Supporting Information

Synthetically amenable amide derivatives of tosylated-amino acids asorganocatalysts for enantioselective allylation of aldehydes: computational-rationale for enantioselectivity

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General information

All reactions were performed in oven-dried (150 °C) glassware under an atmosphere of nitrogen with magnetic stirring unless otherwise indicated. 4Å MS was activated at 120 °C for overnight. Different aldehydes and reagents were used as received. All the solvents used in thepresent study were dried following known purification technique.[1] ^{1}H and ^{13}C spectra were taken in $CDCl_3$ and in CD_3COCD_3 in special cases. For ^{1}H NMR (200 and 500 MHz), tetramethylsilane (TMS) served as internal standard (δ = 0 ppm) and data are reported as follows: chemical shift (in ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constant (in Hz), and integration. For ^{13}C NMR (50 MHz and 125 MHz), $CDCl_3$(CD_3COCD_3 in special cases) was used as internal standard and spectra were obtained with complete proton decoupling. FTIR spectra were carried out using KBr. Optical rotations of the allylation products and the catalysts were recorded on an automatic Polari meter. All the products were purified by flash chromatography using silica gel 100-200 mesh. Enantiomeric excess (ee) were determined by HPLC using OD-H, AS-H, IA, IBand IC chiralcolumns with 2-propanol/hexane as eluent.

Characterization data for the Homoallyl Alcohols

(*S*)-1-phenylbut-3-en-1-ol (compound 2a):[2] The product was isolated as a colorless oil (yield 46 mg, 78%) after purification by silica gel chromatography (Hexane/EtOAc = 95:5). Reaction time = 10 h. ^{1}H NMR ($CDCl_3$, 500 MHz,): δ = 2.04 (d, *J* = 3.1 Hz, 1H), 2.46-2.57 (m, 2H), 4.73-4.75 (m, 1H), 5.13-5.19 (m, 2H), 5.77-7.85 (m, 1H), 7.26-7.36 (m, 5H).^{13}C NMR ($CDCl_3$, 50 MHz): δ = 43.8, 73.2, 118.4, 125.8, 127.5, 128.4, 134.4, 143.8. HPLC (Daicel Chiralcel OD-H, hexanes/2-propanol = 95:5, flow rate = 0.4 mL/min, λ = 220 nm) t_{major}(*S*) = 22.1 min, t_{minor}(*R*) = 20.7 min.

(*S*)-1-(4-methoxyphenyl)but-3-en-1-ol (compound 2b):[2,3] The product was isolated as a yellowish oil (yield 50 mg, 70%) after purification by silica gel chromatography (Hexane/EtOAc = 92:8). Reaction time = 14 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 1.99 (br, 1H), 2.48-2.51 (t, *J* = 6.5 Hz, 2H), 3.80 (s, 3H), 4.68-4.70 (t, *J* = 6.5 Hz, 1H), 5.12-5.17 (m, 2H), 5.76-5.84 (m, 1H), 6.87-6.89 (m, 2H), 7.26-7.29 (m, 2H). ^{13}C NMR ($CDCl_3$, 50 MHz): δ = 43.7, 55.2, 73.3, 113.7, 118.2, 127, 134.6, 136.3, 159. Optical Rotation: $[\alpha]^{27}_{D}$ = -60 (c 1.0, $CHCl_3$).[3] HPLC (Daicel Chiralcel OD-H, hexanes/2-propanol = 95:5, flow rate = 0.8 mL/min, λ = 230 nm) t_{major}(*S*) = 13.3 min, t_{minor}(*R*) = 11.9 min.

(4-benzyloxyphenyl)but-3-en-1-ol (compound 2c): The product was isolated as a colorless oil (yield 66 mg, 65%) after purification by silica gel chromatography (Hexane/EtOAc = 90:10). Reaction time = 15 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 1.98 (br, 1H), 2.48-2.51 (t, *J* = 6.5 Hz, 2H), 4.67-4.70 (t, *J* = 6 Hz, 1H), 5.06 (s, 2H), 5.12-5.17 (m, 2H), 5.76-5.84 (m, 1H), 6.95-6.96 (d, *J* = 8.5 Hz, 2H), 7.25-7.44 (m, 7H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 45.1, 71.4, 74.3, 116.1, 119.7, 128.5, 128.9, 129.3, 130, 136, 137.7, 159.6. Optical Rotation:

$[\alpha]^{27}_D$ = -52 (c 1.0, $CHCl_3$). HPLC (Daicel Chiralpak IC column, hexanes/2-propanol = 98:2, flow rate = 0.8 mL/min, λ = 230 nm) t(major) = 33.1 min, t(minor) = 29.5 min.

(*S*)-1-(4-*tert*-Butylphenyl)-3-buten-1-ol (compound 2d):[4] The product was isolated as a colorless oil (yield 58 mg, 71%) after purification by silica gel chromatography (Hexane/EtOAc = 95:5). Reaction time = 15 h. ^{1}H NMR ($CDCl_3$, 200 MHz): δ = 1.30 (s, 9H), 2.45-2.47 (m, 3H), 2.62-2.63 (m, 1H), 5.06-5.12 (m, 2H), 5.72-5.81 (m, 1H), 7.23-7.34 (m, 4H). ^{13}C NMR ($CDCl_3$, 50 MHz): δ = 31.1, 34.2, 43.3, 72.9, 117.7, 125, 125.3, 134.5, 140.7, 150.1. Optical Rotation: $[\alpha]^{27}_D$ = -30.2 (c 1, Et_2O).[4] HPLC (Daicel Chiralpak IA, hexanes/2-propanol = 96:4, flow rate = 0.4 mL/min, λ = 254 nm) t_{major}(*S*) = 18.6 min, t_{minor}(*R*) = 17.3 min.

(*S*)-1-(*p*-tolyl)but-3-en-1-ol (compound 2e):[2] The product was isolated as a colorless oil (yield 42 mg, 65%) after purification by silica gel chromatography (Hexane/EtOAc = 96:4). Reaction time = 15 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.06 (br, 1H), 2.34 (s, 3H), 2.49-2.50 (m, 2H), 4.67-4.70 (t, *J* = 6.5 Hz, 1H), 5.11-5.16 (m, 2H), 5.77-5.82(m, 1H), 5.75-5.83 (m, 1H), 7.14-7.24 (m, 5H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.1, 43.7, 73.1, 118.2, 125.7, 129, 134.5, 140.9. Optical Rotation: $[\alpha]^{27}_D$ = -45.1 (c 1, $CHCl_3$).[5] HPLC (Daicel Chiralcel OD-H, hexanes/2-propanol = 99:1, flow rate = 0.5 mL/min, λ = 220 nm) t_{major}(*S*) = 34.5 min, t_{minor}(*R*) = 32 min. **(*S*)-1-(4-nitrophenyl)but-3-en-1-ol (compound 2f)**:[6] The product was isolated as a pale yellow oil (yield 54 mg, 70%) after purification by silica gel chromatography (Hexane/EtOAc = 90:10). Reaction time = 12 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.17 (br, 1H), 2.42-2.48 (m, 1H), 2.55-2.59 (m, 1H), 4.86-4.88 (m, 1H), 5.17-5.21 (m, 2H), 5.75-5.83 (m, 1H), 7.53-7.55 (d, *J* = 8.5 Hz, 2H), 8.20-8.22 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR ($CDCl_3$, 50 MHz): δ = 43.9, 72.1, 119.6, 123.6, 126.5, 133.1, 151. Optical Rotation: $[\alpha]^{27}_D$ = -56.5 (c 1.0, $CHCl_3$).[7] HPLC (Daicel Chiralpak IA, hexanes/2-propanol = 99:1, flow rate = 1 mL/min, λ = 220 nm) t_{major}(*S*) = 63.3 min, t_{minor}(*R*) = 58.9 min.

(*S*)-1-(4-fluorophenyl)but-3-en-1-ol (compound 2g):[6] The product was isolated as a colorless oil (yield 50 mg, 76%) after purification by silica gel chromatography (Hexane/EtOAc = 92:8). Reaction time = 12 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.04 (br, 1H), 2.43-2.53 (m, 2H), 4.71-4.74 (m, 1H), 5.14-5.17 (m, 2H), 5.74-5.82 (m, 1H), 7.01-7.04 (t, *J* = 8.5), 7.31-7.34 (m, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 45.3, 74, 116.5, 116.7, 120.1, 128.8, 135.5. Optical Rotation: $[\alpha]^{27}_{D}$ = -31.5 (c 1.0, $CHCl_3$).[8] HPLC (Daicel Chiralpak AS-H, hexanes/2-propanol = 99.5:0.5, flow rate = 0.8 mL/min, λ = 220 nm) t_{major}(*S*) = 28.6 min, t_{minor}(*R*) = 26.1 min.

(*S*)-1-(4-chlorophenyl)but-3-en-1-ol (compound 2h):[2,3,6] The product was isolated as a yellowish oil (yield 54 mg, 75%) after purification by silica gel chromatography (Hexane/EtOAc = 95:5). Reaction time = 12 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.15 (br, 1H), 2.41-2.52 (m, 2H), 4.69-4.72 (dd, *J* = 2.5, 5 Hz, 1H), 5.13-5.16 (m, 2H), 5.73-5.81 (m, 1H), 7.26-7.32 (m, 4H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 43.8, 72.5, 118.8, 127.2, 128.5, 131.1, 133.9, 142.2. Optical Rotation: $[\alpha]^{27}_{D}$ = -58 (c 1.0, $CHCl_3$).[3] HPLC (Daicel Chiralpak IC, hexanes/2-propanol = 99:1, flow rate = 0.4 mL/min, λ = 220 nm) t_{major}(*S*) = 28.9 min, t_{minor}(*R*) = 26.0 min.

(*S*)-1-(4-bromophenyl)but-3-en-1-ol (compound 2i):[8] The product was isolated as a yellowish oil (yield 66 mg, 73%) after purification by silica gel chromatography (Hexane/EtOAc = 92:8). Reaction time = 12 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.02-2.03 (br, 1H), 2.42-2.51 (m, 2H), 4.68-4.71 (dd, *J* = 2,5, 5 Hz, 1H), 5.13-5.16 (m, 2H), 5.72-5.80 (m, 1H), 7.21-7.24 (m, 2H), 7.45-7.46 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 45.2, 73.9, 120.3, 128.9, 132.9, 135.3, 144.2. Optical Rotation: $[\alpha]^{27}_{D}$ = -18 (c 3.0, C_6H_6).[8] HPLC (Daicel Chiralpak IA, hexanes/2-propanol = 99:1, flow rate = 0.5 mL/min, λ = 230 nm) t_{major}(*S*) = 44.5 min, t_{minor}(*R*) = 42.3 min.

(S)-1-(3-methoxyphenyl)but-3-en-1-ol (compound 2j):[7,9] The product was isolated as a sight yellowish oil (yield 53.5 mg, 75%) after purification by silica gel chromatography (Hexane/EtOAc = 94:6). Reaction time = 14 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.02 (d, *J* = 3 Hz,1H), 2.44-2.54 (m, 2H), 3.80 (s, 3H), 4.7-4.72 (m, 1H), 5.12-5.17 (m, 2H), 5.75-5.84 (m, 1H), 6.79-6.81 (dd, *J* = 2.5, 5.5 Hz, 1H), 6.91-6.92 (m, 2H), 7.23-7.26 (m, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 45.2, 56.6, 74.6, 112.7, 114.4, 119.5, 119.8, 130.8, 135.8, 147, 161.1. Optical Rotation: $[\alpha]^{27}_{D}$ = -44.2 (c 0.88, C_6H_6).[7] HPLC (Daicel Chiralpak IA, hexanes/2-propanol = 98:2, flow rate = 0.6 mL/min, λ = 220 nm) t_{major}(*S*) = 25.3 min, t_{minor}(*R*) = 24.3 min.

(*S*)-1-(*m*-tolyl)but-3-en-1-ol (compound 2k):[10] The product was isolated as a colorless oil (yield 40 mg, 65%) after purification by silica gel chromatography (Hexane/EtOAc = 95:5). Reaction time = 16 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.05 (br, 1H), 2.35 (s, 3H), 2.46-2.53 (m, 2H), 4.67-4.71 (m, 1H), 5.13-5.18 (m, 2H), 5.77-5.85 (m, 1H), 7.08-7.09 (d, *J* = 7.5 Hz, 1H), 7.13-7.17 (m, 2H), 7.22-7.25 (t, *J* = 7.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.7, 44, 73.5, 118.5, 123.1, 126.7 128.5, 134.8, 138.3, 144. Optical Rotation: $[\alpha]^{27}_{D}$ = -44.3 (c 1.1, $CHCl_3$).[7] HPLC (Daicel Chiralcel OD-H, hexanes/2-propanol = 98:2, flow rate = 0.4 mL/min, λ = 220 nm) t_{major}(*S*) =31.6 min, t_{minor}(*R*) = 26.7 min.

(*S*)-1-(2-methoxyphenyl)but-3-en-1-ol (compound 2l):[2] The product was isolated as a colorless oil (yield 57 mg, 80%) after purification by silica gel chromatography (Hexane/EtOAc = 95:5). Reaction time = 14 h. ^{1}H NMR ($CDCl_3$, 500 MHz,): δ = 2.47–2.61 (m, 3H), 3.84 (s, 3H), 4.94-4.97 (td, *J* = 5.5, 7.5 Hz, 1H), 5.09-5.15 (m, 2H), 5.8-5.89 (m, 1H), 6.87-6.88 (d, *J* = 8 Hz, 1H), 6.94-6.97 (t, *J* = 7.5 Hz, 1H), 7.22-7.26 (m, 1H), 7.32-7.34 (m, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz,): δ = 41.8, 55.2, 69.6, 110.4, 117.5, 120.6, 126.8, 128.3, 131.7, 135.2, 156.3. Optical Rotation: $[\alpha]^{27}_{D}$ = -39.5 (c 1.1, C_6H_6).[5] HPLC (Daicel

Chiralcel OD-H, hexanes/2-propanol = 96:4, flow rate = 0.6 mL/min, λ = 230 nm) t_{major}(*S*) = 14.4 min, t_{minor}(*R*) = 15.7 min.

(*S*)-1-(*o*-tolyl)but-3-en-1-ol (compound 2m):[7,11] The product was isolated as a colorless oil (yield 35 mg, 55%) after purification by silica gel chromatography (Hexane/EtOAc = 95:5). Reaction time = 16 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.03 (br, 1H), 2.33 (s, 3H), 2.39-2.52 (m, 2H), 4.95-4.98 (q, *J* = 4 Hz, 1H), 5.14-5.19 (m, 2H), 5.81-5.89 (m, 1H), 7.12-7.13 (d, *J* = 7 Hz, 1H), 7.15-7.18 (t, *J* = 7.5 Hz, 1H), 7.21-7.24 (m, 1H), 7.47-7.48 (d, *J* = 7.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 19, 42.6, 69.6, 118.2, 125.1, 126.2, 127.2, 130.3, 134.3, 134.7, 141.9. Optical Rotation: $[\alpha]^{27}_D$ = -48.4 (c 1, C_6H_6).[7] HPLC (Daicel Chiralcel OD-H, hexanes/2-propanol = 99:1, flow rate = 0.5 mL/min, λ = 220 nm) t_{major}(*S*) = 35.4 min, t_{minor}(*R*) = 32.2 min.

(*S*)-1-(2-fluorophenyl)but-3-en-1-ol (compound 2n):[8] The product was isolated as a colorless oil (yield 45 mg, 68%) after purification by silica gel chromatography (Hexane/EtOAc = 96:4). Reaction time = 16 h. ^{1}H NMR ($CDCl_3$, 200 MHz): δ = 2.16-2.17 (d, *J* = 4 Hz, 1H), 2.45-2.61 (m, 2H), 5.04-5.07 (m, 1H), 5.14-5.18 (m, 2H), 5.78-5.85 (m, 1H), 7.00-7.03 (m, 1H), 7.13-7.16 (d, *J* = 7.5 Hz, 1H), 7.22-7.26 (m, 1H), 7.46-7.49 (m, 1H). ^{13}C NMR ($CDCl_3$, 50 MHz): δ = 42.5, 67.2, 115, 115.4, 118.6, 124.1, 124.2, 127.1, 127.2, 128.7, 128.9, 130.6, 134, 157.2. Optical Rotation: $[\alpha]^{27}_D$ = -38.2 (c 1.5, $CHCl_3$).[8] HPLC (Daicel Chiralpak AS-H, hexanes/2-propanol = 99.5:0.5, flow rate = 0.5 mL/min, λ = 220 nm) t_{major}(*S*) = 34.6 min, t_{minor}(*R*) = 32.7 min.

(*S*)-1-(naphthalen-1-yl)but-3-en-1-ol (compound 2o):[2] The product was isolated as a colourless oil (yield 71 mg, 90%) after purification by silica gel chromatography (Hexane/EtOAc = 94:6). Reaction time = 8 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.21 (d, *J* = 3 Hz, 1H), 2.56-2.62 (m, 1H), 2.73-2.78 (m, 1H), 5.16-5.22 (m, 2H), 5.5-5.53 (m, 1H), 5.87-5.96 (m, 1H), 7.45-7.52 (m, 3H), 7.64-7.66 (d, *J* = 7 Hz, 1H), 7.76-7.78 (d, *J* = 8 Hz, 1H),

7.86-7.87 (d, *J* = 8 Hz, 1H), 8.05-8.07 (d, *J* = 8.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 44.3, 71.4, 119.7, 124.2, 124.2, 126.9, 127.4, 129.4, 130.4, 135.2, 136.2, 140.8. Optical Rotation: $[\alpha]^{27}_D$ = -62.5 (c 1.1, $CHCl_3$).[3] HPLC (Daicel Chiralpak IA, hexanes/2-propanol = 95:5, flow rate = 0.6 mL/min, λ = 220 nm) t_{major}(*S*) = 16.7 min, t_{minor}(*R*) = 19.1 min.

(*S*)-1-(naphthalen-2-yl)but-3-en-1-ol (compound 2p):[2] The product was isolated as a pale yellow oil (yield 67 mg, 85%) after purification by silica gel chromatography (Hexane/EtOAc = 90:10). Reaction time = 9 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.14-2.15 (d, *J* = 3.5 Hz, 1H), 2.55-2.65 (m, 2H), 4.9-4.93 (m, 1H), 5.14-5.21 (m, 2H), 5.79-5.87 (m, 1H), 7.44-7.49 (m, 3H), 7.81-7.84 (m, 4H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 45.1, 74.8, 120, 125.4, 125.9, 127.2, 127.5, 129.1, 129.3, 129.6, 135.7, 142.6. Optical Rotation: $[\alpha]^{27}_D$ = -48 (c 1, $CHCl_3$).[3] HPLC (Daicel Chiralpak IA, hexanes/2-propanol = 90:10, flow rate = 0.5 mL/min, λ = 220 nm) t_{major}(*S*) = 16.3 min, t_{minor}(*R*) = 15.3 min.

(*S*)-1-(thiophen-2-yl)but-3-en-1-ol (compound 2q):[2] The product was isolated as a yellowish oil (yield 49 mg, 80%) after purification by silica gel chromatography (Hexane/EtOAc = 94:6). Reaction time = 10 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.19-2.2 (d, *J* = 4Hz, 1H), 2.6-2.64 (m, 2H), 4.97-5.01 (m, 1H), 5.15-5.21 (m, 2H), 5.79-5.87 (m, 1H), 6.96-6.98 (m, 2H), 7.24-7.25 (m, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 45.2, 70.8, 120.2, 125.1, 126, 128, 135.2. HPLC (Daicel Chiralcel OD-H, hexanes/2-propanol = 97:3, flow rate = 0.6 mL/min, λ = 220 nm) t_{major}(*S*) = 18.7 min, t_{minor}(*R*) = 17.1 min.

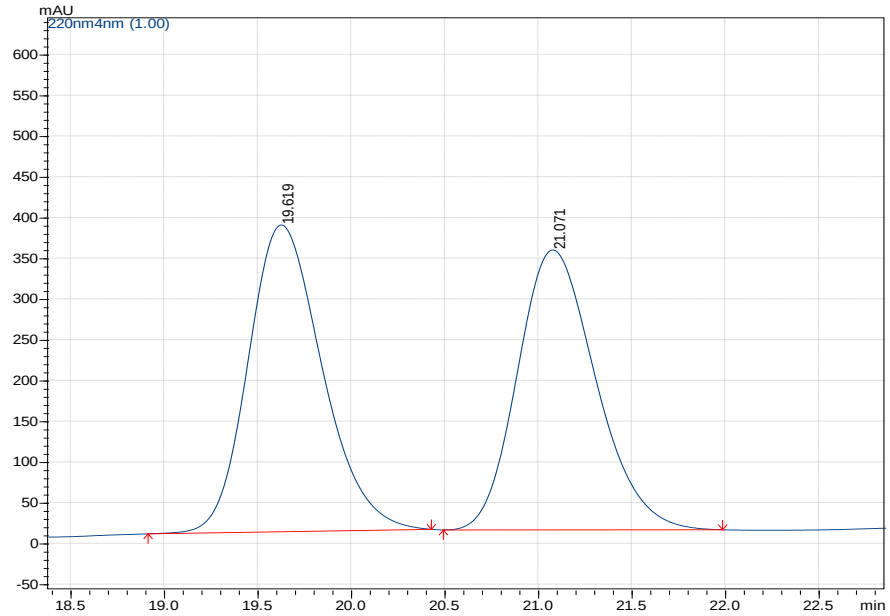
(1*E*,3*R*)-1-Phenyl-1,5-hexadiene-3-ol (compound 2r):[3] The product was isolated as a yellow oil (yield 56.5 mg, 82%) after purification by silica gel chromatography (Hexane/EtOAc = 90:10). Reaction time = 10 h. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 1.84 (br, 1H), 2.35-2.47 (m, 2H), 4.34-4.38 (m, 1H), 5.15-5.2 (m, 2H), 5.81-5.90 (m, 1H), 6.22-6.26 (dd, *J* = 6, 10 Hz, 1H), 6.59-6.62 (d, *J* = 15.5 Hz, 1H), 7.22-7.25 (m, 1H), 7.3-7.33 (t, *J* = 8 Hz, 2H), 7.37-7.39 (d, *J* = 7 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 41.5, 71.2, 118,

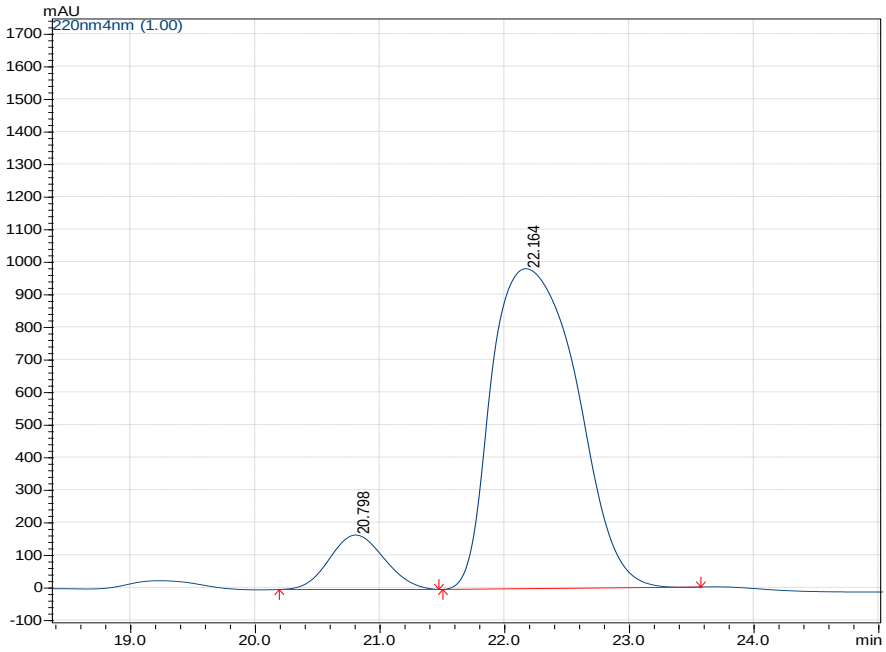
125.9, 127.1, 128, 129.8, 131, 133.5, 136.1. Optical Rotation: $[\alpha]^{27}_{D}$ = +29 (c 1, $CHCl_3$).[3] HPLC (Daicel Chiralpak IA, hexanes/2-propanol = 95:5, flow rate = 0.7 mL/min, λ = 254 nm) t_{major}(*R*) = 14.6 min, t_{minor}(*S*) = 13.6 min.

(1*E*,3*R*)-2-Methyl-1-phenyl-1,5-hexadiene-3-ol (compound 2s):[3] The product was isolated as a yellow oil (yield 65 mg, 87%) after purification by silica gel chromatography (Hexane/EtOAc = 90:10). Reaction time = 10 h. ^{1}H NMR ($CDCl_3$, 200 MHz): δ = 1.82-1.84 (m, 1H), 1.88 (s, 3H), 2.38-2.43 (m, 2H), 4.22 (m, 1H), 5.12-5.22 (m, 2H), 5.73-5.90 (m, 1H), 6.52 (s, 1H), 7.21-7.33 (m, 5H). ^{13}C NMR ($CDCl_3$, 50 MHz): δ = 13.1, 39.5, 76, 117.5, 125.2, 125.9, 127.6, 128.4, 134, 137, 139. Optical Rotation: $[\alpha]^{27}_{D}$ = +2.5 (c 0.9, $CHCl_3$).[3] HPLC (Daicel Chiralcel IC, hexanes/2-propanol = 95:5, flow rate = 0.8 mL/min, λ = 220 nm) t_{major}(*R*) = 8.2 min, t_{minor}(*S*) = 7.5 min.

HPLC chromatograms of the Homoallylic Alcohols

(*S*)-1-phenylbut-3-en-1-ol (compound 2a)





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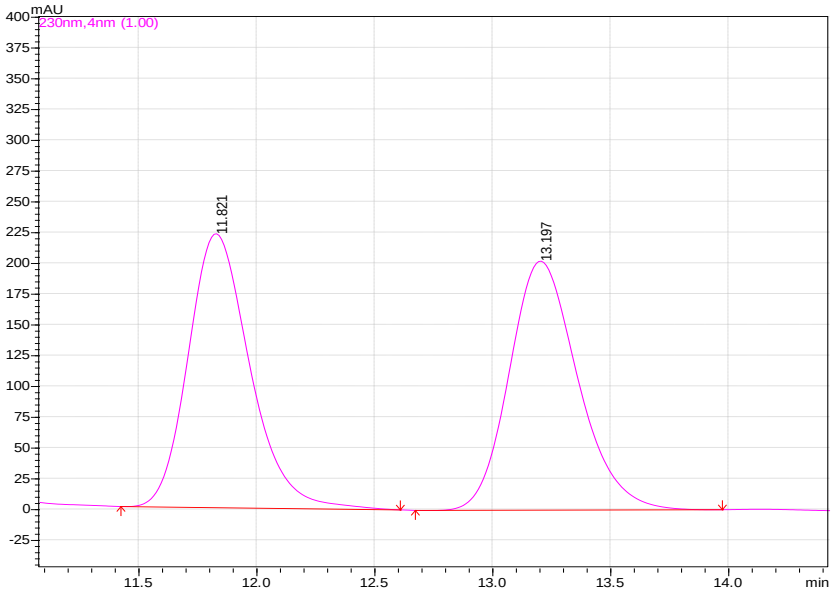
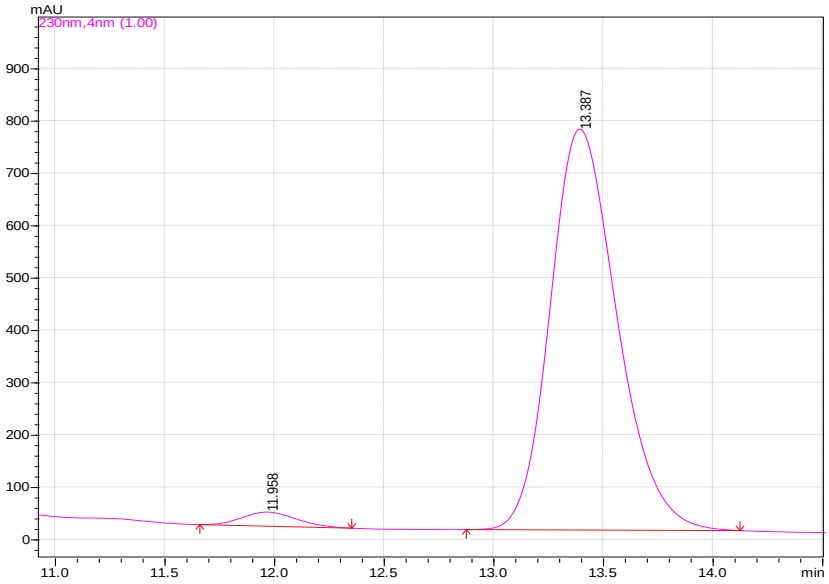
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	20.798	5115327	20.192	21.472	9.8360
2	22.164	46891066	21.504	23.573	90.1640

(*S*)-1-(4-methoxyphenyl)but-3-en-1-ol (compound 2b)





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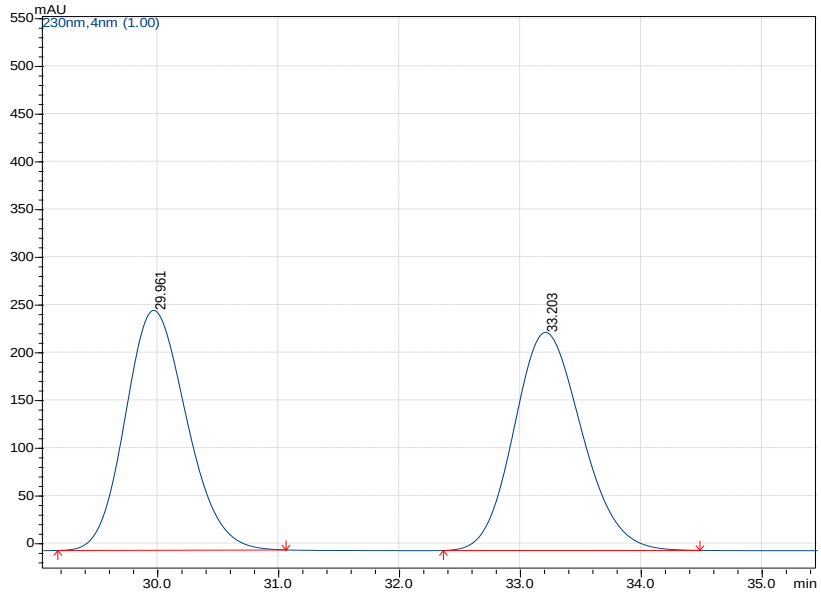
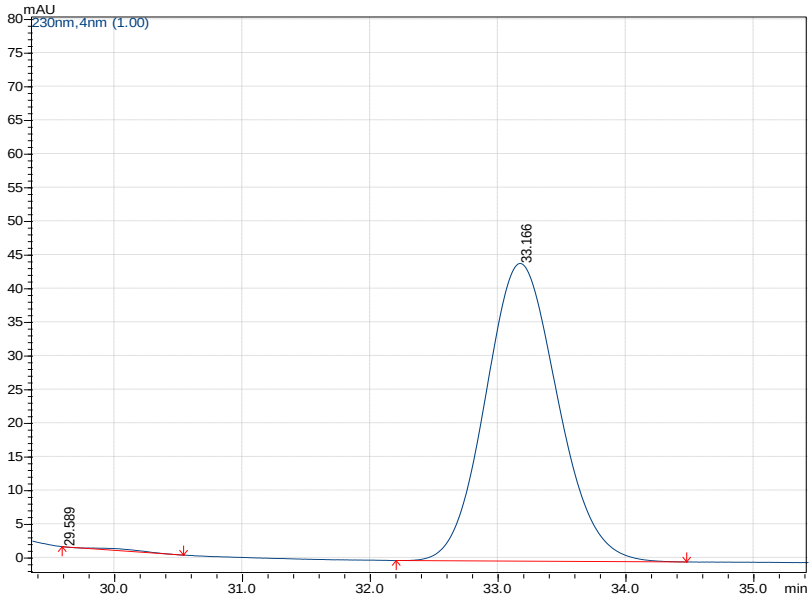
1	11.821	4059344	11.424	12.608	49.8443
2	13.197	4084705	12.672	13.973	50.1557

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	11.958	464430	11.659	12.352	2.7754
2	13.387	16269373	12.875	14.123	97.2246

(4-benzyloxyphenyl)but-3-en-1-ol (compound 2c)

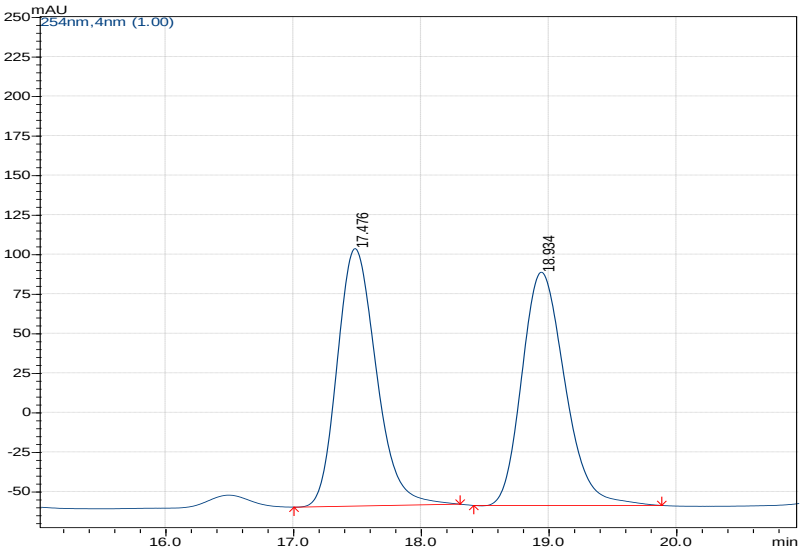


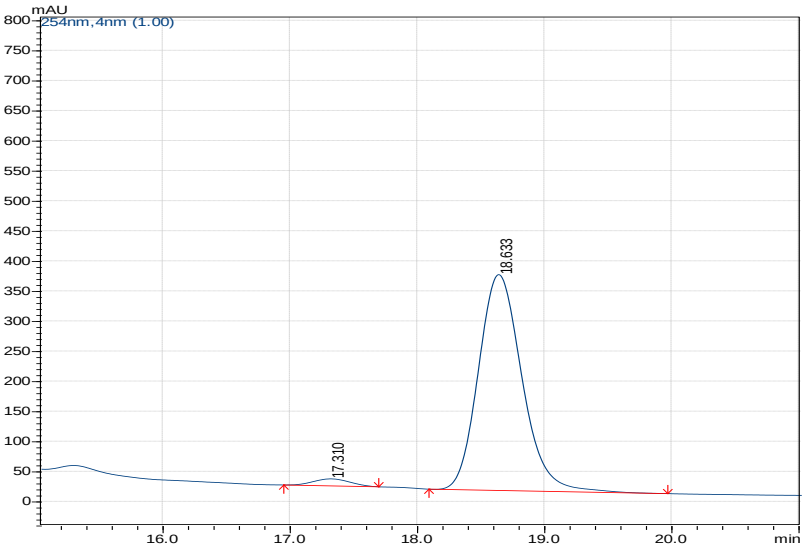


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	29.961	8926091	29.152	31.200	49.9755
2	33.203	8934860	32.309	34.421	50.0245

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	29.589	5542	29.589	30.539	0.3186
2	33.166	1733980	32.203	34.475	99.6814

(*S*)-1-(4-*tert*-Butylphenyl)-3-buten-1-ol (compound 2d)

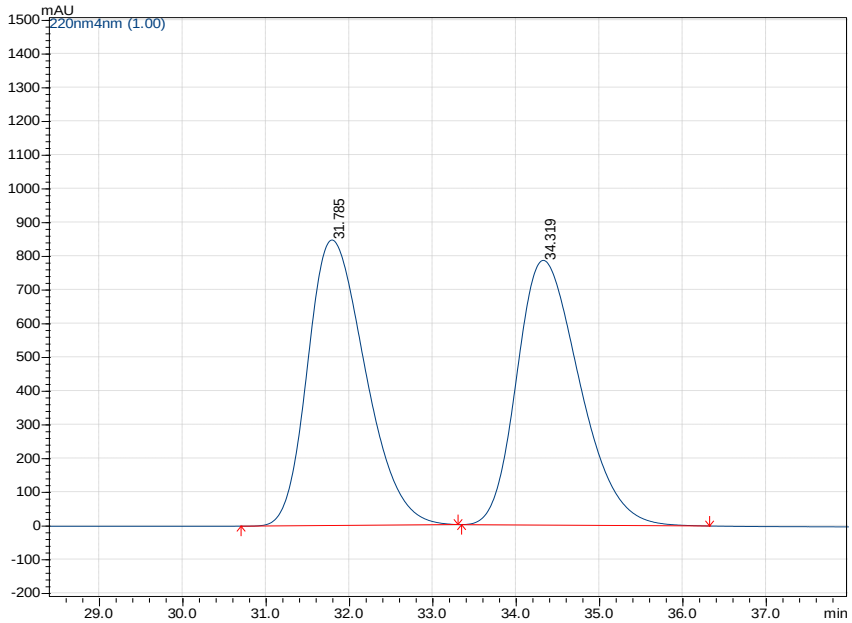


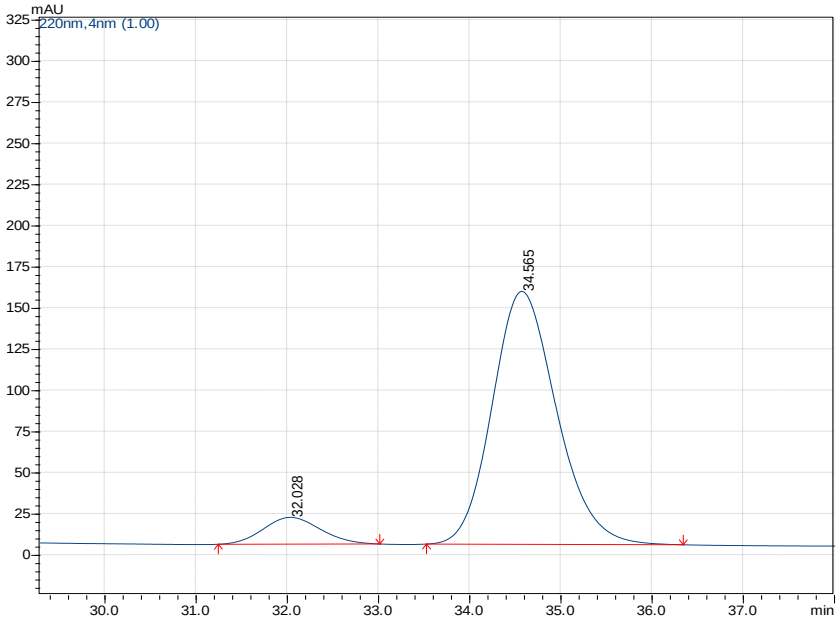


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	17.476	3457839	17.003	18.304	50.0846
2	18.934	3446159	18.411	19.883	49.9154

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	17.310	231851	16.949	17.696	2.6431
2	18.633	8540149	18.091	19.968	97.3569

(*S*)-1-(*p*-tolyl)but-3-en-1-ol (compound 2e)

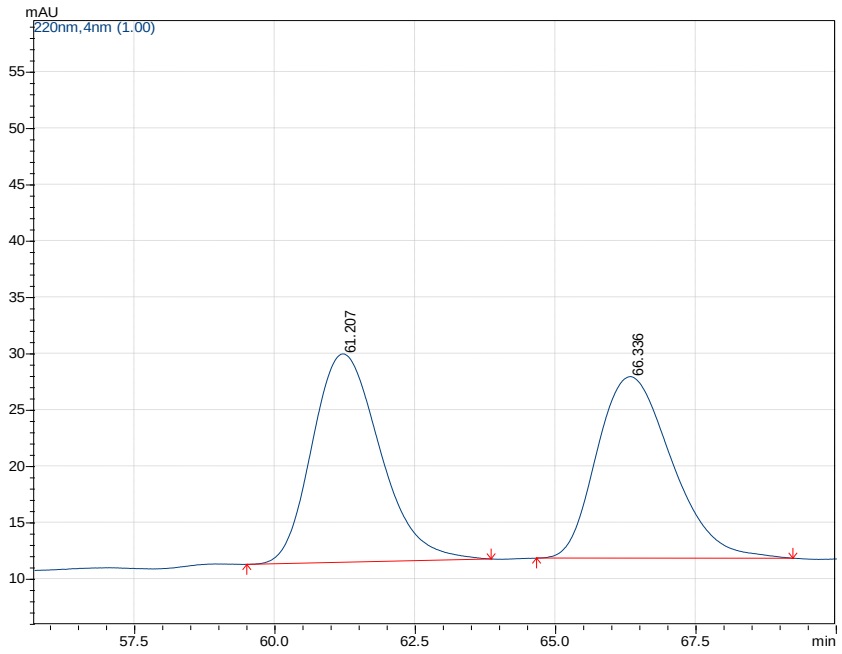


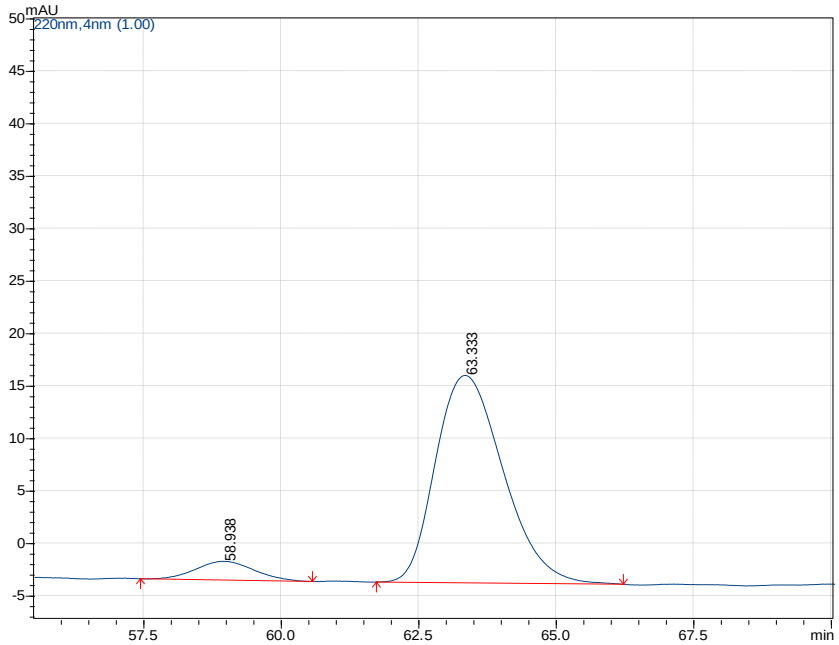


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	31.785	40727300	30.699	33.301	49.7284
2	34.319	41172171	33.344	36.320	50.2716

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	32.028	711150	31.243	33.013	8.6186
2	34.565	7540202	33.525	36.341	91.3814

(*S*)-1-(4-nitrophenyl)but-3-en-1-ol (compound 2f)

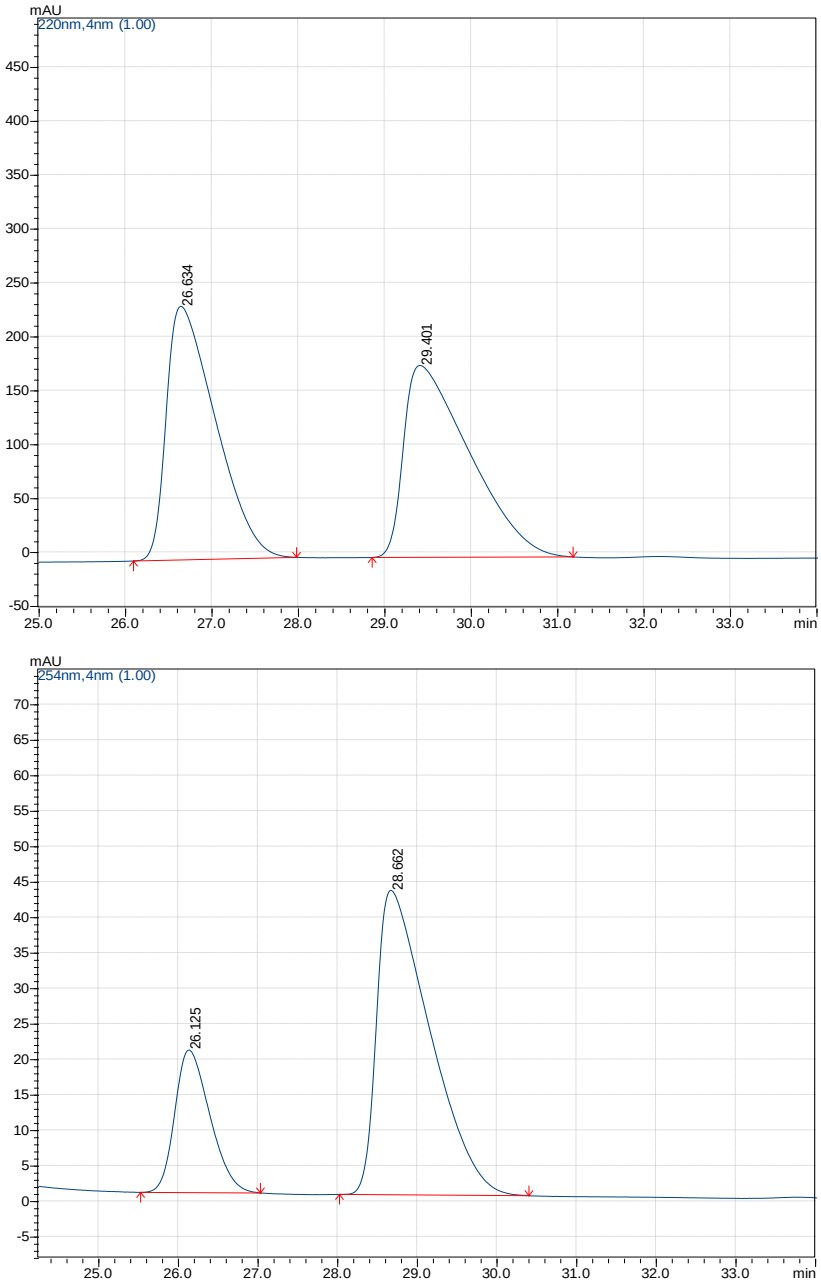




Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	61.207	1555059	59.499	63.851	51.0594
2	66.336	1490530	64.661	69.227	48.9406

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	58.938	131687	57.440	60.565	7.2229
2	63.333	1691508	61.728	66.219	92.7771

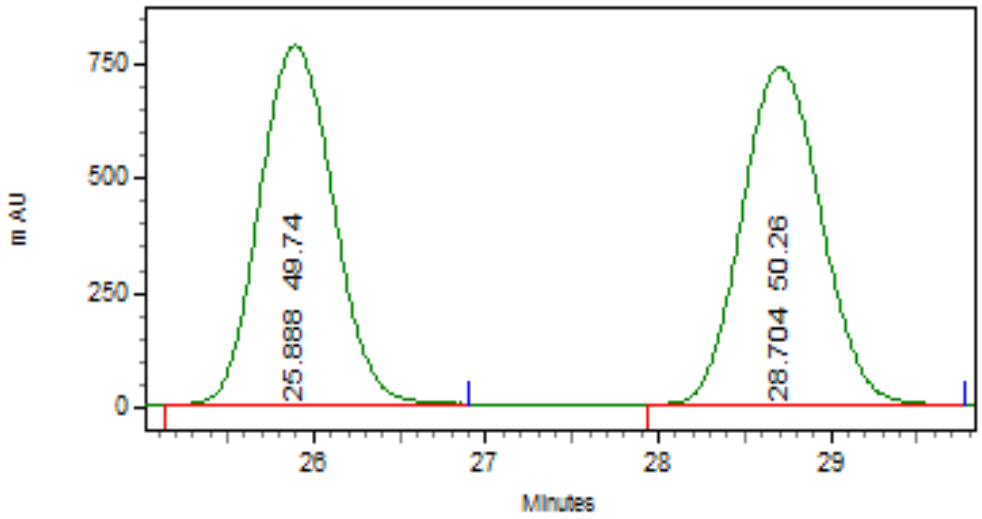
(*S*)-1-(4-fluorophenyl)but-3-en-1-ol (compound 2g)

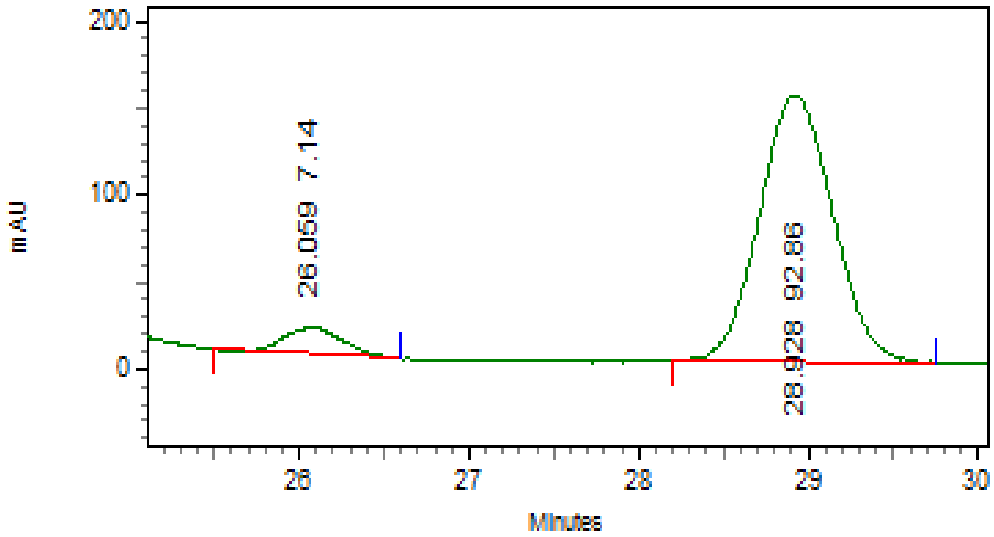


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	26.634	9305374	26.091	27.979	49.7672
2	29.401	9392428	28.853	31.179	50.2328

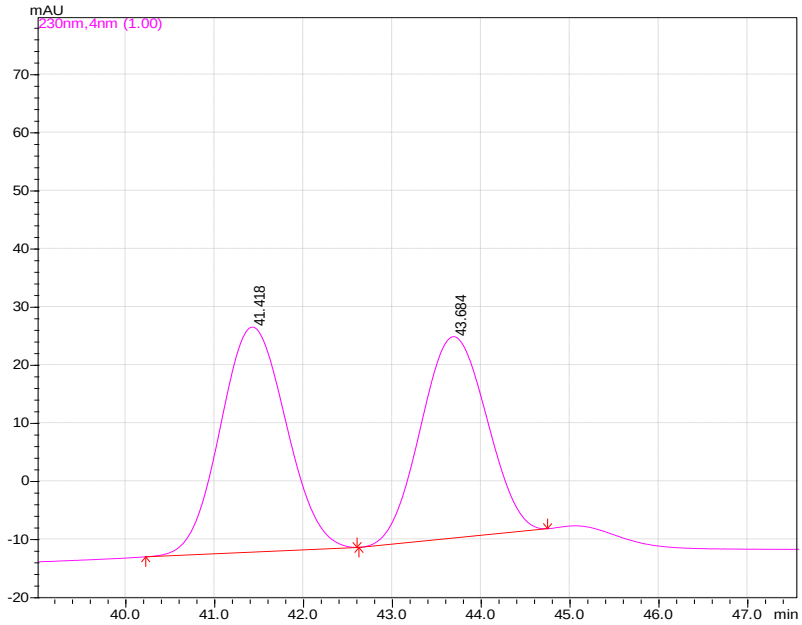
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	26.125	615645	25.525	27.029	23.5862
2	28.662	1994546	28.021	30.400	76.4138

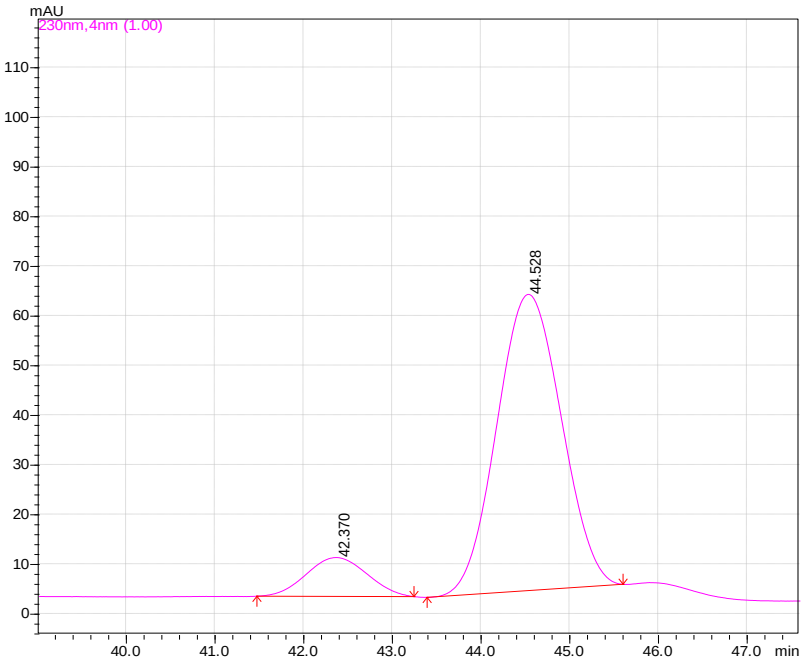
(*S*)-1-(4-chlorophenyl)but-3-en-1-ol (compound 2h)





(*S*)-1-(4-bromophenyl)but-3-en-1-ol (compound 2i)

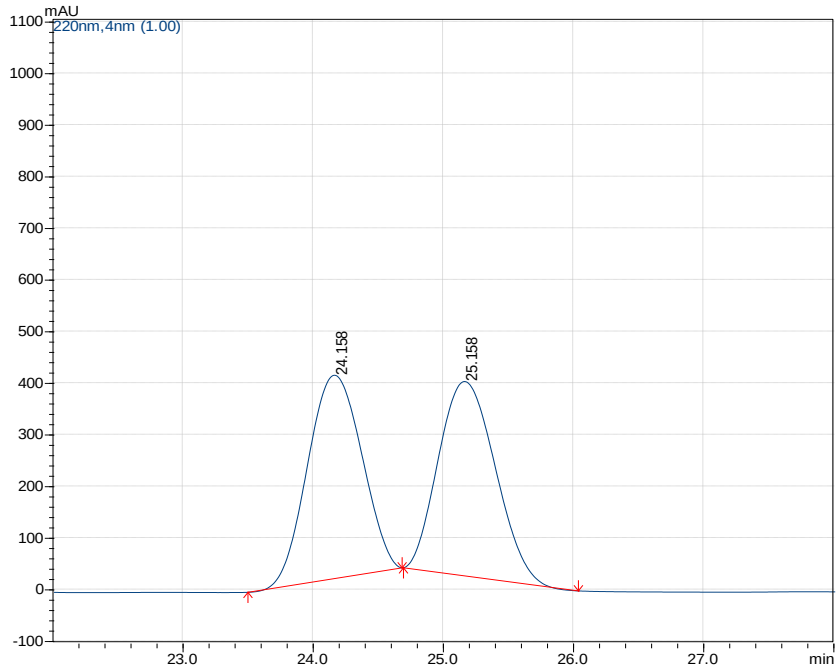


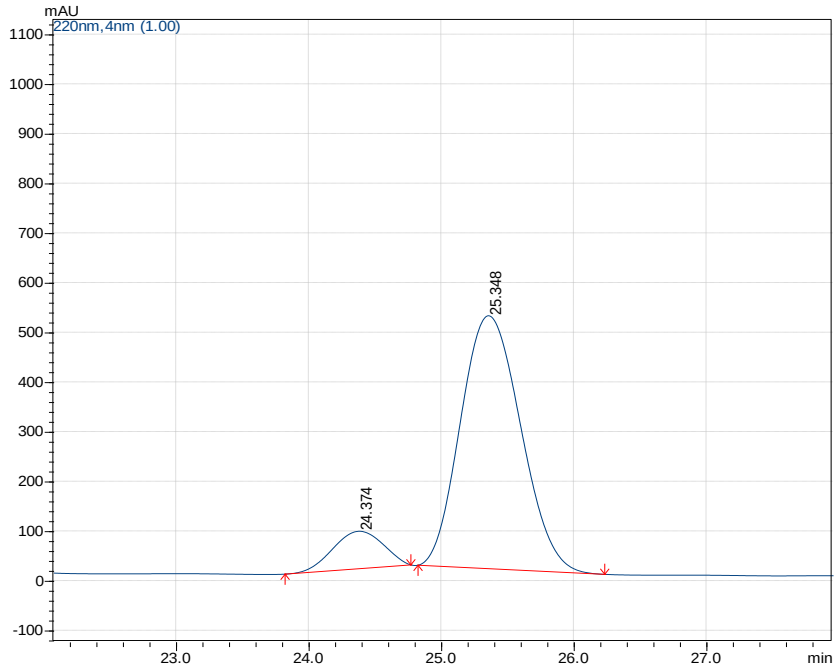


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	41.418	1996744	40.224	42.603	52.7797
2	43.684	1786423	42.624	44.747	47.2203

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	42.370	371295	41.472	43.243	10.9736
2	44.528	3012227	43.328	45.771	89.0264

(S)-1-(3-methoxyphenyl)but-3-en-1-ol (compound 2j)

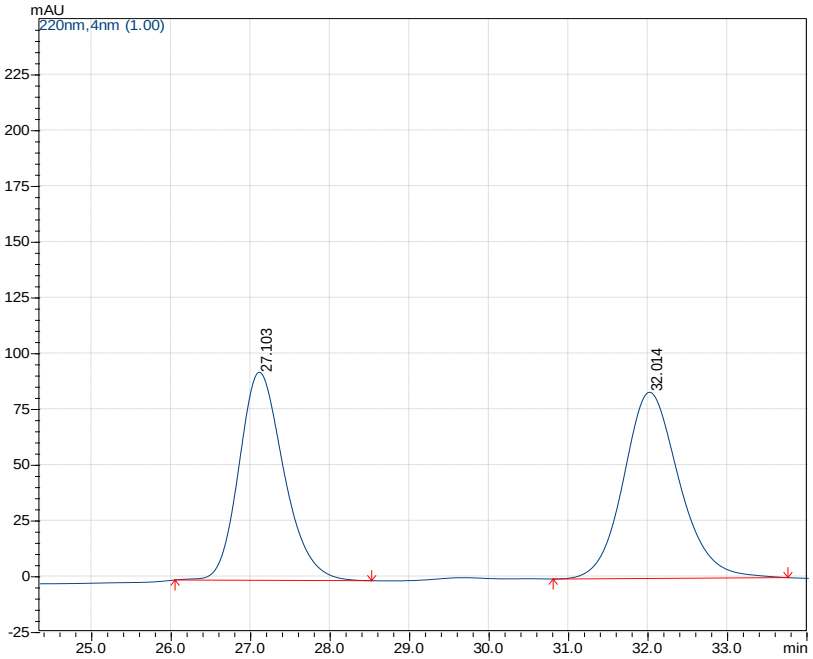


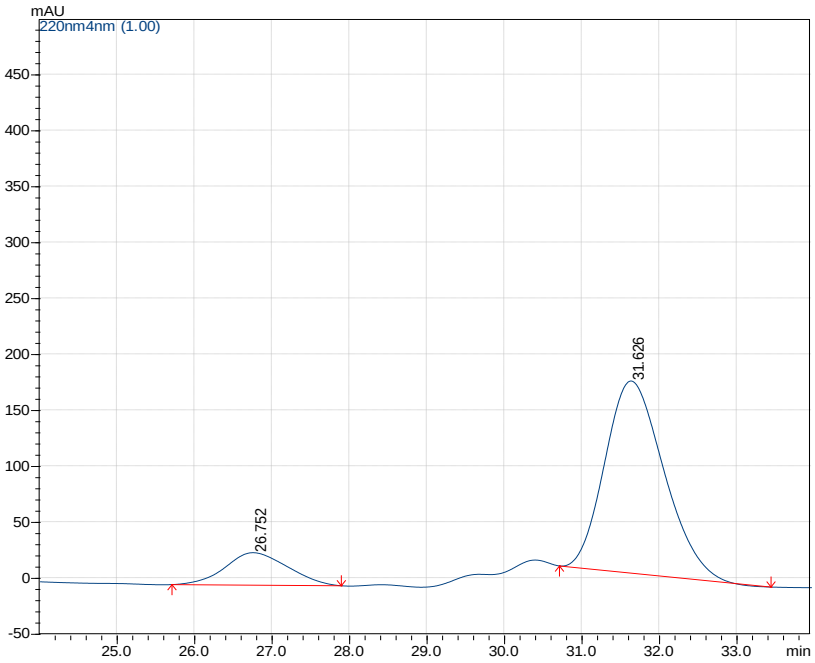


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	24.158	11404118	23.499	24.683	49.9716
2	25.158	11417082	24.693	26.037	50.0284

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	24.374	1991570	23.819	24.768	11.0335
2	25.348	16058634	24.821	26.229	88.9665

(*S*)-1-(*m*-tolyl)but-3-en-1-ol (compound 2k)

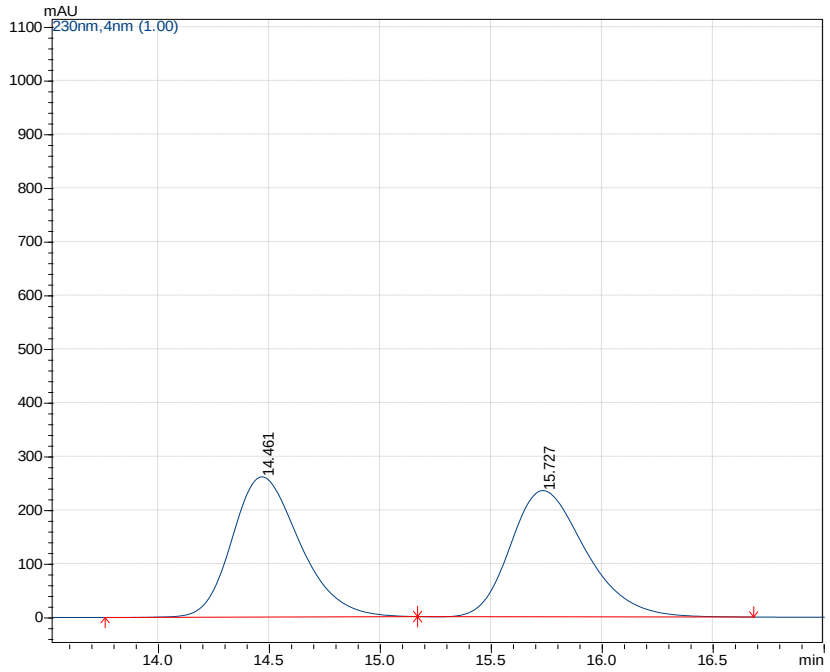


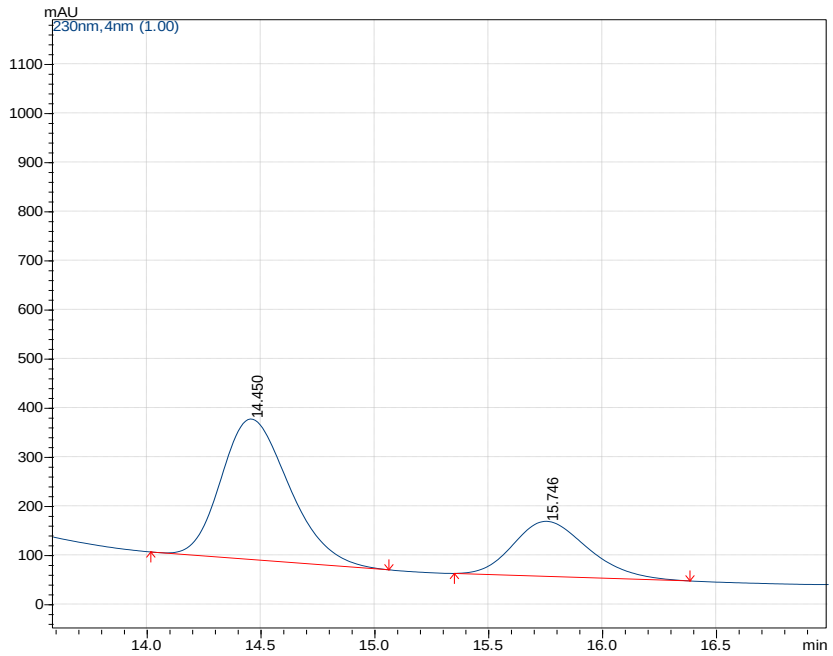


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	27.103	3658696	26.048	28.523	47.3621
2	32.014	4066256	30.805	33.760	52.6379

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	26.752	1631123	25.707	27.893	15.2056
2	31.626	9095995	30.709	33.440	84.7944

(*S*)-1-(2-methoxyphenyl)but-3-en-1-ol (compound 2l)

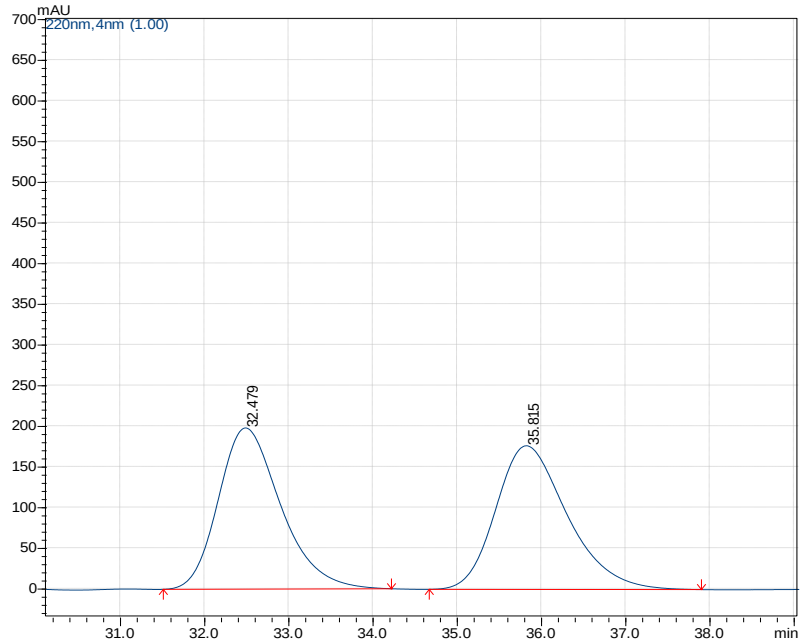


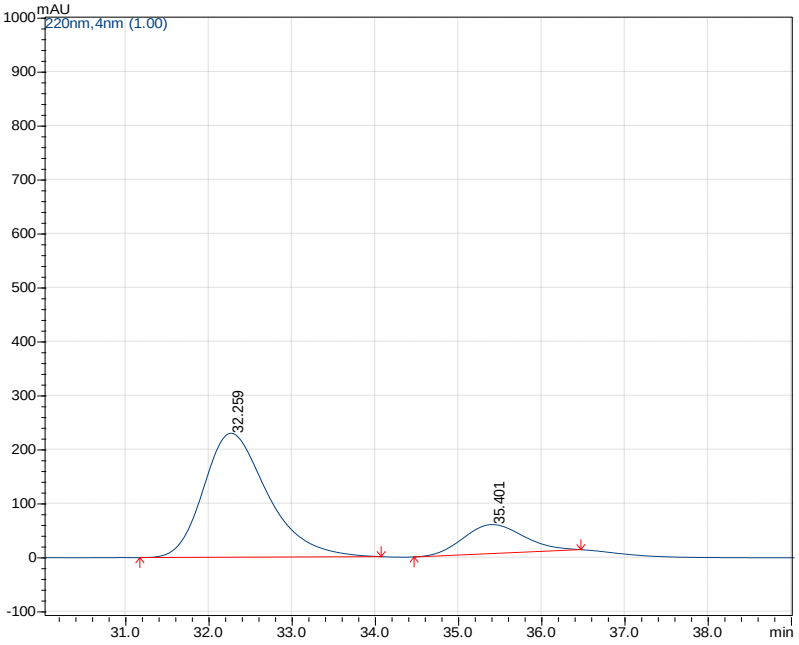


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	14.461	19206379	13.760	15.168	50.0494
2	15.727	19168499	15.168	16.683	49.9506

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	14.450	5940613	14.016	15.061	69.9479
2	15.746	2552294	15.349	16.384	30.0521

(*S*)-1-(*o*-tolyl)but-3-en-1-ol (compound 2m)

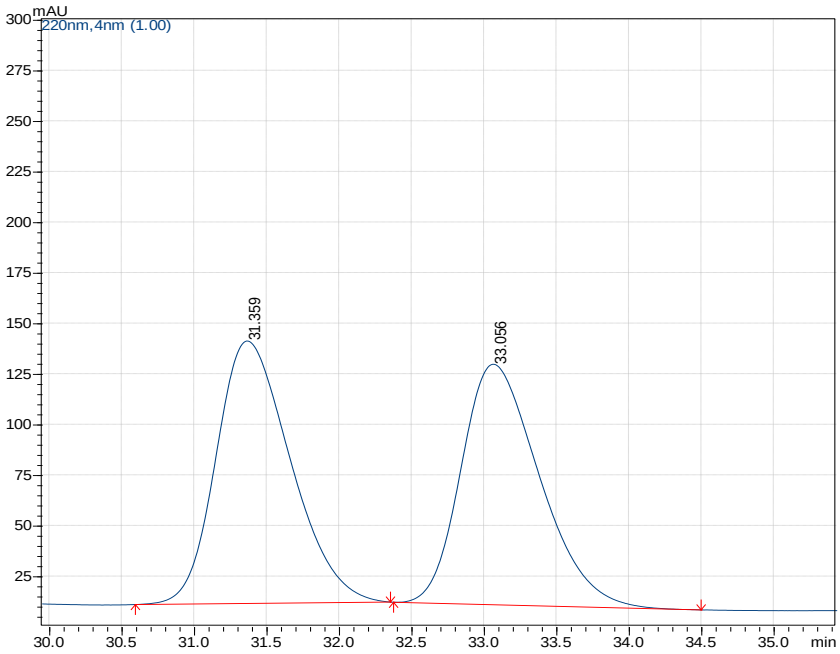


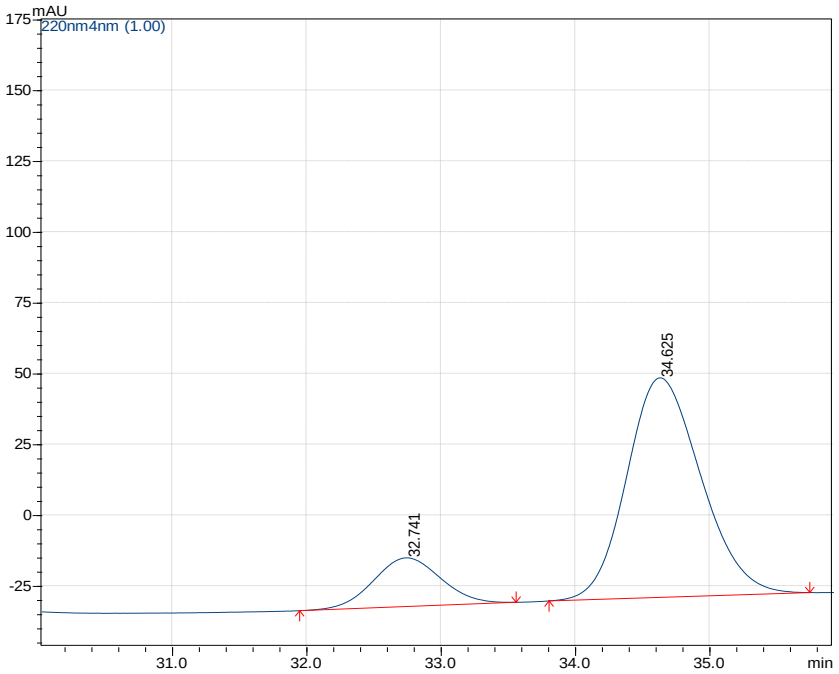


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	32.479	10202178	31.509	34.219	49.4997
2	35.815	10408411	34.667	37.899	50.5003

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	32.259	12324422	31.168	34.069	81.9234
2	35.401	2719420	34.464	36.469	18.0766

(*S*)-1-(2-fluorophenyl)but-3-en-1-ol (compound 2n)

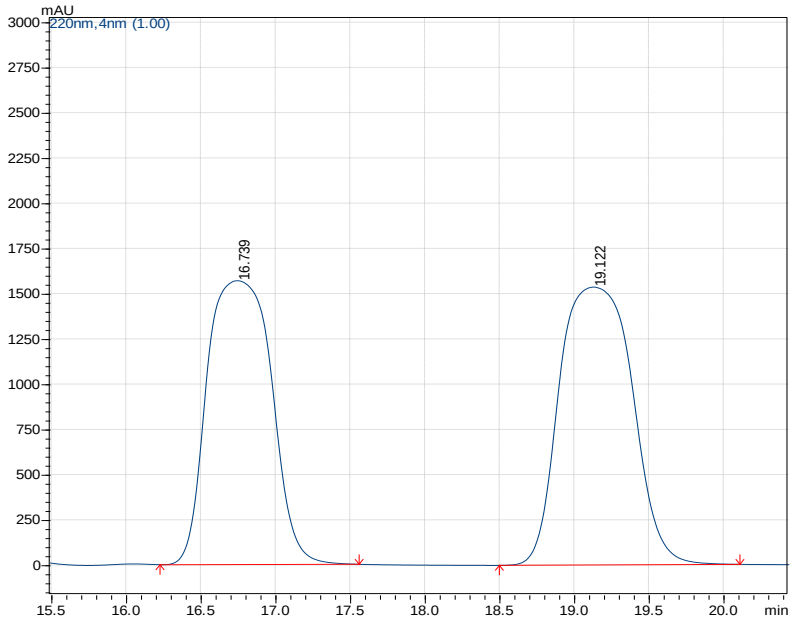


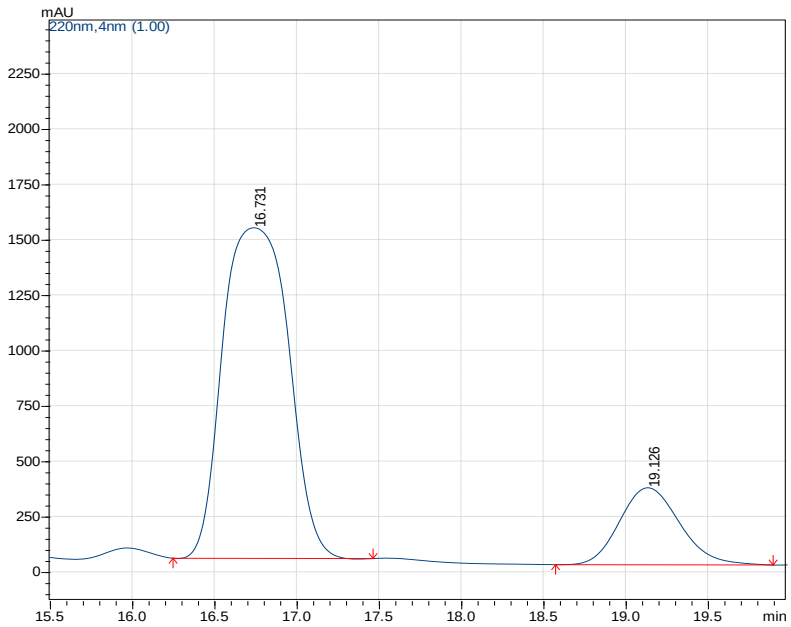


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	31.359	4627708	30.592	32.352	50.9127
2	33.056	4461793	32.373	34.496	49.0873

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	32.741	598991	31.947	33.557	16.7455
2	34.625	2978030	33.803	35.744	83.2545

(*S*)-1-(naphthalen-1-yl)but-3-en-1-ol (compound 2o)

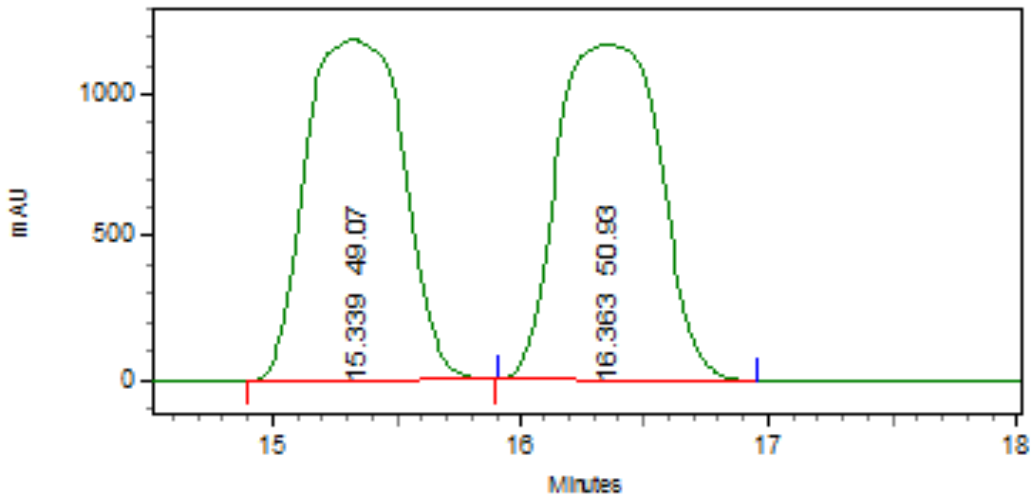


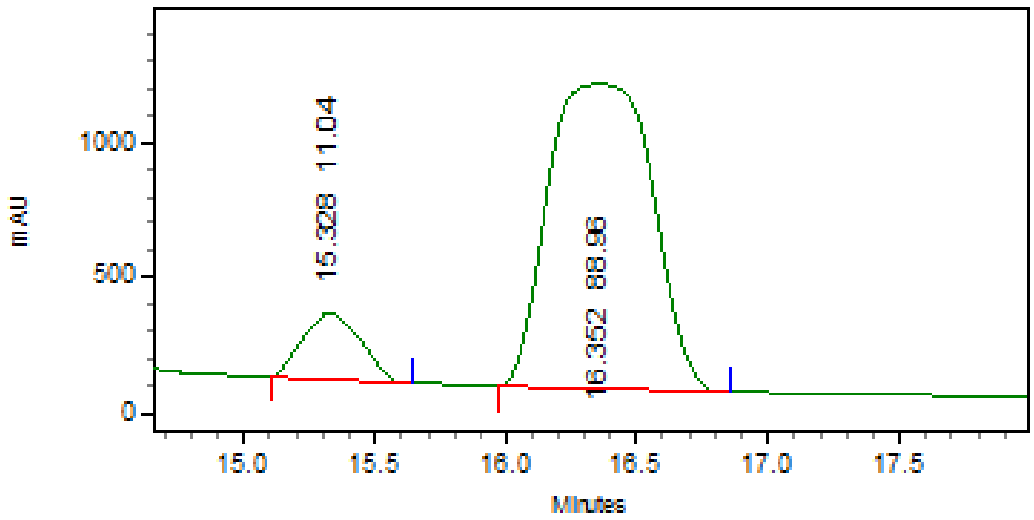


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	16.739	47124829	16.224	17.557	47.4385
2	19.122	52214059	18.496	20.107	52.5615

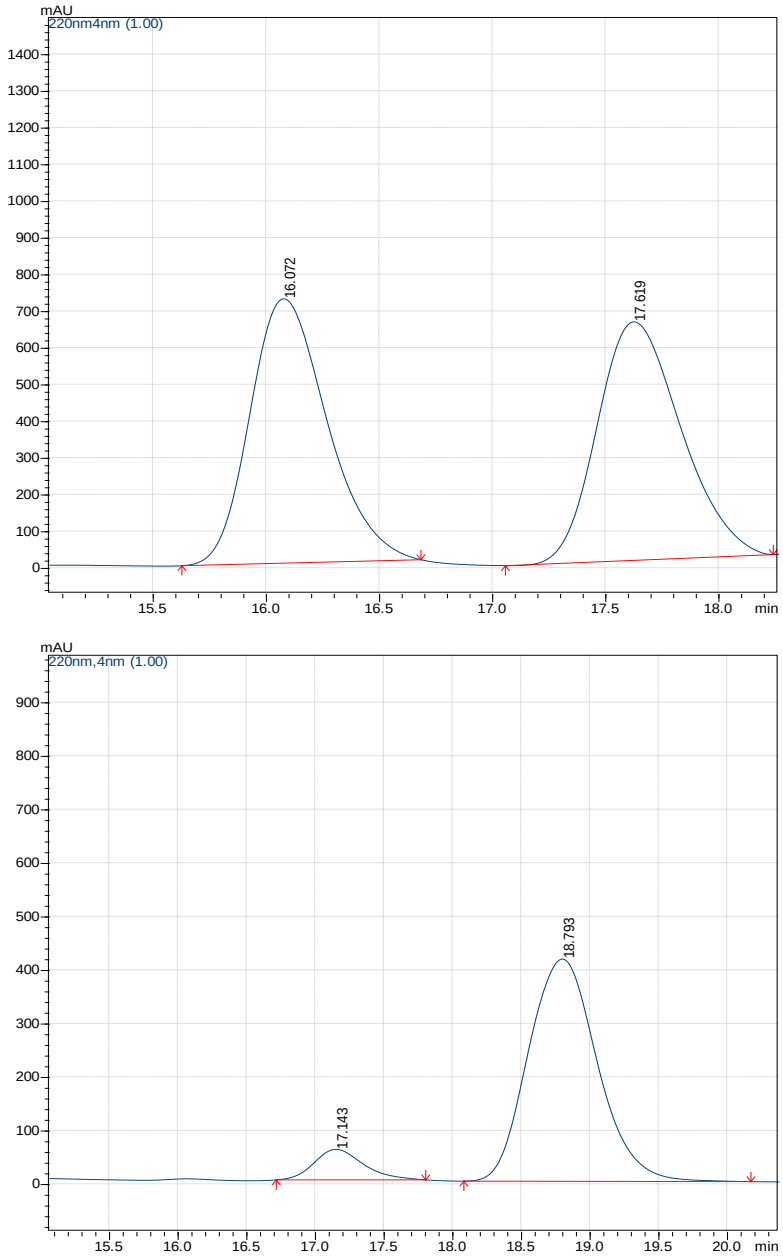
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	16.731	41661560	16.245	17.461	82.4916
2	19.126	8842468	18.571	19.893	17.5084

(*S*)-1-(naphthalen-2-yl)but-3-en-1-ol (compound 2p)





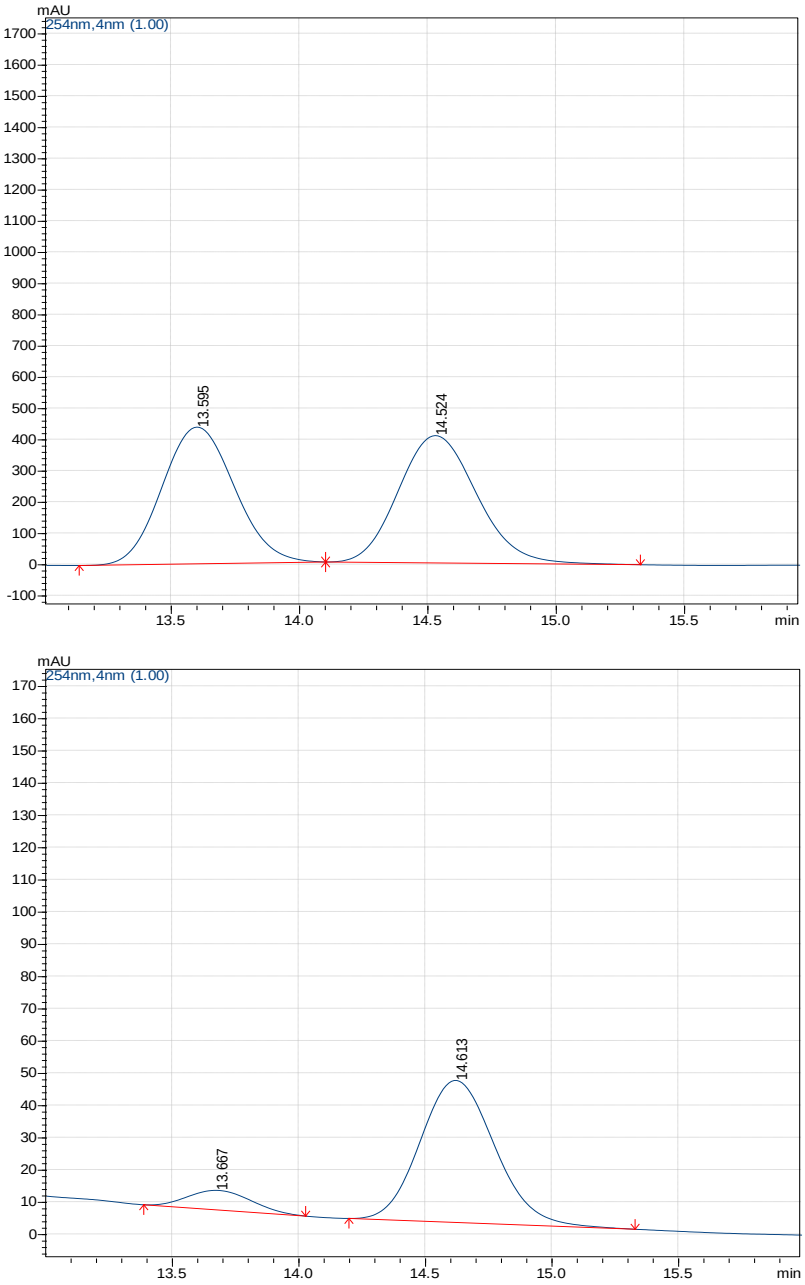
(*S*)-1-(thiophen-2-yl)but-3-en-1-ol (compound 2q)



Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	16.072	17061150	15.627	16.683	50.5413
2	17.619	16695718	17.056	18.240	49.4587

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	17.143	1426400	16.715	17.803	8.9628
2	18.793	14488260	18.080	20.171	91.0372

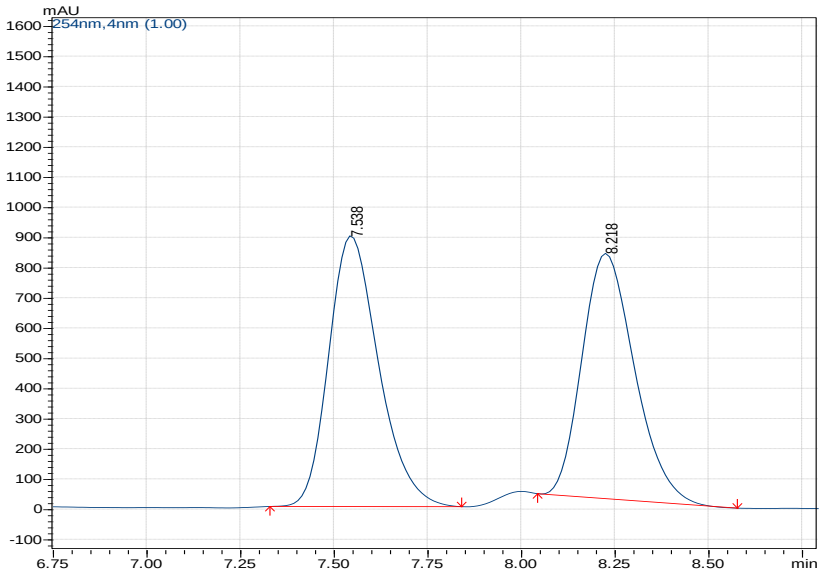
(1*E*,3*R*)-1-Phenyl-1,5-hexadiene-3-ol (compound 2r)

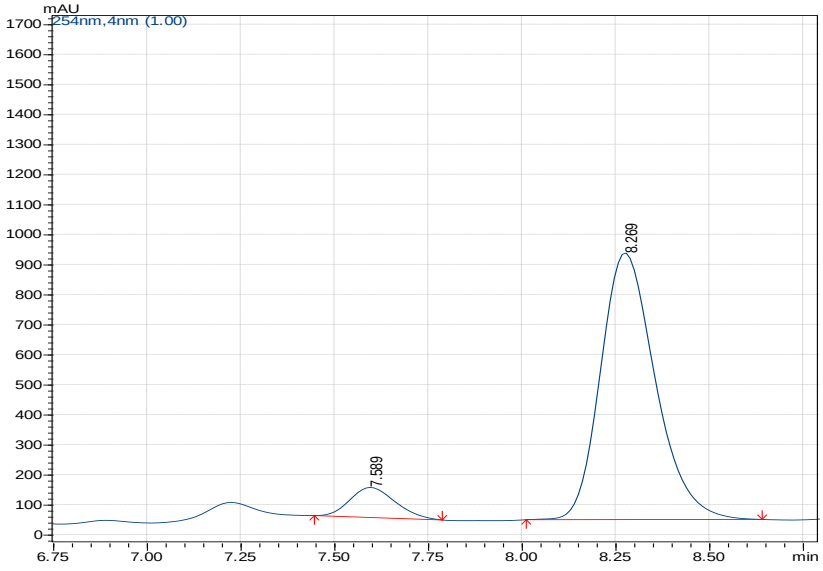


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	13.595	8587514	13.141	14.101	49.8409
2	14.524	8642334	14.101	15.328	50.1591

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	13.667	104866	13.387	14.027	10.3996
2	14.613	903496	14.197	15.328	89.6004

(1*E*,3*R*)-2-Methyl-1-phenyl-1,5-hexadiene-3-ol (compound 2s)



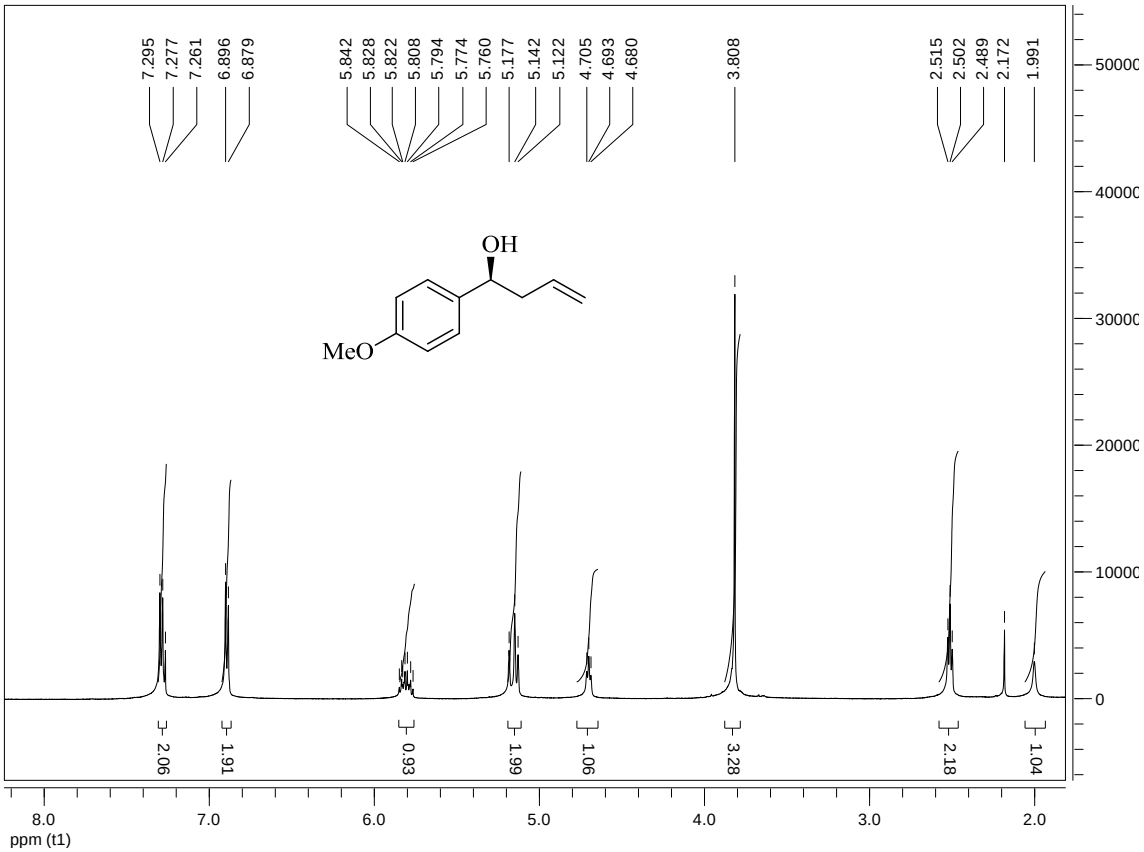


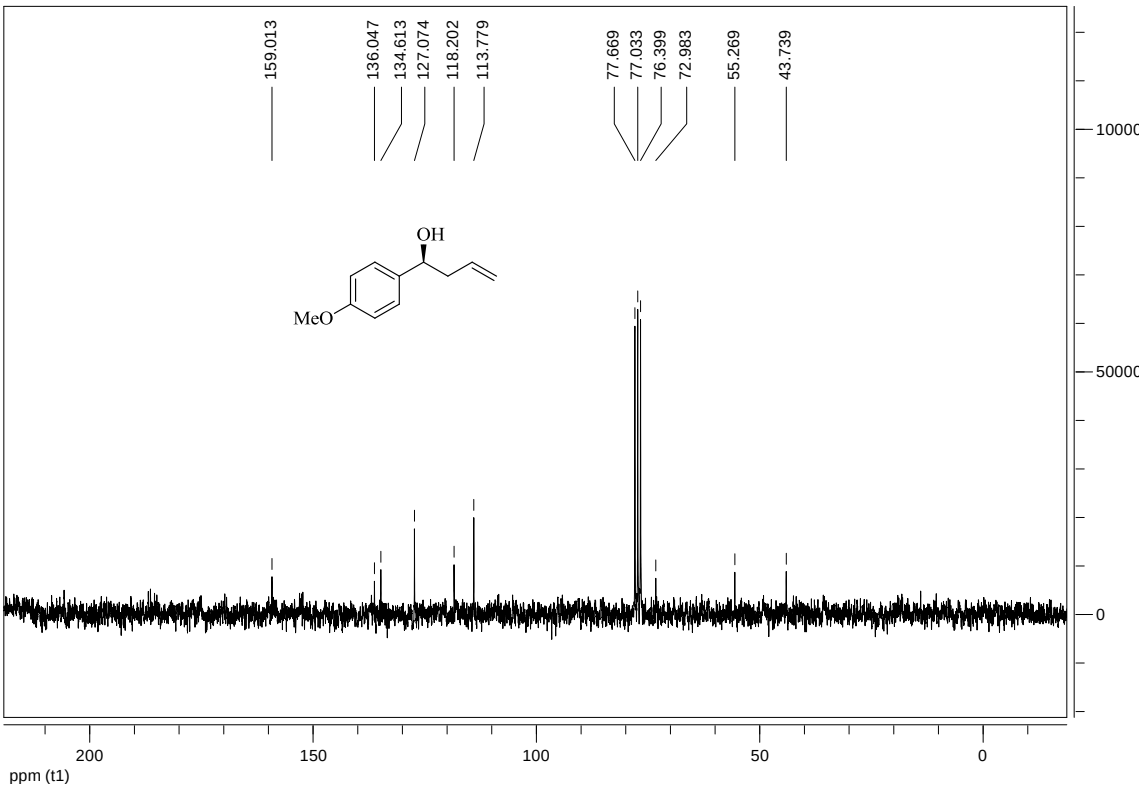
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	7.538	8315913	7.328	7.840	51.2392
2	8.218	7913667	8.043	8.576	48.7608

Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	7.589	836743	7.445	7.787	8.4874
2	8.269	9021876	8.011	8.640	91.5126

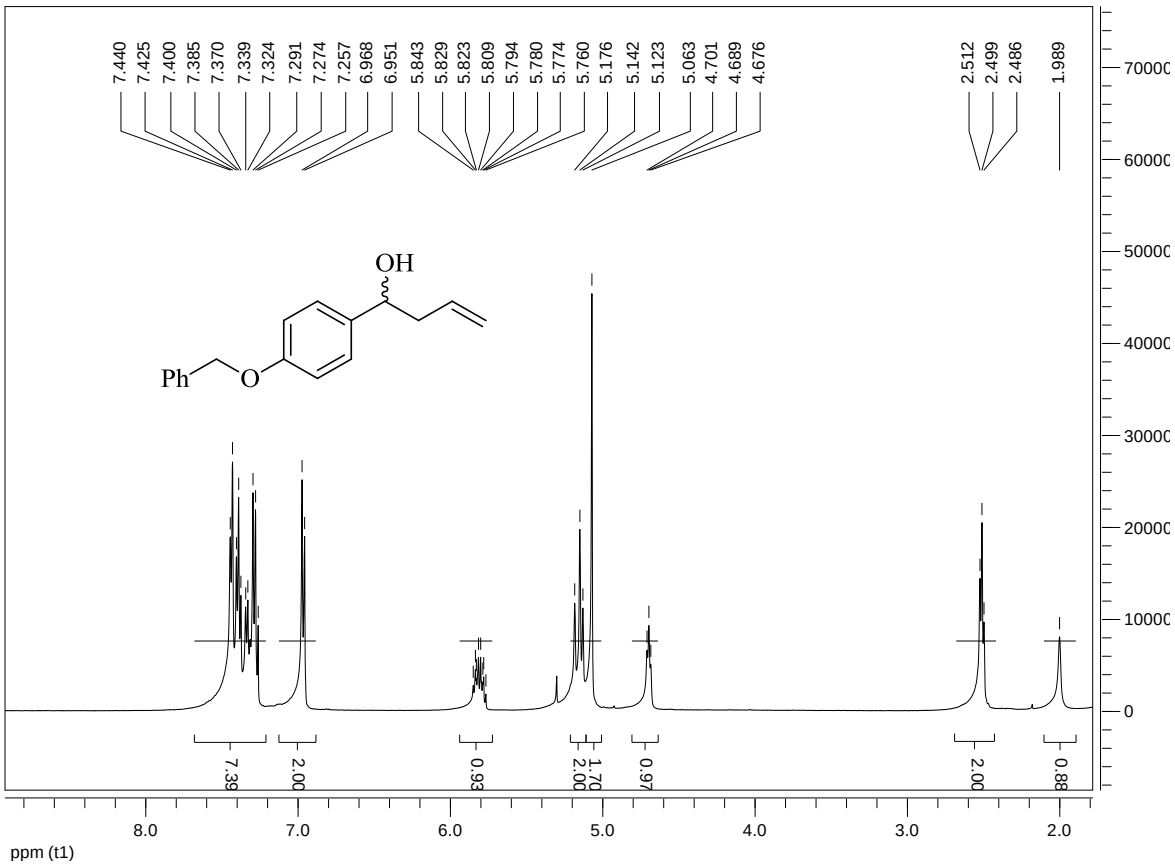
Copy of ^{1}H and ^{13}C spectra of homoallyl alcohol products

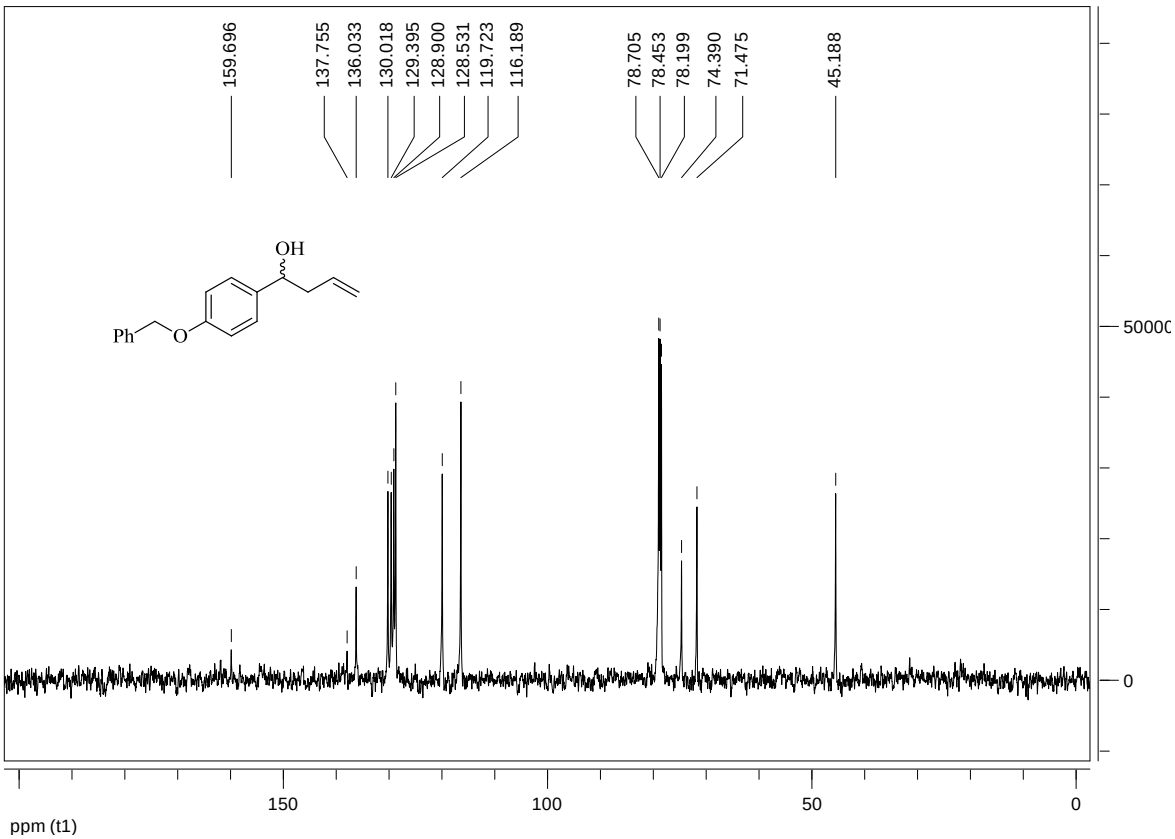
(*S*)-1-(4-methoxyphenyl)but-3-en-1-ol (compound 2b)



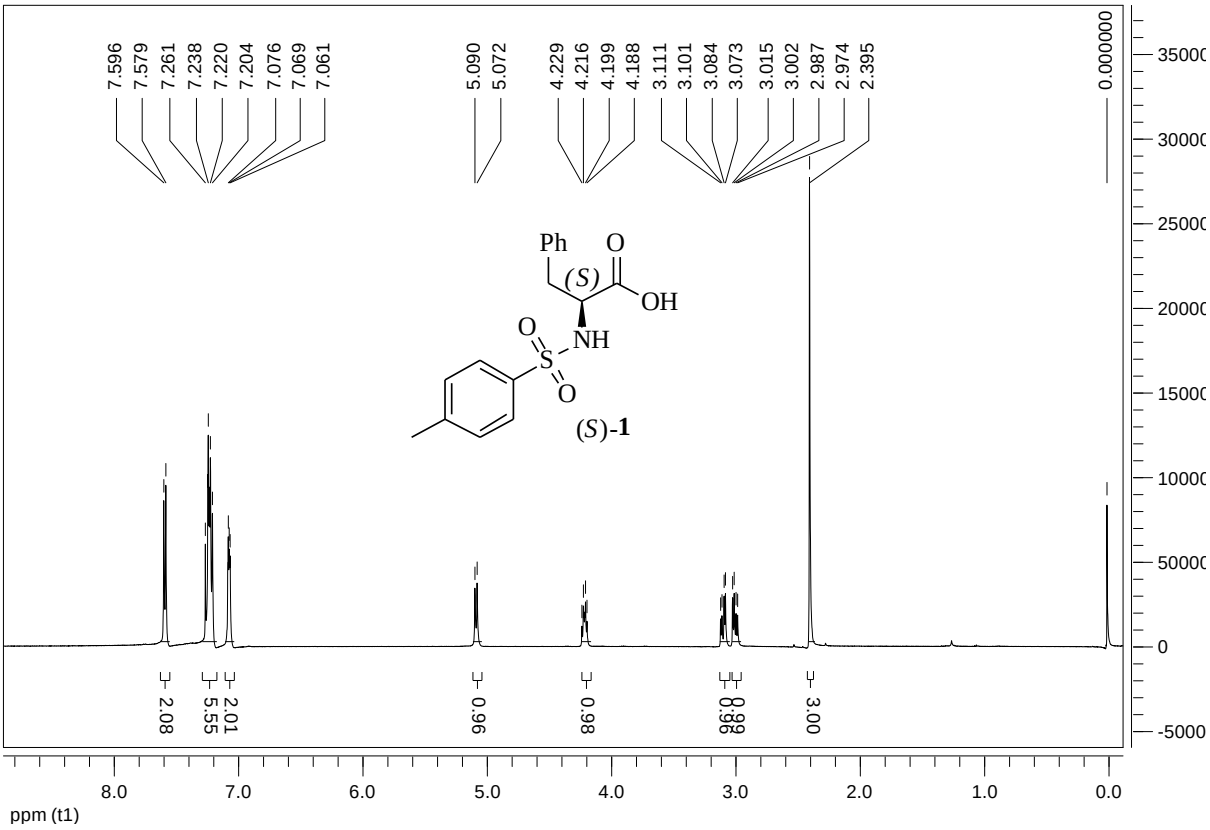


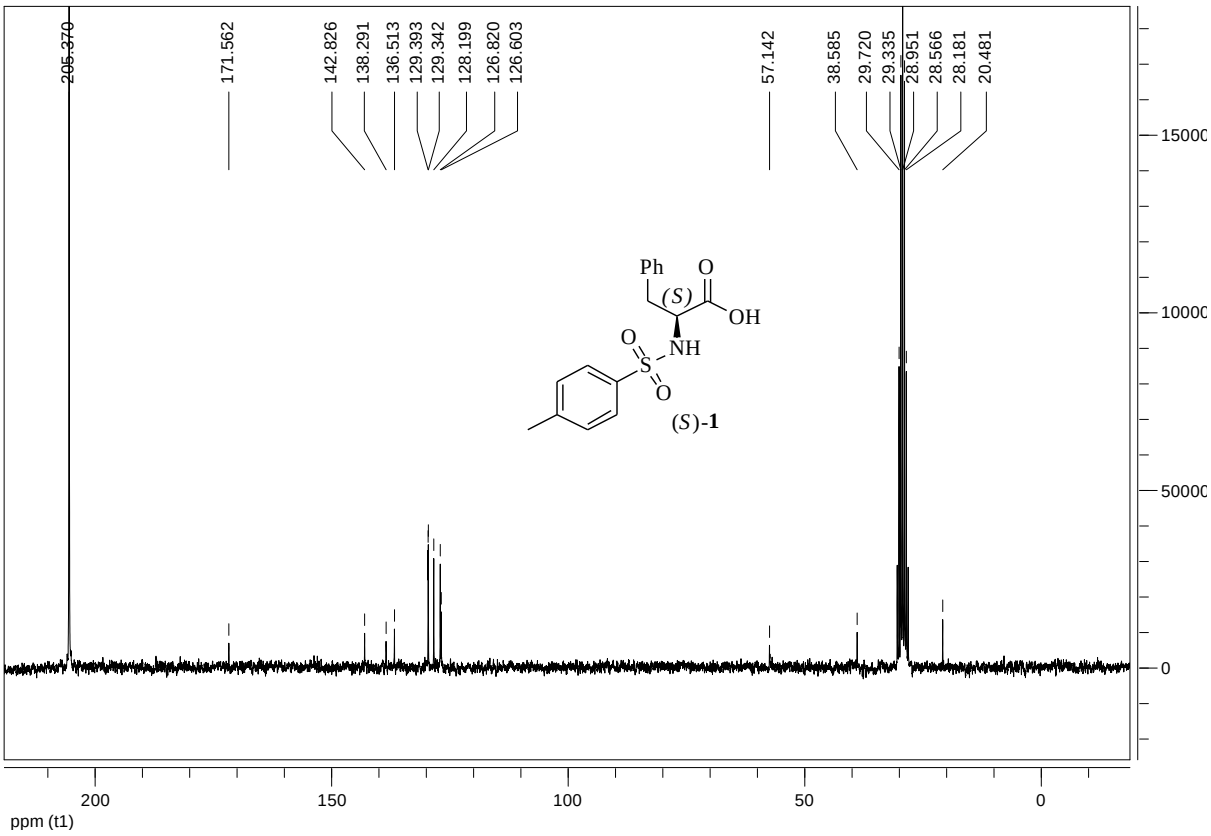
(4-benzyloxyphenyl)but-3-en-1-ol (compound 2c)

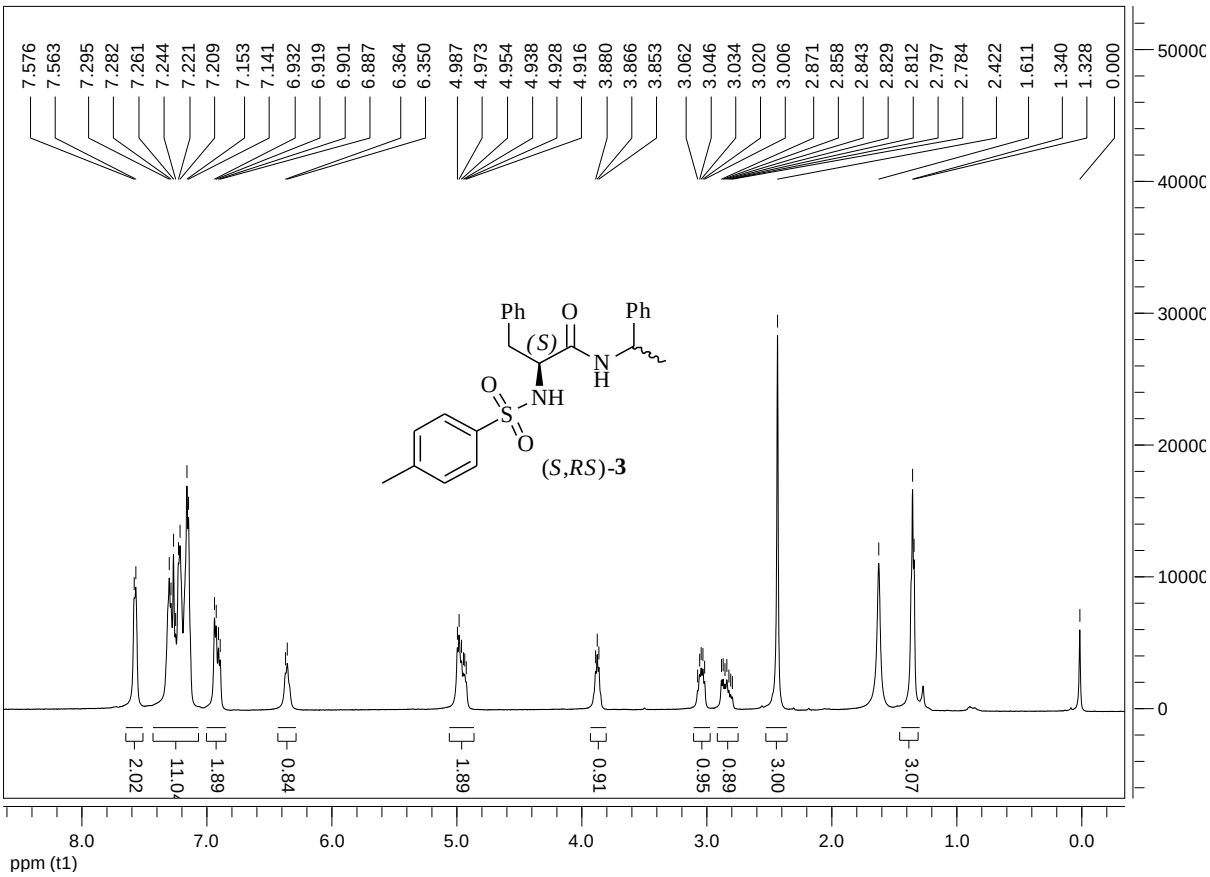


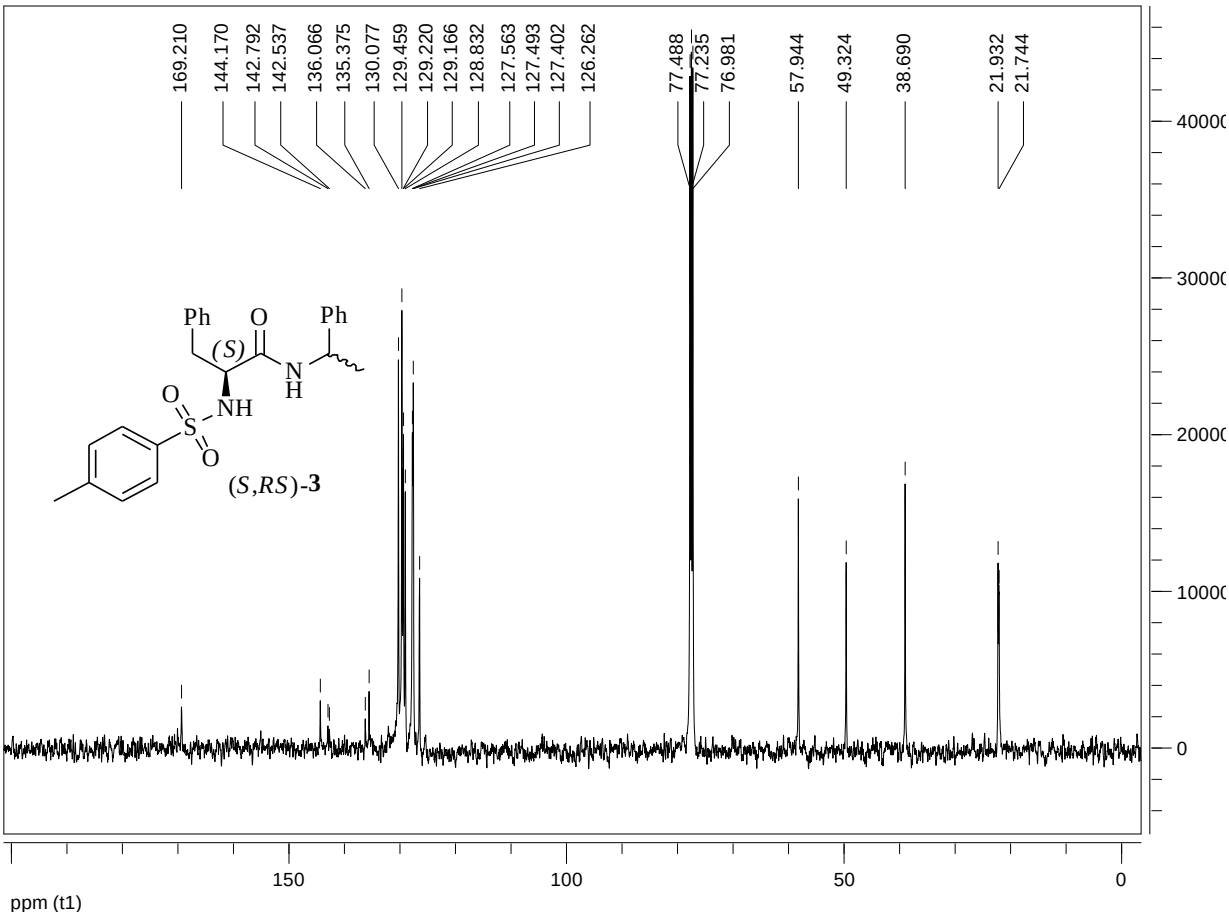


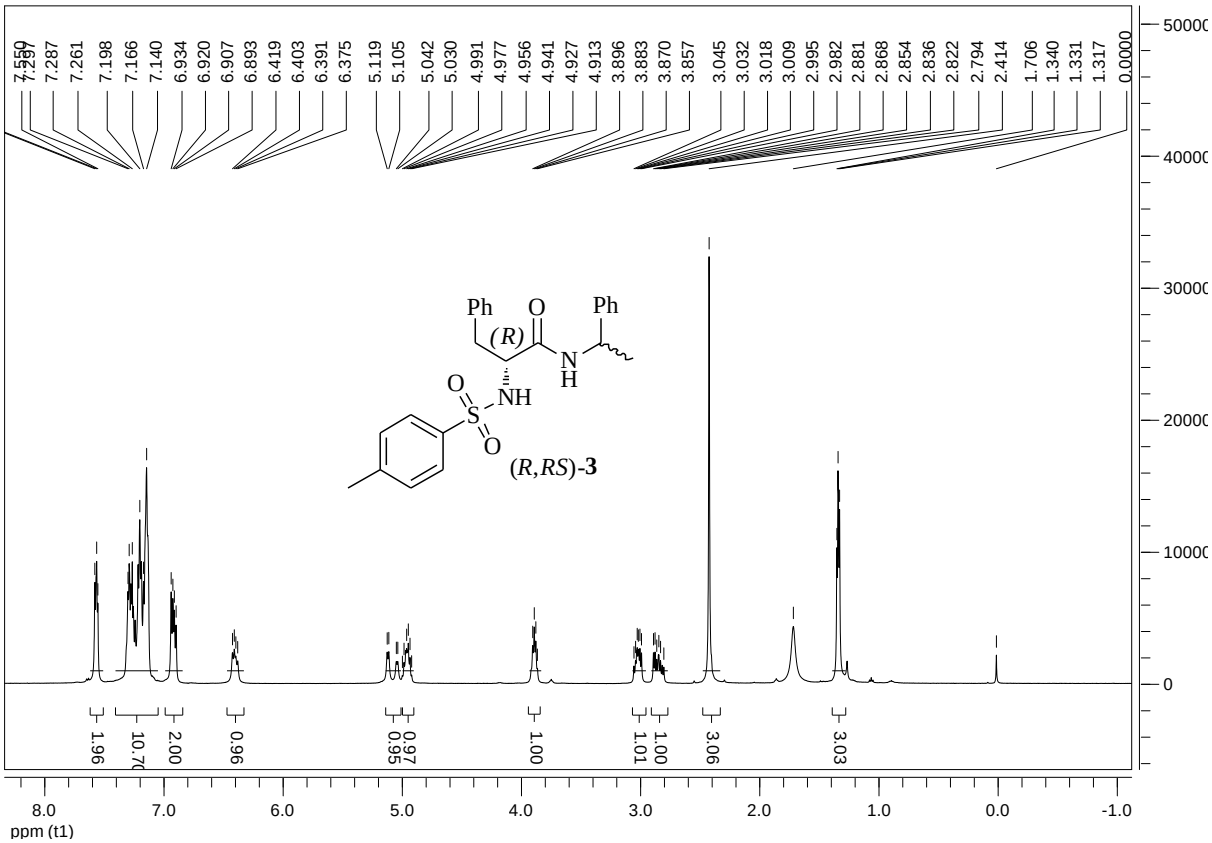
Copy of ^{1}H and ^{13}C spectra of all catalysts

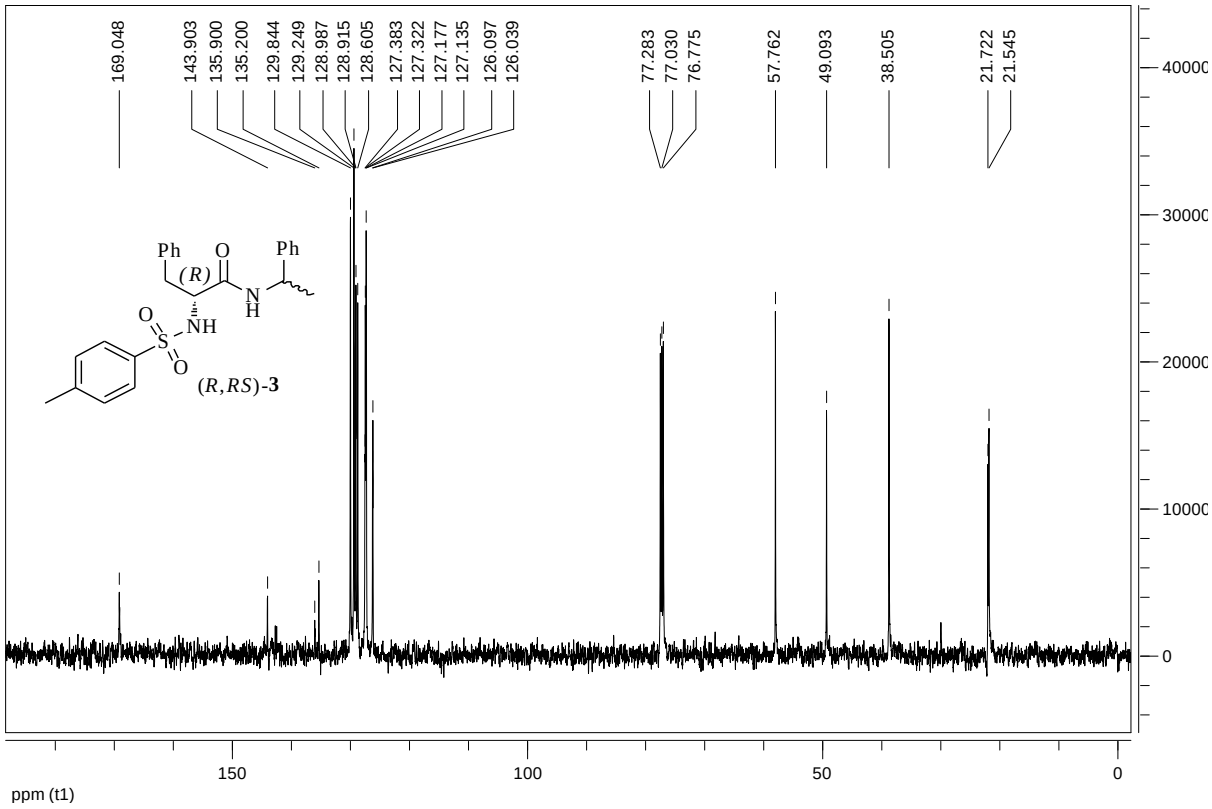


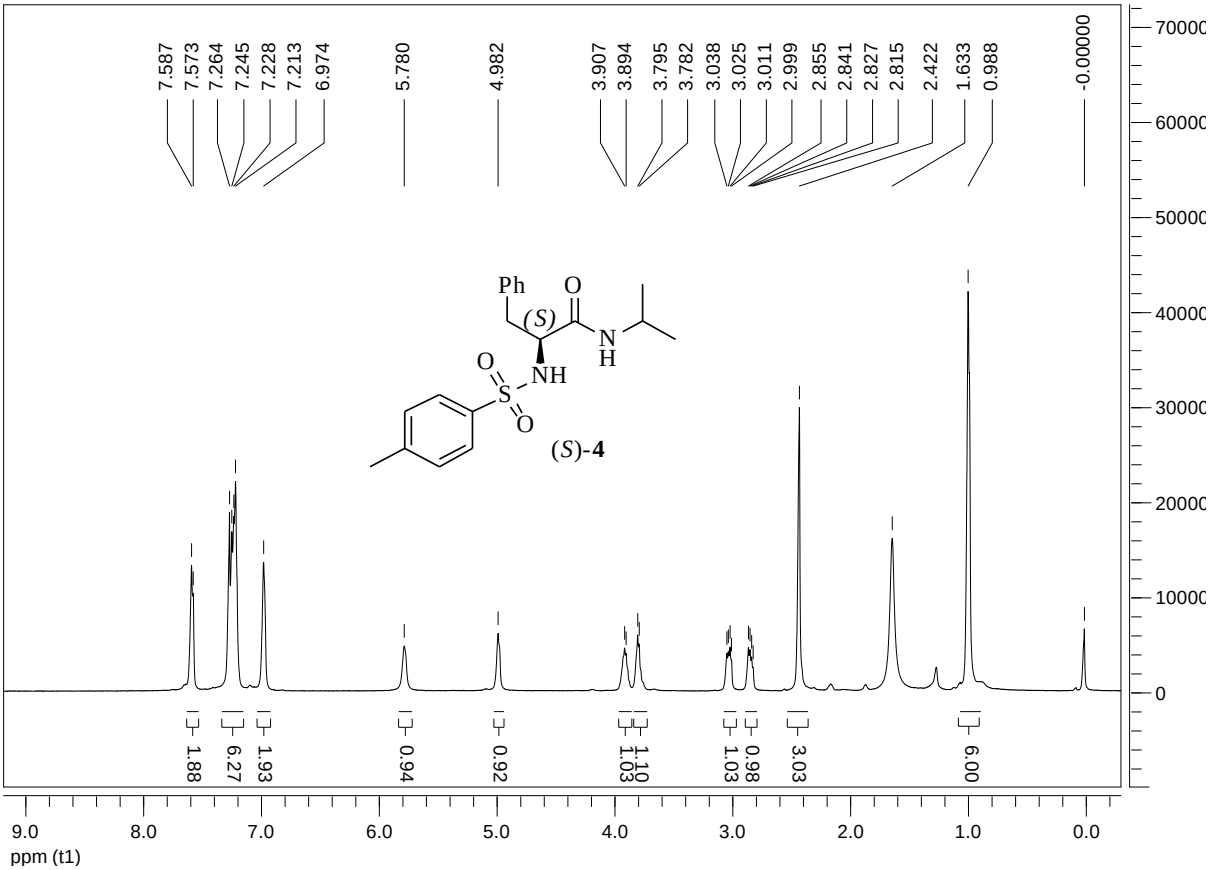


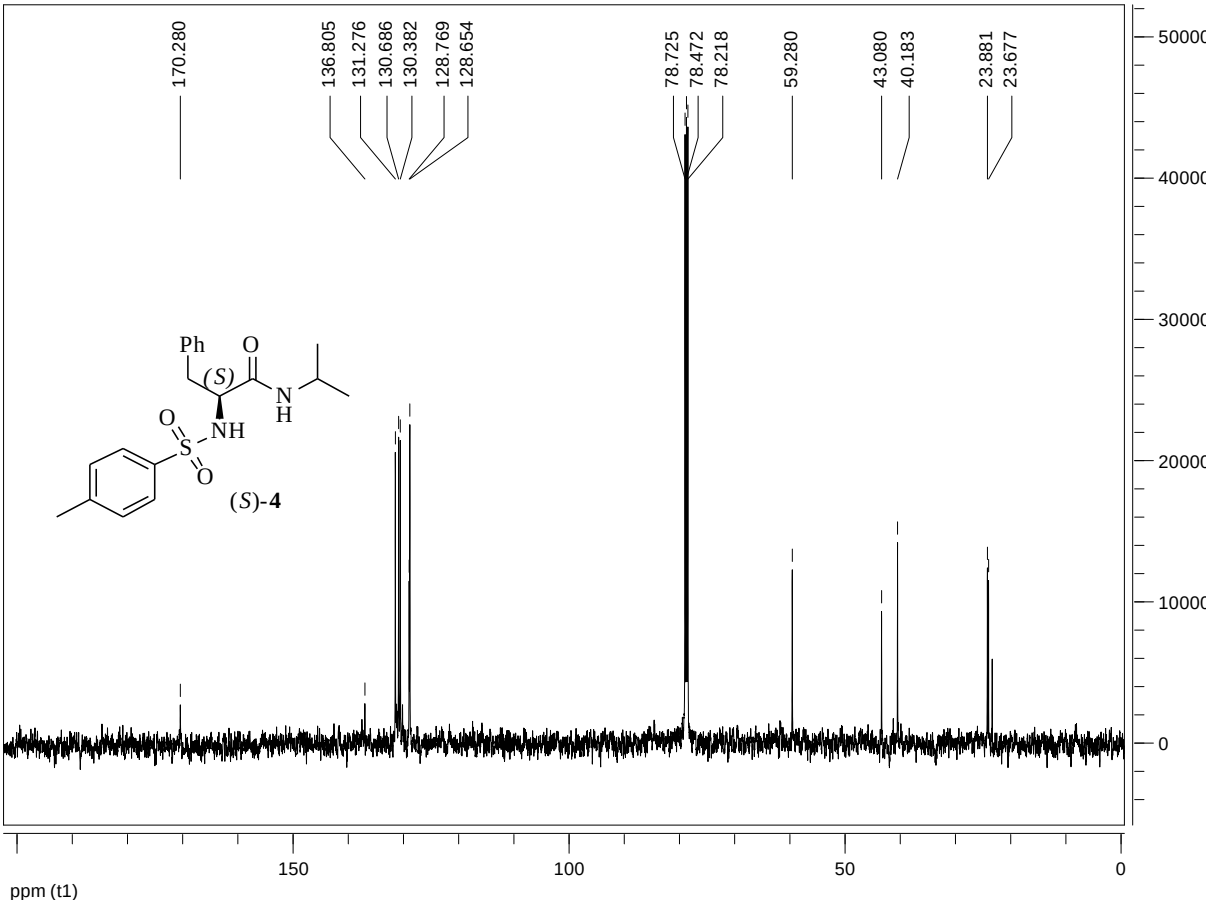


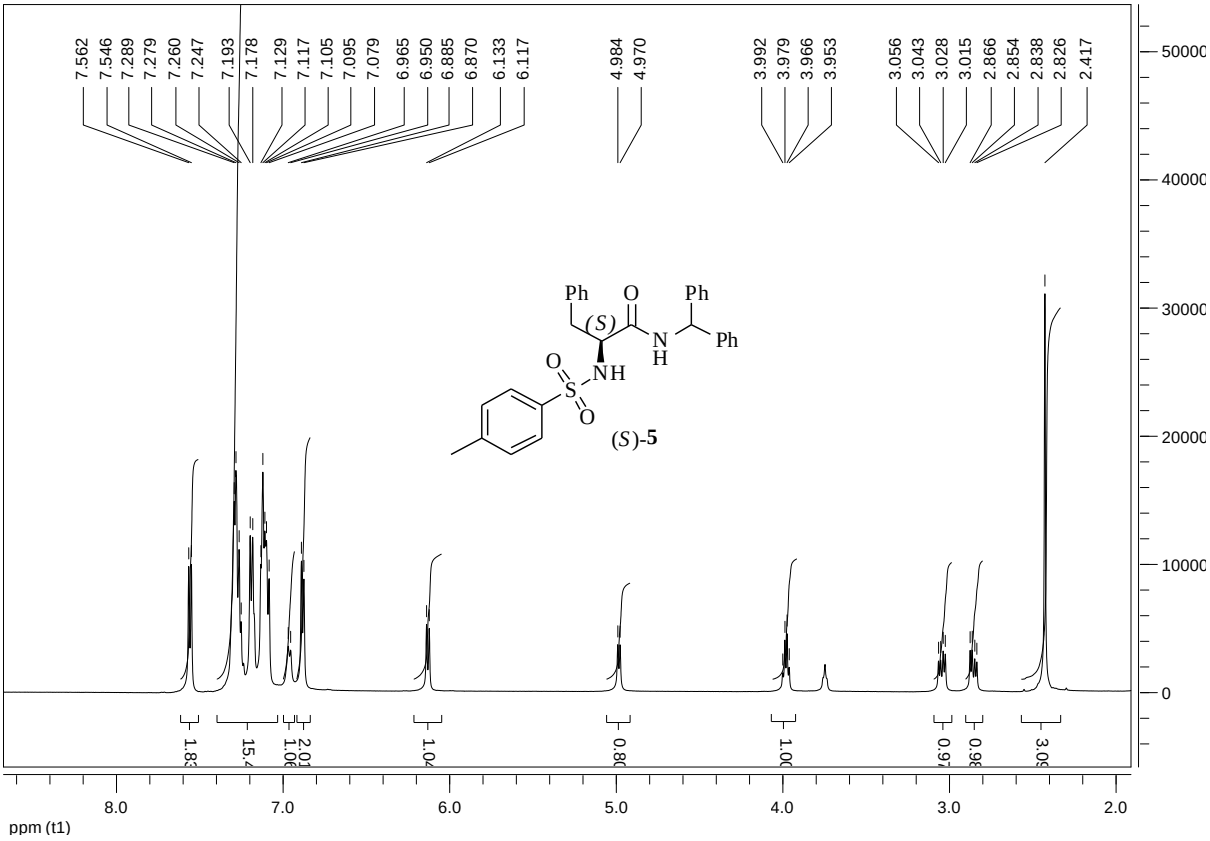


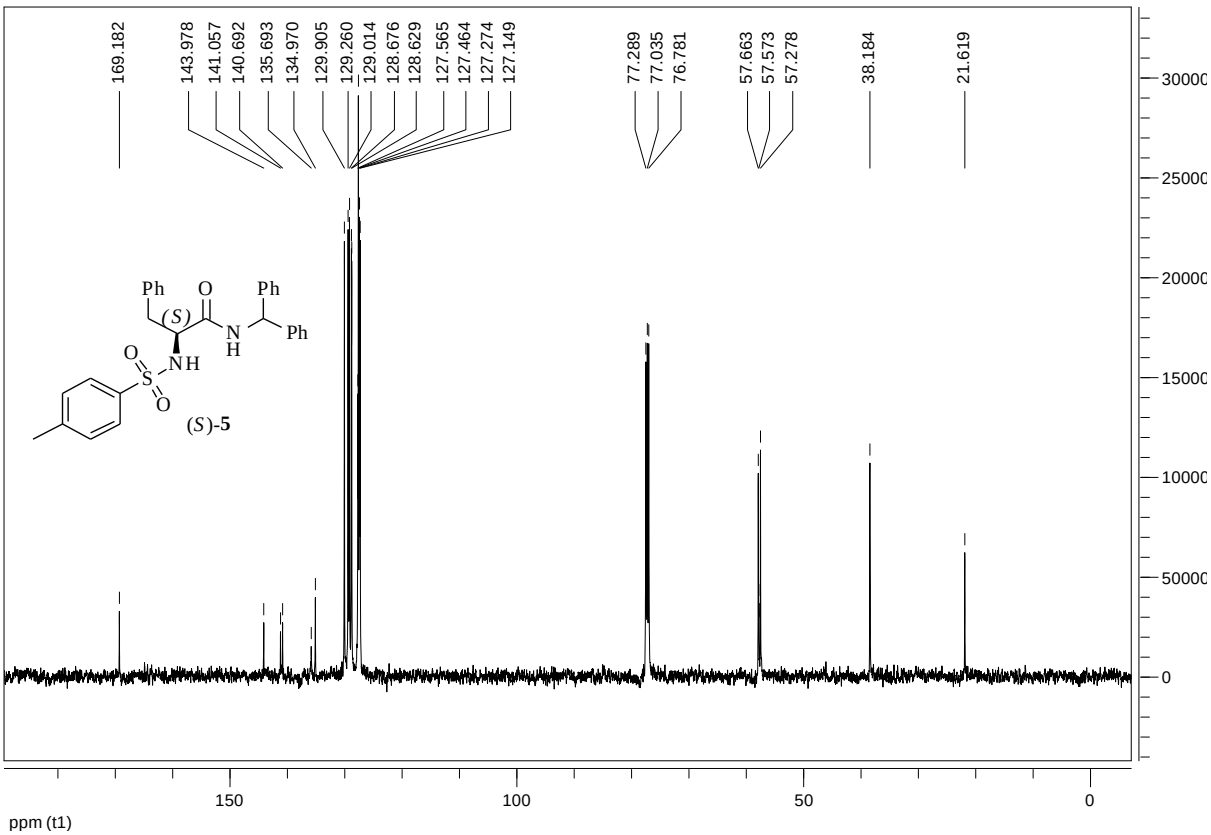


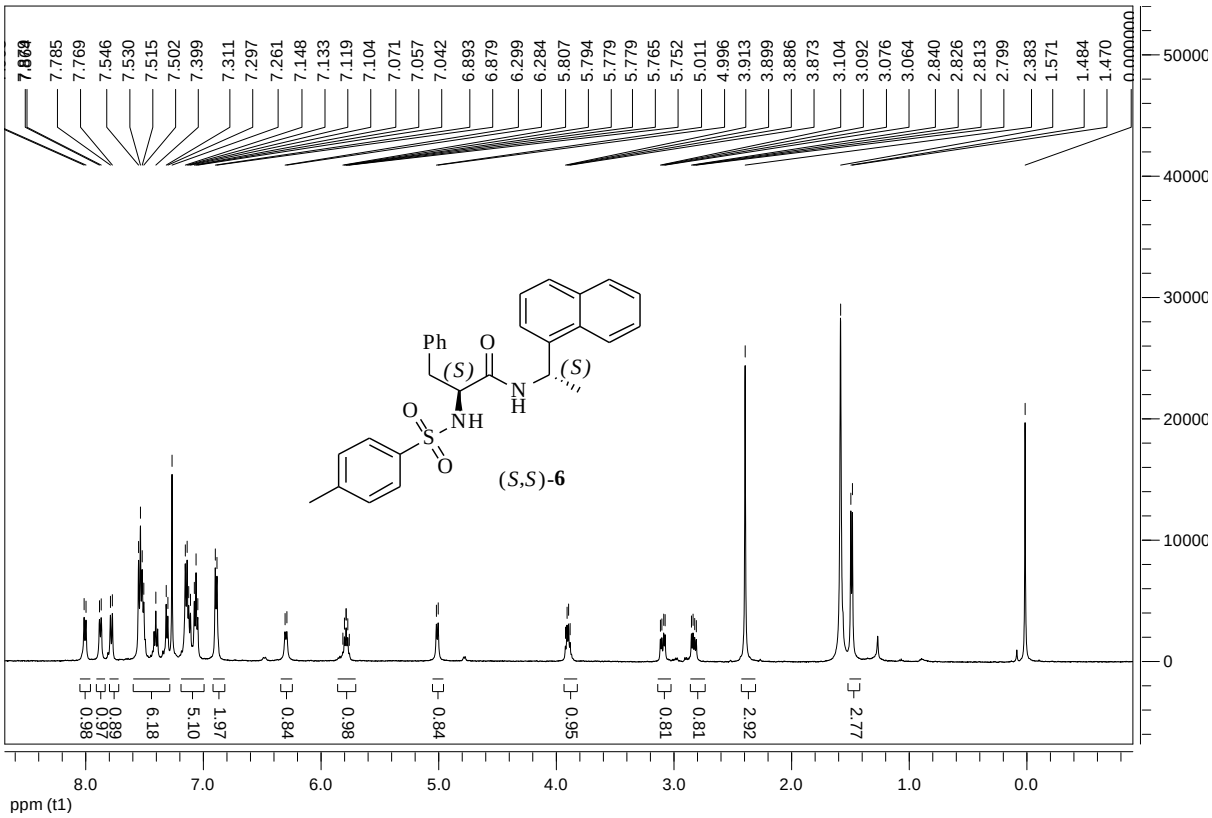


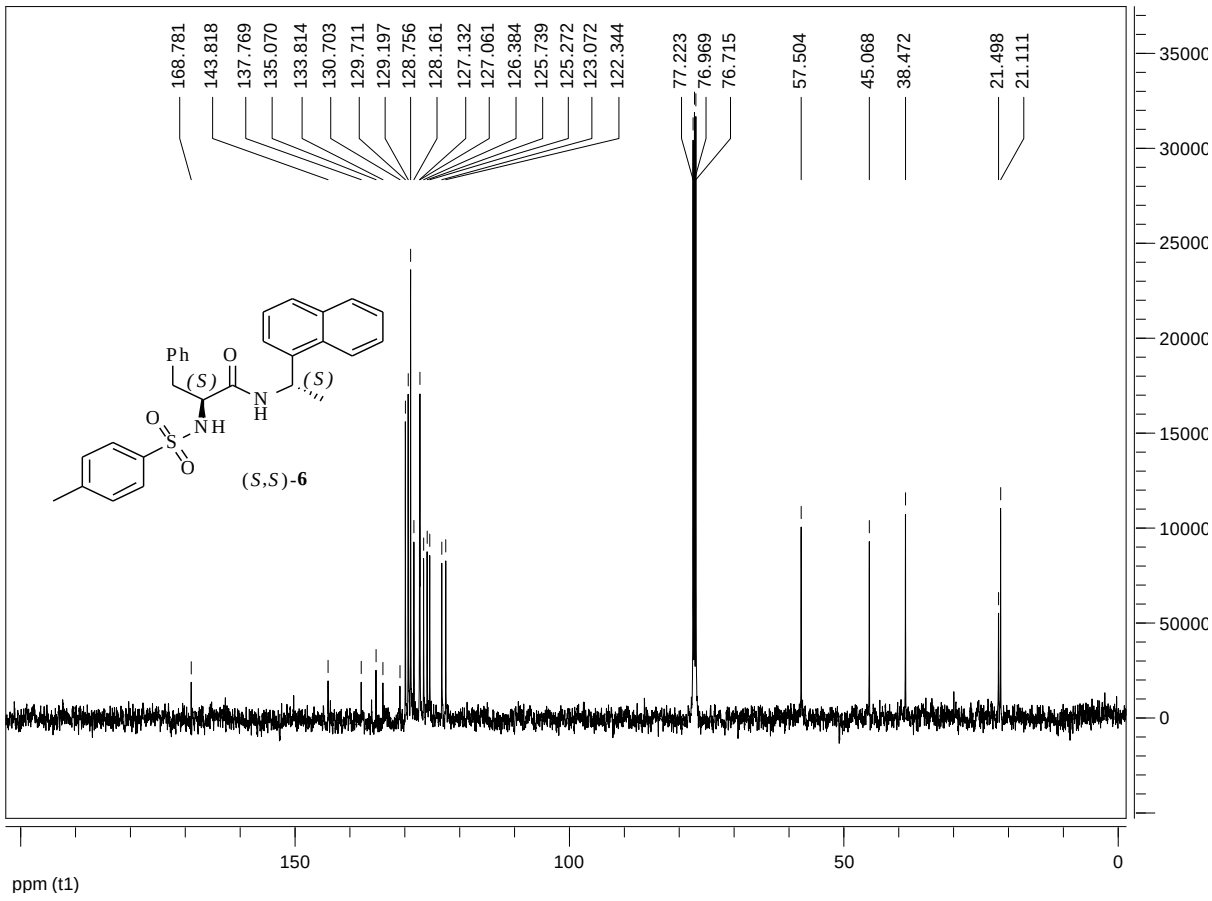




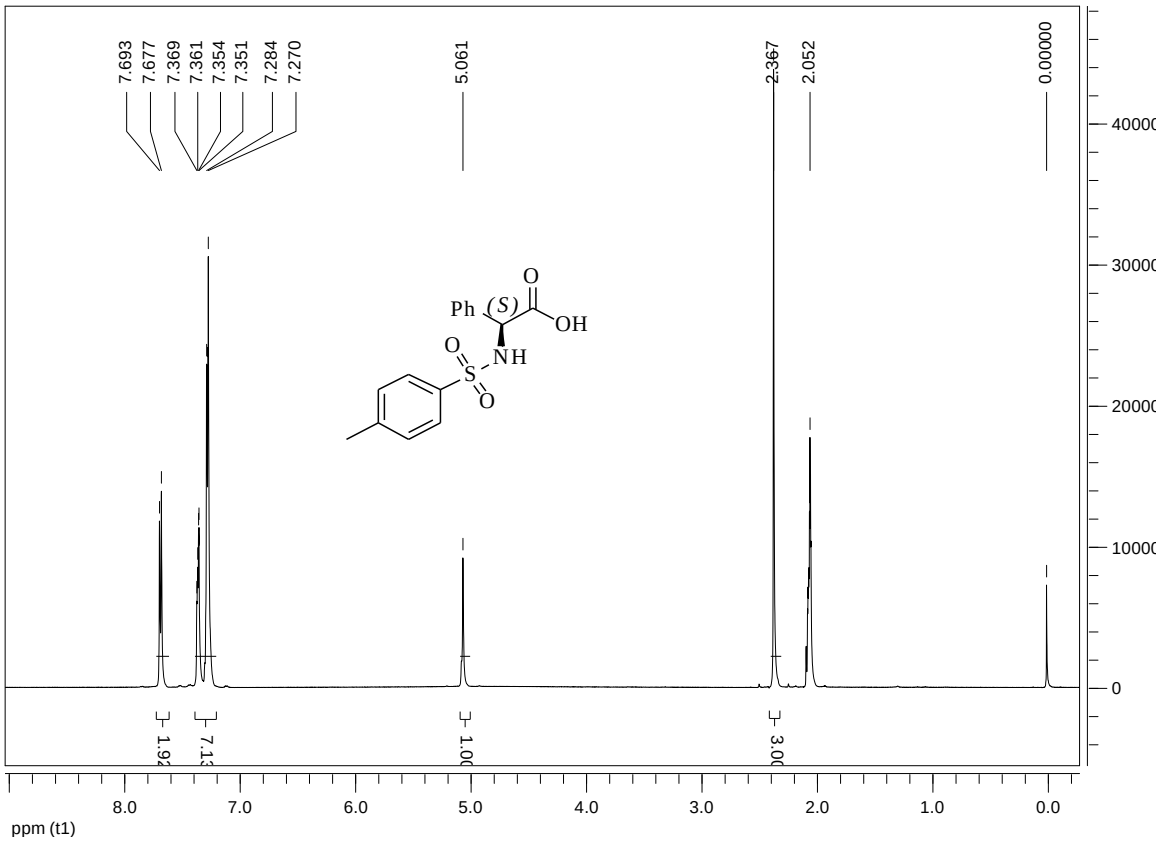


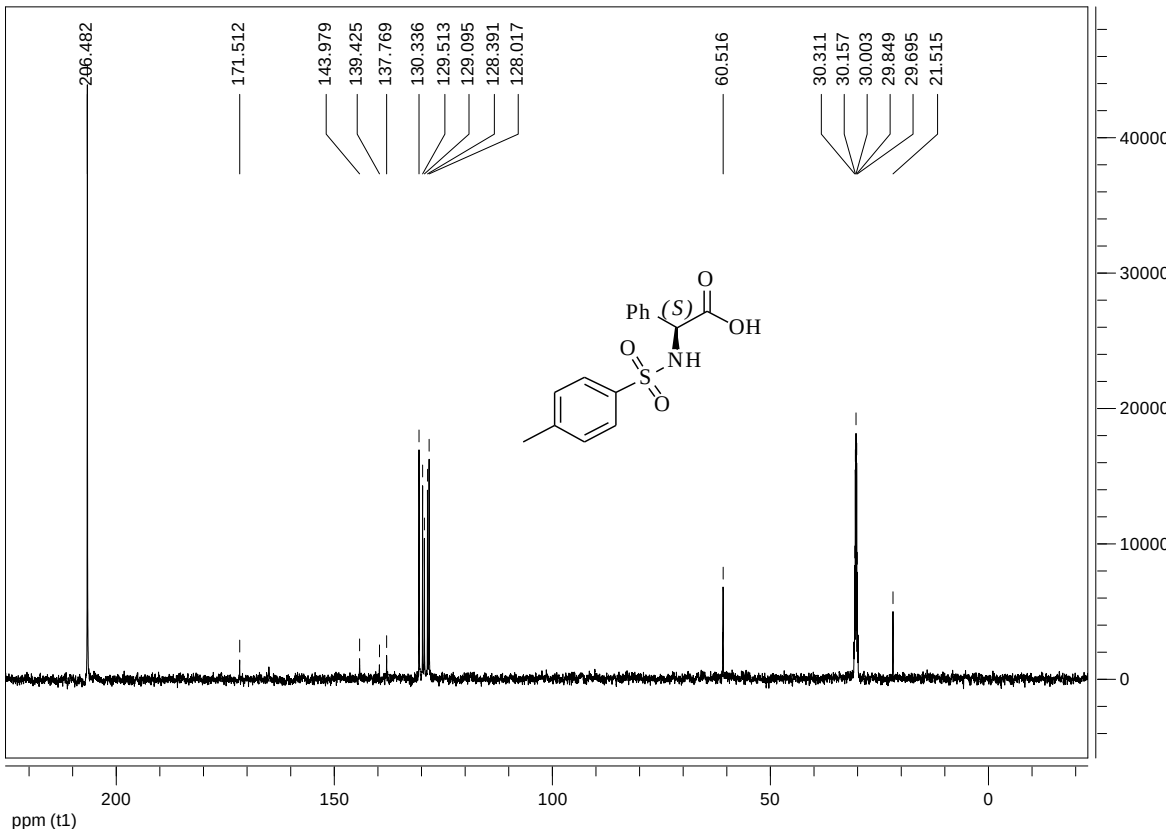


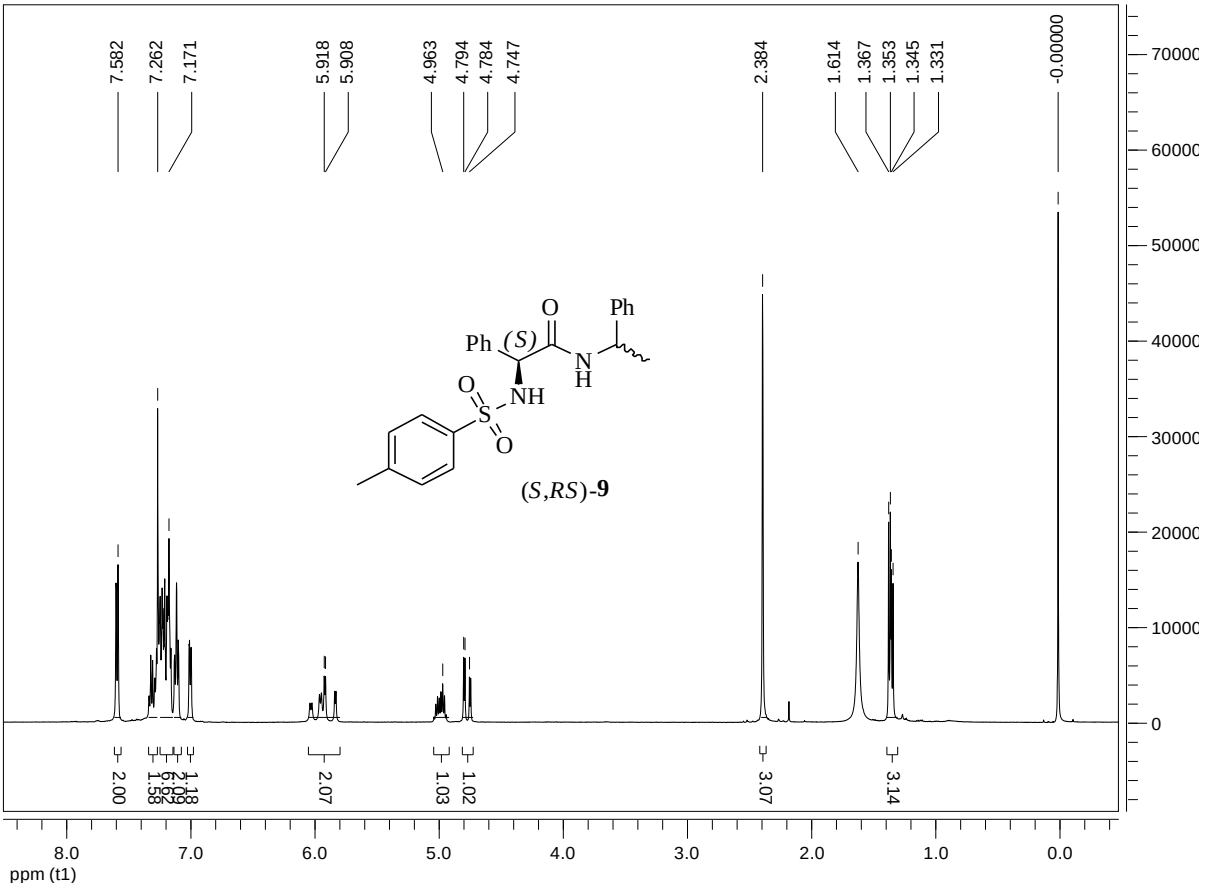


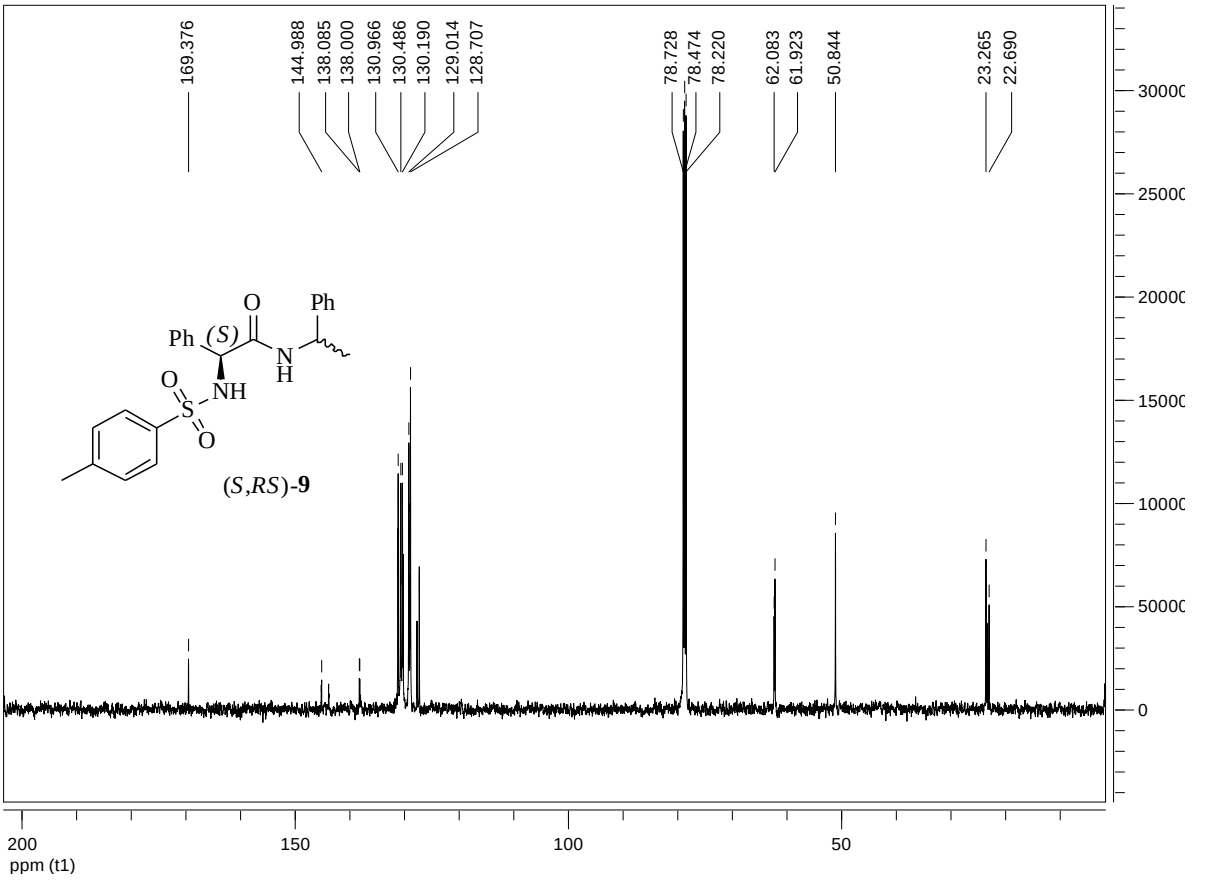


Copy of ^{1}H and ^{13}C spectra of pre-catalyst: N-tosyl-protected L-phenylglycine

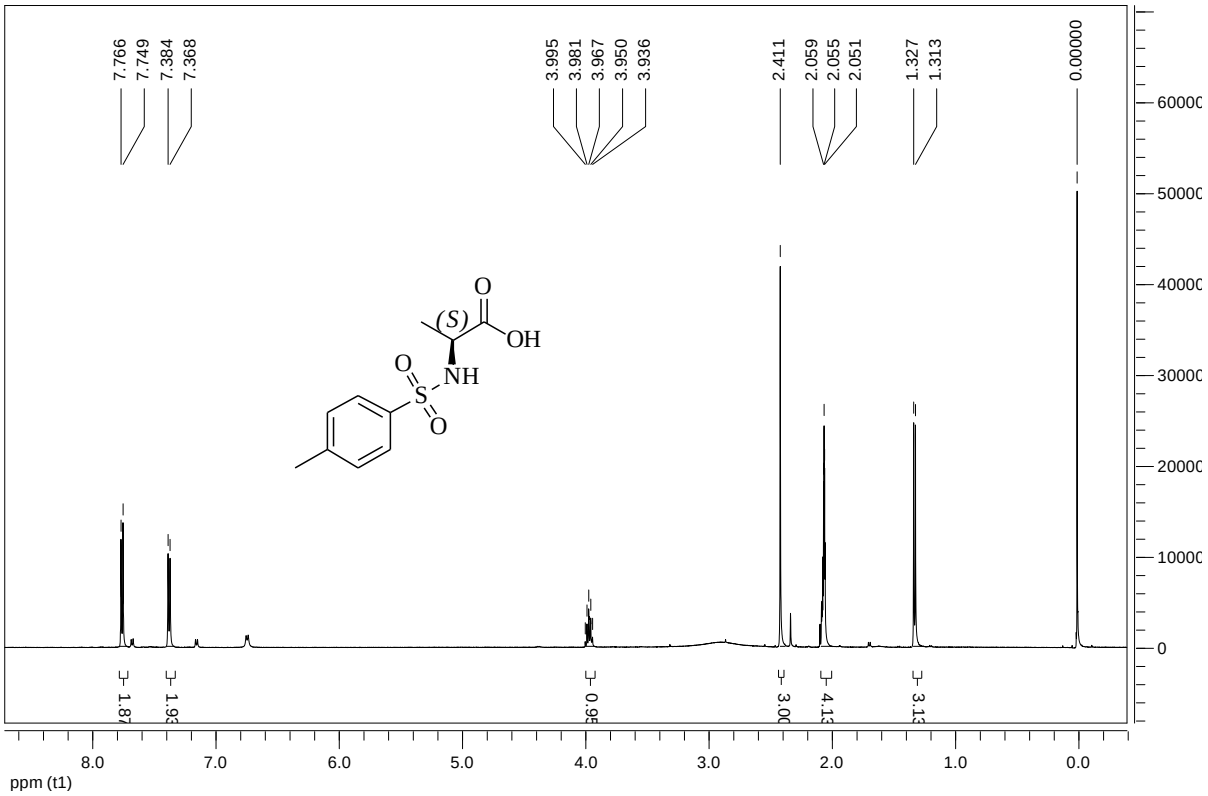


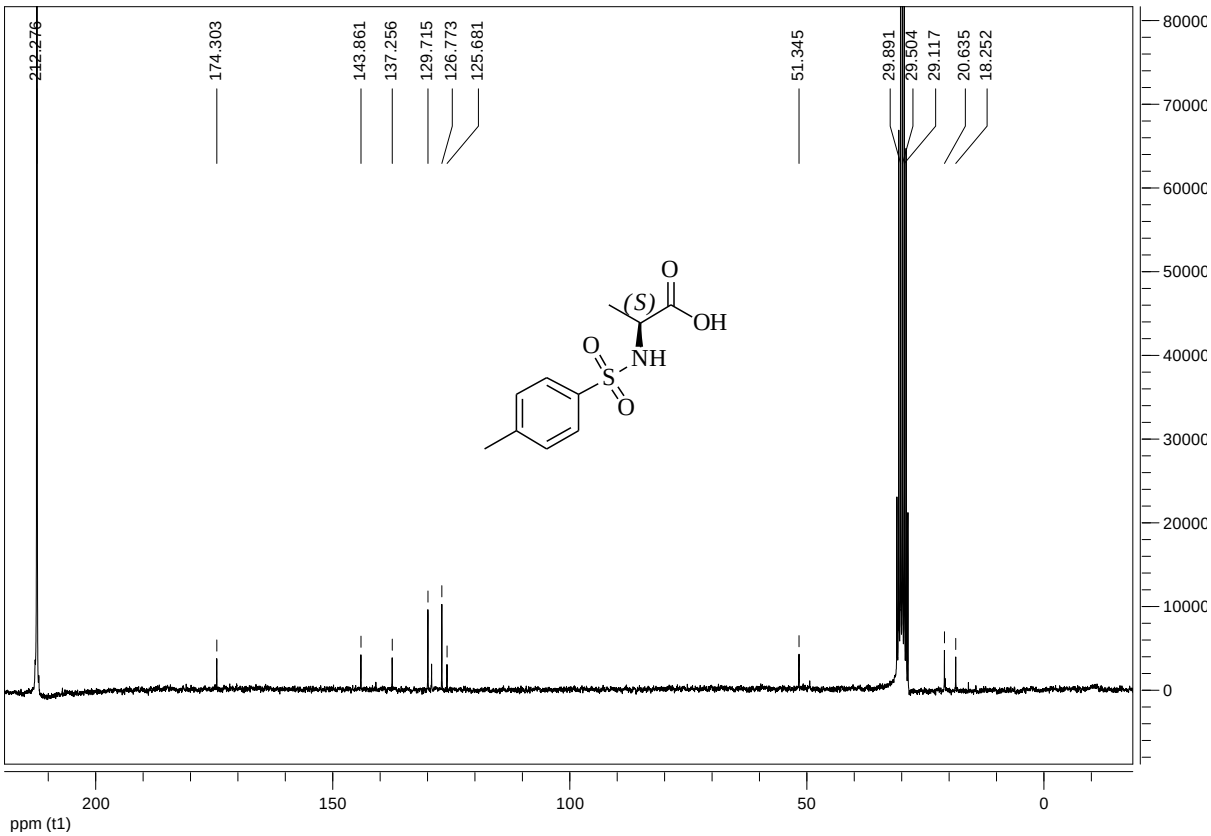


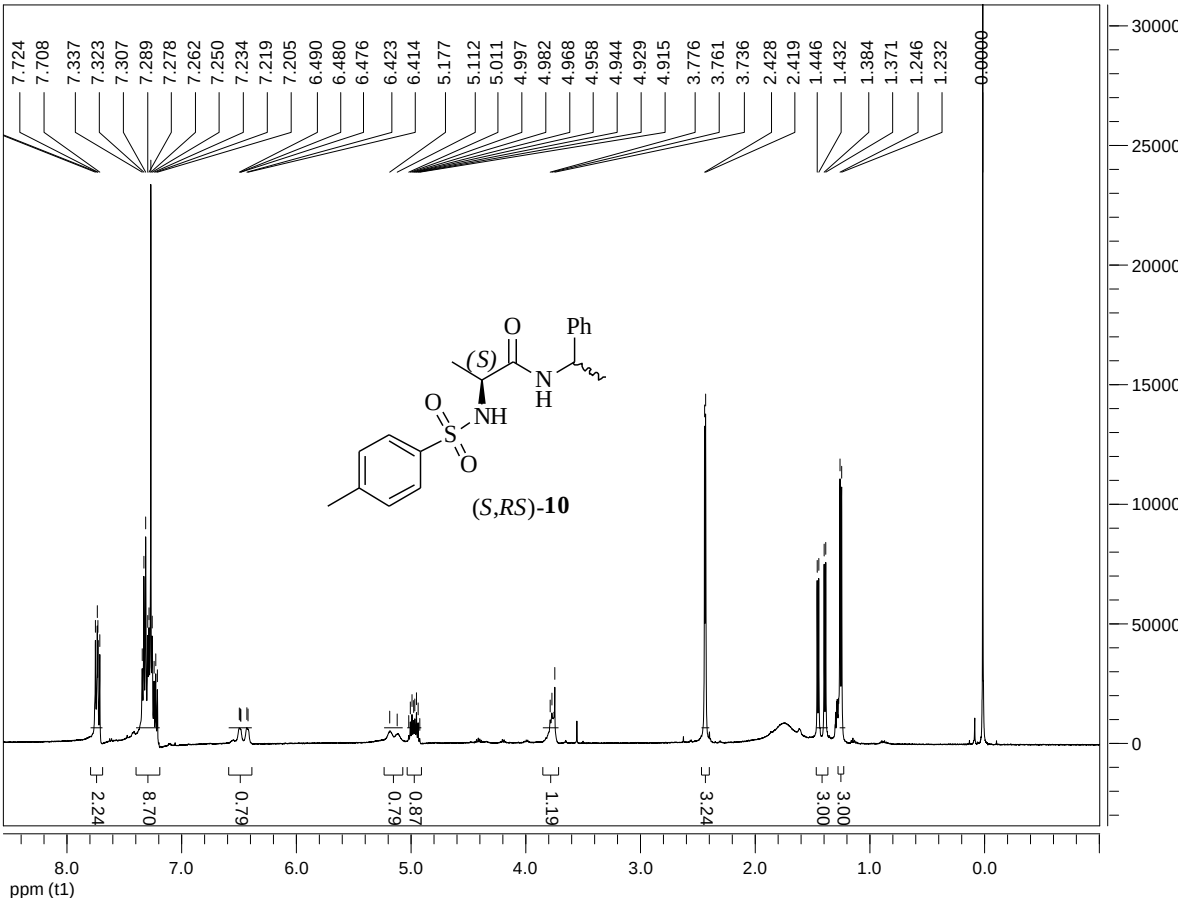


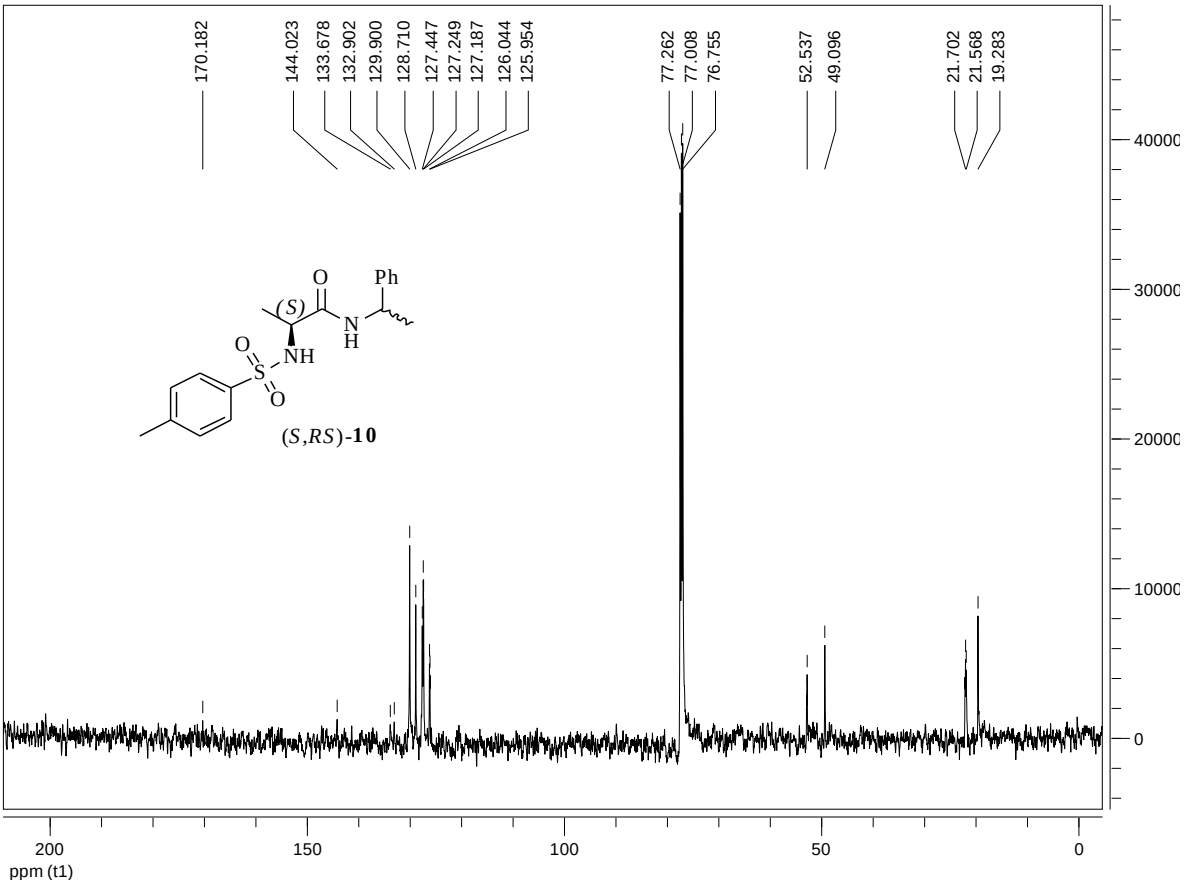


Copy of ^{1}H and ^{13}C spectra of pre-catalyst: N-tosyl protected L-alanine



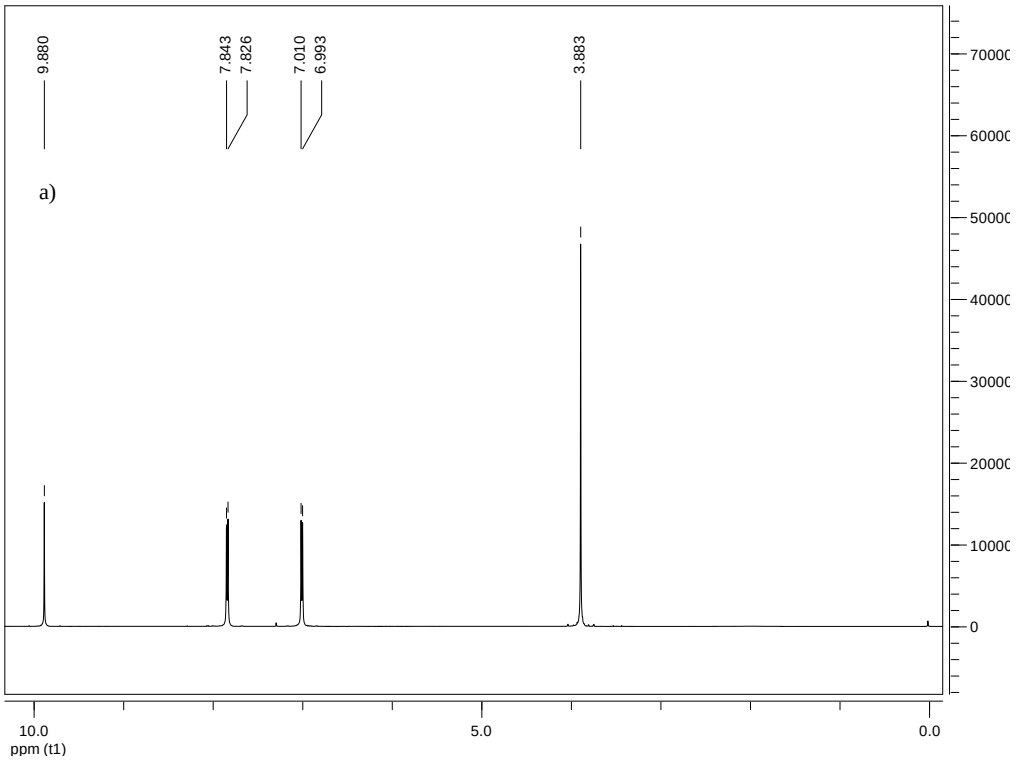




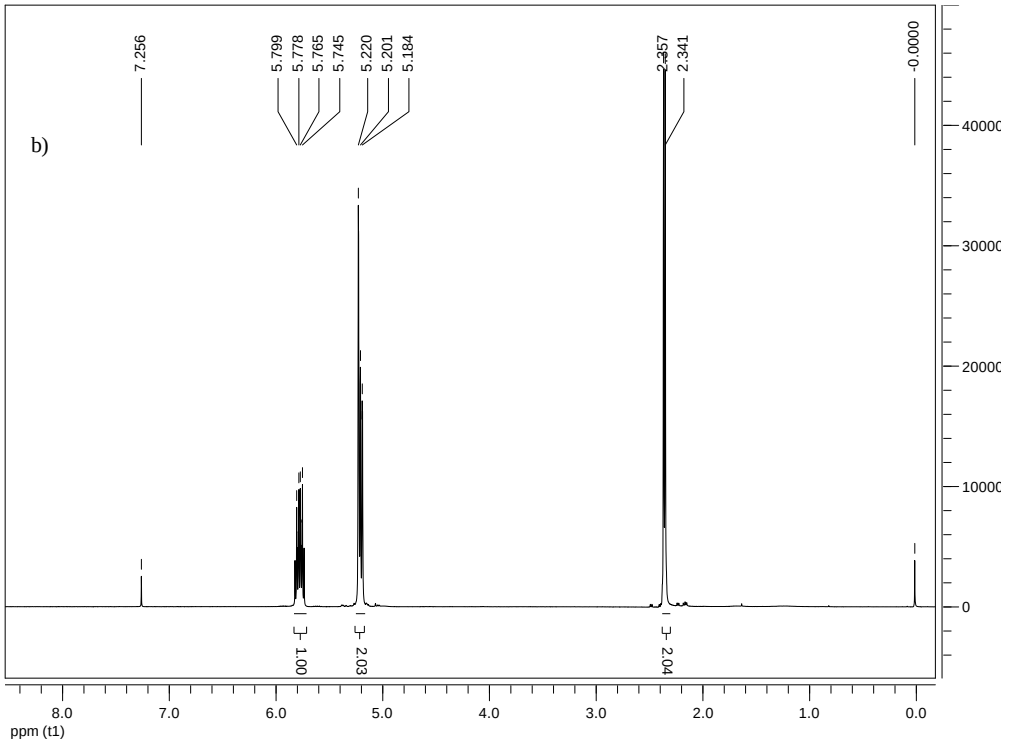


NMR experiments for mechanistic interpretation

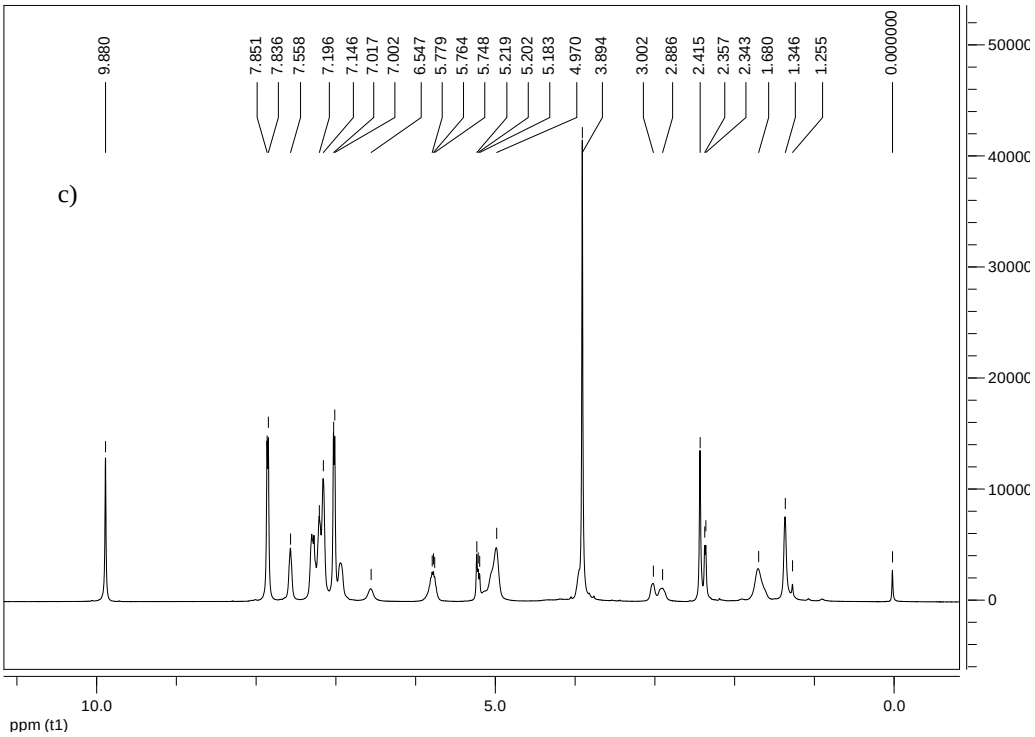
a) ^{1}H spectrum of 4-MeO-benzaldehyde taken in $CDCl_3$



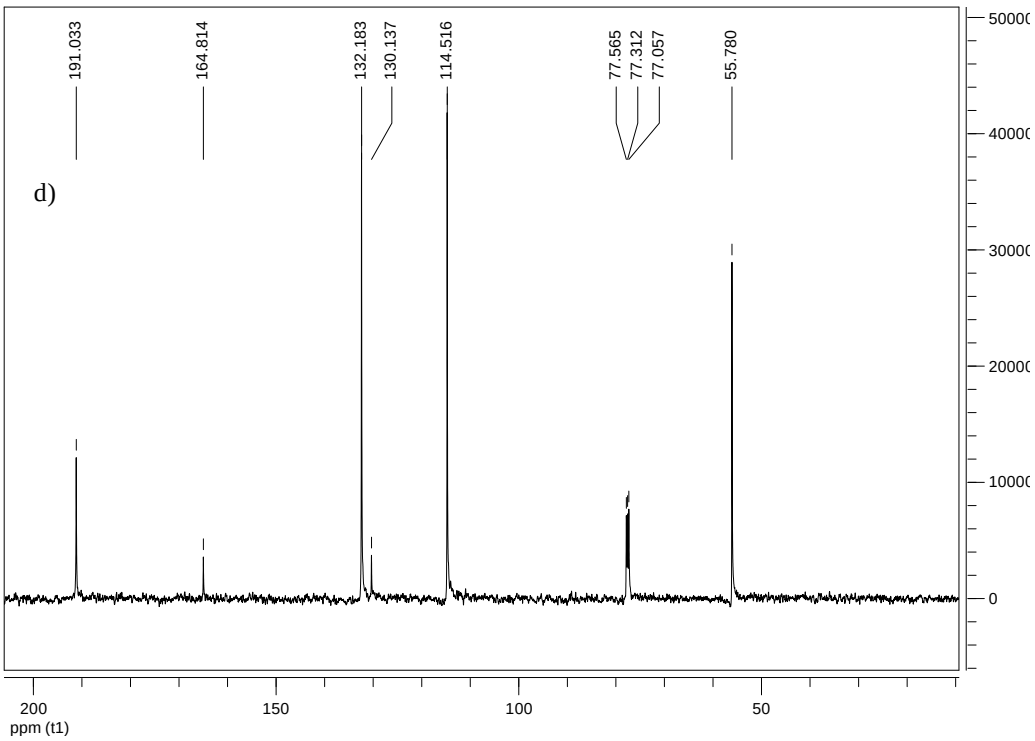
b) ^{1}H spectrum of allyltrichlorosilane taken in $CDCl_3$



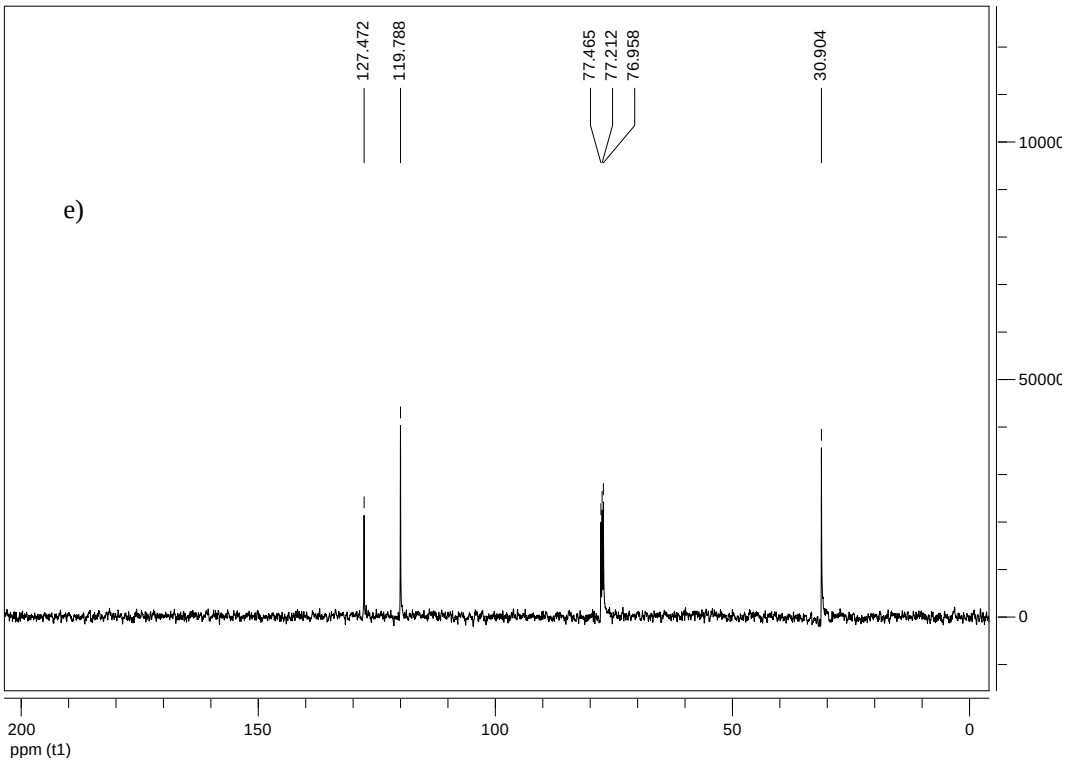
c) ^{1}H spectrum of catalyst (*S,RS*)-**3** after interaction with allyltrichlorosilane and 4-MeO-benzaldehyde (in $CDCl_3$)



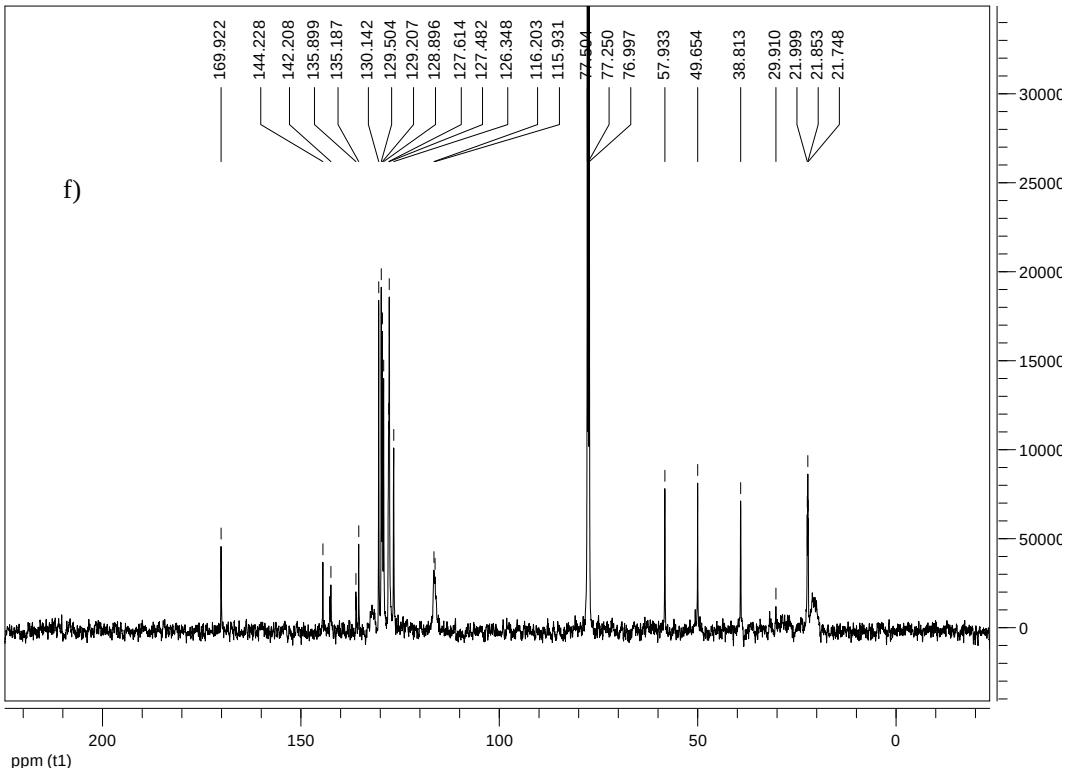
d) ^{13}C spectrum of 4-MeO-benzaldehyde taken in $CDCl_3$



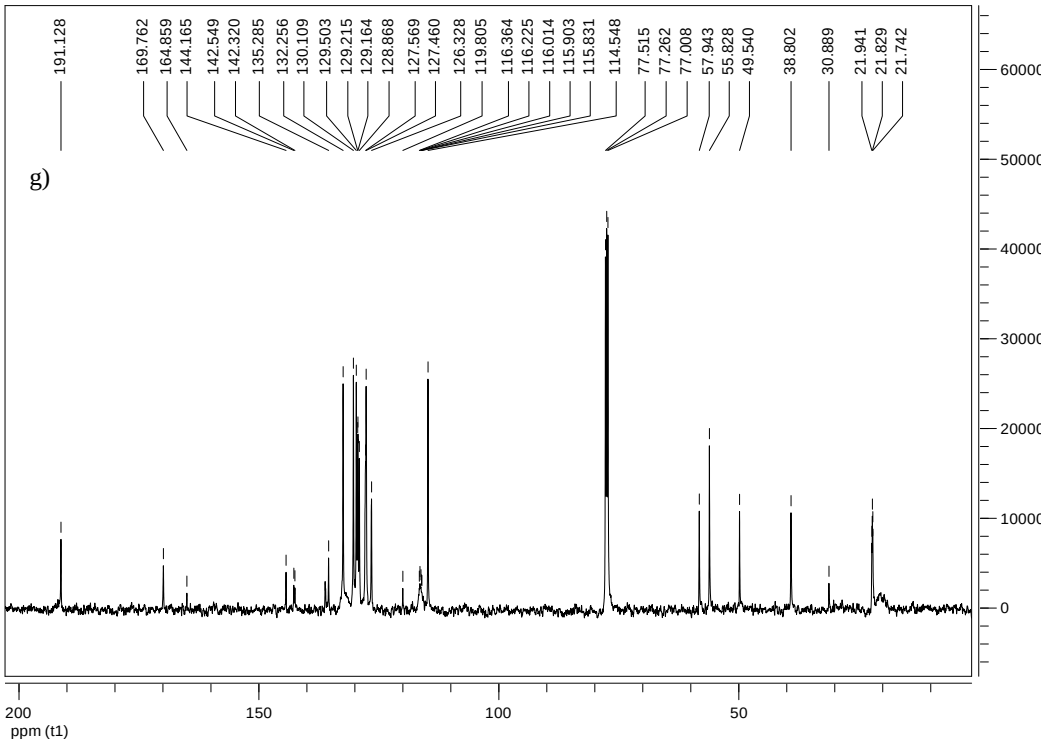
e) ^{13}C spectrum of allyltrichlorosilane taken in $CDCl_3$



f) ^{13}C spectrum of catalyst (*S*,*RS*)-**3** after interaction with allyltrichlorosilane (in $CDCl_3$)



g) ^{13}C spectrum of catalyst (*S*,*RS*)-**3** after interaction with allyltrichlorosilane and 4-MeO-benzaldehyde (in $CDCl_3$)



Quantum chemical calculation details:

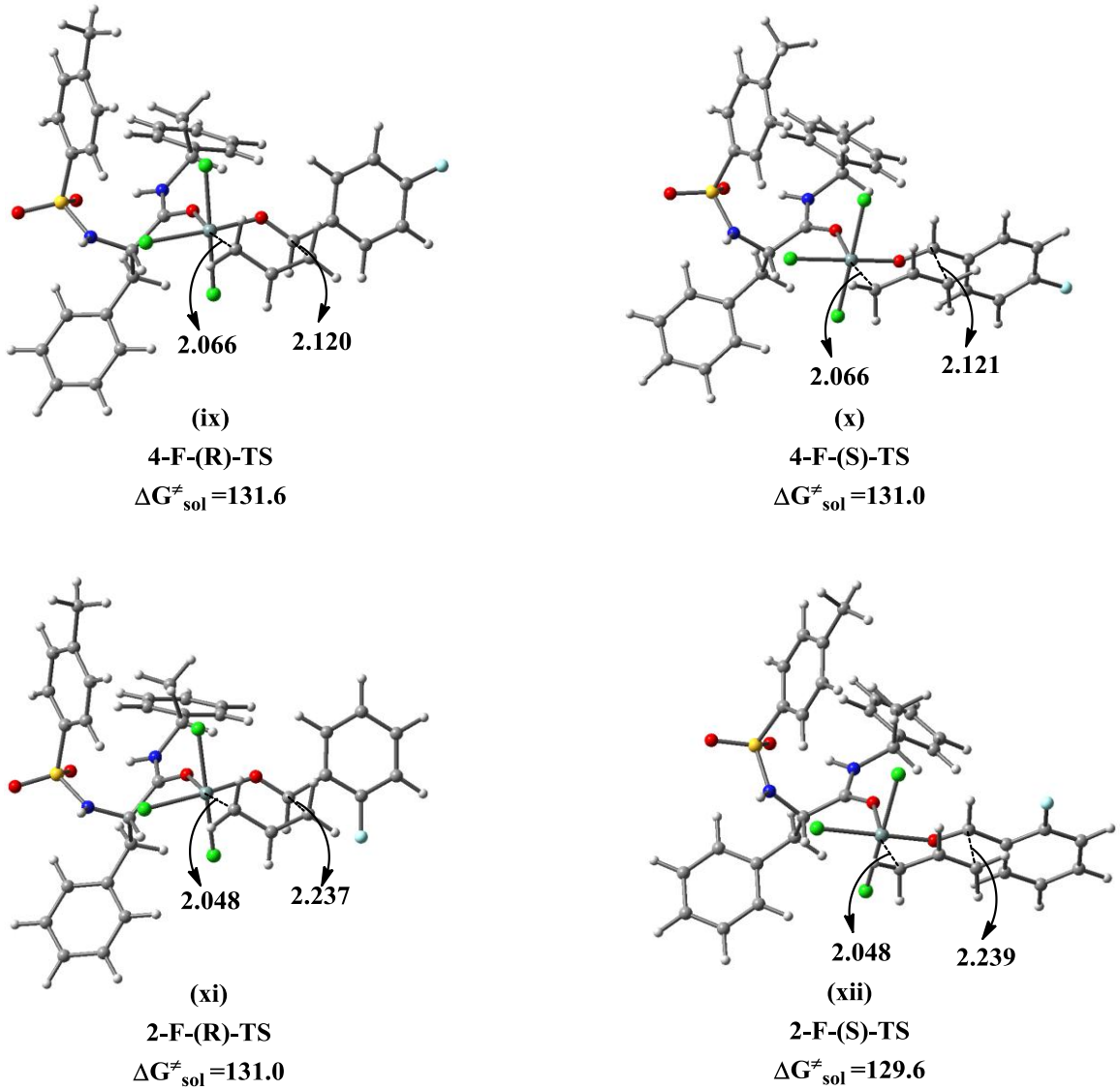


Figure I: PBEPBE/6-31G(d) optimized transition state geometries and corresponding their free energy of activation (kJ/mole) from reactants to transition state in CH_2Cl_2 solvent catalyzed by catalyst (*S*,*R*)-**3**. All distances are in Å. [Gray = carbon; white = hydrogen; red = oxygen; blue = nitrogen; yellow = sulfur; green = chlorine; greenish blue = silicon; sky blue = fluorine].

Table I. PBEPBE/6-31G(d) and B97D/6-31G//PBEPBE/6-31G(d) calculated electronic energy difference (kJ/mol) between *R* and *S* transition states for fluoro substituted benzaldehydes.

Substance	PBEPBE/6-31G(d)	B97D/6-31G//PBEPBE/6-31G(d)
para-flurobenzaldehyde$_{\Delta E^*}$	0.6	0.6

ortho-fluro benzaldehyde $_{\Delta E^*}$	0.7	0.9

$\Delta E^* = E_{R\text{-TS}} - E_{S\text{-TS}}$

Table II. Total electronic energies (kJ/mol) of all the systems calculated at the PBEPBE/6-31G(d) level of theory in gas phase and solvent phase.

Substance	E_{Gas} (Hartree)	E_{Sol}(Hartree)
para-fluro benzaldehyde	-444.29522132	-444.30585396
ortho-fluro benzaldehyde	-444.29295398	-444.30316666
para-methoxy benzaldehyde	-459.54272588	-459.55584222
ortho-methoxy benzaldehyde	-459.53891804	-459.55164121
allyltrichlorosillanes	-1786.61477272	-1786.62601104
Catalyst(*S*,*S*)-3	-1661.79787308	-1661.83383009
TS-*para*-Fluoro(*R*)	-3892.70770480	-3892.76282779
TS-*para*-Fluoro(*S*)	-3892.70797212	-3892.76305621
TS-*ortho*-Fluoro(*R*)	-3892.70753792	-3892.7621240
TS-*ortho*-Fluoro(*S*)	-3892.70769761	-3892.7623876
TS-*para*-methoxy(*R*)	-3907.95480456	-3908.01236640
TS-*para*-methoxy(*S*)	-3907.95523555	-3908.01259639
TS-*ortho*-methoxy(*R*)	-3907.95395382	-3908.01080620
TS-*ortho*-methoxy(*S*)	-3907.95375423	-3908.01085911
PC-*para*-methoxy(*R*)	-3907.98760439	-3908.04629692
PC-*para*-methoxy(*S*)	-3907.98740713	-3908.04700549

Table III. PBEPBE/6-31G(d) calculated Gibbs free energies (kJ/mol) for all the systems in gas phase.

Substance	G_{gas}(Hartree)
para-fluro benzaldehyde	-444.228049
ortho-fluro benzaldehyde	-444.225626
para-methoxy benzaldehyde	-459.437771
ortho-methoxy benzaldehyde	-459.433868
allyltrichlorosillanes	-1786.576841
Catalyst(*S*,*S*)-3	-1661.415370
TS-*para*-Fluoro(*R*)	-3892.168201
TS-*para*-Fluoro(*S*)	-3892.168416
TS-*ortho*-Fluoro(*R*)	-3892.167264
TS-*ortho*-Fluoro(*S*)	-3892.168144
TS-*para*-methoxy(*R*)	-3907.377576
TS-*para*-methoxy(*S*)	-3907.378858
TS-*ortho*-methoxy(*R*)	-3907.376395
TS-*ortho*-methoxy(*S*)	-3907.376791
PC-*para*-methoxy(*R*)	-3907.413025
PC-*para*-methoxy(*S*)	-3907.413932

Table IV. Coordinates for the structures optimized at the PBEPBE/6-31G(d) level of theory.

ortho-fluoro benzaldehyde				*para*-fluoro benzaldehyde			
	Coordinates				Coordinates		
at. no.	x	y	z	at. no.	x	y	z
6	-0.382366	0.966771	0.000099	6	0.156648	1.353469	0.000574
6	0.539253	-0.097363	-0.000070	6	0.996155	0.222173	-0.000357
6	0.028429	-1.413076	-0.000157	6	0.428737	-1.070471	0.000400
6	-1.347015	-1.647642	-0.000057	6	-0.955674	-1.233532	0.000336
6	-2.240330	-0.560124	0.000073	6	-1.764332	-0.087067	-0.000250
6	-1.763168	0.757145	0.000121	6	-1.233315	1.208442	0.000091
6	2.004417	0.133733	0.000143	6	2.465881	0.389068	-0.000277
8	2.833042	-0.772576	0.000088	8	3.275068	-0.533022	-0.000144
1	-2.437339	1.617701	0.000342	1	0.602303	2.355283	0.000375
1	-1.731643	-2.671810	-0.000233	1	-1.908208	2.068296	-0.000316
1	0.755818	-2.231245	-0.000231	1	-1.424653	-2.221211	0.000476
1	2.322308	1.205137	0.000030	1	1.103938	-1.931887	-0.000065
1	-3.320579	-0.737615	0.000228	1	2.809948	1.460044	0.000136
9	0.079087	2.240197	-0.000195	9	-3.105386	-0.239871	-0.000284

ortho-methoxy benzaldehyde				*para*-methoxy benzaldehyde			
	Coordinates				Coordinates		
at. no.	x	y	z	at. no.	x	y	z
6	-1.215582	1.205293	-0.000006	6	-0.841449	1.048923	0.000033
6	-0.660923	-0.089337	0.000057	6	0.535776	1.293281	0.000013
6	0.752856	-0.250721	0.000130	6	1.463005	0.236082	-0.000025
6	1.573343	0.893006	0.000059	6	0.986560	-1.095776	-0.000041
6	1.026542	2.177245	-0.000011	6	-0.376386	-1.356409	-0.000021
6	-0.370006	2.323244	-0.000040	6	-1.301695	-0.284340	0.000017
1	-2.298515	1.349585	-0.000015	1	-1.543065	1.886274	0.000060
1	2.655496	0.725753	0.000116	1	0.902139	2.327329	0.000026
1	1.675089	3.058375	-0.000023	1	1.720322	-1.908016	-0.000070
1	-0.816135	3.323597	-0.000070	1	-0.767884	-2.377881	-0.000032
6	1.389166	-1.589898	0.000233	6	2.910613	0.515650	-0.000046
8	2.606927	-1.763707	-0.000369	8	3.793943	-0.338232	-0.000083
1	0.686519	-2.457997	-0.000453	1	3.168496	1.611375	-0.000033
8	-1.401371	-1.236886	0.000085	8	-2.614135	-0.650820	0.000031
6	-2.823883	-1.114749	0.000026	6	-3.596279	0.385902	0.000093
1	-3.184193	-0.587128	-0.902675	1	-3.515553	1.020332	-0.902242
1	-3.207531	-2.144832	0.000023	1	-4.568307	-0.127164	0.000117
1	-3.184266	-0.587109	0.902688	1	-3.515484	1.020290	0.902451

Allyltrichlorosilanes				Catalyst(*S*,*S*)-**3**			
	Coordinates				Coordinates		
at. no.	x	y	z	at. no.	x	y	z
6	3.400841	-0.286515	-0.327104	7	-1.638904	1.033610	0.521241
6	2.358585	0.510600	-0.613007	6	-1.826035	-0.324950	1.097666

1	3.398370	-1.353727	-0.576947	6	-0.530365	-0.984103	1.642729
1	4.297093	0.102382	0.165227	7	0.349931	-1.463794	0.716471
1	2.400044	1.573303	-0.340913	6	1.589774	-2.136991	1.135514
6	1.086384	0.050070	-1.270326	8	-0.376892	-1.129072	2.862522
1	0.782605	0.723405	-2.094860	6	2.634524	-2.068502	0.033171
1	1.192459	-0.965684	-1.693528	6	2.339192	-2.481587	-1.281382
14	-0.372283	-0.009946	-0.076880	6	3.936597	-1.621137	0.319599
17	-2.100139	-0.500540	-1.112324	6	3.316426	-2.432118	-2.285060
17	-0.067957	-1.426043	1.397606	6	4.921413	-1.585047	-0.678094
17	-0.651520	1.833326	0.825304	6	4.612215	-1.985178	-1.985989
				6	1.298203	-3.588893	1.565162
				16	-0.715482	1.332490	-0.882789
				8	-0.435406	0.076008	-1.642543
				8	-1.407619	2.454946	-1.554837
				6	0.850012	1.902784	-0.214456
				6	2.036594	1.485704	-0.830650
				6	0.865271	2.835403	0.834941
				6	3.255239	2.005758	-0.376337
				6	2.091527	3.341656	1.272514
				6	3.304932	2.936941	0.677022
				6	4.623378	3.472354	1.182325
				6	-2.656287	-1.296718	0.207334
				6	-4.042999	-0.759691	-0.075138
				6	-4.307826	-0.015189	-1.242477
				6	-5.086280	-0.945352	0.854499
				6	-5.581151	0.526939	-1.473476

	6	-6.359215	-0.408329	0.623880
	6	-6.609949	0.331811	-0.541671
	1	0.228197	-1.199520	-0.267130
	1	1.961908	-1.592254	2.022390
	1	1.334845	-2.845567	-1.527615
	1	4.177687	-1.293542	1.337289
	1	3.065534	-2.748966	-3.302690
	1	5.931087	-1.238104	-0.433255
	1	5.377257	-1.952112	-2.768586
	1	0.558577	-3.586510	2.381417
	1	0.902700	-4.175993	0.718928
	1	2.221398	-4.075195	1.923138
	1	2.005642	0.753787	-1.641933
	1	-0.070743	3.139757	1.310543
	1	4.185224	1.669284	-0.846727
	1	2.110242	4.063820	2.096423
	1	5.434415	3.304967	0.455167
	1	4.566721	4.554410	1.390778
	1	4.916657	2.977274	2.126589
	1	-2.551636	1.472831	0.335341
	1	-2.400221	-0.129462	2.018855
	1	-2.114843	-1.480883	-0.734530
	1	-2.722493	-2.258211	0.748578
	1	-3.511422	0.128770	-1.981688
	1	-4.896733	-1.525931	1.765516
	1	-5.767515	1.100130	-2.387603

1	-7.158959	-0.571097	1.354172
1	-7.604814	0.751323	-0.723591

TS-*para*-fluoro(*S*) Coordinates				TS-*para*-fluoro(*R*) Coordinates			
at. no.	x	y	z	at. no.	x	y	z
6	-6.462524	-1.733493	-0.551708	7	2.341973	1.160484	0.147312
6	-5.558417	-0.704784	-0.213801	6	0.967277	1.454853	-0.309228
6	-5.806036	0.612409	-0.658056	6	0.176221	0.155168	-0.537768
6	-6.938992	0.897972	-1.422309	7	0.687127	-0.746455	-1.370392
6	-7.819554	-0.144467	-1.739269	6	0.088958	-2.072783	-1.644058
6	-7.599021	-1.460877	-1.317471	8	-0.984968	-0.053918	-0.037308
6	-4.344330	-1.027422	0.566207	6	1.141634	-3.149590	-1.399036
8	-3.390511	-0.149706	0.567695	6	2.194228	-3.371939	-2.307889
14	-1.864684	-0.075197	1.607427	6	1.080216	-3.920456	-0.222476
17	-1.661945	-2.339390	1.534214	6	3.162415	-4.351377	-2.049626
17	0.052096	0.092999	2.720471	6	2.045850	-4.905835	0.031864
17	-2.081550	2.156297	1.437693	6	3.087718	-5.124488	-0.881537
6	-3.005910	-0.145556	3.319477	6	-0.519845	-2.093037	-3.054364
6	-4.061743	-1.123063	3.191334	16	3.700482	0.986594	-0.843241
6	-5.258215	-0.881284	2.541691	8	3.186140	0.315184	-2.079129
1	-6.268216	-2.758161	-0.215108	8	4.507999	2.215627	-1.002568
1	-8.308957	-2.243875	-1.596058	6	4.669109	-0.163796	0.139844
1	-7.149831	1.908777	-1.781395	6	6.012067	0.146703	0.393950

1	-5.090676	1.399869	-0.402087	6	4.105300	-1.373707	0.575064
1	-2.258915	-0.403983	4.082252	6	6.794948	-0.769119	1.107040
1	-3.358052	0.889607	3.428583	6	4.905646	-2.273439	1.283605
1	-3.821933	-2.160843	3.455944	6	6.257885	-1.987306	1.564844
1	-6.028792	-1.656442	2.482395	6	7.098451	-2.955238	2.362242
1	-5.597723	0.147262	2.380034	6	0.792169	2.412333	-1.522972
1	-4.079482	-2.092036	0.675357	6	1.290497	3.823431	-1.266509
7	2.292836	1.223430	0.245330	6	2.358123	4.353526	-2.012717
6	0.898613	1.491658	-0.169198	6	0.672234	4.636788	-0.295573
6	0.167199	0.187438	-0.533146	6	2.801390	5.665951	-1.795961
7	0.725993	-0.608039	-1.438848	6	1.117130	5.946760	-0.075967
6	0.191812	-1.926452	-1.847670	6	2.183014	6.466259	-0.826233
8	-0.993890	-0.114375	-0.077340	1	1.608698	-0.518599	-1.789087
6	1.286797	-2.976298	-1.681612	1	-0.715466	-2.190320	-0.901101
6	2.359578	-3.077529	-2.588584	1	2.268832	-2.774170	-3.223178
6	1.242560	-3.848608	-0.577315	1	0.274317	-3.735100	0.497191
6	3.362851	-4.037451	-2.399712	1	3.976622	-4.511354	-2.763875
6	2.243329	-4.813763	-0.392599	1	1.979017	-5.505385	0.945950
6	3.304842	-4.911551	-1.304107	1	3.840229	-5.895463	-0.684893
6	-0.391677	-1.838823	-3.266043	1	-1.312857	-1.331651	-3.135500
16	3.647325	1.212802	-0.768068	1	0.234584	-1.889872	-3.833361
8	3.156699	0.629354	-2.057283	1	-0.961215	-3.082857	-3.255979
8	4.389611	2.491137	-0.819903	1	6.424496	1.094527	0.037896
6	4.682015	0.029221	0.101586	1	3.055888	-1.607217	0.376537
6	6.021839	0.366145	0.336181	1	7.844673	-0.532009	1.312391
6	4.171410	-1.227266	0.465755	1	4.467967	-3.218989	1.621084

6	6.857322	-0.572480	0.954249	1	8.175545	-2.791687	2.194899
6	5.023499	-2.148779	1.079057	1	6.911501	-2.839091	3.445948
6	6.375775	-1.838821	1.335674	1	6.863712	-4.001874	2.105082
6	7.273800	-2.838151	2.024322	1	2.578308	1.599656	1.041643
6	0.661859	2.564482	-1.271319	1	0.487664	1.932331	0.557130
6	1.102807	3.961162	-0.870491	1	1.287125	1.984731	-2.410566
6	2.125774	4.619924	-1.575840	1	-0.294253	2.434447	-1.731517
6	0.476769	4.632942	0.198906	1	2.854039	3.728872	-2.762506
6	2.516828	5.919623	-1.223852	1	-0.169798	4.241496	0.284090
6	0.869919	5.929805	.553392	1	3.636160	6.059693	-2.385184
6	1.890882	6.578545	-0.157392	1	0.623951	6.566076	0.680837
1	1.637897	-0.300363	-1.827125	1	2.529104	7.491136	-0.655081
1	-0.618584	-2.147033	-1.135119	6	-6.632033	0.649672	-0.763546
1	2.422909	-2.400829	-3.448096	6	-5.586107	-0.138387	-0.239670
1	0.420546	-3.759884	0.142127	6	-5.617193	-1.539182	-0.412963
1	4.191788	-4.102718	-3.111981	6	-6.676381	-2.142567	-1.093785
1	2.188915	-5.492153	0.465466	6	-7.701524	-1.333287	-1.600546
1	4.085479	-5.666513	-1.162720	6	-7.696653	0.058142	-1.448530
1	-1.213056	-1.104143	-3.293040	6	-4.453432	0.518292	0.448301
1	0.366955	-1.534488	-4.007129	8	-3.371225	-0.178137	0.606685
1	-0.788865	-2.821865	-3.567878	14	-1.870550	0.202291	1.617832
1	6.391310	1.351971	0.041432	17	-1.674715	-2.017829	1.866587
1	3.121840	-1.477351	0.289456	17	0.022625	0.549631	2.733228
1	7.904987	-0.314783	1.144660	17	-2.060352	2.413705	1.112460
1	4.627333	-3.130240	1.360936	6	-3.045276	0.391936	3.299447
1	7.044081	-2.897768	3.104131	6	-4.238189	1.151283	3.007715

1	7.139522	-3.852497	1.610980	6	-5.368587	0.610172	2.422486
1	8.336766	-2.564630	1.926000	1	-6.605357	1.737998	-0.638129
1	2.521636	1.614085	1.164014	1	-8.513350	0.650908	-1.868417
1	0.405843	1.849474	0.746678	1	-6.721068	-3.224565	-1.243809
1	1.162601	2.256136	-2.204230	1	-4.793826	-2.139237	-0.013709
1	-0.427640	2.559375	-1.464353	1	-4.362599	1.611773	0.341070
1	2.628851	4.106582	-.401788	1	-3.231340	-0.651805	3.588477
1	-0.330547	4.138683	0.751279	1	-2.363613	0.893470	3.999613
1	3.317379	6.414134	-1.783966	1	-6.249223	1.230848	2.228819
1	0.370546	6.437310	1.385631	1	-5.541849	-0.470470	2.460453
1	2.196282	7.593239	0.119305	1	-4.170110	2.244320	3.078685
9	-8.915229	0.127795	-2.480960	9	-8.726204	-1.913826	-2.262324

TS-*para*-methoxy(*R*)				TS-*para*-methoxy(*S*)			
Coordinates				Coordinates			
at. no.	x	y	z	at. no.	x	y	z
7	2.341973	1.160484	0.147312	6	-6.243828	-1.920516	-0.272548
6	0.967277	1.454853	-0.309228	6	-5.343379	-0.880227	0.050729
6	0.176221	0.155168	-0.537768	6	-5.642012	0.431693	-0.365975
7	0.687127	-0.746455	-1.370392	6	-6.807579	0.707985	-1.086043
6	0.088958	-2.072783	-1.644058	6	-7.699803	-0.339229	-1.400324
8	-0.984968	-0.053918	-0.037308	6	-7.406405	-1.658817	-0.990048
6	1.141634	-3.149590	-1.399036	6	-4.103594	-1.184670	0.793661
6	2.194228	-3.371939	-2.307889	8	-3.161875	-0.282692	0.765464
6	1.080216	-3.920456	-0.222476	14	-1.610621	-0.190460	1.733534
6	3.162415	-4.351377	-2.049626	17	-1.345130	-2.445855	1.614274
6	2.045850	-4.905835	0.031864	17	0.347568	0.008541	2.779558

6	3.087718	-5.124488	-0.881537	17	-1.877694	2.041517	1.620155
6	-0.519845	-2.093037	-3.054364	6	-2.669583	-0.318253	3.503499
16	3.700482	0.986594	-0.843241	6	-3.699776	-1.319617	3.387469
8	3.186140	0.315184	-2.079129	6	-4.913663	-1.099547	2.754690
8	4.507999	2.215627	-1.002568	1	-6.019834	-2.947112	0.040006
6	4.669109	-0.163796	0.139844	1	-8.107871	-2.455425	-1.253383
6	6.012067	0.146703	0.393950	8	-8.863863	-0.187416	-2.095067
6	4.105300	-1.373707	0.575064	1	-7.011754	1.733571	-1.402661
6	6.794948	-0.769119	1.107040	1	-4.937768	1.234267	-0.125522
6	4.905646	-2.273439	1.283605	1	-1.884025	-0.569561	4.228312
6	6.257885	-1.987306	1.564844	1	-3.041840	0.706708	3.638588
6	7.098451	-2.955238	2.362242	1	-3.426274	-2.355291	3.626396
6	0.792169	2.412333	-1.522972	1	-5.668445	-1.891320	2.712916
6	1.290497	3.823431	-1.266509	1	-5.289078	-0.077181	2.640055
6	2.358123	4.353526	-2.012717	1	-3.803605	-2.244143	0.853105
6	0.672234	4.636788	-0.295573	6	-9.212306	1.128545	-2.526554
6	2.801390	5.665951	-1.795961	1	-10.174820	1.024218	-3.047041
6	1.117130	5.946760	-0.075967	1	-9.330208	1.817660	-1.669614
6	2.183014	6.466259	-0.826233	1	-8.459473	1.539081	-3.225164
1	1.608698	-0.518599	-1.789087	7	2.468135	1.238642	0.236886
1	-0.715466	-2.190320	-0.901101	6	1.050370	1.482496	-0.107606
1	2.268832	-2.774170	-3.223178	6	0.337255	0.169518	-0.476744
1	0.274317	-3.735100	0.497191	7	0.880414	-0.585378	-1.426708
1	3.976622	-4.511354	-2.763875	6	0.367402	-1.907799	-1.848040
1	1.979017	-5.505385	0.945950	8	-0.794665	-0.175787	0.016758
1	3.840229	-5.895463	-0.684893	6	1.488584	-2.936263	-1.724717

1	-1.312857	-1.331651	-3.135500	6	2.537146	-3.008736	-2.662331
1	0.234584	-1.889872	-3.833361	6	1.493362	-3.817881	-0.626839
1	-0.961215	-3.082857	-3.255979	6	3.563599	-3.950746	-2.510521
1	6.424496	1.094527	0.037896	6	2.517504	-4.764465	-0.478731
1	3.055888	-1.607217	0.376537	6	3.553801	-4.834829	-1.421292
1	7.844673	-0.532009	1.312391	6	-0.250288	-1.808441	-3.250956
1	4.467967	-3.218989	1.621084	16	3.775119	1.304453	-0.834048
1	8.175545	-2.791687	2.194899	8	3.247329	0.740963	-2.117405
1	6.911501	-2.839091	3.445948	8	4.472768	2.608031	-0.879927
1	6.863712	-4.001874	2.105082	6	4.887093	0.132331	-0.047590
1	2.578308	1.599656	1.041643	6	6.218899	0.517481	0.156403
1	0.487664	1.932331	0.557130	6	4.443016	-1.159021	0.280387
1	1.287125	1.984731	-2.410566	6	7.114706	-0.407704	0.706218
1	-0.294253	2.434447	-1.731517	6	5.354757	-2.066341	0.825587
1	2.854039	3.728872	-2.762506	6	6.700887	-1.708407	1.049736
1	-0.169798	4.241496	0.284090	6	7.664199	-2.694340	1.665637
1	3.636160	6.059693	-2.385184	6	0.736129	2.576726	-1.168009
1	0.623951	6.566076	0.680837	6	1.160904	3.974926	-0.755269
1	2.529104	7.491136	-0.655081	6	2.112549	4.684546	-1.509650
6	-6.632033	0.649672	-0.763546	6	0.588535	4.598832	0.371583
6	-5.586107	-0.138387	-0.239670	6	2.486949	5.986792	-1.149424
6	-5.617193	-1.539182	-0.412963	6	0.965441	5.898338	0.734278
6	-6.676381	-2.142567	-1.093785	6	1.915617	6.597528	-0.025207
6	-7.701524	-1.333287	-1.600546	1	1.765693	-0.240720	-1.843985
6	-7.696653	0.058142	-1.448530	1	-0.421407	-2.159312	-1.121623
6	-4.453432	0.518292	0.448301	1	2.562444	-2.323468	-3.516928

8	-3.371225	-0.178137	0.606685	1	0.691661	-3.750550	0.117433
14	-1.870550	0.202291	1.617832	1	4.372807	-3.994096	-3.246792
17	-1.674715	-2.017829	1.866587	1	2.501117	-5.449987	0.375208
17	0.022625	0.549631	2.733228	1	4.352274	-5.576011	-1.309246
17	-2.060352	2.413705	1.112460	1	-1.088304	-1.092377	-3.245908
6	-3.045276	0.391936	3.299447	1	0.484148	-1.473779	-4.003248
6	-4.238189	1.151283	3.007715	1	-0.632457	-2.794638	-3.561812
6	-5.368587	0.610172	2.422486	1	6.535544	1.529359	-0.110163
1	-6.605357	1.737998	-0.638129	1	3.399789	-1.449340	0.128181
1	-8.513350	0.650908	-1.868417	1	8.156655	-0.112206	0.871637
1	-6.721068	-3.224565	-1.243809	1	5.010474	-3.074849	1.078681
1	-4.793826	-2.139237	-0.013709	1	7.485581	-2.795414	2.752041
1	-4.362599	1.611773	0.341070	1	7.548158	-3.699783	1.226014
1	-3.231340	-0.651805	3.588477	1	8.711181	-2.378244	1.530073
1	-2.363613	0.893470	3.999613	1	2.726249	1.601188	1.159302
1	-6.249223	1.230848	2.228819	1	0.590681	1.802302	0.838811
1	-5.541849	-0.470470	2.460453	1	1.198582	2.304986	-2.131519
1	-4.170110	2.244320	3.078685	1	-0.361103	2.547747	-1.308317
9	-8.726204	-1.913826	-2.262324	1	2.571697	4.209267	-2.382699
1	-1.949207	1.093878	4.134318	1	-0.165271	4.065641	0.962032
1	-5.888927	1.461514	2.488845	1	3.231802	6.521184	-1.748420
1	-5.209214	-0.245043	2.744745	1	0.508585	6.368301	1.611776
1	-3.767147	2.455191	3.253682	1	2.208214	7.614121	0.258410

TS-*ortho*-fluoro(*R*) Coordinates				TS-*ortho*-fluoro(*S*) Coordinates			
at. no.	x	y	z	at. no.	x	y	z
7	2.236123	1.206038	0.177850	6	-6.636142	-1.302818	-0.697180
6	0.853259	1.433888	-0.295084	6	-5.600746	-0.368163	-0.500228
6	0.145011	0.096748	-0.574330	6	-5.687550	0.864058	-1.184202
7	0.732525	-0.757263	-1.406556	6	-6.766166	1.133035	-2.031088
6	0.228887	-2.115302	-1.713075	6	-7.778278	0.174405	-2.210867
8	-1.017026	-0.187900	-0.115244	6	-7.719077	-1.055236	-1.539064
6	1.343485	-3.122652	-1.446121	6	-4.440777	-0.699849	0.349852
6	2.426429	-3.278346	-2.332960	8	-3.459771	0.139273	0.355114
6	1.309573	-3.892005	-0.267312	14	-1.989417	0.215355	1.498070
6	3.452228	-4.190190	-2.050233	17	-1.883367	-2.051629	1.567330
6	2.332980	-4.810111	0.011290	17	-0.139180	0.376528	2.715942
6	3.405781	-4.961852	-0.879767	17	-2.082949	2.433833	1.156604
6	-0.336112	-2.156553	-3.140729	6	-3.242913	0.306475	3.116686
16	3.617925	1.154024	-0.798201	6	-4.332516	-0.640130	2.993303
8	3.178418	0.452116	-2.045667	6	-5.499156	-0.389522	2.302265
8	4.324547	2.446107	-0.938254	1	-8.493953	-1.817657	-1.653687
6	4.658200	0.078621	0.196055	1	-6.818680	2.090074	-2.558378
6	5.951817	0.512625	0.514775	1	-4.883097	1.590444	-1.034594
6	4.197160	-1.189226	0.586111	1	-2.559535	0.074512	3.945630
6	6.789181	-0.336972	1.248390	1	-3.562932	1.357769	3.141253
6	5.050507	-2.020631	1.315574	1	-4.141334	-1.670401	3.319500
6	6.355056	-1.610247	1.662297	1	-6.280811	-1.151392	2.226355
6	7.250956	-2.510563	2.478338	1	-5.785223	0.637573	2.052592

6	0.643253	2.416757	-1.482145	1	-4.240217	-1.758788	0.568426
6	1.031815	3.850451	-1.166129	7	2.317125	1.129999	0.263187
6	2.052605	4.493263	-1.888916	6	0.964037	1.498737	-0.207833
6	0.355589	4.572154	-0.161864	6	0.150298	0.244506	-0.570250
6	2.392267	5.826377	-1.617715	7	0.672229	-0.604493	-1.450353
6	0.697616	5.902499	0.112458	6	0.055537	-1.891980	-1.840754
6	1.716722	6.535059	-0.615275	8	-1.033750	0.024867	-0.132262
1	1.650319	-0.468584	-1.794943	6	1.079920	-3.006501	-1.652852
1	-0.587113	-2.294718	-0.995368	6	2.159341	-3.171544	-2.542247
1	2.479915	-2.680993	-3.249947	6	0.966897	-3.872005	-0.548162
1	0.479014	-3.757326	0.435320	6	3.102850	-4.186625	-2.336048
1	4.289534	-4.298349	-2.747317	6	1.907435	-4.893194	-0.346432
1	2.287535	-5.409174	0.926991	6	2.976489	-5.053376	-1.240317
1	4.204072	-5.679918	-0.664124	6	-0.516496	-1.792130	-3.263196
1	-1.175848	-1.448718	-3.235585	16	3.702177	1.006267	-0.702023
1	0.424335	-1.891554	-3.894870	8	3.217093	0.427253	-1.994957
1	-0.703656	-3.170794	-3.367601	8	4.529635	2.231262	-0.752417
1	6.284775	1.502866	0.192540	6	4.625668	-0.224585	0.226054
1	3.184807	-1.520161	0.338509	6	5.956101	0.056904	0.563460
1	7.800500	-0.002497	1.504568	6	4.039449	-1.462046	0.538452
1	4.692790	-3.010405	1.619038	6	6.703669	-0.917259	1.237039
1	7.189614	-3.557924	2.136719	6	4.804333	-2.419405	1.208709
1	8.304601	-2.192014	2.424974	6	6.143642	-2.164121	1.572186
1	6.954896	-2.501402	3.543598	6	6.944578	-3.201249	2.322062
1	2.433710	1.651796	1.078684	6	0.849683	2.563506	-1.336050
1	0.333692	1.854904	0.577433	6	1.381350	3.929893	-0.940525

1	1.192396	2.054747	-2.367329	6	2.467635	4.503187	-1.625343
1	-0.435794	2.370347	-1.723135	6	0.776552	4.659476	0.102881
1	2.594495	3.941398	-2.663815	6	2.941641	5.776410	-1.278505
1	-0.452516	4.091056	0.401081	6	1.252534	5.929640	0.452447
1	3.191850	6.308181	-2.190161	6	2.336286	6.493232	-0.237691
1	0.159601	6.448673	0.894620	1	1.614241	-0.370661	-1.816835
1	1.982190	7.575855	-0.401506	1	-0.770263	-2.048592	-1.129056
6	-6.766494	0.030640	-0.864320	1	2.274680	-2.500898	-3.401041
6	-5.584686	-0.625456	-0.467704	1	0.139639	-3.733862	0.157707
6	-5.434813	-1.983168	-0.824697	1	3.938506	-4.300862	-3.034093
6	-6.430030	-2.641566	-1.552109	1	1.800265	-5.565746	0.511248
6	-7.593784	-1.954385	-1.938237	1	3.709887	-5.851628	-1.084687
6	-7.769675	-0.606788	-1.592644	1	-1.286057	-1.004071	-3.306825
6	-4.522722	0.108708	0.248445	1	0.263713	-1.553663	-4.005909
8	-3.403933	-0.510575	0.431999	1	-0.978484	-2.751474	-3.548734
14	-1.968178	-0.033805	1.518128	1	6.386483	1.027264	0.301944
17	-1.613100	-2.240546	1.724916	1	2.999517	-1.672472	0.274853
17	-0.146520	0.424682	2.705691	1	7.743239	-0.703502	1.508669
17	-2.303704	2.160790	1.040749	1	4.349754	-3.385992	1.451032
6	-3.218974	0.023497	3.142916	1	8.020405	-2.962591	2.321659
6	-4.457474	0.704631	2.829940	1	6.618194	-3.266218	3.376336
6	-5.543681	0.096027	2.235617	1	6.814630	-4.205563	1.883460
1	-8.665679	-0.047080	-1.873230	1	2.541618	1.517874	1.184272
1	-6.299328	-3.692792	-1.825341	1	0.468549	1.911825	0.682686
1	-4.516455	-2.494148	-0.520586	1	1.356497	2.201184	-2.245926
1	-4.521142	1.206812	0.191347	1	-0.229827	2.637898	-1.567086

1	-3.343397	-1.035921	3.407806	1	2.954461	3.942039	-2.429607
1	-2.604858	0.554913	3.883320	1	-0.080125	4.232402	0.636751
1	-6.447001	0.667238	2.001168	1	3.790560	6.204435	-1.821911
1	-5.638404	-0.994837	2.243121	1	0.768923	6.483586	1.264100
1	-4.462549	1.799305	2.907608	1	2.706691	7.487144	0.035085
1	-8.372581	-2.467980	-2.510529	1	-8.622145	0.382422	-2.876041
9	-6.941367	1.326593	-0.500608	9	-6.585011	-2.478469	-0.020078

TS-*ortho*-methoxy(*R*)				TS-*ortho*-methoxy(*S*)			
Coordinates				Coordinates			
at. no.	x	y	z	at. no.	x	y	z
7	2.353925	1.248445	0.183133	6	-6.508858	-0.854906	-0.669459
6	0.958167	1.430241	-0.270608	6	-5.433538	0.058710	-0.482225
6	0.298701	0.071029	-0.564450	6	-5.426916	1.265109	-1.208708
7	0.908693	-0.742682	-1.421534	6	-6.450714	1.565572	-2.111933
6	0.455305	-2.113107	-1.749571	6	-7.497297	0.650480	-2.298328
8	-0.843981	-0.266754	-0.095467	6	-7.532531	-0.556762	-1.585186
6	1.604115	-3.084450	-1.491889	6	-4.315659	-0.284615	0.419995
6	2.674446	-3.225063	-2.396184	8	-3.272010	0.489636	0.380607
6	1.613810	-3.835156	-0.300386	14	-1.815635	0.515314	1.511404
6	3.729503	-4.104974	-2.118932	17	-1.859345	-1.745823	1.705448
6	2.666374	-4.721053	-0.027083	17	0.039837	0.601055	2.743883
6	3.725930	-4.858998	-0.936197	17	-1.724336	2.713955	1.060404
6	-0.105603	-2.152371	-3.178621	6	-3.055006	0.786277	3.131038

16	3.726625	1.268514	-0.804561	6	-4.205109	-0.082797	3.035233
8	3.304326	0.571334	-2.060505	6	-5.327177	0.205401	2.280352
8	4.381175	2.589544	-0.928213	1	-8.359528	-1.253035	-1.742721
6	4.819027	0.218898	0.161373	1	-6.429950	2.504036	-2.673560
6	6.097108	0.699528	0.475912	1	-4.587825	1.949478	-1.051377
6	4.413974	-1.073695	0.531774	1	-2.392473	0.548392	3.974284
6	6.976016	-0.128801	1.184705	1	-3.293327	1.858411	3.089686
6	5.308093	-1.883191	1.236715	1	-4.098676	-1.103227	3.425060
6	6.598471	-1.426517	1.577986	1	-6.166167	-0.495474	2.240372
6	7.539431	-2.304292	2.367531	1	-5.535199	1.237899	1.980717
6	0.696489	2.419888	-1.441234	1	-4.174569	-1.343115	0.679863
6	1.032644	3.864019	-1.113663	7	2.564675	0.989647	0.242855
6	2.015797	4.553946	-1.845253	6	1.245668	1.481861	-0.213777
6	0.345198	4.548370	-0.091056	6	0.322058	0.303301	-0.567862
6	2.308061	5.896322	-1.564999	7	0.757065	-0.574799	-1.469441
6	0.639808	5.888281	0.192082	6	0.029742	-1.799430	-1.868946
6	1.621813	6.567777	-0.544467	8	-0.861666	0.170058	-0.101028
1	1.810166	-0.411714	-1.813779	6	0.916815	-3.014099	-1.605343
1	-0.355467	-2.331970	-1.036798	6	1.925637	-3.411839	-2.503623
1	2.694575	-2.642734	-3.324011	6	0.743692	-3.738736	-0.409834
1	0.793113	-3.711142	0.415797	6	2.740019	-4.515988	-2.216039
1	4.555941	-4.202219	-2.830523	6	1.554996	-4.846542	-0.125274
1	2.653594	-5.306580	0.898402	6	2.554346	-5.238877	-1.028478
1	4.546903	-5.552536	-0.725265	6	-0.462090	-1.664610	-3.317389
1	-0.972156	-1.476302	-3.262453	16	3.926155	0.765065	-0.737472
1	0.644212	-1.844472	-3.927205	8	3.385772	0.222900	-2.024057

1	-0.433574	-3.175952	-3.423451	8	4.843301	1.924005	-0.797410
1	6.385538	1.708502	0.169303	6	4.765783	-0.532217	0.180403
1	3.413277	-1.441173	0.288273	6	6.104413	-0.333088	0.542525
1	7.975638	0.241603	1.437441	6	4.105452	-1.739178	0.462263
1	4.994074	-2.892246	1.524540	6	6.784743	-1.359420	1.210183
1	7.510483	-3.348624	2.012739	6	4.803993	-2.749583	1.127016
1	8.579885	-1.946824	2.301942	6	6.149803	-2.577842	1.514626
1	7.260663	-2.319623	3.437405	6	6.879233	-3.672927	2.255051
1	2.542456	1.674812	1.095133	6	1.214932	2.553046	-1.339759
1	0.432670	1.817589	0.613860	6	1.876198	3.865575	-0.957336
1	1.248588	2.090451	-2.337267	6	2.974223	4.351023	-1.689879
1	-0.382858	2.333765	-1.669886	6	1.383269	4.636245	0.115040
1	2.565629	4.031906	-2.635191	6	3.569223	5.577492	-1.362698
1	-0.433856	4.030036	0.479842	6	1.980878	5.859501	0.445606
1	3.079233	6.414621	-2.144545	6	3.075345	6.335034	-0.292471
1	0.093980	6.404824	0.988891	1	1.712087	-0.419044	-1.843512
1	1.850302	7.615782	-0.323185	1	-0.840296	-1.852026	-1.195850
6	-6.599844	-0.234528	-0.776426	1	2.084491	-2.858316	-3.435377
6	-5.394669	-0.872953	-0.369230	1	-0.029313	-3.424088	0.301262
6	-5.183307	-2.220680	-0.718725	1	3.520839	-4.812648	-2.923935
6	-6.131533	-2.927232	-1.463963	1	1.399862	-5.406220	0.803253
6	-7.308687	-2.282683	-1.872032	1	3.185647	-6.106796	-0.810107
6	-7.548109	-0.942500	-1.535023	1	-1.153662	-0.810642	-3.402654
6	-4.360675	-0.113796	0.363514	1	0.369814	-1.501595	-4.023326
8	-3.204298	-0.690551	0.506617	1	-0.994749	-2.580807	-3.621046
14	-1.779121	-0.179669	1.556080	1	6.594022	0.614487	0.302481

17	-1.325002	-2.373300	1.726783	1	3.059842	-1.886990	0.178767
17	0.053339	0.329037	2.720735	1	7.830562	-1.209833	1.500208
17	-2.195575	2.014321	1.131011	1	4.290416	-3.692087	1.345369
6	-2.983595	-0.187203	3.225617	1	7.964787	-3.486674	2.289960
6	-4.254435	0.434021	2.933598	1	6.520676	-3.752157	3.297776
6	-5.306044	-0.218855	2.316693	1	6.714271	-4.656978	1.783301
1	-8.473665	-0.460518	-1.858052	1	2.828112	1.346581	1.166315
1	-5.952016	-3.972410	-1.732385	1	0.799240	1.934462	0.682953
1	-4.247995	-2.689119	-0.397934	1	1.672346	2.145700	-2.256922
1	-4.397749	0.983285	0.310463	1	0.143335	2.726725	-1.554123
1	-3.048300	-1.254534	3.479704	1	3.374343	3.756818	-2.517921
1	-2.376910	0.369053	3.952955	1	0.516330	4.281064	0.683982
1	-6.244276	0.305647	2.112903	1	4.425214	5.936483	-1.943755
1	-5.345580	-1.313092	2.317907	1	1.583374	6.446772	1.280265
1	-4.315926	1.525579	3.030584	1	3.540121	7.292440	-0.033816
1	-8.056535	-2.823945	-2.460843	1	-8.302029	0.872149	-3.006994
8	-6.752662	1.062521	-0.369258	8	-6.466203	-1.987944	0.096477
6	-7.909376	1.771646	-0.815741	6	-7.485326	-2.968340	-0.102937
1	-7.807812	2.787526	-0.408788	1	-7.489750	-3.339120	-1.144570
1	-7.951845	1.818666	-1.919516	1	-7.238200	-3.793722	0.579466
1	-8.838887	1.311938	-0.431319	1	-8.485419	-2.569086	0.148918

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