A DFT Calculation-inspiring Rh(I)-catalyzed Reaction via Suppression of α-H Shift in α-Alkyldiazoacetates

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General Remarks and Materials:

All reactions and manipulations were carried out under an argon atmosphere, in a flame-dried or oven-dried flask containing magnetic stir bar. All ^{1}H NMR, and ^{13}C NMR spectra were recorded using a Brucker 400 MHz or 500 MHz spectrometer in $CDCl_3$. Tetramethylsilane (TMS) served as an internal standard (δ = 0) for ^{1}H NMR, and $CDCl_3$ was used as internal standard (δ 77.0) for ^{13}C NMR. Chemical shifts are reported in parts per million as follows: chemical shift, multiplicity (s =singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad). HRMS (ESI) Mass spectra were recorded on IonSpec FT-ICR mass spectrometer. HPLC analysis was performed on Dalian Elite (UV230+ UV/Vis Detector and P230P High Pressure Pump). Chiralpak AD-H, IA was purchased from Daicel Chemical Industries, LTD. The racemic standards used in HPLC studies were prepared according to the general procedure by using racemic BINOL derived phosphoric acid catalysts. Dichloromethane (DCM), 1, 2-dichloroethane (DCE) and toluene was distilled over calcium hydride. Hayashi chiral diene ligand was prepared according to the literature procedure.[1]

General Procedure for catalyst screening and optimization of reaction conditions (Table 1):
A mixture of metal catalyst (0.01 mmol), aldehyde **3a** (0.12 mmol) in 1.0 mL of solvent under an argon atmosphere was stirred under the indicated temperature in table 1. Diazo compound **1a** (0.20 mmol) and amine **2a** (0.1 mmol) in 1.0 mL of solvent was then added over 1 h via a syringe pump. After completion of the addition, the reaction mixture was filtrated and evaporated *in vacuo* to give the crude product. The crude product was purified by flash chromatography on silica gel (eluent: EtOAc/light petroleum ether = 1:20 ~ 1:5) to give the pure product.

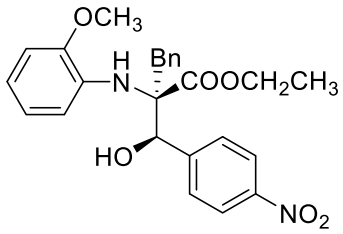
General Procedure for the *threo*-Selective three-component Aldol-type reactions catalyzed by $[Rh(COD)Cl]_2$ (Table 2):
A mixture of $[Rh(COD)Cl]_2$ (0.004 mmol), aldehyde **3** (0.10 mmol) in 1.0 mL of dichloromethane under an argon atmosphere was stirred under rt. Diazo compound **1** (0.20 mmol) and amine **2** (0.12 mmol) in 1.0 mL of dichloromethane was then added over 1 h via a syringe pump. After completion of the addition, the reaction mixture was filtrated and evaporated *in vacuo* to give the crude product. The crude product was purified by flash chromatography on silica gel (eluent: EtOAc/light petroleum ether = 1:20 ~ 1:5) to give the pure product.

General Procedure for Rhodium(I)-catalyzed asymmetric three-component Aldol-type reactions (Table 3):
A mixture of $[Rh(C_2H_2)_2Cl]_2$ (0.0025 mmol) and chiral diene complexin 1.0 mL of solvent of toluene and cyclohexane (1:1) was stirred under room temperature for 1 hour. Aldehyde **3** (0.12 mmol) was added. Diazo compound **1** (0.20 mmol) and amine **2** (0.10 mmol) in 1.0 mL of dichloromethane was then added in -20 ℃ over 1 h via a syringe pump. After completion of the addition, the reaction mixture was filtrated and evaporated *in vacuo* to give the crude product. The crude product was purified by flash chromatography on silica gel (eluent: EtOAc/light petroleum ether = 1:20 ~ 1:5) to give the pure product.

References: [1] S. Abele; R. Inauen; D. Spielvogel; C. Moessner, *J. Org. Chem.* **2012**, *77*, 4765-4773.

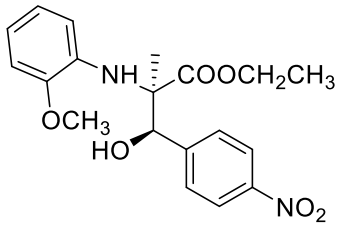
^{1}H NMR, ^{13}C NMR and HPLC data for new compounds:

Ethyl (2*R*, 3*R*)-2-benzyl-3-hydroxy-2-((2-methoxyphenyl) amino)-3-(4-nitrophenyl) propanoate (4a)



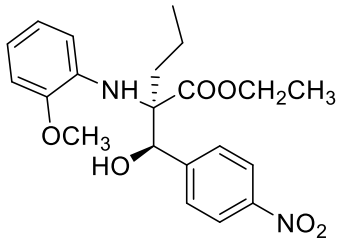
^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) δ 8.16 (d, J = 7.0 Hz, 2H), 7.54 (d, J = 7.0 Hz, 2H), 7.21 (m, J = 2.8 Hz, 3H), 7.00 (m, 2H), 6.89-6.86 (m, 2H), 6.85-6.78 (m, 2H), 5.69 (s, 1H), 5.14(s, 1H), 4.57 (s, 1H), 4.02-3.96 (m, 1H), 3.85 (d, J = 6.0 Hz, 1H), 3.81 (s, 3H), 3.49 (d, J = 11.3 Hz, 1H), 3.00 (d, J = 11.3 Hz, 1H), 0.87 (t, J = 5.7Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) δ 174.17, 147.70, 147.41, 146.34, 135.10, 134.54, 129.95, 128.69, 128.05, 126.96, 122.48, 120.85, 112.98, 110.42, 74.14, 68.04, 61.69, 55.70, 37.61, 13.34. **HRMS** (ESI) Calcd for $C_{25}H_{26}N_2O_6$ $(M+Na)^+$ 473.1477, Found: 473.1783. **HPLC** (Chiral OD-H, λ = 254 nm, hexane/2-propanol = 5:1, Flow rate = 0.8 mL/min), t_R= 11.58 min, 12.70 min.

Ethyl (2*R, 3*R**) -3-hydroxy-2-((2-methoxyphenyl)amino)-2-methyl-3 -(4-nitrophenyl) propanoate (4b)**



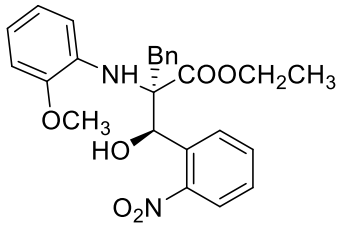
^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) δ 8.10(d, J = 8.0 Hz, 2H), 7.41(d, J = 8.0 Hz, 2H), 6.86-6.76(m, J = 8.0 Hz, 3H), 6.68 (m, 2H), 5.60 (d, J = 4.0 Hz, 1H), 4.45(m, 2H), 4.22-4.16 (d, J = 8.0 Hz, 2H), 3.80 (s, 3H), 1.39 (s, 3H), 1.11 (t, J = 8.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) δ 176.59, 147.41, 146.06, 134.51, 128.54, 122.40, 121.01, 118.60, 112.40, 110.20, 73.11, 63.13, 62.00, 55.50, 19.45, 13.81. **HRMS** (ESI) Calcd for $C_{19}H_{22}N_2O_6$ $(M+Na)^+$ 397.1376 , Found: 397.1385.

Ethyl(2*R,3*R**)-2-propyl-3-hydroxy-2-((2-methoxyphenyl)amino)-2-methyl-3 -(4-nitrophenyl) propanoate (4c)**



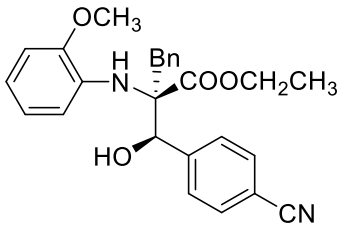
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS) δ 8.12 (d, *J* = 8.4 Hz, 2H), 7.43 (d, J = 8.3 Hz, 2H), 6.82-6.72 (m, *J* = 8.0 Hz, 3H), 6.43 (m, 2H), 5.42 (s, 1H), 5.34 (d, *J* = 8.3 Hz, 1H), 4.20 (q, *J* = 7.0 Hz, 2H), 3.85 (s, 3H), 3.71 (d, *J* = 8.5 Hz, 1H), 2.16 – 1.99 (m, 2H), 1.25 (m, *J* = 4.1 Hz, 5H), 0.79 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) *δ* 173.41, 147.95, 147.95, 134.25, 128.19, 122.82, 120.76, 118.36, 113.49, 110.10, 75.09, 69.21, 62.36, 55.78, 34.80, 29.70, 14.07. **HRMS** (ESI) Calcd for $C_{21}H_{26}N_2O_6$ $(M+Na)^+$ 425.1325 , Found: 425.1342.

Ethyl (2*R*, 3*R*)-2-benzyl-3-hydroxy-2-((2-methoxyphenyl)amino)-3-(2-nitrophenyl) propanoate (4d)



^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) *δ* 7.94 (s, 1H), 7.82 (s, 1H), 7.57 (s, 1H), 7.44 (s, 1H), 7.25(s, 1H), 6.84-7.11 (m, 9H), 6.31 (s, 1H), 5.57 (s, 1H), 3.86 (s, 1H), 3.78 (s, 3H), 3.75 (s, 1H), 3.42 (dd, *J* = 7.5 Hz, 1H), 3.20 (dd, *J* = 12 Hz, 1H), 0.86 (t, *J* = 8.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) *δ* 172.26, 149.43, 148.42, 135.61, 134.28, 133.76, 131.94, 130.58, 129.94, 128.51, 128.02, 126.79, 124.09, 121.06, 118.94, 114.60, 110.45, 70.35, 61.70, 59.91, 36.54, 29.69, 13.34. **HRMS** (ESI) Calcd for $C_{21}H_{26}N_2O_6$ $(M+Na)^+$ 473.1655 Found: 473.1689 **HPLC** (Chiral IA, λ = 254 nm, hexane/2-propanol = 5:1, Flow rate = 0.8 mL/min), t_R= 11.98 min, 15.46 min.

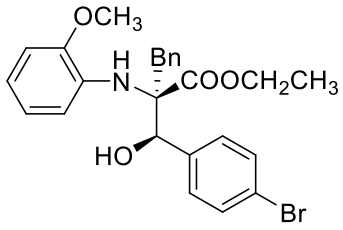
Ethyl (2*R, 3*R**)-2-benzyl-3-(4-cyanophenyl)-3-hydroxy-2-((2-methoxyphenyl) amino) propanoate (4e)**



^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) *δ* 7.58 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.18 (m, 3H), 6.97 (s, 2H), 6.84-6.81 (m, 2H), 6.78-6.73 (m, 2H), 5.61 (s, 1H), 5.10 (s, 1H), 4.49 (s, 1H), 3.96 (m, *J* = 4.0 Hz, 1H), 3.77(s, 3H), 3.46 (d, *J* = 16.0 Hz, 1H), 2.96 (d, *J* = 16.0 Hz, 1H), 0.84 (t, *J* =

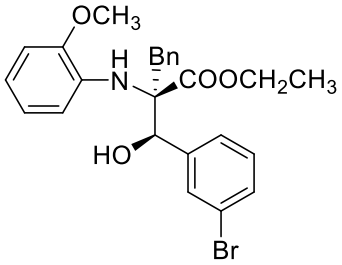
8.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) δ 174.16, 147.66, 144.30, 135.16, 134.55, 131.17, 129.95, 128.54, 128.06, 126.95, 120.84, 118.85, 118.30, 112.98, 111.39, 110.36, 74.27, 68.03, 61.64, 55.69, 37.53, 13.34. **HRMS** (ESI) Calcd for $C_{26}H_{26}N_2O_4$ $(M+Na)^+$ 453.1790, Found: 453.1768.

Ethyl (2*R, 3*R**)-2-benzyl-3-(4-bromophenyl)-3-hydroxy-2-((2-methoxyphenyl) amino)propanoate (4f)**



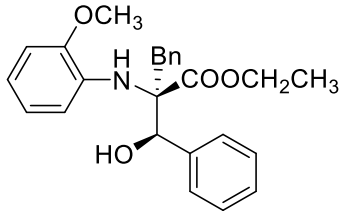
^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) δ 7.36 (d, J = 12.0 Hz, 2H), 7.14 (d, J = 12.0 Hz, 2H),7.08 (m, 3H), 6.94 (m, 2H), 6.81-6.84 (m, 2H), 6.71-6.76 (m, 2H), 5.26-5.32 (m, 2H), 4.04-3.97 (m, 2H), 3.85 (d, J = 8.0 Hz, 1H), 3.72-3.68 (m, 4H), 3.53-3.49 (d, J = 8.0 Hz, 1H),1.05 (t, J = 8.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) δ 172.54, 147.86, 138.86, 135.66, 134.73, 130.77, 130.19, 128.78, 127.89, 126.68, 121.75, 120.90, 117.75, 113.40, 110.47, 74.45, 69.65, 61.93, 55.78, 37.76, 13.75. **HRMS** (ESI) Calcd for $C_{25}H_{26}BrNO_4$ $(M+Na)^+$ 506.0943 , Found: 506.0952. **HPLC** (Chiral IA, λ = 254 nm, hexane/2-propanol = 5:1, Flow rate = 0.8 mL/min), t_R= 9.83 min, 10.57 min.

Ethyl (2*R, 3*R**)-2-benzyl-3-(3-bromophenyl)-3-hydroxy-2-((2-methoxyphenyl) amino)propanoate (4g)**



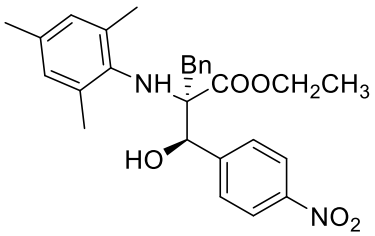
^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) δ 7.47-7.42 (m, 2H), 7.29 (s, 1H), 7.16 (d, J = 7.4 Hz, 4H), 7.00 (s, 2H), 6.86-6.82 (m, 2H), 6.79-6.73 (m, J = 6.5 Hz, 4H), 5.47 (s, 1H), 5.15 (s, 1H), 4.27 (s, 1H), 3.98-3.96 (m, 1H), 3.87-3.80 (m, 4H), 3.46 (d, J = 14.2 Hz, 1H), 3.03 (d, J = 16 Hz, 4H), 0.91 (t, J= 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) δ 173.23, 146.80, 140.17, 133.63, 129.84, 129.10, 128.06, 127.05, 125.84, 125.49, 120.83, 119.86, 117.24, 112.18, 109.40, 73.28, 67.31, 60.66, 54.75, 48.28, 36.57, 34.60, 28.69, 27.46, 12.44. **HRMS** (ESI) Calcd. for $C_{25}H_{26}BrNO_4$ $(M+Na)^+$ 506.0943, Found: 506.0936.

Ethyl (2*R, 3*R**)-2-benzyl-3-hydroxy-2-((2-methoxyphenyl)amino)-3 -phenylpropanoate (4h)**



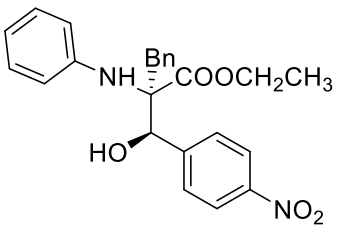
^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) δ 7.48-7.39 (m, 2H), 7.29 (s, 1H), 7.18 (dd, J = 6.0, 2.1 Hz, 4H), 7.00 (dd, J = 6.4, 2.8 Hz, 2H), 6.87-6.80 (m, 2H), 6.76 (dd, J = 15.4, 7.0 Hz, 2H), 5.47 (s, 1H), 5.15 (s, 1H), 4.26 (s, 1H), 3.98 (dd, J = 10.7, 7.2 Hz, 1H), 3.86 (dt, J = 6.6, 5.5 Hz, 1H), 3.80 (s, 3H), 3.46 (d, J = 14.2 Hz, 1H), 3.03 (d, J = 14.2 Hz, 1H), 0.91 (t, J = 7.2 Hz, 4H). **^{13}C NMR** (100 MHz, CDCl3, 25 ℃, TMS) δ 172.19, 146.18, 135.54, 128.27, 127.37, 125.81, 120.12, 116.53, 109.52, 108.93, 59.90, 56.81, 54.48, 37.86, 13.05. **HRMS** (ESI) Calcd. for $C_{25}H_{27}NO_4$ $(M+Na)^+$ 428.1838, Found: 428.1828.

Ethyl (2*R, 3*R**)-2-benzyl-3-hydroxy-2-(mesitylamino)-3-(4-nitrophenyl) propanoate (4i)**



^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) δ 8.20 (d, J = 8.0 Hz, 2H), 7.60 (d, J = 8.0 Hz, 2H), 7.05 (d, J = 4.0 Hz, 1H), 6.92-6.96 (m, J = 8.0 Hz, 2H), 6.72(s, 2H), 6.55 (d, J = 8.0 Hz, 2H), 5.12(s, 1H), 4.74(s, 2H), 4.11-4.07 (m, 1H), 3.88-3.83 (m, 1H), 3.34 (d, J = 16.0 Hz, 1H), 3.00 (d, J = 16.0 Hz, 1H), 2.24 (s, 3H), 2.11 (s, 6H), 0.97 (t, J=8.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) δ 172.13, 148.19, 147.31, 139.32, 135.11, 133.66, 133.64, 129.84, 129.75, 128.51, 127.51, 126.51, 122.67, 72.36, 61.67, 38.78, 20.47, 19.96, 13.44. **HRMS** (ESI) Calcd for $C_{27}H_{30}N_2O_5$ $(M+Na)^+$, Found: 428.1828.

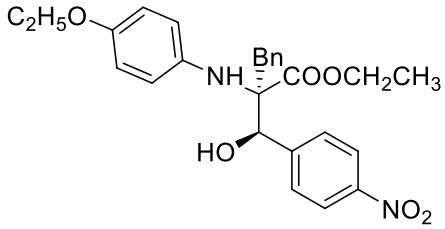
Ethyl (2*R, 3*R**)-2-benzyl-3-hydroxy-3-(4-nitrophenyl)-2-(phenylamino) propanoate (4j)**



^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) δ 8.09(d, J = 7.0 Hz, 2H), 7.41 (d, J = 7.0 Hz, 2H), 7.23 (m, J =13.1 Hz, 2H), 7.17-7.15 (m, 3H), 6.97 (m, 2H),

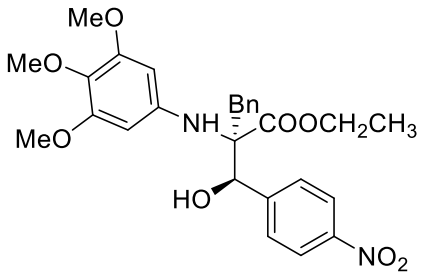
6.83(m,*J* = 5.8 Hz, 2H), 5.59 (d, *J* =7.3 Hz, 1H), 4.58(s, 1H), 4.06-3.99 (m, 3H), 3.83 (d, *J* = 11.3 Hz, 1H), 3.56 (d, *J* = 11.3 Hz, 1H), 1.09 (t, *J* = 5.7Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) *δ* 172.02, 147.50, 147.34, 144.08, 135.23, 130.19, 129.64, 128.17, 127.97, 127.07, 122.85, 118.69, 115.73, 73.89, 69.84, 62.51, 36.71, 29.69, 13.88. **HRMS** (ESI) Calcd for $C_{24}H_{24}N_2O_5$ $(M+Na)^+$ 443.1583, Found: 443.1568 .

Ethyl (2*R, 3*R**)-2-benzyl-2-((4-ethoxyphenyl)amino)-3-hydroxy-3-(4-nitrophenyl) propanoate (4k)**



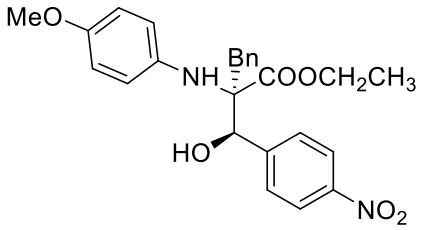
^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) *δ* 8.10 (d, *J* = 8.8 Hz, 2H), 7.49 (d, *J* = 8.7 Hz, 2H), 7.13 (d, *J* = 3.0 Hz, 3H), 6.91-6.86 (m, 2H), 6.75-6.70 (m, 2H), 6.63-6.58 (m, 2H), 5.51 (s, 1H), 4.26 (s, 1H), 4.21 (s, 1H), 3.96-3.88 (m, 3H), 3.77 (m, 1H), 3.36 (d, *J* = 14.2 Hz, 1H), 2.94 (d, *J* = 14.2 Hz, 1H), 1.33 (t, *J* = 7.0 Hz, 3H), 0.83 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) *δ* 172.91, 151.66, 146.55, 145.60, 136.99, 134.19, 129.00, 127.79, 127.26, 126.11, 121.65, 116.85, 115.43, 114.69, 114.60, 112.38, 73.77, 67.81, 62.92, 60.79, 36.49, 28.69, 13.94, 12.49. **HRMS** (ESI) Calcd for $C_{26}H_{28}N_2O_6$ $(M+Na)^+$ 487.1845, Found: 487.1859.

Ethyl (2R, 3R)-2-benzyl-3-hydroxy-3-(4-nitrophenyl)-2-((3,4,5-trimethoxyphenyl) amino) propanoate (4l)



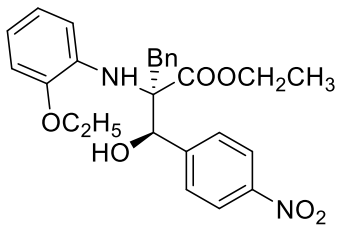
^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) δ 8.10 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 8.8 Hz, 2H), 7.14(t, J =3.2 Hz, 3H), 6.91(t, J =3.2 Hz, 2H), 5.92(s, 2H), 5.55(d, J = 2.4 Hz, 1H), 4.33 (s, 1H), 4.02 (d, J = 2.4 Hz, 1H), 3.72-3.97 (m, 2H), 3.73 (s,6H), 3.72 (s, 3H), 3.38 (d, J = 14.0 Hz, 1H), 3.06 (d, J = 14.0 Hz, 1H), 0.91 (t, J = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) δ 172.87, 152.89, 146.62, 145.39, 140.07, 134.11, 130.48, 129.04, 127.78, 127.32, 127.21, 126.22, 121.75, 93.15, 74.17, 67.74, 61.06, 60.10, 55.12, 36.68, 12.64. **HPLC** (Chiral IA, λ = 254 nm, hexane/2-propanol = 5:1, Flow rate = 0.8 mL/min), t_R= 13.06 min, 15.35 min. **HRMS** (ESI) Calcd for $C_{27}H_{30}N_2O_8$ $(M+Na)^+$ 511.2080 Found: 511.2043

Ethyl (2*R, 3*R**)-2-benzyl-3-hydroxy-2-((4-methoxyphenyl)amino)-3 -(4 -nitrophenyl) propanoate (4m)**



^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) δ 8.14 (d, J = 8.0 Hz, 2H), 7.54 (d, J = 8.7 Hz, 2H), 7.20(d, J = 4.0 Hz, 3H), 6.96(s, 2H), 6.81-6.78 (m, 2H), 6.69 (m, 2H), 5.58(s, 1H), 4.40 (s, 1H), 4.33 (s, 1H), 4.01-3.96 (m, 1H), 3.87-3.82 (m, 1H), 3.76 (s,3H), 3.41 (d, J = 12.0 Hz, 1H), 3.04 (d, J = 12.0 Hz, 1H), 0.90 (t, J = 8.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) δ 173.79, 153.13, 147.37, 146.58, 137.99, 135.13, 129.90, 128.70, 128.17, 127.02, 122.57, 117.69, 114.71, 74.65, 68.73, 61.75, 55.33, 37.33, 13.44. **HRMS** (ESI) Calcd for $C_{25}H_{26}N_2O_6$ $(M+Na)^+$ 473.1689, Found: 473.1694 .

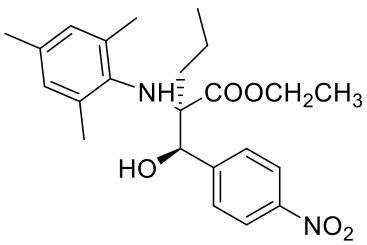
Ethyl (2*R, 3*R**)-2-benzyl-2-((2-ethoxyphenyl)amino)-3-hydroxy-3 -(4 -nitrophenyl) propanoate(4n)**



^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) δ 8.09 (d, J = 8.6 Hz, 2H), 7.43 (d, J = 8.6 Hz, 2H), 7.16 (d, J = 5.1 Hz, 3H), 6.98-6.93 (m, 2H), 6.88-6.74 (m, 4H), 5.50 (d, J = 8.8 Hz, 1H), 5.35 (s, 1H), 4.27 (d, J = 8.9 Hz, 1H), 4.02 –

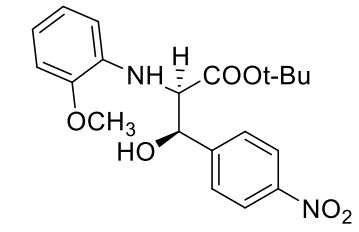
3.87 (m, 4H), 3.75 (d, *J* = 14.0 Hz, 1H), 3.52 (d, *J* = 14.0 Hz, 1H), 1.22 (t, *J* = 6.9 Hz, 3H), 1.01 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) *δ* 171.55, 146.51, 146.28, 134.27, 133.51, 129.25, 127.20, 127.01, 125.92, 121.69, 119.93, 117.29, 112.45, 110.64, 73.43, 68.56, 63.20, 61.12, 36.17, 28.69, 13.83, 12.69. **HRMS** (ESI) Calcd for $C_{26}H_{28}N_2O_6$ $(M+Na)^+$ 487.1845 , Found: 487.1861.

Ethyl (*R)-2-((*R**)-hydroxy(4-nitrophenyl)methyl)-2-(mesitylamino) pentanoate (4o)**



^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS) *δ* 7.69 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 6.35(s, 2H), 4.70 (s, 1H), 4.38 (dd, *J* = 12 Hz, 1H), 3.54-3.49 (m, 1H), 3.07-3.03 (m, 1H), 1.81 (s, 6H), 1.75 (s, 3H), 0.37-0.33 (m, 4H), 0.18 (s, 1H), 0.74-0.58 (m, 1H), 0.00-0.02 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) *δ* 172.61, 148.27, 147.37, 139.12, 133.46, 133.03, 129.76, 128.18, 122.75, 71.63, 63.31, 33.75, 20.52, 19.91, 17.18, 14.40, 13.44. **HRMS** (ESI) Calcd for $C_{23}H_{30}N_2O_5$ $(M+Na)^+$ 435.1896 , Found: 435.1793.

***tert*-Butyl (2*R**, 3*R**)-3-hydroxy-2-((2-methoxyphenyl)amino)-3-(4-nitrophenyl) propanoate (4p)**

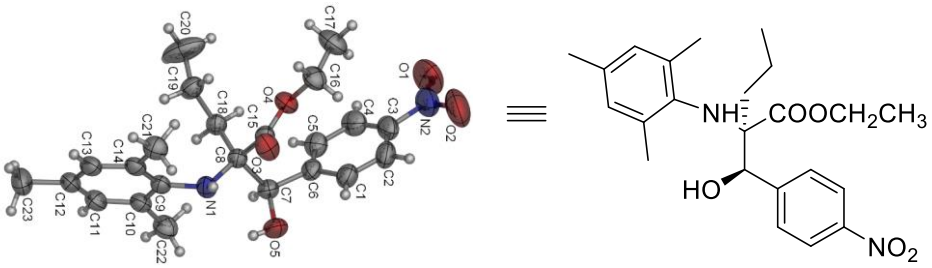


Chemical Formula: $C_{20}H_{24}N_2O_6$
Exact Mass: 388.16

^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃, TMS)*δ* 8.22 (dd, *J* = 12.0, 8.8 Hz, 2H), 7.62 (d, *J* = 8.1 Hz, 2H), 6.85-6.69 (m, 3H), 6.44 (d, *J* = 8.3 Hz, 1H), 5.15 (dd, *J* = 41.7, 24.8 Hz, 2H), 3.87 (s, 3H), 3.43 (d, *J* = 5.2 Hz, 1H), 1.33 (s, 6H), 1.24 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ℃, TMS) *δ* 170.59, 147.72, 147.67, 147.46, 136.15, 127.59, 127.11, 123.43, 123.35, 121.01, 118.93, 111.65, 110.08, 83.16, 73.46, 73.13, 63.82, 55.62, 27.88. **HRMS** (ESI) Calcd for $C_{20}H_{24}N_2O_6$ $(M+Na)^+$ 413.1689 , Found: 413.1529.

Single Crystal X-ray Structure Determinations of Compound *threo*-4o

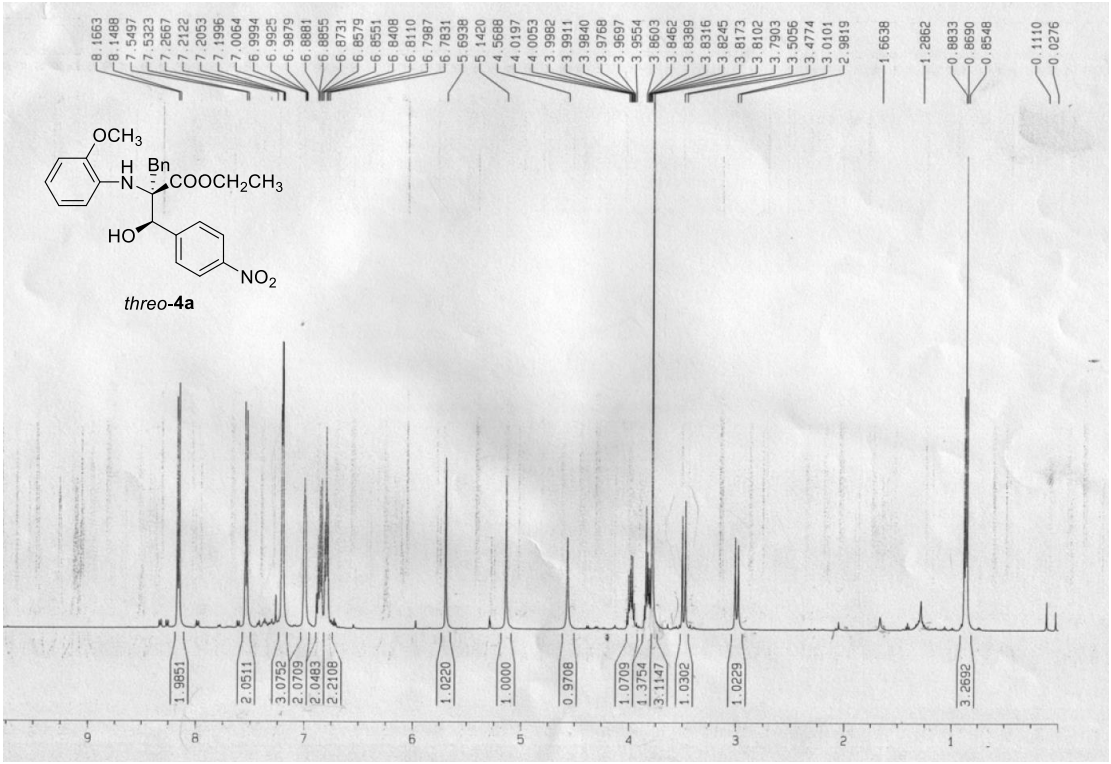
CCDC No.: 984118

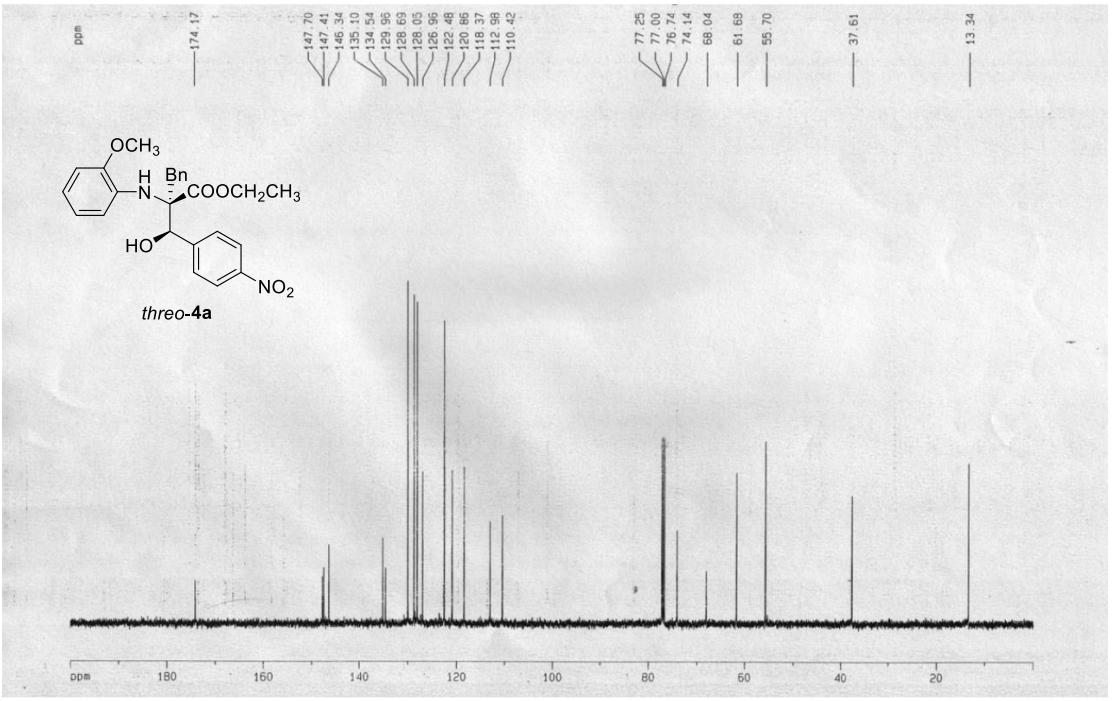


(2*R**, 3*R**)-*threo*-**4o**

Bond precision:	C-C = 0.0032 A	Wavelength=0.71073
Cell: a=12.0803(4)	b=14.8270(5)	c=13.7314(5)
alpha=90	beta=114.984(1)	gamma=90
Temperature: 296 K		
	Calculated	Reported
Volume	2229.35(13)	2229.35(13)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C23 H30 N2 O5	?
Sum formula	C23 H30 N2 O5	C23 H30 N2 O5
Mr	414.49	414.49
Dx,g cm-3	1.235	1.235
Z	4	4
Mu (mm-1)	0.087	0.087
F000	888.0	888.0
F000'	888.43	
h,k,lmax	14,17,16	14,17,16
Nref	3934	3936
Tmin,Tmax	0.973, 0.983	0.973,0.983
Correction method= MULTI-SCAN		
Data completeness= 1.001		Theta(max)= 25.000
R(reflections)= 0.0470(2847)		wR2(reflections)= 0.1483(3936)
S = 1.038		Npar= 276

^{1}H NMR and ^{13}C NMR spectra for new compounds

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120.86
118.37
112.98
110.42
77.25
77.00
76.74
74.14
68.04
61.69
55.70
37.61
13.34
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HO
NO2
threo-4a
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120
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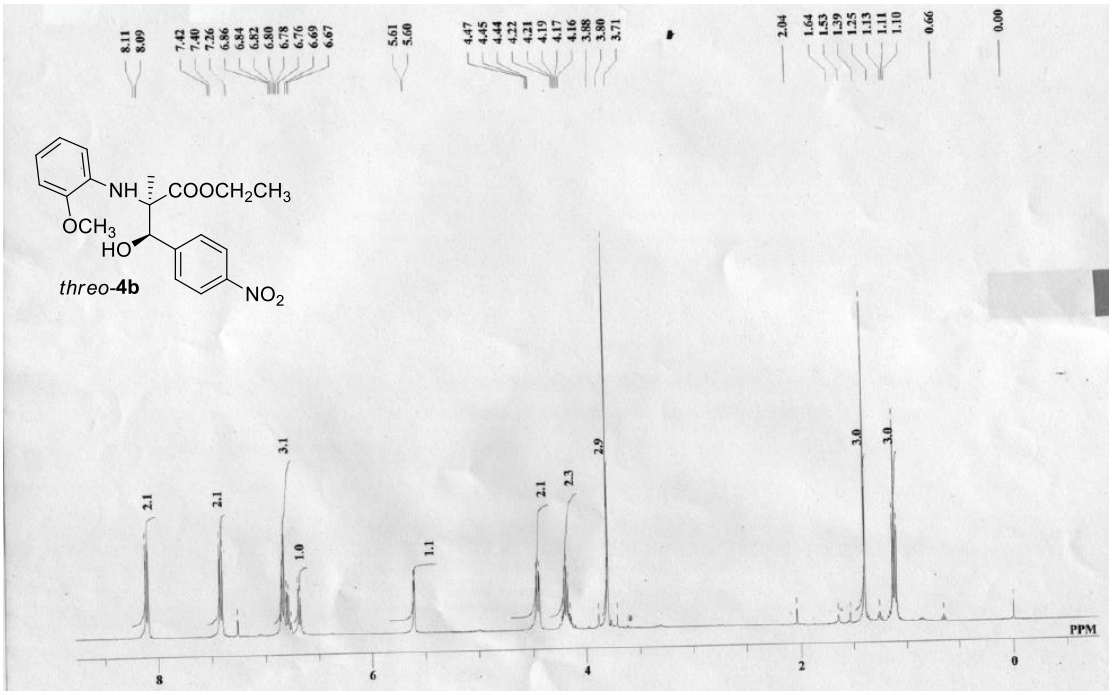
80
60
40
20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6.82
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6.67
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5.60
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4.45
4.44
4.22
4.21
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4.17
4.16
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3.80
3.71
2.04
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0.00
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OCH3
HO
NO2
threo-4b
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2.1
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3.0
PPM
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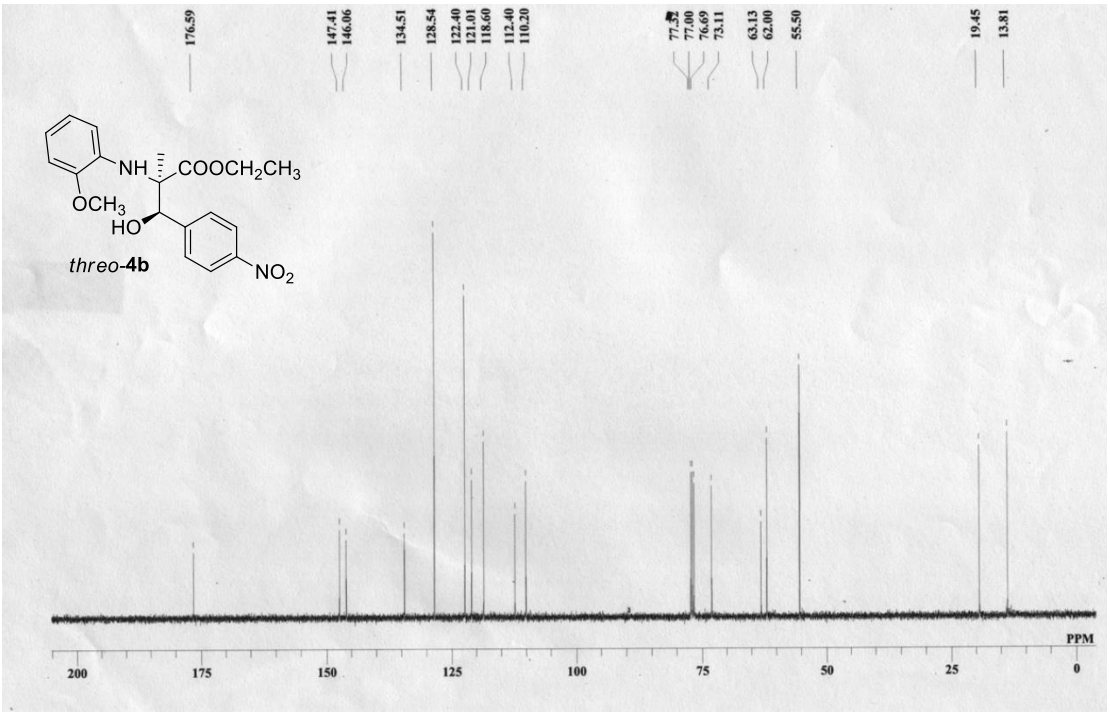
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73.11
63.13
62.00
55.50
19.45
13.81
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HO
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threo-4b
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75
50
25
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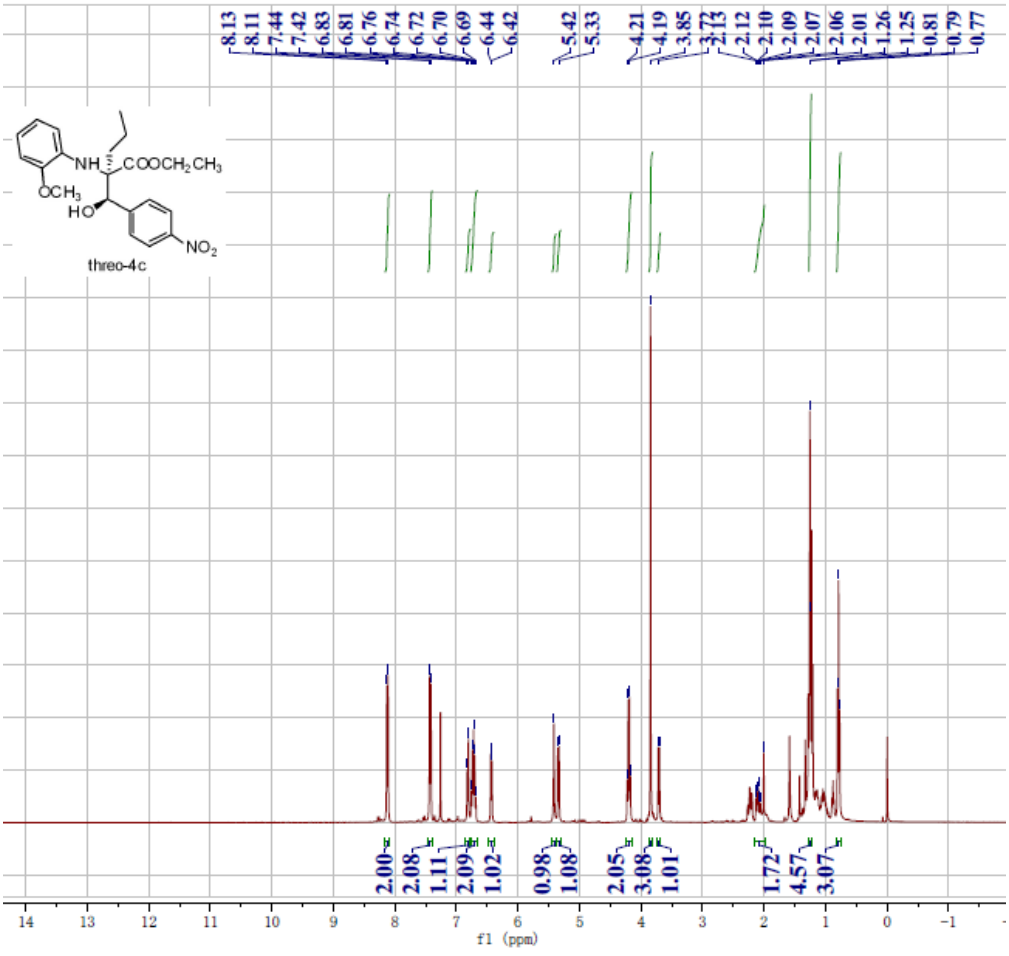
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6.42
5.42
5.33
4.21
4.19
3.85
3.72
2.13
2.12
2.10
2.09
2.07
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2.01
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COOCH2CH3
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HO
NO2
threo-4c
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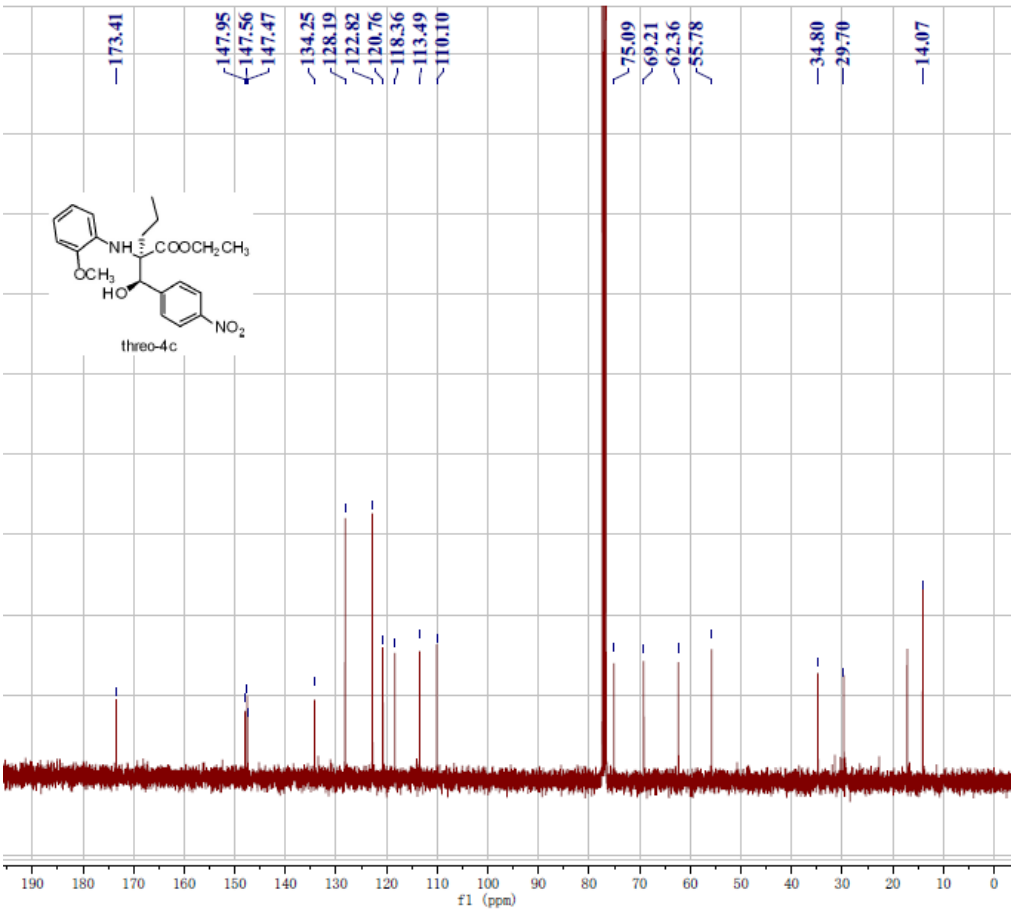
f1 (ppm)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62.36
55.78
34.80
29.70
14.07
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HO
NO2
threo-4c
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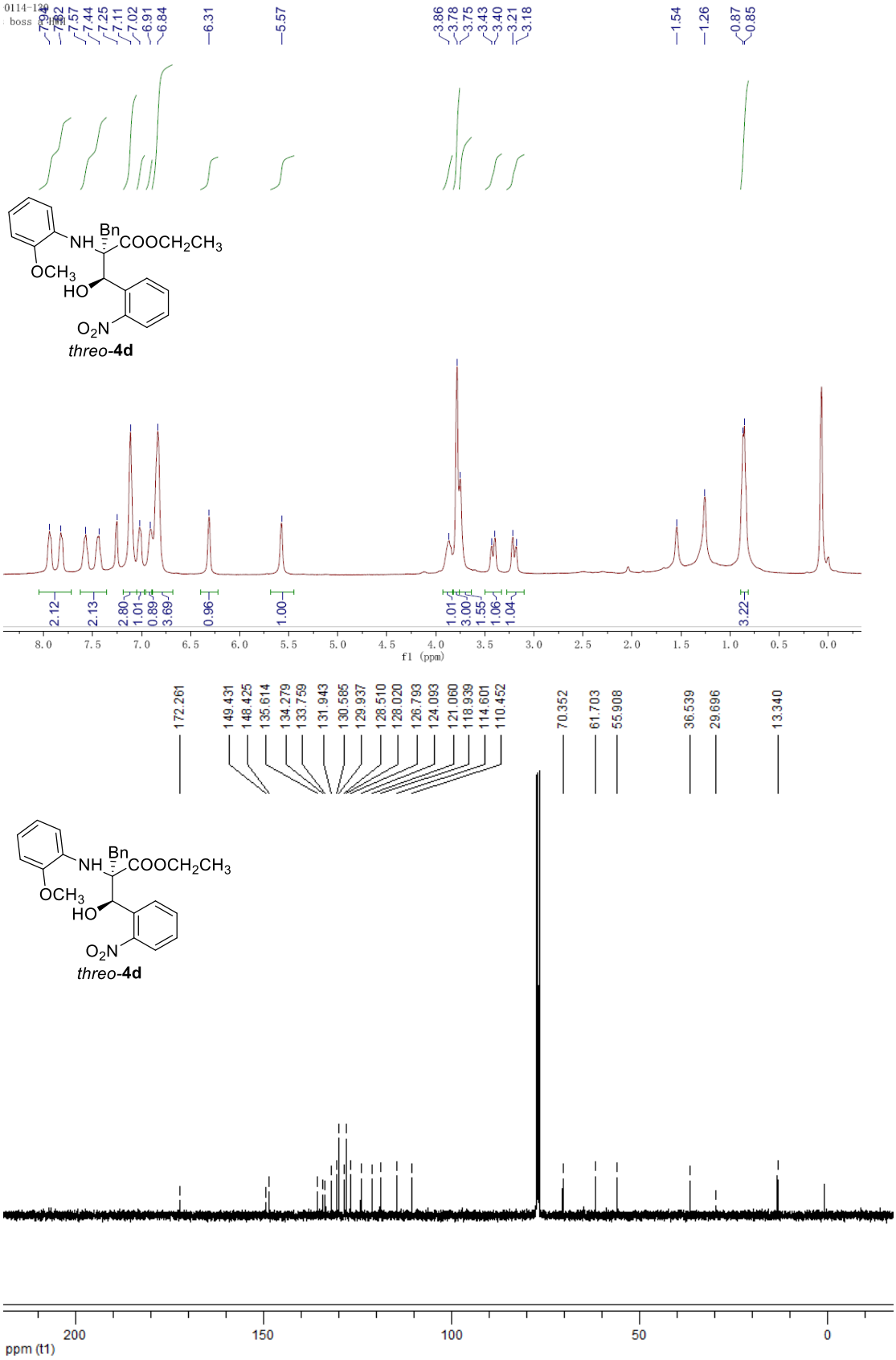
f1 (ppm)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3.75
3.43
3.40
3.21
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Bn
COOCH2CH3
OCH3
HO
O2N
threo-4d
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2.13
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1.01
3.00
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1.06
1.04
3.22
f1 (ppm)
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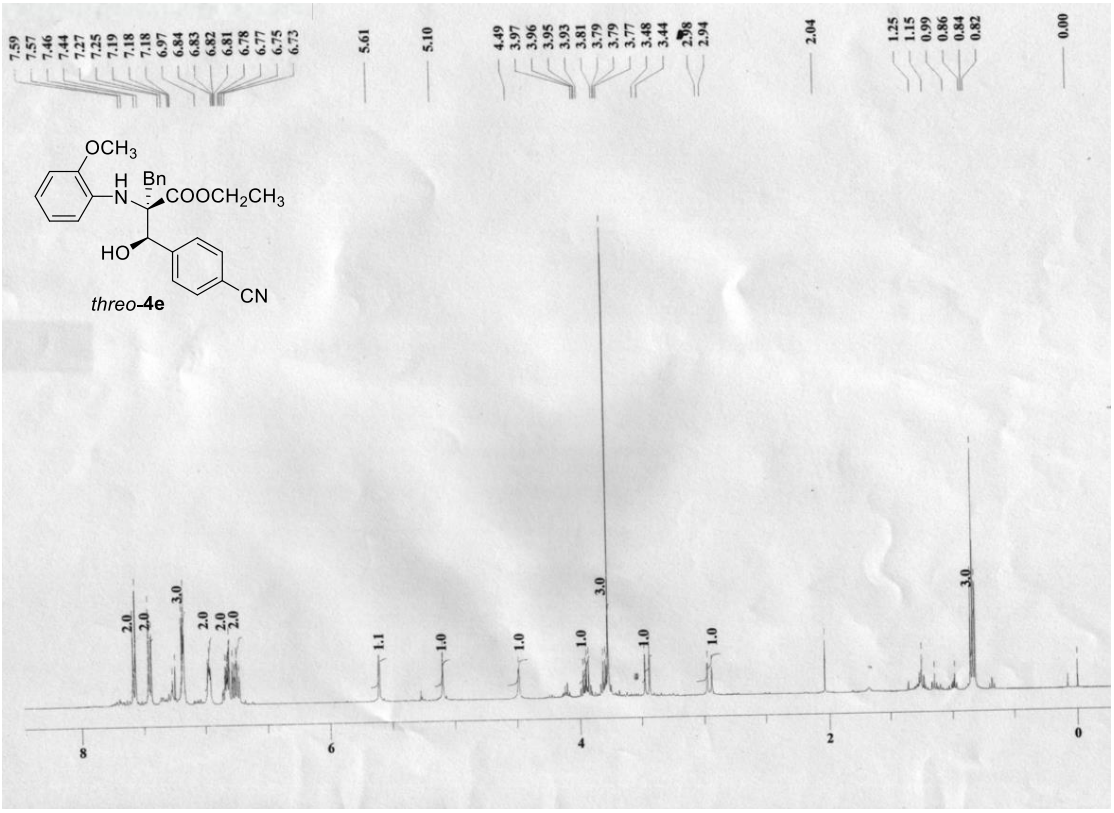
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0.84
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H
Bn
N
COOCH2CH3
HO
CN
threo-4e
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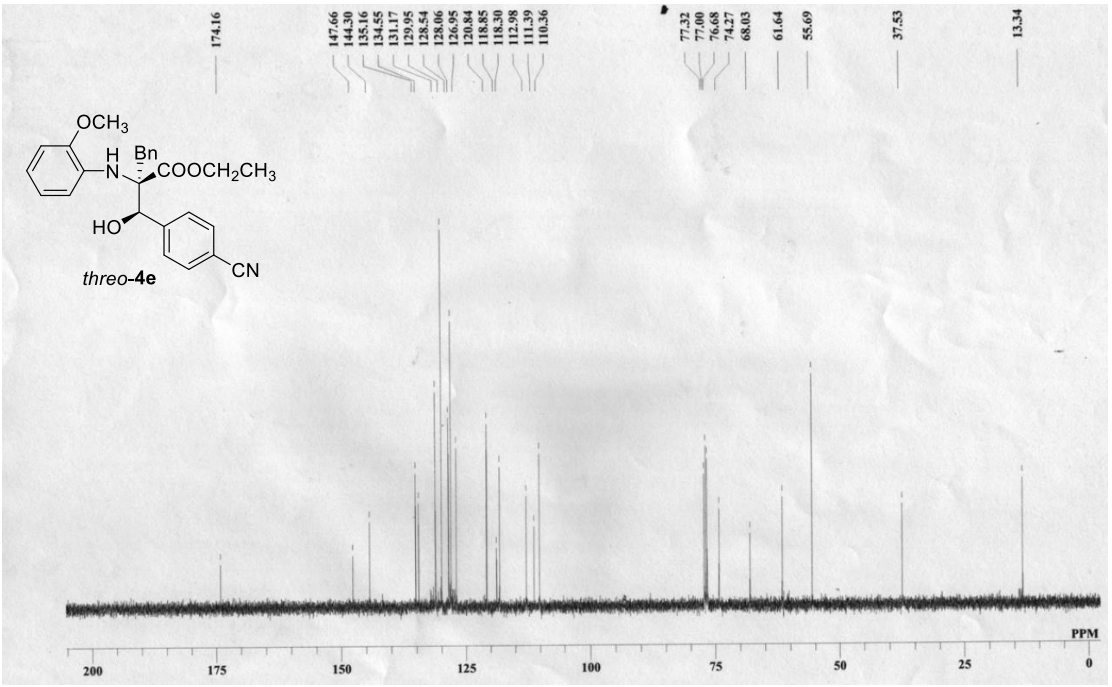
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13.34
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HO
CN
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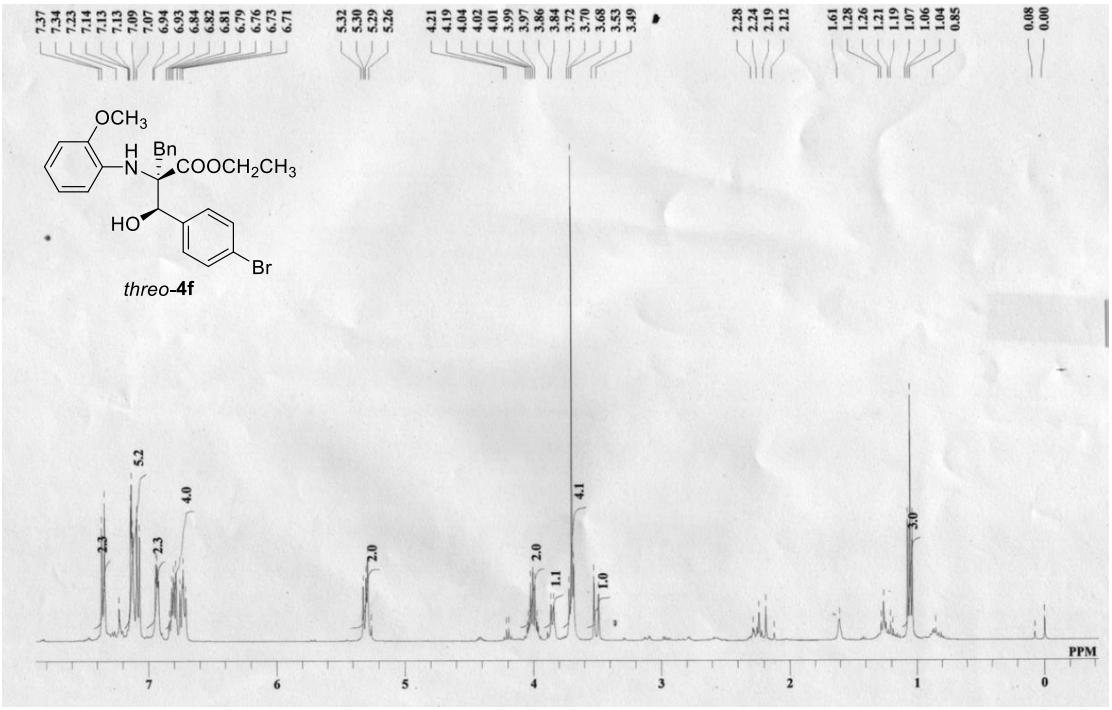
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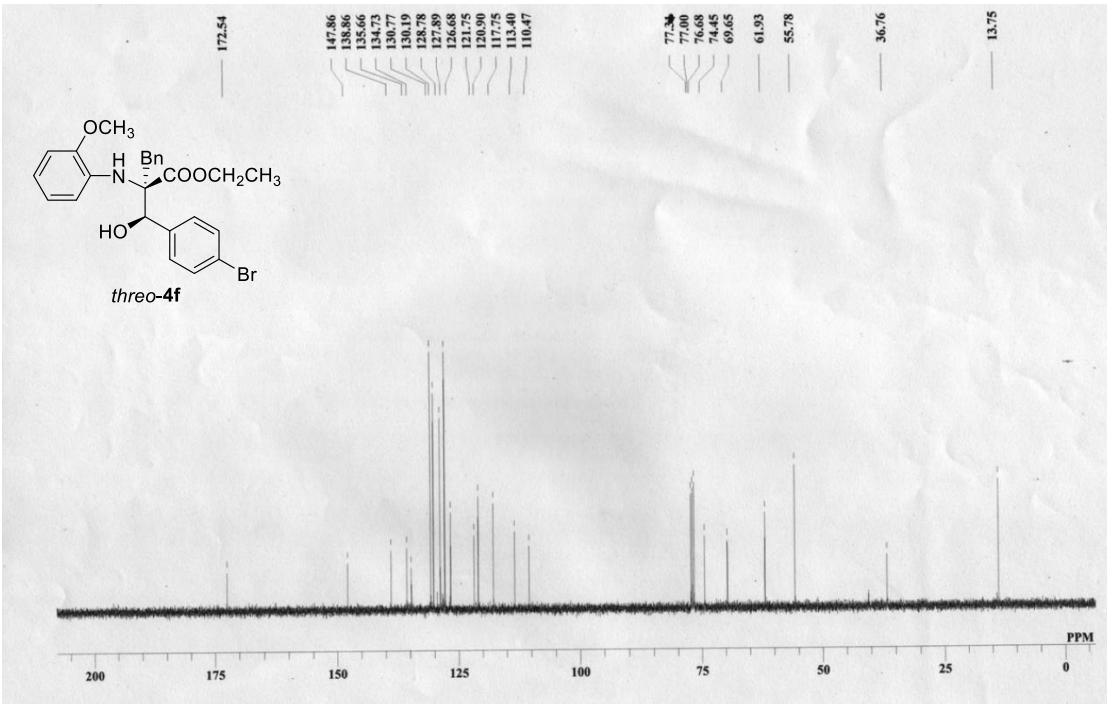
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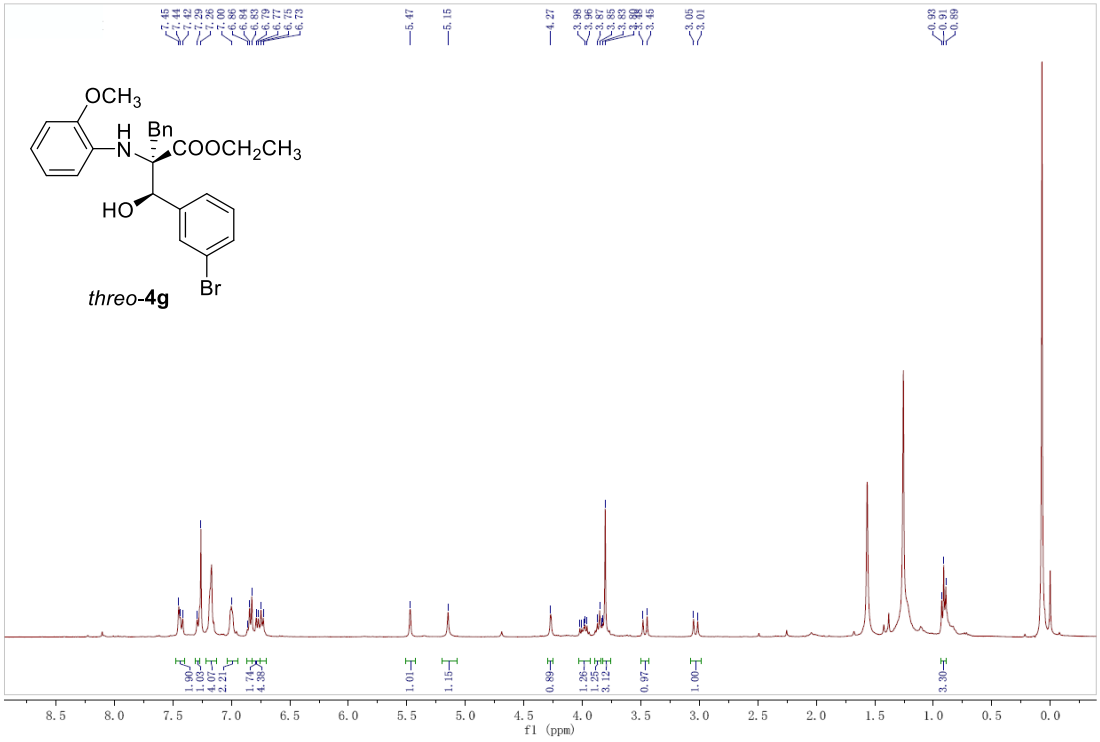
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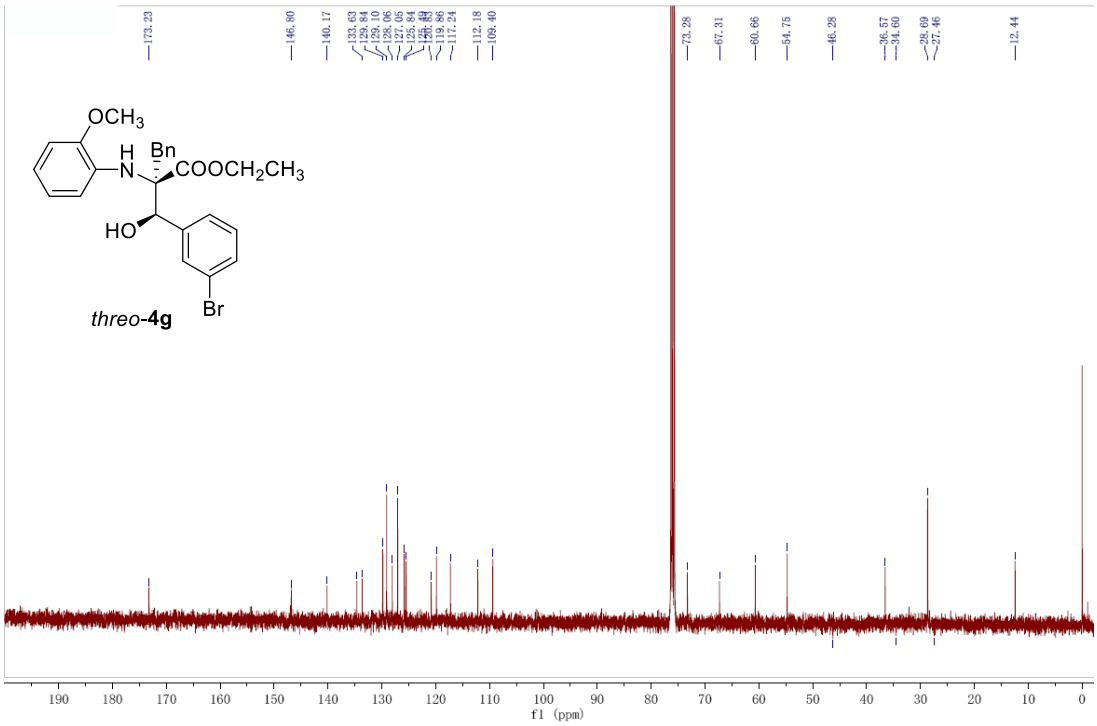
HO
Br
threo-4g
f1 (ppm)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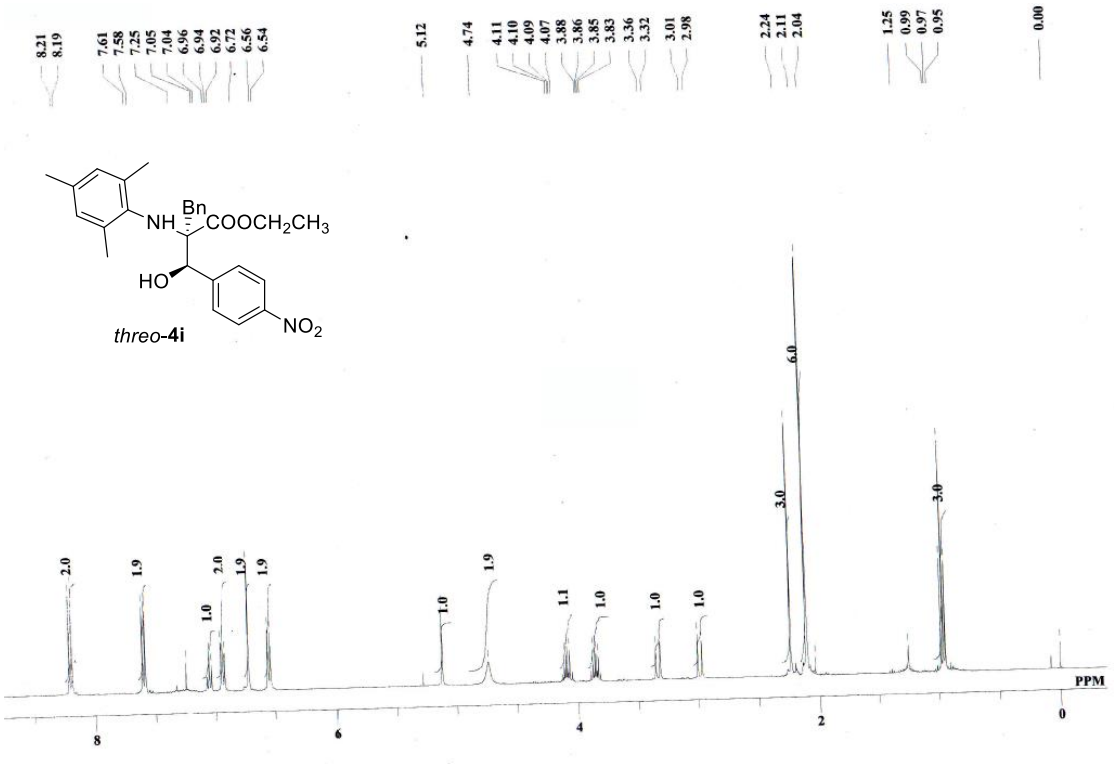
Bn
COOCH2CH3
HO
Br
threo-4g
f1 (ppm)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Bn
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HO
NO2
threo-4i
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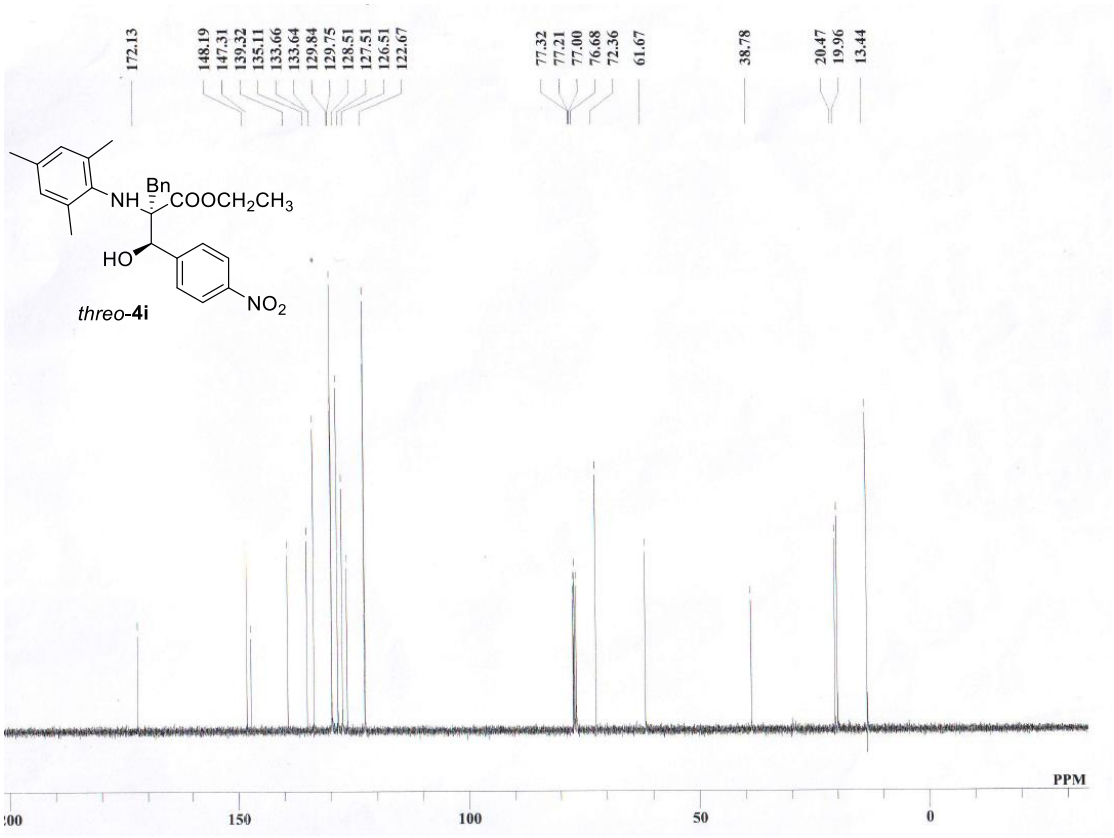
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threo-4i
PPM
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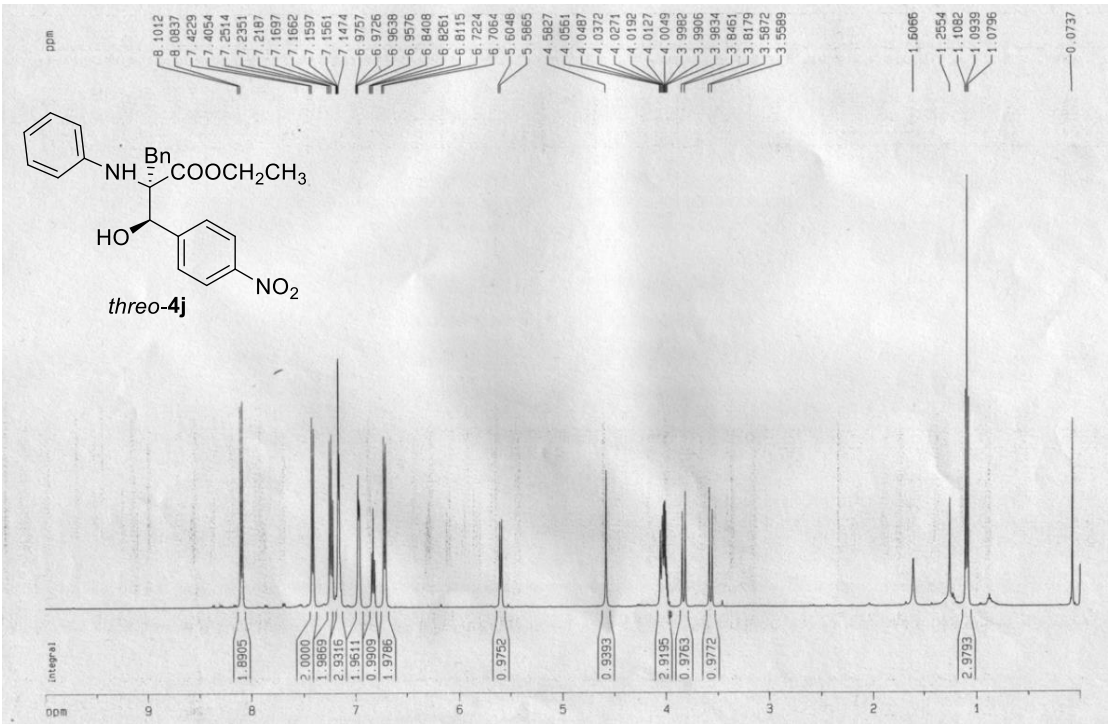
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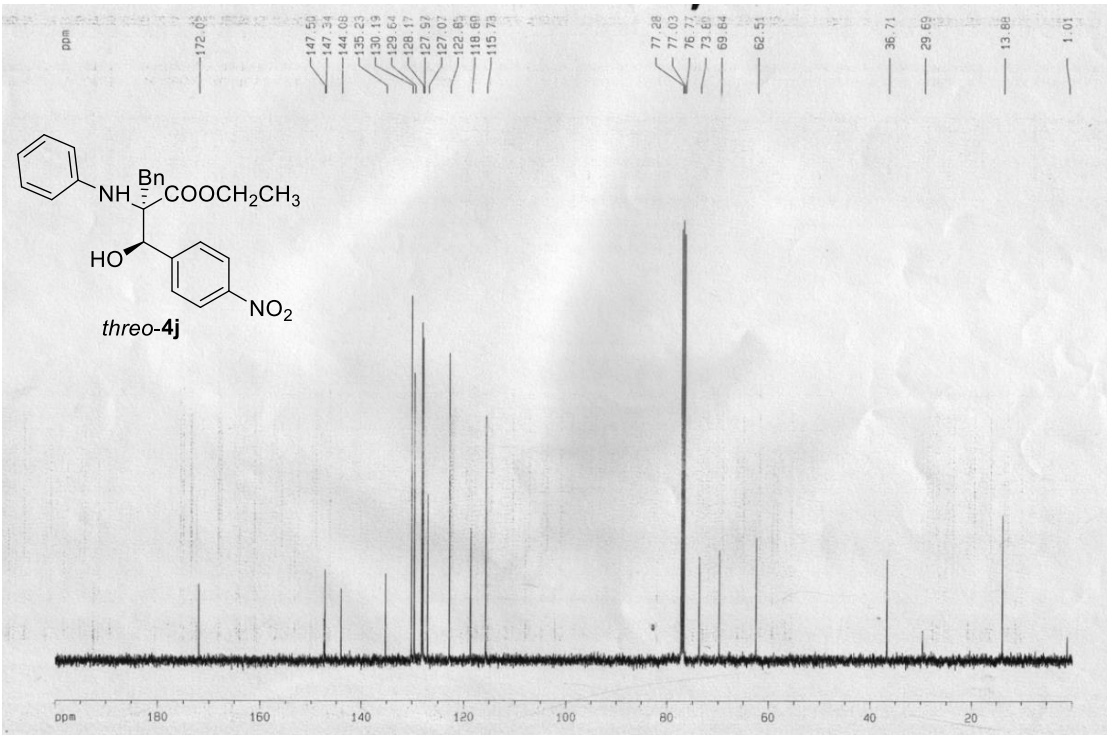
threo-4j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Bn
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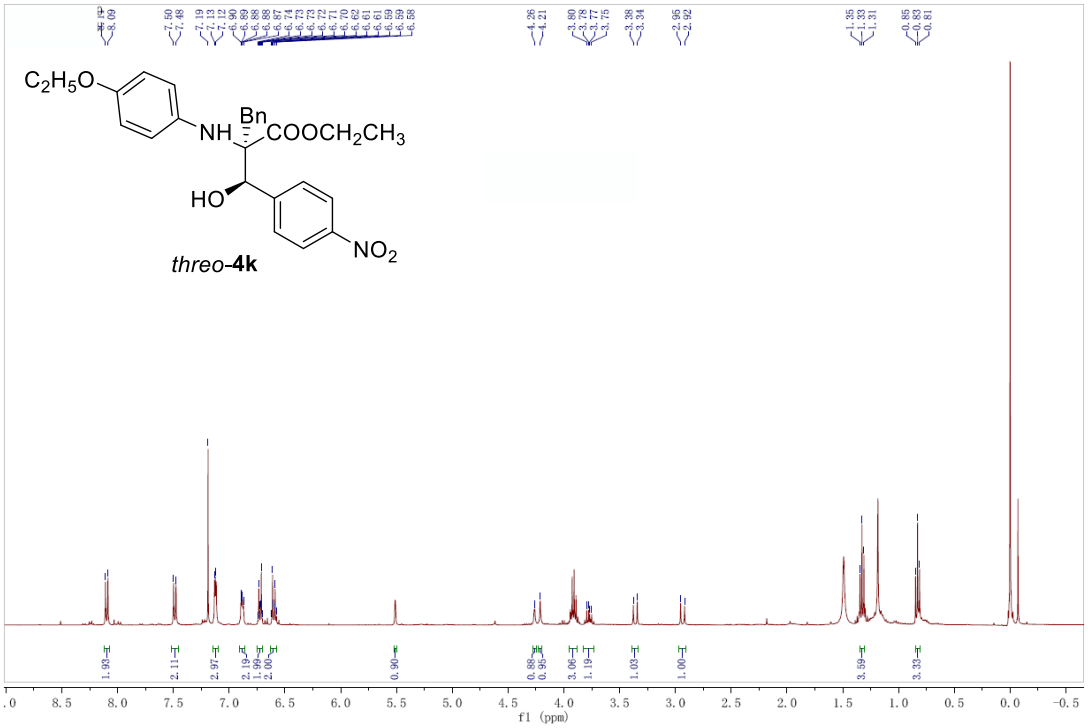
HO
NO2
threo-4j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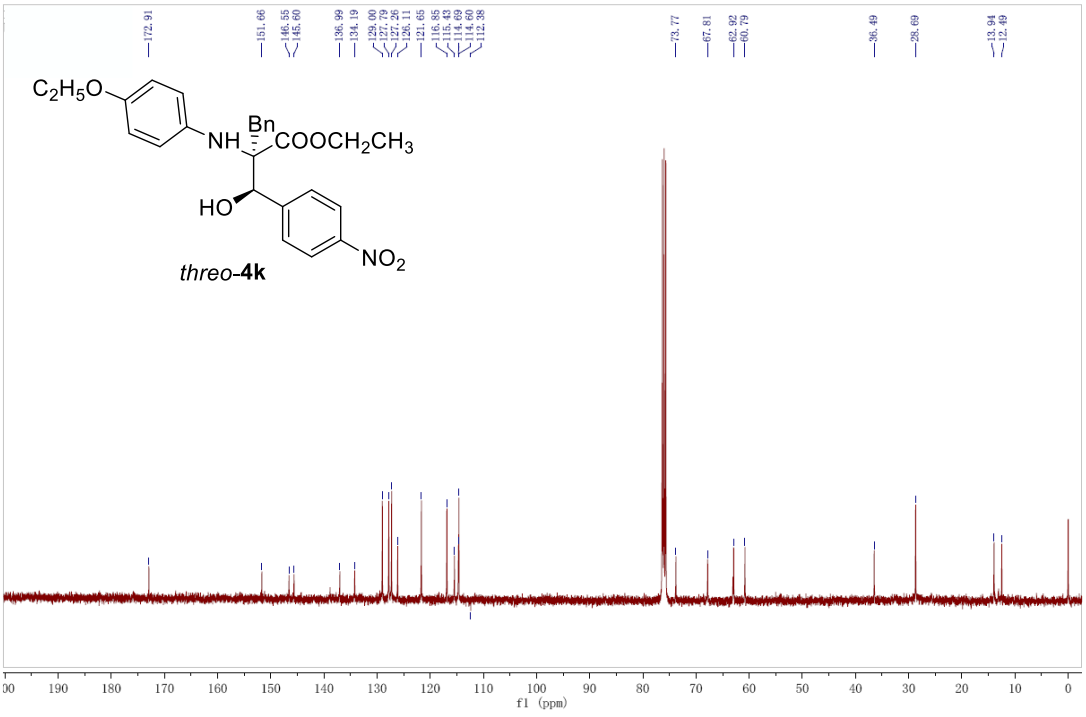
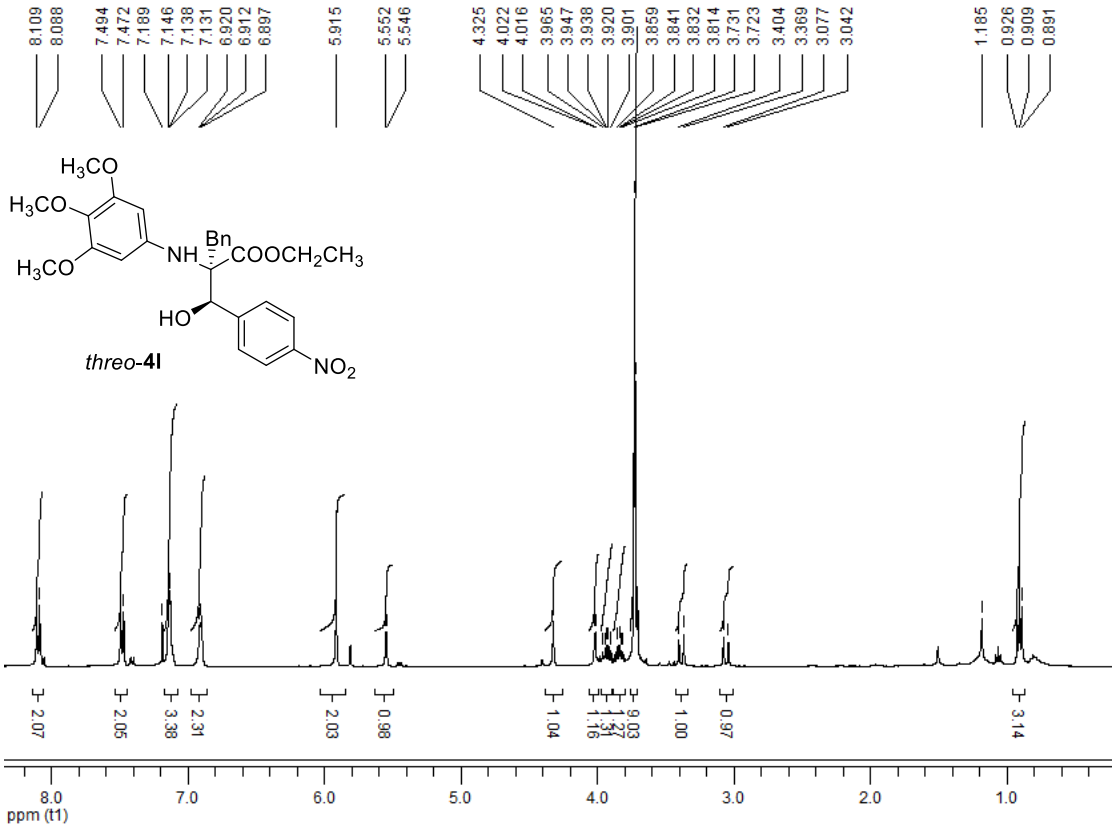
HO
NO2
threo-4k
f1 (ppm)


C2H5O
NH
Bn
COOCH2CH3
HO
NO2
threo-4k
f1 (ppm)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H3CO
H3CO
NH
Bn
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HO
NO2
threo-4l
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2.05
3.38
2.31
2.03
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1.04
9.03
1.00
0.97
3.14
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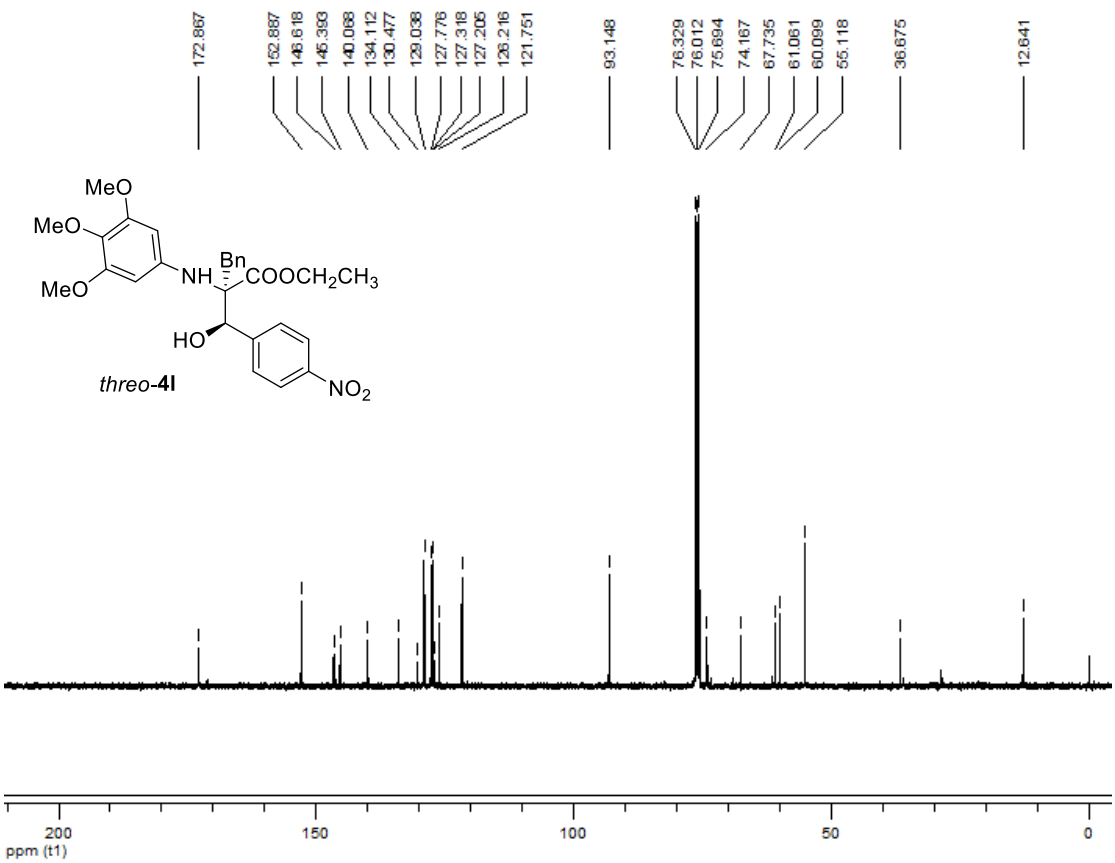
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)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145.393
140.068
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130.477
129.038
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127.318
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126.216
121.751
93.148
76.329
76.012
75.694
74.167
67.735
61.061
60.099
55.118
36.675
12.641
MeO
MeO
MeO
NH
Bn
COOCH2CH3
HO
NO2
threo-4l
200
150
100
50
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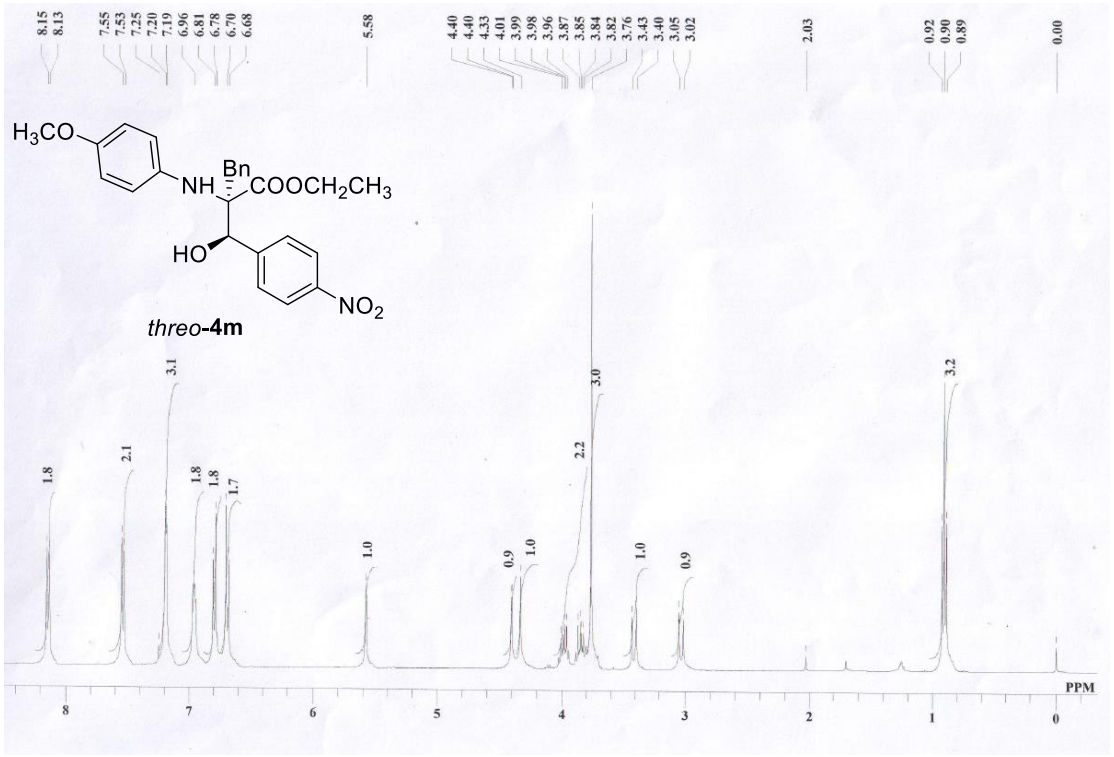
ppm (t1)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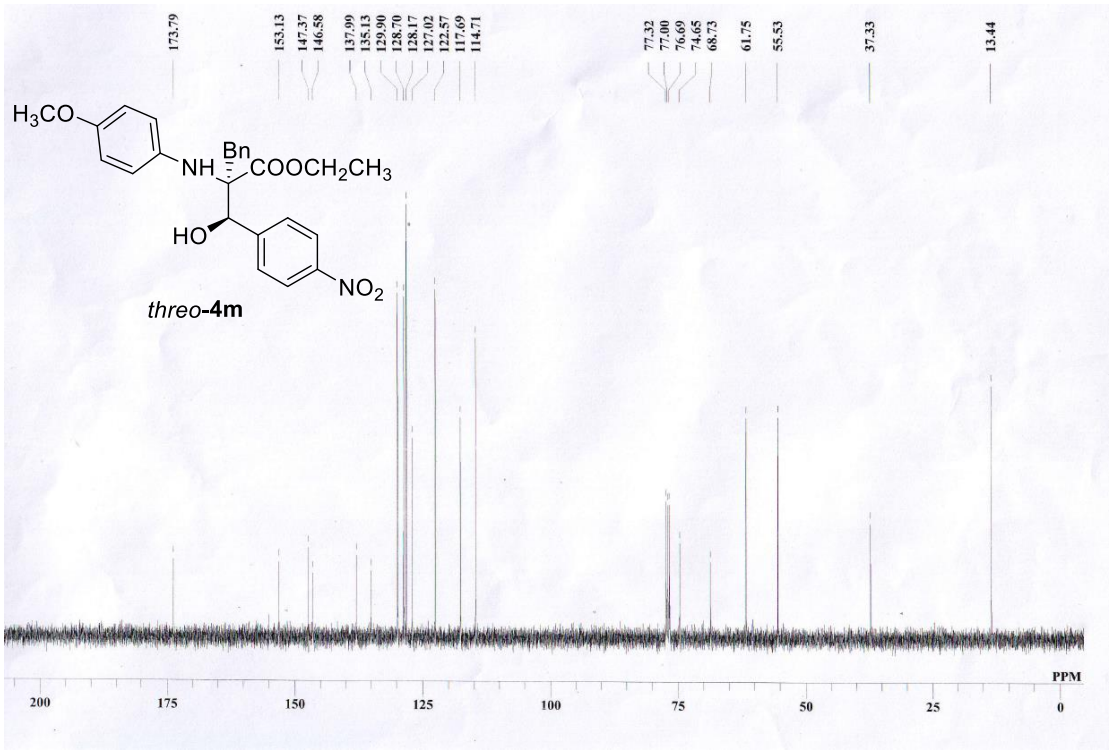
6.78
6.70
6.68
5.58
4.40
4.40
4.33
4.01
3.99
3.98
3.96
3.87
3.85
3.84
3.82
3.76
3.43
3.40
3.05
3.02
2.03
0.92
0.90
0.89
0.00
H3CO
NH
Bn
COOCH2CH3
HO
NO2
threo-4m
3.1
3.0
3.2
2.1
2.2
1.8
1.8
1.8
1.7
1.0
0.9
1.0
1.0
0.9
PPM
8
7
6
5
4
3
2
1
0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128.70
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127.02
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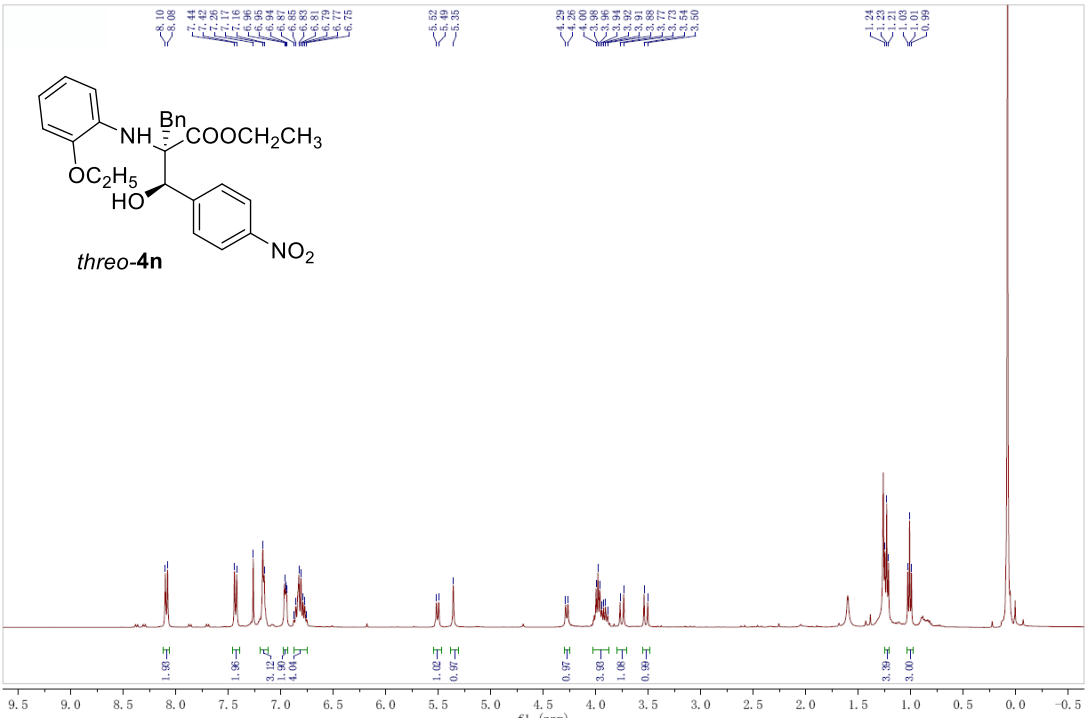
114.71
77.32
77.00
76.69
74.65
68.73
61.75
55.53
37.33
13.44
H3CO
NH
Bn
COOCH2CH3
HO
NO2
threo-4m
PPM
200
175
150
125
100
75
50
25
0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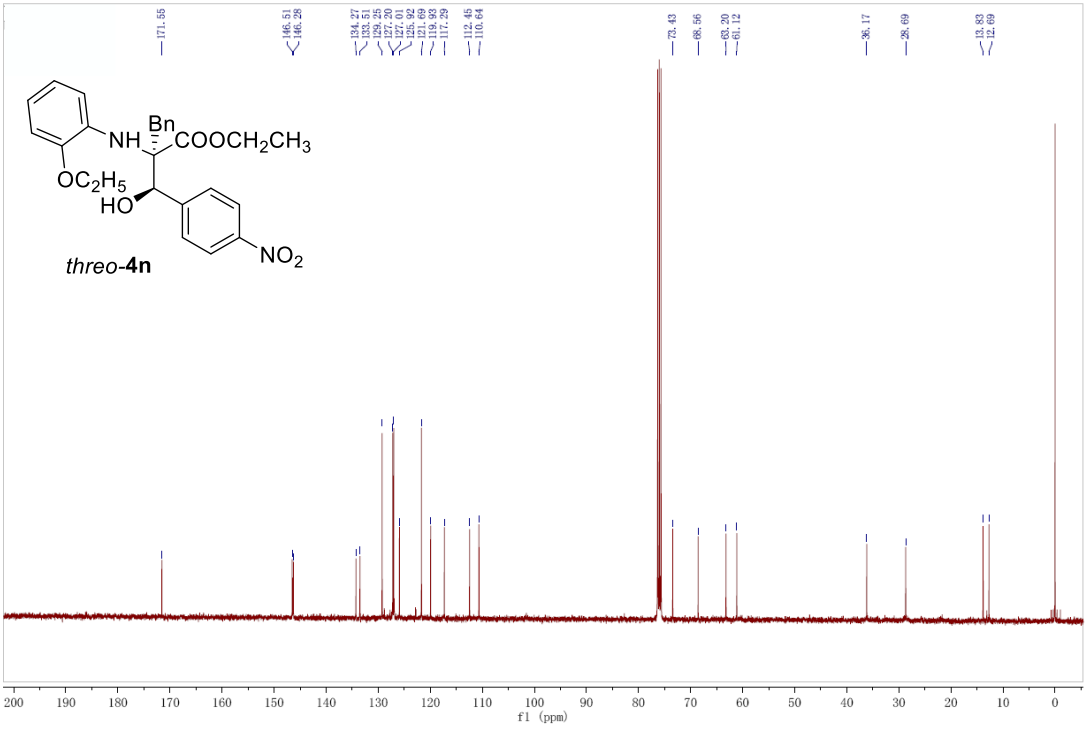
NH
COOCH2CH3
OC2H5
HO
NO2
threo-4n


Bn
NH
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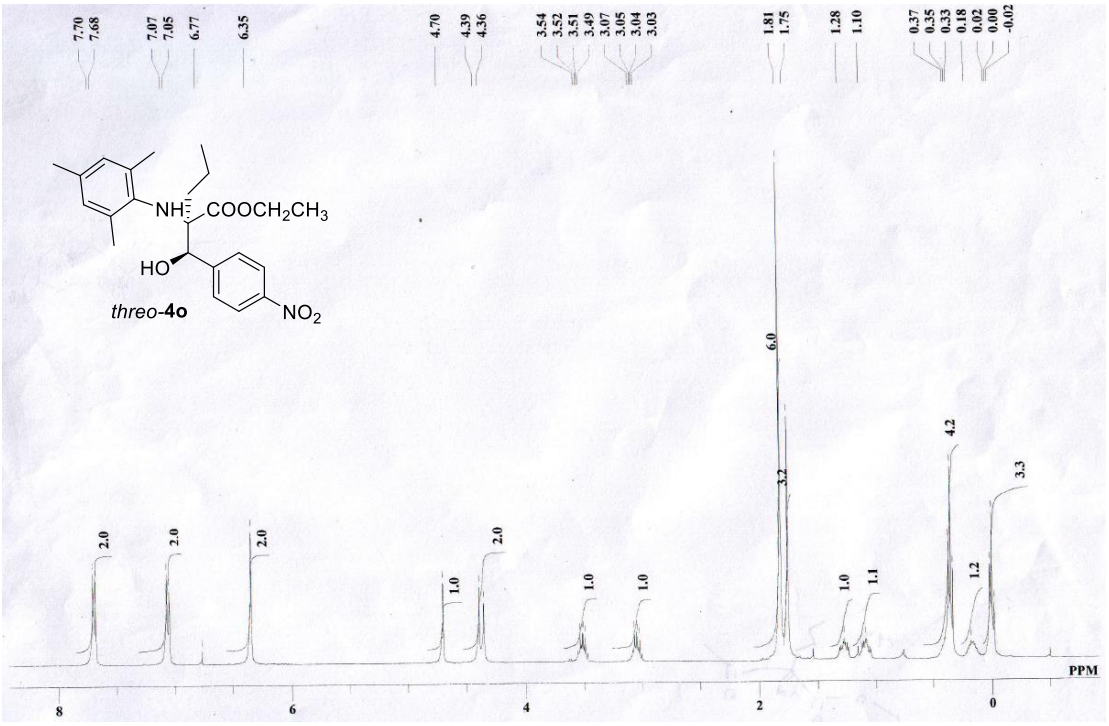
OC2H5
HO
NO2
threo-4n
f1 (ppm)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4.39
4.36
3.54
3.52
3.51
3.49
3.07
3.05
3.04
3.03
1.81
1.75
1.28
1.10
0.37
0.35
0.33
0.18
0.02
0.00
-0.02
NH
COOCH2CH3
HO
NO2
threo-4o
2.0
2.0
2.0
1.0
2.0
1.0
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1.0
1.1
4.2
1.2
3.3
PPM
8
6
4
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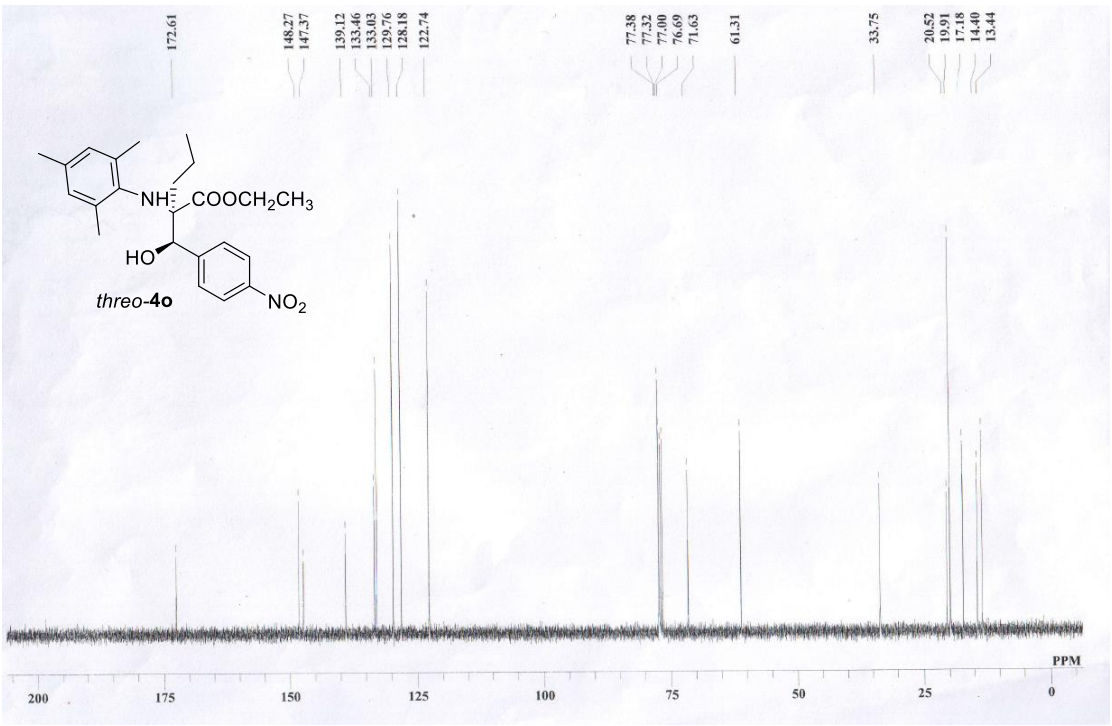
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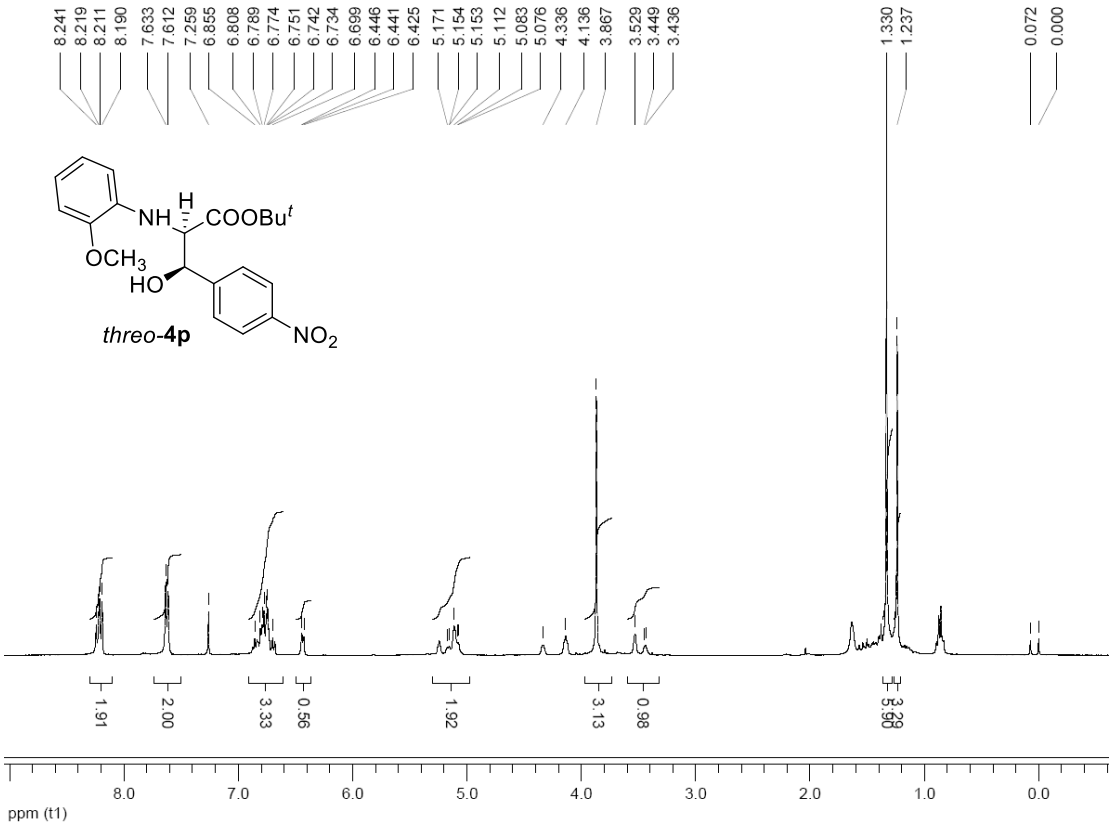
76.69
71.63
61.31
33.75
20.52
19.91
17.18
14.40
13.44
NH
COOCH2CH3
HO
NO2
threo-4o
PPM
200
175
150
125
100
75
50
25
0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6.742
6.734
6.699
6.446
6.441
6.425
5.171
5.154
5.153
5.112
5.083
5.076
4.336
4.136
3.867
3.529
3.449
3.436
1.330
1.237
0.072
0.000
NH
H
COOBu^t
OCH$_3$
HO
NO$_2$
threo-4p
1.91
2.00
3.33
0.56
1.92
3.13
0.98
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2.29
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7.0
6.0
5.0
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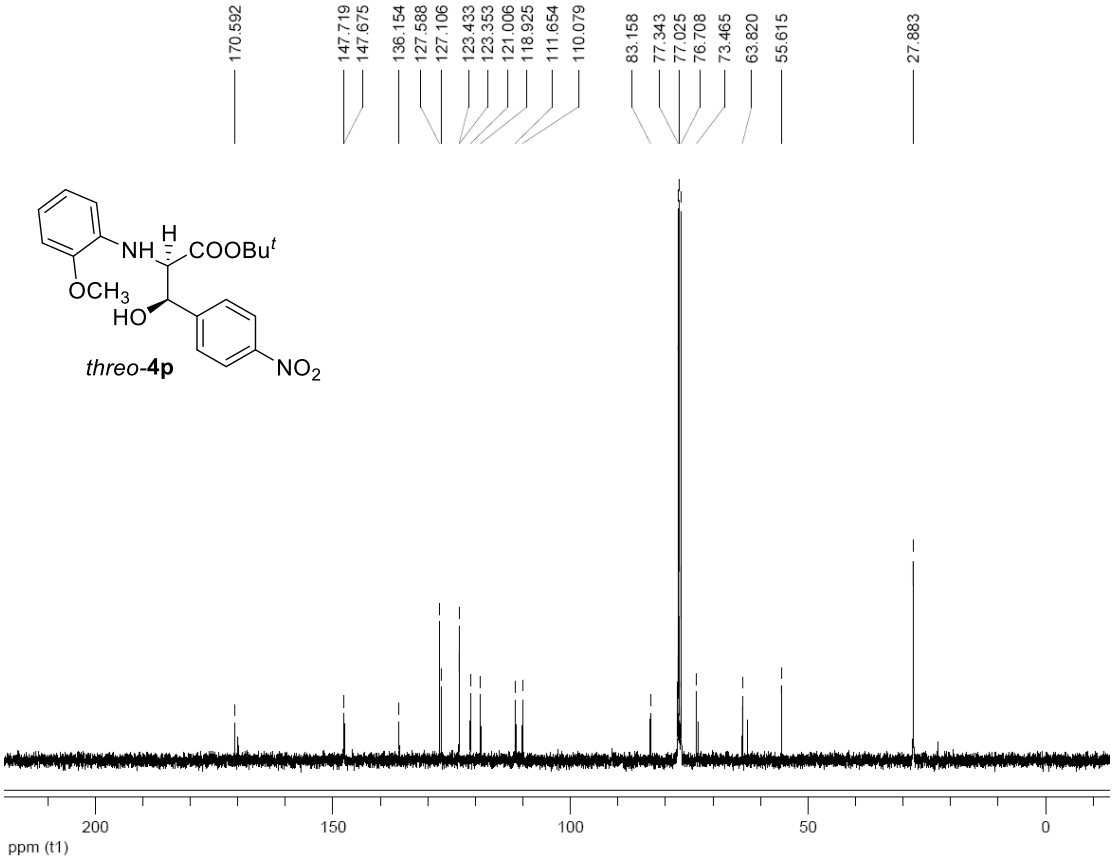
3.0
2.0
1.0
0.0
ppm (t1)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136.154
127.588
127.106
123.433
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118.925
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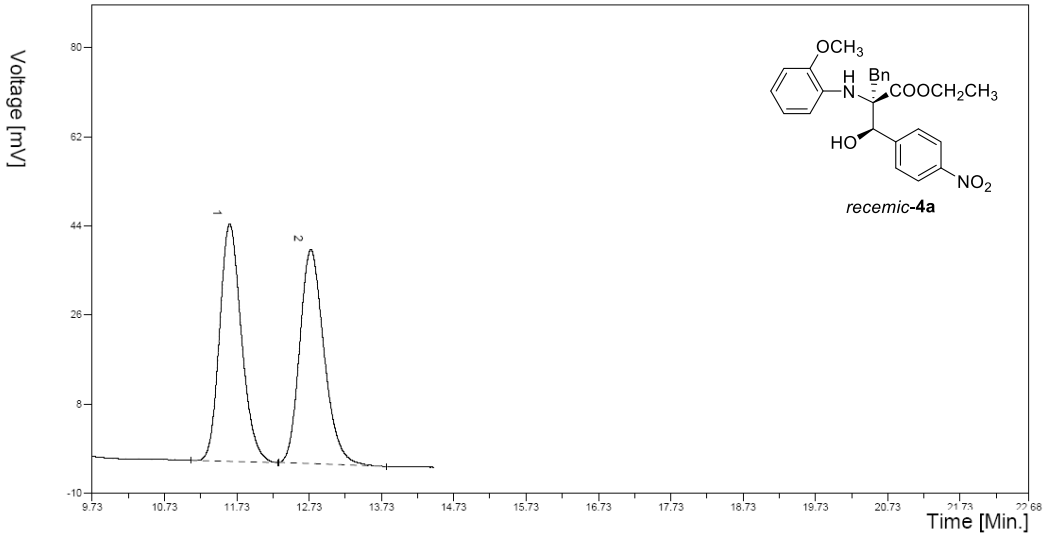
110.079
83.158
77.343
77.025
76.708
73.465
63.820
55.615
27.883
NH
H
COOBu^t
OCH$_3$
HO
NO$_2$
threo-4p
200
150
100
50
0
ppm (t1)

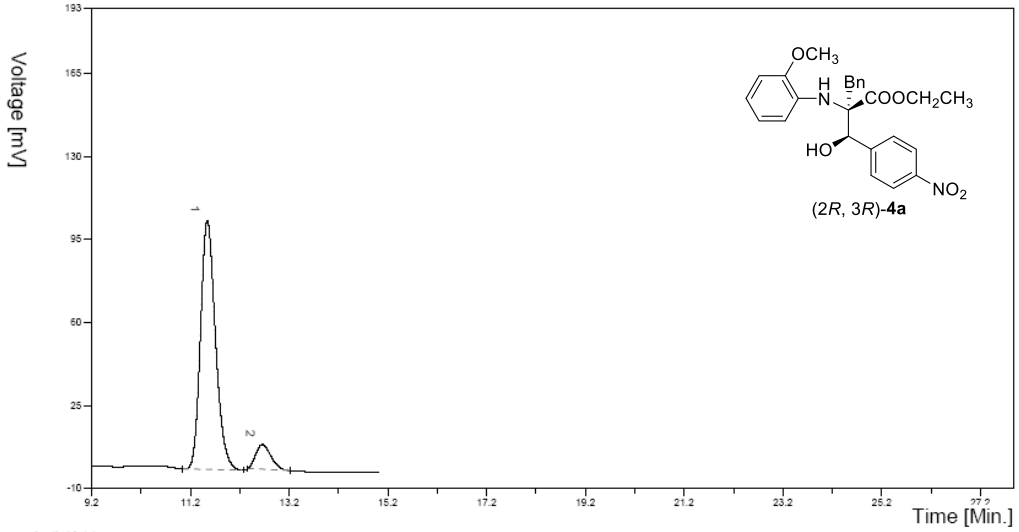
HPLC spectra of compounds

Chiralpak Column: OD-H
M.P: *n*-Hex/*i*-PrOH=5:1
UV: 254nm
0.8 ml/min
Injection Volume: 20μl



积分结果

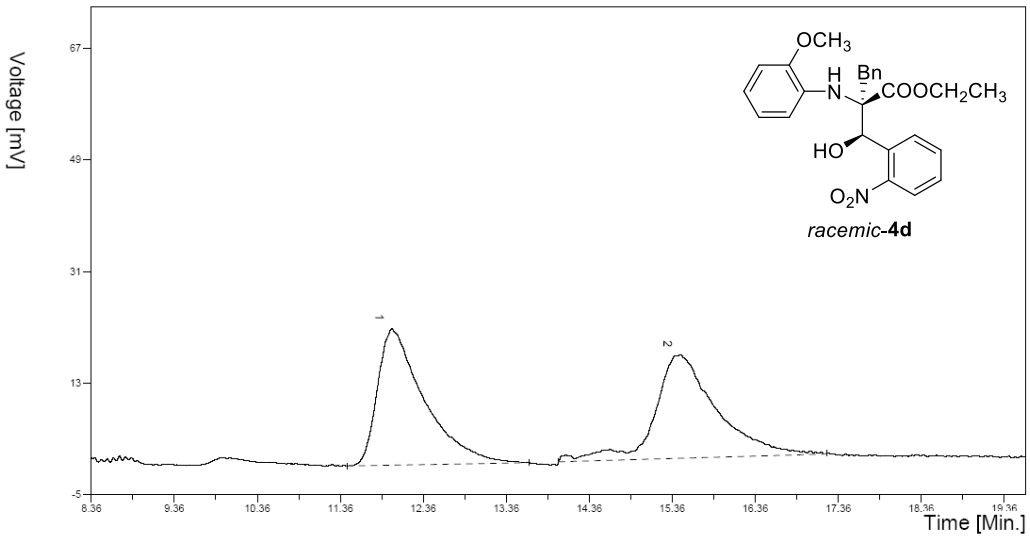
#	组分名	保留时间(min)	峰高(mv)	峰面积(mv.sec)	面积百分比(%)
1	Unknown	11.63	47.97	1006.29	49.8596
2	Unknown	12.75	43.21	1011.96	50.1404
合计			91.18	2018.25	100



积分结果

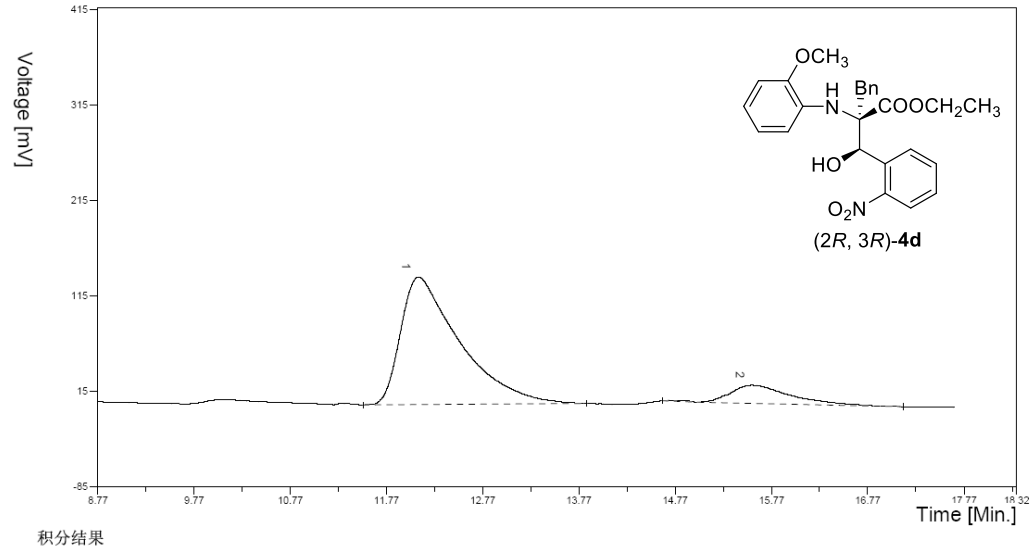
#	组分名	保留时间(min)	峰高(mv)	峰面积(mv.sec)	面积百分比(%)
1	Unknown	11.58	104.87	2203.27	90.7988
2	Unknown	12.70	10.50	223.27	9.2012
合计			115.37	2426.54	100

Chiralpak Column: IA
M.P: *n*-Hex/*i*-PrOH=5:1
UV: 254nm
0.8 ml/min
Injection Volume: 20μl



积分结果

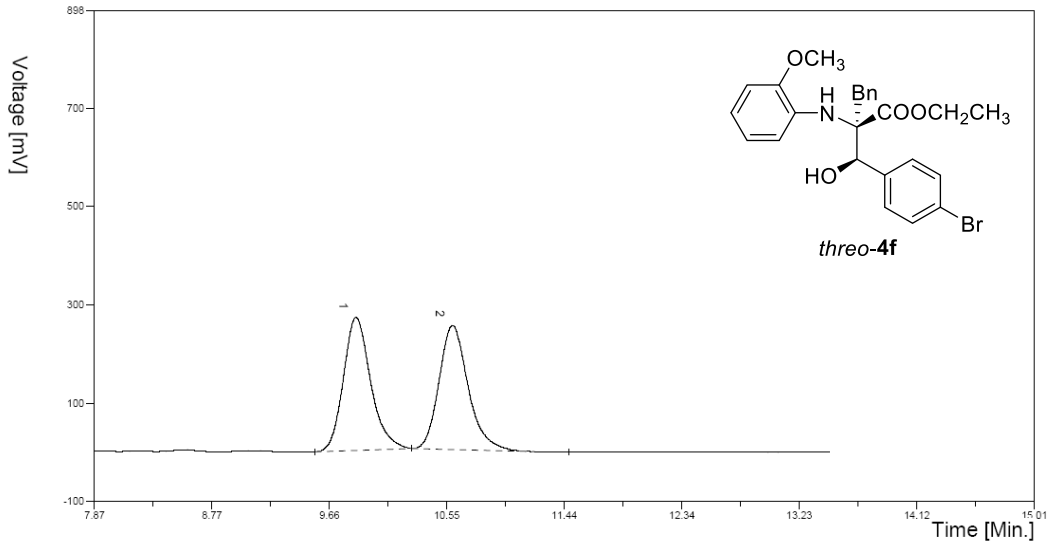
#	组分名	保留时间(min)	峰高(mv)	峰面积(mv.sec)	面积百分比(%)
1	Unknown	11.98	22.03	854.77	49.8967
2	Unknown	15.46	16.70	858.31	50.1033
合计			38.73	1713.08	100



积分结果

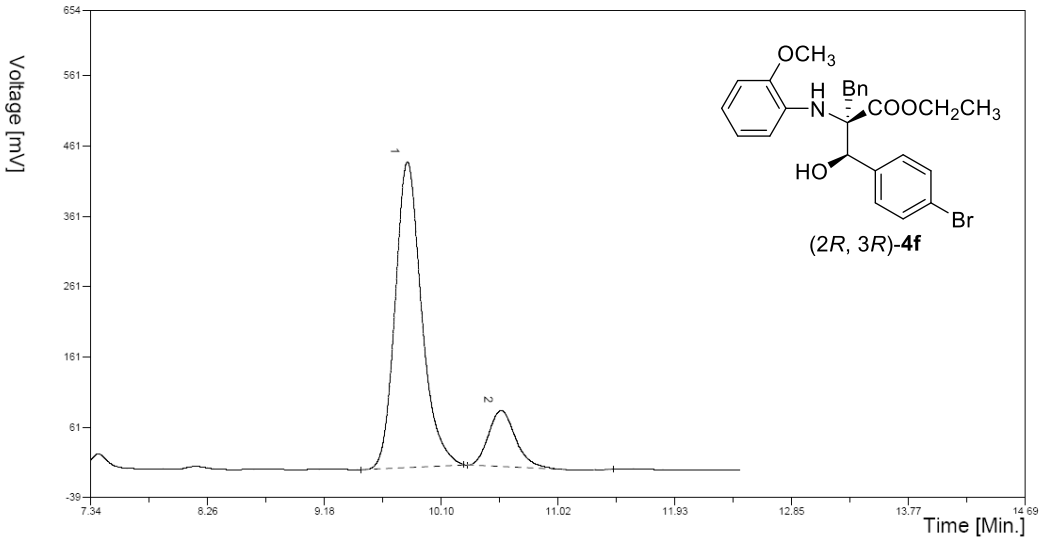
#	组分名	保留时间(min)	峰高(mv)	峰面积(mv.sec)	面积百分比(%)
1	Unknown	12.10	133.45	5669.87	87.6914
2	Unknown	15.57	18.68	795.84	12.3086
合计			152.14	6465.71	100

Chiralpak Column: IA
M.P: *n*-Hex/*i*-PrOH=5:1
UV: 254nm
0.8 ml/min
Injection Volume: 20μl



积分结果

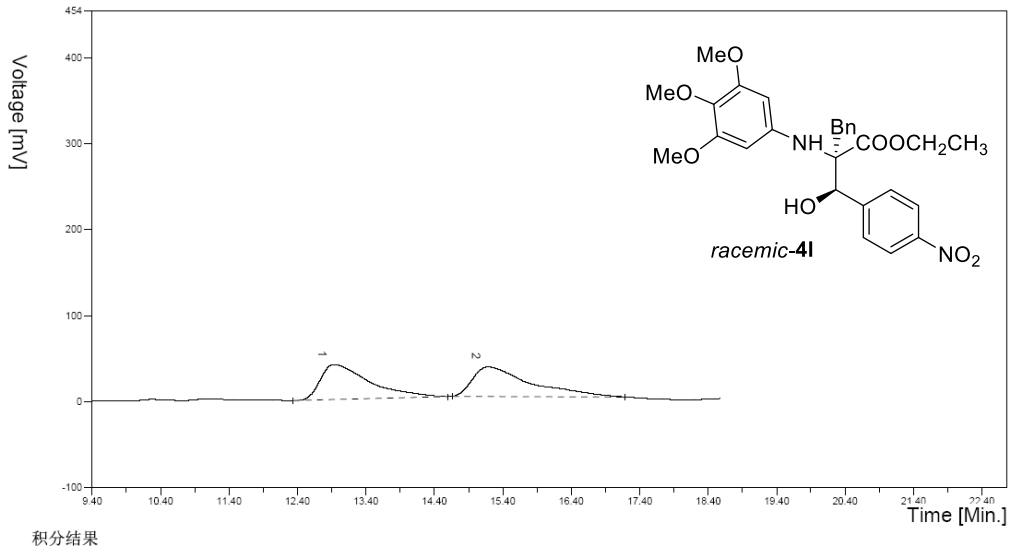
#	组分名	保留时间(min)	峰高(mv)	峰面积(mv.sec)	面积百分比(%)
1	Unknown	9.86	270.50	3886.20	50.3582
2	Unknown	10.59	252.13	3830.91	49.6418
合计			522.63	7717.11	100



积分结果

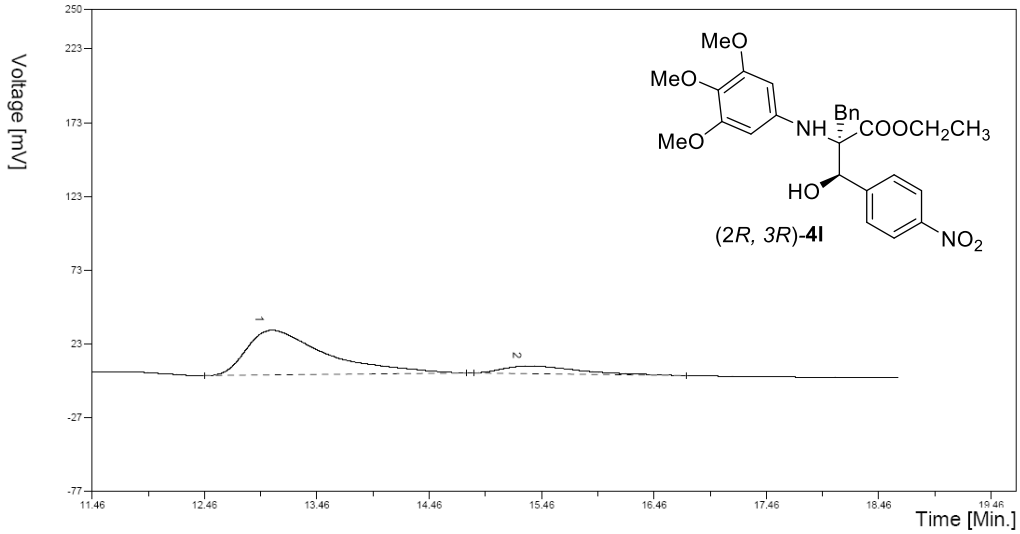
#	组分名	保留时间(min)	峰高(mv)	峰面积(mv.sec)	面积百分比(%)
1	Unknown	9.83	434.92	6280.18	85.5787
2	Unknown	10.57	78.47	1058.30	14.4213
合计			513.39	7338.49	100

Chiralpak Column: IA
M.P: *n*-Hex/*i*-PrOH=5:1
UV: 254nm
0.8 ml/min
Injection Volume: 20μl



积分结果

#	组分名	保留时间(min)	峰高(mv)	峰面积(mv.sec)	面积百分比(%)
1	Unknown	12.94	40.64	2014.36	49.8618
2	Unknown	15.19	34.26	2025.52	50.1382
合计			74.91	4039.88	100



积分结果

#	组分名	保留时间(min)	峰高(mv)	峰面积(mv.sec)	面积百分比(%)
1	Unknown	13.06	30.22	1489.60	86.1703
2	Unknown	15.35	5.22	239.07	13.8297
合计			35.44	1728.67	100

DFT calculation details

The Density Functional Theory (DFT) calculations were carried out by using the quantum chemical calculation software Gaussian09.[1] The geometrical structures of transition states and intermediates are optimized at the level of the M06/Lanl2dz+6-31G* method,[2] which means that the Lanl2dz basis set[3] is used for the description of metal element Rh and the 6-31G* basis is used for the nonmetal elements C, O, N and H. The frequency analyses are performed based on the optimized structures obtained in gas phase to verify the nature of stationary points on the potential surfaces. The solvent effects of CH_2Cl_2 for the reactions are evaluated using the integral equation formalism model (PCM).[4] The intrinsic reaction coordinate (IRC)[5] calculations are conducted to assure that the transition states connect the correct products in the forward directions and reactants in the reverse directions.

References

1. Gaussian09, Revision **B.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.

2. Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc*. **2008**, *120*, 215.

3. a) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299; b) Wadt, W. R.; Hay, P. J. *J. Chem. Phys.* **1985**, *82*, 284.

4. Scalmani, G.; Frisch, M. J. *J. Chem. Phys.* **2010**, *132*, 114110.

5. Fukui, K. *Acc. Chem. Res.* **1981**, *14*, 363.

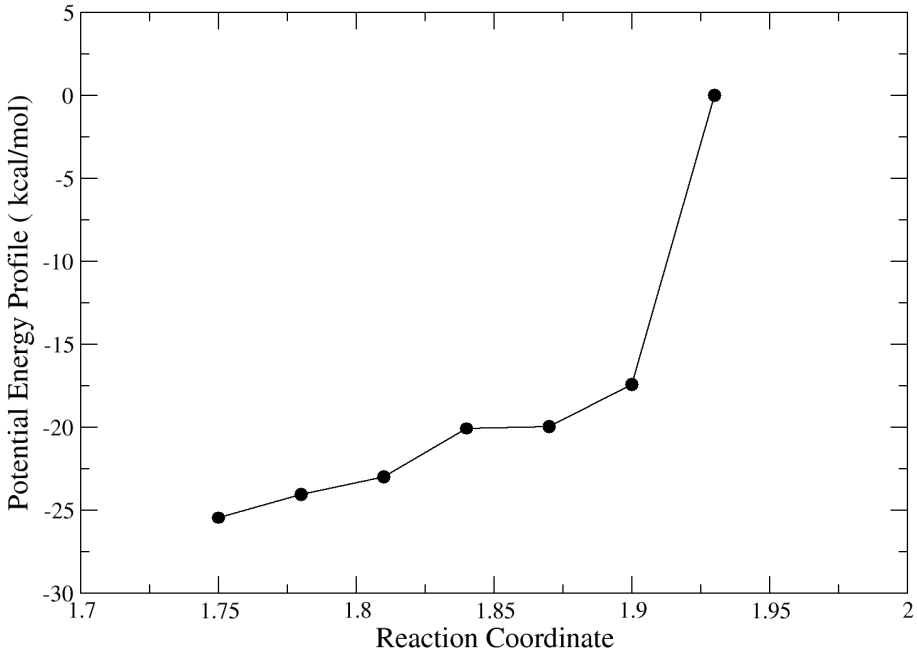
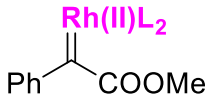
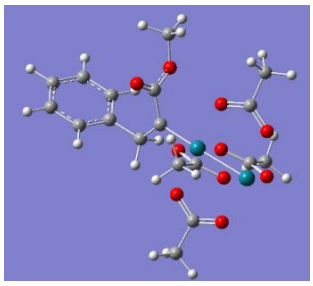


Figure S1 The constrained optimization results indicate that the attack of **A9** by aldehyde is a process that has no energy barrier. The C-C distance between the attached carbon atom in **A9** and the carbon in aldehyde is set as the reaction coordinate, with the discrete values 1.93, 1.90, 1.87, 1.84, 1.81, 1.78 and 1.75 Å adopted in the calculations, respectively. The hydrogen transfer from the NH_2 group of **A9** to the carbonyl oxygen atom of aldehyde takes place spontaneously at the distance 1.90 Å along the reaction coordinate.

Optimized structures and coordinates in Scheme 2

A3: 



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C	-0.61424600	-2.39879400	-1.22261700
C	-1.77584000	1.95610400	1.52036400
C	-2.17355000	0.90147500	-1.99203000
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O	-0.93150600	1.07271300	-1.76090600
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H	-0.15934800	-3.31760500	-3.09319800

H	0.70310600	-4.01211500	-1.71774800
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H	3.02885400	4.61657900	0.45787300
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C	4.17286700	0.64842500	-0.92668000
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C	4.47351600	0.87169300	-2.27070800
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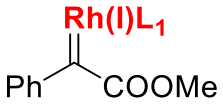
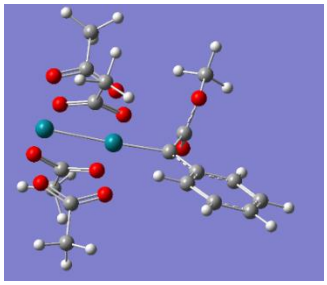
A5: 



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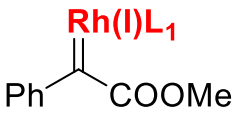
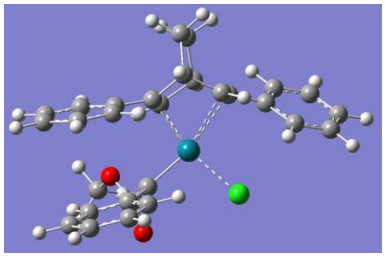
O	2.35681900	2.59194900	0.77542600
Rh	-2.33403400	-0.61750300	0.44653600
Rh	-0.00243600	0.03997300	-0.02562700
C	-0.40064700	-1.50785400	2.42228300
C	-0.82808800	-2.50828900	-1.17216800
C	-1.55639100	1.96103400	1.52957800
C	-1.97626000	0.90818200	-1.98567200
O	0.50569300	-0.91069700	1.75229200
O	0.19824100	-1.76263100	-1.03471500
O	-0.41760400	1.80988500	0.97753700
O	-0.72278100	0.88598300	-1.76364800

O	-1.62193200	-1.58694700	2.13865500
O	-1.97327200	-2.31464800	-0.69285000
O	-2.51097300	1.14424900	1.53166600
O	-2.88045100	0.40546500	-1.26886100
C	0.06278400	-2.15859100	3.69635900
H	-0.68046500	-2.87766400	4.05040300
H	1.03122000	-2.64595900	3.54607100
H	0.19874400	-1.38444600	4.46143000
C	-1.75598600	3.27670100	2.23104600
H	-1.85510700	4.07018900	1.47984900
H	-2.66016300	3.25207900	2.84463800
H	-0.88160600	3.51179100	2.84757300
C	-2.38564500	1.61578900	-3.24689800
H	-2.04244600	2.65564500	-3.20905400
H	-1.89257300	1.14554900	-4.10502900
H	-3.47053100	1.58153700	-3.37330500
C	-0.62636800	-3.73050300	-2.02476400
H	-1.42262000	-4.45788000	-1.84686900
H	-0.64832400	-3.43273000	-3.08032400
H	0.35425800	-4.17594500	-1.82983000
C	2.23503400	4.00772100	0.88865100
H	2.91978100	4.51615900	0.20149900
H	1.20556200	4.30837400	0.66170700
C	3.05159500	-0.17008900	-0.47628800
C	3.04040200	-1.54428500	-0.14203200
C	4.26372400	0.40973400	-0.92827900
C	4.19869600	-2.29556800	-0.24397000
H	2.11464300	-1.98361400	0.21524300
C	5.40613500	-0.35571600	-1.05623500
H	4.27970900	1.46377100	-1.20258500
C	5.37483400	-1.70738200	-0.70660500
H	4.18941300	-3.34801100	0.03185800
H	6.32828300	0.09312800	-1.41943900
H	6.28010500	-2.30648800	-0.79288700
H	2.48415900	4.24716300	1.92406200

A5*(Conformer of A5): 



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O	1.97817900	3.03942000	0.94102800
O	2.71934900	0.92968900	1.24550000
C	4.04977100	1.44176000	1.16176400
H	4.22726000	1.88687700	0.17707600
H	4.21929600	2.20549800	1.92825800
Rh	-0.30027700	0.47691300	-0.40215400
C	0.82737700	-3.11267900	-2.00636800
C	1.02363200	-1.57735800	-1.94601500
C	-1.04525200	-2.21875200	-0.57540900
C	-0.41882800	-3.49780700	-1.18713100
H	0.72409200	-3.42225100	-3.05615400
H	1.72779600	-3.60347900	-1.61273400
H	-1.16797300	-3.99878800	-1.81402100
H	-0.16281700	-4.18886800	-0.37152200
C	-0.24328900	-0.91988200	-2.46736500
C	-1.32880800	-1.23364900	-1.68983300
H	-2.34887900	-0.96819600	-1.96137500
H	-1.94951200	-2.45544200	-0.00488900
H	1.91212200	-1.25895700	-2.49992600
C	0.02191700	-1.56089400	0.28873900
C	1.12061700	-1.15956000	-0.49486600
H	2.08794700	-0.91540900	-0.05998100
Cl	-1.77752800	2.25008800	-1.10905400
C	0.05820700	-1.75987800	1.75081400
C	-1.12198800	-1.74514700	2.50364200
C	1.27348100	-1.92431900	2.42624400
C	-1.08893100	-1.87741700	3.88538600
H	-2.07756000	-1.58623800	2.00288000
C	1.30711500	-2.06247100	3.80901700
H	2.20205100	-1.94515100	1.85732700
C	0.12664200	-2.03696600	4.54481000
H	-2.01854000	-1.84243400	4.45159900
H	2.26339800	-2.19580000	4.31299800
H	0.15288900	-2.14288200	5.62816800
C	-0.29095100	-0.23359600	-3.76678800
C	0.70453700	-0.46562200	-4.72496600

C	-1.36168300	0.60511300	-4.10992000
C	0.63265600	0.11504900	-5.98580500
H	1.53943200	-1.12776500	-4.49985500
C	-1.42499100	1.19192600	-5.36482300
H	-2.12006300	0.84052800	-3.36581900
C	-0.43123100	0.94843100	-6.30997600
H	1.41438100	-0.08565100	-6.71672200
H	-2.25514700	1.85447800	-5.60301500
H	-0.48563200	1.41113800	-7.29403000
H	4.71007500	0.58716200	1.32185200
C	-0.34211700	1.47746200	2.38625600
C	0.34926100	1.51088900	3.61390400
C	-1.74876900	1.56458400	2.39411800
C	-0.34465500	1.59465500	4.80938500
H	1.43605900	1.42906100	3.62222800
C	-2.43364400	1.69126800	3.59266500
H	-2.27113800	1.57819000	1.43775000
C	-1.73524700	1.69499400	4.79882000
H	0.19667600	1.59499300	5.75370800
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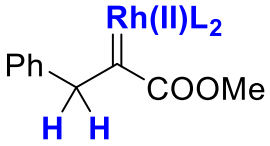
H	-2.27717700	1.78257700	5.73953300



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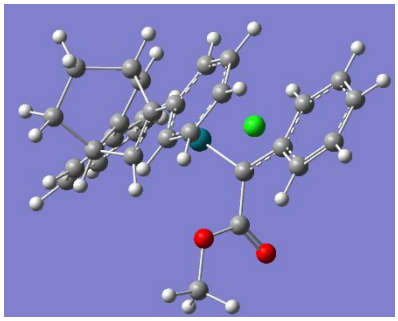
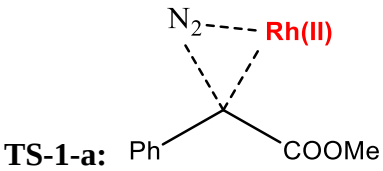


C	0.37810400	1.32214400	1.14330400
C	1.75806600	1.86201800	1.09530900
O	1.97817900	3.03942000	0.94102800
O	2.71934900	0.92968900	1.24550000
C	4.04977100	1.44176000	1.16176400
H	4.22726000	1.88687700	0.17707600
H	4.21929600	2.20549800	1.92825800
Rh	-0.30027700	0.47691300	-0.40215400
C	0.82737700	-3.11267900	-2.00636800
C	1.02363200	-1.57735800	-1.94601500

C	-1.04525200	-2.21875200	-0.57540900
C	-0.41882800	-3.49780700	-1.18713100
H	0.72409200	-3.42225100	-3.05615400
H	1.72779600	-3.60347900	-1.61273400
H	-1.16797300	-3.99878800	-1.81402100
H	-0.16281700	-4.18886800	-0.37152200
C	-0.24328900	-0.91988200	-2.46736500
C	-1.32880800	-1.23364900	-1.68983300
H	-2.34887900	-0.96819600	-1.96137500
H	-1.94951200	-2.45544200	-0.00488900
H	1.91212200	-1.25895700	-2.49992600
C	0.02191700	-1.56089400	0.28873900
C	1.12061700	-1.15956000	-0.49486600
H	2.08794700	-0.91540900	-0.05998100
Cl	-1.77752800	2.25008800	-1.10905400
C	0.05820700	-1.75987800	1.75081400
C	-1.12198800	-1.74514700	2.50364200
C	1.27348100	-1.92431900	2.42624400
C	-1.08893100	-1.87741700	3.88538600
H	-2.07756000	-1.58623800	2.00288000
C	1.30711500	-2.06247100	3.80901700
H	2.20205100	-1.94515100	1.85732700
C	0.12664200	-2.03696600	4.54481000
H	-2.01854000	-1.84243400	4.45159900
H	2.26339800	-2.19580000	4.31299800
H	0.15288900	-2.14288200	5.62816800
C	-0.29095100	-0.23359600	-3.76678800
C	0.70453700	-0.46562200	-4.72496600
C	-1.36168300	0.60511300	-4.10992000
C	0.63265600	0.11504900	-5.98580500
H	1.53943200	-1.12776500	-4.49985500
C	-1.42499100	1.19192600	-5.36482300
H	-2.12006300	0.84052800	-3.36581900
C	-0.43123100	0.94843100	-6.30997600
H	1.41438100	-0.08565100	-6.71672200
H	-2.25514700	1.85447800	-5.60301500
H	-0.48563200	1.41113800	-7.29403000
H	4.71007500	0.58716200	1.32185200
C	-0.34211700	1.47746200	2.38625600
C	0.34926100	1.51088900	3.61390400
C	-1.74876900	1.56458400	2.39411800
C	-0.34465500	1.59465500	4.80938500
H	1.43605900	1.42906100	3.62222800
C	-2.43364400	1.69126800	3.59266500

H	-2.27113800	1.57819000	1.43775000
C	-1.73524700	1.69499400	4.79882000
H	0.19667600	1.59499300	5.75370800
H	-3.51761200	1.78754300	3.58890800
H	-2.27717700	1.78257700	5.73953300



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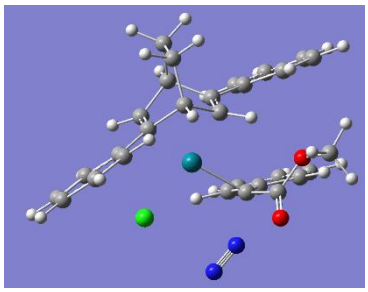

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C	1.04820900	-0.97937200	2.24414900
O	0.41840700	-1.53975700	3.11067200
O	1.79836400	0.11494400	2.47443300
C	1.73385400	0.61259000	3.80748500
H	0.70002000	0.85687800	4.07996800
H	2.11423100	-0.12894500	4.51781800
Rh	-0.53408700	-0.36059200	-0.17299000
C	-1.94601700	3.38196100	0.11774300
C	-1.85458100	1.95556800	0.70433300
C	-0.56336300	2.04925000	-1.51425100
C	-1.14892700	3.44536900	-1.19913600
H	-3.00500700	3.62987500	-0.04485800
H	-1.55641000	4.10045700	0.85188400
H	-1.78521200	3.76567100	-2.03475900
H	-0.32015000	4.16457500	-1.12868900
C	-2.40530800	0.97531600	-0.31860000
C	-1.65998200	1.00729800	-1.49570000
H	-1.99341900	0.53289600	-2.41657000
H	-0.02166300	2.05121700	-2.46631300
H	-2.36277400	1.88346000	1.66949000
C	0.33324400	1.64005400	-0.35355500
C	-0.40645200	1.54163800	0.84013400
H	0.07258400	1.54391600	1.81748600
Cl	-1.43250500	-2.34716400	-1.25566600
C	1.79007800	1.84553200	-0.44539700

C	2.49481300	1.45356000	-1.59003500
C	2.49435500	2.47340700	0.58761200
C	3.86315900	1.66594900	-1.68968400
H	1.96513700	0.94557200	-2.39681800
C	3.86369200	2.69025500	0.48786600
H	1.95362800	2.80744400	1.47288000
C	4.55304000	2.28629000	-0.65119400
H	4.39629800	1.33610200	-2.58017700
H	4.39230900	3.18862200	1.29949800
H	5.62559200	2.45617700	-0.73188000
C	-3.73324000	0.35384300	-0.16870200
C	-4.56073800	0.67026500	0.91707600
C	-4.23629200	-0.52304900	-1.14242400
C	-5.83626600	0.12891600	1.03112000
H	-4.22049900	1.35941600	1.68724100
C	-5.50536800	-1.06624900	-1.02608600
H	-3.60616400	-0.81732700	-1.97779300
C	-6.31395500	-0.74383800	0.06188800
H	-6.45674200	0.39385400	1.88576100
H	-5.86410400	-1.75578500	-1.78818900
H	-7.30983100	-1.17436000	0.15323300
H	2.35811700	1.50982500	3.81680600
C	2.29840900	-1.50198100	0.01400600
C	3.56826300	-1.23877300	0.54372000
C	2.20413600	-1.97722400	-1.30500100
C	4.70641000	-1.42122500	-0.23321500
H	3.66885100	-0.85597700	1.55528000
C	3.34577200	-2.18955200	-2.06396100
H	1.21684700	-2.19505500	-1.71574300
C	4.60181100	-1.90558400	-1.53232300
H	5.68383900	-1.19113500	0.18800700
H	3.25288000	-2.57477400	-3.07795900
H	5.49799600	-2.06416000	-2.13038900
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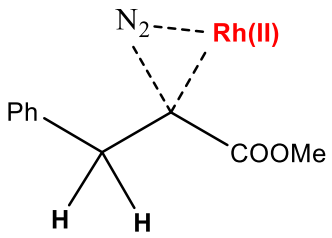
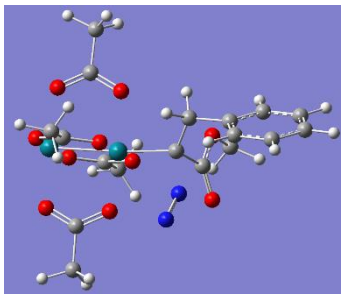
TS-1-b:





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C	2.06441100	1.41991200	-0.78738300
O	2.20147200	1.66225400	-1.96102800
O	2.16056400	2.31753300	0.20289800
Rh	-2.82498000	-0.20495900	0.29787200
Rh	-0.40168400	-0.04281000	-0.04175000
C	-1.30781600	0.38550500	2.70011200
C	-1.34623400	-2.70483900	0.60894700
C	-1.86804400	2.45317500	-0.37143800
C	-1.94231500	-0.63954300	-2.43521100
O	-0.24803900	0.34439000	1.99327300
O	-0.26949000	-2.07491500	0.33650700
O	-0.68746300	1.97624900	-0.41719800
O	-0.74677700	-0.45167900	-2.03367000
O	-2.48743700	0.20886500	2.30168800
O	-2.50567800	-2.22330600	0.67072900
O	-2.92848200	1.82862900	-0.10877500
O	-2.98424400	-0.60760100	-1.73127200
C	-1.09793500	0.68367500	4.15891000
H	-2.04501100	0.63646400	4.70179300
H	-0.38506000	-0.03198000	4.58337300
H	-0.65929100	1.68241400	4.26752600
C	-1.97607100	3.92581900	-0.65825500
H	-1.51783100	4.14616100	-1.62918700
H	-3.02121700	4.24438000	-0.65577100
H	-1.41844600	4.48557400	0.10227700
C	-2.09487200	-0.90201300	-3.90670000
H	-2.01392300	0.04844500	-4.44814600
H	-1.28782000	-1.55223100	-4.25965600
H	-3.07062600	-1.34750400	-4.11671300
C	-1.18450900	-4.17705200	0.86854100
H	-2.13272200	-4.61775200	1.18567700
H	-0.83831200	-4.67159700	-0.04668200
H	-0.41890200	-4.33790700	1.63545200
C	2.27077500	3.66978300	-0.23637200
H	3.22868500	3.82952900	-0.74378500
H	1.45426200	3.90603000	-0.92657000

H	2.20701500	4.28239300	0.66468500
C	2.46326900	-0.50776300	0.89001700
H	2.21334200	0.12303100	1.76082600
H	2.04194500	-1.49854100	1.11250600
C	3.94973200	-0.57030500	0.65752000
C	4.76829600	0.53941800	0.88173800
C	4.52854500	-1.75026000	0.18606700
C	6.13389100	0.47126200	0.63004100
H	4.32457000	1.46144100	1.25754700
C	5.89418600	-1.81889700	-0.06931100
H	3.89955300	-2.62797300	0.02656700
C	6.70006100	-0.70665700	0.15084700
H	6.76094000	1.34209900	0.81459400
H	6.33006400	-2.74683900	-0.43605800
H	7.76954700	-0.75899100	-0.04541400
N	2.01463900	-0.95473400	-1.63990000
N	1.72112500	-1.62328000	-2.47369300

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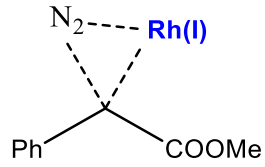

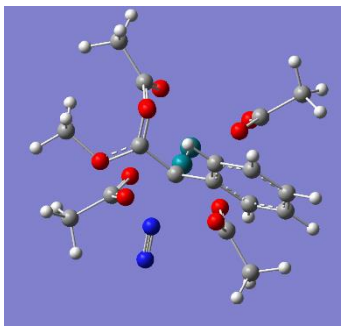

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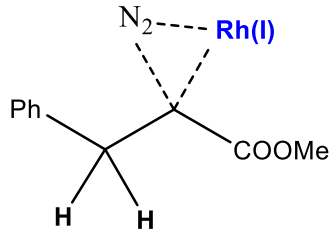
C	2.01043900	2.13534100	-0.20074000
O	2.37955900	2.34199300	-1.33393600
O	1.54290400	3.07666600	0.62439300
Rh	-2.36840400	-0.70178600	-0.39913300
Rh	-0.09108700	0.06306400	0.08267400
C	-1.01551700	-2.19313300	1.69344500
C	-0.31137300	-1.97272000	-1.98747700
C	-2.17376400	1.32850900	1.67096100
C	-1.51208800	1.56623600	-1.97140600
O	0.01956700	-1.48070300	1.47701800
O	0.53546800	-1.20976200	-1.42379300
O	-0.90682700	1.25926200	1.56694900

O	-0.43975900	1.57417600	-1.28875400
O	-2.12837600	-2.09551600	1.11679700
O	-1.54936000	-2.03326700	-1.75625100
O	-3.02258900	0.69435000	0.99034600
O	-2.45674400	0.73742200	-1.88144600
C	-0.86180100	-3.27446800	2.72653200
H	-1.84126000	-3.61391700	3.07324600
H	-0.33722700	-4.12574300	2.27484900
H	-0.25787200	-2.91833300	3.56684600
C	-2.69125200	2.25335900	2.73773000
H	-2.12750300	3.19171200	2.73036200
H	-3.75793300	2.44403900	2.59470400
H	-2.54257100	1.78691400	3.71934500
C	-1.66412000	2.68597900	-2.96261200
H	-2.16678500	3.52877500	-2.47101900
H	-0.68355200	3.02375400	-3.31159900
H	-2.28619900	2.36608900	-3.80333300
C	0.24299100	-2.88013300	-3.05008800
H	1.17937100	-3.33095800	-2.70553900
H	-0.48346500	-3.65251700	-3.31475900
H	0.47562000	-2.28475900	-3.94124500
C	1.36570300	4.35531100	0.02183500
H	2.31599900	4.73885100	-0.36482300
H	0.64622700	4.28178400	-0.80129300
C	3.08780600	-0.14239300	0.15071400
C	2.99036200	-1.48585900	0.54657300
C	4.29334600	0.31449200	-0.40740000
C	4.06825300	-2.34432300	0.39090600
H	2.05735500	-1.84035600	0.97963100
C	5.36057000	-0.55499200	-0.58007200
H	4.37899500	1.34663400	-0.73552500
C	5.25294200	-1.88329400	-0.17754400
H	3.98168000	-3.38256200	0.70640700
H	6.28508900	-0.19111200	-1.02457600
H	6.09471400	-2.56173800	-0.30771000
H	0.98247200	5.00496100	0.81075000
N	1.57821800	0.79220500	3.14465000
N	1.90228600	1.00504200	2.10362200

Optimized structures and coordinates in Scheme 3



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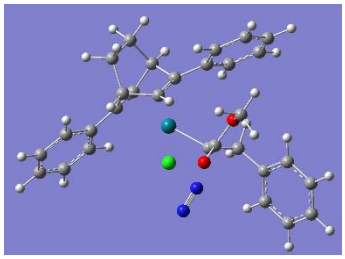
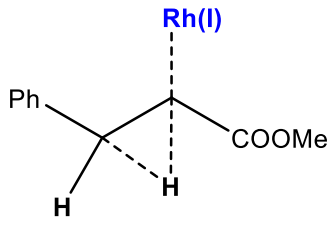
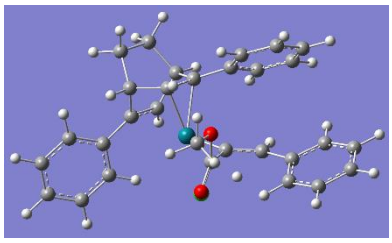


C	1.18303800	-0.73033600	0.15194200
C	1.65121400	-0.24742500	1.49230900
O	1.44244300	-0.76105900	2.56605800
O	2.30217100	0.91244900	1.32683300
C	2.80687100	1.49501500	2.52495400
H	1.99728000	1.68184700	3.24004700
H	3.54092300	0.82485400	2.98731300
Rh	-0.70901300	-0.16304700	-0.38542600
C	-3.16503600	2.74194400	0.87499900
C	-2.53359900	1.35450100	1.13009400
C	-1.79532300	2.22402800	-1.17768900
C	-2.71132100	3.27022300	-0.50019800
H	-4.26012600	2.65466600	0.92389300
H	-2.86119900	3.42564400	1.68022800
H	-3.57131700	3.47378000	-1.15178400
H	-2.15223200	4.21211500	-0.39894200
C	-2.92837100	0.41903800	-0.00290500
C	-2.49532100	0.88313200	-1.23674000
H	-2.83592900	0.45705500	-2.17888100
H	-1.46162100	2.55813100	-2.16705700
H	-2.81018200	0.95136200	2.10918400
C	-0.61209200	1.97422600	-0.24861000
C	-1.02843100	1.44984200	0.99271600
H	-0.39284700	1.48029400	1.88010400
Cl	-0.80895400	-2.12832100	-1.85682500
C	0.65092600	2.70199700	-0.47577700
C	1.38742500	2.51947600	-1.65162300
C	1.11806600	3.61254000	0.47525000
C	2.59510600	3.18041600	-1.83822300
H	1.01785800	1.82044000	-2.40491800
C	2.31642200	4.29186100	0.27999400

H	0.52871300	3.78324100	1.37780000
C	3.06748800	4.06328000	-0.86857100
H	3.17001300	3.00952100	-2.74710500
H	2.66579300	5.00214300	1.02889100
H	4.01187600	4.58390100	-1.01840700
C	-3.89818100	-0.67146300	0.19402800
C	-4.74324200	-0.67506200	1.31181200
C	-4.04956100	-1.69059000	-0.75821300
C	-5.71041600	-1.66058700	1.47358600
H	-4.66558900	0.11302600	2.05988800
C	-5.00963800	-2.67692700	-0.58942700
H	-3.36908600	-1.73756800	-1.60705500
C	-5.84566400	-2.66726500	0.52483600
H	-6.35902300	-1.63966900	2.34796600
H	-5.09880300	-3.46754800	-1.33252900
H	-6.59690400	-3.44477900	0.65429500
H	3.27202300	2.43439800	2.21846600
C	2.23307900	-0.86635200	-0.92756700
H	1.76169300	-1.33901700	-1.79978300
H	2.43866200	0.17984900	-1.20777800
C	3.50210300	-1.57477200	-0.53318400
C	3.62263200	-2.94763000	-0.76199100
C	4.55859000	-0.89703200	0.08122200
C	4.76766700	-3.63346900	-0.37118700
H	2.80853400	-3.47546000	-1.26350500
C	5.70483100	-1.58162300	0.47053100
H	4.47583000	0.17865200	0.24349100
C	5.80991900	-2.95198800	0.24973800
H	4.84875400	-4.70302200	-0.55822700
H	6.52344900	-1.04187200	0.94459400
H	6.70775000	-3.48751200	0.55393400
N	0.90087200	-2.40615300	0.65668700
N	0.47941200	-3.36944100	1.00238800

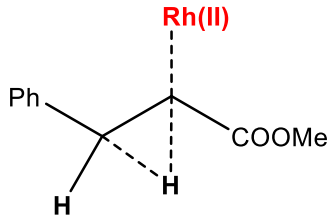
TS-4:





C	1.11600600	-0.86652700	-0.04048500
C	1.14634600	-1.79485400	1.11188800
O	0.87241800	-2.97235700	1.07094600
O	1.50647600	-1.14094200	2.23092200
C	1.56287500	-1.95866500	3.39660400
H	0.59732800	-2.44227300	3.57847300
H	2.32948100	-2.73432200	3.28101100
Rh	-0.73324800	-0.08506000	-0.41319200
C	-2.97093000	2.60406000	1.52775200
C	-2.44905000	1.15587900	1.42040300
C	-1.58004500	2.52359800	-0.57556400
C	-2.43671200	3.42626700	0.33931800
H	-4.07037100	2.59310200	1.53838200
H	-2.64417300	3.03328100	2.48482700
H	-3.26051200	3.85058200	-0.24987900
H	-1.82046300	4.26894900	0.68335600
C	-2.87631700	0.56609400	0.08114300
C	-2.37294400	1.29764400	-0.98738300
H	-2.71887700	1.15673700	-2.01054700
H	-1.21688000	3.08108100	-1.44509900
H	-2.78356800	0.53693400	2.25984300
C	-0.44030300	1.92433500	0.24186800
C	-0.93683100	1.14971100	1.31638800
H	-0.32611900	0.86638700	2.17309700
Cl	-0.75593500	-1.61531000	-2.35254700
C	0.94896100	2.39858200	0.09600100
C	1.43765700	2.77332300	-1.16376700
C	1.83173100	2.43359400	1.18238500
C	2.75832800	3.17118600	-1.33153400
H	0.77952800	2.72217200	-2.03127900
C	3.15573400	2.82138300	1.01401300
H	1.47403200	2.15929100	2.17369100
C	3.62545100	3.19692800	-0.24142800
H	3.11201300	3.46228600	-2.31987900
H	3.82321700	2.83966600	1.87409500
H	4.66071900	3.50942100	-0.36927500
C	-3.93088200	-0.45571700	-0.02104700
C	-4.85791300	-0.61949800	1.01587600

C	-4.06807900	-1.24623000	-1.17120700
C	-5.89570400	-1.53810700	0.90640300
H	-4.78688700	-0.00695600	1.91426000
C	-5.09912300	-2.16844600	-1.27323500
H	-3.32473300	-1.17005200	-1.96422800
C	-6.01930400	-2.31767700	-0.23798800
H	-6.61061400	-1.64380000	1.72102900
H	-5.17555700	-2.78596900	-2.16651500
H	-6.82536500	-3.04485800	-0.32200400
H	1.82175400	-1.29080400	4.22035900
C	2.25885600	-0.65191400	-0.80006600
H	1.19406800	-1.49484400	-1.17004600
H	2.13758400	0.04008200	-1.64194600
C	3.63474200	-1.11253800	-0.57405900
C	3.96859900	-2.28022500	0.12464800
C	4.65757800	-0.29948900	-1.07769800
C	5.30235200	-2.60575300	0.32978200
H	3.18885300	-2.95389600	0.47641400
C	5.98916000	-0.61835800	-0.84973600
H	4.39176100	0.60493300	-1.62624700
C	6.31341300	-1.77385100	-0.14535300
H	5.55513500	-3.52115400	0.86160300
H	6.77525400	0.03059400	-1.23119400
H	7.35679400	-2.03346000	0.02526600



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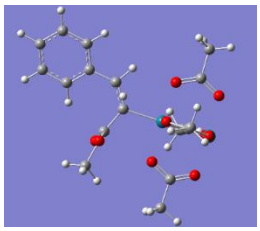
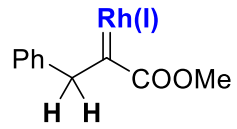


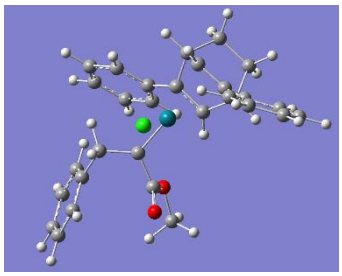
C	1.72625900	0.28026600	-0.07823800
C	2.10123400	1.68852500	-0.31195800
O	2.22240700	2.16498200	-1.41681300
O	2.19074700	2.36797000	0.83698900
Rh	-2.75115700	-0.37842700	0.01319400
Rh	-0.33057400	-0.01402300	-0.02820700
C	-1.51339700	0.06568400	2.62081800

C	-1.12561700	-2.79292900	0.26404200
C	-1.92993500	2.39681900	-0.26955600
C	-1.55211700	-0.45887300	-2.62637500
O	-0.38388100	0.16253100	2.04058100
O	-0.08115700	-2.06319200	0.18958000
O	-0.71814800	2.01028700	-0.21709400
O	-0.42580600	-0.23482300	-2.07936600
O	-2.62990200	-0.12722000	2.07322900
O	-2.32004200	-2.40429300	0.23611200
O	-2.95912000	1.67420500	-0.21460800
O	-2.66466600	-0.58677400	-2.04818300
C	-1.49313000	0.16438500	4.12182900
H	-2.44822500	0.55083900	4.48860200
H	-1.34880400	-0.83881000	4.54231800
H	-0.66546400	0.79628400	4.45665200
C	-2.12271300	3.88252200	-0.40779000
H	-1.58491500	4.23995600	-1.29335100
H	-3.18387000	4.13063700	-0.48722700
H	-1.68970900	4.38797600	0.46387200
C	-1.53256400	-0.56045900	-4.12644600
H	-1.37189100	0.43849800	-4.54951500
H	-0.69597500	-1.18881000	-4.44879900
H	-2.47938200	-0.96045500	-4.49821300
C	-0.87491800	-4.27181300	0.38093100
H	-1.80190800	-4.80183200	0.61291100
H	-0.47378700	-4.64530800	-0.56907100
H	-0.12330900	-4.46659600	1.15349300
C	2.26998600	3.78399000	0.68430500
H	3.15932600	4.06565300	0.11043800
H	1.37497300	4.14531000	0.16554900
H	2.32119300	4.19114500	1.69539400
C	2.64568000	-0.75506700	0.09921000
H	2.06718300	-0.14144800	1.11394300
H	2.18404200	-1.74054500	0.25379000
C	4.11450000	-0.74002100	0.01323400
C	4.82395700	0.25781800	-0.66687100
C	4.81388700	-1.79338600	0.61482500
C	6.21017800	0.20282200	-0.72337000
H	4.29046400	1.05410300	-1.18206100
C	6.19971400	-1.83881100	0.56400700
H	4.25711900	-2.57763700	1.12843200
C	6.89883600	-0.83697800	-0.10400500
H	6.75670200	0.97414600	-1.26243000
H	6.73519400	-2.65747700	1.04066600

H	7.98574200	-0.87307200	-0.15194000

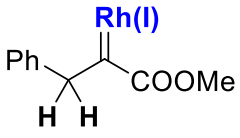
A7:





C	0.31467500	1.40953000	1.03224500
C	1.66497200	2.00558500	0.90260200
O	1.85475300	3.12213900	0.48468300
O	2.61640700	1.17682600	1.35875300
C	3.90406900	1.77972600	1.49503200
H	4.27727000	2.12328000	0.52476500
H	3.84481000	2.63481700	2.17903700
Rh	-0.36035900	0.40872300	-0.38232400
C	0.93434800	-3.12273100	-1.99112700
C	1.05070300	-1.57918000	-1.94168000
C	-0.98244400	-2.31575700	-0.56511700
C	-0.28211400	-3.56606200	-1.15657700
H	0.83703000	-3.44510900	-3.03761000
H	1.86304600	-3.56337000	-1.60370900
H	-1.00200000	-4.12550900	-1.76785900
H	0.02054700	-4.22219200	-0.32777600
C	-0.25232400	-0.99134500	-2.45964700
C	-1.32181500	-1.36491400	-1.69190700
H	-2.35313300	-1.14587100	-1.96227100
H	-1.86880000	-2.59530300	0.01404800
H	1.91626400	-1.21682600	-2.50538500
C	0.05235600	-1.59470300	0.29435200
C	1.13520700	-1.15154800	-0.49088600
H	2.09394700	-0.86732100	-0.05783300
Cl	-1.96263900	2.12902200	-0.93886400
C	0.07927200	-1.81262600	1.75416800
C	-1.10725700	-1.75829600	2.49900000
C	1.27422600	-2.09471000	2.42441000
C	-1.09913000	-1.98208100	3.86952900
H	-2.04292700	-1.51208700	1.99443100
C	1.28232200	-2.32299500	3.79678300

H	2.20296100	-2.15439100	1.85794300
C	0.09699900	-2.27121000	4.52394200
H	-2.03066300	-1.93118300	4.43077600
H	2.22145200	-2.55012500	4.29905100
H	0.10328200	-2.45536400	5.59684800
C	-0.33281700	-0.28045600	-3.74371000
C	0.64158000	-0.49250200	-4.72732200
C	-1.41069300	0.56571200	-4.04116400
C	0.53989300	0.11323200	-5.97408000
H	1.48047300	-1.15956500	-4.53154800
C	-1.50313800	1.17734800	-5.28274300
H	-2.15059000	0.78615800	-3.27271300
C	-0.53188100	0.95235700	-6.25566700
H	1.30438700	-0.07124100	-6.72715300
H	-2.33702100	1.84625400	-5.48773900
H	-0.60904700	1.43503800	-7.22855400
H	4.55456600	1.00647700	1.90735900
C	-0.45219700	1.82340500	2.24134200
H	-1.13340300	2.60531200	1.84568900
H	-1.11757700	0.99938300	2.54293300
C	0.38605000	2.32976400	3.38538600
C	0.73183700	3.67902700	3.47450100
C	0.89662100	1.43373900	4.32604400
C	1.56694000	4.12719400	4.49331400
H	0.34962600	4.37921200	2.73141000
C	1.73110700	1.88072700	5.34452600
H	0.63588300	0.37633100	4.25423700
C	2.06816900	3.22892400	5.43065100
H	1.82505900	5.18319400	4.55442400
H	2.12064100	1.17198100	6.07423600
H	2.72004300	3.57965500	6.22936900



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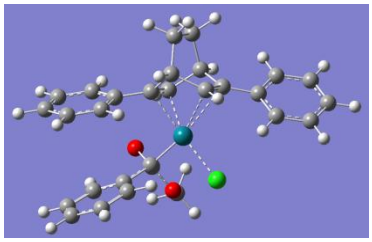

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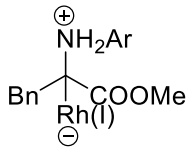
C	1.05414800	-1.67262600	1.78219700

O	0.54022100	-2.90018200	1.85448900
O	1.37986600	-1.00151800	2.74227900
Rh	-0.36423500	-0.34813100	-0.28567000
C	-2.05713800	3.12084700	1.06133400
C	-1.94584400	1.57992700	1.17159400
C	-0.64426600	2.37524500	-0.88862000
C	-1.27595600	3.59899800	-0.17713300
H	-3.11764400	3.40310500	0.99558800
H	-1.65972000	3.57340800	1.97991700
H	-1.93173600	4.12527400	-0.88294900
H	-0.47232300	4.29523500	0.10209700
C	-2.47343300	0.97512800	-0.11929200
C	-1.73497600	1.37456600	-1.20293200
H	-2.02097500	1.15417600	-2.22975300
H	-0.09926100	2.67844900	-1.78869200
H	-2.47038800	1.19583200	2.05186600
C	0.26455800	1.68973800	0.12325000
C	-0.47945700	1.20554000	1.21729600
H	-0.01346900	0.92658400	2.16284200
Cl	-1.00507900	-2.07197400	-1.85722000
C	1.71522800	1.95832300	0.13445900
C	2.44140800	1.99716600	-1.06259800
C	2.40078800	2.16821700	1.33613500
C	3.80948200	2.23322300	-1.05832200
H	1.93019000	1.80486200	-2.00671000
C	3.77032700	2.40590700	1.34067000
H	1.85203700	2.14951000	2.27647800
C	4.48022900	2.43893500	0.14461800
H	4.35718900	2.24513500	-1.99965400
H	4.28362800	2.57124600	2.28670900
H	5.55256900	2.62752000	0.14835800
C	-3.74777700	0.24379200	-0.17848600
C	-4.70183100	0.40595500	0.83444600
C	-4.07213500	-0.56771100	-1.27560700
C	-5.94298200	-0.21472100	0.75281400
H	-4.48925100	1.04498100	1.69051800
C	-5.30706100	-1.19480300	-1.34855400
H	-3.32764900	-0.74912800	-2.04867100
C	-6.24967000	-1.01944300	-0.33814500
H	-6.67268200	-0.06709800	1.54742000
H	-5.53125000	-1.83470100	-2.20016800
H	-7.21828500	-1.51278700	-0.40055200
C	2.44783900	-1.34543600	-0.27944300
C	3.64125100	-1.45351900	0.46451300

C	2.51491500	-1.35554900	-1.68778100
C	4.86311400	-1.53169400	-0.18310100
H	3.59581100	-1.42738700	1.55235400
C	3.73872000	-1.47919500	-2.32580800
H	1.58223600	-1.31210000	-2.24990100
C	4.91156800	-1.55352800	-1.57663100
H	5.78270000	-1.58753300	0.39641900
H	3.78216500	-1.51397300	-3.41265300
H	5.87322700	-1.63555800	-2.08149400
C	0.34993700	-3.40765600	3.17311000
H	-0.08228200	-4.40141700	3.04691200
H	1.30542400	-3.46735700	3.70559200
H	-0.33143400	-2.76164800	3.73675300

Optimized structures and coordinates in Scheme 4



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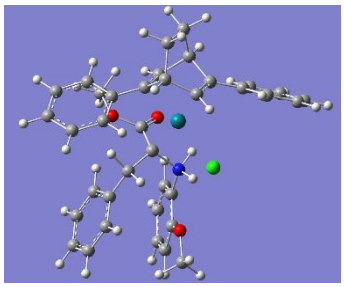
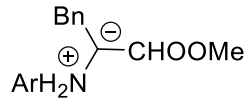
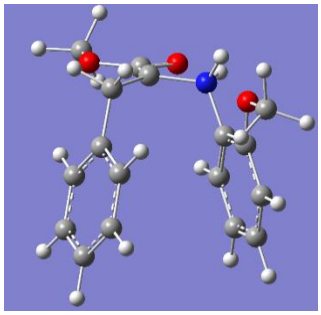


C	0.10427400	1.32557000	-0.25622900
C	0.70318100	1.26819600	-1.59171700
O	0.09172300	1.02488700	-2.62673300
O	2.03837300	1.46453000	-1.58504300
C	2.66647100	1.42866900	-2.85614400
H	2.53717300	0.45233100	-3.34023500
H	2.24990300	2.19811200	-3.51745200
Rh	0.12378100	-0.80000100	0.40081000
C	1.95384600	-4.13099100	-0.73346400
C	0.97089200	-2.98666800	-1.05704900
C	1.91292400	-2.67626800	1.32113900
C	2.56209300	-3.91212900	0.66485000
H	1.41476100	-5.08746600	-0.78636800
H	2.73582700	-4.16302100	-1.50457900
H	2.40558200	-4.78920500	1.30714600
H	3.64796000	-3.74775000	0.60400100
C	-0.12060100	-2.94292300	0.00678400

C	0.40331000	-2.77347100	1.29162100
H	-0.19042800	-2.88688500	2.19724200
H	2.29583300	-2.51746900	2.33568200
H	0.55029200	-3.09749500	-2.06262200
C	2.17479100	-1.46222200	0.42918500
C	1.63555700	-1.63817000	-0.86426100
H	1.95251500	-1.04434300	-1.72089100
Cl	-1.92793000	-0.36313700	1.74560600
C	-2.83428700	5.02823400	-0.10311800
C	-2.39336400	3.74055400	0.19253600
C	-1.84686300	2.95793600	-0.83327800
C	-1.77383800	3.43025200	-2.13369000
C	-2.21945300	4.71690300	-2.42303200
C	-2.73721900	5.50888000	-1.40627600
H	-3.24434800	5.66002400	0.68061500
H	-1.35105000	2.78873300	-2.90418400
H	-2.16037300	5.09415400	-3.44135700
H	-3.08167700	6.51847400	-1.62334900
N	-1.38515100	1.61073800	-0.48928400
H	-1.88213500	1.25062500	0.35667600
H	-1.62531800	0.97666700	-1.26300000
O	-2.44720900	3.15497400	1.40420200
C	-3.03614700	3.86224900	2.46987700
H	-2.99438100	3.19327300	3.33250800
H	-2.47704600	4.78461100	2.68770800
H	-4.08445000	4.11137700	2.24953000
H	3.72600300	1.62151100	-2.66823100
C	3.22593100	-0.49887100	0.79995300
C	4.20189100	-0.09688800	-0.11664200
C	3.26794400	0.03527700	2.09505200
C	5.17156600	0.83430700	0.23677400
H	4.20137500	-0.53196600	-1.11579200
C	4.23622800	0.96489400	2.45011800
H	2.49719600	-0.25169600	2.81218700
C	5.18892200	1.37333700	1.51935500
H	5.92259300	1.13644900	-0.49244500
H	4.24249100	1.38105100	3.45627300
H	5.94590700	2.10512800	1.79609400
C	-1.51917600	-3.27946500	-0.30782400
C	-2.08833000	-2.86907900	-1.52119300
C	-2.31702000	-3.98261800	0.59949200
C	-3.41651200	-3.14912400	-1.81299700
H	-1.48883500	-2.29152900	-2.22720000
C	-3.64439900	-4.26613500	0.30582100

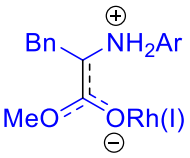
H	-1.88709600	-4.31508400	1.54331900
C	-4.19995700	-3.85037400	-0.90023400
H	-3.84388800	-2.81364100	-2.75690100
H	-4.24976400	-4.81585600	1.02477400
H	-5.24118500	-4.07217700	-1.12891000
C	0.74256100	2.16200600	0.83742400
H	0.29849500	1.85923800	1.79780500
H	1.78886000	1.82322800	0.88486800
C	0.73905100	3.67596400	0.76479900
C	0.43013200	4.40425200	1.91633700
C	1.08120700	4.38725900	-0.38830700
C	0.44216400	5.79548300	1.91845800
H	0.17531900	3.86237400	2.82924800
C	1.08657200	5.77775700	-0.39504000
H	1.34557900	3.84723300	-1.29762500
C	0.76421700	6.48975200	0.75692700
H	0.19870500	6.33834600	2.83187400
H	1.34674800	6.31022200	-1.30925100
H	0.76985200	7.57863800	0.74941400

C1: 



C	-6.76574500	0.45010800	1.13877500
C	-5.54356800	0.69025500	0.52038100
O	-5.39002700	0.73321600	-0.72306900
O	-4.48824300	0.86375400	1.36952800
C	-3.23663800	1.01776300	0.73054300
H	-2.97860000	0.13367700	0.13448800
H	-3.23107700	1.88973700	0.06547200
C	-11.00594100	2.28577200	0.24954600
C	-10.09961300	1.22959700	0.30174600
C	-8.76091500	1.47065800	-0.00709800
C	-8.31032100	2.73359700	-0.34128800
C	-9.21532300	3.78752400	-0.38815700
C	-10.55486100	3.55651800	-0.09621600

H	-12.05507000	2.12719000	0.48572600
H	-7.24869200	2.86964600	-0.54640100
H	-8.87382700	4.78576100	-0.65038400
H	-11.26743100	4.37833400	-0.12932300
N	-7.80739800	0.36456400	0.08989400
H	-8.34033600	-0.51166400	0.13776900
H	-7.18122600	0.35282000	-0.75670200
O	-10.40291800	-0.05060300	0.64884200
C	-11.73034200	-0.33053400	1.03204800
H	-11.75873700	-1.39134000	1.29117600
H	-12.02388200	0.26546300	1.90854300
H	-12.43435400	-0.13852500	0.20976200
H	-2.50293700	1.15286000	1.53046600
C	-7.18574800	0.55481400	2.56148300
H	-6.31468800	0.27466500	3.17169000
H	-7.96729000	-0.19189500	2.79406700
C	-7.67269900	1.92354000	2.99512400
C	-9.00919900	2.16371800	3.30473900
C	-6.77319200	2.99197400	3.05021400
C	-9.44565300	3.43881700	3.65662500
H	-9.72095800	1.33527500	3.25922200
C	-7.19992100	4.26214800	3.41291100
H	-5.72818200	2.80875700	2.79646200
C	-8.54110900	4.49196000	3.71554000
H	-10.49813300	3.60836300	3.88302100
H	-6.48328100	5.08137500	3.46033500
H	-8.87712700	5.48921700	3.99573000



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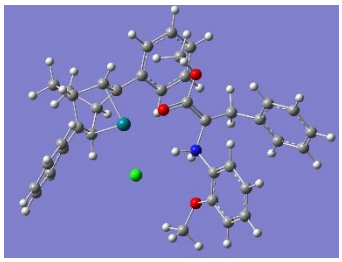
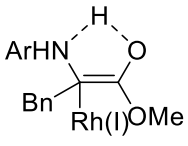


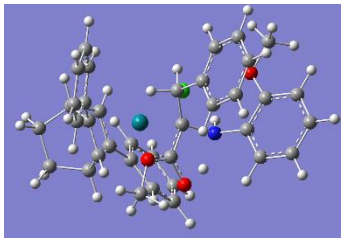
C	-2.25101100	1.05106100	0.63416500
C	-1.12557300	1.73484200	1.02964500
O	-0.03479500	1.81003700	0.37857200
O	-1.24732100	2.40212000	2.21307500
C	-0.19655300	3.28279000	2.54327500

H	0.78367200	2.80690500	2.43018700
H	-0.21662100	4.17971600	1.90870700
Rh	1.39825200	0.22134800	-0.01963100
C	4.62824700	-1.06121800	1.82587500
C	3.93103900	0.03658800	0.99868100
C	2.27327000	-1.88840900	1.47401500
C	3.62401400	-2.18289000	2.15497200
H	5.47770900	-1.44822000	1.24506300
H	5.04223500	-0.61979700	2.74265100
H	3.99710600	-3.15920900	1.81692900
H	3.45933800	-2.26177000	3.23920600
C	3.37065900	-0.57954000	-0.28215400
C	2.45208200	-1.61244900	-0.00479100
H	2.11107400	-2.31061300	-0.76956800
H	1.54700700	-2.68807900	1.66041800
H	4.61400800	0.86490200	0.77918200
C	1.74904000	-0.53521500	1.95373700
C	2.65749700	0.50749700	1.67205000
H	2.58860600	1.49248200	2.13563900
Cl	0.49856300	-0.06216700	-2.31216200
C	-4.05970300	0.17948300	-3.82674600
C	-3.28543600	-0.17600100	-2.72573800
C	-2.98961600	0.79258300	-1.76535400
C	-3.42755200	2.09523900	-1.88973700
C	-4.21344200	2.44450600	-2.98319900
C	-4.52316400	1.48764500	-3.94289600
H	-4.30006300	-0.55871900	-4.58873200
H	-3.16500000	2.81503700	-1.11718000
H	-4.58161800	3.46328300	-3.07948200
H	-5.13369900	1.75808900	-4.80267200
N	-2.10815600	0.38313400	-0.66070100
H	-2.17958400	-0.64275600	-0.58983500
H	-1.12784400	0.52953300	-1.00937400
O	-2.79196400	-1.41644800	-2.48536600
C	-2.51801000	-2.23592400	-3.60304800
H	-1.91454800	-3.06888900	-3.23463100
H	-3.44246100	-2.62890500	-4.05032800
H	-1.94327700	-1.67889900	-4.35481400
C	0.63725200	-0.45147900	2.91806900
C	0.72220100	0.36580000	4.05012000
C	-0.52774100	-1.20702900	2.72778500
C	-0.32685500	0.43535400	4.95952800
H	1.63272200	0.93951400	4.22420500
C	-1.57096400	-1.14695800	3.64148300

H	-0.61309400	-1.83541500	1.83887500
C	-1.47625000	-0.32228000	4.76028300
H	-0.24095700	1.07738100	5.83508600
H	-2.46968200	-1.73995200	3.47602900
H	-2.29600200	-0.27314000	5.47497600
C	4.01799400	-0.35231400	-1.58565700
C	4.26771700	-1.41431200	-2.45924400
C	4.40388500	0.93718500	-1.97017700
C	4.88656500	-1.19519300	-3.68417200
H	3.98403400	-2.42478400	-2.16658500
C	5.01617100	1.15751600	-3.19573300
H	4.18170900	1.77891000	-1.31324800
C	5.26254300	0.09097600	-4.05666500
H	5.07738800	-2.03497300	-4.35061900
H	5.29557900	2.16925600	-3.48533800
H	5.74430600	0.26339300	-5.01780400
H	-0.35545900	3.56500800	3.58840500
C	-3.50772700	0.80508700	1.40136100
H	-3.28291600	0.99599800	2.46061300
H	-3.78173000	-0.26649000	1.34078400
C	-4.70004700	1.63858900	0.98619700
C	-5.79525000	1.07702900	0.33503000
C	-4.68659600	3.01783600	1.21185200
C	-6.84969200	1.87408200	-0.10414800
H	-5.80906100	0.00160600	0.14558900
C	-5.73679600	3.81713300	0.77834300
H	-3.82286100	3.45555100	1.71627300
C	-6.82191300	3.24679900	0.11388300
H	-7.69297600	1.41950400	-0.62260100
H	-5.71221800	4.89115100	0.95948800
H	-7.64487700	3.87274500	-0.22813000

TS-5:





C	0.88560200	-0.11084700	0.40250200
C	0.56397900	0.24938300	1.73318700

O	0.27852400	-0.70920100	2.55612500
O	0.59476200	1.49697800	2.16502700
C	0.35087400	1.70924000	3.55247200
H	-0.62326800	1.30688400	3.85322900
H	1.13249800	1.23261000	4.15453700
Rh	-1.31612700	0.02418800	-0.31906200
C	-4.79908600	1.56705500	0.78686200
C	-3.62942400	0.60580300	1.07834600
C	-3.20331000	1.84318000	-1.14276700
C	-4.51894900	2.34371900	-0.51299300
H	-5.72761100	0.98392400	0.70970200
H	-4.92242600	2.25138100	1.63746600
H	-5.33555900	2.21489700	-1.23610600
H	-4.42928600	3.42256000	-0.32018700
C	-3.44967600	-0.34911100	-0.09640200
C	-3.21167800	0.33773600	-1.29700100
H	-3.24028700	-0.14760600	-2.27133500
H	-3.00012700	2.35001800	-2.09257900
H	-3.78626600	0.06398800	2.01774600
C	-2.06613900	2.04201200	-0.14172700
C	-2.30588600	1.34130000	1.06085100
H	-1.78651000	1.57989500	1.98733200
Cl	-0.79372300	-1.78690600	-1.91610700
C	4.62213100	-2.71570600	-0.31094000
C	3.30261600	-2.29742700	-0.47060900
C	2.52146500	-1.99991500	0.65933500
C	3.07210700	-2.14617900	1.92594600
C	4.39210200	-2.55985500	2.08810800
C	5.16059100	-2.83992600	0.96740400
H	5.23732800	-2.93176800	-1.18123600
H	2.45822900	-1.92302600	2.79744600
H	4.81044300	-2.66805600	3.08674100
H	6.19418700	-3.16381300	1.07824000
N	1.15440200	-1.57088600	0.49503200
H	0.69578700	-2.05064700	-0.29127800
H	0.51247500	-1.51453500	1.79128900
O	2.68398700	-2.13128700	-1.65754300
C	3.37582600	-2.47473300	-2.83086900
H	2.67458400	-2.30404500	-3.65172000
H	4.26867200	-1.84504600	-2.96922300
H	3.67762700	-3.53301500	-2.82400200
H	0.37591600	2.79291400	3.68904700
C	-1.10383900	3.14341400	-0.31280000
C	-0.71568200	3.94542700	0.76563100

C	-0.54471900	3.40423900	-1.57157400
C	0.21760200	4.96142100	0.59869000
H	-1.16087100	3.77031300	1.74480200
C	0.38759500	4.41921900	-1.74000400
H	-0.81311900	2.76758400	-2.41581400
C	0.77526500	5.19994600	-0.65359700
H	0.50705700	5.57496100	1.45087800
H	0.82323600	4.59466200	-2.72225800
H	1.50921300	5.99323900	-0.78414500
C	-3.76765200	-1.78150300	0.02130200
C	-3.37687100	-2.49507400	1.16179600
C	-4.43943800	-2.46040700	-0.99858900
C	-3.64691400	-3.85151000	1.27471100
H	-2.81516600	-1.98423600	1.94581000
C	-4.71507300	-3.81702400	-0.88253000
H	-4.74987800	-1.91497300	-1.88889100
C	-4.31990400	-4.51680500	0.25297600
H	-3.32447700	-4.39560400	2.16113100
H	-5.23926300	-4.33147300	-1.68635400
H	-4.53258400	-5.58097700	0.34115000
C	1.64103100	0.79672600	-0.54276900
H	1.37572200	0.51422100	-1.57196100
H	1.23244800	1.80961500	-0.39737500
C	3.14972900	0.87408800	-0.44775800
C	3.90487700	0.85643100	-1.62147400
C	3.82229000	1.01495000	0.76713700
C	5.29212800	0.95725800	-1.58820400
H	3.38870500	0.75357700	-2.57783900
C	5.20884700	1.10993300	0.80831800
H	3.25373200	1.03869800	1.69790700
C	5.95080000	1.07704100	-0.36899500
H	5.85992500	0.93820000	-2.51826100
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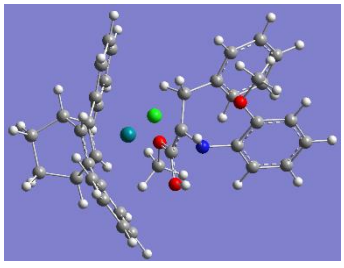

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O	0.63924200	1.61531100	1.98309400
C	0.56632900	1.91953600	3.37016200
H	-0.39419300	1.61574100	3.80271900
H	1.37826700	1.42195300	3.91495100
Rh	-1.34314200	0.11540200	-0.32966100
C	-4.85808600	1.50030000	0.87324200
C	-3.65621600	0.56708600	1.11937200
C	-3.28925500	1.90622100	-1.05390300
C	-4.61415200	2.33879000	-0.39544700
H	-5.76796700	0.89096800	0.77901200
H	-4.99653100	2.14473900	1.75212000
H	-5.43192100	2.21377200	-1.11781900
H	-4.55760000	3.41090100	-0.15848200
C	-3.45011000	-0.33527400	-0.09164200
C	-3.24709000	0.40889000	-1.26864500
H	-3.27063600	-0.03657100	-2.26194700
H	-3.10690600	2.45658600	-1.98349900
H	-3.78840300	-0.01355000	2.03888700
C	-2.14796400	2.09521200	-0.05595200
C	-2.35474400	1.34141100	1.12099300
H	-1.83243000	1.55098500	2.05290800
Cl	-0.78128200	-1.50795200	-2.10384200
C	4.58285900	-2.82874700	-0.17465500
C	3.28429300	-2.38934900	-0.41737300
C	2.45503800	-2.00098000	0.65192600
C	2.95223400	-2.08002100	1.94754600
C	4.25425900	-2.50963800	2.19492900
C	5.06406800	-2.88300600	1.13212500
H	5.23036800	-3.11189000	-1.00124700
H	2.31005300	-1.78826400	2.77845800
H	4.62550400	-2.56039700	3.21679900
H	6.08269800	-3.22393300	1.31024700
N	1.12142500	-1.55201800	0.38897700
H	0.76170500	-1.96387000	-0.47752400
O	2.72321500	-2.27455600	-1.64301800
C	3.47492700	-2.65922100	-2.76436300
H	2.82749600	-2.49775500	-3.63036700
H	4.38513900	-2.04716700	-2.86712700
H	3.75846600	-3.72173400	-2.71568500
H	0.68290400	3.00399600	3.43383600
C	-1.19732900	3.21005600	-0.20296400

C	-0.82881900	3.99982600	0.89033000
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C	0.09855700	5.02476600	0.74743800
H	-1.28571400	3.80816800	1.86114600
C	0.30009700	4.51362200	-1.59627700
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H	0.37313100	5.63070500	1.61029700
H	0.74607200	4.70452200	-2.57087700
H	1.39992500	6.08182200	-0.60710900
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C	-3.31694100	-2.51482500	1.10194600
C	-4.31361400	-2.46030600	-1.08911700
C	-3.52722100	-3.88492800	1.16617900
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C	-4.13867900	-4.54715000	0.10477400
H	-3.20813000	-4.44123000	2.04616700
H	-5.00751900	-4.34225500	-1.85571800
H	-4.30576300	-5.62176800	0.15487300
C	1.64665700	0.77093600	-0.63713900
H	1.36613400	0.43060000	-1.64477100
H	1.25534900	1.79615600	-0.53703900
C	3.15726600	0.81421100	-0.55231800
C	3.90826200	0.72318000	-1.72519300
C	3.83707700	0.98231800	0.65516900
C	5.29812900	0.78364700	-1.69715900
H	3.38689700	0.59138600	-2.67501500
C	5.22556800	1.03767600	0.69119000
H	3.27210700	1.05444100	1.58581200
C	5.96321000	0.93601300	-0.48510000
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H	5.73572000	1.15622900	1.64651100
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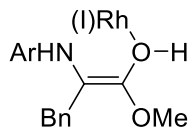

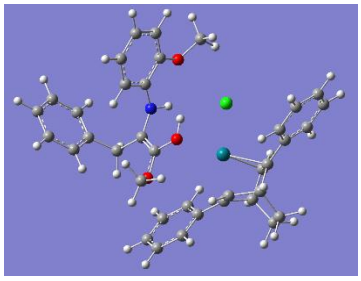

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O	-1.23545800	1.61771100	2.00470600
C	-0.81727700	2.97423100	1.96910400
H	0.17990600	3.07561300	1.52114400
H	-1.53247400	3.58595500	1.39807600
Rh	1.30244900	-0.09800800	0.01174900
C	4.76976700	-0.50079900	1.84465000
C	3.86886700	0.31597500	0.89661400
C	2.57354000	-1.73650200	1.78997400
C	3.98102600	-1.69417300	2.41692400
H	5.65009500	-0.84079500	1.28085500
H	5.13735100	0.15244500	2.64739300
H	4.49751400	-2.64297600	2.21890800
H	3.87238700	-1.61077700	3.50774600
C	3.36996300	-0.58856100	-0.22568000
C	2.64254000	-1.69227000	0.27880600
H	2.39274300	-2.55695200	-0.33656300
H	1.99611500	-2.59461600	2.15165500
H	4.39609200	1.19197000	0.50389200
C	1.85751400	-0.42006500	2.08091800
C	2.56024600	0.68545900	1.56588000
H	2.34467000	1.70911000	1.87562800
Cl	0.35919900	-0.78931800	-2.12336100
C	-3.33856800	0.84206400	-4.27729500
C	-3.12564500	0.09820500	-3.12621600
C	-3.17027900	0.71518000	-1.85686600
C	-3.46036400	2.07698400	-1.78598200
C	-3.68898100	2.81519100	-2.94648800
C	-3.62290000	2.20648500	-4.19028900
H	-3.28652700	0.35902600	-5.25089700
H	-3.52089200	2.55518000	-0.80776300
H	-3.91814200	3.87637000	-2.86419300
H	-3.79193400	2.78026400	-5.09951400
N	-2.92174900	-0.08450300	-0.73901000
H	-2.54835800	-1.00032800	-0.96864600

O	-2.86990700	-1.23947200	-3.10390900
C	-2.35119600	-1.81915500	-4.27542000
H	-2.00716400	-2.82001200	-4.00056500
H	-3.11935800	-1.90503900	-5.05973500
H	-1.49776500	-1.23944700	-4.65569700
C	0.79953400	-0.34236200	3.10175200
C	0.83531400	0.64166200	4.09459500
C	-0.25810400	-1.25930000	3.09990600
C	-0.16982400	0.72059600	5.05084700
H	1.67141900	1.34107800	4.12028900
C	-1.26897300	-1.17243600	4.04710800
H	-0.30488100	-2.01888200	2.31788800
C	-1.23028100	-0.17951800	5.02343300
H	-0.12311000	1.48704700	5.82334000
H	-2.09724400	-1.87931100	4.02012200
H	-2.02153800	-0.11500200	5.76856100
C	3.91696900	-0.49449400	-1.58997100
C	4.24648000	-1.64630400	-2.31062900
C	4.12283500	0.75401500	-2.18927900
C	4.76826800	-1.55358300	-3.59465400
H	4.10466500	-2.62493900	-1.85369200
C	4.63791400	0.84682400	-3.47414100
H	3.83796900	1.65951300	-1.65255300
C	4.96458700	-0.30766900	-4.18097900
H	5.02357800	-2.46051700	-4.14027200
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C	-4.88058800	1.30534200	1.31817400
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H	-6.01598900	-0.01707800	0.06205900
C	-5.74633800	3.55946200	1.51780700
H	-3.95566000	2.84937800	2.49253900
C	-6.80527100	3.23450300	0.67343200
H	-7.72954700	1.68623500	-0.50392400
H	-5.66579600	4.56420200	1.93125100
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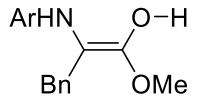
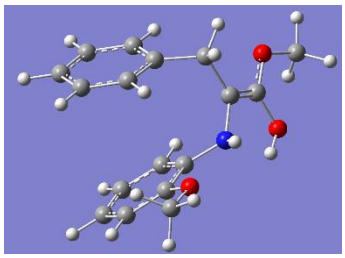
B2: 



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O	-0.15009100	1.95296200	0.45119900
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C	-0.15870500	2.70513800	2.91386800
H	0.67450000	1.99184400	2.92808300
H	0.14386700	3.59238300	2.34573400
C	-3.95766000	0.99399100	-3.89836400
C	-3.26691100	0.37825700	-2.86353000
C	-2.75140600	1.13631900	-1.79624300
C	-2.93999400	2.51268500	-1.80212200
C	-3.64260200	3.13043300	-2.83279900
C	-4.14708900	2.37610200	-3.88142300
H	-4.36202100	0.40507100	-4.71850500
H	-2.55730900	3.09512300	-0.96472400
H	-3.79398700	4.20785100	-2.80722600
H	-4.69306600	2.85224200	-4.69349800
N	-2.03939000	0.47756600	-0.76867400
H	-2.07723700	-0.52998200	-0.90478800
O	-3.05956000	-0.97108300	-2.75893500
C	-3.65590400	-1.79639000	-3.72475400
H	-3.41577100	-2.82652900	-3.44791500
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H	-3.26008500	-1.59448500	-4.73159700
H	-0.41601700	2.99136800	3.93646300
C	-3.49600000	0.45995100	1.31248600
H	-3.39147200	0.69551500	2.38032300
H	-3.61861800	-0.63499200	1.23925600
C	-4.71857200	1.13645700	0.74235700
C	-5.47534800	0.52704300	-0.25654500
C	-5.04615400	2.43417700	1.13626600
C	-6.52586600	1.20502500	-0.86611500
H	-5.20642500	-0.47931000	-0.58670000
C	-6.10093800	3.11223800	0.53805300
H	-4.44600000	2.91891600	1.90885600

C	-6.84092200	2.50036900	-0.47039200
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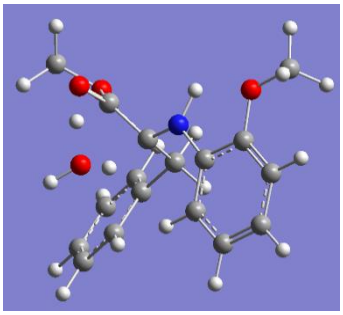
H	-0.25148500	1.47795100	-0.40089900

TS-6:



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O	-6.08595900	0.31452800	-0.16999900
O	-5.01734500	1.08263200	1.64356300
C	-3.80074900	0.93842500	0.91764600
H	-3.62937900	-0.10978100	0.65253500
H	-3.81921000	1.53835500	0.00161100
C	-12.01708900	-0.24053600	1.90122000
C	-10.65191200	-0.46829100	1.86607000
C	-9.74590200	0.57911200	1.57383300
C	-10.27339500	1.84771300	1.33820000
C	-11.64890200	2.07425900	1.37100900
C	-12.52315200	1.03850300	1.65091800
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H	-9.59538400	2.66790700	1.10963800
H	-12.02796500	3.07642100	1.17839800
H	-13.59738700	1.20803400	1.68101700
N	-8.39570000	0.27634900	1.53487300
H	-8.18636800	-0.63364700	1.93045900
O	-10.05810800	-1.67750400	2.10573200
C	-10.89123700	-2.75867300	2.42815100
H	-10.23633200	-3.61631700	2.60418800
H	-11.47845800	-2.55930200	3.33787400
H	-11.58192600	-2.99634800	1.60478200
H	-3.01608500	1.29660000	1.58732500
C	-7.26116300	2.07376100	2.88924900

H	-6.80711700	1.47511700	3.69752600
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C	-6.51455100	3.37538600	2.75553200
C	-6.95341800	4.36189400	1.86852700
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C	-4.69174200	4.84214300	3.39841500
H	-5.01309800	2.86956600	4.20235100
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H	-6.64339000	6.32849500	1.05536800
H	-3.80439900	5.02319900	4.00358200
H	-4.61168500	6.76255100	2.42049500
H	-7.03619400	0.84811600	-0.75581700
O	-7.87422200	1.69018300	-0.91532500
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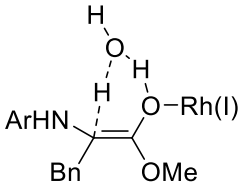
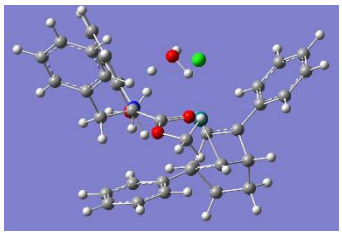
H	-7.45432000	2.43242900	-1.37629200

TS-7:





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O	-0.04732700	2.27754500	1.24103600
O	-0.84707300	3.46725900	2.97817300
C	0.35256000	4.21316100	2.90865100
H	1.23079700	3.57219000	3.05763600
H	0.45995500	4.72234900	1.94269800
Rh	0.38504600	0.24508800	0.33973600
C	3.56109900	-1.94111200	1.15135900
C	2.97298000	-0.63932200	0.57767700
C	1.07138200	-2.13725000	1.46928200
C	2.42828200	-2.82234900	1.71130500
H	4.10924100	-2.46002700	0.35224900
H	4.29288600	-1.69385300	1.93232100
H	2.42388300	-3.81104100	1.23244100

H	2.55326100	-2.99105600	2.79040700
C	1.94819500	-0.96246600	-0.50374000
C	0.89334800	-1.75867700	0.00925600
H	0.19469500	-2.29283600	-0.63606500
H	0.24150200	-2.76120700	1.81648000
H	3.76262600	0.02145300	0.20482100
C	1.05974100	-0.75375300	2.12010100
C	2.08434200	0.06188300	1.58224700
H	2.39000500	1.00756800	2.02923200
Cl	-0.88200100	0.57483800	-1.80626500
C	-4.39101100	-1.68309300	-0.57664900
C	-3.38911600	-1.21849000	0.25979500
C	-3.35696600	0.13472500	0.66392400
C	-4.37331700	0.97894900	0.21925400
C	-5.37703200	0.50953500	-0.62869800
C	-5.38936900	-0.81527900	-1.02790600
H	-4.40306000	-2.72209100	-0.89653900
H	-4.39524400	2.01586500	0.55394800
H	-6.15421300	1.19465600	-0.96248000
H	-6.16853700	-1.19116300	-1.68798300
N	-2.28593900	0.55528000	1.44891700
H	-1.91677400	-0.20018100	2.02447600
O	-2.36740900	-1.99035900	0.74790600
C	-2.27046900	-3.29652300	0.24674300
H	-1.37665200	-3.74343200	0.69595700
H	-3.14556300	-3.90673200	0.51948400
H	-2.16310100	-3.29371900	-0.84942000
C	0.29915500	-0.45024500	3.34695700
C	0.59361400	0.68368200	4.12029300
C	-0.77789800	-1.25220200	3.75600900
C	-0.16573000	1.01605900	5.23323600
H	1.43909300	1.31469500	3.85058900
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H	-1.05454100	-2.13209100	3.17622200
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H	0.08183000	1.91187600	5.80141200
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C	1.80932100	-1.69801900	-2.89002600
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C	2.08440000	-1.50881000	-4.23807500
H	1.24226300	-2.57238900	-2.57365800
C	3.26278900	0.52133900	-3.71238200

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H	1.72570700	-2.23303700	-4.96772900
H	3.82507300	1.39807700	-4.02992900
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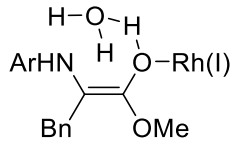

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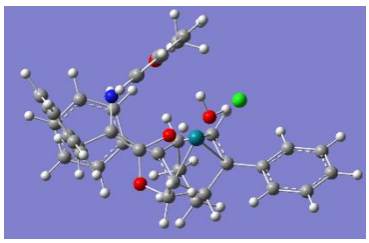

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C	0.83339500	3.12188100	-0.10508400
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Rh	1.11565200	-0.82646700	-0.70278800
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C	3.77303200	-0.71655500	-0.05451000
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H	5.47249100	-2.04194000	0.07672200
H	5.16410200	-1.12936800	1.55592300
H	4.24347200	-3.81723900	0.96230200
H	3.83555000	-2.85835600	2.38831300
C	3.09392000	-1.47565800	-1.19011200
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H	1.94642500	-3.34601700	-1.35956900
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C	-0.17898900	-2.19577300	2.52617500
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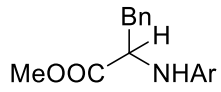
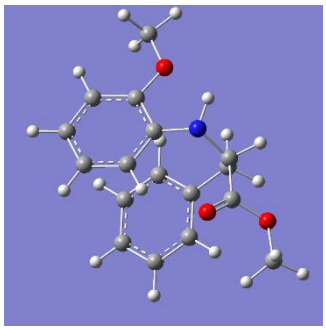
B5: 



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C	-10.18834100	1.15127100	0.31961300
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H	-12.17021600	1.98726300	0.48768900
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H	-8.47684900	-0.56357800	0.04520900
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H	-12.14321000	0.18093400	1.90435400
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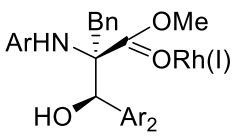
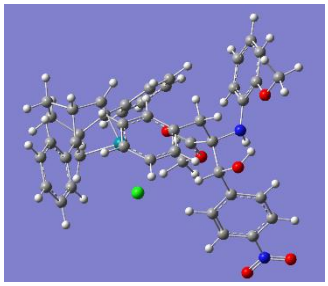
A11: 



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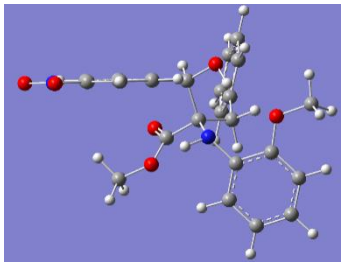

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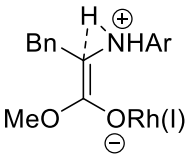
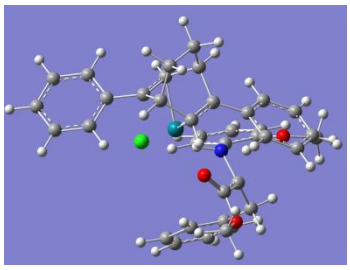
O	-3.06776700	-3.66923400	4.70850900
C	-2.60542300	-4.80099300	4.00771900
H	-3.42857200	-5.48840400	3.76527600
H	-2.16663300	-4.42612600	3.07992900
H	-1.83870300	-5.34237800	4.58070100
H	-5.07997500	-1.91518100	8.30417100
C	-6.60289400	-1.28635400	3.30438100
C	-6.09177100	-1.18839300	2.00701900
C	-7.95011900	-0.99203500	3.51488100
C	-6.90634200	-0.79081100	0.95221900
H	-5.04045800	-1.42318100	1.83278000
C	-8.76757100	-0.59912900	2.46263400
H	-8.35873300	-1.06679300	4.52270500
C	-8.24705700	-0.49621900	1.17665000
H	-6.49098600	-0.71710000	-0.05176200
H	-9.81651500	-0.37327200	2.64809500
H	-8.88617800	-0.19070700	0.34975400
H	-6.36033700	-2.22686000	5.21237400
H	-3.52781200	-0.78432300	6.71599100
H	-5.07495900	-2.56034100	4.05574200
H	-4.63884900	0.47323500	3.33779800
O	-3.13285600	-0.88197800	3.41419900
H	-2.89773400	-1.56042700	4.08029800

TS-8:





C	-2.21381500	0.86182100	-0.60175200
C	-1.21067200	1.13481300	-1.56150000
O	0.01162100	0.90113000	-1.50189500
O	-1.68923900	1.78618000	-2.64612200
C	-0.71683400	2.24377400	-3.56857900
H	-0.01371100	2.93487000	-3.08552500
H	-0.15076900	1.40934000	-3.99761900
Rh	1.62176000	0.09320800	-0.31953700
C	5.12441300	1.63806600	0.58254100
C	4.20462100	0.97580200	-0.45999300
C	2.91999100	1.29391100	1.75828200
C	4.34352900	1.86748200	1.89044200
H	5.99295700	0.98513600	0.74865300
H	5.50868000	2.58485500	0.17932600
H	4.84714800	1.38754700	2.74052200
H	4.27183600	2.93849100	2.12641900
C	3.67649100	-0.34722900	0.09573700
C	2.95518400	-0.15146000	1.29413500
H	2.68549100	-0.97412300	1.95660800
H	2.36072000	1.40814800	2.69295600
H	4.72218800	0.83300900	-1.41505900
C	2.20147000	1.94489300	0.57656800
C	2.91194800	1.74874800	-0.62802000
H	2.69297500	2.29775000	-1.54426800
Cl	0.62032000	-2.14615900	-0.33872100
C	-4.45997600	-0.63920100	2.98216200
C	-3.52443200	0.02827800	2.19769700
C	-2.64648200	-0.70370200	1.38417600
C	-2.67689300	-2.09307000	1.41132000
C	-3.59232600	-2.75929800	2.21975700
C	-4.48955800	-2.03265500	2.99083600
H	-5.15494900	-0.07820300	3.60273100
H	-1.98130000	-2.64044500	0.77581900
H	-3.61406500	-3.84669900	2.22415900
H	-5.22216700	-2.54511000	3.61178900
N	-1.70304900	-0.03275300	0.56006800
H	-1.70043100	1.19001100	0.57501200

H	-0.90710800	-0.62700500	0.27722700
O	-3.38383300	1.38175200	2.14993600
C	-4.42492100	2.16917800	2.66923100
H	-4.18252200	3.20676600	2.41862300
H	-5.39098600	1.90188900	2.21186400
H	-4.50638600	2.07226300	3.76236100
C	1.05990100	2.86294700	0.74024500
C	0.80397500	3.88323200	-0.18473100
C	0.15689300	2.69176900	1.79880700
C	-0.32138900	4.68976900	-0.06769400
H	1.50247900	4.05181500	-1.00375300
C	-0.96098300	3.50736600	1.92389600
H	0.30955000	1.88416500	2.51492000
C	-1.21020700	4.50648900	0.98729800
H	-0.49988000	5.47264600	-0.80353900
H	-1.64408700	3.34783700	2.75580000
H	-2.09022400	5.14117100	1.07982400
C	4.19371700	-1.64314200	-0.37680300
C	4.47278600	-2.67809100	0.52075500
C	4.41115200	-1.86473100	-1.74205600
C	4.95188900	-3.90088100	0.06788500
H	4.32064400	-2.51827100	1.58749200
C	4.88639900	-3.08686900	-2.19544000
H	4.16640000	-1.07951400	-2.45805600
C	5.16004300	-4.11002800	-1.29136200
H	5.16363000	-4.69463400	0.78250100
H	5.03616800	-3.24601100	-3.26214700
H	5.53315100	-5.06888100	-1.64748800
H	-1.27302200	2.76266100	-4.35315200
C	-3.66071100	0.72985700	-0.95891800
H	-3.83588700	1.39949800	-1.81194600
H	-4.30575100	1.10553900	-0.15084800
C	-4.07535200	-0.68336000	-1.30821200
C	-5.29579200	-1.18861400	-0.86050300
C	-3.23679800	-1.51756300	-2.04934000
C	-5.67732900	-2.49405700	-1.14987300
H	-5.93961800	-0.55216300	-0.24949400
C	-3.61172500	-2.82492700	-2.33833400
H	-2.26135500	-1.15437700	-2.37718800
C	-4.83455100	-3.31750800	-1.89061100
H	-6.63028900	-2.87450600	-0.78370300
H	-2.93827100	-3.46450700	-2.90681800
H	-5.12493900	-4.34381000	-2.11072000

Biological activity test:

PTP1B inhibitory assay

Recombinant human PTP1B catalytic domain was expressed and purified according to procedures described previously. In a typical 100 μL assay, mixture containing 50mM MOPS(3-[N-morpholino]propane-sulfonic acid), pH 6.5, 2mM pNPP and recombinant enzymes, PTP1B activities were continuously monitored on a VERSAmax microplate reader(Molecular Devices) at 405nm for 2min at 30 ℃ and the initial rate of the hydrolysis was determined using the early linear region of the enzymatic reaction kinetic curve. For the 50% inhibition concentration (IC_{50}) calculation, inhibition assays were performed with 30 nM recombinant enzyme, 2 mM pNPP in 50 mM MOPs at pH 6.5, and the inhibitors diluted around the estimated IC_{50} values. IC_{50} was calculated from the nonlinear curve fitting of percent inhibition (inhibition (%)) versus inhibitor concentration [I] using Graphpad Prisim 5.0 according to the formula: % Inhibition = $100/(1+[IC_{50}/[I]]k)$, where k is the Hill coefficient.

To study the inhibition selectivity on other PTP family members, human TCPTP, SHP1and LAR were prepared and assays were performed according to procedures described previously.