Supporting information for

Mechanistic implications of the enantioselective addition of alkylzinc reagents to aldehydes catalyzed by nickel complexes with α-amino amide ligands

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1. GENERAL REMARKS.

All reactions were carried out using standard Schlenk techniques unless specified other otherwise. All reagents were purchased from commercial suppliers and used without further purification. Dry hexane, CH_3CN and toluene were prepared by distillation from sodium and stored over sodium wire under N_2 atmosphere. Dry tetrahydrofuran (THF) was freshly distilled from sodium and benzophenone as a moisture indicator under N_2 atmosphere before use. All liquid aldehydes were freshly distilled under reduced pressure. Degassed dry solvents were used for all experiments. The NMR experiments were carried out on a Varian INOVA 500 spectrometer (500 MHz for ^{1}H and 125 MHz for ^{13}C). Chemical shifts (δ, ppm) are relative to the resonance of the deuterated solvent as the internal standard ($CDCl_3$, δ = 7.26 ppm for proton NMR, δ = 77.00 ppm for carbon NMR). The data are reported as (s=singlet, d=doublet, t=triplet, q=quartet, m=multiplet or unresolved, br s=broad singlet, coupling constant(s) in Hz, integration). Infrared spectra were recorded with a Perkin-Elmer 2000 spectrometer. Chiral HPLC was performed using Diacel chiralcel OD column. Optical rotations were measured using a JASCO P-1020 polarimeter. Mass spectra (ESI) were recorded with a Micromass Quattro LC spectrometer equipped with an electrospray ionization source and a triple-quadrupole analyzer. Melting points were measured with a STUART SMP10 melting point apparatus.

2. SYNTHESIS AND CHARACTERIZATION OF α-AMINO AMIDE LIGANDS.

2.1. General procedure for the preparation of H-hydroxysuccinimide ester of N-Cbz-*L*-amino amides. The N-Cbz-*L*-amino acid (1 mmol) and N-hidroxysuccinimide (1 mmol) were dissolved in dry THF at 0°C. Once a clear solution had been obtained, DCC (1 mmol) in anhydrous THF was added in several aliquots and the resulting solution was stirred at 0-5 °C for 3 h. The dicyclohexylurea formed was filtered off and the filtrate was concentrated to dryness. The crude product was recrystallized from 2-propanol to furnish the pure product.

2.2. General procedure for the preparation of N-Cbz-*L*-amino amides. The N-hydroxysuccinimide ester of N-Cbz-*L*-amino acid (1 mmol) was dissolved in anhydrous THF (40 mL) and N-benzylamine (1 mmol) was added dropwise with stirring. The reaction mixture was stirred at 50-60 ºC for 8 h. The white solid formed was filtered and washed with cold basic water (3×10 mL) and then with cold water. The solid was dried under reduced pressure (60-70 ºC) for 24 h.

2.3. General procedure for the deprotection of N-Cbz-*L*-amino amides. The N-Cbz-amino amide was treated with a solution of HBr/AcOH (33%) and the mixture was stirred at rt until CO_2 evolution ceased. At this point, dry diethyl ether was added to the clear solution, which led to the deposition of a precipitate. This was filtered and washed with additional ether and dissolved in distilled water; the resulting solution was extracted with chloroform (3×10 mL). Solid NaOH was then added up to a pH value of 12 and the resulting solution was saturated with NaCl and extracted with chloroform (3×10 mL). The organic phase was dried over anhydrous $MgSO_4$ and evaporated under vacuum to obtain a white solid.

2.3.1. (*S*)-2-amino-N-benzyl-3-phenylpropanamide (7a). Yield = 63%; Mp = 179.1-180.4 ºC; $[\alpha]_D^{20}$ = +21.1º (c = 0.1, MeOH); ESI-MS m/z = 255.3 ($M + H^+$), 277.3 ($M + Na^+$); IR (KBr) ν_{max}: 3320, 2895, 1953, 1667, 1542, 1257 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ_H: 2.74-2.82 (dd, 1H, *J* = 8.7, 13.7 Hz, C<u>H</u>$_2$Ph), 3.26-3.32 (dd, 1H, *J* = 7.0, 12.6 Hz, C<u>H</u>$_2$Ph) 3.66-3.70 (m, 2H,

NHC<u>H</u>$_2$Ph, CH*), 4.43-4.45 (d, 1H, *J* = 6.5 Hz, NHC<u>H</u>$_2$Ph), 6.85-6.88 (m, 2H, Ar-H), 6.87-6.98 (m, 2H, Ar-H), 7.11-7.14 (m, 6H, Ar-H), 7.57 (s, 1H, NH); ^{13}C NMR (125 MHz, $CDCl_3$) δ_C: 41.0, 43.2, 56.5, 126.8, 127.0, 127.4, 127.8, 128.7, 129.4, 137.8, 138.4, 174.0; Anal. Calcd for $C_{16}H_{18}N_2O$: C, 75.56; H, 7.13; N, 11.01. Found: C, 75.49; H, 7.27; N, 11.22.

2.3.2. (*S*)-2-amino-N-benzyl-3-methylbutanamide (7b). Yield = 87%; Mp = 115.1-116.0 ºC; $[\alpha]_D^{20}$ = +37.4º (c = 0.1, MeOH); ESI-MS m/z = 207.1 (M + H$^+$); IR (KBr) ν_{max}: 3320, 2895, 1953, 1667, 1542, 1257 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ_H: 1.01-1.04 (d, 6H, *J* = 6.9 Hz, CH_3), 2.18 (m, 1H, C<u>H</u>$(CH_3)_2$), 3.68 (d, 1H, *J* = 5.7 Hz, CH*), 4.36-4.50 (dd, 2H, *J* = 14.7, 27.0 Hz, NHC<u>H</u>$_2$Ph), 7.26-7.34 (m, 10H, Ar-H); ^{13}C NMR (125 MHz, $CDCl_3$) δ_C: 16.8 (CH_3), 17.7, 30.4, 43.2, 58.7, 127.4, 128.3, 128.5, 138.2, 168.3; Anal. Calcd for $C_{12}H_{18}N_2O$: C, 69.87; H, 8.80; N, 13.58. Found: C, 70.01; H, 8.89; N, 13.42.

2.3.3. (*S*)-2-amino-N-benzyl-4-methylpentanamide (7c). Yield = 83%; Mp = 189.1-190.4 ºC; $[\alpha]_D^{20}$ = +27.9º (*c* = 0.1, MeOH); ESI-MS m/z = 221.3 (M + H$^+$); IR (KBr) ν_{max}: 3310, 2955, 1979, 1655, 1522, 1252 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ_H: 0.90-0.95 (d, 6H, *J* = 6.6 Hz, CH_3), 1.34-1.58 (m, 2H, C<u>H</u>$_2$CH$(CH_3)_2$), 1.61-1.72 (m, 1H, C<u>H</u>$(CH_3)_2$), 3.33-3.36 (d, 1H, *J* = 7.3 Hz, CH*), 4.37 (d, 2H, *J* = 7.2 Hz, NHC<u>H</u>$_2$Ph), 7.27-7.31 (m, 5H, Ar-H); ^{13}C NMR (125 MHz, $CDCl_3$) δ_C: 22.8, 23.5, 26.1, 44.2, 45.9, 54.8, 128.5, 128.8, 129.7, 140.1, 178.1; Anal. Calcd for $C_{13}H_{20}N_2O$: C, 70.87; H, 9.15; N, 12.72. Found: C, 71.04; H, 9.22; N, 12.82.

2.3.5. (2*S*,3*S*)-2-amino-N-benzyl-3-methylpentanamide (7d). Yield = 88%; Mp = 164.1-166.0 ºC; $[\alpha]_D^{20}$ = +7.2º (c = 0.1, MeOH); ESI-MS m/z = 221.1 (M + H$^+$); IR (KBr) ν_{max}: 3290, 2935, 1953, 1684, 1532, 1257 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ_H: 0.92-1.01 (m, 6H, CH_3) 1.58-1.61 (m, 2H, CH_2), 1.87-1.96 (m, 1H, CH), 3.73 (d, 1H, *J* = 5.4 Hz, CH*), 4.34-4.50 (dd, 2H, *J* = 14.4 Hz, NHC<u>H</u>$_2$Ph), 7.28-7.33 (m, 5H, Ar-H); ^{13}C NMR (125 MHz, $CDCl_3$) δ_C: 10.5, 14.0, 24.3, 36.9, 43.1, 57.9, 127.4, 128.3, 128.5, 138.5, 168.1; Anal. Calcd for $C_{13}H_{20}N_2O$: C, 70.87; H, 9.15; N, 12.72. Found: C, 70.98; H, 9.19; N, 12.78.

2.3.4. (*S*)-2-amino-N-benzylpropanamide (7e). Yield = 92%; Mp = 179.0-180.5 ºC; $[\alpha]_D^{20}$ = +2.1º (c = 0.1, MeOH); ESI-MS m/z = 179.3 (M + H$^+$); IR (KBr) ν_{max}: 3294, 2937, 1955, 1682,

1534, 1260 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ_H: 1.31-1.34 (d, 3H, J = 7.2 Hz, CH_3), 3.86-3.92 (dd, 1H, J = 6.9 Hz, CH*), 4.15-4.30 (dd, 2H, J = 15.3 Hz, NHC$\underline{H_2}$Ph), 7.11-7.21 (m, 5H, Ar-H); ^{13}C NMR (125 MHz, $CDCl_3$) δ_C: 19.1, 45.7, 51.7, 129.9, 130.3, 131.5, 138.3, 172.7; Anal. Calcd for $C_{10}H_{14}N_2O$: C, 67.39; H, 7.92; N, 15.72. Found: C, 67.31; H, 7.97; N, 17.87.

2.3.7. (*S*)-2-amino-N-benzyl-3-(1H-indol-3-yl)propanamide (7f). Yield = 89%; Mp = 189.1-190.9 ºC; $[\alpha]_D^{20}$ = +10.8º (c = 0.1, MeOH); ESI-MS m/z = 294.7 ($M + H^+$); IR (KBr) ν_{max}: 3325, 2897, 1963, 1667, 1540, 1258 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ_H: 3.14-3.38 (ddd, 2H, J = 6.8, 11.8 Hz, C$\underline{H_2}$Ind), 4.20-4.34 (dd, 2H, J = 8.9 Hz, NHC$\underline{H_2}$Ph), 4.51 (m, 1H, CH*), 6.85-6.90 (m, 3H, Ar-H), 7-10-7.40 (m, 5H, Ar-H), 7.70 (br, 1H, Ar-H), 8.01 (br, 1H, Ar-H); ^{13}C NMR (125 MHz, $CDCl_3$) δ_C: 43.7, 55.2, 107.2, .112.1, 118.5, 120.5, 125.0, 127.1, 127.3, 127.5, 128.5, 128.8, 131.3, 135.2, 136.6, 169.7; Anal. Calcd for $C_{18}H_{19}N_3O$: C, 73.69; H, 6.53; N, 14.32. Found: C, 73.89; H, 6.64; N, 14.21.

2.3.6. (*S*)-2-amino-N-benzyl-3,3-dimethylbutanamide (7g). Yield = 89%; Mp = 125.1-126.7 ºC; $[\alpha]_D^{20}$ = +13.6º (c = 0.1, MeOH); ESI-MS m/z = 221.3 ($M + H^+$); IR (KBr) ν_{max}: 3312, 2895, 1962, 1669, 1544, 1255 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ_H: 0.95 (s, 3H, $-(CH_3)_3$), 3.27 (s, 1H, CH*), 4.53 (m, 1H, NHC$\underline{H_2}$Ph), 7-23-7.28 (m, 2H, Ar-H), 7.32-7.35 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ_C: 25.6, 39.4, 43.7, 60.9, 126.6, 127.0, 128.6, 136.4, 170.0; Anal. Calcd for $C_{12}H_{16}N_2O$: C, 70.87; H, 9.15; N, 12.72. Found: C, 70.99; H, 9.04; N, 12.61.

2.3.8. (*S*)-2-amino-N-benzyl-2-phenylacetamide (7h). Yield = 84%; Mp = 173-175 ºC; $[\alpha]_D^{20}$ = +34.8º (c = 0.1, MeOH); ESI-MS m/z = 240.3 ($M + H^+$); IR (KBr) ν_{max}: 3332, 2893, 1962, 1669, 1545, 1258 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ_H: 4.20 (d, 2H, J = 8.9 Hz, NHC$\underline{H_2}$Ph), 4.81 (s, 1H, CH*), 6.88-6.94 (m, 4H, Ar-H), 7-13-7.35 (m, 6H, Ar-H); ^{13}C NMR (125 MHz, $CDCl_3$) δ_C: 43.7, 55.2, 126.6, 127.0, 127.8, 128.5, 128.6, 130.3, 133.2, 136.3, 169.7; Anal. Calcd for $C_{18}H_{19}N_3O$: C, 80.20; H, 7.02; N, 8.13. Found: C, 80.29; H, 7.18; N, 8.08

3. CONDITIONS FOR THE ANALYSIS OF CHIRAL SECONDARY ALCOHOLS.

Chiral Capillary GC column VF-5 ms; 30 m × 0.25 mm, 0.25 μm. Carrier Gas: H_2 (5 mL·min^{-1}). Inyector 230 ºC, Detector (FID) 300 ºC, oven 60-130 ºC, 10 ºC min^{-1}. Chiral HPLC: Chiralcel OD columm; 254 nm UV detector. The racemic alcohols products were obtained by addition of Et_2Zn and Me_2Zn to aldehydes.

1-Phenylpropanol: IR (KBr) ν_{max} = 3354, 2927, 2876, 1493, 1450, 760, 742, 698 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 0.93 (t, 3H, *J* = 6.9 Hz), 1.73-1.83 (m, 2H), 2.90 (s, 1H), 4.57-4.63 (t, 1H, *J* = 6.9 Hz), 7.19-7.51 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 10.2 (CH_3), 31.9 (CH_2), 75.8 (CH), 126.1 (CH Ar), 127.6 (CH Ar), 128.5 (CH Ar), 144.6 (C). Retention times: t_r = 11.4 min for (*S*)-isomer and t_r = 9.5 min for (*R*)-isomer

1-(1-Naphtyl)-1-propanol: IR (KBr) ν_{max} = 3384, 2963, 2876, 1612, 1455, 1088, 782, 702 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 0.90-0.94 (t, 3H, J = 7.4 Hz), 1.75-1.97 (m, 2H), 2.52 (bs, 1H), 5.25 (t, 1H, *J* = 6.1 Hz), 7.34-7.44 (m, 3H), 7.53 (d, 1H, *J* = 7.0 Hz), 7.69 (d, 1H, *J* = 8.2 Hz), 7.77-7.82 (m, 1H), 7.99-8.04 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 11.1 (CH_3), 31.7 (CH_2), 73.1 (CH), 123.5 (CH Ar), 123.9 (CH Ar), 126.0 (CH Ar), 126.2 (CH Ar), 126.6 (CH Ar), 128.4 (CH Ar), 129.5 (CH Ar), 131.1 (C), 134.5 (C), 140.9 (C). Retention times: t_r = 27.5 min for (*S*)-isomer and t_r = 16.5 min for (*R*)-isomer

1-(2-Naphtyl)-1-propanol: IR (KBr) ν_{max} = 3388, 2955, 2878, 1612, 1456, 1091, 775, 712 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 0.90-0.94 (t, 3H, J = 7.4 Hz), 1.75-1.97 (m, 2H), 2.70 (bs, 1H), 5.25 (t, 1H, *J* = 6.1 Hz), 7.34-7.44 (m, 3H), 7.53 (d, 1H, *J* = 7.0 Hz), 7.69 (d, 1H, *J* = 8.2 Hz), 7.77-7.82 (m, 1H), 7.99-8.04 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 11.4 (CH_3), 31.76 (CH_2), 73.7 (CH), 123.5 (C), 124.9 (CH Ar), 126.0 (CH Ar), 126.2 (CH Ar), 127.1 (CH Ar), 128.4 (CH Ar), 128.9 (CH Ar), 129.5 (C), 131.1 (C), 133.4 (CH Ar). Retention times: t_r = 14.6 min for (*S*)-isomer and t_r = 16.8 min for (*R*)-isomer

1-(*p*-Methoxyphenyl)propanol: IR (KBr) ν_{max} = 3389, 2963, 2931, 1612, 1512, 1248, 1032, 833 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ = 0.89 (t, 3H, J = 7.4 Hz), 1.66-1.89 (m, 2H), 2.16 (s, 1H), 3.80 (s, 3H), 4.52-4.55 (t, 1H, *J* = 6.7 Hz), 6.87-6.90 (d, 2H, *J* = 8.5 Hz), 7.25-7.29 (d, 2H, *J* = 8.5 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 10.1 (CH_3), 31.2 (CH_2), 55.3 (CH_3), 75.3 (CH), 117.1 (CH Ar), 136.7 (CH Ar), 144.1 (CH Ar), 157.6 (C). Retention times: t_r = 20.8 min for (*S*)-isomer and t_r = 18.3 min for (*R*)-isomer

1-(*p*-Chloroxyphenyl)propanol: IR (KBr) ν_{max} = 3348, 2963, 2928, 1593, 1491, 1090, 1012, 822 cm-1; ^1H NMR (300 MHz, $CDCl_3$) δ = 0.84 (t, 3H, *J* = 7.4 Hz), 1.55-1.81 (m, 2H), 2.90 (bs, 1H), 4.47 (t, 1H, *J* = 6.6 Hz), 7.17-7.28 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 10.0 (CH_3), 31.9 (CH_2), 75.2 (CH), 127.3 (CH Ar), 128.4 (CH Ar), 133.0 (C), 143.1 (C). Retention times: t_r = 27.2 min for (*S*)-isomer and t_r = 28.9 min for (*R*)-isomer

1-(*o*-Tolyl)propanol: IR (KBr) ν_{max} = 3367, 2963, 2931, 2873. 1458, 970, 751, 729 cm-1; ^1H NMR (300 MHz, $CDCl_3$) δ = 0.96-1.01 (t, 3H, *J* = 7.4 Hz), 1.72-1.94 (m, 2H), 2.04 (bs, 1H), 2.34 (s, 3H), 4.85-4.89 (m, 1H), 7.14-7.23 (m, 3H), 7.45-7.48 (d, 1H, *J* = 7.1 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 10.2 (CH_3), 19.1 (CH_3), 30.7 (CH_2), 71.9 (CH), 125.1 (CH Ar), 126.1 (CH Ar), 127.0 (CH Ar), 130.2 (CH Ar), 134.5 (C), 142.6 (C). Retention times: t_r = 18.9 min for (*S*)-isomer and t_r = 15.6 min for (*R*)-isomer

1-(*m*-Tolyl)propanol: IR (KBr) ν_{max} = 3358, 2963, 2929, 2873. 1612, 1455, 785, 702 cm-1; ^1H NMR (300 MHz, $CDCl_3$) δ = 0.90-0.94 (t, 3H, *J* = 7.4 Hz), 1.71-1.85 (m, 2H), 2.36 (s, 3H), 4.54-4.59 (m, 1H), 7.08-7.24 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 10.1 (CH3), 21.4 (CH_3), 31.6 (CH_2), 76.0 (C), 123.0 (CH Ar), 126.6 (CH Ar), 128.2 (CH Ar), 138.0 (C), 144.5 (C). Retention times: t_r = 11.5 min for (*S*)-isomer and t_r = 7.9 min for (*R*)-isomer

1-(*p*-Tolyl)propanol: IR (KBr) ν_{max} = 3362, 2963, 2927, 2873. 1509, 1455, 815, 539 cm-1; ^1H NMR (300 MHz, $CDCl_3$) δ = 0.88-0.93 (t, 3H, *J* = 7.4 Hz), 1.71-1.85 (m, 2H), 2.55 (s, 3H), 4.54-4.59 (m, 1H), 7.14-7.17 (d, 2H, *J* = 7.9 Hz), 7.21-7.25 (d, 2H, *J* = 8.1 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 10.1 (CH3), 21.3 (CH_3), 31.7 (CH_2), 75.8 (CH), 125.9 (CH Ar), 129.1 (CH

Ar), 137.0 (C), 141.5 (C). Retention times: t_r = 12.7 min for (*S*)-isomer and t_r = 8.9 min for (*R*)-isomer.

1-Cyclohexyl-1-propanol: IR (KBr) ν_{max} = 3369, 2973, 2930, 2867. 1503, 1456, 817, 542 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 0.91-0.96 (t, 3H, *J* = 7.4 Hz), 1.27-1.85 (m, 13H), 3.20-3.33 (m, 1H), 3.57 (1H, s); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 10.1 (CH_3), 26.2 (CH_2), 26.4 (CH_2), 26.5 (CH_2), 26.8 (CH_2), 29.2 (CH_2), 44.3 (CH_2), 77.6 (CH). Retention times: t_r = 29.5 min for (*S*)-isomer and t_r = 34.9 min for (*R*)-isomer.

3-Octanol: IR (KBr) ν_{max} = 3375, 2974, 2863, 1510, 1455, 813, 540 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 0.85-0.92 (m, 6H), 1.25-1.49 (m, 10H), 3.21-3.25 (m, 1H), 3.72 (1H, s); 13C NMR (75 MHz, $CDCl_3$) δ = 10.1 (CH_3), 14.2 (CH_3), 22.2 (CH_2), 24.9 (CH_2), 30.5 (CH_2), 32.8 (CH_2), 37.3 (CH_2), 74.6 (CH). Retention times: t_r = 29.5 min for (*S*)-isomer and t_r = 34.9 min for (*R*)-isomer.

1-Phenylethanol: IR (KBr) ν_{max} = 3356, 2929, 2876, 1492, 1450, 760, 742, 698 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 1.24-1.27 (d, 3H, *J* = 7.3 Hz), 2.63-2.64 (m, 1H), 2.90 (s, 1H), 7.19-7.51 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 22.7 (CH_3), 69.4. (CH), 125.7 (CH Ar), 127.2 (CH Ar), 128.5 (CH Ar), 144.1 (C). Retention times: t_r = 12.9 min for (*S*)-isomer and t_r = 11.2 min for (*R*)-isomer

1-(*p*-Methoxyphenyl)etanol: IR (KBr) ν_{max} = 3389, 2963, 2931, 1612, 1512, 1248, 1032, 833 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 1.47-1.49 (d, 3H, *J* = 7.6 Hz), 2.16 (s, 1H), 3.82 (s, 3H), 4.63-4.65 (m, 1H), 6.91-6.94 (d, 2H, *J* = 8.5 Hz), 7.25-7.29 (d, 2H, J = 8.5 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 22.7 (CH_3), 55.3 (CH_3), 69.4 (CH), 113.5 (CH Ar), 127.1 (CH Ar), 138.7 (C), 159.2 (C). Retention times: t_r = 36.9 min for (*S*)-isomer and t_r = 34.1 min for (*R*)-isomer

.**1-(*p*-Tolyl)ethanol:** IR (KBr) ν_{max} = 3362, 2963, 2927, 2873. 1509, 1455, 815, 539 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 1.42-1.44 (d, 3H, J = 7.4 Hz), 2.36 (s, 3H), 3.63 (bs, 1H), 4.54-4.59 (m, 1H), 7.14-7.17 (d, 2H, *J* = 7.9 Hz), 7.21-7.25 (d, 2H, *J* = 8.1 Hz); ^{13}C NMR (75 MHz,

$CDCl_3$) δ = 21.3 (CH_3), 32.7 (CH_3), 68.8 (CH), 125.9 (CH Ar), 129.1 (CH Ar), 137.2 (C), 143.5 (C). Retention times: t_r = 43.0 min for (*S*)-isomer and t_r = 36.9 min for (*R*)-isomer

1-(*p*-Chloroxyphenyl)ethanol: IR (KBr) ν_{max} = 3348, 2963, 2928, 1593, 1491, 1090, 1012, 822 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 1.44-1.46 (d, 3H, *J* = 7.7 Hz), 2.90 (bs, 1H), 4.67 (m, 1H), 7.17-7.28 (d, 2H, *J* = 7.9 Hz), 7.46 (d, 2H, *J* = 8.4 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 22.9 (CH_3), 71.2 (CH), 127.3 (CH Ar), 128.5 (CH Ar), 133.2 (C), 144.3 (C). Retention times: t_r = 47.5 min for (*S*)-isomer and t_r = 44.3 min for (*R*)-isomer.

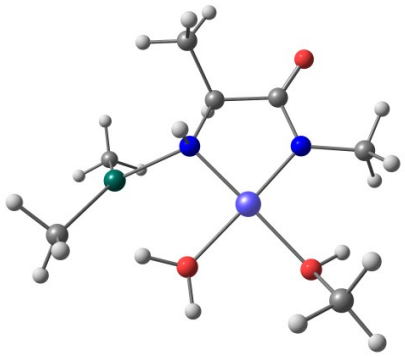
1-(2'-Tolyl)-1-ethanol: IR (KBr) ν_{max} = 3367, 2963, 2931, 2873. 1458, 970, 751, 729 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 1.42-1.54 (m, 2H), 2.36 (s, 3H), 4.85-4.89 (m, 1H), 5.56 (s, 1H), 7.14-7.23 (m, 3H), 7.45-7.48 (d, 1H, *J* = 7.3 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 19.1 (CH3), 23.7 (CH_3), 70.9 (CH), 125.2 (CH Ar), 126.1 (CH Ar), 127.1 (CH Ar), 130.2 (CH Ar), 134.5 (C), 144.6 (C). Retention times: t_r = 66.5 min for (*S*)-isomer and t_r = 62.8 min for (*R*)-isomer.

1-(2'-Naphtyl)-1-ethanol: IR (KBr) ν_{max} = 3388, 2955, 2878, 1612, 1456, 1091, 775, 712 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 1.55-1.58 (d, 3H, *J* = 7.2 Hz), 2.70 (bs, 1H), 4.56 (bs, 1H), 5.03 (t, 1H, *J* = 6.0 Hz), 7.37-7.44 (m, 3H), 7.55 (d, 1H, *J* = 7.0 Hz), 7.69 (d, 1H, *J* = 8.2 Hz), 7.77-7.84 (m, 1H), 7.98-8.01 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 22.4 (CH_3), 70.7 (CH), 123.5 (C), 124.9 (CH Ar), 126.0 (CH Ar), 126.2 (C), 127.1 (CH Ar), 127.5 (CH Ar), 128.4 (CH Ar), 128.9 (CH Ar), 129.5 (C), 131.1 (CH Ar), 133.7 (C). Retention times: t_r = 47.5 min for (*S*)-isomer and t_r = 44.3 min for (*R*)-isomer.

1-Cyclohexyl-1-ethanol: IR (KBr) ν_{max} = 3369, 2973, 2930, 2867. 1503, 1456, 817, 542 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 1.16-1.19 (d, 3H, *J* = 7.4 Hz), 1.44-1.58 (m, 10H), 3.36-3.39 (m, 1H), 3.57 (1H, s); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 23.1 (CH_3), 26.1 (CH_2), 26.1 (CH_2), 28.8 (CH_2), 29.6 (CH_2), 46.3 (CH_2), 73.6 (CH). Retention times: t_r = 16.5 min for (*S*)-isomer and t_r = 17.6 min for (*R*)-isomer.

2-Heptanol: IR (KBr) ν_{max} = 3375, 2974, 2863, 1510, 1455, 813, 540 cm-1; ^{1}H NMR (300 MHz, $CDCl_3$) δ = 0.88-0.91 (t, 3H, *J* = 8.6 Hz), 1.11-1.15 (d, 3H, *J* = 7.4 Hz), 1.26-1.41 (m, 8H), 3.57 (s, 1H), 4.01-4.05 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 14.2 (CH_3), 22.5 (CH_2), 23.5 (CH_3), 24.9 (CH_2), 32.2 (CH_2), 40.1 (CH_2), 68.5 (CH). Retention times: t_r = 21.2 min for (*S*)-isomer and t_r = 23.8 min for (*R*)-isomer.

4. CARTESIAN COORDENATES FOR OPTIMIZED STRUCTURES.



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H	4.753955000	1.384058000	2.587604000
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C	2.298294000	1.848013000	-0.173117000
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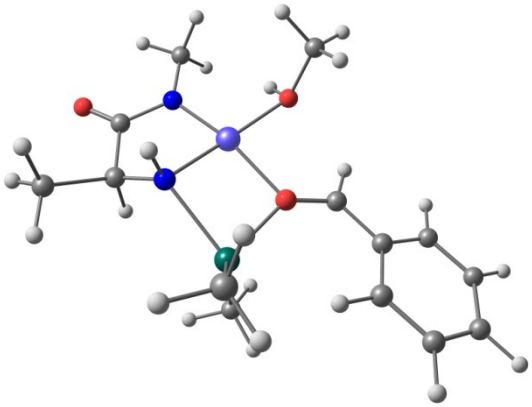

Reactive complex anti trans

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H	2.489948000	-1.141297000	-0.338600000
H	-1.695904000	0.304418000	-1.456819000
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H	-2.101640000	-4.118253000	-0.092403000
C	-1.802826000	2.736336000	2.226270000
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C	1.431873000	1.231432000	1.453549000
O	0.387921000	1.156443000	0.740383000
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H	-1.643304000	3.622410000	-1.938552000
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C	2.462073000	4.839379000	1.714759000
C	3.923311000	3.460830000	3.083742000
C	3.540076000	4.718122000	2.598415000
H	4.762655000	3.371662000	3.766932000
H	1.832226000	0.294337000	1.853453000
N	-1.878015000	0.377174000	-0.449823000
C	-2.935361000	-1.812571000	-0.132977000
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C	-4.232608000	0.064059000	-1.237282000
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H	1.616711000	-2.627194000	-0.801231000
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H	-0.903204000	-3.798126000	1.159974000
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C	2.123689000	2.442088000	1.805213000
C	3.223072000	2.330120000	2.688225000
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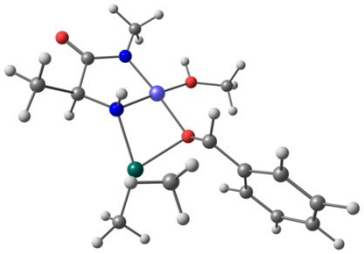

TS *anti trans*

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H	-3.389940000	-2.021713000	2.134919000
H	-2.952900000	-3.284511000	0.958555000
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H	1.173533000	2.819718000	-0.656559000
H	-1.395530000	-0.925294000	1.432900000
H	-3.225627000	3.125462000	0.834300000
H	-4.746111000	2.279502000	0.483889000
C	0.727753000	-2.930184000	-2.042233000
H	0.729511000	-3.973632000	-1.702737000
C	1.484124000	0.191388000	0.695133000
O	0.676866000	0.436702000	-0.316956000
H	2.438001000	-2.471937000	0.891443000
H	0.765073000	-2.861095000	1.411752000
C	3.457463000	0.467355000	-0.821535000
C	4.830431000	0.612717000	-1.015524000
C	5.191763000	0.457986000	1.371138000
C	5.701056000	0.606958000	0.077342000
H	5.864056000	0.458657000	2.224840000
H	1.136514000	0.452623000	1.696985000
N	-1.525108000	-0.922566000	0.417123000
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C	2.939795000	0.308427000	0.474606000
C	3.821295000	0.311493000	1.568962000
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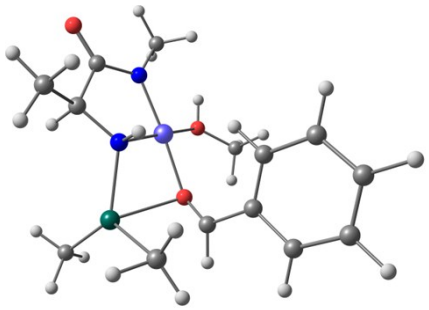

TS *anti cis*

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H	-2.397147000	2.142938000	-2.670945000	O	-0.551201000	-2.127787000	1.986943000
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H	-1.857634000	-3.685735000	-0.055528000	H	-3.083874000	-3.087347000	1.108851000
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C	4.039465000	0.272239000	-0.129890000	C	2.209808000	-1.157097000	-0.814087000
C	4.912431000	-0.454326000	-0.936806000	H	4.410841000	1.110939000	0.453657000
C	3.082788000	-1.881344000	-1.621964000	H	1.157152000	-1.426932000	-0.771040000
C	4.435785000	-1.532683000	-1.686001000	H	5.962656000	-0.180358000	-0.981307000
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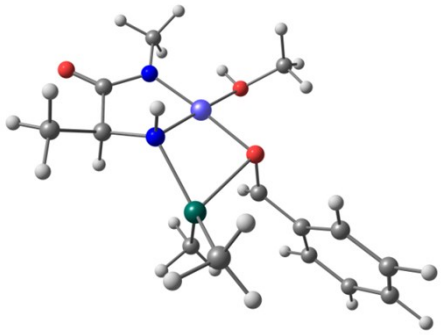

TS *syn trans*

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H	3.781261000	2.689810000	-0.857574000
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H	-0.796361000	-2.296252000	2.126073000
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H	-1.933592000	-0.998414000	2.417852000
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H	-1.063082000	1.110577000	1.438135000
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C	-5.100844000	0.848901000	1.252734000
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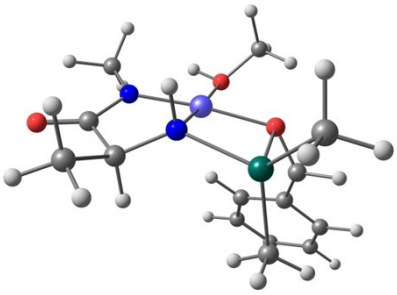

TS *syn cis*

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H	3.191911000	2.052583000	-2.052388000	O	-0.188760000	-2.262347000	1.626667000
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H	2.501095000	-3.327604000	1.329565000	Zn	0.419415000	2.367252000	0.209119000
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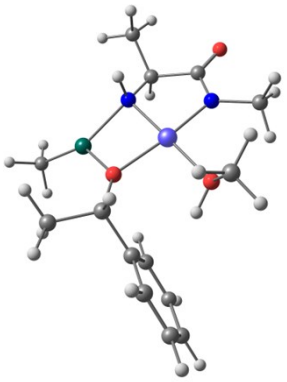
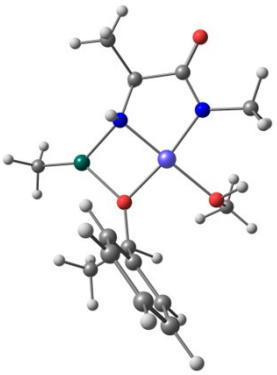
H	0.041175000	4.534101000	1.702128000	H	1.481972000	3.672562000	2.263893000
H	1.561625000	4.681236000	0.812335000	C	-2.621176889	0.067866673	-0.132963095
C	-2.218474889	-1.104214327	-0.794206095	C	-3.967890889	0.461541673	-0.207864095
C	-3.144870889	-1.864839327	-1.502471095	H	-1.176675889	-1.408691327	-0.767269095
C	-4.895779889	-0.303824327	-0.911560095	H	-4.286315889	1.372080673	0.294485905
C	-4.485380889	-1.469840327	-1.561002095	H	-2.820391889	-2.765081327	-2.017022095
H	-5.934782889	0.010232673	-0.955548095	H	-5.204459889	-2.066562327	-2.115462095
H	-2.182654889	1.794274673	1.101581905				



(*S*)- product forming **9**



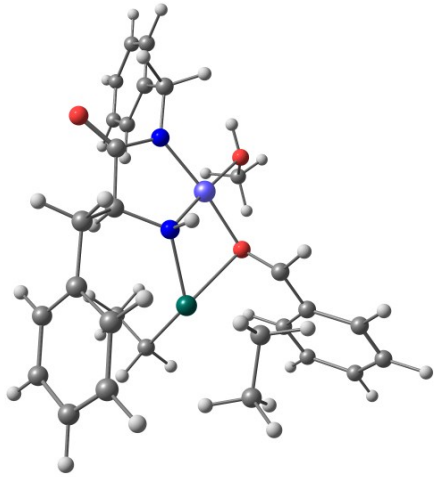
(*R*)- product forming **9**

(*S*)- product forming **9**

Ni	-0.972140000	0.529070000	-0.412376000
N	-2.137191000	-0.533841000	0.637835000
N	-2.162537000	1.930075000	-0.089838000
C	-3.342291000	1.607198000	0.501041000
O	-4.255399000	2.388211000	0.780365000
C	-3.469180000	0.094326000	0.755389000
H	-4.097961000	-0.300449000	-0.055463000
C	-4.153860000	-0.198163000	2.088433000
H	-3.525639000	0.129429000	2.927730000
H	-5.091581000	0.361738000	2.139565000
H	-4.361356000	-1.268065000	2.207113000
O	0.312709000	1.616302000	-1.484109000
C	1.349319000	2.348710000	-0.803830000
H	0.849874000	3.032563000	-0.118648000
H	2.008047000	1.677430000	-0.242124000
H	1.931140000	2.920340000	-1.533368000
H	-1.686333000	-0.462536000	1.555375000
C	-1.972883000	3.328103000	-0.455763000
H	-1.479552000	3.903900000	0.343364000
H	-1.364571000	3.398444000	-1.361622000
H	-2.944831000	3.796754000	-0.638244000
Zn	-1.626041000	-2.313217000	-0.275124000
C	-2.213535000	-4.193247000	-0.747744000
H	-1.634922000	-4.937747000	-0.187224000
H	-3.273016000	-4.348363000	-0.513885000
H	-2.071877000	-4.397170000	-1.815859000
C	1.311419000	-1.362957000	-1.102361000
H	0.721281000	1.013877000	-2.136717000
O	-0.027760000	-1.139510000	-0.736014000
C	1.614146000	-0.940781000	-2.544202000
C	2.906684000	-0.525748000	-2.904472000
C	0.625240000	-0.987744000	-3.538617000
C	3.206599000	-0.178002000	-4.222360000
H	3.684674000	-0.480262000	-2.144314000
C	0.922947000	-0.636315000	-4.858409000
H	-0.380267000	-1.293012000	-3.266134000
C	2.213790000	-0.233089000	-5.204436000
H	4.212591000	0.141216000	-4.481692000
H	0.143822000	-0.677776000	-5.614799000
H	2.444100000	0.042406000	-6.229810000
H	1.972929000	-0.772557000	-0.444019000
C	1.671513000	-2.843523000	-0.895877000
H	2.722152000	-3.034338000	-1.141314000
H	1.504158000	-3.126337000	0.149993000
H	1.050593000	-3.480254000	-1.536363000

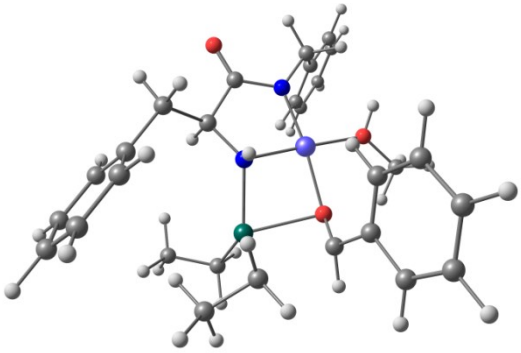
(*R*)- product forming **9**

Ni	-0.288001000	-0.657013000	0.520107000
N	-1.666067000	-0.136189000	-0.665494000
N	-1.261563000	-2.240663000	0.751461000
C	-2.541738000	-2.234628000	0.289180000
O	-3.358044000	-3.154483000	0.379522000
C	-2.903767000	-0.890093000	-0.371275000
H	-3.471346000	-0.318786000	0.377167000
C	-3.787342000	-1.091786000	-1.600898000
H	-3.233745000	-1.609492000	-2.395436000
H	-4.642549000	-1.717653000	-1.332355000
H	-4.146102000	-0.134134000	-1.995046000
O	1.139466000	-1.195137000	1.810710000
C	0.914380000	-0.786213000	3.177760000
H	1.756335000	-1.108360000	3.798365000
H	0.862127000	0.302190000	3.166405000
H	-0.024788000	-1.197039000	3.561012000
H	-1.307473000	-0.480578000	-1.561401000
C	-0.787304000	-3.467589000	1.371124000
H	0.169692000	-3.795558000	0.931985000
H	-0.656255000	-3.369022000	2.461696000
H	-1.517762000	-4.264569000	1.205090000
Zn	-1.280162000	1.897167000	-0.459434000
C	-2.102261000	3.742695000	-0.600862000
H	-2.242874000	4.031836000	-1.649432000
H	-3.084898000	3.772044000	-0.115077000
H	-1.467004000	4.498691000	-0.125377000
C	1.810863000	1.436540000	0.318967000
H	2.147782000	1.205901000	1.342152000
C	2.718233000	0.667282000	-0.637753000
C	4.017711000	0.318025000	-0.249697000
C	2.294185000	0.331880000	-1.929430000
C	4.875711000	-0.345743000	-1.128446000
H	4.360985000	0.567584000	0.752893000
C	3.147167000	-0.333714000	-2.811803000
H	1.285508000	0.589454000	-2.239207000
C	4.441818000	-0.674900000	-2.414437000
H	5.879894000	-0.610871000	-0.807252000
H	2.800223000	-0.586772000	-3.810557000
H	5.105399000	-1.195532000	-3.099688000
H	1.177888000	-2.165858000	1.780844000
O	0.453459000	1.074424000	0.180311000
C	1.958529000	2.952250000	0.113551000
H	2.998944000	3.267541000	0.249596000
H	1.650775000	3.231845000	-0.901264000
H	1.332761000	3.495740000	0.830801000



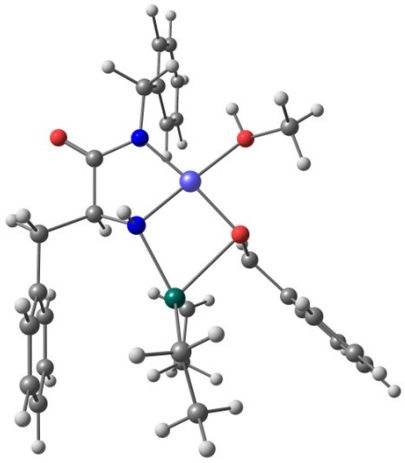
TS *anti trans* Phe

Ni	-1.033098000	-0.614352000	-0.731624000
N	-2.515366000	0.473784000	-1.063795000
O	-3.175113000	2.691197000	-1.042988000
H	-0.962422000	2.145057000	0.690197000
H	-1.077872000	4.250842000	-0.677236000
O	-2.024028000	-2.350714000	-0.783996000
H	-2.444005000	-4.183029000	0.110334000
H	-2.632870000	-2.757415000	1.187868000
C	-3.856490000	0.053605000	-1.471120000
H	-4.330201000	0.881668000	-2.009460000
C	2.122954000	0.680352000	2.321593000
H	2.726342000	-0.160677000	2.686696000
H	-2.932260000	-2.201911000	-1.090084000
C	3.120860000	-0.044388000	-1.314187000
H	2.855402000	0.884961000	-1.843929000
C	2.648956000	-3.164300000	0.939357000
C	3.601090000	-4.072611000	1.394074000
C	4.413898000	-4.366737000	-0.867342000
C	4.485996000	-4.674721000	0.493699000
H	5.095440000	-4.837479000	-1.570244000
H	1.458261000	-1.815747000	-2.010330000
C	2.127046000	3.694969000	-1.187816000
C	3.392669000	3.945285000	-0.648959000
C	2.392419000	4.372452000	1.513189000
C	3.525501000	4.282353000	0.700493000
H	2.496440000	4.632112000	2.558688000
C	-4.754886000	-0.331187000	-0.324138000
C	-6.071012000	-0.736137000	-0.603570000
H	-3.309824000	-0.010156000	1.272706000
H	-6.428720000	-0.763216000	-1.625673000
H	-4.840452000	-0.669163000	3.073583000
H	-7.157720000	-1.376808000	2.555860000
H	1.089716000	0.844849000	4.209871000
H	0.245932000	-0.155289000	2.955633000
H	4.197128000	0.993125000	0.239509000
H	5.214097000	0.469059000	-1.159099000
N	-0.025199000	0.972873000	-0.757030000
C	-2.324566000	1.813359000	-0.888153000
C	-0.898012000	2.113014000	-0.406597000
C	-0.371155000	3.455325000	-0.934396000
H	-0.335275000	3.420664000	-2.032423000
C	-2.040376000	-3.202973000	0.382109000
H	-1.002645000	-3.299575000	0.695339000
H	0.217169000	1.074053000	-1.747923000
H	-3.786190000	-0.790085000	-2.177518000
Zn	1.671622000	0.420323000	0.345266000
H	2.706184000	1.594996000	2.486301000
C	1.557928000	-1.901284000	-0.926430000
O	0.538058000	-1.628663000	-0.188822000
H	3.349235000	-0.778784000	-2.086390000
C	2.579133000	-2.841037000	-0.426260000
C	3.466334000	-3.453913000	-1.325224000
H	1.959349000	-2.691498000	1.630956000
H	3.409847000	-3.214304000	-2.384309000
H	3.655314000	-4.312722000	2.452306000
H	5.227558000	-5.383506000	0.851848000
C	0.983066000	3.771906000	-0.374786000
C	1.125419000	4.117180000	0.980108000
H	2.042419000	3.424094000	-2.232875000
H	0.256593000	4.181800000	1.623354000
H	4.271273000	3.872407000	-1.276762000
H	4.506270000	4.472904000	1.116483000
C	-4.317575000	-0.309088000	1.016028000
C	-5.183505000	-0.685770000	2.047135000
C	-6.932968000	-1.110505000	0.431599000
C	-6.489590000	-1.085540000	1.755728000
H	-7.945017000	-1.421301000	0.206542000
C	0.850957000	0.759077000	3.128761000
H	0.264321000	1.646091000	2.812988000
C	4.372008000	0.180497000	-0.495254000
H	4.635298000	-0.750110000	0.049064000



TS *anti cis* Phe

i	1.031629000	0.579923000	-0.068739000
N	1.977726000	-0.518677000	-1.238059000
O	1.842843000	-2.544034000	-2.347044000
H	0.011729000	-2.524761000	-0.254108000
H	-1.078724000	-1.535987000	-2.949752000
O	2.602205000	1.725619000	0.386124000
H	2.679271000	3.723190000	1.004523000
H	3.729397000	2.579779000	1.910760000
C	3.366354000	-0.346167000	-1.663749000
H	3.525838000	-0.952292000	-2.561475000
C	-1.443185000	-1.401407000	3.132683000
H	-0.452101000	-1.426758000	3.603527000
H	3.305430000	1.784072000	-0.276216000
C	-3.101330000	1.222908000	0.658725000
H	-3.065377000	1.087359000	-0.427029000
C	-2.035500000	4.455232000	0.440181000
C	-2.195400000	5.478374000	-0.491571000
C	-0.754246000	4.294724000	-2.028357000
C	-1.555244000	5.400524000	-1.731058000
H	-0.256152000	4.226771000	-2.991851000
H	-1.516121000	2.559556000	2.159362000
C	4.006856000	-1.219942000	0.649931000
C	4.984269000	-1.579125000	1.583051000
C	6.718289000	-1.021751000	-0.008724000
C	6.338140000	-1.480752000	1.254335000
H	7.767710000	-0.944841000	-0.262281000
C	-2.418480000	-2.527993000	-1.597171000
C	-2.647397000	-3.596346000	-0.713521000
H	-3.342943000	-0.876345000	-2.653579000
H	-1.833051000	-4.244361000	-0.414220000
H	-5.602122000	-1.313330000	-1.766471000
H	-5.987760000	-3.197926000	-0.203359000
H	-1.171826000	-3.254891000	2.075504000
H	-2.894057000	-2.809233000	2.394507000
H	-3.644541000	-0.834458000	1.028297000
H	-5.040340000	0.302204000	0.911979000
N	-0.465327000	-0.495947000	-0.450531000
C	1.354933000	-1.663091000	-1.636698000
C	-0.064575000	-1.781423000	-1.060518000
C	-1.043244000	-2.276848000	-2.137964000
H	-0.644631000	-3.195870000	-2.579185000
C	2.760803000	2.711821000	1.417359000
H	1.952376000	2.538555000	2.124331000
H	-0.973732000	0.042312000	-1.156527000
H	3.543514000	0.704715000	-1.948299000
Zn	-1.351547000	-0.297697000	1.422233000
H	-2.145590000	-0.970161000	3.856549000
C	-1.079040000	2.293933000	1.193849000
O	-0.024404000	1.524718000	1.275199000
H	-3.526212000	2.203956000	0.872524000
C	-1.233015000	3.337589000	0.152873000
C	-0.593404000	3.271600000	-1.095320000
H	-2.531767000	4.520426000	1.405879000
H	0.029395000	2.413921000	-1.337430000
H	-2.816583000	6.336610000	-0.250735000
H	-1.679759000	6.195977000	-2.460594000
C	4.379901000	-0.755880000	-0.628233000
C	5.745371000	-0.660289000	-0.945431000
H	2.966371000	-1.302260000	0.935434000
H	6.056026000	-0.303818000	-1.920024000
H	4.691228000	-1.933178000	2.563024000
H	7.092595000	-1.759348000	1.978648000
C	-3.495426000	-1.707637000	-1.976534000
C	-4.777905000	-1.951601000	-1.475639000
C	-3.931173000	-3.835255000	-0.213641000
C	-4.995351000	-3.013346000	-0.593614000
H	-4.100432000	-4.657123000	0.469900000
C	-1.868941000	-2.814305000	2.818091000
H	-1.859507000	-3.430212000	3.742045000
C	-4.002535000	0.181739000	1.288118000
H	-3.995875000	0.301048000	2.391229000



TS *syn trans* Phe

Ni	1.167856000	0.428118000	-0.940960000
N	2.602088000	-0.769672000	-0.858507000
O	3.089225000	-2.941259000	-0.229816000
H	0.703768000	-1.872314000	0.987811000
H	0.328654000	-3.789955000	-1.383845000
O	2.279185000	2.089872000	-1.104048000
H	2.229038000	2.597778000	-3.143420000
H	2.545051000	3.950036000	-2.002232000
C	4.010868000	-0.522008000	-1.171184000
H	4.461502000	-1.460701000	-1.512627000
C	-1.630449000	0.260836000	1.766089000
H	-1.009795000	-0.624282000	1.975657000
O	-0.413710000	1.566436000	-0.849728000
H	-0.013988000	2.031046000	1.103607000
C	-2.070720000	3.660775000	1.633811000
C	-3.104595000	4.586154000	1.751826000
C	-3.783935000	4.113602000	-0.523142000
C	-3.966710000	4.810971000	0.674695000
H	-4.450269000	4.290517000	-1.362814000
C	-3.420047000	-0.440164000	-1.714009000
H	-3.460788000	-1.438812000	-2.167725000
C	-2.216027000	-3.802952000	-0.773219000
C	-3.539127000	-3.898158000	-0.330687000
C	-2.785127000	-3.774751000	1.965645000
C	-3.823616000	-3.882826000	1.037104000
H	-3.006621000	-3.760510000	3.024901000
C	4.821586000	-0.014225000	-0.006192000
C	6.202546000	0.180487000	-0.177972000
H	3.178181000	0.163400000	1.410997000
H	6.670753000	-0.038623000	-1.129902000
H	4.577465000	0.994887000	3.247898000
H	7.012220000	1.319313000	2.923763000
H	-5.554098000	-0.138475000	-1.807321000
H	-4.698026000	0.836159000	-0.544855000
H	-3.698618000	0.853790000	1.885359000
H	-3.154077000	-0.259527000	3.206746000
N	0.070431000	-1.095039000	-0.839552000
C	2.292050000	-2.017903000	-0.402938000
C	0.793576000	-2.133559000	-0.076578000
C	0.251840000	-3.550336000	-0.314165000
H	0.888455000	-4.272550000	0.207474000
C	1.983607000	3.025105000	-2.165165000
H	0.914471000	3.219838000	-2.105548000
H	0.046720000	-1.417756000	-1.812952000
H	4.085110000	0.196313000	-2.002944000
Zn	-1.835297000	-0.290632000	-0.415913000
H	-1.277694000	1.042930000	2.437892000
H	3.215996000	1.843666000	-1.150939000
C	-0.770661000	1.990447000	0.317920000
C	-1.888127000	2.948738000	0.437295000
C	-2.748302000	3.190476000	-0.646336000
H	-1.400942000	3.484531000	2.472031000
H	-2.599407000	2.646835000	-1.572968000
H	-3.239010000	5.131747000	2.681601000
H	-4.775920000	5.530123000	0.767418000
H	-3.270515000	0.279646000	-2.530789000
C	-1.165925000	-3.686021000	0.153536000
C	-1.461010000	-3.676565000	1.527822000
H	-2.013641000	-3.805514000	-1.837035000
H	-0.666435000	-3.588234000	2.258330000
H	-4.344748000	-3.977672000	-1.049047000
H	-4.848651000	-3.952153000	1.377311000
C	4.239786000	0.287422000	1.242230000
C	5.030337000	0.765037000	2.292042000
C	6.988143000	0.657894000	0.875402000
C	6.402780000	0.949062000	2.109543000
H	8.051367000	0.803082000	0.734079000
C	-4.742949000	-0.151230000	-1.049014000
H	-4.965256000	-0.936976000	-0.298129000
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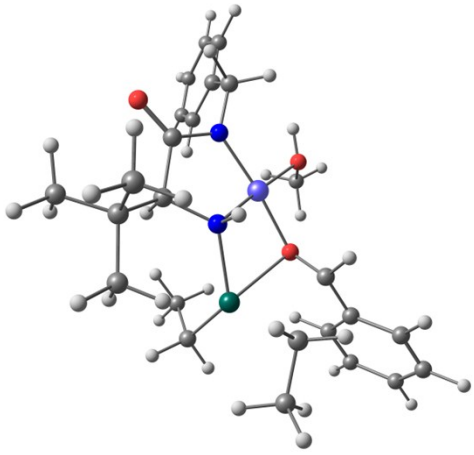

TS *anti trans* terbut

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H	-1.344900000	1.857262000	1.066247000
O	-0.920875000	-2.406968000	-0.989574000
H	-0.712511000	-4.380238000	-0.360762000
H	-1.378894000	-3.261670000	0.877267000
C	-3.411975000	-0.644853000	-1.466082000
H	-4.126106000	0.044746000	-1.928500000
C	1.993529000	1.288028000	2.598791000
H	2.982910000	0.894448000	2.864623000
H	-1.824830000	-2.520987000	-1.321850000
C	3.244108000	1.412669000	-1.042505000
H	2.727315000	2.303939000	-1.436340000
C	3.760540000	-1.987910000	0.734918000
C	4.942883000	-2.636772000	1.079949000
C	5.758131000	-2.376090000	-1.184966000
C	5.944022000	-2.831908000	0.122716000
H	6.531385000	-2.531026000	-1.932119000
H	2.169327000	-0.660383000	-2.028743000
C	-3.732157000	-1.437949000	0.941964000
C	-4.433050000	-2.191997000	1.888012000
C	-5.959620000	-2.942603000	0.168352000
C	-5.545608000	-2.942968000	1.502198000
H	-6.821234000	-3.525768000	-0.130016000
C	0.935720000	0.461408000	3.288091000
H	-0.067914000	0.874026000	3.056088000
C	4.383063000	1.845188000	-0.146981000
H	4.900494000	0.952611000	0.261178000
C	0.187669000	4.111174000	0.445772000
H	0.283128000	5.218769000	0.430585000
C	-1.273810000	4.141340000	-1.578051000
H	-1.211799000	5.249958000	-1.635236000
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H	-2.265329000	3.984841000	1.747972000
N	-0.103001000	1.351976000	-0.498290000
C	-2.547601000	1.425098000	-0.607119000
C	-1.289724000	2.101320000	-0.005374000
C	-1.168323000	3.668531000	-0.122669000
C	-0.663064000	-3.369579000	0.055770000
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H	0.070289000	1.620355000	-1.470925000
H	-3.069395000	-1.331159000	-2.257998000
Zn	1.697704000	1.198529000	0.578208000
H	1.939159000	2.318181000	2.973289000
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O	1.270544000	-1.001352000	-0.218555000
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C	3.571543000	-1.518103000	-0.575806000
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H	2.979281000	-1.830769000	1.471281000
H	4.432940000	-1.366735000	-2.550142000
H	5.086567000	-2.991622000	2.096747000
H	6.865221000	-3.339526000	0.395271000
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H	-0.451029000	3.727323000	-2.197159000
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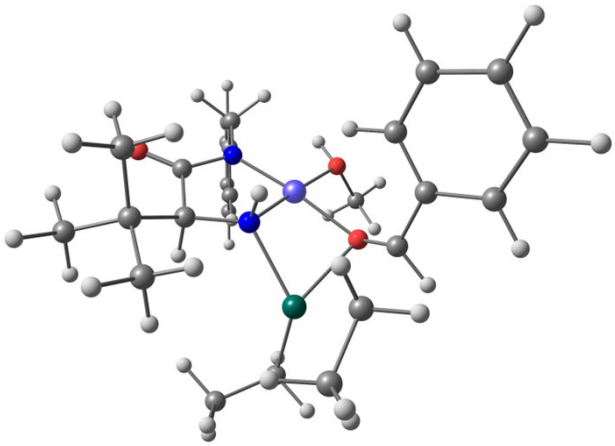

TS *anti cis* terbut

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H	1.660820000	-3.824733000	-2.092767000
H	2.266430000	-2.150230000	-2.335211000
C	2.938614000	-0.965605000	1.450695000
H	3.335221000	-0.559799000	2.386968000
C	-0.988409000	2.143246000	-3.040180000
H	-0.062716000	1.717919000	-3.449316000
H	1.998699000	-2.655816000	-0.051168000
C	-3.684178000	0.581799000	-0.715468000
H	-3.694497000	0.613985000	0.379851000
C	-4.213929000	-2.685549000	-0.195476000
C	-4.810074000	-3.432222000	0.817800000
C	-2.875518000	-3.060975000	2.219847000
C	-4.143030000	-3.619304000	2.030938000
H	-2.350504000	-3.207477000	3.159775000
H	-2.903552000	-1.425061000	-2.077956000
C	3.908175000	-0.236326000	-0.798413000
C	4.953318000	-0.238633000	-1.727147000
C	6.277904000	-1.614650000	-0.242898000
C	6.136868000	-0.926327000	-1.449894000
H	7.195049000	-2.148201000	-0.029238000
C	-0.755723000	3.601340000	-2.727787000
H	-0.448707000	4.143698000	-3.646948000
C	-4.107081000	1.930703000	-1.264444000
H	-4.100248000	1.899106000	-2.373792000
C	-0.449022000	2.379916000	3.321564000
H	-1.162817000	1.531581000	3.270260000
C	0.797884000	4.141193000	2.071132000
H	1.727891000	3.866559000	2.607217000
C	-1.465456000	3.462356000	1.316019000
H	-1.296138000	3.836566000	0.284094000
N	-0.488561000	0.852064000	0.450881000
C	1.722607000	1.101397000	1.506926000
C	0.477868000	1.854178000	0.974496000
C	-0.154400000	2.946208000	1.926056000
C	1.439464000	-2.761465000	-1.959494000
H	0.520541000	-2.501026000	-2.480606000
H	-1.106641000	0.549278000	1.206785000
H	2.658843000	-2.013394000	1.648867000
Zn	-1.547681000	1.129762000	-1.352415000
H	-1.760549000	2.066850000	-3.816338000
C	-2.344508000	-1.365548000	-1.141454000
O	-1.077892000	-1.157168000	-1.276145000
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C	-2.278208000	-2.315630000	1.205863000
H	-4.732721000	-2.546622000	-1.140988000
H	-1.288419000	-1.893728000	1.359845000
H	-5.792288000	-3.869100000	0.661189000
H	-4.606357000	-4.199714000	2.823963000
C	4.040170000	-0.928057000	0.422954000
C	5.235624000	-1.616738000	0.688932000
H	3.000911000	0.299287000	-1.044852000
H	5.359027000	-2.157324000	1.619476000
H	4.844284000	0.292088000	-2.664160000
H	6.944184000	-0.926731000	-2.170782000
H	0.043444000	3.695388000	-1.963745000
H	-1.689855000	4.051265000	-2.332552000
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H	0.480222000	2.020773000	3.811758000
H	0.319463000	4.958777000	2.653447000
H	1.073777000	4.549098000	1.074639000
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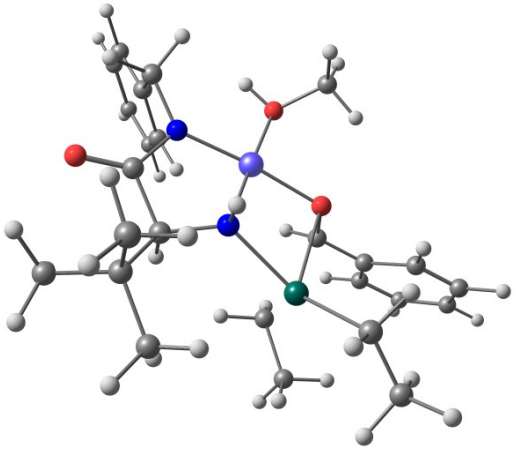

TS *syn trans* terbut

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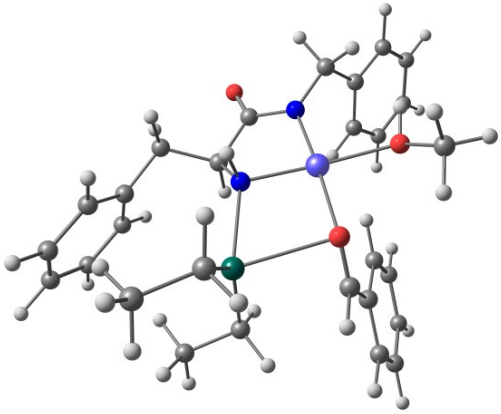
H	-1.118698000	1.553221000	1.359073000	C	-1.277374000	3.491946000	0.396217000
O	-1.180782000	-2.237494000	-1.412685000	C	-0.520230000	-2.772002000	-2.607378000
H	-0.879367000	-2.246071000	-3.498581000	H	0.537782000	-2.566780000	-2.455655000
H	-0.665813000	-3.866745000	-2.762270000	H	-0.297232000	1.877187000	-1.413577000
C	-3.772229000	-0.344215000	-1.228787000	H	-3.729550000	-0.898977000	-2.179443000
H	-4.512041000	0.447496000	-1.392089000	Zn	1.836763000	1.243041000	-0.076867000
C	1.807152000	0.272478000	1.963809000	H	1.744329000	-0.690409000	2.470097000
H	0.909863000	0.834957000	2.265560000	H	-2.140192000	-2.308711000	-1.471102000
O	1.169164000	-0.880440000	-0.911157000	C	1.636646000	-1.350958000	0.198242000
H	0.932422000	-1.787612000	0.908808000	C	3.019379000	-1.867555000	0.247954000
C	3.425486000	-2.668995000	1.327193000	C	3.924657000	-1.603317000	-0.792838000
C	4.718420000	-3.184004000	1.374514000	H	2.724916000	-2.884824000	2.130247000
C	5.218363000	-2.116542000	-0.739930000	H	3.605912000	-0.992424000	-1.630438000
C	5.619423000	-2.904631000	0.342942000	H	5.024275000	-3.802264000	2.213817000
H	5.915972000	-1.902273000	-1.544777000	H	6.629571000	-3.303051000	0.381140000
C	3.285657000	2.163092000	-1.205165000	H	3.414415000	1.595242000	-2.137144000
H	2.976445000	3.178111000	-1.486127000	C	-4.104979000	-1.301682000	-0.117971000
C	-3.221203000	-1.550590000	0.952041000	C	-5.332931000	-1.983535000	-0.158823000
C	-3.569369000	-2.456768000	1.958432000	H	-2.260962000	-1.055534000	1.013186000
C	-5.675960000	-2.888188000	0.850449000	H	-6.025438000	-1.813087000	-0.974166000
C	-4.795416000	-3.123946000	1.908575000	H	-2.886305000	-2.643495000	2.777056000
H	-6.624826000	-3.407439000	0.811303000	H	-5.062140000	-3.825176000	2.688700000
C	4.614202000	2.236170000	-0.494251000	H	5.389007000	2.641745000	-1.178604000
H	4.531111000	2.901782000	0.389322000	H	4.914705000	1.221008000	-0.162173000
C	3.044619000	0.973380000	2.474372000	H	3.949079000	0.421104000	2.145207000
H	3.077678000	2.005077000	2.072532000	H	3.025244000	1.020630000	3.583665000
C	-2.459496000	3.978906000	1.254743000	H	-2.199083000	4.901679000	1.729694000
H	-3.315826000	4.128153000	0.630780000	H	-2.684930000	3.245232000	2.000269000
C	0.043754000	3.986481000	1.014003000	H	0.835742000	3.867913000	0.304353000
H	-0.049438000	5.019945000	1.275106000	H	0.262890000	3.415192000	1.891793000
C	-1.416465000	4.049728000	-1.032468000	H	-1.478248000	5.117257000	-0.994129000
H	-0.564191000	3.762380000	-1.612093000	H	-2.303601000	3.657104000	-1.483847000



TS *syn cis* terbut

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H	0.541731000	-1.308651000	-1.329094000
H	1.716147000	-3.432311000	0.549395000
O	-2.675172000	0.553885000	1.896297000
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H	-3.746226000	1.674821000	3.285740000
C	-2.914121000	-2.356797000	0.962465000
H	-3.193088000	-2.112999000	2.001165000
C	2.331059000	1.980547000	-0.988268000
H	1.565317000	1.756645000	-1.741776000
O	-0.082667000	1.603268000	1.590801000
C	3.197702000	0.760378000	2.580375000
H	2.802019000	0.001319000	3.269180000
C	-1.670562000	2.426965000	-0.823371000
C	-2.336302000	2.963123000	-1.918093000
C	-0.906746000	4.924146000	-1.843732000
C	-1.955340000	4.210220000	-2.429901000
H	-0.612569000	5.889883000	-2.243353000
H	0.898257000	3.317232000	1.317931000
C	3.180305000	-2.135615000	-2.238978000
C	4.443539000	-1.744849000	-2.690453000
C	5.316985000	-1.970719000	-0.445470000
C	5.512088000	-1.664392000	-1.794409000
H	6.146826000	-1.901461000	0.247340000
C	-4.003960000	-1.888139000	0.030398000
C	-5.317593000	-2.336525000	0.244377000
H	-2.746323000	-0.654510000	-1.244363000
H	-5.537709000	-3.012239000	1.063031000
H	-4.584551000	0.084066000	-2.696521000
H	-6.897100000	-0.712304000	-2.294456000
H	5.081371000	1.283158000	1.672080000
H	4.790016000	-0.476036000	1.799158000
H	4.477062000	1.867277000	-0.855790000
H	3.843124000	2.328065000	-2.484168000
N	0.793584000	-0.854932000	0.695547000
C	-0.810466000	-2.501378000	-0.197307000
C	0.570720000	-1.850444000	-0.373139000
C	1.638558000	-2.956119000	-0.438482000
H	1.285147000	-3.728718000	-1.129537000
C	-2.729976000	1.299889000	3.131502000
H	-2.039729000	2.133204000	3.022319000
H	1.017282000	-1.387982000	1.543487000
H	-2.858377000	-3.448241000	0.895211000
Zn	2.171972000	0.832221000	0.783030000
H	2.296049000	3.059388000	-0.791147000
H	-3.273196000	-0.206727000	1.966454000
C	0.124018000	2.643629000	0.926968000
H	3.138314000	1.729432000	3.099147000
C	-0.608468000	3.135367000	-0.227767000
C	-0.234740000	4.389281000	-0.749120000
H	-1.966996000	1.467706000	-0.416186000
H	0.587071000	4.934219000	-0.292796000
H	-3.152265000	2.412877000	-2.377084000
H	-2.478098000	4.624161000	-3.287726000
C	2.977116000	-2.453244000	-0.885135000
C	4.052268000	-2.357419000	0.013232000
H	2.363260000	-2.209045000	-2.947561000
H	3.912606000	-2.568638000	1.067018000
H	4.594857000	-1.505982000	-3.736088000
H	6.491103000	-1.361195000	-2.144959000
C	-3.747472000	-1.011344000	-1.041683000
C	-4.788806000	-0.590358000	-1.873780000
C	-6.355651000	-1.913201000	-0.590904000
C	-6.091719000	-1.039762000	-1.648261000
H	-7.366349000	-2.262220000	-0.417235000
C	4.664631000	0.486641000	2.319050000
H	5.223564000	0.460697000	3.275864000
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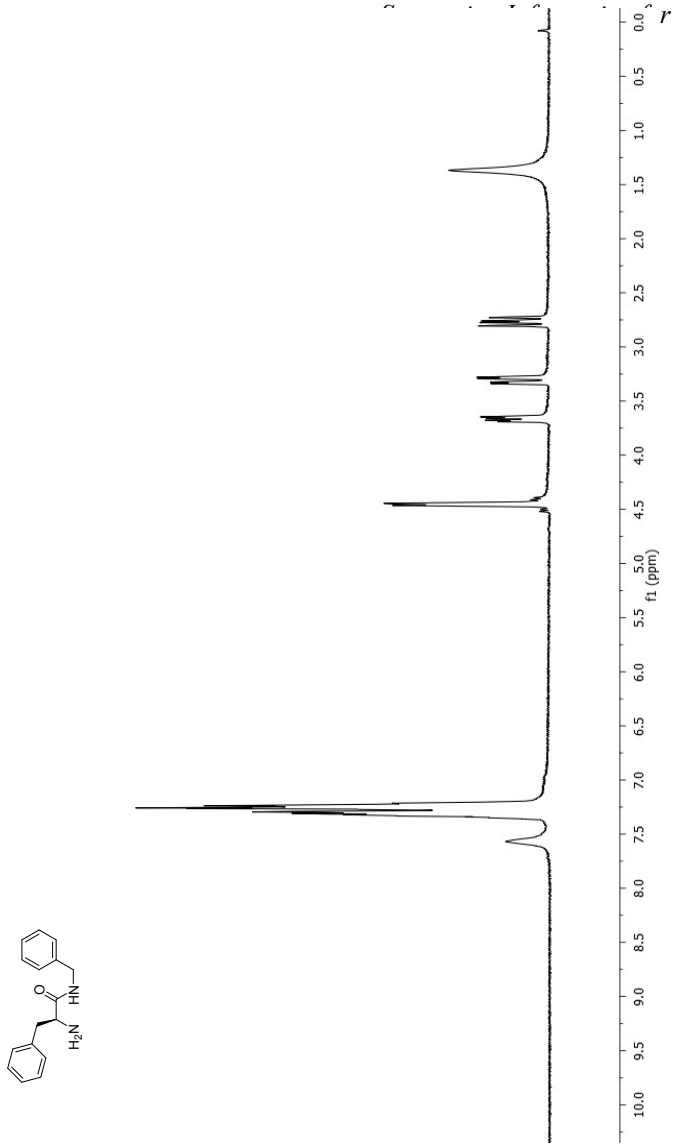
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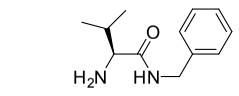
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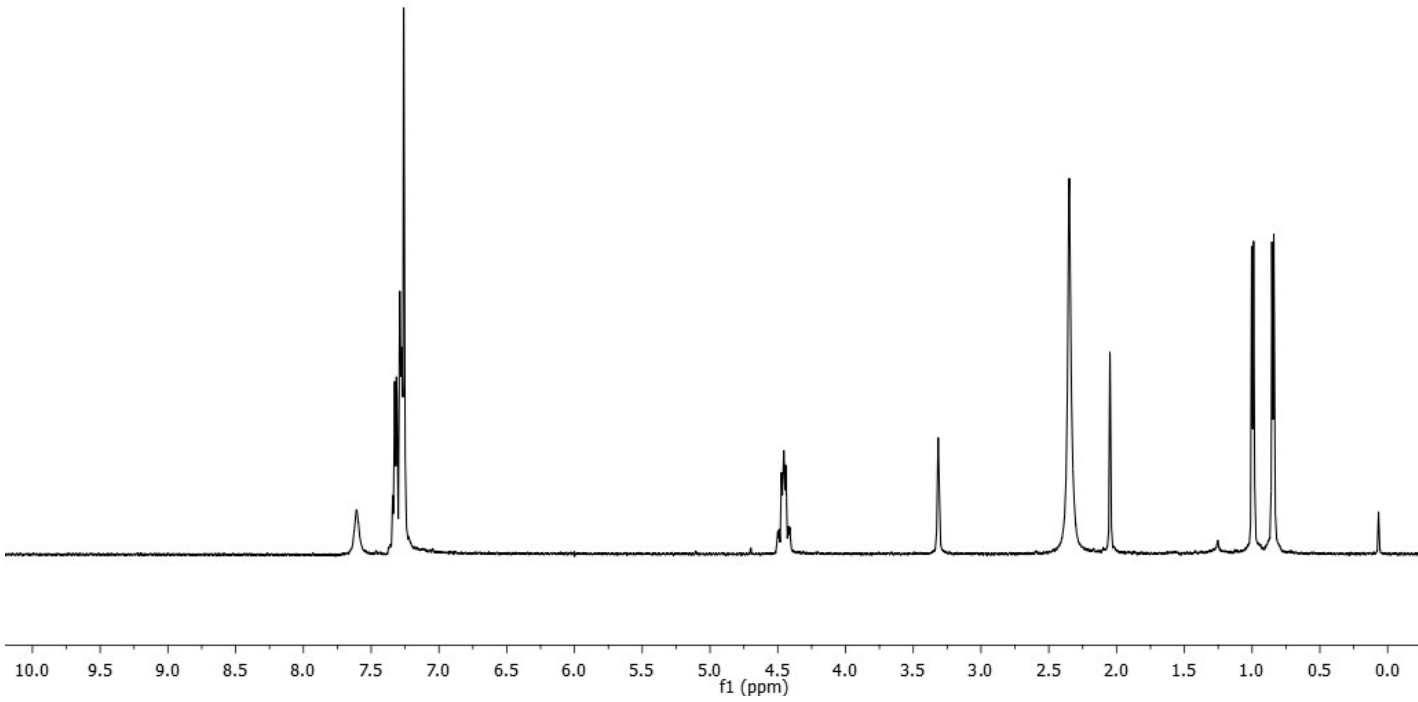
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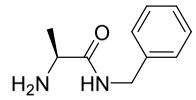
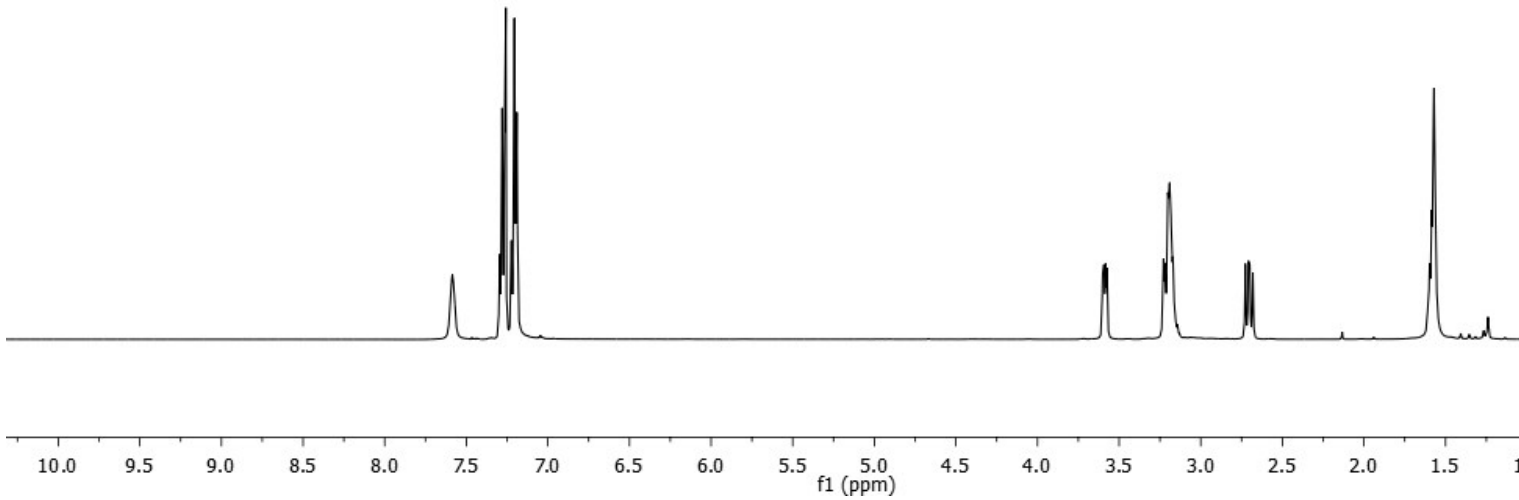
1.5
1.0
0.5
0.0
f1 (ppm)


O
H_2N
HN


10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)

O
HN
H2N
0
1
2
3
4
5
6
7
8
9
10