Supporting Information

Asymmetric Rh(I)-Catalyzed Intramolecular [3+2] Cycloaddition of 1-Yne-vinylcyclopropanes for Bicyclo[3.3.0] Compounds with a Chiral Quaternary Carbon Stereocenter and Density Functional Theory Study of the Origins of Enantioselectivity

Mu Lin, Guan-Yu Kang, Yi-An Guo, and Zhi-Xiang Yu*

Beijing National Laboratory for Molecular Sciences (BNLMS), Key Laboratory of Bioorganic Chemistry and Molecular Engineering of Ministry of Education, College of Chemistry, Peking University, Beijing 100871, P. R. China

E-mail: yuzx@pku.edu.cn

Contents

1. General

Air and moisture sensitive reactions were carried out in oven-dried glassware sealed with rubber septa under a positive pressure of dry argon. Similarly sensitive liquids and solutions were transferred via syringe. Reactions were stirred using Teflon-coated magnetic stir bars. Elevated temperatures were maintained using Thermostat-controlled silicone oil baths. Organic solutions were concentrated using a Büchi rotary evaporator with a desktop vacuum pump. Tetrahydrofuran, diethyl ether, and toluene were distilled from sodium and benzophenone prior to use. Dichloromethane was distilled from CaH_2 prior to use. 1,2-Dichloroethane (DCE) was distilled from P_2O_5 prior to use. Synthetic reagents were purchased from Acros, Aldrich, and Alfa Aesar and used without further purification, unless otherwise indicated. Analytical TLC was performed with 0.25 mm silica gel G plates with a 254 nm fluorescent indicator. The TLC plates were visualized by ultraviolet light and treatment with phosphomolybdic acid stain followed by gentle heating. Purification of products was accomplished by flash chromatography on silica gel and the purified compounds showed a single spot by analytical TLC.

NMR spectra were measured on Bruker ARX 400 (^{1}H at 400 MHz, ^{13}C at 100 MHz) and Bruker AVANCE 600 (^{1}H at 600 MHz, ^{13}C at 150 MHz) nuclear magnetic resonance spectrometers. Data for ^{1}H-NMR spectra are reported as follows: chemical shift (ppm, referenced to TMS; s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, dm = doublet of multiplet, ddd = doublet of doublet of doublets, tdd = triplet of doublet of doublets, m = multiplet), coupling constant (Hz), and integration. Data for ^{13}C-NMR are reported in terms of chemical shift (ppm) relative to residual solvent peak ($CDCl_3$: 77.0 ppm, C_6D_6: 128.0 ppm). 2D NMR experiments were conducted on a Bruker AVANCE 600 nuclear magnetic resonance spectrometer. Infrared spectra were recorded on Mettler-Toledo ReactIR iC10 system with a SiComp probe and are reported in wavenumbers (cm^{-1}). High-resolution mass spectra (HRMS) were recorded on a Bruker Apex IV FTMS mass spectrometer (ESI). Optical rotations were measured on a Perkin-Elmer 341 LC spectrometer. The enatiomeric excesses (*ee*) of the products were determined by chiral HPLC analysis using Aglient HP 1100 instrument.

Abbreviations:

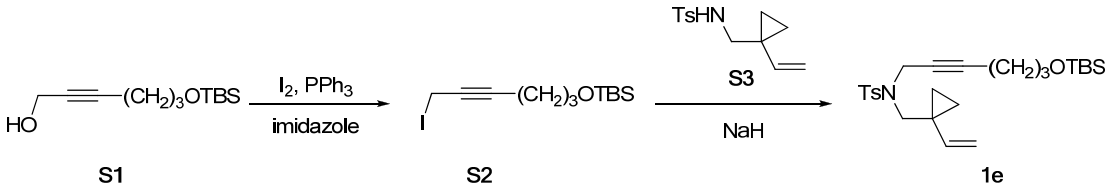
Bn = benzyl
DCE = 1,2-dichloroethane
DCM = dichloromethane
DMF = N,N-dimethylformamide
EA = ethyl acetate
LDA = lithium diisopropylamide
PE = petroleum ether
Ns = 4-nitrobenzenesulfonyl
TBAF = tetrabutylammonium fluoride
TBS = *tert*-butyldimethylsilyl
TFA = trifluoroacetic acid
THF = tetrahydrofuran
TLC = thin layer chromatography
TMS = trimethylsilyl
Ts = *p*-toluenesulfonyl

2. Experimental Procedures and Characterization Data

2.1 Synthesis of Substrates

Substrates **1a-d**, **1g-i**, **1n**, **1o**, **1p** and **1q** are known compounds and were synthesized according to the literature (Jiao, L.; Lin, M.; Yu, Z.-X. *Chem. Commun.* **2010**, *46*, 1059. Jiao, L.; Lin, M.; Zhuo, L.-G., Yu, Z.-X. *Org. Lett.* **2010**, *12*, 2528. Lin, M.; Li, F.; Jiao, L.; Yu, Z.-X. *J. Am. Chem. Soc.* **2011**, *133*, 1690).The synthesis of the other new substrates are shown below.

1-Yne-VCP (1e)

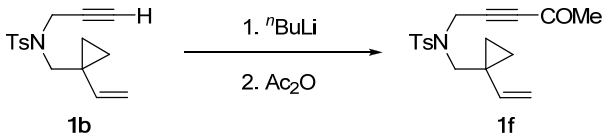


S1 to **1e**: To a stirred solution of alcohol **S1**[1] (1.14 g, 5.0 mmol), triphenylphosphine (1.44 g, 5.4 mmol), and imidazole (0.68 g, 10.0 mmol) at 0 ºC in DCM (10 mL) was added iodine (1.27 g, 5.0 mmol) in three potions. After the stirred solution turned orange, saturated aqueous $Na_2S_2O_3$ was added. The mixture was extracted with CH_2Cl_2, and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by a thin pad of silica gel eluted with pantene to afford the crude iodide **S2**. To a suspension of NaH (96 mg, 6.0 mmol) in DMF (5 mL) was added a solution of tosylamide **S3**[2] (500 mg, 2.0 mmol) in DMF (3 mL) at 0 ºC. After stirred for 5 min, iodide **S2** was added and the reaction mixture was allowed to warm to room temperature and stirred for 1.5 h. Then saturated NH_4Cl solution (4 mL) was added to quench the reaction. The resulting mixture was washed with water (10 mL), extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 30:1 to 20:1) to afford 1-yne-VCP **1e** (849 mg, two steps 37%).

1e: White solid: TLC R_f (5% EA/PE) = 0.45, m.p. 40-41 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 2H), 5.82 (dd, *J* = 17.4 and 10.8 Hz, 1H), 5.11 (dd, *J* = 17.4 and 1.1 Hz, 1H), 4.96 (dd, *J* = 10.8 and 1.0 Hz, 1H), 4.20 (t, *J* = 2.2 Hz, 2H), 3.47 (t, *J* = 6.1 Hz, 2H), 3.21 (s, 2H), 2.40 (s, 3H), 1.93 (tt, *J* = 7.1 and 2.2 Hz, 2H), 1.43–1.37 (m, 2H), 0.88 (s, 9H), 0.71 (d, *J* = 1.0 Hz, 4H), 0.02 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): *δ* 142.9, 140.0, 135.9, 129.1, 127.8, 112.2, 86.0, 72.3, 61.3, 51.3, 35.9, 31.3, 25.8, 21.4, 19.5, 18.1, 14.7, 12.66, -5.5. IR (neat): *v* 2939, 2864, 1646, 1605, 1356, 1259, 1166, 1106 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{40}NNaO_3SSi$ (M+Na): 462.2493. Found: 462.2499.

[1] Lindsay, K. B.; Pyne, S. G. *J. Org. Chem*. **2002**, *67*, 7774.
[2] Lin, M.; Li, F.; Jiao, L.; Yu, Z.-X. *J. Am. Chem. Soc.* **2011**, *133*, 1690.

1-Yne-VCP (1f)

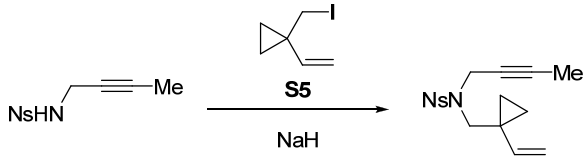


1b **1f**

1b to **1f**: To a stirred solution of 1-yne-VCP **1b**[3] (289 mg, 1.0 mmol) in THF (4 mL) at -78 ºC was added ^{n}BuLi (0.5 mL, 2.4 M in hexanes, 1.2 mmol) dropwise. After stirred for 30 min, acetic anhydride (306 mg, 3.0 mmol) was added. The reaction mixture was allowed to warm to room temperature and stirred for 2 h. Water was added to quench the reaction, and the mixture was extracted with ether. The combined extract was washed with 1 M aqueous Na_2SO_4, dried over $MgSO_4$, and concentrated. The residue was purified by flash column chromatography on silica gel (eluted with PE/EA 30:1 to 10:1) to afford 1-yne-VCP **1f** (176 mg, 53%).

1f: Light yellow solid: TLC R_f (20% EA/PE) = 0.32, m.p. 73-75 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.1 Hz, 2H), 7.30 (d, J = 8.1 Hz, 2H), 5.79 (dd, J = 17.3 and 10.8 Hz, 1H), 5.11 (d, J = 17.3 Hz, 1H), 4.99 (d, J = 10.8 Hz, 1H), 4.38 (s, 2H), 3.24 (s, 2H), 2.41 (s, 3H), 2.06 (s, 3H), 0.77–0.72 (m, 2H), 0.70–0.66 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 183.2, 144.1, 139.9, 135.7, 129.8, 128.0, 113.0, 85.3, 84.5, 52.4, 36.0, 32.5, 21.7, 19.9, 13.2. IR (neat): ν 2998, 2261, 1687, 1430, 1348, 1225, 1170, 1102 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{22}NO_3S$ (M+H): 332.1315. Found: 332.1312.

1-Yne-VCP (1j)



S4 **1j**

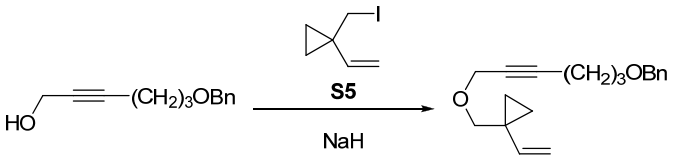
S4 to **1j**: To a suspension of NaH (72 mg, 3.0 mmol) in DMF (5 mL) was added a solution of nosylamide **S4**[4] (480 mg, 2.0 mmol) in DMF (3 mL) at 0 ºC. After stirred for 5 min, iodide **S5**[2] (312 mg, 1.5 mmol) was added and the reaction mixture was allowed to warm to room temperature and stirred for 7 h. Then saturated NH_4Cl solution (4 mL) was added to quench the reaction. The resulting mixture was washed with water (10 mL), extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 50:1) to afford 1-yne-VCP **1j** (256 mg, 51%).

1j: Light yellow solid: TLC R_f (20% EA/PE) = 0.54, m.p. 112-114 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36–8.31 (m, 2H), 8.05–8.00 (m, 2H), 5.81 (dd, J = 17.3 and 10.8 Hz, 1H), 5.11 (dd, J = 17.4 and 0.9 Hz, 1H), 4.99 (dd, J = 10.8 and 0.9 Hz, 1H), 4.23 (q, J = 2.4 Hz, 2H), 3.23 (s, 2H), 1.47 (t, J = 2.4 Hz, 3H), 0.78–0.66 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.1, 144.8, 139.7,

[3] Jiao, L.; Lin, M.; Zhuo, L.-G., Yu, Z.-X. *Org. Lett.* **2010**, *12*, 2528.
[4] Zhang, D.-H.; Yao, L.-F.; Wei, Y.; Shi, M. *Angew. Chem. Int. Ed.* **2011**, *50*, 2583.

129.2, 123.8, 112.9, 82.6, 71.2, 51.9, 36.3, 19.8, 12.9, 3.2. IR (neat): ν 1531, 1352, 1170, 1102 cm^{-1}. HRMS (ESI) calcd for $C_{16}H_{19}N_2O_4S$ (M+H): 335.1060. Found: 335.1061.

1-Yne-VCP (1k)

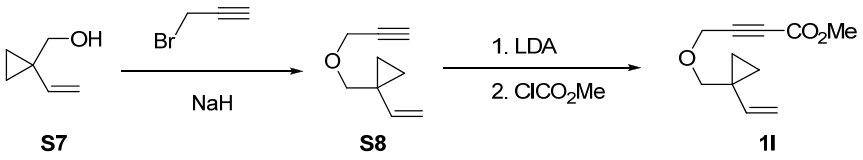


S6 **1k**

S6 to **1k**: To a suspension of NaH (72 mg, 3.0 mmol) in DMF (5 mL) was added a solution of **S6**[5] (398 mg, 1.95 mmol) at 0 ºC. After stirred for 5 min, iodide **S5**[2] (208 mg, 1.0 mmol) was added and the reaction mixture was allowed to warm to 50 ºC and stirred for 4 h. Then saturated NH_4Cl solution (4 mL) was added to quench the reaction. The resulting mixture was washed with water (10 mL), extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 30:1) to afford 1-yne-VCP **1k** (241 mg, 85%).

1k: Colorless oil: TLC R_f (20% EA/PE) = 0.58. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43–7.15 (m, 5H), 5.64 (dd, J = 17.4 and 10.7 Hz, 1H), 5.10 (dd, J = 17.4 and 1.2 Hz, 1H), 4.96 (dd, J = 10.7, 1.2 Hz, 1H), 4.51 (s, 2H), 4.14 (t, J = 2.1 Hz, 2H), 3.56 (t, J = 6.2 Hz, 2H), 3.49 (s, 2H), 2.35 (tt, J = 7.0 and 2.1 Hz, 2H), 1.82 (quint, J = 6.7 Hz, 2H), 0.83–0.48 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.6, 138.5, 128.4, 127.6, 111.5, 86.2, 74.4, 73.0, 68.8, 58.2, 28.8, 22.3, 15.7, 12.7. IR (neat): ν 2939, 2864, 1639, 1456, 1363, 1084, 1028 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{24}NaO_2$ (M+Na): 307.1669. Found: 307.1668.

1-Yne-VCP (1l)



S7 **S8** **1l**

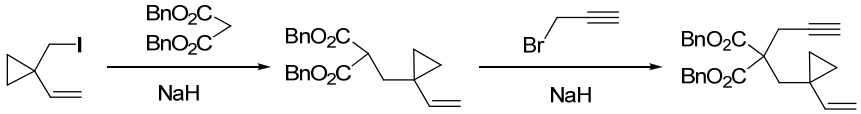
S7 to **1l**: To a suspension of NaH (240 mg, 10.2 mmol) in DMF (20 mL) was added a solution of **S7**[2] (580 mg, 5.1 mmol) at 0 ºC. After stirred for 5 min, propargyl bromide (1.08 g, 7.7 mmol) was added and the reaction mixture was allowed to warm to 20 ºC and stirred for 23 h. Then saturated NH_4Cl solution (10 mL) was added to quench the reaction. The resulting mixture was washed with water (20 mL), extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated to afford crude **S8**. To 1/4 part of above **S8** in THF (5 mL) at -78 ºC was added LDA (0.7 mL, 2.0 M in hexanes, 1.5 mmol) dropwise. After stirred for 30 min, methyl carbonochloridate (141 mg, 1.5 mmol) was added. The reaction mixture was allowed to warm to room temperature and stirred for 5 h. Water was added to quench the reaction, and the mixture was

[5] Schomaker, J. M.; Pulgam, V. R.; Borhan, B. *J. Am. Chem. Soc.* **2004**, *126*, 13600.

extracted with ether. The combined extract was washed with 1 M aqueous Na_2SO_4, dried over $MgSO_4$, and concentrated. The residue was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford 1-yne-VCP **1l** (148 mg, two steps 63%).

1l: Light yellow oil: TLC R_f (20% EA/PE) = 0.67. ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.62 (dd, J = 17.4 and 10.7 Hz, 1H), 5.07 (dd, J = 17.4 and 1.1 Hz, 1H), 4.97 (dd, J = 10.7 and 1.1 Hz, 1H), 4.30 (s, 2H), 3.78 (s, 3H), 3.53 (s, 2H), 0.79–0.65 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.6, 141.1, 111.8, 83.7, 77.8, 75.3, 57.4, 52.8, 22.2, 12.7. IR (neat): ν 2961, 2250, 1721, 1441, 1255, 1102, 1065 cm^{-1}. HRMS (ESI) calcd for $C_{11}H_{14}NaO_3$ (M+Na): 217.0835. Found: 217.0834.

1-Yne-VCP (1m)



S5 **S9** **1m**

S5 to **S9**: To a suspension of NaH (0.18 g, 7.5 mmol) in DMF (20 mL) was added a solution of dibenzyl malonate (1.70 g, 6.0 mmol) at 0 ºC. After stirred for 5 min, a solution of iodide **S5** (1.22 g, 5.0 mmol) was added and the reaction mixture was allowed to warm to room temperature and stirred for 3 h. Then saturated NH_4Cl solution (4 mL) and water (20 mL) was added to quench the reaction. The resulting mixture was extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 30:1) to afford **S9** (1.50 g, 69%).

S9: Colorless oil: TLC R_f (20% EA/PE) = 0.71. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.36–7.26 (m, 10H), 5.58 (dd, J = 17.3 and 10.6 Hz, 1H), 5.13 (s, 4H), 4.96–4.94 (m, 2H), 3.71 (t, J = 7.1 Hz, 1H), 2.12 (d, J = 7.1 Hz, 2H), 0.52 (d, J = 3.3 Hz, 4H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 169.5, 141.8, 135.5, 128.7, 128.4, 128.3, 112.7, 67.2, 50.4, 35.3, 21.3, 13.5. IR (neat): ν 2261, 1732, 1229, 1162 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{24}NaO_4$ (M+Na): 387.1567. Found: 387.1574.

S9 to **1m**: To a suspension of NaH (34 mg, 1.4 mmol) in DMF (3 mL) was added a solution of **S9** (255 mg, 0.7 mmol) at 0 ºC. After stirred for 5 min, a solution of propargyl bromide (106 mg, 0.9 mmol) was added and the reaction mixture was allowed to warm to room temperature and stirred for 3 h. Then saturated NH_4Cl solution (4 mL) and water (5 mL) were added to quench the reaction. The resulting mixture was extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 30:1) to afford **1m** (237 mg, 84%).

1m: Light yellow oil: TLC R_f (5% EA/PE) = 0.42. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.31–7.28 (m, 5H), 7.27–7.24 (m, 5H), 5.90 (dd, J = 17.1 and 10.4 Hz, 1H), 5.10 (d, J = 12.3 Hz, 2H), 5.04 (d, J = 12.3 Hz, 2H), 4.81 (d, J = 17.1 Hz, 1H), 4.76 (d, J = 10.4 Hz, 1H), 2.97 (d, J = 2.5 Hz, 2H), 2.28 (s, 2H), 1.68 (s, 1H), 0.63–0.57 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 170.1, 141.2, 135.3, 128.4, 128.2, 112.0, 79.3, 74.0, 67.0, 57.7, 38.7, 23.1, 19.7, 13.2, 3.4. IR (neat): ν 1736, 1460, 1278, 1203 cm^{-1}. HRMS (ESI) calcd for $C_{26}H_{26}NaO_4$ (M+Na): 425.1723. Found: 425.1727.

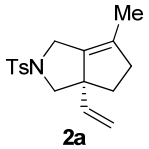
2.2 Experimental Details for Asymmetric Rh(I)-Catalyzed [3+2] Cycloadditions

Preparation of the cationic Rh(I) catalyst solution: Anhydrous DCE (5.0 mL) was added to a mixture of $[Rh(CO)_2Cl]_2$ (9.9 mg, 25.4 μmol) and $AgSbF_6$ (21.0 mg, 61.1 μmol, 1.2 equiv. to Rh) under argon. The mixture was stirred at room temperature for 10 min. The resulting yellow suspension was left to stand until the formed AgCl precipitated. The supernatant was used in the [3+2] cycloaddition reactions as the catalyst precursor ($[Rh(I)^+]$ = 10.2 μmol/mL).

General procedure for the asymmetric [3+2] cycloaddition reaction: Under argon, the above $Rh(I)^+$ solution (5 mL per mmol substrate, 5 mol %) was added to flame-dried reaction tube containing (*R*)-ligand **B** (*R*)-(+)-2,2'-Bis(diphenylphosphino)-5,5',6,6',7,7',8,8'-octahydro-1,1'-binaphthyl ((*R*)-H_8-BINAP) (42 mg per mmol substrate, 6.5 mol %). The resulting light yellow solution was stirred at room temperature for 10 min, and then a solution of the 1-yne-VCP substrate in DCE (ca. 15 mL per mmol substrate, 0.05 M) was added. The reaction tube was immersed into an oil bath and heated at the indicated temperature. When TLC indicated the disappearance of the starting material, the reaction mixture was cooled to room temperature and filtered through a thin pad of silica gel. The filter cake was washed with PE/EA, and the combined filtrate was concentrated. The crude product was purified by flash column chromatography on silica gel to afford the corresponding [3+2] cycloadduct.

Experimental Data for Asymmetric Rh(I)-Catalyzed [3+2] Cycloaddition

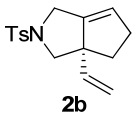
Product (2a)



2a

Substrate concentration: 0.05 M, temperature: 70 ºC, reaction time: 1 h. Following the general procedure, 1-yne-VCP **1a**[6] (37.1 mg, 0.12 mmol) was converted to product **2a**[6] (33.4 mg, 0.109 mmol) in 90% yield and 97% *ee* as determined by HPLC analysis (Chiral OJ-H, hexane: ^{i}PrOH = 90:10, 1.2 mL/min, 230 nm), t_r 15.2 min (minor), 16.6 min (major); $[\alpha]^{20}_D$ = +21.3° (c = 1.16, $CHCl_3$).

Product (2b)

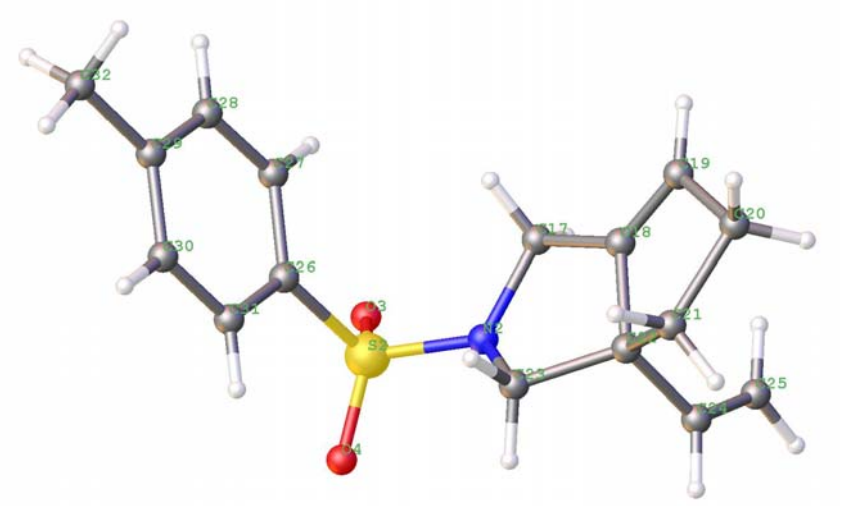


2b

Substrate concentration: 0.05 M, temperature: 50 ºC, reaction time: 3 h. Following the general procedure, 1-yne-VCP **1b**[6] (34.9 mg, 0.12 mmol) was converted to product **2b**[6] (31.3 mg, 0.107 mmol) in 90% yield and 87% *ee* as determined by HPLC analysis (Chiral OJ-H, hexane: ^{i}PrOH = 95:5, 1.0 mL/min, 230 nm), t_r 30.1 min (minor), 32.1 min (major); $[\alpha]^{20}_D$ = +40.4° (c = 0.48, $CHCl_3$). **2b**'s structure was further confirmed by X-ray analysis. For the Cambridge X-ray data,

[6] Jiao, L.; Lin, M.; Yu, Z.-X. *Chem. Commun.* **2010**, *46*, 1059.

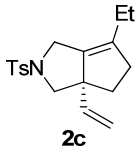
see CCDC number: 821941.[7]



Empirical formula	$C_{16}H_{19}NO_2S$
Formula weight	289.38
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C2
Unit cell dimensions	a = 16.901(3) Å α = 90.00 deg.
	b = 9.2889(19)Å β = 106.99(3) deg.
	c = 19.688(4) Å γ = 90.00 deg.
Volume	2955.9(10) $Å^3$
Z, Calculated density	8, 1.301 Mg/m^3
Absorption coefficient	0.220 mm^{-1}
F(000)	1232
Crystal size	0.38 x 0.34 x 0.24 mm
Theta range for data collection	1.08 to 27.48 deg.
Limiting indices	$-21 \le h \le 21$, $-12 \le k \le 12$, $-25 \le l \le 25$
Reflections collected / unique	20508 / 6742 [R(int) = 0.0431]
Completeness to theta = 25.00	99.7 %
Absorption correction	Numerical
Max. and min. transmission	0.9475 and 0.9054
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6742 / 1 / 361
Goodness-of-fit on F^2	1.090
Final R indices [I>2sigma(I)]	R1 = 0.0531, wR^2 =0.1308
R indices (all data)	R1 = 0.0568, wR^2 = 0.1336
Absolute structure parameter	0.04(8)
Largest diff. peak and hole	0.445 and -0.258 e $Å^{-3}$

[7] Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339.

Product (2c)

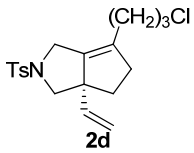


2c

Substrate concentration: 0.05 M, temperature: 70 ºC, reaction time: 2.5 h. Following the general procedure, 1-yne-VCP **1c**[2] (18.7 mg, 0.06 mmol) was converted to product **2c** (16.8 mg, 0.051 mmol) in 90% yield and 93% *ee* as determined by HPLC analysis (Chiral OJ-H, hexane: ^{i}PrOH = 90:10, 1.2 mL/min, 230 nm), t_r 9.7 min (minor), 10.6 min (major); $[\alpha]^{20}_{D}$ = +31.1°(c = 0.045, $CHCl_3$).

2c: Colorless oil: TLC R_f (20% EA/PE) = 0.37. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, J = 8.3 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 5.67 (dd, J = 17.3 and 10.4 Hz, 1H), 4.89–4.81 (m, 2H), 3.81 (dd, J = 13.0 and 1.1 Hz, 1H), 3.72 (ddd, J = 13.0, 4.1 and 1.5 Hz, 1H), 3.61 (d, J = 9.2 Hz, 1H), 2.83 (d, J = 9.2 Hz, 1H), 2.72–2.59 (m, 1H), 2.43 (s, 3H), 2.26 (dd, J = 15.6 and 8.6 Hz, 1H), 2.11–1.93 (m, 2H), 1.87 (dd, J = 12.3 and 6.6 Hz, 1H), 1.69 (ddd, J = 12.3, 10.3 and 8.7 Hz, 1H), 0.96 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.1, 139.4, 137.9, 136.2, 134.6, 129.5, 127.4, 111.9, 60.8, 57.9, 44.8, 37.9, 35.6, 22.6, 21.5, 12.5. IR (neat): ν 2972, 2257, 1602, 1460, 1345, 1162, 1099 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{24}NO_2S$ (M+H): 318.1522. Found: 318.1521.

Product (2d)

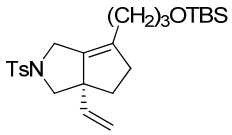


2d

Substrate concentration: 0.05 M, temperature: 60 ºC, reaction time: 10 h. Following the general procedure, 1-yne-VCP **1d**[2] (21.2 mg, 0.06 mmol) was converted to product **2d** (15.7 mg, 0.043 mmol) in 74% yield and 94% *ee* as determined by HPLC analysis (Chiral AD-H, hexane: ^{i}PrOH = 95:5, 1.0 mL/min, 230 nm), t_r 19.1 min (minor), 21.4 min (major); $[\alpha]^{20}_{D}$ = +6.8°(c = 0.355, $CHCl_3$).

2d: Colorless oil: TLC R_f (20% EA/PE) = 0.40. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, J = 8.3 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 5.70 (dd, J = 17.3 and 10.4 Hz, 1H), 4.90–4.84 (m, 2H), 3.80 (dd, J = 13.2 and 1.5 Hz, 1H), 3.74 (ddd, J = 13.3, 3.9 and 1.2 Hz, 1H), 3.63 (d, J = 9.1 Hz, 1H), 3.40 (td, J = 6.5 and 1.3 Hz, 2H), 2.81 (d, J = 9.2 Hz, 1H), 2.71–2.58 (m, 1H), 2.43 (s, 3H), 2.30–2.10 (m, 3H), 1.91 (dd, J = 12.4 and 6.6 Hz, 1H), 1.87–1.66 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.3, 139.2, 139.1, 134.3, 129.6, 127.4, 112.2, 60.8, 58.0, 44.8, 44.1, 38.0, 35.7, 30.1, 26.4, 21.5. IR (neat): ν 2942, 2861, 2261, 1602, 1460, 1345, 1166, 1099 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{25}ClNO_2S$ (M+H): 366.1289. Found: 366.1294.

Product (2e)

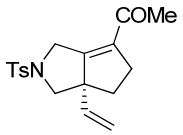


2e

Substrate concentration: 0.05 M, temperature: 70 ºC, reaction time: 10 h. Following the general procedure, 1-yne-VCP **1e** (27.2 mg, 0.06 mmol) was converted to product **2e** (17.1 mg, 0.037 mmol) in 63% yield and 95% *ee* as determined by HPLC analysis (Chiral AS-H, hexane: ^{i}PrOH = 95:5, 1.0 mL/min, 230 nm), t_r 13.2 min (major), 16.7 min (minor); $[\alpha]^{20}_{D}$ = -16.0°(c = 0.025, $CHCl_3$).

2e: Colorless oil: TLC R_f (20% EA/PE) = 0.71. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 7.9 Hz, 2H), 5.67 (dd, J = 17.3 and 10.4 Hz, 1H), 4.92–4.78 (m, 2H), 3.79 (d, J = 13.0 Hz, 1H), 3.70 (dd, J = 12.9 and 2.2 Hz, 1H), 3.61 (d, J = 9.2 Hz, 1H), 3.53 (t, J = 6.3 Hz, 2H), 2.83 (d, J = 9.2 Hz, 1H), 2.73–2.59 (m, 1H), 2.42 (s, 3H), 2.26 (dd, J = 15.5 and 8.6 Hz, 1H), 2.14–1.97 (m, 2H), 1.88 (dd, J = 12.3 and 6.6 Hz, 1H), 1.70 (dd, J = 20.9 and 10.3 Hz, 1H), 1.63–1.48 (m, 2H), 0.89 (s, 9H), 0.03 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.1, 139.5, 137.6, 136.1, 135.0, 129.5, 127.4, 112.0, 62.4, 60.9, 58.0, 44.9, 38.3, 35.8, 30.9, 25.9, 25.7, 21.5, 18.3, -5.3. IR (neat): ν 2939, 2861, 1602, 1475, 1348, 1259, 1162, 1095 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{40}NO_3SSi$ (M+H): 462.2493. Found: 462.2503.

Product (2f)

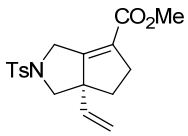


2f

Substrate concentration: 0.05 M, temperature: 70 ºC, reaction time: 1 h. Following the general procedure, 1-yne-VCP **1f** (19.7 mg, 0.06 mmol) was converted to product **2f** (13.8 mg, 0.042 mmol) in 70% yield and 98% *ee* as determined by HPLC analysis (Chiral OD-H, hexane: ^{i}PrOH = 95:5, 1.0 mL/min, 230 nm), t_r 44.3 min (minor), 16.7 min (major); $[\alpha]^{20}_{D}$ = +21.1°(c = 0.455, $CHCl_3$).

2f: Colorless oil: TLC R_f (20% EA/PE) = 0.21. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.1 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 5.77 (dd, J = 17.4 and 10.4 Hz, 1H), 5.02 (s, 1H), 4.99 (d, J = 5.9 Hz, 1H), 4.17–4.03 (m, 2H), 3.74 (d, J = 9.2 Hz, 1H), 2.95–2.80 (m, 2H), 2.76 (dd, J = 15.8 and 8.6 Hz, 1H), 2.43 (s, 3H), 2.20 (s, 3H), 2.01 (dd, J = 12.6 and 6.4 Hz, 1H), 1.78 (dd, J = 21.1 and 10.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.3, 157.7, 143.7, 137.5, 134.2, 134.1, 129.8, 127.5, 113.9, 62.4, 56.9, 47.1, 35.2, 34.9, 29.2, 21.5. IR (neat): ν 2954, 2265, 1669, 1352, 1166, 1099, 1050 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{22}NO_3S$ (M+H): 332.1315. Found: 332.1313.

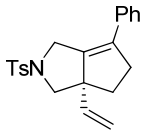
Product (2g)



2g

Substrate concentration: 0.05 M, temperature: 70 ºC, reaction time: 1 h. Following the general procedure, 1-yne-VCP **1g**[6] (20.1 mg, 0.06 mmol) was converted to product **2g**[6] (12.4 mg, 0.036 mmol) in 62% yield and 99% *ee* as determined by HPLC analysis (Chiral OD-H, hexane: ^{i}PrOH = 95:5, 1.0 mL/min, 230 nm), t_r 26.0 min (minor), 29.2 min (major); $[\alpha]^{20}_{D}$ = +10.0°(c = 0.120, $CHCl_3$).

Product (2h)

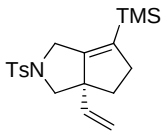


2h

Substrate concentration: 0.05 M, temperature: 60 ºC, reaction time: 1 h. Following the general procedure, 1-yne-VCP **1h**[3] (43.8 mg, 0.12 mmol) was converted to product **2h** (30.3 mg, 0.083 mmol) in 69% yield and 48% *ee* as determined by HPLC analysis (Chiral OJ-H, hexane: ^{i}PrOH = 90:10, 1.2 mL/min, 230 nm), t_r 27.6 min (major), 37.4 min (minor); $[\alpha]^{20}_{D}$ = -32.3°(c = 0.352, $CHCl_3$).

2h: Colorless oil: TLC R_f (20% EA/PE) = 0.49. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.2 Hz, 2H), 7.42 – 7.18 (m, 7H), 5.82 (dd, J = 17.3 and 10.4 Hz, 1H), 5.01 (d, J = 17.3 Hz, 1H), 4.95 (d, J = 10.4 Hz, 1H), 4.24 – 4.15 (m, 1H), 3.98 (d, J = 14.2 Hz, 1H), 3.73 (d, J = 9.0 Hz, 1H), 3.08 – 2.88 (m, 2H), 2.83 (d, J = 9.0 Hz, 1H), 2.40 (s, 3H), 2.04 (dd, J = 12.4 and 5.1 Hz, 1H), 1.91 – 1.78 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.3, 140.1, 139.2, 134.8, 134.4, 133.8, 129.7, 128.6, 127.6, 127.4, 127.0, 112.8, 62.2, 57.2, 46.7, 36.6, 34.7, 21.4. IR (neat): ν 2924, 1356, 1166, 1095 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{24}NO_2S$ (M+H): 366.1522. Found: 366.1522.

Product (2i)

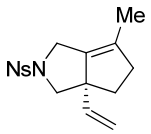


2i

Substrate concentration: 0.05 M, temperature: 70 ºC, reaction time: 120 h. Following the general procedure, 1-yne-VCP **1i**[2] (22.5 mg, 0.06 mmol) was converted to product **2i** (9.6 mg, 0.027 mmol) in 43% yield. Flash column chromatography also recovered 6.4 mg of 1-yne-VCP **1i** (72% conversion). The yield of **2i** was 60% based on the recovered starting material and 61% *ee* as determined by HPLC analysis (Chiral AD-H, hexane: ^{i}PrOH = 95:5, 1.0 mL/min, 230 nm), t_r 7.5 min (minor), 8.5 min (major); $[\alpha]^{20}_{D}$ = +18.3°(c = 0.230, $CHCl_3$).

2i: Colorless oil: TLC R_f (20% EA/PE) = 0.53. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 5.66 (dd, J = 17.3 and 10.4 Hz), 4.88 – 4.82 (m, 2H), 3.87 – 3.74 (m, 2H), 3.65 (d, J = 9.2 Hz, 1H), 2.82 (d, J = 9.2 Hz, 1H), 2.71 – 2.58 (m, 1H), 2.50 (dd, J = 15.7 and 8.2 Hz, 1H), 2.43 (s, 3H), 1.88 (dd, J = 12.2 and 6.2 Hz, 1H), 1.60 (ddd, J = 12.1, 10.6 and 8.3 Hz, 1H), 0.05 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.2, 143.2, 138.6, 135.0, 134.5, 129.5, 127.4, 127.4, 112.2, 63.2, 57.5, 46.1, 39.9, 36.5, 21.5, -1.5. IR (neat): ν 2965, 1352, 1255, 1166, 1095, 1035 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{27}NNaO_2SSi$ (M+Na): 384.1424. Found: 384.1429.

Product (2j)

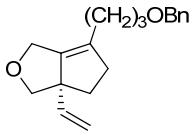


2j

Substrate concentration: 0.05 M, temperature: 70 ºC, reaction time: 1 h. Following the general procedure, 1-yne-VCP **1j** (20.0 mg, 0.06 mmol) was converted to product **2j** (17.3 mg, 0.052 mmol) in 87% yield and 96% *ee* as determined by HPLC analysis (Chiral OD-H, hexane: ^{i}PrOH = 95:5, 1.0 mL/min, 230 nm), t_r 28.9 min (minor), 30.6 min (major); $[\alpha]^{20}_D$ = +30.0°(c = 0.510, $CHCl_3$).

2j: Colorless oil: TLC R_f (20% EA/PE) = 0.44. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, J = 8.8 Hz, 2H), 8.00 (d, J = 8.8 Hz, 2H), 5.66 (dd, J = 17.3 and 10.4 Hz, 1H), 4.86–4.80 (m, 2H), 3.83 (d, J = 12.8 Hz, 1H), 3.73 (dd, J = 12.9 and 1.7 Hz, 1H), 3.67 (d, J = 9.3 Hz, 1H), 2.91 (d, J = 9.4 Hz, 1H), 2.77–2.61 (m, 1H), 2.27 (dd, J = 15.8 and 8.7 Hz, 1H), 1.89 (dd, J = 12.4 and 6.9 Hz, 1H), 1.79–1.71 (m, 1H), 1.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.0, 143.9, 139.3, 136.3, 133.5, 128.4, 124.2, 112.5, 60.9, 58.5, 45.1, 40.3, 35.9, 14.6. IR (neat): ν 2942, 1535, 1356, 1170, 1099 cm^{-1}. HRMS (ESI) calcd for $C_{16}H_{18}N_2NaO_4S$ (M+Na): 357.0880. Found: 357.0886.

Product (2k)



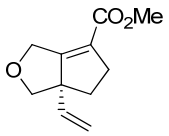
2k

Substrate concentration: 0.05 M, temperature: 70 ºC, reaction time: 5 h. Following the general procedure, 1-yne-VCP **1k** (17.0 mg, 0.06 mmol) was converted to product **2k** (10.4 mg, 0.037 mmol) in 61% yield and 93% *ee* as determined by HPLC analysis (Chiral OD-H, hexane: ^{i}PrOH = 95:5, 1.0 mL/min, 230 nm), t_r 7.6 min (major), 8.3 min (minor); $[\alpha]^{20}_D$ = -7.6°(c = 0.170, $CHCl_3$).

2k: Colorless oil: TLC R_f (5% EA/PE) = 0.19. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39–7.26 (m, 5H), 5.94 (dd, J = 17.3 and 10.4 Hz, 1H), 5.07 (dd, J = 17.3 and 1.1 Hz, 1H), 5.02 (d, J = 10.4 Hz, 1H), 4.49 (s, 2H), 4.25 (d, J = 12.2 Hz, 1H), 4.10 (dd, J = 12.3 and 2.9 Hz, 1H), 3.93 (d, J = 7.8 Hz, 1H), 3.45 (t, J = 6.4 Hz, 2H), 3.36 (d, J = 7.8 Hz, 1H), 2.92–2.77 (m, 1H), 2.42 (dd, J = 15.5 and 8.3 Hz, 1H), 2.25–2.09 (m, 2H), 1.90 (dd, J = 12.2 and 6.7 Hz, 1H), 1.86–1.66 (m, 3H). ^{13}C

NMR (100 MHz, $CDCl_3$): δ 142.8, 140.3, 138.5, 133.8, 128.4, 127.6, 127.6, 111.8, 73.0, 69.7, 63.3, 63.0, 39.9, 34.7, 28.0, 26.3. IR (neat): ν 2928, 2864, 1639, 1460, 1367, 1102, 1028 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{24}NaO_2$ (M+Na): 307.1669. Found: 307.1666.

Product (2l)

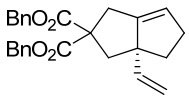


2l

Substrate concentration: 0.05 M, temperature: 70 ºC, reaction time: 2 h. Following the general procedure, 1-yne-VCP **1l** (10.1 mg, 0.06 mmol) was converted to product **2j** (4.0 mg, 0.021 mmol) in 40% yield and 97% *ee* as determined by HPLC analysis (Chiral OD-H, hexane: ^{i}PrOH = 90:10, 1.0 mL/min, 230 nm), t_r 7.1 min (minor), 7.6 min (major); $[\alpha]^{20}_D$ = +15.0°(c = 0.020, $CHCl_3$).

2l: Colorless oil: TLC R_f (20% EA/PE) = 0.49. ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.97 (dd, J = 17.4 and 10.5 Hz, 1H), 5.17−5.12 (m, 2H), 4.59 (d, J = 16.3 Hz, 1H), 4.43 (ddd, J = 16.3, 4.1 and 1.3 Hz, 1H), 4.01 (d, J = 8.2 Hz, 1H), 3.74 (s, 3H), 3.48 (d, J = 8.2 Hz, 1H), 3.13–2.98 (m, 1H), 2.91 (dd, J = 15.7 and 8.2 Hz, 1H), 2.02 (dd, J = 12.3 and 6.3 Hz, 1H), 1.97–1.86 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.4, 165.0, 138.3, 124.3, 113.6, 76.3, 65.3, 64.3, 51.5, 36.5, 34.1. IR (neat): ν 2961, 2864, 1721, 1441, 1333, 1278, 1203, 1117, 1021 cm^{-1}. HRMS (ESI) calcd for $C_{11}H_{15}O_3$ (M+H): 195.1016. Found: 195.1017.

Product (2m)



2m

Substrate concentration: 0.05 M, temperature: 50 ºC, reaction time: 1 h. Following the general procedure, 1-yne-VCP **1m** (25.0 mg, 0.06 mmol) was converted to product **2m** (6.6 mg, 0.016 mmol) in 26% yield. Flash column chromatography also recovered 8.9 mg of 1-yne-VCP **1m** (64% conversion). The yield of **2m** was 41% based on the recovered starting material and 90% *ee* as determined by HPLC analysis (Chiral OD-H, hexane: ^{i}PrOH = 95:5, 1.0 mL/min, 230 nm), t_r 7.8 min (minor), 8.5 min (major); $[\alpha]^{20}_D$ = +34.0°(c = 0.100, $CHCl_3$).

2m: Colorless oil: TLC R_f (20% EA/PE) = 0.74. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33–7.21 (m, 10H), 5.76 (dd, J = 17.3 and 10.4 Hz, 1H), 5.43 (s, 1H), 5.14–5.01 (m, 4H), 4.87 (dd, J = 17.3 and 1.5 Hz, 1H), 4.85 (dd, J = 10.4 and 1.5 Hz, 1H), 2.95 (ddt, J = 7.0, 4.5 and 2.0 Hz, 1H), 2.81 (d, J = 16.2 Hz, 1H), 2.62–2.47 (m, 2H), 2.41–2.33 (m, 1H), 2.21 (d, J = 13.6 Hz, 1H), 1.92 (dd, J = 12.1 and 6.1 Hz, 1H), 1.75–1.83 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.9, 171.3, 149.7, 141.4, 135.50, 135.49, 128.48, 128.45, 128.2, 128.1, 127.90, 127.89, 121.6, 111.4, 67.25, 67.18, 62.7, 61.5, 44.2, 39.9, 35.0, 32.9. IR (neat): ν 2957, 1739, 1460, 1248, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{26}H_{27}O_4$ (M+H): 403.1904. Found: 403.1906.

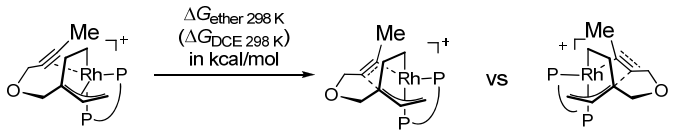
3. DFT Study

3.1 Computational Details

All calculations were performed with the Gaussian 09 program.[8] Density functional theory calculations using the B3LYP method were used to locate all the stationary points involved. The 6-31G(d) basis set was applied for all elements except for Rh, for which the LANL2DZ basis set and pseudopotential were used. The keyword "5D" in Gaussian 09 program was used to specify that five (instead of six) d-type STO orbitals were used as basis sets in all elements of the calculations. Single-point energies based on the structures obtained at the B3LYP level using the same basic set were obtained by M06 method in order to take the dispersion energies into consideration. Solvation energies were evaluated by a self-consistent reaction field (SCRF) using the CPCM model, where UFF radii were used. Solvation calculations were carried out on the gas-phase optimized structures. The reported energies are zero-point energy-corrected enthalpies (ΔH_{gas}), Gibbs free energies ($\Delta G_{gas\ 298K}$), and Gibbs free energies in 1,2-dichloroethane (DCE) solution[9] ($\Delta G_{sol\ 298K}$, where the entropies in solution were approximated by the computed gas phase entropies at 298 K). Unless specifically mentioned, all discussed relative energies in this paper and the Supporting Information are referred to $\Delta G_{sol\ 298K}$.

[8] Full citation of Gaussian 09: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A. Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C. ; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision A.02; Gaussian Inc.: Wallingford CT, 2009.

[9] We have also computed how ether solvent affects the reactivity, but calculations (M06//B3LYP) found that DCE and ether are very similar in giving enantioselectivity, even though experiments in DCE and DME gave different *ee* values.



3.2 The DFT Computed Energy Surface by B3LYP Method

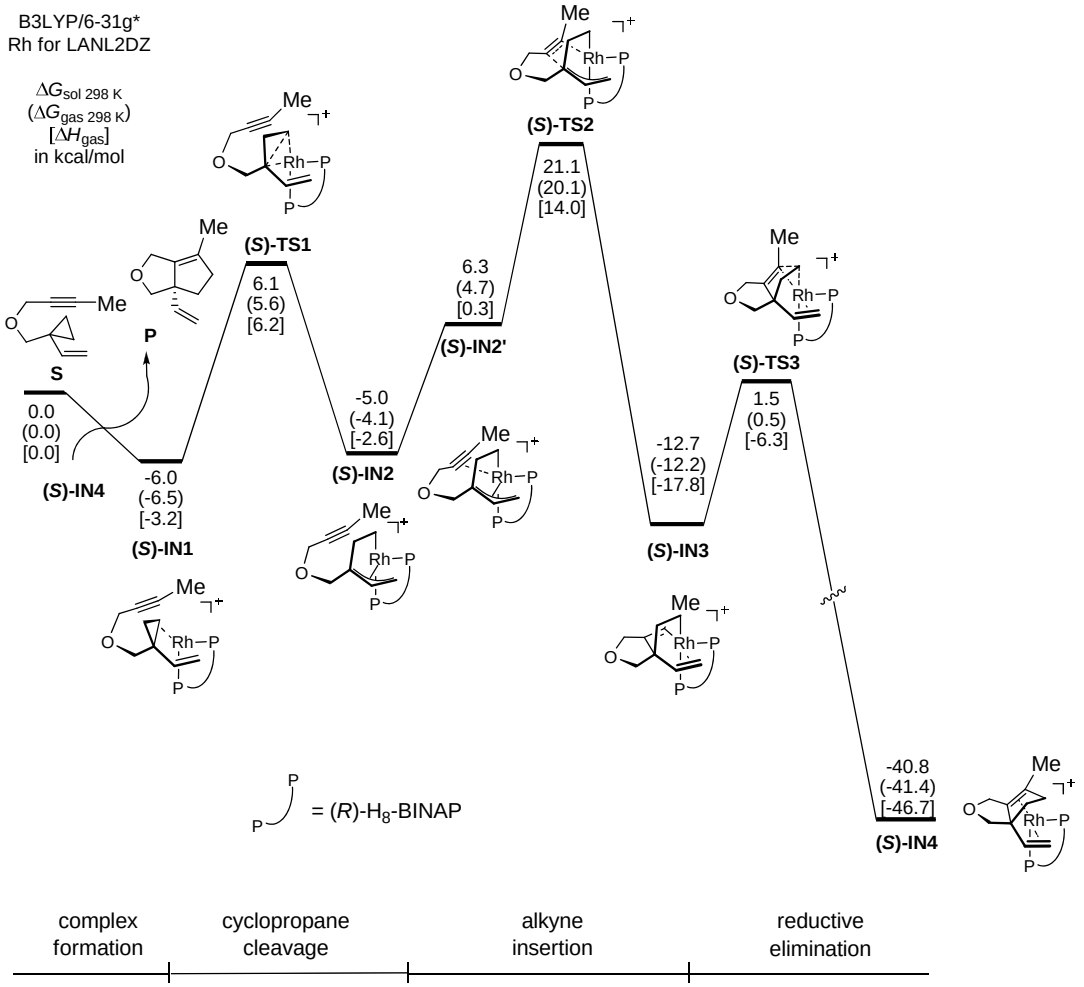


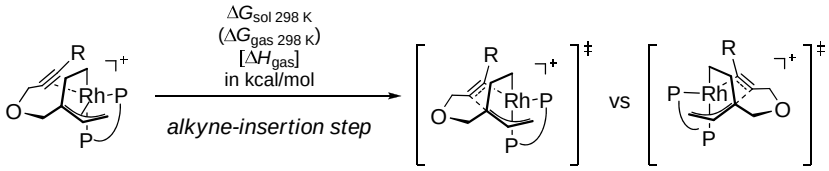
Figure S1. B3LYP computed potential energy surface of the asymmetric [3+2] reactions.

The B3LYP energy surface of the asymmetric reaction in Figure S1 is similar to the M06//B3LYP surface shown in Figure 3. The major difference is the relative energies of the rate-determining step: B3LYP predicted that the activation free energy is 27.1 kcal/mol (from **(*S*)-IN1** to **(*S*)-TS2**), while M06//B3LYP predicted that the activation free energy is 22.3 kcal/mol (from **S** to **(*S*)-TS2**).

3.3 Enantioselectivity Predictions by M06 and B3LYP Functionals

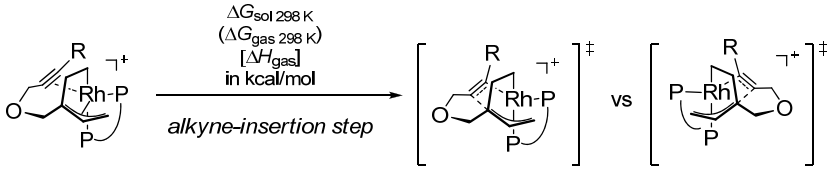
Figures S2 and S3 give the predicted ee values at 298 K for the asymmetric [3+2] cycloadditions in solution using M06//B3LYP and B3LYP methods, respectively. Comparison of Figures S3 and S4 finds that both M06 and B3LYP methods predict the same trend in the enantioselectivity of the [3+2] reactions in terms of the computed activation enthalpies. But in solution, M06 method gave much better results than B3LYP method did. The M06 predictions are consistent with experimental results. Therefore, all discussed energies in the paper are the

M06//B3LYP energies in solution.



entry					predicted *ee* value by M06//B3LYP
1	0.0 (0.0) [0.0]	R = H	15.9 (16.4) [16.0]	17.2 (18.1) [18.3]	80%
2	0.0 (0.0) [0.0]	R = Me	15.7 (16.2) [14.7]	18.6 (19.4) [18.4]	98%
3	0.0 (0.0) [0.0]	R = TMS	16.7 (16.9) [14.8]	22.0 (22.4) [21.1]	~100%
4	0.0 (0.0) [0.0]	R = CO_2Me	11.7 (12.4) [11.0]	15.4 (16.8) [16.8]	99.6%
5	0.0 (0.0) [0.0]	R = Ph	14.0 (14.1) [12.5]	17.4 (17.7) [17.1]	99.3%

Figure S2. M06//B3LYP computed energies of **(*S*)-TS2** and **(*R*)-TS2** with different substituents.



entry					predicted *ee* value by B3LYP
1	0.0 (0.0) [0.0]	R = H	13.4 (13.9) [13.6]	12.5 (13.4) [13.7]	-64%
2	0.0 (0.0) [0.0]	R = Me	14.5 (15.4) [13.7]	16.1 (16.8) [15.7]	46%
3	0.0 (0.0) [0.0]	R = TMS	18.2 (18.4) [16.3]	21.3 (21.7) [20.5]	99%
4	0.0 (0.0) [0.0]	R = CO_2Me	8.8 (9.5) [8.1]	10.7 (12.1) [12.0]	92%
5	0.0 (0.0) [0.0]	R = Ph	13.3 (13.5) [12.0]	12.8 (15.6) [15.0]	-40%

Figure S3. B3LYP computed energies of **(*S*)-TS2** and **(*R*)-TS2** with different substituents.

3.4 The DFT Computed Energy Surfaces of the Asymmetric [3+2] Cycloaddition of TMS-substituted 1-Yne-VCP

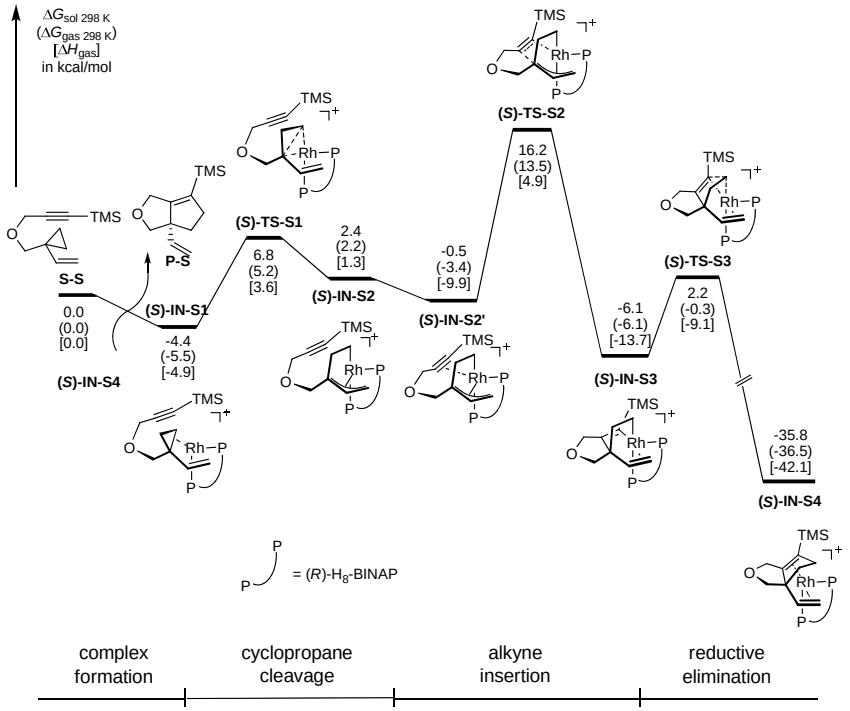


Figure S4. M06//B3LYP computed potential energy surface of the asymmetric [3+2] cycloaddition of TMS-substituted 1-yne-VCP.

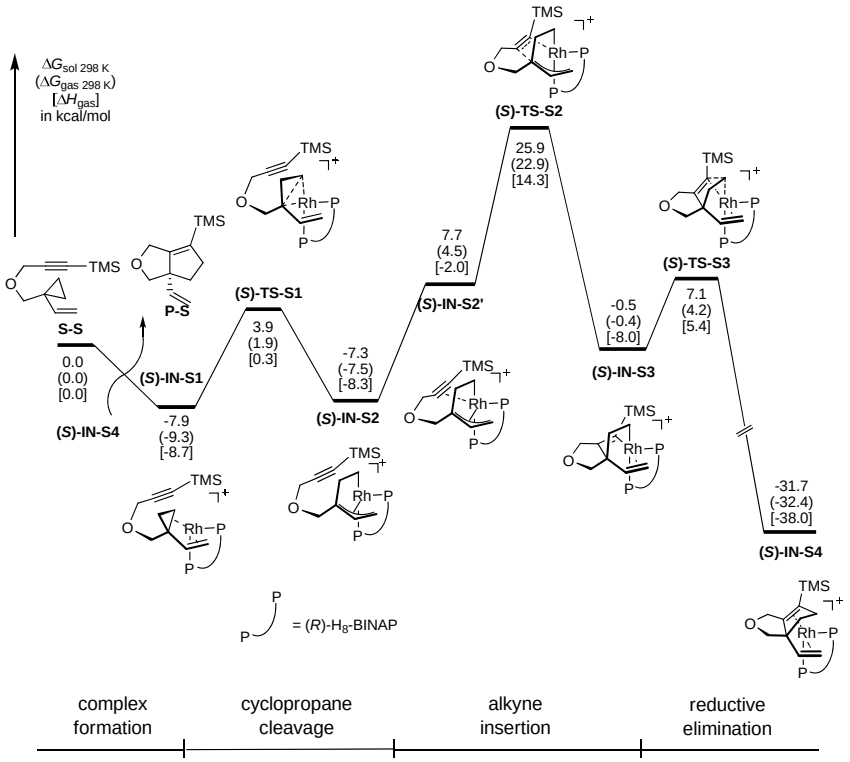


Figure S5. B3LYP computed potential energy surface of the asymmetric [3+2] cycloaddition of TMS-substituted 1-yne-VCP.

The asymmetric [3+2] catalytic cycle of TMS-substituted 1-yne-VCP starts with the ligand exchange between the product-Rh(I) complex **(*S*)-IN-S4**, which is generated in the previous catalytic cycle, and the TMS-substituted substrate 1-yne-VCP **S-S** (Figure S4). The M06//B3LYP computed energy surface (Figure S4) shows that the ligand exchange reaction is exergonic by 4.4 kcal/mol, giving a 16-electron Rh(I) complex **(*S*)-IN-S1**, in which the VCP moiety binds to the rhodium center by both the vinyl group and the cyclopropane unit. The CP ring-opening reaction from **(*S*)-IN-S1** to **(*S*)-IN-S2**, via the transition state **(*S*)-TS-S1**, is facile with an activation free energy in the DCE solution of 11.2 kcal/mol. The followed step is the alkyne complexation to the Rh center, transforming the 16-e complex **(*S*)-IN-S2** to 18-e complex **(*S*)-IN-S2′**. Subsequent alkyne insertion into the Rh-C bond via **(*S*)-TS-S2** generates **(*S*)-IN-S3**, and this whole step from **(*S*)-IN-S2** to **(*S*)-TS-S2** requires an activation free energy of 16.7 kcal/mol. The final step of this asymmetric [3+2] catalytic cycle is an easy reductive elimination reaction with an activation free energy of 8.3 kcal/mol, converting intermediate **(*S*)-IN-S3** to the product-catalyst complex **(*S*)-IN-S4** via transition state **(*S*)-TS-S3**.

The rate-determining step of the asymmetric [3+2] cycloadditions is the alkyne insertion step. The activation free energy for this [3+2] reaction is 20.6 kcal/mol in the DCE solution (from **(*S*)-IN-S1** to **(*S*)-TS-S2**). DFT calculations found that the alkyne insertion step is irreversible, suggesting that the alkyne insertion step is the rate- and stereochemistry-determining step of this asymmetric [3+2] reaction.

As mentioned above, in terms of computing enantioselectivity, M06 is better than B3LYP. But in terms of comparing reactivities of substrates with different substituents, B3LYP gave a better result. For example, if we compare Figure S4 and Figure 3, we can find that, TMS-substituted substrate is easier to undergo the [3+2] reaction because the activation free energy of this reaction is 20.6 kcal/mol, 1.7 kcal/mol lower than the [3+2] reaction of Me-substituted substrate **S**. This is contradictory to the experimental observations (see Table 2). However, comparing the B3LYP results in Figures S1 and S5 reveals that TMS-substituted substrate is difficult than Me-substituted substrate **S** to undergo the asymmetric [3+2] reaction, in accord with experiments. The inaccuracy of computing solvation energy and weak interaction energy such as dispersion energy is responsible for some of the discrepancies in computing the relative reactivity and ee values in the present Rh chemistry. Further study of how substituent affects the reactivity of substrates in the Rh-catalyzed [3+2] reactions and other related chemistry will be reported in due course.

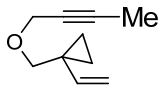
3.5 Computed Energies of All Stationary Points

Table S1. Electronic energy (*E*, in Hartree, M06), sum of electronic (M06) and thermal enthalpy corrections (B3LYP) (*H*, in Hartree), sum of electronic (M06) and thermal free energy corrections (B3LYP) (*G*, in Hartree), entropy (B3LYP) (*S*, in cal/mol), thermal correction to Gibbs free energy (B3LYP) (TCGFE, in Hartree), total free energy in solution (M06) (E_{sol}, in hartree), and thermo corrected Gibbs free energy in dichloroethane solution (G_{sol}, which equals to E_{sol} + TCGFE, in Hartree). Relative energies (ΔH_{gas}, ΔG_{gas}, and ΔG_{sol}) are reported in kcal/mol.

Structure	TCGFE	*E*	*H*	*G*	*S*	E_{sol}	G_{sol}	ΔH_{gas}	ΔG_{gas}	ΔG_{sol}
Manuscript										
S	0.172749	-464.223601	-463.995399	-464.050852	116.711	-464.228594	-464.055845	0.0	0.0	0.0
P	0.183331	-464.301723	-464.071367	-464.118392	98.973	-464.305691	-464.122360	-	-	-
(*S*)-IN1	0.840168	-2955.722986	-2954.731277	-2954.882818	318.945	-2955.768417	-2954.928249	3.1	-0.2	0.2
(*S*)-TS1	0.843174	-2955.706563	-2954.716114	-2954.863389	309.967	-2955.751836	-2954.908662	12.6	12.0	12.5
(*S*)-IN2	0.843132	-2955.713571	-2954.721739	-2954.870439	312.966	-2955.760556	-2954.917424	9.1	7.6	7.0
(*S*)-IN2'	0.853751	-2955.728199	-2954.735186	-2954.874448	293.102	-2955.771783	-2954.918032	0.6	5.1	6.6
(*S*)-TS2	0.854343	-2955.702875	-2954.711856	-2954.848532	287.659	-2955.747347	-2954.893004	15.3	21.3	22.3
(*S*)-IN3	0.855943	-2955.749912	-2954.756662	-2954.893969	288.987	-2955.796568	-2954.940625	-12.8	-7.2	-7.6
(*S*)-TS3	0.856592	-2955.742338	-2954.750374	-2954.885746	284.915	-2955.786956	-2954.930364	-8.9	-2.0	-1.1
(*S*)-IN4	0.856391	-2955.806441	-2954.812188	-2954.950050	290.155	-2955.851481	-2954.995090	-47.7	-42.4	-41.7
(*S*)-TS2-H	0.826295	-2916.414519	-2915.454296	-2915.588224	281.875	-2916.459359	-2915.633064	0.0	0.0	0.0
(*R*)-TS2-H	0.825441	-2916.410969	-2915.450640	-2915.585528	283.896	-2916.456447	-2915.631006	2.3	1.7	1.3
(*S*)-TS2-Me	0.854343	-2955.702875	-2954.711856	-2954.848532	287.659	-2955.747347	-2954.893004	0.0	0.0	0.0
(*R*)-TS2-Me	0.853674	-2955.697121	-2954.705885	-2954.843447	289.524	-2955.742099	-2954.888425	3.7	3.2	2.9
(*S*)-TS2-N	0.969061	-3754.470398	-3753.338580	-3753.501337	342.551	-3754.519720	-3753.550659	0.0	0.0	0.0
(*R*)-TS2-N	0.969237	-3754.465129	-3753.332761	-3753.495892	343.338	-3754.514095	-3753.544858	3.7	3.4	3.6
(*S*)-TS2-C	0.930138	-2998.369661	-2997.296028	-2997.439523	302.011	-2998.411302	-2997.481164	0.0	0.0	0.0
(*R*)-TS2-C	0.929757	-2998.366929	-2997.292840	-2997.437172	303.773	-2998.409168	-2997.479411	2.0	1.5	1.1
(*S*)-IN2'-TMS	0.921141	-3324.995019	-3323.921554	-3324.073878	320.593	-3325.038204	-3324.117063	0.0	0.0	0.0
(*S*)-TS2-TMS	0.922866	-3324.969749	-3323.898030	-3324.046883	313.288	-3325.01332	-3324.090454	14.8	16.9	16.7
(*R*)-TS2-TMS	0.921807	-3324.959955	-3323.887868	-3324.038148	316.291	-3325.003881	-3324.082074	21.1	22.4	22.0
(*S*)-IN2'-E	0.865428	-3144.199722	-3143.189057	-3143.334294	305.677	-3144.244815	-3143.379387	0.0	0.0	0.0
(*S*)-TS2-E	0.865815	-3144.180417	-3143.171543	-3143.314602	301.093	-3144.226611	-3143.360796	11.0	12.4	11.7
(*R*)-TS2-E	0.863916	-3144.171401	-3143.162332	-3143.307485	305.500	-3144.218702	-3143.354786	16.8	16.8	15.4
(*S*)-IN2'-Ph	0.902943	-3147.314447	-3146.265415	-3146.411504	307.470	-3147.358521	-3146.455578	0.0	0.0	0.0
(*S*)-TS2-Ph	0.903374	-3147.292462	-3146.245416	-3146.389088	302.383	-3147.336705	-3146.433331	12.5	14.1	14.0
(*R*)-TS2-Ph	0.902517	-3147.285795	-3146.238099	-3146.383278	305.555	-3147.330332	-3146.427815	17.1	17.7	17.4
Supporting Information										
S-S	0.238327	-833.487446	-833.178461	-833.249119	148.712	-833.4927378	-833.254411	0.0	0.0	0.0
P-S	0.249038	-833.556396	-833.245571	-833.307358	130.042	-833.5605386	-833.311501	-	-	-
(*S*)-IN-S1	0.909128	-3324.986369	-3323.913626	-3324.077241	344.357	-3325.032401	-3324.123273	-4.9	-5.5	-4.4
(*S*)-TS-S1	0.910916	-3324.971117	-3323.900045	-3324.060201	337.077	-3325.016303	-3324.105387	3.6	5.2	6.8
(*S*)-IN-S2	0.911295	-3324.976323	-3323.903712	-3324.065028	339.518	-3325.023811	-3324.112516	1.3	2.2	2.4
(*S*)-IN-S2'	0.921141	-3324.995019	-3323.921554	-3324.073878	320.593	-3325.038204	-3324.117063	-9.9	-3.4	-0.5
(*S*)-TS-S2	0.922866	-3324.969749	-3323.898030	-3324.046883	313.288	-3325.01332	-3324.090454	4.9	13.5	16.2
(*S*)-IN-S3	0.923796	-3325.002028	-3323.927728	-3324.078232	316.763	-3325.049725	-3324.125929	-13.7	-6.1	-6.1
(*S*)-TS-S3	0.924316	-3324.993276	-3323.920368	-3324.068960	312.738	-3325.037141	-3324.112825	-9.1	-0.3	2.2
(*S*)-IN-S4	0.920872	-3325.047569	-3323.972951	-3324.126697	323.586	-3325.094240	-3324.173368	-42.1	-36.5	-35.8

3.6 Coordinates of All Stationary Points

S



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	4.323709	-0.319255	-0.491930
4	1	0	5.276085	-0.795921	-0.275895
5	1	0	4.280319	0.297693	-1.385753
6	6	0	1.740521	1.398450	-0.663253
7	6	0	1.625973	1.441396	0.843022
8	6	0	0.811358	-0.917337	0.086252
9	1	0	0.821842	1.499009	-1.232624
10	1	0	2.614892	1.848629	-1.123904
11	1	0	2.439086	1.894919	1.403311
12	1	0	0.636310	1.569943	1.269647
13	1	0	0.947797	-1.559275	-0.801805
14	1	0	0.881410	-1.572472	0.974134
15	6	0	-1.522285	-1.227623	-0.021019
16	1	0	-1.480215	-1.909798	0.846339
17	1	0	-1.417475	-1.857398	-0.921913
18	6	0	1.916625	0.130454	0.132523
19	6	0	-2.805257	-0.529175	-0.044905
20	6	0	-3.879218	0.024913	-0.064835
21	8	0	-0.457297	-0.290716	0.045095
22	6	0	-5.170424	0.706961	-0.086634
23	1	0	-5.654144	0.620366	-1.067164
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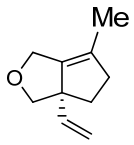
P



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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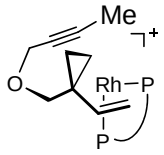
4	6	0	1.309559	-1.525262	0.547056
5	6	0	1.620126	-0.190228	-0.120016
6	6	0	0.115358	1.941639	-0.544465
7	6	0	-1.391750	1.040343	1.013057
8	6	0	-1.621188	-0.694399	-0.771957
9	6	0	-1.898464	-1.961053	-1.087392
10	1	0	-0.670466	-2.175411	1.337005
11	1	0	0.100206	-0.861623	2.224958
12	1	0	2.082778	-1.812881	1.271944
13	1	0	1.258172	-2.339149	-0.192234
14	1	0	-0.027800	2.146759	-1.613557
15	1	0	0.851742	2.663267	-0.159229
16	1	0	-2.475230	0.963719	1.144065
17	1	0	-0.924847	1.238232	1.991685
18	1	0	-2.064586	0.100634	-1.372564
19	1	0	-2.552416	-2.197030	-1.922854
20	1	0	-1.497605	-2.810068	-0.540483
21	8	0	-1.158108	2.125940	0.104872
22	6	0	3.006251	0.191574	-0.543558
23	1	0	3.052927	1.221544	-0.912702
24	1	0	3.716760	0.092522	0.288459
25	1	0	3.371485	-0.465341	-1.345714

(*S*)-IN1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	-1.967975	-1.220786	0.981809
3	6	0	-2.729104	-1.587029	2.099372
4	6	0	-4.093003	-1.323281	2.132856
5	6	0	-1.831510	-0.374846	-1.389971

6	6	0	-0.871292	0.654143	-1.511206
7	6	0	-0.094951	0.726412	-2.682949
8	6	0	-0.314853	-0.150548	-3.732135
9	1	0	-2.261994	-2.076780	2.946078
10	1	0	-4.672464	-1.623985	3.002846
11	1	0	0.678731	1.479650	-2.780470
12	1	0	0.280793	-0.060516	-4.637777
13	6	0	-4.658886	0.470624	-1.190311
14	6	0	-6.230496	-0.415683	1.181354
15	6	0	-6.756365	0.623820	0.186822
16	6	0	-6.187387	0.345779	-1.206269
17	1	0	-4.397351	1.531627	-1.068499
18	1	0	-4.242740	0.177833	-2.157871
19	1	0	-6.748711	-1.371026	1.007271
20	1	0	-6.478408	-0.127357	2.210287
21	1	0	-7.851917	0.606056	0.176512
22	1	0	-6.456144	1.630830	0.507839
23	1	0	-6.478527	-0.664880	-1.526592
24	1	0	-6.601499	1.041499	-1.945169
25	6	0	-4.734786	-0.666474	1.078993
26	6	0	-3.988284	-0.299431	-0.060475
27	6	0	-1.462927	-2.087504	-4.834596
28	6	0	-2.755923	-2.904873	-4.785868
29	6	0	-2.915152	-3.513881	-3.392194
30	6	0	-3.054114	-2.413279	-2.332267
31	1	0	-1.404110	-1.503715	-5.761772
32	1	0	-3.617457	-2.260005	-5.008532
33	1	0	-2.734438	-3.682277	-5.557668
34	1	0	-3.792026	-4.170011	-3.346217
35	1	0	-2.039054	-4.136543	-3.166728
36	1	0	-4.066442	-1.991207	-2.401025
37	1	0	-2.988685	-2.850679	-1.330862
38	1	0	-0.604705	-2.775942	-4.858990
39	6	0	-2.033589	-1.287689	-2.463383
40	6	0	-1.286564	-1.153952	-3.648943
41	6	0	-1.769177	2.357405	0.883263
42	6	0	-2.771123	3.172841	0.330482
43	6	0	-1.789863	2.098407	2.260425
44	6	0	-3.784549	3.689455	1.137247
45	1	0	-2.753758	3.425971	-0.724275
46	6	0	-2.803260	2.618130	3.067300
47	1	0	-0.995956	1.499466	2.695099
48	6	0	-3.804475	3.411696	2.506722
49	1	0	-4.550256	4.322827	0.698107

50	1	0	-2.804935	2.409110	4.133358
51	1	0	-4.588935	3.824902	3.134307
52	6	0	0.125907	3.342561	-0.996606
53	6	0	1.041670	4.232604	-0.415699
54	6	0	-0.527041	3.740872	-2.179327
55	6	0	1.313344	5.470533	-1.001534
56	1	0	1.544980	3.977046	0.505791
57	6	0	-0.256329	4.978884	-2.762404
58	1	0	-1.243732	3.082909	-2.658301
59	6	0	0.668005	5.846911	-2.178806
60	1	0	2.029936	6.138421	-0.532333
61	1	0	-0.770271	5.262062	-3.676619
62	1	0	0.879948	6.808827	-2.636243
63	6	0	0.299315	-2.704028	-0.198977
64	6	0	1.409742	-2.531851	-1.037217
65	6	0	-0.428835	-3.904310	-0.259427
66	6	0	1.793010	-3.545382	-1.918461
67	1	0	1.968147	-1.599921	-1.002665
68	6	0	-0.040575	-4.917468	-1.136397
69	1	0	-1.292318	-4.049472	0.384124
70	6	0	1.071024	-4.739126	-1.966286
71	1	0	2.654134	-3.402116	-2.565034
72	1	0	-0.602426	-5.846661	-1.170099
73	1	0	1.372157	-5.530415	-2.646943
74	6	0	0.300976	-2.117780	2.654311
75	6	0	0.122445	-1.332451	3.810811
76	6	0	0.900463	-3.380376	2.787424
77	6	0	0.512484	-1.806140	5.062805
78	1	0	-0.334377	-0.350657	3.732673
79	6	0	1.298019	-3.848144	4.042638
80	1	0	1.059559	-4.005384	1.916114
81	6	0	1.105111	-3.066367	5.181570
82	1	0	0.355128	-1.191192	5.944471
83	1	0	1.757727	-4.828813	4.126168
84	1	0	1.414012	-3.434151	6.155681
85	15	0	-0.342262	1.766622	-0.131216
86	15	0	-0.130103	-1.390934	1.010208
87	45	0	1.209754	0.589968	1.014297
88	1	0	3.144655	2.504331	0.299533
89	6	0	3.038573	1.825333	1.140291
90	6	0	2.213501	2.163424	2.206382
91	1	0	1.693680	3.114368	2.237921
92	1	0	2.307040	1.679820	3.177944
93	6	0	3.725128	-0.540480	2.058461

94	6	0	4.842211	0.407514	2.380617
95	6	0	4.651423	0.405103	-0.190060
96	1	0	3.965866	-1.518095	1.652051
97	1	0	2.864497	-0.542979	2.725873
98	1	0	4.724024	1.069558	3.233151
99	1	0	5.860713	0.072761	2.205045
100	1	0	5.278608	-0.495816	-0.127698
101	1	0	3.880160	0.226883	-0.960304
102	6	0	6.106875	1.403892	-1.789110
103	1	0	6.555187	2.385538	-1.973684
104	1	0	5.373843	1.218280	-2.592568
105	6	0	7.137845	0.360154	-1.800506
106	6	0	7.990154	-0.498999	-1.809563
107	6	0	4.005528	0.689520	1.152458
108	8	0	5.430727	1.534504	-0.538275
109	6	0	9.037174	-1.517387	-1.832803
110	1	0	9.541743	-1.588750	-0.861971
111	1	0	8.633162	-2.507318	-2.075856
112	1	0	9.798748	-1.274907	-2.583393

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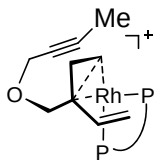

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	-1.680292	-1.376390	0.978121
3	6	0	-2.492053	-1.831256	2.026571
4	6	0	-3.873546	-1.859953	1.884678
5	6	0	-1.430502	-0.634341	-1.425023
6	6	0	-0.732284	0.589410	-1.525260
7	6	0	0.142414	0.785576	-2.611393
8	6	0	0.262510	-0.171956	-3.605497
9	1	0	-2.050856	-2.165859	2.957878
10	1	0	-4.485683	-2.226859	2.705567
11	1	0	0.720278	1.699880	-2.689525
12	1	0	0.924501	0.012819	-4.448676
13	6	0	-4.362521	-0.414885	-1.613383

14	6	0	-6.011491	-1.485430	0.625459
15	6	0	-6.607673	-0.642306	-0.505924
16	6	0	-5.815856	-0.868903	-1.795908
17	1	0	-4.346376	0.682693	-1.546997
18	1	0	-3.772648	-0.661175	-2.500259
19	1	0	-6.295493	-2.538084	0.474312
20	1	0	-6.443753	-1.197896	1.591806
21	1	0	-7.664812	-0.897006	-0.641170
22	1	0	-6.567040	0.422266	-0.237250
23	1	0	-5.845700	-1.935163	-2.062416
24	1	0	-6.265524	-0.322600	-2.633135
25	6	0	-4.495655	-1.415802	0.714836
26	6	0	-3.699221	-0.961710	-0.356235
27	6	0	-0.269939	-2.378779	-4.670933
28	6	0	-1.356258	-3.456532	-4.711513
29	6	0	-1.555607	-4.025262	-3.305901
30	6	0	-2.050088	-2.937400	-2.343331
31	1	0	-0.214102	-1.843739	-5.627169
32	1	0	-2.299747	-3.025136	-5.074047
33	1	0	-1.074509	-4.243355	-5.420183
34	1	0	-2.275692	-4.851711	-3.313929
35	1	0	-0.604341	-4.436205	-2.942924
36	1	0	-3.114137	-2.751335	-2.546358
37	1	0	-2.010091	-3.306477	-1.313698
38	1	0	0.709460	-2.863795	-4.540571
39	6	0	-1.290188	-1.619349	-2.442813
40	6	0	-0.454748	-1.372184	-3.548495
41	6	0	-2.255630	2.134684	0.665461
42	6	0	-3.365879	2.679201	-0.001725
43	6	0	-2.331424	1.929205	2.049615
44	6	0	-4.533318	2.978063	0.699476
45	1	0	-3.314469	2.893229	-1.064529
46	6	0	-3.499117	2.232512	2.752173
47	1	0	-1.463805	1.543420	2.575850
48	6	0	-4.603321	2.753758	2.077524
49	1	0	-5.383198	3.403241	0.172827
50	1	0	-3.542056	2.068849	3.825292
51	1	0	-5.510141	2.998713	2.623121
52	6	0	-0.504582	3.475021	-1.101192
53	6	0	0.025725	4.594037	-0.438323
54	6	0	-1.029592	3.657099	-2.393514
55	6	0	0.056827	5.847370	-1.052078
56	1	0	0.398620	4.503991	0.574609
57	6	0	-0.997981	4.910570	-3.006733

58	1	0	-1.462219	2.820353	-2.930890
59	6	0	-0.449499	6.008413	-2.341927
60	1	0	0.473593	6.696416	-0.517895
61	1	0	-1.406763	5.026551	-4.006590
62	1	0	-0.424278	6.982160	-2.822207
63	6	0	0.875779	-2.583094	0.210034
64	6	0	1.972044	-2.329017	-0.625509
65	6	0	0.360489	-3.889361	0.279706
66	6	0	2.558878	-3.361404	-1.361278
67	1	0	2.358619	-1.317790	-0.711146
68	6	0	0.950951	-4.920962	-0.450572
69	1	0	-0.497864	-4.101304	0.911173
70	6	0	2.054562	-4.659359	-1.268751
71	1	0	3.408713	-3.149345	-2.003983
72	1	0	0.550750	-5.928495	-0.380601
73	1	0	2.514497	-5.465056	-1.833975
74	6	0	0.439883	-1.753135	2.973519
75	6	0	-0.007052	-0.914475	4.012895
76	6	0	1.179214	-2.896259	3.310813
77	6	0	0.253469	-1.225602	5.346165
78	1	0	-0.569452	-0.015358	3.780080
79	6	0	1.448085	-3.201494	4.648902
80	1	0	1.552203	-3.555901	2.536027
81	6	0	0.985014	-2.372519	5.668956
82	1	0	-0.111377	-0.571234	6.132979
83	1	0	2.022141	-4.092270	4.887757
84	1	0	1.193393	-2.612910	6.707399
85	15	0	-0.640682	1.863515	-0.186728
86	15	0	0.151361	-1.224040	1.223327
87	45	0	1.220028	1.005622	0.999945
88	1	0	2.403826	3.358479	0.210033
89	6	0	2.530518	2.691790	1.057543
90	6	0	1.676127	2.760472	2.180274
91	1	0	0.925424	3.540348	2.240632
92	1	0	1.975199	2.363747	3.147612
93	6	0	3.068904	0.064547	2.043798
94	6	0	4.208753	1.052142	2.139446
95	6	0	4.168312	1.397019	-0.384742
96	1	0	3.301907	-0.871684	1.547696
97	1	0	2.468560	-0.033853	2.945584
98	1	0	4.215118	1.661384	3.043246
99	1	0	5.205578	0.666349	1.928540
100	1	0	4.318434	0.316176	-0.520972
101	1	0	3.523651	1.758637	-1.200733

102	6	0	6.210256	1.818359	-1.542476
103	1	0	7.066487	2.493246	-1.446069
104	1	0	5.655856	2.113455	-2.448173
105	6	0	6.662555	0.428185	-1.655843
106	6	0	7.050887	-0.714122	-1.754363
107	6	0	3.546238	1.677826	0.966838
108	8	0	5.413149	2.073134	-0.381240
109	6	0	7.553213	-2.080064	-1.880507
110	1	0	7.423921	-2.637117	-0.944917
111	1	0	7.034183	-2.629586	-2.674857
112	1	0	8.623270	-2.081009	-2.119064

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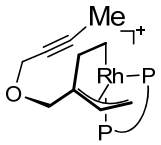

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.319878	0.916577	0.099241
2	6	0	2.387112	-0.178110	-0.799072
3	6	0	3.352784	-0.163556	-1.816415
4	6	0	4.205086	0.922366	-1.961526
5	6	0	1.414952	0.853934	1.302947
6	6	0	0.019598	1.079516	1.199660
7	6	0	-0.785183	0.877432	2.340547
8	6	0	-0.209848	0.568194	3.565916
9	1	0	3.445962	-0.998894	-2.500370
10	1	0	4.950624	0.912501	-2.753477
11	1	0	-1.860888	0.999582	2.278155
12	1	0	-0.846452	0.456693	4.440866
13	6	0	3.047472	3.251740	0.831269
14	6	0	5.102650	3.175650	-1.324587
15	6	0	4.714900	4.469379	-0.602438
16	6	0	4.286711	4.155319	0.832712
17	1	0	2.188184	3.839977	0.478758
18	1	0	2.796106	2.951719	1.851992
19	1	0	6.089549	2.846650	-0.964983
20	1	0	5.223994	3.353844	-2.400174
21	1	0	5.557285	5.169908	-0.618964

22	1	0	3.883899	4.956102	-1.130890
23	1	0	5.112894	3.659938	1.362613
24	1	0	4.064823	5.075156	1.386008
25	6	0	4.123678	2.031832	-1.115144
26	6	0	3.176105	2.031984	-0.072027
27	6	0	1.740978	0.103594	5.076123
28	6	0	3.246554	0.357970	5.181240
29	6	0	3.953492	-0.312223	4.002369
30	6	0	3.496313	0.297978	2.669582
31	1	0	1.191591	0.682150	5.829104
32	1	0	3.445948	1.438661	5.170912
33	1	0	3.623164	-0.024726	6.136366
34	1	0	5.041608	-0.211963	4.086523
35	1	0	3.733791	-1.387169	4.012772
36	1	0	4.007823	1.260906	2.534234
37	1	0	3.833428	-0.330596	1.838802
38	1	0	1.541505	-0.954169	5.306746
39	6	0	1.991919	0.522935	2.558056
40	6	0	1.173244	0.414285	3.701611
41	6	0	0.032066	2.448435	-1.556282
42	6	0	0.183784	3.818865	-1.286553
43	6	0	0.430056	1.955939	-2.806641
44	6	0	0.752439	4.665826	-2.237331
45	1	0	-0.165113	4.231849	-0.345104
46	6	0	0.997150	2.804274	-3.759454
47	1	0	0.282360	0.905733	-3.036707
48	6	0	1.163274	4.159807	-3.474190
49	1	0	0.859835	5.724762	-2.019162
50	1	0	1.299589	2.408371	-4.724787
51	1	0	1.595497	4.824221	-4.216967
52	6	0	-2.335853	2.377742	-0.029287
53	6	0	-3.381217	2.381435	-0.968506
54	6	0	-2.412997	3.262788	1.059443
55	6	0	-4.480673	3.227010	-0.816339
56	1	0	-3.324568	1.744853	-1.846900
57	6	0	-3.517342	4.103227	1.215282
58	1	0	-1.612546	3.303587	1.790606
59	6	0	-4.554687	4.086212	0.281619
60	1	0	-5.273523	3.217098	-1.558765
61	1	0	-3.559875	4.778608	2.065180
62	1	0	-5.408501	4.746752	0.402601
63	6	0	2.068127	-2.636382	0.692743
64	6	0	1.461719	-2.832034	1.940691
65	6	0	3.344581	-3.182908	0.465807

66	6	0	2.093698	-3.595821	2.925556
67	1	0	0.499159	-2.381930	2.154047
68	6	0	3.976282	-3.940083	1.451462
69	1	0	3.844808	-3.025921	-0.485223
70	6	0	3.346714	-4.158075	2.680376
71	1	0	1.602989	-3.751170	3.882311
72	1	0	4.958042	-4.362751	1.258194
73	1	0	3.834702	-4.758231	3.442984
74	6	0	1.441685	-2.643384	-2.156049
75	6	0	1.313703	-2.047880	-3.423912
76	6	0	1.557269	-4.041337	-2.083327
77	6	0	1.330461	-2.823009	-4.582762
78	1	0	1.216116	-0.970748	-3.511795
79	6	0	1.565102	-4.816431	-3.246024
80	1	0	1.649439	-4.534223	-1.121928
81	6	0	1.456629	-4.211758	-4.497890
82	1	0	1.244828	-2.340948	-5.552571
83	1	0	1.661115	-5.895529	-3.167094
84	1	0	1.468843	-4.815437	-5.400579
85	15	0	-0.866702	1.315064	-0.409837
86	15	0	1.248671	-1.631953	-0.624552
87	45	0	-1.062603	-1.196528	-0.378301
88	1	0	-3.515240	-0.345338	-1.727155
89	6	0	-3.054297	-1.296820	-1.481475
90	6	0	-1.884698	-1.736012	-2.216686
91	1	0	-1.561370	-1.113143	-3.047018
92	1	0	-1.729872	-2.798179	-2.396051
93	6	0	-1.408477	-3.206036	0.162654
94	6	0	-2.927207	-3.331732	0.009031
95	6	0	-4.534104	-1.354724	0.548031
96	1	0	-1.096742	-3.308291	1.204009
97	1	0	-0.845861	-3.915126	-0.449356
98	1	0	-3.217869	-4.033063	-0.782943
99	1	0	-3.408040	-3.687605	0.924886
100	1	0	-4.163431	-1.285405	1.587427
101	1	0	-4.812546	-0.343130	0.223789
102	6	0	-6.690385	-1.912194	1.397894
103	1	0	-6.303352	-1.930229	2.430577
104	1	0	-7.411289	-2.730163	1.300320
105	6	0	-7.332502	-0.622955	1.125177
106	6	0	-7.855866	0.445087	0.902714
107	6	0	-3.460700	-1.943407	-0.331653
108	8	0	-5.638695	-2.240181	0.486368
109	6	0	-8.506164	1.726519	0.642482

110	1	0	-7.775220	2.543686	0.612484
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112	1	0	-9.234013	1.961137	1.428259

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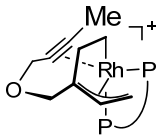

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3	6	0	-1.233030	-1.802660	2.577935
4	6	0	-2.360351	-1.449143	3.306864
5	6	0	-2.011179	-0.145278	-0.764182
6	6	0	-1.258323	0.920000	-1.307412
7	6	0	-1.318668	1.149748	-2.695228
8	6	0	-2.129595	0.381544	-3.513987
9	1	0	-0.501236	-2.460645	3.030941
10	1	0	-2.491080	-1.844347	4.312061
11	1	0	-0.725227	1.938177	-3.144005
12	1	0	-2.171904	0.598268	-4.579136
13	6	0	-4.205627	0.846734	0.878724
14	6	0	-4.530815	-0.235531	3.638977
15	6	0	-5.313144	0.981392	3.136820
16	6	0	-5.543723	0.858756	1.629303
17	1	0	-3.776382	1.858973	0.905378
18	1	0	-4.372732	0.628993	-0.180007
19	1	0	-5.201967	-1.107601	3.662400
20	1	0	-4.203727	-0.085627	4.675371
21	1	0	-6.263544	1.061342	3.676367
22	1	0	-4.747167	1.899517	3.345445
23	1	0	-6.098289	-0.067218	1.419739
24	1	0	-6.161007	1.684874	1.257641
25	6	0	-3.326659	-0.586476	2.780909
26	6	0	-3.174735	-0.111392	1.463902
27	6	0	-3.743585	-1.488561	-3.953093
28	6	0	-4.830557	-2.308684	-3.254842
29	6	0	-4.213770	-3.063192	-2.076514

30	6	0	-3.656178	-2.084846	-1.034109
31	1	0	-4.179789	-0.819876	-4.705538
32	1	0	-5.627970	-1.644276	-2.893453
33	1	0	-5.292923	-2.999438	-3.968917
34	1	0	-4.952997	-3.714286	-1.595671
35	1	0	-3.409242	-3.714954	-2.441913
36	1	0	-4.499203	-1.653616	-0.475199
37	1	0	-3.064977	-2.632384	-0.294246
38	1	0	-3.082030	-2.172221	-4.506857
39	6	0	-2.824797	-0.947548	-1.618926
40	6	0	-2.891869	-0.671261	-2.996530
41	6	0	-0.616522	2.315581	1.311370
42	6	0	-1.518290	3.372298	1.525914
43	6	0	-0.151561	1.600958	2.423264
44	6	0	-1.944860	3.692604	2.816288
45	1	0	-1.879792	3.963907	0.692873
46	6	0	-0.581220	1.915732	3.711935
47	1	0	0.557981	0.796877	2.276195
48	6	0	-1.478937	2.966014	3.913122
49	1	0	-2.634731	4.519177	2.961391
50	1	0	-0.213239	1.342131	4.558100
51	1	0	-1.806344	3.221201	4.916972
52	6	0	-0.075175	3.605656	-1.159308
53	6	0	1.007884	4.480791	-0.977232
54	6	0	-1.232007	4.101178	-1.788378
55	6	0	0.950208	5.800507	-1.428631
56	1	0	1.903989	4.138801	-0.474676
57	6	0	-1.287105	5.419916	-2.242428
58	1	0	-2.097627	3.462576	-1.923859
59	6	0	-0.195633	6.272686	-2.068725
60	1	0	1.802561	6.456959	-1.278459
61	1	0	-2.189514	5.780137	-2.728248
62	1	0	-0.240938	7.297935	-2.424184
63	6	0	-0.015876	-3.126400	-0.724420
64	6	0	0.202702	-3.143808	-2.108119
65	6	0	-0.650631	-4.234653	-0.133114
66	6	0	-0.178718	-4.244766	-2.881671
67	1	0	0.661416	-2.295162	-2.599004
68	6	0	-1.031829	-5.332726	-0.902710
69	1	0	-0.842873	-4.242596	0.935602
70	6	0	-0.791470	-5.343274	-2.280376
71	1	0	0.005044	-4.239013	-3.952455
72	1	0	-1.514845	-6.181546	-0.426805
73	1	0	-1.083485	-6.201833	-2.878375

74	6	0	1.624142	-2.544361	1.560141
75	6	0	1.936183	-1.940345	2.792788
76	6	0	2.289105	-3.736841	1.224204
77	6	0	2.848655	-2.525921	3.671378
78	1	0	1.455000	-1.012626	3.082725
79	6	0	3.214129	-4.314755	2.098330
80	1	0	2.079646	-4.230060	0.281180
81	6	0	3.492985	-3.716624	3.327497
82	1	0	3.055630	-2.049594	4.625877
83	1	0	3.708326	-5.240565	1.817244
84	1	0	4.203701	-4.172306	4.010715
85	15	0	0.014150	1.918833	-0.392691
86	15	0	0.521064	-1.692529	0.332856
87	6	0	4.027362	-0.137824	-1.761725
88	6	0	4.667521	-0.658779	1.142687
89	6	0	5.061683	-1.058887	-1.162352
90	6	0	4.423561	1.316307	-2.007423
91	6	0	3.299432	2.176935	-1.432486
92	45	0	2.094996	0.676919	-0.606349
93	1	0	5.368514	1.511252	-1.493554
94	1	0	4.590315	1.485730	-3.080453
95	1	0	2.735985	2.746316	-2.171752
96	1	0	3.647388	2.840703	-0.641005
97	1	0	5.271371	-0.552669	2.050047
98	1	0	4.186939	-1.643771	1.166315
99	1	0	5.925594	-1.119511	-1.835731
100	1	0	4.654545	-2.073227	-1.032118
101	6	0	2.836446	-0.656093	-2.266974
102	6	0	1.766763	0.185545	-2.699795
103	1	0	1.980029	1.077099	-3.283387
104	1	0	0.823336	-0.282768	-2.954651
105	1	0	2.649957	-1.717335	-2.117753
106	6	0	3.652494	0.424668	1.159586
107	6	0	3.065412	1.465719	1.473005
108	8	0	5.586818	-0.576403	0.066754
109	6	0	2.823153	2.736628	2.183374
110	1	0	2.372572	2.553561	3.163694
111	1	0	3.780526	3.247520	2.340568
112	1	0	2.155438	3.408547	1.642057

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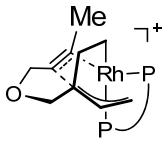

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3	6	0	-1.104521	-1.751207	2.641185
4	6	0	-2.274463	-1.502169	3.347135
5	6	0	-2.023250	-0.341864	-0.774732
6	6	0	-1.324494	0.746104	-1.342941
7	6	0	-1.299341	0.879546	-2.743977
8	6	0	-2.012258	0.012423	-3.554624
9	1	0	-0.303610	-2.296130	3.127083
10	1	0	-2.368263	-1.865184	4.368428
11	1	0	-0.720924	1.671638	-3.205651
12	1	0	-2.002939	0.156944	-4.632830
13	6	0	-4.341452	0.472070	0.816521
14	6	0	-4.579056	-0.542386	3.610781
15	6	0	-5.485974	0.560768	3.057895
16	6	0	-5.682487	0.362435	1.553483
17	1	0	-4.023033	1.524708	0.816535
18	1	0	-4.468544	0.206935	-0.236783
19	1	0	-5.147844	-1.483635	3.656989
20	1	0	-4.286545	-0.322183	4.644876
21	1	0	-6.446547	0.550903	3.585175
22	1	0	-5.030356	1.543609	3.240220
23	1	0	-6.129942	-0.625330	1.371767
24	1	0	-6.381436	1.102981	1.147767
25	6	0	-3.330565	-0.783930	2.778325
26	6	0	-3.220824	-0.347918	1.443287
27	6	0	-3.502683	-1.965708	-3.956916
28	6	0	-4.566424	-2.816024	-3.259025
29	6	0	-3.951725	-3.475648	-2.024166
30	6	0	-3.495617	-2.418149	-1.009310
31	1	0	-3.946071	-1.364482	-4.760402
32	1	0	-5.414413	-2.184486	-2.959373
33	1	0	-4.959455	-3.566414	-3.954098
34	1	0	-4.667741	-4.149829	-1.540165
35	1	0	-3.095415	-4.091159	-2.329632
36	1	0	-4.381813	-2.031126	-0.487039

37	1	0	-2.883114	-2.890310	-0.235010
38	1	0	-2.777191	-2.633336	-4.446592
39	6	0	-2.733278	-1.245901	-1.618474
40	6	0	-2.746371	-1.048498	-3.011128
41	6	0	-0.958336	2.332335	1.231898
42	6	0	-1.971172	3.304212	1.320481
43	6	0	-0.478021	1.758335	2.414474
44	6	0	-2.486410	3.679513	2.561953
45	1	0	-2.349710	3.787236	0.426607
46	6	0	-0.992409	2.132138	3.655654
47	1	0	0.297715	1.007585	2.357067
48	6	0	-1.997342	3.097528	3.733282
49	1	0	-3.262944	4.437600	2.611711
50	1	0	-0.607054	1.670671	4.560481
51	1	0	-2.391957	3.399772	4.699180
52	6	0	-0.367140	3.548533	-1.233988
53	6	0	0.552412	4.543829	-0.860247
54	6	0	-1.434021	3.908561	-2.075030
55	6	0	0.435042	5.846637	-1.343548
56	1	0	1.356401	4.308908	-0.171888
57	6	0	-1.548535	5.213804	-2.559533
58	1	0	-2.190425	3.181659	-2.346456
59	6	0	-0.611650	6.183979	-2.203565
60	1	0	1.159663	6.598059	-1.043216
61	1	0	-2.379742	5.469859	-3.210406
62	1	0	-0.702918	7.197660	-2.582620
63	6	0	0.254285	-3.014531	-0.658562
64	6	0	0.480737	-3.013808	-2.040395
65	6	0	-0.262917	-4.180681	-0.064311
66	6	0	0.224973	-4.152623	-2.810590
67	1	0	0.844407	-2.119371	-2.528472
68	6	0	-0.518502	-5.317136	-0.830451
69	1	0	-0.457853	-4.204174	1.003766
70	6	0	-0.268721	-5.308308	-2.206500
71	1	0	0.413268	-4.132535	-3.880453
72	1	0	-0.910453	-6.210903	-0.353174
73	1	0	-0.461391	-6.196644	-2.801268
74	6	0	1.827153	-2.261930	1.625310
75	6	0	2.103516	-1.602362	2.836882
76	6	0	2.587415	-3.400339	1.307154
77	6	0	3.074612	-2.083970	3.714730
78	1	0	1.545288	-0.713343	3.111857
79	6	0	3.569512	-3.875987	2.180597
80	1	0	2.409351	-3.933081	0.379703

81	6	0	3.813392	-3.224812	3.389802
82	1	0	3.252948	-1.568175	4.654388
83	1	0	4.136056	-4.764096	1.914708
84	1	0	4.568901	-3.601148	4.073349
85	15	0	-0.211597	1.895444	-0.409353
86	15	0	0.640987	-1.533771	0.397611
87	6	0	4.046354	0.252144	-1.380126
88	6	0	5.145952	-0.221088	1.032631
89	6	0	5.288784	-0.620125	-1.194411
90	6	0	4.256644	1.733525	-1.699331
91	6	0	2.976466	2.456788	-1.259570
92	45	0	1.873636	0.811685	-0.512795
93	1	0	5.136341	2.094065	-1.159456
94	1	0	4.465598	1.850103	-2.772034
95	1	0	2.426369	2.941593	-2.066373
96	1	0	3.166451	3.184668	-0.471556
97	1	0	5.644474	0.289397	1.863449
98	1	0	4.917420	-1.254121	1.338973
99	1	0	5.938744	-0.503237	-2.068528
100	1	0	4.997382	-1.679871	-1.109661
101	6	0	2.964220	-0.405071	-2.121758
102	6	0	2.062310	0.227213	-2.947582
103	1	0	2.208352	1.234068	-3.315240
104	1	0	1.286446	-0.346372	-3.442052
105	1	0	2.868275	-1.478219	-1.972173
106	6	0	3.885524	0.502950	0.687242
107	6	0	2.966730	1.246625	1.199750
108	8	0	6.029818	-0.211273	-0.069800
109	6	0	2.841134	2.109163	2.410341
110	1	0	2.381219	3.072293	2.166513
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112	1	0	3.828404	2.299469	2.848604

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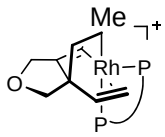

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

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4	6	0	-3.017757	-0.926037	3.178824
5	6	0	-2.052372	0.076589	-0.880308
6	6	0	-1.056899	0.954662	-1.374542
7	6	0	-0.859315	1.053708	-2.767224
8	6	0	-1.684921	0.372463	-3.648113
9	1	0	-1.280027	-2.170523	3.166135
10	1	0	-3.311059	-1.245253	4.176532
11	1	0	-0.073033	1.686113	-3.164099
12	1	0	-1.538831	0.492346	-4.719201
13	6	0	-4.265170	1.448525	0.461336
14	6	0	-5.040205	0.560021	3.199349
15	6	0	-5.603023	1.831659	2.557900
16	6	0	-5.670590	1.658107	1.039119
17	1	0	-3.717136	2.400410	0.517001
18	1	0	-4.328594	1.210620	-0.604155
19	1	0	-5.812679	-0.223697	3.177947
20	1	0	-4.817243	0.727146	4.260322
21	1	0	-6.592380	2.051015	2.974502
22	1	0	-4.957293	2.687355	2.798288
23	1	0	-6.307624	0.795127	0.797750
24	1	0	-6.131937	2.531589	0.564108
25	6	0	-3.799943	0.018617	2.506731
26	6	0	-3.443397	0.397614	1.197430
27	6	0	-3.576435	-1.177880	-4.203573
28	6	0	-4.870463	-1.743701	-3.613783
29	6	0	-4.544968	-2.521157	-2.337977
30	6	0	-3.942592	-1.594516	-1.272437
31	1	0	-3.789360	-0.492065	-5.032938
32	1	0	-5.567003	-0.925407	-3.383688
33	1	0	-5.366497	-2.383822	-4.351704
34	1	0	-5.441726	-2.999861	-1.928632
35	1	0	-3.836690	-3.326107	-2.573127
36	1	0	-4.754130	-1.004267	-0.824872
37	1	0	-3.528735	-2.191046	-0.453093
38	1	0	-2.992623	-2.002681	-4.640225
39	6	0	-2.873079	-0.641103	-1.795187
40	6	0	-2.706101	-0.464007	-3.183732
41	6	0	-0.545668	2.401294	1.265005
42	6	0	-1.318459	3.576754	1.275633
43	6	0	-0.296544	1.750760	2.479424
44	6	0	-1.836809	4.071540	2.472573

45	1	0	-1.505596	4.120609	0.356533
46	6	0	-0.809708	2.248996	3.676367
47	1	0	0.304840	0.853273	2.487431
48	6	0	-1.581836	3.411476	3.676402
49	1	0	-2.428091	4.982729	2.463181
50	1	0	-0.602123	1.731248	4.608385
51	1	0	-1.974249	3.806563	4.609031
52	6	0	0.567568	3.434224	-1.112323
53	6	0	1.712851	4.119327	-0.669925
54	6	0	-0.294829	4.073903	-2.017382
55	6	0	2.000146	5.400712	-1.138181
56	1	0	2.382426	3.655065	0.048148
57	6	0	-0.001711	5.356877	-2.486536
58	1	0	-1.202497	3.584167	-2.352562
59	6	0	1.146211	6.020622	-2.053193
60	1	0	2.891117	5.913531	-0.787847
61	1	0	-0.678208	5.836952	-3.187813
62	1	0	1.371511	7.017507	-2.420449
63	6	0	-0.466127	-3.114404	-0.430569
64	6	0	-0.476526	-3.040921	-1.830994
65	6	0	-0.963667	-4.275533	0.187752
66	6	0	-0.931976	-4.117330	-2.597996
67	1	0	-0.139795	-2.137698	-2.330064
68	6	0	-1.421841	-5.347166	-0.577839
69	1	0	-0.984058	-4.349826	1.270791
70	6	0	-1.397580	-5.274799	-1.973573
71	1	0	-0.918702	-4.049346	-3.682327
72	1	0	-1.794760	-6.240106	-0.084322
73	1	0	-1.743993	-6.114835	-2.568755
74	6	0	1.092636	-2.475638	1.936104
75	6	0	1.266760	-1.867988	3.192390
76	6	0	1.843261	-3.631300	1.651984
77	6	0	2.139961	-2.408670	4.137553
78	1	0	0.705504	-0.977400	3.452782
79	6	0	2.722081	-4.166340	2.595893
80	1	0	1.735328	-4.130545	0.694540
81	6	0	2.872636	-3.559598	3.843401
82	1	0	2.243594	-1.928602	5.106632
83	1	0	3.282477	-5.065292	2.354704
84	1	0	3.551062	-3.980371	4.579598
85	15	0	0.197106	1.808431	-0.322838
86	15	0	0.118665	-1.674460	0.583666
87	6	0	4.619919	-0.439062	-1.016926
88	6	0	5.815219	0.394515	0.956082

89	6	0	6.102762	-0.872602	-0.926477
90	6	0	4.311318	0.575659	-2.136956
91	6	0	2.921521	1.206573	-1.930184
92	45	0	1.731883	0.072257	-0.582122
93	1	0	5.092083	1.343890	-2.126224
94	1	0	4.378168	0.076316	-3.112411
95	1	0	2.320522	1.198993	-2.849475
96	1	0	3.007011	2.235775	-1.593461
97	1	0	6.041654	1.396155	1.335395
98	1	0	5.950753	-0.325607	1.781563
99	1	0	6.615790	-0.880039	-1.891444
100	1	0	6.191760	-1.872820	-0.469471
101	6	0	3.622954	-1.563523	-1.026599
102	6	0	2.671190	-1.791783	-1.968281
103	1	0	2.632733	-1.247696	-2.906606
104	1	0	2.025199	-2.657104	-1.885186
105	1	0	3.680305	-2.245466	-0.178641
106	6	0	4.438472	0.264238	0.322542
107	6	0	3.227943	0.651002	0.723188
108	8	0	6.720888	0.112181	-0.107262
109	6	0	2.975169	1.370706	2.016490
110	1	0	2.346162	2.258116	1.907329
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112	1	0	3.929879	1.693933	2.452853

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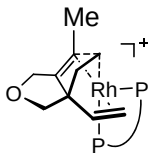

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4	6	0	-2.278789	-0.832152	3.558041
5	6	0	-2.271244	-0.007789	-0.651329
6	6	0	-1.333944	0.796133	-1.334358
7	6	0	-1.342945	0.806260	-2.742042
8	6	0	-2.314065	0.113752	-3.446314
9	1	0	-0.499479	-1.964984	3.210487

10	1	0	-2.314583	-1.103903	4.610720
11	1	0	-0.601779	1.376758	-3.291103
12	1	0	-2.321755	0.161281	-4.533064
13	6	0	-4.232636	1.343454	1.106713
14	6	0	-4.354441	0.517445	3.965966
15	6	0	-5.130847	1.722257	3.424555
16	6	0	-5.500298	1.489601	1.957527
17	1	0	-3.733412	2.321970	1.052562
18	1	0	-4.492680	1.092605	0.075313
19	1	0	-5.056464	-0.313022	4.136409
20	1	0	-3.922358	0.745166	4.948151
21	1	0	-6.025462	1.890720	4.034455
22	1	0	-4.514501	2.628144	3.504390
23	1	0	-6.116275	0.582768	1.873464
24	1	0	-6.105118	2.317755	1.570448
25	6	0	-3.257457	0.020034	3.039046
26	6	0	-3.224888	0.349427	1.668516
27	6	0	-4.317779	-1.383188	-3.626008
28	6	0	-5.508730	-1.903949	-2.818138
29	6	0	-4.996460	-2.614681	-1.564542
30	6	0	-4.246444	-1.633464	-0.654111
31	1	0	-4.653938	-0.726103	-4.438008
32	1	0	-6.162126	-1.068660	-2.529736
33	1	0	-6.111688	-2.578058	-3.436693
34	1	0	-5.822017	-3.066073	-1.002297
35	1	0	-4.327134	-3.433393	-1.859165
36	1	0	-4.987094	-1.003455	-0.142685
37	1	0	-3.731197	-2.182669	0.140509
38	1	0	-3.818254	-2.232970	-4.115458
39	6	0	-3.248369	-0.740671	-1.383847
40	6	0	-3.287041	-0.647130	-2.787152
41	6	0	-0.465868	2.420980	1.102101
42	6	0	-1.311595	3.542340	1.154434
43	6	0	0.059669	1.919101	2.301190
44	6	0	-1.634670	4.129029	2.378809
45	1	0	-1.706329	3.975289	0.241662
46	6	0	-0.263833	2.505205	3.524725
47	1	0	0.731869	1.069183	2.270378
48	6	0	-1.112047	3.612942	3.566710
49	1	0	-2.284411	4.999421	2.400823
50	1	0	0.153130	2.100721	4.442593
51	1	0	-1.355119	4.079047	4.517321
52	6	0	0.207810	3.259163	-1.524100
53	6	0	1.379028	4.028339	-1.443352

54	6	0	-0.878453	3.784104	-2.249784
55	6	0	1.480508	5.259781	-2.092089
56	1	0	2.214902	3.681417	-0.853643
57	6	0	-0.776435	5.016374	-2.897427
58	1	0	-1.812013	3.237638	-2.313888
59	6	0	0.405068	5.755537	-2.828834
60	1	0	2.400914	5.831582	-2.015227
61	1	0	-1.627921	5.397693	-3.453938
62	1	0	0.482731	6.712419	-3.336597
63	6	0	-0.542893	-2.844189	-0.743928
64	6	0	-0.401919	-2.780929	-2.136739
65	6	0	-1.288014	-3.897938	-0.183490
66	6	0	-0.956374	-3.770518	-2.952490
67	1	0	0.127266	-1.948225	-2.587326
68	6	0	-1.835492	-4.888587	-0.998526
69	1	0	-1.432654	-3.950821	0.891875
70	6	0	-1.662373	-4.831758	-2.384926
71	1	0	-0.833206	-3.710537	-4.030186
72	1	0	-2.395613	-5.704949	-0.551397
73	1	0	-2.082559	-5.608391	-3.017647
74	6	0	1.311213	-2.563959	1.498643
75	6	0	1.983598	-1.893863	2.539029
76	6	0	1.588927	-3.924602	1.293787
77	6	0	2.878115	-2.570762	3.366208
78	1	0	1.812945	-0.834770	2.702407
79	6	0	2.498337	-4.598056	2.115340
80	1	0	1.101547	-4.470368	0.494465
81	6	0	3.140767	-3.927584	3.155270
82	1	0	3.374199	-2.037606	4.172449
83	1	0	2.698346	-5.650997	1.938505
84	1	0	3.842358	-4.454255	3.795558
85	15	0	0.065776	1.698337	-0.521701
86	15	0	0.231105	-1.579583	0.361984
87	45	0	1.788620	0.081733	-0.556639
88	6	0	4.775812	-0.505868	-0.803881
89	6	0	5.760544	0.457377	1.220837
90	6	0	6.209765	-0.996450	-0.497627
91	6	0	4.605985	0.439006	-2.008966
92	6	0	3.319619	1.251237	-1.775600
93	1	0	5.472875	1.106992	-2.046755
94	1	0	4.575571	-0.105599	-2.960371
95	1	0	2.553528	1.094561	-2.550442
96	1	0	3.485492	2.323378	-1.717461
97	1	0	6.031217	1.455470	1.578245

98	1	0	5.688415	-0.215731	2.093447
99	1	0	6.838329	-1.099702	-1.385534
100	1	0	6.186550	-1.963076	0.031800
101	6	0	3.707963	-1.555637	-0.755483
102	6	0	2.771708	-1.799177	-1.720405
103	1	0	2.825704	-1.359030	-2.710269
104	1	0	2.107747	-2.647176	-1.614032
105	1	0	3.696720	-2.171456	0.141156
106	6	0	4.510268	0.420261	0.375445
107	6	0	3.400020	1.173204	0.304705
108	8	0	6.783476	0.014588	0.328554
109	6	0	3.240255	2.435919	1.118299
110	1	0	2.211097	2.741641	1.292841
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112	1	0	3.768631	3.274545	0.643528

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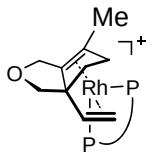

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	-1.725013	-1.504511	2.545416
4	6	0	-2.994583	-1.207015	3.025455
5	6	0	-1.978847	-0.256582	-1.033386
6	6	0	-1.062001	0.750268	-1.404181
7	6	0	-0.652677	0.839872	-2.748386
8	6	0	-1.211634	0.014761	-3.710690
9	1	0	-1.018230	-2.005971	3.196238
10	1	0	-3.261476	-1.496136	4.039574
11	1	0	0.093438	1.567874	-3.047738
12	1	0	-0.902775	0.118466	-4.748438
13	6	0	-4.564684	0.645896	0.082058
14	6	0	-5.304635	-0.245372	2.827506
15	6	0	-6.096005	0.823666	2.067740
16	6	0	-6.018770	0.558333	0.562526
17	1	0	-4.244697	1.697041	0.131104
18	1	0	-4.494475	0.370187	-0.973265

19	1	0	-5.877970	-1.184943	2.823266
20	1	0	-5.196056	0.030828	3.883527
21	1	0	-7.135607	0.831704	2.413947
22	1	0	-5.679762	1.817356	2.282979
23	1	0	-6.426967	-0.438764	0.343974
24	1	0	-6.630175	1.277974	0.005933
25	6	0	-3.931788	-0.530021	2.240468
26	6	0	-3.589500	-0.169733	0.920658
27	6	0	-2.740866	-1.816754	-4.482954
28	6	0	-4.007154	-2.573798	-4.075583
29	6	0	-3.777538	-3.249278	-2.722891
30	6	0	-3.524934	-2.202500	-1.629788
31	1	0	-2.925266	-1.193175	-5.366654
32	1	0	-4.854443	-1.877659	-4.003533
33	1	0	-4.265536	-3.308936	-4.845826
34	1	0	-4.638534	-3.865083	-2.438353
35	1	0	-2.914493	-3.923663	-2.797884
36	1	0	-4.485871	-1.738196	-1.368239
37	1	0	-3.179121	-2.692490	-0.713809
38	1	0	-1.970443	-2.542874	-4.783503
39	6	0	-2.535872	-1.111308	-2.024986
40	6	0	-2.168975	-0.949694	-3.374436
41	6	0	-1.151768	2.334154	1.247101
42	6	0	-2.211180	3.246081	1.095425
43	6	0	-0.782099	1.933454	2.537946
44	6	0	-2.898066	3.720638	2.212320
45	1	0	-2.488184	3.605826	0.109683
46	6	0	-1.467770	2.413400	3.655138
47	1	0	0.045863	1.244782	2.664216
48	6	0	-2.527722	3.306165	3.494645
49	1	0	-3.711732	4.428543	2.081502
50	1	0	-1.169005	2.092770	4.649118
51	1	0	-3.055879	3.688072	4.363670
52	6	0	0.010861	3.456492	-1.061566
53	6	0	0.902752	4.417567	-0.554310
54	6	0	-0.848917	3.841279	-2.106501
55	6	0	0.965516	5.700826	-1.097832
56	1	0	1.541599	4.185855	0.288270
57	6	0	-0.786873	5.127384	-2.647316
58	1	0	-1.578207	3.144910	-2.502769
59	6	0	0.126158	6.058708	-2.153497
60	1	0	1.667122	6.421690	-0.687957
61	1	0	-1.460704	5.397901	-3.455305
62	1	0	0.174870	7.057105	-2.578015

63	6	0	0.236305	-2.775002	-0.592364
64	6	0	0.962831	-2.684255	-1.787366
65	6	0	-0.571266	-3.904519	-0.372413
66	6	0	0.913956	-3.712960	-2.731133
67	1	0	1.553233	-1.795562	-1.984854
68	6	0	-0.611744	-4.937190	-1.310370
69	1	0	-1.170257	-3.977197	0.531027
70	6	0	0.135862	-4.845980	-2.488339
71	1	0	1.481871	-3.628327	-3.653468
72	1	0	-1.229065	-5.811295	-1.123005
73	1	0	0.104173	-5.651720	-3.216174
74	6	0	1.209775	-2.215795	2.119491
75	6	0	1.737904	-1.363657	3.106518
76	6	0	1.353479	-3.601880	2.287842
77	6	0	2.372616	-1.880077	4.236424
78	1	0	1.654855	-0.287893	2.981073
79	6	0	1.995976	-4.118279	3.416556
80	1	0	0.977924	-4.287504	1.537277
81	6	0	2.503818	-3.261946	4.394333
82	1	0	2.765844	-1.204533	4.991180
83	1	0	2.099147	-5.194031	3.527269
84	1	0	3.000801	-3.667101	5.270989
85	15	0	-0.137453	1.810733	-0.206418
86	15	0	0.381276	-1.429768	0.659411
87	45	0	1.745434	0.549815	0.167427
88	6	0	4.512271	1.233922	-0.486830
89	6	0	3.817506	-0.305795	-2.260188
90	6	0	5.045746	1.622371	-1.894629
91	6	0	5.563917	0.956527	0.624192
92	6	0	5.115840	-0.373589	1.292799
93	1	0	6.541833	0.802021	0.154858
94	1	0	5.665741	1.785463	1.331205
95	1	0	4.549810	-0.226526	2.221711
96	1	0	5.969897	-1.006754	1.564924
97	1	0	3.930958	-1.328837	-2.627912
98	1	0	2.876936	0.115340	-2.651267
99	1	0	6.097320	1.920094	-1.893517
100	1	0	4.452611	2.440804	-2.330031
101	6	0	3.341540	2.103375	-0.041592
102	6	0	2.843330	2.094245	1.259487
103	1	0	3.348839	1.553899	2.056130
104	1	0	2.186102	2.881579	1.614678
105	1	0	3.018789	2.882206	-0.727081
106	6	0	3.953437	-0.170057	-0.762552

107	6	0	4.288606	-1.058359	0.213462
108	8	0	4.938651	0.451691	-2.716541
109	6	0	4.171858	-2.549761	0.169993
110	1	0	5.177661	-2.979811	0.060986
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112	1	0	3.555538	-2.901899	-0.660433

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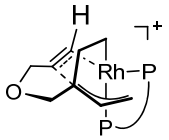

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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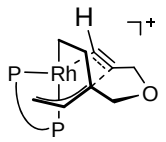
3	6	0	-1.022244	-1.786461	2.625332
4	6	0	-2.210908	-1.598561	3.319195
5	6	0	-1.961922	-0.393600	-0.788588
6	6	0	-1.294527	0.729227	-1.322836
7	6	0	-1.227525	0.881376	-2.720802
8	6	0	-1.877262	-0.005721	-3.562180
9	1	0	-0.202948	-2.297547	3.116981
10	1	0	-2.298410	-1.972809	4.336955
11	1	0	-0.666556	1.702140	-3.153737
12	1	0	-1.837464	0.149261	-4.638210
13	6	0	-4.343337	0.286973	0.776132
14	6	0	-4.562767	-0.753818	3.561951
15	6	0	-5.521469	0.299840	2.999854
16	6	0	-5.686789	0.098187	1.492050
17	1	0	-4.082314	1.355311	0.793335
18	1	0	-4.440308	0.028580	-0.281930
19	1	0	-5.080808	-1.724152	3.601847
20	1	0	-4.293448	-0.518974	4.599132
21	1	0	-6.486851	0.235675	3.514380
22	1	0	-5.122989	1.305522	3.191559
23	1	0	-6.075326	-0.912024	1.299043

24	1	0	-6.420207	0.800907	1.079974
25	6	0	-3.294045	-0.928435	2.743108
26	6	0	-3.190882	-0.480181	1.411462
27	6	0	-3.268019	-2.039268	-4.033508
28	6	0	-4.308648	-2.952783	-3.381660
29	6	0	-3.704220	-3.592940	-2.131352
30	6	0	-3.342278	-2.524003	-1.091419
31	1	0	-3.716401	-1.448622	-4.842089
32	1	0	-5.199728	-2.370968	-3.107450
33	1	0	-4.635727	-3.715154	-4.097527
34	1	0	-4.400018	-4.309969	-1.680543
35	1	0	-2.804841	-4.157436	-2.410490
36	1	0	-4.267392	-2.181955	-0.606274
37	1	0	-2.742613	-2.972403	-0.293474
38	1	0	-2.495287	-2.662193	-4.509551
39	6	0	-2.610032	-1.314345	-1.662692
40	6	0	-2.585868	-1.100907	-3.052987
41	6	0	-0.996370	2.260178	1.315185
42	6	0	-2.091391	3.135020	1.428500
43	6	0	-0.423724	1.748148	2.486664
44	6	0	-2.601041	3.473817	2.682297
45	1	0	-2.538096	3.571781	0.541772
46	6	0	-0.931334	2.089523	3.740588
47	1	0	0.415548	1.069903	2.414131
48	6	0	-2.020671	2.955651	3.842089
49	1	0	-3.443809	4.155847	2.751219
50	1	0	-0.474452	1.679479	4.636857
51	1	0	-2.410769	3.231290	4.817675
52	6	0	-0.491497	3.573069	-1.119383
53	6	0	0.349252	4.610008	-0.678702
54	6	0	-1.547210	3.892068	-1.989905
55	6	0	0.166791	5.918005	-1.125417
56	1	0	1.138930	4.401817	0.034517
57	6	0	-1.727102	5.203553	-2.436556
58	1	0	-2.244062	3.128213	-2.314031
59	6	0	-0.867661	6.217648	-2.014149
60	1	0	0.830284	6.702870	-0.773859
61	1	0	-2.548575	5.429198	-3.110615
62	1	0	-1.009806	7.235919	-2.364131
63	6	0	0.441443	-2.933528	-0.688794
64	6	0	0.727846	-2.891336	-2.058510
65	6	0	-0.055168	-4.130677	-0.141227
66	6	0	0.546319	-4.019563	-2.864305
67	1	0	1.079881	-1.970542	-2.504845

68	6	0	-0.236212	-5.256855	-0.943066
69	1	0	-0.293064	-4.185775	0.917026
70	6	0	0.069828	-5.205756	-2.306940
71	1	0	0.778717	-3.968284	-3.924420
72	1	0	-0.613863	-6.175686	-0.503335
73	1	0	-0.065362	-6.086063	-2.928884
74	6	0	1.940209	-2.160514	1.635766
75	6	0	2.166009	-1.523014	2.869920
76	6	0	2.758803	-3.252592	1.299584
77	6	0	3.145061	-1.983637	3.750465
78	1	0	1.563642	-0.668641	3.160156
79	6	0	3.749152	-3.705608	2.175608
80	1	0	2.619515	-3.768346	0.356066
81	6	0	3.942577	-3.078517	3.406437
82	1	0	3.283507	-1.486996	4.706998
83	1	0	4.361212	-4.558293	1.895085
84	1	0	4.704160	-3.438266	4.092192
85	15	0	-0.255492	1.906129	-0.346494
86	15	0	0.738454	-1.463305	0.405037
87	6	0	4.142211	0.541651	-1.168666
88	6	0	5.147696	0.176765	1.323507
89	6	0	5.432286	-0.229999	-0.896927
90	6	0	4.249311	2.037969	-1.469024
91	6	0	2.887021	2.656387	-1.122268
92	45	0	1.856371	0.928544	-0.461648
93	1	0	5.056731	2.467025	-0.869565
94	1	0	4.523360	2.178735	-2.524157
95	1	0	2.361457	3.107917	-1.964538
96	1	0	2.966557	3.387638	-0.319331
97	1	0	5.562860	0.739471	2.165207
98	1	0	4.991561	-0.867450	1.637505
99	1	0	6.124733	-0.073276	-1.731345
100	1	0	5.219687	-1.308201	-0.812469
101	6	0	3.167391	-0.191648	-1.986486
102	6	0	2.293800	0.378711	-2.885135
103	1	0	2.393283	1.398175	-3.232985
104	1	0	1.607243	-0.245582	-3.446201
105	1	0	3.137355	-1.270714	-1.847395
106	6	0	3.842695	0.776601	0.914378
107	6	0	2.775780	1.371153	1.307397
108	1	0	2.440022	1.907869	2.182465
109	8	0	6.075293	0.249657	0.261224

(*R*)-TS2-H



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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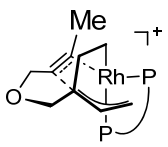
3	6	0	-1.295086	-1.776156	2.596577
4	6	0	-2.590948	-1.683408	3.085579
5	6	0	-1.796378	-0.538838	-0.971455
6	6	0	-1.191572	0.646400	-1.444717
7	6	0	-1.012664	0.807114	-2.832785
8	6	0	-1.466460	-0.149184	-3.727061
9	1	0	-0.528613	-2.205028	3.230332
10	1	0	-2.808660	-2.042395	4.089149
11	1	0	-0.517312	1.690130	-3.221420
12	1	0	-1.340119	0.014060	-4.795118
13	6	0	-4.446561	-0.077792	0.163641
14	6	0	-5.012819	-1.048635	2.924664
15	6	0	-5.957787	-0.104108	2.176949
16	6	0	-5.864431	-0.367788	0.672893
17	1	0	-4.290737	1.010524	0.162483
18	1	0	-4.354026	-0.384116	-0.881766
19	1	0	-5.445217	-2.060822	2.925030
20	1	0	-4.931361	-0.760606	3.980049
21	1	0	-6.983153	-0.239751	2.538729
22	1	0	-5.681183	0.939116	2.382539
23	1	0	-6.128940	-1.415367	0.469441
24	1	0	-6.581464	0.249793	0.119710
25	6	0	-3.620121	-1.127799	2.320692
26	6	0	-3.342214	-0.704233	1.006452
27	6	0	-2.527600	-2.345188	-4.313841
28	6	0	-3.505802	-3.385598	-3.763366
29	6	0	-2.968986	-3.931931	-2.439908
30	6	0	-2.877106	-2.817103	-1.390169
31	1	0	-2.959707	-1.817458	-5.173232
32	1	0	-4.490999	-2.926326	-3.601657
33	1	0	-3.646665	-4.188161	-4.495935
34	1	0	-3.610476	-4.733478	-2.055881

35	1	0	-1.975931	-4.371549	-2.602188
36	1	0	-3.892000	-2.587044	-1.035870
37	1	0	-2.335330	-3.179784	-0.511797
38	1	0	-1.635128	-2.862512	-4.697625
39	6	0	-2.228409	-1.533379	-1.896800
40	6	0	-2.078202	-1.325497	-3.280483
41	6	0	-1.261995	2.197907	1.191817
42	6	0	-2.523398	2.816672	1.155203
43	6	0	-0.666097	1.952110	2.433894
44	6	0	-3.181411	3.149018	2.338378
45	1	0	-2.982846	3.064191	0.203507
46	6	0	-1.323633	2.289021	3.618945
47	1	0	0.323143	1.510438	2.469286
48	6	0	-2.584229	2.884081	3.573860
49	1	0	-4.153681	3.631822	2.294786
50	1	0	-0.846698	2.094401	4.575615
51	1	0	-3.093557	3.154873	4.494257
52	6	0	-0.622237	3.546813	-1.169917
53	6	0	0.048009	4.648519	-0.609594
54	6	0	-1.584714	3.791206	-2.164113
55	6	0	-0.194136	5.944012	-1.063141
56	1	0	0.740515	4.502442	0.211221
57	6	0	-1.825900	5.090631	-2.617509
58	1	0	-2.167330	2.979080	-2.581409
59	6	0	-1.124566	6.168846	-2.079364
60	1	0	0.339430	6.777612	-0.615650
61	1	0	-2.572902	5.254919	-3.388941
62	1	0	-1.312934	7.177329	-2.435727
63	6	0	0.809934	-2.883703	-0.351733
64	6	0	1.390290	-2.885980	-1.626451
65	6	0	0.278343	-4.084998	0.152131
66	6	0	1.450575	-4.062833	-2.379800
67	1	0	1.793122	-1.966935	-2.032945
68	6	0	0.342588	-5.258830	-0.597549
69	1	0	-0.181070	-4.104403	1.136148
70	6	0	0.931883	-5.251029	-1.866013
71	1	0	1.904930	-4.048201	-3.366798
72	1	0	-0.066027	-6.180065	-0.191767
73	1	0	0.984485	-6.167110	-2.447553
74	6	0	1.790500	-1.869395	2.149201
75	6	0	1.723391	-1.166064	3.367307
76	6	0	2.765382	-2.873059	2.019907
77	6	0	2.582854	-1.471818	4.423087
78	1	0	0.979635	-0.387490	3.504444

79	6	0	3.633778	-3.170350	3.074354
80	1	0	2.847651	-3.435078	1.096158
81	6	0	3.544822	-2.474916	4.280151
82	1	0	2.497891	-0.927593	5.359775
83	1	0	4.373878	-3.956191	2.951136
84	1	0	4.214515	-2.712372	5.101451
85	15	0	-0.334170	1.890611	-0.379331
86	15	0	0.773619	-1.346181	0.686371
87	6	0	4.286130	1.012853	-0.097038
88	6	0	4.580821	-0.613437	-2.262200
89	6	0	5.529291	0.161300	-0.345105
90	6	0	4.277873	2.441193	-0.638947
91	6	0	2.806311	2.857045	-0.764203
92	45	0	1.848572	1.072116	-0.165556
93	1	0	4.797895	2.464954	-1.600311
94	1	0	4.841426	3.091066	0.046221
95	1	0	2.540407	3.679993	-0.103742
96	1	0	2.512932	3.113657	-1.782491
97	1	0	4.669674	-0.586187	-3.352631
98	1	0	4.480698	-1.665158	-1.941379
99	1	0	6.405723	0.695171	0.038584
100	1	0	5.444889	-0.801641	0.184130
101	6	0	3.691687	0.814005	1.226372
102	6	0	3.029913	1.761596	1.973892
103	1	0	3.057664	2.820651	1.753817
104	1	0	2.659503	1.481075	2.954056
105	1	0	3.775104	-0.186964	1.642341
106	6	0	3.371949	0.152374	-1.837517
107	6	0	2.165132	0.486366	-2.099584
108	1	0	1.471145	0.459799	-2.926858
109	8	0	5.749070	-0.038404	-1.723346

(*S*)-TS2-Me



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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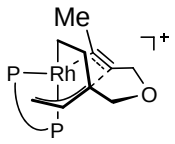
3	6	0	-1.104521	-1.751207	2.641185
4	6	0	-2.274463	-1.502169	3.347135
5	6	0	-2.023250	-0.341864	-0.774732
6	6	0	-1.324494	0.746104	-1.342941
7	6	0	-1.299341	0.879546	-2.743977
8	6	0	-2.012258	0.012423	-3.554624
9	1	0	-0.303610	-2.296130	3.127083
10	1	0	-2.368263	-1.865184	4.368428
11	1	0	-0.720924	1.671638	-3.205651
12	1	0	-2.002939	0.156944	-4.632830
13	6	0	-4.341452	0.472070	0.816521
14	6	0	-4.579056	-0.542386	3.610781
15	6	0	-5.485974	0.560768	3.057895
16	6	0	-5.682487	0.362435	1.553483
17	1	0	-4.023033	1.524708	0.816535
18	1	0	-4.468544	0.206935	-0.236783
19	1	0	-5.147844	-1.483635	3.656989
20	1	0	-4.286545	-0.322183	4.644876
21	1	0	-6.446547	0.550903	3.585175
22	1	0	-5.030356	1.543609	3.240220
23	1	0	-6.129942	-0.625330	1.371767
24	1	0	-6.381436	1.102981	1.147767
25	6	0	-3.330565	-0.783930	2.778325
26	6	0	-3.220824	-0.347918	1.443287
27	6	0	-3.502683	-1.965708	-3.956916
28	6	0	-4.566424	-2.816024	-3.259025
29	6	0	-3.951725	-3.475648	-2.024166
30	6	0	-3.495617	-2.418149	-1.009310
31	1	0	-3.946071	-1.364482	-4.760402
32	1	0	-5.414413	-2.184486	-2.959373
33	1	0	-4.959455	-3.566414	-3.954098
34	1	0	-4.667741	-4.149829	-1.540165
35	1	0	-3.095415	-4.091159	-2.329632
36	1	0	-4.381813	-2.031126	-0.487039
37	1	0	-2.883114	-2.890310	-0.235010
38	1	0	-2.777191	-2.633336	-4.446592
39	6	0	-2.733278	-1.245901	-1.618474
40	6	0	-2.746371	-1.048498	-3.011128
41	6	0	-0.958336	2.332335	1.231898
42	6	0	-1.971172	3.304212	1.320481
43	6	0	-0.478021	1.758335	2.414474
44	6	0	-2.486410	3.679513	2.561953
45	1	0	-2.349710	3.787236	0.426607

46	6	0	-0.992409	2.132138	3.655654
47	1	0	0.297715	1.007585	2.357067
48	6	0	-1.997342	3.097528	3.733282
49	1	0	-3.262944	4.437600	2.611711
50	1	0	-0.607054	1.670671	4.560481
51	1	0	-2.391957	3.399772	4.699180
52	6	0	-0.367140	3.548533	-1.233988
53	6	0	0.552412	4.543829	-0.860247
54	6	0	-1.434021	3.908561	-2.075030
55	6	0	0.435042	5.846637	-1.343548
56	1	0	1.356401	4.308908	-0.171888
57	6	0	-1.548535	5.213804	-2.559533
58	1	0	-2.190425	3.181659	-2.346456
59	6	0	-0.611650	6.183979	-2.203565
60	1	0	1.159663	6.598059	-1.043216
61	1	0	-2.379742	5.469859	-3.210406
62	1	0	-0.702918	7.197660	-2.582620
63	6	0	0.254285	-3.014531	-0.658562
64	6	0	0.480737	-3.013808	-2.040395
65	6	0	-0.262917	-4.180681	-0.064311
66	6	0	0.224973	-4.152623	-2.810590
67	1	0	0.844407	-2.119371	-2.528472
68	6	0	-0.518502	-5.317136	-0.830451
69	1	0	-0.457853	-4.204174	1.003766
70	6	0	-0.268721	-5.308308	-2.206500
71	1	0	0.413268	-4.132535	-3.880453
72	1	0	-0.910453	-6.210903	-0.353174
73	1	0	-0.461391	-6.196644	-2.801268
74	6	0	1.827153	-2.261930	1.625310
75	6	0	2.103516	-1.602362	2.836882
76	6	0	2.587415	-3.400339	1.307154
77	6	0	3.074612	-2.083970	3.714730
78	1	0	1.545288	-0.713343	3.111857
79	6	0	3.569512	-3.875987	2.180597
80	1	0	2.409351	-3.933081	0.379703
81	6	0	3.813392	-3.224812	3.389802
82	1	0	3.252948	-1.568175	4.654388
83	1	0	4.136056	-4.764096	1.914708
84	1	0	4.568901	-3.601148	4.073349
85	15	0	-0.211597	1.895444	-0.409353
86	15	0	0.640987	-1.533771	0.397611
87	6	0	4.046354	0.252144	-1.380126
88	6	0	5.145952	-0.221088	1.032631
89	6	0	5.288784	-0.620125	-1.194411

90	6	0	4.256644	1.733525	-1.699331
91	6	0	2.976466	2.456788	-1.259570
92	45	0	1.873636	0.811685	-0.512795
93	1	0	5.136341	2.094065	-1.159456
94	1	0	4.465598	1.850103	-2.772034
95	1	0	2.426369	2.941593	-2.066373
96	1	0	3.166451	3.184668	-0.471556
97	1	0	5.644474	0.289397	1.863449
98	1	0	4.917420	-1.254121	1.338973
99	1	0	5.938744	-0.503237	-2.068528
100	1	0	4.997382	-1.679871	-1.109661
101	6	0	2.964220	-0.405071	-2.121758
102	6	0	2.062310	0.227213	-2.947582
103	1	0	2.208352	1.234068	-3.315240
104	1	0	1.286446	-0.346372	-3.442052
105	1	0	2.868275	-1.478219	-1.972173
106	6	0	3.885524	0.502950	0.687242
107	6	0	2.966730	1.246625	1.199750
108	8	0	6.029818	-0.211273	-0.069800
109	6	0	2.841134	2.109163	2.410341
110	1	0	2.381219	3.072293	2.166513
111	1	0	2.214650	1.646640	3.178693
112	1	0	3.828404	2.299469	2.848604

(*R*)-TS2-Me



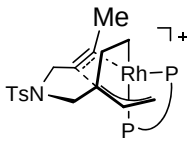
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.043161	-0.846334	0.568453
2	6	0	-0.976104	-1.433207	1.290969
3	6	0	-1.241994	-1.966047	2.561315
4	6	0	-2.505424	-1.857372	3.126641
5	6	0	-1.890272	-0.510449	-0.892033
6	6	0	-1.283291	0.674071	-1.366698
7	6	0	-1.214484	0.881022	-2.755875
8	6	0	-1.762525	-0.027212	-3.646834
9	1	0	-0.464683	-2.472883	3.118902

10	1	0	-2.685581	-2.279840	4.112882
11	1	0	-0.727883	1.763249	-3.151188
12	1	0	-1.716212	0.176555	-4.714529
13	6	0	-4.448061	-0.002546	0.415705
14	6	0	-4.900564	-1.108976	3.147889
15	6	0	-5.842310	-0.083996	2.510290
16	6	0	-5.845594	-0.265589	0.991178
17	1	0	-4.248332	1.077629	0.457346
18	1	0	-4.427088	-0.261018	-0.646704
19	1	0	-5.376255	-2.101011	3.115883
20	1	0	-4.748237	-0.887362	4.211485
21	1	0	-6.850627	-0.196470	2.924250
22	1	0	-5.505868	0.932707	2.755083
23	1	0	-6.165343	-1.288904	0.747271
24	1	0	-6.566192	0.409800	0.515613
25	6	0	-3.548236	-1.207615	2.460964
26	6	0	-3.324519	-0.713186	1.161278
27	6	0	-2.910784	-2.178156	-4.232028
28	6	0	-3.868890	-3.220282	-3.650079
29	6	0	-3.253632	-3.820579	-2.385696
30	6	0	-3.065306	-2.744402	-1.309085
31	1	0	-3.392013	-1.610407	-5.038186
32	1	0	-4.832167	-2.750853	-3.406203
33	1	0	-4.074371	-3.994931	-4.397332
34	1	0	-3.884112	-4.622372	-1.984152
35	1	0	-2.283445	-4.272907	-2.631028
36	1	0	-4.049199	-2.501247	-0.883017
37	1	0	-2.479923	-3.150691	-0.479364
38	1	0	-2.059452	-2.697336	-4.698083
39	6	0	-2.415946	-1.460951	-1.816129
40	6	0	-2.364360	-1.207048	-3.198964
41	6	0	-1.273230	2.166291	1.276275
42	6	0	-2.458659	2.922085	1.287584
43	6	0	-0.759440	1.709048	2.495143
44	6	0	-3.111714	3.198791	2.488965
45	1	0	-2.865639	3.316929	0.363112
46	6	0	-1.411644	1.985355	3.697287
47	1	0	0.158602	1.136613	2.498271
48	6	0	-2.589743	2.733200	3.697791
49	1	0	-4.021280	3.792836	2.479507
50	1	0	-0.996773	1.621043	4.633063
51	1	0	-3.092927	2.960366	4.633300
52	6	0	-0.667400	3.557901	-1.087083
53	6	0	0.055008	4.648947	-0.574585

54	6	0	-1.693405	3.822841	-2.011592
55	6	0	-0.194080	5.949522	-1.011276
56	1	0	0.795887	4.491943	0.198559
57	6	0	-1.942568	5.126090	-2.448419
58	1	0	-2.319929	3.022748	-2.385785
59	6	0	-1.186376	6.192075	-1.962073
60	1	0	0.383096	6.772773	-0.600184
61	1	0	-2.739047	5.303299	-3.165636
62	1	0	-1.380538	7.203748	-2.306084
63	6	0	0.736900	-2.843276	-0.593784
64	6	0	1.308601	-2.716308	-1.866014
65	6	0	0.193078	-4.083469	-0.214197
66	6	0	1.343185	-3.805156	-2.742506
67	1	0	1.733908	-1.766728	-2.166900
68	6	0	0.230169	-5.169725	-1.087659
69	1	0	-0.251807	-4.202890	0.769466
70	6	0	0.806750	-5.032902	-2.354640
71	1	0	1.791445	-3.692495	-3.725930
72	1	0	-0.187526	-6.123985	-0.779008
73	1	0	0.838551	-5.881300	-3.032434
74	6	0	1.812199	-2.103281	1.958858
75	6	0	1.794641	-1.538283	3.249311
76	6	0	2.775710	-3.089362	1.686360
77	6	0	2.688169	-1.961221	4.234092
78	1	0	1.068063	-0.770906	3.497711
79	6	0	3.679328	-3.502917	2.669589
80	1	0	2.822019	-3.549211	0.705073
81	6	0	3.637909	-2.944763	3.947196
82	1	0	2.641300	-1.521157	5.226476
83	1	0	4.409323	-4.272345	2.433937
84	1	0	4.334765	-3.272930	4.712780
85	15	0	-0.357493	1.891603	-0.317256
86	15	0	0.751806	-1.422332	0.593593
87	6	0	4.255063	1.042806	0.310033
88	6	0	4.780383	-0.588388	-1.787981
89	6	0	5.519905	0.190463	0.208881
90	6	0	4.316390	2.476315	-0.210238
91	6	0	2.869965	2.890107	-0.506404
92	45	0	1.868442	1.076154	-0.102659
93	1	0	4.946895	2.508933	-1.102549
94	1	0	4.793803	3.116734	0.545696
95	1	0	2.516053	3.677909	0.154590
96	1	0	2.705078	3.200452	-1.539013
97	1	0	4.989696	-0.584329	-2.863176

98	1	0	4.628445	-1.632402	-1.463497
99	1	0	6.345220	0.728647	0.688155
100	1	0	5.372996	-0.768426	0.731303
101	6	0	3.500755	0.818171	1.540582
102	6	0	2.725806	1.735981	2.209341
103	1	0	2.754781	2.799829	2.016367
104	1	0	2.244517	1.431982	3.132094
105	1	0	3.552131	-0.186315	1.949268
106	6	0	3.552520	0.215655	-1.519861
107	6	0	2.463376	0.636440	-2.055230
108	8	0	5.893820	-0.022760	-1.132893
109	6	0	1.945033	0.798987	-3.441033
110	1	0	1.080136	0.157512	-3.626380
111	1	0	1.630369	1.834011	-3.616228
112	1	0	2.727432	0.556484	-4.170961

(*S*)-TS2-N



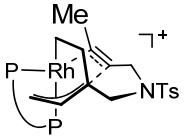
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.315597	-0.388003	0.937341
2	6	0	-2.216395	-1.075583	1.509057
3	6	0	-2.260437	-1.401191	2.872292
4	6	0	-3.338670	-1.014792	3.657439
5	6	0	-3.426307	-0.223854	-0.557688
6	6	0	-2.740118	0.774378	-1.284385
7	6	0	-2.871420	0.805795	-2.685592
8	6	0	-3.715719	-0.074595	-3.340990
9	1	0	-1.451565	-1.959004	3.329206
10	1	0	-3.354203	-1.283829	4.711484
11	1	0	-2.310803	1.526262	-3.270474
12	1	0	-3.824686	-0.008381	-4.421386
13	6	0	-5.530395	0.860063	1.157432
14	6	0	-5.547215	0.112602	4.043567
15	6	0	-6.451385	1.209903	3.474004
16	6	0	-6.799342	0.889004	2.018779
17	1	0	-5.163786	1.889537	1.034990

18	1	0	-5.770595	0.514852	0.147989
19	1	0	-6.153211	-0.785777	4.236276
20	1	0	-5.142319	0.411521	5.018388
21	1	0	-7.356071	1.300456	4.085694
22	1	0	-5.935378	2.178758	3.519843
23	1	0	-7.306783	-0.085190	1.970981
24	1	0	-7.498829	1.627566	1.610266
25	6	0	-4.401229	-0.278601	3.124905
26	6	0	-4.397414	0.032169	1.751167
27	6	0	-5.327985	-1.994841	-3.421225
28	6	0	-6.335835	-2.744845	-2.547112
29	6	0	-5.610879	-3.337803	-1.338347
30	6	0	-5.009047	-2.228819	-0.464519
31	1	0	-5.838274	-1.429591	-4.211110
32	1	0	-7.122454	-2.056915	-2.206836
33	1	0	-6.830268	-3.526239	-3.134992
34	1	0	-6.291643	-3.943630	-0.729255
35	1	0	-4.814634	-4.009261	-1.685204
36	1	0	-5.818217	-1.757828	0.111463
37	1	0	-4.338388	-2.668808	0.279949
38	1	0	-4.691621	-2.727792	-3.940491
39	6	0	-4.267878	-1.147582	-1.244258
40	6	0	-4.430072	-1.052351	-2.638402
41	6	0	-1.979421	2.503836	1.099445
42	6	0	-2.941011	3.523983	1.212840
43	6	0	-1.379913	2.016670	2.266374
44	6	0	-3.294620	4.028493	2.464670
45	1	0	-3.404192	3.943408	0.326594
46	6	0	-1.731324	2.521942	3.518224
47	1	0	-0.640635	1.231305	2.191051
48	6	0	-2.689384	3.531308	3.620901
49	1	0	-4.034640	4.820914	2.532849
50	1	0	-1.255802	2.127567	4.411856
51	1	0	-2.957605	3.933684	4.593613
52	6	0	-1.577599	3.496563	-1.501074
53	6	0	-0.546014	4.432148	-1.311150
54	6	0	-2.702178	3.885950	-2.248593
55	6	0	-0.617557	5.703434	-1.879637
56	1	0	0.314478	4.174958	-0.703518
57	6	0	-2.770223	5.159040	-2.819699
58	1	0	-3.537389	3.208075	-2.381043
59	6	0	-1.727038	6.068325	-2.644340
60	1	0	0.193189	6.408836	-1.721347
61	1	0	-3.647446	5.438561	-3.396289

62	1	0	-1.782624	7.057046	-3.090333
63	6	0	-1.296030	-3.058001	-0.363476
64	6	0	-1.287160	-3.193464	-1.757141
65	6	0	-1.744616	-4.142366	0.413355
66	6	0	-1.684421	-4.388828	-2.364701
67	1	0	-0.985492	-2.360537	-2.378526
68	6	0	-2.143177	-5.333768	-0.190596
69	1	0	-1.774839	-4.059269	1.495649
70	6	0	-2.106332	-5.463296	-1.582731
71	1	0	-1.661513	-4.476297	-3.447443
72	1	0	-2.479472	-6.162965	0.425459
73	1	0	-2.408365	-6.395453	-2.051588
74	6	0	0.549074	-2.149479	1.640974
75	6	0	0.941914	-1.417656	2.775919
76	6	0	1.271138	-3.313816	1.325466
77	6	0	1.991747	-1.852584	3.585388
78	1	0	0.413979	-0.509646	3.048579
79	6	0	2.332166	-3.741884	2.127729
80	1	0	1.002848	-3.903038	0.455260
81	6	0	2.692883	-3.017370	3.263963
82	1	0	2.260461	-1.280499	4.469457
83	1	0	2.874079	-4.644611	1.861475
84	1	0	3.512425	-3.355327	3.891207
85	15	0	-1.452406	1.897574	-0.572039
86	15	0	-0.730902	-1.494573	0.468745
87	6	0	2.517531	-0.173885	-1.899048
88	6	0	3.893471	-0.458397	0.451174
89	6	0	3.695301	-1.133564	-1.810095
90	6	0	2.772300	1.249139	-2.400626
91	6	0	1.613114	2.109918	-1.877813
92	45	0	0.513906	0.641206	-0.824412
93	1	0	3.739071	1.594550	-2.025710
94	1	0	2.836230	1.240282	-3.497730
95	1	0	0.990755	2.557474	-2.653436
96	1	0	1.959668	2.894649	-1.206274
97	1	0	4.493543	0.125120	1.159921
98	1	0	3.656937	-1.426028	0.917541
99	1	0	4.199721	-1.173736	-2.780098
100	1	0	3.336136	-2.146368	-1.567745
101	6	0	1.300831	-0.810172	-2.430472
102	6	0	0.353331	-0.194135	-3.211830
103	1	0	0.515057	0.763971	-3.687274
104	1	0	-0.513777	-0.749157	-3.551852
105	1	0	1.152085	-1.853116	-2.160903

106	6	0	2.650376	0.297645	0.143403
107	6	0	1.842292	1.150012	0.674432
108	1	0	9.005317	2.375340	-0.923455
109	6	0	8.607022	1.590316	-0.285669
110	6	0	9.014881	1.518530	1.057822
111	6	0	7.712394	0.668276	-0.817766
112	6	0	10.012050	2.508939	1.608373
113	6	0	8.496913	0.493146	1.859791
114	6	0	7.207880	-0.340130	0.010111
115	1	0	7.416461	0.717079	-1.860415
116	1	0	9.788394	3.528691	1.276288
117	1	0	11.026592	2.272495	1.262799
118	1	0	10.026213	2.500617	2.702238
119	6	0	7.597612	-0.442008	1.345731
120	1	0	8.807628	0.417502	2.898445
121	16	0	6.084065	-1.546760	-0.672322
122	1	0	7.213924	-1.248780	1.961036
123	8	0	5.896433	-2.617587	0.316213
124	8	0	6.460351	-1.851197	-2.054270
125	7	0	4.634680	-0.628067	-0.804909
126	6	0	1.906771	2.123991	1.803034
127	1	0	1.345366	3.035858	1.580578
128	1	0	1.480949	1.701686	2.719299
129	1	0	2.947978	2.396954	2.014150

(*R*)-TS2-N



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	-2.843780	-1.816499	2.569148
4	6	0	-4.123454	-1.603510	3.064487
5	6	0	-3.196566	-0.381530	-0.930579
6	6	0	-2.483743	0.744815	-1.397426
7	6	0	-2.324192	0.907441	-2.785679
8	6	0	-2.877792	0.010103	-3.683707

9	1	0	-2.139556	-2.374806	3.172848
10	1	0	-4.387943	-1.998617	4.043019
11	1	0	-1.772350	1.753450	-3.174477
12	1	0	-2.757664	0.179990	-4.751553
13	6	0	-5.768881	0.359304	0.235261
14	6	0	-6.450525	-0.670456	2.950708
15	6	0	-7.274203	0.415349	2.252721
16	6	0	-7.211477	0.213493	0.737421
17	1	0	-5.486558	1.421062	0.278331
18	1	0	-5.710934	0.084359	-0.821848
19	1	0	-6.999761	-1.623059	2.902953
20	1	0	-6.338400	-0.445869	4.018700
21	1	0	-8.308828	0.387124	2.612620
22	1	0	-6.873186	1.406550	2.505040
23	1	0	-7.596196	-0.785430	0.486594
24	1	0	-7.851336	0.935786	0.217326
25	6	0	-5.075852	-0.883109	2.338530
26	6	0	-4.746573	-0.426843	1.047401
27	6	0	-4.141595	-2.071428	-4.280840
28	6	0	-5.217834	-3.011123	-3.732698
29	6	0	-4.730674	-3.622109	-2.418436
30	6	0	-4.512333	-2.533949	-1.359325
31	1	0	-4.521676	-1.495515	-5.133841
32	1	0	-6.149802	-2.454899	-3.559834
33	1	0	-5.444789	-3.788361	-4.470983
34	1	0	-5.449495	-4.355586	-2.035005
35	1	0	-3.790347	-4.161489	-2.593890
36	1	0	-5.493747	-2.200912	-0.992445
37	1	0	-4.005657	-2.962705	-0.489678
38	1	0	-3.308022	-2.673644	-4.673126
39	6	0	-3.737183	-1.319225	-1.859709
40	6	0	-3.585794	-1.111999	-3.242566
41	6	0	-2.528323	2.344616	1.196352
42	6	0	-3.619811	3.229021	1.139431
43	6	0	-2.150347	1.832401	2.444223
44	6	0	-4.312314	3.579121	2.299652
45	1	0	-3.924736	3.667060	0.195927
46	6	0	-2.842773	2.180652	3.603886
47	1	0	-1.308523	1.155918	2.505686
48	6	0	-3.925829	3.058034	3.535666
49	1	0	-5.146918	4.271642	2.235421
50	1	0	-2.533668	1.769019	4.560696
51	1	0	-4.459086	3.340643	4.438880
52	6	0	-1.725013	3.569073	-1.226458

53	6	0	-0.872134	4.630946	-0.886446
54	6	0	-2.790068	3.835881	-2.108036
55	6	0	-1.045406	5.901418	-1.437756
56	1	0	-0.077072	4.480906	-0.170776
57	6	0	-2.963104	5.106804	-2.658293
58	1	0	-3.497987	3.057312	-2.366233
59	6	0	-2.086519	6.142783	-2.333565
60	1	0	-0.366523	6.702275	-1.158947
61	1	0	-3.791635	5.284414	-3.338124
62	1	0	-2.221599	7.130367	-2.764862
63	6	0	-0.755994	-2.842941	-0.494822
64	6	0	-0.138222	-2.732362	-1.746861
65	6	0	-1.372824	-4.057602	-0.145737
66	6	0	-0.126522	-3.814231	-2.632299
67	1	0	0.340903	-1.801826	-2.025513
68	6	0	-1.360250	-5.136482	-1.029013
69	1	0	-1.854715	-4.163626	0.822005
70	6	0	-0.734618	-5.017421	-2.274441
71	1	0	0.361615	-3.716000	-3.598014
72	1	0	-1.833584	-6.071940	-0.744058
73	1	0	-0.719678	-5.861094	-2.958643
74	6	0	0.232919	-2.182143	2.116883
75	6	0	0.171615	-1.635442	3.413924
76	6	0	1.163040	-3.208418	1.878667
77	6	0	0.988591	-2.116647	4.437801
78	1	0	-0.525660	-0.833172	3.634888
79	6	0	1.992109	-3.679068	2.901035
80	1	0	1.243604	-3.653714	0.892937
81	6	0	1.905084	-3.140229	4.184739
82	1	0	0.908947	-1.689192	5.433627
83	1	0	2.701614	-4.473710	2.688770
84	1	0	2.543468	-3.512758	4.980414
85	15	0	-1.546949	1.946077	-0.333199
86	15	0	-0.713038	-1.433809	0.703707
87	6	0	2.938849	0.783280	0.671006
88	6	0	3.448765	-0.928772	-1.419209
89	6	0	4.135531	-0.158006	0.709472
90	6	0	3.146203	2.208453	0.164924
91	6	0	1.758921	2.732451	-0.226518
92	45	0	0.596142	0.995835	0.076802
93	1	0	3.836727	2.194999	-0.681735
94	1	0	3.616877	2.808820	0.957287
95	1	0	1.417062	3.531840	0.429482
96	1	0	1.694118	3.071448	-1.260948

97	1	0	3.702454	-0.960869	-2.482761
98	1	0	3.160098	-1.946487	-1.104440
99	1	0	4.937686	0.337124	1.270960
100	1	0	3.875681	-1.087751	1.236278
101	6	0	2.073051	0.628871	1.843146
102	6	0	1.324813	1.601080	2.458970
103	1	0	1.435929	2.660439	2.272608
104	1	0	0.750695	1.330300	3.338287
105	1	0	2.017570	-0.375127	2.249376
106	6	0	2.319084	0.009586	-1.207028
107	6	0	1.308568	0.522194	-1.815318
108	1	0	9.448398	0.349202	2.204507
109	6	0	8.961020	0.434506	1.236984
110	6	0	9.402990	1.401397	0.324560
111	6	0	7.913232	-0.431491	0.921665
112	6	0	10.554848	2.317976	0.657706
113	6	0	8.764955	1.485538	-0.925647
114	6	0	7.296419	-0.318212	-0.324739
115	1	0	7.587736	-1.194972	1.620167
116	1	0	11.452795	2.036411	0.093207
117	1	0	10.325381	3.357812	0.399281
118	1	0	10.806369	2.278036	1.721469
119	6	0	7.719240	0.632503	-1.260255
120	1	0	9.100959	2.224959	-1.648182
121	16	0	5.982811	-1.443699	-0.758402
122	1	0	7.243967	0.689278	-2.233863
123	8	0	6.069608	-1.795075	-2.177354
124	8	0	5.900160	-2.486187	0.274066
125	7	0	4.597338	-0.421321	-0.654162
126	6	0	0.908763	0.725901	-3.234598
127	1	0	0.019797	0.143538	-3.489598
128	1	0	0.676961	1.780279	-3.424837
129	1	0	1.726144	0.432885	-3.905229

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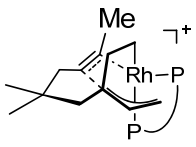

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-2.267916	-0.705081	0.682860
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3	6	0	-1.302865	-1.808556	2.615928
4	6	0	-2.487559	-1.611990	3.313674
5	6	0	-2.243238	-0.390155	-0.791338
6	6	0	-1.584318	0.735536	-1.332328
7	6	0	-1.562805	0.902263	-2.729929
8	6	0	-2.236683	0.025002	-3.562546
9	1	0	-0.484545	-2.324323	3.104703
10	1	0	-2.575984	-1.988041	4.330758
11	1	0	-1.016697	1.728118	-3.171645
12	1	0	-2.230146	0.194079	-4.637212
13	6	0	-4.604032	0.313201	0.786826
14	6	0	-4.829661	-0.744019	3.565923
15	6	0	-5.773887	0.328749	3.015921
16	6	0	-5.947298	0.140814	1.507366
17	1	0	-4.326608	1.377323	0.806700
18	1	0	-4.710121	0.059964	-0.271628
19	1	0	-5.361894	-1.706995	3.597900
20	1	0	-4.554720	-0.522915	4.604669
21	1	0	-6.738489	0.275341	3.533280
22	1	0	-5.359037	1.326507	3.213884
23	1	0	-6.352371	-0.861913	1.309049
24	1	0	-6.671322	0.857640	1.102935
25	6	0	-3.565314	-0.928740	2.742511
26	6	0	-3.459782	-0.473479	1.413632
27	6	0	-3.636607	-2.006915	-4.016208
28	6	0	-4.666584	-2.918180	-3.344690
29	6	0	-4.032925	-3.572700	-2.116632
30	6	0	-3.635572	-2.515303	-1.077640
31	1	0	-4.100565	-1.408903	-4.810461
32	1	0	-5.545281	-2.331952	-3.041407
33	1	0	-5.018686	-3.672219	-4.057602
34	1	0	-4.720798	-4.289273	-1.652994
35	1	0	-3.145518	-4.140683	-2.425344
36	1	0	-4.544343	-2.172911	-0.562818
37	1	0	-3.015913	-2.975236	-0.301965
38	1	0	-2.879392	-2.631894	-4.514125
39	6	0	-2.913325	-1.303539	-1.657693
40	6	0	-2.926905	-1.078051	-3.045964
41	6	0	-1.268590	2.268761	1.282023
42	6	0	-2.320924	3.193457	1.403518
43	6	0	-0.756667	1.684374	2.446295

44	6	0	-2.841852	3.514855	2.657903
45	1	0	-2.726649	3.682571	0.525086
46	6	0	-1.276660	2.003440	3.700397
47	1	0	0.048192	0.966998	2.363847
48	6	0	-2.319832	2.924222	3.810300
49	1	0	-3.649136	4.238045	2.732433
50	1	0	-0.866035	1.533934	4.589867
51	1	0	-2.719279	3.184276	4.786451
52	6	0	-0.752721	3.571062	-1.155410
53	6	0	0.126554	4.596575	-0.767458
54	6	0	-1.843173	3.903295	-1.977160
55	6	0	-0.054910	5.904756	-1.215107
56	1	0	0.949824	4.378204	-0.096703
57	6	0	-2.021829	5.213878	-2.426596
58	1	0	-2.567939	3.149325	-2.261182
59	6	0	-1.126118	6.216388	-2.054428
60	1	0	0.639142	6.680210	-0.903735
61	1	0	-2.870585	5.448326	-3.062867
62	1	0	-1.267574	7.234292	-2.405816
63	6	0	0.118597	-3.002466	-0.672526
64	6	0	0.396892	-3.005561	-2.044786
65	6	0	-0.404146	-4.173275	-0.092449
66	6	0	0.183270	-4.150360	-2.818944
67	1	0	0.770953	-2.109894	-2.522094
68	6	0	-0.616443	-5.316369	-0.862047
69	1	0	-0.638175	-4.194906	0.967729
70	6	0	-0.317793	-5.309763	-2.228313
71	1	0	0.410491	-4.131934	-3.881270
72	1	0	-1.013599	-6.213322	-0.395065
73	1	0	-0.478000	-6.202703	-2.825862
74	6	0	1.639243	-2.210101	1.633604
75	6	0	1.901436	-1.524023	2.833769
76	6	0	2.397997	-3.359376	1.353616
77	6	0	2.855838	-1.990659	3.737318
78	1	0	1.345353	-0.625473	3.080509
79	6	0	3.363339	-3.820473	2.253527
80	1	0	2.232688	-3.911853	0.435593
81	6	0	3.591911	-3.143314	3.451133
82	1	0	3.023572	-1.453015	4.666617
83	1	0	3.927934	-4.718266	2.017231
84	1	0	4.334197	-3.508077	4.155225
85	15	0	-0.513047	1.906386	-0.374310
86	15	0	0.451850	-1.511080	0.388040
87	6	0	3.828549	0.462069	-1.456970

88	6	0	4.830391	-0.216850	1.029092
89	6	0	5.129001	-0.339263	-1.373893
90	6	0	3.895935	1.955686	-1.799161
91	6	0	2.604502	2.601527	-1.285816
92	45	0	1.613384	0.910344	-0.520513
93	1	0	4.776891	2.411728	-1.347143
94	1	0	4.015945	2.060029	-2.886787
95	1	0	1.996431	3.075909	-2.056923
96	1	0	2.799541	3.326905	-0.495909
97	1	0	5.205964	0.143707	1.996749
98	1	0	4.484837	-1.246560	1.191158
99	1	0	5.744986	-0.046696	-2.236363
100	1	0	4.891073	-1.401564	-1.508450
101	6	0	2.745814	-0.250214	-2.156675
102	6	0	1.780349	0.324810	-2.950651
103	1	0	1.857910	1.334530	-3.331849
104	1	0	1.017767	-0.292647	-3.411757
105	1	0	2.713180	-1.325990	-1.999413
106	6	0	3.662848	0.623103	0.639014
107	6	0	2.739240	1.362527	1.158695
108	6	0	5.923973	-0.188453	-0.053558
109	6	0	6.734762	1.120502	0.027418
110	1	0	7.385768	1.104951	0.909266
111	1	0	7.375717	1.246173	-0.852811
112	1	0	6.097299	2.005444	0.114062
113	6	0	6.888458	-1.376972	0.104039
114	1	0	7.642118	-1.378396	-0.691909
115	1	0	7.420385	-1.324505	1.060853
116	1	0	6.355572	-2.334492	0.066619
117	6	0	2.625440	2.235817	2.360429
118	1	0	2.421586	3.270898	2.060479
119	1	0	1.810897	1.939489	3.024609
120	1	0	3.561870	2.229819	2.931922

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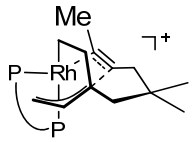


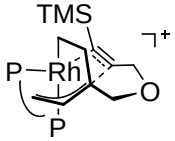
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-2.283514	-0.895068	0.475122
2	6	0	-1.242784	-1.430215	1.273485
3	6	0	-1.568652	-1.955757	2.532651
4	6	0	-2.869476	-1.893334	3.013693
5	6	0	-2.048472	-0.569586	-0.977369
6	6	0	-1.441177	0.624852	-1.427014
7	6	0	-1.270467	0.809714	-2.810557
8	6	0	-1.733733	-0.123454	-3.723716
9	1	0	-0.808975	-2.422194	3.147003
10	1	0	-3.095961	-2.310420	3.992670
11	1	0	-0.765120	1.690962	-3.183965
12	1	0	-1.612478	0.063983	-4.788552
13	6	0	-4.705346	-0.150165	0.159169
14	6	0	-5.290854	-1.253597	2.866697
15	6	0	-6.235572	-0.281475	2.154813
16	6	0	-6.125762	-0.472748	0.640912
17	1	0	-4.555598	0.937689	0.208367
18	1	0	-4.601075	-0.409897	-0.897785
19	1	0	-5.716846	-2.267350	2.817803
20	1	0	-5.219972	-1.013332	3.934791
21	1	0	-7.263361	-0.442059	2.499427
22	1	0	-5.969029	0.752591	2.412463
23	1	0	-6.381704	-1.511194	0.385519
24	1	0	-6.841933	0.165855	0.110865
25	6	0	-3.892724	-1.297433	2.271822
26	6	0	-3.604879	-0.807890	0.983122
27	6	0	-2.800248	-2.304381	-4.353895
28	6	0	-3.775351	-3.355846	-3.819804
29	6	0	-3.226457	-3.933316	-2.514747
30	6	0	-3.123299	-2.844062	-1.439466
31	1	0	-3.237839	-1.756862	-5.198043
32	1	0	-4.758249	-2.899053	-3.638079
33	1	0	-3.924404	-4.141019	-4.569536
34	1	0	-3.864619	-4.743542	-2.143356
35	1	0	-2.235310	-4.369226	-2.697783
36	1	0	-4.133942	-2.625393	-1.066902
37	1	0	-2.570333	-3.228024	-0.577079
38	1	0	-1.910927	-2.813804	-4.755163
39	6	0	-2.481930	-1.546643	-1.921346
40	6	0	-2.342875	-1.308840	-3.300844
41	6	0	-1.676367	2.140410	1.184507
42	6	0	-2.889292	2.844764	1.083999
43	6	0	-1.242139	1.735221	2.451751

44	6	0	-3.646293	3.121744	2.222536
45	1	0	-3.237034	3.201320	0.120190
46	6	0	-1.998573	2.012006	3.591441
47	1	0	-0.304265	1.204150	2.545762
48	6	0	-3.202966	2.707470	3.480521
49	1	0	-4.575857	3.675781	2.125939
50	1	0	-1.643516	1.688446	4.566029
51	1	0	-3.787250	2.934673	4.367666
52	6	0	-0.931285	3.541145	-1.119323
53	6	0	-0.343648	4.651971	-0.488085
54	6	0	-1.825046	3.783627	-2.176506
55	6	0	-0.586924	5.950080	-0.933337
56	1	0	0.278978	4.509943	0.386755
57	6	0	-2.068038	5.085418	-2.623217
58	1	0	-2.361870	2.969805	-2.646770
59	6	0	-1.440396	6.171627	-2.015460
60	1	0	-0.116388	6.787749	-0.426528
61	1	0	-2.761917	5.244205	-3.443923
62	1	0	-1.629946	7.181704	-2.366714
63	6	0	0.616837	-2.805674	-0.480630
64	6	0	1.219722	-2.670301	-1.737025
65	6	0	0.110009	-4.062171	-0.102932
66	6	0	1.322617	-3.766243	-2.599343
67	1	0	1.612562	-1.707176	-2.037287
68	6	0	0.216913	-5.155976	-0.960856
69	1	0	-0.361488	-4.188289	0.867383
70	6	0	0.825020	-5.010339	-2.212146
71	1	0	1.794040	-3.645802	-3.570962
72	1	0	-0.172679	-6.122371	-0.653144
73	1	0	0.910260	-5.864258	-2.878367
74	6	0	1.522414	-1.999955	2.119561
75	6	0	1.411226	-1.420433	3.398519
76	6	0	2.530003	-2.958234	1.917642
77	6	0	2.257465	-1.803124	4.439800
78	1	0	0.648794	-0.672445	3.592612
79	6	0	3.386473	-3.331249	2.957440
80	1	0	2.645705	-3.427856	0.946891
81	6	0	3.252434	-2.759483	4.222642
82	1	0	2.138768	-1.352615	5.421434
83	1	0	4.151921	-4.080854	2.776159
84	1	0	3.912383	-3.056640	5.032376
85	15	0	-0.629494	1.880486	-0.330735
86	15	0	0.525302	-1.368140	0.685503
87	6	0	3.990186	1.246533	0.607527

88	6	0	4.555212	-0.687156	-1.299882
89	6	0	5.329183	0.508221	0.665488
90	6	0	3.957853	2.683381	0.083882
91	6	0	2.518671	2.987558	-0.342651
92	45	0	1.591164	1.139653	0.040221
93	1	0	4.656860	2.802994	-0.744099
94	1	0	4.307197	3.351602	0.884868
95	1	0	2.063194	3.778318	0.248667
96	1	0	2.425961	3.250785	-1.397481
97	1	0	4.706211	-0.934939	-2.360040
98	1	0	4.282906	-1.624507	-0.792913
99	1	0	6.066672	1.218249	1.066674
100	1	0	5.246742	-0.302050	1.399225
101	6	0	3.144193	0.996687	1.778336
102	6	0	2.261213	1.871246	2.367862
103	1	0	2.242225	2.933867	2.165891
104	1	0	1.731976	1.548104	3.257591
105	1	0	3.225496	0.004184	2.210790
106	6	0	3.413019	0.263065	-1.201499
107	6	0	2.366289	0.658462	-1.838771
108	6	0	5.829343	-0.099827	-0.668315
109	6	0	6.859567	-1.204857	-0.375120
110	1	0	7.185702	-1.692221	-1.301162
111	1	0	7.751127	-0.790940	0.109984
112	1	0	6.445397	-1.976280	0.285117
113	6	0	6.471435	0.936982	-1.611003
114	1	0	5.745062	1.653769	-2.005184
115	1	0	7.262457	1.498585	-1.101135
116	1	0	6.927083	0.432247	-2.470833
117	6	0	1.956746	0.755258	-3.266512
118	1	0	1.086426	0.130929	-3.482473
119	1	0	1.689395	1.787826	-3.521638
120	1	0	2.781860	0.451057	-3.922910

(*R*) -TS2 -TMS



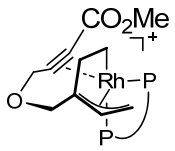
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.487380	-0.626593	-0.168079
2	6	0	1.716725	-1.644429	-0.782317
3	6	0	2.329992	-2.450418	-1.752805
4	6	0	3.637839	-2.207719	-2.153780
5	6	0	1.979749	0.049589	1.076402
6	6	0	1.032333	1.096328	1.074184
7	6	0	0.595823	1.605085	2.310986
8	6	0	1.136269	1.155011	3.503607
9	1	0	1.795114	-3.279617	-2.197712
10	1	0	4.092248	-2.850817	-2.904554
11	1	0	-0.157288	2.381338	2.345777
12	1	0	0.808327	1.599771	4.440530
13	6	0	4.594940	0.802315	-0.012744
14	6	0	5.799918	-0.932238	-2.118533
15	6	0	6.384079	0.433182	-1.743539
16	6	0	6.105532	0.726065	-0.267739
17	1	0	4.209613	1.730259	-0.458996
18	1	0	4.398555	0.890666	1.059477
19	1	0	6.436822	-1.723031	-1.693723
20	1	0	5.828704	-1.080896	-3.205187
21	1	0	7.459592	0.447542	-1.953075
22	1	0	5.926203	1.216837	-2.362546
23	1	0	6.551612	-0.065079	0.351999
24	1	0	6.573926	1.667856	0.040862
25	6	0	4.379823	-1.149653	-1.621741
26	6	0	3.807815	-0.359769	-0.605784
27	6	0	2.629594	-0.321524	4.873105
28	6	0	3.908830	-1.155046	4.770345
29	6	0	3.722985	-2.227567	3.696756
30	6	0	3.507001	-1.586877	2.319581
31	1	0	2.783526	0.556189	5.513417
32	1	0	4.758379	-0.509867	4.506286
33	1	0	4.141149	-1.603266	5.742868
34	1	0	4.592648	-2.893192	3.649593
35	1	0	2.857641	-2.852738	3.953967
36	1	0	4.473432	-1.212209	1.954367
37	1	0	3.200117	-2.352385	1.600450
38	1	0	1.851018	-0.921473	5.368096
39	6	0	2.496459	-0.443820	2.312075
40	6	0	2.093056	0.135567	3.527363
41	6	0	1.364998	1.877640	-1.856311
42	6	0	2.282474	2.935933	-1.980727
43	6	0	1.311654	0.920593	-2.878627
44	6	0	3.118023	3.025706	-3.095815

45	1	0	2.339269	3.706448	-1.220827
46	6	0	2.146941	1.008264	-3.991481
47	1	0	0.614614	0.097811	-2.797331
48	6	0	3.052060	2.064820	-4.105726
49	1	0	3.812349	3.857300	-3.177078
50	1	0	2.089958	0.251959	-4.769375
51	1	0	3.695150	2.143054	-4.977726
52	6	0	0.064903	3.622407	-0.050058
53	6	0	-0.789873	4.415449	-0.832868
54	6	0	0.911415	4.270522	0.868707
55	6	0	-0.831231	5.801351	-0.676078
56	1	0	-1.419502	3.959558	-1.583437
57	6	0	0.868244	5.657350	1.024964
58	1	0	1.615410	3.700838	1.463329
59	6	0	-0.008862	6.427608	0.260498
60	1	0	-1.505566	6.389543	-1.291971
61	1	0	1.529541	6.133256	1.743572
62	1	0	-0.042160	7.505968	0.385567
63	6	0	-0.091556	-2.653686	1.275412
64	6	0	-0.903743	-2.175868	2.310732
65	6	0	0.689822	-3.802381	1.493938
66	6	0	-0.941509	-2.836507	3.542575
67	1	0	-1.502367	-1.285870	2.153629
68	6	0	0.647029	-4.462877	2.721031
69	1	0	1.323518	-4.187131	0.699780
70	6	0	-0.170736	-3.980665	3.748530
71	1	0	-1.573246	-2.454959	4.339772
72	1	0	1.248489	-5.354434	2.875352
73	1	0	-0.205917	-4.497718	4.703385
74	6	0	-0.710502	-3.175840	-1.476201
75	6	0	-0.526192	-3.128425	-2.872409
76	6	0	-1.514047	-4.205028	-0.955972
77	6	0	-1.094017	-4.089626	-3.709656
78	1	0	0.073137	-2.339504	-3.316446
79	6	0	-2.094676	-5.159000	-1.796461
80	1	0	-1.683502	-4.275768	0.112798
81	6	0	-1.883020	-5.110362	-3.174306
82	1	0	-0.920326	-4.038346	-4.781003
83	1	0	-2.705337	-5.948009	-1.366301
84	1	0	-2.326407	-5.858451	-3.824861
85	15	0	0.183448	1.802883	-0.419366
86	15	0	-0.095599	-1.813418	-0.370465
87	6	0	-3.878698	-0.247505	-1.769848
88	6	0	-4.819882	-1.279160	0.495442

89	6	0	-5.012630	-1.281552	-1.752868
90	6	0	-4.269732	1.227406	-1.878204
91	6	0	-3.047283	2.043567	-1.439837
92	45	0	-1.743781	0.501548	-0.850793
93	1	0	-5.140059	1.417386	-1.244453
94	1	0	-4.572023	1.445226	-2.912762
95	1	0	-2.605630	2.607031	-2.262339
96	1	0	-3.247954	2.722827	-0.612819
97	1	0	-5.344535	-1.049139	1.424752
98	1	0	-4.394784	-2.295400	0.568456
99	1	0	-5.700853	-1.070519	-2.578100
100	1	0	-4.599738	-2.294379	-1.884542
101	6	0	-2.760549	-0.676703	-2.615183
102	6	0	-1.965705	0.115827	-3.401318
103	1	0	-2.185684	1.147867	-3.637983
104	1	0	-1.193259	-0.352634	-4.001459
105	1	0	-2.545605	-1.740198	-2.602133
106	6	0	-3.715501	-0.290976	0.262934
107	6	0	-2.955729	0.537195	0.903723
108	8	0	-5.752335	-1.200852	-0.557315
109	14	0	-3.348987	1.488264	2.508879
110	6	0	-5.220258	1.397040	2.795506
111	1	0	-5.559334	0.405394	3.115265
112	1	0	-5.487880	2.095885	3.598469
113	1	0	-5.794527	1.683999	1.907466
114	6	0	-2.919471	3.315144	2.304572
115	1	0	-3.045536	3.824103	3.268596
116	1	0	-1.904781	3.510414	1.950673
117	1	0	-3.608120	3.791704	1.596942
118	6	0	-2.509445	0.701362	4.006620
119	1	0	-1.430739	0.578066	3.890141
120	1	0	-2.689251	1.325226	4.891531
121	1	0	-2.944394	-0.283896	4.213522

(*S*) -IN2’ -E



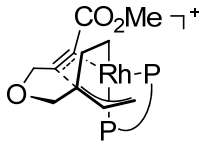
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-2.142147	0.312289	0.829133
2	6	0	-1.414307	-0.734684	1.445970
3	6	0	-1.572923	-0.942273	2.824441
4	6	0	-2.394317	-0.113046	3.576234
5	6	0	-2.193601	0.442431	-0.671565
6	6	0	-1.178303	1.056441	-1.438663
7	6	0	-1.333384	1.112344	-2.836981
8	6	0	-2.477554	0.630395	-3.451386
9	1	0	-1.054297	-1.753142	3.321077
10	1	0	-2.505611	-0.298598	4.642392
11	1	0	-0.551202	1.534760	-3.456367
12	1	0	-2.578700	0.711734	-4.531428
13	6	0	-3.652803	2.365689	0.961991
14	6	0	-3.950886	1.832447	3.879659
15	6	0	-4.324849	3.176955	3.249322
16	6	0	-4.787057	2.959445	1.807121
17	1	0	-2.895891	3.144422	0.789908
18	1	0	-4.026356	2.099237	-0.030344
19	1	0	-4.872526	1.273552	4.102686
20	1	0	-3.453671	1.981959	4.846027
21	1	0	-5.106112	3.662226	3.845181
22	1	0	-3.454120	3.846652	3.255990
23	1	0	-5.653552	2.282569	1.799887
24	1	0	-5.120936	3.900898	1.355616
25	6	0	-3.072418	0.962584	2.995314
26	6	0	-2.953165	1.176291	1.608611
27	6	0	-4.721867	-0.491089	-3.447490
28	6	0	-5.925916	-0.743826	-2.537216
29	6	0	-5.472321	-1.538343	-1.311928
30	6	0	-4.454878	-0.738126	-0.488114
31	1	0	-4.980153	0.206020	-4.254358
32	1	0	-6.363481	0.212654	-2.218740
33	1	0	-6.705116	-1.280033	-3.090488
34	1	0	-6.324748	-1.797703	-0.673353
35	1	0	-5.023307	-2.485290	-1.638937
36	1	0	-4.993244	0.041082	0.069800
37	1	0	-4.005796	-1.383224	0.272912
38	1	0	-4.445578	-1.434273	-3.943201
39	6	0	-3.355036	-0.079569	-1.314841
40	6	0	-3.502672	0.034721	-2.708858
41	6	0	0.211906	2.476350	0.843682
42	6	0	-0.224443	3.813907	0.862107
43	6	0	0.512145	1.857750	2.062429

44	6	0	-0.358060	4.501306	2.068974
45	1	0	-0.444546	4.332725	-0.063804
46	6	0	0.386703	2.545891	3.270143
47	1	0	0.842255	0.828152	2.076127
48	6	0	-0.049338	3.871306	3.277150
49	1	0	-0.691913	5.535190	2.060945
50	1	0	0.641110	2.044384	4.198626
51	1	0	-0.140807	4.412356	4.214780
52	6	0	0.981942	3.050354	-1.808792
53	6	0	2.317313	3.475543	-1.704481
54	6	0	0.089075	3.834957	-2.560521
55	6	0	2.756877	4.622709	-2.366755
56	1	0	3.010592	2.923597	-1.082549
57	6	0	0.532725	4.981542	-3.222844
58	1	0	-0.959400	3.568829	-2.624755
59	6	0	1.868847	5.374216	-3.137304
60	1	0	3.795508	4.928873	-2.277106
61	1	0	-0.173977	5.570497	-3.800664
62	1	0	2.211515	6.264518	-3.656587
63	6	0	-1.401683	-2.993133	-0.348870
64	6	0	-1.389991	-3.221739	-1.730904
65	6	0	-2.320118	-3.711236	0.440014
66	6	0	-2.248318	-4.161017	-2.311088
67	1	0	-0.723418	-2.658726	-2.371087
68	6	0	-3.175866	-4.648714	-0.136446
69	1	0	-2.360997	-3.543967	1.512248
70	6	0	-3.137480	-4.881704	-1.514890
71	1	0	-2.218574	-4.325617	-3.384603
72	1	0	-3.871907	-5.198713	0.490661
73	1	0	-3.800105	-5.616893	-1.962538
74	6	0	0.605339	-2.865736	1.708618
75	6	0	1.311307	-2.298423	2.787275
76	6	0	0.675333	-4.259977	1.535413
77	6	0	2.024331	-3.099723	3.680799
78	1	0	1.309412	-1.225648	2.946192
79	6	0	1.400300	-5.059474	2.423773
80	1	0	0.152676	-4.733974	0.712077
81	6	0	2.071276	-4.484538	3.503629
82	1	0	2.544809	-2.635556	4.513834
83	1	0	1.429698	-6.134900	2.272090
84	1	0	2.625428	-5.107459	4.199760
85	15	0	0.470941	1.596171	-0.772977
86	15	0	-0.236808	-1.785769	0.453183
87	6	0	3.260975	-1.948991	-2.154358

88	6	0	4.012621	-2.630876	0.690039
89	6	0	3.921043	-3.188615	-1.610621
90	6	0	4.155317	-0.769430	-2.519835
91	6	0	3.485249	0.482056	-1.954593
92	45	0	1.882290	-0.395353	-0.912365
93	1	0	5.138112	-0.927583	-2.067399
94	1	0	4.299810	-0.730586	-3.609195
95	1	0	3.110522	1.173506	-2.707970
96	1	0	4.112909	1.015715	-1.243087
97	1	0	4.695914	-2.831755	1.525763
98	1	0	3.149941	-3.299371	0.812206
99	1	0	4.604153	-3.594431	-2.366991
100	1	0	3.175863	-3.962081	-1.371060
101	6	0	1.914354	-1.983572	-2.513976
102	6	0	1.203813	-0.820692	-2.938088
103	1	0	1.682026	-0.103829	-3.599192
104	1	0	0.134729	-0.908461	-3.091714
105	1	0	1.358743	-2.888096	-2.277344
106	6	0	3.570537	-1.235099	0.820411
107	6	0	3.196376	-0.053557	0.930722
108	8	0	4.745551	-2.932169	-0.479883
109	6	0	3.465641	1.111689	1.799031
110	8	0	3.422033	1.045255	3.007550
111	8	0	3.786670	2.207727	1.098695
112	6	0	4.102306	3.376677	1.891924
113	1	0	3.235288	3.664779	2.489368
114	1	0	4.950883	3.168308	2.546743
115	1	0	4.351343	4.152542	1.169286

(*S*) -TS2-E



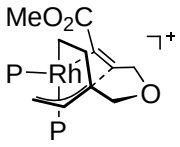
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.202813	0.065550	0.897288
2	6	0	-1.270821	-0.804596	1.517239
3	6	0	-1.312837	-0.959863	2.909756
4	6	0	-2.229833	-0.247255	3.671703

5	6	0	-2.327807	0.106539	-0.605410
6	6	0	-1.435364	0.822165	-1.435172
7	6	0	-1.578865	0.726146	-2.832117
8	6	0	-2.625914	0.013227	-3.391486
9	1	0	-0.628330	-1.637659	3.406768
10	1	0	-2.251209	-0.388661	4.750193
11	1	0	-0.864820	1.211963	-3.487407
12	1	0	-2.733936	-0.020870	-4.473462
13	6	0	-4.041592	1.829189	1.029835
14	6	0	-4.095536	1.403515	3.979653
15	6	0	-4.739610	2.622687	3.313347
16	6	0	-5.224358	2.250410	1.910719
17	1	0	-3.445192	2.721709	0.791248
18	1	0	-4.403160	1.456260	0.067667
19	1	0	-4.887381	0.701541	4.282516
20	1	0	-3.585351	1.693035	4.906659
21	1	0	-5.566157	2.990346	3.931788
22	1	0	-4.006639	3.437743	3.240757
23	1	0	-5.951505	1.428705	1.980861
24	1	0	-5.745963	3.091613	1.439695
25	6	0	-3.119435	0.657186	3.084517
26	6	0	-3.112120	0.814451	1.684261
27	6	0	-4.666153	-1.439467	-3.269110
28	6	0	-5.814254	-1.810369	-2.327784
29	6	0	-5.239866	-2.424268	-1.050533
30	6	0	-4.364373	-1.409819	-0.302468
31	1	0	-5.032623	-0.858937	-4.124838
32	1	0	-6.400076	-0.914487	-2.078896
33	1	0	-6.496643	-2.506115	-2.828728
34	1	0	-6.040096	-2.766258	-0.384023
35	1	0	-4.643983	-3.309404	-1.308869
36	1	0	-5.021346	-0.689059	0.204447
37	1	0	-3.813402	-1.915610	0.496043
38	1	0	-4.240335	-2.362230	-3.692379
39	6	0	-3.389158	-0.644086	-1.190740
40	6	0	-3.548692	-0.667750	-2.588605
41	6	0	-0.200459	2.519968	0.771471
42	6	0	-0.911292	3.732317	0.802198
43	6	0	0.343898	2.030282	1.963719
44	6	0	-1.081404	4.423060	2.002422
45	1	0	-1.316360	4.152843	-0.112071
46	6	0	0.172417	2.719140	3.164372
47	1	0	0.898919	1.101658	1.953148
48	6	0	-0.539373	3.919486	3.186634

49	1	0	-1.626560	5.362692	2.007240
50	1	0	0.594633	2.316710	4.080969
51	1	0	-0.664570	4.463770	4.118396
52	6	0	0.345566	3.170010	-1.911880
53	6	0	1.549556	3.872878	-1.720985
54	6	0	-0.626763	3.712299	-2.768626
55	6	0	1.788694	5.063560	-2.406310
56	1	0	2.285565	3.510517	-1.010531
57	6	0	-0.379281	4.905128	-3.452810
58	1	0	-1.586489	3.225707	-2.896866
59	6	0	0.830840	5.577696	-3.282861
60	1	0	2.723757	5.592893	-2.246858
61	1	0	-1.141814	5.309533	-4.112497
62	1	0	1.020113	6.504089	-3.817505
63	6	0	-0.961615	-3.109467	-0.182502
64	6	0	-0.949066	-3.431294	-1.545026
65	6	0	-1.713667	-3.917329	0.690709
66	6	0	-1.646131	-4.543445	-2.027225
67	1	0	-0.405300	-2.807512	-2.241629
68	6	0	-2.408813	-5.027062	0.212166
69	1	0	-1.748923	-3.683723	1.750680
70	6	0	-2.371859	-5.347146	-1.148820
71	1	0	-1.618945	-4.778210	-3.087704
72	1	0	-2.977964	-5.643901	0.901959
73	1	0	-2.908562	-6.215924	-1.519181
74	6	0	1.128953	-2.540500	1.700462
75	6	0	1.811588	-1.813580	2.693198
76	6	0	1.435809	-3.904954	1.554372
77	6	0	2.736367	-2.435030	3.532479
78	1	0	1.625152	-0.753536	2.823889
79	6	0	2.370912	-4.524432	2.387833
80	1	0	0.937087	-4.498973	0.796916
81	6	0	3.019849	-3.795228	3.384596
82	1	0	3.238345	-1.851573	4.299060
83	1	0	2.582001	-5.582509	2.260050
84	1	0	3.739073	-4.279597	4.038749
85	15	0	0.096506	1.677167	-0.850312
86	15	0	0.012710	-1.678900	0.494385
87	6	0	3.481436	-1.364089	-1.928251
88	6	0	4.796249	-1.661480	0.423475
89	6	0	4.452154	-2.512830	-1.658970
90	6	0	4.031216	-0.091880	-2.579479
91	6	0	3.069898	1.048335	-2.212779
92	45	0	1.693667	-0.019464	-1.008743

93	1	0	5.042112	0.092978	-2.205538
94	1	0	4.114631	-0.249031	-3.664232
95	1	0	2.545076	1.497250	-3.056526
96	1	0	3.550564	1.833372	-1.634230
97	1	0	5.540024	-1.163380	1.053353
98	1	0	4.354568	-2.494554	0.993700
99	1	0	4.964963	-2.773360	-2.591254
100	1	0	3.902459	-3.397404	-1.298541
101	6	0	2.157791	-1.789919	-2.397001
102	6	0	1.350961	-1.080508	-3.259190
103	1	0	1.712270	-0.253659	-3.855339
104	1	0	0.379998	-1.472199	-3.540186
105	1	0	1.791650	-2.735565	-2.003110
106	6	0	3.726032	-0.691775	0.055032
107	6	0	3.099058	0.373958	0.425068
108	8	0	5.448379	-2.129466	-0.738059
109	6	0	3.451653	1.519307	1.287103
110	8	0	3.439138	2.674534	0.914786
111	8	0	3.823785	1.122915	2.518642
112	6	0	4.247152	2.185847	3.404814
113	1	0	3.433859	2.900339	3.550167
114	1	0	4.505379	1.692412	4.341245
115	1	0	5.114222	2.702761	2.987835

(*R*) –TS2 -E



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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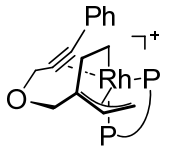
3	6	0	1.897972	-2.052477	-2.385987
4	6	0	3.238445	-1.910057	-2.719782
5	6	0	1.843934	-0.397155	1.035331
6	6	0	1.099134	0.769086	1.318299
7	6	0	0.727451	1.029054	2.650039
8	6	0	1.129216	0.190599	3.676755
9	1	0	1.255500	-2.623093	-3.045102
10	1	0	3.612062	-2.372817	-3.630725

11	1	0	0.108435	1.882602	2.887827
12	1	0	0.854581	0.434137	4.701107
13	6	0	4.575179	0.179553	0.180372
14	6	0	5.567925	-1.051190	-2.348372
15	6	0	6.340070	0.045601	-1.609519
16	6	0	6.063911	-0.051517	-0.107776
17	1	0	4.347531	1.244348	0.027928
18	1	0	4.363060	-0.014718	1.235455
19	1	0	6.063525	-2.018111	-2.172449
20	1	0	5.608715	-0.890556	-3.432896
21	1	0	7.411283	-0.047262	-1.820919
22	1	0	6.025945	1.032907	-1.975068
23	1	0	6.365976	-1.044534	0.254978
24	1	0	6.659446	0.680746	0.449596
25	6	0	4.116212	-1.176918	-1.916214
26	6	0	3.638691	-0.627282	-0.710538
27	6	0	2.266160	-1.846947	4.596366
28	6	0	3.385621	-2.838918	4.271614
29	6	0	3.066388	-3.542868	2.952339
30	6	0	3.020686	-2.536620	1.794852
31	1	0	2.540319	-1.211849	5.448125
32	1	0	4.344171	-2.308282	4.185884
33	1	0	3.494343	-3.559911	5.089635
34	1	0	3.811845	-4.314427	2.727361
35	1	0	2.097827	-4.053261	3.037568
36	1	0	4.050802	-2.253130	1.536117
37	1	0	2.618225	-3.022366	0.901055
38	1	0	1.374078	-2.407812	4.914587
39	6	0	2.221479	-1.272811	2.095230
40	6	0	1.878895	-0.962322	3.423652
41	6	0	1.518089	2.123719	-1.375930
42	6	0	2.647656	2.947401	-1.223537
43	6	0	1.256880	1.571996	-2.635342
44	6	0	3.493995	3.196736	-2.304170
45	1	0	2.859522	3.415958	-0.268317
46	6	0	2.102400	1.821777	-3.716942
47	1	0	0.384297	0.946002	-2.767270
48	6	0	3.223634	2.636301	-3.554477
49	1	0	4.357016	3.842910	-2.170406
50	1	0	1.882696	1.383611	-4.686578
51	1	0	3.877088	2.841489	-4.397598
52	6	0	0.425690	3.609793	0.737135
53	6	0	-0.190780	4.624558	-0.015277
54	6	0	1.191174	3.984259	1.853634

55	6	0	-0.095212	5.961746	0.365549
56	1	0	-0.721778	4.378790	-0.927174
57	6	0	1.286507	5.325102	2.233666
58	1	0	1.733569	3.242446	2.425904
59	6	0	0.634266	6.316306	1.501607
60	1	0	-0.584799	6.725945	-0.231263
61	1	0	1.881164	5.590042	3.103263
62	1	0	0.707651	7.357302	1.802389
63	6	0	-0.561962	-2.879400	0.425335
64	6	0	-1.267696	-2.697927	1.621591
65	6	0	0.034691	-4.128191	0.171454
66	6	0	-1.388152	-3.745411	2.540248
67	1	0	-1.720760	-1.741526	1.848586
68	6	0	-0.088638	-5.172014	1.087193
69	1	0	0.590476	-4.288123	-0.748019
70	6	0	-0.804571	-4.983660	2.274182
71	1	0	-1.941464	-3.587468	3.461816
72	1	0	0.371890	-6.132745	0.874434
73	1	0	-0.903967	-5.799437	2.984774
74	6	0	-1.217801	-2.313990	-2.314410
75	6	0	-0.995465	-1.812886	-3.612008
76	6	0	-2.184893	-3.321069	-2.155339
77	6	0	-1.693107	-2.318602	-4.709637
78	1	0	-0.261435	-1.029775	-3.774458
79	6	0	-2.892302	-3.818760	-3.253615
80	1	0	-2.384352	-3.730824	-1.171217
81	6	0	-2.647222	-3.324100	-4.534776
82	1	0	-1.489218	-1.926919	-5.702447
83	1	0	-3.628473	-4.603628	-3.103530
84	1	0	-3.190604	-3.717817	-5.388662
85	15	0	0.351252	1.888530	0.049106
86	15	0	-0.435766	-1.520780	-0.828083
87	6	0	-4.047519	0.758680	-1.258566
88	6	0	-4.820861	-0.789238	0.830963
89	6	0	-5.269871	-0.158056	-1.306473
90	6	0	-4.252495	2.211069	-0.827587
91	6	0	-2.891264	2.723847	-0.339189
92	45	0	-1.753876	0.948898	-0.491113
93	1	0	-5.013539	2.250321	-0.043255
94	1	0	-4.641512	2.786676	-1.680046
95	1	0	-2.474390	3.498532	-0.978486
96	1	0	-2.889406	3.076420	0.691486
97	1	0	-5.186000	-0.730979	1.860953
98	1	0	-4.564176	-1.839811	0.608723

99	1	0	-6.036456	0.307416	-1.935526
100	1	0	-4.996860	-1.131537	-1.744045
101	6	0	-3.090846	0.518729	-2.337485
102	6	0	-2.255855	1.447295	-2.916644
103	1	0	-2.368490	2.515661	-2.793039
104	1	0	-1.613348	1.127001	-3.729359
105	1	0	-3.027779	-0.504294	-2.695831
106	6	0	-3.601317	0.055502	0.692969
107	6	0	-2.616140	0.574319	1.344334
108	8	0	-5.838298	-0.325121	-0.026271
109	6	0	-2.493596	0.933879	2.771968
110	8	0	-2.159403	2.025696	3.179922
111	8	0	-2.876702	-0.089658	3.562833
112	6	0	-2.882745	0.192454	4.980676
113	1	0	-3.252185	-0.717089	5.453115
114	1	0	-1.871477	0.422644	5.323622
115	1	0	-3.540220	1.037381	5.196374

(*S*) -IN2’ -Ph



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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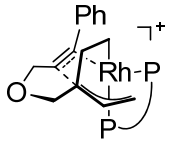
2	6	0	1.413841	0.434267	1.619660
3	6	0	1.405809	0.539580	3.018681
4	6	0	1.932705	-0.473330	3.808633
5	6	0	2.277553	-0.756350	-0.453969
6	6	0	1.308429	-1.130033	-1.411339
7	6	0	1.677913	-1.143962	-2.770170
8	6	0	2.970298	-0.843474	-3.166655
9	1	0	0.986910	1.413948	3.501599
10	1	0	1.919242	-0.366041	4.891230
11	1	0	0.949074	-1.400816	-3.529792
12	1	0	3.229004	-0.886995	-4.222358
13	6	0	3.081635	-3.015084	1.203887
14	6	0	3.016372	-2.708074	4.169502

15	6	0	3.219474	-4.064636	3.488765
16	6	0	3.935726	-3.867809	2.151020
17	1	0	2.229572	-3.617665	0.857765
18	1	0	3.652589	-2.772109	0.303209
19	1	0	3.981146	-2.359599	4.568678
20	1	0	2.353862	-2.805875	5.038435
21	1	0	3.789163	-4.729887	4.147438
22	1	0	2.245913	-4.542322	3.313686
23	1	0	4.904721	-3.378185	2.324725
24	1	0	4.152153	-4.831588	1.675646
25	6	0	2.469376	-1.634021	3.243743
26	6	0	2.523493	-1.748415	1.841498
27	6	0	5.341794	-0.146891	-2.738180
28	6	0	6.411587	-0.171109	-1.643998
29	6	0	5.910615	0.615591	-0.432136
30	6	0	4.654603	-0.036435	0.160094
31	1	0	5.602095	-0.831175	-3.555338
32	1	0	6.624754	-1.208487	-1.350387
33	1	0	7.348019	0.248006	-2.029075
34	1	0	6.682183	0.676113	0.344207
35	1	0	5.685669	1.646389	-0.735519
36	1	0	4.956995	-0.938424	0.711089
37	1	0	4.212212	0.627628	0.908361
38	1	0	5.313088	0.857970	-3.186652
39	6	0	3.600891	-0.423944	-0.872694
40	6	0	3.948793	-0.483414	-2.233862
41	6	0	-0.676309	-2.382298	0.508496
42	6	0	-0.508736	-3.778478	0.523899
43	6	0	-1.042967	-1.742601	1.699397
44	6	0	-0.690217	-4.503166	1.702962
45	1	0	-0.252604	-4.313359	-0.382961
46	6	0	-1.219669	-2.464935	2.878458
47	1	0	-1.196289	-0.672188	1.704959
48	6	0	-1.045618	-3.849195	2.883939
49	1	0	-0.563204	-5.582129	1.691656
50	1	0	-1.507754	-1.945492	3.787356
51	1	0	-1.196491	-4.416173	3.798302
52	6	0	-0.983227	-2.717872	-2.301828
53	6	0	-2.337137	-2.874137	-2.637633
54	6	0	-0.064674	-3.655523	-2.811356
55	6	0	-2.760265	-3.910531	-3.472412
56	1	0	-3.075681	-2.188501	-2.245832
57	6	0	-0.487285	-4.689974	-3.647216
58	1	0	0.986793	-3.586352	-2.556570

59	6	0	-1.835413	-4.818764	-3.986083
60	1	0	-3.814176	-4.004108	-3.718478
61	1	0	0.242129	-5.398514	-4.029419
62	1	0	-2.161313	-5.623241	-4.638885
63	6	0	2.073893	2.745395	0.017435
64	6	0	2.306308	3.044666	-1.331262
65	6	0	2.973596	3.243877	0.978183
66	6	0	3.389072	3.842791	-1.713669
67	1	0	1.653533	2.646945	-2.097868
68	6	0	4.052791	4.040886	0.599058
69	1	0	2.824759	3.016312	2.029624
70	6	0	4.259947	4.348602	-0.749402
71	1	0	3.547419	4.066799	-2.764949
72	1	0	4.731390	4.423384	1.356360
73	1	0	5.097304	4.974969	-1.043539
74	6	0	-0.209336	2.884608	1.755858
75	6	0	-1.140127	2.401025	2.695238
76	6	0	-0.025466	4.275695	1.668177
77	6	0	-1.827451	3.272615	3.541187
78	1	0	-1.322372	1.335435	2.785455
79	6	0	-0.726336	5.148727	2.505153
80	1	0	0.676683	4.688617	0.952505
81	6	0	-1.624614	4.651725	3.449465
82	1	0	-2.520365	2.871598	4.276236
83	1	0	-0.558813	6.218879	2.421195
84	1	0	-2.159989	5.329565	4.107869
85	15	0	-0.500288	-1.413651	-1.067623
86	15	0	0.608475	1.732585	0.551412
87	6	0	-2.389943	2.674460	-2.519320
88	6	0	-3.401105	3.226588	0.235585
89	6	0	-2.894015	3.975195	-1.946536
90	6	0	-3.420144	1.729165	-3.127233
91	6	0	-3.103165	0.334403	-2.593256
92	45	0	-1.562926	0.800365	-1.244482
93	1	0	-4.414526	2.053201	-2.809576
94	1	0	-3.387694	1.790335	-4.224513
95	1	0	-2.743711	-0.359702	-3.351427
96	1	0	-3.934720	-0.105497	-2.043467
97	1	0	-4.205093	3.348069	0.969202
98	1	0	-2.528277	3.792395	0.585556
99	1	0	-3.374546	4.555552	-2.743987
100	1	0	-2.066056	4.573438	-1.536116
101	6	0	-1.019524	2.467952	-2.678274
102	6	0	-0.474520	1.223175	-3.102950

103	1	0	-0.963150	0.653402	-3.887877
104	1	0	0.603304	1.112837	-3.087902
105	1	0	-0.353909	3.226707	-2.273513
106	6	0	-3.089157	1.774754	0.168631
107	6	0	-3.249387	0.565611	0.423397
108	8	0	-3.902084	3.783801	-0.966424
109	6	0	-3.934164	-0.487544	1.145374
110	6	0	-4.412709	-0.181548	2.436721
111	6	0	-4.195821	-1.758764	0.612273
112	6	0	-5.130878	-1.125430	3.166253
113	1	0	-4.219528	0.801670	2.855320
114	6	0	-4.921420	-2.696548	1.343648
115	1	0	-3.826445	-2.015269	-0.371853
116	6	0	-5.389068	-2.386273	2.621972
117	1	0	-5.495310	-0.873558	4.158151
118	1	0	-5.117943	-3.674522	0.914135
119	1	0	-5.952320	-3.120604	3.190296

(*S*) -Ph-TS2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	-1.257201	-0.660899	1.639157
3	6	0	-1.191493	-0.747432	3.036879
4	6	0	-1.974881	0.077944	3.833266
5	6	0	-2.442150	0.214849	-0.427017
6	6	0	-1.587899	0.795826	-1.390267
7	6	0	-1.903513	0.646115	-2.754205
8	6	0	-3.065917	0.006891	-3.150695
9	1	0	-0.529596	-1.460721	3.513357
10	1	0	-1.912753	-0.011424	4.915740
11	1	0	-1.241296	1.045492	-3.514267
12	1	0	-3.302749	-0.065371	-4.210060
13	6	0	-3.847093	2.166972	1.244827
14	6	0	-3.661620	1.898658	4.208050
15	6	0	-4.267980	3.130815	3.530611
16	6	0	-4.907868	2.727029	2.200658

17	1	0	-3.209927	2.995063	0.902866
18	1	0	-4.323537	1.773923	0.342492
19	1	0	-4.474287	1.281609	4.620764
20	1	0	-3.046547	2.192529	5.067632
21	1	0	-5.002487	3.597332	4.196707
22	1	0	-3.483677	3.877085	3.344798
23	1	0	-5.685435	1.971302	2.383062
24	1	0	-5.405975	3.582198	1.729201
25	6	0	-2.834495	1.028604	3.275341
26	6	0	-2.941158	1.115039	1.873362
27	6	0	-5.200289	-1.238553	-2.715445
28	6	0	-6.259496	-1.442779	-1.630062
29	6	0	-5.599589	-2.052174	-0.392827
30	6	0	-4.546957	-1.099644	0.191021
31	1	0	-5.608553	-0.669542	-3.560015
32	1	0	-6.720689	-0.479758	-1.369914
33	1	0	-7.061556	-2.086489	-2.008285
34	1	0	-6.343899	-2.278202	0.379457
35	1	0	-5.128432	-3.005271	-0.665755
36	1	0	-5.066170	-0.300708	0.738400
37	1	0	-3.948319	-1.625972	0.940971
38	1	0	-4.914809	-2.219926	-3.124399
39	6	0	-3.623033	-0.467830	-0.845421
40	6	0	-3.945132	-0.546520	-2.212182
41	6	0	-0.031531	2.560031	0.533828
42	6	0	-0.636627	3.829761	0.541611
43	6	0	0.563986	2.092889	1.711936
44	6	0	-0.655693	4.598009	1.706033
45	1	0	-1.079865	4.233292	-0.361780
46	6	0	0.541914	2.859893	2.876597
47	1	0	1.055938	1.129713	1.714791
48	6	0	-0.067235	4.114984	2.876998
49	1	0	-1.121034	5.579640	1.692218
50	1	0	1.012854	2.479778	3.778228
51	1	0	-0.073688	4.719179	3.779887
52	6	0	0.214418	2.952759	-2.261942
53	6	0	1.483229	3.514406	-2.480446
54	6	0	-0.896990	3.564075	-2.870154
55	6	0	1.643263	4.631277	-3.301513
56	1	0	2.356532	3.086406	-2.004645
57	6	0	-0.734733	4.680176	-3.693142
58	1	0	-1.896179	3.179338	-2.700748
59	6	0	0.534962	5.214117	-3.916782
60	1	0	2.635731	5.044497	-3.457080

61	1	0	-1.607188	5.134042	-4.154610
62	1	0	0.658359	6.081441	-4.558715
63	6	0	-1.296056	-3.042798	0.022286
64	6	0	-1.497680	-3.354747	-1.327651
65	6	0	-1.981904	-3.795471	0.993884
66	6	0	-2.334041	-4.410475	-1.703916
67	1	0	-1.019271	-2.761397	-2.095433
68	6	0	-2.817711	-4.847002	0.620959
69	1	0	-1.855174	-3.565027	2.047516
70	6	0	-2.989554	-5.163434	-0.730550
71	1	0	-2.470786	-4.640197	-2.757031
72	1	0	-3.333116	-5.421690	1.385384
73	1	0	-3.634156	-5.988662	-1.019546
74	6	0	0.985988	-2.598605	1.700689
75	6	0	1.765167	-1.912193	2.649281
76	6	0	1.190445	-3.982365	1.556752
77	6	0	2.675733	-2.592797	3.458953
78	1	0	1.658030	-0.839716	2.773096
79	6	0	2.116024	-4.660182	2.354734
80	1	0	0.616186	-4.546215	0.830067
81	6	0	2.855324	-3.970987	3.316236
82	1	0	3.243095	-2.042894	4.204937
83	1	0	2.246513	-5.731458	2.229391
84	1	0	3.562739	-4.499938	3.948287
85	15	0	0.058562	1.572395	-1.031518
86	15	0	-0.144625	-1.680956	0.549926
87	6	0	3.024209	-1.828750	-2.230338
88	6	0	4.508703	-2.274315	-0.034890
89	6	0	3.851935	-3.100574	-2.039951
90	6	0	3.673605	-0.667033	-2.986356
91	6	0	2.927467	0.602370	-2.554995
92	45	0	1.554882	-0.248016	-1.190404
93	1	0	4.735116	-0.623160	-2.728510
94	1	0	3.610492	-0.854407	-4.067441
95	1	0	2.386478	1.107364	-3.355519
96	1	0	3.586532	1.315065	-2.060510
97	1	0	5.371024	-1.854784	0.493963
98	1	0	4.040196	-3.042078	0.601421
99	1	0	4.217902	-3.435655	-3.016617
100	1	0	3.227234	-3.896740	-1.602841
101	6	0	1.614745	-2.084366	-2.556010
102	6	0	0.825078	-1.295677	-3.360401
103	1	0	1.227648	-0.534089	-4.014718
104	1	0	-0.211001	-1.563535	-3.532044

105	1	0	1.171553	-2.964723	-2.096086
106	6	0	3.532215	-1.178575	-0.325795
107	6	0	3.158473	-0.022428	0.123071
108	8	0	4.978751	-2.845999	-1.238124
109	6	0	3.734731	0.943611	1.060307
110	6	0	3.658575	2.327737	0.833222
111	6	0	4.455789	0.487709	2.182984
112	6	0	4.299502	3.226768	1.683486
113	1	0	3.092958	2.696352	-0.014167
114	6	0	5.084529	1.390701	3.038746
115	1	0	4.509987	-0.576367	2.388212
116	6	0	5.014182	2.763245	2.789813
117	1	0	4.234836	4.292476	1.483698
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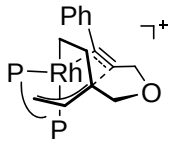
119	1	0	5.509652	3.465159	3.454144

(*R*) -Ph-TS2



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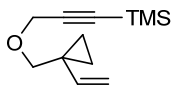
3	6	0	2.530143	-2.674428	-1.116958
4	6	0	3.858573	-2.453021	-1.456895
5	6	0	1.851054	0.328003	1.096769
6	6	0	0.878206	1.309498	0.805414
7	6	0	0.304553	2.023177	1.873484
8	6	0	0.724731	1.824054	3.177243
9	1	0	2.064954	-3.603912	-1.419498
10	1	0	4.396907	-3.212119	-2.020497
11	1	0	-0.475786	2.747753	1.690111
12	1	0	0.273897	2.409008	3.975608
13	6	0	4.530976	0.967797	0.095435
14	6	0	5.966808	-1.091462	-1.515565
15	6	0	6.470457	0.348683	-1.384625
16	6	0	6.059415	0.917342	-0.024552
17	1	0	4.153090	1.771421	-0.552313
18	1	0	4.242257	1.251982	1.111446

19	1	0	6.590335	-1.747401	-0.889150
20	1	0	6.094463	-1.454462	-2.543019
21	1	0	7.558671	0.375006	-1.511075
22	1	0	6.039692	0.967704	-2.183520
23	1	0	6.478196	0.289344	0.774945
24	1	0	6.468487	1.923951	0.120621
25	6	0	4.517055	-1.273711	-1.097739
26	6	0	3.834113	-0.323748	-0.313770
27	6	0	2.113419	0.704534	4.938727
28	6	0	3.421741	-0.068149	5.122310
29	6	0	3.388301	-1.326477	4.254987
30	6	0	3.299745	-0.960227	2.767538
31	1	0	2.170025	1.690913	5.416089
32	1	0	4.274198	0.560866	4.829761
33	1	0	3.561578	-0.319149	6.179830
34	1	0	4.280370	-1.941967	4.419463
35	1	0	2.522784	-1.940283	4.537426
36	1	0	4.287455	-0.609056	2.436537
37	1	0	3.096911	-1.860174	2.178944
38	1	0	1.304966	0.166434	5.456580
39	6	0	2.258553	0.107908	2.446131
40	6	0	1.709287	0.880443	3.484984
41	6	0	1.413884	1.483496	-2.188254
42	6	0	2.343944	2.516623	-2.399185
43	6	0	1.437983	0.377775	-3.047409
44	6	0	3.273216	2.434273	-3.437334
45	1	0	2.336625	3.398947	-1.769120
46	6	0	2.367930	0.293629	-4.083617
47	1	0	0.723170	-0.420926	-2.902579
48	6	0	3.288240	1.323678	-4.283149
49	1	0	3.977382	3.247292	-3.590345
50	1	0	2.370510	-0.574537	-4.736818
51	1	0	4.005313	1.266723	-5.097145
52	6	0	-0.122944	3.478663	-0.913029
53	6	0	-0.904574	4.012250	-1.951207
54	6	0	0.557103	4.374639	-0.068714
55	6	0	-1.041272	5.391191	-2.114727
56	1	0	-1.395094	3.353114	-2.654488
57	6	0	0.420074	5.754539	-0.234129
58	1	0	1.203800	4.005567	0.718075
59	6	0	-0.386253	6.268742	-1.249941
60	1	0	-1.655029	5.776399	-2.923990
61	1	0	0.954083	6.426075	0.432318
62	1	0	-0.492099	7.342441	-1.374934

63	6	0	-0.111454	-2.426156	1.700004
64	6	0	-0.895704	-1.699847	2.604243
65	6	0	0.586913	-3.557227	2.159396
66	6	0	-1.000779	-2.104764	3.938127
67	1	0	-1.408642	-0.806253	2.270039
68	6	0	0.477101	-3.963686	3.488710
69	1	0	1.208419	-4.128027	1.475217
70	6	0	-0.322463	-3.240568	4.380385
71	1	0	-1.610801	-1.529422	4.629333
72	1	0	1.014192	-4.844535	3.829322
73	1	0	-0.410260	-3.561473	5.414618
74	6	0	-0.504360	-3.458747	-0.956401
75	6	0	-0.190034	-3.658387	-2.315366
76	6	0	-1.353381	-4.392422	-0.336651
77	6	0	-0.676713	-4.763436	-3.014921
78	1	0	0.446718	-2.950653	-2.836720
79	6	0	-1.850712	-5.492328	-1.041281
80	1	0	-1.624634	-4.272047	0.706509
81	6	0	-1.510920	-5.686589	-2.380328
82	1	0	-0.403951	-4.900947	-4.057653
83	1	0	-2.497733	-6.202789	-0.534236
84	1	0	-1.890541	-6.546491	-2.924255
85	15	0	0.123344	1.636070	-0.858954
86	15	0	-0.019757	-1.899994	-0.070373
87	6	0	-3.785002	-0.836917	-1.868533
88	6	0	-4.752759	-1.278230	0.619360
89	6	0	-4.855738	-1.884991	-1.562909
90	6	0	-4.253356	0.550459	-2.300571
91	6	0	-3.084420	1.505856	-2.035607
92	45	0	-1.747494	0.186107	-1.077873
93	1	0	-5.143989	0.824037	-1.729031
94	1	0	-4.545656	0.520247	-3.360427
95	1	0	-2.631120	1.886802	-2.950551
96	1	0	-3.347989	2.345869	-1.394954
97	1	0	-5.316928	-0.788275	1.420331
98	1	0	-4.349738	-2.231841	1.001887
99	1	0	-5.531606	-1.957007	-2.422165
100	1	0	-4.386412	-2.868177	-1.398314
101	6	0	-2.623213	-1.385913	-2.563700
102	6	0	-1.820162	-0.742952	-3.473667
103	1	0	-2.071260	0.197738	-3.944081
104	1	0	-1.006155	-1.298660	-3.925567
105	1	0	-2.368695	-2.409194	-2.309317
106	6	0	-3.637573	-0.382089	0.191651

107	6	0	-2.928490	0.614911	0.600121
108	8	0	-5.638185	-1.510409	-0.453284
109	6	0	-3.055213	1.574590	1.699780
110	6	0	-3.385224	1.116450	2.989740
111	6	0	-2.951709	2.960207	1.483729
112	6	0	-3.598544	2.018737	4.031720
113	1	0	-3.471525	0.049596	3.174266
114	6	0	-3.175766	3.857939	2.526685
115	1	0	-2.695587	3.333698	0.498035
116	6	0	-3.495682	3.392363	3.804843
117	1	0	-3.851103	1.646212	5.020520
118	1	0	-3.100468	4.925174	2.338619
119	1	0	-3.667698	4.094559	4.615244

S-S



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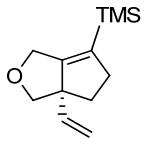
1	1	0	-5.202376	-0.954752	-1.163576
2	6	0	-5.029585	-0.320949	-0.290514
3	6	0	-6.055387	-0.054880	0.520398
4	1	0	-7.051387	-0.439136	0.317497
5	1	0	-5.942454	0.557165	1.411557
6	6	0	-3.318631	1.414396	0.646595
7	6	0	-3.212377	1.428645	-0.860841
8	6	0	-2.627087	-0.989877	-0.080428
9	1	0	-2.390066	1.432062	1.208503
10	1	0	-4.141330	1.953012	1.107543
11	1	0	-3.981847	1.952976	-1.420939
12	1	0	-2.218338	1.455829	-1.295817
13	1	0	-2.815937	-1.601604	0.819024
14	1	0	-2.769513	-1.647756	-0.957092
15	6	0	-0.336358	-1.525401	0.030141
16	1	0	-0.444719	-2.225550	-0.816908
17	1	0	-0.493634	-2.116668	0.949450
18	6	0	-3.624036	0.160710	-0.133072
19	6	0	1.010525	-0.958801	0.031133

20	6	0	2.144365	-0.515779	0.032671
21	8	0	-1.301454	-0.490409	-0.060317
22	6	0	4.975522	-1.003918	-0.934238
23	1	0	6.005654	-0.626449	-0.958718
24	1	0	4.996455	-1.999122	-0.475358
25	1	0	4.637576	-1.120867	-1.970332
26	6	0	3.810109	1.868804	-0.811155
27	1	0	3.452802	1.793515	-1.844565
28	1	0	3.146658	2.560126	-0.279263
29	1	0	4.811807	2.316541	-0.834909
30	6	0	4.453237	0.339407	1.810934
31	1	0	4.481758	-0.634490	2.313261
32	1	0	5.465232	0.762694	1.844424
33	1	0	3.797358	0.996312	2.393719
34	14	0	3.851868	0.175377	0.026092

P-S



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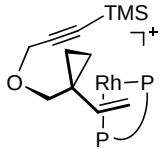
3	6	0	-1.477021	-1.283330	1.283017
4	6	0	-0.051203	-1.646051	0.783608
5	6	0	0.472565	-0.327501	0.191531
6	6	0	-0.838437	1.906851	-0.401717
7	6	0	-2.618915	1.100317	0.886413
8	6	0	-2.662028	-0.621339	-0.919553
9	6	0	-2.955968	-1.871134	-1.283668
10	1	0	-2.157265	-2.139204	1.320551
11	1	0	-1.405569	-0.878300	2.300084
12	1	0	0.583565	-2.026298	1.594024
13	1	0	-0.083528	-2.434751	0.017315
14	1	0	-0.776458	2.125292	-1.475505
15	1	0	-0.149079	2.585660	0.119814
16	1	0	-3.712124	1.082076	0.854077
17	1	0	-2.292905	1.287379	1.922730
18	1	0	-2.962512	0.196705	-1.574966

19	1	0	-3.485044	-2.070807	-2.211835
20	1	0	-2.692595	-2.740320	-0.687432
21	8	0	-2.193279	2.156134	0.014705
22	6	0	2.587133	1.705554	-0.870617
23	1	0	2.042874	1.827007	-1.814602
24	1	0	2.278167	2.514508	-0.198431
25	1	0	3.653154	1.849936	-1.086268
26	6	0	2.966168	-1.333640	-1.285439
27	1	0	4.043279	-1.207798	-1.452325
28	1	0	2.809924	-2.343033	-0.886223
29	1	0	2.469661	-1.283428	-2.261806
30	6	0	3.234427	-0.116885	1.542298
31	1	0	3.097135	-1.094554	2.019672
32	1	0	4.311962	0.027203	1.393440
33	1	0	2.892066	0.648415	2.249070
34	14	0	2.302245	-0.004486	-0.106527

(*S*)-IN-S1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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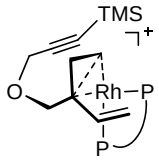
3	6	0	-3.347528	-1.574920	2.158166
4	6	0	-4.730156	-1.454534	2.089647
5	6	0	-2.356444	-0.688274	-1.403183
6	6	0	-1.496667	0.414126	-1.609425
7	6	0	-0.663842	0.424134	-2.743697
8	6	0	-0.734714	-0.592076	-3.682249
9	1	0	-2.888874	-1.914437	3.079759
10	1	0	-5.331636	-1.714870	2.957733
11	1	0	0.035429	1.237408	-2.901281
12	1	0	-0.099226	-0.549941	-4.563995
13	6	0	-5.259541	-0.124269	-1.450743
14	6	0	-6.882074	-0.887914	0.929847
15	6	0	-7.443725	-0.033039	-0.210220
16	6	0	-6.764018	-0.412147	-1.527967
17	1	0	-5.113854	0.965540	-1.446127

18	1	0	-4.755334	-0.481980	-2.352568
19	1	0	-7.293177	-1.905760	0.849628
20	1	0	-7.219865	-0.507527	1.901707
21	1	0	-8.529518	-0.166018	-0.273389
22	1	0	-7.263327	1.030378	-0.001088
23	1	0	-6.933053	-1.478657	-1.734477
24	1	0	-7.198113	0.143460	-2.367214
25	6	0	-5.365413	-0.991616	0.933672
26	6	0	-4.588772	-0.681896	-0.202627
27	6	0	-1.620639	-2.757892	-4.582474
28	6	0	-2.829308	-3.691853	-4.489764
29	6	0	-3.006345	-4.143975	-3.039872
30	6	0	-3.311369	-2.945481	-2.131288
31	1	0	-1.564867	-2.287508	-5.572173
32	1	0	-3.735207	-3.170020	-4.828547
33	1	0	-2.689405	-4.549361	-5.157297
34	1	0	-3.816086	-4.877344	-2.950984
35	1	0	-2.087416	-4.641103	-2.701633
36	1	0	-4.355678	-2.644313	-2.293586
37	1	0	-3.256827	-3.251141	-1.081433
38	1	0	-0.699859	-3.351982	-4.480341
39	6	0	-2.402847	-1.741790	-2.358983
40	6	0	-1.605287	-1.674901	-3.517140
41	6	0	-2.713421	2.295702	0.490658
42	6	0	-3.747691	2.939556	-0.209502
43	6	0	-2.804848	2.186926	1.885026
44	6	0	-4.859334	3.433702	0.472751
45	1	0	-3.682624	3.077512	-1.283613
46	6	0	-3.916467	2.684219	2.566807
47	1	0	-1.988248	1.721976	2.428506
48	6	0	-4.947820	3.305081	1.861463
49	1	0	-5.649668	3.933854	-0.079978
50	1	0	-3.972169	2.592891	3.647904
51	1	0	-5.809927	3.700886	2.390707
52	6	0	-0.797773	3.235701	-1.394547
53	6	0	-0.004441	4.276879	-0.889598
54	6	0	-1.413121	3.418093	-2.648400
55	6	0	0.185654	5.453827	-1.616285
56	1	0	0.465597	4.189184	0.079478
57	6	0	-1.224036	4.595439	-3.372183
58	1	0	-2.036065	2.637837	-3.071704
59	6	0	-0.420420	5.616159	-2.861492
60	1	0	0.808077	6.242429	-1.203473
61	1	0	-1.706695	4.711411	-4.338461

62	1	0	-0.271668	6.530677	-3.428050
63	6	0	-0.076334	-2.601081	0.161696
64	6	0	1.035431	-2.389750	-0.665554
65	6	0	-0.644576	-3.884167	0.237056
66	6	0	1.578321	-3.445561	-1.401488
67	1	0	1.468371	-1.395526	-0.738303
68	6	0	-0.097351	-4.938014	-0.494978
69	1	0	-1.507044	-4.061364	0.873970
70	6	0	1.015198	-4.719818	-1.314208
71	1	0	2.439667	-3.272078	-2.040279
72	1	0	-0.535778	-5.929414	-0.423617
73	1	0	1.440840	-5.542886	-1.881227
74	6	0	-0.302197	-1.687608	2.919701
75	6	0	-0.682361	-0.828733	3.970816
76	6	0	0.485825	-2.809630	3.223126
77	6	0	-0.303955	-1.098749	5.285389
78	1	0	-1.288353	0.047729	3.762880
79	6	0	0.870612	-3.071780	4.540467
80	1	0	0.801330	-3.485066	2.436104
81	6	0	0.477483	-2.221138	5.573703
82	1	0	-0.618324	-0.432437	6.083789
83	1	0	1.477525	-3.946620	4.755653
84	1	0	0.776652	-2.429195	6.596810
85	15	0	-1.170401	1.738844	-0.360226
86	15	0	-0.718164	-1.216999	1.182368
87	45	0	0.388032	0.894947	1.039429
88	1	0	2.185926	2.931267	0.286782
89	6	0	2.053725	2.347711	1.193037
90	6	0	1.075090	2.705395	2.112449
91	1	0	0.455068	3.582365	1.962213
92	1	0	1.102678	2.354130	3.143453
93	6	0	2.938582	0.248604	2.513980
94	6	0	3.886651	1.380234	2.773047
95	6	0	3.945240	0.981827	0.224738
96	1	0	3.343015	-0.731715	2.280397
97	1	0	2.021447	0.215631	3.099043
98	1	0	3.599121	2.134824	3.498938
99	1	0	4.952771	1.175712	2.729402
100	1	0	4.686081	0.209707	0.476715
101	1	0	3.284174	0.572035	-0.559139
102	6	0	5.368417	1.952322	-1.421649
103	1	0	5.683878	2.953433	-1.733731
104	1	0	4.740652	1.535873	-2.227937
105	6	0	6.539698	1.094401	-1.210790

106	6	0	7.512351	0.381604	-1.035449
107	6	0	3.141031	1.360434	1.453922
108	8	0	4.584683	2.154987	-0.247629
109	14	0	9.029527	-0.651858	-0.799981
110	6	0	8.656894	-2.409983	-1.384610
111	1	0	9.537409	-3.052178	-1.259542
112	1	0	7.834684	-2.858585	-0.815083
113	1	0	8.380598	-2.427960	-2.445068
114	6	0	9.470047	-0.645189	1.037372
115	1	0	10.376573	-1.236016	1.217696
116	1	0	9.658572	0.372176	1.398330
117	1	0	8.666958	-1.074838	1.647279
118	6	0	10.421439	0.108096	-1.823821
119	1	0	11.343088	-0.477227	-1.717284
120	1	0	10.166128	0.136781	-2.889157
121	1	0	10.638037	1.133457	-1.503696

(*S*)-TS-S1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.572120	-1.381745	-0.189693
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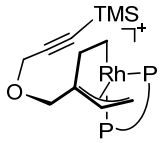
3	6	0	-2.634047	-2.130430	2.118618
4	6	0	-3.970427	-2.476268	1.963683
5	6	0	-1.781224	-0.937715	-1.390708
6	6	0	-1.379812	0.404468	-1.566505
7	6	0	-0.549036	0.726049	-2.657443
8	6	0	-0.193195	-0.239011	-3.585631
9	1	0	-2.153849	-2.300465	3.074755
10	1	0	-4.505685	-2.919890	2.800294
11	1	0	-0.194412	1.741847	-2.793218
12	1	0	0.426477	0.039323	-4.435282
13	6	0	-4.677923	-1.394844	-1.626970
14	6	0	-6.106648	-2.664607	0.659609
15	6	0	-6.846435	-2.041826	-0.528377
16	6	0	-5.994579	-2.163932	-1.794035
17	1	0	-4.899820	-0.317886	-1.636870

18	1	0	-4.027525	-1.565815	-2.488932
19	1	0	-6.147544	-3.761029	0.571404
20	1	0	-6.615075	-2.424047	1.601381
21	1	0	-7.818192	-2.531309	-0.658412
22	1	0	-7.047910	-0.980900	-0.326115
23	1	0	-5.786620	-3.224676	-1.994928
24	1	0	-6.532631	-1.778051	-2.667611
25	6	0	-4.646548	-2.254669	0.760789
26	6	0	-3.943644	-1.701278	-0.328610
27	6	0	-0.189211	-2.571831	-4.508458
28	6	0	-0.999016	-3.870259	-4.479954
29	6	0	-1.088516	-4.379074	-3.040519
30	6	0	-1.837612	-3.375046	-2.154583
31	1	0	-0.242249	-2.099824	-5.497534
32	1	0	-2.009462	-3.691579	-4.873497
33	1	0	-0.531932	-4.615081	-5.134034
34	1	0	-1.599503	-5.347848	-2.996596
35	1	0	-0.075313	-4.535862	-2.647758
36	1	0	-2.911777	-3.452831	-2.374178
37	1	0	-1.734400	-3.657425	-1.102104
38	1	0	0.873173	-2.808957	-4.345733
39	6	0	-1.397794	-1.926839	-2.339128
40	6	0	-0.618789	-1.565632	-3.454438
41	6	0	-3.272683	1.696941	0.498771
42	6	0	-4.462757	1.947203	-0.205004
43	6	0	-3.328848	1.543028	1.890481
44	6	0	-5.681458	2.008100	0.470003
45	1	0	-4.439655	2.118620	-1.276382
46	6	0	-4.548552	1.606528	2.566363
47	1	0	-2.406579	1.385781	2.440857
48	6	0	-5.727444	1.835842	1.856424
49	1	0	-6.594055	2.207503	-0.084796
50	1	0	-4.575666	1.485271	3.645602
51	1	0	-6.676998	1.895281	2.380688
52	6	0	-1.830745	3.279980	-1.350217
53	6	0	-1.571526	4.536251	-0.778989
54	6	0	-2.366678	3.240689	-2.650463
55	6	0	-1.814956	5.714405	-1.487196
56	1	0	-1.197372	4.608853	0.234418
57	6	0	-2.610677	4.418810	-3.357820
58	1	0	-2.590931	2.289133	-3.120053
59	6	0	-2.330986	5.659182	-2.781853
60	1	0	-1.604141	6.673305	-1.022450
61	1	0	-3.022438	4.363812	-4.361655

62	1	0	-2.519787	6.574357	-3.335303
63	6	0	0.873416	-2.180498	0.384929
64	6	0	1.897941	-1.713698	-0.449633
65	6	0	0.681658	-3.566891	0.519221
66	6	0	2.730097	-2.611081	-1.123503
67	1	0	2.034802	-0.644734	-0.583379
68	6	0	1.518224	-4.462508	-0.147376
69	1	0	-0.116618	-3.946237	1.151141
70	6	0	2.546757	-3.985749	-0.966285
71	1	0	3.520512	-2.235707	-1.766949
72	1	0	1.367795	-5.531711	-0.027534
73	1	0	3.198743	-4.684784	-1.482358
74	6	0	0.181268	-1.336777	3.092547
75	6	0	-0.477679	-0.573923	4.076056
76	6	0	1.155392	-2.257395	3.505589
77	6	0	-0.191850	-0.748613	5.428870
78	1	0	-1.226015	0.157090	3.784770
79	6	0	1.448196	-2.423886	4.862932
80	1	0	1.694052	-2.850452	2.775699
81	6	0	0.775294	-1.676207	5.827466
82	1	0	-0.721457	-0.158509	6.171602
83	1	0	2.205749	-3.143322	5.160580
84	1	0	1.002584	-1.809564	6.881076
85	15	0	-1.617637	1.749758	-0.317900
86	15	0	-0.176082	-0.982731	1.311559
87	45	0	0.353391	1.423633	0.964430
88	1	0	1.022353	3.889223	-0.036228
89	6	0	1.268902	3.352451	0.874718
90	6	0	0.389195	3.341453	1.978511
91	1	0	-0.512389	3.943245	1.959670
92	1	0	0.738248	3.106905	2.981162
93	6	0	2.319921	0.996390	2.117048
94	6	0	3.217999	2.210889	2.129971
95	6	0	3.193385	2.306194	-0.413320
96	1	0	2.762952	0.092681	1.711746
97	1	0	1.723575	0.850083	3.015482
98	1	0	3.066128	2.886919	2.971416
99	1	0	4.280458	2.030526	1.968606
100	1	0	3.585419	1.279245	-0.422187
101	1	0	2.516842	2.426131	-1.272720
102	6	0	5.230020	2.957432	-1.475423
103	1	0	5.884897	3.834423	-1.492993
104	1	0	4.747436	2.885004	-2.463438
105	6	0	6.009121	1.745545	-1.201607

106	6	0	6.663075	0.744161	-0.965686
107	6	0	2.477338	2.572835	0.893325
108	8	0	4.255280	3.244680	-0.468919
109	6	0	9.358084	-0.490834	-1.562979
110	1	0	10.031553	-1.338682	-1.387256
111	1	0	9.186730	-0.418839	-2.642872
112	1	0	9.877648	0.419797	-1.244675
113	6	0	8.045464	-0.810224	1.240608
114	1	0	8.541623	0.095659	1.606461
115	1	0	7.109149	-0.928819	1.798301
116	1	0	8.688631	-1.664454	1.485535
117	6	0	6.842121	-2.278921	-1.211958
118	1	0	5.894638	-2.422072	-0.679214
119	1	0	6.625882	-2.230795	-2.285677
120	1	0	7.459068	-3.169015	-1.037488
121	14	0	7.740069	-0.722877	-0.621084

(*S*)-IN-S2



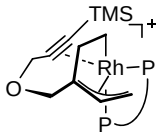
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.920199	1.052331	0.075637
2	6	0	3.055094	-0.058321	-0.794392
3	6	0	4.013448	-0.007312	-1.817641
4	6	0	4.789289	1.129187	-1.998826
5	6	0	2.036349	0.961984	1.292803
6	6	0	0.629445	1.100568	1.207551
7	6	0	-0.142401	0.895883	2.370064
8	6	0	0.470006	0.659790	3.593271
9	1	0	4.160608	-0.853443	-2.477993
10	1	0	5.529656	1.147400	-2.795447
11	1	0	-1.224017	0.957688	2.324668
12	1	0	-0.144228	0.543039	4.483410
13	6	0	3.490970	3.449669	0.739545
14	6	0	5.525798	3.459834	-1.438254
15	6	0	5.047073	4.743434	-0.753761
16	6	0	4.657521	4.444460	0.695537
17	1	0	2.582545	3.959735	0.388901

18	1	0	3.280696	3.159226	1.772237
19	1	0	6.536701	3.216578	-1.077262
20	1	0	5.626177	3.611699	-2.520034
21	1	0	5.833461	5.504909	-0.802157
22	1	0	4.176788	5.147922	-1.288299
23	1	0	5.524401	4.030627	1.230470
24	1	0	4.372058	5.362342	1.222288
25	6	0	4.634638	2.255007	-1.184735
26	6	0	3.697015	2.218543	-0.133552
27	6	0	2.468777	0.344102	5.079011
28	6	0	3.959342	0.685308	5.150342
29	6	0	4.683656	0.024403	3.976709
30	6	0	4.169607	0.569563	2.636416
31	1	0	1.900247	0.911149	5.826492
32	1	0	4.097086	1.774809	5.108698
33	1	0	4.372686	0.349876	6.108042
34	1	0	5.765469	0.188975	4.038152
35	1	0	4.526597	-1.060746	4.020080
36	1	0	4.622521	1.555513	2.463814
37	1	0	4.527685	-0.063176	1.817713
38	1	0	2.333371	-0.716602	5.340522
39	6	0	2.653172	0.704546	2.546759
40	6	0	1.861806	0.584431	3.707481
41	6	0	0.509593	2.374568	-1.590472
42	6	0	0.579614	3.760486	-1.371617
43	6	0	0.919789	1.863414	-2.829405
44	6	0	1.080509	4.606355	-2.360778
45	1	0	0.219893	4.185060	-0.439493
46	6	0	1.418799	2.710284	-3.820763
47	1	0	0.835775	0.798044	-3.018599
48	6	0	1.503789	4.082938	-3.586107
49	1	0	1.125050	5.676965	-2.181176
50	1	0	1.731362	2.299550	-4.776678
51	1	0	1.882625	4.745754	-4.358850
52	6	0	-1.822182	2.203121	-0.011834
53	6	0	-2.898772	2.085717	-0.906270
54	6	0	-1.917135	3.141334	1.030402
55	6	0	-4.044227	2.868463	-0.757518
56	1	0	-2.832665	1.401754	-1.747204
57	6	0	-3.067178	3.918066	1.183937
58	1	0	-1.095873	3.270734	1.727608
59	6	0	-4.133802	3.782543	0.293765
60	1	0	-4.864129	2.764304	-1.461834
61	1	0	-3.123742	4.635618	1.997719

62	1	0	-5.025434	4.391165	0.413399
63	6	0	2.861891	-2.484349	0.780471
64	6	0	2.243394	-2.668829	2.024363
65	6	0	4.169416	-2.968861	0.594415
66	6	0	2.895114	-3.365267	3.045326
67	1	0	1.254646	-2.261995	2.205181
68	6	0	4.820440	-3.659582	1.615871
69	1	0	4.678671	-2.817127	-0.352707
70	6	0	4.179457	-3.870248	2.840110
71	1	0	2.395587	-3.513623	3.998600
72	1	0	5.826263	-4.036385	1.454069
73	1	0	4.682945	-4.419513	3.630502
74	6	0	2.288855	-2.619794	-2.079906
75	6	0	2.126731	-2.074670	-3.366624
76	6	0	2.508257	-4.002231	-1.963536
77	6	0	2.210605	-2.881372	-4.500762
78	1	0	1.950166	-1.011005	-3.489061
79	6	0	2.582948	-4.809816	-3.101593
80	1	0	2.629653	-4.457414	-0.987104
81	6	0	2.439072	-4.253627	-4.372155
82	1	0	2.096639	-2.436834	-5.485448
83	1	0	2.758849	-5.875719	-2.988505
84	1	0	2.502949	-4.882040	-5.255574
85	15	0	-0.296967	1.224610	-0.392476
86	15	0	2.009551	-1.575408	-0.583300
87	45	0	-0.322212	-1.300805	-0.363784
88	1	0	-2.850304	-0.697112	-1.783616
89	6	0	-2.298576	-1.590649	-1.508525
90	6	0	-1.065991	-1.906564	-2.206919
91	1	0	-0.792292	-1.253443	-3.032213
92	1	0	-0.807414	-2.948081	-2.389198
93	6	0	-0.513210	-3.333284	0.161842
94	6	0	-2.014444	-3.594594	0.001997
95	6	0	-3.870936	-1.827955	0.438362
96	1	0	-0.195849	-3.418979	1.203426
97	1	0	0.107180	-3.990026	-0.452159
98	1	0	-2.235579	-4.343753	-0.769054
99	1	0	-2.464972	-3.969971	0.925225
100	1	0	-3.549213	-1.635492	1.478299
101	1	0	-4.306254	-0.898862	0.045815
102	6	0	-5.898355	-2.728852	1.320769
103	1	0	-5.514918	-2.579281	2.344158
104	1	0	-6.427363	-3.687444	1.302588
105	6	0	-6.815002	-1.640774	0.966729

106	6	0	-7.594584	-0.747952	0.684332
107	6	0	-2.687822	-2.280945	-0.381398
108	8	0	-4.807730	-2.891450	0.414120
109	6	0	-7.974461	1.878315	-0.774663
110	1	0	-7.125238	2.315259	-0.236760
111	1	0	-7.601925	1.457418	-1.715930
112	1	0	-8.669155	2.689643	-1.024199
113	6	0	-9.456576	1.315775	1.890905
114	1	0	-10.202837	2.094867	1.691924
115	1	0	-9.927669	0.560189	2.529618
116	1	0	-8.639544	1.772898	2.460821
117	6	0	-10.252037	-0.230665	-0.688425
118	1	0	-10.749719	-1.008364	-0.098279
119	1	0	-11.006615	0.519440	-0.955652
120	1	0	-9.895604	-0.692106	-1.616300
121	14	0	-8.836040	0.560764	0.275040

(*S*)-IN-S2'/(*S*) -IN2' -TMS



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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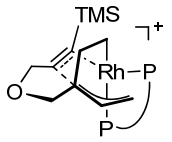
3	6	0	1.649835	0.878018	2.889248
4	6	0	2.341454	-0.012416	3.698934
5	6	0	2.321288	-0.633716	-0.545994
6	6	0	1.313874	-1.188062	-1.367409
7	6	0	1.561914	-1.308078	-2.748341
8	6	0	2.777441	-0.932487	-3.295006
9	1	0	1.189086	1.748038	3.341744
10	1	0	2.414651	0.183850	4.766560
11	1	0	0.796215	-1.702177	-3.406617
12	1	0	2.946043	-1.060139	-4.362061
13	6	0	3.493408	-2.653882	1.196172
14	6	0	3.675809	-2.095605	4.119483
15	6	0	3.951510	-3.481960	3.530660
16	6	0	4.513837	-3.338465	2.115081
17	1	0	2.677485	-3.360989	0.987131

18	1	0	3.950210	-2.440782	0.225597
19	1	0	4.633428	-1.624422	4.388805
20	1	0	3.112197	-2.177718	5.057134
21	1	0	4.646120	-4.029547	4.177644
22	1	0	3.020001	-4.063386	3.495689
23	1	0	5.441512	-2.749148	2.149021
24	1	0	4.779264	-4.316447	1.696977
25	6	0	2.938085	-1.162399	3.173293
26	6	0	2.874167	-1.392131	1.785342
27	6	0	5.091772	0.026006	-3.167189
28	6	0	6.251966	0.206386	-2.185676
29	6	0	5.785235	1.062020	-1.007406
30	6	0	4.656933	0.362593	-0.237316
31	1	0	5.345062	-0.707392	-3.942793
32	1	0	6.591052	-0.773407	-1.821256
33	1	0	7.104731	0.667351	-2.696665
34	1	0	6.612696	1.269611	-0.319004
35	1	0	5.432872	2.032949	-1.379722
36	1	0	5.093907	-0.446499	0.365254
37	1	0	4.217670	1.058419	0.483208
38	1	0	4.922118	0.975958	-3.696866
39	6	0	3.560931	-0.222721	-1.122059
40	6	0	3.790951	-0.387012	-2.499739
41	6	0	-0.392022	-2.348457	0.843013
42	6	0	-0.055527	-3.702206	1.011558
43	6	0	-0.751494	-1.603371	1.973768
44	6	0	-0.065925	-4.284707	2.280569
45	1	0	0.197933	-4.316449	0.155296
46	6	0	-0.747134	-2.180517	3.243673
47	1	0	-1.046777	-0.569359	1.854488
48	6	0	-0.406849	-3.525464	3.401286
49	1	0	0.186309	-5.335905	2.388678
50	1	0	-1.014285	-1.580645	4.109066
51	1	0	-0.416130	-3.980491	4.387669
52	6	0	-0.901317	-3.040848	-1.871844
53	6	0	-2.264120	-3.320752	-2.055641
54	6	0	0.039998	-3.962647	-2.366700
55	6	0	-2.677761	-4.471937	-2.729119
56	1	0	-3.010668	-2.643602	-1.662540
57	6	0	-0.374448	-5.112119	-3.040957
58	1	0	1.101523	-3.789439	-2.228355
59	6	0	-1.733836	-5.368850	-3.228909
60	1	0	-3.738661	-4.665018	-2.860720
61	1	0	0.369845	-5.808692	-3.416401

62	1	0	-2.053496	-6.262929	-3.756175
63	6	0	1.857941	2.905038	-0.273598
64	6	0	1.964025	3.144728	-1.649982
65	6	0	2.771049	3.540605	0.588571
66	6	0	2.936566	4.013888	-2.154849
67	1	0	1.299193	2.646824	-2.344277
68	6	0	3.740932	4.407310	0.087047
69	1	0	2.719895	3.362835	1.658613
70	6	0	3.822591	4.651518	-1.287560
71	1	0	2.997509	4.189065	-3.225375
72	1	0	4.432275	4.893971	0.769337
73	1	0	4.574700	5.331779	-1.676912
74	6	0	-0.307679	2.944130	1.611800
75	6	0	-1.114015	2.441707	2.650497
76	6	0	-0.284951	4.335577	1.410543
77	6	0	-1.837512	3.299631	3.479856
78	1	0	-1.170962	1.373512	2.828068
79	6	0	-1.021346	5.193237	2.232748
80	1	0	0.318472	4.761516	0.616530
81	6	0	-1.794735	4.680678	3.274483
82	1	0	-2.435178	2.886178	4.287750
83	1	0	-0.979563	6.265067	2.060090
84	1	0	-2.358000	5.348516	3.919737
85	15	0	-0.428736	-1.571699	-0.842861
86	15	0	0.540225	1.792658	0.426949
87	6	0	-2.751327	2.214456	-2.443091
88	6	0	-3.659926	2.797278	0.355825
89	6	0	-3.367040	3.477168	-1.893187
90	6	0	-3.689631	1.134776	-2.975334
91	6	0	-3.203484	-0.194117	-2.399849
92	45	0	-1.674662	0.494430	-1.147755
93	1	0	-4.703826	1.359557	-2.634517
94	1	0	-3.700267	1.151730	-4.074554
95	1	0	-2.801318	-0.890431	-3.135238
96	1	0	-3.959516	-0.688193	-1.791663
97	1	0	-4.409418	2.930269	1.143420
98	1	0	-2.799590	3.433139	0.597777
99	1	0	-3.958226	3.963285	-2.678895
100	1	0	-2.587008	4.180597	-1.563568
101	6	0	-1.375541	2.148128	-2.651929
102	6	0	-0.720517	0.942640	-3.047561
103	1	0	-1.172779	0.304845	-3.802403
104	1	0	0.362978	0.937193	-3.068708
105	1	0	-0.777998	2.985550	-2.298513

106	6	0	-3.277999	1.362978	0.354681
107	6	0	-3.315563	0.147020	0.624737
108	8	0	-4.286755	3.232429	-0.838237
109	6	0	-6.150952	-0.789200	0.741570
110	1	0	-6.905476	-1.407834	1.243429
111	1	0	-6.454187	0.258562	0.844487
112	1	0	-6.176507	-1.040409	-0.325362
113	6	0	-4.428241	-0.620994	3.318650
114	1	0	-5.148907	-1.234653	3.873226
115	1	0	-3.443888	-0.777045	3.772807
116	1	0	-4.707801	0.429059	3.459842
117	6	0	-4.008756	-2.922934	1.293875
118	1	0	-3.957873	-3.244002	0.249493
119	1	0	-3.067208	-3.191683	1.778412
120	1	0	-4.806921	-3.506596	1.771407
121	14	0	-4.443527	-1.103105	1.491198

(S)-TS-S2/(*S*) -S2-TMS



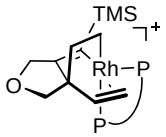
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.377833	1.020800	0.614697
2	6	0	-2.650181	-0.218403	1.249674
3	6	0	-3.208801	-0.197759	2.536817
4	6	0	-3.476087	1.003979	3.179460
5	6	0	-1.968015	1.049810	-0.838313
6	6	0	-0.633630	1.086455	-1.312703
7	6	0	-0.415427	1.068874	-2.705127
8	6	0	-1.464492	1.048648	-3.605187
9	1	0	-3.431065	-1.129759	3.045081
10	1	0	-3.911507	0.992164	4.176681
11	1	0	0.595003	1.113950	-3.094037
12	1	0	-1.256622	1.049933	-4.672766
13	6	0	-2.386913	3.571199	0.571681
14	6	0	-3.551282	3.509051	3.318258
15	6	0	-2.916212	4.768297	2.721566
16	6	0	-3.106405	4.770320	1.203399

17	1	0	-1.304094	3.759839	0.599566
18	1	0	-2.647188	3.498669	-0.489905
19	1	0	-4.645717	3.625152	3.315891
20	1	0	-3.268110	3.395534	4.372277
21	1	0	-3.360626	5.661049	3.175990
22	1	0	-1.842651	4.790956	2.954757
23	1	0	-4.179797	4.726744	0.970581
24	1	0	-2.726255	5.698207	0.760049
25	6	0	-3.206223	2.232548	2.568159
26	6	0	-2.667058	2.244754	1.267427
27	6	0	-3.902088	1.072294	-4.194947
28	6	0	-5.224044	1.627011	-3.660408
29	6	0	-5.558655	0.934894	-2.338983
30	6	0	-4.482595	1.208058	-1.279741
31	1	0	-3.569163	1.629092	-5.079455
32	1	0	-5.139741	2.711813	-3.505216
33	1	0	-6.018938	1.472716	-4.398841
34	1	0	-6.528684	1.270651	-1.954257
35	1	0	-5.644041	-0.145875	-2.507459
36	1	0	-4.613667	2.232205	-0.898726
37	1	0	-4.646117	0.555277	-0.420053
38	1	0	-4.061905	0.036495	-4.531894
39	6	0	-3.045441	1.077832	-1.777659
40	6	0	-2.790235	1.068137	-3.161363
41	6	0	0.805646	1.704173	1.365479
42	6	0	1.158351	2.993926	1.800585
43	6	0	0.374458	0.772160	2.321836
44	6	0	1.081030	3.333583	3.153999
45	1	0	1.495868	3.739751	1.091701
46	6	0	0.289325	1.114948	3.669767
47	1	0	0.075878	-0.220878	2.015192
48	6	0	0.648521	2.397285	4.092225
49	1	0	1.363717	4.334038	3.469006
50	1	0	-0.061293	0.380740	4.388992
51	1	0	0.591406	2.662096	5.144063
52	6	0	1.710802	2.757798	-1.155348
53	6	0	3.093108	2.979854	-1.074139
54	6	0	0.897020	3.758263	-1.714523
55	6	0	3.654117	4.167471	-1.545034
56	1	0	3.730486	2.223282	-0.635625
57	6	0	1.460819	4.944314	-2.187266
58	1	0	-0.175109	3.616592	-1.783838
59	6	0	2.839186	5.151637	-2.106838
60	1	0	4.727314	4.320621	-1.475446

61	1	0	0.818584	5.706864	-2.618493
62	1	0	3.274781	6.074395	-2.478978
63	6	0	-3.770523	-2.268317	-0.521879
64	6	0	-3.643606	-2.765380	-1.827198
65	6	0	-5.053093	-2.190158	0.047265
66	6	0	-4.766044	-3.187561	-2.546043
67	1	0	-2.658195	-2.831200	-2.282237
68	6	0	-6.175193	-2.605844	-0.669718
69	1	0	-5.173568	-1.809242	1.057545
70	6	0	-6.033301	-3.109170	-1.967025
71	1	0	-4.648976	-3.579888	-3.552655
72	1	0	-7.160266	-2.543469	-0.215252
73	1	0	-6.907589	-3.439478	-2.521049
74	6	0	-2.238798	-3.080004	1.760292
75	6	0	-1.480969	-2.887466	2.930099
76	6	0	-2.866632	-4.325256	1.584044
77	6	0	-1.375492	-3.887801	3.896516
78	1	0	-0.980730	-1.939567	3.104529
79	6	0	-2.753629	-5.330201	2.547188
80	1	0	-3.454331	-4.516109	0.692433
81	6	0	-2.012058	-5.116141	3.709065
82	1	0	-0.794868	-3.705773	4.797070
83	1	0	-3.255038	-6.281078	2.387963
84	1	0	-1.930401	-5.896495	4.460274
85	15	0	0.994579	1.225023	-0.410389
86	15	0	-2.220682	-1.821638	0.393286
87	6	0	3.467722	-2.397541	-2.206868
88	6	0	5.548232	-2.845949	-0.585052
89	6	0	4.356813	-3.639867	-2.328036
90	6	0	3.795731	-1.218548	-3.126050
91	6	0	3.219470	0.053667	-2.488780
92	1	0	4.881335	-1.158446	-3.249017
93	1	0	3.376982	-1.420859	-4.121980
94	1	0	2.551317	0.604253	-3.153267
95	1	0	4.007097	0.729270	-2.162847
96	1	0	6.517967	-2.435051	-0.298002
97	1	0	5.276980	-3.651903	0.118741
98	1	0	4.419364	-3.927573	-3.383028
99	1	0	3.927646	-4.478896	-1.756326
100	6	0	2.043543	-2.718719	-2.056306
101	6	0	1.000977	-1.984054	-2.565874
102	1	0	1.138335	-1.230800	-3.329628
103	1	0	-0.021261	-2.272348	-2.344057
104	1	0	1.806940	-3.590140	-1.446094

105	6	0	4.495465	-1.764844	-0.529912
106	6	0	4.186487	-0.723526	0.165629
107	8	0	5.661410	-3.350969	-1.892302
108	45	0	2.248518	-0.751052	-0.777682
109	6	0	1.577375	-1.813020	0.814705
110	8	0	1.435541	-2.568814	1.661422
111	6	0	6.759031	-0.604507	1.813905
112	1	0	7.349219	-0.363551	0.921959
113	1	0	7.261292	-0.135593	2.669501
114	1	0	6.800477	-1.687690	1.973804
115	6	0	5.058165	1.934780	1.663988
116	1	0	5.599274	2.315585	0.790644
117	1	0	4.069470	2.401538	1.695780
118	1	0	5.606835	2.270469	2.553454
119	6	0	4.003985	-0.529405	3.211568
120	1	0	2.989042	-0.119718	3.224277
121	1	0	3.933420	-1.622112	3.256082
122	1	0	4.508234	-0.194197	4.126716
123	14	0	4.986379	0.052022	1.709374

(*S*)-IN-S3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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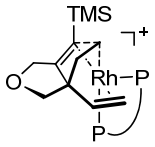
2	6	0	-2.037479	-0.536391	1.381307
3	6	0	-2.394438	-0.604906	2.735719
4	6	0	-3.218517	0.365287	3.292706
5	6	0	-2.319232	0.509111	-0.897941
6	6	0	-1.095033	0.890015	-1.494398
7	6	0	-0.969625	0.793135	-2.893717
8	6	0	-2.030184	0.369717	-3.677783
9	1	0	-2.028563	-1.412669	3.359438
10	1	0	-3.496961	0.289937	4.341589
11	1	0	-0.044768	1.070999	-3.382896
12	1	0	-1.908879	0.324321	-4.757716
13	6	0	-3.786644	2.735295	0.351988

14	6	0	-4.584496	2.470930	3.212530
15	6	0	-4.702607	3.790753	2.444079
16	6	0	-4.963020	3.507137	0.962890
17	1	0	-2.925822	3.415311	0.269574
18	1	0	-4.021399	2.436950	-0.673544
19	1	0	-5.586774	2.029058	3.320537
20	1	0	-4.227334	2.648106	4.234469
21	1	0	-5.503750	4.401182	2.875589
22	1	0	-3.771531	4.364897	2.546321
23	1	0	-5.888481	2.922629	0.859801
24	1	0	-5.115975	4.438694	0.405814
25	6	0	-3.686744	1.446181	2.538636
26	6	0	-3.345099	1.531004	1.173695
27	6	0	-4.371506	-0.455628	-4.029719
28	6	0	-5.753932	-0.439241	-3.373169
29	6	0	-5.667738	-1.109668	-2.001752
30	6	0	-4.728855	-0.329744	-1.072137
31	1	0	-4.362857	0.155623	-4.940724
32	1	0	-6.103943	0.596214	-3.259006
33	1	0	-6.478484	-0.949221	-4.017782
34	1	0	-6.656922	-1.180440	-1.534783
35	1	0	-5.298986	-2.136784	-2.123065
36	1	0	-5.247473	0.580482	-0.739309
37	1	0	-4.543949	-0.908446	-0.162181
38	1	0	-4.142996	-1.482033	-4.355000
39	6	0	-3.400968	0.064626	-1.710831
40	6	0	-3.255445	0.008492	-3.109652
41	6	0	0.064008	2.406481	0.895584
42	6	0	-0.201147	3.782831	0.789204
43	6	0	0.114688	1.836714	2.175670
44	6	0	-0.416314	4.555577	1.931846
45	1	0	-0.214870	4.269872	-0.177656
46	6	0	-0.100458	2.607423	3.317291
47	1	0	0.310726	0.777858	2.286832
48	6	0	-0.364558	3.972579	3.198941
49	1	0	-0.610194	5.619294	1.827186
50	1	0	-0.056781	2.140026	4.296568
51	1	0	-0.520604	4.578848	4.086537
52	6	0	1.221524	2.578330	-1.760064
53	6	0	2.605175	2.601775	-1.981043
54	6	0	0.417758	3.524841	-2.426669
55	6	0	3.175089	3.552032	-2.832889
56	1	0	3.238340	1.869980	-1.494166
57	6	0	0.990326	4.477080	-3.268521

58	1	0	-0.660945	3.507920	-2.308855
59	6	0	2.372324	4.494525	-3.473411
60	1	0	4.249283	3.549488	-2.994820
61	1	0	0.353788	5.199009	-3.772034
62	1	0	2.816191	5.232829	-4.134910
63	6	0	-1.861137	-2.867790	-0.365902
64	6	0	-1.430086	-3.249557	-1.643909
65	6	0	-3.082382	-3.372753	0.115227
66	6	0	-2.182751	-4.137903	-2.415357
67	1	0	-0.510359	-2.840389	-2.047126
68	6	0	-3.831082	-4.265519	-0.652637
69	1	0	-3.448374	-3.069604	1.092124
70	6	0	-3.379451	-4.654557	-1.917252
71	1	0	-1.833344	-4.424681	-3.403236
72	1	0	-4.767132	-4.656524	-0.263799
73	1	0	-3.961989	-5.352121	-2.512206
74	6	0	-0.314116	-2.761648	2.117753
75	6	0	0.642189	-2.213073	2.992652
76	6	0	-0.760882	-4.069737	2.357835
77	6	0	1.116818	-2.934863	4.086849
78	1	0	1.026266	-1.209701	2.824341
79	6	0	-0.277634	-4.797720	3.449688
80	1	0	-1.481526	-4.532723	1.693483
81	6	0	0.656156	-4.233741	4.318645
82	1	0	1.848313	-2.485598	4.752647
83	1	0	-0.635903	-5.809523	3.616961
84	1	0	1.027687	-4.801818	5.166425
85	15	0	0.459600	1.364299	-0.584776
86	15	0	-0.823128	-1.736494	0.659175
87	6	0	3.972962	-2.008976	-1.277921
88	6	0	5.963961	-0.644455	-0.903400
89	6	0	5.313444	-2.706823	-1.606490
90	6	0	3.103383	-1.753046	-2.519005
91	6	0	1.924375	-0.827955	-2.196757
92	45	0	1.594647	-0.683441	-0.129540
93	1	0	3.736184	-1.307080	-3.294666
94	1	0	2.745682	-2.711934	-2.916339
95	1	0	0.968093	-1.193902	-2.578777
96	1	0	2.100837	0.175957	-2.575727
97	1	0	6.322778	0.310942	-1.293295
98	1	0	6.532593	-0.882206	0.008774
99	1	0	5.265945	-3.360333	-2.481244
100	1	0	5.674920	-3.294608	-0.745311
101	6	0	3.164760	-2.658282	-0.176103

102	6	0	1.943276	-3.231402	-0.301374
103	1	0	1.462696	-3.367175	-1.262643
104	1	0	1.474394	-3.715954	0.546412
105	1	0	3.650672	-2.691405	0.797895
106	6	0	4.454374	-0.691423	-0.662823
107	6	0	3.579347	0.083317	0.002908
108	8	0	6.201458	-1.638081	-1.897552
109	6	0	6.029770	1.347992	1.547492
110	1	0	6.463390	0.384455	1.834453
111	1	0	6.547916	1.704501	0.651188
112	1	0	6.260807	2.057451	2.352881
113	6	0	3.494024	0.613819	3.019325
114	1	0	2.408326	0.692333	3.122234
115	1	0	3.779246	-0.437553	3.146978
116	1	0	3.937982	1.177815	3.849201
117	6	0	3.628343	3.115191	1.184806
118	1	0	4.122299	3.584621	0.327008
119	1	0	2.555044	3.289437	1.090665
120	1	0	3.967744	3.646840	2.083579
121	14	0	4.138196	1.301809	1.369376

(*S*)-TS-S3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	-1.458536	-1.048543	2.875894
4	6	0	-2.306903	-0.336458	3.714699
5	6	0	-2.570970	0.212114	-0.528276
6	6	0	-1.585904	0.785176	-1.360199
7	6	0	-1.758473	0.726062	-2.756231
8	6	0	-2.911473	0.189967	-3.304869
9	1	0	-0.785714	-1.780567	3.306063
10	1	0	-2.288422	-0.535939	4.783904
11	1	0	-0.999607	1.127992	-3.418077
12	1	0	-3.037202	0.185887	-4.385433

13	6	0	-4.090730	1.998526	1.280228
14	6	0	-4.072458	1.382221	4.194384
15	6	0	-4.678732	2.671085	3.630535
16	6	0	-5.224839	2.419158	2.223146
17	1	0	-3.440514	2.868408	1.106806
18	1	0	-4.490211	1.733518	0.298275
19	1	0	-4.886808	0.701533	4.486114
20	1	0	-3.514854	1.587956	5.116408
21	1	0	-5.466749	3.033519	4.300193
22	1	0	-3.910919	3.455592	3.587000
23	1	0	-5.992631	1.633187	2.262761
24	1	0	-5.713596	3.316582	1.826663
25	6	0	-3.171567	0.643091	3.218037
26	6	0	-3.215920	0.879236	1.828867
27	6	0	-5.154694	-0.922791	-3.167709
28	6	0	-6.319068	-1.165466	-2.204701
29	6	0	-5.801768	-1.897848	-0.965712
30	6	0	-4.782804	-1.034720	-0.209548
31	1	0	-5.457434	-0.260522	-3.988583
32	1	0	-6.768707	-0.207343	-1.908680
33	1	0	-7.104109	-1.742139	-2.706471
34	1	0	-6.623827	-2.157453	-0.288717
35	1	0	-5.333034	-2.841885	-1.272437
36	1	0	-5.330508	-0.261200	0.345389
37	1	0	-4.278222	-1.639054	0.551699
38	1	0	-4.876422	-1.877358	-3.639619
39	6	0	-3.738048	-0.371330	-1.101441
40	6	0	-3.920266	-0.346685	-2.495796
41	6	0	-0.224214	2.395049	0.824653
42	6	0	-0.853197	3.649543	0.886039
43	6	0	0.310434	1.857681	2.004251
44	6	0	-0.955777	4.334826	2.098482
45	1	0	-1.242863	4.114904	-0.011178
46	6	0	0.196806	2.535128	3.217635
47	1	0	0.832273	0.908986	1.962888
48	6	0	-0.435331	3.778951	3.268249
49	1	0	-1.434096	5.309965	2.122832
50	1	0	0.612614	2.097035	4.120551
51	1	0	-0.509810	4.316871	4.209032
52	6	0	0.237646	2.899497	-1.980145
53	6	0	1.503350	3.297012	-2.427080
54	6	0	-0.881307	3.635218	-2.421392
55	6	0	1.657547	4.388933	-3.285383
56	1	0	2.379946	2.758354	-2.104050

57	6	0	-0.727863	4.728945	-3.272045
58	1	0	-1.881283	3.346175	-2.116841
59	6	0	0.542958	5.109791	-3.709286
60	1	0	2.651690	4.671684	-3.619734
61	1	0	-1.605565	5.279945	-3.597844
62	1	0	0.659992	5.958503	-4.376774
63	6	0	-1.377333	-2.863008	-0.550313
64	6	0	-1.426333	-2.878630	-1.950776
65	6	0	-2.197205	-3.754303	0.166284
66	6	0	-2.236431	-3.797017	-2.623526
67	1	0	-0.848965	-2.158638	-2.519962
68	6	0	-3.001805	-4.673824	-0.506508
69	1	0	-2.201554	-3.736590	1.252288
70	6	0	-3.014044	-4.704960	-1.904258
71	1	0	-2.257700	-3.799377	-3.709681
72	1	0	-3.617882	-5.365872	0.060613
73	1	0	-3.634147	-5.427643	-2.426986
74	6	0	0.715000	-2.783405	1.491526
75	6	0	1.572874	-2.179220	2.430635
76	6	0	0.746160	-4.181362	1.364447
77	6	0	2.405842	-2.950164	3.240071
78	1	0	1.596468	-1.098910	2.529139
79	6	0	1.594810	-4.951633	2.165896
80	1	0	0.112691	-4.681369	0.641224
81	6	0	2.421174	-4.341926	3.108903
82	1	0	3.045203	-2.463451	3.971365
83	1	0	1.601937	-6.031747	2.050585
84	1	0	3.073833	-4.942956	3.735321
85	15	0	0.032714	1.494368	-0.778284
86	15	0	-0.279586	-1.692005	0.374715
87	45	0	1.484843	-0.388219	-0.790533
88	6	0	4.182988	-1.687549	-1.184223
89	6	0	5.383051	-1.122258	0.858196
90	6	0	5.450220	-2.537772	-0.929319
91	6	0	4.212406	-0.744294	-2.398122
92	6	0	3.157741	0.347985	-2.170917
93	1	0	5.210664	-0.299938	-2.468647
94	1	0	4.035354	-1.291295	-3.331827
95	1	0	2.360847	0.374948	-2.925859
96	1	0	3.598281	1.339702	-2.130551
97	1	0	5.921030	-0.302969	1.335092
98	1	0	5.059765	-1.830181	1.642551
99	1	0	6.024138	-2.743419	-1.836177
100	1	0	5.189582	-3.495903	-0.451672

101	6	0	2.893248	-2.433039	-1.091158
102	6	0	1.884288	-2.404903	-2.016516
103	1	0	2.010414	-1.979939	-3.005886
104	1	0	1.038222	-3.067417	-1.893086
105	1	0	2.775668	-3.063039	-0.212958
106	6	0	4.199720	-0.711818	0.004165
107	6	0	3.359673	0.343861	-0.015799
108	8	0	6.266306	-1.756250	-0.060416
109	6	0	4.073841	1.572575	2.730948
110	1	0	4.604872	0.646623	2.974012
111	1	0	4.595590	2.393076	3.239746
112	1	0	3.069486	1.508488	3.163469
113	6	0	5.724621	2.285170	0.167027
114	1	0	6.193631	3.104392	0.726666
115	1	0	6.410118	1.433074	0.187504
116	1	0	5.648582	2.616401	-0.876706
117	6	0	3.090236	3.584189	0.646859
118	1	0	3.153596	3.967909	-0.374911
119	1	0	2.045481	3.594717	0.955374
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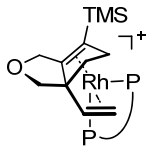
121	14	0	3.991654	1.941029	0.870553

(*S*)-IN-S4



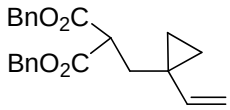
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.623320	-0.913030	0.383176
2	6	0	-1.569186	-1.380663	1.208165
3	6	0	-1.866780	-1.838914	2.497877
4	6	0	-3.176719	-1.826819	2.962187
5	6	0	-2.331775	-0.559512	-1.050810
6	6	0	-1.627094	0.616272	-1.391543
7	6	0	-1.215132	0.807715	-2.724592
8	6	0	-1.586943	-0.091214	-3.710463
9	1	0	-1.078572	-2.206623	3.145072
10	1	0	-3.391627	-2.201601	3.960487

11	1	0	-0.605310	1.662932	-2.994692
12	1	0	-1.281999	0.087162	-4.739057
13	6	0	-5.057915	-0.228171	0.052964
14	6	0	-5.634148	-1.363246	2.745568
15	6	0	-6.627522	-0.464512	2.001823
16	6	0	-6.467412	-0.645241	0.490390
17	1	0	-4.970455	0.863420	0.156514
18	1	0	-4.912564	-0.431854	-1.011060
19	1	0	-5.991648	-2.403350	2.701538
20	1	0	-5.603150	-1.105958	3.811444
21	1	0	-7.649336	-0.698707	2.320832
22	1	0	-6.445572	0.587156	2.262790
23	1	0	-6.647207	-1.696727	0.224312
24	1	0	-7.209194	-0.050953	-0.055552
25	6	0	-4.223142	-1.329624	2.180532
26	6	0	-3.945873	-0.857118	0.881294
27	6	0	-2.720258	-2.166998	-4.541322
28	6	0	-3.823073	-3.162090	-4.172622
29	6	0	-3.489133	-3.809162	-2.827808
30	6	0	-3.456264	-2.757024	-1.711134
31	1	0	-3.006273	-1.572769	-5.418185
32	1	0	-4.789795	-2.643820	-4.105298
33	1	0	-3.922479	-3.916917	-4.960568
34	1	0	-4.221159	-4.583148	-2.570011
35	1	0	-2.512282	-4.305343	-2.898012
36	1	0	-4.490913	-2.493143	-1.452411
37	1	0	-3.030730	-3.193080	-0.801847
38	1	0	-1.818332	-2.723832	-4.837308
39	6	0	-2.694330	-1.485773	-2.068017
40	6	0	-2.345922	-1.227920	-3.407789
41	6	0	-2.037398	2.065123	1.303155
42	6	0	-3.263088	2.738710	1.157085
43	6	0	-1.598038	1.724305	2.588479
44	6	0	-4.039832	3.037442	2.275660
45	1	0	-3.602956	3.051167	0.174618
46	6	0	-2.374634	2.029921	3.707496
47	1	0	-0.644683	1.222775	2.708783
48	6	0	-3.596894	2.684586	3.553555
49	1	0	-4.982784	3.562067	2.150020
50	1	0	-2.020094	1.760990	4.698456
51	1	0	-4.197118	2.931037	4.424727
52	6	0	-1.116812	3.492618	-0.927996
53	6	0	-0.547898	4.584787	-0.246486
54	6	0	-1.907420	3.756734	-2.059498

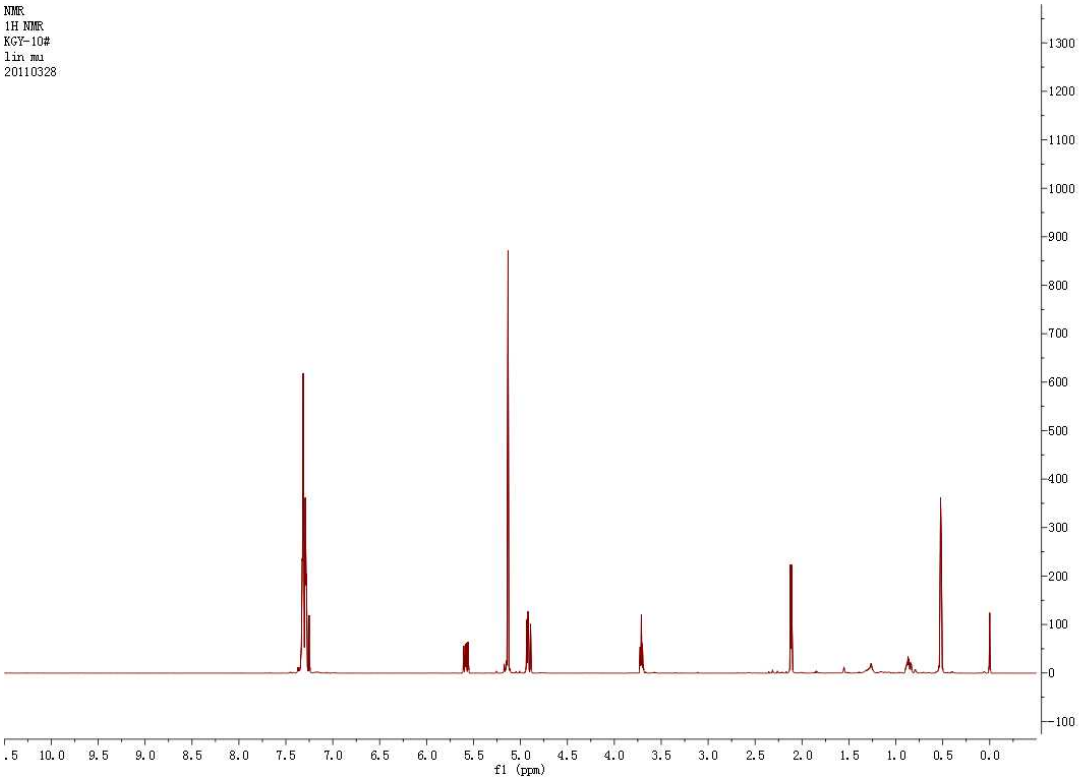
55	6	0	-0.720865	5.888887	-0.707420
56	1	0	0.013148	4.429438	0.668487
57	6	0	-2.082304	5.065455	-2.517046
58	1	0	-2.407124	2.952151	-2.584466
59	6	0	-1.481860	6.133577	-1.852384
60	1	0	-0.267550	6.713510	-0.164955
61	1	0	-2.697543	5.243912	-3.394309
62	1	0	-1.617213	7.149061	-2.212709
63	6	0	0.334334	-2.622407	-0.612339
64	6	0	1.081185	-2.412606	-1.778385
65	6	0	-0.273370	-3.874277	-0.409083
66	6	0	1.234667	-3.434418	-2.718632
67	1	0	1.538192	-1.445412	-1.955679
68	6	0	-0.108888	-4.898384	-1.342041
69	1	0	-0.871971	-4.050231	0.480272
70	6	0	0.647016	-4.680499	-2.498275
71	1	0	1.816588	-3.256283	-3.618437
72	1	0	-0.572293	-5.865424	-1.167671
73	1	0	0.773754	-5.479335	-3.223408
74	6	0	1.184980	-1.895034	2.087626
75	6	0	1.464392	-0.992156	3.130776
76	6	0	1.673671	-3.207325	2.190095
77	6	0	2.181701	-1.397247	4.256196
78	1	0	1.117560	0.034612	3.059314
79	6	0	2.399448	-3.608914	3.314299
80	1	0	1.491727	-3.923456	1.397180
81	6	0	2.649594	-2.710164	4.352201
82	1	0	2.377725	-0.687761	5.055328
83	1	0	2.767960	-4.628911	3.375969
84	1	0	3.210247	-3.027512	5.226636
85	15	0	-0.946058	1.808641	-0.164174
86	15	0	0.196689	-1.283798	0.646328
87	45	0	1.115081	0.960102	0.211184
88	6	0	3.639863	2.481147	-0.687468
89	6	0	3.434259	0.589159	-2.206299
90	6	0	3.659572	2.899648	-2.186920
91	6	0	4.858312	2.892986	0.186703
92	6	0	5.228789	1.609605	0.978772
93	1	0	5.695702	3.157218	-0.469456
94	1	0	4.653790	3.754985	0.829587
95	1	0	4.757917	1.576569	1.971306
96	1	0	6.307932	1.545880	1.165525
97	1	0	3.915523	-0.305086	-2.607151
98	1	0	2.338535	0.483885	-2.303858

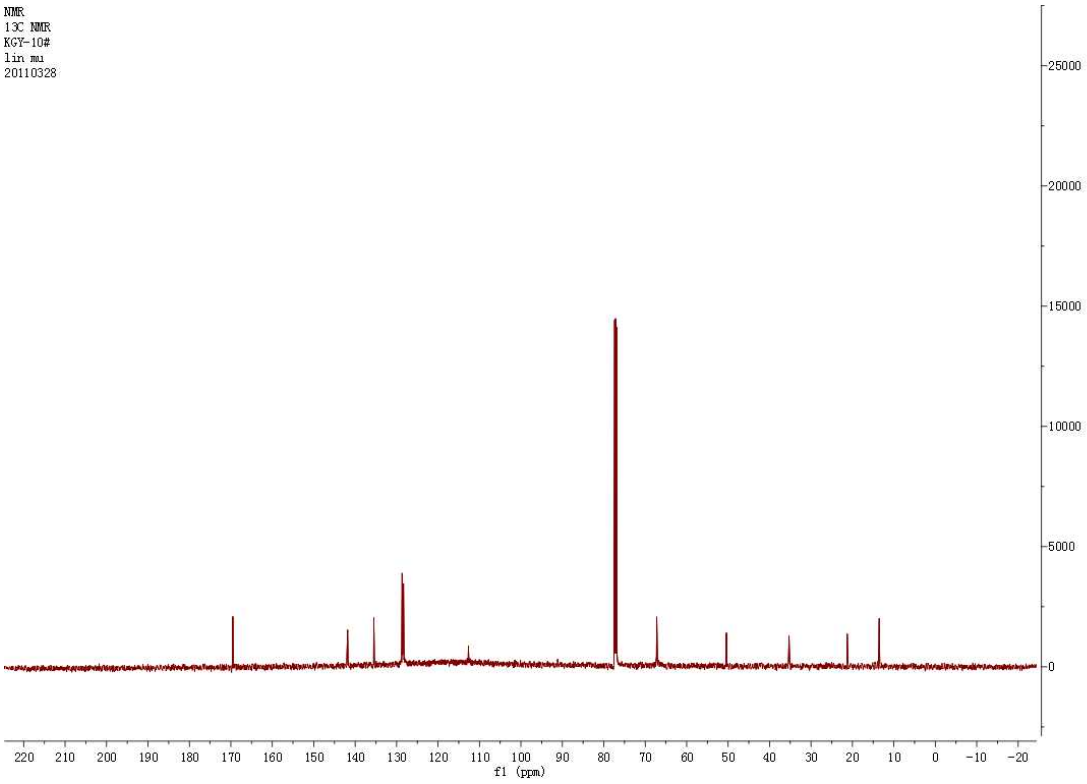
99	1	0	4.465813	3.598956	-2.425780
100	1	0	2.704429	3.357150	-2.484515
101	6	0	2.304392	2.836506	-0.037514
102	6	0	1.986659	2.598772	1.302745
103	1	0	2.695141	2.116110	1.974467
104	1	0	1.227269	3.187087	1.810720
105	1	0	1.714502	3.576841	-0.570023
106	6	0	3.858814	0.963364	-0.810600
107	6	0	4.745864	0.463831	0.079775
108	8	0	3.887074	1.712602	-2.962402
109	6	0	7.347858	-0.958367	-0.579176
110	1	0	7.912077	-0.180418	-0.051717
111	1	0	7.934540	-1.883609	-0.521584
112	1	0	7.287763	-0.668513	-1.634558
113	6	0	5.792516	-1.693317	1.994312
114	1	0	4.816432	-1.848331	2.467073
115	1	0	6.361533	-2.625833	2.094702
116	1	0	6.325336	-0.924074	2.565761
117	6	0	4.720275	-2.579098	-0.774816
118	1	0	3.689861	-2.711021	-0.428489
119	1	0	4.693620	-2.389743	-1.853952
120	1	0	5.240560	-3.534262	-0.629997
121	14	0	5.628465	-1.218607	0.171560

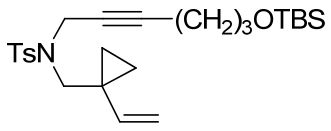
4. ^{1}H and ^{13}C-NMR Spectra for New Compounds



S9







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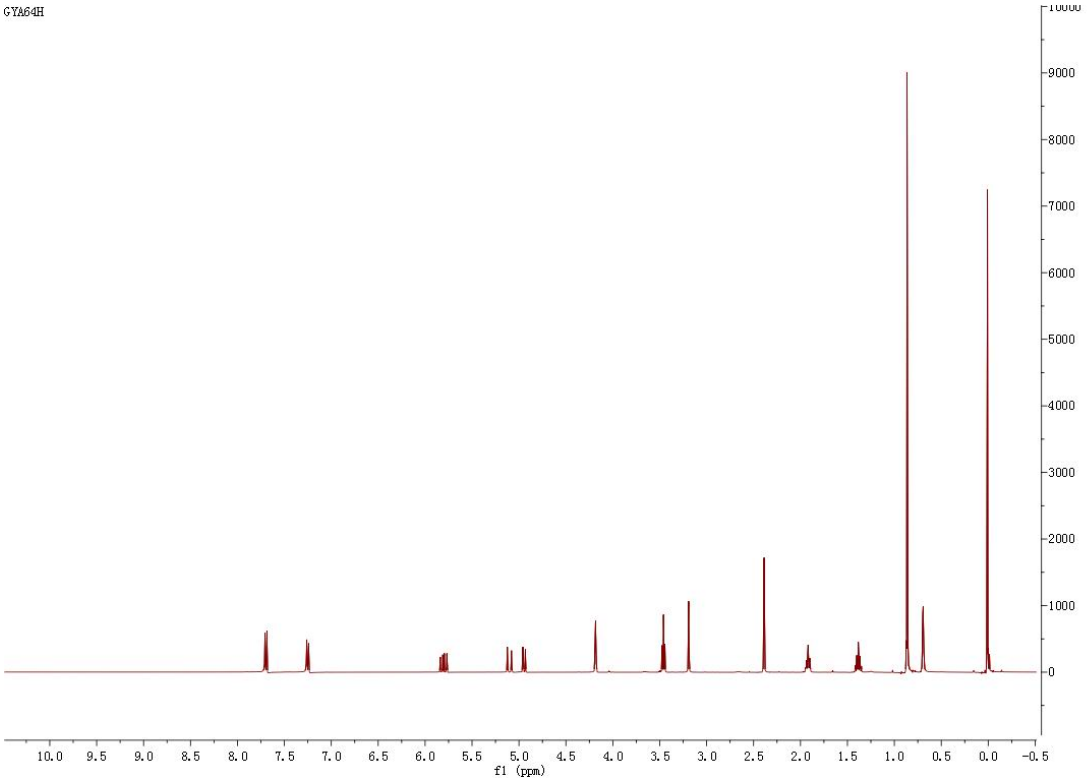

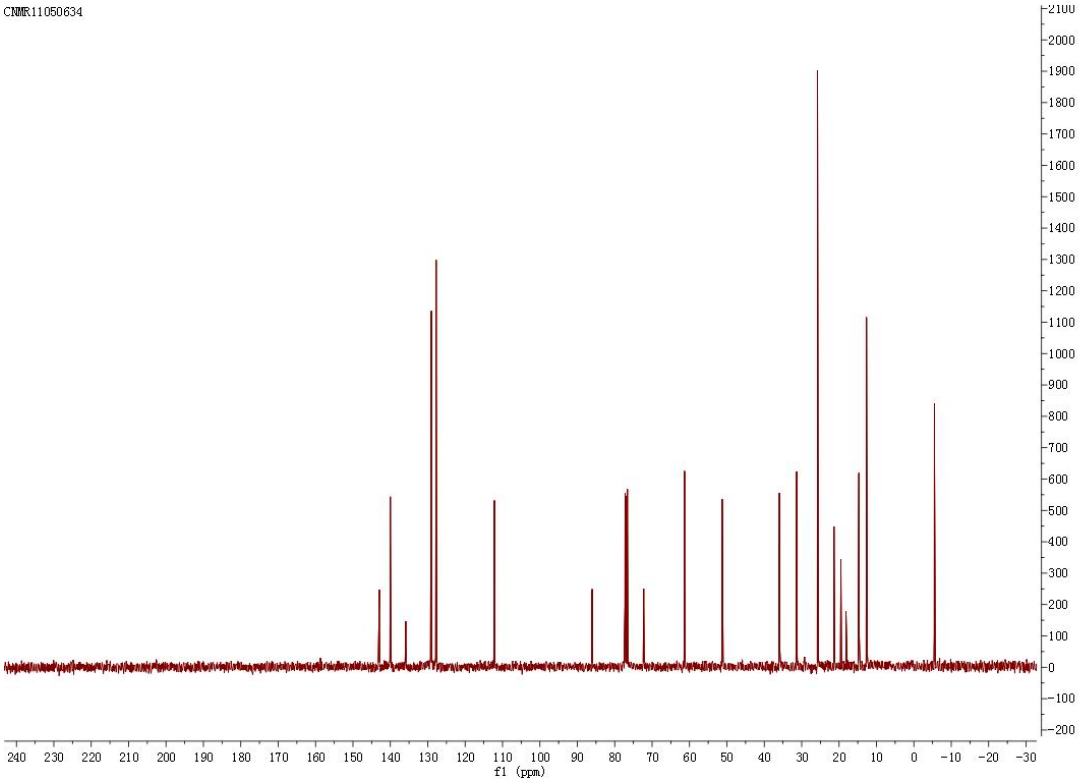

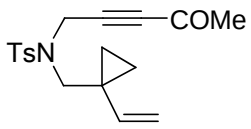

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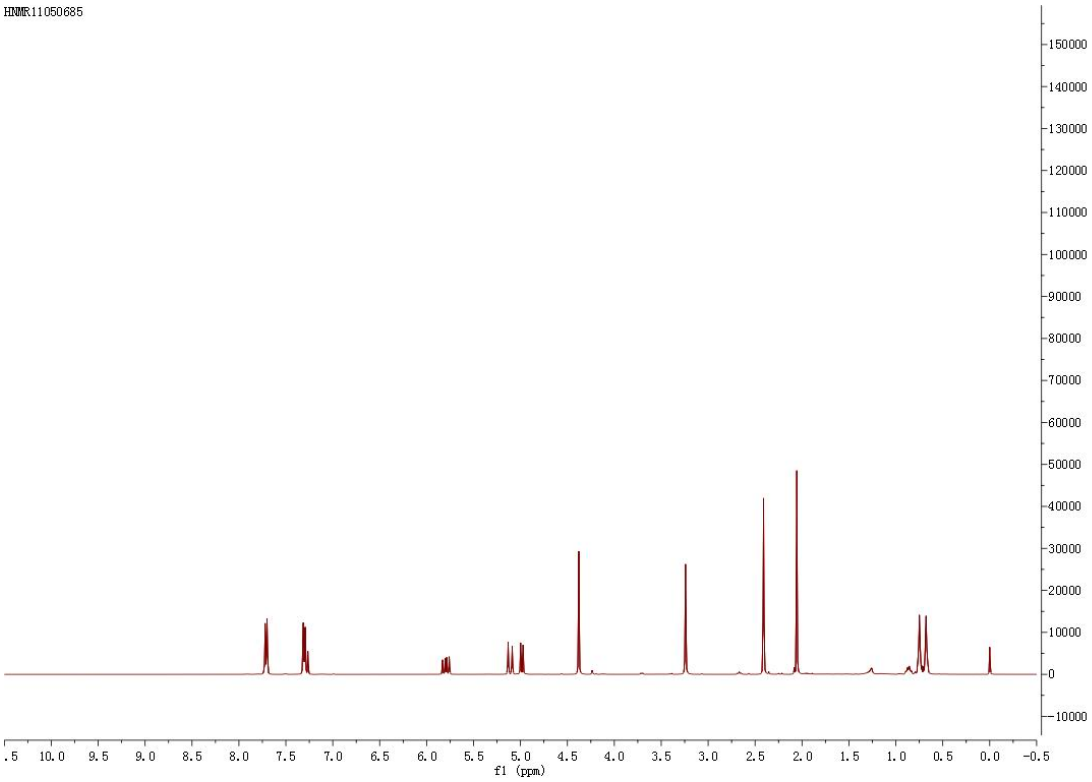

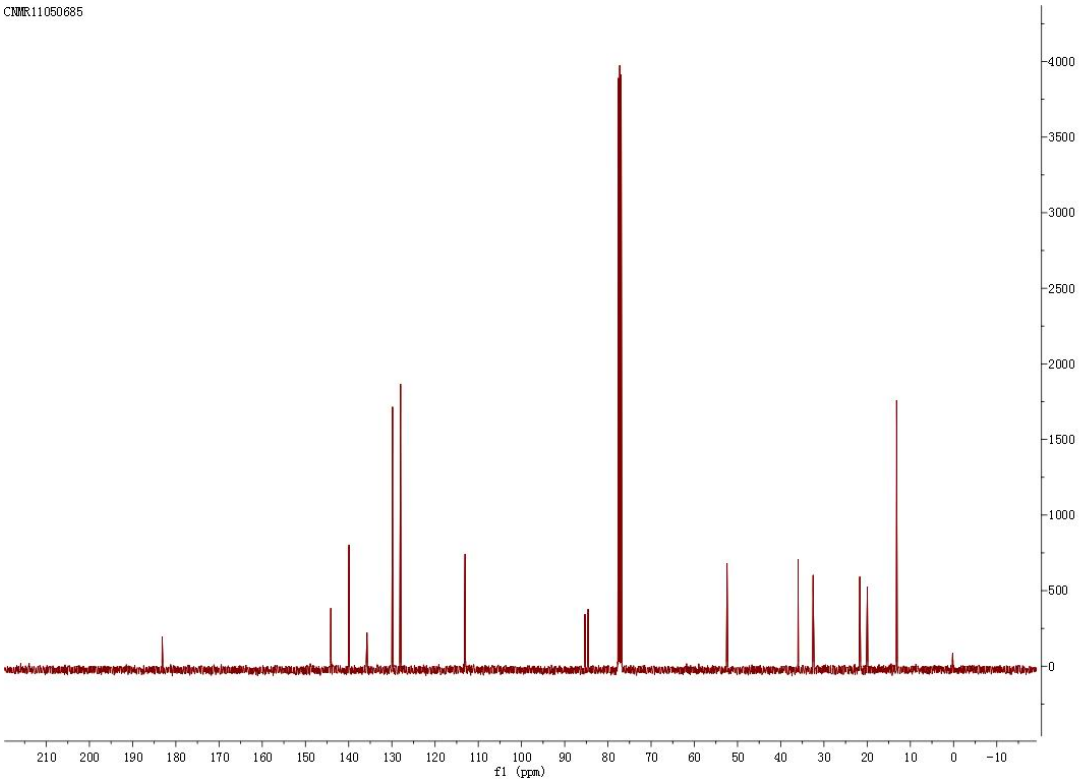

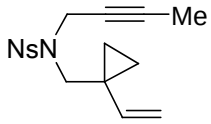

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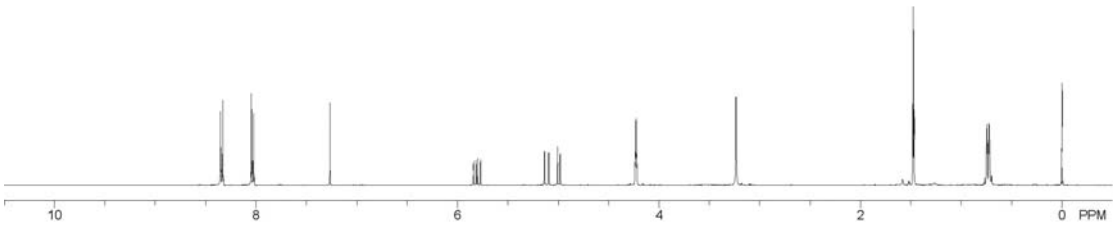

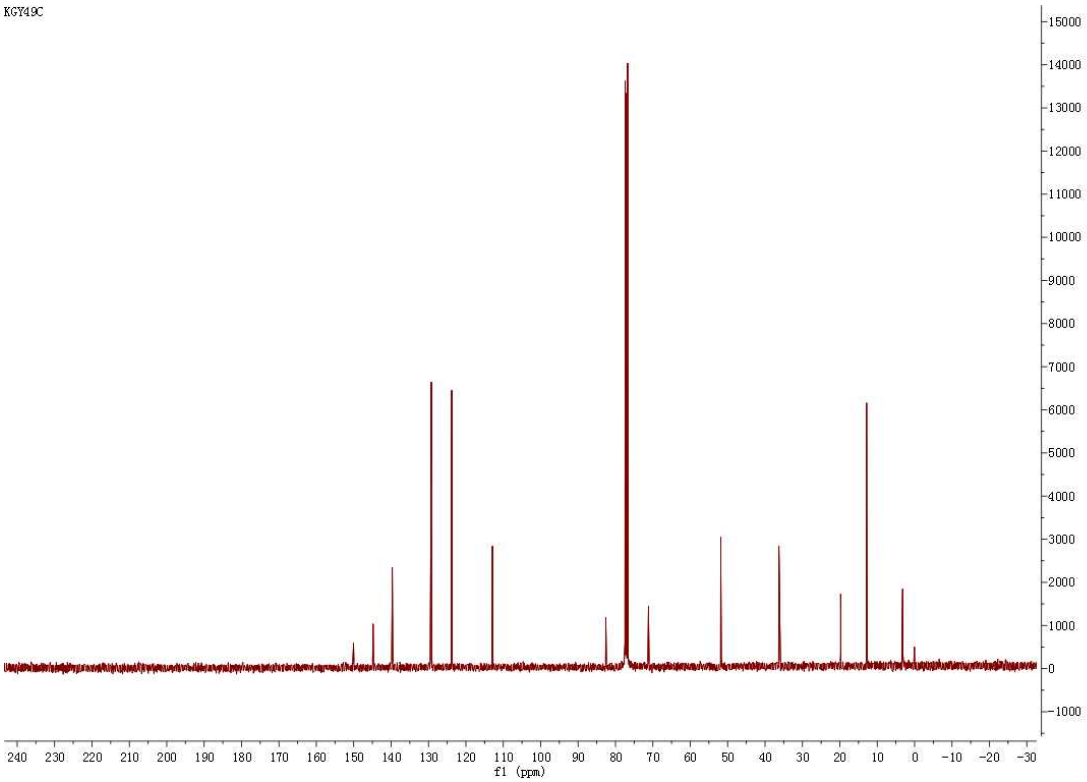

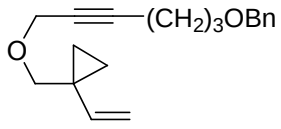

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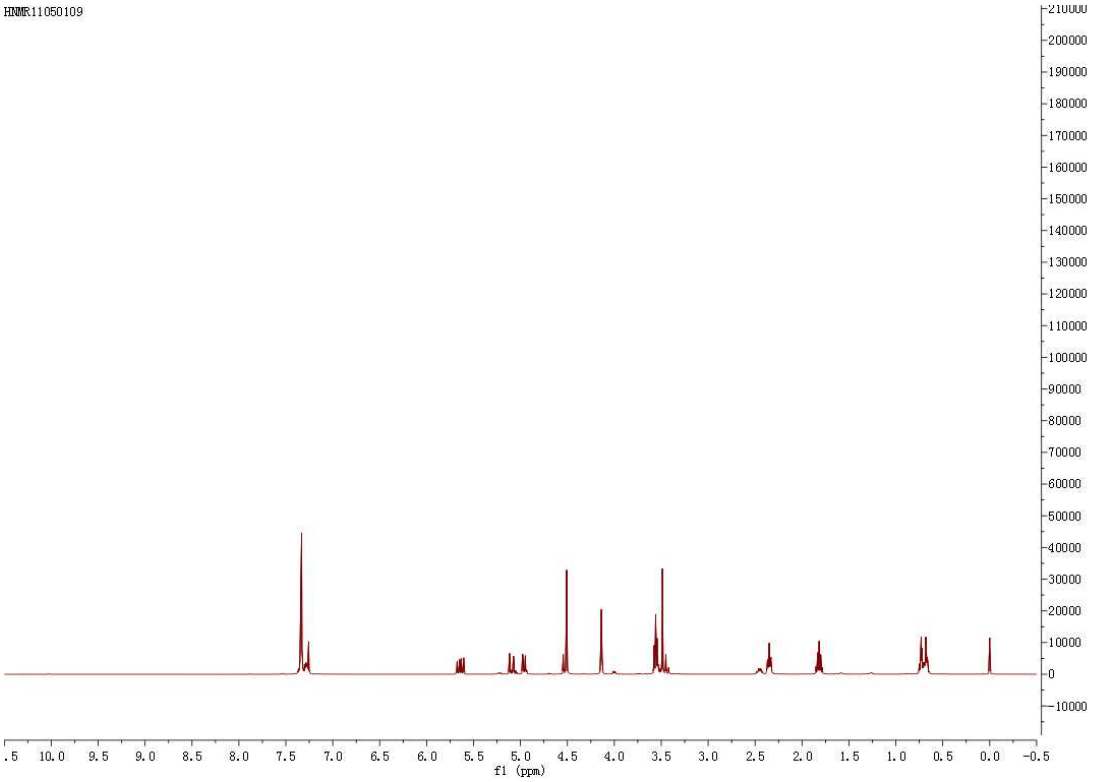
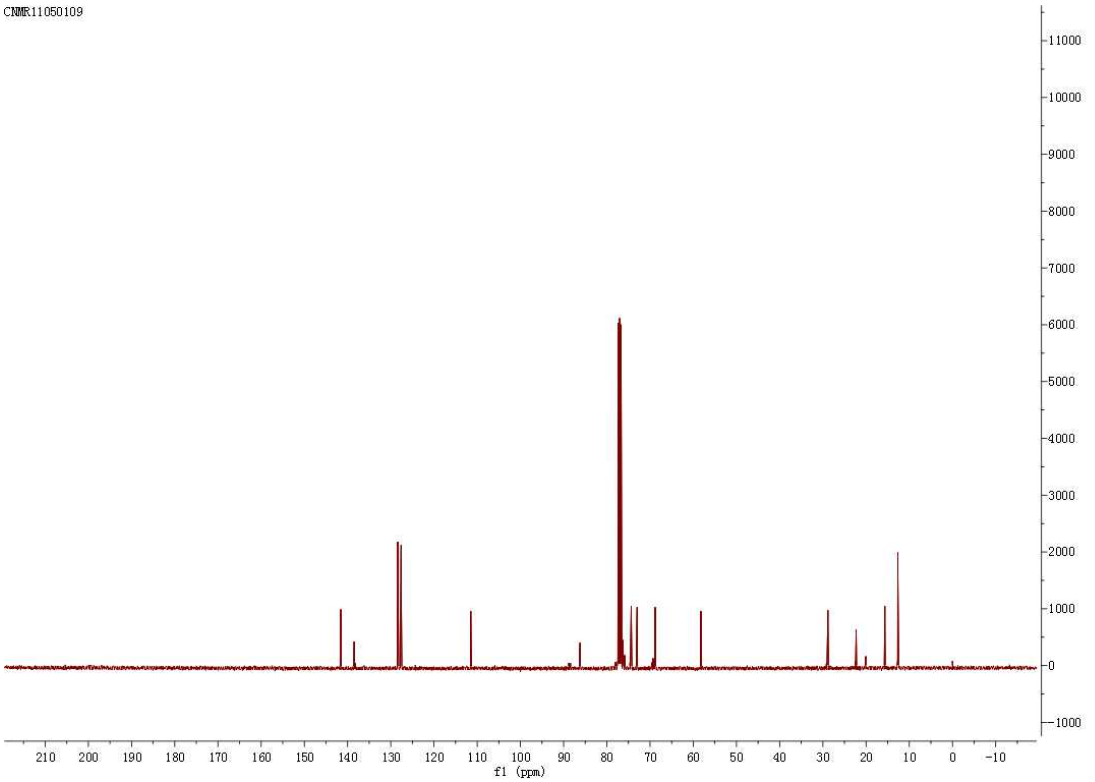
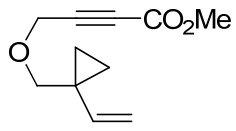
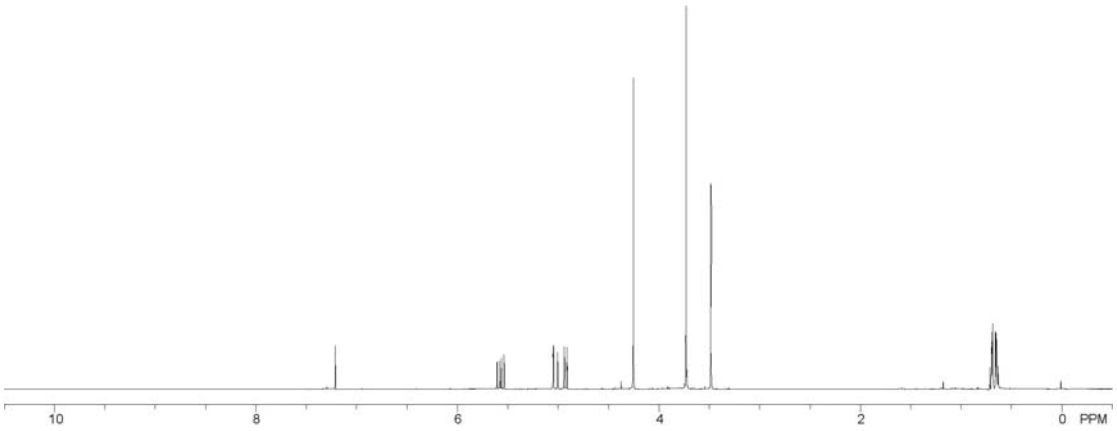
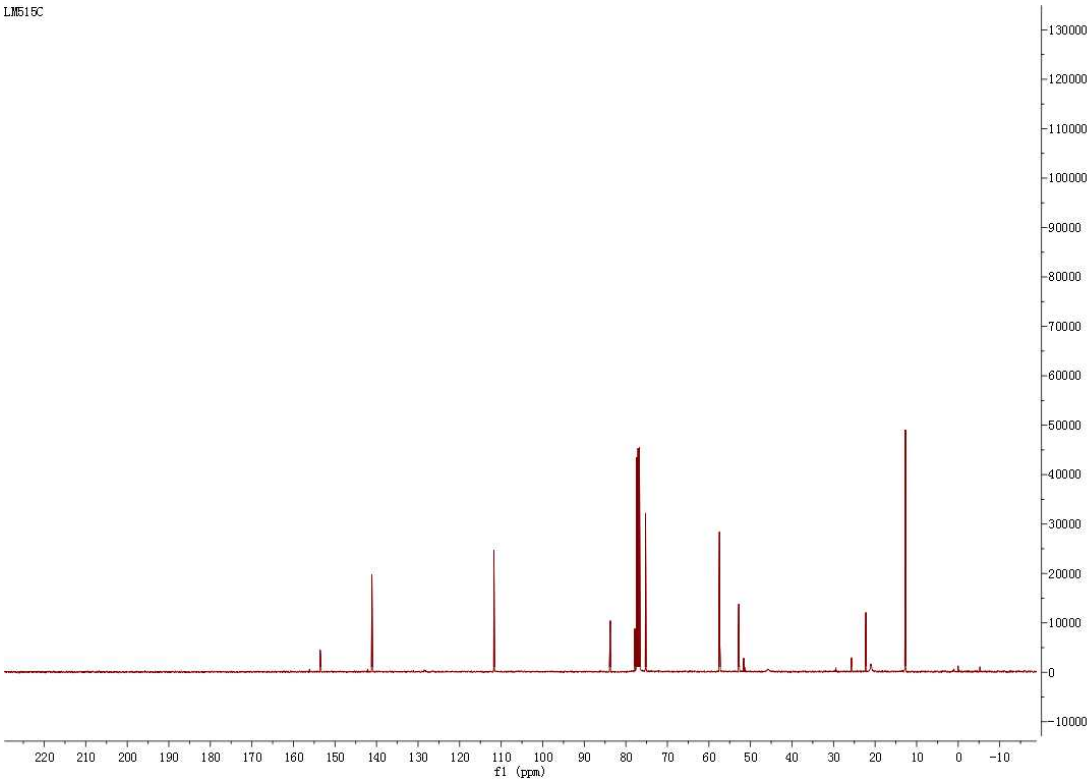


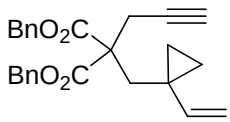



CO2Me
O

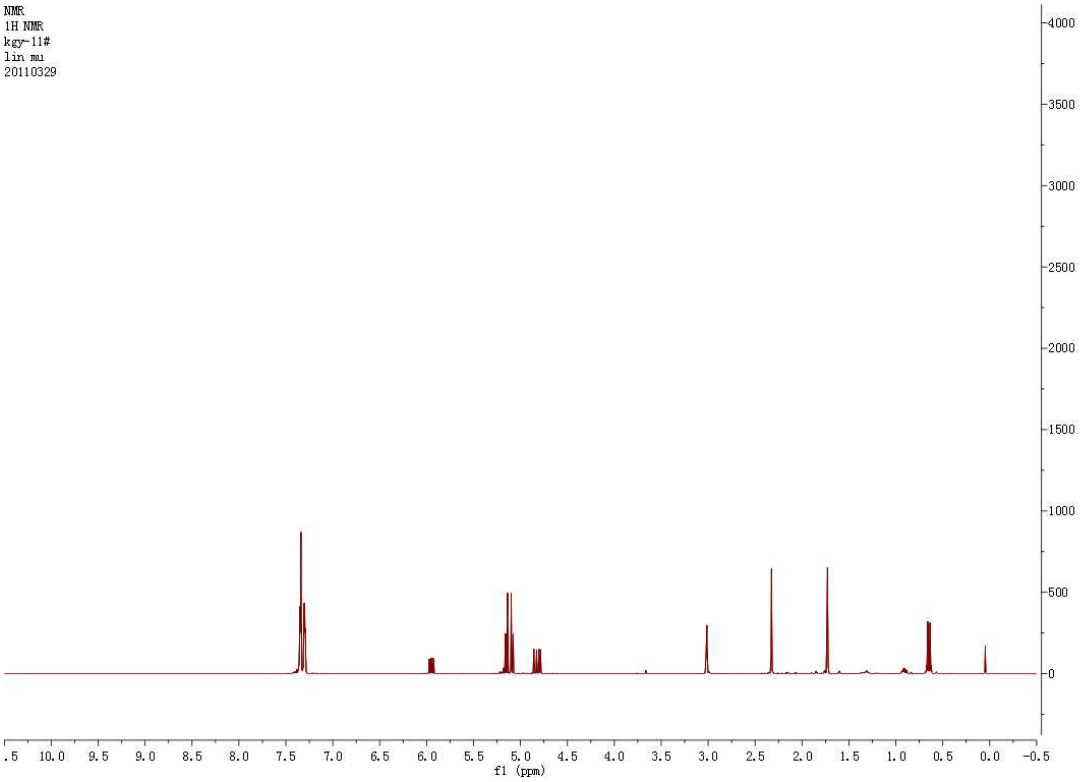
1j


10
8
6
4
2
0 PPM


LM515C
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


BnO2C
BnO2C

1k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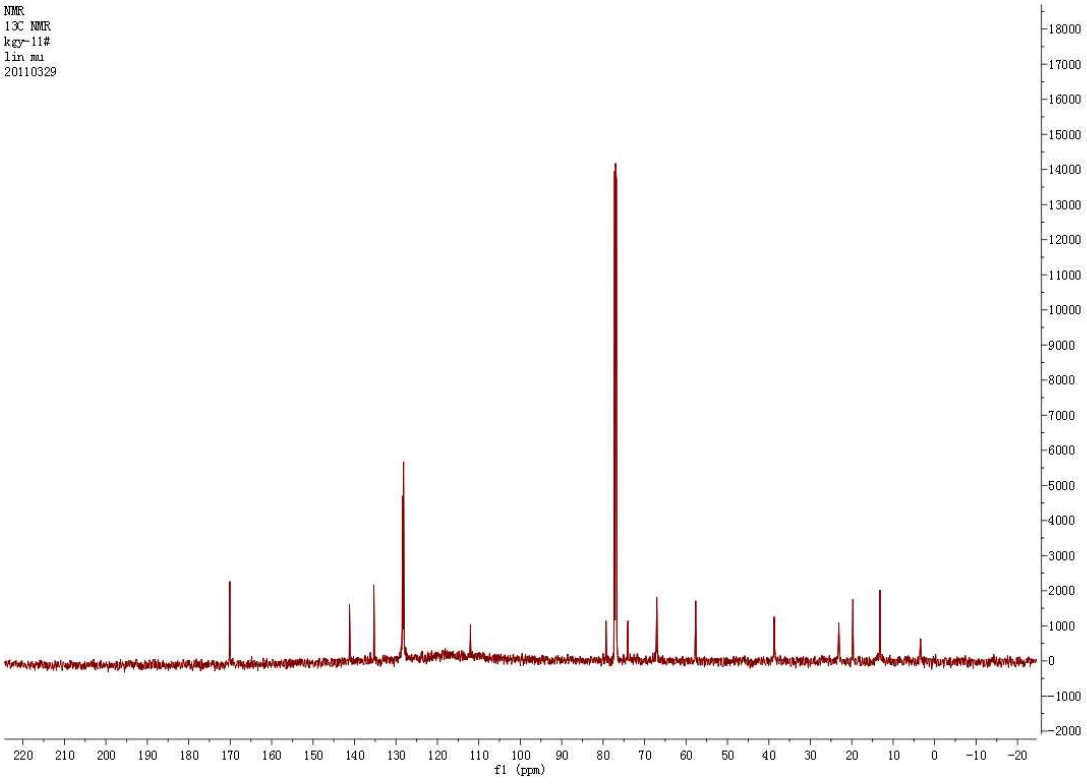
1H NMR
kgy-11#
lin mu
20110329
f1 (ppm)


NMR
13C NMR
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20110329
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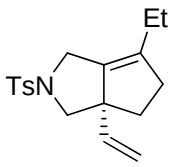

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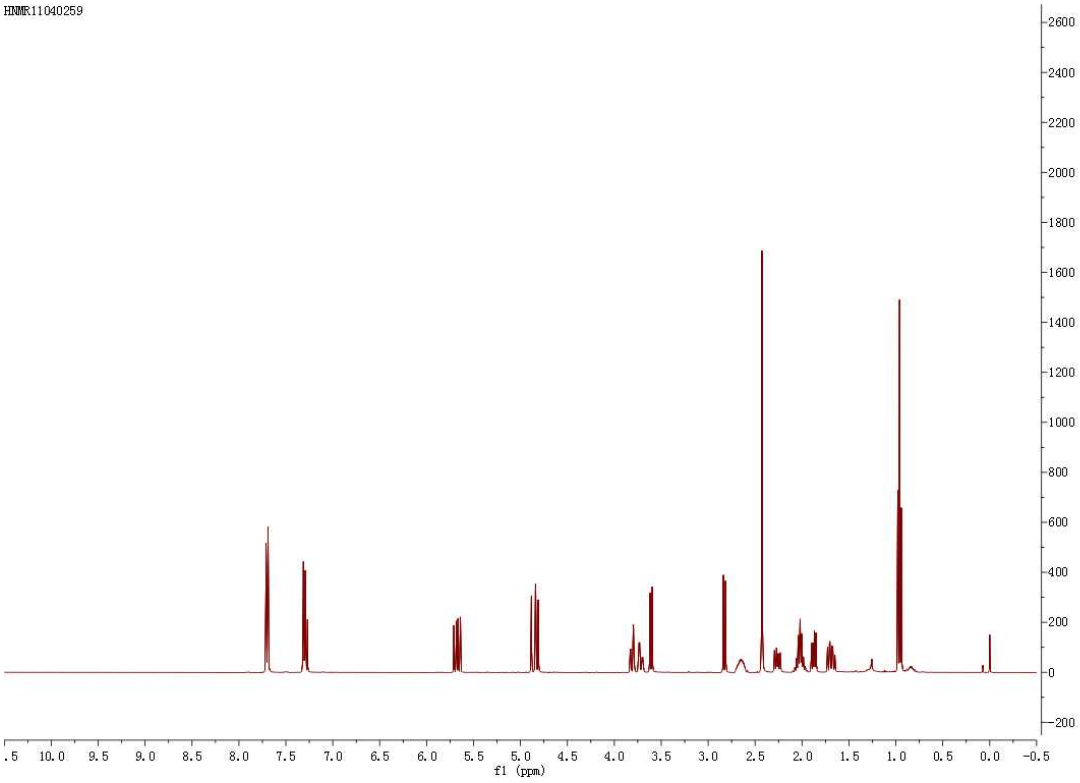
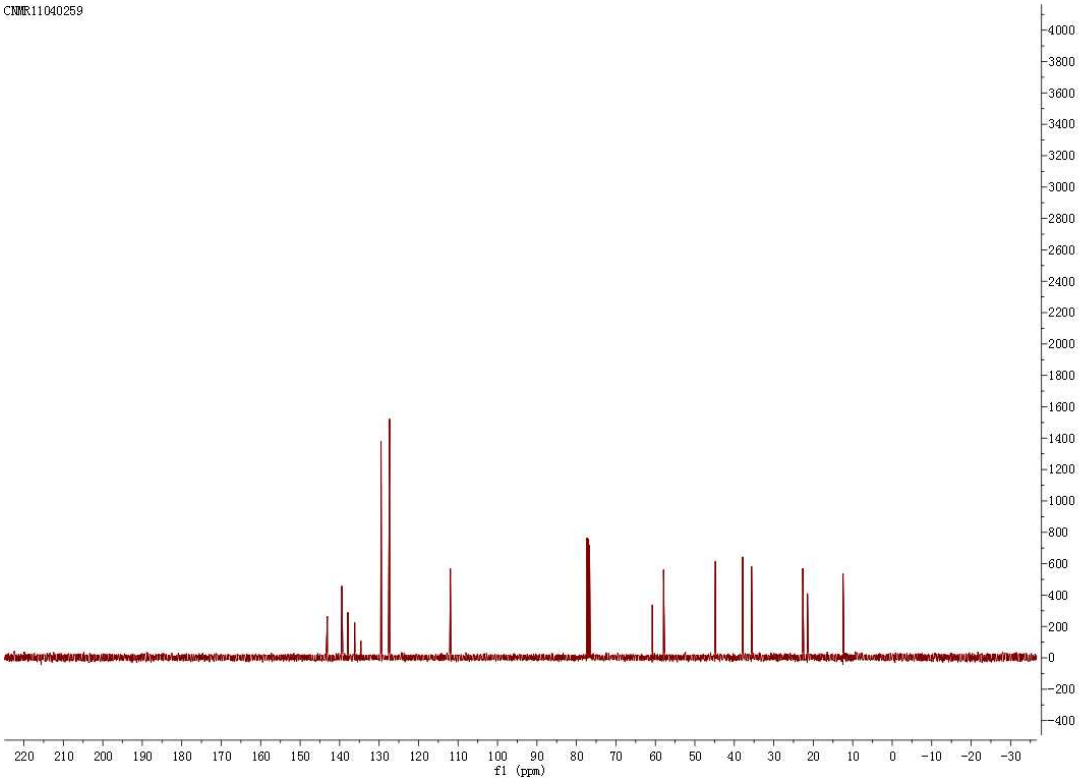
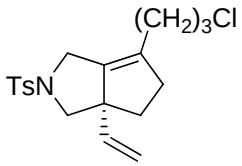
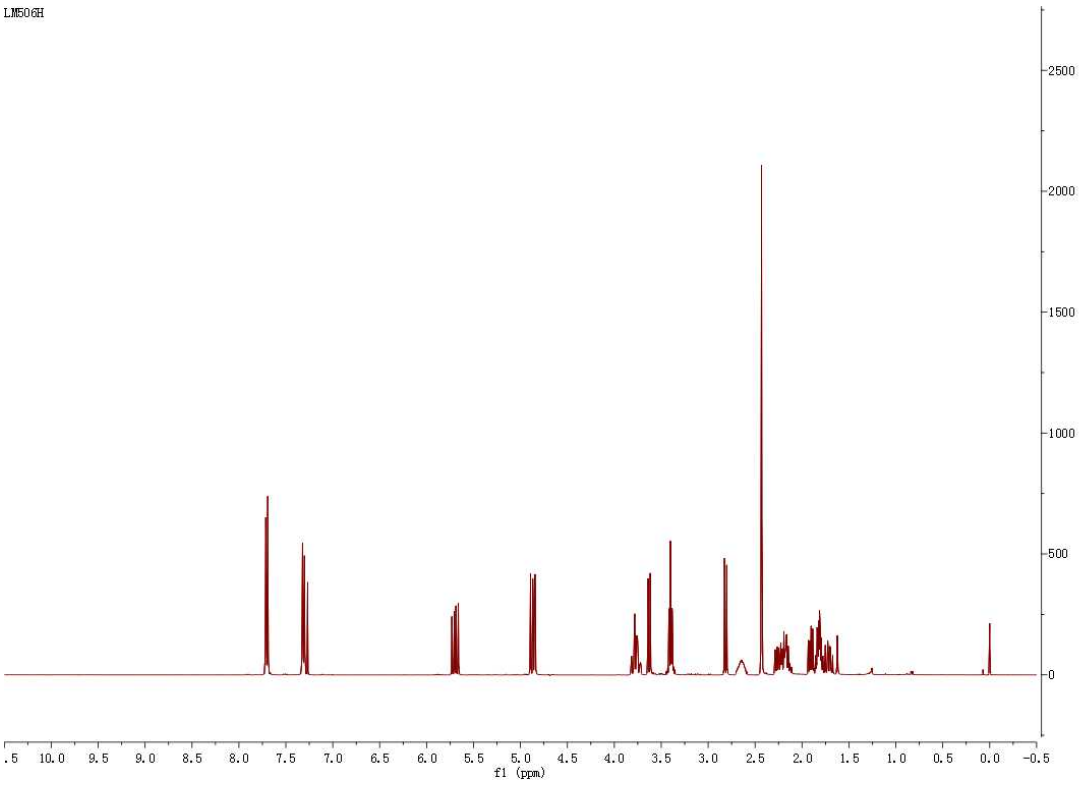
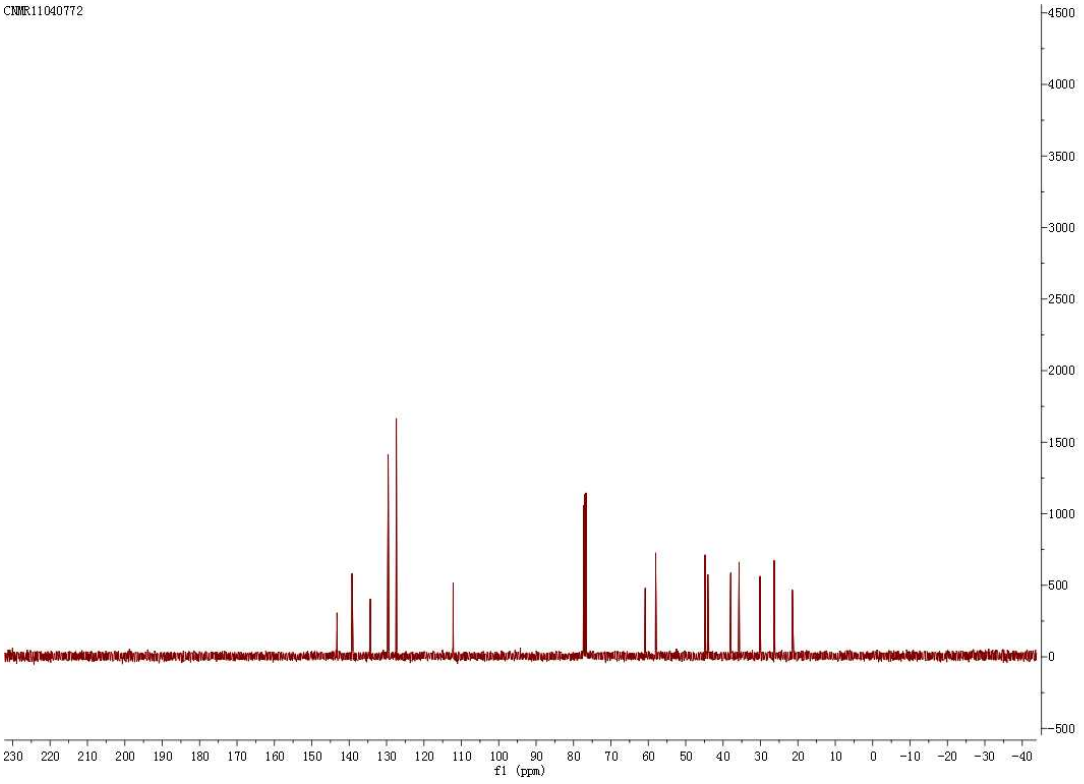


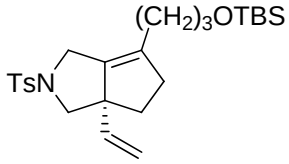



(CH2)3Cl
TsN

2d


LM506H
2500
2000
1500
1000
500
0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


CNMR11040772
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40
f1 (ppm)



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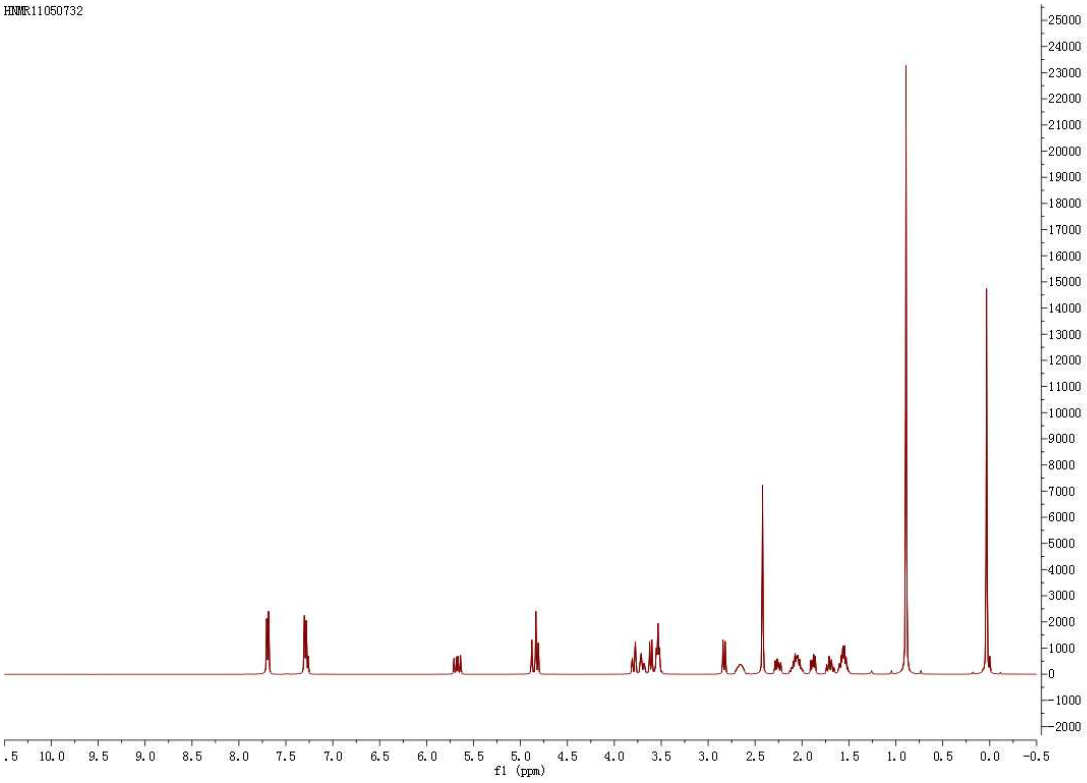

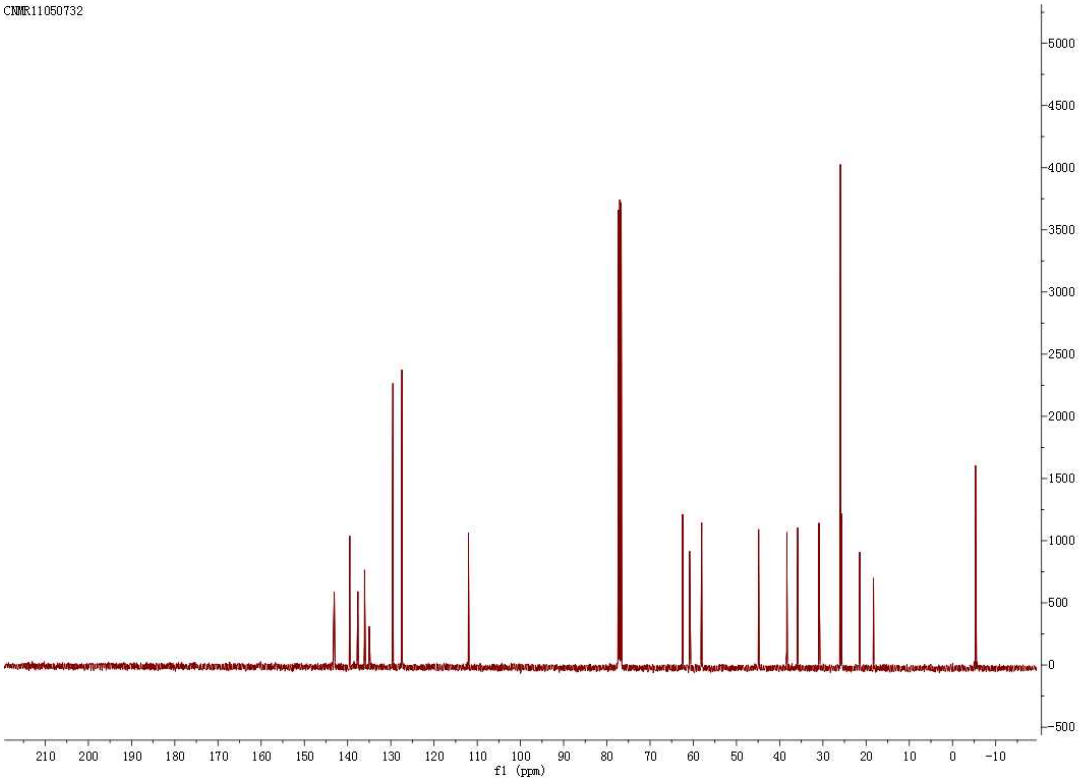

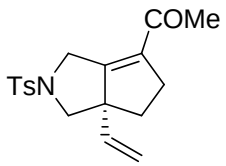

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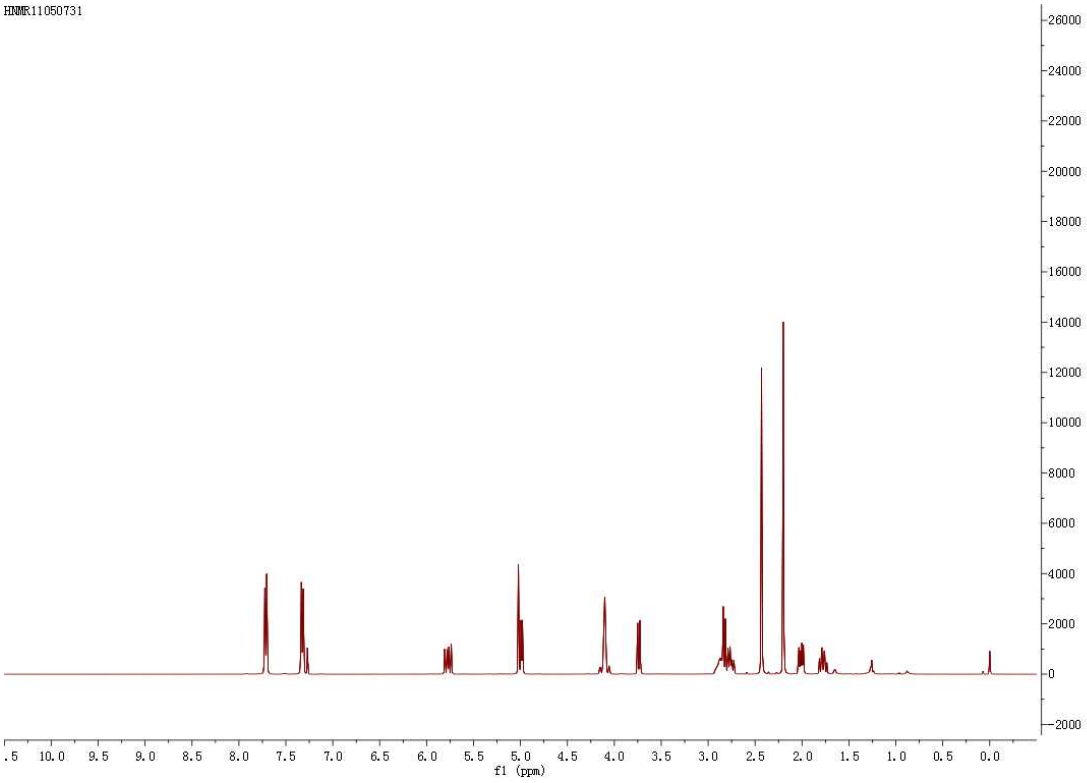

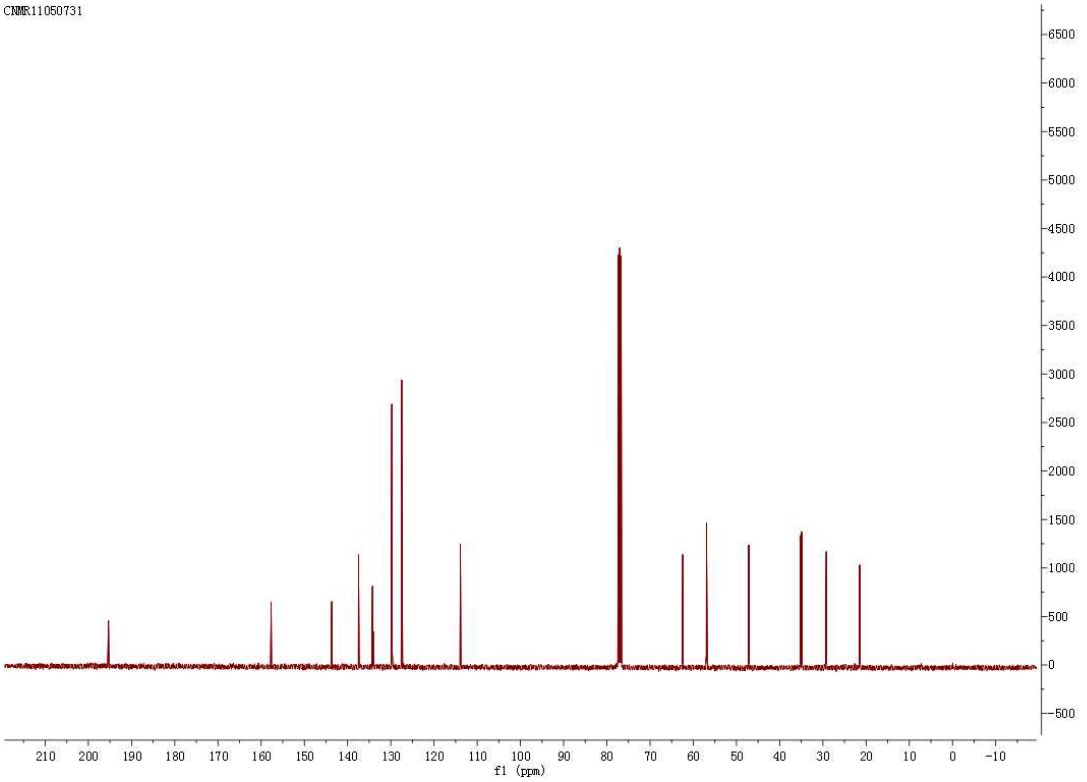

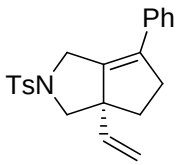

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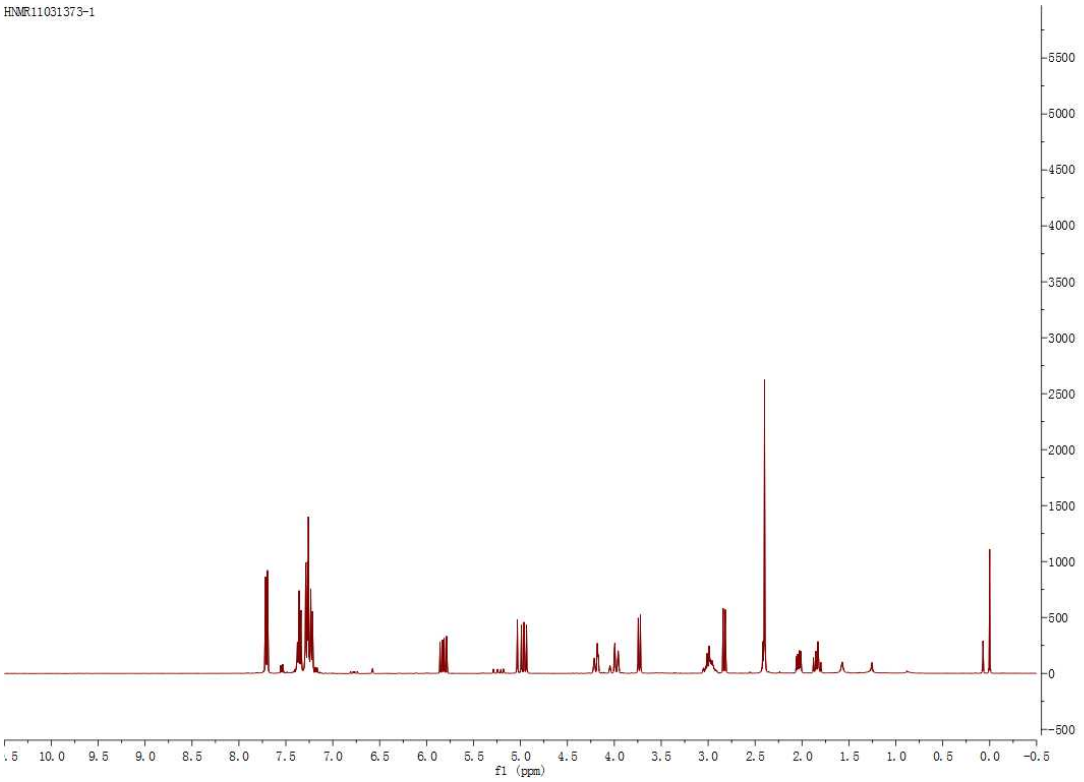

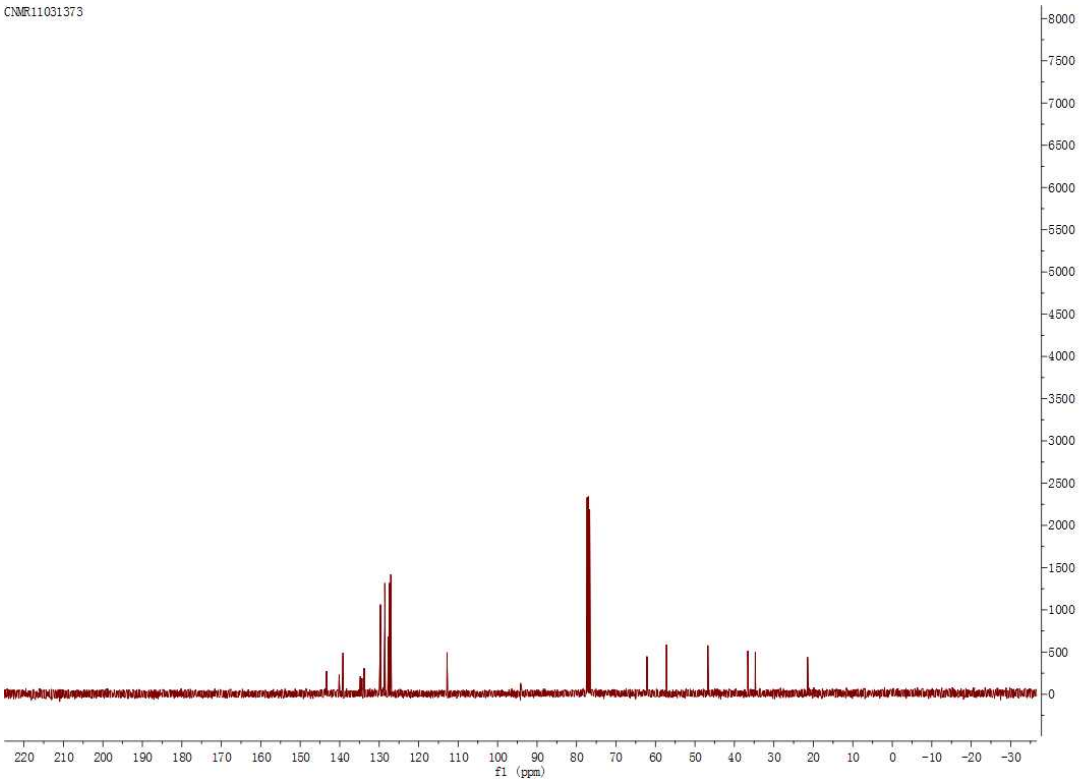

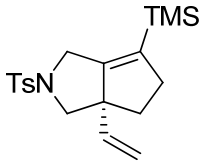

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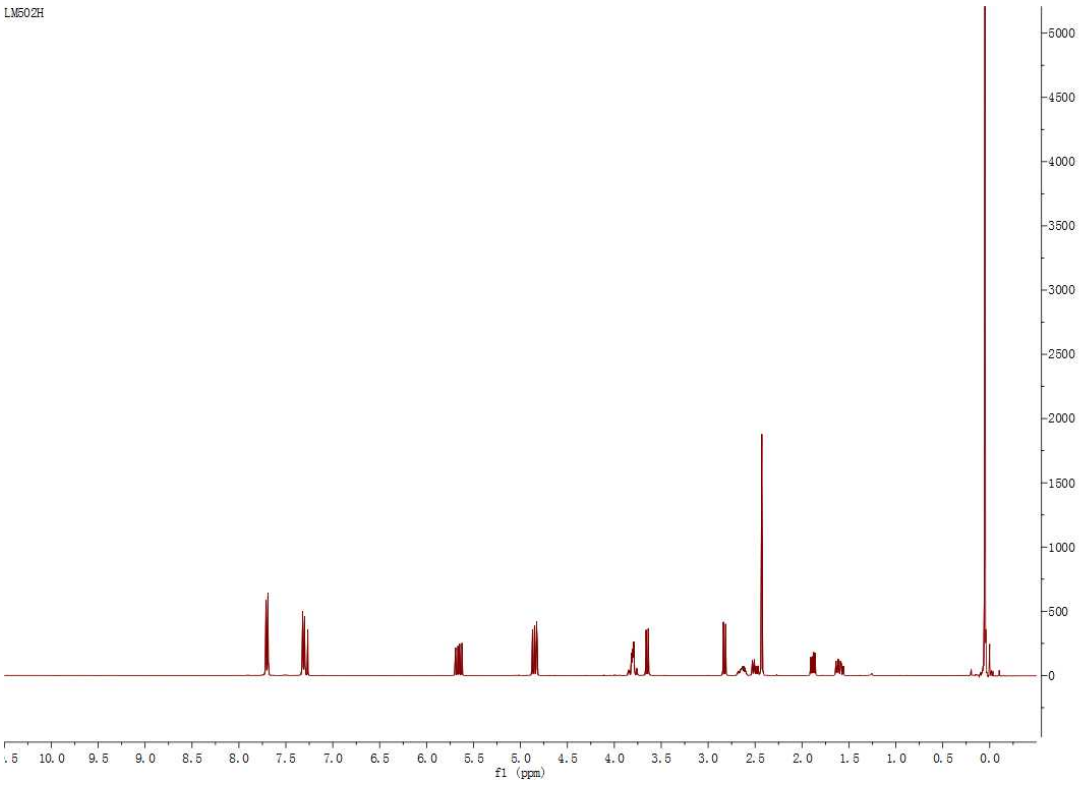

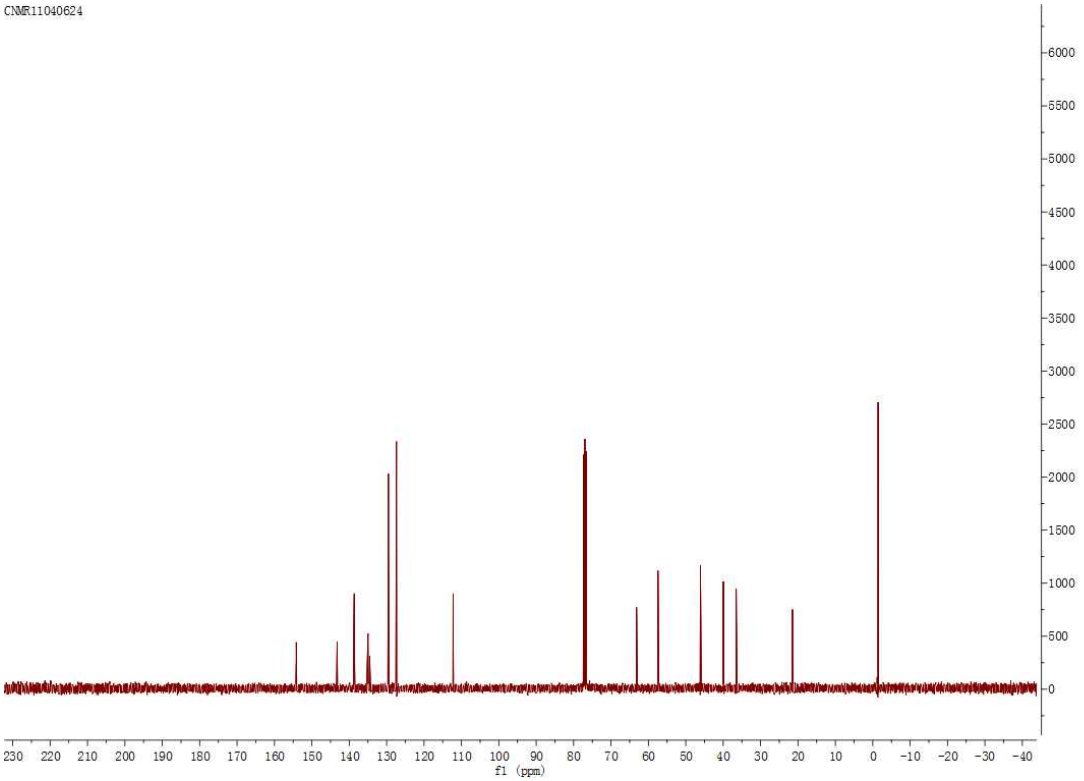

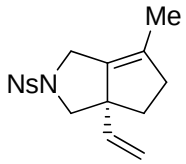

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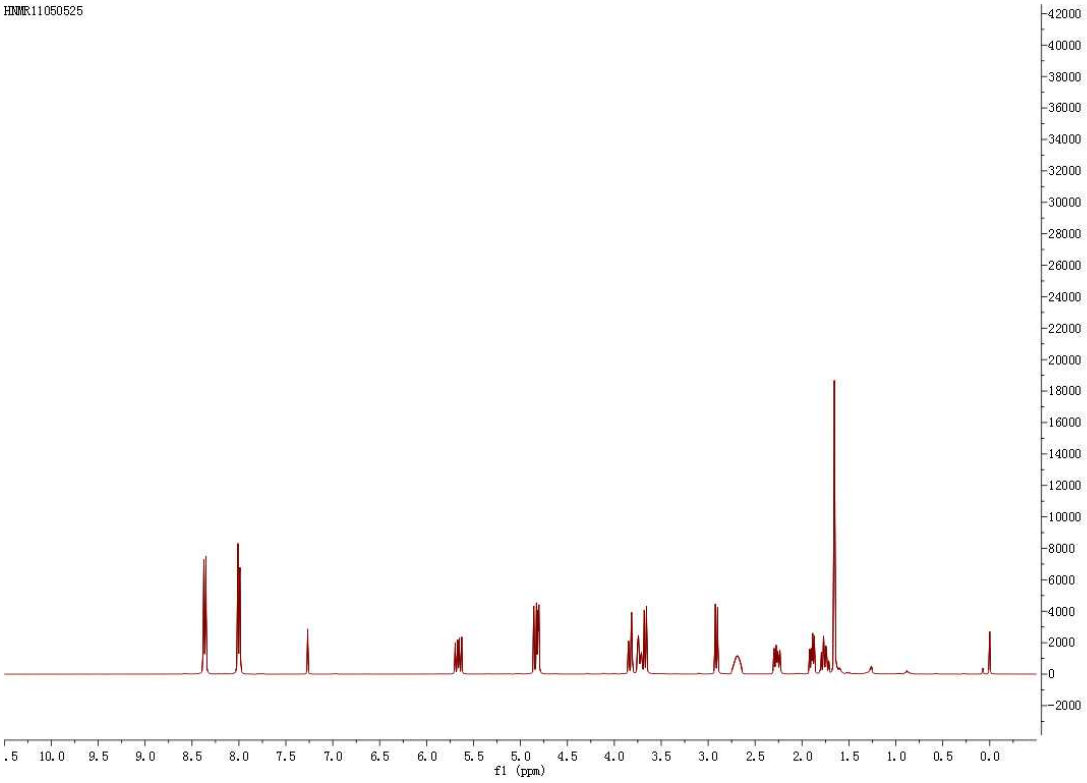

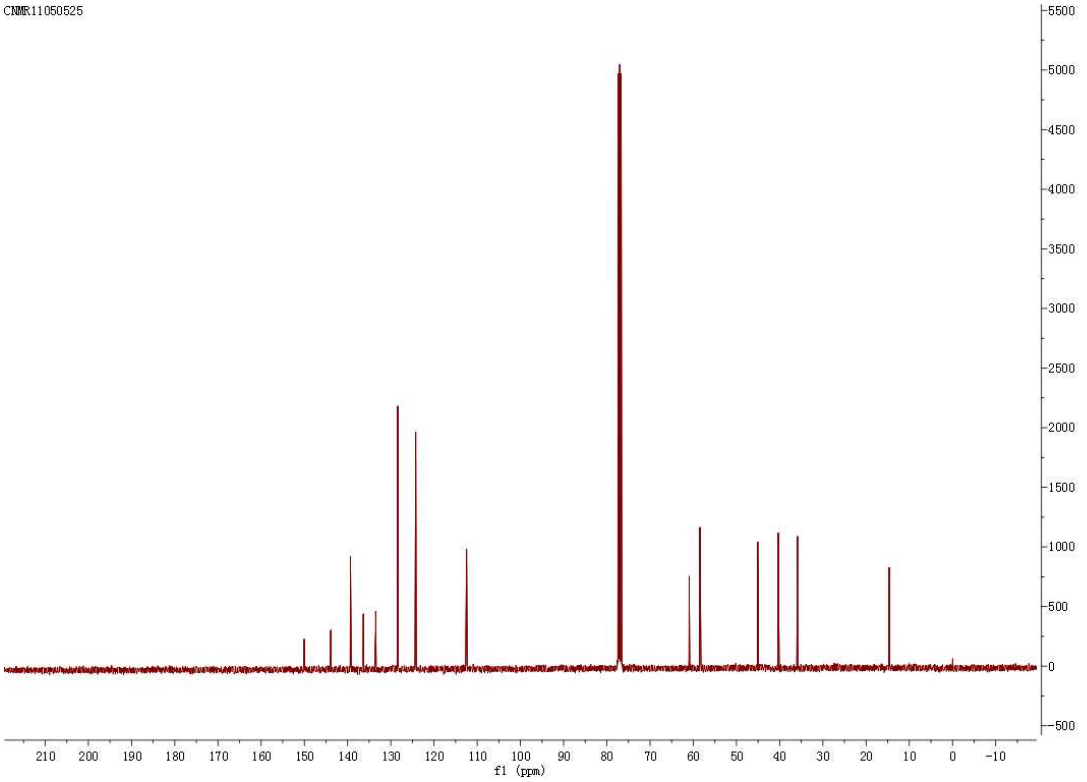

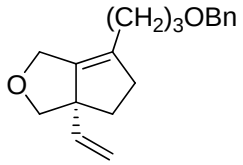

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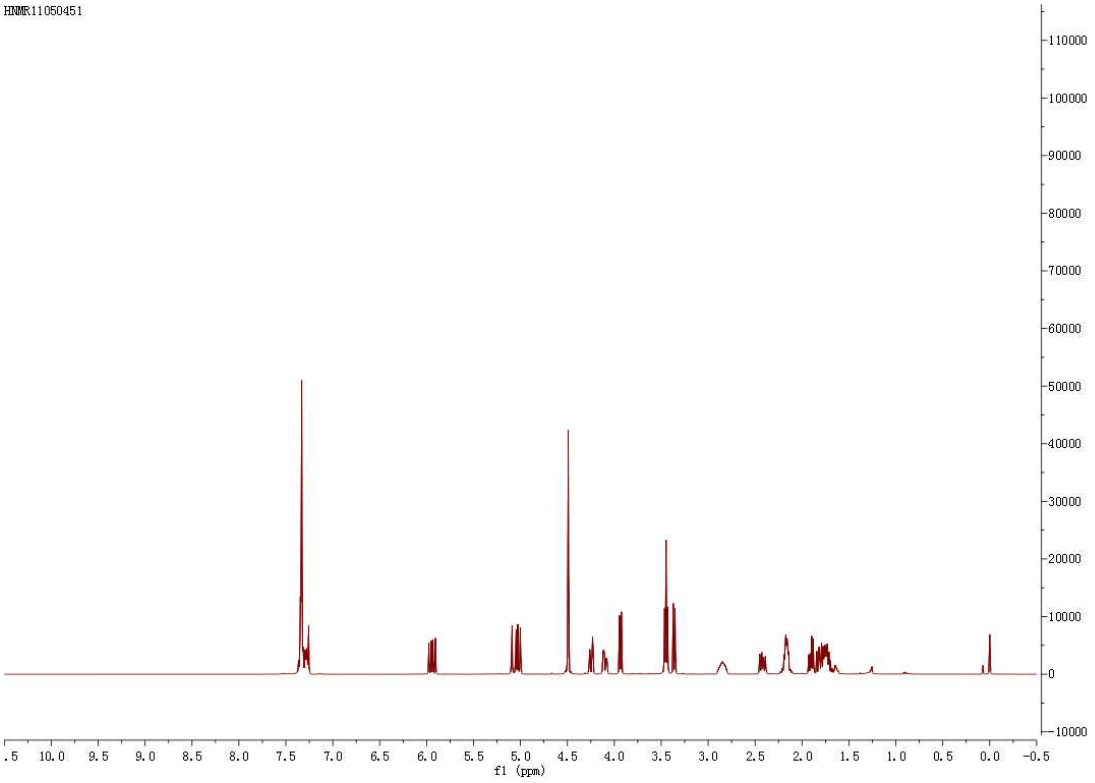

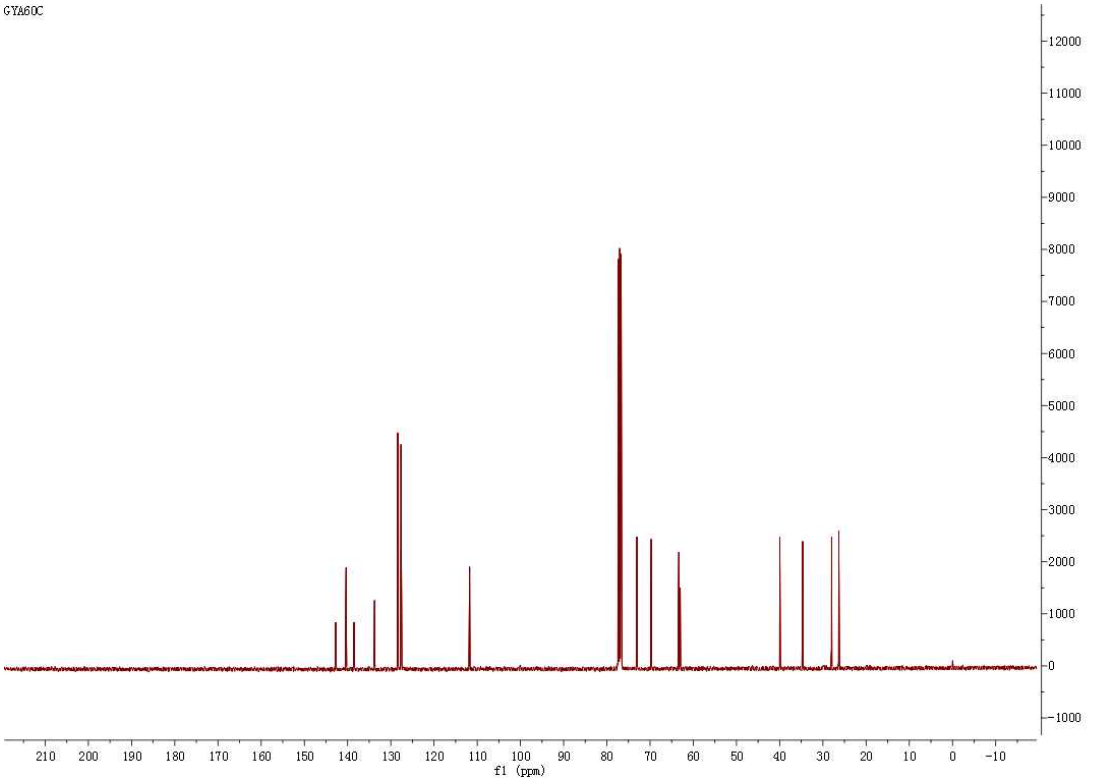

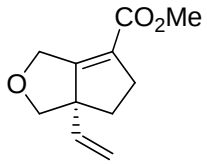

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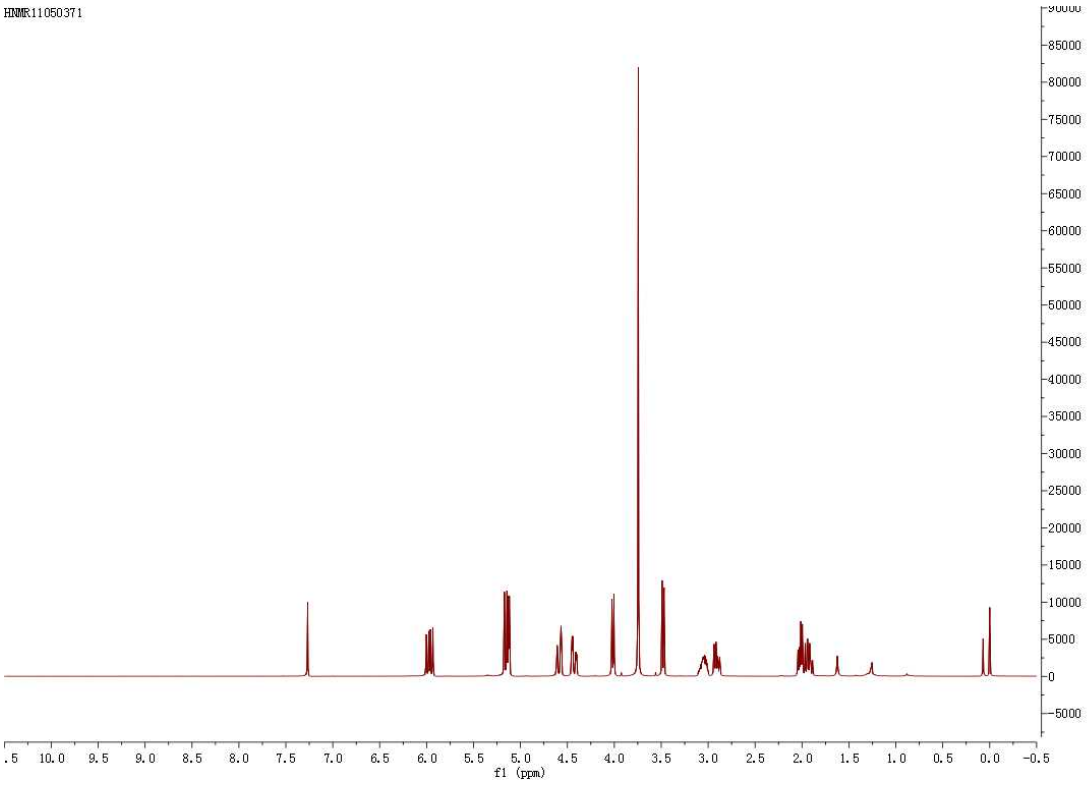
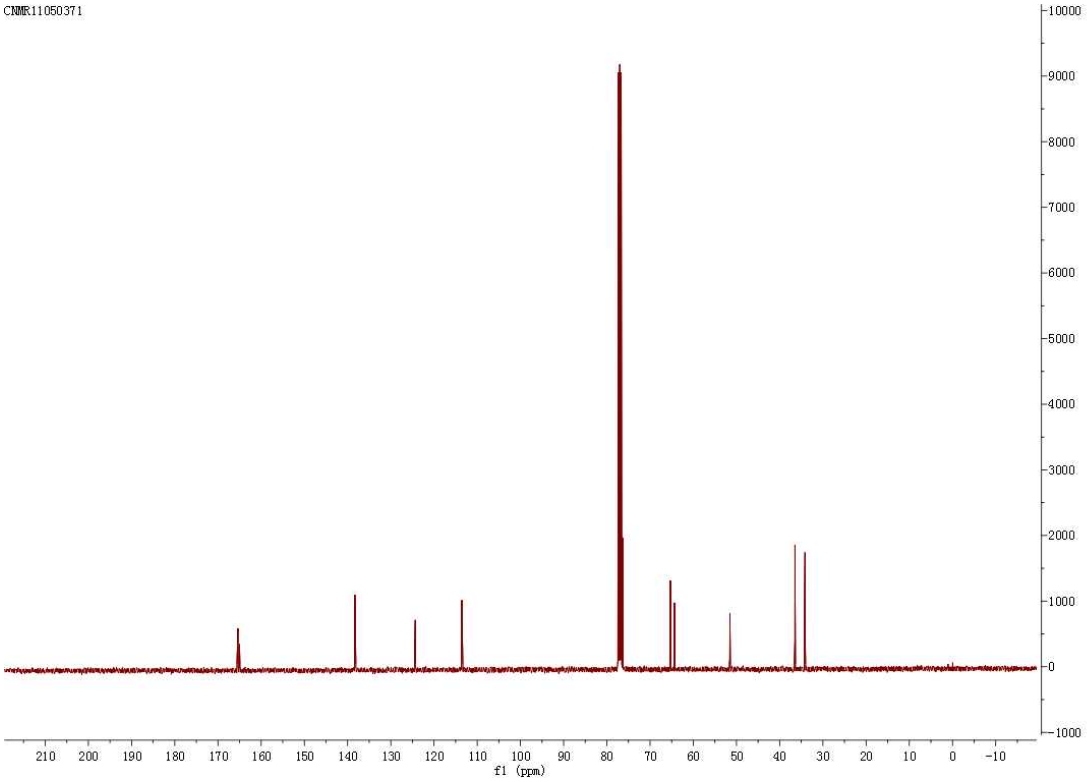
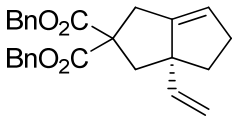
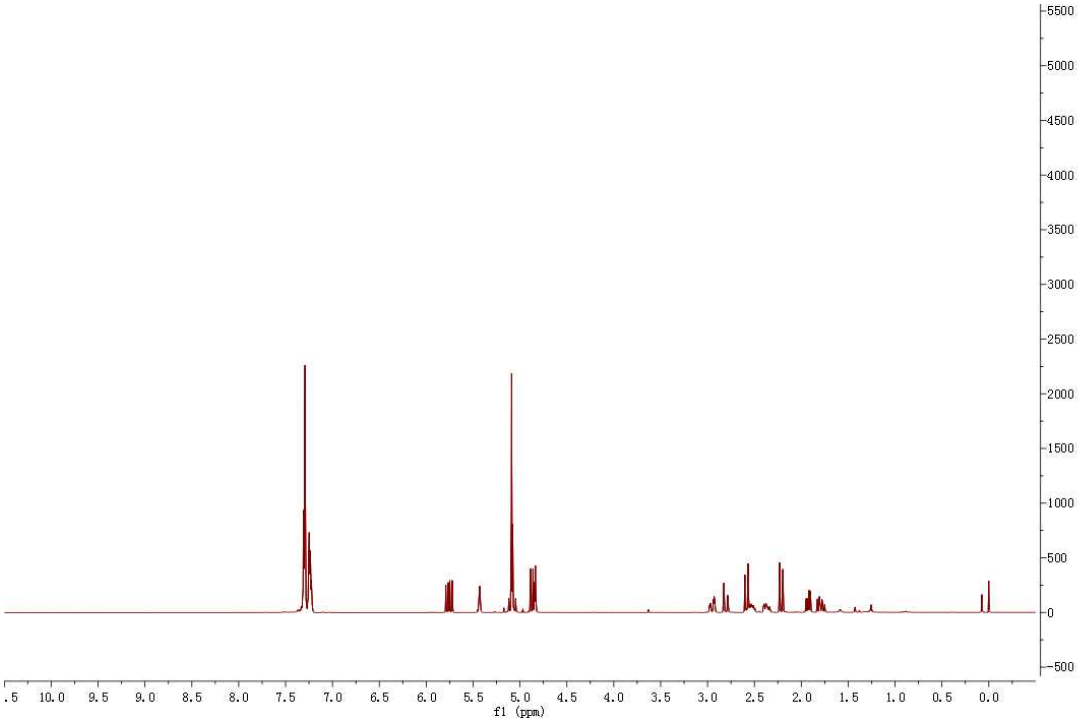
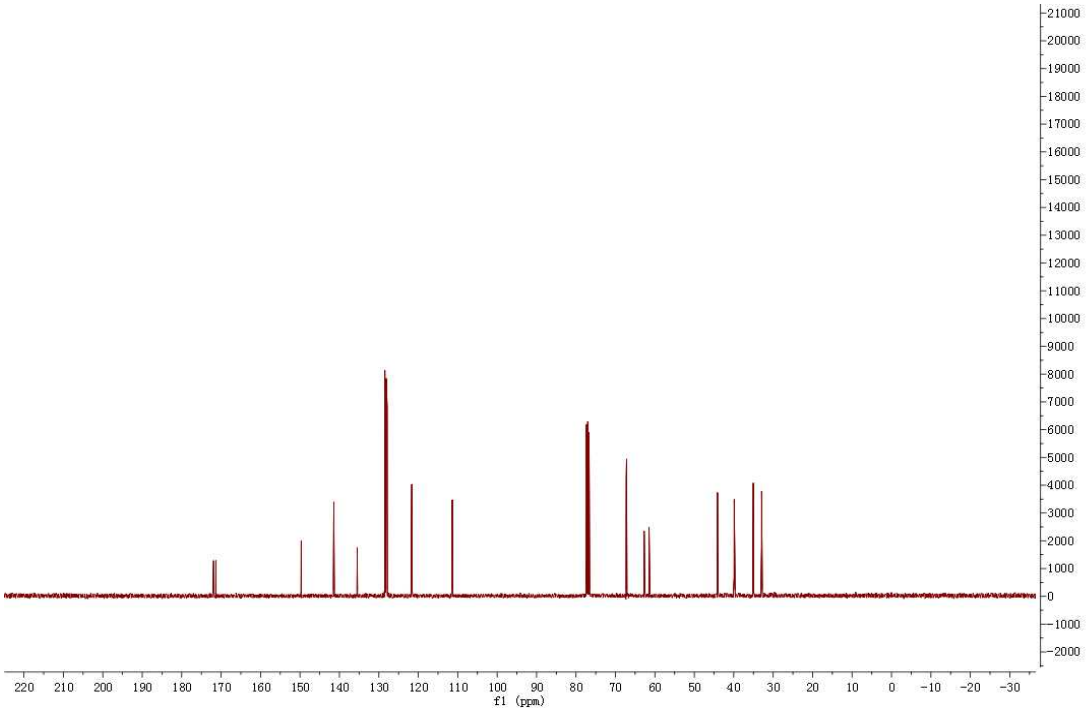




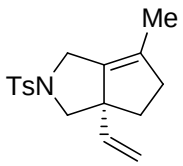


2m



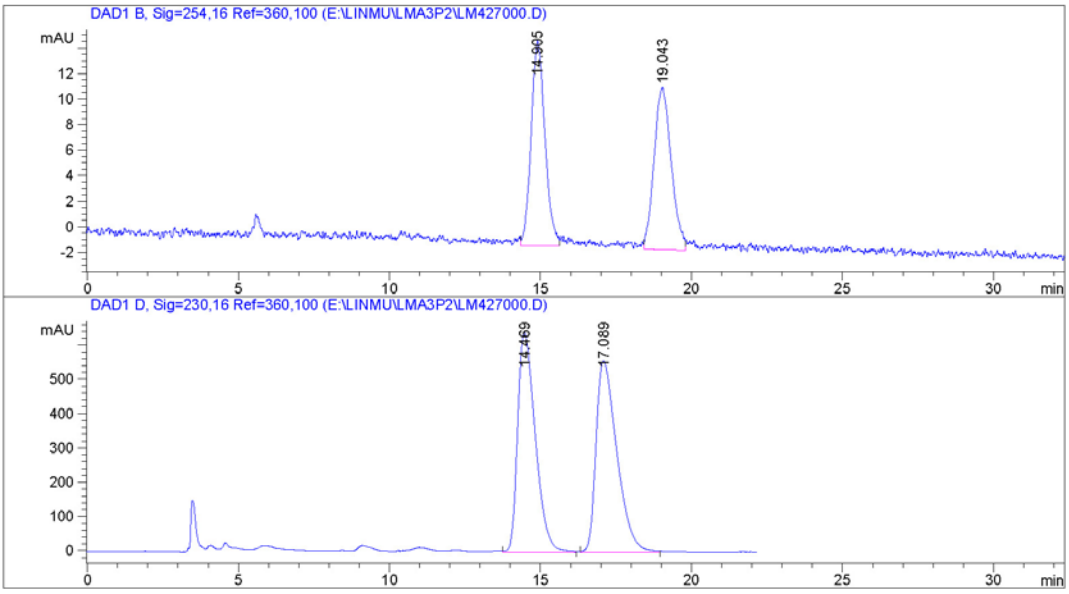


5. HPLC Data for the Asymmetric [3+2] Cycloadducts

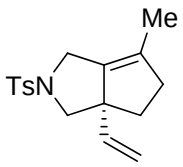


racemic **2a**

```
Data File E:\LINMU\LMA3P2\LM427000.D
 Sample Name: LM427

    ========================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-3-22 10:26:10
    Acq. Method     : C:\HPCHEM\1\METHODS\DEF LC.M
    Last changed    : 2011-3-22 10:12:55  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OJ-H, 1.2 ml/min, nHexane:iPrOH = 90:10
```

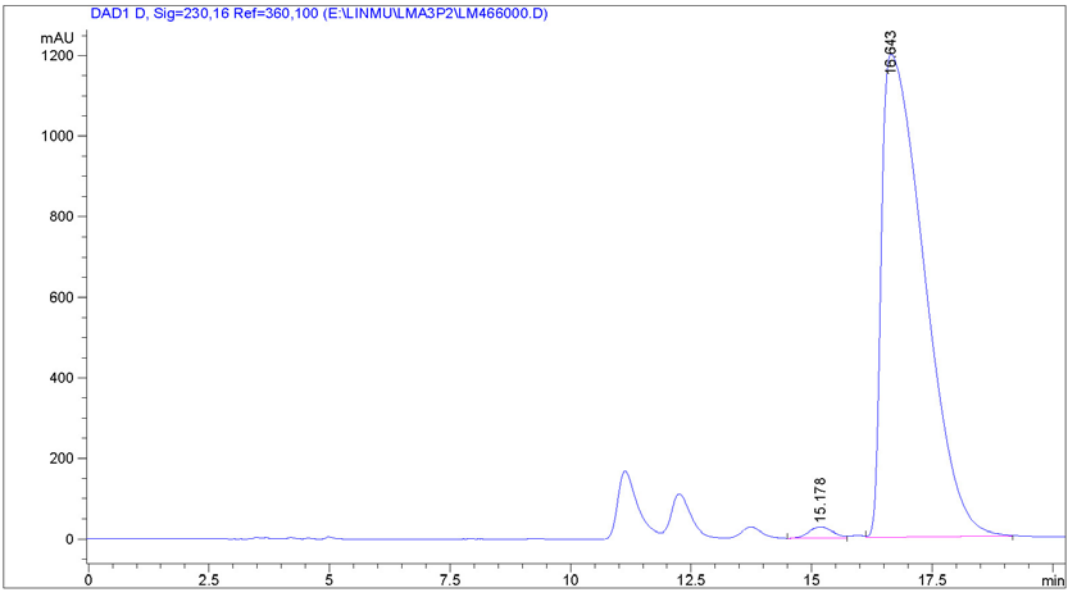



```
    ========================================================================
                              Area Percent Report
    ========================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs

Data File E:\LINMU\LMA3P2\LM427000.D
 Sample Name: LM427


    Signal 2: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  14.469 VB    0.5840 2.59221e4   640.72009  49.2432
       2  17.089 BV    0.6935 2.67188e4   557.11230  50.7568

    Totals :                  5.26409e4  1197.83240
```

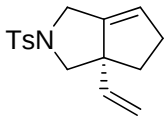


2a

```
Data File E:\LINMU\LMA3P2\LM466000.D
 Sample Name: LM466

    ======================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :    -
    Injection Date  : 2011-3-16 6:18:10
    Acq. Method     : C:\HPCHEM\1\METHODS\DEF LC.M
    Last changed    : 2011-3-16 3:41:30  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OJ-H, 1.2 ml/min, nHexane:iPrOH = 90:10
```

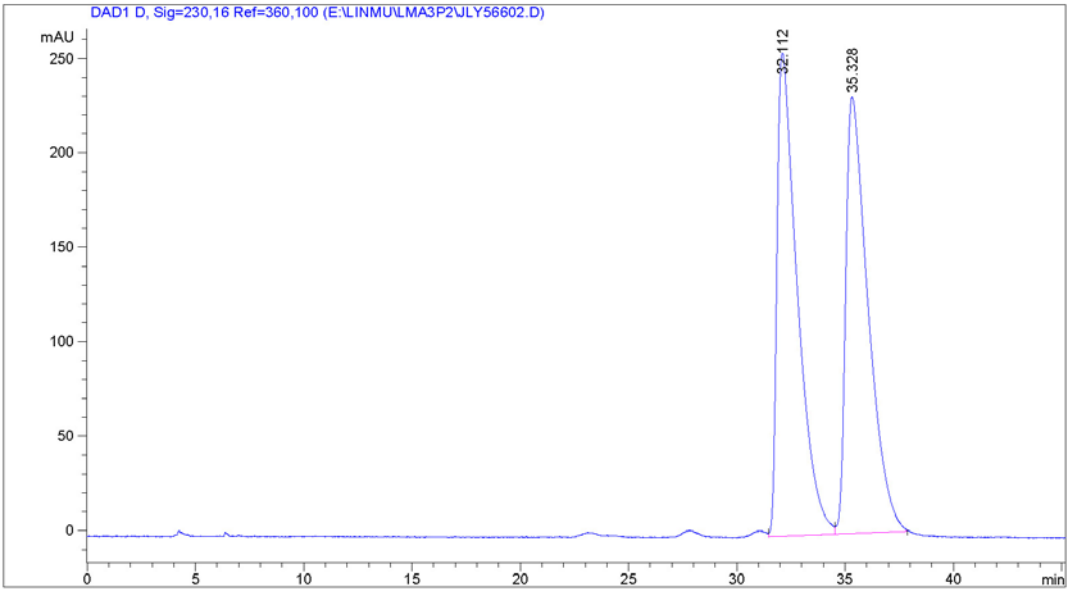



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  15.178 VV    0.4371  951.88763   27.41724   1.2773
       2  16.643 VB    0.7220 7.35734e4  1198.77039  98.7227

    Totals :                  7.45253e4  1226.18763

    ======================================================================
                              *** End of Report ***

Instrument 1 2011-5-18 19:57:47                          Page   1 of 1
```

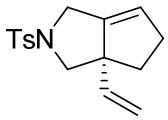


racemic **2b**

```
Data File E:\LINMU\LMA3P2\JLY56602.D
 Sample Name: JLY566

    ==================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-3-25 7:05:50
    Acq. Method     : C:\HPCHEM\1\METHODS\DEF LC.M
    Last changed    : 2011-3-25 6:54:13  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OJ-H, 1.0 ml/min, nHexane:iPrOH = 95:5
```

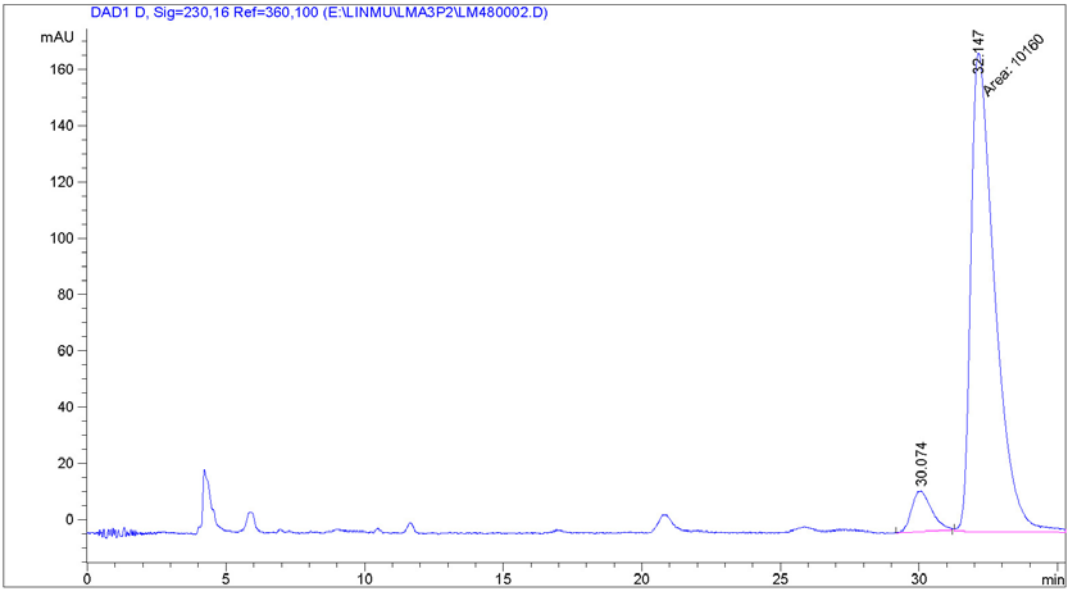



```
    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  32.112 VV    0.8625 1.66670e4   255.69180  50.1673
       2  35.328 VB    0.9376 1.65558e4   231.15012  49.8327

    Totals :                  3.32228e4   486.84192


    ==================================================================
                            *** End of Report ***

Instrument 1 2011-5-18 19:50:06                          Page   1 of 1
```

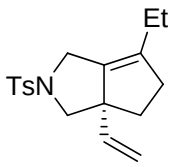


2b

```
Data File E:\LINMU\LMA3P2\LM480002.D
 Sample Name: LM480

    ======================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-3-29 7:43:02
    Acq. Method     : C:\HPCHEM\1\METHODS\DEF LC.M
    Last changed    : 2011-3-29 7:04:24  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OJ-H, 1.0 ml/min, nHexane:iPrOH = 95:5
```

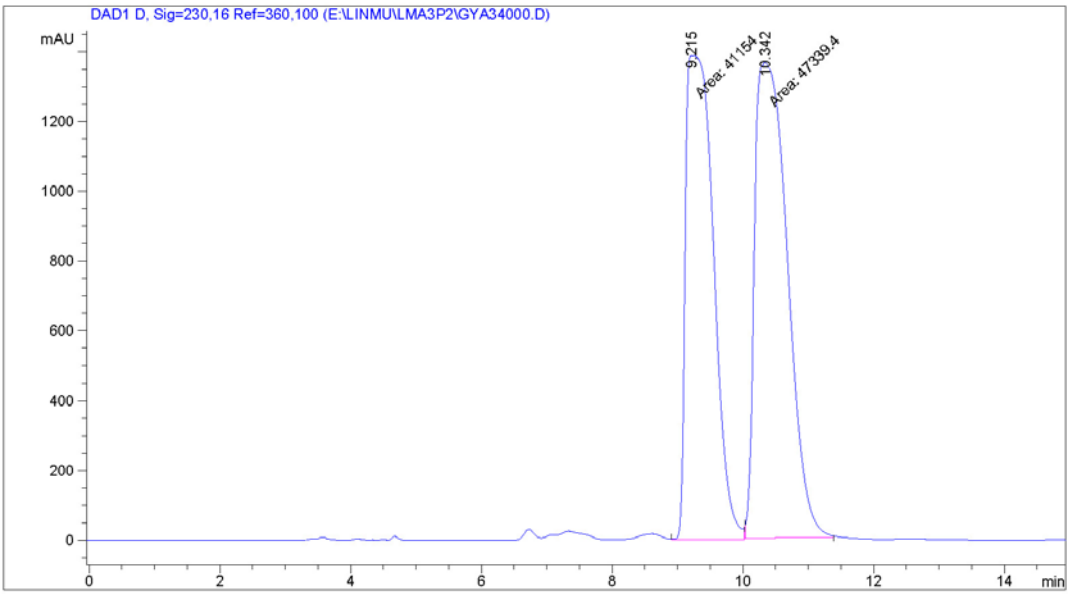



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  30.074 VV    0.5886  712.50146   14.46673   6.5532
       2  32.147 MM    0.9964 1.01600e4   169.94279  93.4468

    Totals :                  1.08725e4   184.40952


    ======================================================================
                              *** End of Report ***

Instrument 1 2011-5-18 19:55:21                          Page   1 of 1
```

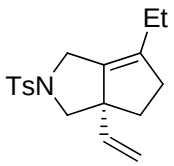


racemic **2c**

```
Data File E:\LINMU\LMA3P2\GYA34000.D
 Sample Name: GYA34

    ==================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-4-8 8:30:15
    Acq. Method     : C:\HPCHEM\1\METHODS\DEF_LC.M
    Last changed    : 2011-4-8 8:05:29  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OJ-H, 1.2 ml/min, nHexane:iPrOH = 90:10
```

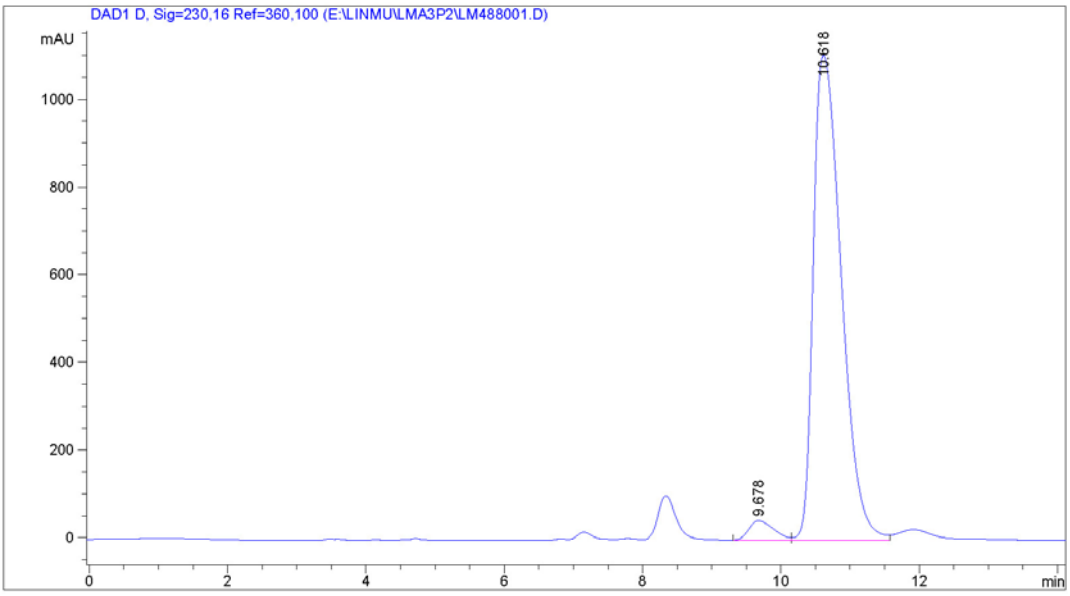



```
    ==================================================================
                          Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.215 MM    0.4936 4.11540e4  1389.57825  46.5052
       2  10.342 MM    0.5769 4.73394e4  1367.55103  53.4948

    Totals :                  8.84934e4  2757.12927

    ==================================================================
                          *** End of Report ***
```

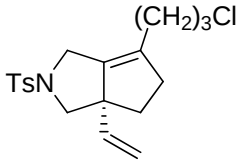


2c

```
Data File E:\LINMU\LMA3P2\LM488001.D
 Sample Name: LM488

    ==================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-4-8 9:29:33
    Acq. Method     : C:\HPCHEM\1\METHODS\DEF_LC.M
    Last changed    : 2011-4-8 8:05:29  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OJ-H, 1.2 ml/min, nHexane:iPrOH = 90:10
```

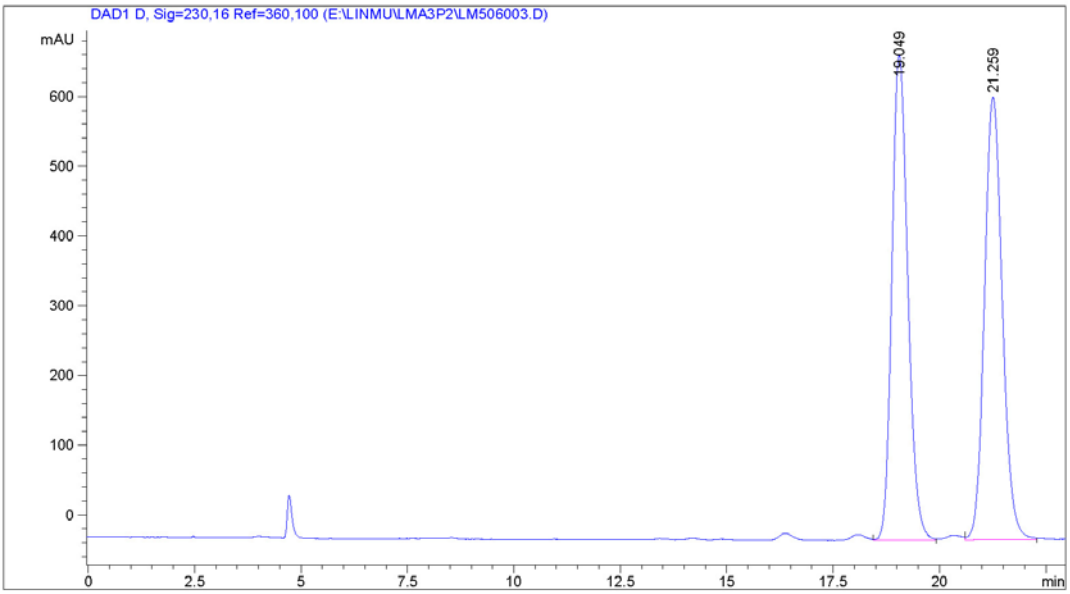



```
    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.678 BV    0.3300 1063.97107   44.01767   3.3230
       2  10.618 VV    0.4387 3.09548e4  1105.33667  96.6770

    Totals :                  3.20188e4  1149.35434

    ==================================================================
                            *** End of Report ***

Instrument 1 2011-5-18 20:03:05                          Page   1 of 1
```

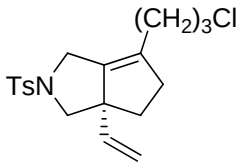


racemic **2d**

```
Data File E:\LINMU\LMA3P2\LM506003.D
 Sample Name: LM506

    ========================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-4-29 9:21:39
    Acq. Method     : E:\DATA\LM-YU\DEF LC.M
    Last changed    : 2011-4-29 9:07:55  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : AD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```



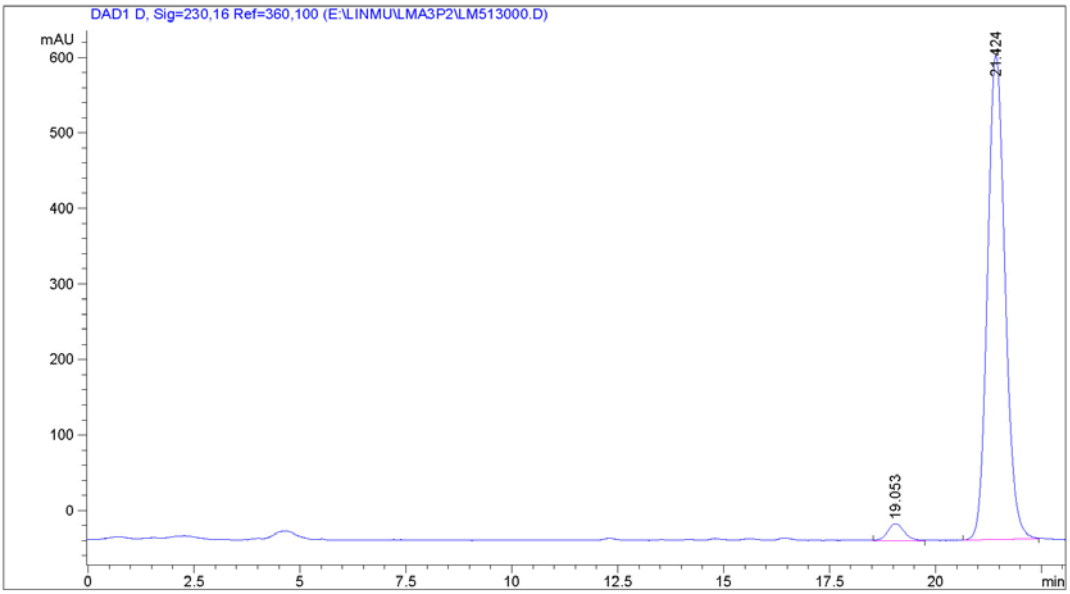

```
    ========================================================================
                              Area Percent Report
    ========================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  19.049 VV    0.3972 1.80658e4   695.12781  49.4454
       2  21.259 VB    0.4477 1.84711e4   634.43158  50.5546

    Totals :                  3.65368e4  1329.55939

    ========================================================================
                              *** End of Report ***
```



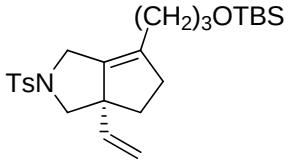
2d

Data File E:\LINMU\LMA3P2\LM513000.D
Sample Name: LM513

```
==========================================================================
Acq. Operator   : LM
Acq. Instrument : Instrument 1                    Location :   -
Injection Date  : 2011-4-29 10:33:42
Acq. Method     : E:\DATA\LM-YU\DEF LC.M
Last changed    : 2011-4-29 9:07:55  by LM
                  (modified after loading)
Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
Last changed    : 2004-4-7 0:10:12
Sample Info     : AD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```

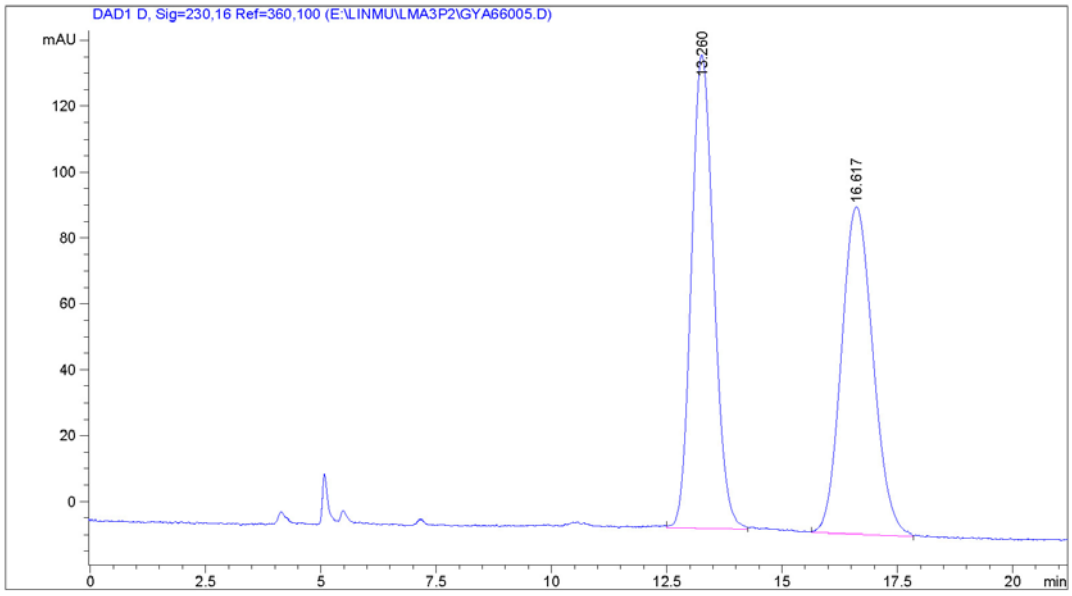



```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  19.053 VV    0.3525  580.35406   22.23727   3.0506
   2  21.424 BB    0.4455 1.84437e4   641.39636  96.9494

Totals :                  1.90240e4   663.63363

==========================================================================
                        *** End of Report ***
```

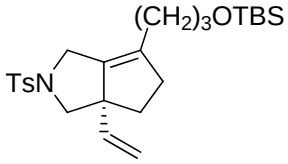


racemic **2e**

```
Data File E:\LINMU\LMA3P2\GYA66005.D
 Sample Name: GYA66

    ========================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-5-20 9:14:46
    Acq. Method     : E:\DATA\LM-YU\DEF LC.M
    Last changed    : 2011-5-20 8:05:30  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : AS-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```



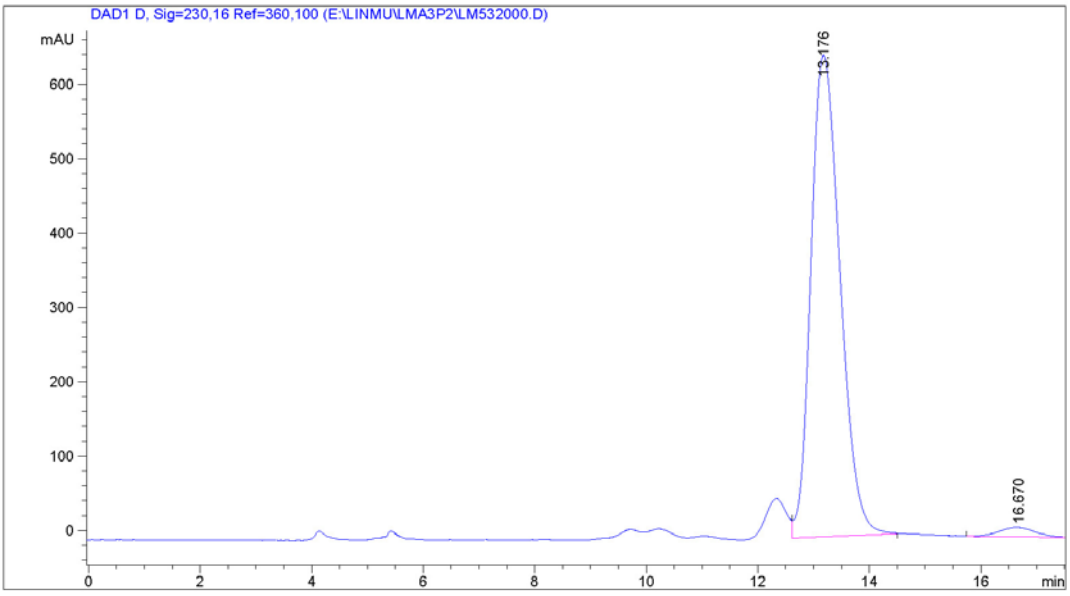

```
    ========================================================================
                              Area Percent Report
    ========================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  13.260 VB    0.5060 4849.36182  143.60808  50.6143
       2  16.617 BV    0.5721 4731.65039   99.26756  49.3857

    Totals :                  9581.01221  242.87563

    ========================================================================
                              *** End of Report ***
```



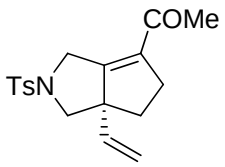
2e

Data File E:\LINMU\LMA3P2\LM532000.D
Sample Name: LM532

```
==========================================================================
Acq. Operator   : LM
Acq. Instrument : Instrument 1                    Location :   -
Injection Date  : 2011-5-20 9:38:00
Acq. Method     : E:\DATA\LM-YU\DEF LC.M
Last changed    : 2011-5-20 8:05:30  by LM
                  (modified after loading)
Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
Last changed    : 2004-4-7 0:10:12
Sample Info     : AS-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```

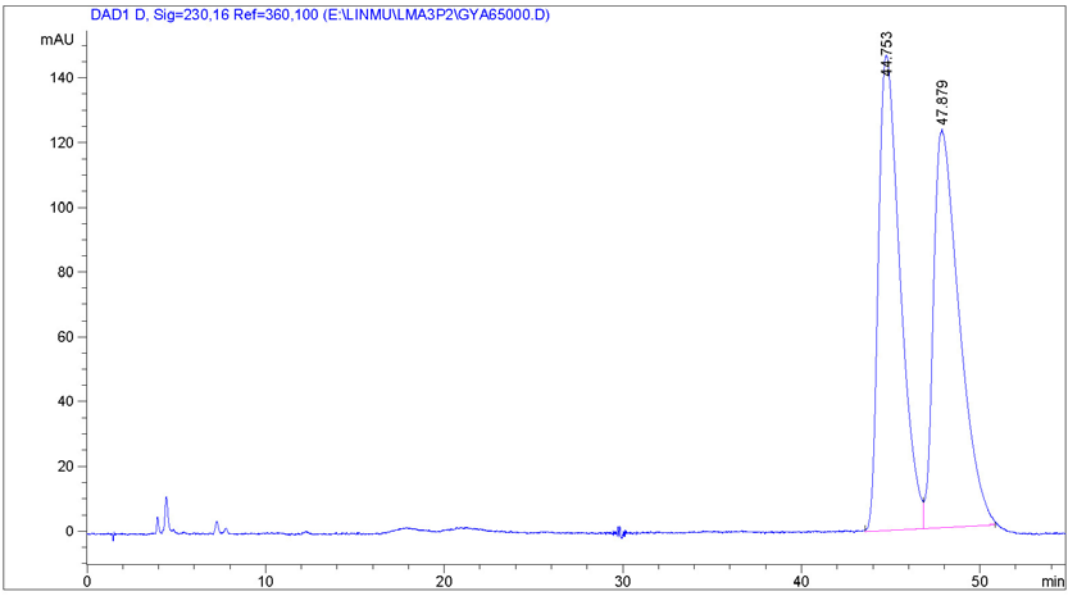



```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.176 VB    0.5600 2.35160e4   647.06238  97.6336
   2  16.670 VBA   0.5396  569.97021   12.55695   2.3664

Totals :                  2.40859e4   659.61932

==========================================================================
                        *** End of Report ***
```

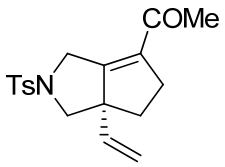


racemic **2f**

```
Data File E:\LINMU\LMA3P2\GYA65000.D
 Sample Name: GYA65

    ==================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-5-21 9:49:13
    Acq. Method     : E:\DATA\LM-YU\DEF LC.M
    Last changed    : 2011-4-20 10:08:55  by LM
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```

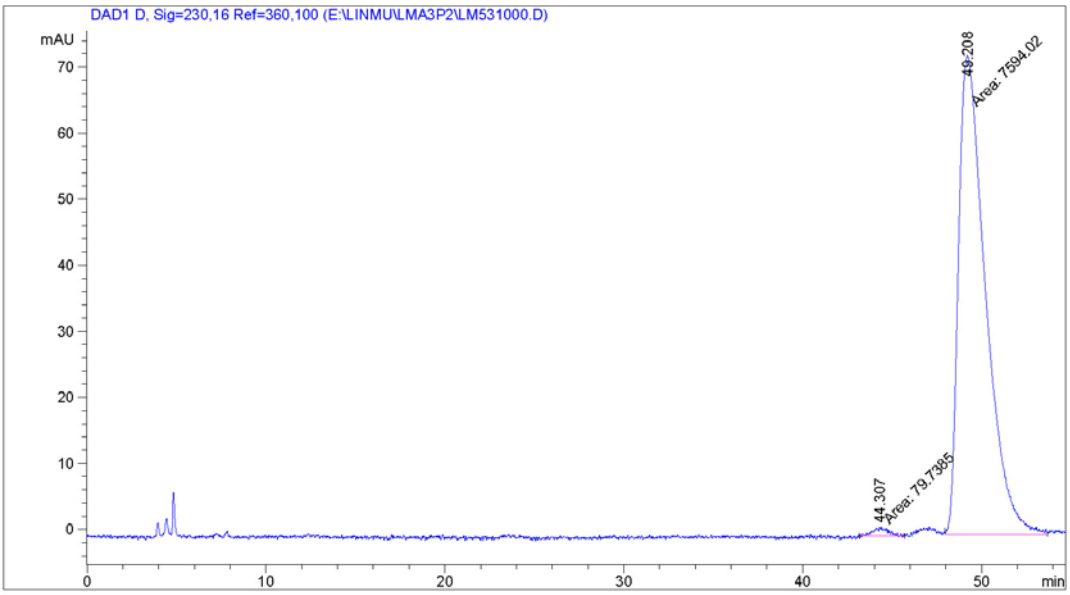



```
    ==================================================================
                          Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  44.753 VV    1.0071 1.24195e4   146.79349  50.0935
       2  47.879 VB    1.1880 1.23732e4   122.95770  49.9065

    Totals :                  2.47927e4   269.75119

    ==================================================================
                          *** End of Report ***
```

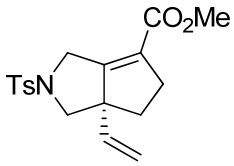


2f

```
Data File E:\LINMU\LMA3P2\LM531000.D
 Sample Name: LM531

    ==================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-5-21 10:45:00
    Acq. Method     : E:\DATA\LM-YU\DEF LC.M
    Last changed    : 2011-4-20 10:08:55  by LM
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```



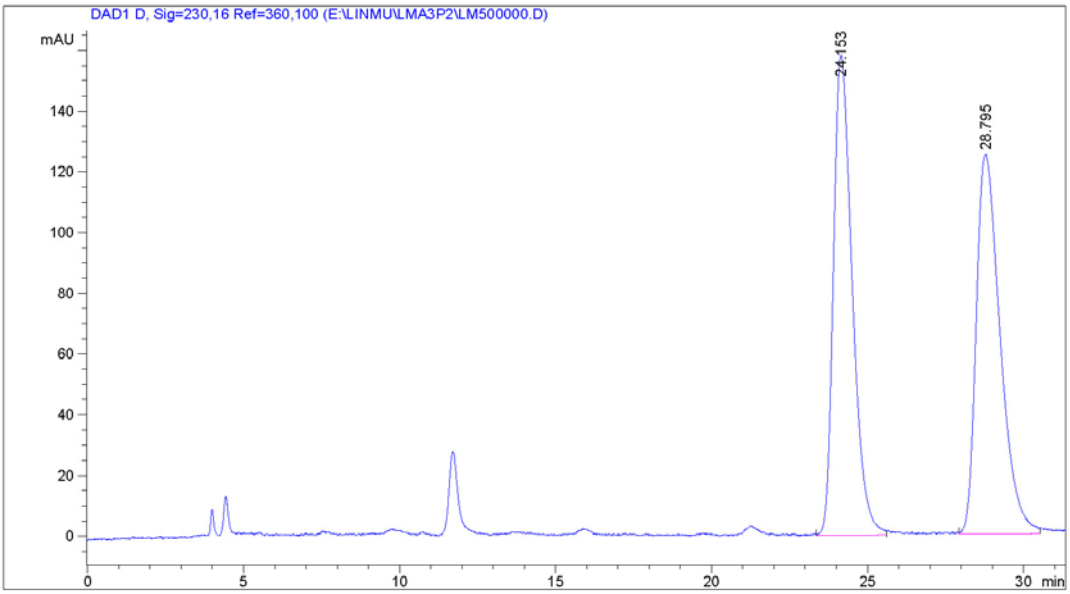

```
    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  44.307 MM    0.9668   79.73850    1.37462   1.0391
       2  49.208 MM    1.7441 7594.01904   72.57001  98.9609

    Totals :                  7673.75755   73.94464

    ==================================================================
                            *** End of Report ***
```



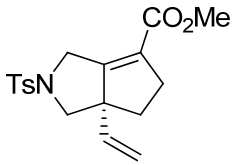
racemic **2g**

Data File E:\LINMU\LMA3P2\LM500000.D
Sample Name: LM500

```
==========================================================================
Acq. Operator   : LM
Acq. Instrument : Instrument 1                    Location :   -
Injection Date  : 2011-4-16 11:58:15
Acq. Method     : C:\HPCHEM\1\METHODS\DEF LC.M
Last changed    : 2011-4-16 11:28:57  by LM
                  (modified after loading)
Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
Last changed    : 2004-4-7 0:10:12
Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```



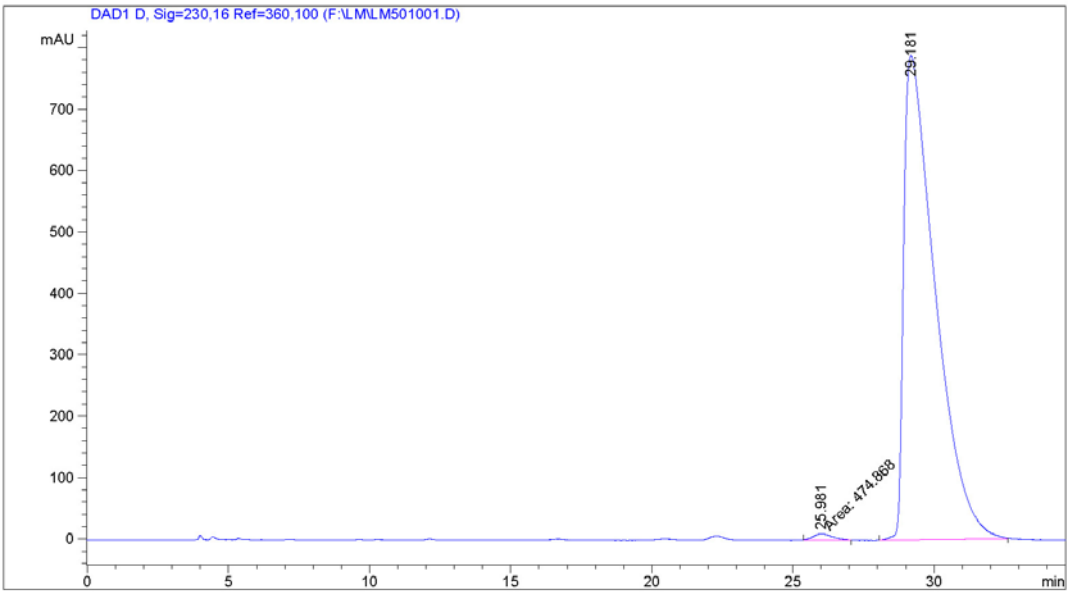

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  24.153 VV    0.5664 6618.02588  158.08757  49.8872
   2  28.795 VV    0.6375 6647.96484  125.20493  50.1128

Totals :                 1.32660e4   283.29250

==========================================================================
                        *** End of Report ***
```



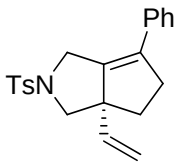
2g

Data File F:\LM\LM501001.D
Sample Name: LM501

```
==========================================================================
Acq. Operator   : LM
Acq. Instrument : Instrument 1                    Location :   -
Injection Date  : 2011-4-16 13:07:33
Acq. Method     : C:\HPCHEM\1\METHODS\DEF LC.M
Last changed    : 2011-4-16 11:28:57  by LM
                  (modified after loading)
Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
Last changed    : 2004-4-7 0:10:12
Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```

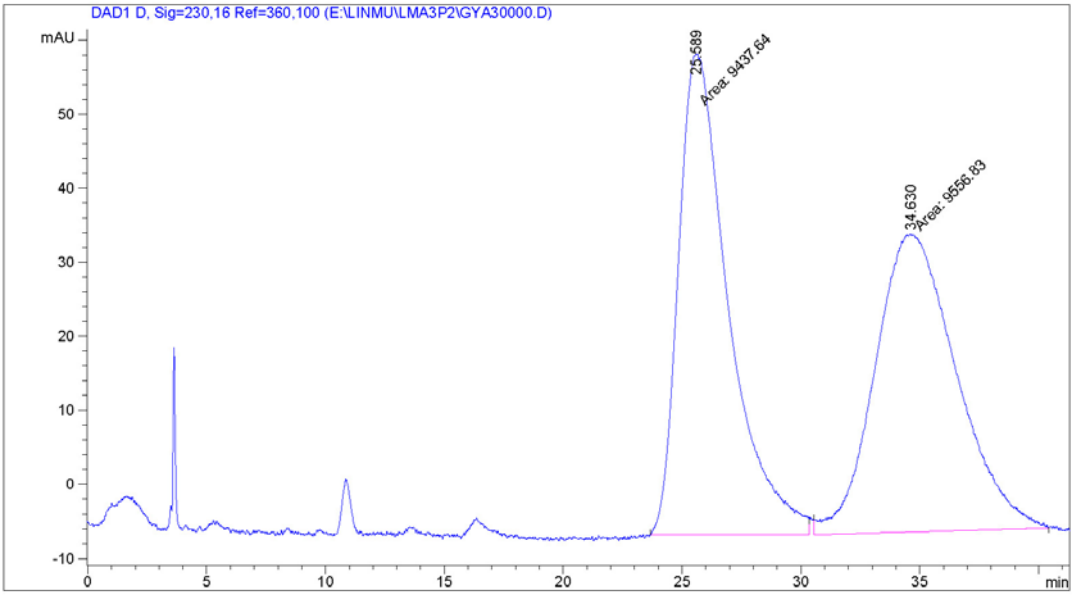



```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  25.981 MM    0.7872  474.86804   10.05356   0.7715
   2  29.181 VB    1.0069 6.10735e4   789.11871  99.2285

Totals :                  6.15483e4   799.17228

==========================================================================
                        *** End of Report ***
```

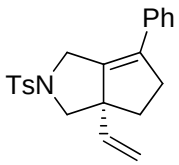


racemic **2h**

```
Data File E:\LINMU\LMA3P2\GYA30000.D
 Sample Name: GYA30

    ==================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-4-8 9:44:40
    Acq. Method     : C:\HPCHEM\1\METHODS\DEF_LC.M
    Last changed    : 2011-4-8 8:05:29  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OJ-H, 1.2 ml/min, nHexane:iPrOH = 90:10
```

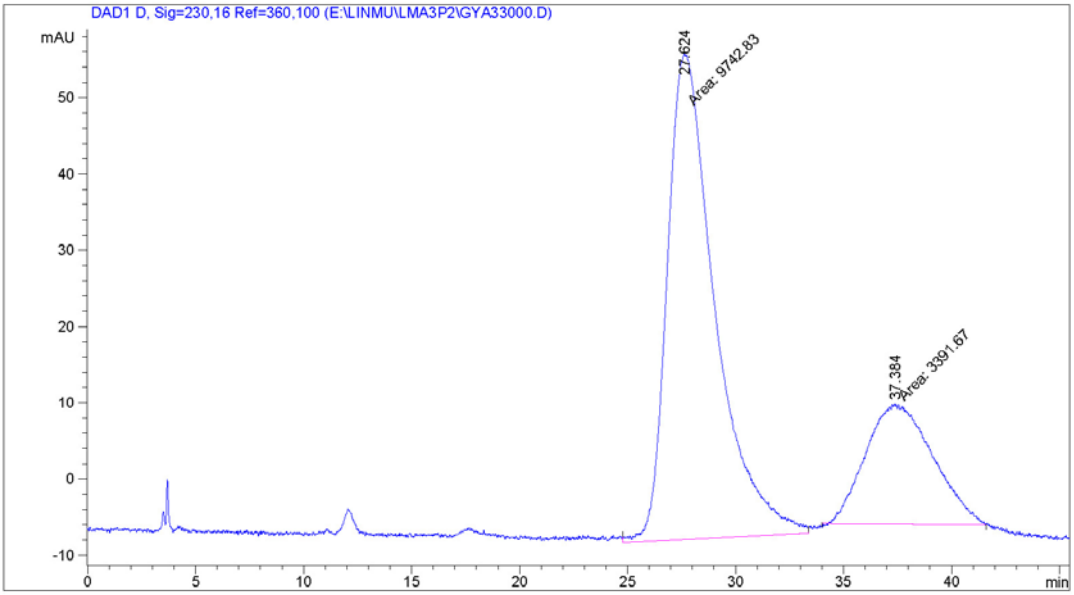



```
    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  25.589 PM    2.4219 9437.63867   64.94610  49.6862
       2  34.630 MM    3.9597 9556.83203   40.22510  50.3138

    Totals :                  1.89945e4   105.17120

    ==================================================================
                            *** End of Report ***
```

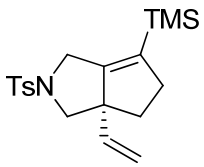


2h

```
Data File E:\LINMU\LMA3P2\GYA33000.D
 Sample Name: GYA33

    ==================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-4-8 10:27:16
    Acq. Method     : C:\HPCHEM\1\METHODS\DEF_LC.M
    Last changed    : 2011-4-8 8:05:29  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OJ-H, 1.2 ml/min, nHexane:iPrOH = 90:10
```



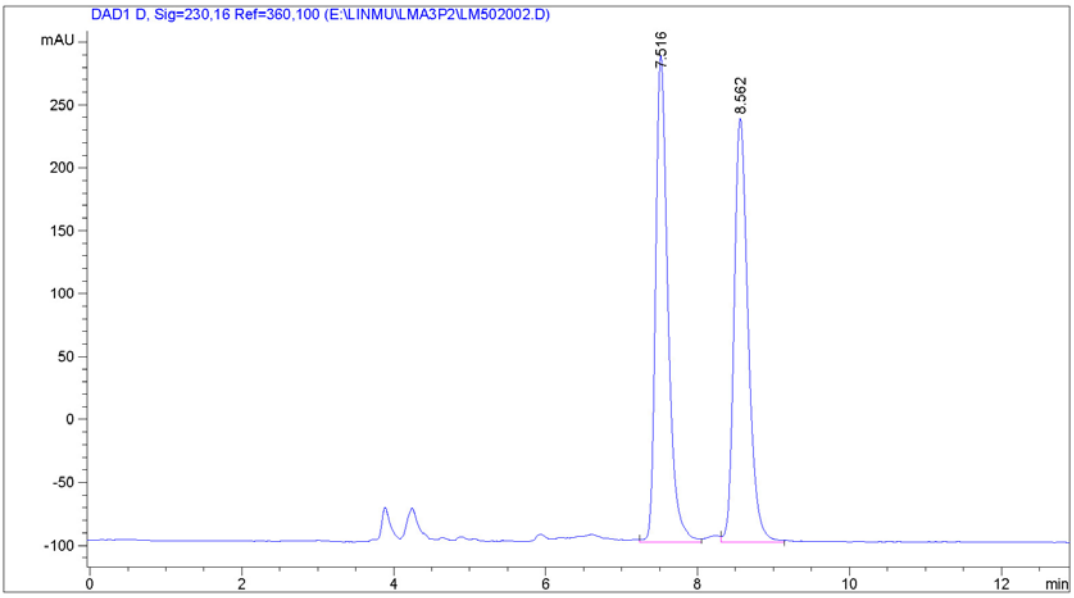

```
    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]    [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  27.624 MM T  2.6385 9742.83008   63.70629  74.1774
       2  37.384 MM T  3.5939 3391.66846   15.72896  25.8226

    Totals :                  1.31345e4    79.43525

    ==================================================================
                            *** End of Report ***
```



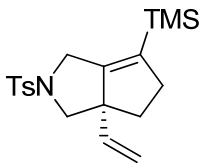
racemic **2i**

Data File E:\LINMU\LMA3P2\LM502002.D
Sample Name: LM502

```
Acq. Operator   : LM
Acq. Instrument : Instrument 1                    Location :   -
Injection Date  : 2011-4-26 10:13:39
Acq. Method     : E:\DATA\LM-YU\DEF LC.M
Last changed    : 2011-4-26 9:36:23  by LM
                  (modified after loading)
Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
Last changed    : 2004-4-7 0:10:12
Sample Info     : AD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```

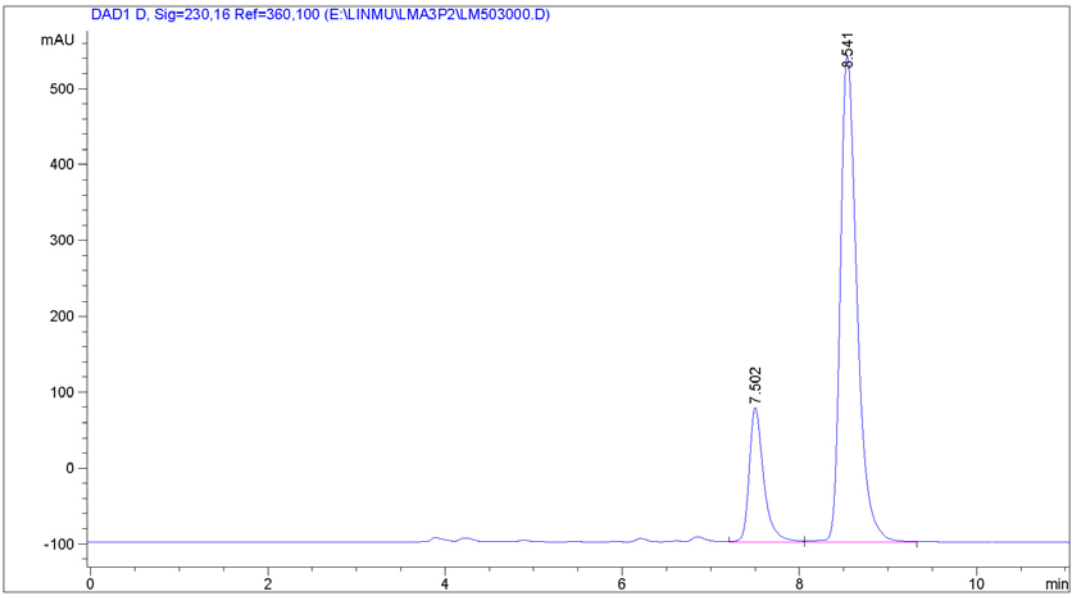



```
=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   7.516 VB    0.1692 4357.13916  387.36292  50.2374
   2   8.562 VV    0.1975 4315.96484  336.87546  49.7626

Totals :                   8673.10400  724.23837

=====================================================================
                      *** End of Report ***
```

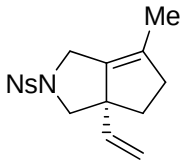


2i

```
Data File E:\LINMU\LMA3P2\LM503000.D
 Sample Name: LM503

    ======================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :    -
    Injection Date  : 2011-4-26 10:27:55
    Acq. Method     : E:\DATA\LM-YU\DEF LC.M
    Last changed    : 2011-4-26 9:36:23  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : AD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```

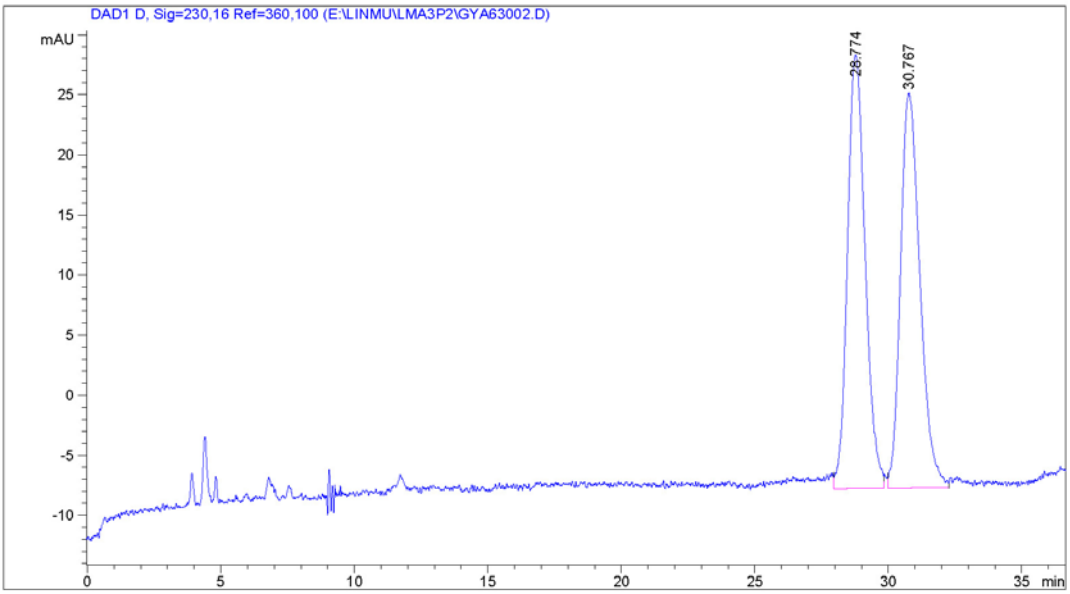



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]    [mAU*s]     [mAU]      %
    ----|-------|----|-------|----------|----------|--------|
       1   7.502 VV    0.1688 2013.60669  176.92795  19.3688
       2   8.541 VB    0.1984 8382.52832  641.73688  80.6312

    Totals :                   1.03961e4   818.66483

    ======================================================================
                              *** End of Report ***
```

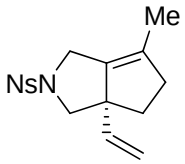


racemic **2j**

```
Data File E:\LINMU\LMA3P2\GYA63002.D
 Sample Name: GYA63

    ========================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-5-27 9:14:56
    Acq. Method     : E:\DATA\LM-YU\DEF LC.M
    Last changed    : 2011-5-27 8:51:45  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```



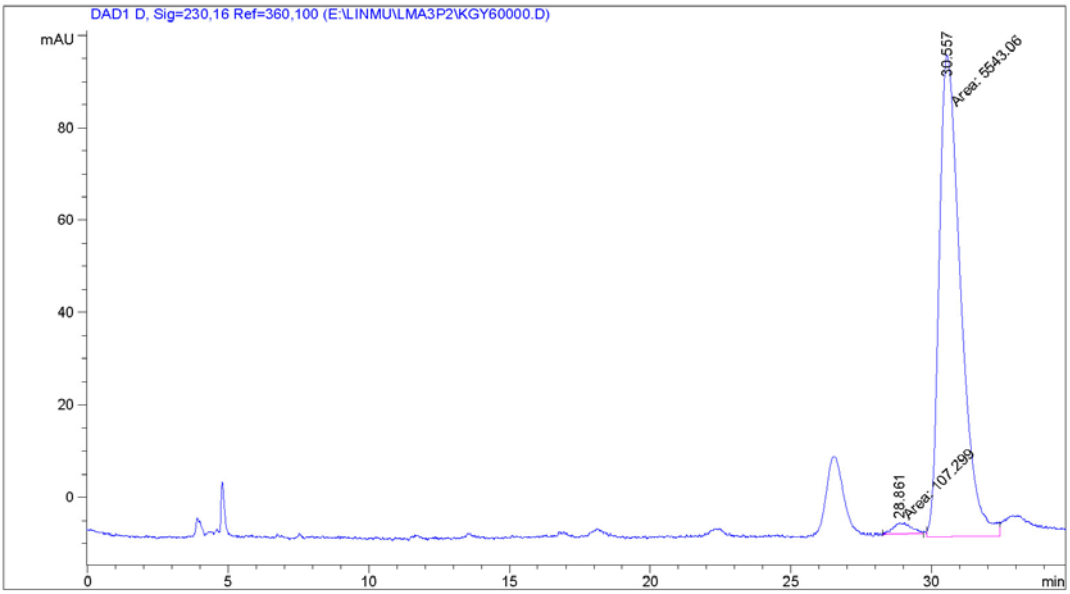

```
    ========================================================================
                              Area Percent Report
    ========================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  28.774 VV    0.5497 1662.07446   36.06300  49.8858
       2  30.767 BV    0.6010 1669.68689   32.84714  50.1142

    Totals :                  3331.76135   68.91013

    ========================================================================
                              *** End of Report ***
```



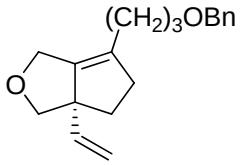
2j

Data File E:\LINMU\LMA3P2\KGY60000.D
Sample Name: KGY60

```
==========================================================================
Acq. Operator   : LM
Acq. Instrument : Instrument 1                    Location :   -
Injection Date  : 2011-5-27 9:52:25
Acq. Method     : E:\DATA\LM-YU\DEF LC.M
Last changed    : 2011-5-27 8:51:45  by LM
                  (modified after loading)
Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
Last changed    : 2004-4-7 0:10:12
Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```

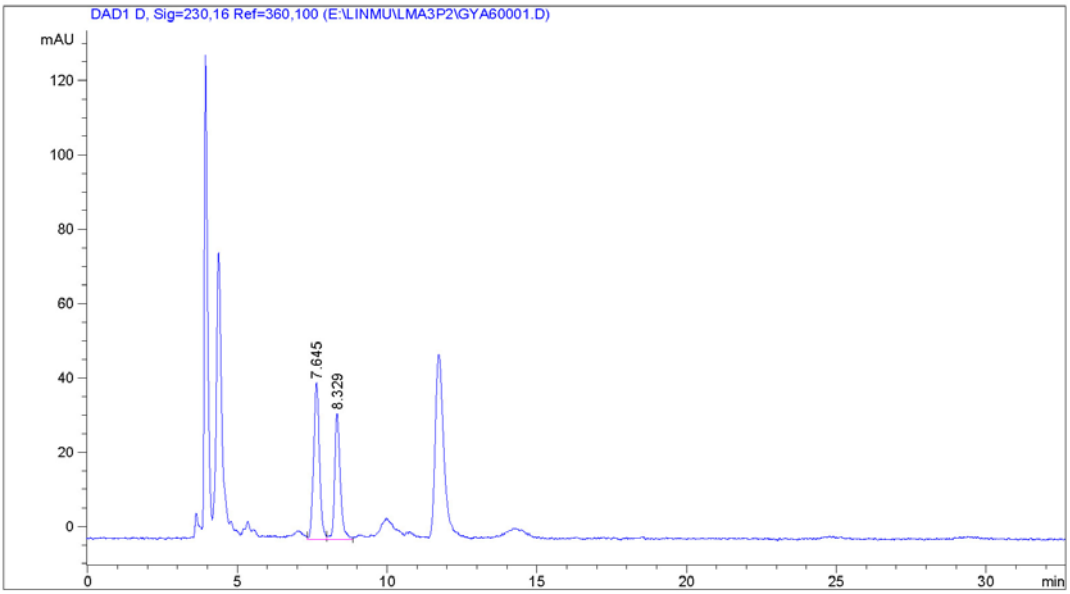



```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  28.861 MM    0.7385  107.29913    2.42145   1.8990
   2  30.557 MM    0.8867 5543.05566  104.19244  98.1010

Totals :                  5650.35479  106.61389

==========================================================================
                          *** End of Report ***
```

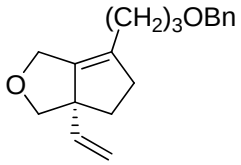


racemic **2k**

```
Data File E:\LINMU\LMA3P2\GYA60001.D
 Sample Name: GYA60

    ========================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :    -
    Injection Date  : 2011-5-13 10:07:43
    Acq. Method     : E:\DATA\LM-YU\DEF LC.M
    Last changed    : 2011-5-13 8:30:11  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```



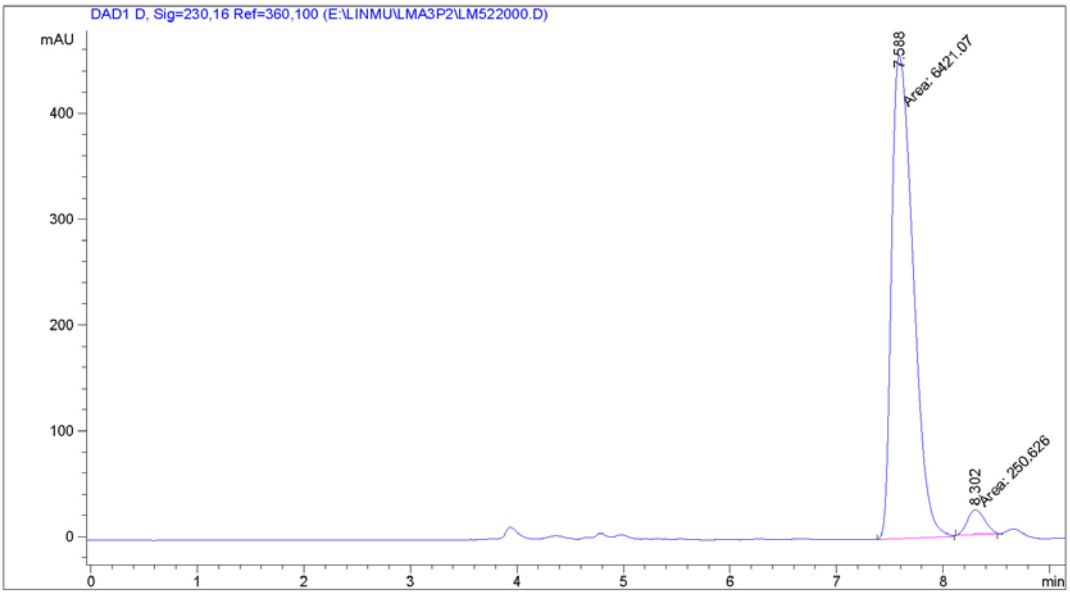

```
    ========================================================================
                              Area Percent Report
    ========================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   7.645 VV    0.2008  565.28296   42.06378  56.3575
       2   8.329 VV    0.1916  437.74829   33.68930  43.6425

    Totals :                  1003.03125   75.75308

    ========================================================================
                              *** End of Report ***
```



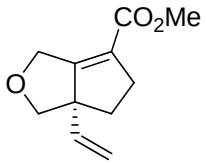
2k

Data File E:\LINMU\LMA3P2\LM522000.D
Sample Name: LM522

```
==========================================================================
Acq. Operator   : LM
Acq. Instrument : Instrument 1                    Location :   -
Injection Date  : 2011-5-13 10:48:39
Acq. Method     : E:\DATA\LM-YU\DEF LC.M
Last changed    : 2011-5-13 8:30:11  by LM
                  (modified after loading)
Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
Last changed    : 2004-4-7 0:10:12
Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```

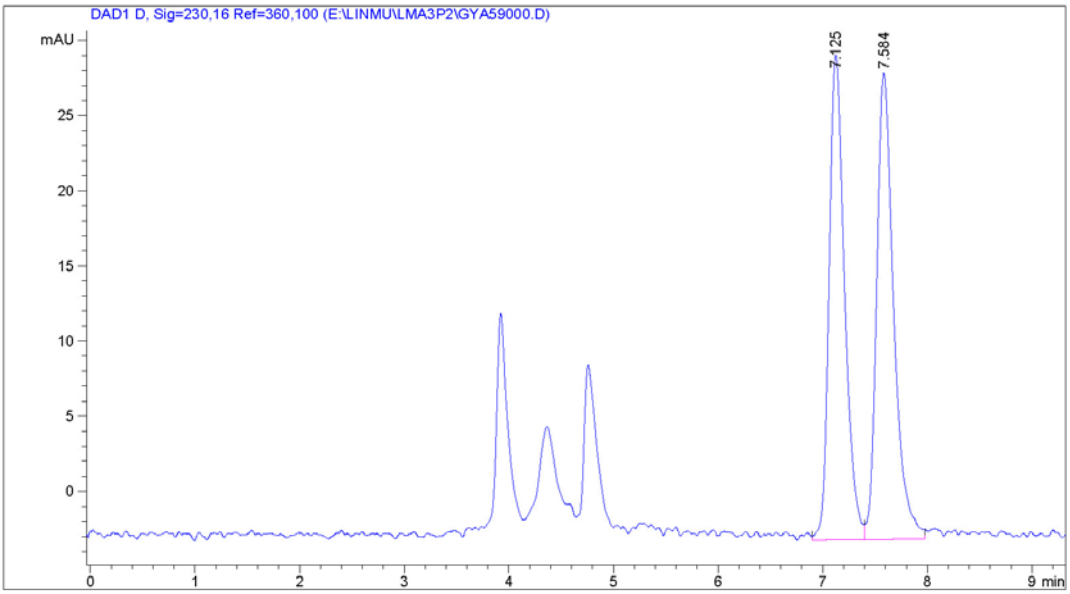



```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   7.588 MM    0.2341 6421.06592  457.09598  96.2434
   2   8.302 MM    0.1812  250.62595   23.05603   3.7566

Totals :                  6671.69186  480.15201

==========================================================================
                        *** End of Report ***
```

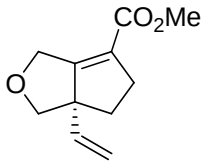


racemic **2l**

```
Data File E:\LINMU\LMA3P2\GYA59000.D
 Sample Name: GYA59

    ==================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-5-13 9:07:21
    Acq. Method     : E:\DATA\LM-YU\DEF LC.M
    Last changed    : 2011-5-13 8:30:11  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```



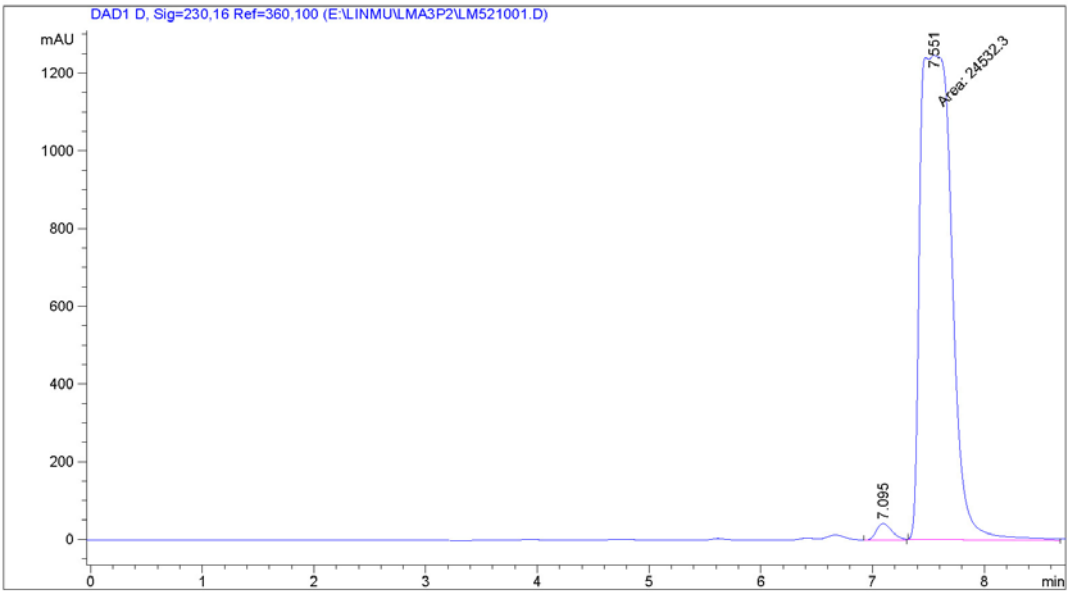

```
    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   7.125 VV    0.1560  331.95941   32.26163  48.6765
       2   7.584 VB    0.1697  350.01065   31.00667  51.3235

    Totals :                    681.97006   63.26830

    ==================================================================
                              *** End of Report ***
```



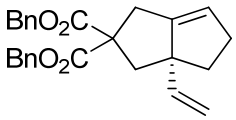
2l

Data File E:\LINMU\LMA3P2\LM521001.D
Sample Name: LM521

```
==========================================================================
Acq. Operator   : LM
Acq. Instrument : Instrument 1                    Location :   -
Injection Date  : 2011-5-13 9:34:16
Acq. Method     : E:\DATA\LM-YU\DEF LC.M
Last changed    : 2011-5-13 8:30:11  by LM
                  (modified after loading)
Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
Last changed    : 2004-4-7 0:10:12
Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```

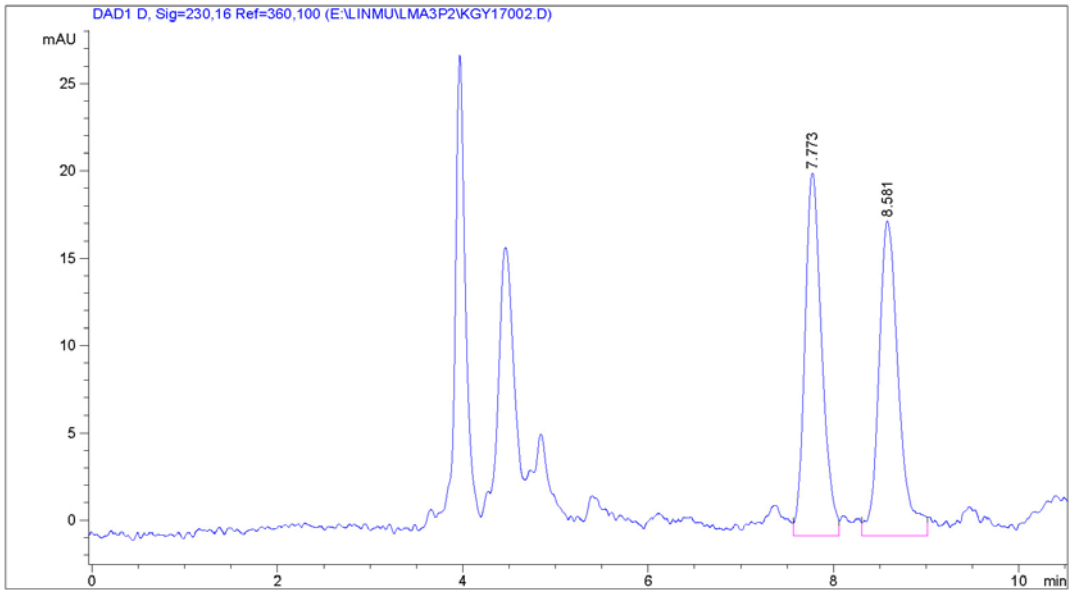



```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.095 VV    0.1440  396.47617   42.04183   1.5904
   2   7.551 MM    0.3282 2.45323e4  1245.85388  98.4096

Totals :                  2.49288e4  1287.89571

==========================================================================
                        *** End of Report ***
```

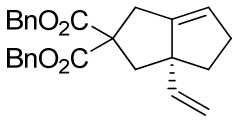


racemic **2m**

```
Data File E:\LINMU\LMA3P2\KGY17002.D
 Sample Name: KGY17

    ==================================================================
    Acq. Operator   : LM
    Acq. Instrument : Instrument 1                    Location :   -
    Injection Date  : 2011-5-21 13:11:30
    Acq. Method     : E:\DATA\LM-YU\DEF LC.M
    Last changed    : 2011-5-21 13:10:59  by LM
                      (modified after loading)
    Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
    Last changed    : 2004-4-7 0:10:12
    Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```



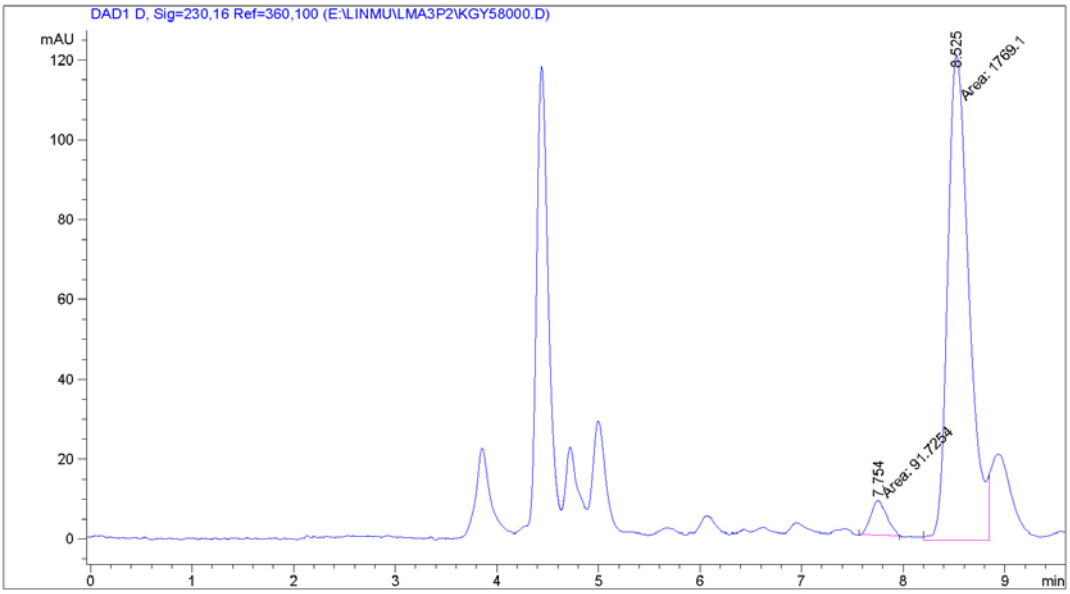

```
    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 D, Sig=230,16 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   7.773 VV    0.1852  261.83633   20.75694  49.7585
       2   8.581 VB    0.2114  264.37845   17.99048  50.2415

    Totals :                    526.21478   38.74741

    ==================================================================
                              *** End of Report ***
```



2m

Data File E:\LINMU\LMA3P2\KGY58000.D
Sample Name: KGY58

```
==========================================================================
Acq. Operator   : LM
Acq. Instrument : Instrument 1                    Location :   -
Injection Date  : 2011-5-21 13:23:54
Acq. Method     : E:\DATA\LM-YU\DEF LC.M
Last changed    : 2011-5-21 13:10:59  by LM
                  (modified after loading)
Analysis Method : C:\Chem32\1\METHODS\DEF_LC.M
Last changed    : 2004-4-7 0:10:12
Sample Info     : OD-H, 1.0 mL/min, nHexane:iPrOH = 95:5
```




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :      1.00000  [ng/ul]   (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.754 MM    0.1804   91.72541    8.47197   4.9293
   2   8.525 MM    0.2428 1769.10156  121.41713  95.0707

Totals :                  1860.82697  129.88910

==========================================================================
                          *** End of Report ***
```