
58	1	0	6.450046	1.699114	-1.725797
59	6	0	5.181454	-1.399871	-2.095623
60	8	0	3.926886	-1.543421	0.065139
61	6	0	2.662484	2.829538	3.054003
62	1	0	2.323271	0.869435	2.235471
63	6	0	2.826196	4.636724	1.441107
64	1	0	2.609944	4.093981	-0.622338
65	1	0	5.322393	0.376452	-3.344417
66	1	0	6.805586	-0.570756	-3.350467
67	1	0	5.774595	-2.323243	-2.027280
68	1	0	4.280415	-1.654281	-2.669707
69	14	0	4.352250	-2.553545	1.387776
70	6	0	2.851263	4.186340	2.765609
71	1	0	2.697904	2.481290	4.081556
72	1	0	2.999532	5.685661	1.221255
73	6	0	5.608496	-3.829666	0.823013
74	6	0	2.707725	-3.347609	1.855707
75	6	0	5.021354	-1.510429	2.803138

76	1	0	3.033310	4.890276	3.572271
77	1	0	1.948296	-2.593221	2.098558
78	1	0	2.824056	-3.988432	2.737653
79	1	0	2.323899	-3.977642	1.044267
80	1	0	5.957254	-1.011001	2.529300
81	1	0	4.308948	-0.738233	3.117914
82	1	0	5.231776	-2.140164	3.676408
83	1	0	5.879096	-4.494591	1.652417
84	1	0	5.220758	-4.456050	0.011457
85	1	0	6.534146	-3.358547	0.472604

TS1-trans (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.384693	-4.082366	-0.910239
2	6	0	3.157713	-3.190411	-0.622934
3	7	0	3.757218	-1.860142	-0.353499
4	6	0	5.037549	-1.952793	-0.510706
5	8	0	5.508476	-3.148944	-0.843118
6	29	0	2.691171	-0.249269	0.175552
7	7	0	4.367163	0.842150	0.261207
8	6	0	4.394132	2.276373	0.639733
9	6	0	5.883749	2.654956	0.493927
10	8	0	6.523469	1.390646	0.132274
11	6	0	5.579453	0.463801	0.017362
12	6	0	6.111058	-0.895035	-0.381287
13	6	0	6.830585	-0.757788	-1.758067
14	6	0	7.130722	-1.358728	0.703813
15	1	0	6.086712	3.361527	-0.312563
16	1	0	6.350961	3.002107	1.416184
17	1	0	3.742829	2.847355	-0.026062
18	1	0	4.023165	2.388514	1.660880
19	1	0	7.557879	-2.320732	0.414784
20	1	0	7.935385	-0.625674	0.785637
21	1	0	6.651718	-1.466199	1.682589
22	1	0	7.637437	-0.027229	-1.675997
23	1	0	7.255108	-1.721612	-2.045200
24	1	0	6.137581	-0.431236	-2.540433
25	1	0	2.476055	-3.115684	-1.473172
26	1	0	2.586089	-3.521493	0.247180
27	1	0	4.392569	-4.527637	-1.905763

28	1	0	4.560264	-4.853596	-0.158422
29	6	0	-0.203562	-0.815464	0.028712
30	6	0	0.400039	1.263430	1.262600
31	8	0	0.978660	-1.184094	-0.196325
32	8	0	1.635568	1.200840	1.028557
33	8	0	-0.069642	2.211768	2.055367
34	6	0	0.857497	3.168208	2.624800
35	1	0	0.239961	3.830846	3.228204
36	1	0	1.587939	2.650481	3.249067
37	1	0	1.357324	3.725167	1.830244
38	8	0	-1.214780	-1.562865	-0.389459
39	6	0	-0.929874	-2.793266	-1.097075
40	1	0	-1.907228	-3.214323	-1.325778
41	1	0	-0.376542	-2.580603	-2.014128
42	1	0	-0.360900	-3.469233	-0.456217
43	6	0	-0.616245	0.382829	0.728870
44	1	0	-2.655649	-0.363546	1.136888
45	6	0	-2.085693	0.562501	1.112985
46	6	0	-2.076569	1.263653	-0.169886
47	1	0	-2.224153	1.163776	2.007035
48	6	0	-5.305110	0.983406	-0.533156
49	6	0	-2.063612	2.689659	-0.418484
50	1	0	-2.189370	0.628485	-1.042615
51	6	0	-5.784501	1.555046	-1.840091
52	6	0	-5.315610	-0.370222	-0.551729
53	6	0	-1.871051	3.134875	-1.747282
54	6	0	-2.325479	3.644932	0.589760
55	6	0	-5.772183	0.331484	-2.799432
56	1	0	-5.159336	2.379407	-2.208033
57	1	0	-6.796794	1.972843	-1.730457
58	6	0	-5.790751	-0.916475	-1.882601
59	8	0	-4.946848	-1.154691	0.483744
60	6	0	-1.925690	4.488494	-2.056254
61	1	0	-1.688806	2.405945	-2.533147
62	6	0	-2.387080	4.997478	0.273565
63	1	0	-2.511118	3.323607	1.608503
64	1	0	-5.157154	-1.732423	-2.251061
65	1	0	-6.804143	-1.332123	-1.780789
66	14	0	-5.715500	-2.564545	1.114766
67	6	0	-2.182588	5.421599	-1.044852
68	1	0	-1.782172	4.819648	-3.079958
69	1	0	-2.609974	5.724539	1.048360
70	6	0	-7.531489	-2.181050	1.395537
71	6	0	-4.789216	-2.852745	2.721936
72	6	0	-5.472697	-4.009297	-0.069001

73	1	0	-2.237975	6.478909	-1.286577
74	1	0	-3.717511	-3.010294	2.549967
75	1	0	-5.172115	-3.743278	3.234464
76	1	0	-4.903236	-2.005017	3.406819
77	1	0	-5.995736	-3.869474	-1.021046
78	1	0	-4.411429	-4.182955	-0.286385
79	1	0	-5.864603	-4.929048	0.383175
80	1	0	-8.029553	-3.033186	1.874199
81	1	0	-7.658729	-1.313057	2.052345
82	1	0	-8.066265	-1.976469	0.461011
83	1	0	-4.848361	0.336127	-3.389248
84	1	0	-6.604409	0.344317	-3.507277
85	1	0	-5.091699	1.577128	0.349631

TS2-cis (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.786623	-3.364840	1.114990
2	6	0	-3.382063	-2.934860	0.640963
3	7	0	-3.583688	-1.529596	0.204670
4	6	0	-4.835118	-1.233004	0.356688
5	8	0	-5.611633	-2.185397	0.851971
6	29	0	-2.121951	-0.386262	-0.520831
7	7	0	-3.411223	1.109626	-0.776871
8	6	0	-3.025710	2.432612	-1.330271
9	6	0	-4.363307	3.201461	-1.375103
10	8	0	-5.320918	2.255684	-0.801223
11	6	0	-4.680806	1.129244	-0.523075
12	6	0	-5.569761	0.052083	0.053237
13	6	0	-6.195153	0.586601	1.378422
14	6	0	-6.699605	-0.258032	-0.976789
15	1	0	-4.386224	4.099743	-0.757013
16	1	0	-4.708532	3.436593	-2.383037
17	1	0	-2.286568	2.899383	-0.674945
18	1	0	-2.577229	2.301944	-2.316640
19	1	0	-7.372463	-1.011688	-0.563564
20	1	0	-7.269283	0.651395	-1.176174
21	1	0	-6.289433	-0.631396	-1.920898
22	1	0	-6.762368	1.496243	1.172378
23	1	0	-6.871607	-0.164501	1.790564
24	1	0	-5.424049	0.812890	2.122222

25	1	0	-2.635955	-2.969669	1.437422
26	1	0	-3.016046	-3.528416	-0.199442
27	1	0	-4.852983	-3.572100	2.184064
28	1	0	-5.216498	-4.192530	0.549711
29	6	0	1.261297	-0.714321	-0.795011
30	6	0	0.412176	-1.865683	-0.524518
31	6	0	0.556555	0.433392	-1.362490
32	8	0	-0.837035	-1.853070	-0.324234
33	8	0	-0.673944	0.692781	-1.275200
34	8	0	1.341959	1.276337	-2.000987
35	6	0	0.763257	2.429706	-2.657814
36	1	0	1.604489	2.930990	-3.133020
37	1	0	0.038693	2.105448	-3.407383
38	1	0	0.288321	3.081671	-1.923016
39	8	0	1.051688	-3.016245	-0.425991
40	6	0	0.306033	-4.229492	-0.159668
41	1	0	1.054451	-5.019714	-0.157230
42	1	0	-0.187115	-4.163785	0.811985
43	1	0	-0.426430	-4.397403	-0.951312
44	6	0	3.397607	3.485723	0.650122
45	14	0	1.927721	2.903223	1.658728
46	8	0	1.357595	1.352862	1.077038
47	6	0	2.345497	2.696586	3.475419
48	6	0	0.422529	3.990206	1.394008
49	6	0	1.780617	0.097541	1.159145
50	1	0	1.488468	2.341397	4.058720
51	1	0	2.640254	3.668142	3.891912
52	1	0	3.184077	2.012129	3.646943
53	1	0	0.620500	5.006004	1.756515
54	1	0	-0.447079	3.609393	1.941688
55	1	0	0.156774	4.071773	0.333316
56	6	0	3.254750	-0.259969	1.001418
57	6	0	1.142849	-0.769451	2.249794
58	6	0	3.378588	-1.621304	1.718454
59	6	0	3.704722	-0.153434	-0.475602
60	1	0	3.812532	0.488073	1.585248
61	6	0	2.341384	-1.542202	2.855780
62	1	0	0.642469	-0.110718	2.966798
63	1	0	0.373179	-1.447871	1.871349
64	6	0	2.683129	-0.968639	-1.301311
65	1	0	3.128386	-2.443189	1.040749
66	1	0	4.393240	-1.797661	2.081356
67	6	0	5.158558	-0.513599	-0.732353
68	1	0	3.581545	0.897958	-0.755077
69	1	0	2.751093	-0.974968	3.698842

70	1	0	2.054065	-2.525168	3.238914
71	1	0	2.772843	-0.701979	-2.358177
72	1	0	2.900790	-2.032704	-1.227941
73	6	0	6.083504	0.512184	-0.975986
74	6	0	5.621251	-1.838727	-0.728868
75	6	0	7.431500	0.229662	-1.199905
76	1	0	5.744324	1.545990	-0.998982
77	6	0	6.968361	-2.125481	-0.954068
78	1	0	4.934869	-2.662723	-0.553928
79	6	0	7.878108	-1.092522	-1.188403
80	1	0	8.129323	1.040163	-1.388779
81	1	0	7.306682	-3.157583	-0.949702
82	1	0	8.925432	-1.317437	-1.365896
83	1	0	3.183449	3.507984	-0.424209
84	1	0	4.291562	2.872553	0.806705
85	1	0	3.654477	4.509349	0.952029

TS2-trans (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.421908	-3.954359	-0.346206
2	6	0	-2.220613	-2.993752	-0.475124
3	7	0	-2.845953	-1.649844	-0.384020
4	6	0	-4.121860	-1.805386	-0.226450
5	8	0	-4.563414	-3.053981	-0.181474
6	29	0	-1.820373	0.051566	-0.555073
7	7	0	-3.496832	1.095272	-0.285148
8	6	0	-3.542877	2.579500	-0.275830
9	6	0	-5.032483	2.887143	-0.013521
10	8	0	-5.652330	1.562604	0.027606
11	6	0	-4.702336	0.650995	-0.122814
12	6	0	-5.214233	-0.770344	-0.087701
13	6	0	-5.946741	-1.001794	1.268994
14	6	0	-6.218723	-0.956403	-1.267642
15	1	0	-5.227216	3.363850	0.948417
16	1	0	-5.521517	3.448266	-0.810562
17	1	0	-2.885222	2.965212	0.506259
18	1	0	-3.192595	2.959645	-1.237374
19	1	0	-6.629339	-1.967434	-1.239193
20	1	0	-7.036609	-0.240806	-1.164541
21	1	0	-5.732463	-0.800066	-2.236221

22	1	0	-6.767154	-0.288459	1.366122
23	1	0	-6.355342	-2.013629	1.294474
24	1	0	-5.267044	-0.874576	2.117964
25	1	0	-1.490947	-3.114114	0.328580
26	1	0	-1.697718	-3.091709	-1.428480
27	1	0	-3.389061	-4.597960	0.533806
28	1	0	-3.610965	-4.554837	-1.237131
29	6	0	1.460327	0.865396	-1.107600
30	6	0	1.010120	-0.524473	-1.027705
31	6	0	0.395221	1.842798	-1.254306
32	8	0	-0.139998	-0.942353	-0.708639
33	8	0	-0.826311	1.688513	-0.959618
34	8	0	0.789905	3.031047	-1.680347
35	6	0	-0.187601	4.080483	-1.882851
36	1	0	0.385398	4.923181	-2.265392
37	1	0	-0.931795	3.760213	-2.614494
38	1	0	-0.666824	4.339767	-0.936749
39	8	0	1.957196	-1.386343	-1.295913
40	6	0	1.713078	-2.810040	-1.240191
41	1	0	2.697598	-3.258321	-1.358224
42	1	0	1.275816	-3.081926	-0.278712
43	1	0	1.051464	-3.099594	-2.059814
44	1	0	6.477616	-2.258495	-3.226145
45	6	0	6.002323	-1.984830	-2.288629
46	6	0	5.337751	-0.764225	-2.180302
47	6	0	6.076823	-2.841566	-1.186897
48	6	0	4.721781	-0.372463	-0.980336
49	1	0	5.311606	-0.097957	-3.040477
50	6	0	5.482463	-2.459945	0.015971
51	1	0	6.608276	-3.785648	-1.261537
52	6	0	4.035727	0.994037	-0.953179
53	6	0	4.810395	-1.237092	0.116901
54	1	0	5.551381	-3.108356	0.885509
55	6	0	3.636814	1.558820	0.420658
56	6	0	2.770395	1.112556	-1.861563
57	1	0	4.771779	1.692236	-1.371757
58	1	0	4.352928	-0.970327	1.063701
59	6	0	3.668480	3.102078	0.497080
60	6	0	2.223360	1.201671	0.916930
61	1	0	4.307692	1.164118	1.195329
62	1	0	2.734577	2.118462	-2.278866
63	1	0	2.857552	0.423689	-2.705721
64	6	0	2.745948	3.445192	1.675362
65	1	0	4.688379	3.471838	0.632573
66	1	0	3.281019	3.542049	-0.429455

67	6	0	1.568570	2.455248	1.518794
68	8	0	2.059934	0.032669	1.514154
69	1	0	2.411678	4.486190	1.678539
70	1	0	3.261349	3.262393	2.625326
71	14	0	1.331598	-0.543598	2.997521
72	6	0	1.703471	-2.375787	2.949201
73	6	0	-0.527175	-0.225184	2.940128
74	6	0	2.174551	0.316926	4.433291
75	1	0	-0.782093	0.837848	2.868672
76	1	0	-0.992334	-0.608622	3.857023
77	1	0	-0.986096	-0.754556	2.095773
78	1	0	1.825412	-0.124522	5.375375
79	1	0	1.970998	1.391642	4.486614
80	1	0	3.261171	0.178345	4.397755
81	1	0	1.065896	2.224459	2.460426
82	1	0	0.812315	2.885912	0.859462
83	1	0	1.350730	-2.858773	3.868534
84	1	0	2.779274	-2.565956	2.871829
85	1	0	1.212219	-2.874146	2.105860

TS3-cis (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.332164	-3.039935	1.370011
2	6	0	3.961144	-2.651343	0.777376
3	7	0	4.148402	-1.229364	0.391735
4	6	0	5.377800	-0.901259	0.631543
5	8	0	6.146369	-1.841708	1.161126
6	29	0	2.698536	-0.104738	-0.377848
7	7	0	3.955752	1.430174	-0.529816
8	6	0	3.564743	2.756441	-1.071087
9	6	0	4.891625	3.544513	-1.067909
10	8	0	5.837854	2.617459	-0.445946
11	6	0	5.210959	1.473285	-0.214344
12	6	0	6.093998	0.408114	0.393665
13	6	0	7.288534	0.144909	-0.574365
14	6	0	6.628529	0.935440	1.760790
15	1	0	5.274674	3.774406	-2.063481
16	1	0	4.876413	4.448630	-0.458541
17	1	0	3.142843	2.638482	-2.071163
18	1	0	2.803398	3.200882	-0.426221

19	1	0	7.296868	0.192814	2.200574
20	1	0	7.186177	1.860287	1.601134
21	1	0	5.810437	1.132806	2.461258
22	1	0	7.843105	1.072401	-0.727757
23	1	0	7.957403	-0.596855	-0.134029
24	1	0	6.943205	-0.224220	-1.545619
25	1	0	3.698192	-3.234649	-0.107637
26	1	0	3.146675	-2.735922	1.499875
27	1	0	5.828268	-3.862145	0.853516
28	1	0	5.314389	-3.233114	2.443843
29	6	0	0.293949	-1.709521	-0.825542
30	6	0	-0.027352	0.727331	-1.082902
31	8	0	1.518434	-1.658116	-0.521786
32	8	0	1.188869	1.023982	-0.914885
33	8	0	-0.873219	1.677263	-1.425209
34	6	0	-0.386325	3.026495	-1.618735
35	1	0	-1.266241	3.601509	-1.901018
36	1	0	0.042340	3.407516	-0.689502
37	1	0	0.355332	3.045225	-2.419324
38	8	0	-0.253821	-2.878686	-1.083741
39	6	0	0.561323	-4.076612	-1.034659
40	1	0	-0.114427	-4.883337	-1.312004
41	1	0	1.382197	-3.998327	-1.749729
42	1	0	0.944358	-4.225076	-0.023096
43	6	0	-0.651591	-0.586104	-0.878267
44	1	0	-2.442199	0.109282	-1.816032
45	6	0	-2.018573	-0.857799	-1.547955
46	6	0	-2.944897	-1.558478	-0.511215
47	1	0	-1.913636	-1.448571	-2.461920
48	6	0	-2.600789	-0.990023	0.876916
49	6	0	-4.434260	-1.540447	-0.859605
50	1	0	-2.645660	-2.612062	-0.473349
51	6	0	-2.205057	-1.875587	2.060205
52	6	0	-3.143449	0.188235	1.391222
53	1	0	-1.259030	-0.521375	0.313625
54	6	0	-5.321971	-2.259562	-0.042274
55	6	0	-4.957628	-0.875005	-1.974893
56	6	0	-2.020165	-0.874050	3.222320
57	1	0	-1.303788	-2.472017	1.871666
58	1	0	-3.008112	-2.592533	2.283420
59	6	0	-2.993698	0.276958	2.891406
60	8	0	-3.722825	1.097027	0.650993
61	6	0	-6.688706	-2.294108	-0.314700
62	1	0	-4.939599	-2.810459	0.814337
63	6	0	-6.327614	-0.913263	-2.256498

64	1	0	-4.308308	-0.325752	-2.649199
65	1	0	-2.209285	-1.316804	4.203024
66	1	0	-0.991721	-0.492035	3.227190
67	1	0	-2.661503	1.262976	3.232260
68	1	0	-3.982627	0.101460	3.341614
69	14	0	-4.878670	2.381920	0.968896
70	6	0	-7.198958	-1.616204	-1.425656
71	1	0	-7.353107	-2.861174	0.331096
72	1	0	-6.708315	-0.398123	-3.134037
73	6	0	-6.365471	1.602511	1.801024
74	6	0	-5.247503	2.998169	-0.757636
75	6	0	-4.038287	3.692065	2.023630
76	1	0	-8.261468	-1.649146	-1.647208
77	1	0	-4.350720	3.389423	-1.251979
78	1	0	-5.986004	3.808160	-0.727444
79	1	0	-5.656747	2.194779	-1.379296
80	1	0	-3.854564	3.365116	3.052778
81	1	0	-3.084506	4.015541	1.590351
82	1	0	-4.683725	4.577791	2.080047
83	1	0	-7.184464	2.331215	1.847792
84	1	0	-6.726807	0.736519	1.234890
85	1	0	-6.163090	1.282569	2.829300

TS3-trans (A)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.060081	-2.411032	2.438571
2	6	0	-3.708466	-2.261497	1.708864
3	7	0	-3.933497	-1.098884	0.812888
4	6	0	-5.167979	-0.726935	0.931128
5	8	0	-5.907568	-1.404990	1.796834
6	29	0	-2.519995	-0.328139	-0.355871
7	7	0	-3.808438	1.023855	-1.042532
8	6	0	-3.448737	2.064259	-2.039015
9	6	0	-4.791606	2.777148	-2.305809
10	8	0	-5.716318	2.121737	-1.379780
11	6	0	-5.062935	1.155954	-0.750371
12	6	0	-5.920491	0.370956	0.215602
13	6	0	-6.492008	1.357302	1.279550
14	6	0	-7.091305	-0.281503	-0.583206
15	1	0	-4.791785	3.840434	-2.064050

16	1	0	-5.183541	2.625428	-3.312768
17	1	0	-2.690717	2.726276	-1.614725
18	1	0	-3.033538	1.593473	-2.932555
19	1	0	-7.742836	-0.824144	0.104444
20	1	0	-7.672880	0.498445	-1.078106
21	1	0	-6.719505	-0.978745	-1.341170
22	1	0	-7.074131	2.134233	0.780520
23	1	0	-7.144638	0.814530	1.965719
24	1	0	-5.691276	1.832026	1.856095
25	1	0	-2.879504	-2.052730	2.388543
26	1	0	-3.449176	-3.135408	1.107607
27	1	0	-5.021136	-2.167416	3.501595
28	1	0	-5.542788	-3.378440	2.297372
29	6	0	-0.129397	-2.022786	-0.320897
30	6	0	0.173624	0.194686	-1.377605
31	8	0	-1.339395	-1.847206	-0.003668
32	8	0	-1.024335	0.570969	-1.243194
33	8	0	1.007679	0.945281	-2.066825
34	6	0	0.534866	2.177406	-2.660869
35	1	0	1.411281	2.608900	-3.140590
36	1	0	-0.238563	1.961781	-3.400431
37	1	0	0.149516	2.843548	-1.886298
38	8	0	0.402283	-3.217886	-0.159588
39	6	0	-0.418358	-4.301255	0.343729
40	1	0	0.231726	-5.173867	0.324049
41	1	0	-0.738186	-4.082973	1.364594
42	1	0	-1.281728	-4.449327	-0.307250
43	6	0	0.805343	-1.000413	-0.805448
44	1	0	2.214291	-2.542993	-1.330903
45	6	0	2.120263	-1.467099	-1.472809
46	6	0	3.310449	-0.724938	-0.789107
47	1	0	2.114414	-1.279503	-2.549224
48	6	0	2.953292	-0.558546	0.692091
49	6	0	4.663121	-1.372069	-1.048731
50	1	0	3.345285	0.285872	-1.205457
51	6	0	3.058035	-1.678929	1.731913
52	6	0	3.093536	0.654410	1.368315
53	6	0	5.729253	-0.576287	-1.491835
54	6	0	4.890547	-2.743677	-0.857529
55	6	0	2.652277	-0.986924	3.052019
56	1	0	4.092893	-2.041106	1.779403
57	1	0	2.432333	-2.547301	1.503726
58	6	0	3.104238	0.475945	2.867117
59	8	0	3.216972	1.812846	0.761762
60	6	0	6.986684	-1.129544	-1.736643

61	1	0	5.570434	0.487561	-1.655390
62	6	0	6.147281	-3.300428	-1.100402
63	1	0	4.086802	-3.392644	-0.518262
64	1	0	4.137276	0.617723	3.219230
65	1	0	2.485550	1.210883	3.392408
66	14	0	3.736504	3.404794	1.286161
67	6	0	7.199474	-2.495077	-1.540484
68	1	0	7.796991	-0.496060	-2.085808
69	1	0	6.303298	-4.364671	-0.949010
70	6	0	2.454043	4.100023	2.471284
71	6	0	3.766362	4.342595	-0.333628
72	6	0	5.438244	3.236315	2.052611
73	1	0	8.175786	-2.929559	-1.733146
74	1	0	4.453330	3.882292	-1.052342
75	1	0	4.102643	5.373552	-0.171325
76	1	0	2.772569	4.391516	-0.793766
77	1	0	5.426313	2.731932	3.024789
78	1	0	6.124637	2.692990	1.393309
79	1	0	5.865206	4.234071	2.215034
80	1	0	2.677499	5.157032	2.663986
81	1	0	1.442224	4.055169	2.051253
82	1	0	2.445647	3.593945	3.442479
83	1	0	3.096206	-1.456145	3.933083
84	1	0	1.562392	-1.018411	3.175922
85	1	0	1.489754	-0.562440	0.284161

1 (B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.373690	-1.628668	-0.221461
2	6	0	2.362544	-1.878432	-1.181365
3	6	0	3.670091	-2.183004	-0.795862
4	6	0	4.005073	-2.242860	0.558015
5	6	0	3.025459	-1.996522	1.523733
6	6	0	1.720561	-1.692887	1.136870
7	6	0	-0.045812	-1.349503	-0.619448
8	6	0	-0.400457	-0.541530	-1.823067
9	6	0	-0.658921	0.056324	-0.444760
10	6	0	-2.092224	0.200002	-0.008835
11	8	0	-2.786609	-0.939697	-0.223192
12	6	0	-4.220493	-0.995945	0.066080

13	6	0	0.246542	1.127847	0.121573
14	8	0	1.018512	1.687551	-0.826910
15	6	0	2.026286	2.687365	-0.461657
16	8	0	0.275085	1.397387	1.303237
17	8	0	-2.563177	1.228895	0.427372
18	1	0	5.022110	-2.479441	0.859274
19	1	0	4.424768	-2.376076	-1.553934
20	1	0	3.278855	-2.036280	2.579794
21	1	0	2.104773	-1.839972	-2.236371
22	1	0	0.965410	-1.483311	1.889377
23	1	0	-0.749557	-2.137664	-0.363168
24	1	0	-4.450803	-2.027172	-0.220431
25	6	0	-4.498489	-0.826990	1.558290
26	6	0	-5.015197	-0.048326	-0.830087
27	1	0	2.470545	2.899988	-1.439356
28	6	0	1.375469	3.961686	0.071650
29	6	0	3.102143	2.101500	0.450028
30	1	0	-1.273435	-0.833255	-2.397986
31	1	0	0.396649	-0.074222	-2.390751
32	1	0	3.931025	2.814760	0.530014
33	1	0	2.710612	1.904388	1.449524
34	1	0	3.492921	1.167237	0.034217
35	1	0	2.135495	4.747156	0.157351
36	1	0	0.599068	4.312661	-0.616261
37	1	0	0.927090	3.795607	1.052963
38	1	0	-5.549476	-1.065296	1.759184
39	1	0	-3.877538	-1.513646	2.143361
40	1	0	-4.299768	0.195078	1.885992
41	1	0	-6.085772	-0.250845	-0.710082
42	1	0	-4.823631	0.994871	-0.572196
43	1	0	-4.757424	-0.207980	-1.882748

C (B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.102959	-4.099967	-0.641648
2	6	0	-1.082359	-3.026642	-0.207901
3	7	0	-1.891928	-1.781186	-0.183748
4	6	0	-3.123800	-2.089974	-0.440601
5	8	0	-3.369881	-3.367415	-0.686073
6	29	0	-1.132949	0.010025	0.204085

7	7	0	-2.931268	0.831734	0.044021
8	6	0	-3.188036	2.285275	0.211743
9	6	0	-4.725086	2.383143	0.116506
10	8	0	-5.132121	1.019580	-0.228171
11	6	0	-4.058942	0.244941	-0.207896
12	6	0	-4.350135	-1.208984	-0.500548
13	6	0	-5.381043	-1.730188	0.547777
14	6	0	-4.959583	-1.306010	-1.933718
15	1	0	-5.213270	2.634528	1.059630
16	1	0	-5.086798	3.038736	-0.675806
17	1	0	-2.799508	2.625689	1.173588
18	1	0	-2.677503	2.836014	-0.581679
19	1	0	-5.212501	-2.345421	-2.151401
20	1	0	-5.869547	-0.704964	-1.983037
21	1	0	-4.257402	-0.946777	-2.693141
22	1	0	-6.291999	-1.131821	0.489798
23	1	0	-5.628304	-2.770460	0.328413
24	1	0	-4.983331	-1.669386	1.566095
25	1	0	-0.670285	-3.208365	0.787261
26	1	0	-0.253534	-2.920085	-0.911079
27	1	0	-2.226903	-4.916870	0.069616
28	1	0	-1.928806	-4.500885	-1.641543
29	1	0	5.777559	-2.810909	-2.988941
30	6	0	5.271343	-2.003772	-2.468054
31	6	0	5.730846	-1.582748	-1.218027
32	6	0	4.175544	-1.367767	-3.060427
33	6	0	5.090643	-0.537784	-0.550362
34	1	0	6.600304	-2.054779	-0.770383
35	6	0	3.543016	-0.316785	-2.400931
36	1	0	3.831319	-1.677085	-4.042670
37	6	0	3.986721	0.103115	-1.133734
38	1	0	5.476150	-0.200179	0.406494
39	1	0	2.712237	0.198314	-2.879208
40	6	0	3.335617	1.276821	-0.501646
41	6	0	2.056129	1.120925	0.546060
42	1	0	3.079336	2.076080	-1.192837
43	6	0	1.693511	-0.242569	0.984600
44	6	0	0.958303	2.074515	0.291406
45	8	0	0.569565	-0.775299	0.790403
46	8	0	-0.263435	1.778251	0.227286
47	8	0	1.368726	3.300672	0.111958
48	6	0	0.424226	4.421166	-0.192085
49	1	0	-0.403215	3.976167	-0.749035
50	8	0	2.651089	-0.886387	1.585064
51	6	0	2.452281	-2.280169	2.101532

52	1	0	1.819912	-2.783243	1.367008
53	6	0	3.442501	1.680163	0.904093
54	1	0	3.460885	2.739138	1.136842
55	1	0	4.009369	1.052126	1.581997
56	6	0	-0.048623	5.006590	1.129679
57	1	0	-0.731176	5.839625	0.932062
58	1	0	-0.579890	4.264282	1.733717
59	1	0	0.795763	5.393539	1.708352
60	6	0	1.213127	5.386148	-1.059577
61	1	0	1.553814	4.908024	-1.982791
62	1	0	0.571835	6.230301	-1.332374
63	1	0	2.081115	5.779261	-0.521429
64	6	0	3.837516	-2.898370	2.145621
65	1	0	3.753343	-3.934524	2.488632
66	1	0	4.304021	-2.898828	1.157335
67	1	0	4.484910	-2.361813	2.846464
68	6	0	1.765537	-2.191680	3.456660
69	1	0	2.376964	-1.624280	4.165205
70	1	0	0.778182	-1.725626	3.384491
71	1	0	1.635538	-3.201656	3.859122

2 (B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.671825	-1.628818	0.396490
2	6	0	-2.674769	-2.409905	1.213714
3	6	0	-3.342239	-3.316960	0.153118
4	6	0	-3.060424	-2.632549	-1.215044
5	6	0	-1.869504	-1.749448	-0.924536
6	8	0	-0.748889	-0.896925	1.082064
7	14	0	0.340814	0.286673	0.558472
8	6	0	1.733526	-0.544874	-0.409012
9	6	0	-0.597807	1.540724	-0.499172
10	6	0	0.980070	1.021915	2.209395
11	6	0	1.670295	-0.096063	3.022137
12	6	0	1.991041	2.158071	1.944795
13	6	0	-0.200659	1.582900	3.031288
14	1	0	-4.410043	-3.471218	0.337265
15	1	0	-2.864062	-4.302860	0.168264
16	1	0	-2.868723	-3.367241	-2.008033
17	1	0	-3.922658	-2.035727	-1.551951

18	1	0	-1.300831	-1.242710	-1.696454
19	1	0	-2.196759	-2.971714	2.025400
20	1	0	-3.391096	-1.722326	1.688666
21	1	0	2.322242	2.595485	2.897544
22	1	0	2.887076	1.796862	1.426974
23	1	0	1.554255	2.968012	1.347315
24	1	0	0.160947	1.956830	4.000122
25	1	0	-0.691871	2.419606	2.521438
26	1	0	-0.955645	0.814697	3.232798
27	1	0	2.040449	0.305561	3.976640
28	1	0	0.977798	-0.913801	3.250535
29	1	0	2.527588	-0.519678	2.486340
30	6	0	2.801200	0.180366	-0.975916
31	6	0	3.839153	-0.461034	-1.654632
32	6	0	3.836339	-1.851320	-1.781542
33	6	0	2.792565	-2.592236	-1.225136
34	6	0	1.756925	-1.945996	-0.546961
35	1	0	2.832562	1.263820	-0.889054
36	1	0	4.649267	0.124420	-2.082144
37	1	0	4.643057	-2.353331	-2.309511
38	1	0	2.783575	-3.675323	-1.318565
39	1	0	0.951309	-2.539872	-0.125587
40	6	0	-0.093078	2.049617	-1.709799
41	6	0	-0.807568	2.987152	-2.459553
42	6	0	-2.053595	3.433136	-2.017668
43	6	0	-2.583570	2.931887	-0.826530
44	6	0	-1.863922	1.998385	-0.080384
45	1	0	0.864633	1.701547	-2.086364
46	1	0	-0.392693	3.363331	-3.391372
47	1	0	-2.612154	4.161080	-2.600536
48	1	0	-3.559081	3.265090	-0.481262
49	1	0	-2.302338	1.611752	0.836109

I-cis (B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.305402	-3.732651	-0.332879
2	6	0	5.015712	-2.885025	-0.333115
3	7	0	5.520092	-1.491263	-0.320142
4	6	0	6.809469	-1.528524	-0.363606
5	8	0	7.371580	-2.734970	-0.392345

6	29	0	4.296309	0.106615	-0.250444
7	7	0	5.921255	1.297956	-0.272876
8	6	0	5.833089	2.776394	-0.208703
9	6	0	7.300854	3.228990	-0.353818
10	8	0	8.046637	1.972130	-0.366101
11	6	0	7.168332	0.972078	-0.342275
12	6	0	7.810112	-0.395691	-0.395918
13	6	0	8.631489	-0.504865	-1.716020
14	6	0	8.760635	-0.539381	0.830672
15	1	0	7.516573	3.741832	-1.293143
16	1	0	7.674081	3.820428	0.483101
17	1	0	5.189643	3.144166	-1.009726
18	1	0	5.387468	3.068059	0.745090
19	1	0	9.261995	-1.508253	0.792358
20	1	0	9.513820	0.250232	0.802983
21	1	0	8.208408	-0.465744	1.773370
22	1	0	9.384115	0.285385	-1.743367
23	1	0	9.133907	-1.473289	-1.754630
24	1	0	7.986739	-0.407420	-2.595708
25	1	0	4.401509	-3.037555	-1.222781
26	1	0	4.389689	-3.057292	0.544977
27	1	0	6.417133	-4.379364	-1.204202
28	1	0	6.456377	-4.313067	0.579070
29	6	0	1.523953	-0.713324	-0.403501
30	6	0	1.878861	1.633683	0.132832
31	8	0	2.763810	-1.034642	-0.489475
32	8	0	3.159288	1.631692	0.051493
33	8	0	1.275940	2.796761	0.426892
34	6	0	2.049861	4.034036	0.542445
35	1	0	3.016310	3.777363	0.982371
36	8	0	0.619526	-1.662443	-0.671229
37	6	0	1.047719	-2.995447	-1.098249
38	1	0	1.940948	-3.251367	-0.523559
39	6	0	0.997542	0.549608	-0.057611
40	1	0	-0.757378	1.698061	-0.488779
41	6	0	-0.498978	0.779673	0.051806
42	6	0	-0.994400	0.924631	1.518308
43	1	0	-1.024153	-0.037953	-0.443163
44	6	0	-2.388150	1.637057	1.635241
45	6	0	-0.926924	-0.363324	2.329766
46	1	0	-0.322625	1.643772	1.998658
47	6	0	-2.792834	2.026187	3.079539
48	6	0	-3.617225	0.954887	1.092357
49	1	0	-2.315041	2.550094	1.017797
50	6	0	-0.096232	-0.434813	3.456951

51	6	0	-1.697352	-1.490941	2.005544
52	6	0	-4.333887	2.057797	3.079511
53	1	0	-2.349485	2.978864	3.379957
54	1	0	-2.433961	1.260247	3.774816
55	6	0	-4.716160	0.926994	2.102887
56	8	0	-3.689255	0.552289	-0.102137
57	6	0	-0.036810	-1.590942	4.240119
58	1	0	0.505454	0.428578	3.732122
59	6	0	-1.651128	-2.644020	2.791016
60	1	0	-2.332522	-1.487081	1.123946
61	1	0	-4.764320	1.906466	4.071743
62	1	0	-4.709434	3.013890	2.697516
63	1	0	-5.713788	0.982156	1.663155
64	1	0	-4.627698	-0.054376	2.601827
65	14	0	-5.079876	-0.154125	-1.103005
66	6	0	-0.819125	-2.698548	3.912412
67	1	0	0.610770	-1.618883	5.111874
68	1	0	-2.270623	-3.497319	2.528388
69	6	0	-4.240942	-0.327405	-2.804826
70	1	0	-0.786075	-3.593722	4.526427
71	6	0	1.262035	4.928318	1.489352
72	1	0	0.271464	5.153262	1.079458
73	1	0	1.139286	4.453148	2.467751
74	1	0	1.791646	5.875363	1.633966
75	6	0	2.237009	4.637702	-0.845571
76	1	0	2.810833	5.568241	-0.776993
77	1	0	2.772063	3.949516	-1.507335
78	1	0	1.267513	4.869965	-1.298792
79	6	0	-0.093723	-3.932741	-0.731267
80	1	0	-0.311207	-3.879002	0.339215
81	1	0	-1.001251	-3.676248	-1.289173
82	1	0	0.178397	-4.963295	-0.981619
83	6	0	1.360306	-2.976457	-2.591156
84	1	0	2.176086	-2.283517	-2.816998
85	1	0	1.653936	-3.977467	-2.925815
86	1	0	0.477405	-2.673837	-3.164206
87	6	0	-3.093548	-1.360007	-2.848952
88	1	0	-2.312229	-1.159514	-2.105754
89	1	0	-3.456345	-2.382958	-2.708957
90	1	0	-2.617404	-1.324031	-3.837706
91	6	0	-5.344547	-0.761868	-3.803212
92	1	0	-6.159056	-0.031966	-3.864456
93	1	0	-4.911503	-0.851077	-4.807740
94	1	0	-5.774912	-1.737654	-3.547336
95	6	0	-3.687114	1.053752	-3.230598

96	1	0	-4.461633	1.827662	-3.243071
97	1	0	-2.874531	1.389796	-2.575689
98	1	0	-3.280703	0.982656	-4.247722
99	6	0	-5.583907	-1.692638	-0.164139
100	6	0	-6.784605	-1.720236	0.577364
101	6	0	-4.781050	-2.854502	-0.151693
102	6	0	-7.172210	-2.858588	1.285575
103	1	0	-7.431903	-0.848629	0.600921
104	6	0	-5.166407	-3.991646	0.558459
105	1	0	-3.845466	-2.881421	-0.700638
106	6	0	-6.365400	-3.997512	1.275284
107	1	0	-8.105645	-2.856390	1.840785
108	1	0	-4.537443	-4.877326	0.542615
109	1	0	-6.670113	-4.885908	1.820752
110	6	0	-6.376560	1.194854	-1.086442
111	6	0	-7.708418	0.879510	-1.430418
112	6	0	-6.063051	2.548929	-0.850944
113	6	0	-8.684876	1.873216	-1.519470
114	1	0	-7.994469	-0.149348	-1.634218
115	6	0	-7.039116	3.542352	-0.933747
116	1	0	-5.043317	2.844457	-0.613600
117	6	0	-8.352980	3.205158	-1.266598
118	1	0	-9.703056	1.605761	-1.786087
119	1	0	-6.774141	4.579059	-0.746885
120	1	0	-9.112780	3.978068	-1.334173

I-trans (B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.857297	4.125202	0.122436
2	6	0	4.628264	3.194339	0.183686
3	7	0	5.184651	1.865161	-0.163705
4	6	0	6.460843	1.990368	-0.312719
5	8	0	6.964217	3.212730	-0.153789
6	29	0	4.043304	0.212064	-0.340951
7	7	0	5.717034	-0.853453	-0.685388
8	6	0	5.700564	-2.319705	-0.904036
9	6	0	7.187423	-2.665393	-1.131078
10	8	0	7.859598	-1.371256	-1.035149
11	6	0	6.937794	-0.445559	-0.780066
12	6	0	7.503780	0.950083	-0.652365

13	6	0	8.582139	0.945607	0.472177
14	6	0	8.160642	1.339589	-2.011621
15	1	0	7.617720	-3.310871	-0.363635
16	1	0	7.406247	-3.071729	-2.119745
17	1	0	5.275308	-2.814008	-0.027845
18	1	0	5.069232	-2.551420	-1.763729
19	1	0	8.609821	2.331199	-1.928316
20	1	0	8.941274	0.617764	-2.259844
21	1	0	7.423479	1.353282	-2.821226
22	1	0	9.364621	0.225996	0.224673
23	1	0	9.027952	1.938430	0.555321
24	1	0	8.147976	0.673190	1.439815
25	1	0	4.177225	3.146375	1.177865
26	1	0	3.848849	3.465336	-0.529816
27	1	0	6.082094	4.635257	1.060033
28	1	0	5.825178	4.850335	-0.693033
29	6	0	1.258804	0.825723	0.137600
30	6	0	1.704598	-1.492858	-0.428749
31	8	0	2.464134	1.253522	0.035152
32	8	0	2.968054	-1.360768	-0.608249
33	8	0	1.174379	-2.702202	-0.646878
34	6	0	1.995509	-3.800504	-1.158269
35	1	0	2.974205	-3.729521	-0.678013
36	8	0	0.306120	1.725837	0.444109
37	6	0	0.653082	3.136420	0.612454
38	1	0	1.634614	3.177541	1.090278
39	6	0	0.791866	-0.490347	-0.032893
40	1	0	-1.289358	-0.138964	-0.436395
41	6	0	-0.677947	-0.817410	0.164710
42	6	0	-1.179753	-0.747398	1.640840
43	1	0	-0.854526	-1.822878	-0.223853
44	6	0	-2.599906	-1.376297	1.825300
45	6	0	-0.212327	-1.401102	2.621891
46	1	0	-1.258900	0.309385	1.917950
47	6	0	-3.086722	-1.549538	3.288988
48	6	0	-3.782541	-0.719363	1.162405
49	6	0	0.402009	-0.633070	3.619072
50	6	0	0.079595	-2.772570	2.561832
51	6	0	-4.610388	-1.727868	3.173665
52	1	0	-2.847823	-0.643983	3.860789
53	1	0	-2.591955	-2.385212	3.784543
54	6	0	-4.995332	-0.763342	2.038533
55	8	0	-3.736997	-0.221892	0.002763
56	6	0	1.286898	-1.212619	4.532550
57	1	0	0.182356	0.430366	3.686641

58	6	0	0.958538	-3.356468	3.474771
59	1	0	-0.378197	-3.394035	1.795930
60	1	0	-5.131057	0.264269	2.417320
61	1	0	-5.903564	-1.002575	1.476913
62	14	0	-5.034088	0.573409	-1.047298
63	6	0	1.566423	-2.577732	4.463882
64	1	0	1.745521	-0.599576	5.303409
65	1	0	1.163161	-4.422372	3.421097
66	6	0	-3.993671	1.200950	-2.509609
67	1	0	2.242742	-3.035004	5.180190
68	1	0	-5.139476	-1.506392	4.102921
69	1	0	-4.858532	-2.756935	2.889336
70	1	0	-2.587878	-2.380515	1.357725
71	6	0	-0.403453	3.716557	1.542557
72	1	0	-1.399816	3.645872	1.092234
73	1	0	-0.413548	3.191186	2.502732
74	1	0	-0.192416	4.773661	1.733549
75	6	0	0.697290	3.819629	-0.750791
76	1	0	0.957078	4.877444	-0.633016
77	1	0	1.440046	3.350801	-1.403023
78	1	0	-0.279268	3.763935	-1.243009
79	6	0	1.289995	-5.077505	-0.724372
80	1	0	1.859832	-5.949637	-1.060660
81	1	0	1.202490	-5.124681	0.365287
82	1	0	0.287578	-5.137563	-1.161558
83	6	0	2.131359	-3.669222	-2.671920
84	1	0	1.147050	-3.703319	-3.150761
85	1	0	2.619333	-2.729051	-2.946341
86	1	0	2.728769	-4.497702	-3.067875
87	6	0	-4.979493	1.845743	-3.517682
88	1	0	-5.520980	2.695991	-3.085780
89	1	0	-4.418526	2.223334	-4.382148
90	1	0	-5.712569	1.126177	-3.898642
91	6	0	-3.280037	0.009944	-3.190515
92	1	0	-2.739297	0.368360	-4.076157
93	1	0	-2.546536	-0.465319	-2.528955
94	1	0	-3.985307	-0.757999	-3.525853
95	6	0	-2.948241	2.256915	-2.090416
96	1	0	-2.234630	1.872811	-1.351122
97	1	0	-2.369589	2.561592	-2.972837
98	1	0	-3.417845	3.159387	-1.685205
99	6	0	-6.178477	-0.835694	-1.498725
100	6	0	-7.405328	-0.551211	-2.136732
101	6	0	-5.842342	-2.189173	-1.298112
102	6	0	-8.263506	-1.575632	-2.538880

103	1	0	-7.700771	0.476973	-2.330892
104	6	0	-6.700981	-3.214293	-1.697147
105	1	0	-4.894069	-2.460005	-0.839389
106	6	0	-7.914962	-2.908785	-2.315320
107	1	0	-9.202535	-1.331545	-3.026640
108	1	0	-6.420605	-4.250456	-1.530996
109	1	0	-8.583396	-3.705977	-2.626575
110	6	0	-5.791565	1.855798	0.084971
111	6	0	-4.990959	2.838703	0.707734
112	6	0	-7.175392	1.867550	0.355204
113	6	0	-5.551331	3.795895	1.553021
114	1	0	-3.917625	2.859186	0.537726
115	6	0	-7.738445	2.832408	1.192358
116	1	0	-7.824184	1.115825	-0.083498
117	6	0	-6.928483	3.798548	1.790952
118	1	0	-4.917325	4.543445	2.021251
119	1	0	-8.808337	2.826364	1.378645
120	1	0	-7.366538	4.548983	2.442494

TS1-cis (B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.411473	2.498130	0.840868
2	6	0	5.910485	2.157280	0.723209
3	7	0	5.909550	0.701786	0.436586
4	6	0	7.135145	0.290856	0.428629
5	8	0	8.070823	1.207018	0.654847
6	29	0	4.234744	-0.363358	0.125543
7	7	0	5.348837	-2.007948	-0.175974
8	6	0	4.775928	-3.331849	-0.522985
9	6	0	6.008943	-4.259809	-0.547701
10	8	0	7.126290	-3.348495	-0.306717
11	6	0	6.632855	-2.133056	-0.094520
12	6	0	7.691903	-1.097835	0.210240
13	6	0	8.443630	-1.530618	1.506591
14	6	0	8.689482	-1.049235	-0.986691
15	1	0	6.021537	-5.003978	0.250580
16	1	0	6.186905	-4.744929	-1.508101
17	1	0	4.036880	-3.623135	0.225591
18	1	0	4.274344	-3.265772	-1.491727
19	1	0	9.487563	-0.337375	-0.768397

20	1	0	9.128891	-2.037180	-1.135576
21	1	0	8.189137	-0.743658	-1.911506
22	1	0	8.890706	-2.515206	1.356891
23	1	0	9.236532	-0.812666	1.724815
24	1	0	7.764920	-1.578401	2.364526
25	1	0	5.356691	2.346042	1.645351
26	1	0	5.414452	2.692768	-0.089495
27	1	0	7.709534	2.876084	1.819722
28	1	0	7.779883	3.164561	0.059327
29	6	0	1.858561	1.343241	0.524633
30	6	0	1.385061	-0.958338	-0.322195
31	8	0	3.115214	1.212438	0.535817
32	8	0	2.578703	-1.366635	-0.256377
33	8	0	0.423216	-1.775361	-0.713997
34	6	0	0.702918	-3.198228	-1.021973
35	1	0	1.702351	-3.231865	-1.461158
36	8	0	1.302421	2.434955	1.017598
37	6	0	2.137499	3.466476	1.680428
38	1	0	3.061475	3.537470	1.102524
39	6	0	0.919964	0.374048	0.003267
40	1	0	-1.190256	-0.238701	0.196746
41	6	0	-0.581315	0.647903	0.038569
42	6	0	-0.343378	1.007768	-1.359993
43	1	0	-0.849287	1.455882	0.713152
44	6	0	-3.137061	0.023521	-2.587934
45	6	0	-0.235798	2.322767	-1.947907
46	1	0	-0.293929	0.171835	-2.049034
47	6	0	-3.465242	1.015116	-3.673194
48	6	0	-3.898941	0.230851	-1.485575
49	1	0	-2.485897	-0.836016	-2.716400
50	6	0	0.215727	2.425947	-3.285205
51	6	0	-0.651460	3.495288	-1.277547
52	6	0	-4.290523	2.100830	-2.927974
53	1	0	-4.054209	0.536409	-4.470602
54	1	0	-2.577869	1.436629	-4.164548
55	6	0	-4.838177	1.405711	-1.658737
56	8	0	-3.840377	-0.530628	-0.373803
57	6	0	0.261412	3.657967	-3.926108
58	1	0	0.521182	1.527101	-3.815010
59	6	0	-0.615245	4.723966	-1.927606
60	1	0	-1.028865	3.435144	-0.263215
61	1	0	-3.627868	2.923084	-2.635964
62	1	0	-5.083237	2.525980	-3.548483
63	1	0	-5.862292	1.035008	-1.800170
64	1	0	-4.864489	2.060355	-0.780128

65	14	0	-5.062848	-0.950749	0.768221
66	6	0	-0.155145	4.808988	-3.247515
67	1	0	0.605982	3.725061	-4.953220
68	1	0	-0.958820	5.617499	-1.415319
69	6	0	-4.388477	-2.583136	1.513771
70	1	0	-0.134169	5.770958	-3.751048
71	6	0	-4.241848	-3.667956	0.425352
72	1	0	-3.588856	-3.338959	-0.393215
73	1	0	-3.803762	-4.577633	0.859884
74	1	0	-5.208267	-3.949146	-0.005282
75	6	0	-3.007290	-2.327723	2.155954
76	1	0	-3.048204	-1.555630	2.932643
77	1	0	-2.637114	-3.249480	2.627706
78	1	0	-2.266366	-2.017589	1.407398
79	6	0	-5.361479	-3.095380	2.600484
80	1	0	-4.998975	-4.048801	3.008464
81	1	0	-5.446309	-2.396305	3.439799
82	1	0	-6.366557	-3.274059	2.200559
83	6	0	-6.683918	-1.143497	-0.163614
84	6	0	-7.869631	-0.509374	0.256338
85	6	0	-6.744391	-1.936690	-1.329841
86	6	0	-9.067112	-0.676423	-0.442240
87	1	0	-7.862608	0.132346	1.132248
88	6	0	-7.937517	-2.100310	-2.033352
89	1	0	-5.848885	-2.427352	-1.702412
90	6	0	-9.104045	-1.474255	-1.586458
91	1	0	-9.968764	-0.179926	-0.094787
92	1	0	-7.959159	-2.716707	-2.927901
93	1	0	-10.035024	-1.604576	-2.130881
94	6	0	-5.123131	0.417394	2.063801
95	6	0	-4.205443	1.484816	2.041560
96	6	0	-6.063536	0.395625	3.114639
97	6	0	-4.229029	2.488168	3.012254
98	1	0	-3.462241	1.535227	1.249210
99	6	0	-6.091026	1.395551	4.088623
100	1	0	-6.792103	-0.408290	3.180443
101	6	0	-5.173883	2.446690	4.038715
102	1	0	-3.514075	3.306272	2.967336
103	1	0	-6.829885	1.354496	4.883884
104	1	0	-5.197356	3.227647	4.793440
105	6	0	-0.348266	-3.609323	-2.039902
106	1	0	-0.280470	-3.003573	-2.948999
107	1	0	-0.194448	-4.656598	-2.318865
108	1	0	-1.355403	-3.512252	-1.622308
109	6	0	0.650774	-3.992696	0.276297

110	1	0	1.403766	-3.644139	0.990264
111	1	0	-0.336766	-3.911024	0.741009
112	1	0	0.840926	-5.050546	0.066279
113	6	0	1.350012	4.762839	1.592691
114	1	0	1.928496	5.568376	2.056054
115	1	0	1.153004	5.036675	0.552897
116	1	0	0.397815	4.681066	2.127343
117	6	0	2.419829	3.018933	3.109333
118	1	0	2.971223	2.074198	3.134864
119	1	0	3.019827	3.780115	3.619166
120	1	0	1.486250	2.896202	3.667700

TS1-trans (B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.582859	-4.577503	0.134033
2	6	0	4.469414	-3.508565	0.138720
3	7	0	5.221548	-2.231586	0.089972
4	6	0	6.479749	-2.506148	-0.016455
5	8	0	6.806716	-3.794530	-0.031494
6	29	0	4.347067	-0.428535	0.161525
7	7	0	6.143078	0.450701	0.007680
8	6	0	6.339776	1.920062	0.031343
9	6	0	7.860720	2.079366	-0.179772
10	8	0	8.349410	0.701557	-0.191767
11	6	0	7.301477	-0.111555	-0.101078
12	6	0	7.669060	-1.578714	-0.137992
13	6	0	8.382221	-1.873188	-1.493026
14	6	0	8.643237	-1.868971	1.044207
15	1	0	8.132071	2.526883	-1.137589
16	1	0	8.374840	2.598953	0.629557
17	1	0	5.748725	2.387046	-0.760095
18	1	0	5.997843	2.313547	0.991372
19	1	0	8.950344	-2.915973	1.014778
20	1	0	9.529289	-1.238501	0.950122
21	1	0	8.169256	-1.668302	2.010677
22	1	0	9.267366	-1.240716	-1.583428
23	1	0	8.691779	-2.919618	-1.522242
24	1	0	7.720613	-1.677653	-2.343347
25	1	0	3.810528	-3.572736	-0.730247
26	1	0	3.851391	-3.541786	1.038718

27	1	0	5.530619	-5.278266	-0.699862
28	1	0	5.675328	-5.126163	1.073088
29	6	0	1.424620	-0.636638	-0.088380
30	6	0	2.254631	1.526753	0.839745
31	8	0	2.561173	-1.182342	-0.186491
32	8	0	3.482804	1.232562	0.764273
33	8	0	1.889964	2.671286	1.396362
34	6	0	2.902742	3.532111	2.055395
35	1	0	3.793917	3.504046	1.424855
36	8	0	0.336867	-1.312813	-0.423812
37	6	0	0.434074	-2.723047	-0.871782
38	1	0	1.398171	-2.823792	-1.374926
39	6	0	1.162902	0.705625	0.375864
40	1	0	-0.974450	0.350599	0.735449
41	6	0	-0.279405	1.169519	0.557159
42	6	0	-0.222408	1.615853	-0.840355
43	1	0	-0.376559	1.947698	1.309575
44	6	0	-3.441250	2.363698	-0.522431
45	6	0	-0.016326	2.931029	-1.370732
46	1	0	-0.350074	0.821964	-1.571223
47	6	0	-3.778189	3.370769	-1.589681
48	6	0	-4.145398	1.217167	-0.687606
49	6	0	0.201706	3.061176	-2.766575
50	6	0	-0.111742	4.105436	-0.584167
51	6	0	-4.529107	2.525776	-2.655108
52	1	0	-2.897967	3.878234	-2.006743
53	1	0	-4.420746	4.166658	-1.181951
54	6	0	-5.051509	1.281488	-1.899350
55	8	0	-4.067690	0.156005	0.139687
56	6	0	0.333232	4.313450	-3.350563
57	1	0	0.257220	2.166354	-3.381169
58	6	0	0.010102	5.355424	-1.176638
59	1	0	-0.306444	4.030066	0.478914
60	1	0	-5.027717	0.366255	-2.500291
61	1	0	-6.091144	1.408369	-1.566419
62	14	0	-5.295167	-0.928777	0.674089
63	6	0	0.238978	5.462353	-2.555227
64	1	0	0.496654	4.402409	-4.419860
65	1	0	-0.086374	6.252761	-0.573262
66	6	0	-4.559137	-1.618400	2.304677
67	1	0	0.329227	6.443581	-3.011956
68	1	0	-3.824099	2.209372	-3.432368
69	1	0	-5.328053	3.083978	-3.149371
70	1	0	-2.834161	2.576586	0.351154
71	6	0	-3.244433	-2.368150	1.993833

72	1	0	-2.497191	-1.702590	1.541533
73	1	0	-2.813899	-2.772238	2.921180
74	1	0	-3.408586	-3.209305	1.310104
75	6	0	-5.560575	-2.603374	2.948529
76	1	0	-5.152484	-2.991006	3.892030
77	1	0	-6.517225	-2.121220	3.180921
78	1	0	-5.760393	-3.466383	2.303692
79	6	0	-4.264036	-0.479737	3.304366
80	1	0	-5.177680	0.039998	3.611171
81	1	0	-3.803767	-0.889735	4.214192
82	1	0	-3.573423	0.263235	2.887133
83	6	0	-5.468507	-2.292035	-0.617518
84	6	0	-6.441582	-3.304787	-0.495177
85	6	0	-4.601672	-2.359225	-1.725187
86	6	0	-6.549904	-4.328409	-1.438891
87	1	0	-7.132819	-3.300934	0.343645
88	6	0	-4.706591	-3.379440	-2.673432
89	1	0	-3.836538	-1.597690	-1.853185
90	6	0	-5.683319	-4.366893	-2.532582
91	1	0	-7.312918	-5.092710	-1.321264
92	1	0	-4.032877	-3.400122	-3.526514
93	1	0	-5.771214	-5.158975	-3.270821
94	6	0	-6.874005	0.067745	0.896662
95	6	0	-6.853645	1.275598	1.626939
96	6	0	-8.103996	-0.339313	0.343461
97	6	0	-8.011890	2.030723	1.810309
98	1	0	-5.921964	1.639490	2.052392
99	6	0	-9.266413	0.411630	0.530047
100	1	0	-8.159684	-1.246608	-0.250478
101	6	0	-9.223271	1.596239	1.266259
102	1	0	-7.971457	2.956062	2.378524
103	1	0	-10.203272	0.073291	0.096384
104	1	0	-10.126980	2.181301	1.411807
105	6	0	-0.708012	-2.928973	-1.852265
106	1	0	-0.664847	-3.949183	-2.247251
107	1	0	-1.679010	-2.795397	-1.366457
108	1	0	-0.633418	-2.236338	-2.696767
109	6	0	0.363418	-3.621547	0.355820
110	1	0	0.430151	-4.670187	0.047071
111	1	0	1.184359	-3.414423	1.049564
112	1	0	-0.585034	-3.482643	0.883700
113	6	0	2.310117	4.930858	2.081769
114	1	0	3.023881	5.616374	2.549442
115	1	0	2.101233	5.292188	1.071204
116	1	0	1.386015	4.955299	2.668916

117	6	0	3.199403	2.968281	3.439449
118	1	0	2.291562	2.945007	4.050858
119	1	0	3.613769	1.957630	3.381571
120	1	0	3.930693	3.607662	3.944995

TS2-cis (B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.463538	2.558972	2.227624
2	6	0	4.075028	2.540745	1.553963
3	7	0	4.144611	1.359058	0.658353
4	6	0	5.333083	0.853978	0.745576
5	8	0	6.169793	1.451963	1.583283
6	29	0	2.623713	0.759538	-0.485943
7	7	0	3.758264	-0.701088	-1.228809
8	6	0	3.276771	-1.659466	-2.256282
9	6	0	4.489470	-2.588520	-2.469000
10	8	0	5.506608	-2.039249	-1.570268
11	6	0	4.982462	-0.998357	-0.935965
12	6	0	5.936081	-0.332691	0.029639
13	6	0	6.376911	-1.380670	1.096352
14	6	0	7.180507	0.158579	-0.772578
15	1	0	4.313562	-3.621176	-2.164174
16	1	0	4.903900	-2.564019	-3.477648
17	1	0	2.400886	-2.187055	-1.875831
18	1	0	2.996089	-1.114441	-3.160055
19	1	0	7.898443	0.614997	-0.088711
20	1	0	7.654381	-0.692167	-1.265755
21	1	0	6.900740	0.895387	-1.532776
22	1	0	6.846182	-2.231325	0.598444
23	1	0	7.100835	-0.927107	1.775954
24	1	0	5.523476	-1.740479	1.680712
25	1	0	3.258401	2.416145	2.268506
26	1	0	3.877281	3.434747	0.958792
27	1	0	5.442054	2.347973	3.298045
28	1	0	6.041714	3.464480	2.040394
29	6	0	-0.641230	1.666170	-0.691680
30	6	0	0.374068	2.621376	-0.248201
31	6	0	-0.096422	0.580544	-1.524623
32	8	0	1.597304	2.360556	-0.038528
33	8	0	1.071630	0.104772	-1.465736

34	8	0	-0.948084	0.101704	-2.398865
35	6	0	-0.528593	-0.853924	-3.455619
36	1	0	0.052542	-1.632858	-2.955623
37	8	0	-0.072866	3.830662	0.007646
38	6	0	0.833392	4.924571	0.439622
39	1	0	1.579397	4.472071	1.096767
40	14	0	-1.709750	-2.179003	1.291859
41	8	0	-1.042627	-0.592634	0.942189
42	6	0	-1.850040	-2.425130	3.198084
43	6	0	-1.302060	0.699905	1.121962
44	6	0	-2.723049	1.253984	0.995964
45	6	0	-0.586495	1.367509	2.308144
46	6	0	-2.708484	2.530468	1.865776
47	6	0	-3.133203	1.422967	-0.487949
48	1	0	-3.386349	0.508064	1.455562
49	6	0	-1.661357	2.266039	2.965821
50	1	0	-0.226903	0.577690	2.974007
51	1	0	0.297932	1.938104	2.016680
52	6	0	-1.990720	2.224189	-1.147362
53	1	0	-2.407000	3.396889	1.271193
54	1	0	-3.697993	2.751048	2.272312
55	6	0	-4.521001	2.002695	-0.712859
56	1	0	-3.127954	0.418301	-0.924862
57	1	0	-2.121708	1.738041	3.806589
58	1	0	-1.237453	3.190737	3.368632
59	1	0	-2.086618	2.176609	-2.234819
60	1	0	-2.054165	3.275093	-0.872925
61	6	0	-5.567400	1.144032	-1.080240
62	6	0	-4.804643	3.370164	-0.569778
63	6	0	-6.858518	1.630408	-1.289036
64	1	0	-5.368865	0.082809	-1.206517
65	6	0	-6.094831	3.859906	-0.778596
66	1	0	-4.020520	4.071610	-0.299113
67	6	0	-7.127210	2.991490	-1.137320
68	1	0	-7.652784	0.947099	-1.576079
69	1	0	-6.291986	4.922079	-0.665054
70	1	0	-8.130061	3.373854	-1.302738
71	6	0	-0.440430	-2.409856	3.836704
72	1	0	-0.527013	-2.593371	4.915405
73	1	0	0.211187	-3.184697	3.422228
74	1	0	0.065413	-1.443809	3.713159
75	6	0	-2.465091	-3.831652	3.417771
76	1	0	-1.863709	-4.622825	2.955788
77	1	0	-2.507568	-4.045702	4.493574
78	1	0	-3.484858	-3.906314	3.026532

79	6	0	-2.721233	-1.384525	3.933896
80	1	0	-2.333862	-0.366292	3.830842
81	1	0	-3.763922	-1.385007	3.603997
82	1	0	-2.731392	-1.613264	5.007624
83	6	0	-0.337930	-3.299456	0.645909
84	6	0	-0.607018	-4.637575	0.293935
85	6	0	1.011260	-2.897395	0.677347
86	6	0	0.420218	-5.532039	-0.017553
87	1	0	-1.632012	-4.996739	0.266439
88	6	0	2.042587	-3.791648	0.381162
89	1	0	1.258108	-1.878669	0.966023
90	6	0	1.750065	-5.112700	0.030875
91	1	0	0.181358	-6.557948	-0.282182
92	1	0	3.079135	-3.468079	0.453346
93	1	0	2.550994	-5.814673	-0.184438
94	6	0	-3.311660	-2.466340	0.347688
95	6	0	-4.584046	-2.199160	0.894316
96	6	0	-3.272799	-3.039152	-0.941095
97	6	0	-5.756042	-2.491290	0.194562
98	1	0	-4.677646	-1.768572	1.885420
99	6	0	-4.441367	-3.333915	-1.645950
100	1	0	-2.315915	-3.286119	-1.391733
101	6	0	-5.687801	-3.062254	-1.077763
102	1	0	-6.720623	-2.282300	0.647911
103	1	0	-4.380573	-3.789978	-2.630279
104	1	0	-6.598544	-3.303424	-1.618213
105	6	0	0.305277	-0.114705	-4.496320
106	1	0	1.219124	0.308699	-4.070374
107	1	0	0.588732	-0.811548	-5.292133
108	1	0	-0.277971	0.692340	-4.951325
109	6	0	-1.822831	-1.408189	-4.026384
110	1	0	-1.589917	-2.175636	-4.771519
111	1	0	-2.441588	-1.855720	-3.246183
112	1	0	-2.399426	-0.618376	-4.518155
113	6	0	-0.045606	5.898425	1.206972
114	1	0	0.566921	6.727353	1.575543
115	1	0	-0.826332	6.313175	0.561771
116	1	0	-0.518945	5.415972	2.067445
117	6	0	1.488488	5.528030	-0.795755
118	1	0	2.139933	6.355554	-0.495871
119	1	0	2.096589	4.791980	-1.330597
120	1	0	0.730931	5.925000	-1.478734

TS2-trans (B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.102733	-1.684371	-3.690149
2	6	0	2.866427	-1.549481	-2.775615
3	7	0	3.409311	-0.901098	-1.556585
4	6	0	4.675666	-0.704611	-1.732645
5	8	0	5.182583	-1.103644	-2.892752
6	29	0	2.315588	-0.523889	0.084427
7	7	0	3.870470	0.440127	0.877771
8	6	0	3.776535	1.227526	2.130706
9	6	0	5.221145	1.727557	2.343342
10	8	0	5.931464	1.237111	1.162059
11	6	0	5.080173	0.524883	0.432606
12	6	0	5.699532	-0.102224	-0.795863
13	6	0	6.514292	0.977909	-1.564266
14	6	0	6.656595	-1.242698	-0.324808
15	1	0	5.323205	2.813269	2.354792
16	1	0	5.716982	1.301239	3.217159
17	1	0	3.059350	2.040819	1.990050
18	1	0	3.424531	0.586036	2.938919
19	1	0	7.141154	-1.693610	-1.193643
20	1	0	7.426651	-0.823709	0.326973
21	1	0	6.114070	-2.020741	0.222074
22	1	0	7.278477	1.395783	-0.907263
23	1	0	7.001343	0.523424	-2.428279
24	1	0	5.871670	1.792336	-1.914203
25	1	0	2.081561	-0.923153	-3.206848
26	1	0	2.427043	-2.512860	-2.513371
27	1	0	4.040610	-1.111073	-4.616247
28	1	0	4.383224	-2.714973	-3.912630
29	6	0	-0.727770	-1.591328	1.261920
30	6	0	-0.283502	-1.864386	-0.114523
31	6	0	0.340715	-1.159921	2.159450
32	8	0	0.753466	-1.407909	-0.678908
33	8	0	1.419142	-0.586496	1.824668
34	8	0	0.088287	-1.339178	3.441845
35	6	0	1.077958	-0.989329	4.488081
36	1	0	1.555263	-0.059220	4.170406
37	8	0	-1.069641	-2.681179	-0.771774
38	6	0	-0.654115	-3.287641	-2.062235
39	1	0	-0.159707	-2.499963	-2.633660
40	1	0	-5.269330	-5.706599	-0.482391

41	6	0	-5.040848	-4.645591	-0.529989
42	6	0	-4.278130	-4.055912	0.477302
43	6	0	-5.537634	-3.866667	-1.579309
44	6	0	-3.982670	-2.682230	0.459766
45	1	0	-3.931500	-4.669403	1.306915
46	6	0	-5.253244	-2.502230	-1.610065
47	1	0	-6.150654	-4.317547	-2.354065
48	6	0	-3.230172	-2.102919	1.657179
49	6	0	-4.478761	-1.918474	-0.601927
50	1	0	-5.642792	-1.883245	-2.413991
51	6	0	-3.215002	-0.573972	1.808552
52	6	0	-1.754414	-2.579080	1.827346
53	1	0	-3.769186	-2.487959	2.532369
54	1	0	-4.271425	-0.855262	-0.651255
55	6	0	-3.200342	-0.116129	3.284900
56	6	0	-2.019522	0.175393	1.177402
57	1	0	-4.101201	-0.146086	1.325343
58	1	0	-1.554207	-2.701067	2.890977
59	1	0	-1.628928	-3.561537	1.367216
60	6	0	-2.619633	1.303099	3.250025
61	1	0	-4.203085	-0.156378	3.719784
62	1	0	-2.559676	-0.776156	3.880205
63	6	0	-1.514100	1.231890	2.174323
64	8	0	-2.098284	0.498615	-0.109079
65	1	0	-2.232181	1.635898	4.217470
66	1	0	-3.385342	2.021514	2.938199
67	14	0	-1.843518	1.981943	-1.029539
68	6	0	-2.259356	1.486154	-2.832644
69	1	0	-1.352575	2.184289	1.670167
70	1	0	-0.559579	0.961194	2.628077
71	6	0	-1.931840	-3.739791	-2.745350
72	1	0	-2.463493	-4.473051	-2.132801
73	1	0	-2.605477	-2.901515	-2.932050
74	1	0	-1.678976	-4.203519	-3.704599
75	6	0	0.301486	-4.436747	-1.758092
76	1	0	0.621202	-4.903463	-2.695872
77	1	0	1.193848	-4.098322	-1.220813
78	1	0	-0.197330	-5.203069	-1.156476
79	6	0	2.096415	-2.116911	4.597650
80	1	0	2.646774	-2.256036	3.662040
81	1	0	2.817636	-1.882484	5.387644
82	1	0	1.602773	-3.057729	4.860899
83	6	0	0.268773	-0.772464	5.756717
84	1	0	-0.254385	-1.688188	6.049627
85	1	0	0.941470	-0.489737	6.572593

86	1	0	-0.466279	0.027943	5.629630
87	6	0	-1.634225	0.141312	-3.255494
88	1	0	-0.537904	0.154561	-3.236316
89	1	0	-1.978400	-0.673701	-2.612343
90	1	0	-1.933563	-0.095242	-4.285356
91	6	0	-1.769690	2.614019	-3.774050
92	1	0	-2.074456	2.388542	-4.804149
93	1	0	-2.209766	3.584529	-3.516364
94	1	0	-0.680327	2.726910	-3.769102
95	6	0	-3.795955	1.367127	-2.983841
96	1	0	-4.039380	1.116442	-4.024633
97	1	0	-4.215009	0.576032	-2.352344
98	1	0	-4.308670	2.301992	-2.740675
99	6	0	-0.061727	2.601632	-0.786945
100	6	0	0.220017	3.659056	0.101737
101	6	0	1.015532	2.108685	-1.553647
102	6	0	1.500509	4.208361	0.212809
103	1	0	-0.577705	4.092811	0.697427
104	6	0	2.297454	2.656635	-1.452465
105	1	0	0.847410	1.314515	-2.274123
106	6	0	2.543412	3.713768	-0.571919
107	1	0	1.672555	5.041594	0.888603
108	1	0	3.093883	2.285091	-2.092136
109	1	0	3.529756	4.167463	-0.520339
110	6	0	-3.058287	3.261351	-0.387734
111	6	0	-2.854436	4.630838	-0.659941
112	6	0	-4.262894	2.897549	0.247450
113	6	0	-3.800034	5.591380	-0.295557
114	1	0	-1.950454	4.961229	-1.165211
115	6	0	-5.208113	3.855270	0.617520
116	1	0	-4.485021	1.851763	0.440718
117	6	0	-4.976022	5.206152	0.349840
118	1	0	-3.618394	6.638832	-0.518200
119	1	0	-6.129011	3.547335	1.104526
120	1	0	-5.712058	5.952377	0.634034

TS3-cis (B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.770258	1.677374	-2.166577
2	6	0	5.398359	1.868897	-1.486211

3	7	0	5.102031	0.523866	-0.932172
4	6	0	6.054956	-0.278386	-1.281922
5	8	0	7.038516	0.248537	-1.999182
6	29	0	3.502051	0.128174	0.190979
7	7	0	4.029111	-1.792977	0.269451
8	6	0	3.238734	-2.825128	0.986105
9	6	0	4.028279	-4.123474	0.716515
10	8	0	5.209065	-3.661411	-0.012967
11	6	0	5.085172	-2.356572	-0.220674
12	6	0	6.236318	-1.750876	-0.990953
13	6	0	7.532967	-1.923389	-0.139695
14	6	0	6.387787	-2.509355	-2.343536
15	1	0	4.380933	-4.630734	1.615077
16	1	0	3.508595	-4.832778	0.069978
17	1	0	3.190442	-2.567664	2.046499
18	1	0	2.219467	-2.856916	0.594164
19	1	0	7.239267	-2.106143	-2.894465
20	1	0	6.562754	-3.568962	-2.149407
21	1	0	5.489504	-2.408118	-2.961408
22	1	0	7.702669	-2.984161	0.055264
23	1	0	8.386295	-1.525886	-0.692662
24	1	0	7.456129	-1.396498	0.817170
25	1	0	5.420606	2.604913	-0.680526
26	1	0	4.610674	2.152983	-2.188218
27	1	0	7.586155	2.216671	-1.682440
28	1	0	6.773647	1.883779	-3.237290
29	6	0	1.715493	2.414737	0.310753
30	6	0	1.090441	0.550323	1.762377
31	8	0	2.849606	1.956478	-0.022445
32	8	0	2.115816	-0.157530	1.529783
33	8	0	0.364647	0.312819	2.829502
34	6	0	0.812170	-0.667547	3.854736
35	1	0	1.171232	-1.544390	3.310090
36	8	0	1.436656	3.681586	0.109098
37	6	0	2.430957	4.613897	-0.479855
38	1	0	3.008848	4.036175	-1.205048
39	6	0	0.613840	1.639873	0.901736
40	1	0	-1.230684	1.755958	1.967697
41	6	0	-0.649816	2.409420	1.314432
42	6	0	-1.467617	2.711249	0.023038
43	1	0	-0.423667	3.323413	1.869631
44	6	0	-1.252056	1.533249	-0.950168
45	6	0	-2.914698	3.140042	0.256341
46	1	0	-0.975180	3.561977	-0.463135
47	6	0	-0.640608	1.762253	-2.337688

48	6	0	-2.027410	0.367566	-1.026455
49	1	0	-0.080868	1.108049	-0.169331
50	6	0	-3.726845	3.431976	-0.852474
51	6	0	-3.445205	3.348889	1.534809
52	6	0	-0.608242	0.353910	-2.964719
53	1	0	0.351693	2.227682	-2.295382
54	1	0	-1.275453	2.441803	-2.924368
55	6	0	-1.813677	-0.365727	-2.330792
56	8	0	-2.851466	-0.030824	-0.090540
57	6	0	-5.029997	3.899374	-0.689713
58	1	0	-3.329797	3.309918	-1.858186
59	6	0	-4.750778	3.823668	1.702011
60	1	0	-2.846883	3.157861	2.419983
61	1	0	-0.651869	0.367785	-4.056504
62	1	0	0.318567	-0.160773	-2.678870
63	1	0	-1.679100	-1.442913	-2.194550
64	1	0	-2.723240	-0.240220	-2.935623
65	14	0	-3.905247	-1.448184	-0.006976
66	6	0	-5.549202	4.096309	0.592970
67	1	0	-5.636103	4.123414	-1.563073
68	1	0	-5.137830	3.982790	2.704463
69	6	0	-4.817231	-1.249166	1.655804
70	1	0	-6.561186	4.467649	0.723241
71	6	0	-3.860101	-1.088563	2.854345
72	1	0	-3.279866	-1.999794	3.037489
73	1	0	-3.167755	-0.248709	2.719959
74	1	0	-4.441133	-0.892482	3.765336
75	6	0	-5.687683	-2.511481	1.870882
76	1	0	-5.086352	-3.426197	1.937869
77	1	0	-6.246027	-2.416612	2.811351
78	1	0	-6.425667	-2.643706	1.071560
79	6	0	-5.736608	-0.007745	1.581694
80	1	0	-5.169256	0.919425	1.450571
81	1	0	-6.463146	-0.081245	0.766192
82	1	0	-6.302768	0.080771	2.518650
83	6	0	1.928754	-0.042113	4.681532
84	1	0	2.238060	-0.744970	5.462144
85	1	0	2.804992	0.193772	4.071107
86	1	0	1.578006	0.871904	5.171313
87	6	0	-0.426454	-0.999157	4.668151
88	1	0	-0.811122	-0.108004	5.173806
89	1	0	-1.219597	-1.414269	4.041675
90	1	0	-0.168742	-1.739756	5.431979
91	6	0	3.323605	5.134557	0.638604
92	1	0	3.873603	4.323144	1.125582

93	1	0	4.050461	5.842726	0.227051
94	1	0	2.729971	5.660291	1.393000
95	6	0	1.614683	5.693132	-1.171710
96	1	0	0.969028	5.268570	-1.946305
97	1	0	0.993238	6.235884	-0.452620
98	1	0	2.290792	6.410758	-1.647421
99	6	0	-2.725636	-2.924733	-0.109272
100	6	0	-2.801602	-3.878139	-1.143866
101	6	0	-1.717895	-3.103356	0.861414
102	6	0	-1.933518	-4.971689	-1.194171
103	1	0	-3.546362	-3.770508	-1.926172
104	6	0	-0.850001	-4.196176	0.817647
105	1	0	-1.612627	-2.386686	1.671093
106	6	0	-0.960075	-5.138341	-0.208651
107	1	0	-2.025642	-5.696794	-1.997775
108	1	0	-0.108943	-4.330123	1.602921
109	1	0	-0.301120	-6.002064	-0.234493
110	6	0	-5.101615	-1.345782	-1.447770
111	6	0	-5.853578	-2.470626	-1.846069
112	6	0	-5.370883	-0.119024	-2.088129
113	6	0	-6.812154	-2.379942	-2.857279
114	1	0	-5.705307	-3.431360	-1.359446
115	6	0	-6.326505	-0.027292	-3.101363
116	1	0	-4.851022	0.784875	-1.778964
117	6	0	-7.045244	-1.159015	-3.492058
118	1	0	-7.378273	-3.261148	-3.144964
119	1	0	-6.518161	0.929574	-3.579022
120	1	0	-7.790673	-1.087259	-4.278709

TS3-trans (B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.703257	1.271114	-1.939740
2	6	0	-5.280197	1.660259	-1.488749
3	7	0	-4.825335	0.465590	-0.734101
4	6	0	-5.732929	-0.450614	-0.839726
5	8	0	-6.819743	-0.128874	-1.529343
6	29	0	-3.113618	0.395267	0.285577
7	7	0	-3.483291	-1.496721	0.784982
8	6	0	-2.571348	-2.307778	1.631744
9	6	0	-3.210087	-3.708978	1.586112

10	8	0	-4.493262	-3.477408	0.917534
11	6	0	-4.506981	-2.225508	0.478011
12	6	0	-5.751795	-1.862979	-0.299591
13	6	0	-5.893877	-2.844490	-1.501899
14	6	0	-6.978953	-2.012588	0.651696
15	1	0	-2.652570	-4.419459	0.972357
16	1	0	-3.426533	-4.143057	2.562166
17	1	0	-1.562231	-2.295015	1.216714
18	1	0	-2.542989	-1.879182	2.636525
19	1	0	-7.895686	-1.795476	0.100226
20	1	0	-7.026808	-3.037004	1.026110
21	1	0	-6.909506	-1.328896	1.504112
22	1	0	-5.948865	-3.869436	-1.130590
23	1	0	-6.809141	-2.619095	-2.052345
24	1	0	-5.043356	-2.762902	-2.186972
25	1	0	-4.600751	1.835778	-2.326566
26	1	0	-5.262253	2.539728	-0.842883
27	1	0	-6.860373	1.307208	-3.017956
28	1	0	-7.496195	1.822042	-1.430482
29	6	0	-1.461470	2.738978	-0.249756
30	6	0	-0.719433	1.333399	1.633262
31	8	0	-2.565186	2.136236	-0.413595
32	8	0	-1.658666	0.486081	1.574855
33	8	0	0.023255	1.413422	2.711111
34	6	0	-0.278917	0.621588	3.932247
35	1	0	-0.496407	-0.395455	3.596010
36	8	0	-1.245891	3.879280	-0.865675
37	6	0	-2.282351	4.510483	-1.719272
38	1	0	-2.823270	3.696848	-2.208015
39	6	0	-0.333963	2.255859	0.555561
40	1	0	0.756035	4.079850	0.216819
41	6	0	0.836469	3.203486	0.859224
42	6	0	2.145905	2.418295	0.541739
43	1	0	0.830649	3.550552	1.894205
44	6	0	1.878733	1.651139	-0.763653
45	6	0	3.403168	3.273616	0.531870
46	1	0	2.269040	1.661396	1.323759
47	6	0	1.854378	2.340192	-2.133001
48	6	0	2.240565	0.316425	-0.976485
49	6	0	4.539462	2.832224	1.225649
50	6	0	3.474903	4.498569	-0.149067
51	6	0	1.646330	1.175900	-3.124434
52	1	0	2.815686	2.838707	-2.310616
53	1	0	1.078958	3.107956	-2.215661
54	6	0	2.337836	-0.020431	-2.443529

55	8	0	2.465467	-0.540793	-0.002430
56	6	0	5.714530	3.584754	1.236816
57	1	0	4.499875	1.893000	1.773611
58	6	0	4.649186	5.253486	-0.141445
59	1	0	2.612065	4.879024	-0.689447
60	1	0	3.407178	-0.061355	-2.699409
61	1	0	1.918781	-0.998809	-2.696662
62	14	0	3.042916	-2.198017	-0.024513
63	6	0	5.773264	4.798797	0.550345
64	1	0	6.579966	3.227147	1.787457
65	1	0	4.683505	6.200356	-0.672651
66	6	0	3.349117	-2.544543	1.827277
67	1	0	6.684652	5.389102	0.559539
68	1	0	2.049292	1.384108	-4.118380
69	1	0	0.575610	0.963673	-3.239721
70	1	0	0.471562	1.538761	-0.337026
71	6	0	3.943129	-3.963719	1.987270
72	1	0	4.139854	-4.165404	3.048424
73	1	0	3.257417	-4.742666	1.634349
74	1	0	4.893325	-4.074755	1.452832
75	6	0	4.336023	-1.519853	2.428454
76	1	0	5.321730	-1.573787	1.954644
77	1	0	3.968059	-0.490846	2.336674
78	1	0	4.480256	-1.726948	3.497320
79	6	0	2.007273	-2.468087	2.588665
80	1	0	2.172190	-2.649493	3.659440
81	1	0	1.540930	-1.480204	2.485579
82	1	0	1.294397	-3.221049	2.232639
83	6	0	-1.479261	1.234653	4.642412
84	1	0	-2.380876	1.198622	4.024560
85	1	0	-1.676535	0.676980	5.563919
86	1	0	-1.274828	2.274716	4.916198
87	6	0	0.997212	0.666044	4.755950
88	1	0	0.861730	0.072234	5.665449
89	1	0	1.844768	0.254635	4.201594
90	1	0	1.233905	1.693194	5.050548
91	6	0	-1.517942	5.340921	-2.737158
92	1	0	-0.847543	4.717658	-3.336631
93	1	0	-2.226367	5.827902	-3.414848
94	1	0	-0.928880	6.120086	-2.243304
95	6	0	-3.209656	5.326147	-0.828318
96	1	0	-3.972576	5.814256	-1.443793
97	1	0	-3.715172	4.695618	-0.090090
98	1	0	-2.651755	6.105809	-0.300293
99	6	0	4.565389	-2.233459	-1.112243

100	6	0	4.743129	-3.198242	-2.122971
101	6	0	5.586717	-1.275793	-0.927693
102	6	0	5.898855	-3.218047	-2.905899
103	1	0	3.971857	-3.938617	-2.314464
104	6	0	6.738072	-1.289699	-1.714652
105	1	0	5.483364	-0.501929	-0.170750
106	6	0	6.898181	-2.265348	-2.702167
107	1	0	6.016097	-3.974202	-3.676811
108	1	0	7.510819	-0.542859	-1.556466
109	1	0	7.797028	-2.279941	-3.311722
110	6	0	1.616728	-3.242767	-0.692655
111	6	0	1.764655	-4.633003	-0.878124
112	6	0	0.361072	-2.682190	-0.996255
113	6	0	0.716166	-5.422622	-1.355333
114	1	0	2.711810	-5.116661	-0.654867
115	6	0	-0.689208	-3.466136	-1.482435
116	1	0	0.198738	-1.614527	-0.864583
117	6	0	-0.514229	-4.840095	-1.664927
118	1	0	0.864457	-6.489444	-1.494964
119	1	0	-1.638293	-3.000254	-1.740298
120	1	0	-1.322705	-5.450513	-2.057648

9.3. Computed energies of all stationary points

Table S2. <S2> value, sum of electronic and thermal enthalpies (*H*, in Hartree), sum of electronic and thermal free energies (*G*, in Hartree), thermal correction to Enthalpy (*TCH*, in Hartree), thermal correction to Gibbs free energy (*TCGFE*, in Hartree), electronic energy (*E*, in Hartree), and total free energy in solution (E_S, in Hartree, solvent = dichloromethane).

Structure	*<S2>*[a]	*H*[a]	*G*[a]	*TCH*[a]	*TCGFE*[a]	*E*[b]	E_S[b]
Cu^{2+}L2	0.75666	-806.607682	-806.664586	0.245628	0.188724	-807.013061	-807.25766
1 (A)	0	-804.412111	-804.475532	0.266894	0.203473	-804.9059501	-804.905886
C (A)	0.752346	-1611.203267	-1611.302356	0.518389	0.419301	-1612.102187	-1612.260821
2 (A)	0	-679.017814	-679.072668	0.238636	0.183781	-679.4017848	-679.391416
TS1-cis (A)	0.752358	-2290.233316	-2290.371244	0.757536	0.619608	-2291.514797	-2291.643823
I-cis (A)	0.752383	-2290.27613	-2290.410214	0.760459	0.626374	-2291.558465	-2291.676233
TS2-cis (A)	0.752338	-2290.251276	-2290.379946	0.759848	0.631178	-2291.531632	-2291.664261
TS3-cis (A)	0.752342	-2290.240617	-2290.371351	0.755612	0.624878	-2291.51844	-2291.646809
D-cis (A)	0.752264	-2290.262423	-2290.388085	0.761616	0.635954	-2291.543247	-2291.678314
P-cis (A)	0	-1483.466977	-1483.559231	0.509904	0.41765	-1484.343581	-1484.3319
TS1-trans (A)	0.753023	-2290.233155	-2290.373207	0.756932	0.61688	-2291.514119	-2291.641511
I-trans (A)	0.752388	-2290.277176	-2290.41074	0.760288	0.626724	-2291.559847	-2291.676233
TS2-trans (A)	0.75235	-2290.244681	-2290.37349	0.75973	0.630921	-2291.524157	-2291.659843
TS3-trans (A)	0.752354	-2290.244728	-2290.376886	0.755749	0.623592	-2291.523241	-2291.650377
D-trans (A)	0.752289	-2290.257773	-2290.382939	0.761612	0.636447	-2291.538539	-2291.673481
P-trans (A)	0	-1483.47138	-1483.562666	0.510376	0.419091	-1484.348797	-1484.335259
1 (B)	0	-961.558274	-961.633305	0.385339	0.310308	-962.2147801	-962.21074
C (B)	0.752348	-1768.365169	-1768.477593	0.636405	0.523981	-1769.425634	-1769.567599
2 (B)	0	-1180.201362	-1180.280108	0.442968	0.364222	-1180.911897	-1180.900978
TS1-cis (B)	0.7537	-2948.577385	-2948.750122	1.079574	0.906837	-2950.345818	-2950.453957
I-cis (B)	0.75243	-2948.622752	-2948.79079	1.083273	0.915235	-2950.393284	-2950.487674
TS2-cis (B)	0.752372	-2948.590748	-2948.752781	1.082695	0.920663	-2950.35818	-2950.462103

TS3-cis (B)	0.75238	-2948.582675	-2948.748794	1.077864	0.911745	-2950.347723	-2950.447921
TS1-trans (B)	0.754924	-2948.575306	-2948.748135	1.079464	0.906635	-2950.344082	-2950.452374
I-trans (B)	0.752413	-2948.622223	-2948.791071	1.082821	0.913973	-2950.392635	-2950.487385
TS2-trans (B)	0.752328	-2948.584998	-2948.74368	1.082548	0.923866	-2950.350618	-2950.460857
TS3-trans (B)	0.752386	-2948.591704	-2948.755671	1.078227	0.914261	-2950.357072	-2950.454491

[a] Computed at the (U)B3LYP/6-31G(d)-LANL2DZ level.

[b] Computed at the (U)B3LYP/6-311G(d,p)-LANL2DZ level.

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