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Supporting Information

Hydroxy-Directed Ruthenium-Catalyzed Alkene/Alkyne Coupling: Increased Scope, Stereochemical Implications, and Mechanistic Rationale

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Crystallographic Information

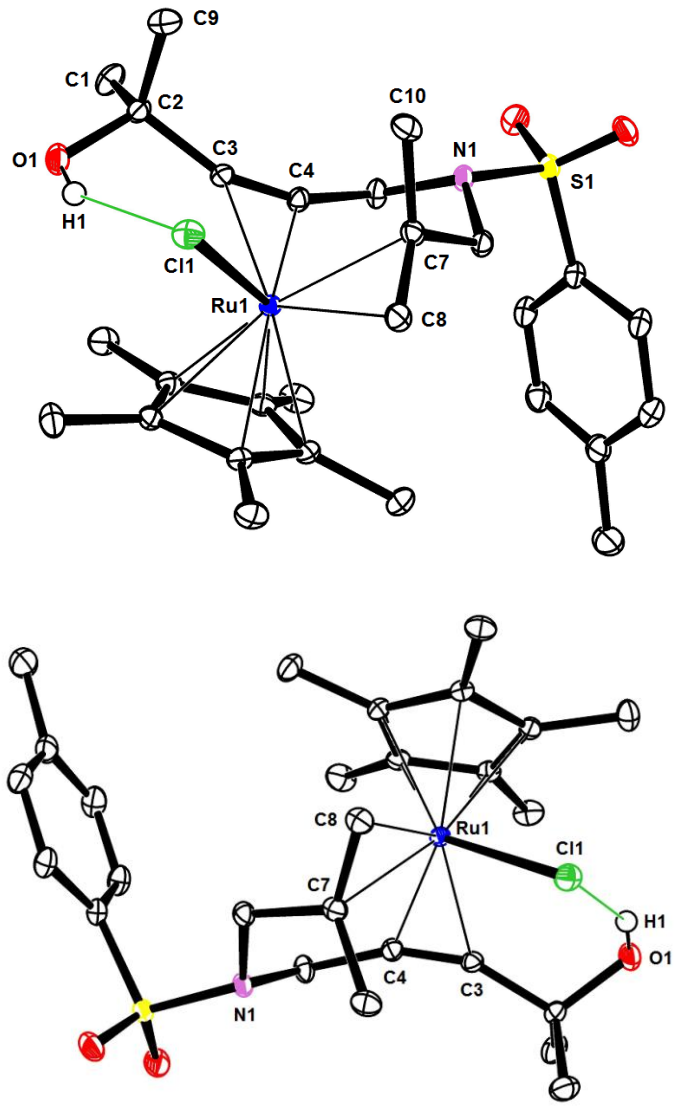


Figure S-1. Structure of complex **20** in the solid state in two different projections; hydrogen atoms, except the one engaged in hydrogen bonding to the chloride ligand, are omitted for clarity.

X-ray Crystal Structure Analysis of Complex 20: $C_{27}H_{38}ClNO_3RuS$, M_r = 593.16 g · mol^{-1}, orange prism, crystal size 0.25 x 0.10 x 0.10 mm, monoclinic, space group $P2_1/c$, a = 8.3708(10) Å, b = 13.6799(16) Å, c = 22.994(3) Å, β = 97.387(2)°, V = 2611.2(5) Å^3, T = 100 K, Z = 4, D_{calc} = 1.509 g · cm^3, λ = 0.71073 Å, μ(*Mo-K*$_\alpha$) = 0.812 mm^{-1}, Empirical absorption correction (T_{min} = 0.78, T_{max} = 0.91), Bruker-AXS Kappa Mach3 APEX-II diffractometer, 2.453 < θ < 36.315°, 101515 measured reflections, 12637 independent reflections, 11846 reflections with $I > 2\sigma(I)$, Structure solved by direct methods and refined by full-matrix least-squares against F^2 to R_1 = 0.032 [$I > 2\sigma(I)$], wR_2 = 0.083, 317 parameters, H atoms riding, absolute structure parameter = 0.0(2), S = 1.107, residual electron density 6.1 (0.78 Å from Ru1)/ -0.8 e Å^{-3}. **CCDC-1523566**.

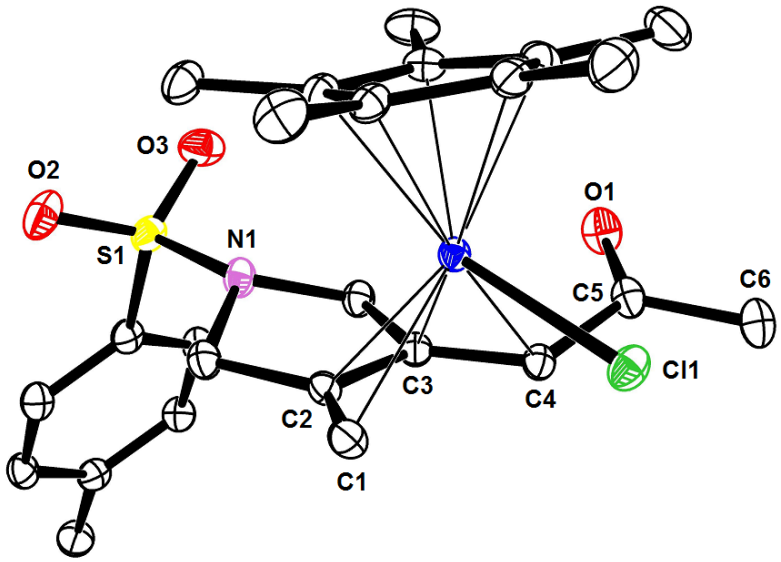
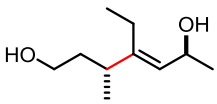


Figure S-2. Structure of complex **18** in the solid state; hydrogen atoms are omitted for clarity

X-ray Crystal Structure Analysis of Complex 18: C_{25} H_{32} Cl N O_3 Ru S, M_r = 563.09 g · mol^{-1}, orange prism, crystal size 0.04 x 0.04 x 0.02 mm, orthorhombic, space group $P2_12_12_1$, a = 8.9882(10) Å, b = 10.6912(9) Å, c = 24.9109(12) Å, V = 2393.8(4) Å^3, T = 100 K, Z = 4, D_{calc} = 1.562 g · cm^3, λ = 0.71073 Å, $\mu(MoK_\alpha)$ = 0.881 mm^{-1}, Empirical absorption correction (T_{min} = 0.96, T_{max} = 0.98), Bruker AXS Enraf-Nonius KappaCCD diffractometer, 3.271 < θ < 34.975°, 61936 measured reflections, 10512 independent reflections, 9746 reflections with $I > 2\sigma(I)$, Structure solved by direct methods and refined by full-matrix least-squares against F^2 to R_1 = 0.037 [$I > 2\sigma(I)$], wR_2 = 0.095, 308 parameters, absolute structure parameter = -0.035(14), H atoms riding, S = 1.066, residual electron density 0.8 (1.16 Å from C13)/ -2.5 e Å^{-3}. **CCDC-1523565**.

General. Unless stated otherwise, all reactions were carried out under Argon atmosphere in flame-dried glassware. The solvents were purified by distillation over the indicated drying agents under Argon: THF, Et_2O (Mg/anthracene), CH_3CN (CaH_2), hexane, toluene (Na/K), EtOH, MeOH (Mg). CH_2Cl_2 was stored over molecular sieves and degassed via freeze-pump-thaw procedure (3 x). Flash chromatography: Merck silica gel 60 (40-63 µm). NMR spectra were recorded on Bruker DPX 300, AMX 300, AV 400 or AVIII 600 spectrometers in the solvents indicated; chemical shifts (δ) are given in ppm relative to TMS, coupling constants (J) in Hz. The solvent signals were used as references and the chemical shifts converted to the TMS scale ($CDCl_3$: δ_C = 77.16 ppm; residual $CHCl_3$ in $CDCl_3$: δ_H = 7.26 ppm; CD_2Cl_2: δ_C = 54.0 ppm; residual $CHDCl_2$ in CD_2Cl_2: δ_H = 5.32 ppm); proton and carbon assignments were established using NOESY, HSQC, and HMBC experiments. MS (EI): Finnigan MAT 8200 (70 eV), ESI-MS: ESQ 3000 (Bruker). Accurate mass determinations: Bruker APEX III FT-MS (7 T magnet) or MAT 95 (Finnigan). Optical rotations were measured on a Perkin Elmer Polarimeter 343+. Diastereomeric ratios were determined by HPLC. Unless stated otherwise, all commercially available compounds (ABCR, Acros, Aldrich) were used as received. (Homo-)propargylic alcohols were purified by flash chromatography before use. Crotyl alcohol (*E/Z* ≈ 20/1) was purchased from Sigma Aldrich and used without further purification. 2-Methylnon-4-yn-3-ol[1], undec-6-yn-5-ol[2], 5-methylhex-3-yn-2-ol[3], 2-(hex-1-yn-1-yl)cyclopentan-1-ol[4], and 3-methylnon-4-yn-2-ol[5] were prepared according to literature procedures. [{Cp*Ru(CH_3CN)$_3$}PF_6],[6] [{Cp*RuCl}$_4$],[7] were prepared according to literature procedures and stored under Argon.

Representative Procedures for the Ruthenium-Catalyzed En/Yne Coupling of Propargylic Alcohols and Allylic Alcohols. (*E*)-4-Ethyl-3-methylhept-4-ene-1,6-diol. Method A. Hex-3-yn-2-ol (108 µL, 1.0 mmol, 1.0 equiv) and crotyl alcohol (170 µL, 2.0 mmol, 2.0 equiv) were added to a stirred orange/brown solution of [{Cp*RuCl}$_4$] (27.2 mg, 0.025 mmol, 2.5 mol%) in CH_2Cl_2 (5 mL) in a flame-dried Schlenk tube under argon at 0 °C. The resulting dark violet mixture was stirred for 4 h at 0 °C, during which the color changed to orange/brown. The mixture was then warmed to ambient temperature and diluted with MeOH (5 mL) before $NaBH_4$ (75.7 mg, 2.0 mmol, 2.0 equiv) was added in one portion. After stirring for another 1 h, the mixture was filtered through a plug of SiO_2 (CH_2Cl_2/MeOH, 5/1), the combined filtrates were concentrated and the residue was purified by flash chromatography (hexane/EtOAc: 2/1 → 0/1) to give the title compound as a colorless oil (118.0 mg, 69%, d.r. 12/1).



Method B. Hex-3-yn-2-ol (22 µL, 0.20 mmol, 1.0 equiv) and crotyl alcohol (34 µL, 0.40 mmol, 2.0 equiv) were added to a stirred solution of [{Cp*Ru(CH_3CN)$_3$}$^+PF_6^-$] (10.1 mg, 0.02 mmol, 10 mol%) in CH_2Cl_2 (1.0 mL) in a flame-dried Schlenk tube under argon at 0 °C. The mixture was stirred for 2 h at 0 °C before it was warmed to ambient temperature and diluted with MeOH (1.0 mL). $NaBH_4$ (15.1 mg, 0.40 mmol, 2.0 equiv) was added in one portion and stirring continued for 1 h, before the mixture was filtered through a plug of SiO_2 (eluent: CH_2Cl_2/MeOH: 5/1). The combined filtrates were concentrated and the residue was purified by flash chromatography (hexane/EtOAc, 2/1 → 0/1) to give the title compound as a colorless oil (23.9 mg, 69%, d.r. 6/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 5.19 (d, J = 8.8 Hz, 1H), 4.60 (dq, J = 8.9, 6.2 Hz, 1H), 3.60 (t, J = 6.6 Hz, 2H), 2.31 – 2.21 (m, 1H), 2.19 – 2.06 (m, 1H), 2.05 – 1.93 (m, 1H), 1.81 – 1.62 (m, 3H), 1.61 – 1.50 (m, 1H), 1.24 (d, J = 6.2 Hz, 3H), 1.03 (d, J = 6.9 Hz, 3H), 1.00 (t, J = 7.6 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 147.7, 128.2, 64.5, 61.3, 38.4, 37.2, 24.1, 22.4, 20.6, 15.2; **IR** (ν_{max} /cm^{-1}): 3308, 2963, 2930, 2873, 1457, 1374, 1144, 1048; **ESI-MS** calcd for $C_{10}H_{20}O_2Na$ (MNa^+) 195.13555; found 195.13557.

(*E*)-3-Heptyl-4-methylhex-2-ene-1,6-diol. Prepared according to the general procedure using [(Cp*RuCl)$_4$] (2.5 mol%) as the catalyst; colorless oil (77.4 mg, 68%, regioisomeric ratio ≈ 10:1 in the crude product). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 5.40 (t, *J* = 6.9 Hz, 1H), 4.17 (d, *J* = 6.9 Hz, 2H), 3.62 (t, *J* = 6.6 Hz, 2H), 2.27 (h, *J* = 7.0 Hz, 1H), 2.09 – 1.93 (m, 2H), 1.77 – 1.63 (m, 1H), 1.62 – 1.51 (m, 1H), 1.50 – 1.38 (bs, 2H), 1.37 – 1.17 (m, 10H), 1.04 (d, *J* = 6.9 Hz, 3H), 0.93 – 0.82 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 148.5, 123.0, 61.4, 59.4, 38.6, 37.2, 32.0, 30.3, 30.2, 29.9, 29.3, 22.8, 20.5, 14.3; **IR** (ν_{max} /cm^{-1}): 3318, 2955, 2924, 2855, 1457, 1377, 1041, 1000; **ESI-MS** calcd for $C_{14}H_{28}O_2Na$ (MNa$^+$) 251.19815; found 251.19799.

(*E*)-3,4-Diethylhept-4-ene-1,6-diol. Prepared according to the general procedure using [(Cp*RuCl)$_4$] (2.5 mol%) as the catalyst; isolated as mixture of diastereomers (d.r. = 13:1) in the form of a colorless oil (125.0 mg, 67%); (regioisomeric ratio = 5:1 in the crude product). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 5.18 (d, *J* = 9.0 Hz, 1H), 4.61 (dq, *J* = 9.0, 6.2 Hz, 1H), 3.68 – 3.48 (m, 2H), 2.14 – 1.85 (m, 5H), 1.70 – 1.53 (m, 2H), 1.38 (p, *J* = 7.2 Hz, 2H), 1.25 (d, *J* = 6.2 Hz, 3H), 1.00 (t, *J* = 7.6 Hz, 3H), 0.82 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 145.0, 130.4, 64.5, 61.3, 45.8, 36.5, 27.2, 24.1, 21.9, 15.2, 12.2; **IR** (ν_{max} /cm^{-1}): 3313, 2963, 2928, 2873, 1462, 1374, 1289, 1143, 1052; **ESI-MS** calcd for $C_{11}H_{22}O_2Na$ (MNa$^+$) 209.15120; found 209.15151.

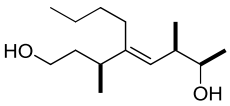
(*E*)-4-Butyl-3-methyldec-4-ene-1,6-diol. Prepared according to the general procedure using [(Cp*RuCl)$_4$] (2.5 mol%) as the catalyst; isolated as mixture of diastereomers (d.r. = 12:1) in form of a colorless oil (163.1 mg, 67%); (regioisomeric ratio = 6:1 in the crude product). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 5.16 (d, *J* = 9.1 Hz, 1H), 4.36 (dt, *J* = 9.1, 6.4 Hz, 1H), 3.62 (t, *J* = 6.6 Hz, 2H), 2.24 (h, *J* = 7.0 Hz, 1H), 2.13 – 1.96 (m, 2H), 1.77 – 1.65 (m, 1H), 1.65 – 1.51 (m, 2H), 1.50 – 1.17 (m, 11H), 1.04 (d, *J* = 6.9 Hz, 3H), 0.90 (t, *J* = 7.0 Hz, 3H), 0.90 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 147.8, 127.2, 68.4, 61.5, 38.8, 37.6, 36.9, 32.5, 30.0, 27.9, 23.3, 22.8, 20.7, 14.3, 14.1; **IR** (ν_{max} /cm^{-1}): 3314, 2956, 2929, 2860, 1458, 1377, 1049, 1021, 996; **ESI-MS** calcd for $C_{15}H_{30}O_2Na$ (MNa$^+$) 265.21380; found 265.21364.

(*E*)-4-Butyl-3,7-dimethyloct-4-ene-1,6-diol. Prepared according to the general procedure using [(Cp*RuCl)$_4$] (3.75 mol%) as the catalyst; isolated as mixture of diastereomers (d.r. = 9:1) in form of a colorless oil (80.0 mg, 70%); (regioisomeric ratio = 6:1 in the crude product). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 5.20 (d, *J* = 9.3 Hz, 1H), 4.05 (dd, *J* = 9.3, 6.9 Hz, 1H), 3.63 (t, *J* = 6.7 Hz, 2H), 2.26 (h, *J* = 7.0 Hz, 1H), 2.12 – 1.98 (m, 2H), 1.79 – 1.62 (m, 2H), 1.62 – 1.51 (m, 1H), 1.48 – 1.22 (m, 6H), 1.04 (d, *J* = 6.9 Hz, 3H), 0.96 (d, *J* = 6.6 Hz, 3H), 0.91 (t, *J* = 7.0 Hz, 3H), 0.85 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 148.8, 125.2, 73.3, 61.5, 39.0, 36.8, 34.6, 32.4, 30.2, 23.4, 20.8, 18.64, 18.62, 14.2; **IR** (ν_{max} /cm^{-1}): 3328, 2955, 2930, 2871, 1466, 1379, 1051, 1005; **ESI-MS** calcd for $C_{14}H_{28}O_2Na$ (MNa$^+$) 251.19815; found 251.19796.

(*E*)-4-Isopropyl-3-methylhept-4-ene-1,6-diol. Prepared according to the general procedure using [(Cp*RuCl)$_4$] (2.5 mol%) as the catalyst; isolated as mixture of regioisomers (8:1) in form of a colorless oil (151.5 mg, 81%). The minor diastereomer of the major regioisomer was isolated in a separate fraction as a colorless oil (12.8 mg, 7%); **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 5.17 (d, *J* = 8.5 Hz, 1H), 4.73 (dq, *J* = 8.6, 6.2 Hz, 1H), 3.60 (t, *J* = 6.7 Hz, 2H), 2.83 (hept, *J* = 7.0 Hz, 1H), 2.27 (h, *J* = 7.0 Hz, 1H), 1.76 – 1.64 (m, 1H), 1.64 – 1.53 (m, 1H), 1.50 – 1.31 (bs, 2H), 1.22 (d, *J* = 6.2 Hz, 3H), 1.03 (d, *J* = 6.8 Hz, 3H), 1.03 (d, *J* = 6.9 Hz, 3H), 1.00 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 152.1, 127.2, 64.1, 61.6, 40.7, 30.5, 29.8, 24.3, 23.1, 21.7,

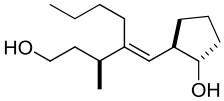
21.6; **IR** (ν_{max} /cm^{-1}): 3324, 2960, 2929, 2870, 1456, 1367, 1047, 1007; **ESI-MS** calcd for $C_{11}H_{22}O_2Na$ (MNa^+) 209.15120; found 209.15115.

(*E*)-4-Butyl-3,6-dimethyloct-4-ene-1,7-diol. Prepared according to the general procedure using [(Cp*RuCl)$_4$] (2.5 mol%) as the catalyst; isolated as colorless oil (104.6 mg, 92%).



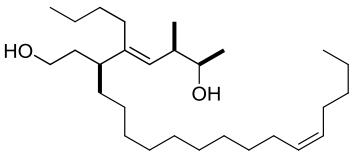
^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.99 (d, *J* = 10.3 Hz, 1H), 3.59 (dt, *J* = 11.3, 6.3 Hz, 3H), 2.47 (dp, *J* = 10.2, 6.7 Hz, 1H), 2.30 – 2.18 (m, 1H), 2.16 – 2.04 (m, 1H), 1.95 – 1.84 (m, 1H), 1.73 – 1.51 (m, 4H), 1.40 – 1.25 (m, 4H), 1.12 (d, *J* = 6.3 Hz, 3H), 1.02 (d, *J* = 6.9 Hz, 3H), 0.97 (d, *J* = 6.7 Hz, 3H), 0.93 – 0.87 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 145.4, 126.0, 72.4, 61.8, 39.3, 38.8, 38.7, 32.5, 29.3, 23.5, 21.0, 20.3, 17.5, 14.2; **IR** (ν_{max} /cm^{-1}): 3329, 2957, 2929, 2870, 1455, 1370, 1081, 1050, 1000; **ESI-MS** calcd for $C_{14}H_{28}O_2Na$ (MNa^+) 251.19815; found 251.19822.

2-((*E*)-2-(4-Hydroxybutan-2-yl)hex-1-en-1-yl)cyclopentan-1-ol. Prepared according to the general procedure using [(Cp*RuCl)$_4$] (2.5 mol%) as the catalyst; isolated as colorless oil (103.9 mg, 86%); (regioisomeric ratio = 11:1 in the crude product).



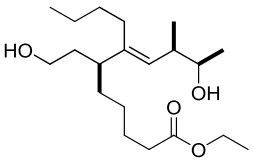
^{1}H NMR (400 MHz, $CDCl_3$): δ = 5.01 (d, *J* = 9.8 Hz, 1H), 3.77 (q, *J* = 7.1 Hz, 1H), 3.71 – 3.54 (m, 2H), 2.54 (tt, *J* = 9.8, 7.4 Hz, 1H), 2.24 (dp, *J* = 8.6, 6.7 Hz, 1H), 2.18 – 2.06 (m, 1H), 2.02 – 1.80 (m, 3H), 1.80 – 1.49 (m, 6H), 1.40 – 1.22 (m, 6H), 1.02 (d, *J* = 6.9 Hz, 3H), 0.95 – 0.86 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 146.2, 126.9, 79.9, 62.0, 47.2, 39.1, 38.7, 33.4, 33.0, 30.6, 29.1, 23.5, 21.3, 20.8, 14.2; **IR** (ν_{max} /cm^{-1}): 3322, 1954, 1931, 2870, 1455, 1372, 1341, 1083, 1049; **ESI-MS** calcd for $C_{15}H_{28}O_2Na$ (MNa^+) 263.19815; found 263.19820.

(*E*)-4-Butyl-6-methyl-3-((*Z*)-pentadec-10-en-1-yl)oct-4-ene-1,7-diol. Prepared according to the general procedure using [(Cp*RuCl)$_4$] (2.5 mol%) as the catalyst; isolated as colorless oil (71.6 mg, 85%).



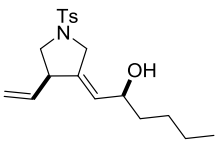
^{1}H NMR (400 MHz, $CDCl_3$): δ = 5.42 – 5.27 (m, 2H), 4.98 (d, *J* = 10.2 Hz, 1H), 3.65 – 3.52 (m, 3H), 2.48 (dp, *J* = 10.2, 6.7 Hz, 1H), 2.10 – 1.92 (m, 6H), 1.90 – 1.79 (m, 1H), 1.67 – 1.56 (m, 4H), 1.39 – 1.27 (m, 12H), 1.27 – 1.15 (m, 12H), 1.13 (d, *J* = 6.3 Hz, 3H), 0.98 (d, *J* = 6.8 Hz, 3H), 0.95 – 0.84 (m, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 143.27, 130.02, 129.98, 127.8, 72.4, 61.9, 45.2, 39.5, 37.1, 34.7, 32.4, 32.1, 29.91, 29.88, 29.8, 29.7, 29.5, 29.2, 27.7, 27.3, 27.1, 23.6, 22.5, 20.4, 17.6, 14.19, 14.17; **IR** (ν_{max} /cm^{-1}): 3341, 2956, 2923, 2854, 1458, 1376, 1081, 1040; **ESI-MS** calcd for $C_{28}H_{54}O_2Na$ (MNa^+) 445.40160; found 445.40220.

Ethyl (*E*)-7-butyl-10-hydroxy-6-(2-hydroxyethyl)-9-methylundec-7-enoate. Prepared according to the general procedure using [(Cp*RuCl)$_4$] (2.5 mol%) as the catalyst; isolated as colorless oil (62.8 mg, 92%).



^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.99 (d, *J* = 10.3 Hz, 1H), 4.11 (q, *J* = 7.1 Hz, 2H), 3.65 – 3.52 (m, 3H), 2.48 (dp, *J* = 10.3, 6.7 Hz, 1H), 2.27 (t, *J* = 7.5 Hz, 2H), 2.13 – 1.98 (m, 2H), 1.90 – 1.78 (m, 1H), 1.73 – 1.65 (bs, 2H), 1.65 – 1.51 (m, 4H), 1.42 – 1.18 (m, 8H), 1.25 (t, *J* = 7.2 Hz, 3H), 1.12 (d, *J* = 6.3 Hz, 3H), 0.97 (d, *J* = 6.7 Hz, 3H), 0.95 – 0.85 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 174.0, 142.9, 128.2, 72.3, 61.8, 60.4, 45.0, 39.4, 37.1, 34.4, 34.3, 32.5, 29.1, 27.2, 25.1, 23.6, 20.4, 17.5, 14.4, 14.2; **IR** (ν_{max} /cm^{-1}): 3354, 2956, 2930, 2864, 1735, 1718, 1458, 1371, 1181, 1086, 1036; **ESI-MS** calcd for $C_{20}H_{38}O_4Na$ (MNa^+) 365.26623; found 365.26662.

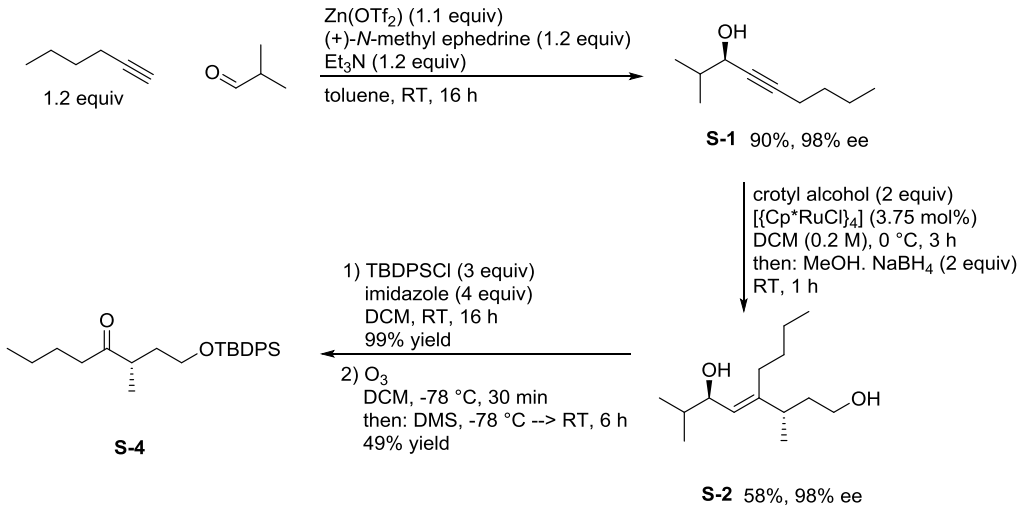
(*Z*)-1-(1-Tosyl-4-vinylpyrrolidin-3-ylidene)hexan-2-ol. [(Cp*RuCl)$_4$] (5.4 mg, 2.5 mol%) was added to a stirred solution of the enyne substrate (67.1 mg, 0.2 mmol, 1.0 equiv) in CH_2Cl_2 (0.2 M) in a flame-dried Schlenk tube under argon at 0 °C. The resulting yellow mixture was stirred for 4 h before it was filtered through a plug of SiO_2 (eluent:



tert-butyl methyl ether). The combined filtrates were concentrated and the residue was purified by flash chromatography (SiO_2, hexane/EtOAc: 4/1) to yield the title compound as a colorless oil (57.8 mg, 0.17 mmol, 86%, d.r.: 11:1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.75 – 7.67 (m, 2H), 7.38 – 7.31 (m, 2H), 5.44 (ddd, *J* = 16.7, 10.3, 8.4 Hz, 1H), 5.23 – 5.06 (m, 3H), 4.14 – 4.04 (m, 1H), 3.99 (ddd, *J* = 14.5, 2.6, 1.4 Hz, 1H), 3.73 (dt, *J* = 14.5, 2.3 Hz, 1H), 3.65 (dd, *J* = 9.3, 7.7 Hz, 1H), 3.26 (q, *J* = 8.7 Hz, 1H), 2.69 (t, *J* = 9.5 Hz, 1H), 2.44 (s, 3H), 1.58 – 1.47 (m, 1H), 1.44 – 1.18 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 144.0, 139.6, 135.3, 132.2, 129.9, 128.0, 126.7, 119.0, 70.0, 52.7, 49.5, 47.9, 39.7, 21.8, 18.7, 14.2; **IR** (ν_{max} /cm^{-1}): 3527, 2957, 2929, 2871, 1597, 1456, 1340, 1158, 1091, 1034, 1015; **ESI-MS** calcd for $C_{18}H_{25}NO_3SNa$ (MNa^+) 358.14474; found 358.14520.

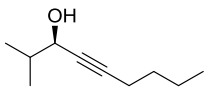
Determination of Relative Stereochemistry

To elucidate the configuration of the newly formed stereocenter, enantiomerically pure propargylic alcohol **S-1** was prepared via Carreira addition of 1-hexyne to 2-methylpropanal.[10] The subsequent enyne coupling proceeded without loss of enantiopurity to give diastereomer **S-2** in 58% yield after separation of the diastereomers via careful flash chromatography. Chemical degradation of this diol afforded known ketone **S-3**,[11] which had previously been made in stereochemically unambiguous form starting from the "chiral pool". Comparison of the optical rotation confirmed an anti-configuration of the alkene-alkyne coupling products.



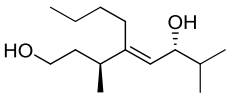
Scheme S-1. Preparation of a reference compound, which allows the configuration of the newly formed stereocenter in the ene/yne coupling process to be determined.

(*R*)-2-Methylnon-4-yn-3-ol (S-1). Triethylamine (0.84 mL, 6 mmol, 1.2 equiv) was added to a stirred suspension of $Zn(OTf)_2$ (2.00 g, 5.5 mmol, 1.1 equiv) and (+)-*N*-methylephedrine (1.08 g, 5.5 mmol, 1.1 equiv) in toluene (15 mL, 0.33 M) at ambient temperature and the resulting mixture was stirred for 2 h. 1-Hexyne (0.69 mL, 6 mmol, 1.2 equiv) was added and stirring continued for 15 min before isobutyraldehyde (0.46 mL, 5 mmol, 1.0 equiv) was added in one portion. The resulting mixture was stirred for 16 h at ambient temperature before sat. NH_4Cl aq. was added. The phases were separated and the aqueous layer was extracted with *tert*-butyl methyl ether (3 times). The combined organic phases were dried over $MgSO_4$ and concentrated, and the residue was purified by flash chromatography (pentane/Et_2O, 20/1) to yield

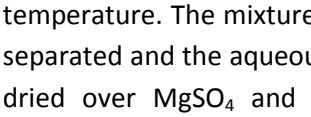


the title compound as colorless oil (694 mg, 4.5 mmol, 90%, 98% ee). $[\boldsymbol{a}]_{\boldsymbol{D}}^{\boldsymbol{20}}$ = –2.1 (c =1.0, $CHCl_3$); $[\boldsymbol{a}]_{\boldsymbol{D}}^{\boldsymbol{20}}$ = +9.7 (c =4.0, hexane) (lit.[8] for (*S*)-enantiomer: $[a]_D^{23}$ = –9.9 (c =5.97, hexane)). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 4.20 – 4.10 (m, 1H), 2.22 (td, *J* = 7.0, 2.0 Hz, 2H), 1.83 (heptd, *J* = 6.8, 5.5 Hz, 1H), 1.74 – 1.62 (bs, 1H), 1.54 – 1.45 (m, 2H), 1.45 – 1.33 (m, 2H), 0.99 (d, *J* = 6.9 Hz, 3H), 0.97 (d, *J* = 6.9 Hz, 3H), 0.91 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 86.4, 79.9, 68.3, 34.8, 30.9, 22.1, 18.5, 18.3, 17.6, 13.7; **IR** (ν_{max} /cm^{-1}): 3360, 2958, 2923, 2872, 1467, 1381. 1366, 1251, 1149, 1021; **ESI-MS** calcd for $C_{10}H_{18}ONa$ (MNa^+) 177.12498; found 177.12497.

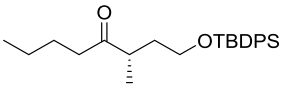
(3*S*,6*R*,*E*)-4-Butyl-3,7-dimethyloct-4-ene-1,6-diol (S-2). Prepared according to the general procedure using [(Cp*RuCl)$_4$] (3.75 mol%) as the catalyst; careful flash chromatography (hexane/EtOAc: 4/1) afforded the title compound as a single diastereomer (107.3 mg, 59%, 98% ee); $[\boldsymbol{a}]_{\boldsymbol{D}}^{\boldsymbol{20}}$ = –5.8 (c =1.0, $CHCl_3$). The NMR data are identical with those of the racemic sample (see above).



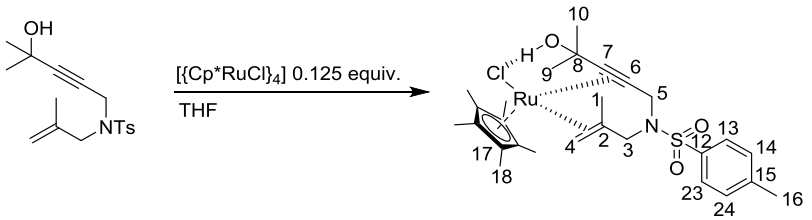
(5*R*,8*S*,*E*)-7-Butyl-5-isopropyl-2,2,8,13,13-pentamethyl-3,3,12,12-tetraphenyl-4,11-dioxa-3,12-disilatetradec-6-ene (S-3). TBDPSCl (0.19 mL, 0.74 mmol, 3 equiv) was added to a stirred solution of diol (56.2 mg, 0.25 mmol, 1.0 equiv) and imidazole (67 mg, 0.1 mmol, 4 equiv) in CH_2Cl_2 (0.5 mL, 0.5 M) at ambient temperature. The mixture was stirred for 16 h, before sat. $NaHCO_3$ aq. was added. The phases were separated and the aqueous layer was extracted with CH_2Cl_2 (3 x). The combined organic phases were dried over $MgSO_4$ and concentrated, and the residue was purified by flash chromatography (hexane/EtOAc: 100/1) to yield the title compound as colorless oil (174 mg, 0.25 mmol, quant.). $[\boldsymbol{a}]_{\boldsymbol{D}}^{\boldsymbol{20}}$ = +19.2 (c =1.0, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.70 – 7.61 (m, 8H), 7.46 – 7.27 (m, 12H), 5.14 (d, *J* = 9.2 Hz, 1H), 4.16 (dd, *J* = 9.2, 4.8 Hz, 1H), 3.59 (t, *J* = 6.5 Hz, 2H), 2.10 (h, *J* = 6.9 Hz, 1H), 1.73 – 1.58 (m, 2H), 1.49 – 1.34 (m, 3H), 1.03 (s, 9H), 1.02 (s, 9H), 1.02 – 0.88 (m, 4H), 0.82 (d, *J* = 6.8 Hz, 3H), 0.79 (d, *J* = 6.8 Hz, 3H), 0.74 (d, *J* = 6.9 Hz, 3H), 0.69 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 145.6, 136.3, 136.2, 135.7, 135.0, 134.7, 134.22, 134.21, 129.63, 129.61, 129.5, 129.3, 127.70, 127.69, 127.5, 127.2, 124.2, 74.6, 62.3, 39.2, 35.7, 34.7, 30.93, 30.85, 27.2, 27.0, 23.3, 20.1, 19.6, 19.3, 18.3, 14.0; **IR** (ν_{max} /cm^{-1}): 3071, 2956, 2930, 2893, 2857, 1471, 1427, 1389, 1362, 1217, 1107, 1047, 1006; **ESI-MS** calcd for $C_{46}H_{64}O_2Si_2Na$ (MNa^+) 727.43371; found 727.43466.



(*S*)-1-((*tert*-Butyldiphenylsilyl)oxy)-3-methyloctan-4-one (S-4). Ozone was bubbled through a stirred solution of bis-silylether **S-3** (73.6 mg, 0.10 mmol, 1.0 equiv) in CH_2Cl_2 (5 mL, 0.02 M) at –78 °C until a deep blue color persisted (ca. 30 min). Dimethylsulfide (0.1 mL, 1.3 mmol, 13 equiv) was added and stirring continued at –78 °C for 3 h and for another 3 h at ambient temperature. All volatile materials were removed and the residue was purified by flash chromatography (hexane/EtOAc; 50:1) to yield the title compound as colorless oil (20.4 mg, 0.05 mmol, 49%). $[\boldsymbol{a}]_{\boldsymbol{D}}^{\boldsymbol{20}}$ = +6.0 (c = 0.34, $CHCl_3$) (lit.: $[a]_D^{26}$ = +8.0 (c = 0.13, $CHCl_3$)). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.64 (dq, *J* = 6.5, 1.4 Hz, 4H), 7.46 – 7.34 (m, 6H), 3.65 (t, *J* = 6.2 Hz, 2H), 2.80 (h, *J* = 6.9 Hz, 1H), 2.52 – 2.34 (m, 2H), 1.94 (dq, *J* = 13.8, 6.4 Hz, 1H), 1.58 – 1.45 (m, 3H), 1.34 – 1.19 (m, 3H), 1.05 (s, 9H), 1.03 (d, *J* = 5.5 Hz, 3H), 0.90 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 214.9, 135.7, 133.9, 133.8, 129.8, 127.8, 61.7, 42.7, 41.2, 35.6, 27.0, 26.0, 22.6, 19.3, 16.5, 14.1; **IR** (ν_{max} /cm^{-1}): 3071, 2958, 2930, 2857, 1711, 1461, 1378, 1258, 1106, 1086, 997; **ESI-MS** calcd for $C_{25}H_{36}O_2SiNa$ (MNa^+) 419.23768; found 419.23812.

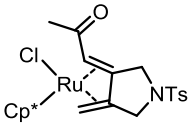


Complex 20.



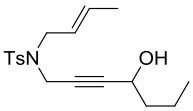
A mixture of [(Cp*RuCl)$_4$] (45.5 mg, 0.042 mmol, 1.0 equiv) and enyne **19** (107.6 mg, 0.335 mmol, 8 equiv) were dissolved in THF (4 mL). The resulting orange/red solution was slowly concentrated at 0 °C to a total volume of ca. 2 mL under a stream of Argon to obtain red crystals suitable for X-ray diffraction. **^{1}H NMR** (400 MHz, 223 K, THF-d_8) δ = 7.68 (d, *J* = 8.3 Hz, 2H, H-13, H-23), 7.43 (m, 2H, H-24, H-14), 4.81 (d, *J* = 13.8 Hz, 1H, H-5'), 4.68 (s, 1H, 11-OH), 4.48 (d, *J* = 12.6 Hz, 1H, H-3'), 3.65 (s, 1H, H-4'), 2.69 (d, *J* = 13.9 Hz, 1H, H-5''), 2.58 (s, 1H, H-4''), 2.40 (d, *J* = 3.5 Hz, 3H, H-16), 1.73 (s, 3H, H-9), 1.66 (d, *J* = 12.5 Hz, 1H, H-3''), 1.40 (s, 3H, H-10), 1.29 (s, 15H, H-18), 1.04 (s, 3H, H-1); **^{13}C NMR** (101 MHz, 223 K, THF) δ = 144.8 (C-15), 133.0 (C-12), 130.4 (C-24, C-14), 128.9 (C-13, C-23), 96.8 (C-17), 82.5 (C-2), 78.1 (C-7), 75.6 (C-6), 70.1 (C-8), 64.4 (C-4), 56.9 (C-3), 36.0 (C-10), 35.6 (C-5), 34.4 (C-9), 21.5 (C-16), 19.3 (C-1), 9.2 (C-18).

Complex 18. [(Cp*RuCl)$_4$] (88.0 mg, 0.081 mmol, 0.27 equiv.) was added to a solution of *N*-allyl-*N*-(4-hydroxypent-2-in-1-yl)-4-methylbenzenesulfonamide (88.0 mg, 0.3 mmol, 1.0 equiv.) in CH_2CL_2 (3 mL) and the resulting mixture was stirred for 2.5 h. All volatile materials were evaporated and the residue was purified by flash chromatography (hexanes/EtOAc, 5:1) to give product **18** as an orange-red waxy solid (58.3 mg, 0.1 mmol, 34%). Single crystals suitable for X-ray diffraction were grown by slow evaporation of a solution of this compound in THF under a stream of Ar. **^{1}H NMR** (400 MHz, CD_2Cl_2): δ = 7.86 – 7.69 (m, 2H), 7.47 – 7.31 (m, 2H), 4.62 (ddd, *J* = 15.1, 1.9, 1.1 Hz, 1H), 4.34 – 4.18 (m, 2H), 3.80 – 3.72 (m, 1H), 3.46 (dd, *J* = 3.5, 0.7 Hz, 1H), 2.49 (s, 1H), 2.45 (s, 3H), 2.12 (d, *J* = 3.4 Hz, 1H), 1.97 (s, 3H), 1.52 (s, 15H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 202.8, 145.0, 132.9, 130.6, 128.3, 107.6, 103.4, 98.5, 59.3, 52.4, 52.1, 48.1, 29.9, 21.9, 8.8.



Preparation of the Substrates

(*E*)-*N*-(But-2-en-1-yl)-*N*-(4-hydroxyhept-2-yn-1-yl)-4-methylbenzenesulfonamide (12). *n*-BuLi (1.6 M in hexanes, 1.4 mL, 1.1 equiv) was slowly added to a stirred solution of (*E*)-*N*-(but-2-en-1-yl)-4-methyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide (527 mg, 2.0 mmol, 1.0 equiv)[12] in THF (4 mL, 0.5 M) at –78 °C and the resulting mixture was stirred for 30 min at –78 °C before butanal (0.54 mL, 6.1 mmol, 3 equiv) was added dropwise. After 30 min at –78 °C the mixture was warmed to ambient temperature and stirring was continued for 2.5 h. The reaction was quenched with water and the aqueous phase extracted with *tert*-butyl methyl ether (3 x). The combined organic phases were dried over $MgSO_4$ and concentrated, and the residue was purified by flash chromatography (hexane/EtOAc: 5/1) to yield the title compound as pale yellow oil (479 mg, 1.4 mmol, 71%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.75 – 7.71 (m, 2H), 7.33 – 7.28 (m, 2H), 5.68 (dqt, *J* = 15.4, 6.5, 1.2 Hz, 1H), 5.37 (dtq, *J* = 15.2, 6.8, 1.6 Hz, 1H), 4.12 – 4.02 (m, 3H), 3.80 – 3.68 (m, 2H), 2.43 (s, 3H), 1.69 (dq, *J* = 6.6, 1.2 Hz, 3H), 1.51 – 1.30 (m, 3H), 1.25 (dtd, *J* = 8.6, 7.3, 6.1 Hz, 2H), 0.87 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 143.6, 136.4, 131.7, 129.5,



128.0, 124.7, 86.7, 77.7, 62.0, 48.5, 39.7, 35.8, 21.7, 18.4, 17.9, 13.8; **IR** (ν_{max} /cm^{-1}): 3500, 2959, 2934, 2872, 1446, 1329, 1157, 1091, 1055, 1019; **ESI-MS** calcd for $C_{18}H_{25}NO_3SNa$ (MNa^+) 358.14474; found 358.14445.

***N*-(4-Hydroxy-4-methylpent-2-yn-1-yl)-4-methyl-*N*-(2-methylallyl)benzenesulfonamide (19)**. *n*-BuLi (1.6 M in hexanes, 1.5 mL, 1.2 equiv) was slowly added to a stirred solution of 4-methyl-*N*-(2-methylallyl)-*N*-(prop-2-yn-1-yl)benzenesulfonamide (527 mg, 2.0 mmol, 1.0 equiv)[13] in THF (4 mL, 0.5 M) at –78 °C and the resulting mixture was stirred for 30 min at –78 °C before acetone (0.44 mL, 6.0 mmol, 3 equiv) was added dropwise. After 1 h at –78 °C, stirring was continued at ambient temperature for 30 min before the reaction was quenched with water. The phases were separated and the aqueous layer was extracted with *tert*-butyl methyl ether (3 x). The combined organic phases were dried over $MgSO_4$ and concentrated, and the residue was purified by flash chromatography (hexane/EtOAc: 2/1) to yield the title compound as pale yellow oil that solidified upon standing (521 mg, 1.6 mmol, 81%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.78 – 7.72 (m, 2H), 7.35 – 7.30 (m, 2H), 5.01 – 4.91 (m, 2H), 4.05 (s, 2H), 3.73 (s, 2H), 2.43 (s, 3H), 1.78 (dd, *J* = 1.5, 0.9 Hz, 3H), 1.42 (s, 1H), 1.24 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 143.6, 139.3, 136.5, 129.6, 128.1, 115.7, 90.6, 74.7, 64.9, 52.7, 35.8, 31.1, 21.6, 19.9; **IR** (ν_{max} /cm^{-1}): 3515, 2981, 2925, 1442, 1347, 1329, 1161, 1098, 905; **ESI-MS** calcd for $C_{17}H_{23}NO_3SNa$ (MNa^+) 344.12909; found 344.12893.

Ethyl (2*E*,13*Z*)-octadeca-2,13-dienoate. *cis*-11-Hexadecenal (1.00 g, 4,2 mmol, 1.0 equiv) was added to a stirred solution of (carbethoxymethylen)-triphenylphosphorane (1.75 g, 5.0 mmol, 1.2 equiv) in CH_2Cl_2 (4 mL) and the resulting mixture was stirred at reflux temperature for 3 h. The mixture was concentrated and the residue was purified by flash chromatography (hexane/EtOAc: 30/1) to yield the title compound (*E*/*Z* > 20/1) as colorless oil (1.22 g, 4.0 mmol, 95%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 6.96 (dt, *J* = 15.6, 6.9 Hz, 1H), 5.80 (dt, *J* = 15.6, 1.6 Hz, 1H), 5.42 – 5.27 (m, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 2.18 (qd, *J* = 7.1, 1.6 Hz, 2H), 2.07 – 1.92 (m, 4H), 1.50 – 1.38 (m, 2H), 1.38 – 1.18 (m, 19H), 0.95 – 0.83 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 167.0, 149.7, 130.0, 121.3, 60.3, 32.4, 32.1, 29.9, 29.6, 29.5, 29.4, 29.3, 28.1, 27.3, 27.1, 22.5, 14.4, 14.2; **IR** (ν_{max} /cm^{-1}): 2924, 2854, 1721, 1654, 1464, 1367, 1308, 1264, 1178, 1043; **ESI-MS** calcd for $C_{20}H_{36}O_2Na$ (MNa^+) 331.26075; found 331.26067.

(2*E*,13*Z*)-Octadeca-2,13-dien-1-ol. DIBAL (1 M in CH_2Cl_2, 10.7 mL, 2.5 equiv) was slowly added to a stirred solution of ethyl (2*E*,13*Z*)-octadeca-2,13-dienoate (1.32 g, 4.3 mmol, 1.0 equiv) in CH_2Cl_2 (8 mL) at –78 °C. The mixture was stirred for 2 h at –78 °C before MeOH (5 mL) was carefully added. The mixture was then warmed to ambient temperature before sat. potassium sodium tartrate aq. was added. After vigorous stirring, the phases could be separated, the aqueous layer was extracted with CH_2Cl_2 (3 x) and the combined organic phases were dried over $MgSO_4$ and concentrated. The residue was purified by flash chromatography (hexane/EtOAc, 10/1) to yield the title compound as colorless oil (1.09 g, 4.1 mmol, 97%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 5.77 – 5.55 (m, 2H), 5.42 – 5.28 (m, 2H), 4.13 – 4.03 (m, 2H), 2.13 – 1.93 (m, 6H), 1.58 – 1.43 (bs, 1H), 1.43 – 1.19 (m, 18H), 0.99 – 0.83 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 133.8, 130.02, 130.00, 128.9, 64.0, 32.4, 32.1, 29.91, 29.72, 29.68, 29.63, 29.44, 29.34, 29.27, 27.3, 27.1, 22.5, 14.2; **IR** (ν_{max} /cm^{-1}): 3312, 2922, 2853, 1463, 1089, 1002, 968; **ESI-MS** calcd for $C_{18}H_{34}ONa$ (MNa^+) 289.25018; found 289.24978.

Ethyl (*E*)-8-hydroxyoct-6-enoate. Grubbs 2nd generation catalyst (59 mg, 0.07 mmol, 1 mol%) was added to a stirred solution of ethyl 6-heptenoate (1.23 mL, 7 mmol, 1.0

equiv) and *trans*-crotonaldehyde (2.9 mL, 35 mmol, 5 equiv) and the resulting mixture was stirred at reflux temperature for 5 h. The mixture was concentrated and the residue was purified by flash chromatography (hexane/EtOAc: 5/1).

The resulting aldehyde was dissovled in MeOH (20 mL) and sodium borohydride (330 mg, 8.7 mmol, 1.2 equiv) was added in one portion. The mixture was stirred for 1 h before sat. NH_4Cl aq. was added. The aqueous layer was extracted with EtOAc (3 x), the combined organic phases were washed with brine, dried over $MgSO_4$ and concentrated, and the residue was purified by flash chromatography (hexane/EtOAc: 5/1) to yield the title compound as colorless oil (0.97 g, 5.2 mmol, 74%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 5.74 – 5.56 (m, 2H), 4.19 – 4.04 (m, 4H), 2.29 (t, *J* = 7.4 Hz, 2H), 2.13 – 2.01 (m, 2H), 1.70 – 1.57 (m, 2H), 1.52 – 1.47 (bs, 1H), 1.48 – 1.36 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 173.9, 132.8, 129.4, 63.9, 60.4, 34.3, 31.9, 28.7, 24.6, 14.4; **IR** *(ν_{max}* /cm^{-1}): 3408, 2981, 2933, 2859, 1732, 1373, 1181, 1150, 1094, 1008, 969; **ESI-MS** calcd for $C_{10}H_{18}O_3Na$ (MNa^+) 209.11481; found 209.11477.

References

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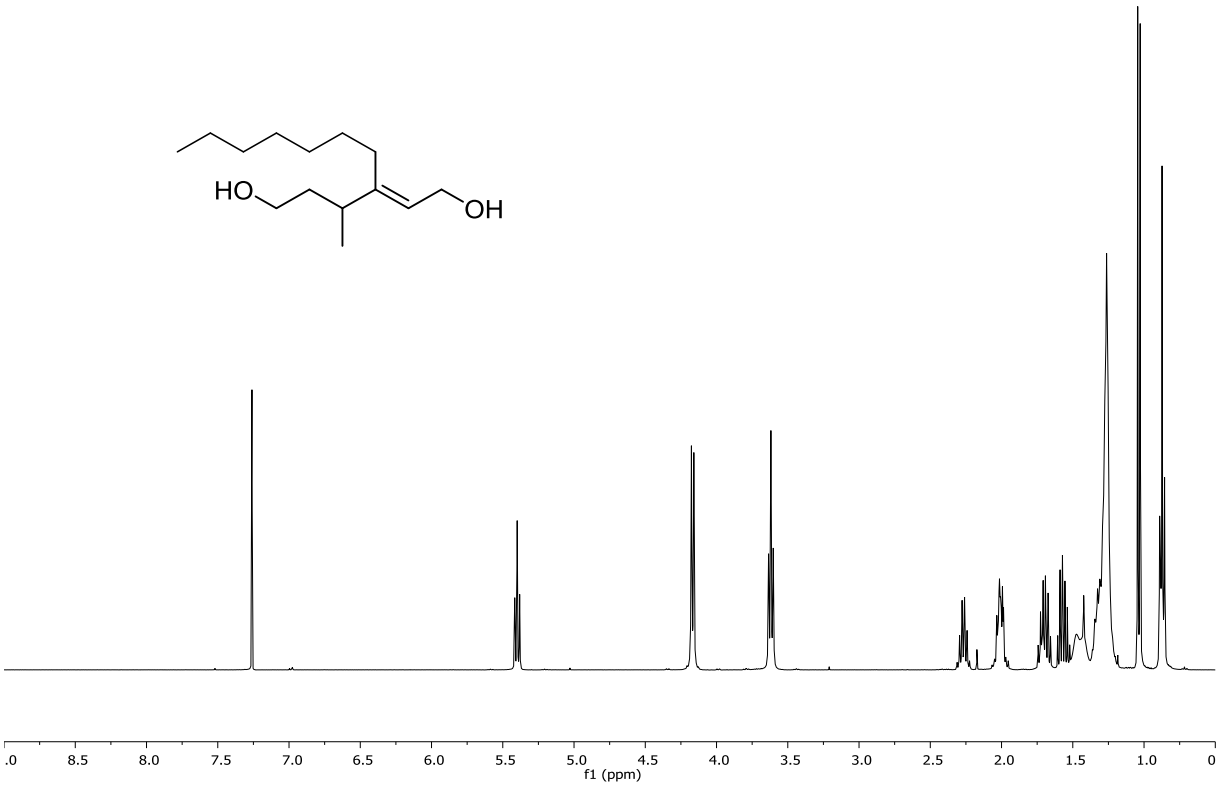
HO
OH
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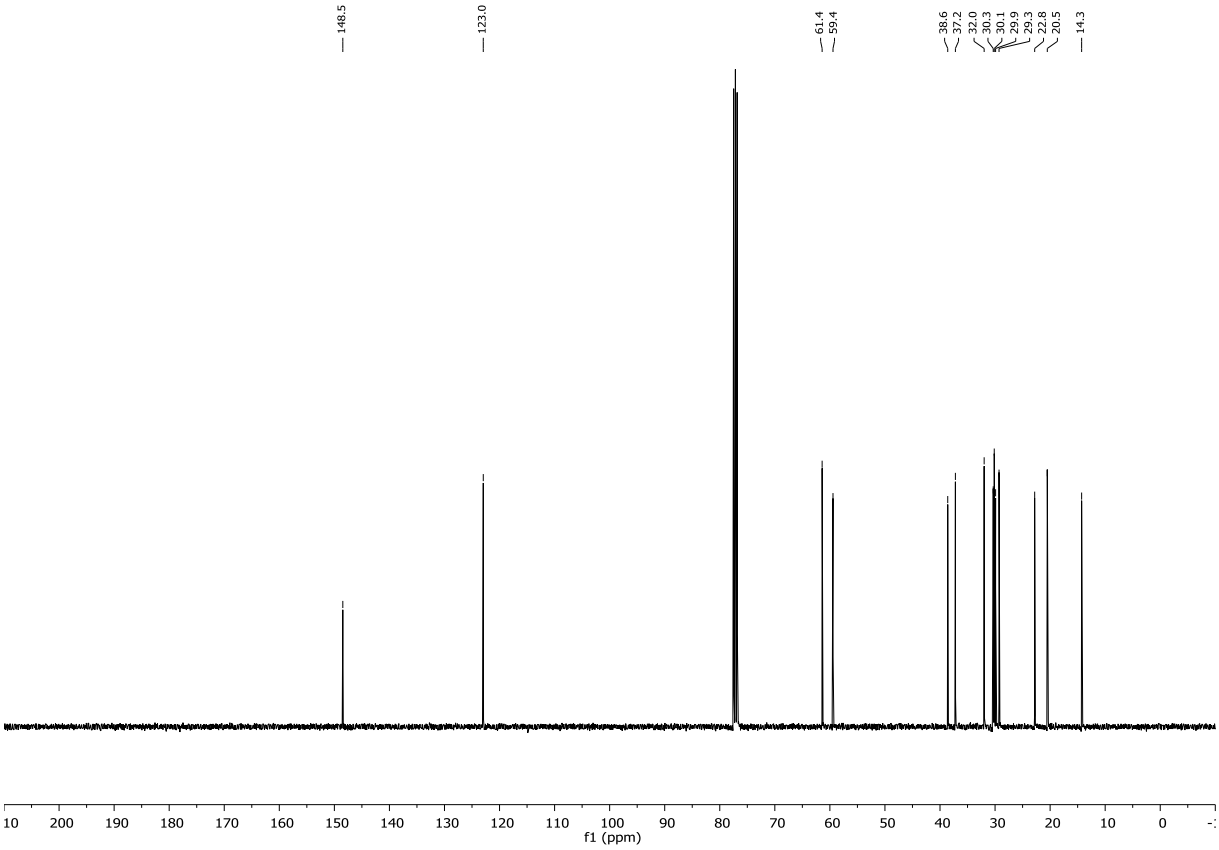
f1 (ppm)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37.2
32.0
30.3
30.1
29.9
29.3
22.8
20.5
14.3
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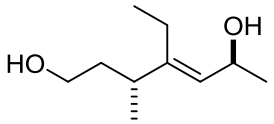
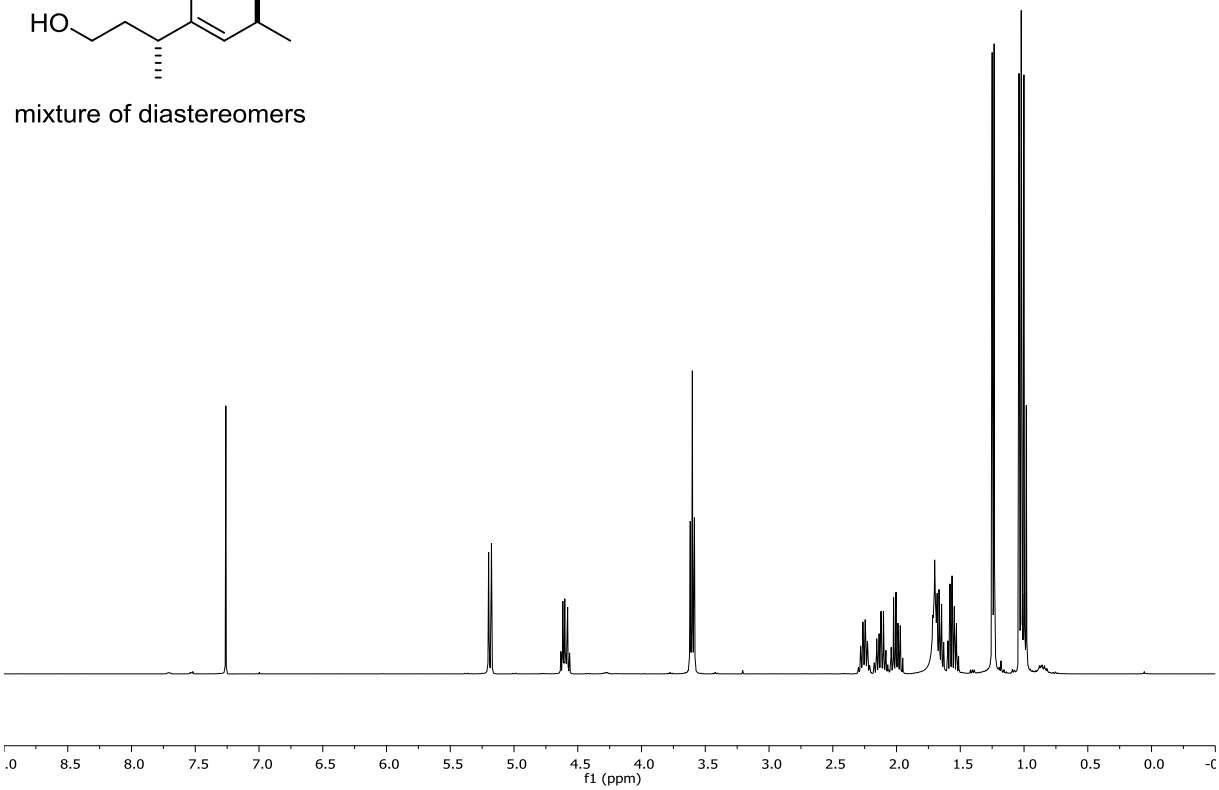
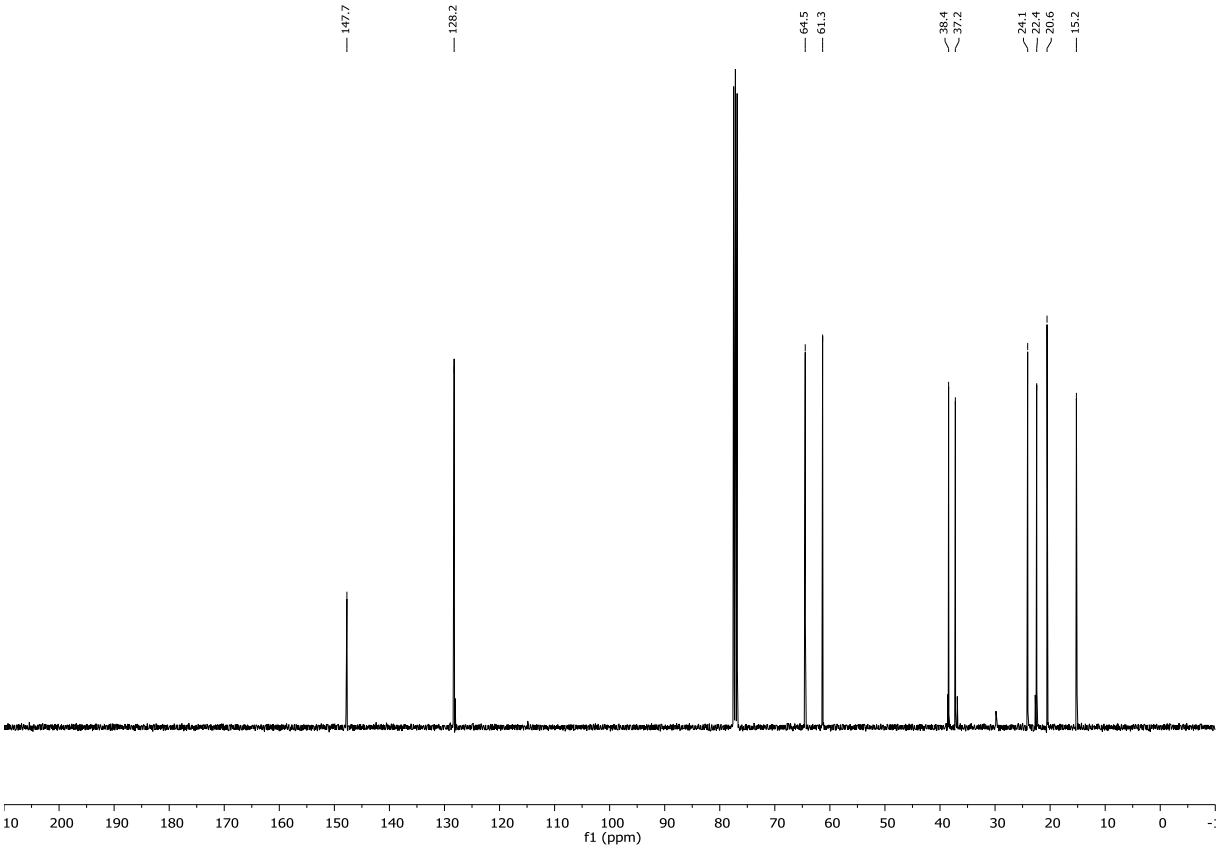
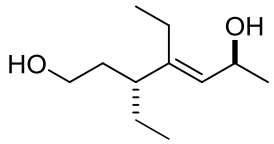
f1 (ppm)



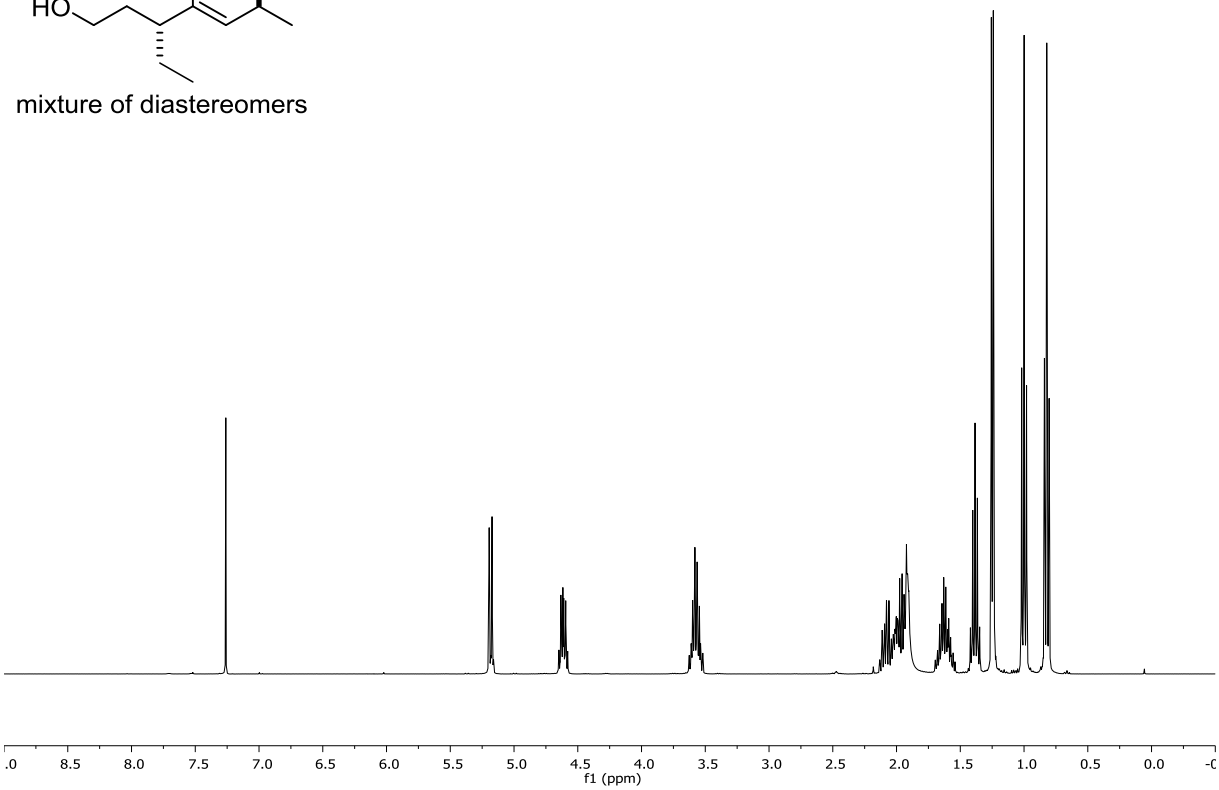
mixture of diastereomers

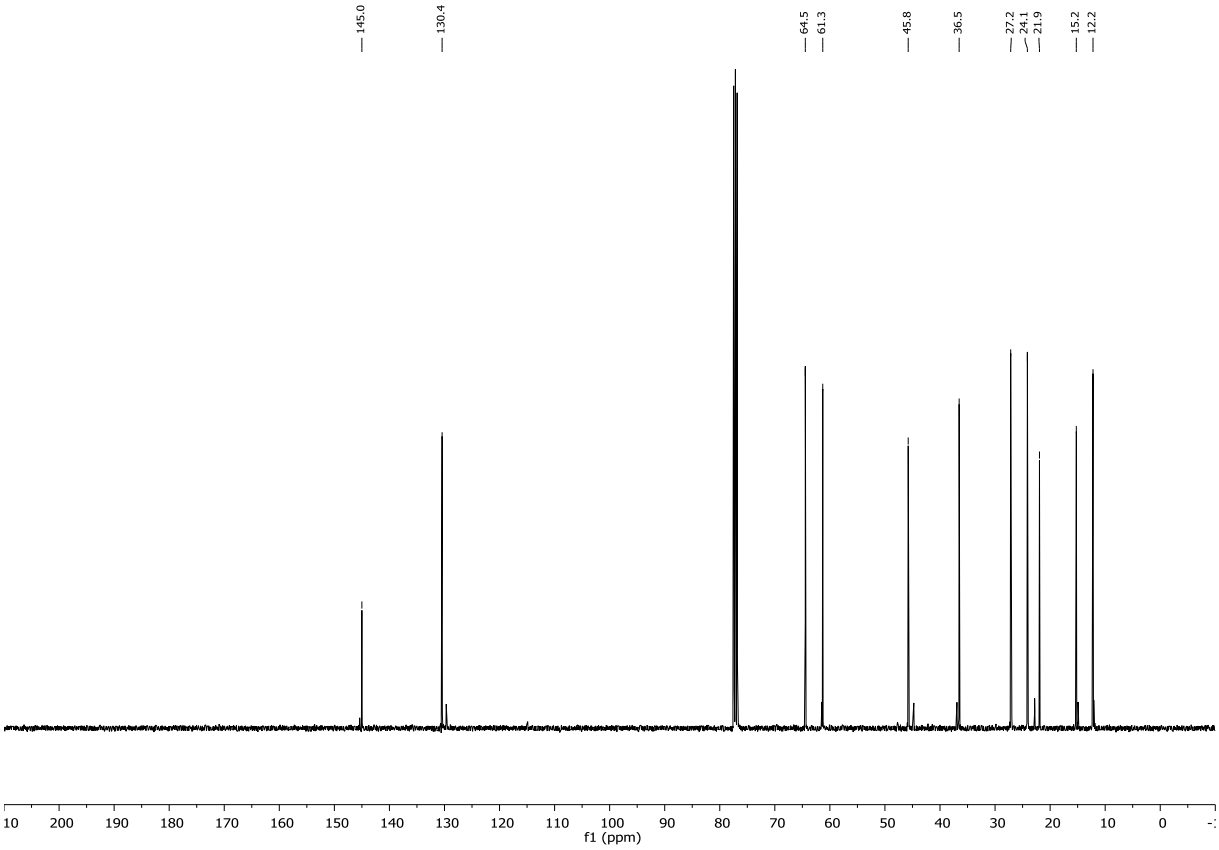


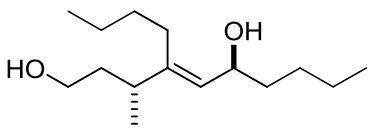




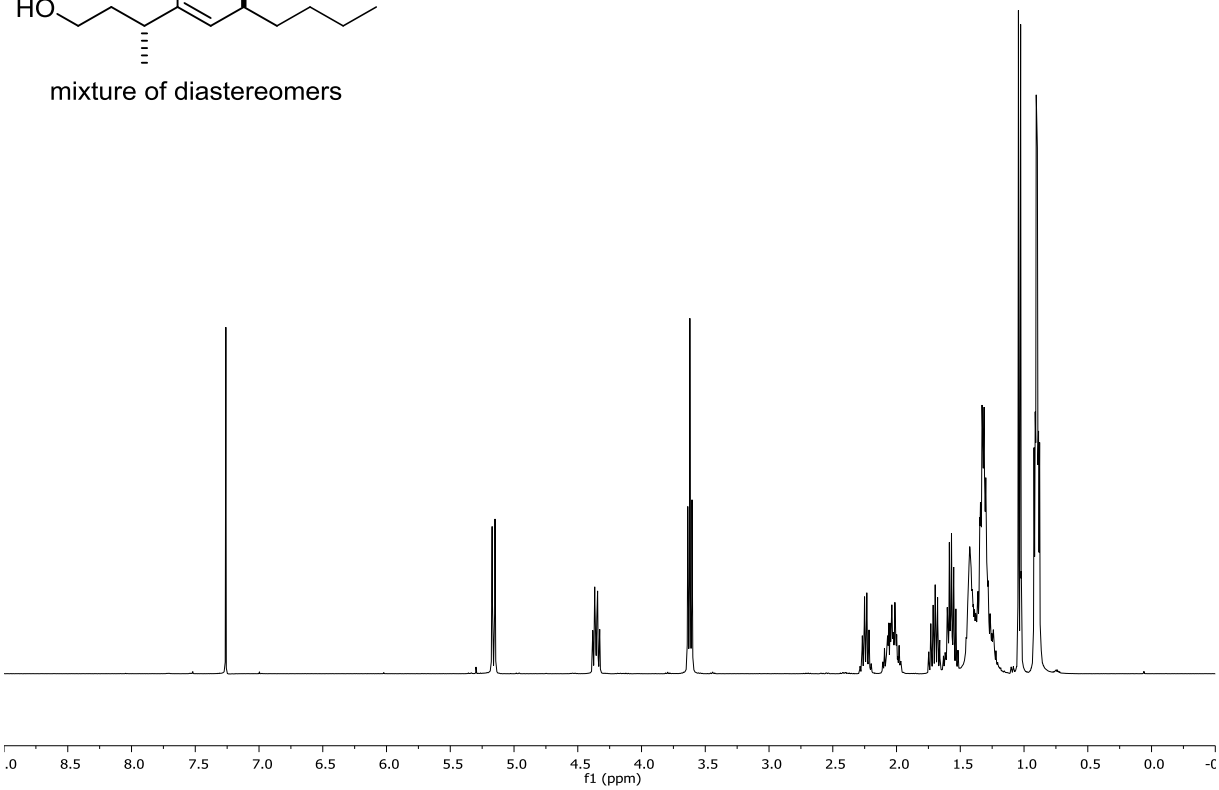
mixture of diastereomers

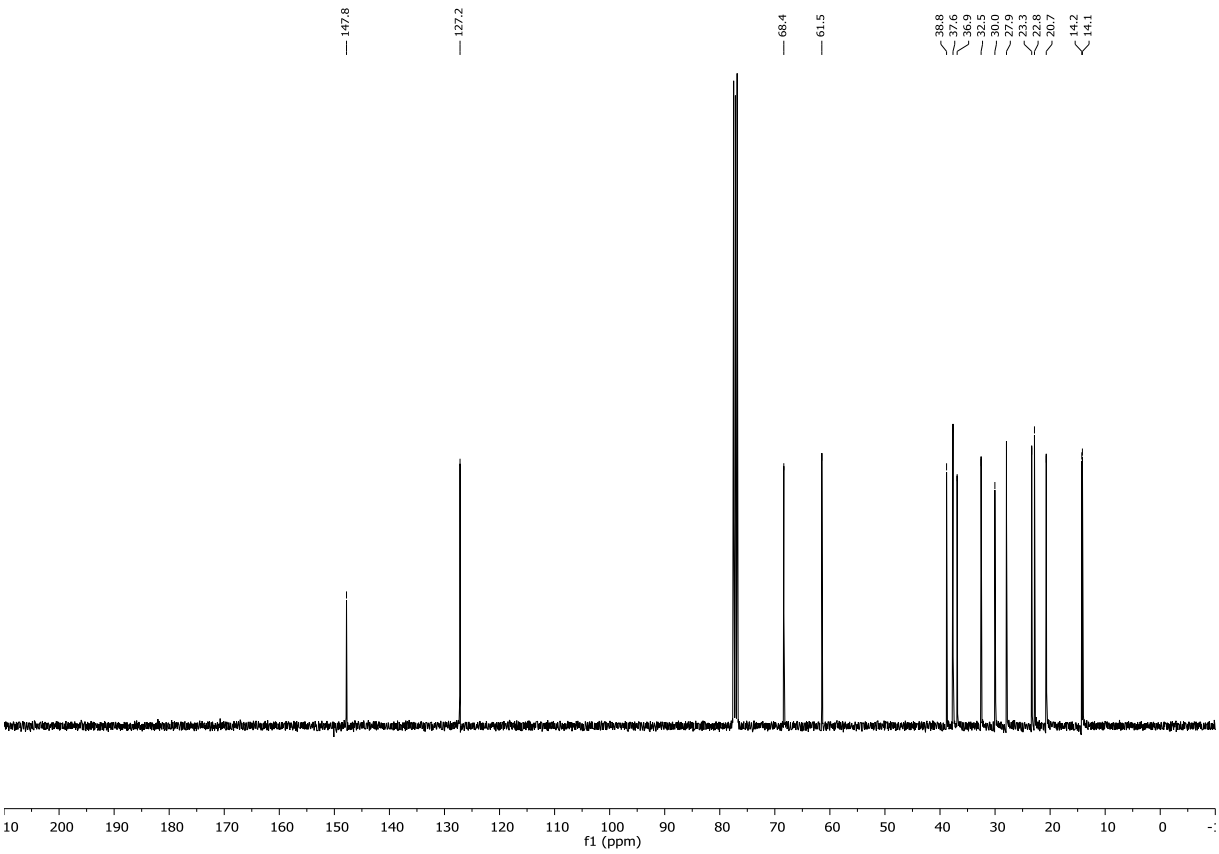


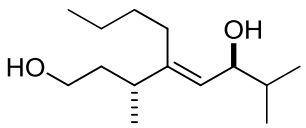




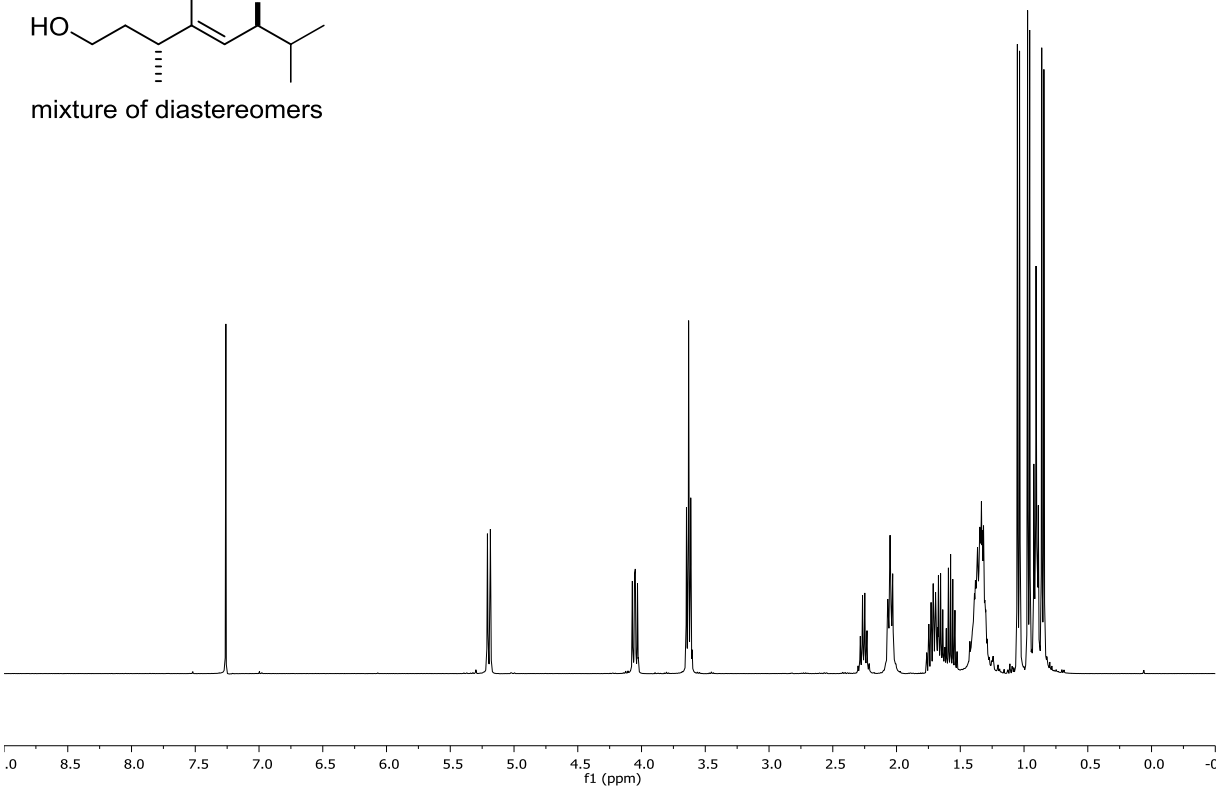
mixture of diastereomers

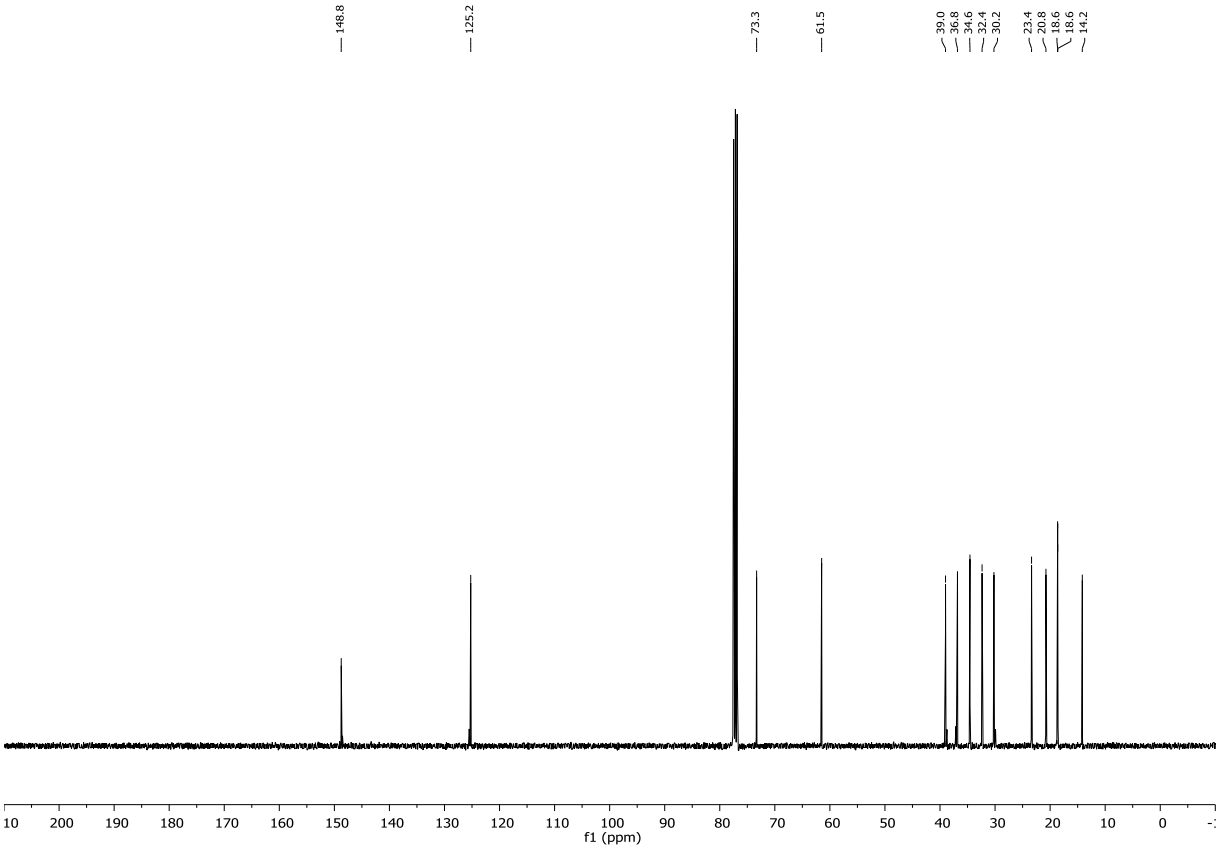


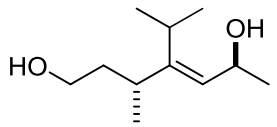




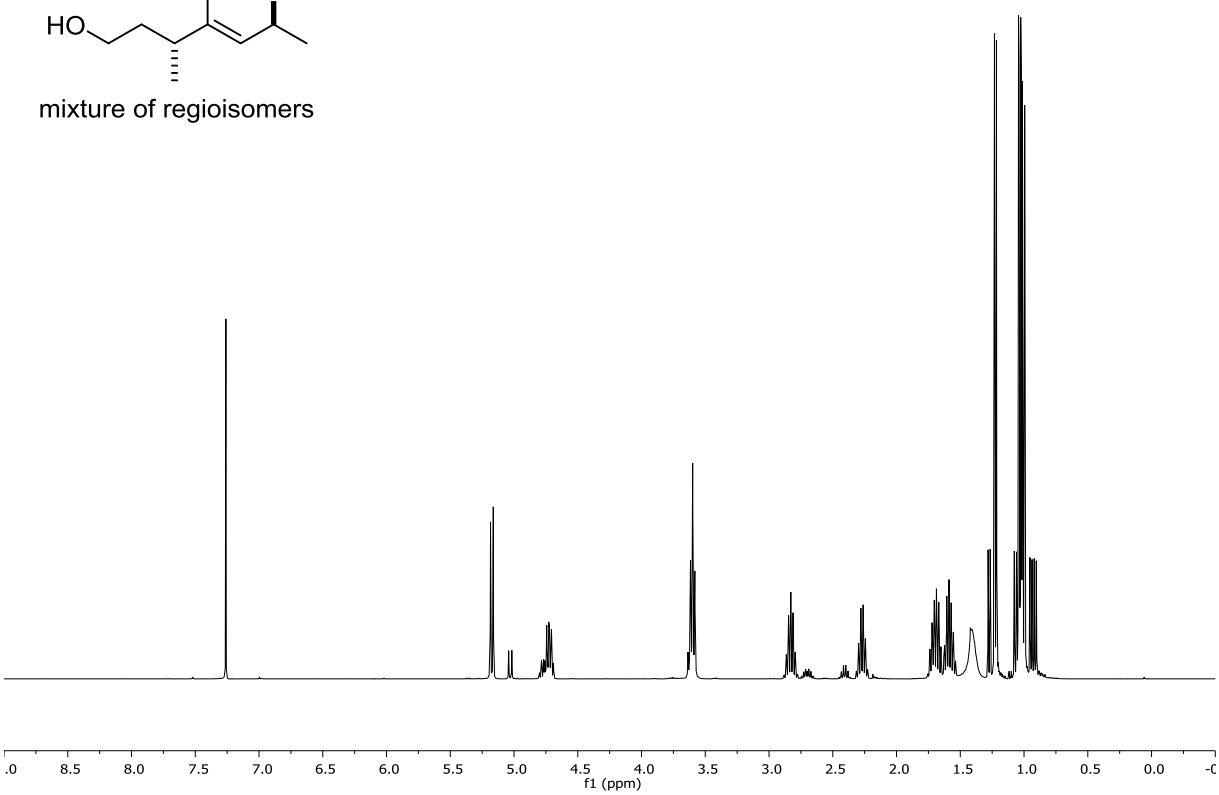
mixture of diastereomers

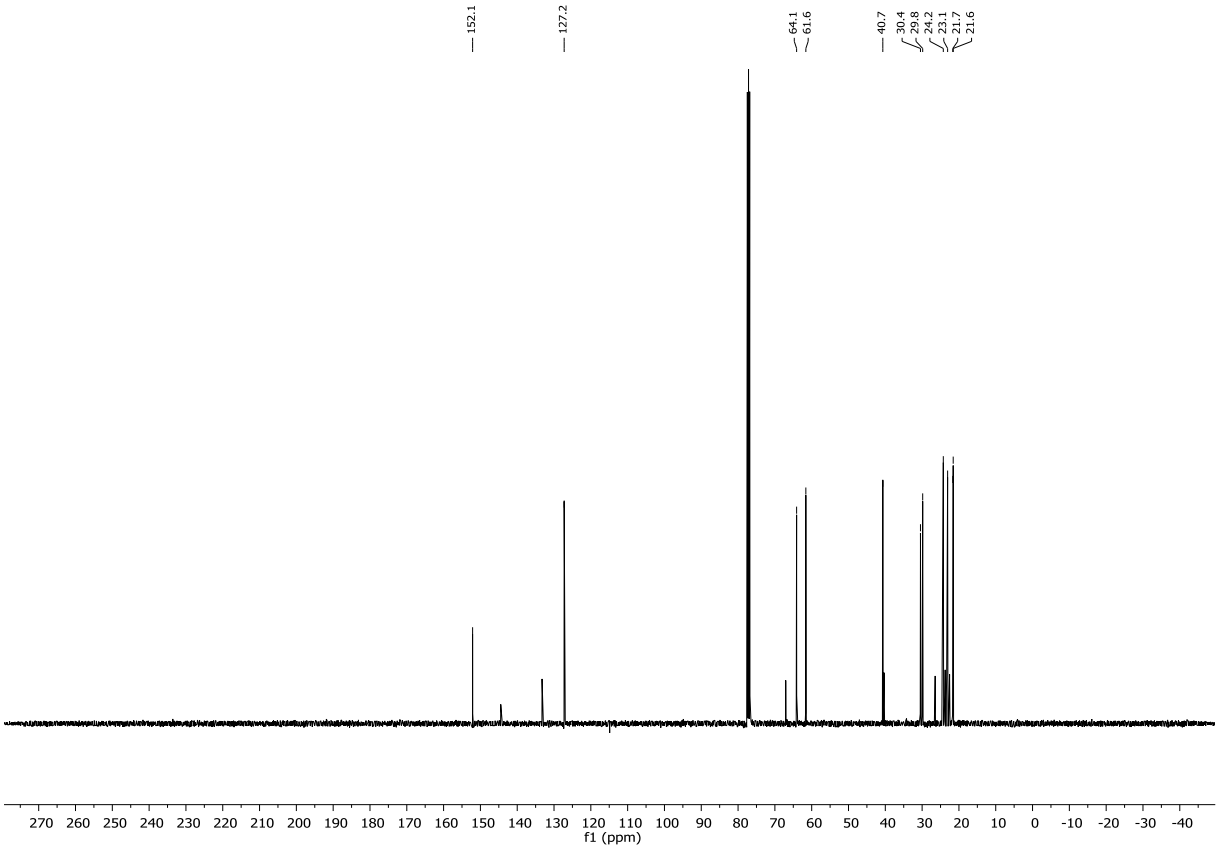


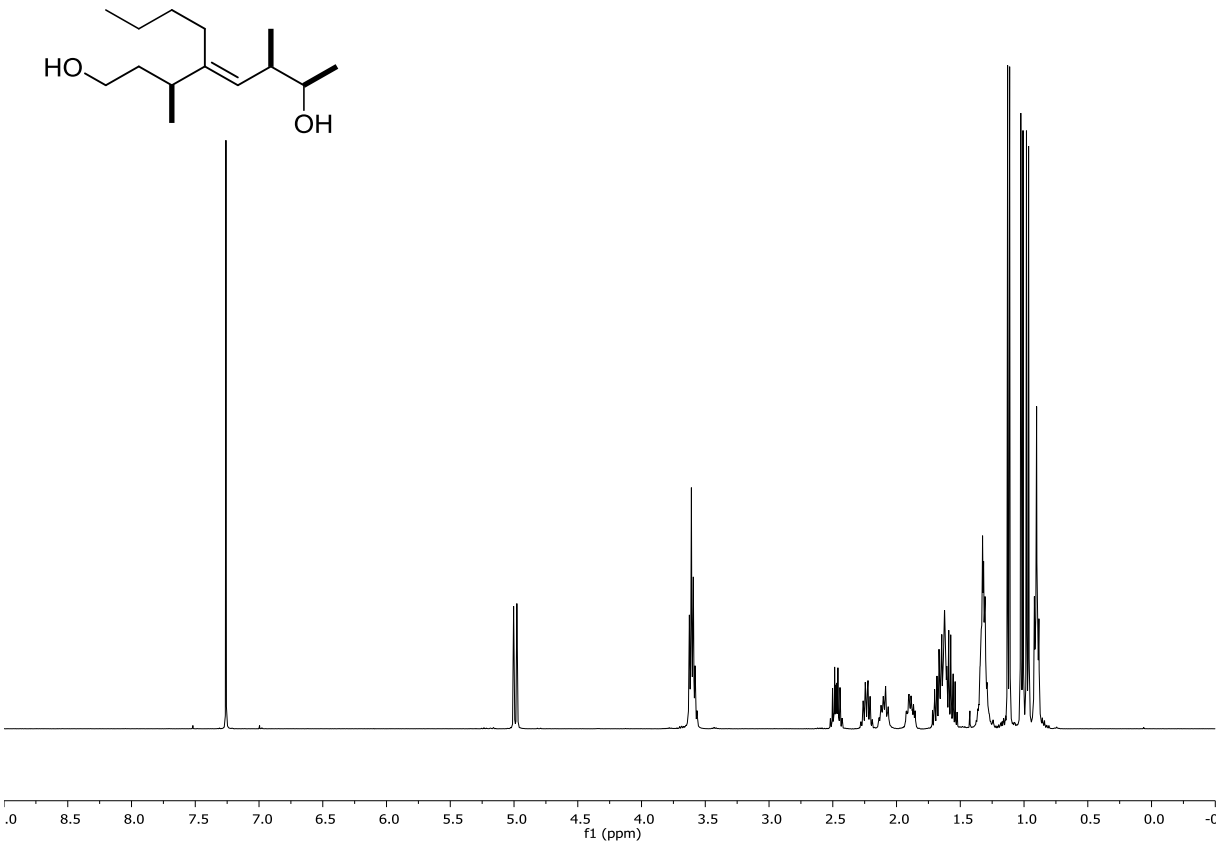




mixture of regioisomers



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OH
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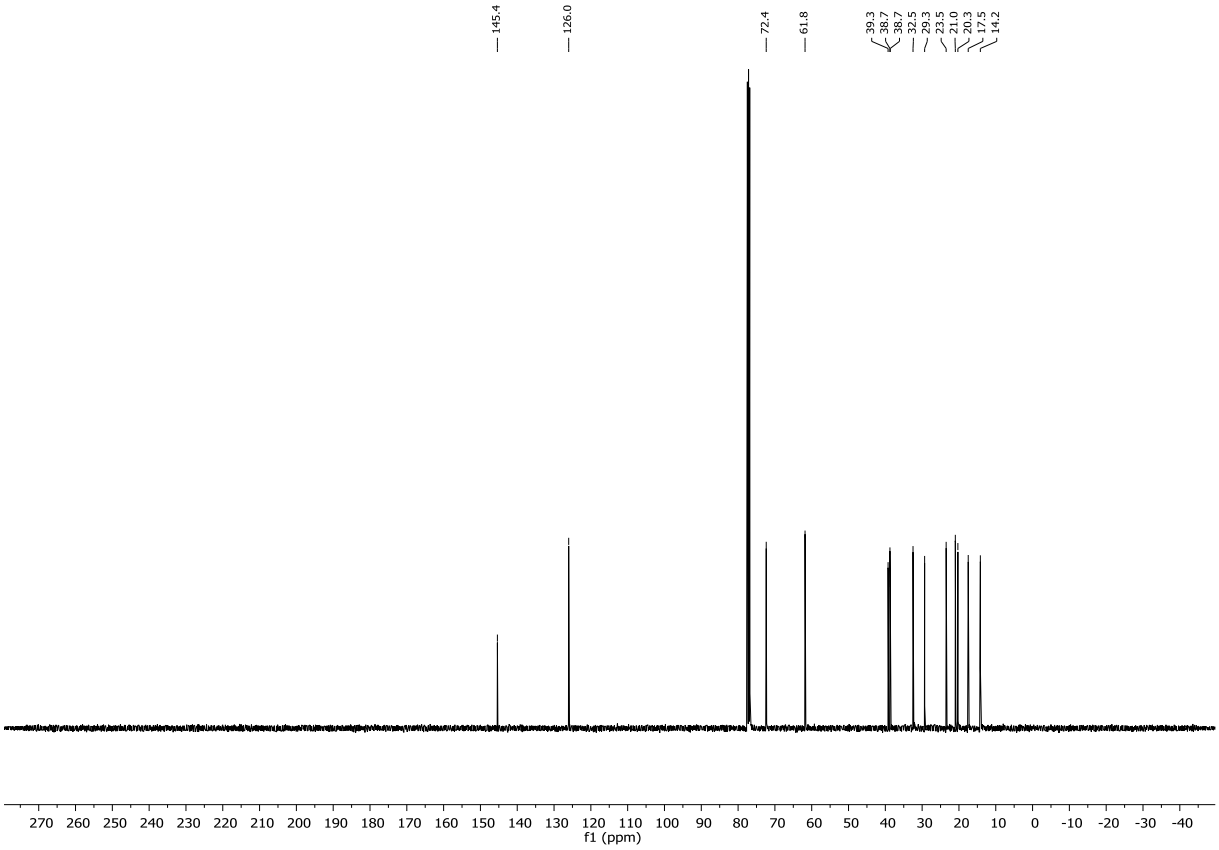
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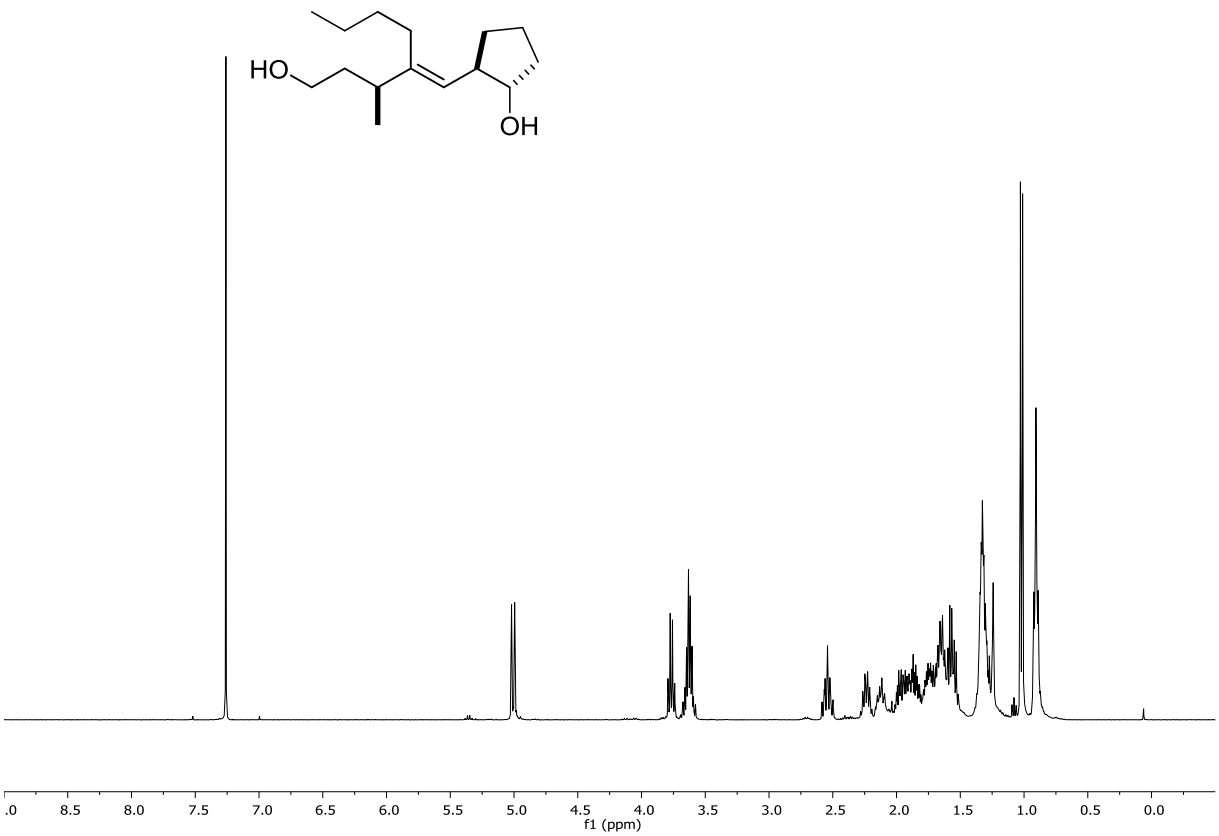
72.4
61.8
39.3
38.7
38.7
32.5
29.3
23.5
21.0
20.3
17.5
14.2
f1 (ppm)


HO
OH
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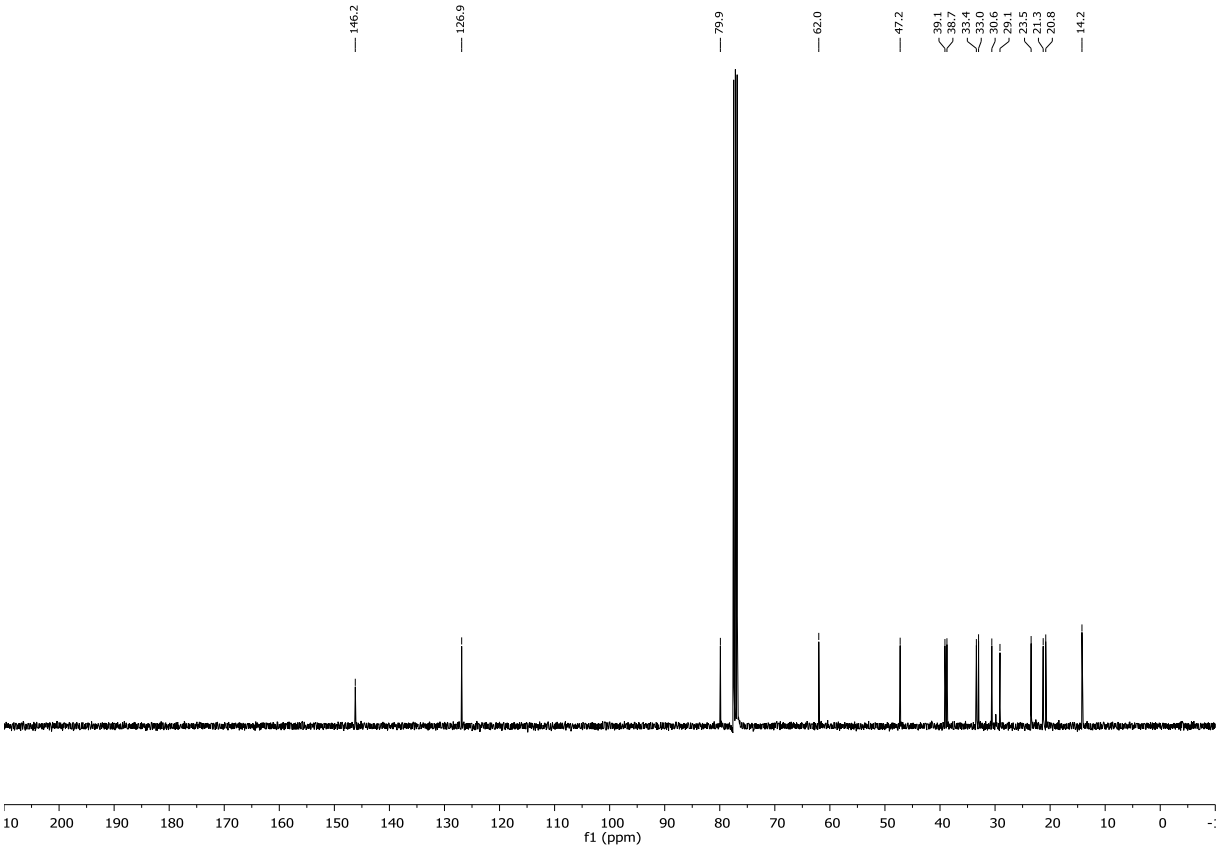
f1 (ppm)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38.7
33.4
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29.1
23.5
21.3
20.8
14.2
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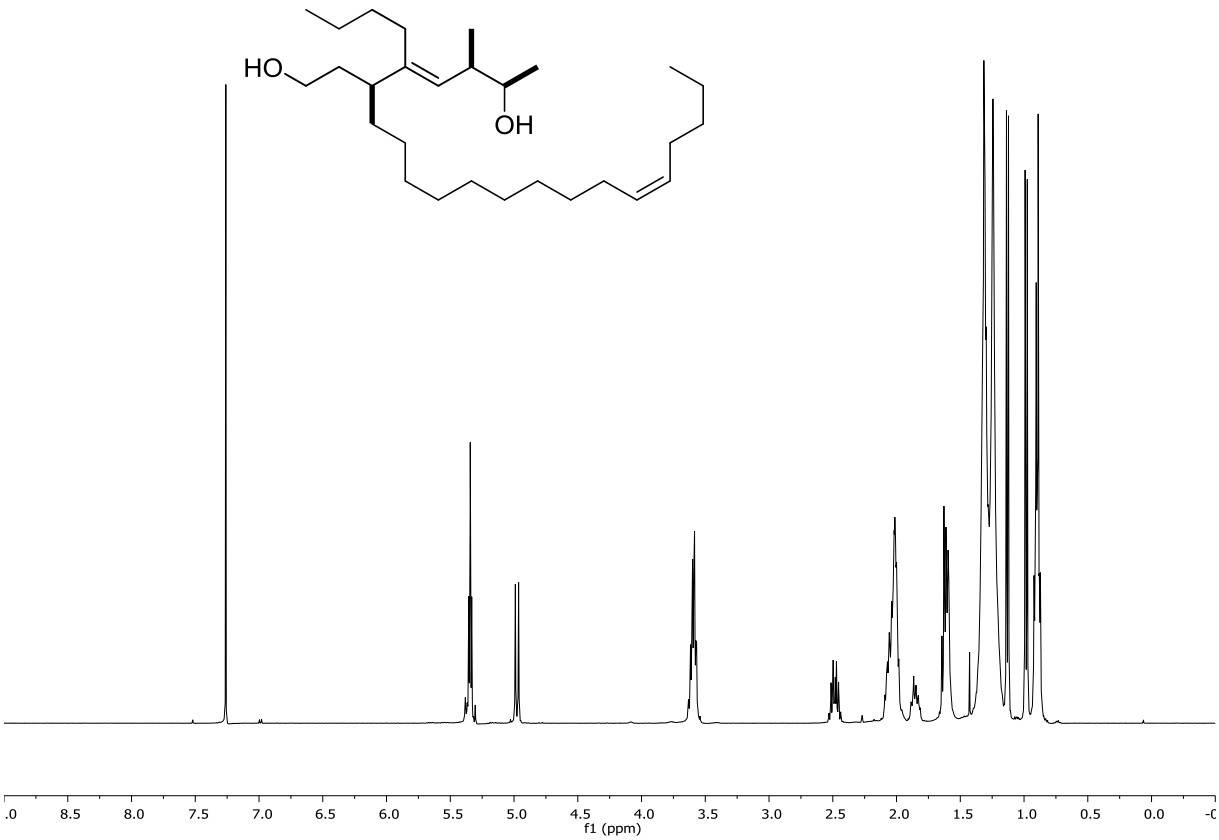
f1 (ppm)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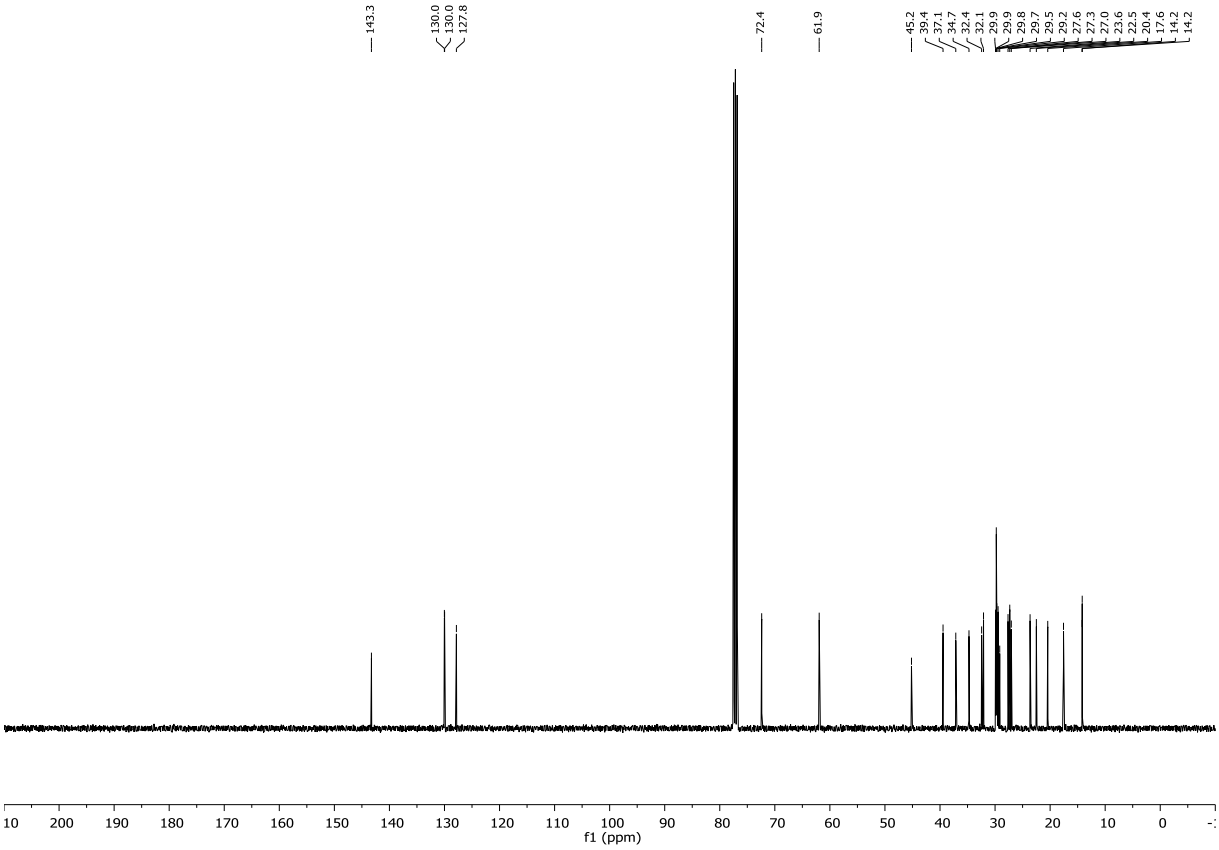
OH
f1 (ppm)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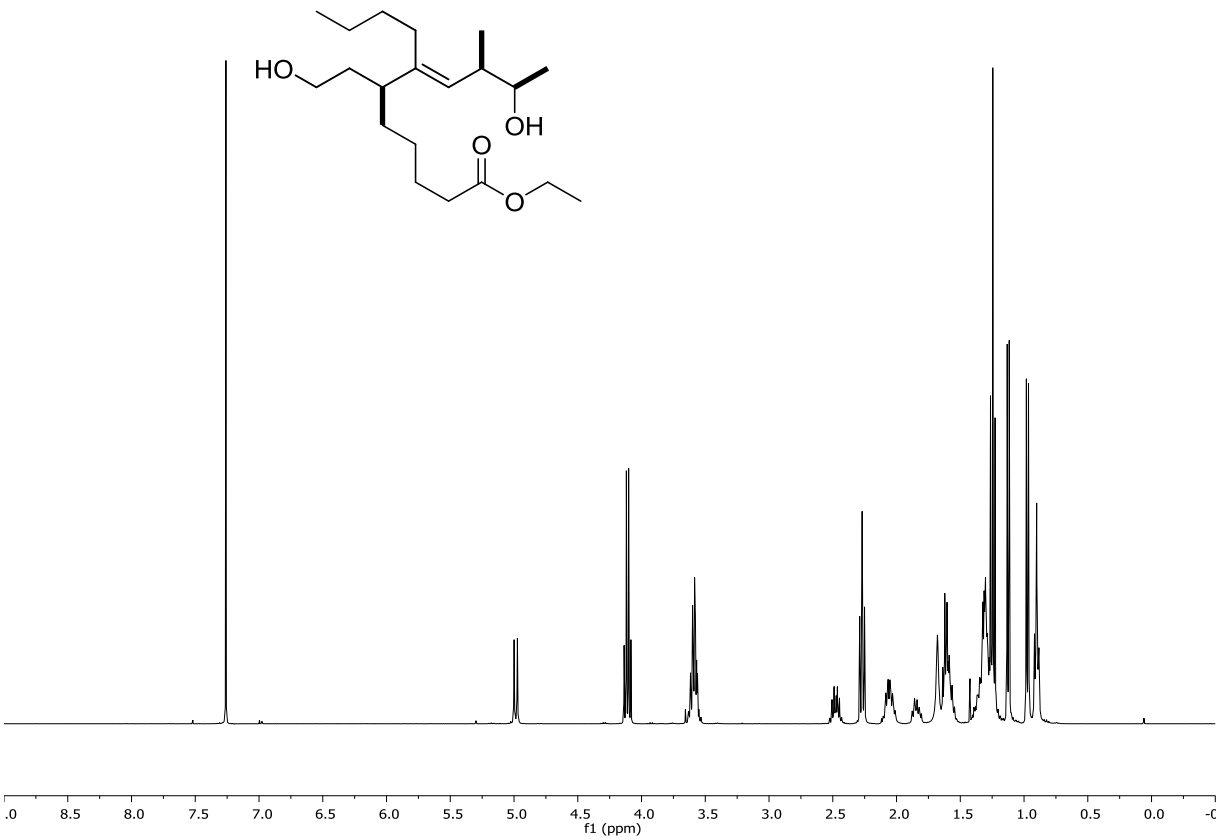
130.0
127.8
72.4
61.9
45.2
39.4
37.1
34.7
32.4
32.1
29.9
29.9
29.8
29.7
29.5
29.2
27.6
27.3
27.0
23.6
22.5
20.4
17.6
14.2
14.2
f1 (ppm)


HO
OH
O
O
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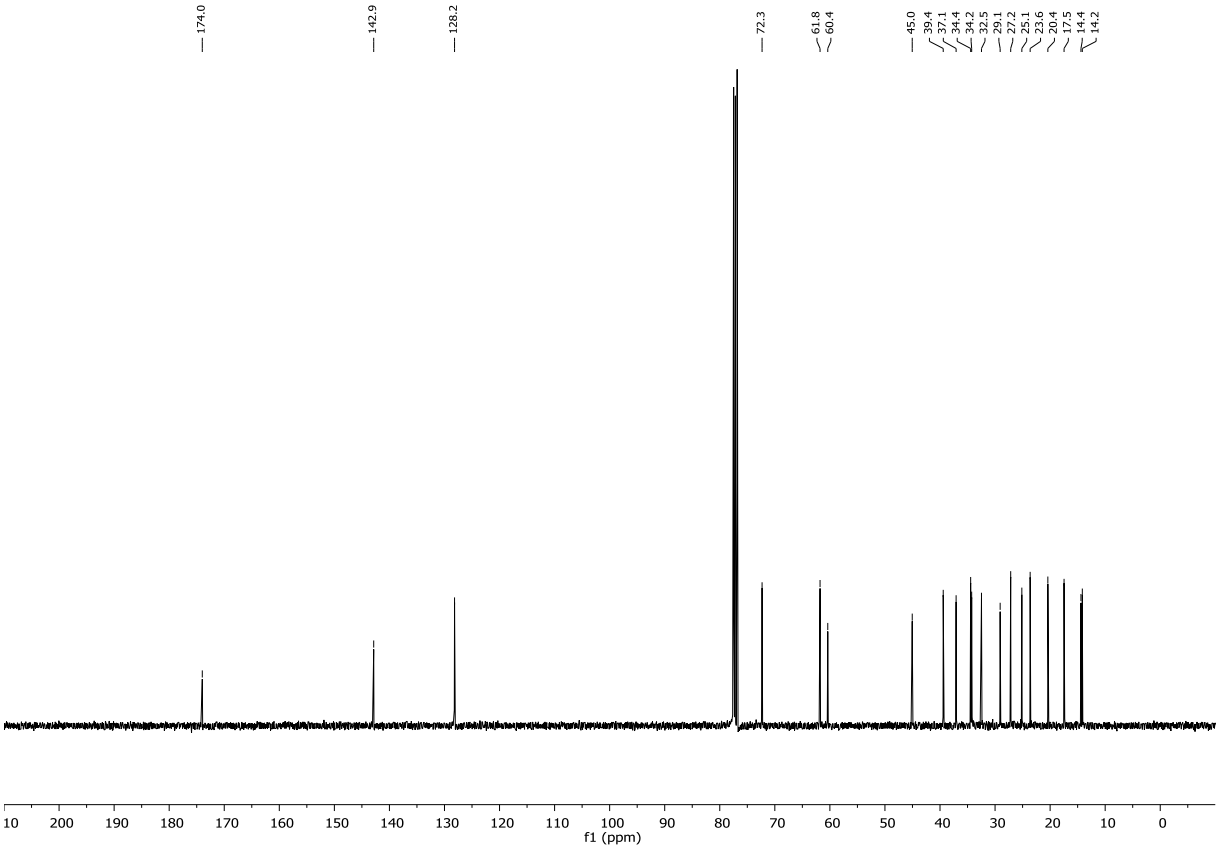
f1 (ppm)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72.3
61.8
60.4
45.0
39.4
37.1
34.4
34.2
32.5
29.1
27.2
25.1
23.6
20.4
17.5
14.4
14.2
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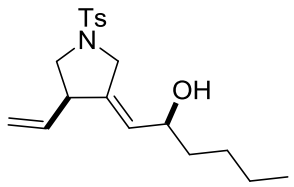
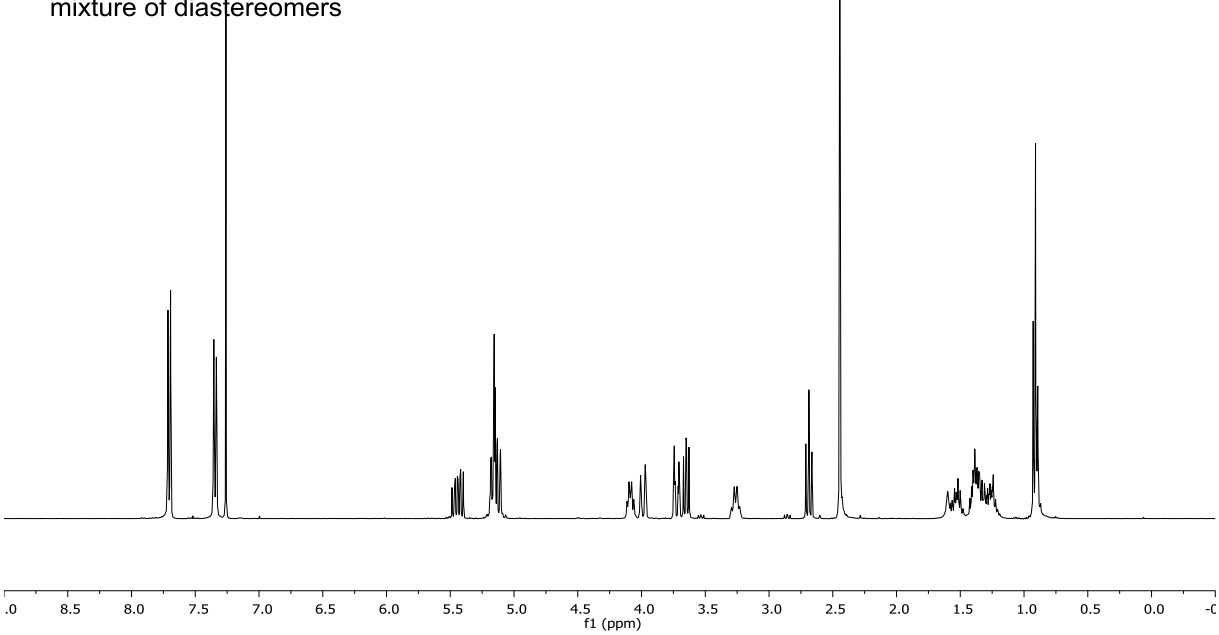
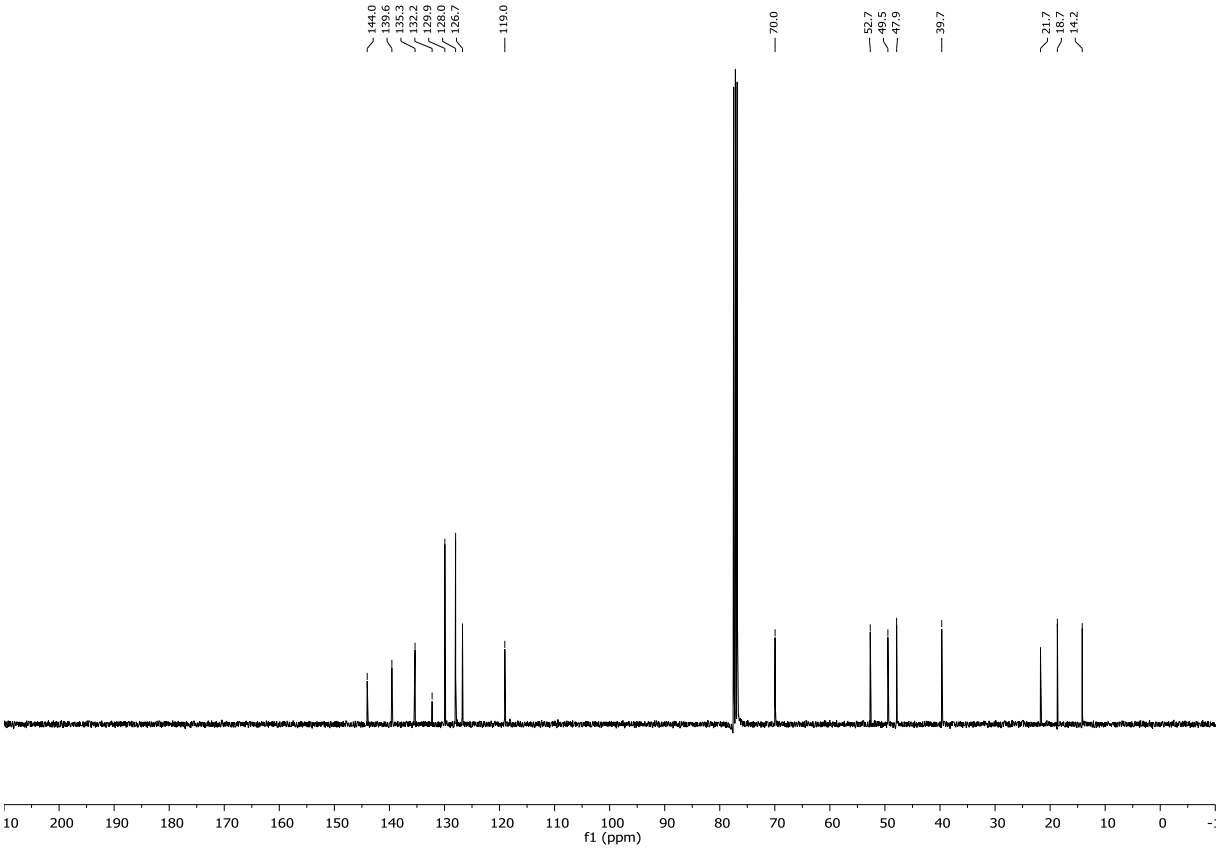
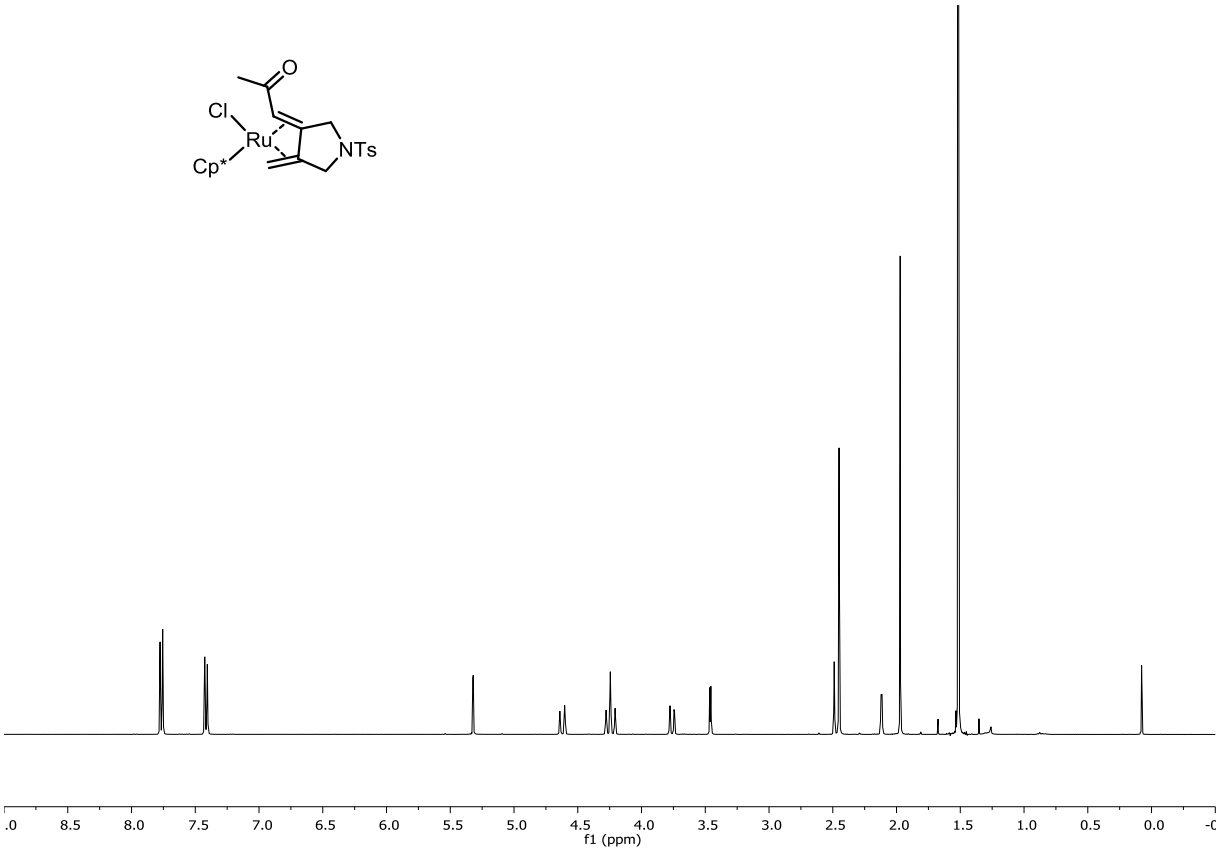
f1 (ppm)

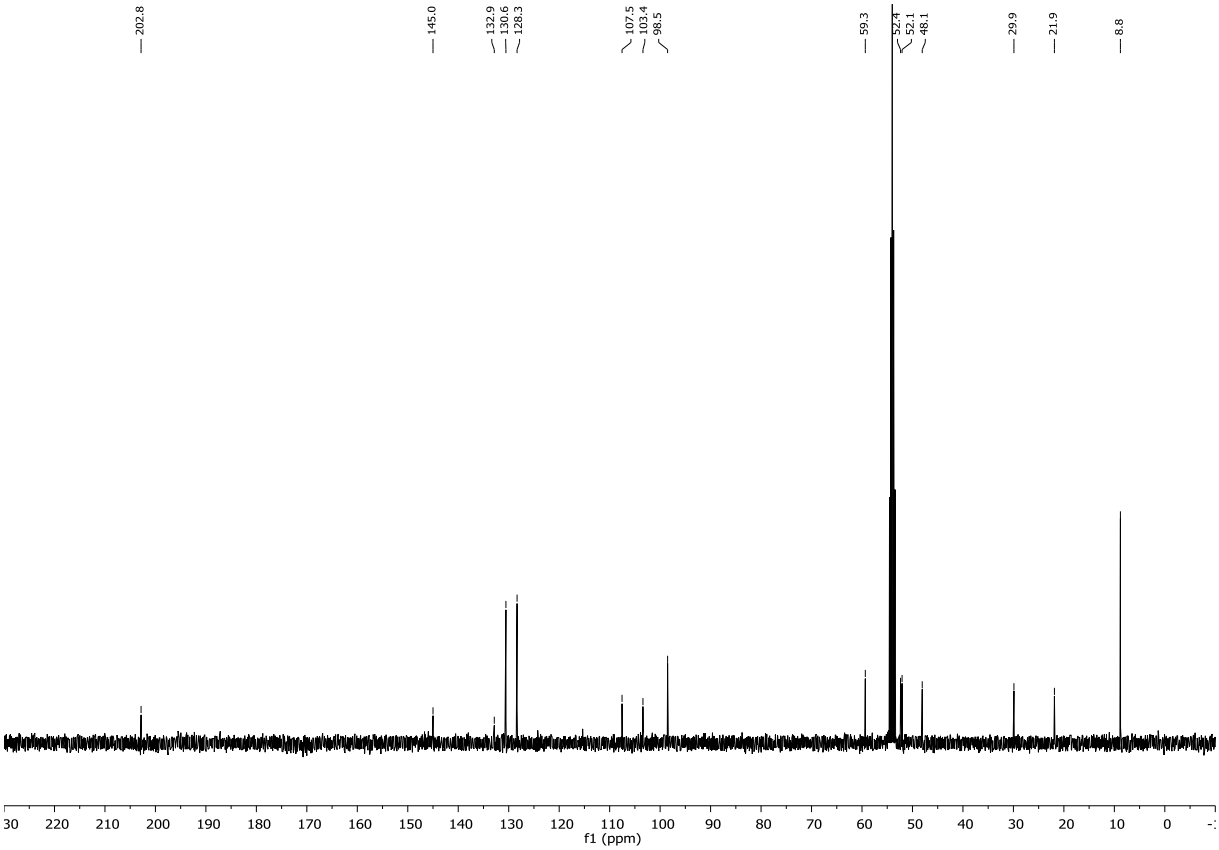


mixture of diastereomers






O
Cl
Ru
Cp*
NTs
f1 (ppm)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52.4
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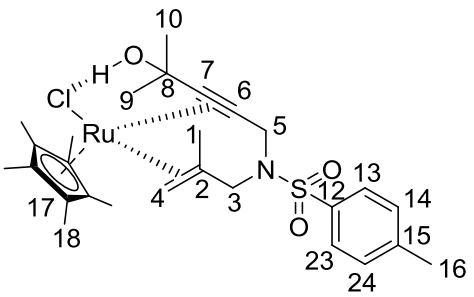
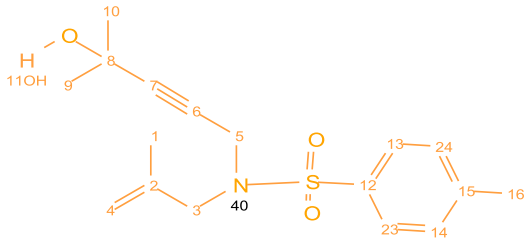
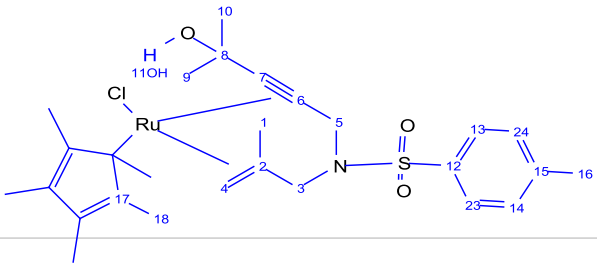
29.9
21.9
8.8
f1 (ppm)

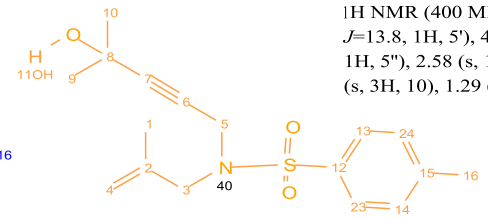


Assignments					
Atom	Chemical Shift	COSY	HSQC	HMBC	NOESY/EXSY
1 C	19.277		1	4', 4'', 3''	
H3	1.04		1	4, 2, 3	11OH, 4'', 9
2 C	82.445			1, 3', 3''	
3 C	56.912		3'', 3'	1, 5', 4', 4''	
H'	4.482	3''	3	5, 2	13, 18
H''	1.664	3'	3	1, 2	
4 C	64.361		4', 4''	1	
H'	3.654	4''	4	1, 3	18, 4''
H''	2.582	4'	4	1, 3	4', 1, 18
5 C	35.636		5', 5''	3'	
H'	4.812	5''	5	3, 6	13, 18, 5''
H''	2.691	5'	5	6, 7	13, 18, 5'
6 C	75.611			5', 5''	
7 C	78.128			11OH, 5'', 9, 10	
8 C	70.086			11OH, 9, 10	
9 C	34.418		9	11OH, 10	
H3	1.727		9	10, 8, 7	11OH, 1
10 C	36.002		10	9	
H3	1.405		10	9, 8, 7	11OH
11OH H	4.684			8, 9, 7	18, 10, 1, 9
12 C	132.949			14	
13 C	128.875		13		
H	7.681	14	13	23, 15	18, 3', 5'', 5'
14 C	130.4		14	16	
H	7.431	13	14	24, 12, 16	16, 18
15 C	144.795			13, 16	
16 C	21.444		16	14	
H3	2.403		16	14, 15, 24	14
17 C	96.778			18	
18 C	9.218				
H3	1.294			17	13, 14, 11OH, 3', 4', 5'', 4'', 5'
23 C	128.875			13	
H	7.681				
24 C	130.4			14, 16	
H	7.431				

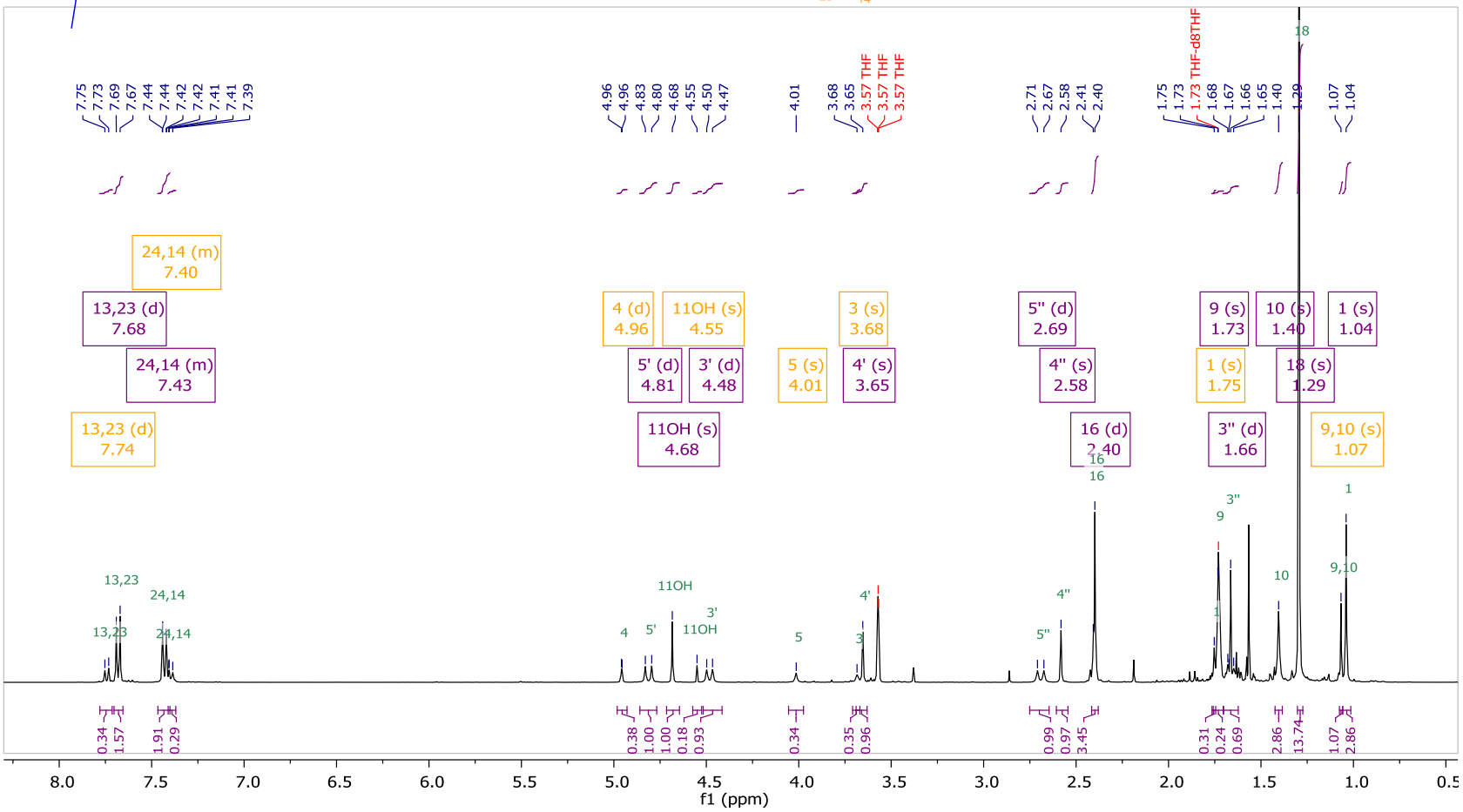


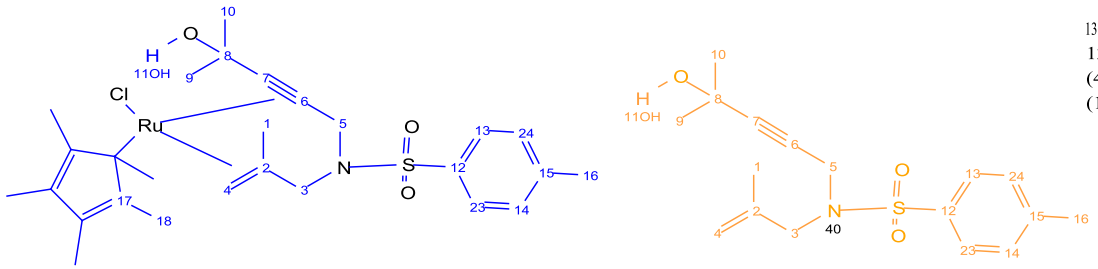
Assignments			
Atom	Chemical Shift	HSQC	HMBC
1 C	20.051	1	4
H3	1.753	1	2, 4, 3
2 C	140.8		3, 1
3 C	52.929	3	4, 5, 1
H2	3.685	3	5, 4, 2
4 C	115.805	4	3, 1
H2	4.957	4	1, 3
5 C	36.115	5	3
H2	4.014	5	3, 6, 7
6 C	73.319		5
7 C	92.585		5, 9, 10
8 C	63.479		9, 10
9 C	31.636	9	11OH, 10
H3	1.067	9	10, 8, 7
10 C	31.636	10	11OH, 9
H3	1.067	10	7, 8, 9
11OH H	4.55		9, 10
12 C	137.227		14
13 C	128.793		
H	7.743		23, 15
14 C	130.456		16
H	7.399		24, 12, 16
15 C	144.193		13, 16
16 C	21.501		14
H3	2.403		15, 14, 24
23 C	128.793		13
H	7.743		
24 C	130.456		14, 16
H	7.399		



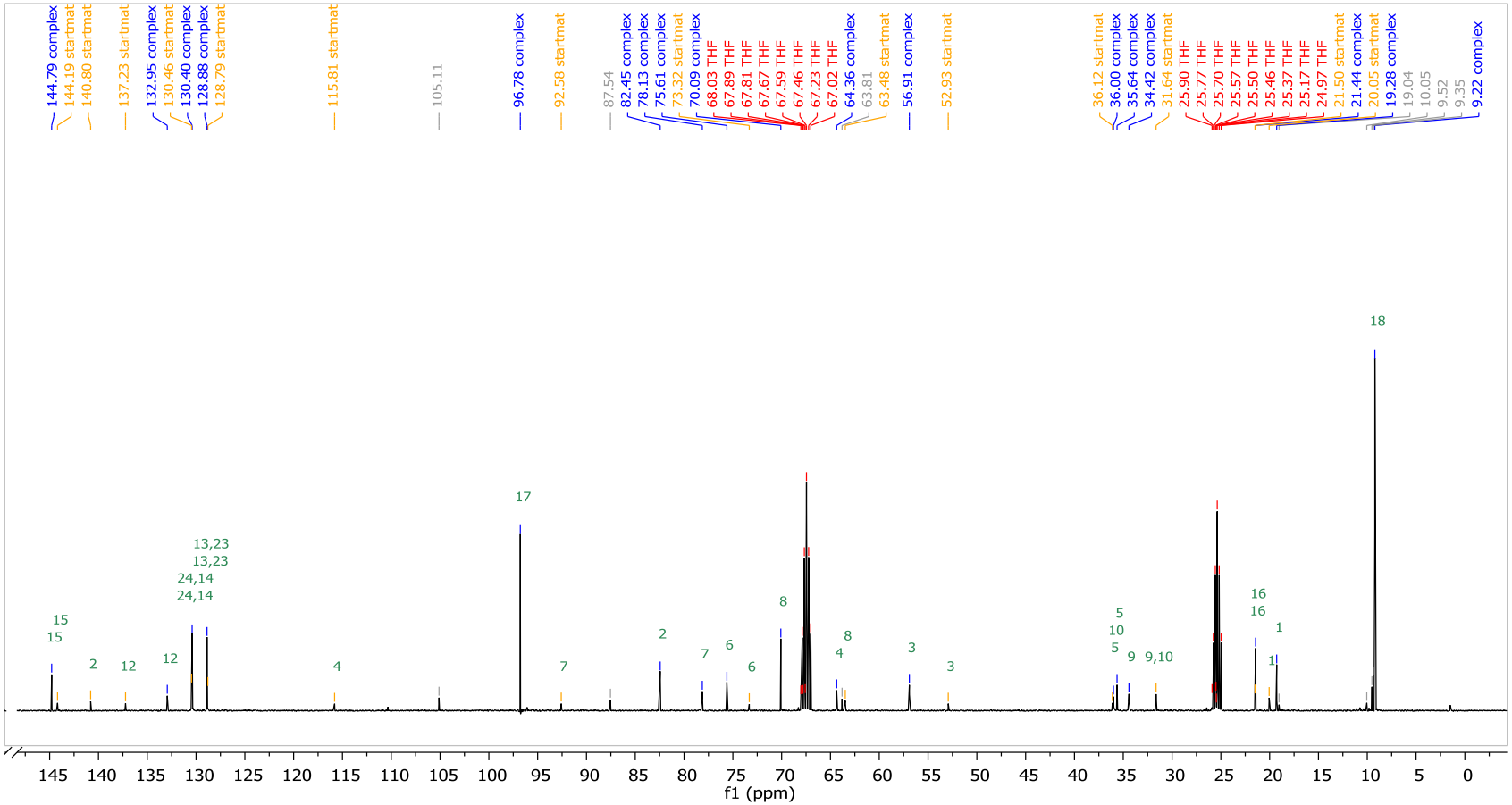


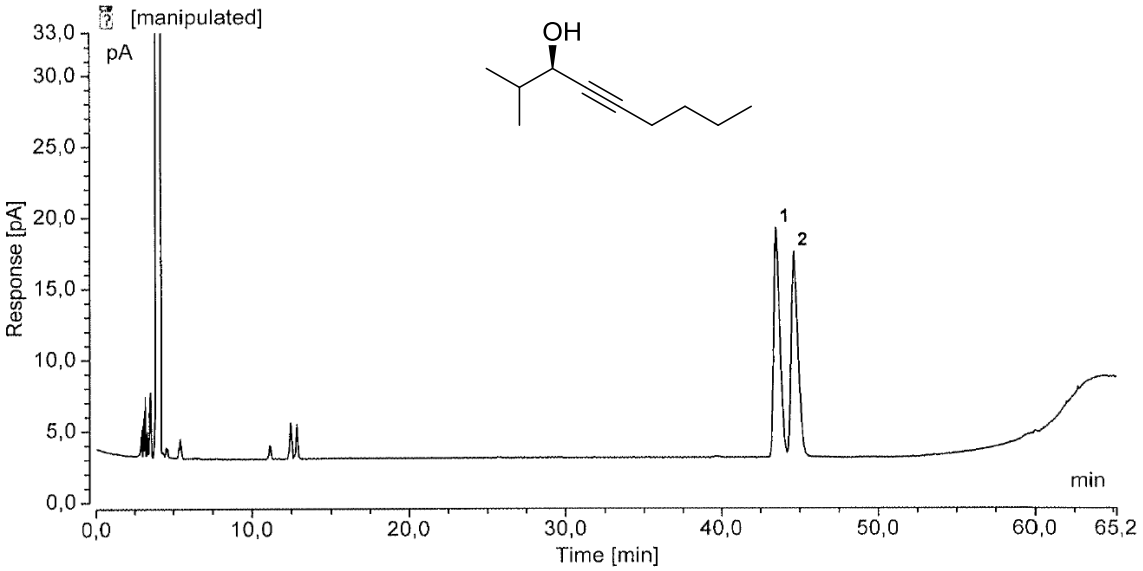
^{1}H NMR (400 MHz, THF-d_8) δ = 7.68 (d, *J*=8.3, 2H, 13, 23), 7.43 (m, 2H, 24, 14), 4.81 (d, *J*=13.8, 1H, 5'), 4.68 (s, 1H, 11OH), 4.48 (d, *J*=12.6, 1H, 3'), 3.65 (s, 1H, 4'), 2.69 (d, *J*=13.9, 1H, 5"), 2.58 (s, 1H, 4"), 2.40 (d, *J*=13.5, 3H, 16), 1.73 (s, 3H, 9), 1.66 (d, *J*=12.5, 1H, 3"), 1.40 (s, 3H, 10), 1.29 (s, 15H, 18), 1.04 (s, 3H, 1).

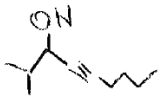


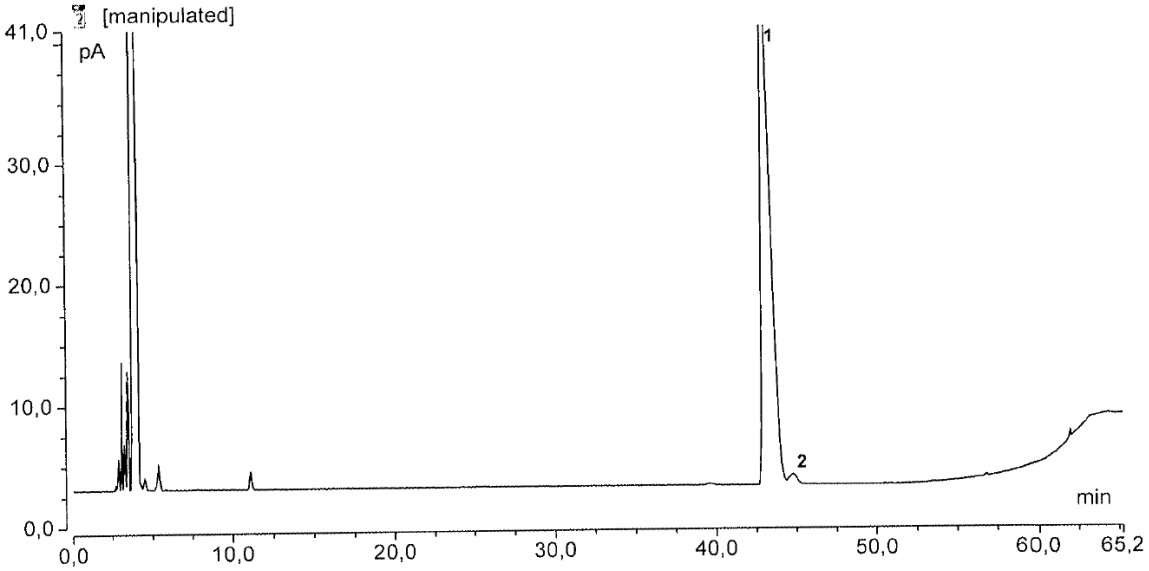


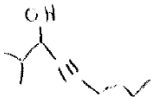
13C NMR (101 MHz, THF) δ= 144.79 (15), 132.95 (12), 130.40 (24, 14
128.88 (13, 23), 96.78 (17), 82.45 (2), 78.13 (7), 75.61 (6), 70.09 (8),
(4), 56.91 (3), 36.00 (10), 35.64 (5), 34.42 (9), 21.50 (16), 19.28 (1), 9
(18)





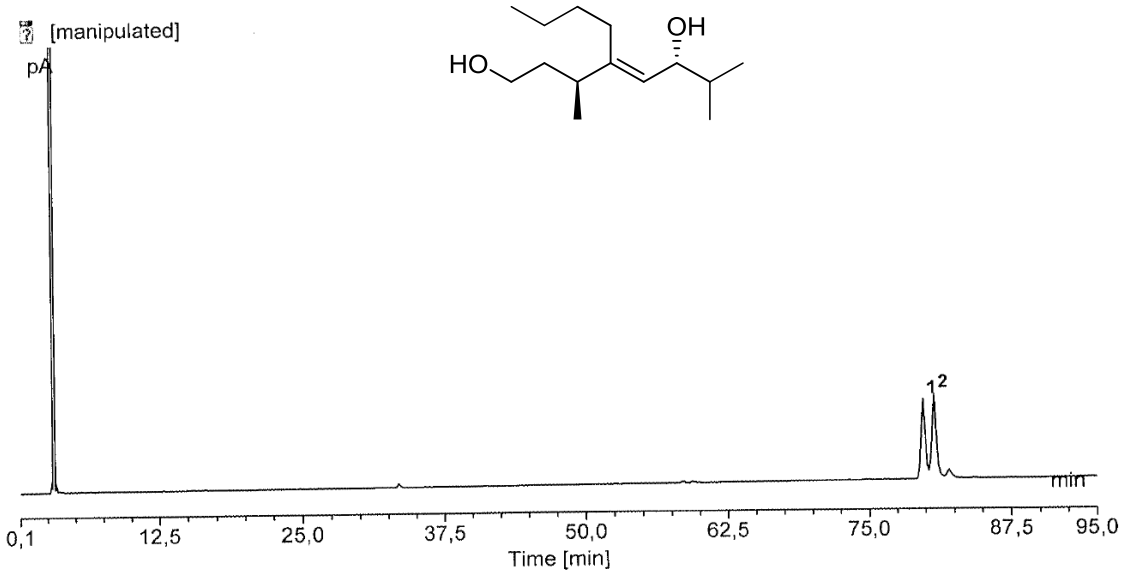
No.	Ret.Time min	area-% %	Peak Name
1	43,51	50,17	
2	44,65	49,83	

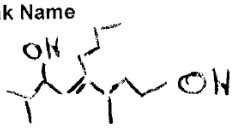


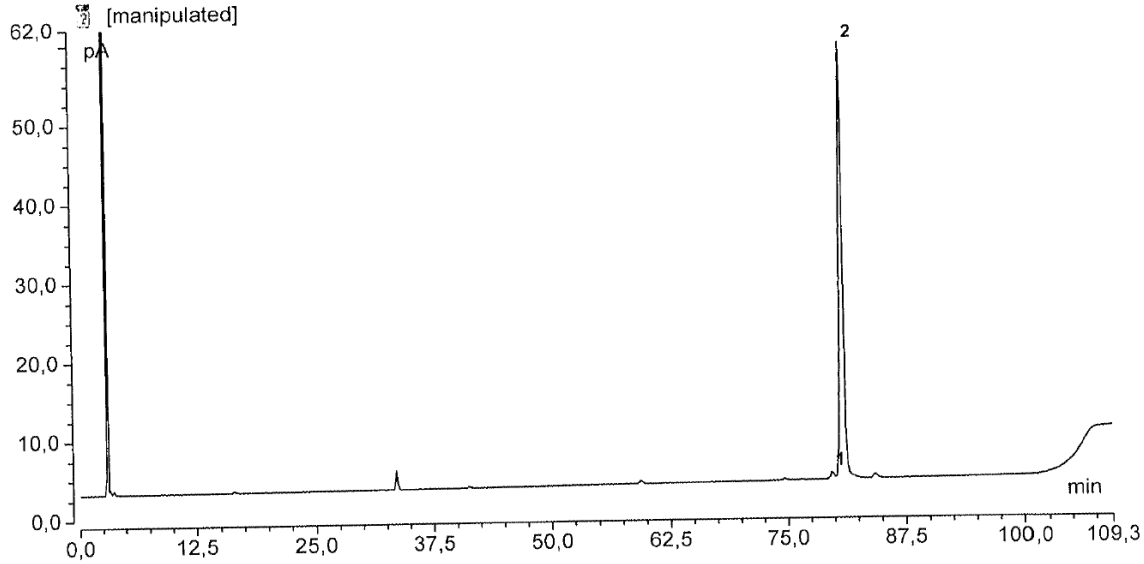
No.	Ret.Time min	area-% %	Peak Name
1	43,03	99,11	
2	44,79	0,89	

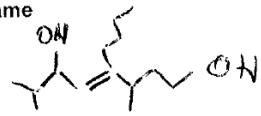
Instrument parameters:

Column:	25,0 m	IVADEX 1/PS086 G 662
Temperature:	100 50 MIN ISO 9/MIn 210 3 MIN ISO	
Gas:	0,40 bar	Hydrogen
Sample size:	1,0 µL	



No.	Ret.Time min	area-% %	Peak Name
1	79,80	49,55	
2	80,78	50,45	



No.	Ret.Time min	area-% %	Peak Name
1	79,72	1,11	
2	80,94	98,89	

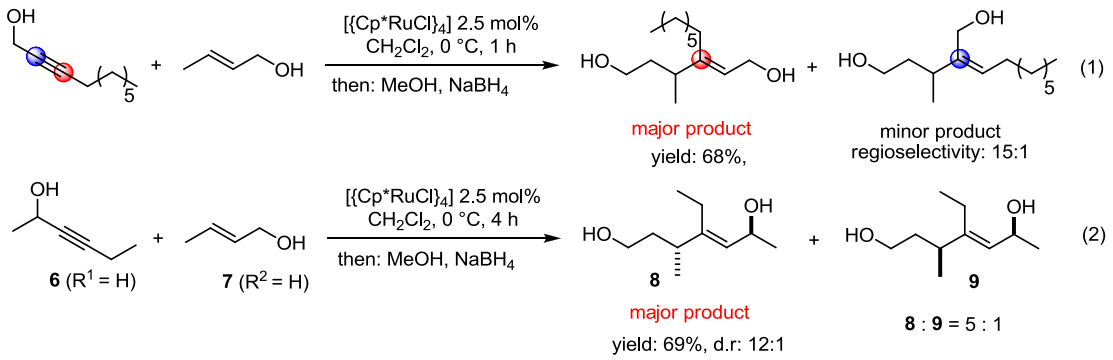
Instrument parameters:

Column:	25,0 m	IVADEX 1/PS086 G 662
Temperature:	120 0,5/MIN 170 8/MIN 220 3 MIN ISO	
Gas:	0,40 bar	Hydrogen
Sample size:	1,0 µL	

COMPUTATIONAL PART

1. Introduction

The Ru-catalyzed alkyne-alkene coupling reaction provides an effective methodology for the synthesis of complex molecules. Recently, the Fürstner group extended the reaction to internal olefins and achieved high regioselectivity and stereoselectivity in product formation. Two examples are listed below. The Ru-catalyzed coupling between achiral dec-2-yn-1-ol and crotyl alcohol (reaction 1) proceeds with a high regioselectivity of 15:1 (unpublished). The coupling reaction between chiral hex-3-yn-2-ol (**6**) and crotyl alcohol (**7**) (reaction 2, see entry 1 in Table 1 of the main paper) generates **8** as the major product in high regioselectivity and diastereoselectivity.



We have applied density functional theory (DFT) to study the mechanism of these reactions and to unravel the origin of the high selectivity observed experimentally. Achiral but-2-yn-1-ol (**1**) and chiral pent-3-yn-2-ol (**2**) were chosen as model substrates for the computational investigation. Please note that the labels **1** and **2** are used for catalyst-substrates complexes in the main paper (Figure 1). Here and in the computational section of the main paper, we use composite labels (such as **1-A1** or **2-TS$_{A1-A2}$**) for the computed species (see e.g. Figures 3-5) to avoid confusion with the notation in the experimental section.

Model substrates used in the computational study:

1 **2**

2. Computational methods

All computations were carried out using the Gaussian09 [1] program. Geometries were optimized using the M06L [2] density functional with the def2-TZVP [3] basis set. For computational efficiency, we employed density fitting; the auxiliary basis set for the def2-TZVP basis set was generated automatically using the auto keyword as implemented in the Gaussian09 program. Harmonic frequency analysis was conducted at the same level of theory to verify the stationary points to be real minima or saddle points and to obtain the thermal corrections at 298.15K. Solvent effects were captured with the SMD[4] approach, by means of single-point SMD-M06L/def2-TZVP calculations at optimized gas-phase geometries. The final Gibbs free energies were obtained by adding the thermal corrections (M06L/def2-TZVP) to these single-point energies. Ultrafine grids and default convergence criteria were used throughout. Molecular pictures were drawn using the visualization software CYLview[5].

3. Reaction mechanism for Ru-catalyzed coupling of but-2-yn-1-ol and crotyl alcohol

The reaction between the simplest model substrate (**1**) and crotyl alcohol was studied in the presence of the catalyst monomer {Cp*RuCl} in its neutral form. The SMD single-point calculations were performed for the solvent used in the experiments (dichloromethane CH_2Cl_2, dielectric constant 8.93).

We first constructed a catalyst-substrates complex **1-A1** such that it has the maximum number of hydrogen bonds between the chloride ligand of the catalyst and the hydroxyl groups of the alkyne and alkene substrates (cf. Figure 1). Starting from this complex **1-A1**, the first step along the reaction coordinate is the C3−C3' coupling between alkyne and alkene via $\mathbf{TS_{A1\text{-}A2}}$ ($\Delta G^{\ddagger}$ = 15.8 kcal mol^{-1}) which yields an unstable ruthenacyclopentene intermediate **1-A2** (Figure S1). The high energy of **1-A2** may be due to steric repulsion between the substituents at the C2 and C3 centers and the presence of a weak sigma bond, d(C3-C3') = 1.63 Å. **1-A2** easily rearranges into a relatively stable intermediate **1-A3** via $\mathbf{1\text{-}TS_{A2\text{-}A3}}$ with a minute activation barrier of 1.6 kcal mol^{-1}. **1-A3** then further converts to an even more stable intermediate **1-A4** through a conformational change in the five-membered ring (from twisted to planar) and a subsequent rotation of the hydroxyl group of the alkyne. In **1-A4**, the hydroxyl group of the alkyne coordinates to Ru, this is the reason for the stabilization. **1-A4** undergoes a facile rotation to yield **1-A5**, in which the methylene group of the alkene forms an agostic interaction with Ru and pre-activates the C−H bond. Finally, a concerted hydrogen shift in **1-A5** from C1' to C2 via $\mathbf{TS_{A5\text{-}A6}}$ ($\Delta G^{\ddagger}$ = 19.1 kcal mol^{-1} relative to **1-A4** or 16.4 kcal mol^{-1} relative to **1-A5**) leads to the highly stable diene product **1-A6**.

An alternative stepwise pathway from **1-A5** to another conformer of the diene product (**1-B3**) consists of a *β*-hydride shift with subsequent Ru−H bond rotation and reductive elimination (Figure S2). The *β*-hydride shift has a barrier of only 7.3 kcal mol^{-1} and generates the intermediate **1-B1**. The direct reductive elimination from **1-B1** is hindered because of an unfavorable orientation of the chloride and enol groups. Therefore, the Ru−H bond rotates inward toward the ruthenacyclopentene plane, thus generating the intermediate **1-B2**, which undergoes a nearly barrier-free reductive elimination to yield a stable diene product **1-B3**. However, the rotation of Ru−H has to overcome a rather high barrier ($\Delta G^{\ddagger}$ = 21. 0 kcal mol^{-1} relative to **1-A4** or 18.3 kcal mol^{-1} relative to **1-A5**). Therefore, starting from **1-A5**, the direct hydrogen transfer to produce a diene product is slightly preferred over the alternative stepwise process.

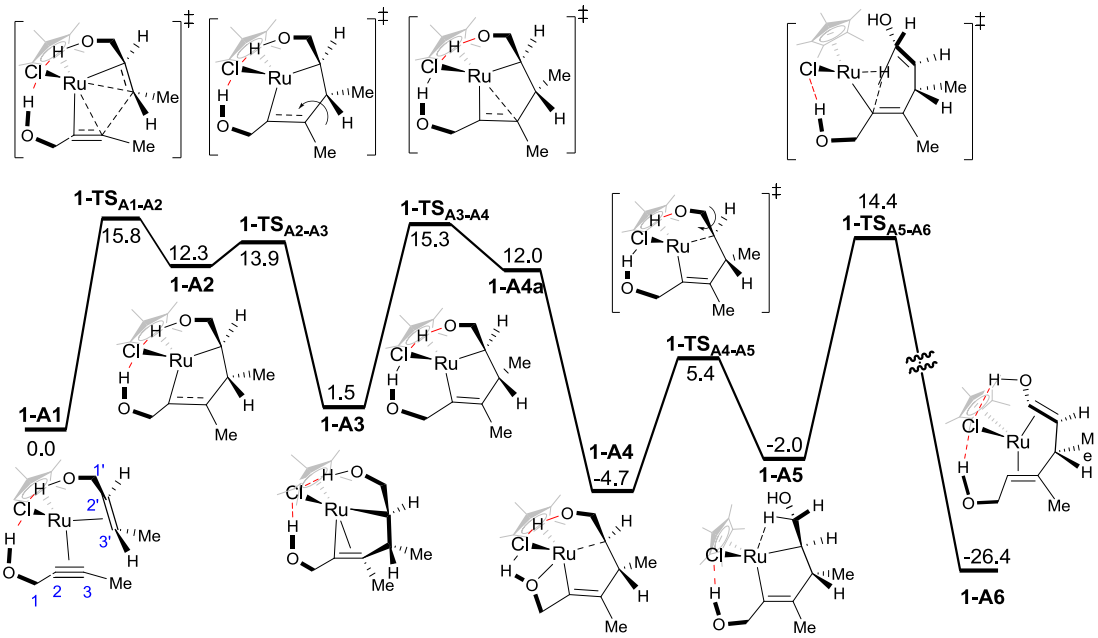


Figure S1. Free energy profile (kcal mol^{-1}) for Ru-catalyzed coupling of but-2-yn-1-ol (**1**) and crotyl alcohol.

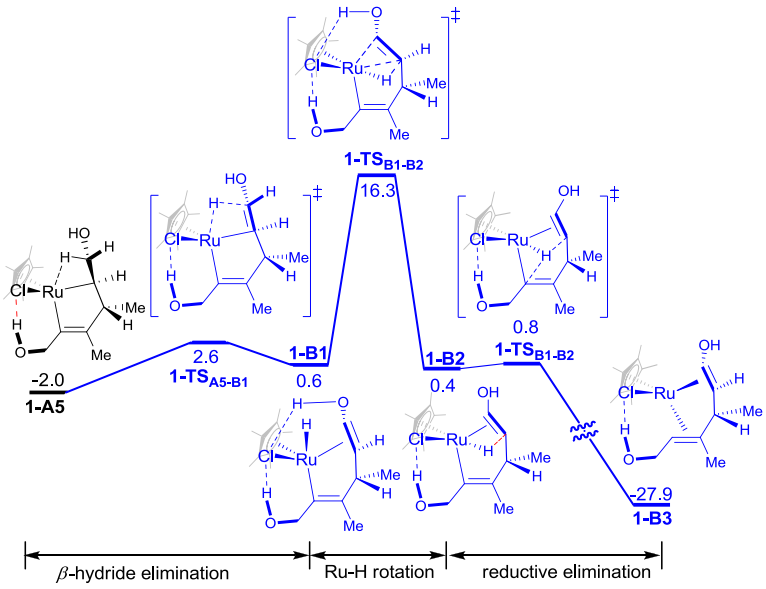


Figure S2. Free energy profile (kcal mol^{-1}) for hydrogen transfer from **1-A5** by a stepwise hydride elimination/reductive elimination process.

4. Structural analysis of key intermediates

In the intermediate **1-A2**, the length of the newly formed C3-C3' bond is 1.63 Å, which is much longer than a normal C-C bond (1.51 Å), thus suggesting that the C3-C3' bond is rather weak. Consequently, the complex **1-A2** has a high energy of 12.3 kcal mol^{-1} and can easily rearrange to a more stable conformer, **1-A3.** In **1-A3**, the ruthenacyclopentene moiety adopts a twisted five-membered ring to avoid the steric repulsion between the substituents at the C2

and C3 centers, and the C3-C3' bond is shortened to 1.53 Å. A further conformational change in **1-A3** leads to a pseudo-planar ruthenacyclopentene intermediate, **1-A4a**, in which the C3-C3' bond is completely formed and the angle ∠C1-Ru-C1' is reduced to 82°. However, because of the constraints imposed by the sp^2 hybridized C2 atom and the hydrogen bonding interaction between the chloride and the hydroxyl group of the alkyne, the methylene group of the alkyne suffers from steric repulsion with the terminal methyl group of the alkyne. Thus **1-A4a** is not stable and rearranges to **1-A4** through an exothermic process. This complex **1-A4** is stabilized by the coordination of the hydroxyl group of the alkyne coordinates to Ru. Furthermore, the binding of O to Ru enlarges the angle ∠C1-C2-C3, which reduces the steric hindrance within the alkyne moiety.

In **1-B1**, the hydride and C2 are located at opposite coordination sites of Ru (∠H-Ru-C2 is 142°). The direct reductive elimination from **1-B1** is not possible because of the wrong orientation of the chloride and the enol group. The angle ∠H-Ru-C2 is 71° in **1-B2,** which can thus undergo a nearly barrier-free reductive elimination to the diene product.

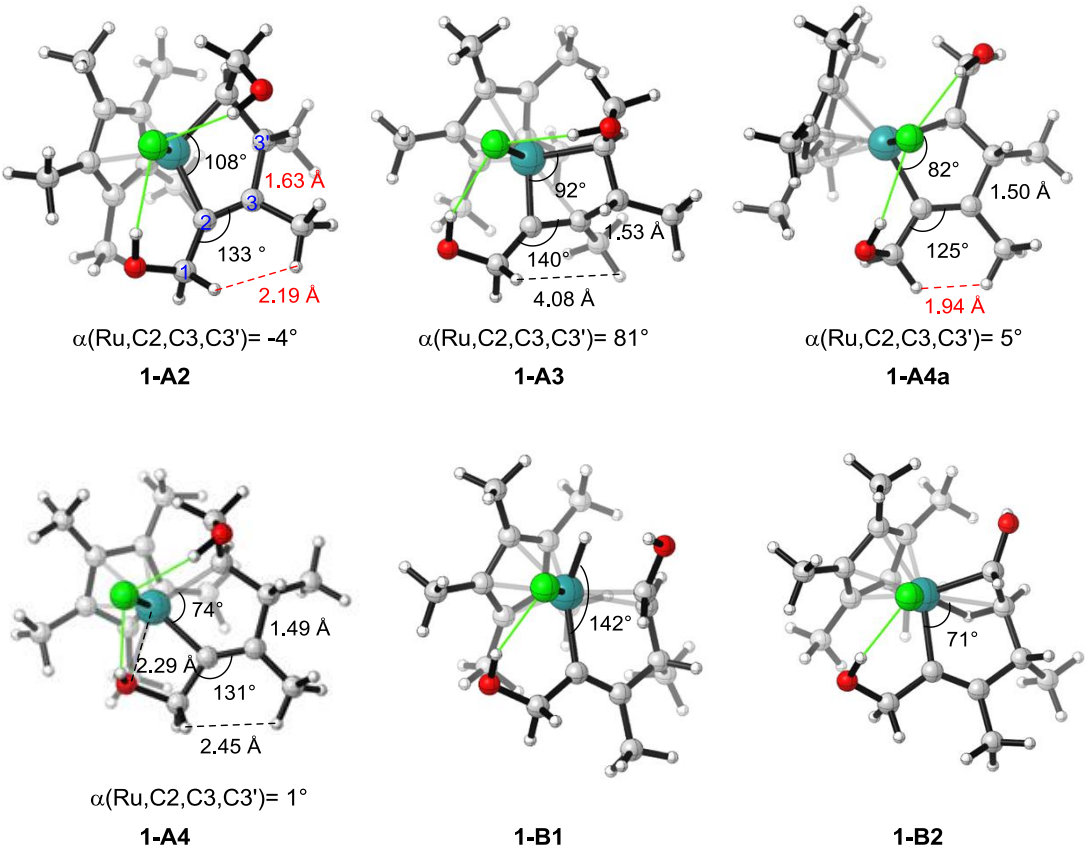


Figure S3. Molecular structures of the intermediates of the coupling reaction with alkyne **1**; interligand hydrogen bonds are indicated by green lines and steric repulsions are indicated by red dashed lines.

5. Regioselectivity

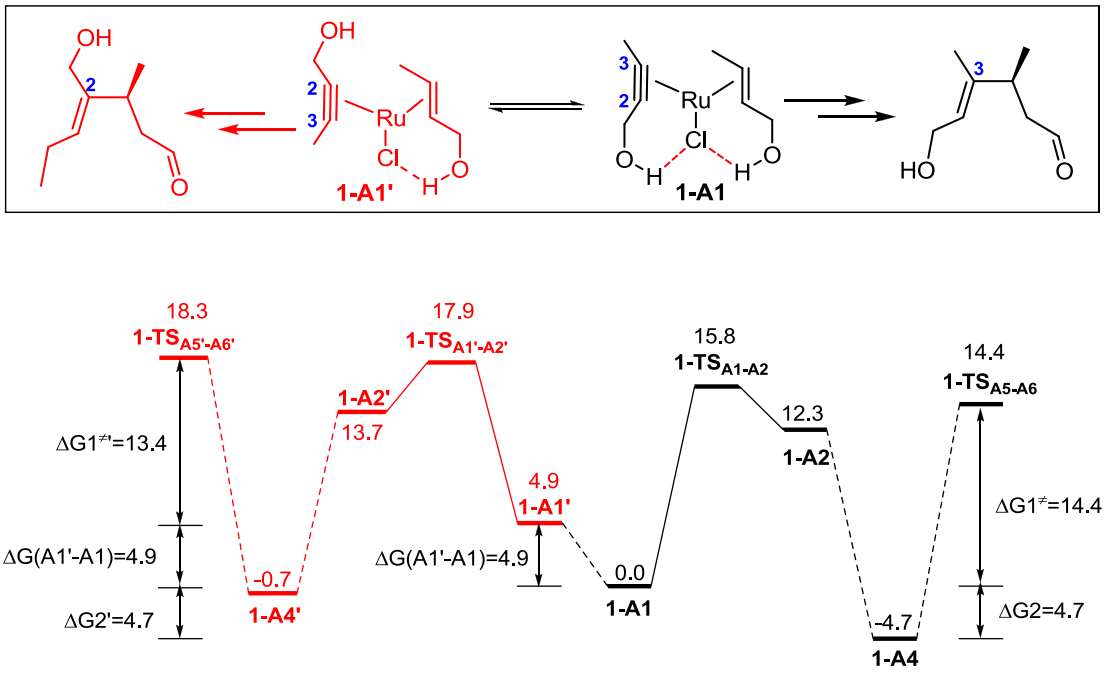


Figure S4. Relative free energies (in kcal mol^{-1}) for key species governing the regioselectivity of the coupling reaction with alkyne **1**; also shown are data from energy decomposition.

Experimentally, C-C coupling preferentially occurs at C3 of the alkyne (see Figure S4, top panel). To identify the origin of regioselectivity with respect to the alkyne, we considered two orientations of the alkyne labeled as **1-A1** and **1-A1'**. The catalyst-substrates complex **1-A1'** is less stable than **1-A1** by 4.9 kcal mol^{-1} since **1-A1**' lacks the hydrogen bonding interaction between the chloride and the hydroxyl group of the alkyne. The rate-limiting transition state **1-TS$_{A5'-A6'}$**, is 3.9 kcal mol^{-1} higher in free energy than its counterpart **1-TS$_{A5-A6}$**, implying that the reaction via the latter is preferred, which is in agreement with experiment.

A more detailed energy decomposition indicates (see Figure S4, bottom panel) that the barrier from complex **1-A1** to **1-TS$_{A5-A6}$** ($\Delta G1^{\neq}$=14.4 kcal mol^{-1}) is comparable to that from **1-A1'** to **1-TS$_{A5'-A6'}$** ($\Delta G1'^{\neq}$=13.4 kcal mol^{-1}), and thus the difference in the free energies of the relevant transition states is mainly due to the different stability of the coordinated complexes **1-A1** and **1-A1'**. Hence, we conclude that the initial equilibrium generated between **1-A1** and **1-A1'** governs the regioselectivity. The additional hydrogen bonding interaction between the chloride and the hydroxyl group of the alkyne stabilizes both **1-A1** and **1-TS$_{A5-A6}$**.

6. Stereoselectivity

In the initial step of the coupling reaction (via **1-TS$_{A1-A2}$**) the alkyne may approach the *Re*-face or the *Si*-face of the crotyl alcohol (Figure S5). In the former case (**1-TS$_{A1-A2}$-cf1**) the hydrogen bond between crotyl alcohol and [Ru-Cl] is retained, whereas it is lost in the latter case (**1-TS$_{A1-A2}$-cf2**). Given the significant enthalpic penalty for *Si*-face attack (7.6 kcal mol^{-1}), we considered only the *Re*-face approach in our analysis of diastereoselectivity (Figure S6).

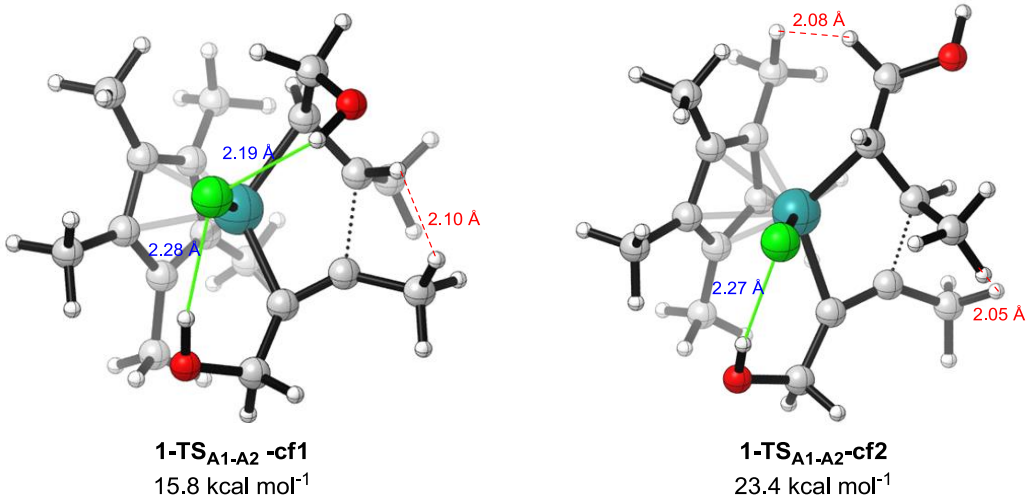


Figure S5. Molecular structures of **1-TS$_{A1-A2}$-cf1** and **1-TS$_{A1-A2}$-cf2**; interligand hydrogen bonds are indicated by green lines and steric repulsions are indicated by red dashed lines. Free energies are given relative to **1-A1**.

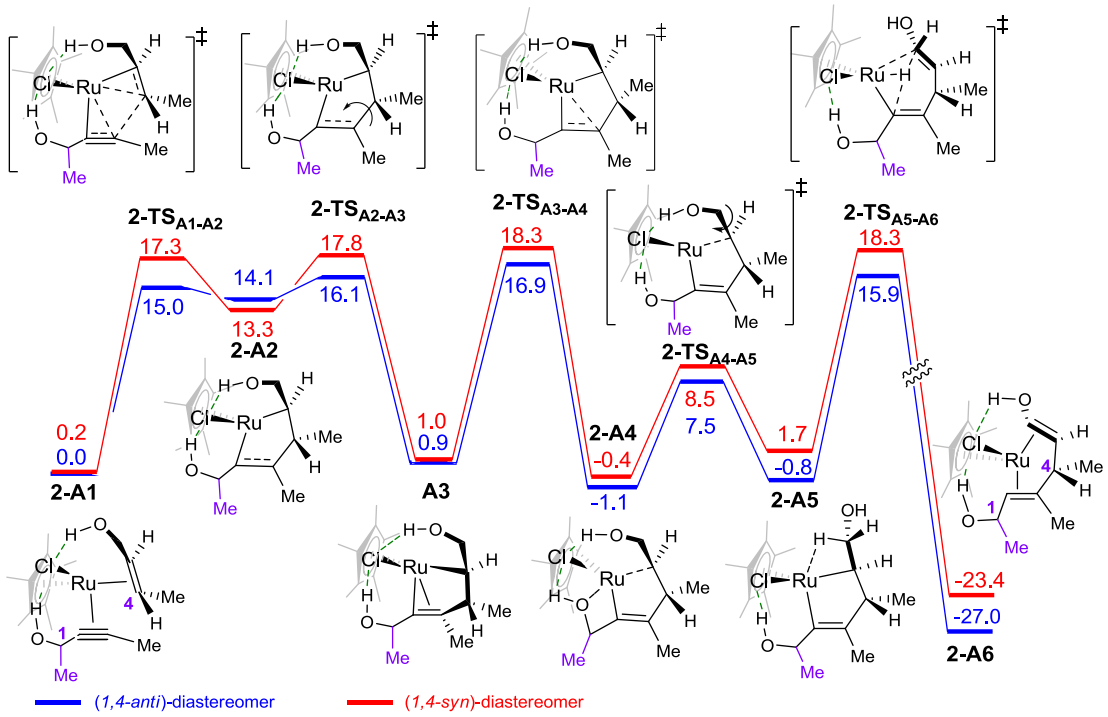


Figure S6. Free energy profile (kcal mol^{-1}) for the diastereoselective Ru-catalyzed coupling of pent-3-yn-2-ol (**2**) and crotyl alcohol.

To identify the origin of diastereoselectivity, we studied the Ru-catalyzed coupling of pent-3-yn-2-ol (**2**) and crotyl alcohol (reaction 2). We assumed that the mechanistic steps for the reaction of chiral alkyne **2** are generally analogous to those for the achiral alkyne **1**. There is one exception: the methyl group in **2** increases the steric repulsion between alkyne and the Cp* ligand as well as within the alkyne moiety. Therefore, the intermediate **2-A4a** does not exist, and **2-A3** directly connects to **2-A4** via **TS$_{A3-A4}$**. As discussed in the main paper,

incorporation of a methyl substituent at the propargylic position spreads the diastereomeric pathways in energetic terms: all transition states are lower in free energy on the route leading to the (1,4-*anti*)-diastereomer. This consistent trend is important because the free energies of the individual transition states are quite similar, and hence the reaction rate might not solely depend on a single step. According to the calculated free energy profiles (Figure S6) formation of the (*1,4-anti*)-diastereomer is clearly favored, in agreement with experiment.

Analyzing this preference, it is essentially the steric repulsion between the propargylic Me-group and the Cp* ring which renders the formation of the (*1,4-syn*)-isomer less favorable. The situation in the diastereomeric transition states **2-TS$_{A5-A6}$** is representative (Figure S7): the sp^2 hybridized C2 atom constrains C1 to be co-planar with the ruthenacyclopentene plane; moreover, the hydrogen bond between the hydroxyl group and the chloride further restricts the rotation around C1. In **(*1,4-anti*)-2-TS$_{A5-A6}$**, the methyl group at the chiral C1 atom occupies the less crowded upper face of the ruthenacyclopentene plane (*anti* to the methyl group at the newly formed chiral center) so that it avoids steric interactions with the Cp* ligand and the terminal methyl group. In contrast, the methyl group at the chiral C2 atom is oriented downward in **(*1,4-syn*)-2-TS$_{A5-A6}$** (*syn* to the methyl group at the newly formed chiral center) and thus "squeezes in" between the planes of the Cp* ring and the ruthenacyclopentene. This results in steric repulsion with the Cp* ligand and the terminal methyl group, as indicated by the C5-C6 distance (3.18 Å) and the short distances between the H-atoms shown in Figure S7. Therefore, the transition state **(*1,4-syn*)-2-TSA$_{5-A6}$** is energetically less favorable than the diastereomeric transition state **(*1,4-anti*)-2-TS$_{A5-A6}$**.

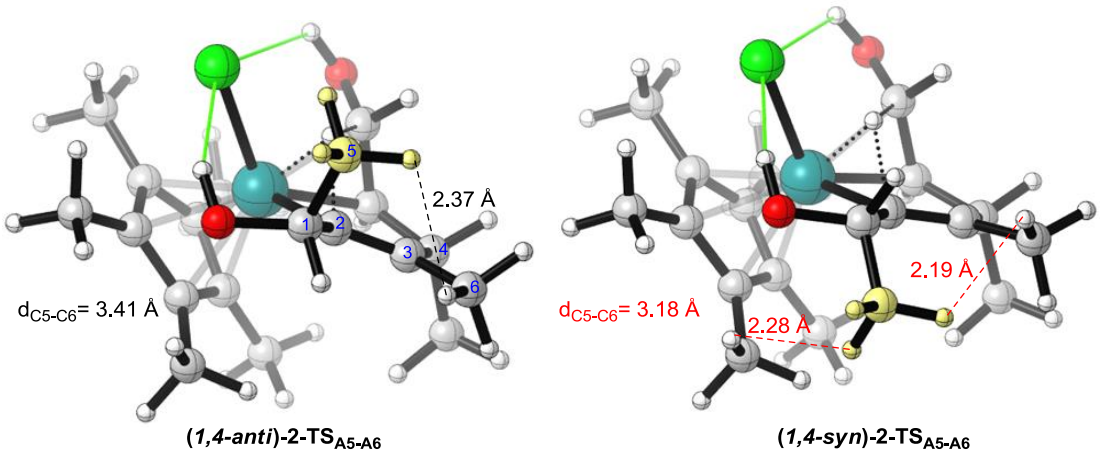


Figure S7. Molecular structures of **(*1,4-anti*)-2-TS$_{A5-A6}$** and **(*1,4-syn*)-2-TS$_{A5-A6}$**; interligand hydrogen bonds are indicated by green lines and steric repusions are indicated by red dashed lines.

In the transition states of the C-C coupling step (**2-TS$_{A1-A2}$**), the methyl group suffers from steric repulsion with the Cp* ligand in **(*1,4-syn*)-2-TS$_{A1-A2}$**. To minimize the steric interactions of the methyl group with the neighboring groups, **(*1,4-syn*)-2-TS$_{A1-A2}$** adjusts its structure which however causes other adverse effects. For example, the distance between O-H and chloride becomes larger, and the alkyne plane is more distorted in **(*1,4-syn*)-2-TS$_{A1-A2}$** compared to **(*1,4-anti*)-2-TS$_{A1-A2}$** (Figure S8).

In **2-TS$_{A2-A3}$** and **2-TS$_{A3-A4}$**, constraints from the sp^2 hybridized C2 atom and the hydrogen bonding interaction between the hydroxyl group and chloride restrict the rotation around C1. In **(*1,4-syn*)-2-TS$_{A2-A3}$** and **(*1,4-syn*)-2-TS$_{A3-A4}$**, the methyl group at the chiral C1 atom is oriented downward (*syn* to the methyl group at the newly formed chiral center) and "squeezes" in between the Cp* and ruthenacyclopentene planes, which leads to severe steric repulsions as indicated by the short distances presented in Figure S8.

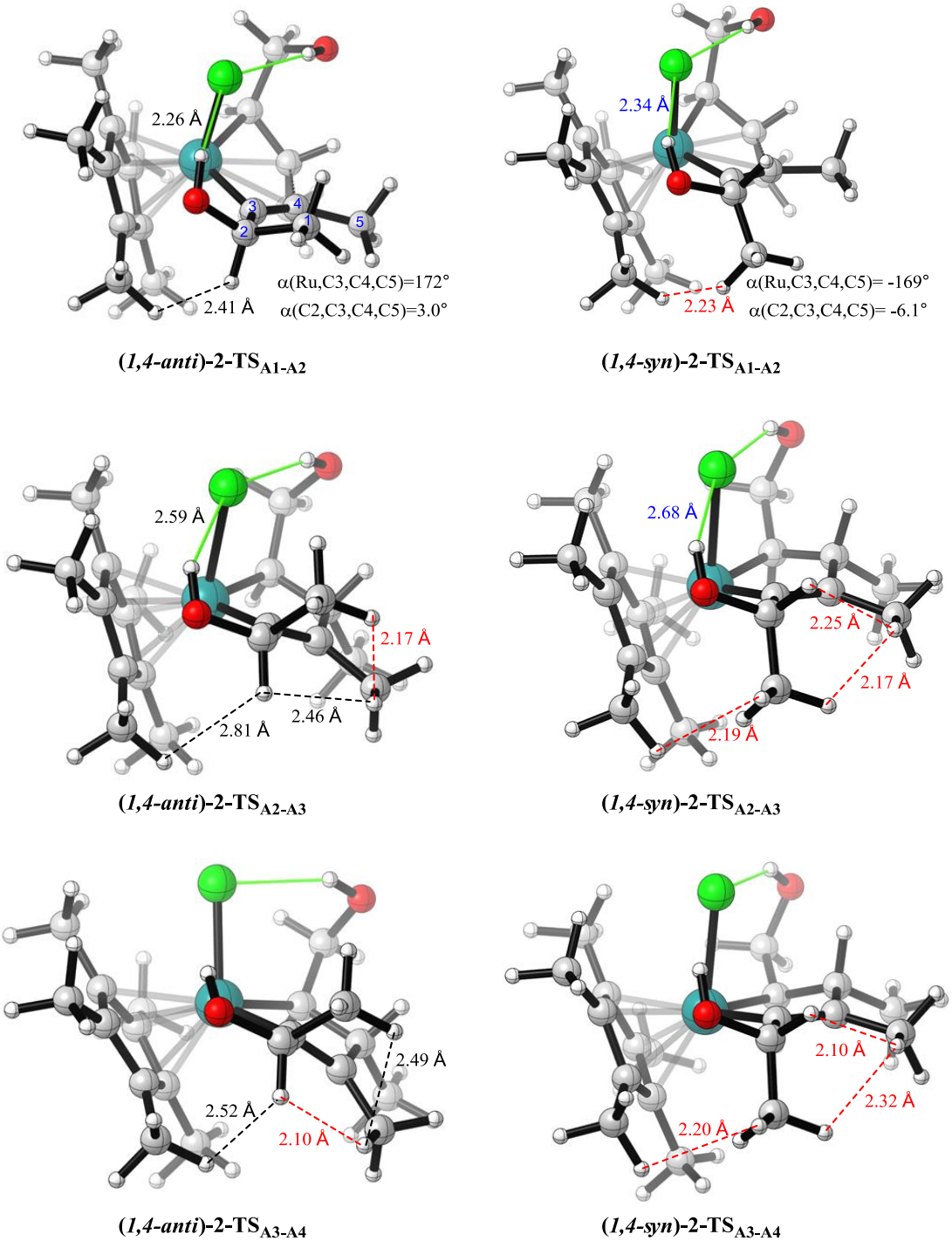


Figure S8. Molecular structures of **2-TS$_{A1-A2}$**, **2-TS$_{A2-A3}$** and **2-TSA$_{3-A4}$**. interligand hydrogen bonds are indicated by green lines and steric repusions are indicated by red dashed lines.

7. Coupling reaction with *Z*-crotyl alcohol

The activation barrier of the C-C coupling step for *Z*-crotyl alcohol is calculated to be 23.0 kcal mol^{-1}, which is significantly higher than the value of 15.0 kcal mol^{-1} computed for *E*-crotyl alcohol (Figure S9). For the *Z*-configured substrate, the terminal methyl group has severe steric repulsions with the methylene group and the alkyne, which leads to distortions in the ruthenacyclopentene ring. The dihedral angle α(Ru,C2,C3,C4) is 35.7°, which makes the orbital overlap between alkyne and alkene less favorable compared to the case of the *E*-alkene (α(Ru,C2,C3,C4) = 2.2 °).

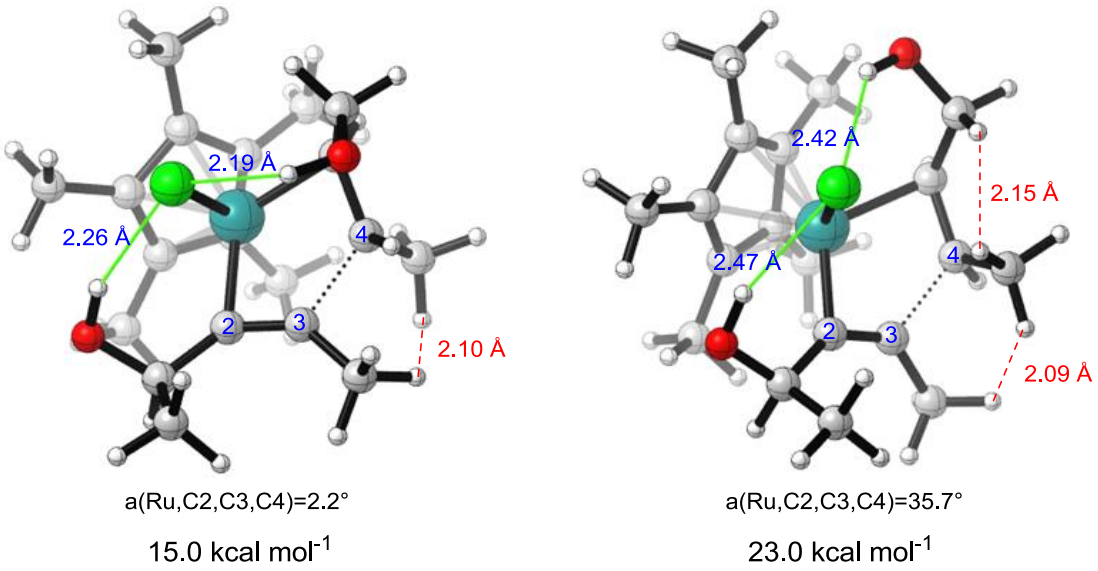


Figure S9. Transition states **2-TS$_{A1-A2}$** for the Ru-catalyzed coupling of (*E*)- and (*Z*)-crotyl alcohol with pent-3-yn-2-ol (**2**). Also given are the computed free energies relative to **2-A1**.

8. Energy table for the coupling reaction of but-2-yn-1-ol (1) and crotyl alcohol.

Table S1. Listed are the zero-point vibrational energy (ZPVE), enthalpy correction (H_{corr}), and Gibbs free energy correction (G_{corr}) determined at the gas-phase geometries. Single-point solvent (DCM) corrected SCF energies are also presented. All values are given in Hartree.

	ZPVE	H_{corr}	G_{corr}	SCF_{DCM}
1-A1	0.434640	0.380993	0.380993	-1409.27266
1-TS$_{A1-A2}$ (1-TS$_{A1-A2}$-cf1)	0.435253	0.461726	0.38303	-1409.249578
1-A2	0.435436	0.463418	0.382107	-1409.254241
1-TS$_{A2-A3}$	0.434602	0.462287	0.380772	-1409.250315
1-A3	0.434616	0.462857	0.380033	-1409.269299
1-TS$_{A3-A4}$	0.435425	0.462808	0.382485	-1409.249736
1-A4	0.433761	0.462152	0.379163	-1409.251685
1-A4	0.436424	0.464322	0.382316	-1409.281536
1-TS$_{A4-A5}$	0.434238	0.46233	0.379425	-1409.262487
1-A5	0.435668	0.463548	0.382029	-1409.276858
1-TS$_{A5-A6}$	0.431272	0.459298	0.376011	-1409.244704
1-A6	0.436998	0.464509	0.384823	-1409.318494
1-TS$_{A5-B1}$	0.432075	0.459554	0.378976	-1409.266422
1-B1	0.433626	0.461443	0.379629	-1409.270418
1-TS$_{B1-B2}$	0.431394	0.459376	0.377689	-1409.243357
1-B2	0.43492	0.462589	0.381286	-1409.272307
1-TS$_{B2-B3}$	0.432509	0.459915	0.379853	-1409.270245
1-B3	0.437457	0.464676	0.386024	-1409.322123
1-TS$_{A1-A2}$-cf2	0.434444	0.462373	0.380783	-1409.235185
1-A'	0.434674	0.463472	0.380296	-1409.26417
1-TS$_{A1'-A2'}$	0.434404	0.462346	0.381216	-1409.244348
1-TS$_{A5'-A6'}$	0.430668	0.45882	0.376187	-1409.238767

9. Energy table for the coupling reaction of pent-3-yn-2-ol (2) and crotyl alcohol.

Table S2. Listed are the zero-point vibrational energy (ZPVE), enthalpy correction (H_{corr}), and Gibbs free energy correction (G_{corr}) determined on the gas-phase geometries. Single-point solvent (DCM) corrected SCF energies are also presented. All values are given in Hartree.

	ZPE	H_{corr}	G_{corr}	SCF_{DCM}
(*1,4-anti*)-2-A1	0.462768	0.492792	0.407639	-1448.598642
(*1,4-anti*)-2-TS$_{A1-A2}$	0.463154	0.492031	0.409182	-1448.576234
(*1,4-anti*)-2-A2	0.463337	0.492755	0.408500	-1448.576972
(*1,4-anti*)-2-TS$_{A2-A3}$	0.463171	0.491918	0.408541	-1448.573916
(*1,4-anti*)-2-A3	0.462406	0.49234	0.405598	-1448.595125
(*1,4-anti*)-2-TS$_{A3-A4}$	0.462097	0.491232	0.406452	-1448.570558
(*1,4-anti*)-2-A4	0.46433	0.493751	0.408241	-1448.601062
(*1,4-anti*)-2-TS$_{A4-A5}$	0.463145	0.4921	0.40874	-1448.587778
(*1,4-anti*)-2-A5	0.463632	0.492827	0.409025	-1448.601364
(*1,4-anti*)-2-TS$_{A5-A6}$	0.459865	0.488942	0.405136	-1448.57078
(*1,4-anti*)-2-A6	0.464998	0.493899	0.41142	-1448.64538
(*1,4-syn*)-2-A1	0.462576	0.492764	0.40643	-1448.59713
(*1,4-syn*)-2-TS$_{A1-A2}$	0.463089	0.492100	0.409275	-1448.572778
(*1,4-syn*)-2-A2	0.463336	0.492879	0.408222	-1448.577974
(*1,4-syn*)-2-TS$_{A2-A3}$	0.463837	0.492374	0.409283	-1448.571848
(*1,4-syn*)-2-A3	0.463001	0.492618	0.406989	-1448.596371
(*1,4-syn*)-2-TS$_{A3-A4}$	0.462284	0.491496	0.406853	-1448.568681
(*1,4-syn*)-2-A4	0.464411	0.493731	0.408666	-1448.600261
(*1,4-syn*)-2-TS$_{A4-A5}$	0.463216	0.492138	0.408471	-1448.585903
(*1,4-syn*)-2-A5	0.463796	0.492796	0.409541	-1448.597741
(*1,4-syn*)-2-TS$_{A5-A6}$	0.459681	0.48866	0.40488	-1448.566758
(*1,4-syn*)-2-A6	0.465394	0.494248	0.412154	-1448.640412

10. Optimized Cartesian coordinates (in Å)

1-A1

Ru	0.027407	-0.012260	0.124999
C	1.609294	-1.420360	0.594270
C	1.712861	-0.507945	1.447412
C	2.362653	0.140416	2.588660
C	1.971355	-2.702886	-0.030377
C	0.741227	0.912327	-1.734954
C	1.459932	1.459134	-0.644487
C	0.519880	2.107626	0.246317
C	-0.760828	2.062017	-0.394843
C	-0.641891	1.300193	-1.577974
C	1.306542	0.220578	-2.919738
H	0.617751	-0.535884	-3.295375
H	2.246287	-0.274631	-2.684252
H	1.490323	0.930518	-3.731034
C	2.939350	1.425902	-0.521143
H	3.327417	0.407860	-0.561475
H	3.285380	1.883278	0.402362
H	3.389080	1.980287	-1.346618
C	0.840866	2.947335	1.431040
H	0.143271	2.772061	2.250883
H	0.789547	4.011449	1.185618
H	1.841523	2.750747	1.807929
C	-1.968050	2.801201	0.052950
H	-2.892254	2.285151	-0.200457
H	-1.999024	3.778398	-0.435422
H	-1.964295	2.983526	1.125827
C	-1.699705	1.050973	-2.589581
H	-1.807466	-0.013758	-2.799313
H	-1.436142	1.544501	-3.527615
H	-2.666979	1.437916	-2.276752
H	1.204088	-3.448242	0.215676
H	2.914096	-3.054434	0.398342
H	1.664590	0.678860	3.226526
H	3.119424	0.855463	2.260537
H	2.870834	-0.601791	3.207557
Cl	-0.891650	-1.949790	-1.234909
C	-1.104756	-1.031845	1.827443
C	-1.916059	-0.066474	1.243559
C	-3.160137	-0.389594	0.437869
C	-0.586627	-0.898241	3.219013
H	-1.315414	-1.319959	3.916653
H	-0.439545	0.145856	3.499506
H	0.346213	-1.436839	3.379712
H	-3.101780	0.033315	-0.573298
H	-3.996456	0.117301	0.932028
H	-1.975741	0.879832	1.776227
H	-1.245967	-2.054033	1.487615
O	2.168650	-2.613895	-1.422733
H	1.282746	-2.461147	-1.790147
O	-3.499996	-1.746372	0.394232
H	-2.844020	-2.169746	-0.182348

1-TS$_{A1-A2}$ (1-TS$_{A1-A2}$-cf1)

Ru	-0.008862	-0.114662	-0.031144
C	0.344142	1.708603	0.858965
C	1.459304	1.214855	1.257045
C	2.685094	1.771868	1.869646
C	-0.287367	3.048207	0.788795
C	-2.070488	-0.046716	-0.759257
C	-2.146654	0.113616	0.646622
C	-1.538263	-1.018157	1.273846
C	-1.170496	-1.938930	0.237543
C	-1.447395	-1.326601	-1.028787
C	-2.654241	0.844101	-1.791881
H	-1.999564	0.925839	-2.657883
H	-2.824093	1.846664	-1.407300
H	-3.610476	0.439787	-2.133837
C	-2.820635	1.218082	1.373900
H	-2.858721	2.129308	0.781967
H	-2.331298	1.437400	2.321812
H	-3.846957	0.923250	1.607446
C	-1.521021	-1.266298	2.739866
H	-0.968261	-2.168039	2.994619
H	-2.536147	-1.389434	3.125536
H	-1.070054	-0.435749	3.284067
C	-0.744260	-3.346368	0.453146
H	-0.275336	-3.771443	-0.431992
H	-1.615800	-3.963605	0.683415
H	-0.047792	-3.457700	1.283541
C	-1.282958	-1.921464	-2.380288
H	-0.948572	-1.168501	-3.093537
H	-2.222542	-2.339045	-2.751532
H	-0.543706	-2.721012	-2.378841
H	-0.960130	3.206815	1.636473
H	0.508655	3.802233	0.885398

H	3.063644	1.164228	2.693197
H	2.480093	2.770326	2.254857
H	3.486442	1.849224	1.131026
Cl	0.701642	1.215544	-2.089235
C	2.066683	-0.630021	0.895830
C	1.681874	-1.348731	-0.312911
C	2.595213	-1.234712	-1.518229
C	1.997078	-1.349339	2.216562
H	2.869278	-1.996236	2.332712
H	1.112442	-1.978770	2.280373
H	1.978385	-0.674006	3.071540
H	2.013269	-1.327583	-2.443579
H	3.289300	-2.083609	-1.499291
H	1.377843	-2.376257	-0.136762
H	3.023411	-0.154135	0.707571
O	-1.043615	3.259996	-0.376283
H	-0.549188	2.845581	-1.106912
O	3.393068	-0.078809	-1.532614
H	2.798589	0.643882	-1.798026

1-A2

Ru	-0.076976	-0.138572	-0.061324
C	0.778702	1.517539	0.730689
C	1.855296	0.844884	1.084617
C	3.133214	1.429271	1.598478
C	0.469153	2.965602	0.697182
C	-2.128085	0.303881	-0.654219
C	-2.093763	0.534503	0.742617
C	-1.675469	-0.665192	1.390810
C	-1.539775	-1.687405	0.390094
C	-1.791822	-1.090797	-0.887962
C	-2.578176	1.260833	-1.694345
H	-2.055682	1.099414	-2.634591
H	-2.403439	2.290520	-1.389111
H	-3.648434	1.135831	-1.878818
C	-2.470872	1.791961	1.435076
H	-2.299296	2.663483	0.807102
H	-1.920258	1.922392	2.365601
H	-3.532650	1.765943	1.693683
C	-1.605169	-0.844947	2.864734
H	-1.218763	-1.823763	3.140915
H	-2.598119	-0.752265	3.311303
H	-0.973334	-0.089789	3.334295
C	-1.308902	-3.129212	0.666038
H	-0.953470	-3.657851	-0.216442
H	-2.236743	-3.611408	0.981778
H	-0.579214	-3.286840	1.460734
C	-1.821458	-1.758808	-2.214501
H	-1.357403	-1.129818	-2.974061
H	-2.845915	-1.966640	-2.534278
H	-1.281917	-2.704450	-2.197617
H	-0.098204	3.263685	1.584870
H	1.410824	3.534684	0.735682
H	3.448338	0.959336	2.533007
H	3.039225	2.497540	1.780322
H	3.936928	1.270880	0.874749
Cl	0.717327	0.921076	-2.222227
C	2.020184	-0.762590	0.888723
C	1.382920	-1.555045	-0.278148
C	2.281197	-1.725368	-1.490195
C	1.919167	-1.472668	2.229525
H	2.374942	-2.461634	2.174049
H	0.884119	-1.602370	2.537490
H	2.427275	-0.921518	3.020532
H	1.660003	-1.867341	-2.384657
H	2.863519	-2.646253	-1.366112
H	1.038107	-2.530036	0.064679
H	3.060982	-0.731291	0.553829
O	-0.301634	3.348044	-0.419106
H	0.020132	2.821160	-1.172256
O	3.221582	-0.699957	-1.674915
H	2.713171	0.073921	-1.973666

1-TS$_{A2-A3}$

Ru	-0.125223	-0.009066	0.037904
C	0.577438	1.841460	-0.059794
C	1.774862	1.514189	0.436766
C	2.646041	2.571773	1.058715
C	-0.025982	3.155996	-0.372107
C	-2.216557	-0.092595	-0.391723
C	-2.054378	0.435290	0.929011
C	-1.421472	-0.580871	1.726185
C	-1.285237	-1.759196	0.928586
C	-1.713625	-1.457973	-0.386112
C	-2.929730	0.523842	-1.539261
H	-2.380653	0.368737	-2.468167
H	-3.057847	1.594573	-1.404610
H	-3.916615	0.069939	-1.662781

C	-2.544404	1.750335	1.419792
H	-2.637880	2.463090	0.602177
H	-1.875457	2.179775	2.165032
H	-3.526394	1.649423	1.888764
C	-1.082414	-0.467126	3.168567
H	-0.203960	-1.058671	3.425129
H	-1.903164	-0.823252	3.796638
H	-0.882847	0.564947	3.451612
C	-0.773003	-3.069750	1.402227
H	-0.233421	-3.605788	0.622517
H	-1.601608	-3.708296	1.716713
H	-0.108748	-2.967886	2.259100
C	-1.785147	-2.388809	-1.540246
H	-1.457520	-1.900491	-2.457112
H	-2.810497	-2.734754	-1.693679
H	-1.161343	-3.268292	-1.391008
H	-0.535942	3.583652	0.498234
H	0.757143	3.873411	-0.657424
H	2.781838	2.428383	2.132254
H	2.218352	3.561005	0.913916
H	3.642377	2.567073	0.609854
Cl	0.534910	0.101721	-2.390355
C	2.447707	0.079510	0.387463
C	1.580939	-1.170985	0.321011
C	2.048417	-2.264299	-0.622898
C	3.418111	-0.112160	1.554098
H	3.907650	-1.080651	1.461758
H	2.891513	-0.095477	2.510525
H	4.199718	0.643014	1.586855
H	1.176960	-2.863310	-0.933668
H	2.693173	-2.952340	-0.061060
H	1.442092	-1.605067	1.314816
H	3.017111	0.106320	-0.548071
O	-0.993915	3.046037	-1.398544
H	-0.680384	2.346399	-1.993730
O	2.801680	-1.853490	-1.725874
H	2.231141	-1.257968	-2.242656

1-A3

Ru	-0.096143	-0.001010	-0.025923
C	0.661298	1.546403	-0.741892
C	1.503642	1.422527	0.364236
C	1.521086	2.381161	1.514746
C	0.468918	2.386441	-1.921880
C	-2.350464	-0.153865	-0.229574
C	-2.039457	0.839969	0.721257
C	-1.312096	0.212499	1.804441
C	-1.269469	-1.197422	1.549997
C	-1.856274	-1.419957	0.289606
C	-3.119955	0.000044	-1.488976
H	-2.663144	-0.572329	-2.297631
H	-3.166740	1.039837	-1.806314
H	-4.144885	-0.362667	-1.373934
C	-2.412663	2.277961	0.642320
H	-2.466598	2.618153	-0.390862
H	-1.696348	2.912415	1.163424
H	-3.388274	2.455380	1.101083
C	-0.950596	0.842174	3.101395
H	-0.017264	0.447401	3.502331
H	-1.725294	0.645548	3.847001
H	-0.849160	1.922061	3.022687
C	-0.699584	-2.218487	2.465292
H	-0.359741	-3.101735	1.927057
H	-1.443212	-2.548858	3.194685
H	0.147734	-1.830216	3.029443
C	-2.043508	-2.730397	-0.382374
H	-1.881484	-2.653389	-1.456216
H	-3.061844	-3.094138	-0.224799
H	-1.360898	-3.486294	0.001289
H	1.422256	2.351681	-2.481476
H	0.356240	3.434372	-1.614542
H	1.634898	1.871854	2.472914
H	0.615881	2.984988	1.559957
H	2.371100	3.062937	1.422293
Cl	0.169693	-1.041796	-2.264024
C	2.656337	0.424369	0.194692
C	1.838788	-0.790775	0.552059
C	2.303670	-2.131312	0.004917
C	3.929711	0.672570	0.974724
H	4.629156	-0.145226	0.801476
H	3.744252	0.725205	2.048729
H	4.427754	1.595943	0.674859
H	1.471037	-2.851190	-0.004375
H	3.056882	-2.545438	0.688135
H	1.744618	-0.852178	1.642672
H	2.903004	0.356480	-0.870328
O	-0.629617	2.052193	-2.716442
H	-0.593372	1.086369	-2.832787

O	2.932259	-2.062181	-1.249071
H	2.241504	-1.815524	-1.883559

1-TS$_{A3-A4}$

Ru	-0.163450	0.014078	0.128710
C	1.029717	1.583608	0.010836
C	2.318540	1.250217	0.305790
C	3.322743	2.261086	0.754017
C	0.560820	2.966745	-0.329090
C	-2.284453	0.238055	-0.541077
C	-2.152916	0.848812	0.727329
C	-1.727774	-0.187546	1.631506
C	-1.722423	-1.455330	0.957212
C	-2.018948	-1.194367	-0.389483
C	-2.785403	0.863750	-1.787863
H	-2.166225	0.586046	-2.642519
H	-2.792131	1.948565	-1.715548
H	-3.802879	0.527331	-2.003838
C	-2.488836	2.250166	1.087038
H	-2.316004	2.921035	0.247319
H	-1.892543	2.604181	1.927755
H	-3.537917	2.338815	1.382200
C	-1.423480	0.009359	3.074433
H	-0.737960	-0.746850	3.454407
H	-2.337712	-0.055574	3.670658
H	-0.987675	0.989385	3.266212
C	-1.468868	-2.770121	1.599156
H	-1.349931	-3.561095	0.861908
H	-2.298883	-3.054998	2.250265
H	-0.569709	-2.761065	2.217287
C	-2.146030	-2.190362	-1.480683
H	-1.813398	-1.776751	-2.430876
H	-3.188159	-2.498213	-1.599956
H	-1.555620	-3.084871	-1.286562
H	1.399663	3.604748	-0.639965
H	0.107496	3.451468	0.543937
H	3.701248	2.036110	1.753154
H	2.925120	3.272337	0.769142
H	4.193696	2.245494	0.092827
Cl	0.405179	-0.207223	-2.231707
C	2.765562	-0.183142	0.163221
C	1.610914	-1.103282	0.448669
C	1.746253	-2.520533	-0.052934
C	4.007964	-0.555164	0.971663
H	4.291548	-1.584773	0.760701
H	3.823836	-0.472407	2.044453
H	4.864512	0.073278	0.730525
H	0.789505	-3.048376	0.073649
H	2.472572	-3.069321	0.562793
H	1.424783	-1.111769	1.538142
H	3.025590	-0.301768	-0.899188
O	-0.425202	2.953004	-1.344826
H	-0.245889	2.175658	-1.896368
O	2.218278	-2.626190	-1.373378
H	1.671920	-2.029469	-1.909531

1-A4a

Ru	-0.167189	-0.034562	0.170913
C	1.144748	1.512071	0.241731
C	2.450958	1.158067	0.298590
C	3.598158	2.102753	0.461040
C	0.641532	2.908144	0.073109
C	-2.242077	0.185956	-0.719557
C	-2.249163	0.927995	0.480070
C	-1.870708	0.020515	1.510124
C	-1.790518	-1.329012	0.968174
C	-1.990541	-1.222448	-0.418988
C	-2.615351	0.725036	-2.048695
H	-2.205045	0.129467	-2.859707
H	-2.269060	1.750229	-2.171971
H	-3.704056	0.728156	-2.150847
C	-2.642055	2.350287	0.635326
H	-2.240484	2.963366	-0.169937
H	-2.297136	2.764531	1.581190
H	-3.730852	2.448479	0.622167
C	-1.704481	0.365061	2.948513
H	-0.998391	-0.297985	3.447106
H	-2.655938	0.271645	3.478808
H	-1.355693	1.388118	3.081199
C	-1.630309	-2.567153	1.775150
H	-1.417605	-3.431073	1.149084
H	-2.542839	-2.788366	2.334478
H	-0.824770	-2.486234	2.506406
C	-2.023980	-2.317794	-1.418725
H	-1.482053	-2.035790	-2.322113
H	-3.048778	-2.555533	-1.714844
H	-1.570659	-3.230099	-1.034448
H	1.452327	3.648447	0.096156

H	-0.043245	3.175990	0.886612
H	4.073342	1.999360	1.439535
H	3.303680	3.142468	0.351061
H	4.375329	1.890761	-0.277352
Cl	0.474394	-0.027392	-2.171942
C	2.782972	-0.302428	0.181038
C	1.553378	-1.133119	0.420545
C	1.618188	-2.586638	0.045642
C	3.956217	-0.751211	1.058357
H	4.171392	-1.806584	0.901608
H	3.733787	-0.604614	2.116788
H	4.864201	-0.195916	0.829932
H	0.669959	-3.076768	0.306371
H	2.399616	-3.111726	0.611542
H	1.201729	-0.989185	1.481170
H	3.076568	-0.476668	-0.865074
O	-0.082766	3.054901	-1.144739
H	0.174663	2.315278	-1.715697
O	1.935764	-2.769712	-1.314517
H	1.435843	-2.101382	-1.811019

1-A4

Ru	-0.331585	0.142710	-0.216778
C	2.562595	1.036585	-0.000166
C	1.305028	1.354576	-0.290356
C	-1.654271	1.081286	1.129281
C	-0.917173	0.093722	1.848042
C	-1.297045	-1.189218	1.300358
C	-2.295300	-0.996445	0.300494
C	-2.506253	0.385832	0.168082
Cl	-0.157691	-0.632913	-2.580377
C	2.760835	-0.382515	0.407438
C	1.410831	-1.132740	0.364596
H	1.163572	-1.411992	1.384990
H	3.402030	-0.843762	-0.356408
C	-1.707344	2.535552	1.426434
H	-2.525641	2.758692	2.116263
H	-0.786049	2.881943	1.891602
H	-1.875374	3.124000	0.525317
C	-3.431819	1.054026	-0.780393
H	-3.016036	1.990070	-1.149261
H	-3.653393	0.424398	-1.639767
H	-4.378704	1.289683	-0.288495
C	-2.925354	-2.080018	-0.492482
H	-2.208238	-2.865489	-0.726915
H	-3.748006	-2.542135	0.058796
H	-3.322488	-1.711324	-1.435263
C	-0.948413	-2.521328	1.859128
H	-0.097892	-2.486556	2.535131
H	-1.798443	-2.900125	2.431796
H	-0.733766	-3.255792	1.084615
C	-0.077082	0.330539	3.049057
H	-0.689835	0.378333	3.952870
H	0.652058	-0.464286	3.197037
H	0.474456	1.266292	2.971919
C	0.729878	2.543066	-0.951626
H	0.450359	3.355570	-0.276463
H	1.315821	2.977584	-1.769022
C	3.740045	1.943040	-0.138263
H	4.178114	2.192918	0.832182
H	4.535751	1.470645	-0.720696
H	3.482292	2.883994	-0.623879
C	1.505504	-2.425715	-0.436603
H	2.058812	-3.156997	0.170302
H	0.506247	-2.854428	-0.598041
C	3.462456	-0.557977	1.750500
H	4.464439	-0.126492	1.739353
H	2.905992	-0.073082	2.555361
H	3.569716	-1.613436	2.005720
O	-0.548128	2.036375	-1.481485
H	-0.358206	1.550923	-2.310965
O	2.213647	-2.337300	-1.643627
H	1.676020	-1.785104	-2.233661

1-TS$_{A4-A5}$

Ru	-0.236354	0.073198	-0.241821
C	2.749251	0.167083	-0.220111
C	1.658229	0.946912	-0.150301
C	-0.747588	0.171969	1.846615
C	-0.798762	-1.207085	1.495187
C	-1.820622	-1.392357	0.496958
C	-2.434739	-0.145016	0.250387
C	-1.771940	0.826048	1.080875
Cl	-0.773015	1.715159	-1.910685
C	2.520365	-1.309026	-0.281881
C	1.062775	-1.539583	-0.631620
H	0.686289	-2.510249	-0.307986
H	3.123609	-1.745718	-1.095964

C	0.098157	0.804680	2.888152
H	-0.414607	0.816118	3.853392
H	1.038146	0.270036	3.013688
H	0.336602	1.831079	2.613893
C	-2.170825	2.248849	1.205852
H	-1.376827	2.859347	1.626224
H	-2.464499	2.674306	0.247521
H	-3.037294	2.312323	1.870840
C	-3.571241	0.142210	-0.658168
H	-3.746554	-0.676964	-1.353412
H	-4.495367	0.301493	-0.097864
H	-3.382576	1.041448	-1.245763
C	-2.200603	-2.708347	-0.068650
H	-1.326882	-3.293623	-0.352536
H	-2.756708	-3.292323	0.669617
H	-2.823207	-2.609860	-0.954145
C	-0.138715	-2.317257	2.226155
H	-0.877370	-2.791387	2.878020
H	0.246483	-3.098648	1.573274
H	0.674518	-1.970784	2.857166
C	1.822534	2.440796	-0.014382
H	2.610275	2.658136	0.713641
H	2.163312	2.863251	-0.971724
C	4.167301	0.657246	-0.166819
H	4.546602	0.710331	0.859000
H	4.839238	-0.010623	-0.709202
H	4.283865	1.650783	-0.597201
C	0.783792	-1.381796	-2.131272
H	0.915732	-0.342802	-2.457686
C	2.977657	-1.995861	1.000188
H	4.056106	-1.900989	1.124247
H	2.513872	-1.534681	1.871835
H	2.738490	-3.060724	1.004369
O	0.689322	3.149676	0.450754
H	0.024392	3.067250	-0.248150
H	1.573240	-1.941304	-2.651260
O	-0.462288	-1.895605	-2.566858
H	-1.054465	-1.142999	-2.686223

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Ru	-0.260990	-0.007990	-0.297925
C	2.743652	0.299814	-0.192614
C	1.601124	1.005359	-0.208394
C	-1.797954	0.841422	1.007325
C	-0.807725	0.214829	1.819057
C	-0.838374	-1.178072	1.507886
C	-1.833688	-1.407156	0.495767
C	-2.436019	-0.166975	0.185770
Cl	-0.846447	1.731353	-1.934779
C	2.614388	-1.186535	-0.117332
C	1.191529	-1.525075	-0.492705
H	0.850915	-2.497469	-0.139997
H	3.273607	-1.673715	-0.854655
C	-2.251756	2.249969	1.105986
H	-3.198422	2.277758	1.652532
H	-1.536562	2.873382	1.634700
H	-2.433887	2.686291	0.123943
C	-3.575690	0.084735	-0.729712
H	-3.389597	0.960159	-1.352067
H	-3.756655	-0.761119	-1.390030
H	-4.494099	0.266328	-0.166298
C	-2.177001	-2.741783	-0.055254
H	-2.757466	-3.324314	0.664452
H	-2.764194	-2.662311	-0.967461
H	-1.283719	-3.319974	-0.293664
C	-0.178052	-2.255939	2.286172
H	0.668184	-1.894935	2.862912
H	-0.902859	-2.668069	2.993219
H	0.160069	-3.086488	1.668695
C	0.020068	0.881719	2.854861
H	-0.511017	0.929546	3.808761
H	0.954805	0.348835	3.021371
H	0.268971	1.896038	2.546596
C	1.669782	2.510854	-0.175815
H	2.533076	2.825994	0.417604
C	4.125735	0.888939	-0.131757
H	4.233209	1.772563	-0.759535
H	4.402676	1.188489	0.884025
H	4.876972	0.168675	-0.459096
C	0.811772	-1.346059	-1.913428
H	0.022658	-0.512742	-2.058838
H	1.635796	-0.925884	-2.505123
C	3.031776	-1.710417	1.250856
H	4.093033	-1.534290	1.423794
H	2.488303	-1.193241	2.041921
H	2.854208	-2.782553	1.353007
O	0.258242	-2.517249	-2.461124
H	-0.113405	-2.304984	-3.323264

H	1.834261	2.892948	-1.193610
O	0.559925	3.162904	0.412281
H	-0.162434	3.050619	-0.223219

1-TS$_{A5-A6}$

Ru	-0.223387	0.013401	-0.288265
C	2.746005	0.342743	-0.261006
C	1.609936	1.055177	-0.159755
C	-1.804595	0.691131	1.135618
C	-0.752101	0.150303	1.908028
C	-0.609898	-1.218523	1.531826
C	-1.638316	-1.541847	0.560323
C	-2.370410	-0.374590	0.312750
Cl	-1.117660	1.693838	-1.882730
C	2.640212	-1.148090	-0.447854
C	1.197880	-1.513417	-0.757635
H	0.858589	-2.492834	-0.437285
H	3.248155	-1.446582	-1.316663
C	-2.382955	2.052402	1.249944
H	-3.327415	2.004176	1.798522
H	-1.717704	2.731334	1.776490
H	-2.600976	2.480195	0.271210
C	-3.555217	-0.223919	-0.565534
H	-3.529212	0.721683	-1.105639
H	-3.615864	-1.025822	-1.299586
H	-4.476230	-0.244282	0.022700
C	-1.907021	-2.901188	0.028159
H	-2.457963	-3.497937	0.759933
H	-2.496949	-2.868457	-0.884529
H	-0.991435	-3.445513	-0.199643
C	0.185660	-2.234981	2.264219
H	0.987155	-1.789602	2.847661
H	-0.468721	-2.763097	2.963273
H	0.619255	-2.991178	1.611606
C	0.067466	0.867086	2.917504
H	-0.352388	0.748160	3.919119
H	1.088348	0.486351	2.940093
H	0.119061	1.929690	2.689247
C	1.630206	2.549602	0.041860
H	2.378808	2.811526	0.794991
C	4.128178	0.907540	-0.131523
H	4.160296	1.981893	-0.297483
H	4.557133	0.720727	0.857751
H	4.809333	0.446071	-0.850575
C	0.643402	-1.039273	-1.993447
H	0.704627	0.375403	-1.565239
H	1.372184	-0.595167	-2.688687
C	3.209919	-1.896748	0.751926
H	4.285915	-1.745202	0.827287
H	2.767429	-1.540684	1.681532
H	3.035471	-2.971312	0.678603
O	-0.321189	-1.787478	-2.652731
H	-0.884209	-1.166512	-3.130766
H	1.947701	3.039103	-0.891767
O	0.422887	3.116407	0.502336
H	-0.234846	2.951100	-0.191359

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Ru	0.075069	0.088344	-0.160779
C	-2.032564	-0.788329	-0.309480
C	-1.147287	-1.496606	-1.131397
C	1.923146	-0.429319	0.928583
C	0.820342	-0.837627	1.713854
C	0.036047	0.337868	2.005114
C	0.706377	1.470596	1.429979
C	1.850376	1.005869	0.737794
Cl	1.512875	-0.303002	-2.241421
C	-2.680295	0.466963	-0.898269
C	-1.577924	1.488499	-0.761201
H	-1.681489	2.265982	-0.012563
H	-2.876217	0.285409	-1.960285
C	3.033327	-1.306115	0.483680
H	3.788048	-1.372975	1.272536
H	2.681688	-2.313990	0.269835
H	3.514916	-0.922099	-0.412178
C	2.867160	1.842623	0.052730
H	3.229041	1.357880	-0.853803
H	2.460317	2.814502	-0.222272
H	3.728890	2.017630	0.701819
C	0.309389	2.893920	1.581294
H	0.951787	3.392196	2.310911
H	0.401238	3.436744	0.640494
H	-0.715467	2.996735	1.934269
C	-1.074503	0.435933	2.990460
H	-1.504716	-0.534655	3.222721
H	-0.706729	0.857325	3.929501
H	-1.880016	1.084984	2.645624
C	0.637255	-2.209528	2.255858

H	1.305960	-2.373989	3.105091
H	-0.375112	-2.386203	2.613582
H	0.874322	-2.961954	1.503965
C	-0.711460	-2.909960	-0.885448
H	-0.980615	-3.234881	0.122881
H	-1.268164	-3.564771	-1.573993
C	-2.683886	-1.413699	0.883889
H	-2.021474	-2.083972	1.422946
H	-3.069224	-0.681182	1.587241
H	-3.541204	-2.009846	0.554462
C	-0.627494	1.585947	-1.752570
H	-1.099947	-1.197992	-2.176433
H	-0.732151	0.984732	-2.650643
C	-3.969849	0.929824	-0.251634
H	-4.740623	0.160555	-0.276618
H	-3.819351	1.216135	0.790394
H	-4.357099	1.805302	-0.771562
O	0.674556	-3.140536	-1.039867
H	1.038017	-2.408566	-1.566164
O	0.237011	2.633815	-1.846923
H	1.011985	2.287464	-2.318408

1-TS$_{A5-B1}$

Ru	-0.270919	-0.121759	-0.310709
C	2.701327	0.430948	-0.168370
C	1.510332	1.044595	-0.160501
C	-1.950785	0.845722	0.885162
C	-0.927365	0.490814	1.798780
C	-0.721433	-0.920336	1.697230
C	-1.642519	-1.445902	0.723179
C	-2.394478	-0.344879	0.207850
Cl	-0.741987	1.457576	-2.183982
C	2.719363	-1.060677	-0.137597
C	1.329464	-1.564786	-0.467421
H	1.063566	-2.520034	-0.015579
H	3.400594	-1.446887	-0.911857
C	-2.566530	2.181782	0.700433
H	-3.586475	2.170988	1.092547
H	-2.009552	2.961436	1.211110
H	-2.631624	2.444494	-0.356452
C	-3.513142	-0.387752	-0.769370
H	-3.412655	0.406539	-1.509400
H	-3.544393	-1.336504	-1.301811
H	-4.475952	-0.256467	-0.270122
C	-1.846845	-2.887012	0.425531
H	-2.322180	-3.035124	-0.541987
H	-0.905579	-3.435368	0.411245
H	-2.480336	-3.355194	1.182913
C	0.080120	-1.747424	2.634576
H	0.853343	-1.167968	3.132247
H	-0.573161	-2.151724	3.412503
H	0.555188	-2.596345	2.145821
C	-0.224483	1.393780	2.745007
H	-0.691940	1.352936	3.731920
H	0.819336	1.104293	2.864581
H	-0.242412	2.421438	2.392179
C	1.478397	2.554828	-0.102226
H	2.141635	2.895621	0.700536
C	4.018477	1.150174	-0.108014
H	4.015254	2.065311	-0.700176
H	4.280732	1.440979	0.914056
H	4.833324	0.524586	-0.474931
C	0.813463	-1.410948	-1.781300
H	-0.655096	-0.906879	-1.641505
C	3.245364	-1.580295	1.196009
H	4.291742	-1.307935	1.330470
H	2.689047	-1.148055	2.026979
H	3.177318	-2.667440	1.264800
H	1.301342	-0.703504	-2.450862
O	0.329365	-2.561906	-2.396765
H	-0.092592	-2.310718	-3.225966
O	0.233905	3.160983	0.160107
H	-0.327181	2.934531	-0.598633
H	1.904378	2.953198	-1.036224

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Ru	-0.305303	-0.135459	-0.350640
C	2.642485	0.462282	-0.005570
C	1.442928	1.059046	0.030542
C	-1.902931	0.639479	1.075603
C	-0.818192	0.202905	1.874836
C	-0.580419	-1.178591	1.592270
C	-1.539323	-1.610369	0.614344
C	-2.356576	-0.472285	0.287646
Cl	-0.905036	1.609149	-2.035249
C	2.725080	-0.998370	-0.325987
C	1.401101	-1.439351	-0.922045
H	1.141123	-2.493270	-0.857020

H	3.470720	-1.132975	-1.125270
C	-2.570373	1.964053	1.090904
H	-3.573836	1.863864	1.511669
H	-2.017976	2.691918	1.676370
H	-2.683465	2.360270	0.080646
C	-3.548402	-0.436876	-0.598414
H	-3.525480	0.440034	-1.244938
H	-3.603124	-1.317607	-1.234648
H	-4.465986	-0.391460	-0.007372
C	-1.754682	-3.017272	0.188932
H	-2.292752	-3.075093	-0.754757
H	-0.812240	-3.547558	0.062275
H	-2.333469	-3.563384	0.938160
C	0.257579	-2.099889	2.399592
H	1.025828	-1.573166	2.959339
H	-0.374888	-2.615260	3.128071
H	0.738491	-2.866948	1.795948
C	-0.078856	1.004953	2.880880
H	-0.463726	0.802297	3.883319
H	0.982504	0.756179	2.880384
H	-0.173678	2.069141	2.681207
C	1.376313	2.544447	0.289902
H	1.954925	2.787322	1.188869
C	3.931864	1.182919	0.272672
H	4.078417	1.355837	1.343162
H	4.795782	0.617960	-0.078253
H	3.964308	2.163515	-0.204424
C	0.990661	-0.758373	-2.072995
H	-1.069462	-0.912234	-1.493987
C	3.237509	-1.820916	0.849369
H	4.286562	-1.595402	1.039575
H	2.693650	-1.599342	1.763340
H	3.165775	-2.892583	0.656225
H	1.492103	0.168589	-2.335891
H	1.882287	3.067229	-0.538075
O	0.098386	3.093412	0.502240
H	-0.408427	2.906161	-0.305458
O	0.387143	-1.406271	-3.112829
H	-0.073863	-0.733247	-3.631262

1-TS$_{B1-B2}$

Ru	0.310081	0.018395	-0.277820
C	-2.610999	0.378707	0.375626
C	-1.515660	-0.341810	0.649742
C	1.917836	-0.689467	1.066626
C	1.300814	0.446277	1.656716
C	1.488968	1.535774	0.756617
C	2.380015	1.089386	-0.324428
C	2.608584	-0.270229	-0.149683
Cl	0.170951	-2.347197	-1.143470
C	-2.497968	1.496217	-0.619997
C	-1.281179	1.296601	-1.482808
H	-0.865129	2.203614	-1.919847
H	-3.367239	1.457498	-1.294664
C	2.065651	-2.041192	1.665409
H	3.102614	-2.199673	1.971593
H	1.442867	-2.168223	2.547885
H	1.807521	-2.826551	0.955536
C	3.437133	-1.171723	-0.984755
H	2.904200	-2.097770	-1.203346
H	3.711701	-0.709450	-1.930574
H	4.360829	-1.439913	-0.466086
C	2.966353	1.980893	-1.358957
H	3.260156	1.429928	-2.250033
H	2.275513	2.765942	-1.665884
H	3.859294	2.481308	-0.975371
C	1.168338	2.959649	1.040982
H	0.351678	3.052853	1.753279
H	2.036433	3.465760	1.472723
H	0.890236	3.511665	0.143256
C	0.622024	0.526880	2.975223
H	1.278447	0.988241	3.716777
H	-0.288348	1.122778	2.918670
H	0.345880	-0.456209	3.349184
C	-1.590143	-1.553032	1.544523
H	-2.137996	-1.323390	2.465216
H	-0.588863	-1.876086	1.854368
C	-3.978979	0.114006	0.916567
H	-3.971774	-0.560699	1.768608
H	-4.484152	1.036123	1.216323
H	-4.605522	-0.352267	0.150534
C	-1.078662	0.126977	-2.222511
H	-0.308352	0.086652	-2.989438
H	0.398569	1.367762	-1.055048
C	-2.489860	2.864458	0.050467
H	-3.394140	3.019938	0.636392
H	-1.639917	2.944548	0.728429
H	-2.424279	3.676032	-0.676692

O	-2.278961	-2.637876	0.946112
H	-1.761664	-2.862839	0.158386
O	-2.045750	-0.795163	-2.286437
H	-1.614178	-1.670524	-2.326667

1-B2

Ru	0.236525	0.169286	0.055342
C	-2.668903	-0.423929	0.355398
C	-1.485023	-1.054340	0.434365
C	1.844545	-1.334632	0.384390
C	1.608036	-0.529595	1.545753
C	1.923226	0.840291	1.193760
C	2.367044	0.862609	-0.168482
C	2.275498	-0.463745	-0.666196
Cl	-0.586198	-0.299221	-2.307092
C	-2.695813	1.080284	0.161175
C	-1.355982	1.655671	0.594199
H	-1.415083	2.337290	1.451065
H	-2.800095	1.253578	-0.919145
C	1.866579	-2.820792	0.307092
H	2.857467	-3.162599	0.001426
H	1.653741	-3.270622	1.274635
H	1.140319	-3.213305	-0.405604
C	2.645669	-0.908193	-2.031077
H	2.075898	-1.784272	-2.332333
H	2.471925	-0.131468	-2.772141
H	3.706768	-1.170397	-2.059426
C	2.848415	2.039349	-0.937752
H	2.441210	2.049818	-1.948458
H	2.571280	2.978887	-0.463100
H	3.937426	2.030260	-1.024189
C	1.934856	1.989952	2.137337
H	1.178242	1.883396	2.913676
H	2.901363	2.070041	2.639781
H	1.761840	2.939260	1.631641
C	1.287525	-1.030438	2.908796
H	2.193574	-1.334237	3.439281
H	0.797752	-0.269163	3.513700
H	0.625502	-1.894155	2.872054
C	-1.357187	-2.537365	0.491070
H	-2.271012	-3.003052	0.881320
H	-0.558785	-2.834908	1.182365
C	-4.003120	-1.099814	0.287047
H	-3.927524	-2.181274	0.227659
H	-4.634346	-0.853784	1.144510
H	-4.546328	-0.763085	-0.600387
C	-0.376598	2.167366	-0.398329
H	0.318185	2.900077	0.009385
H	-0.861998	0.795499	1.270148
C	-3.845399	1.791867	0.860958
H	-4.813730	1.455238	0.495638
H	-3.820500	1.617794	1.938602
H	-3.791550	2.867800	0.695551
O	-1.072988	-3.101829	-0.783857
H	-1.064950	-2.370203	-1.421889
O	-0.731832	2.551033	-1.648622
H	-1.009991	1.754841	-2.147431

1-TS$_{B2-B3}$

Ru	-0.212069	-0.153371	0.077635
C	2.705195	0.455023	0.328976
C	1.521922	1.079732	0.415517
C	-1.880737	1.321497	0.256042
C	-1.633217	0.625247	1.483472
C	-1.888375	-0.780170	1.253260
C	-2.329746	-0.930850	-0.104769
C	-2.298283	0.349546	-0.708883
Cl	0.583035	0.239577	-2.305156
C	2.705381	-1.049943	0.157685
C	1.368035	-1.596447	0.597329
H	1.377194	-2.057957	1.588274
H	2.802364	-1.235281	-0.921629
C	-1.962448	2.792426	0.067714
H	-2.994189	3.126764	0.209380
H	-1.344117	3.334366	0.778757
H	-1.643329	3.096164	-0.925311
C	-2.682723	0.648479	-2.108804
H	-3.751584	0.872755	-2.159041
H	-2.141815	1.507103	-2.498981
H	-2.485334	-0.192215	-2.770116
C	-2.774950	-2.183937	-0.769739
H	-2.308333	-2.308735	-1.746935
H	-2.537097	-3.065599	-0.177689
H	-3.856510	-2.180137	-0.922302
C	-1.879509	-1.843132	2.293547
H	-1.174036	-1.618143	3.091931
H	-2.865146	-1.947439	2.752696
H	-1.615955	-2.817969	1.884442

C	-1.348956	1.253032	2.800691
H	-2.277625	1.550026	3.294311
H	-0.826608	0.572881	3.471067
H	-0.738035	2.147843	2.696775
C	1.368049	2.558839	0.458309
H	0.640027	2.855269	1.225005
H	2.308922	3.045549	0.747135
C	4.040819	1.119001	0.224416
H	3.971579	2.200599	0.156500
H	4.685515	0.878050	1.073211
H	4.565459	0.767916	-0.668534
C	0.425699	-2.217465	-0.295648
H	-0.273918	-2.913170	0.160731
H	0.754832	-0.473260	1.330668
C	3.844193	-1.773335	0.864298
H	4.816463	-1.456842	0.491114
H	3.824503	-1.583004	1.939247
H	3.771890	-2.850337	0.714848
O	0.937051	3.091764	-0.784675
H	0.950898	2.362130	-1.423948
O	0.689421	-2.602974	-1.567647
H	0.969543	-1.817396	-2.081824

1-B3

Ru	-0.062250	-0.130825	-0.149655
C	2.278446	-0.082131	-0.177108
C	1.791838	0.842614	0.736621
C	-1.147138	1.070720	1.477425
C	-1.035292	-0.334139	1.773084
C	-1.777022	-1.050642	0.763738
C	-2.222597	-0.105273	-0.206326
C	-1.838707	1.212413	0.262173
Cl	0.052848	1.003867	-2.389324
C	2.379712	-1.561642	0.193261
C	0.981116	-2.039154	-0.088907
H	0.529237	-2.789898	0.552759
H	3.097245	-2.040545	-0.484623
C	-0.683184	2.172078	2.357211
H	-1.462843	2.417255	3.083223
H	0.200991	1.895280	2.930241
H	-0.455630	3.070748	1.789044
C	-2.195683	2.486799	-0.405499
H	-1.526263	3.293018	-0.113761
H	-2.150344	2.390779	-1.488731
H	-3.215876	2.773970	-0.136792
C	-3.071177	-0.374350	-1.394770
H	-2.714035	0.181788	-2.262544
H	-3.073793	-1.434026	-1.644887
H	-4.107756	-0.078047	-1.215883
C	-2.143083	-2.489009	0.819983
H	-1.476656	-3.055086	1.468346
H	-3.150623	-2.593926	1.229233
H	-2.127960	-2.954463	-0.161974
C	-0.526174	-0.904168	3.047829
H	-1.297140	-0.886138	3.823556
H	-0.209870	-1.939714	2.930932
H	0.323105	-0.341207	3.435364
C	1.999943	2.337289	0.569173
H	2.014016	2.799941	1.557788
H	2.999633	2.504283	0.143200
C	3.010736	0.337373	-1.409665
H	2.806860	1.359851	-1.712551
H	4.084656	0.240680	-1.213811
H	2.789985	-0.299426	-2.264437
C	0.476475	-1.833995	-1.383717
H	1.665605	0.515431	1.763350
C	2.828790	-1.836571	1.614401
H	3.801366	-1.390204	1.819092
H	2.120538	-1.443317	2.343178
H	2.908497	-2.909710	1.788483
O	1.027697	3.039061	-0.169341
H	0.815737	2.528663	-0.972533
H	1.133713	-1.451212	-2.158460
O	-0.555580	-2.614268	-1.864840
H	-0.900736	-2.161834	-2.643465

(*Si*)-1-TS$_{A1-A2}$

Ru	-0.007321	-0.045795	-0.078380
C	-0.894835	1.749722	0.494562
C	0.256900	1.980965	1.020148
C	0.747338	2.789507	2.161685
C	-2.232167	2.361930	0.336129
C	-1.772500	-1.073299	0.864028
C	-0.573646	-1.423225	1.554863
C	0.279468	-2.108455	0.634843
C	-0.334295	-2.068900	-0.663246
C	-1.626616	-1.433979	-0.501719
C	-2.985358	-0.498348	1.498702

H	-3.598397	0.042000	0.781633
H	-2.735329	0.174856	2.317636
H	-3.589947	-1.303069	1.924423
C	-0.322645	-1.256126	3.009691
H	-0.677448	-2.120004	3.578558
H	-0.831932	-0.378175	3.404503
H	0.740780	-1.144285	3.219928
C	1.414901	-2.976397	1.044267
H	2.090561	-3.206229	0.225331
H	1.010400	-3.928487	1.398944
H	1.998258	-2.559323	1.862554
C	0.150015	-2.719971	-1.908308
H	-0.096675	-2.115459	-2.780125
H	-0.298626	-3.707192	-2.048800
H	1.231637	-2.847826	-1.896441
C	-2.660739	-1.329585	-1.560939
H	-3.402841	-0.571077	-1.322905
H	-3.174488	-2.287799	-1.674410
H	-2.217559	-1.070705	-2.520372
H	-2.833026	2.242641	1.243557
H	-2.086880	3.444848	0.208592
H	1.665804	3.335611	1.944278
H	0.955838	2.149972	3.023378
H	-0.015394	3.507213	2.463727
Cl	-0.360294	1.010250	-2.333962
C	1.860845	1.412325	0.169430
C	2.035081	0.183236	-0.596534
C	3.137919	-0.701615	-0.120940
C	2.088411	2.675537	-0.632538
H	1.888064	3.588992	-0.077291
H	1.468900	2.667879	-1.525960
H	3.134823	2.685641	-0.941759
H	3.147469	-1.654679	-0.661818
H	3.028161	-0.919746	0.949729
H	2.068001	0.337654	-1.672637
H	2.430016	1.378956	1.097931
O	-2.982593	1.825108	-0.724372
H	-2.349354	1.655780	-1.447289
O	4.357477	0.005525	-0.354296
H	5.088760	-0.582246	-0.144243

1-A1’

Ru	-0.028726	0.011903	-0.155046
C	1.403116	1.131729	-1.422321
C	1.958656	0.056153	-1.106756
C	3.148756	-0.783662	-1.259509
C	1.348690	2.432544	-2.082058
C	-0.250350	1.818570	1.080802
C	0.863872	1.040509	1.533197
C	0.384160	-0.238493	1.969846
C	-1.048427	-0.210360	1.841990
C	-1.429575	1.030865	1.271705
C	-0.261504	3.238646	0.646161
H	-0.829189	3.365286	-0.276589
H	0.741848	3.624279	0.482588
H	-0.733155	3.867111	1.405326
C	2.270723	1.502199	1.630546
H	2.490643	2.289621	0.911718
H	2.973359	0.690151	1.452020
H	2.461405	1.903807	2.628929
C	1.201589	-1.260661	2.674572
H	0.703507	-2.227774	2.704770
H	1.391042	-0.962837	3.709672
H	2.166453	-1.397907	2.187304
C	-2.001990	-1.223798	2.362750
H	-2.854739	-1.355801	1.697326
H	-2.380987	-0.898843	3.334715
H	-1.532417	-2.194598	2.513053
C	-2.812979	1.491739	0.998115
H	-2.877388	1.979783	0.025105
H	-3.128065	2.217438	1.752286
H	-3.521613	0.666563	1.008818
H	1.862726	3.190109	-1.486798
H	1.852760	2.379662	-3.048716
H	3.868966	-0.245111	-1.888724
H	2.898453	-1.715570	-1.782731
Cl	-1.389065	0.829811	-2.114851
C	0.226231	-2.087186	-0.984619
C	-1.091093	-1.941652	-0.544512
C	-2.316143	-1.954092	-1.407113
C	1.135852	-3.031809	-0.251530
H	1.234159	-3.961653	-0.819522
H	0.703180	-3.299596	0.712214
H	-2.682211	-2.987214	-1.420909
H	-1.278360	-2.374059	0.432493
H	0.414662	-1.959322	-2.048972
H	-2.070599	-1.683276	-2.436675
H	0.326540	2.759486	-2.258676

O	3.723617	-1.062792	0.017288
H	4.520652	-1.581032	-0.129775
H	2.136751	-2.657611	-0.056737
O	-3.376543	-1.170412	-0.902493
H	-3.134406	-0.263429	-1.154996

1-TS$_{A1'-A2'}$

Ru	0.120875	-0.035542	-0.094057
C	-1.543343	-0.755957	-1.048360
C	-2.150184	0.261224	-0.553997
C	-3.573706	0.664135	-0.594154
C	-1.841946	-1.877300	-1.943680
C	1.188117	-1.885965	-0.101436
C	0.242395	-1.900908	0.980735
C	0.589385	-0.844792	1.889762
C	1.788285	-0.230829	1.408245
C	2.131875	-0.825087	0.166368
C	1.311569	-2.838543	-1.236018
H	1.396178	-2.305853	-2.184357
H	0.453998	-3.504371	-1.303521
H	2.202317	-3.461593	-1.127037
C	-0.850468	-2.882725	1.221469
H	-0.910760	-3.620105	0.424275
H	-1.825729	-2.399695	1.302751
H	-0.677847	-3.426836	2.152140
C	-0.066555	-0.598312	3.199675
H	0.087382	0.422696	3.546979
H	0.337464	-1.261781	3.969346
H	-1.140085	-0.777651	3.150002
C	2.575200	0.832943	2.083352
H	2.911913	1.588162	1.372970
H	3.458140	0.396161	2.555724
H	2.006685	1.331581	2.866494
C	3.329150	-0.522055	-0.656275
H	3.089931	-0.544379	-1.718814
H	4.112760	-1.262224	-0.474195
H	3.736195	0.459751	-0.422683
H	-1.775243	-2.838997	-1.434941
H	-2.848826	-1.792842	-2.359238
H	-3.974331	0.323481	-1.557759
H	-3.694170	1.754451	-0.558753
Cl	0.593635	0.595192	-2.482539
C	-1.273755	1.830390	0.287083
C	0.163943	2.021800	0.391473
C	0.869476	3.000093	-0.514576
C	-2.042669	2.010663	1.573065
H	-2.054888	3.071553	1.831387
H	-1.545072	1.489704	2.388579
H	0.908360	3.976641	-0.019452
H	0.504246	2.090854	1.422565
H	-1.677213	2.387543	-0.558401
H	0.299422	3.127325	-1.440542
H	-1.127492	-1.891007	-2.768470
O	-4.282532	0.041080	0.478063
H	-5.216346	0.247882	0.367963
H	-3.069581	1.658582	1.542297
O	2.208644	2.649587	-0.790606
H	2.132798	1.928542	-1.439707

1-TS$_{A5'-A6'}$

Ru	0.410818	-0.113881	-0.302056
C	-2.537335	-0.239931	-0.606416
C	-1.471009	-1.029601	-0.381723
C	1.599336	-0.924027	1.379558
C	0.537238	-0.181771	1.951805
C	0.682726	1.169882	1.521332
C	1.892516	1.283908	0.736407
C	2.462624	0.007945	0.654347
Cl	1.400562	-1.832991	-1.764630
C	-2.313549	1.235325	-0.816363
C	-0.824037	1.495823	-0.976490
H	-0.451281	2.457328	-0.637990
H	-2.806584	1.549360	-1.749913
C	1.897342	-2.364906	1.577722
H	2.701599	-2.496136	2.306278
H	1.029356	-2.911240	1.941639
H	2.214346	-2.832500	0.645723
C	3.748524	-0.357998	0.014659
H	3.686620	-1.326542	-0.478290
H	4.050990	0.374564	-0.731736
H	4.541529	-0.413690	0.764942
C	2.435982	2.558606	0.203681
H	2.907376	3.145553	0.996464
H	3.182524	2.386705	-0.568222
H	1.656828	3.180992	-0.236027
C	-0.055439	2.331507	2.078648
H	-0.977300	2.036132	2.572214
H	0.572469	2.822949	2.826967

H	-0.297672	3.087364	1.332905
C	-0.540603	-0.679143	2.846693
H	-0.429564	-0.265500	3.851237
H	-1.531880	-0.402484	2.482763
H	-0.517157	-1.762304	2.939636
C	-1.546102	-2.486875	-0.091320
H	-1.298605	-2.676895	0.955989
H	-2.538254	-2.910755	-0.261857
C	-3.951053	-0.718012	-0.518400
H	-4.058509	-1.708234	-0.976466
H	-4.612663	-0.036008	-1.070019
C	-0.162401	0.947867	-2.124018
H	-0.359140	-0.457507	-1.682243
H	-0.830915	0.526149	-2.890138
C	-2.945767	2.051362	0.304829
H	-4.028732	1.938248	0.303156
H	-2.598833	1.709689	1.278302
H	-2.718227	3.114415	0.206028
O	0.928470	1.599829	-2.679093
H	1.514965	0.915160	-3.025508
O	-4.337584	-0.770086	0.860347
H	-5.251547	-1.069390	0.898457
H	-0.818335	-3.041543	-0.684844

(*1,4-anti*)-2-A1

Ru	0.093233	-0.057970	0.111433
C	-2.010538	-0.483108	0.345553
C	-1.450361	-1.036085	1.324428
C	-1.475094	-1.834759	2.552937
C	-3.231450	-0.127664	-0.418712
C	0.651558	-1.258939	-1.635220
C	0.467086	-2.117981	-0.525115
C	1.419779	-1.749344	0.500605
C	2.269108	-0.740452	-0.057655
C	1.786142	-0.410433	-1.342019
C	-0.058592	-1.317783	-2.936667
H	-0.135410	-0.327853	-3.384303
H	-1.068453	-1.707156	-2.824745
H	0.478653	-1.960450	-3.639645
C	-0.498609	-3.243955	-0.490006
H	-1.480275	-2.941390	-0.853181
H	-0.623314	-3.652345	0.509488
H	-0.144353	-4.053548	-1.131489
C	1.704016	-2.480833	1.763650
H	1.874883	-1.799655	2.598092
H	2.601455	-3.096921	1.663109
H	0.888036	-3.142483	2.042428
C	3.512467	-0.230921	0.573082
H	3.739185	0.792803	0.282048
H	4.358944	-0.849919	0.265218
H	3.468427	-0.273222	1.659719
C	2.402330	0.524837	-2.316344
H	1.686163	1.272598	-2.659601
H	2.740338	-0.029664	-3.194457
H	3.266072	1.040270	-1.902126
H	-3.978154	-0.896822	-0.186455
H	-0.690035	-1.560998	3.255166
H	-1.359510	-2.900088	2.342139
H	-2.431348	-1.713554	3.066059
Cl	-0.617577	1.775685	-1.496139
C	-0.273886	1.599430	1.664082
C	1.069286	1.573807	1.314082
C	1.744830	2.682634	0.528436
C	-0.760773	1.226803	3.021881
H	-0.776661	2.120762	3.651194
H	-0.105105	0.503807	3.508046
H	-1.775551	0.830524	3.016388
H	2.204272	2.299401	-0.391154
H	2.568537	3.052767	1.148913
H	1.730792	1.062749	2.010342
H	-0.893684	2.322460	1.142402
O	-3.042119	-0.225909	-1.816743
H	-2.355747	0.427457	-2.035735
O	0.935316	3.791627	0.256599
H	0.297698	3.502352	-0.415601
C	-3.780435	1.227603	-0.003461
H	-4.709173	1.427210	-0.535780
H	-3.979363	1.257320	1.068187
H	-3.067539	2.014738	-0.243441

(*1,4-anti*)-2-TS$_{A1-A2}$

Ru	0.251216	0.095129	-0.042439
C	-1.596614	-0.472301	0.669064
C	-1.728687	0.727584	1.116599
C	-2.832473	1.506025	1.731146
C	-2.443182	-1.688644	0.470557
C	1.277499	-1.737904	-0.664939
C	1.059540	-1.870246	0.728976

C	1.686798	-0.774344	1.397742
C	2.385244	-0.004167	0.410503
C	2.095021	-0.558925	-0.878388
C	0.906042	-2.701806	-1.730471
H	0.474643	-2.192968	-2.592076
H	0.184255	-3.433167	-1.378003
H	1.796755	-3.233466	-2.074459
C	0.371866	-2.988840	1.421845
H	-0.328796	-3.499365	0.766825
H	-0.165513	-2.645628	2.305063
H	1.113351	-3.715197	1.764690
C	1.772156	-0.626093	2.874872
H	2.250444	0.306416	3.166424
H	2.356569	-1.439643	3.311880
H	0.786637	-0.654721	3.340822
C	3.373290	1.068498	0.697190
H	3.564827	1.691281	-0.174339
H	4.326867	0.622672	0.989868
H	3.066209	1.723721	1.511642
C	2.641413	-0.134859	-2.193445
H	1.884203	-0.226027	-2.971794
H	3.498299	-0.746758	-2.487589
H	2.967855	0.903837	-2.175402
H	-2.486012	2.188334	2.507587
H	-3.564378	0.836355	2.178148
H	-3.341896	2.110390	0.976196
Cl	-1.048132	0.064932	-2.231344
C	-0.428031	2.126225	0.863699
C	0.487897	2.167635	-0.281863
C	0.028543	2.924208	-1.513036
C	0.148073	2.432201	2.223480
H	0.246886	3.511903	2.352333
H	1.139015	1.998558	2.335623
H	-0.462735	2.061687	3.046015
H	0.484965	2.492209	-2.412418
H	0.400110	3.953305	-1.437944
H	1.506338	2.433244	-0.012175
H	-1.284345	2.742059	0.603383
O	-1.983788	-2.487672	-0.602775
H	-1.794456	-1.875094	-1.336585
O	-1.366506	3.023723	-1.644933
H	-1.662468	2.148360	-1.948312
H	-2.358588	-2.326708	1.358011
C	-3.906284	-1.325741	0.265050
H	-4.473989	-2.229001	0.049206
H	-4.337540	-0.852989	1.145855
H	-4.009104	-0.642561	-0.578106

(*1,4-anti*)-2-A2

Ru	-0.255997	-0.141616	-0.085877
C	1.429761	0.682561	0.696157
C	1.864606	-0.492810	1.096675
C	3.174959	-0.819495	1.746784
C	2.029143	2.051922	0.613726
C	-1.704139	1.444454	-0.507290
C	-1.530536	1.474558	0.898484
C	-1.872218	0.194313	1.422347
C	-2.346947	-0.622433	0.342422
C	-2.214947	0.130239	-0.868452
C	-1.584075	2.584032	-1.450769
H	-1.052204	2.295965	-2.357144
H	-1.055878	3.421431	-1.002605
H	-2.578587	2.925635	-1.748425
C	-1.116848	2.634324	1.728463
H	-0.568204	3.369079	1.146758
H	-0.489374	2.325182	2.563902
H	-1.999475	3.117564	2.155649
C	-1.907294	-0.130956	2.872969
H	-2.190085	-1.165049	3.057419
H	-2.636159	0.500015	3.387017
H	-0.942860	0.044307	3.351558
C	-2.986731	-1.956186	0.486240
H	-2.973986	-2.513501	-0.448597
H	-4.032073	-1.847301	0.784299
H	-2.501323	-2.572697	1.242981
C	-2.647538	-0.261765	-2.234493
H	-1.937627	0.093919	-2.980611
H	-3.626777	0.158884	-2.478330
H	-2.717142	-1.343548	-2.337769
H	1.969151	2.533351	1.597770
H	3.074353	-1.642011	2.456219
H	3.583539	0.032660	2.284882
H	3.906497	-1.133933	0.997128
Cl	0.929153	0.418476	-2.243439
C	1.076628	-1.902137	0.780590
C	0.150163	-2.118310	-0.430875
C	0.834454	-2.673516	-1.665320
C	0.544441	-2.539190	2.054456

H	0.539327	-3.625613	1.961363
H	-0.476913	-2.226444	2.257256
H	1.140951	-2.287850	2.930810
H	0.252840	-2.406395	-2.557445
H	0.826671	-3.768581	-1.605068
H	-0.694763	-2.750899	-0.159076
H	1.977528	-2.420199	0.437891
O	1.283913	2.895666	-0.250970
H	1.185558	2.396637	-1.080783
O	2.183287	-2.307222	-1.800864
H	2.177653	-1.367048	-2.050098
C	3.481128	2.020705	0.156639
H	3.833596	3.041350	0.018228
H	4.135544	1.526068	0.870631
H	3.556831	1.496626	-0.796596

(*1,4-anti*)-2-TS$_{A2-A3}$

Ru	0.234791	0.008762	0.019867
C	-1.658365	-0.544168	0.320440
C	-1.995035	0.642322	0.823240
C	-3.181357	0.797245	1.735372
C	-2.420745	-1.816724	0.169943
C	1.513773	-1.702806	-0.248271
C	1.213897	-1.580343	1.143395
C	1.745757	-0.317610	1.588732
C	2.444571	0.289730	0.502428
C	2.249779	-0.512484	-0.647956
C	1.337423	-2.889479	-1.124735
H	0.908212	-2.609285	-2.087979
H	0.691410	-3.635174	-0.669815
H	2.305558	-3.353798	-1.329641
C	0.567069	-2.601558	2.009311
H	-0.067514	-3.262986	1.423047
H	-0.053598	-2.140779	2.777732
H	1.315443	-3.210305	2.523052
C	1.678411	0.199824	2.980413
H	1.753401	1.286006	3.013861
H	2.495022	-0.198978	3.587666
H	0.747119	-0.086039	3.468075
C	3.226073	1.551263	0.555725
H	3.121445	2.136527	-0.357471
H	4.289368	1.332663	0.677387
H	2.934035	2.184034	1.392321
C	2.825231	-0.286594	-1.997707
H	2.119301	-0.572128	-2.776081
H	3.733630	-0.879142	-2.134039
H	3.087434	0.757905	-2.156461
H	-2.665114	-2.229258	1.157508
H	-2.887989	1.045872	2.757123
H	-3.762294	-0.120000	1.782159
H	-3.838829	1.600357	1.389705
Cl	-0.620286	-0.119733	-2.344440
C	-1.268447	2.038500	0.545681
C	0.104892	2.084754	-0.104688
C	0.215823	2.876316	-1.392733
C	-1.230936	2.889582	1.813318
H	-0.797929	3.862681	1.585317
H	-0.612633	2.423614	2.583234
H	-2.215665	3.067838	2.238605
H	0.431638	3.921795	-1.135391
H	0.855525	2.458618	0.593664
H	-1.957036	2.494141	-0.177185
O	-1.624483	-2.811945	-0.457584
H	-1.255740	-2.381115	-1.245884
C	-3.698205	-1.602136	-0.629129
H	-4.217475	-2.550419	-0.756739
H	-4.372537	-0.896336	-0.147126
H	-3.446639	-1.206071	-1.612958
H	1.091421	2.519149	-1.957870
O	-0.932686	2.911424	-2.189971
H	-1.075203	2.000897	-2.500689

(*1,4-anti*)-2-A3

Ru	-0.186475	-0.062231	-0.009772
C	1.035678	1.239483	0.527515
C	1.551244	0.183153	1.279042
C	1.513083	0.126474	2.775217
C	1.303220	2.656961	0.239758
C	-2.305190	0.691360	-0.332889
C	-2.016673	0.704879	1.046666
C	-1.726409	-0.653173	1.456666
C	-1.939673	-1.511599	0.328515
C	-2.243417	-0.693162	-0.775956
C	-2.700070	1.835492	-1.191321
H	-2.194632	1.791528	-2.157395
H	-2.449078	2.788150	-0.729487
H	-3.775449	1.829617	-1.388218
C	-2.026501	1.898855	1.934061

H	-1.746479	2.798967	1.388586
H	-1.335173	1.788552	2.769123
H	-3.018839	2.062309	2.360981
C	-1.550883	-1.131340	2.853168
H	-0.849597	-1.963158	2.916123
H	-2.503262	-1.486951	3.254769
H	-1.196556	-0.346357	3.517312
C	-1.848710	-2.993675	0.347715
H	-1.606979	-3.398291	-0.633625
H	-2.796706	-3.439871	0.658273
H	-1.089213	-3.345206	1.045249
C	-2.553077	-1.143983	-2.156115
H	-2.124728	-0.473296	-2.899222
H	-3.634339	-1.166575	-2.312854
H	-2.171104	-2.143727	-2.353930
H	1.282454	3.199536	1.196945
H	1.282399	-0.874184	3.144184
H	0.781803	0.816707	3.193432
H	2.491893	0.391190	3.185178
Cl	0.364024	0.519977	-2.362179
C	2.459315	-0.785844	0.510466
C	1.330732	-1.610739	-0.051721
C	1.595257	-2.372685	-1.340893
C	3.546738	-1.501061	1.283298
H	4.067748	-2.194991	0.623710
H	3.141861	-2.078428	2.115914
H	4.291713	-0.811571	1.684392
H	0.647990	-2.606111	-1.850658
H	2.051299	-3.339019	-1.088208
H	0.972891	-2.304274	0.718436
H	2.919021	-0.244044	-0.322634
O	0.310091	3.250025	-0.562643
H	0.169963	2.641668	-1.309254
O	2.501947	-1.746627	-2.212085
H	2.053996	-0.951794	-2.540230
C	2.699188	2.797339	-0.370014
H	2.898024	3.848511	-0.566074
H	3.467868	2.408937	0.297469
H	2.748261	2.253151	-1.312545

(*1,4-anti*)-2-TS$_{A3-A4}$

Ru	-0.271454	-0.115390	-0.162439
C	1.310916	1.051026	-0.285859
C	2.375482	0.503745	0.396908
C	3.387922	1.313688	1.132919
C	1.291794	2.497115	-0.706690
C	-2.636111	-0.313583	0.168223
C	-2.300798	1.072896	0.293600
C	-1.315296	1.183908	1.303128
C	-1.038117	-0.149327	1.807156
C	-1.893059	-1.071251	1.094408
C	-3.641324	-0.841889	-0.784019
H	-4.648137	-0.672222	-0.393945
H	-3.523683	-1.909875	-0.950428
H	-3.577544	-0.349148	-1.752520
C	-2.956070	2.175486	-0.451629
H	-3.057885	1.934338	-1.510920
H	-2.393741	3.102666	-0.374231
H	-3.966689	2.359035	-0.075691
C	-0.772150	2.441198	1.882391
H	0.261476	2.318183	2.207850
H	-1.350628	2.741141	2.759790
H	-0.799824	3.254832	1.161157
C	-0.248184	-0.460170	3.029157
H	0.102007	-1.490574	3.040738
H	-0.861931	-0.319010	3.923463
H	0.621301	0.189327	3.127949
C	-1.995256	-2.534720	1.331255
H	-1.070584	-2.944650	1.735030
H	-2.213044	-3.074277	0.410193
H	-2.789092	-2.771455	2.044842
H	1.499790	3.163654	0.141157
H	3.421712	1.028886	2.187668
H	3.213253	2.384463	1.073750
H	4.389299	1.105698	0.744530
Cl	-0.831022	-1.036472	-2.258783
C	2.554636	-0.980055	0.366502
C	1.214946	-1.648535	0.114262
C	1.336668	-2.795080	-0.864046
C	3.266445	-1.576389	1.578049
H	3.358172	-2.655285	1.461480
H	2.704874	-1.392751	2.496241
H	4.272211	-1.178632	1.715643
H	1.999897	-3.559675	-0.435074
H	0.850088	-2.057717	1.062857
H	3.204035	-1.157103	-0.507518
O	0.016920	2.904210	-1.181638
H	-0.386547	2.117184	-1.582502

C	2.345892	2.727650	-1.781763
H	2.300042	3.756265	-2.135144
H	3.351933	2.532457	-1.409654
H	2.166727	2.065469	-2.629186
H	0.363099	-3.275637	-1.019399
O	1.935520	-2.434284	-2.089996
H	1.281251	-1.882069	-2.542130

(*1,4-anti*)-2-A4

Ru	0.361281	0.160700	0.098763
C	-1.468036	0.923652	-0.376216
C	-2.598815	0.247439	-0.568156
C	-3.924040	0.820248	-0.953512
C	-1.198720	2.383732	-0.284088
C	2.476995	0.617357	-0.402746
C	1.595024	0.554592	-1.564110
C	1.119277	-0.786202	-1.671905
C	1.681155	-1.519935	-0.558087
C	2.535993	-0.656812	0.185949
C	3.180262	1.834307	0.075284
H	3.284991	1.836520	1.159347
H	2.650713	2.740403	-0.210293
H	4.183887	1.890346	-0.352810
C	1.383134	1.645691	-2.549167
H	1.368993	2.622662	-2.068133
H	0.442884	1.519755	-3.083392
H	2.184324	1.659552	-3.292780
C	0.372094	-1.354670	-2.821281
H	-0.156847	-2.266427	-2.550138
H	1.050038	-1.605475	-3.641227
H	-0.365246	-0.651276	-3.205287
C	1.623971	-2.990434	-0.346196
H	1.363763	-3.253616	0.678541
H	2.606661	-3.422566	-0.548033
H	0.914610	-3.481313	-1.007709
C	3.287888	-1.043159	1.404427
H	2.723262	-1.750373	2.010171
H	3.510097	-0.182116	2.030565
H	4.236553	-1.519300	1.144001
H	-1.095940	2.868815	-1.261232
H	-4.347048	0.292155	-1.811739
H	-3.865672	1.871959	-1.227039
H	-4.655440	0.723521	-0.145271
Cl	0.171913	0.616708	2.560980
C	-2.499154	-1.210968	-0.270804
C	-1.073023	-1.546747	0.223276
C	-1.099466	-2.210161	1.593027
C	-2.953300	-2.127873	-1.401755
H	-2.817529	-3.177056	-1.133525
H	-2.395446	-1.942199	-2.320913
H	-4.011221	-1.992279	-1.630193
H	-0.080200	-2.326730	1.988453
H	-1.498260	-3.226892	1.462866
H	-0.652710	-2.274971	-0.464988
H	-3.170015	-1.397904	0.580080
O	0.186332	2.399442	0.264478
H	0.107710	2.386263	1.241726
O	-1.940272	-1.601708	2.536774
H	-1.518859	-0.759212	2.770957
C	-2.083216	3.198838	0.623975
H	-1.685873	4.205964	0.753697
H	-3.086812	3.282918	0.214120
H	-2.160885	2.718788	1.600431

(*1,4-anti*)-2-TS$_{\mathbf{A4\text{-}A5}}$

Ru	0.295265	-0.098699	-0.208708
C	-2.556547	0.783279	-0.019195
C	-1.771977	-0.303374	0.094746
C	0.917565	-0.035535	1.853149
C	1.366583	1.184688	1.273163
C	2.311100	0.881626	0.228255
C	2.488001	-0.516512	0.180030
C	1.621588	-1.089925	1.177987
Cl	0.235339	-2.040212	-1.630426
C	-1.881038	2.078402	-0.351561
C	-0.469683	1.766653	-0.808850
H	0.221815	2.599503	-0.679216
H	-2.399590	2.557699	-1.199732
C	0.005473	-0.200524	3.011083
H	0.566827	-0.232864	3.948416
H	-0.707415	0.619760	3.074231
H	-0.562644	-1.124859	2.919526
C	1.571345	-2.529929	1.528616
H	0.667210	-2.785454	2.073160
H	1.634435	-3.165074	0.646276
H	2.431133	-2.765778	2.162827
C	3.411305	-1.281095	-0.692449
H	3.759691	-0.681321	-1.531589

H	4.291594	-1.614058	-0.137776
H	2.921826	-2.166355	-1.098927
C	3.031845	1.905761	-0.564113
H	2.363459	2.692933	-0.910998
H	3.805470	2.382252	0.044009
H	3.512521	1.480728	-1.441544
C	1.160149	2.544135	1.831362
H	2.076115	2.847914	2.345184
H	0.963642	3.301098	1.074085
H	0.355245	2.575096	2.559749
C	-2.387470	-1.641107	0.462840
H	-3.076385	-1.470991	1.299719
C	-4.043736	0.824148	0.164554
H	-4.355341	1.707960	0.725658
H	-4.567241	0.873654	-0.795285
H	-4.431249	-0.045946	0.690622
C	-0.398620	1.297532	-2.266556
H	-0.861551	0.310698	-2.395722
C	-1.952181	3.071019	0.803747
H	-2.978366	3.385839	0.987077
H	-1.586341	2.619991	1.725228
H	-1.367518	3.970436	0.604311
O	-1.454118	-2.576598	0.996295
H	-0.863951	-2.804339	0.262778
H	-1.037909	1.981748	-2.841071
O	0.894549	1.329391	-2.841976
H	1.219620	0.420557	-2.859263
C	-3.164025	-2.268652	-0.683632
H	-2.500100	-2.467829	-1.524311
H	-3.610367	-3.211207	-0.366274
H	-3.958546	-1.611340	-1.034365

(*1,4-anti*)-2-A5

Ru	0.331968	-0.040015	-0.273273
C	-2.578885	0.731858	0.022702
C	-1.757761	-0.333761	0.051299
C	0.942704	-0.169343	1.834614
C	1.395074	1.086004	1.328348
C	2.329279	0.847742	0.260436
C	2.478102	-0.548599	0.113197
C	1.613238	-1.181662	1.088505
Cl	0.253311	-2.060850	-1.682664
C	-1.946124	2.074626	-0.167633
C	-0.535435	1.840788	-0.650344
H	0.143164	2.673021	-0.467519
H	-2.472500	2.645555	-0.950645
C	0.024042	-0.392008	2.978759
H	0.579005	-0.472705	3.916688
H	-0.688379	0.425083	3.081645
H	-0.544556	-1.309090	2.833816
C	1.592665	-2.637452	1.369189
H	0.745463	-2.922186	1.985832
H	1.565871	-3.225828	0.452642
H	2.510316	-2.905732	1.900126
C	3.408996	-1.270133	-0.787946
H	3.795994	-0.621468	-1.571339
H	4.263533	-1.660351	-0.229893
H	2.912795	-2.113484	-1.267878
C	3.042630	1.916456	-0.481872
H	2.367225	2.719023	-0.779706
H	3.825191	2.364638	0.135403
H	3.511079	1.535406	-1.386517
C	1.194210	2.407026	1.975055
H	2.095618	2.654100	2.542136
H	1.042686	3.218253	1.264893
H	0.362524	2.406325	2.673151
C	-2.340414	-1.702406	0.365527
H	-3.042388	-1.570243	1.198193
C	-4.065441	0.714074	0.220589
H	-4.398423	1.550010	0.839553
H	-4.596468	0.810647	-0.731288
H	-4.425231	-0.199379	0.689308
C	-0.363529	1.354227	-2.039286
H	0.069170	0.284264	-2.082502
C	-2.012997	2.915889	1.101322
H	-3.039995	3.187381	1.339820
H	-1.621659	2.359459	1.952683
H	-1.445576	3.843029	1.004903
O	-1.396967	-2.629144	0.887541
H	-0.782817	-2.812837	0.160225
H	-1.329428	1.181347	-2.532533
O	0.511672	2.172246	-2.776314
H	0.722675	1.726418	-3.602844
C	-3.100767	-2.308201	-0.804209
H	-2.435005	-2.465781	-1.651195
H	-3.527688	-3.269292	-0.516632
H	-3.910248	-1.656038	-1.130548

(*1,4-anti*)-2-TS$_{A5-A6}$

Ru	0.294483	-0.034127	-0.262845
C	-2.624020	0.575183	-0.050478
C	-1.753913	-0.440413	0.100966
C	1.708550	-0.913276	1.224589
C	0.914923	0.033083	1.911617
C	1.151880	1.303405	1.307245
C	2.158347	1.145903	0.273939
C	2.502193	-0.209168	0.220632
Cl	0.600339	-2.114348	-1.584206
C	-2.098748	1.908175	-0.522260
C	-0.649951	1.752186	-0.953802
H	-0.006619	2.617942	-0.836983
H	-2.670807	2.219446	-1.410911
C	1.872801	-2.348767	1.561237
H	2.827708	-2.499212	2.071964
H	1.078903	-2.703866	2.212671
H	1.884698	-2.972769	0.667188
C	3.534948	-0.839802	-0.635356
H	3.213818	-1.818297	-0.989148
H	3.762882	-0.228572	-1.507174
H	4.464084	-0.977244	-0.076236
C	2.773909	2.259134	-0.490936
H	3.541476	2.758088	0.106614
H	3.243194	1.908754	-1.407067
H	2.047142	3.020619	-0.771024
C	0.747795	2.614867	1.871897
H	-0.096698	2.529458	2.550459
H	1.583195	3.026311	2.445216
H	0.499845	3.351907	1.109730
C	-0.005901	-0.234128	3.045090
H	0.498013	-0.083990	4.002802
H	-0.868720	0.431114	3.017150
H	-0.378910	-1.255549	3.007347
C	-2.206455	-1.825548	0.515152
H	-2.917579	-1.721758	1.342951
C	-4.094101	0.509422	0.228220
H	-4.404859	-0.441779	0.652285
H	-4.408929	1.292486	0.922122
H	-4.676693	0.661766	-0.685583
C	-0.380611	0.932561	-2.101763
H	-0.800624	-0.302012	-1.431859
H	-1.272686	0.630366	-2.672651
C	-2.302631	3.002192	0.520647
H	-3.357932	3.246145	0.630812
H	-1.939925	2.687130	1.498015
H	-1.785467	3.922001	0.243898
O	-1.165016	-2.620417	1.064862
H	-0.530239	-2.765264	0.345278
O	0.696857	1.221103	-2.926002
H	1.022630	0.379465	-3.269124
C	-2.885396	-2.561766	-0.629956
H	-3.208928	-3.550420	-0.305517
H	-3.753160	-2.014847	-0.997969
H	-2.188249	-2.686858	-1.459537

(*1,4-anti*)-2-A6

Ru	0.235679	0.027394	-0.154055
C	-1.778243	1.091472	0.027590
C	-1.927859	-0.144652	-0.614483
C	1.279111	-1.576592	0.941277
C	0.455488	-0.881029	1.856692
C	0.890214	0.494508	1.872729
C	2.021106	0.611437	0.995267
C	2.248534	-0.648883	0.392428
Cl	0.385938	-1.596120	-2.125668
C	-1.398149	2.292633	-0.841564
C	0.085869	2.094569	-1.028950
H	0.767623	2.754829	-0.504709
H	-1.902866	2.189873	-1.808014
C	1.235495	-3.036434	0.682761
H	1.834478	-3.561295	1.432448
H	0.217974	-3.420012	0.738712
H	1.631682	-3.282751	-0.299188
C	3.357441	-0.998995	-0.530096
H	3.019802	-1.681263	-1.310181
H	3.769150	-0.112622	-1.009899
H	4.171497	-1.490069	0.009004
C	2.851559	1.826291	0.793469
H	3.792082	1.739376	1.342250
H	3.099179	1.971452	-0.258125
H	2.353628	2.725558	1.152528
C	0.476966	1.538322	2.849114
H	-0.460171	1.291788	3.341265
H	1.233451	1.641793	3.631182
H	0.362895	2.518817	2.385705
C	-0.546607	-1.526801	2.743798
H	-0.048860	-2.016383	3.585300

H	-1.252088	-0.813972	3.166132
H	-1.108480	-2.291132	2.207566
C	-2.665691	-1.317553	-0.026211
H	-2.744772	-1.188957	1.058877
C	-2.388289	1.370472	1.366041
H	-2.356485	0.515332	2.034289
H	-1.928416	2.213295	1.873864
H	-3.444279	1.627108	1.230410
C	0.530514	1.291726	-2.054422
H	-1.931178	-0.139826	-1.704230
H	-0.187668	0.877638	-2.755612
C	-1.722414	3.662760	-0.281790
H	-2.784483	3.779357	-0.070034
H	-1.175505	3.862086	0.641063
H	-1.439127	4.435797	-0.995213
O	-2.001024	-2.557793	-0.228154
H	-1.319162	-2.425472	-0.907956
O	1.829979	1.259338	-2.457408
H	1.955301	0.382050	-2.854629
C	-4.072566	-1.396863	-0.597068
H	-4.599685	-2.256881	-0.187000
H	-4.645837	-0.497829	-0.365107
H	-4.037038	-1.509688	-1.680901

(1,4-syn)-2-A1

Ru	-0.238423	0.008824	-0.049974
C	1.731084	0.593004	-0.836615
C	1.078136	0.295573	-1.858029
C	0.942751	0.165193	-3.305604
C	2.944776	1.153373	-0.181958
C	0.283484	-1.284602	1.726696
C	0.843378	-1.86861	0.566589
C	-0.221184	-2.155196	-0.358697
C	-1.450143	-1.797708	0.272606
C	-1.138354	-1.189752	1.533554
C	0.998767	-0.910569	2.970429
H	0.695752	0.075591	3.322024
H	2.076864	-0.903646	2.82874
H	0.767107	-1.626686	3.762636
C	2.267568	-2.221164	0.345656
H	2.93391	-1.597012	0.936474
H	2.545678	-2.10342	-0.701317
H	2.439099	-3.267434	0.610288
C	-0.073971	-2.90058	-1.63574
H	-0.857778	-2.642586	-2.346849
H	-0.124553	-3.98007	-1.470125
H	0.885529	-2.693602	-2.107307
C	-2.803856	-2.219778	-0.172734
H	-3.571664	-1.46485	-0.010412
H	-3.106495	-3.098082	0.403327
H	-2.82283	-2.502824	-1.222308
C	-2.105965	-0.716035	2.557623
H	-1.747896	0.191579	3.043913
H	-2.259047	-1.467906	3.336208
H	-3.079297	-0.496446	2.121598
H	2.821916	2.244986	-0.209964
H	0.582445	-0.818323	-3.611034
H	1.915431	0.319507	-3.776444
H	0.253339	0.902512	-3.718043
Cl	0.35683	2.009349	1.399348
C	-1.571653	0.999199	-1.542023
C	-2.172923	1.127178	-0.283584
C	-2.436262	2.452261	0.381346
C	-2.184084	0.122683	-2.596315
H	-2.725254	0.740454	-3.318712
H	-2.911672	-0.561081	-2.165018
H	-1.472798	-0.469425	-3.167953
H	-2.314947	2.380529	1.468643
H	-3.497831	2.666617	0.20443
H	-2.954235	0.40725	-0.052698
H	-1.070843	1.892366	-1.906245
O	3.132975	0.742016	1.154982
H	2.377536	1.117164	1.640066
O	-1.725971	3.534914	-0.152275
H	-0.830097	3.460859	0.211407
C	4.1875	0.772464	-0.960342
H	5.059344	1.255059	-0.522593
H	4.342874	-0.305126	-0.930393
H	4.104575	1.079808	-2.001227

(1,4-syn)-2-TS$_{A1-A2}$

Ru	-0.259893	-0.059063	0.036
C	1.555765	0.864001	-0.305124
C	0.891565	1.783629	-0.906089
C	1.217779	3.133642	-1.418182
C	2.938411	0.756937	0.263886
C	0.193351	-2.082803	0.730475
C	0.678497	-2.014941	-0.599727

C	-0.404505	-1.684025	-1.46818
C	-1.597781	-1.640851	-0.675912
C	-1.234846	-1.833225	0.696085
C	0.944387	-2.515101	1.935531
H	0.727279	-1.875225	2.790361
H	2.018155	-2.500701	1.766059
H	0.656691	-3.534073	2.206355
C	2.055887	-2.323047	-1.05552
H	2.792366	-2.116063	-0.283239
H	2.318611	-1.755479	-1.946916
H	2.123586	-3.381671	-1.320184
C	-0.31291	-1.635228	-2.951796
H	-1.247359	-1.318304	-3.409724
H	-0.073132	-2.621638	-3.356533
H	0.469714	-0.953632	-3.286479
C	-2.982426	-1.583965	-1.21341
H	-3.705926	-1.301947	-0.451169
H	-3.273348	-2.569678	-1.584173
H	-3.088764	-0.888269	-2.045116
C	-2.141636	-1.931065	1.869029
H	-1.69115	-1.461885	2.74333
H	-2.358	-2.972328	2.122091
H	-3.091627	-1.432028	1.683665
H	3.099549	1.723653	0.767937
H	0.74086	3.358225	-2.373373
H	2.295499	3.223053	-1.552635
H	0.900378	3.903728	-0.710319
Cl	0.261345	0.793182	2.376367
C	-1.081023	1.850489	-1.019216
C	-1.932976	1.226006	-0.014348
C	-2.350799	2.068105	1.174451
C	-1.431655	1.670862	-2.471979
H	-2.229927	2.363062	-2.748379
H	-1.789901	0.664046	-2.672905
H	-0.593813	1.858546	-3.142753
H	-2.517009	1.428531	2.050134
H	-3.315948	2.532781	0.938848
H	-2.772644	0.675705	-0.42857
H	-0.93551	2.886348	-0.730925
O	3.066675	-0.276202	1.21652
H	2.355889	-0.122436	1.862978
O	-1.472232	3.122881	1.472284
H	-0.713077	2.710263	1.918085
C	4.028894	0.587085	-0.771566
H	5.002983	0.612143	-0.285739
H	3.938003	-0.360566	-1.296224
H	3.990576	1.388057	-1.507605

(*1,4-syn*)-2-A2

Ru	-0.249105	0.165648	0.045435
C	1.595707	-0.648596	-0.20975
C	2.054844	0.453353	-0.772018
C	3.490862	0.741605	-1.083276
C	2.327451	-1.834286	0.334574
C	-1.700852	-1.313395	0.727588
C	-1.31179	-1.770579	-0.555214
C	-1.586446	-0.74468	-1.50255
C	-2.249544	0.330457	-0.817476
C	-2.305659	0.000064	0.574109
C	-1.677199	-2.102131	1.983966
H	-1.465288	-1.47348	2.846326
H	-0.924976	-2.887438	1.946732
H	-2.649666	-2.574842	2.145383
C	-0.781214	-3.117705	-0.878561
H	-0.136076	-3.497528	-0.089467
H	-0.221729	-3.116916	-1.812146
H	-1.61236	-3.817124	-1.003637
C	-1.401943	-0.88273	-2.971433
H	-1.635421	0.03757	-3.502592
H	-2.059341	-1.659757	-3.368813
H	-0.380668	-1.168752	-3.226858
C	-2.883649	1.500711	-1.478667
H	-3.081979	2.305623	-0.773558
H	-3.839911	1.215907	-1.92321
H	-2.266829	1.908737	-2.279965
C	-2.954606	0.767828	1.667752
H	-2.350049	0.735395	2.574041
H	-3.939973	0.361159	1.910065
H	-3.086109	1.8147	1.398417
H	3.23221	-1.435109	0.823081
H	3.621106	1.090271	-2.110811
H	4.117997	-0.137197	-0.949334
H	3.86443	1.532936	-0.427523
Cl	0.594939	0.320766	2.427085
C	1.15053	1.765029	-1.054707
C	-0.017099	2.189211	-0.129481
C	0.382538	3.12537	0.99564
C	0.852629	1.917681	-2.537709

H	0.544394	2.938734	-2.765052
H	0.057209	1.251099	-2.861559
H	1.728961	1.696724	-3.147088
H	-0.339711	3.034698	1.817836
H	0.311844	4.157434	0.631359
H	-0.823703	2.634774	-0.710284
H	1.905687	2.496625	-0.751995
O	1.563249	-2.533756	1.300925
H	1.248239	-1.858444	1.926158
O	1.701788	2.968337	1.448336
H	1.713478	2.130981	1.943798
C	2.770931	-2.826471	-0.719535
H	3.312275	-3.647369	-0.25143
H	1.921774	-3.242766	-1.256073
H	3.427611	-2.349225	-1.444983

(*1,4-syn*)-2-TS$_{A2-A3}$

Ru	-0.007896	-0.173497	-0.041593
C	0.902741	1.57211	0.2149
C	-0.066166	2.350355	-0.296418
C	0.240889	3.75499	-0.740288
C	2.267293	1.953638	0.684937
C	1.05783	-1.933926	0.555497
C	1.616113	-1.528504	-0.697124
C	0.565196	-1.583505	-1.667781
C	-0.601093	-2.135562	-1.049239
C	-0.325685	-2.323621	0.323905
C	1.79137	-2.157298	1.827206
H	1.204097	-1.823966	2.682633
H	2.74024	-1.625471	1.837851
H	1.998766	-3.221722	1.967135
C	3.058848	-1.295502	-0.963075
H	3.53484	-0.758686	-0.144553
H	3.221449	-0.734558	-1.881601
H	3.574659	-2.252753	-1.079642
C	0.695119	-1.237601	-3.107361
H	-0.237467	-0.849317	-3.515469
H	0.963636	-2.115411	-3.700956
H	1.466634	-0.486635	-3.269374
C	-1.869443	-2.463614	-1.748504
H	-2.731675	-2.405309	-1.08623
H	-1.833456	-3.481552	-2.143163
H	-2.055344	-1.804039	-2.595351
C	-1.211061	-2.936237	1.346317
H	-1.231657	-2.33943	2.258262
H	-0.854972	-3.934651	1.611758
H	-2.233925	-3.039279	0.989123
H	0.190524	3.881199	-1.823762
H	1.230206	4.067779	-0.417081
H	-0.484162	4.449329	-0.308863
Cl	-0.614879	0.340932	2.33466
C	-1.577534	1.975107	-0.407581
C	-1.946163	0.504211	-0.480689
C	-3.192141	0.094006	0.283282
C	-2.248024	2.665574	-1.598717
H	-3.307604	2.414101	-1.616005
H	-1.81046	2.332573	-2.542094
H	-2.173787	3.74999	-1.558684
H	-3.124835	-0.975692	0.53399
H	-2.054895	0.184745	-1.521677
H	-2.018622	2.373376	0.5135
O	2.77853	0.94901	1.555562
H	2.036652	0.67683	2.117255
H	-4.05582	0.186397	-0.387871
O	-3.506365	0.858957	1.411758
H	-2.746336	0.781788	2.013438
H	2.179474	2.896208	1.24971
C	3.278714	2.157729	-0.424573
H	4.276599	2.258818	0.000647
H	3.057669	3.057732	-0.994408
H	3.281831	1.317786	-1.11437

(*1,4-syn*)-2-A3

Ru	0.146466	-0.108748	0.02056
C	-1.025431	1.335241	0.169819
C	-1.70121	0.648397	-0.841572
C	-1.832557	1.144498	-2.248752
C	-1.18724	2.525834	1.019107
C	2.348564	0.373254	0.28113
C	1.907242	0.897734	-0.950788
C	1.444039	-0.203997	-1.767088
C	1.703323	-1.420876	-1.055724
C	2.208225	-1.073444	0.211731
C	2.943713	1.110774	1.422997
H	2.561633	0.733912	2.37281
H	2.717798	2.174213	1.375308
H	4.031099	0.999054	1.443495
C	1.941738	2.327888	-1.358672

H	1.830675	2.987943	-0.499479
H	1.149466	2.567821	-2.067249
H	2.889236	2.572908	-1.844844
C	1.066766	-0.134795	-3.203139
H	0.290001	-0.855525	-3.457806
H	1.930431	-0.361735	-3.833523
H	0.711927	0.852413	-3.489955
C	1.470654	-2.789442	-1.582648
H	1.298636	-3.508453	-0.783527
H	2.333107	-3.139947	-2.15491
H	0.610595	-2.826898	-2.250359
C	2.63316	-2.007541	1.284384
H	2.356568	-1.634364	2.269098
H	3.718683	-2.132351	1.268826
H	2.187036	-2.993269	1.167023
H	-1.739657	0.338959	-2.978815
H	-1.089069	1.903565	-2.487609
H	-2.820566	1.589004	-2.399935
Cl	-0.064234	-0.400602	2.475087
C	-2.595369	-0.499972	-0.357386
C	-1.481532	-1.512068	-0.266886
C	-1.667815	-2.669301	0.701933
C	-3.806486	-0.858033	-1.191737
H	-4.304218	-1.726018	-0.759293
H	-3.532401	-1.112371	-2.216836
H	-4.5381	-0.049438	-1.231202
H	-0.694573	-3.113279	0.961268
H	-1.270736	-1.903331	-1.269116
H	-2.924337	-0.276936	0.663294
O	-0.093314	2.759857	1.867757
H	0.110532	1.90913	2.293684
H	-2.23796	-3.459836	0.196291
O	-2.406746	-2.351886	1.853416
H	-1.853707	-1.744809	2.369611
H	-2.097549	2.298687	1.610286
C	-1.446264	3.790864	0.21815
H	-1.600497	4.625622	0.898179
H	-2.327154	3.682921	-0.411183
H	-0.590097	4.023723	-0.413198

(*1,4-syn*)-2-TS$_{A3-A4}$

Ru	-0.209372	0.027101	-0.057697
C	1.322794	1.283385	-0.272921
C	2.453502	0.620438	0.084100
C	3.743862	1.326129	0.363487
C	1.259692	2.737627	-0.628591
C	-2.273388	-1.009042	-0.198749
C	-2.244544	0.400500	-0.542289
C	-1.913190	1.152935	0.654374
C	-1.588966	0.184654	1.652041
C	-1.865609	-1.131946	1.129624
C	-2.652898	-2.089967	-1.141205
H	-2.058039	-2.038088	-2.054780
H	-3.702924	-2.001386	-1.428073
H	-2.511374	-3.078030	-0.707904
C	-2.735643	0.967674	-1.823399
H	-2.359356	0.398953	-2.673344
H	-2.425787	2.004489	-1.940742
H	-3.828369	0.940091	-1.867815
C	-2.157377	2.605849	0.853520
H	-1.727573	2.964562	1.786921
H	-3.233214	2.796683	0.904637
H	-1.748895	3.202806	0.040368
C	-1.213465	0.467849	3.062043
H	-0.527591	-0.281434	3.455900
H	-2.094568	0.462634	3.710103
H	-0.737762	1.441603	3.163969
C	-1.768728	-2.373755	1.939696
H	-1.923622	-3.269700	1.343732
H	-2.528343	-2.366492	2.724674
H	-0.805416	-2.471823	2.441072
H	4.026510	1.274482	1.417770
H	3.711362	2.375442	0.082692
H	4.558652	0.854160	-0.191423
Cl	0.350149	-0.818611	-2.283409
C	2.475176	-0.897349	0.215361
C	1.143186	-1.510016	0.586851
C	0.938504	-2.943278	0.126243
C	3.520708	-1.418636	1.210139
H	3.512875	-2.507099	1.216349
H	3.310761	-1.072599	2.223594
H	4.529158	-1.102061	0.949519
H	1.260507	-3.622696	0.926078
H	0.976914	-1.432039	1.666705
H	2.765966	-1.275557	-0.771430
O	0.124966	2.992084	-1.462266
H	0.069935	2.249630	-2.079068
C	1.156286	3.649361	0.575230

H	2.093963	3.662620	1.128516
H	0.925506	4.667964	0.264791
H	0.374551	3.308223	1.251215
H	2.164523	3.010023	-1.194551
O	1.670309	-3.320525	-1.007990
H	1.363439	-2.743207	-1.727287
H	-0.133558	-3.135169	-0.016835

(*1,4-syn*)-2-A4

Ru	0.331064	0.099012	0.142886
C	-2.695464	0.258875	-0.151283
C	-1.555122	0.88904	0.119578
C	1.145001	-0.337518	-1.801523
C	1.677255	-1.334727	-0.895465
C	2.494358	-0.691892	0.077464
C	2.439914	0.691522	-0.164916
C	1.597584	0.930915	-1.329986
Cl	0.210257	-0.16214	2.671561
C	-2.49897	-1.129691	-0.656384
C	-1.090398	-1.594425	-0.239115
H	-0.653144	-2.161476	-1.057693
H	-3.208009	-1.792098	-0.140612
C	0.503852	-0.610178	-3.110656
H	1.263436	-0.772844	-3.880486
H	-0.122155	-1.500209	-3.082298
H	-0.119723	0.220123	-3.435981
C	1.422728	2.241394	-2.004214
H	0.530582	2.252478	-2.627675
H	1.338845	3.053801	-1.283609
H	2.278253	2.461931	-2.648473
C	3.107881	1.742196	0.643739
H	3.168509	1.460845	1.694408
H	4.128208	1.90477	0.288664
H	2.583179	2.692845	0.580188
C	3.209772	-1.373288	1.182736
H	2.681277	-2.26921	1.503669
H	4.212132	-1.675907	0.869323
H	3.312493	-0.728	2.052537
C	1.632381	-2.810078	-1.076649
H	2.635211	-3.177963	-1.30426
H	1.29693	-3.330101	-0.179616
H	0.985069	-3.108399	-1.897501
C	-1.323403	2.229652	0.71119
C	-4.072428	0.806387	0.020434
H	-4.60323	0.893815	-0.932069
H	-4.673071	0.143535	0.648839
H	-4.076366	1.791551	0.485198
C	-1.166155	-2.522811	0.965473
C	-2.78253	-1.238474	-2.149694
H	-3.832113	-1.03579	-2.366331
H	-2.191638	-0.518571	-2.715192
H	-2.561795	-2.237607	-2.531468
O	0.137994	2.193654	0.996632
H	0.229868	1.887476	1.922859
H	-1.558526	-3.486637	0.611133
C	-1.588772	3.411021	-0.181661
H	-1.246481	4.338731	0.276852
H	-2.657466	3.495106	-0.372783
H	-1.09011	3.28897	-1.141492
H	-1.826668	2.363098	1.676453
H	-0.166504	-2.725222	1.374673
O	-2.053124	-2.107751	1.970054
H	-1.622056	-1.363936	2.421312

(*1,4-syn*)-2-TS$_{A4-A5}$

Ru	-0.331909	-0.033346	0.264422
C	2.559474	0.729652	0.402376
C	1.751339	-0.34644	0.355259
C	-0.613824	-0.01466	-1.859746
C	-1.503393	0.989395	-1.36713
C	-2.507119	0.379895	-0.546954
C	-2.238398	-0.995092	-0.497279
C	-1.047496	-1.26271	-1.286268
Cl	-0.603161	-1.451556	2.207856
C	1.921712	2.074049	0.258637
C	0.435847	1.921008	0.486429
H	-0.142369	2.70848	0.011561
H	2.31281	2.752262	1.035867
C	0.395991	0.117821	-2.9425
H	0.071521	-0.428721	-3.831312
H	0.540773	1.155581	-3.234063
H	1.364945	-0.281921	-2.646309
C	-0.575653	-2.6088	-1.689995
H	0.46156	-2.597717	-2.011035
H	-0.648217	-3.331485	-0.882226
H	-1.186632	-2.966213	-2.525751
C	-3.052786	-2.026829	0.189171
H	-3.534718	-1.6393	1.084301

H	-3.835925	-2.38698	-0.482929
H	-2.450887	-2.880959	0.48809
C	-3.624458	1.096945	0.113718
H	-3.296095	2.050783	0.524731
H	-4.432237	1.304506	-0.592881
H	-4.049768	0.510663	0.926621
C	-1.550182	2.401904	-1.817419
H	-2.241962	2.484681	-2.659424
H	-1.91422	3.071436	-1.039107
H	-0.580265	2.76384	-2.152935
C	2.385967	-1.734964	0.352237
C	4.053988	0.719076	0.537817
H	4.560518	0.868336	-0.42083
H	4.387983	1.532687	1.186454
H	4.436268	-0.211216	0.953855
C	0.042781	1.867319	1.958175
H	0.337562	0.920929	2.428314
C	2.244242	2.729643	-1.079958
H	3.317193	2.873619	-1.202159
H	1.904426	2.106348	-1.906497
H	1.769484	3.708481	-1.170979
O	1.496627	-2.825334	0.487956
H	0.926571	-2.642948	1.248147
H	0.650726	2.626382	2.470392
O	-1.325161	2.150268	2.20057
H	-1.734327	1.331669	2.504164
C	3.150633	-2.009049	-0.930843
H	3.60422	-2.999091	-0.890617
H	3.932888	-1.274603	-1.104866
H	2.475863	-1.990817	-1.787068
H	3.106353	-1.76345	1.18782

(*1,4-syn*)-2-A5

Ru	-0.376282	0.055559	0.275065
C	2.579845	0.684193	0.417647
C	1.725289	-0.352975	0.354417
C	-0.783415	-0.8119	-1.722351
C	-1.114711	0.576955	-1.732127
C	-2.175173	0.800949	-0.783741
C	-2.495815	-0.443841	-0.180947
C	-1.6365	-1.440418	-0.772917
Cl	-0.495806	-1.422389	2.27132
C	2.020672	2.027345	0.066874
C	0.525921	1.958809	0.256678
H	-0.03496	2.700793	-0.310667
H	2.407723	2.809337	0.740377
C	0.169921	-1.494922	-2.629724
H	-0.330931	-1.799884	-3.552303
H	0.996223	-0.840941	-2.90403
H	0.587767	-2.380755	-2.156236
C	-1.723356	-2.895377	-0.505332
H	-0.828468	-3.421099	-0.825917
H	-1.881801	-3.100656	0.552415
H	-2.577633	-3.305449	-1.051188
C	-3.568948	-0.725404	0.804889
H	-3.92523	0.18598	1.281733
H	-4.427329	-1.205206	0.328505
H	-3.209524	-1.392157	1.589009
C	-2.861173	2.099589	-0.573158
H	-2.158039	2.931051	-0.536249
H	-3.558195	2.301625	-1.390336
H	-3.42562	2.113739	0.356253
C	-0.654037	1.568021	-2.73675
H	-1.379992	1.614873	-3.552928
H	-0.571589	2.574997	-2.331299
H	0.305016	1.299626	-3.171244
C	2.258774	-1.782156	0.382323
C	4.05264	0.625694	0.698599
H	4.665068	0.708857	-0.204471
H	4.346844	1.458764	1.34202
H	4.345529	-0.293475	1.202721
C	0.044171	1.90311	1.652934
H	-0.445815	0.884783	1.913682
C	2.424037	2.425281	-1.348185
H	3.502176	2.561562	-1.423226
H	2.146025	1.643156	-2.055768
H	1.951624	3.358785	-1.660364
O	1.268239	-2.78754	0.224811
H	0.641997	-2.674614	0.956187
H	0.875091	1.883611	2.370555
O	-0.919209	2.888275	1.929408
H	-1.300685	2.70661	2.794404
C	3.249598	-2.061076	-0.736192
H	3.534435	-3.112456	-0.713886
H	4.150685	-1.461702	-0.658161
H	2.796821	-1.855679	-1.704995
H	2.769213	-1.93519	1.34872

(*1,4-syn*)-2-TS$_{A5-A6}$

Ru	0.333418	-0.042247	0.271585
C	-2.605432	-0.598253	0.476947
C	-1.745368	0.433299	0.354981
C	1.644913	1.249509	-0.992029
C	0.739434	0.603817	-1.861875
C	0.944702	-0.801957	-1.725907
C	2.058765	-1.016225	-0.81864
C	2.487629	0.236546	-0.364146
Cl	0.858327	1.496958	2.170338
C	-2.056275	-1.997664	0.361005
C	-0.552325	-1.969653	0.550807
H	0.023506	-2.75544	0.074217
H	-2.477728	-2.624373	1.162362
C	1.837973	2.712546	-0.843822
H	2.690604	3.034829	-1.447837
H	0.961509	3.269235	-1.165107
H	2.049268	2.985336	0.189434
C	3.632049	0.523439	0.533363
H	3.392646	1.317556	1.239461
H	3.924892	-0.355728	1.104991
H	4.502505	0.845628	-0.043887
C	2.687794	-2.330236	-0.533849
H	3.417049	-2.579533	-1.309147
H	3.204778	-2.333235	0.42261
H	1.962005	-3.141767	-0.513214
C	0.388616	-1.848422	-2.619276
H	-0.533453	-1.532171	-3.100321
H	1.109196	-2.06845	-3.411929
H	0.194969	-2.786695	-2.101513
C	-0.232455	1.264083	-2.766638
H	0.212913	1.443932	-3.748313
H	-1.119813	0.650111	-2.916321
H	-0.553564	2.220867	-2.359284
C	-2.217617	1.87847	0.328025
C	-4.091218	-0.49731	0.656185
H	-4.391124	0.443941	1.114211
H	-4.640453	-0.586552	-0.285465
H	-4.452339	-1.304598	1.297569
C	-0.079945	-1.513005	1.824508
H	-0.579815	-0.145397	1.607911
H	-0.863676	-1.395571	2.589614
C	-2.485489	-2.628691	-0.958446
H	-3.565255	-2.769321	-0.988287
H	-2.217575	-1.986438	-1.796866
H	-2.023022	-3.605573	-1.110487
O	-1.165261	2.814948	0.156173
H	-0.514079	2.654066	0.856614
O	1.107045	-1.987485	2.35723
H	1.480753	-1.268433	2.884219
H	-2.72834	2.085137	1.285298
C	-3.186611	2.179264	-0.801935
H	-4.117162	1.628096	-0.711506
H	-3.418578	3.243488	-0.803742
H	-2.741666	1.930595	-1.763525

(*1,4-syn*)-2-A6

Ru	0.240384	-0.004597	0.228373
C	-1.78352	-1.027167	0.080679
C	-1.90908	0.089835	0.90757
C	1.121283	1.523941	-1.179976
C	0.466682	0.563825	-1.975298
C	1.049986	-0.719934	-1.680733
C	2.14734	-0.513078	-0.771066
C	2.169909	0.854242	-0.430754
Cl	0.304698	1.794161	1.980498
C	-1.325979	-2.312725	0.780291
C	0.131057	-2.014285	1.066838
H	0.878698	-2.668779	0.629831
H	-1.884451	-2.424979	1.717598
C	0.909526	2.994407	-1.199244
H	1.762568	3.495782	-1.663112
H	0.023345	3.271382	-1.768927
H	0.813604	3.39544	-0.18821
C	3.181415	1.522887	0.424023
H	2.758373	2.372165	0.955948
H	3.595034	0.837223	1.162247
H	4.012531	1.884301	-0.187749
C	3.137758	-1.532428	-0.339695
H	4.079154	-1.39629	-0.877002
H	3.348111	-1.463224	0.726095
H	2.797456	-2.545656	-0.545537
C	0.832522	-1.975706	-2.447633
H	-0.177127	-2.057435	-2.843279
H	1.512819	-2.020455	-3.302697
H	1.026912	-2.860844	-1.84367
C	-0.528334	0.854507	-3.040563
H	-0.033117	1.342936	-3.883431

H	-0.991612	-0.051501	-3.423172
H	-1.32085	1.515538	-2.693223
C	-2.665878	1.373838	0.638187
C	-2.470121	-1.107003	-1.244527
H	-2.607551	-0.119785	-1.676916
H	-1.953571	-1.738682	-1.964266
H	-3.463293	-1.547451	-1.107696
C	0.496302	-1.152564	2.0973
H	-1.834805	-0.094108	1.975094
H	-0.253234	-0.791734	2.795177
C	-1.498156	-3.586191	-0.020951
H	-2.543085	-3.772759	-0.265333
H	-0.941024	-3.553052	-0.957179
H	-1.133176	-4.442911	0.544749
O	-2.221545	2.073448	-0.519334
H	-1.298244	2.293148	-0.328752
O	1.780749	-1.109464	2.578718
H	1.881203	-0.221651	2.954981
H	-2.487047	2.009062	1.513896
C	-4.158668	1.163689	0.496444
H	-4.553974	0.624186	1.355994
H	-4.669192	2.123269	0.432031
H	-4.399097	0.595951	-0.400781

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