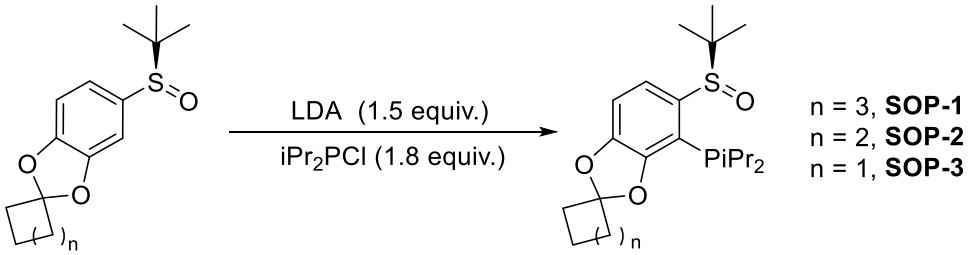
Supporting Information

General information

All the commercially available reagents were used directly without further purification. Solvents used in catalytic reactions were freshly distilled in appropriate method. Solvents employed for column chromatography were purchased in technical grade quality without distillation. All the catalytic reactions were operated in glovebox. NMR spectras were obtained on a Bruker 400 spectrometer in $CDCl_3$ operating at 400 MHz for ^{1}H NMR, 101 MHz for ^{13}CNMR, 162 MHz for ^{31}P NMR, and 376 MHz for ^{19}F NMR. The coupling constants are in Hertz (Hz). The following abbreviations are used for spin multiplicity: s = singlet, d = doublet, dd = doublet of doublet, t = triplet, tt = triplet of triplet, brs = broad singlet and m = multiplet. Optical rotation was recorded on PE polarmeter 341, and reported as $[\alpha]_{\lambda}^{T}$ (c: g/100 mL, in solvent). Enantiomerical excesses were measured by HPLC analysis on Chiralcel OD-H, OZ-H, AS-H, IC chiral column (Daicel Chemical Industries, LTD). Electrospray ionization high-resolution mass spectra (ESI-HRMS (M/Z, ESI)) were recorded on a Waters Vion® IMS Q-TOf mass spectrometer. Liquid chromatography was performed using forced flow (flash chromatography) on silicagel (300-400 mesh). The deactivated silica gel (35 wt% H_2O) was prepared by mixing silica gel and deionized water (65:35 by weight), followed by vigorous shaking and stirring. After the mixture turned to a fluffy powder, it was allowed to sit overnight prior to use.

1. General procedures for synthesis of Ligands

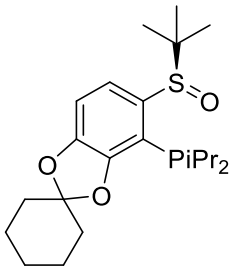
All commercially available reagents were used as received without further purification. Chiral sulfoxide phosphine ligands (**SOP) SOP-1**, **SOP-2**, **SOP-3**, **SOP-4**, **S0P-5**, **SOP-6** were prepared according to the literature procedure reported by our group.[1]



Under argon atmosphere and at -78 ℃, LDA (5.1 mL, 2.0 M in hexane, 10.2 mmol) was added to a solution of *(R)-5-(tert-butylsulfinyl)spiro[benzo[d][1,3]dioxole-2,1'-cyclohexane* (2 g, 6.8 mmol) in tetrahydrofuran (10 mL), the mixture was stirred for 1 hour at -45℃, then iPr_2PCl (1.86 g, 12.2 mmol) in THF (1 mL) was added dropwise. The mixture was warmed to room temperature and stirred overnight, then quenched with saturated NH_4Cl aqueous solution (2 mL). The organic phase was separated and aqueous layer was extracted with ethyl acetate (3 x 10 mL). The combined organic layer was dried over Na_2SO_4 and concentrated. Flash chromatography of the crude material with petroleum ether (PE)/ethyl acetate (EA) = (3/1) afforded (*R*)-(6-(*tert*-butylsulfinyl)-2, 3-dimethoxyphenyl) diphenylphosphane **SOP-1** as a white solid (1.24 g, 44% yield).

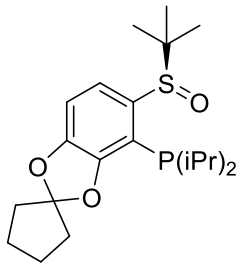
(*R*)-(5-(tert-butylsulfinyl)spiro[benzo[d][1,3]dioxole-2,1'-cyclohexan]-4-yl)diisopropylphosphane

(**SOP-1**)



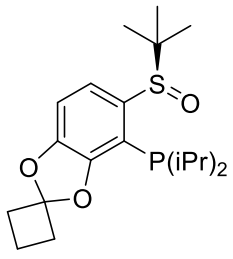
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.44 (dd, *J* = 2.6, 8.2 Hz, 1H), 6.91 (d, *J* = 8.2 Hz, 1H), 2.97-2.88 (m, 1H), 2.18-2.10 (m, 1H), 1.99-1.76 (m, 6H),1.74-1.69 (m, 2H), 1.64-1.58 (m, 1H), 1.53-1.44 (m, 1H),1.28 (s, 9H), 1.23-1.15 (m, 6H), 1.03-0.98 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 150.2 (d, *J* = 4 Hz), 148.8, 139.6 (d, *J* = 23 Hz), 121.1 (d, *J* = 6 Hz), 119.2, 117.0 (d, *J* = 32 Hz), 109.2, 58.9, 35.4 (d, *J* = 12 Hz), 26.6 (d, *J* = 14 Hz), 24.4, 23.9 (d, *J* = 5 Hz), 23.2, 21.3 (d, *J* = 10 Hz), 21.0 (d, *J* = 13 Hz), 20.8 (d, *J* = 4 Hz), 20.7 (d, *J* = 10 Hz), 19.4 (d, *J* = 3 Hz); ^{31}P NMR (162 MHz, $CDCl_3$) δ = 0.87; HRMS (M/Z, ESI) Calcd. for $C_{22}H_{35}O_3PS$ [M+H]: 411.2123, Found: 411.2112; Optical Rotation: $[\alpha]_D^{25}$ 153.8 (c 1.05, $CHCl_3$).

(*R*)-(5-(tert-butylsulfinyl)spiro[benzo[d][1,3]dioxole-2,1'-cyclopentan]-4-yl)diisopropylphosphane (**SOP-2**)



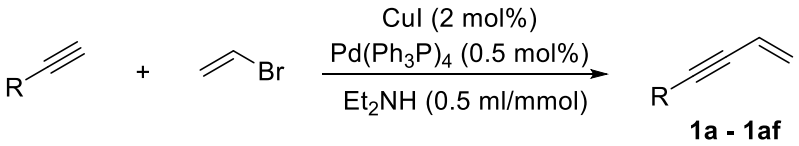
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ= 7.45 (dd, *J* = 2.6, 8.2Hz, 1H), 6.91 (d, *J* = 8.2 Hz, 1H), 2.95-2.86 (m, 1H), 2.16-2.04 (m, 5H), 1.88-1.86 (m, 4H), 1.28 (s, 9H), 1.22-1.14 (m, 6H), 1.02-0.97 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 150.3 (d, *J* = 3 Hz), 148.8, 139.7 (d, *J* = 12 Hz), 127.6, 121.1 (d, *J* = 6 Hz), 117.0 (d, *J* = 33 Hz), 108.9, 58.9, 37.0 (d, *J* = 27 Hz), 26.6 (d, *J* = 13 Hz), 23.8 (d, *J* = 5 Hz), 23.0 (d, *J* = 2 Hz), 21.3 (d, *J* = 10 Hz), 20.9 (d, *J* = 7 Hz), 20.8 (d, *J* = 6 Hz), 20.7 (d, *J* = 2 Hz), 19.3 (d, *J* = 3 Hz); ^{31}P NMR (162 MHz, $CDCl_3$) δ = 1.25; HRMS (M/Z, ESI) Calcd. for $C_{21}H_{33}O_3PS$ [M+H]: 397.1966, Found: 397.1961; Optical Rotation: $[\alpha]_D^{25}$ 179.7 (c 0.79, $CHCl_3$).

(*R*)-(5-(tert-butylsulfinyl)spiro[benzo[d][1,3]dioxole-2,1'-cyclobutan]-4-yl)diisopropylphosphane (**SOP-3**)



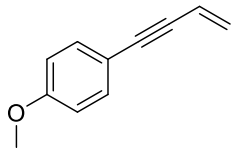
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.47 (dd, *J* = 2.6, 8.2 Hz, 1H), 6.93 (d, *J* = 8.2 Hz, 1H), 3.02-2.93 (m, 1H), 2.72-2.56 (m, 4H), 2.18-2.10 (m, 1H), 1.93-1.85 (m, 2H), 1.28 (s, 9H), 1.22-1.16 (m, 6H), 1.04-0.97 (m, 6H), ^{13}C NMR (101 MHz, $CDCl_3$) δ = 150.0 (d, *J* = 3 Hz), 148.4, 140.0 (d, *J* = 2.3 Hz), 121.3 (d, *J* = 6.3 Hz), 117.9, 117.0 (d, *J* = 33 Hz), 108.9, 58.9, 37.0 (d, *J* = 35 Hz), 26.6 (d, *J* = 14 Hz), 23.8 (d, *J* = 4.7 Hz), 21.2 (d, *J* = 10 Hz), 21.0, 20.8 (d, *J* = 1.5 Hz), 20.6 (d, *J* = 4.5 Hz), 19.4 (d, *J* = 3 Hz), 10.8; ^{31}P NMR (162 MHz, $CDCl_3$) δ = 1.37; HRMS (M/Z, ESI) Calcd. for $C_{21}H_{33}O_3PS$ [M+H]: 383.1804, Found: 383.1804; Optical Rotation: $[\alpha]_D^{25}$ 195.7 (c 0.42, $CHCl_3$).

2. General procedures for the synthesis of substrates (1a – 1af)[2]



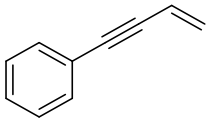
CuI (2 mol%) and $Pd(PPh_3)_4$ (0.5 mol%) were dissolved in anhydrous/degassed diethyl amine and cooled to 0 ℃. The alkyne (10 mmol, 1.0 equiv.) was added into the mixture, and vinyl bromide (1 M in THF, 1.3 equiv.) was added into the mixture slowly. After addition, the mixture was warmed to room temperature and stirred for 4 hours. The reaction mixture was filtrated a celite pad, the solvent was removed under vaccum, flash chromatography of the crude product with PE/EA from 1:0 to 20:1 afforded the products.

1-(but-3-en-1-yn-1-yl)-4-methoxybenzene (**1a**)



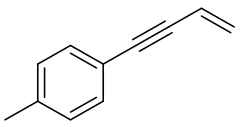
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.41 (d, *J* = 8.1 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.03 (dd, *J* = 11.2, 17.5 Hz, 1H), 5.72 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.52 (dd, *J* = 2.0, 11.2 Hz, 1H), 3.83 (s, 3H).

but-3-en-1-yn-1-ylbenzene (**1b**)



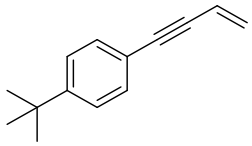
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.49-7.47(m, 2H), 7.35-7.33(m, 3H), 6.05 (dd, *J* = 11.1, 17.5 Hz, 1H), 5.77 (dd, *J* = 2.1, 17.5 Hz, 1H), 5.58 (dd, *J* = 2.1, 11.1 Hz, 1H).

1-(but-3-en-1-yn-1-yl)-4-methylbenzene (**1c**)



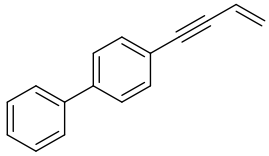
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.37 (d, *J* = 8.1 Hz, 2H), 7.15 (d, *J* = 7.9 Hz, 2H), 6.05 (dd, *J* = 11.1, 17.5 Hz, 1H), 5.75 (dd, *J* = 2.1, 17.5 Hz, 1H), 5.55 (dd, *J* = 2.1, 11.2 Hz, 1H).

1-(but-3-en-1-yn-1-yl)-4-(tert-butyl)benzene (**1d**)



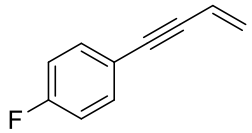
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.48-7.35 (m, 4H), 6.04 (dd, *J* = 11.1, 17.5 Hz, 1H), 5.74 (dd, *J* = 2.1, 17.5 Hz, 1H), 5.62 (dd, *J* = 2.1, 11.1 Hz, 1H), 1.34 (s, 9H).

4-(but-3-en-1-yn-1-yl)-1,1'-biphenyl (**1e**)



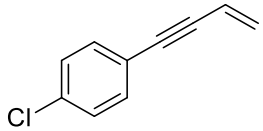
White solid. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.64-7.54 (m, 6H), 7.50-7.46 (m, 2H), 7.41-7.37 (m, 1H), 6.08 (dd, *J* = 11.2, 17.5 Hz, 1H), 5.79 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.59 (dd, *J* = 2.0, 11.2 Hz, 1H).

1-(but-3-en-1-yn-1-yl)-4-fluorobenzene (**1f**)



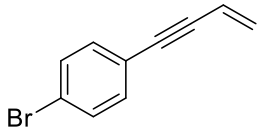
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.46-7.43 (m, 2H), 7.06-7.01 (m, 2H), 6.03 (dd, *J* = 11.1, 17.5 Hz, 1H), 5.75 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.57 (dd, *J* = 2.0, 11.1 Hz, 1H).

1-(but-3-en-1-yn-1-yl)-4-chlorobenzene (**1g**)



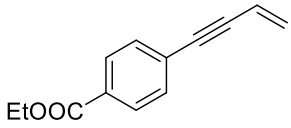
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ =7.40-7.38 (m, 2H), 7.33-7.30 (m, 2H),6.03 (dd, *J* = 11.1, 17.5 Hz, 1H), 5.77 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.59 (dd, *J* = 2.0, 11.1 Hz, 1H).

bromo-4-(but-3-en-1-yn-1-yl)benzene (**1h**)



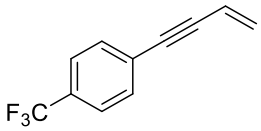
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.47 (d, *J* = 8.5 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 6.02 (dd, *J* = 11.2, 17.6 Hz, 1H), 5.77 (dd, *J* = 2.0, 17.6 Hz, 1H), 5.59 (dd, *J* = 2.0, 11.2 Hz, 1H).

ethyl 4-(but-3-en-1-yn-1-yl)benzoate (**1i**)



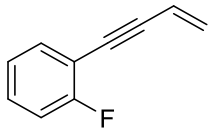
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 8.01 (d, *J* = 8.5 Hz, 2H), 7.51 (d,*J* = 8.5 Hz,2H), 6.05 (dd, *J* = 11.2, 17.5 Hz, 1H), 5.80 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.62 (dd, *J* = 2.0, 11.2 Hz, 1H), 4.40 (q,*J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H).

1-(but-3-en-1-yn-1-yl)-4-(trifluoromethyl)benzene (**1j**)



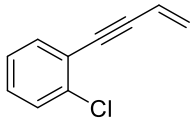
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.61-7.55 (m, 4H), 6.05 (dd, *J* = 11.2, 17.5 Hz, 1H), 5.82 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.64 (dd, *J* = 2.0, 11.2 Hz, 1H).

1-(but-3-en-1-yn-1-yl)-2-fluorobenzene (**1k**)



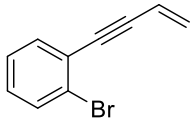
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.48-7.44 (m, 1H), 7.33-7.28 (m, 1H), 7.14-7.07 (m, 2H), 6.08 (dd, *J* = 11.2, 17.5 Hz, 1H), 5.81 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.62 (dd, *J* = 2.0, 11.2 Hz, 1H).

1-(but-3-en-1-yn-1-yl)-2-chlorobenzene (**1l**)



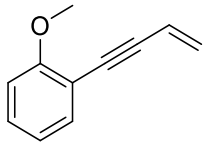
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.51-7.49 (m, 1H), 7.43-7.41 (m, 1H), 7.29-7.23 (m, 2H), 6.10 (dd, *J* = 11.2, 17.5 Hz, 1H), 5.83 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.63 (dd, *J* = 2.0, 11.2 Hz, 1H).

bromo-2-(but-3-en-1-yn-1-yl)benzene (**1m**)



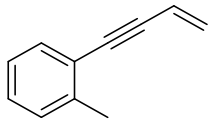
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.62-7.60 (m, 1H), 7.51-7.48 (m, 1H), 7.30-7.26 (m, 1H), 7.20-7.16 (m, 1H), 6.09 (dd, *J* = 11.2, 17.6 Hz, 1H), 5.84 (dd, *J* = 2.1, 17.6 Hz, 1H), 5.64 (dd, *J* = 2.1, 11.2 Hz, 1H).

1-(but-3-en-1-yn-1-yl)-2-methoxybenzene (**1n**)



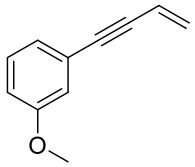
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.45-7.43 (m, 1H), 7.33-7.28 (m, 1H), 6.96-6.89 (m, 2H), 6.10 (dd, *J* = 11.2, 17.5 Hz, 1H), 5.77 (dd, *J* = 2.1, 17.5 Hz, 1H), 5.56 (dd, *J* = 2.1, 11.2 Hz, 1H).

1-(but-3-en-1-yn-1-yl)-2-methylbenzene (**1o**)



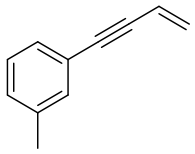
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.44 (d,*J* = 7.6 Hz,1H), 7.27-7.22 (m, 2H), 7.19-7.14 (m, 1H), 6.09 (dd, *J* = 11.1, 17.5 Hz, 1H), 5.76 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.57 (dd, *J* = 2.1, 11.1 Hz, 1H), 2.48 (s, 3H).

1-(but-3-en-1-yn-1-yl)-3-methoxybenzene (**1p**)



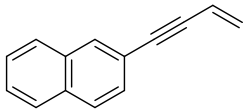
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.28-7.23 (m, 1H), 7.08-7.06 (m, 1H), 7.0 (s, 1H), 6.91-6.89 (m, 1H), 6.05 (dd, *J* = 11.2, 17.5 Hz, 1H), 5.77 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.58 (dd, *J* = 2.0, 11.2 Hz, 1H), 3.83 (s, 3H).

1-(but-3-en-1-yn-1-yl)-3-methylbenzene (**1q**)



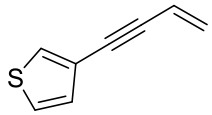
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.31-7.21 (m, 3H), 7.16-7.14 (m, 1H), 6.05 (dd, *J* = 11.1, 17.5 Hz, 1H), 5.76 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.56 (dd, *J* = 2.0, 11.1 Hz, 1H), 2.36 (s, 3H).

2-(but-3-en-1-yn-1-yl)naphthalene (**1r**)



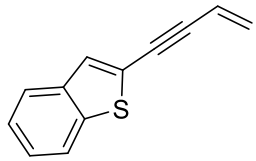
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 8.01 (s, 1H), 7.85-7.80 (m, 3H), 7.54-7.50 (m, 3H), 6.11 (dd, *J* = 11.2, 17.5 Hz, 1H), 5.82 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.61 (dd, *J* = 2.0, 11.2 Hz, 1H).

3-(but-3-en-1-yn-1-yl)thiophene (**1s**)



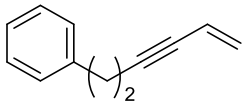
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.48-7.47 (m, 1H), 7.30-7.28 (m, 1H), 7.15-7.14 (m, 1H), 6.02 (dd, *J* = 11.2, 17.5 Hz, 1H), 5.74 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.56 (dd, *J* = 2.1, 11.2 Hz, 1H).

2-(but-3-en-1-yn-1-yl)benzo[*b*]thiophene (**1t**)



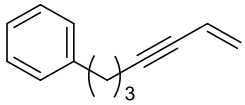
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.99 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 7.8 Hz, 1H), 7.64 (s, 1H), 7.50-7.41(m, 2H), 6.14 (dd, *J* = 11.2, 17.5 Hz, 1H), 5.85 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.64 (dd, *J* = 2.0, 11.2 Hz, 1H).

hex-5-en-3-yn-1-ylbenzene (**1u**)



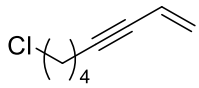
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.39-7.35 (m, 2H), 7.31-7.29 (m, 3H), 5.89-5.81 (m, 1H), 5.65-5.60 (m, 1H), 5.47-5.44 (m, 1H), 2.94-2.90 (m, 2H), 2.68-2.64 (m, 2H).

hept-6-en-4-yn-1-ylbenzene (**1v**)



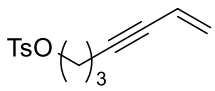
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.34-7.30 (m, 2H), 7.24-7.21 (m, 3H), 5.87-5.80 (m, 1H), 5.63-5.58 (m, 1H), 5.43 (dd, *J* = 1.9, 11.0 Hz, 1H), 2.77(t, *J* = 7.6 Hz, 2H), 2.37-2.34 (m, 2H), 1.93-1.86 (m, 2H).

8-chlorooct-1-en-3-yne (**1w**)



Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 5.83-5.75 (m, 1H), 5.58 (dd, *J* = 2.1, 17.5 Hz, 1H), 5.41 (dd, *J* = 2.1, 11.0 Hz, 1H), 3.60 (t, *J* = 6.6 Hz, 2H), 2.40-2.36 (m, 2H), 1.96-1.89 (m, 2H), 1.75-1.68 (m, 2H).

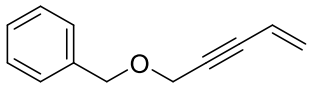
hept-6-en-4-yn-1-yl 4-methylbenzenesulfonate (**1x**)



Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.82 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H),

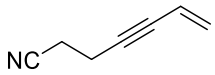
5.73-5.65 (m, 1H), 5.52-5.47 (m, 1H), 5.39 (dd, *J* = 2.0, 11.0 Hz, 1H), 4.16 (t, *J* = 6.1 Hz, 2H), 2.46 (s, 3H), 2.41-2.37 (m, 2H), 1.88 (t, *J* = 6.4 Hz, 2H).

((pent-4-en-2-yn-1-yloxy)methyl)benzene (**1y**)



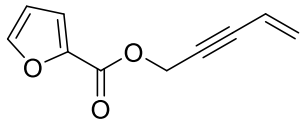
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.41-7.32 (m, 5H), 5.92-5.84 (m, 1H), 5.74-5.76 (m, 1H), 5.54 (dd, *J* = 2.2, 11.0 Hz, 1H), 4.64 (s, 2H), 4.33-4.32 (m, 2H).

hept-6-en-4-ynenitrile (**1z**)



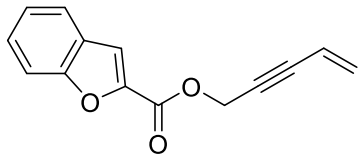
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 5.82-5.74 (m, 1H), 5.63 (dd, *J* = 2.2, 17.6 Hz, 1H), 5.48 (dd, *J* = 2.2, 11.0 Hz, 1H), 2.71 (m, 2H), 2.61-2.57 (m, 2H).

pent-4-en-2-yn-1-yl furan-2-carboxylate (**1aa**)



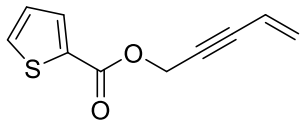
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.62 (s, 1H), 7.27-7.26 (m, 1H), 6.55-6.54 (m, 1H), 5.88-5.81 (m, 1H), 5.75-5.70 (m, 1H), 5.58-5.55 (m, 1H), 5.05 (s, 2H).

hept-6-en-4-yn-1-yl benzofuran-2-carboxylate (**1ab**)



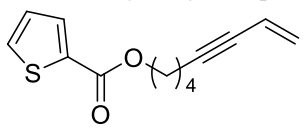
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.72-7.70 (m, 1H), 7.63-7.61 (m, 1H), 7.56-7.55 (m,1H), 7.50-7.46 (m, 1H), 7.35-7.31 (m, 1H), 5.83-5.75 (m, 1H), 5.59 (dd, *J* = 2.2, 17.5 Hz, 1H), 5.42 (dd, *J* = 2.2, 11.0 Hz, 1H), 4.52 (t, *J* = 6.3 Hz,2H), 2.57-2.53 (m, 2H), 2.10-2.03 (m, 2H).

pent-4-en-2-yn-1-yl thiophene-2-carboxylate (**1ac**)



Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.88-7.86 (m, 1H), 7.62-7.60 (m, 1H), 7.15-7.12 (m, 1H), 5.89-5.81 (m, 1H), 5.75-5.70 (m, 1H), 5.56 (dd, *J* = 2.2, 11.0 Hz, 1H), 5.04 (s, 2H).

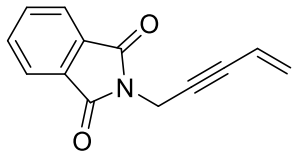
oct-7-en-5-yn-1-yl thiophene-2-carboxylate (**1ad**)



Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.83-7.81 (m, 1H), 7.58-7.56 (m, 1H), 7.13-7.11

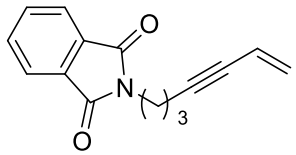
(m, 1H), 5.84-5.76 (m, 1H), 5.57 (dd, *J* = 2.0, 17.5 Hz, 1H), 5.41 (dd, *J* = 2.0, 11.0 Hz, 1H), 4.35 (t, *J* = 6.4 Hz, 2H), 2.44-2.40 (m, 2H), 1.94-1.87 (m, 2H), 1.74-1.67 (m, 2H).

2-(pent-4-en-2-yn-1-yl)isoindoline-1,3-dione (**1ae**)



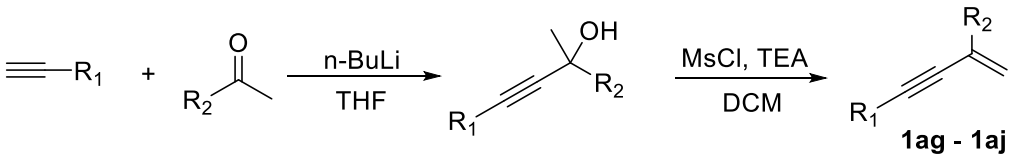
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.91-7.89 (m, 2H), 7.77-7.75 (m, 2H), 5.80-5.73 (m, 1H), 5.68-5.63 (m, 1H), 5.51-5.47 (m, 1H), 4.59 (s, 2H).

2-(hept-6-en-4-yn-1-yl)isoindoline-1,3-dione (**1af**)



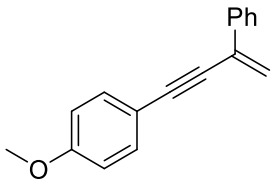
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.86-7.84 (m, 2H), 7.73-7.71 (m, 2H), 5.66-5.58 (m, 1H), 5.44 (dd, *J* = 1.6, 17.5 Hz, 1H), 5.30 (dd, *J* = 2.0, 11.0 Hz, 1H), 3.81(t, *J* = 7.1 Hz, 2H), 2.42-2.39 (m, 2H), 2.00-1.93 (m, 2H).

3. General procedures for the synthesis of substrates (1ag – 1aj)[2i, 3]



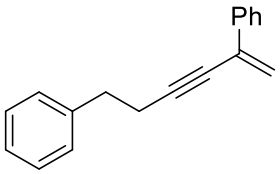
Under argon atmosphere, *n*-BuLi (8.0 mL, 2.5 M in hexane, 20 mmol) was added dropwise to a solution of alkyne (20 mmol) in andydrous THF (50 mL) at -78 ℃. After addition, the resulting mixture was stirred at 0 ℃ for one hour. Then, cooled to -78 ℃, ketone (20 mmol) in 8 mL THF was added slowly. The reaction mixture was warmed slowly to room temperature and stirred for another 6 hours, then quenched with Sat. NH_4Cl (10 mL), and extracted with EtOAc three times. The combined organic layer was dried over Na_2SO4 and concentrated under reduced pressure to afford the crude material. The crude was dissolved in dry DCM (40 mL), and the mixture was cooled to 0 ℃. TEA (100 mmol, 5 equiv) was added to this solution and methylsulfonyl chloride (50 mmol, 2.5 equiv) sequentially. After one hour the reaction was quenched with saturated aqueous NH_4Cl (40 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layer was dried over Na_2SO4 filtered, and concentrated under reduced pressure. The crude material was purified by flash chromatography to yield the product.

1-methoxy-4-(3-phenylbut-3-en-1-yn-1-yl)benzene (**1ag**)



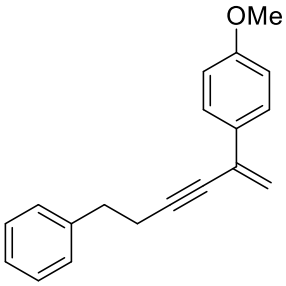
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.78-7.75 (m, 2H), 7.52-7.50 (m, 2H), 7.44-7.34 (m, 3H), 6.93-6.90 (m, 2H), 5.98 (d, *J* = 0.9 Hz, 1H), 5.76 (d, *J* = 0.9 Hz, 1H), 3.86 (s, 3H).

hex-5-en-3-yne-1,5-diyldibenzene (**1ah**)



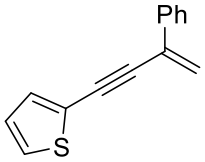
Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.60-7.58 (m, 2H), 7.38-7.26 (m, 8H), 5.88 (s, 1H), 5.60 (s, 1H), 2.97 (t, *J* = 7.4 Hz, 2H), 2.76 (t, *J* = 7.4 Hz, 2H).

1-methoxy-4-(6-phenylhex-1-en-3-yn-2-yl)benzene (**1ai**)



Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.54-7.52 (m, 2H), 7.37-7.27 (m, 5H), 6.88-6.86 (m, 2H), 5.76 (s, 1H), 5.50 (s, 1H), 3.85(s, 3H), 2.96 (t, *J* = 7.4 Hz, 2H), 2.75 (t, *J* = 7.4 Hz, 2H).

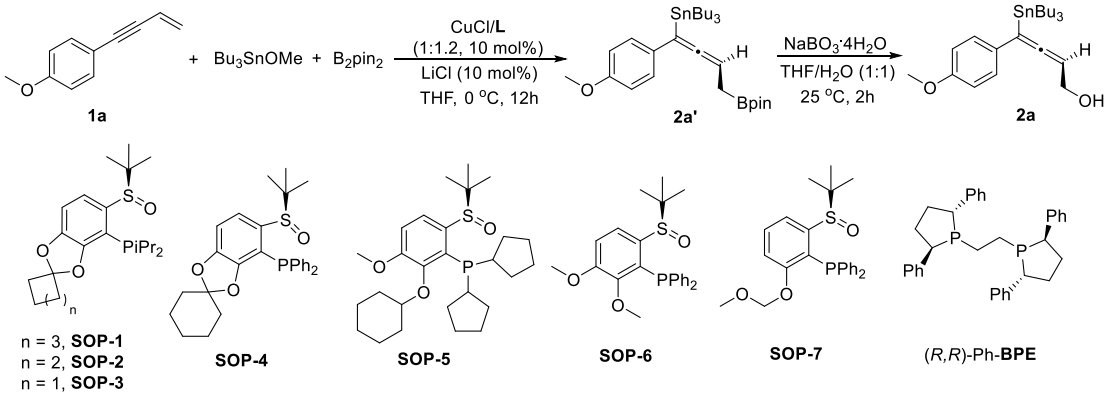
3-(3-phenylbut-3-en-1-yn-1-yl)thiophene (**1aj**)



Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.75-7.73 (m, 2H), 7.56-7.55 (m, 1H), 7.43-7.32 (m, 4H), 7.24-7.22 (m, 1H), 6.00 (d, *J* = 0.8 Hz, 1H), 5.77 (d, *J* = 0.8 Hz, 1H).

4. Optimization of reaction conditions

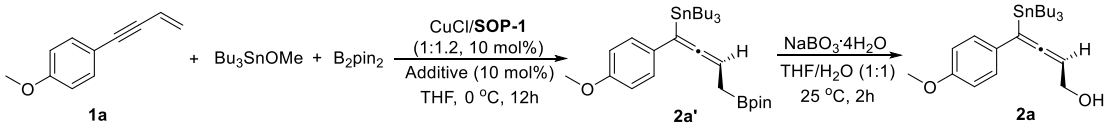
Table S1. Screening of ligands[a]



Entry	Ligand	Yield (%)[b]	*ee*(%)[c]
1	**SOP-1**	**97(73[d])**	**94(76[d])**
2	**SOP-2**	95(65)	91(75)
3	**SOP-3**	94(65)	88(83)
4	**SOP-4**	75(90)	82(75)
5	**SOP-5**	80(58)	88(84)
6	**SOP-6**	84(68)	92(82)
7	**SOP-7**	82(64)	85(79)
8	(*R*,*R*)-Ph-**BPE**	n.r.	n.d.

[a]Reactions were carried out with **1a** (0.2 mmol), Bu_3SnOMe (0.3 mmol), $(Bpin)_2$ (0.3 mmol), **L** (12 mol%), CuCl (10 mol%), with or without LiCI (10 mol%) in THF (1.0 mL) at 0°C for 12 h. [b]The yield of **2a'** was determined by crude ^1H NMR analysis with 2-methylnaphthalene as internal standard, n.r. = no reaction, n.d. = not determined. [c]The *ee* value of **2a** was determined by chiral HPLC analysis. [d]data in parenthese, no LiCI was added.

Table S2. Screening of additives[a]

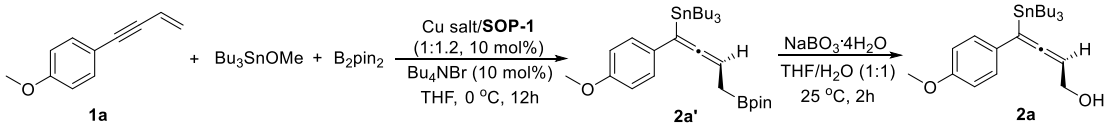


entry	additive	Yield (%)[b]	ee (%)[c]
1	LiCl	97	94
2	Ph_3PO	72	70
3	LiBr	95	92
4	KCl	64	80
5	$FeCl_2$	80	77
6	$MgCl_2$	54	78
7	$Bu_4NF{\cdot}3H_2O$	74	94
8	$Bu_4NCl{\cdot}H_2O$	95	96
9	**Bu_4NBr**	**99**	**96**
10	Bu_4NI	99	95

[a]Reactions were carried out with **1a** (0.2 mmol), Bu_3SnOMe (0.3 mmol), $(Bpin)_2$ (0.3 mmol), **SOP-1** (12 mol%), CuCl (10 mol%), additive (10 mol%) in THF (1.0 mL) at 0°C for 12 h. [b]The

yield of **2a'** was determined by crude ^{1}H NMR analysis with 2-methylnaphthalene as internal standard.[c]The *ee* value of **2a** was determined by chiral HPLC analysis.

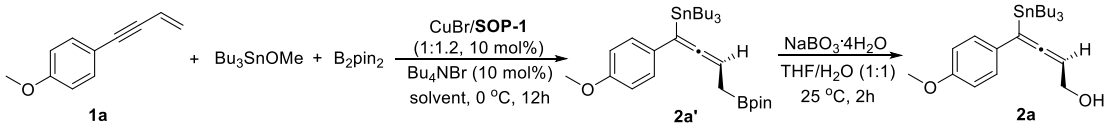
Table S3. Screening of copper salt[a]



Entry	Cu salt	Yield (%)[b]	ee (%)[c]
1	CuCl	99	96
2	**CuBr**	**99**	**97**
3	CuI	99	96
4	CuTc	97	95
5	$CuPF_6{\cdot}4CH_3CN$	98	96
6	$(CuOTf)_2{\cdot}C_7H_8$	80	96
7	CuOAc	98	96
8	$CuCl_2$	n.r.	n.d.

[a]Reactions were carried out with **1a** (0.2 mmol), Bu_3SnOMe (0.3 mmol), $(Bpin)_2$ (0.3 mmol), **SOP-1** (12 mol%), Cu salt (10 mol%), Bu_4NBr (10 mol%) in THF (1.0 mL) at 0^{o}C for 12 h. [b]The yield of **2a'** was determined by crude ^{1}H NMR analysis with 2-methylnaphthalene as internal standard, n.r. = no reaction, n.d. = not determined. [c]The *ee* value of **2a** was determined by chiral HPLC analysis.

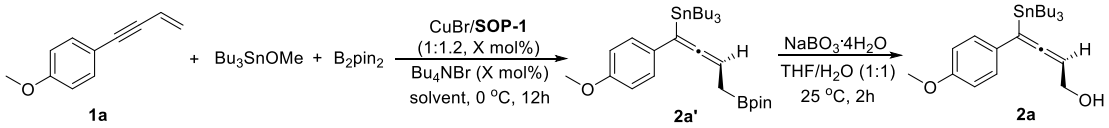
Table S4. Screening of solvent[a]



Entry	Solvent	Yield (%)[b]	ee (%)[c]
1	**THF**	**99**	**97**
2	2-Me-THF	99	96
3	CH_3CN	99	94
4	Toluene	99	96
5	1,4-Dioxane	99	96
6	$CHCl_3$	97	95
7	CH_2Cl_2	99	94
8	DMF	99	96
9	MTBE	99	97
10	DCE	99	92

[a]Reactions were carried out with **1a** (0.2 mmol), Bu_3SnOMe (0.3 mmol), $(Bpin)_2$ (0.3 mmol), **SOP-1** (12 mol%), CuBr (10 mol%), Bu_4NBr (10 mol%) in solvent (1.0 mL) at 0^{o}C for 12 h. [b]The yield of **2a'** was determined by crude ^{1}H NMR analysis with 2-methylnaphthalene as internal standard. [c]The *ee* value of **2a** was determined by chiral HPLC analysis.

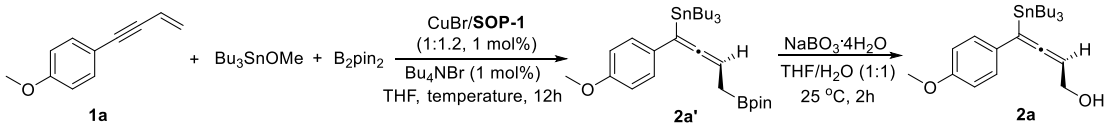
Table S5. Screening of catalyst loading[a]



entry	X	Yield (%)[b]	ee (%)[c]
1	10	99	97
2	5	99	97
3	2	99	97
4	**1**	**99**	**97**

[a]Reactions were carried out with **1a** (0.2 mmol), Bu_3SnOMe (0.3 mmol), $(Bpin)_2$ (0.3 mmol), **SOP-1** (1.2Xmol%), CuBr (X mol%), Bu_4NBr (X mol%) in THF (1.0 mL) at 0°C for 12 h. [b]The yield of **2a'** was determined by crude ^1H NMR analysis with 2-methylnaphthalene as internal standard. [c]The *ee* value of **2a** was determined by chiral HPLC analysis.

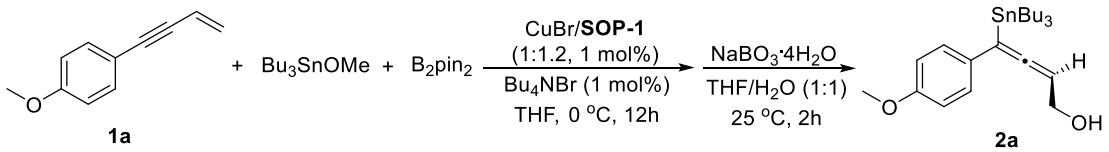
Table S6. Screening of reaction temperature[a]



Entry	Temperature	Yield (%)[b]	ee (%)[c]
1	25 °C	99	94
2	10°C	99	96
3	**0°C**	**99**	**97**
4	-10°C	99	96
5	-20°C	87	95

[a]Reactions were carried out with **1a** (0.2 mmol), Bu_3SnOMe (0.3 mmol), $(Bpin)_2$ (0.3 mmol), **SOP-1** (1.2 mol%), CuBr (1 mol%), Bu_4NBr (1 mol%) in THF (1.0 mL) for 12 h. [b]The yield of **2a'** was determined by crude ^1H NMR analysis with 2-methylnaphthalene as internal standard. [c]The *ee* value of **2a** was determined by chiral HPLC analysis.

5. General procedure for enantioselective 1,4-Borylstannation



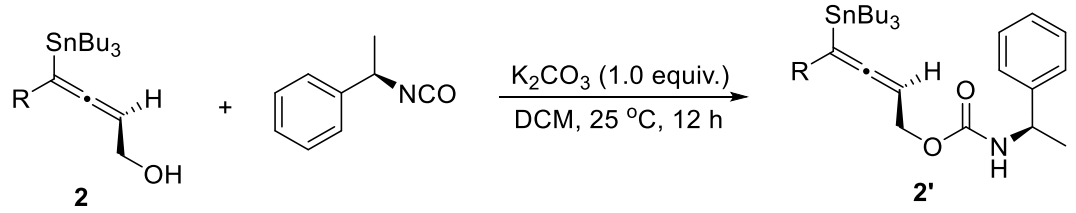
Step 1: In an argon-filled glovebox, a Schlenktube (**labeled asVial A**) equipped with magnetic stir bar was charged with CuB (2.8 mg, 0.02 mmol), **SOP-1** (9.8mg, 0.024 mmol), Bu_4NBr (6.3 mg, 0.02 mmol) and 1.0 mL dry THF, then the mixture was stirred at 40 ℃ for 30 minutes.

Step 2: The in-situ generated complex (0.1 mL, 1 mol%) (in **Vial A**), B_2pin_2 (75 mg, 0.3 mmol, 1.5 equiv.) and THF (0.9 mL) were added to anther tube (**labeled as Vial B**), then the mixture was removed from the glovebox and cooled to 0 ℃, **1** (0.2mmol) and Bu_3SnOMe (96 mg, 0.3 mmol, 1.5 equiv.) were added, and the resulting mixture was stirred for 12 hours at 0 °C. The reaction

mixture was filtrated through a celite pad, concentrated.Then, a 10 mL vial with a stir bar was charged the products, 2.0 mL THF, 2.0 mL H_2O and $NaBO_3 \cdot 4H_2O$ (200 mg, 1.3 mmol, 6.5 equiv.) were added, then stirred at 25 ℃ for 2hours. After the reaction was completed, the mixture was extracted with EtOAc (3*10 mL), dried over Na_2SO_4. The combined organic phase was evaporated under vacuo, purified by preparative TLC (silica gel, 20 × 20 cm, 2 mm), petro ether/Acetate (5/1) to get the product.

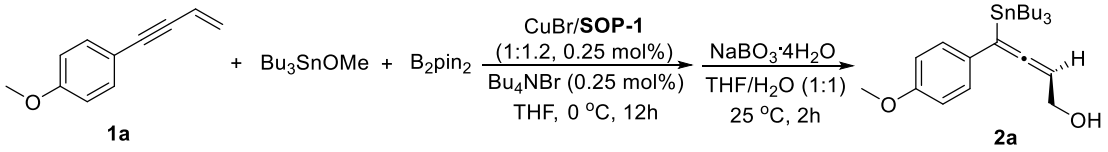
Note: Since the allene products are unstable, procedures involving allenes should be performed under 25 ℃

The ee values of part of products 2, which could not be directly determined, was determined by chiral HPLC analysis after a derivatization to 2'.



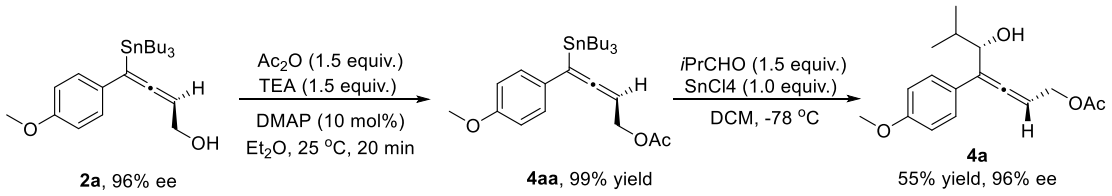
General procedure: 2 was added K_2CO_3 (1.0 equiv.), (*R*)-(1-isocyanatoethyl)benzene (2.0 equiv.) and CH_2Cl_2 (1.0 mL), the mixture was stirred at room temperature for 12 hours.The reaction mixture was filtrated through a celite pad, concentrated, and purified by preparative TLC (silica gel, 20 ×20 cm, 2 mm), petro ether/Acetate (6/1) to get the product **2'**.

6. Procedure for gram scale experiment



In an argon-filled glovebox, a Schlenk tube equipped with magnetic stir bar was charged with CuBr (2.8 mg, 0.02 mmol, 0.25 mol%), **SOP-1** (9.8 mg, 0.024 mmol,0.3 mol%), Bu_4NBr (6.3 mg, 0.02 mmol, 0.25 mol%) and 4.0 mL dry THF, then the mixture was stirred at 40 ℃ for 30 minutes. The in-situ generated complex was added B_2pin_2 (3 g, 1.5equiv.), **1a** (1.26 g, 8 mmol), and removed from the glovebox and cooled to 0 ℃, then Bu_3SnOMe (3.85 g, 1.5 equiv.) was added dropwise. The reaction was stirred at 0 ℃ for 24 hours. The reaction mixture was filtrated through a celite pad, concentrated, the crude product was added THF (30 mL), H_2O (30 mL) and $NaBO_3 \cdot 4H_2O$ (6.0 g, 39.2 mmol, 4.9 equiv.), and stirred at 25 ℃ for 2 hours. After the reaction was completed, the mixture was extracted with EtOAc (3*50 mL), dried over Na_2SO_4. The combined organic phase was evaporated under vacuo, purified by rapid silica gel chromatography on deactivated silica gel (PE/EA = 10/1)to give the desired product **2a** (3.45 g, 93% yield, 96% *ee*).

7. Procedure for Transformation[4]



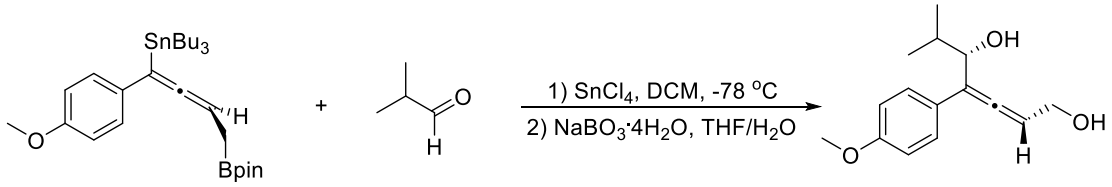
2a, 96% ee

4aa, 99% yield

4a
55% yield, 96% ee

2a (200 mg, 0.43 mmol, 96% *ee*) was added ether (2.0 mL), triethylamine (65 mg, 1.5 equiv.), 4-dimethylaminopyridine (5.2 mg, 10 mol%) and Ac_2O (65 mg, 1.5 equiv.) sequencently, then the mixture was stirred at 25 ^oC for 20 minutes. After the reaction was completed, the mixture wasconcentrated, the crude product was purified by flash column chromatography on silica gel (PE/EA = 10/1) to give the product **3a** (217 mg, 99% yield).

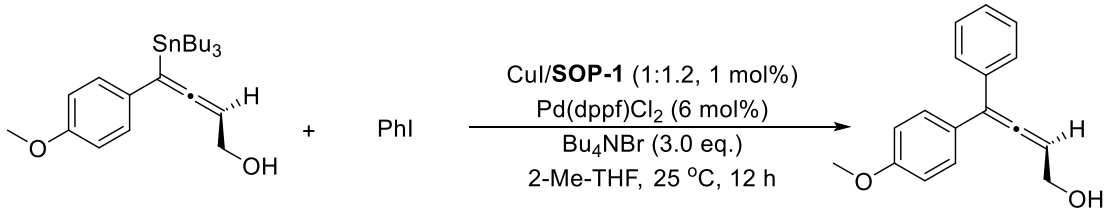
To a solution of **3a** (180 mg, 0.35 mmol) in CH_2Cl_2 (2 mL) was added $SnCl_4$ (1 M in hexane) (0.35 mL, 1.0 equiv.) at -78 ^oC. After 30 minutes, isobutyraldehyde (41 mg, 1.5 equiv.) was added. The mixture was stirred for 30 minutes at -78 ^oC, then quenched with saturated aqueous NH_4Cl (3 mL) and extracted with DCM (3*10 mL), dried over Na_2SO_4. The combined organic phase was evaporated under vacuo, purified by flash column chromatography on silica gel (PE/EA = 5/1) to give the product **4a** (56 mg, 55% yield, 96% *ee*)



2a', 96% *ee*

3a
63% yield, 96% *ee*, 4:1 dr

To a stirred solution of chiral bronic ester **2a'** (170 mg, 0.3 mmol) in DCM (2 mL), was added $SnCl_4$ (0.3 mL, 1.0 M in hexane, 0.3 mmol) dropwise at -78 ^oC. After 30 min., iPrCHO (33 mg, 0.45 mmol) in DCM (0.5 mL) was added, then, the reaction mixture was continued to stir at -78 ^oC for 30 min. Then the reaction was quenched with saturated aqueous NH_4Cl (3 mL) and extracted with DCM (3*10 mL), dried over Na_2SO_4. The combined organic phase was evaporated under vacuo, the crude product was added THF (3 mL), H_2O (3 mL) and $NaBO_3$ $4H_2O$ (180 mg, 1.2 mmol), and stirred at 25 ℃ for 2 hours. After the reaction was completed, the mixture was extracted with EtOAc (3*50 mL), dried over Na_2SO_4. The combined organic phase was evaporated under vacuo, purified by flash column chromatography on silica gel (PE/EA = 5:1 to 1/1) to give the product (47 mg, 63% yield, 96% ee, 4:1 dr).



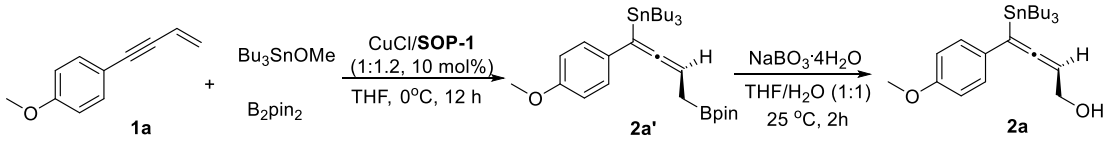
2a, 96% ee

5a, 53%, 60% ee

In an argon-filled glovebox, a Schlenk tube equipped with magnetic stir bar was charged with CuI (1.9 mg, 0.01 mmol, 1 mol%), **SOP-1** (4.9 mg, 0.012 mmol, 1.2 mol%), 1.0 mL dry 2-Me-THF,then the mixture was stirred at 40 ℃ for 30 minutes. The in-situ generated complex was added **2a** (47mg, 0.1 mmol), PhI (41 mg, 0.2 mmol, 2.0 eq.), $Pd(dppf)Cl_2$ (4.4 mg, 0.06 mmol,

6 mol%), Bu_4NBr (92 mg, 0.3 mmol, 3.0 eq.), the resulting mixture was then removed out from the glove-box, and stirred at 25 °C for 12 h. The reaction mixture was filtrated through a celite pad, concentrated, and purified by preparative TLC (silica gel, 20 × 20 cm, 2 mm), petro ether/Acetate (5/1) to get the product.

8. Control experiments



Experiment A: + 10 mol% **KBr** 48% yield, 78% ee

Experiment B: + 10 mol% **KBr** & 10 mol% **18-C-6** 87% yield, 96% ee

[a] Reactions were carried out with **1a** (0.2 mmol), Bu_3SnOMe (0.3 mmol), $(Bpin)_2$ (0.3 mmol), **SOP-1** (1.2 mol%), CuCl (10 mol%), KBr (10 mol%) in THF (1.0 mL) at 0 °C for 12 h. [b]The yield of **2a'** was determined by crude ^1H NMR analysis with 2-methylnaphthalene as internal standard. [c]The *ee* value of **2a** was determined by chiral HPLC analysis.

General procedure:

In an argon-filled glovebox, a Schlenk tube equipped with magnetic stir bar was charged with CuCl (2 mg, 0.02 mmol, 10 mol%), **SOP-1** (9.8 mg, 0.024 mmol, 10 mol%), KBr (2.4 mg, 10 mol%) and 1.0 mL dry THF, then the mixture was stirred at 40 ℃ for 30 minutes. The in-situ generated complex was added B_2pin_2 (75 mg, 1.5 equiv.) **with or without** 18-crown-6 (5.0 mg, 10 mol%), then the mixture was removed from the glovebox and cooled to 0 ℃, **1a** (32 mg, 0.2 mmol) and Bu_3SnOMe (96 mg, 1.5 equiv.) were added, and the resulting mixture was stirred for 12 hours at 0 °C. The reaction mixture was filtrated through a celite pad, concentrated, then the NMR yield of **2a'**was determined by crude ^1H NMR analysis with 2-methylnaphthalene as internal standard. The ee value was determined after oxidation to the oxidized allene product: a 10 mL vial with a stir bar was charged the crude product, 2.0 mL THF, 2.0 mL H_2O and $NaBO_3$ $4H_2O$ (200 mg, 1.3 mmol, 6.5 equiv.) were added, then stirred at 25 ℃ for 2 hours. After the reaction was completed, the mixture was extracted with EtOAc (3*10 mL), dried over Na_2SO_4. The combined organic phase was evaporated under vacuo, purified by preparative TLC (silica gel, 20 × 20 cm, 2 mm), petro ether/Acetate (5/1) to get the pure product.

9. Experimental Procedures for the Kinetic Studies

Procedures for determining the rate order of the reactants.

Step 1. In an argon-filled glovebox, a Schlenk tube equipped with magnetic stir bar was charged with CuBr (2.8 mg, 0.02 mmol), **SOP-1** (9.8 mg, 0.024 mmol), Bu_4NBr (6.3 mg, 0.02 mmol) and 1.0 mL dry THF, then the mixture was stirred at 40 ℃ for 30 minutes. (In-situ generated chiral complex, 0.02 M, in THF)

Step 2. 50 μL (1 mol%) of the above stock solution was added to a screw-capped vial, the solvent was evaporated. Then, THF-d8 (0.5 mL), **1a** (16 mg, 0.1 mmol), B_2pin_2 (38 mg, 0.15 mmol, 1.5 equiv.) were added.

Step 3. Bu_3SnOMe (48 mg, 0.15 mmol, 1.5 equiv.) was added to the vial. This time was set as time 0.

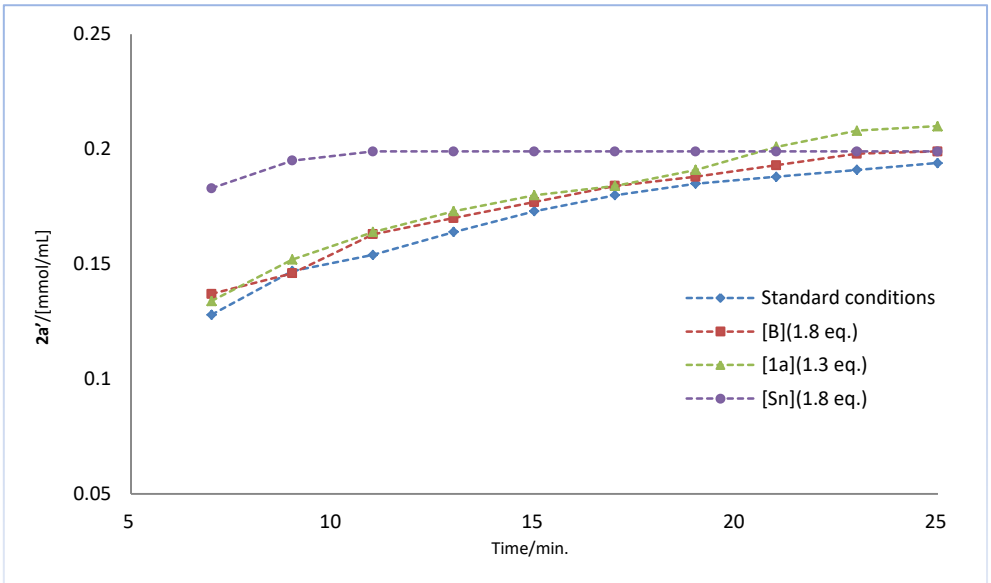
Step 4. Immediately after, 500 μL of the reaction mixture was then transferred into a NMR tube. Then, the NMR tube was removed out from the glovebox.

Step 5. ^1H NMR was recorded automatically at an internal of 25/26 seconds (NS = 4; DS = 2). The first data point was normally recorded at ~7 min.

Step 6. Step 2-5 were repeated, with a changed amount of **1a**, or Bu_3SnOMe, or B_2pin_2.

These procedures were conducted at 17 °C. Qualitatively identical conclusions could be drawn from these results.

Reaction profile of the 1,4-addition.



Procedures for determining the rate order of the chiral complex.

Step 1. In an argon-filled glovebox, a Schlenk tube equipped with magnetic stir bar was charged with CuBr (2.8 mg, 0.02 mmol), **SOP-1** (9.8 mg, 0.024 mmol), Bu_4NBr (6.3 mg, 0.02 mmol) and 1.0 mL dry THF, then the mixture was stirred at 40 ℃ for 30 minutes. (Chiral complex, 0.02 M, in THF)

Step 2. 50 μL (1 mol%) of the above stock solution was added to a screw-capped vial, the solvent was evaporated. Then, THF-d8 (0.5 mL), **1a** (16 mg, 0.1 mmol), B_2pin_2 (38 mg, 0.15 mmol, 1.5 equiv.) were added.

Step 3. Bu_3SnOMe (48 mg, 0.15 mmol, 1.5 equiv.) was added to the vial. This time was set as time 0.

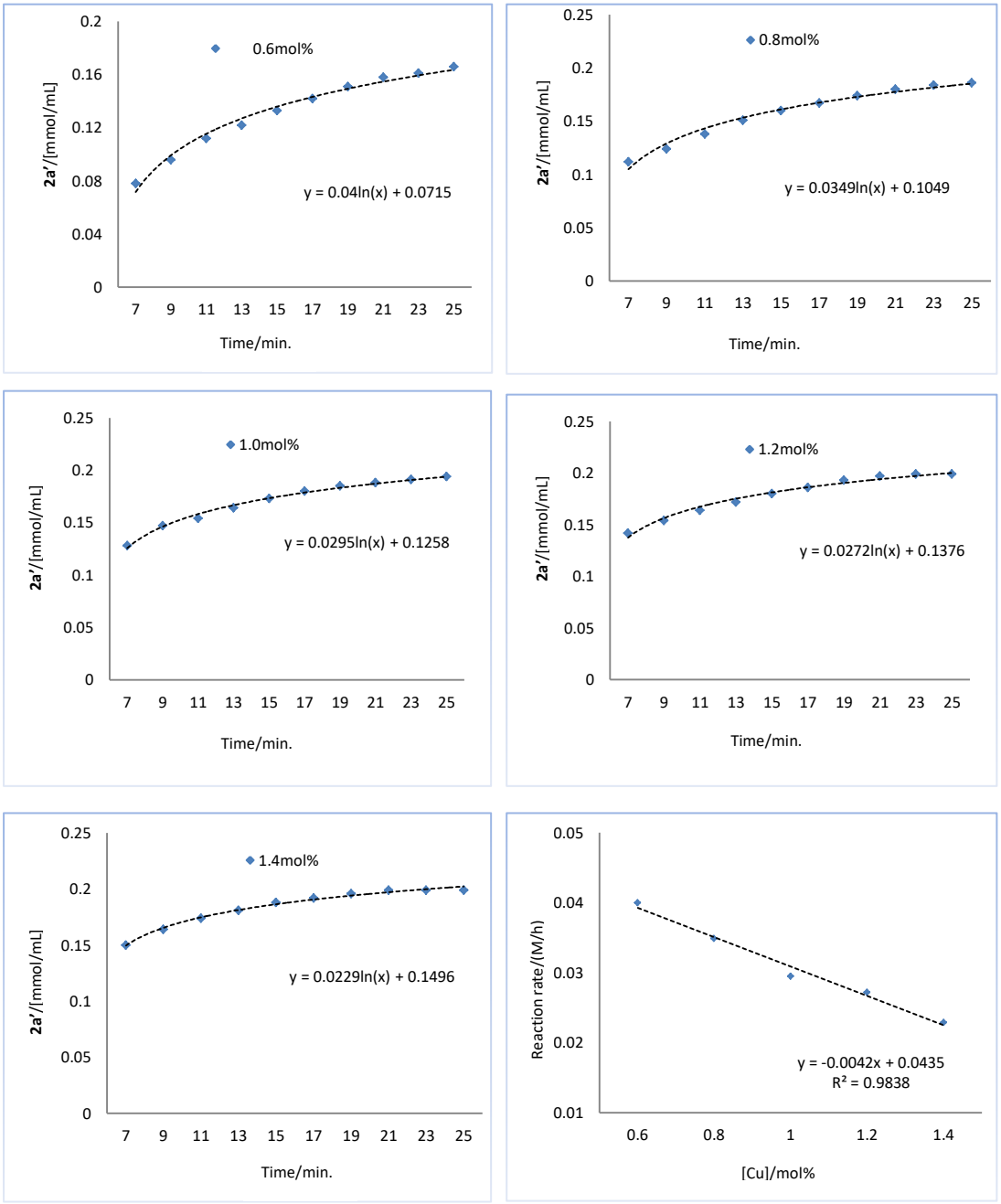
Step 4. Immediately after, 500 μL of the reaction mixture was then transferred into a NMR tube. Then, the NMR tube was removed out from the glovebox.

Step 5. ^1H NMR was recorded automatically at an internal of 25/26 seconds (NS = 4; DS = 2). The first data point was normally recorded at ~7 min.

Step 6. Step 2-5 was repeated, with a changed amount of catalyst loading.

These procedures were conducted at 17 °C. Qualitatively identical conclusions could be drawn from these results.

Rates determined while varying CuBr + SOP-1+Bu_4NBr together (1:1.2:1 molar ratio)



Procedures for reaction kinetics on Bu_4NBr.

Step 1. In an argon-filled glovebox, a Schlenk tube equipped with magnetic stir bar was charged with CuBr (2.8 mg, 0.02 mmol), **SOP-1** (9.8 mg, 0.024 mmol) and 1.0 mL dry THF, then the mixture was stirred at 40 ℃ for 30 minutes. (Chiral complex, 0.02 M, in THF)

In another a Schlenk tube, Bu_4NBr (6.3 mg, 0.02 mmol) and CH_3CN (1.0 mL) were added, the solution of Bu_4NBr in CH_3CN was prepared (0.02 M, in CH_3CN).

Step 2. 50 μL (1 mol%) of the above **SOP**/Cu solution in THF and 50 μL (1 mol%) Bu_4NBr solution in CH_3CN were added to a screw-capped vial, the solvent was evaporated. Then, THF-d8 (0.5 mL), **1a** (16 mg, 0.1 mmol), B_2pin_2 (38 mg, 0.15 mmol, 1.5 equiv.) were added.

Step 3. Bu_3SnOMe (48 mg, 0.15 mmol, 1.5 equiv.) was added to the vial. This time was set as

time 0.

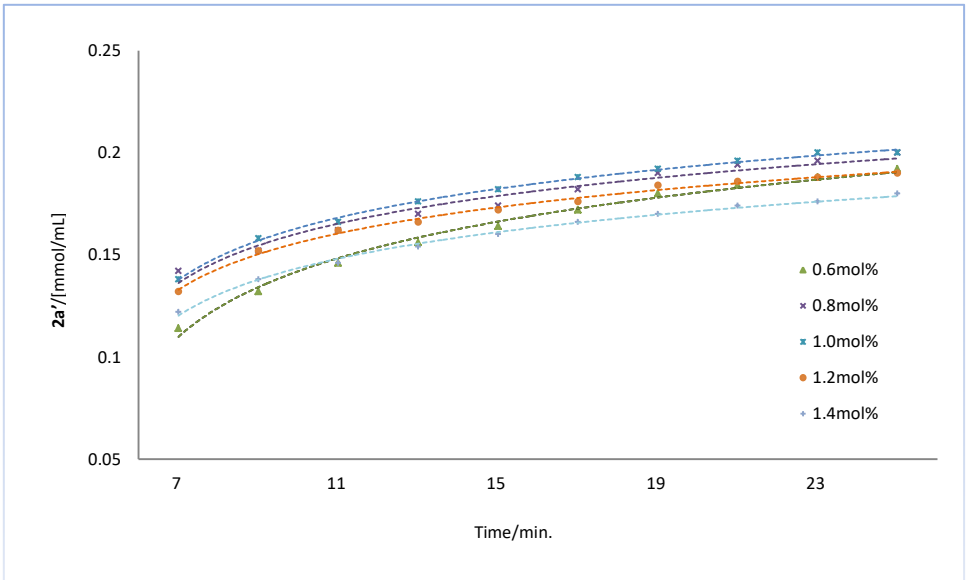
Step 4. Immediately after, 500 μL of the reaction mixture was then transferred into a NMR tube. Then, the NMR tube was removed out from the glovebox.

Step 5. ^{1}H NMR was recorded automatically at an internal of 25/26 seconds (NS = 4; DS = 2). The first data point was normally recorded at ~7 min.

Step 6. Steps 2-5 were repeated, with a changed amount of Bu_4NBr.

These procedures were conducted at 23 ^{o}C. Qualitatively identical conclusions could be drawn from these results.

Reaction profile on Bu_4NBr



Procedures for nonlinear effect experiments

Step 1: A Schlenktube (**labeled asVial A**) equipped with magnetic stir bar was charged with CuBr (2.8 mg, 0.02 mmol), **SOP-1** or/and (*S*)-**SOP-1** (9.8 mg in total, 0.024 mmol), Bu_4NBr (6.3 mg, 0.02 mmol) and 1.0 mL dry THF, then the mixture was stirred at 40 ℃ for 30 minutes.

Step 2: The in-situ generated complex (0.1 mL, 1 mol%) (in **Vial A**), B_2pin_2 (75 mg, 0.3 mmol, 1.5 equiv.) and THF (0.9 mL) were added to anther tube (**labeled as Vial B**), then the mixture was removed from the glovebox and cooled to 0 ℃, **1** (0.2mmol) and Bu_3SnOMe (96 mg, 0.3 mmol, 1.5 equiv.) were added, and the resulting mixture was stirred for 12 hours at 0 ^{o}C. The reaction mixture was filtrated through a celite pad, concentrated. The yield was determined by crude ^{1}H NMR. Then, a 10 mL vial with a stir bar was charged the products, 2.0 mL THF, 2.0 mL H_2O and $NaBO_3 \cdot 4H_2O$ (200 mg, 1.3 mmol, 6.5 equiv.) were added, then stirred at 25 ℃ for 2 hours. After the reaction was completed, the mixture was extracted with EtOAc (3*10 mL), dried over Na_2SO_4. The combined organic phase was evaporated under vacuo, purified by preparative TLC (silica gel, 20 × 20 cm, 2 mm), petro ether/Acetate (5/1) to get the product to determine the ee value.

Step 3. Steps 1-2 were repeated, with a changed amount of **SOP-1** and (*S*)-**SOP-1**.

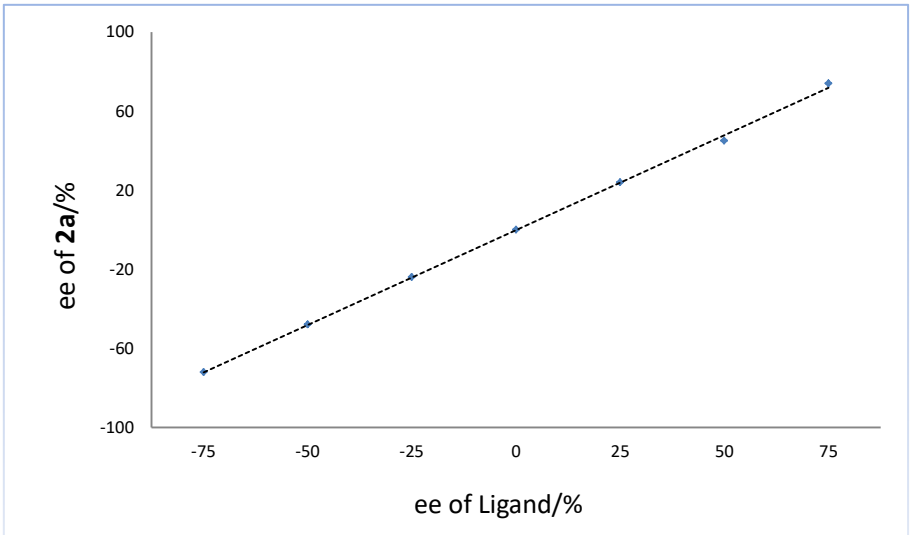
Qualitatively identical conclusions could be drawn from these results.

ee values and yields with different ee values of ligand

Entry	ee of ligand (%)	Yield of **2a'** (%)	ee of 2a (%)
1	75 (*R*)	>99	74 (*S*)
2	50	>99	45

3	25	>99	24
4	0	>99	0
5	-25	>99	-24
6	-50	>99	-48
7	-75 (*S*)	>99	-72 (*R*)

Nonlinear effect of the 1,4-addition



Reference

1 a) D. Wang, P. Cao, B. Wang, T. Jia, Y. Lou, M. Wang, J. Liao, *Org. Lett.* **2015**, *17*, 2420. b) Y. Lou, P. Cao, T. Jia, Y. Zhang, M. Wang, J. Liao, *Angew. Chem. Int. Ed.* **2015**, *54*, 12134. c) T. Jia, P. Cao, B. Wang, Y. Z. Lou, X. M. Yin, M. Wang, J. Liao, *J. Am. Chem. Soc.* **2015**, *137*, 13760. d) F. Lang, G. Chen, L. Li, J. Xing, F. Han, L. Cun, J. Liao, *Chem. Eur. J.* **2011**, *17*, 5242.

2 a) F. Meng, F. Haeffner, A.-H. Hoveyda, *J. Am. Chem. Soc.* **2014**, *136*, 11304. b) Y. Lan, X. Chang, P. Fan, C. Shan, Z. Liu, T.-P. Loh, Y.-He. Xu, *ACS Catal.* **2017**, *7*, 7120. c) Y. Zhang, B. Yu, B. Gao, T. Zhang, H. Huang, *Org. Lett.* **2019**, *21*, 535. d) N. Adamson, H. Jeddi, S.-J. Malcolmson, *J. Am. Chem. Soc.* **2019**, *141*, 8574. e) L.-B. Romero, S.-L. Buchwald, *J. Am. Chem. Soc.* **2019**, *141*, 13788. f) H.-L. Sang, S. Yu, S. Ge, *Org. Chem. Front.* **2018**, *5*, 1284. g) A. Tikad, A. Hamze, O. Provot, J.-D. Brion, M. Alami, *Eur. J. Org. Chem.* **2010**, 725. h) X. Chang, Z. Liu, Y. Luo, C. Yang, X. Liu, B. Da, J. Li, T. Ahmad, T. Loh, Y. Xu, *Chem. Commun.* **2017**, *53*, 9344. i) Y. Liao, X. M. Yin, X. H. Wang, W. Z. Yu, D. M. Fang, L. R. Hu, M. Wang, J. Liao, *Angew. Chem. Int. Ed.* **2020**, *59*, 1176 –1180.

3. X. Zhu, W. Deng, M. Chiou, C. Ye, W. Jian, Y. Zeng, Y. Jiao, L. Ge. Y. Li, X. Zhang, H. Bao, *J. Am. Chem. Soc.* **2019**, *141*, 548.

4. J. A. Marshall, J. Perkins, *J. Org. Chem.* **1994**, *59*, 3509.

10.Density functional theory (DFT) calculations

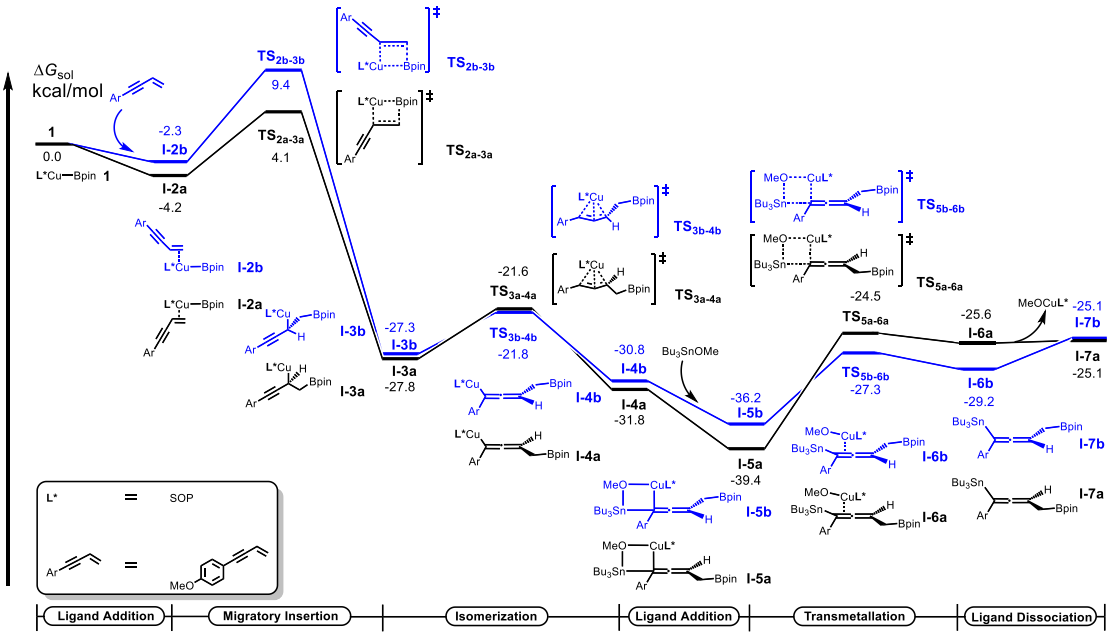


Figure X1. DFT-calculated energy profile of the enantioselective 1,4-addition reaction of 1,3-enynes without additives (**1** has been set as the zero point of energy)

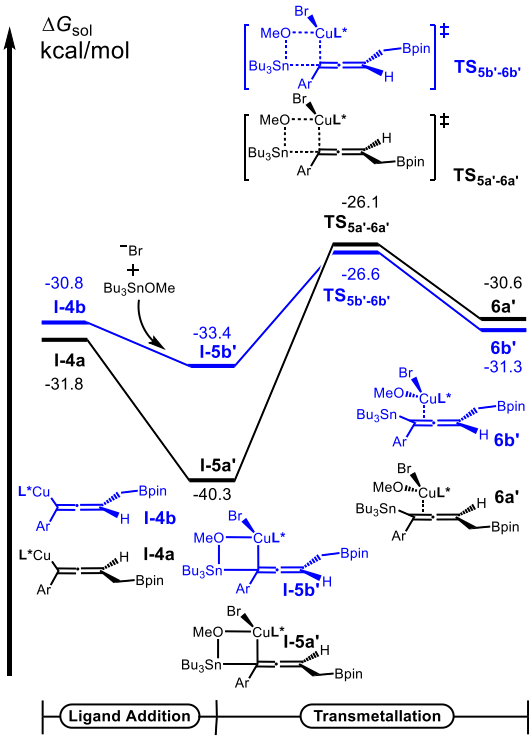


Figure X2. DFT-calculated energy profile of the enantioselective 1,4-addition reaction of 1,3-enynes with bromide anion (**1** has been set as the zero point of energy)

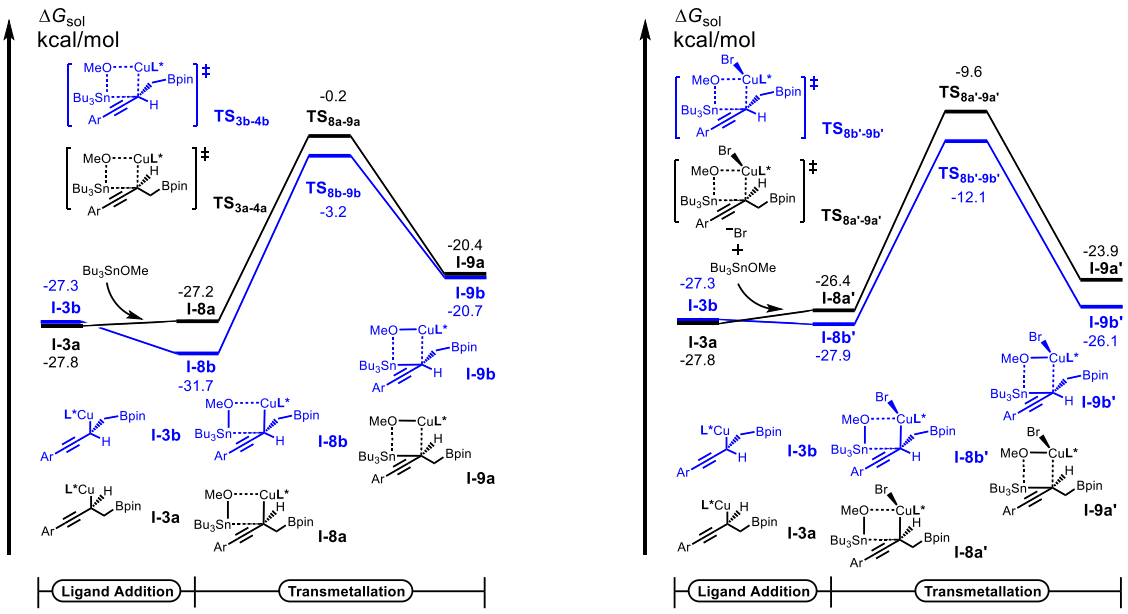


Figure X3. DFT-calculated energy profile of transmetallation happened before isomerization with and without bromide anion (**1** has been set as the zero point of energy)

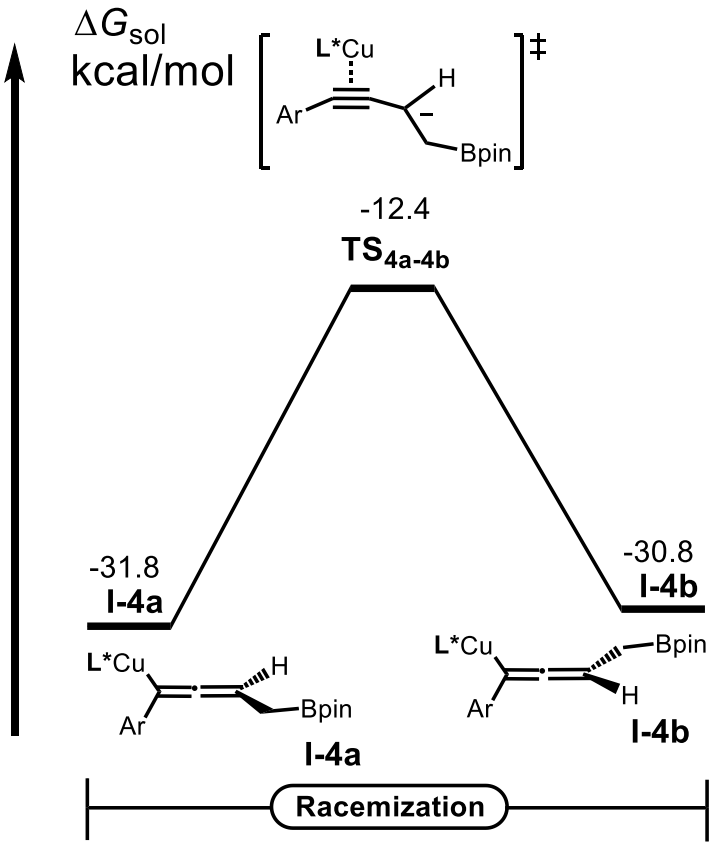


Figure X4. DFT-calculated energy profile of axially chiral allenylcopper intermediate **4a** racemization without bromide anion (**1** has been set as the zero point of energy)

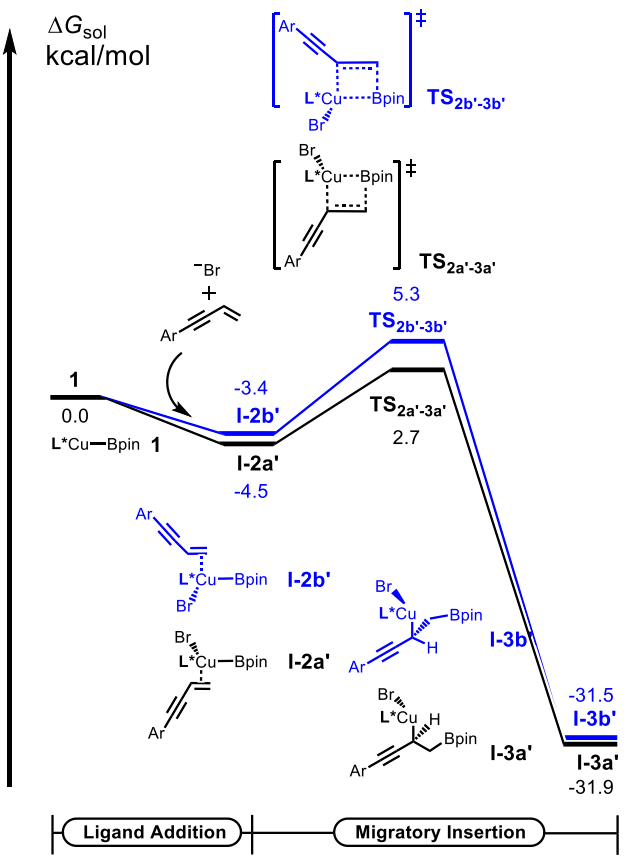
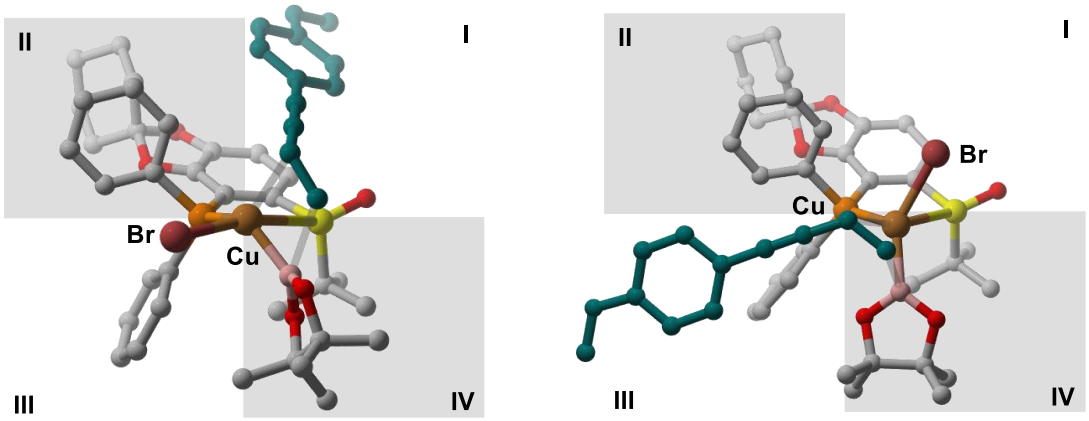


Figure X5. DFT-calculated energy profile of enantio-determining step with bromide anion (**1** has been set as the zero point of energy)



$TS_{2\text{-}3a'}$-favored
(*Re*)-face attack
$\Delta G_{sol}^{\ddagger}$= 2.7 kcal/mol

$TS_{2\text{-}3b'}$-disfavored
(*Si*)-face attack
$\Delta G_{sol}^{\ddagger}$= 5.3 kcal/mol

Figure X6. Enatioselectivity-determining migratory insertion step transition states with bromide anion

DFT calculation has been conducted to give more details on the mechanism and origin of chemoselectivity. Figure X1 shows the most preferred enantioselective 1,4-addition energy profile

of 1,3-enyne without additives. Calculation results revealed that the initial 1,3-enyne migratory insertion is irreversible. Thus, it is the enantio-determining step for this reaction. The migratory insertion transition state (**$TS_{2a\text{-}3a}$**) leading to the preferential formation of the (S)-propargylcopper intermediate **I-3a** has an activation free energy that is 5.3 kcal/mol lower than the disfavored transition state **$TS_{2b\text{-}3b}$**. Previous research works also proposed a similar enantioselective hydrocupration step of 1,3-enyne in their theoretical calculations.[*J. Am. Chem. Soc.* **2018**, *140*, 2643−2655.; *Science* **2016**, *353*, 144-150.; *Commun. Chem.*, **2018**, *1*, 64. *Angew. Chem. Int. Ed.* **2020**, *59*, 1176–1180.] Then the highly enantioenriched propargylcopper **I-3a** isomerized to an axially chiral allenylcopper intermediate **I-4a** in a stereospecific fashion. Finally, coordination of **I-4a** with Bu_3SnOMe complex followed by transmetallation and afforded the final product of axially chiral allenylpalladium **I-6a**. DFT calculations show that the reaction leading to the major diastereomer **I-6a** is an exothermic process with ca. 25.6 kcal/mol, and the rate-limiting step of the mechanism is the transmetallation of **I-5a** with an energy barrier of 14.9 kcal/mol. And the minor diastereomer **I-6b** has been predicted energetically unfavorable for the enantio-determining step (e.g., the migratory insertion transition states **$TS_{2b\text{-}3b}$** is energetically higher than **$TS_{2a\text{-}3a}$** of 5.3 kcal/mol).

Owing to the experimental results show that the significant role of bromide anion played in promoting enantioselective and yield of this reaction. The effect of bromide anion on the reaction mechanism has been carefully analyzed and presented in Figure X1 and X2. It shows that bromide anion will stabilize **I-5a** with 0.9 kcal/mol after coordinating an additional bromide anion and forming **I-5a'**. Synergistically **I-5b** has been destabilized with 2.8 kcal/mol after coordinating with a bromide anion (energy rising from -36.2 kcal/mol for **I-5b** to -33.4 kcal/mol for **I-5b'**). The synergistic stabilization and destabilization effects can also be observed at transmetallation transition states and products. Moreover, bromide anion will also reduce the energy barrier from **I-5a** to **I-6a** with 0.7 kcal/mol (transmetallation energy barriers with bromide anion reducing from 14.9 kcal/mol for without bromide anion to 14.2 kcal/mol), which is the rate-determine step for this reaction. All these effects of bromide anion make the formation of desired product **I-6a'** much easier both thermodynamically and kinetically.

In addition, we also calculated the potential epimerization pathways from **I-4a** to **I-4b** (Figure X4). It turns out that the racemization steps have much higher energy barriers

(19.4 kcal/mol from **I-4a** to **I-4b**) than the rate-limiting step of the enantioselective 1,4-addition reactions. Thus, the racemization process of **I-4a** is energetically unfavorable and the **I-3a** generated from the enantio-determining step will proceed in a stereospecific fashion to produce the final enantioselective product **I-7a**. And the potential pathways of transmetallation that happened before isomerization with and without bromide anion (Figure X3) have also been carefully checked to be unfavorable in comparison with isomerization from **I-3a** to **I-4a**.

1. Computational details

If there are no special statements, all structures were optimized at B3LYP[S1] level of theory in gas phase with Def2SVP[S2] basis set for all atoms in combination with the corresponding Stuttgart relativistic small-core ECP[S3] basis set for tin. Empirical dispersion correction has been considered by using Grimme's DFT empirical dispersion correction with the Becke-Jonson (D3BJ) damping function.[S4] Optimized minima and transition states (TSs) were verified at the same level of theory by harmonic vibrational analysis to have no and one proper imaginary frequency, respectively. To refine the calculated energy, single point calculation with larger basis set were then done based on these optimized structures, by using MN15 functional[S5] with the Def2TZVPP basis set for all atoms in combination with the corresponding Stuttgart relativistic small-core ECP basis set for tin. The solvent effect was modelled in these single point calculations by employing SMD continuum solvation model,[S6] taking tetrahydrofuran as the solvent for each reaction. The reported free energies in this work were based on the electronic energy of single point calculations, including the Gibbs free energy thermal correction obtained from vibrational analysis in gas phase at 0℃, as well as DFT-D3(BJ) empirical dispersion correction.[S4] The protocol introduced by Martin and coworkers[S7], which has been proved to be very robust and given reasonable results in a lot of theoretical calculations,[S8] has been used to reduce the overestimation of entropy. These corrections are based on the consideration of a pressure at which the ideal gas density matches that for the solvent used in experiments (in this case, tetrahydrofuran). Martin and coworkers proposed to determine the pressure (from $P = nRT/V = \rho RT/M$) applicable at the concentration of the solvent used from its experimental density. By applying this approximation for the solvent tetrahydrofuran (ρ = 889.2 kg m^{-3}) with reaction temperature 0℃ we obtained a pressure of 276.4 atm, which is

used for adjusting the solvent concentration of the gas-phase entropies. Thus, the pressure 276.4 atm is incorporated then to the calculation of the translational partition function in equation 1, which has been used to calculate the translational entropy S_{trans} in electronic-structure calculations. All DFT geometry optimizations and single point calculations were performed with Gaussian 09 program.[S9]

$$q_{trans} = \left(\frac{2\pi mRT}{h^2}\right)^{1.5} \frac{RT}{P} \qquad \text{eq. 1}$$

CAM-B3LYP/Def2SVP[S10] has been adopted to optimize all the structures for the ECD spectrum calculations in combination with D3 dispersion corrections with Becke-Johnson damping scheme (D3BJ).[S4] Solvent effect was included by using polarizable continuum model[S11] (PCM) with solvent parameters of methanol. CD spectra were calculated by TDDFT at the CAM-B3LYP/Def2SVP level.

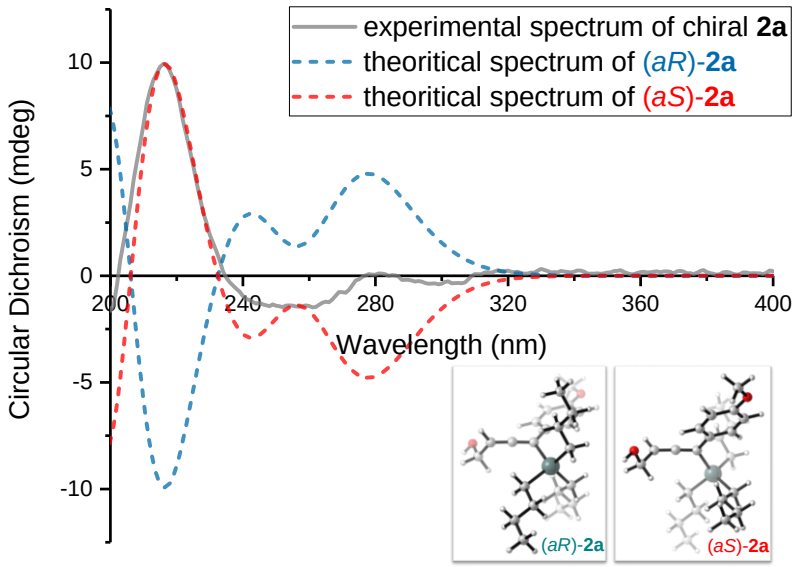


Figure X7. Experimental *vs* simulated ECD Spectra of chiral-**2a**.

(S1) (a) Lee, C. T.; Yang, W. T.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785–798. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648–5652.

(S2) Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.

(S3) (a) Andrae, D.; Haeussermann, U.; Dolg, M.; Stoll, H.; Preuss, H. *Theor. Chim. Acta*, **1990**, *77*, 123–141. (b) Eichkorn, K.; Weigend, F.; Treutler, O.; Ahlrichs, R. *Theor. Chem. Acc.* **1997**, *97*, 119–124. (c) Peterson, K. A.; Figgen, D.; Goll, E.; Stoll, H.; Dolg, M. *J. Chem. Phys.* **2003**, *119*, 11113–11123.

(S4) (a) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104; (b) Grimme, S.; Ehrlich, S.; Goerigk, L. *J. Compt. Chem.* **2011**, *32*, 1456–1465.

(S5) Yu, H. S.; He, X.; Li, S. L.; Truhlar, D. G. *Chem. Sci.* **2016**, *7*, 5032−5051.

(S6) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378–6396.

(S7) Martin, R. L.; Hay, P. J.; Pratt, L. R. *J. Phys. Chem. A* **1998**, *102*, 3565−3573.

(S8) (a) González Fabra, J.; Castro-Gómez, F.; Sameera, W. M. C.; Nyman, G.; Kleij, A. W.; Bo, C. *Catal. Sci. Technol.* **2019**, *9*, 5433−5440. (b) Maquilón, C.; Limburg, B.; Laserna, V.; Garay-Ruiz, D.; Gonzáez-Fabra, J.; Bo, C.; Martínez Belmonte, M.; Escudero-Adán, E. C.; Kleij, A. W. *Organometallics* **2020,** *39*, 1642−1651. (c) Qu, S.; Dang, Y.; Song, C.; Wen, M.; Huang, K.-W.; Wang, Z.-X. *J. Am. Chem. Soc.* **2014**, *136*, 4974−4991. (d) Wang, Y.; Ling, B.; Liu, P.; Bi, S. *Organometallics* **2018,** *37*, 3035−3044.

(S9) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc.: Wallingford, CT, 2009.

(S10) (a) Yanai, T.; Tew, D. P.; Handy, N. C. *Chem. Phys. Lett.* **2004**, *393*, 51−57.

(S11) (a) Cancès, E.; Mennucci, B.; Tomasi, J. *J. Chem. Phys.* **1997**, *107*, 3032−3041. (b) Tomasi, J.; Mennucci, B.; Cancès, E. *J. Mol. Struct. (Theochem)* **1999**, *464*, 211−226.

2. Cartesian coordinates for the optimized structures

1				C	6.55344500	-0.82232900	6.10836000
Cu	7.78138500	4.77353600	5.03292000	C	7.80924000	-0.97792400	5.54594100
C	5.99174000	0.46674500	6.07126200	C	8.49058500	0.09835400	4.96389800

C	7.97626900	1.38765900	4.93192200	C	10.38345500	-2.58857900	3.93213600
C	6.67673700	1.52871600	5.48533900	C	10.84313300	-1.60037700	6.22355400
O	4.92808000	3.07991000	6.78238000	C	10.68792300	-3.98691300	4.48164600
P	8.96548200	2.88568500	4.50577700	H	11.29336100	-2.13485600	3.50613900
B	7.44654100	6.64332900	4.39259800	H	9.62095400	-2.61845600	3.13909300
S	5.91754300	3.18129100	5.64266900	C	11.14639500	-3.00007900	6.76610500
O	9.69635500	-0.33493800	4.50523000	H	11.76383500	-1.10045100	5.88171000
O	8.58112400	-2.09443100	5.47727100	H	10.39692900	-0.95051500	6.99181800
H	6.03826200	-1.66008800	6.57992200	C	11.66704700	-3.92431600	5.65956900
H	5.02929200	0.67351600	6.54265700	H	11.08806200	-4.62164600	3.67543100
C	4.85638000	3.29056900	4.05883200	H	9.74367000	-4.45072900	4.81300700
C	4.13580900	4.63204300	4.22382900	H	11.87453000	-2.92989600	7.58950000
H	3.58200100	4.66242200	5.17297000	H	10.22239800	-3.42483900	7.19321700
H	3.42048400	4.75621600	3.39476200	H	11.84415900	-4.93566700	6.05923200
H	4.85017000	5.46650000	4.18790700	H	12.64467100	-3.55184000	5.30243900
C	3.87596700	2.12620400	4.07058900	C	10.56806500	2.45973000	5.28736700
H	4.37581700	1.16519200	3.88162100	C	11.77038200	2.35890000	4.57710700
H	3.12467700	2.28076300	3.27922900	C	10.56987700	2.25983600	6.67810300
H	3.35201700	2.07556000	5.03665100	C	12.95532700	2.03932400	5.24682900
C	5.77202200	3.29670200	2.84314800	H	11.78109200	2.51729400	3.49773700
H	6.45349800	4.15948000	2.86299500	C	11.75164500	1.93247000	7.34188900
H	5.15470000	3.39106000	1.93442200	H	9.63735900	2.35329000	7.24171500
H	6.35478000	2.36844200	2.75230600	C	12.94885000	1.81817300	6.62619600
C	6.93574100	8.14597300	2.69614900	H	13.88863600	1.95984400	4.68396300
C	7.11325700	8.90736800	4.05729100	H	11.74063700	1.77236100	8.42269300
O	7.72833500	7.90309500	4.89334900	H	13.87612300	1.56607800	7.14614400
O	6.84381900	6.77377800	3.13235100	C	9.26717100	2.84419100	2.69847800
C	8.02461300	10.12763500	3.99772600	C	9.60234900	1.67402100	1.99589400
H	7.62789100	10.88252800	3.30002000	C	9.13446400	4.05634200	2.00067600
H	8.09271100	10.58625800	4.99557100	C	9.80448200	1.72289400	0.61531900
H	9.04091700	9.85662800	3.68417100	H	9.71432000	0.72993500	2.52910700
C	5.77932100	9.28132600	4.71184400	C	9.34243800	4.09824700	0.61998100
H	5.97270300	9.59929300	5.74668800	H	8.84072100	4.95986800	2.54042000
H	5.27494900	10.10338100	4.18134300	C	9.67681400	2.93351700	-0.07455100
H	5.10234800	8.41559500	4.74772000	H	10.06313400	0.80945400	0.07399900
C	5.67874800	8.50434800	1.91257400	H	9.23206700	5.04624000	0.08827500
H	5.67618600	9.57050500	1.63492100	H	9.83475000	2.96587300	-1.15541700
H	5.63790600	7.91020000	0.98687300				
H	4.77020100	8.28946500	2.48950900	**I-2a**			
C	8.16583800	8.24205600	1.78686800	Cu	5.02278300	10.04246300	9.71829000
H	8.05631700	7.51195700	0.97044000	C	3.08352400	5.65921400	8.80494100
H	8.27829600	9.24330900	1.34402900	C	3.68488300	4.40279100	8.62835100
H	9.08269100	7.99661000	2.34197300	C	5.05162600	4.39172100	8.42730700
C	9.89576100	-1.66458600	5.03129100	C	5.79953000	5.57466400	8.37932900

C	5.23672800	6.83308000	8.56081200	H	1.73111300	6.03544500	11.83901900
C	3.83069800	6.83285000	8.75959300	H	5.87983800	4.91441800	12.09387300
O	1.75755800	7.97016900	10.01571000	H	5.28665500	2.54540700	11.77366900
P	6.23327700	8.37510900	8.69755300	O	2.72484000	1.66346400	11.39980100
B	4.87542600	11.79596000	8.71568700	C	3.68811100	0.64996200	11.23004500
S	2.95084200	8.37098400	9.16813500	H	4.37761600	0.87984000	10.39695100
O	7.10355300	5.26356300	8.13317600	H	3.13836000	-0.27173100	10.99751500
O	5.87702800	3.32383900	8.25952200	H	4.28358000	0.48870900	12.14689500
H	3.11142100	3.47856000	8.69147000	C	2.15417200	3.92285900	11.69961300
H	2.02233600	5.73332100	9.03884500	C	2.49461400	5.25711600	11.86463600
C	2.20675600	8.85052000	7.48137100	C	3.84931100	5.64241900	11.99278600
C	1.39781500	10.10872000	7.81092800	C	4.83104600	4.63398600	11.98237100
H	0.66307200	9.89575200	8.60078900	C	4.49468500	3.29274900	11.80347900
H	0.85222700	10.42628200	6.90682600	C	3.14962100	2.93139100	11.64001600
H	2.05001100	10.93642400	8.12132300	C	4.22832700	7.00968600	12.04536900
C	1.29485700	7.72678700	7.00651100	C	4.60960300	8.16794800	11.97442200
H	1.86039600	6.83782300	6.69350500	C	5.14617100	9.47245900	11.84907300
H	0.71318300	8.08160300	6.14010600	C	4.41611900	10.63846400	11.62681100
H	0.58889200	7.44423900	7.80142400	H	4.87737500	11.60830300	11.81477300
C	3.34678800	9.13867700	6.51484700	H	3.32405500	10.60909100	11.59247800
H	4.02866300	9.89648200	6.92266300	H	6.21608300	9.56693500	12.07452800
H	2.93161300	9.53407600	5.57329800	C	7.23512400	3.84006700	8.30838300
H	3.92148700	8.23349000	6.27279600	C	8.04110900	3.24747500	7.16876800
C	5.54300300	13.85421900	7.87607500	C	7.83717100	3.54706400	9.67796900
C	4.15273900	13.45399700	7.26682300	C	8.25800800	1.74367500	7.37334600
O	3.75321300	12.36232800	8.12628300	H	9.00590000	3.77975400	7.14171900
O	5.97873400	12.61249800	8.47652500	H	7.51642400	3.45857100	6.22469600
C	3.08675400	14.54102100	7.32065200	C	8.04937800	2.04431400	9.87832400
H	3.40019800	15.42854700	6.74827400	H	8.79157000	4.09375500	9.74043200
H	2.15134200	14.16409300	6.88043800	H	7.17315300	3.97210400	10.44379000
H	2.87326500	14.84484600	8.35322300	C	8.88517900	1.44658300	8.74058300
C	4.25731300	12.88913900	5.84641100	H	8.88836100	1.34628100	6.56228100
H	3.29329400	12.43467700	5.57490100	H	7.28323600	1.23290200	7.29823200
H	4.49129300	13.67207900	5.10931700	H	8.53041500	1.86161400	10.85238000
H	5.02605000	12.10581000	5.78557400	H	7.06517100	1.54633700	9.91030800
C	6.58547300	14.30321600	6.85933400	H	8.99691700	0.35899200	8.87811800
H	6.25248100	15.20841100	6.32729600	H	9.90391400	1.87398400	8.77545800
H	7.52890400	14.53698800	7.37506300	C	7.77891300	7.77146600	9.49308300
H	6.79003600	13.51942400	6.11879300	C	9.03242600	7.87526500	8.87652500
C	5.43228000	14.88325500	9.00442000	C	7.68710400	7.20316700	10.77402300
H	6.40052600	14.94446300	9.52264100	C	10.17637600	7.40399200	9.52701400
H	5.17546800	15.88408900	8.62560800	H	9.11703300	8.31052100	7.87995100
H	4.67334000	14.57970800	9.73970300	C	8.82974400	6.72517400	11.41539100
H	1.11358500	3.61710300	11.57506200	H	6.71500800	7.12179500	11.26229100

C	10.07929900	6.82252900	10.79367800	H	4.03041700	8.03435200	6.10987300
H	11.14899900	7.48816300	9.03584600	C	4.92905800	14.15475100	8.51182900
H	8.74320500	6.27749600	12.40870200	C	4.99149200	13.60830600	7.04103800
H	10.97502600	6.45236300	11.29838100	O	4.72301700	12.20323300	7.23074600
C	6.76524600	8.75427700	6.98233100	O	5.28580000	12.98837300	9.28451500
C	7.12202700	10.08078300	6.69254600	C	3.95057700	14.18833200	6.09101500
C	6.83095700	7.78483100	5.97018200	H	4.07312700	15.27827400	5.98713500
C	7.54294700	10.42714000	5.40570000	H	4.06626400	13.73482900	5.09485900
H	7.05091500	10.85089000	7.46305000	H	2.93003300	13.98066100	6.43713800
C	7.23874400	8.14009400	4.68263600	C	6.38710100	13.71619900	6.41740000
H	6.57020900	6.74900500	6.18545500	H	6.40269200	13.12555100	5.48910000
C	7.59582200	9.46150400	4.39711900	H	6.65248100	14.75544000	6.17101200
H	7.82082100	11.46184700	5.19099500	H	7.15184200	13.30760500	7.09355100
H	7.27848600	7.37989700	3.89867200	C	5.91151300	15.27729600	8.82386000
H	7.91378000	9.73727200	3.38868500	H	5.72118600	16.15682100	8.18811500
				H	5.79932500	15.58498800	9.87443800
I-2b				H	6.95064500	14.95530000	8.67838100
Cu	5.08365400	9.93742500	9.22831400	C	3.51518200	14.56181500	8.93970800
C	2.99292900	5.72291000	8.86221400	H	3.50753700	14.71492300	10.02887900
C	3.47840000	4.40643800	8.77926400	H	3.18827000	15.49382800	8.45397000
C	4.82978000	4.25344900	8.53083500	H	2.79002600	13.76883300	8.70651300
C	5.67129200	5.35524400	8.34274600	H	1.31957500	3.50546400	11.92856700
C	5.22882500	6.66804500	8.43468600	H	1.87344300	5.94562300	12.08897100
C	3.83883500	6.81353000	8.68157800	H	6.06792900	4.97415200	11.97767100
O	1.94652700	8.28477900	9.88666800	H	5.52690800	2.57848400	11.78189900
P	6.33673100	8.14340000	8.46802600	O	2.98086300	1.60640300	11.64919600
B	5.02739100	11.83713200	8.54508700	C	3.95488500	0.63649400	11.33330100
S	3.13339000	8.47024500	8.96292100	H	4.51443300	0.91443800	10.42225400
O	6.93548000	4.91347900	8.08975300	H	3.41620000	-0.30359600	11.15588500
O	5.55544300	3.10477900	8.45197300	H	4.67184600	0.48545800	12.16022900
H	2.83265600	3.54592700	8.94997400	C	2.35547500	3.84892700	11.95024600
H	1.95247000	5.91156500	9.12684800	C	2.66503500	5.19586800	12.04927800
C	2.38203300	8.89339900	7.26633000	C	4.01154800	5.63110900	12.04368300
C	1.72604200	10.25585600	7.50989100	C	5.02409900	4.65804100	11.97207800
H	1.00205000	10.19785900	8.33518600	C	4.71786000	3.30236300	11.86084600
H	1.19353700	10.56323000	6.59543300	C	3.37795000	2.89123200	11.82438800
H	2.48420200	11.01814400	7.73679800	C	4.30305800	7.02061600	12.02746300
C	1.34262500	7.83422500	6.92276800	C	4.49465400	8.21984400	11.90777900
H	1.80612600	6.86998700	6.67017000	C	4.57565300	9.61780400	11.69594000
H	0.76319500	8.17195900	6.04836700	C	5.70809300	10.34686200	11.48927300
H	0.64666200	7.69117400	7.76256400	H	5.65840300	11.43149600	11.38870800
C	3.50284600	8.99030800	6.24165700	H	6.69617500	9.88009600	11.52861100
H	4.22423800	9.77183200	6.51529000	H	3.60727000	10.13327200	11.69230100
H	3.06876200	9.26874100	5.26716700	C	6.95058400	3.48934100	8.30306900

C	7.53489500	2.78908300	7.08854000	C	5.77689200	6.14991100	7.95013400
C	7.71317600	3.18202500	9.58550000	C	4.60023900	5.62368400	8.54949100
C	7.64886400	1.27896600	7.32538300	O	3.26858800	5.41025600	10.85982800
H	8.52927200	3.22838900	6.90565000	P	6.69785500	7.55784600	8.71615400
H	6.90276800	3.01803400	6.21704000	B	5.48127000	8.93122200	13.18846900
C	7.83409600	1.67383600	9.81841000	S	3.83482200	6.48793300	9.95021600
H	8.70825100	3.64518300	9.48762000	O	7.40590800	5.63099100	6.17801100
H	7.20740900	3.69022700	10.41738900	O	6.49782500	3.62203800	5.52419000
C	8.44289800	0.97022100	8.60001900	H	4.22567600	2.65950500	6.85756900
H	8.11655600	0.80021200	6.45071600	H	3.20971800	4.00757200	8.74777300
H	6.63344400	0.85716500	7.41369500	C	2.34022400	7.33464800	9.14002500
H	8.43743700	1.48330100	10.72018600	C	1.75071900	8.13446100	10.30647000
H	6.83119300	1.25870500	10.01477900	H	1.45458000	7.46533300	11.12733400
H	8.48365300	-0.11801600	8.76802900	H	0.85985900	8.68283000	9.96139700
H	9.48743400	1.30721200	8.47004500	H	2.48367800	8.86078600	10.69008600
C	7.82191000	7.47659500	9.32022200	C	1.36893200	6.27474800	8.64211300
C	9.08526500	7.39799700	8.71948100	H	1.74518300	5.76336500	7.74483800
C	7.67021800	7.06256100	10.65394500	H	0.41110900	6.75390800	8.38227600
C	10.17199100	6.88349900	9.43273800	H	1.18055200	5.52991200	9.42969600
H	9.22069300	7.72399900	7.68749100	C	2.85887300	8.24957000	8.03823900
C	8.75408100	6.53924100	11.35928000	H	3.61081700	8.94776300	8.43619600
H	6.69551000	7.14633400	11.13665600	H	2.02308700	8.84493000	7.63615500
C	10.00941600	6.44321500	10.74892500	H	3.30716300	7.68463400	7.20792200
H	11.15192900	6.82319200	8.95254100	C	5.98113700	6.67938700	13.28929000
H	8.61908700	6.21444000	12.39424800	C	6.91528000	7.50659500	14.24350800
H	10.86044200	6.03830300	11.30196200	O	6.22743500	8.78701500	14.31984200
C	6.88693100	8.37285700	6.72997400	O	5.42916500	7.74317100	12.46870300
C	6.95970100	9.68512800	6.23921200	C	7.05646500	6.93777500	15.64633900
C	7.21915800	7.30023300	5.88469800	H	7.50032900	5.93072800	15.61125200
C	7.36959600	9.92282300	4.92468400	H	7.71631100	7.58346800	16.24447500
H	6.65469600	10.51432500	6.87983600	H	6.08621200	6.87736000	16.15575500
C	7.62093900	7.54319900	4.57004900	C	8.28669800	7.78414600	13.62208700
H	7.17722200	6.27707800	6.25854000	H	8.80349800	8.54380800	14.22625700
C	7.69902400	8.85452700	4.08779200	H	8.90929500	6.87814300	13.59111200
H	7.41710000	10.94927300	4.55366700	H	8.18760400	8.17532900	12.59904400
H	7.87504700	6.70399800	3.91761000	C	6.68362900	5.68505300	12.37969500
H	8.01229300	9.04062800	3.05744200	H	7.19466000	4.91000300	12.97118100
				H	5.93464400	5.19120800	11.74276700
I-3a				H	7.42269800	6.17619100	11.73720200
Cu	5.39236000	8.36500300	10.37318800	C	4.79725300	6.01565900	13.99166300
C	4.05942400	4.39187300	8.18246600	H	4.08576900	5.68522300	13.22043500
C	4.62795500	3.63178600	7.14437800	H	5.11787500	5.14273900	14.57936500
C	5.74388600	4.15988700	6.51735700	H	4.28680400	6.72091600	14.66418600
C	6.29370900	5.38713400	6.91159100	H	12.09395300	9.81259100	11.22699000

H	9.75066500	10.10139800	12.02724900	C	8.87118200	3.71182600	6.07036100
H	8.60501500	11.46033600	8.09900200	C	7.95675500	4.80799500	3.97493600
H	10.91201000	11.17869400	7.31208800	C	10.14489900	4.55619600	5.96355100
O	12.95364400	10.19113200	8.86682400	H	8.99568900	2.74436200	5.55655700
C	13.35010200	10.45151900	7.54415500	H	8.61918700	3.50321700	7.12075100
H	12.77439700	9.85111700	6.81484500	C	9.24061900	5.63891500	3.85438600
H	13.23757700	11.51956700	7.28160600	H	8.04396200	3.87234400	3.39889400
H	14.41148000	10.17761600	7.47071800	H	7.08138600	5.35514800	3.59387400
C	11.31497100	10.17933100	10.55542100	C	10.43663800	4.93444700	4.50679700
C	10.00979800	10.34334800	10.99531900	H	10.99230200	4.00602100	6.40076600
C	8.98605000	10.78661200	10.11878000	H	10.01999500	5.46515700	6.57395300
C	9.36535500	11.11193000	8.79794800	H	9.44539000	5.84766400	2.79257100
C	10.67812300	10.94383900	8.35038400	H	9.07576800	6.61457900	4.34031900
C	11.66055900	10.45473300	9.22238200	H	11.32889500	5.57873700	4.45251300
C	7.63041700	10.81412000	10.53055000	H	10.67581700	4.01999400	3.93351800
C	6.44150800	10.63143600	10.79285000				
C	5.09143500	10.29635800	11.08952900	**I-3b**			
C	4.76605800	10.19138800	12.60108300	Cu	3.12229200	8.64430500	9.20722500
H	3.67795000	10.03039200	12.71797900	C	1.85111700	6.07597900	5.56422200
H	5.01250500	11.11137900	13.16226400	C	2.30857400	4.85299600	5.03882200
H	4.37015400	10.91766900	10.53603500	C	3.50920700	4.36701300	5.52865600
C	8.33158600	6.76202700	9.00120200	C	4.22499500	5.04442400	6.52494900
C	9.51211300	7.52042700	8.96550700	C	3.79013400	6.23843400	7.08241800
C	8.40359900	5.40800500	9.37133200	C	2.58780900	6.75607200	6.53032900
C	10.74289500	6.92781800	9.26199200	O	0.42156800	8.28558300	6.93538100
H	9.47915600	8.57665800	8.70496100	P	4.49328600	6.94923100	8.63038900
C	9.63324800	4.82100500	9.67223500	B	3.32274100	11.38912200	10.33410400
H	7.49511800	4.80516900	9.42208600	S	1.91996100	8.34048600	7.12524500
C	10.80858500	5.57723400	9.61238800	O	5.33877400	4.33689000	6.83878900
H	11.64751700	7.53791600	9.22209800	O	4.15990800	3.22188500	5.20322200
H	9.67271200	3.76569500	9.95362300	H	1.74089600	4.30179600	4.28824200
H	11.77117100	5.11531800	9.84425500	H	0.89658700	6.49961100	5.24769200
C	6.99181700	8.78032700	7.37706800	C	2.56601600	9.54246400	5.79452800
C	6.22600100	9.95538200	7.40891300	C	2.20413100	10.90644200	6.39084000
C	7.95216100	8.61482400	6.36688900	H	1.11962700	10.97646100	6.56085400
C	6.39654900	10.93747400	6.43054000	H	2.49841000	11.70647300	5.69243100
H	5.52087000	10.11007600	8.22653600	H	2.72090400	11.06749200	7.34717900
C	8.13145900	9.60397100	5.39957000	C	1.81307200	9.28270300	4.49893200
H	8.56227300	7.71460200	6.34390200	H	2.12318900	8.33779300	4.03013600
C	7.35017400	10.76430700	5.42448500	H	2.01883400	10.09907200	3.78721700
H	5.79742100	11.84993200	6.47077800	H	0.73027300	9.24698300	4.68834600
H	8.88633000	9.46770200	4.62099400	C	4.06953200	9.34772300	5.66759100
H	7.49341100	11.53767200	4.66581000	H	4.55158000	9.33626500	6.65436800
C	7.69410100	4.42797200	5.41953900	H	4.50639100	10.18053300	5.09311000

H	4.31150000	8.41013400	5.14849000	C	5.33286700	4.52375000	9.90146800
C	4.95829500	12.88564700	9.78392600	C	3.14046800	5.39215500	10.46852900
C	5.36134100	11.45233300	9.28658400	C	5.11347000	3.43291200	10.74487700
O	4.07083800	10.77352700	9.33026900	H	6.27345800	4.61280500	9.35877400
O	3.85637000	12.59690200	10.67823100	C	2.92006400	4.29380400	11.30109300
C	5.93963700	11.39752800	7.88281200	H	2.38795300	6.17950700	10.37843300
H	6.84401700	12.02263200	7.82683800	C	3.90651800	3.31201700	11.44037600
H	6.23269400	10.36667600	7.63711500	H	5.89244000	2.67573900	10.86373500
H	5.22584500	11.74857900	7.12821100	H	1.98315700	4.21520200	11.85703000
C	6.27028500	10.71442900	10.26481200	H	3.73953300	2.45889600	12.10240200
H	6.28874200	9.65098100	9.99893700	C	6.28300200	7.14488600	8.33865900
H	7.29979600	11.09926900	10.23368900	C	6.82306000	7.30270000	7.05373900
H	5.88633500	10.79017100	11.28968200	C	7.12307000	7.27160400	9.45978200
C	6.04445400	13.61420900	10.56293700	C	8.18112500	7.58914200	6.89246800
H	6.94104200	13.75681300	9.93986900	H	6.18329100	7.19461700	6.17658300
H	5.67864400	14.60504400	10.87010200	C	8.48054600	7.54656000	9.29223600
H	6.32696800	13.06203000	11.46786700	H	6.71910000	7.15903600	10.46677100
C	4.41322100	13.77385600	8.66324800	C	9.01302100	7.71186000	8.00955100
H	3.93782100	14.65837900	9.11113900	H	8.59229600	7.70926700	5.88706000
H	5.21362900	14.11252400	7.98909300	H	9.11508400	7.63735400	10.17659800
H	3.65479100	13.24447400	8.06850500	H	10.07527100	7.93234400	7.87954500
H	7.06075900	4.61901200	13.21062700	C	5.25037800	3.06804800	6.15463000
H	4.87325800	5.68261000	12.70274900	C	6.53971100	2.79711600	5.40178800
H	6.73793200	9.56292800	12.90749600	C	4.89778600	1.97086500	7.15081300
H	8.89915900	8.51374700	13.40169400	C	6.50518000	1.42094100	4.72742000
O	9.28635600	5.79994500	13.57297700	H	7.36152900	2.85029300	6.13441000
C	10.46629100	6.53260900	13.77739100	H	6.69322600	3.60699300	4.67260400
H	10.73663000	7.13955500	12.89232400	C	4.86335200	0.59902500	6.47009200
H	11.26629000	5.80273600	13.96291900	H	5.66094800	1.99322800	7.94513300
H	10.39000000	7.20783200	14.64990900	H	3.93609000	2.22028500	7.62513300
C	6.97384400	5.70494000	13.13907200	C	6.17703100	0.31196600	5.73386600
C	5.75442100	6.30327400	12.85915500	H	7.47062500	1.22631700	4.23443600
C	5.63023200	7.71261000	12.73641000	H	5.73932900	1.43451700	3.93377500
C	6.79644000	8.47580000	12.96472300	H	4.65774000	-0.18195700	7.21886800
C	8.02831100	7.87701800	13.24400400	H	4.02743200	0.57885400	5.75091400
C	8.13052000	6.48122600	13.32252700	H	6.12148200	-0.66128900	5.22044100
C	4.40517100	8.29854400	12.32471900	H	6.99801000	0.23221500	6.46984300
C	3.38728900	8.70323700	11.76037900				
C	2.27573300	9.16139700	10.99876700	**I-4a**			
C	2.07061200	10.69008100	10.95146000	Cu	6.31960500	8.47111700	9.95043800
H	1.20167800	10.91726400	10.30494800	C	3.87773100	4.68898100	8.42353800
H	1.83773000	11.13785300	11.93801400	C	4.17975600	3.65816900	7.51481400
H	1.35028400	8.60907900	11.22120200	C	5.30916100	3.81956200	6.72924200
C	4.34362800	5.50566400	9.75526400	C	6.11522400	4.95891700	6.83680400

C	5.85350900	5.98825200	7.73011500	H	9.03634800	8.95654500	9.79181400
C	4.67999300	5.82494800	8.51427600	H	7.71282800	12.71408800	11.39934600
O	3.44356200	6.22085400	10.82886200	H	9.99320300	13.62430600	11.18865700
P	7.03487500	7.33028000	8.13299100	O	12.12224500	12.20088500	10.20788300
B	5.62351300	8.82166600	13.61514600	C	12.47081500	13.50541200	10.59771300
S	4.26394100	7.01486100	9.83319800	H	11.91472500	14.27122900	10.02567600
O	7.15593900	4.85408100	5.97260800	H	12.29151700	13.67717600	11.67512600
O	5.83532900	2.97634700	5.80304400	H	13.54423100	13.62090400	10.39378000
H	3.56640900	2.75911600	7.44380200	C	10.54084600	10.47598900	9.98043800
H	3.03407300	4.59931000	9.10965700	C	9.24650500	9.98314300	10.09898500
C	3.04863600	8.18960500	8.97595400	C	8.19088000	10.76466900	10.61671800
C	2.61528200	9.10309800	10.12661100	C	8.50848300	12.08072500	10.99893000
H	2.10976200	8.52372800	10.91171900	C	9.80112200	12.59629900	10.88032000
H	1.91556200	9.86107800	9.73943200	C	10.83185300	11.79267100	10.36796900
H	3.47331900	9.62281300	10.58066300	C	6.82878100	10.20736400	10.72695300
C	1.87948900	7.38436200	8.42764900	C	5.88514700	10.68429100	11.49948800
H	2.16984600	6.77456000	7.55987500	C	4.90202100	10.92483400	12.35260100
H	1.08298000	8.07595700	8.10848600	C	4.76282800	10.13713700	13.64849900
H	1.46869200	6.72668100	9.20802200	H	3.70138700	9.85040900	13.77897700
C	3.80872200	8.95570900	7.90058700	H	5.02557600	10.74633700	14.53256900
H	4.66955700	9.49639700	8.32638600	H	4.13696300	11.67720100	12.11973000
H	3.13815800	9.70582200	7.45097800	C	8.63782700	6.44962000	8.20015600
H	4.16525600	8.29991300	7.09265000	C	9.80099000	7.01964300	7.66245100
C	6.23994200	6.68792900	13.08518300	C	8.73166100	5.24925800	8.92455400
C	7.30010200	7.34101500	14.04656200	C	11.03723100	6.39157200	7.83968900
O	6.59079700	8.50563100	14.53194400	H	9.74178200	7.95691500	7.10632300
O	5.47862100	7.84097100	12.65801500	C	9.96663400	4.62350900	9.09360700
C	7.70269700	6.47578700	15.23218600	H	7.83329900	4.80032500	9.35366300
H	8.16904600	5.53909600	14.88856000	C	11.12444500	5.19360400	8.55309700
H	8.43433200	7.01475400	15.85233300	H	11.93684200	6.84399400	7.41576600
H	6.83916600	6.22828100	15.86286800	H	10.02653100	3.68690100	9.65324500
C	8.53748500	7.85456100	13.30474100	H	12.09172000	4.70482800	8.68953500
H	9.12239100	8.48865800	13.98649600	C	7.16435500	8.44531200	6.68827500
H	9.17965400	7.03046700	12.96020600	C	7.30932600	9.81608000	6.95941500
H	8.25444600	8.46941400	12.43947000	C	7.14401000	7.99795300	5.35662200
C	6.84462600	5.99085400	11.87232900	C	7.44033900	10.72766900	5.90839600
H	7.55946600	5.21553500	12.18805700	H	7.31633800	10.16403600	7.99487100
H	6.04996000	5.50335900	11.29075700	C	7.26345400	8.91623900	4.31215500
H	7.37941100	6.70042200	11.22420000	H	7.04703700	6.93486600	5.13872300
C	5.25614700	5.74782600	13.78413500	C	7.41409600	10.28048200	4.58553100
H	4.42899300	5.55525400	13.08607600	H	7.55841700	11.79062700	6.13035600
H	5.72984000	4.79387500	14.06122700	H	7.24289800	8.56433700	3.27772100
H	4.84401300	6.21062200	14.69287200	H	7.51080300	10.99461500	3.76403800
H	11.34899600	9.85670200	9.58563700	C	7.12887400	3.50555200	5.43231400

C	8.24091500	2.69776900	6.08934300	H	2.38399900	7.23047100	7.46734400
C	7.25941000	3.57935000	3.92279000	C	4.19733300	12.23867800	9.17712800
C	9.61582200	3.24065400	5.68558900	C	3.49259900	12.01074000	10.57126700
H	8.12126600	1.64894200	5.77145600	O	4.61158700	11.70477800	11.43223600
H	8.10206900	2.73337600	7.18089400	O	5.40516100	11.46117300	9.31396900
C	8.63953900	4.11336200	3.51942000	C	2.76619800	13.22794800	11.13073600
H	7.10752300	2.56110500	3.52916700	H	1.95090600	13.53915100	10.45849800
H	6.44569300	4.21000100	3.53324200	H	2.32616900	12.96940400	12.10508700
C	9.76635500	3.29564100	4.16147400	H	3.44640100	14.07689800	11.27974600
H	10.40609500	2.61898800	6.13428400	C	2.56622700	10.79637100	10.57465200
H	9.73515700	4.25074100	6.10768500	H	2.22302300	10.60185100	11.59847600
H	8.73040600	4.10806400	2.42185600	H	1.68639600	10.95561700	9.93496400
H	8.72342900	5.16533900	3.84046700	H	3.09674900	9.89583300	10.23991400
H	10.74455500	3.72513500	3.89233100	C	3.41251500	11.72505200	7.97573100
H	9.75068500	2.26884600	3.75209700	H	2.43675500	12.23078200	7.90390800
				H	3.97215700	11.92402800	7.04959400
I-4a'				H	3.24855100	10.64320600	8.03880400
Cu	4.44987400	6.18470600	10.75669600	C	4.62864400	13.68970100	8.94608700
C	1.30607600	3.58755000	8.26109900	H	5.28873000	13.72811000	8.06660400
C	1.51631300	2.67846100	7.20908600	H	3.76556300	14.34746600	8.76344100
C	2.71119500	2.78865000	6.52170900	H	5.18899900	14.07812500	9.80899200
C	3.66765100	3.74923800	6.86801700	H	2.10671400	10.45910200	14.97871700
C	3.51228400	4.63792900	7.92425500	H	3.97153300	10.08398100	13.35209800
C	2.26112900	4.54524000	8.59070100	H	2.62837900	6.03863400	12.77531000
O	0.69209800	4.89706700	10.72328700	H	0.79022900	6.39758300	14.34935400
P	4.90051400	5.65520700	8.61191400	O	0.32153900	8.77472200	15.65919200
B	5.64004500	11.23810400	10.65322400	C	-0.61919000	7.78101300	15.96147000
S	1.85244800	5.59124000	10.03562900	H	-1.17346400	7.44386400	15.06493900
O	4.72949900	3.63714600	6.01185000	H	-1.33198300	8.22121200	16.67451500
O	3.17060900	2.04294100	5.47212200	H	-0.15336100	6.89180600	16.42717400
H	0.78395100	1.91092300	6.95415900	C	2.23734500	9.49302800	14.48415700
H	0.40833800	3.54311500	8.88130000	C	3.27556400	9.27513500	13.58449700
C	1.02196500	7.08009600	9.16908600	C	3.44077400	8.03320400	12.92777600
C	0.55594300	7.91797400	10.36347800	C	2.52045000	7.01881100	13.24420800
H	-0.14406300	7.34467800	10.98671200	C	1.47634600	7.22166500	14.15298700
H	0.05087400	8.82830400	10.00027700	C	1.32258100	8.46712600	14.77263500
H	1.40196100	8.21720300	10.99692100	C	4.49753800	7.80792700	11.91255400
C	-0.16097900	6.59459200	8.34486100	C	5.58166200	8.54273400	11.88733600
H	0.16222500	6.05603800	7.44188100	C	6.71782100	9.22846900	11.87842600
H	-0.77293700	7.45756500	8.03015800	C	6.94811000	10.56995500	11.19682700
H	-0.79026800	5.92555400	8.95118400	H	7.68090700	10.47876500	10.37104400
C	2.06881500	7.81155500	8.34481100	H	7.40749700	11.27364700	11.92100800
H	2.95920500	8.03497500	8.94990200	H	7.58216100	8.81180600	12.41739900
H	1.65507900	8.76710000	7.98081400	C	4.56940800	2.39601700	5.31321300

C	4.87505200	2.59249700	3.83921300	C	2.72015200	2.52735600	7.29951000
C	5.44271700	1.32508400	5.96046900	C	3.07942200	3.55281500	8.16403300
C	4.79512700	1.26670100	3.07516400	C	1.98963700	4.24671800	8.75655200
H	5.88950800	3.01849900	3.77289100	O	1.04133500	5.59177300	10.87043200
H	4.17204800	3.33762600	3.43693600	P	4.80650100	3.82334600	8.75048400
C	5.35824600	0.00308800	5.19360100	B	9.26202500	8.83772100	11.51582600
H	6.47485300	1.70952500	5.97718700	S	2.28960900	5.52632200	10.01454200
H	5.13474400	1.21028400	7.01039400	O	3.53975600	1.70943500	6.58668600
C	5.69331500	0.19859900	3.71039000	O	1.35544200	1.09378000	6.22319800
H	5.06838800	1.42750800	2.01948600	H	-0.69703100	2.51984000	7.49975200
H	3.74886300	0.91680900	3.08450100	H	-0.11427500	4.42041400	9.08303100
H	6.03447900	-0.73768300	5.64984000	C	2.29143500	7.12771500	8.98212200
H	4.33496400	-0.39869600	5.28626000	C	2.48465400	8.21457600	10.04391300
H	5.59367300	-0.75460200	3.16488100	H	1.68551700	8.17217400	10.79699700
H	6.75043400	0.50802000	3.61384900	H	2.45354800	9.20115600	9.55419300
C	6.34013400	4.54815500	8.29355500	H	3.45416000	8.11053100	10.55225500
C	7.39449900	4.89650000	7.43727200	C	0.93771800	7.24826100	8.29695300
C	6.38984300	3.32502500	8.98456200	H	0.81908800	6.51298500	7.48777000
C	8.47098300	4.02481200	7.25198800	H	0.84324600	8.25543000	7.85964700
H	7.37142400	5.84602800	6.90113600	H	0.12617300	7.11321000	9.02730700
C	7.46573100	2.45710200	8.79095300	C	3.45835200	7.08664400	8.00486300
H	5.59514700	3.07564000	9.69563600	H	4.41925200	6.98497600	8.53030100
C	8.50729400	2.79834100	7.92181800	H	3.48885400	8.03641900	7.44618700
H	9.28503000	4.30773600	6.57868700	H	3.36396300	6.27300900	7.27115800
H	7.49233800	1.50921200	9.33519800	C	9.31861200	10.96041800	12.33084400
H	9.34992700	2.11664900	7.77577100	C	9.61869000	9.93243300	13.48750700
C	5.16767500	7.00633500	7.39133800	O	9.24082300	8.67543700	12.87975400
C	4.96080800	6.87524100	6.00817600	O	9.48315900	10.14229700	11.14807100
C	5.60799200	8.23464000	7.90826200	C	11.10693800	9.83115900	13.83113900
C	5.19554300	7.95709800	5.15728400	H	11.46367800	10.72366600	14.36610100
H	4.63493500	5.92104800	5.59448700	H	11.26147800	8.95345100	14.47556200
C	5.85747300	9.31180100	7.05186200	H	11.71592900	9.69902400	12.92490400
H	5.73486500	8.34918300	8.98925200	C	8.80005100	10.14010600	14.75520900
C	5.64864200	9.17450000	5.67741900	H	9.04167600	9.35231500	15.48403400
H	5.02753400	7.84752500	4.08214100	H	9.03378100	11.11452900	15.21187600
H	6.17909000	10.26120500	7.47992300	H	7.72297500	10.09644600	14.55602000
H	5.83171800	10.02080100	5.00926500	C	7.86717400	11.44865400	12.33078000
Br	4.21792900	3.86177900	11.71756100	H	7.66832000	12.13762900	13.16481300
				H	7.67451100	11.97907400	11.38672100
I-4b				H	7.16372500	10.60565300	12.39399600
Cu	4.78540200	5.24561500	10.48139500	C	10.27752400	12.14053900	12.25495100
C	0.66263800	3.88604900	8.53316400	H	9.99273500	12.79493300	11.41759600
C	0.33629800	2.82430600	7.67025500	H	10.23903400	12.73411900	13.18162000
C	1.38912800	2.15886400	7.06543500	H	11.31140000	11.81134400	12.08960900

H	5.93360100	8.90198600	15.69743800	C	2.72509000	0.62449500	6.09091800
H	6.82977700	8.10587700	13.50191700	C	3.03402400	0.37118600	4.62842500
H	3.05065800	6.20634000	12.68600800	C	2.93134700	-0.60399500	6.96887800
H	2.16595900	6.99459500	14.82560400	C	2.24802700	-0.83414700	4.09959700
O	3.60325300	8.49850200	16.61852300	H	4.11848200	0.18844900	4.55283300
C	2.30074200	8.21628700	17.06348900	H	2.80801800	1.28671100	4.06099800
H	1.53237900	8.62842100	16.38332100	C	2.14626000	-1.80525400	6.43395900
H	2.19277200	8.68934500	18.04932000	H	4.01299200	-0.81410400	6.98522000
H	2.12539400	7.12943000	17.16754400	H	2.64243400	-0.35166100	8.00078000
C	5.31201700	8.32086700	15.01268800	C	2.48277900	-2.07846400	4.96364600
C	5.80091100	7.87917200	13.79054900	H	2.52943700	-1.02767100	3.05260500
C	5.00184900	7.11363700	12.91057600	H	1.17375500	-0.58421700	4.09948700
C	3.69991100	6.80233100	13.33093700	H	2.35640100	-2.69167700	7.05287500
C	3.18911800	7.25354400	14.55353100	H	1.06721900	-1.59793800	6.53029400
C	3.99624500	8.01863600	15.40468600	H	1.88234800	-2.92111900	4.58521500
C	5.51722200	6.66015200	11.60079800	H	3.54159600	-2.38538900	4.88212600
C	6.46220100	7.29681100	10.95419400				
C	7.41671500	7.89149500	10.25443700	**I-4b'**			
C	8.91193800	7.69734400	10.50022900	Cu	4.86907600	4.56764400	10.75813700
H	9.47782100	7.79503000	9.55882800	C	0.92506200	4.29783300	8.10113600
H	9.10525600	6.70319700	10.93027700	C	0.57343500	3.40121000	7.07612300
H	7.14256900	8.67433300	9.53332600	C	1.60910600	2.71785100	6.46519900
C	5.36991500	2.09214000	8.96014800	C	2.93900800	2.90134900	6.85965000
C	6.42190400	1.53401400	8.22480500	C	3.32032200	3.74503000	7.89507100
C	4.70586900	1.31293000	9.92144000	C	2.25275600	4.47721000	8.47980400
C	6.79344300	0.20311400	8.43674500	O	1.16814800	5.80656900	10.52808100
H	6.94383600	2.13415200	7.47789900	P	5.01013500	3.72046100	8.65559200
C	5.07254500	-0.01742200	10.12332100	B	8.96872800	8.96319600	11.28823800
H	3.89375300	1.74952200	10.50956300	S	2.52915700	5.61364700	9.88486700
C	6.11747600	-0.57626700	9.37890400	O	3.74062900	2.12124600	6.07206000
H	7.61527000	-0.22655400	7.85882900	O	1.55443300	1.79709100	5.45652900
H	4.54747300	-0.61815000	10.86970600	H	-0.46485600	3.23668600	6.78395900
H	6.40925100	-1.61661800	9.54080100	H	0.16608500	4.84769300	8.66169400
C	5.77644300	4.51026700	7.36180000	C	2.82939700	7.26132800	8.96000600
C	6.73778200	5.48224500	7.68429500	C	3.01744300	8.24831900	10.11716700
C	5.59627600	4.12802100	6.02174400	H	2.14009300	8.24037300	10.77952900
C	7.51371100	6.06191000	6.67786500	H	3.14581500	9.26535400	9.71003700
H	6.86779000	5.81247100	8.71867400	H	3.90867400	7.99598400	10.70912000
C	6.37231800	4.71580600	5.02089600	C	1.59025000	7.59724500	8.14292300
H	4.86119200	3.36605000	5.76317800	H	1.48691300	6.93894000	7.26745500
C	7.33134900	5.68161800	5.34623500	H	1.65783300	8.63814500	7.78313900
H	8.25217500	6.82160400	6.94369700	H	0.68953700	7.50133900	8.76784700
H	6.22691200	4.41837700	3.97948400	C	4.09037100	7.14719700	8.11825200
H	7.93330400	6.14034800	4.55799100	H	4.94582300	6.81946100	8.72408100

H	4.33946600	8.13737300	7.70005100	C	2.87932400	1.20810300	5.38092900
H	3.96323700	6.45347400	7.27557300	C	3.30152600	1.10359700	3.92653800
C	8.56958600	11.04925900	12.09690200	C	2.88059000	-0.13994700	6.09592500
C	9.22694200	10.16050500	13.21866100	C	2.45487600	0.06987600	3.17662500
O	9.12707900	8.83850600	12.65194900	H	4.36515300	0.81445600	3.91823500
O	8.85033700	10.28427200	10.90614700	H	3.22286400	2.10252900	3.47138400
C	10.71835000	10.45056600	13.41612900	C	2.03374000	-1.16850300	5.34244900
H	10.88542300	11.41498600	13.91947000	H	3.92915900	-0.46842300	6.17338600
H	11.15200600	9.65272000	14.03698600	H	2.52321400	0.00981200	7.12568600
H	11.25024400	10.45937000	12.45335500	C	2.47964700	-1.29194400	3.88078100
C	8.50473700	10.18972400	14.55963500	H	2.81233100	-0.02234000	2.13803300
H	9.00585700	9.50932500	15.26448900	H	1.41529100	0.43566400	3.12526300
H	8.52298800	11.20467000	14.98798500	H	2.09240000	-2.14487500	5.84985200
H	7.46224800	9.86630400	14.46443000	H	0.97673900	-0.85416400	5.37574600
C	7.04528600	11.13263200	12.22642400	H	1.83810400	-2.00942800	3.34252500
H	6.74008200	11.75997700	13.07722600	H	3.50662200	-1.70028500	3.84689000
H	6.63867100	11.57129900	11.30320600	C	6.10708600	4.54635000	7.43061400
H	6.60150900	10.13356100	12.34561800	C	5.87810200	4.58691400	6.04574500
C	9.16933600	12.44123400	11.94508700	C	7.23814100	5.18633900	7.95835600
H	8.65133800	12.97911700	11.13667800	C	6.76953600	5.25805600	5.20620200
H	9.05062100	13.02152800	12.87382900	H	5.01060500	4.08180000	5.62109300
H	10.23641900	12.39567600	11.69054000	C	8.13570900	5.84609300	7.11462700
H	6.08098500	8.45797100	15.73298400	H	7.38901900	5.19785500	9.03925200
H	6.96275300	7.68729600	13.51837200	C	7.90117100	5.88689600	5.73836400
H	3.24540300	5.64715900	12.77818400	H	6.58067900	5.28980500	4.12953800
H	2.35784700	6.44291400	14.91514800	H	9.00504800	6.34834400	7.54415100
O	3.77028700	7.99948100	16.69114100	H	8.59487700	6.41558000	5.07897400
C	2.48848500	7.66491100	17.14743500	C	5.45719900	1.94329000	8.44435100
H	1.69341300	8.04527600	16.47793800	C	4.73243100	0.99680700	9.18907300
H	2.36944700	8.13019600	18.13720800	C	6.50094000	1.51102200	7.61379100
H	2.35330500	6.57138600	17.24918900	C	5.03496800	-0.36134300	9.07485200
C	5.46499600	7.85949500	15.05728400	H	3.95407100	1.33658500	9.88038400
C	5.94776400	7.42586100	13.82649500	C	6.80255400	0.15059500	7.50883800
C	5.15917500	6.63420800	12.95969300	H	7.07158100	2.23710400	7.03317100
C	3.87080800	6.28832600	13.40102500	C	6.06607000	-0.79157100	8.23325700
C	3.36793300	6.73565900	14.62762900	H	4.46449200	-1.08720500	9.66055400
C	4.16472500	7.52425000	15.46547200	H	7.61689500	-0.17348000	6.85464200
C	5.65685400	6.19175800	11.63637300	H	6.30220200	-1.85617400	8.14990100
C	6.46846900	6.94600700	10.94693900	Br	3.41483200	2.88193600	11.87183100
C	7.25920400	7.69798800	10.18920500				
C	8.78361900	7.76220000	10.31019900	**I-5a**			
H	9.24876400	7.94321800	9.32599200	Cu	4.32103000	6.46608800	10.69424700
H	9.18213200	6.82510700	10.72786000	C	1.27180600	3.61570200	8.59850400
H	6.80897700	8.41041300	9.48401400	C	1.42074800	2.63955200	7.59680300

C	2.58700500	2.67706700	6.85178000	H	5.31308900	14.18796100	9.23872800
C	3.58158000	3.63425000	7.09225900	H	3.08070900	11.10600700	15.03719900
C	3.48000100	4.59723400	8.08750300	H	4.57998400	10.49122100	13.13732900
C	2.26109600	4.57103100	8.81742700	H	2.64938700	6.65855100	12.88507500
O	0.95924600	5.07457800	11.09771200	H	1.17824800	7.24464900	14.75413600
P	4.87259000	5.67402100	8.64369000	O	1.26514600	9.65691900	16.06593900
B	5.77738200	11.35039200	10.07993100	C	0.28518300	8.79062600	16.58087000
S	1.99343400	5.72649000	10.19451200	H	-0.46933800	8.52034400	15.81914800
O	4.61076100	3.43208500	6.23030400	H	-0.21295100	9.32680300	17.40020000
O	2.97898900	1.85304700	5.84598700	H	0.72652600	7.85847800	16.97938100
H	0.66178600	1.87662500	7.41974700	C	3.00678900	10.12782100	14.55706300
H	0.39556600	3.62421700	9.24891800	C	3.84446500	9.77483300	13.50770500
C	1.07349300	7.15809300	9.34643100	C	3.75378900	8.51086400	12.87965500
C	0.74370000	8.08325800	10.52014900	C	2.76834200	7.63387900	13.35978000
H	0.11177900	7.56967600	11.25739900	C	1.92304300	7.96838000	14.42375600
H	0.20289200	8.96540900	10.14289900	C	2.03913000	9.22442900	15.03254600
H	1.65429800	8.42627600	11.02771800	C	4.64306900	8.11489000	11.76120400
C	-0.19044100	6.61084700	8.69877800	C	5.75710200	8.76977400	11.53586200
H	0.03199800	5.99850100	7.81326600	C	6.90962300	9.38807300	11.32663500
H	-0.82467600	7.45417700	8.38033800	C	7.11296600	10.62805900	10.47154600
H	-0.75994700	6.00667900	9.42036700	H	7.69025200	10.39015500	9.55829900
C	2.01935200	7.81850000	8.35439500	H	7.73619300	11.35107900	11.03314500
H	2.95064400	8.13299700	8.84517300	H	7.80664800	8.99608000	11.82565800
H	1.53665800	8.71731200	7.93790200	C	4.33972500	2.20294700	5.50711100
H	2.27196100	7.15639100	7.51423300	C	4.45747100	2.47419900	4.01765800
C	4.19044800	12.37308700	8.78097900	C	5.90349000	2.80944100	3.63328500
C	3.66368300	12.19355400	10.25912200	C	6.87221200	1.71745400	4.10148700
O	4.87413500	11.85413800	10.97672100	C	6.74184400	1.47028000	5.60803500
O	5.38287300	11.55314000	8.77977900	C	5.29999100	1.12698000	5.99590000
C	3.05946800	13.44396700	10.88390600	H	5.97231600	2.95178900	2.54326900
H	2.17689600	13.77680200	10.31571300	H	4.11686000	1.56797100	3.49064000
H	2.73926400	13.21774400	11.91151200	H	3.76447600	3.28883600	3.75682400
H	3.78294900	14.26807800	10.92774400	H	6.66022400	0.78137200	3.55272300
C	2.70625000	11.01233300	10.40929700	H	7.90777800	1.99921700	3.85211200
H	2.50231200	10.84407300	11.47448300	H	7.41553100	0.66170100	5.93195600
H	1.75221000	11.19640900	9.89489600	H	7.04904300	2.37261900	6.15808000
H	3.15451300	10.09084600	10.01652800	H	4.98539300	0.17204100	5.54343400
C	3.24864400	11.85845900	7.69910200	H	5.19190900	1.03231100	7.08739600
H	2.28731500	12.39399500	7.73120000	H	6.18369000	3.76967500	4.09827800
H	3.69735300	12.01978100	6.70757000	C	5.16852800	6.89742900	7.31447900
H	3.06040700	10.78374000	7.81090900	C	5.07833300	6.58827200	5.94646600
C	4.63361100	13.80262100	8.46487400	C	5.51294200	8.19945300	7.70985200
H	5.17341700	13.80526600	7.50646200	C	5.32760200	7.57363000	4.99028300
H	3.77483200	14.48485600	8.38228000	H	4.82735700	5.57621200	5.63137500

C	5.76910000	9.18194200	6.74755800	H	4.80108400	6.48662600	14.55535200
H	5.57077200	8.44598500	8.77352600	H	6.01845200	5.69112800	15.57371700
C	5.67420800	8.86919000	5.38968200	C	6.60816700	7.65744000	14.81897000
H	5.25222400	7.32805200	3.92784600	H	7.69501500	7.49561400	14.94605400
H	6.01247700	10.19181100	7.07798100	H	6.49087600	8.23747200	13.89127300
H	5.86701600	9.63893600	4.63798300	C	6.08431100	8.49430300	15.98978400
C	6.29688800	4.52862700	8.51345900	H	6.26654100	7.95667400	16.93864600
C	6.21950600	3.27935900	9.14956700	H	4.99014900	8.58830000	15.89202900
C	7.49663600	4.91517000	7.90052700	C	6.70710200	9.88742300	16.04705400
C	7.31813400	2.42008500	9.14448500	H	6.31399800	10.47445900	16.89253300
H	5.29929100	2.98827700	9.65967300	H	7.80392500	9.83523500	16.15590900
C	8.60354700	4.06205200	7.92117600	H	6.49239500	10.44577100	15.12148700
H	7.57022900	5.88845700	7.41299500	Sn	6.47626200	5.09646800	12.98827100
C	8.51667300	2.81132500	8.53790500	O	4.75941600	4.66009300	11.91341800
H	7.24557100	1.44564900	9.62941800	C	3.76546900	3.91328100	12.58405400
H	9.53651700	4.37708100	7.44776900	H	3.44314200	4.39305800	13.52930300
H	9.37897700	2.14068000	8.54597400	H	2.86668000	3.82673100	11.95527300
C	7.77299000	5.81041600	11.41711200	H	4.11724700	2.89179700	12.82759300
H	7.93392000	4.95153900	10.75013100				
H	7.18507900	6.55575600	10.86314000	**I-5a'**			
C	9.10413400	6.40287600	11.87593200	Cu	4.31583100	7.13367500	11.31249800
H	8.93173100	7.22378100	12.59392900	C	1.53436700	3.56909600	9.23355900
H	9.69786500	5.64595800	12.42203800	C	1.95151400	2.52366800	8.39254000
C	9.93123100	6.93763300	10.70226500	C	3.16986700	2.68516700	7.75968700
H	9.32207300	7.68034100	10.15764800	C	3.96072600	3.81915600	7.97234900
H	10.11282500	6.11357500	9.98911000	C	3.59295700	4.86320100	8.81454500
C	11.25644600	7.56551800	11.12861700	C	2.31101100	4.71056200	9.41365700
H	11.89347300	6.83743900	11.65878400	O	0.46953300	5.21560700	11.28147700
H	11.82688700	7.94009400	10.26366700	P	4.74881800	6.22177500	9.30638900
H	11.09076400	8.41567100	11.81132400	B	4.43442700	12.17795300	10.13083000
C	7.05371300	3.11990100	13.71675800	S	1.59525700	5.94477700	10.56510800
H	6.27444600	2.79218100	14.42580800	O	5.09369700	3.71198400	7.21656500
H	7.97623000	3.24988800	14.30943300	O	3.79261400	1.84350000	6.88326800
C	7.25724800	2.09054800	12.60776200	H	1.35160600	1.62414500	8.24655100
H	8.03669600	2.44432300	11.91061600	H	0.59990700	3.51027000	9.79567300
H	6.33810500	2.01597400	12.00016300	C	0.65754000	7.05699600	9.31454300
C	7.63541700	0.69413800	13.11060200	C	-0.07310500	8.03802000	10.23532900
H	8.55740900	0.76550300	13.71540400	H	-0.72717800	7.49797700	10.93364900
H	6.85082800	0.33457200	13.80056400	H	-0.68658600	8.72330700	9.62689600
C	7.83513800	-0.31962900	11.98442000	H	0.63304500	8.63456800	10.82716600
H	8.63924200	-0.00135200	11.29968300	C	-0.33237200	6.20940600	8.52961100
H	8.10376900	-1.31525700	12.37164900	H	0.17164900	5.55792500	7.80104400
H	6.91618100	-0.43443200	11.38467300	H	-1.02748400	6.86720400	7.97990000
C	5.88175900	6.32051700	14.67816100	H	-0.91863900	5.58384500	9.21968600

C	1.67032400	7.76692800	8.43255500	H	6.00485900	12.82556400	11.48563900
H	2.44742000	8.25302100	9.03884300	H	6.39662800	10.68132300	12.70748400
H	1.16514700	8.54606300	7.83687100	C	5.10357700	2.38955300	6.63738000
H	2.15816500	7.07851300	7.72996600	C	5.34558200	2.51613500	5.14134900
C	3.08103200	12.59672500	8.32787300	C	6.75201500	3.05519500	4.85870400
C	2.22853800	12.53503800	9.65415700	C	7.82232000	2.18998500	5.53408600
O	3.24827200	12.60191000	10.67544500	C	7.56761900	2.07444100	7.04033700
O	4.35586700	12.07316600	8.75897700	C	6.16257500	1.54474000	7.33726300
C	1.26394000	13.69807200	9.85174500	H	6.91973800	3.10767500	3.77048700
H	0.51588800	13.72632200	9.04365900	H	5.21762600	1.51428600	4.69858800
H	0.73172900	13.56880300	10.80563200	H	4.56476800	3.16795900	4.72000900
H	1.78798900	14.66232700	9.88363900	H	7.82012500	1.18290000	5.07557600
C	1.49433900	11.20632600	9.82375100	H	8.82256200	2.61643700	5.35248700
H	1.03352800	11.16732500	10.81827800	H	8.32015000	1.42568800	7.51603300
H	0.70468500	11.07925100	9.06949900	H	7.67322300	3.06479800	7.50444000
H	2.19119000	10.36099100	9.75952700	H	6.04420700	0.50708900	6.98170500
C	2.54545500	11.73635300	7.18960600	H	5.95519100	1.55536100	8.41834800
H	1.52760700	12.05284300	6.91244300	H	6.82041600	4.08591500	5.24486100
H	3.18988500	11.84048700	6.30411000	C	4.87014200	7.32100700	7.83384900
H	2.52552100	10.67515900	7.46322600	C	5.09021800	8.68341600	8.08595900
C	3.33405800	14.02476300	7.83627200	C	4.80521700	6.86914700	6.50583300
H	4.09862300	13.99752300	7.04553400	C	5.27159500	9.57825300	7.02657600
H	2.42191600	14.48163600	7.42389000	H	5.10124500	9.04380000	9.11901700
H	3.70888600	14.66307900	8.64962800	C	4.96780700	7.76706100	5.44904300
H	0.39900600	11.56614100	14.04509500	H	4.64917000	5.81045700	6.29968200
H	2.53608000	11.27613100	12.77607800	C	5.20904700	9.12105400	5.70811100
H	2.07906200	7.00893400	13.02513400	H	5.42766900	10.63357800	7.25033800
H	-0.01874000	7.27364600	14.24597500	H	4.91316800	7.40641300	4.41801100
O	-1.12140400	9.71236200	14.90255700	H	5.34044800	9.82201200	4.87903900
C	-1.88683200	8.62174800	15.34090500	C	6.39512100	5.39725300	9.26871700
H	-2.22401600	7.98505500	14.50142500	C	6.63651200	4.37210600	10.19679500
H	-2.76943900	9.03542000	15.85033100	C	7.45162900	5.86071600	8.47122200
H	-1.33110600	7.98236300	16.05239600	C	7.90874100	3.80902700	10.30220600
C	0.78207700	10.57079700	13.80699000	H	5.83092200	4.05244200	10.86359900
C	1.97159200	10.40199400	13.10705900	C	8.72977400	5.30944600	8.59711400
C	2.47019300	9.11692200	12.79005600	H	7.28310100	6.66545200	7.75530300
C	1.71643700	8.01651000	13.23147600	C	8.96269500	4.28059100	9.51242200
C	0.52307200	8.16961300	13.94395800	H	8.08516300	3.01279800	11.02518500
C	0.04318700	9.45296200	14.23003200	H	9.54523700	5.68911000	7.97547800
C	3.72055600	8.91637900	12.02448300	H	9.96066700	3.84561900	9.61185400
C	4.62876800	9.85657100	11.96396500	C	8.17477800	8.15959800	14.63949900
C	5.60457500	10.75578400	11.94691100	H	8.04726700	9.13765300	14.14586000
C	5.74169500	11.89293500	10.94662100	H	8.09895000	8.35132200	15.72534100
H	6.57979800	11.71267800	10.24492800	C	9.53389400	7.54767300	14.30100800

H	9.63898000	6.56603600	14.79979300
H	9.59139900	7.33248500	13.21949300
C	10.73162400	8.42329000	14.68674300
H	10.68726200	8.63899600	15.77023700
H	10.63568900	9.40216300	14.18267900
C	12.08121000	7.79502100	14.33974400
H	12.16015400	7.59882200	13.25699100
H	12.92544900	8.44490100	14.62420300
H	12.21444000	6.82876300	14.85571900
C	4.72491900	7.67156200	15.17526400
H	4.66751700	7.07877800	16.10615300
H	3.85228200	7.40124300	14.57100000
C	4.76356800	9.16765800	15.46957900
H	4.81967300	9.72403000	14.52080300
H	5.67590000	9.43309600	16.03697100
C	3.53395700	9.65109800	16.24658700
H	2.62730700	9.33081100	15.70960500
H	3.50247800	9.14912400	17.23233400
C	3.50178700	11.16681700	16.43082100
H	3.49078500	11.67257100	15.45197500
H	2.60494900	11.49220600	16.98364800
H	4.38844600	11.52643800	16.98233900
C	7.03368800	4.89946200	14.86604200
H	7.77012800	5.07643900	15.67149900
H	6.12301400	4.48716500	15.32809100
C	7.57968000	3.92576000	13.82886300
H	6.81067400	3.78314800	13.05405700
H	8.45801900	4.35768000	13.31562600
C	7.96198200	2.56677700	14.42582800
H	7.08067600	2.14820400	14.94454200
H	8.72970100	2.71459600	15.20847100
C	8.47098500	1.55844200	13.39576300
H	8.74905200	0.59853500	13.86215000
H	7.70103600	1.34668600	12.63530800
H	9.36068800	1.94115400	12.86709200
Sn	6.45358300	6.87339100	14.13756900
O	6.49338700	7.02560900	12.08869900
C	7.47801500	7.74415800	11.39986400
H	8.35929400	7.11348000	11.16568000
H	7.06338700	8.09857400	10.43997900
H	7.82674400	8.64506800	11.93613200
Br	4.07459000	4.97513500	12.77755200

I-5b

Cu	4.43360300	7.07757400	11.13919100
C	1.27307500	4.94469500	8.46986100
C	1.38124700	3.95798400	7.47303800
C	2.63450200	3.75961000	6.91980100
C	3.74836200	4.50042000	7.33801700
C	3.68649700	5.45663300	8.34289400
C	2.38695500	5.67666900	8.87269800
O	0.87773200	6.43123800	10.94870800
P	5.16906900	6.18045100	9.17759700
B	8.01425500	11.75909300	12.90445800
S	2.15291000	6.85183400	10.23637400
O	4.83749900	4.10136700	6.62729400
O	3.01280400	2.87149400	5.96384400
H	0.52365300	3.36234800	7.15797500
H	0.32455600	5.13047400	8.97668900
C	1.71558000	8.45288100	9.30044300
C	1.44468300	9.45648500	10.42323600
H	0.65589100	9.09381500	11.09665000
H	1.11387200	10.40781400	9.97642400
H	2.34949200	9.64748000	11.01490400
C	0.46409900	8.19154400	8.47371400
H	0.66441200	7.52764000	7.62058700
H	0.08810300	9.14944200	8.07935300
H	-0.32255600	7.74485700	9.09966400
C	2.91580800	8.87196500	8.46294000
H	3.81081600	9.00189800	9.08793200
H	2.69571700	9.84165400	7.98727000
H	3.14015500	8.15337300	7.66209300
C	8.30131200	13.99129900	13.29673300
C	7.30151200	13.37624200	14.35246100
O	7.50135700	11.95463500	14.16559600
O	8.40217500	12.93538000	12.31486700
C	7.60231800	13.73536300	15.80215500
H	7.55905600	14.82583100	15.94868700
H	6.85529200	13.27138800	16.46214800
H	8.59209800	13.37653200	16.11131800
C	5.83426600	13.67055600	14.03199500
H	5.19537200	13.07870400	14.70215300
H	5.59302800	14.73358600	14.17743400
H	5.58677100	13.38793300	12.99878200
C	7.80646700	15.25642900	12.60736500
H	7.63452200	16.06012800	13.34008300
H	8.56287700	15.60461100	11.88829700
H	6.87479700	15.07569600	12.05656700

C	9.70769500	14.21217500	13.85946900	C	5.90569700	7.16635100	6.58885300
H	10.39160300	14.43091800	13.02637200	C	7.29369800	9.32803100	7.70267100
H	9.73711400	15.05522100	14.56526900	H	6.66230700	8.56366200	9.61715400
H	10.07587100	13.31250600	14.37354500	C	6.54238500	8.09377000	5.76123800
H	3.38857100	11.52808600	15.75694600	H	5.38353900	6.31668300	6.14948300
H	4.94694500	10.85785400	13.92484400	C	7.23899600	9.17356600	6.31529700
H	2.33152700	7.59270600	12.92960200	H	7.82453000	10.17307200	8.14728800
H	0.80466500	8.23203100	14.72652700	H	6.49564600	7.97198700	4.67616300
O	1.22085600	10.37315700	16.39912600	H	7.73431700	9.89677300	5.66269600
C	0.04450000	9.66579800	16.70161700	C	6.26892500	4.70885900	9.18659800
H	-0.66631800	9.66409600	15.85476700	C	5.87754700	3.62219300	9.98546500
H	-0.42141700	10.17581100	17.55590200	C	7.44588200	4.62343300	8.43238900
H	0.25426300	8.61693500	16.98184100	C	6.63297000	2.44894700	9.98900300
C	3.17062600	10.66902400	15.11817900	H	4.98916900	3.71137000	10.61415500
C	4.02824200	10.29345000	14.09471100	C	8.21088800	3.45450500	8.45677700
C	3.75987500	9.17613200	13.27118900	H	7.75700700	5.46378600	7.81075100
C	2.58435600	8.45885900	13.54146200	C	7.80150300	2.36141000	9.22542700
C	1.70591600	8.82409800	14.56855000	H	6.31824600	1.60348900	10.60181500
C	1.99678000	9.93582500	15.36875000	H	9.12667800	3.39619300	7.86388000
C	4.69016500	8.75785600	12.19303200	H	8.39583800	1.44462500	9.23739100
C	5.66971800	9.54509700	11.82599600	C	7.56628400	6.45043300	12.37878000
C	6.68811900	10.30240500	11.44858400	H	7.00487600	6.87163600	11.53267400
C	8.03011000	10.37524900	12.17125600	H	8.01226600	7.31153100	12.90050000
H	8.87088800	10.30022700	11.45989000	C	8.63568900	5.46609800	11.91329700
H	8.11034200	9.54998700	12.89388800	H	9.18043600	5.05026800	12.78108600
H	6.54907400	11.01327300	10.62124100	H	8.16826700	4.60485800	11.40819000
C	4.46600700	2.89838800	5.92328200	C	9.64016400	6.11392600	10.95470200
C	5.01833500	1.68592500	6.66273500	H	10.06593400	7.01464200	11.43229300
C	4.71361100	0.38938300	5.90709100	H	9.09390700	6.47608700	10.06598800
C	5.21110900	0.46133600	4.45896000	C	10.76406800	5.17255200	10.52805500
C	4.62683800	1.67731200	3.73083500	H	10.35904300	4.27206600	10.03982200
C	4.92993600	2.97888100	4.48175900	H	11.45562100	5.65780300	9.82066200
H	5.17001300	-0.46363900	6.43361000	H	11.35581600	4.83895200	11.39709400
H	6.10459600	1.83608800	6.76790000	C	6.46043000	3.68092700	14.51065300
H	4.60136300	1.67562300	7.68140900	H	5.67568300	3.47750400	15.25939000
H	6.31448000	0.52892300	4.45506200	H	7.40846500	3.75943500	15.07147500
H	4.95185800	-0.46383100	3.91964000	C	6.53272500	2.55854900	13.47806400
H	5.02003700	1.74282100	2.70412000	H	7.32201200	2.77966700	12.74046000
H	3.53297300	1.56374400	3.64615000	H	5.59262800	2.52609000	12.89964600
H	6.01519300	3.17100500	4.50086100	C	6.79222200	1.17749500	14.08830400
H	4.44497500	3.84579200	4.00789600	H	7.73374300	1.21121400	14.66565500
H	3.62357700	0.22063300	5.91179600	H	5.99795600	0.95223700	14.82279900
C	5.95695600	7.32058700	7.98376900	C	6.86648900	0.05792800	13.05064100
C	6.64955800	8.40959800	8.53540500	H	7.67467600	0.24211300	12.32322400

H	7.05653800	-0.92106000	13.51846900	H	0.52134900	6.18252800	7.90959100
H	5.92319900	-0.02386800	12.48420400	H	-0.64357100	7.41591200	8.47790400
C	5.39327600	6.94194200	15.34103100	H	-0.52197000	5.84229200	9.32863000
H	4.38794300	7.31444200	15.09944000	C	2.07691700	8.14586500	9.04580500
H	5.30459000	6.28673600	16.22395800	H	2.86557700	8.47947800	9.73853800
C	6.35199800	8.10284200	15.61073000	H	1.54476100	9.04585000	8.68239600
H	7.38582500	7.73057400	15.74627500	H	2.54863500	7.66447400	8.17406400
H	6.38177600	8.76449100	14.72911800	C	8.63542800	10.84912100	12.43614700
C	5.96221800	8.92556900	16.84188800	C	8.38521900	10.63715900	10.89245000
H	5.92993000	8.26257100	17.72613900	O	7.09947100	11.27151000	10.69622400
H	4.93504200	9.29983800	16.69994600	O	7.29546400	11.00288700	12.94878400
C	6.90912400	10.09678900	17.09582700	C	9.40013500	11.31479700	9.97689100
H	6.58215400	10.70385600	17.95598700	H	10.41305400	10.90890000	10.14742800
H	7.93271700	9.74362300	17.30997700	H	9.12514700	11.12253000	8.92563500
H	6.96944900	10.75006600	16.21262700	H	9.42481500	12.40521900	10.12757300
Sn	6.04673100	5.67122800	13.71035900	C	8.23903600	9.16334700	10.51178900
O	4.44175800	5.31227500	12.44728000	H	7.90647000	9.10271500	9.46559800
C	3.24853800	4.80666500	13.01116700	H	9.19884500	8.62771900	10.59879700
H	2.91098800	5.39718100	13.88406500	H	7.49815000	8.64638600	11.14371100
H	2.43721400	4.84894800	12.26668400	C	9.29944500	9.66472000	13.12906700
H	3.36791900	3.75490200	13.33778300	H	10.28318300	9.44765500	12.67657100
				H	9.45801800	9.89671200	14.19572900
I-5b'				H	8.66533400	8.76953900	13.05910900
Cu	4.85896000	6.75207200	11.61092800	C	9.38071500	12.14668100	12.76653200
C	1.94052500	3.90606300	8.66111600	H	9.33538500	12.31182600	13.85682500
C	2.32757200	3.12283100	7.56055400	H	10.44054500	12.09792600	12.46282000
C	3.54227100	3.43227300	6.97814800	H	8.91184700	13.01438900	12.27265200
C	4.35371900	4.45400700	7.48009600	H	0.85607800	9.41280800	16.04027100
C	4.01859000	5.23177000	8.58460200	H	2.55688200	9.93815100	14.28147100
C	2.74010000	4.94293000	9.13627100	H	2.74195100	5.76624500	13.24520900
O	0.96358400	4.89815000	11.12709300	H	1.04015200	5.24733600	14.91436700
P	5.22040800	6.40971300	9.36630200	O	-0.10821300	7.11859000	16.58116800
B	6.45726300	11.33083700	11.91046300	C	-0.58141500	5.81809200	16.80367300
S	2.06465400	5.80773000	10.60481400	H	-1.07325000	5.39540900	15.90428200
O	5.47923000	4.53684100	6.70820900	H	-1.32139000	5.88618500	17.61849400
O	4.14351100	2.84587300	5.90034100	H	0.23026700	5.12774300	17.11129400
H	1.70810800	2.30599400	7.18364400	C	1.27737200	8.62434700	15.40946500
H	1.01045600	3.70720300	9.19945600	C	2.22650400	8.90612500	14.43357500
C	1.09430000	7.22146700	9.74766500	C	2.78406200	7.89208500	13.61921500
C	0.42211200	7.92667000	10.93132200	C	2.33140300	6.58200700	13.84272900
H	-0.18827500	7.21764900	11.51401900	C	1.36245900	6.28414500	14.80689700
H	-0.23372500	8.73233400	10.55039500	C	0.83208100	7.30530100	15.60274300
H	1.17014000	8.37608400	11.60324700	C	3.78783900	8.18545300	12.56764400
C	0.05633000	6.62401900	8.80713400	C	3.90656000	9.39514900	12.08581400

C	4.03325300	10.60616800	11.55417200	H	8.83465100	5.91728300	15.31419700
C	4.94616600	11.71562500	12.08711900	H	9.10354600	7.67084400	15.37797100
H	4.73449900	11.93511800	13.15032700	C	8.33901900	6.81033200	17.23134100
H	4.74400800	12.64453000	11.52191500	H	7.93405300	7.76272300	17.62446700
H	3.46341800	10.84601500	10.64311400	H	7.62003600	6.02703400	17.54284400
C	5.43225100	3.46811500	5.74198800	C	9.68500000	6.53410700	17.91502900
C	5.55477000	4.06746800	4.34604900	H	10.40976600	7.31431200	17.61049400
C	6.93572700	4.70253600	4.13942900	H	10.09081600	5.57666700	17.53436600
C	8.05699600	3.69533300	4.42710600	C	9.59273300	6.48400000	19.44162600
C	7.92158100	3.10574600	5.83632700	H	8.89592000	5.69094900	19.77183400
C	6.54338800	2.47051400	6.05270200	H	10.57557000	6.28254200	19.90640100
H	7.01614600	5.09249900	3.10889300	H	9.21797300	7.44166000	19.84930800
H	5.38953300	3.25378700	3.61671900	C	5.73073000	9.16535700	15.15069700
H	4.74430500	4.80418900	4.21320400	H	4.72677300	9.06425700	15.59467000
H	8.01812500	2.88078900	3.67600300	H	5.60364400	9.61538300	14.15813900
H	9.04152800	4.18404600	4.31539000	C	6.65378800	10.01461300	16.02324700
H	8.71091100	2.35643400	6.02269200	H	7.67410000	10.01750700	15.59971300
H	8.06279200	3.90335300	6.58306300	H	6.74381100	9.57928200	17.03833400
H	6.40184800	1.59528400	5.39228500	C	6.18199000	11.46830000	16.14832000
H	6.42272200	2.13226500	7.09535700	H	6.06672100	11.88340300	15.13217700
H	7.03731700	5.56647500	4.82063500	H	5.17725100	11.48696700	16.61350900
C	5.27506200	7.83534300	8.19375000	C	7.14454300	12.34454900	16.95179400
C	5.37713500	9.11001000	8.76417000	H	8.14018200	12.37790700	16.46951800
C	5.23452100	7.71560200	6.79327100	H	6.77922700	13.38482900	17.03616100
C	5.45620600	10.25012100	7.95774900	H	7.28701600	11.95412500	17.97764200
H	5.37858400	9.22231600	9.84978300	C	5.24325600	5.48428300	15.42584600
C	5.29735500	8.85418400	5.98735700	H	4.83776800	5.75514100	16.41928500
H	5.16920600	6.72906600	6.33292400	H	4.40028100	5.41313400	14.72682700
C	5.41252900	10.12461700	6.56771300	C	6.01119700	4.16313900	15.46612100
H	5.55775600	11.22748200	8.43597600	H	6.46934700	3.98167100	14.47811700
H	5.26222700	8.74925600	4.89773300	H	6.83700300	4.20917300	16.20509700
H	5.46717800	11.01458300	5.93183900	C	5.10601600	2.96831000	15.78652400
C	6.83876300	5.58864400	9.03179700	H	4.29023100	2.95264900	15.04171400
C	7.06179800	4.29049700	9.52437100	H	4.63442000	3.11636800	16.77891600
C	7.90992200	6.28661900	8.45366000	C	5.84882600	1.63178200	15.75371500
C	8.33230600	3.71799100	9.45193100	H	5.17876500	0.78473000	15.99187300
H	6.24510200	3.75234500	10.01328200	H	6.27287100	1.45160900	14.74876200
C	9.18433900	5.71360700	8.39258500	H	6.68513100	1.61426000	16.47950800
H	7.75317200	7.28936600	8.05275300	Sn	6.45162300	7.15693600	14.76160000
C	9.40336300	4.42910800	8.89806900	O	6.94904800	7.04165600	12.76132800
H	8.48937500	2.71098600	9.85166300	C	7.91194500	6.09331800	12.36041100
H	10.00954400	6.27897700	7.94711300	H	8.84307600	6.15440600	12.96369500
H	10.40113900	3.98079700	8.85377800	H	7.51605500	5.06131300	12.40992800
C	8.42162300	6.86526000	15.70323500	H	8.18611300	6.29104300	11.30905800

Br	4.71383000	4.20393600	12.11096600	H	2.28346000	12.69514800	10.30656300
				H	1.97270800	11.08465800	9.61657600
I-6a				H	2.85116400	11.22505700	11.15138700
Cu	4.71279400	6.61754300	10.41729700	C	3.73117700	12.13670700	7.92677100
C	1.35890000	3.96072100	8.82941300	H	3.10263900	11.35846500	7.47045200
C	1.46330100	2.84442100	7.98283700	H	3.20234800	13.09786800	7.85162700
C	2.60624800	2.75289200	7.20872900	H	4.66403500	12.20667800	7.34828500
C	3.60269000	3.73798100	7.25176900	H	2.66668000	10.63873000	14.34543400
C	3.52055800	4.86494600	8.05718100	H	4.70003000	9.86745900	13.10549200
C	2.34517400	4.94465300	8.85782700	H	3.15729900	5.85800600	13.10044700
O	1.32093500	5.47324700	11.25665900	H	1.15814100	6.59431100	14.29994000
P	4.84988600	6.13519900	8.18726700	O	0.70638800	9.19275000	15.06604600
B	5.98352600	10.60173600	9.50846800	C	-0.33254300	8.32167700	15.44497800
S	2.20743600	6.14619600	10.22311200	H	-0.79921600	7.83285400	14.57040100
O	4.59308700	3.39914100	6.38331000	H	-1.08697500	8.93436500	15.95664800
O	2.96394800	1.78180100	6.33047600	H	0.02158600	7.53602800	16.13666200
H	0.69807900	2.06795000	7.95775200	C	2.79180100	9.59193500	14.06113400
H	0.53178200	4.04246400	9.53585100	C	3.91602200	9.15620300	13.37293000
C	1.13701400	7.54760300	9.53362200	C	4.08100100	7.80236400	13.01248300
C	0.96714900	8.45809900	10.75347700	C	3.07243500	6.90562300	13.38708000
H	0.46462400	7.92768800	11.57257700	C	1.92893500	7.32790400	14.06905100
H	0.35860200	9.33154800	10.47070100	C	1.78069800	8.67809900	14.41145000
H	1.93643500	8.81948900	11.12681300	C	5.28405000	7.33349100	12.28166300
C	-0.19520600	6.96831800	9.07981000	C	6.00411500	8.14069800	11.51491200
H	-0.08589300	6.35178500	8.17578600	C	6.90764500	8.95708000	10.99232700
H	-0.88817000	7.79387900	8.84884600	C	6.98647800	9.39924800	9.54305800
H	-0.64046400	6.35853100	9.87935900	H	6.69525500	8.57505700	8.87719800
C	1.90233300	8.23594800	8.41574600	H	8.01067100	9.71023900	9.28936700
H	2.86801100	8.62501800	8.76664100	H	7.60989600	9.43275000	11.68888000
H	1.31380200	9.09362900	8.04994600	C	4.34786000	2.02334500	5.98960600
H	2.07093700	7.56744200	7.56035500	C	4.56229500	1.89724900	4.49479500
C	4.00971800	11.75815200	9.38270500	C	6.03786100	2.11800700	4.13883600
C	5.13167800	12.64313800	10.05324200	C	6.95025400	1.17221600	4.92845200
O	6.33637200	11.90312800	9.74306700	C	6.72146900	1.31269900	6.43676100
O	4.62213200	10.44563200	9.36879600	C	5.25020900	1.10295500	6.80374500
C	5.25923500	14.05173400	9.48938600	H	6.17982300	1.98361400	3.05485200
H	4.32465400	14.61554500	9.63354200	H	4.23950100	0.88572700	4.19909700
H	6.06512400	14.58620600	10.01344600	H	3.90415500	2.61789900	3.98572300
H	5.50307400	14.03978100	8.41944600	H	6.75334700	0.12972300	4.61723500
C	5.02278500	12.68837700	11.57880100	H	8.00530000	1.37831700	4.68687800
H	5.94043800	13.13617400	11.98642700	H	7.34833000	0.60099600	6.99667000
H	4.16351500	13.28886900	11.91017500	H	7.02517900	2.31840800	6.75927500
H	4.92494100	11.67675700	11.99516000	H	4.93310400	0.06748000	6.59686700
C	2.70652100	11.68842500	10.16760900	H	5.07416100	1.29458500	7.87438800

H	6.30803600	3.16182500	4.37126200	H	6.36942000	0.36062700	12.44288900
C	4.60050100	7.12827500	6.65845100	C	7.93868700	0.11619700	10.96842200
C	4.28500800	6.51450400	5.43286400	H	8.94641300	0.50214000	10.73783300
C	4.73520300	8.52187700	6.70850000	H	8.02123700	-0.97581100	11.09084400
C	4.11457500	7.28541400	4.28194100	H	7.30721600	0.30732800	10.08342800
H	4.19091600	5.43093800	5.37044200	C	5.90706900	5.81501100	15.03908700
C	4.56894600	9.28968500	5.55248200	H	4.81873000	5.69013400	15.15890900
H	4.93324200	9.01911000	7.65523400	H	6.38242100	5.05832800	15.68461500
C	4.25866500	8.67549900	4.33776000	C	6.32529600	7.23613700	15.42231900
H	3.87015700	6.79653100	3.33574100	H	7.39140500	7.24464300	15.71202200
H	4.67333000	10.37496700	5.60919000	H	6.25746600	7.90899900	14.55196800
H	4.12502700	9.27745500	3.43567900	C	5.48121400	7.84812200	16.54493600
C	6.43367500	5.25483600	7.87763600	H	5.55503400	7.21726200	17.44958000
C	6.92326400	4.42372000	8.89948400	H	4.42142000	7.82000400	16.23589600
C	7.21296300	5.47184400	6.73197000	C	5.87353700	9.28673800	16.87529400
C	8.16880000	3.80912500	8.76535600	H	5.24782500	9.70847800	17.67850400
H	6.33669100	4.29109200	9.81186300	H	6.92589100	9.35313800	17.20009200
C	8.46335000	4.85963500	6.60837100	H	5.75931400	9.93454400	15.98997700
H	6.85106300	6.12071400	5.93432500	Sn	6.31597800	5.22658300	12.94721800
C	8.94453200	4.02853100	7.62318200	O	4.89378600	4.73134200	11.33004100
H	8.53531400	3.16590000	9.56652600	C	4.14873500	3.54994700	11.19390800
H	9.06488800	5.03895700	5.71389900	H	3.06917200	3.73770500	11.32136300
H	9.92367000	3.55374500	7.52555800	H	4.29651900	3.09222500	10.19394600
C	8.23228400	5.82723700	12.07212300	H	4.43996600	2.79376700	11.94089600
H	8.85384400	4.92770400	11.93686700				
H	8.00017300	6.20852600	11.06517400	**I-6a'**			
C	8.97856400	6.88945400	12.87866400	Cu	4.81130600	6.06170900	11.57752800
H	8.29366300	7.70928700	13.15016100	C	1.36056400	3.49737400	8.79779500
H	9.31998000	6.46425400	13.84061400	C	1.75609400	2.48494800	7.90746800
C	10.17949000	7.48537100	12.13744900	C	3.01315300	2.60776700	7.34471000
H	9.82851000	7.89075500	11.17143400	C	3.85797900	3.67358100	7.66908600
H	10.88935700	6.67669400	11.88519200	C	3.51530900	4.67719700	8.56898100
C	10.89612100	8.58050800	12.92560700	C	2.19926300	4.56734200	9.09630100
H	11.27476900	8.19807900	13.88852100	O	0.31602900	5.07862900	10.90509500
H	11.75349700	8.99365500	12.36997000	P	4.73944900	5.88753400	9.24780500
H	10.21234400	9.41593900	13.15323500	B	4.47845000	12.22364100	10.42564700
C	6.62529200	3.04001800	13.25483600	S	1.52435900	5.77510700	10.29003900
H	5.69305400	2.55800500	13.59458700	O	5.02102900	3.54221200	6.96691200
H	7.32039800	2.99452300	14.11265600	O	3.63078200	1.78175000	6.45048200
C	7.21468700	2.30959700	12.05133400	H	1.11112500	1.63665700	7.67398800
H	8.20796500	2.73399200	11.81747600	H	0.39774000	3.45973800	9.31051100
H	6.59969600	2.49607800	11.15460800	C	0.70573600	7.01036800	9.07204800
C	7.36002800	0.79265200	12.21158400	C	0.04630000	8.01989300	10.01373900
H	7.99524900	0.57456300	13.08893800	H	-0.70297300	7.54232000	10.65785500

H	-0.45418400	8.80219000	9.41918400	C	0.28282000	7.97773600	13.38329800
H	0.78514300	8.50612300	10.66542200	C	4.40058500	9.26175000	13.55862100
C	-0.33506400	6.28391100	8.23330400	C	4.80970000	10.44373100	13.17508000
H	0.12806600	5.62542700	7.48425300	C	5.25645900	11.62565600	12.79737400
H	-0.96188300	7.02136400	7.70314500	C	5.69556500	11.97079600	11.38390000
H	-0.98397800	5.67971300	8.88463100	H	6.31288800	11.16401900	10.95492300
C	1.78508500	7.67264600	8.23193800	H	6.33633500	12.87211500	11.39188700
H	2.55873100	8.13232300	8.86260800	H	5.23853400	12.44672000	13.52760400
H	1.33661800	8.47369800	7.62051300	C	4.97073300	2.27994500	6.26631100
H	2.27414100	6.96716700	7.54662100	C	5.23340500	2.53150300	4.78855100
C	3.26760000	12.44741100	8.49764200	C	6.66706400	3.02227300	4.55900200
C	2.32927600	12.55840700	9.75592700	C	7.68866900	2.05352600	5.16553100
O	3.28059100	12.75786400	10.82315700	C	7.41240600	1.82299000	6.65473300
O	4.48279400	11.91689700	9.08028700	C	5.98265800	1.32794000	6.89220400
C	1.35722900	13.73038000	9.73286000	H	6.84661500	3.15610900	3.47976000
H	0.67332600	13.65314200	8.87298500	H	5.05907100	1.58187700	4.25584400
H	0.75325500	13.72246800	10.65221000	H	4.48925000	3.25698200	4.42490700
H	1.88343300	14.69258000	9.68210300	H	7.64361000	1.08973900	4.62408500
C	1.58817100	11.25488700	10.05400800	H	8.70959700	2.44516700	5.02631400
H	1.12806600	11.31535600	11.04897100	H	8.13113100	1.10492900	7.08005200
H	0.79950800	11.05397200	9.31532000	H	7.55320900	2.76515700	7.20426200
H	2.27807500	10.40004800	10.06942200	H	5.82649400	0.33373800	6.44049900
C	2.76285300	11.50317300	7.41466100	H	5.76400400	1.24833000	7.96773600
H	1.77003700	11.82333600	7.06112400	H	6.78392900	4.01354700	5.02814800
H	3.44863100	11.50629600	6.55535400	C	5.04977200	7.07871100	7.86771000
H	2.69282300	10.47236700	7.77878900	C	5.19977900	8.43297400	8.19888700
C	3.62217200	13.80776200	7.89120400	C	5.16519500	6.69233000	6.52106900
H	4.44421800	13.67265800	7.17273300	C	5.48300300	9.38396600	7.21386200
H	2.76622500	14.25163300	7.36113000	H	5.09730600	8.75330800	9.23625200
H	3.95827700	14.51260800	8.66574100	C	5.43212700	7.64385200	5.53473100
H	-0.21979700	10.06892400	13.34293700	H	5.06532000	5.64253600	6.24839000
H	2.16484300	10.83180700	13.42779600	C	5.59829800	8.99019100	5.87928100
H	3.42324400	6.71677100	13.54346200	H	5.59162100	10.42835200	7.50893200
H	1.12713300	5.96640600	13.38447500	H	5.51917300	7.32977600	4.49082800
O	-1.03902400	7.66191000	13.30221900	H	5.81450800	9.73150900	5.10505800
C	-1.39662200	6.29141000	13.36956000	C	6.30186200	4.90146800	9.25209400
H	-0.94042700	5.71541600	12.54818300	C	6.32549200	3.67244000	9.93540700
H	-2.49281800	6.25613600	13.29180600	C	7.49998500	5.42028500	8.74026900
H	-1.09159700	5.84944900	14.33604400	C	7.52604200	2.98054500	10.09440800
C	0.60077700	9.34869800	13.38684000	H	5.40657400	3.27654500	10.37384200
C	1.92608800	9.76528100	13.43580500	C	8.70275600	4.72856700	8.91545300
C	2.98590300	8.83402800	13.49947200	H	7.49938900	6.37225200	8.20800500
C	2.64155500	7.47544100	13.50900200	C	8.72131500	3.50822900	9.59411500
C	1.31733800	7.03715900	13.43951900	H	7.52769700	2.02919300	10.63121300

H	9.62996400	5.15197300	8.52049900	H	7.66684200	8.62850100	11.67384900
H	9.66218400	2.97050500	9.73553400	H	6.97703200	7.67318800	10.35425600
C	7.91237700	8.93625900	14.35038300	H	6.03255400	8.99723000	11.09349800
H	7.79339400	9.74726300	13.61287000	Br	3.62156700	4.09077500	12.27527600
H	8.14378500	9.42399800	15.31234300				
C	9.03434500	7.98462500	13.93606800	**I-6b**			
H	9.25128700	7.28208700	14.76131700	Cu	5.04383500	6.65527400	11.52726900
H	8.69748700	7.35150000	13.09878800	C	1.58150200	5.83717700	8.58168000
C	10.33440800	8.68879900	13.53428900	C	1.52067000	5.01776500	7.43905300
H	10.68791100	9.31705000	14.37315500	C	2.72284200	4.68703400	6.84050800
H	10.11739600	9.38889800	12.70655600	C	3.94561100	5.14274800	7.35323000
C	11.43825700	7.72042600	13.10909000	C	4.04645900	5.91525900	8.50202300
H	11.11103300	7.10296100	12.25561100	C	2.79974700	6.28425200	9.08452000
H	12.36067000	8.24652800	12.81036000	O	1.36520400	6.95427900	11.24439200
H	11.69798200	7.02853700	13.92855400	P	5.64479600	6.20597600	9.36497300
C	5.36673400	8.70477300	16.61252900	B	7.03346900	11.63004400	12.48428700
H	6.10959700	8.27866500	17.31377500	S	2.71838500	7.24970600	10.62775100
H	4.39614700	8.23982800	16.86456000	O	4.95321900	4.69229600	6.56162100
C	5.28540100	10.21979400	16.77162500	O	2.95232200	3.91439800	5.74702400
H	4.55633100	10.62777800	16.04852700	H	0.57258200	4.64520800	7.04944300
H	6.25346200	10.68137400	16.49590100	H	0.67577700	6.10295200	9.12987000
C	4.90171600	10.70166400	18.17659000	C	2.57151000	9.03272300	9.97917000
H	3.93167000	10.25122300	18.45634800	C	2.61515800	9.85801500	11.26777800
H	5.63419700	10.31110900	18.90749900	H	1.85734000	9.51535900	11.98678100
C	4.81538200	12.22356800	18.29746300	H	2.41549900	10.91449200	11.02875400
H	4.06698300	12.63369900	17.59811200	H	3.59934600	9.79462300	11.75108300
H	4.53475900	12.54582200	19.31465000	C	1.23200500	9.16789000	9.26974400
H	5.78170300	12.69690700	18.05178800	H	1.21394100	8.60780700	8.32324000
C	5.84655100	5.84729800	14.90677200	H	1.04812400	10.23043200	9.04153500
H	5.81630800	5.73992800	16.00531000	H	0.42024200	8.80183700	9.91453600
H	4.88453300	5.47469300	14.52494100	C	3.75602800	9.34025000	9.07649600
C	6.98888700	5.02980000	14.30585200	H	4.70983500	9.11926600	9.57424900
H	7.06681100	5.25914100	13.23143200	H	3.75566800	10.41461800	8.82976800
H	7.95262900	5.33864100	14.75122700	H	3.71005000	8.77939800	8.13387900
C	6.81970400	3.51817800	14.48538600	C	6.58988900	13.86153300	12.62828800
H	5.88352800	3.21299400	13.98844600	C	5.55297600	13.04603400	13.49129800
H	6.69578500	3.28283000	15.55958300	O	6.18412000	11.74315000	13.55560000
C	7.99369000	2.72312000	13.91454600	O	7.20957600	12.81910900	11.83174600
H	7.84277700	1.63400000	14.00870200	C	5.34370700	13.55894400	14.90926500
H	8.13169300	2.95299100	12.84573200	H	4.94231200	14.58398900	14.89694700
H	8.93931600	2.97543300	14.42632500	H	4.61920000	12.91532600	15.42998100
Sn	5.93838600	8.00873900	14.55589200	H	6.27680800	13.55216200	15.48643200
O	6.20828700	7.26416500	12.24126700	C	4.20652400	12.85881700	12.78947700
C	6.72611700	8.15779500	11.32147900	H	3.61358900	12.11314200	13.33631600

H	3.63723000	13.79893000	12.75235500	H	3.27002500	2.85660700	3.27503100
H	4.34284900	12.49028600	11.76294200	H	5.98864400	3.84830500	4.32407400
C	5.97592800	14.89501300	11.69421400	H	4.58075500	4.86235500	3.93526800
H	5.41878100	15.65324500	12.26584100	H	3.06791600	1.23098500	5.34295900
H	6.77235600	15.40590900	11.13318900	C	6.61833600	7.31214800	8.28224100
H	5.29594000	14.43068200	10.96894700	C	7.89013300	7.69110500	8.74910300
C	7.70042800	14.49569600	13.46868800	C	6.16371800	7.80975000	7.05438900
H	8.49412700	14.85289100	12.79655200	C	8.68831700	8.55451700	7.99894500
H	7.32852600	15.34972000	14.05337400	H	8.25272500	7.30614700	9.70538800
H	8.14392300	13.76488400	14.16050600	C	6.96217400	8.68222100	6.30909200
H	2.78433700	10.81457900	15.50966100	H	5.18660900	7.50987300	6.67335600
H	4.91526000	10.11946000	14.39457200	C	8.22308000	9.05763900	6.77891900
H	3.27792700	6.20578800	13.71676600	H	9.67452800	8.84111900	8.37143800
H	1.14391800	6.89541500	14.76341700	H	6.59698200	9.06631100	5.35353100
O	0.70023500	9.39826200	15.79614700	H	8.84488500	9.74027100	6.19504100
C	-0.42544200	8.55754700	15.89030000	C	6.55267500	4.61201300	9.22108100
H	-0.77464700	8.22615800	14.89574000	C	6.37154900	3.67621900	10.25193300
H	-1.21864600	9.14596100	16.37115300	C	7.42392200	4.32199600	8.15941400
H	-0.22072600	7.66274300	16.50582600	C	7.03330300	2.44635900	10.19802900
C	2.90902500	9.80528600	15.11090700	H	5.74185900	3.95061700	11.10909900
C	4.09527900	9.40929400	14.50245100	C	8.09121600	3.09680000	8.12085700
C	4.23876300	8.10561500	13.99254300	H	7.57546700	5.04894800	7.36143600
C	3.16816200	7.21070000	14.12971300	C	7.88971800	2.15245200	9.13443800
C	1.96668400	7.60744400	14.71974600	H	6.88967800	1.72544200	11.00659300
C	1.82829700	8.91279200	15.21258000	H	8.77342400	2.87749600	7.29560700
C	5.48711400	7.68846000	13.29411600	H	8.41598800	1.19532500	9.10099300
C	6.03834600	8.39776200	12.29394600	C	8.23014300	5.80535000	12.65317500
C	6.76028700	9.23177300	11.56008100	H	7.64084700	5.89973100	11.72824400
C	7.72704600	10.27798500	12.08734300	H	8.91871000	6.66729800	12.67060900
H	8.49980200	10.46768500	11.32642100	C	8.99889300	4.48706500	12.64923900
H	8.23326800	9.89433700	12.98648500	H	9.59717500	4.38491700	13.57383000
H	6.68478100	9.17445200	10.47130600	H	8.29019200	3.64354800	12.65429300
C	4.38794900	3.68038800	5.70410100	C	9.91887400	4.34056700	11.43273100
C	4.69554500	2.29991900	6.27333000	H	10.63651900	5.18145200	11.41711800
C	4.17020800	1.19389500	5.35356500	H	9.31068100	4.44024400	10.51770200
C	4.69924000	1.36402100	3.92478400	C	10.67402800	3.01374300	11.40071500
C	4.36414700	2.75291000	3.36859400	H	9.97231300	2.16392300	11.39365100
C	4.88718000	3.86495700	4.28500100	H	11.30808400	2.92734800	10.50371700
H	4.45161000	0.20901300	5.75816200	H	11.32446000	2.89941900	12.28432600
H	5.78923100	2.23125600	6.38797900	C	5.73955100	4.43152000	15.08907300
H	4.26558500	2.23204200	7.28501200	H	4.67351500	4.69774700	15.04461900
H	5.79596300	1.22518100	3.92289100	H	6.02840700	4.36676600	16.15186300
H	4.28356400	0.58297200	3.26808800	C	5.99007900	3.12053600	14.34681700
H	4.78308200	2.87934800	2.35782500	H	7.04555500	2.81211600	14.45757700

H	5.81243200	3.29759700	13.27602200	C	1.36950100	7.73830400	9.93076100
C	5.08663300	1.97251400	14.80473400	C	1.08912100	8.63138100	11.14240300
H	5.26434800	1.75800200	15.87462500	H	0.44646000	8.11665300	11.87124700
H	4.03475600	2.30036300	14.72944100	H	0.57799200	9.55215000	10.81396600
C	5.28538200	0.70282100	13.97781300	H	2.02054600	8.91593500	11.65012900
H	6.32790600	0.34596300	14.03667600	C	0.08552900	7.38431800	9.19604100
H	4.63260800	-0.11767900	14.31684200	H	0.28474400	6.80844400	8.28009900
H	5.06006200	0.89101300	12.91432100	H	-0.44313000	8.31000500	8.91113400
C	7.60697700	7.34359700	15.88695200	H	-0.56829600	6.78983300	9.85111800
H	6.82000700	7.38749400	16.65919000	C	2.42101300	8.35094300	9.01925700
H	8.45619800	6.79492900	16.32933800	H	3.38283700	8.46423300	9.53615200
C	8.01504100	8.74915700	15.45424200	H	2.09899800	9.35942100	8.70800200
H	8.82777200	8.68506100	14.70652000	H	2.58169300	7.75274400	8.11215000
H	7.17240700	9.23372500	14.93466400	C	8.69153800	11.48453800	13.25557300
C	8.46323300	9.67528000	16.58879600	C	8.87017500	10.82945500	11.83471100
H	9.32659300	9.22912800	17.11486000	O	7.58074100	11.08964000	11.22551600
H	7.65230000	9.73860200	17.33653100	O	7.26853300	11.35498900	13.46890600
C	8.81604300	11.07888400	16.09368600	C	9.95861800	11.45806900	10.97463100
H	9.09980200	11.74870900	16.92128700	H	10.94173100	11.35863700	11.46104000
H	9.66130100	11.04988300	15.38486700	H	10.00710200	10.94141000	10.00425800
H	7.96124600	11.52926600	15.56376100	H	9.76446600	12.52182000	10.78464600
Sn	6.77168900	6.14992100	14.24414800	C	9.03710200	9.30963600	11.88659200
O	4.50567000	4.92954300	12.27734500	H	9.02544000	8.91401500	10.86096700
C	3.42993400	4.17896000	11.83878700	H	9.99057000	9.01793500	12.34993400
H	2.46568300	4.73039600	11.85831700	H	8.21516200	8.82048500	12.42909600
H	3.54458000	3.80143400	10.79104100	C	9.42567100	10.77892700	14.38504500
H	3.28502600	3.27190000	12.46849700	H	10.51148000	10.76844500	14.20097200
				H	9.24255500	11.30392000	15.33432600
I-6b'				H	9.07777300	9.74810900	14.50019300
Cu	5.09076100	6.24608900	11.73868000	C	9.00689900	12.98322100	13.27026900
C	1.51017000	4.39645900	8.74400700	H	8.64219800	13.40887200	14.21665000
C	1.69902900	3.62995600	7.58025700	H	10.08835200	13.17238200	13.19647200
C	2.93250300	3.72791900	6.96425200	H	8.50132100	13.50517700	12.44446000
C	3.95190000	4.52403900	7.49606300	H	0.56113800	9.61857300	15.19693600
C	3.81189600	5.27140600	8.65960900	H	2.92630900	9.76141000	14.40486900
C	2.51766100	5.21317000	9.24869200	H	2.94397500	5.50926500	13.74388600
O	0.82094800	5.46870800	11.29718600	H	0.61771100	5.36702800	14.45870200
P	5.25190800	6.06331700	9.49457900	O	-0.88046000	7.51810800	15.28080200
B	6.66427800	11.20346000	12.24847100	C	-1.62221700	6.32983100	15.16879800
S	2.06783000	6.15032400	10.75859900	H	-1.61821100	5.93901200	14.13488700
O	5.04741300	4.43915000	6.68739000	H	-2.65471600	6.57154400	15.46019900
O	3.37103300	3.11968000	5.82253700	H	-1.24102400	5.53637100	15.83881800
H	0.91540500	2.98457700	7.18049600	C	1.10340400	8.72470500	14.88091900
H	0.57581700	4.35395000	9.30737000	C	2.42065600	8.79467100	14.44095800

C	3.11539500	7.64229800	14.01821900	H	7.93912600	6.30904600	8.19270100
C	2.44404800	6.41606300	14.08656300	C	8.81754200	3.11407400	8.98385300
C	1.11168000	6.33633200	14.49784100	H	7.51135600	1.67223200	9.93432700
C	0.42969700	7.49287500	14.88961800	H	9.86062800	4.76290800	8.04729200
C	4.49274900	7.75229700	13.45868200	H	9.67025700	2.43249200	8.92697200
C	4.69769800	8.61814400	12.48549800	C	8.40845200	7.21383700	15.20273900
C	4.84624700	9.62708500	11.64435700	H	8.83508400	6.20052300	15.11458600
C	5.11564000	11.07013900	12.05813200	H	8.86643700	7.80105000	14.39395900
H	4.59528600	11.32276100	12.99388700	C	8.74642400	7.80584800	16.56617800
H	4.74926500	11.75001500	11.27092700	H	8.30798000	8.81439600	16.66334600
H	4.86415300	9.43590900	10.56988100	H	8.27413700	7.20838100	17.36756600
C	4.77746300	3.41474600	5.70552700	C	10.25090900	7.90042300	16.84976700
C	5.08178200	3.97307500	4.32457200	H	10.73028900	8.48974900	16.04678800
C	6.57976500	4.25571400	4.16816400	H	10.69562600	6.89067400	16.78346600
C	7.41386400	3.00544600	4.47103100	C	10.57772800	8.52317500	18.20700900
C	7.09833000	2.45598100	5.86597000	H	10.13309400	7.93827000	19.03013300
C	5.60302500	2.17651500	6.03768100	H	11.66444500	8.58052100	18.38680600
H	6.78534700	4.62679200	3.15077800	H	10.17184500	9.54662400	18.28045300
H	4.74696000	3.22777600	3.58395900	C	5.44129200	8.30458400	16.37855700
H	4.47715400	4.88152100	4.17935900	H	5.97001000	8.08204400	17.32122500
H	7.20231300	2.23234100	3.70815900	H	4.38104100	8.04389800	16.52727500
H	8.48819800	3.23977800	4.39175600	C	5.58653100	9.77458100	16.00058000
H	7.67535900	1.53922800	6.06561200	H	5.14926000	9.94619900	15.00309100
H	7.40695800	3.18852200	6.62492500	H	6.65227300	10.03710400	15.87737100
H	5.26929000	1.36746100	5.36601200	C	4.94967500	10.76860500	16.97660200
H	5.37282000	1.87341700	7.07055200	H	3.88119500	10.51357000	17.09991700
H	6.86104300	5.06068600	4.86742100	H	5.40615200	10.64486800	17.97646100
C	5.73115300	7.48726900	8.43920800	C	5.08511400	12.22153600	16.51907500
C	6.54263300	8.45415500	9.05508700	H	4.59333200	12.37402000	15.54360300
C	5.34123500	7.66916300	7.10422800	H	4.63653400	12.92899600	17.23698200
C	6.95537200	9.58885800	8.35177800	H	6.14435200	12.49777900	16.38401600
H	6.82596800	8.32319400	10.10141500	C	5.77594900	4.89920800	15.36155600
C	5.75301000	8.80420000	6.40183700	H	5.89191700	4.83687500	16.45861100
H	4.72103900	6.92060300	6.61133200	H	4.71485300	4.72004700	15.13325300
C	6.55853900	9.76514500	7.02316500	C	6.64648400	3.87148900	14.64268600
H	7.54741100	10.34447400	8.87041100	H	6.57084600	4.04423200	13.55983900
H	5.43955100	8.94078200	5.36320000	H	7.71115400	4.01292300	14.91035900
H	6.86778000	10.65800300	6.47313200	C	6.24664000	2.41790400	14.90630100
C	6.63040300	4.87771200	9.15698400	H	5.17341300	2.31261000	14.67416300
C	6.52269500	3.56066900	9.63379200	H	6.36573600	2.18023900	15.98087900
C	7.83735500	5.29312100	8.57505900	C	7.04084600	1.42968700	14.05278800
C	7.60881300	2.68811700	9.54270900	H	6.74851100	0.38356800	14.24670900
H	5.60128500	3.23784700	10.12361000	H	6.87073800	1.63561300	12.98302200
C	8.92427500	4.41836700	8.49444700	H	8.12595600	1.51507600	14.23976100

Sn	6.23511800	6.94931000	14.77671200	H	0.66390800	14.07673600	7.96790400
O	6.91470900	6.58675900	12.64899200	C	-0.56681100	11.44072200	9.85895500
C	8.06817000	5.97036300	12.17529400	H	-0.75818100	12.07443000	10.73606000
H	8.94165400	6.13723200	12.83531900	H	-1.52146500	11.26910200	9.34000300
H	7.95598700	4.87308500	12.05826000	H	-0.18057200	10.48163600	10.22762500
H	8.34985300	6.36270100	11.17561700	C	0.04568100	10.16152400	7.31337700
Br	4.13548300	3.92438500	12.12149600	H	-0.84097600	10.64126800	6.87070300
				H	0.52912300	9.55102700	6.53653600
I-8a				H	-0.28113500	9.49454700	8.11793100
Cu	4.14949000	8.10045600	10.44167200	C	1.60059100	11.99853200	6.64344700
C	2.98465200	3.54115200	10.04042200	H	2.13501100	11.30129900	5.98317500
C	3.63480000	2.44536800	9.44795800	H	0.81251700	12.49057800	6.05512900
C	4.70107400	2.72634200	8.61163400	H	2.31195100	12.76410700	6.98569900
C	5.11404900	4.04083500	8.36550100	H	-2.65906200	10.81470800	14.31468900
C	4.50243900	5.14716000	8.94201100	H	-0.48125200	11.32389500	13.19483500
C	3.39815300	4.84650700	9.78304100	H	0.54317600	7.14102600	13.33523100
O	1.88207100	5.53957900	11.87363000	H	-1.57388300	6.64504400	14.48354500
P	5.16488800	6.86849000	8.84388200	O	-3.46626000	8.53640400	15.08748000
B	2.51790700	11.36751700	9.54614600	C	-3.83657700	7.24397500	15.49752200
S	2.49880200	6.18042900	10.63556200	H	-3.90877700	6.54410500	14.64445500
O	6.17952700	4.02183100	7.52470400	H	-4.82510900	7.33242300	15.96858400
O	5.51326000	1.85910400	7.95262200	H	-3.12602600	6.82437500	16.23339300
H	3.33196700	1.41803100	9.65121100	C	-1.94038600	10.02249100	14.09537800
H	2.16239200	3.38746600	10.74010100	C	-0.73155700	10.29787600	13.47043700
C	1.05878500	6.45369100	9.41580400	C	0.20040300	9.27168600	13.18485300
C	0.18586000	7.48921000	10.12044100	C	-0.14420400	7.95755400	13.56527400
H	-0.21439100	7.09935400	11.06413400	C	-1.35257000	7.67579300	14.20659300
H	-0.66483600	7.74002300	9.46755700	C	-2.26283000	8.70856900	14.47420900
H	0.74696200	8.40706500	10.33954400	C	1.44026900	9.55099700	12.54112900
C	0.30556700	5.14387000	9.22940100	C	2.51892100	9.72427500	11.98316800
H	0.87025400	4.41816300	8.62805700	C	3.75492900	9.89113400	11.27903400
H	-0.64187600	5.35428900	8.70716800	C	3.81271300	11.16788400	10.40158100
H	0.06259700	4.69673400	10.20482600	H	4.69240900	11.11604400	9.73554200
C	1.64311300	6.99960700	8.12069500	H	3.93939800	12.07406700	11.02504000
H	2.16074200	7.95452400	8.28592400	H	4.58563900	9.91588400	12.00743800
H	0.81901500	7.19028300	7.41544800	C	6.56896900	2.63605900	7.33910300
H	2.32914300	6.28909800	7.63857500	C	6.63818000	2.33926500	5.85135900
C	1.02014000	11.21339000	7.82274000	C	7.77815600	3.11878400	5.18494100
C	0.45217200	12.14383000	8.95863600	C	9.11488900	2.86651100	5.89148500
O	1.62726600	12.38829200	9.75866700	C	9.02001900	3.18938000	7.38615800
O	2.12992200	10.56396000	8.48926800	C	7.89028600	2.40185400	8.05810200
C	-0.10293200	13.47816900	8.47619300	H	7.84027600	2.84284300	4.12047800
H	-0.94842400	13.32492300	7.78735300	H	6.79620700	1.25400500	5.74109700
H	-0.46561200	14.05699100	9.33835100	H	5.66147200	2.57860600	5.40339600

H	9.40359000	1.80759500	5.75908400	H	2.69457300	7.37302700	13.86283000
H	9.90935300	3.46902600	5.42279900	C	3.94202700	8.73188100	15.02715400
H	9.97293500	2.97476500	7.89445800	H	4.21148200	9.30195700	14.12313800
H	8.82923400	4.26510800	7.52153700	H	4.85549500	8.68708300	15.64985200
H	8.09437200	1.31871100	8.03326200	C	2.85930100	9.50328100	15.78832000
H	7.77249100	2.69404100	9.11208800	H	1.91712200	9.44212300	15.22321200
H	7.54533800	4.19650300	5.22021000	H	2.67314900	9.00344900	16.75688100
C	4.95361300	7.43280800	7.11161800	C	3.22041100	10.96958400	16.01276000
C	4.47854600	8.74064200	6.92917800	H	3.33636700	11.49032900	15.04812500
C	5.27339400	6.64955400	5.98910500	H	2.43944800	11.49623900	16.58426600
C	4.34051000	9.26273100	5.63972500	H	4.16930000	11.07435900	16.56688200
H	4.19550200	9.34372600	7.79438800	C	4.60991600	4.07830800	13.27144700
C	5.11887400	7.17190700	4.70432100	H	4.55520000	3.59553200	14.26383500
H	5.65330300	5.63762900	6.12363700	H	3.59412400	4.07416000	12.85224300
C	4.65723200	8.48119000	4.52689400	C	5.60030400	3.33395100	12.37455200
H	3.97972800	10.28489900	5.51143900	H	5.49409000	3.68994300	11.33791600
H	5.36619400	6.55577700	3.83609900	H	6.64137500	3.55519200	12.66460800
H	4.54453400	8.89004800	3.51968000	C	5.40566200	1.81461000	12.40527900
C	6.97216800	6.57179200	8.98661200	H	4.36406200	1.57993400	12.12552800
C	7.45686700	5.70770700	9.98172700	H	5.52248800	1.46448000	13.44678400
C	7.88645700	7.28089200	8.19489900	C	6.37261400	1.05648400	11.49790000
C	8.82847500	5.54795500	10.17200000	H	6.24730600	-0.03405300	11.59166300
H	6.75634200	5.17384800	10.62017500	H	6.22052200	1.31490500	10.43938900
C	9.26209400	7.12435400	8.39345300	H	7.42054200	1.29277700	11.74953600
H	7.52566800	7.95737700	7.41790600	Sn	5.07439300	6.14444300	13.74443200
C	9.73795300	6.25862900	9.38090900	O	5.60319800	7.08390800	11.98287400
H	9.18960300	4.86753700	10.94703400	C	6.64650000	8.03441700	12.04850600
H	9.96378500	7.68308500	7.76939800	H	6.46031800	8.81942300	12.80504200
H	10.81275600	6.13536500	9.53306000	H	7.62375400	7.56837600	12.26748400
C	6.94911800	6.28747100	14.85702800	H	6.73380800	8.53932000	11.07233700
H	7.22146100	7.35538900	14.87649900				
H	6.74768300	6.00086100	15.90316700	**I-8a'**			
C	8.08687100	5.44946500	14.26779000	Cu	3.99906500	7.34303900	11.09649800
H	7.85048000	4.37532500	14.37069900	C	1.87632900	3.17893200	8.92789800
H	8.16792900	5.63059700	13.18132500	C	2.55124400	2.19061400	8.19221400
C	9.45337900	5.71802200	14.90504300	C	3.78668200	2.53596400	7.67696600
H	9.39499600	5.51586900	15.98967300	C	4.34443000	3.79769900	7.90281300
H	9.68586000	6.79401100	14.81097500	C	3.72014700	4.79150700	8.65112900
C	10.57672800	4.89196100	14.28006100	C	2.42588300	4.44328200	9.12738400
H	10.67624600	5.11105200	13.20334100	O	0.32598400	4.64922900	10.73889200
H	11.54986600	5.09945700	14.75251300	P	4.59286300	6.33387000	9.18324800
H	10.38097600	3.81097200	14.37956200	B	2.78582900	11.10296900	10.29457000
C	3.49476900	7.32930900	14.61356000	S	1.37930300	5.56699200	10.13605700
H	3.10691300	6.75619800	15.47345000	O	5.55301200	3.86271500	7.26886800

O	4.63551900	1.78143600	6.91886500	H	-3.27265300	4.27730600	14.01034700
H	2.12931100	1.19660700	8.03628800	C	-2.52265900	8.12524300	12.94479700
H	0.90864000	2.98207800	9.39402900	C	-1.33113900	8.84095200	12.87759000
C	0.42494600	6.46864300	8.74347300	C	-0.07833700	8.18422800	12.90713800
C	-0.49270800	7.40054500	9.54028800	C	-0.08373100	6.78101000	13.06027200
H	-1.13117000	6.83586900	10.23363300	C	-1.27392200	6.06062400	13.13412400
H	-1.14153000	7.95963600	8.84588800	C	-2.50438000	6.72701200	13.06201800
H	0.09298600	8.11921400	10.13092000	C	1.16087600	8.86290000	12.71352200
C	-0.37712000	5.44893300	7.94930700	C	2.31539700	9.05750700	12.32133400
H	0.26874400	4.83139500	7.30760900	C	3.64611100	9.22878300	11.86873700
H	-1.10395100	5.97173100	7.30431900	C	3.97557100	10.55774200	11.15006300
H	-0.92888000	4.79007300	8.63640400	H	4.87593100	10.43798300	10.52099100
C	1.40515800	7.25359300	7.88712600	H	4.22446400	11.34625800	11.88862000
H	1.99363800	7.96316700	8.48615300	H	4.35195500	9.07556800	12.69640100
H	0.84646800	7.84084300	7.14034400	C	5.84603400	2.54606000	6.75429300
H	2.08996000	6.59459300	7.33667600	C	6.18973400	2.66532000	5.27712000
C	1.40906100	11.51223200	8.51423500	C	7.49804300	3.43799300	5.07792400
C	0.88286300	12.25824900	9.79584000	C	8.64192100	2.80592600	5.87931800
O	2.02327600	12.18426700	10.67242900	C	8.28117700	2.70152700	7.36454300
O	2.37857000	10.60185100	9.07345800	C	6.97446300	1.93188600	7.57502700
C	0.51803500	13.72233100	9.58218900	H	7.74714600	3.47907400	4.00491200
H	-0.29286800	13.81982800	8.84288500	H	6.27827900	1.64252300	4.87448400
H	0.16931700	14.15519400	10.53178800	H	5.34486200	3.15139900	4.76514600
H	1.38101800	14.30919200	9.24091200	H	8.85765600	1.79876600	5.47508000
C	-0.26476100	11.51684800	10.48535900	H	9.56297000	3.39879300	5.75500200
H	-0.42322000	11.96274000	11.47768600	H	9.09338900	2.22114100	7.93265400
H	-1.20195900	11.58590400	9.91277600	H	8.16405100	3.71091800	7.78381100
H	-0.01466700	10.45969600	10.64243500	H	7.07731400	0.87933500	7.26104400
C	0.34835300	10.72735700	7.75627500	H	6.67665700	1.94010100	8.63459200
H	-0.44687500	11.40045000	7.39823200	H	7.35059500	4.47823500	5.41323400
H	0.80288800	10.23521200	6.88414800	C	4.72985200	7.36941600	7.66470500
H	-0.10069400	9.95255700	8.38585600	C	4.66533900	8.75455700	7.86147800
C	2.16251700	12.43431500	7.54963800	C	4.91347900	6.86805300	6.36539400
H	2.66215900	11.81606100	6.79011100	C	4.79608700	9.63157800	6.78134400
H	1.48310500	13.13165200	7.03676800	H	4.48082900	9.13542000	8.86613700
H	2.93079100	13.01793600	8.07806500	C	5.03127900	7.74517800	5.28558900
H	-3.49075300	8.62983800	12.89965000	H	4.98012000	5.79308800	6.20165800
H	-1.35613600	9.92782300	12.77989300	C	4.97758100	9.12934400	5.49112600
H	0.86759000	6.24606300	13.06925700	H	4.73828500	10.70765600	6.95599500
H	-1.21302800	4.97479900	13.18519800	H	5.17014300	7.34655400	4.27679100
O	-3.72351700	6.10008800	13.09313800	H	5.07178200	9.81298900	4.64291600
C	-3.73876800	4.69680700	13.09852900	C	6.32353400	5.74393300	9.39508500
H	-3.21415500	4.27341800	12.22193000	C	6.56538600	4.70187600	10.30348400
H	-4.79454700	4.38940200	13.06896200	C	7.41152700	6.41258600	8.81839300

C	7.87186400	4.32392500	10.60813400	H	7.18620300	0.07153600	13.60575500
H	5.72024800	4.21794400	10.79781900	H	6.59553800	1.16597100	12.33128400
C	8.72161100	6.05008200	9.14812600	H	8.23664200	1.36585600	12.98175000
H	7.23905200	7.23018800	8.11701500	Sn	5.93375800	6.60315400	14.17416400
C	8.95658100	5.00448000	10.04304300	O	6.13463300	7.09748500	12.16985500
H	8.04531200	3.50813600	11.31089800	C	6.93197200	8.17934500	11.78230400
H	9.56030600	6.58985600	8.70023200	H	6.69396600	9.11860300	12.32133500
H	9.97941200	4.71704600	10.30001600	H	8.01569300	7.98614200	11.90464700
C	7.92209100	7.38951900	14.74992700	H	6.76032500	8.37967200	10.70925800
H	8.01183100	8.43418000	14.40979900	Br	3.58623900	5.22986600	12.60375600
H	7.99247300	7.40939500	15.85218100				
C	9.03349200	6.52503700	14.14808700	**I-8b**			
H	9.00761500	5.51858500	14.60503900	Cu	5.29777600	7.37076000	10.89141100
H	8.84174500	6.35753500	13.07266700	C	3.54396700	2.67428300	10.42398600
C	10.44736500	7.09535700	14.29895500	C	3.87559500	1.69897800	9.46888500
H	10.67067700	7.24435700	15.37161600	C	4.54479900	2.13250800	8.33758000
H	10.47538400	8.10200800	13.84334400	C	4.88460700	3.47889300	8.15688400
C	11.51995400	6.21321100	13.65974600	C	4.58244700	4.46928700	9.08477500
H	11.32123700	6.07340400	12.58356100	C	3.86745100	4.01528300	10.22568300
H	12.52938900	6.64511500	13.76226400	O	3.26251700	4.25089500	12.80476400
H	11.53660000	5.21044500	14.12002200	P	5.24687300	6.18747500	8.99894900
C	4.36030800	7.79393200	15.08579100	B	5.45766800	11.16292900	13.12211400
H	4.05786800	7.27579200	16.01196600	S	3.43796600	5.14711200	11.58102600
H	3.51037200	7.72359200	14.39299400	O	5.54790800	3.61387000	6.97874200
C	4.73545300	9.24997400	15.36212000	O	4.99391300	1.40072100	7.28558700
H	5.19014300	9.70120400	14.46250200	H	3.63931800	0.64473600	9.61656700
H	5.51341100	9.30700800	16.14696900	H	3.05527000	2.40042800	11.36013600
C	3.53021600	10.10794800	15.76214100	C	1.67215200	5.67326200	11.10147900
H	2.75786000	10.01009700	14.98063600	C	1.22229500	6.49836300	12.30895600
H	3.08474700	9.69742900	16.68735700	H	1.18392900	5.87772800	13.21487000
C	3.87991900	11.58173300	15.96107700	H	0.21891200	6.90526100	12.11208500
H	4.27972500	12.01804400	15.03003800	H	1.89131400	7.35113900	12.48223100
H	2.99712000	12.17507700	16.25084600	C	0.80871400	4.43155800	10.93319500
H	4.64670700	11.71589900	16.74460300	H	1.06358400	3.86942600	10.02362900
C	6.09843600	4.52767700	14.84850800	H	-0.24635400	4.74129400	10.85878400
H	6.73901800	4.55895100	15.74907300	H	0.90994800	3.77038100	11.80674400
H	5.08055600	4.24493100	15.15664200	C	1.76125100	6.52043900	9.84171300
C	6.63808900	3.53698700	13.82555600	H	2.43490100	7.37519800	9.98758300
H	6.01343400	3.59873200	12.92102000	H	0.76497900	6.92982600	9.61310900
H	7.65952200	3.82631200	13.52374300	H	2.09532500	5.93671900	8.97209200
C	6.65623300	2.08399400	14.30869000	C	5.11062500	13.42283500	13.11638200
H	5.62947200	1.78994600	14.59079600	C	4.18943200	12.73105900	14.19782200
H	7.26031800	2.00624300	15.23201700	O	4.76359600	11.40488700	14.28540700
C	7.19651800	1.11682400	13.25484400	O	5.61251800	12.29773000	12.36704000

C	4.22705500	13.38236000	15.57501500	H	5.88745400	2.99941300	3.07711400
H	3.89537300	14.43079000	15.51778500	H	5.40421900	1.16104900	4.70107000
H	3.54899300	12.84838600	16.25636900	H	4.27606300	2.50481800	4.97996600
H	5.23466700	13.35530400	16.00940100	H	7.87469900	1.73967300	3.89402400
C	2.74093900	12.55915500	13.73453900	H	8.30315900	3.43951000	3.65676500
H	2.21493000	11.91482800	14.45287600	H	9.19646100	2.56737700	5.84734200
H	2.21290300	13.52283400	13.68600900	H	8.05062200	3.88590400	6.09207900
H	2.69172500	12.07026300	12.75217900	H	7.41009200	0.88889300	6.38353100
C	4.37698000	14.35651100	12.16105800	H	7.53819500	2.07766200	7.69963300
H	3.90198200	15.18538600	12.70873300	H	6.04706900	4.15888700	4.40390000
H	5.09193000	14.78469600	11.44257700	C	4.37620300	7.02087800	7.61558200
H	3.60703500	13.81951200	11.59313700	C	3.93227900	8.33283400	7.84450000
C	6.32436000	14.13318300	13.72188200	C	4.12928800	6.41463400	6.37226800
H	7.01644000	14.40234800	12.91046600	C	3.24863100	9.02991900	6.84490400
H	6.03812200	15.05186800	14.25495800	H	4.10552100	8.79688500	8.81742200
H	6.86155800	13.47564900	14.42080300	C	3.44255100	7.11452300	5.37835600
H	-1.53342600	9.88183200	9.15200200	H	4.47946400	5.40044600	6.18190700
H	0.95761000	9.75697500	9.20837900	C	3.00050100	8.42152600	5.61220200
H	0.84205000	9.88947300	13.51388900	H	2.90473500	10.04873000	7.03827700
H	-1.61217500	10.01438200	13.45961100	H	3.25025500	6.63625300	4.41464300
O	-3.09575000	10.00840600	11.15027300	H	2.46065800	8.96389200	4.83206300
C	-3.88953200	10.07654600	12.30767300	C	6.95101700	5.89465600	8.38715000
H	-3.75209000	9.19138300	12.95640600	C	7.76293300	4.99839800	9.10183700
H	-4.93542700	10.11228700	11.97339500	C	7.50532100	6.62964300	7.33090700
H	-3.67440900	10.98235500	12.90445000	C	9.10085700	4.82552300	8.75116800
C	-0.99405500	9.88390500	10.10149400	H	7.34722000	4.44435300	9.94398900
C	0.39188400	9.81966200	10.14008900	C	8.85188000	6.46349600	6.99067800
C	1.09714300	9.81737700	11.37019300	H	6.88484400	7.33209900	6.77151400
C	0.32959300	9.89597100	12.55128200	C	9.65220500	5.56183600	7.69636400
C	-1.06519700	9.96007000	12.51831400	H	9.71870800	4.11961600	9.31161100
C	-1.74107900	9.95239500	11.28986300	H	9.27512700	7.04193800	6.16588500
C	2.51031700	9.70004600	11.40329400	H	10.70247900	5.43143700	7.42559000
C	3.73128400	9.55288400	11.40067300	C	7.73115300	6.71257800	15.38641200
C	5.13926900	9.33749500	11.37179700	H	7.90091600	7.74946000	15.05143900
C	5.92657000	9.74617600	12.64907400	H	7.31965800	6.78263600	16.40784000
H	7.00104800	9.74320900	12.40452800	C	9.02927000	5.90410500	15.37407200
H	5.78803100	9.01576700	13.45896400	H	8.82920400	4.86461500	15.69262700
H	5.56750300	9.85918600	10.49842400	H	9.41569100	5.82581500	14.34221400
C	5.79687900	2.27796600	6.46545900	C	10.12675400	6.49352800	16.26612900
C	5.33695800	2.21392800	5.02024100	H	9.74697600	6.56867100	17.30104000
C	6.20821100	3.10364400	4.12563100	H	10.33006800	7.53091400	15.94487700
C	7.69480600	2.76128800	4.27641200	C	11.42161000	5.68282400	16.24691700
C	8.13662200	2.84665200	5.74103800	H	11.83795400	5.62125400	15.22738400
C	7.27489400	1.95306600	6.63821200	H	12.19199400	6.12990500	16.89497100

H	11.25102000	4.65014600	16.59481400	B	3.32633800	11.36428000	12.06094500
C	4.25898600	6.92023200	14.35784800	S	1.45304200	5.98866200	9.75148100
H	3.48671500	6.14282000	14.42842800	O	5.47425500	4.05732700	6.81471600
H	4.11960900	7.42812800	13.39106200	O	4.30680300	2.17122100	6.20605300
C	4.17927700	7.92513600	15.50521800	H	1.70780700	1.80004000	7.19984700
H	5.04272600	8.61210500	15.48653800	H	0.67777000	3.57021400	8.72216200
H	4.22827600	7.40065800	16.47737100	C	0.64182700	7.12381500	8.43351600
C	2.90114900	8.76744500	15.43887600	C	-0.22508000	8.05409700	9.28794800
H	2.90278300	9.31174400	14.48061600	H	-0.96354900	7.47946000	9.86486900
H	2.02428500	8.09522600	15.41696600	H	-0.76265500	8.75576300	8.62797800
C	2.77854000	9.76146600	16.59007500	H	0.38043000	8.63266500	9.99985500
H	3.63233800	10.45568900	16.58431900	C	-0.21810500	6.28059500	7.50377300
H	1.85750100	10.36186900	16.51035200	H	0.39098700	5.67164100	6.81984200
H	2.75795800	9.24985700	17.56741200	H	-0.85931100	6.94195400	6.89622800
C	6.22456600	3.73618400	13.89093200	H	-0.86521200	5.61401400	8.09338700
H	6.84026600	3.30722000	14.69827900	C	1.72733800	7.89506600	7.70200400
H	5.18887900	3.38785200	14.00619900	H	2.40360500	8.39505100	8.40766000
C	6.76508600	3.35298600	12.51244100	H	1.26706600	8.67312700	7.06938600
H	6.18829000	3.87810400	11.73553600	H	2.32502500	7.24619500	7.04796900
H	7.80457900	3.70961700	12.39677600	C	1.64667300	12.81821300	11.56383900
C	6.71730000	1.85139400	12.22340200	C	1.86353500	12.77155200	13.12790600
H	5.66959300	1.51104400	12.29302500	O	2.75762700	11.65542900	13.28108400
H	7.27000100	1.30623300	13.00969900	O	2.85114400	12.20203000	11.06825800
C	7.28384300	1.49745200	10.84902700	C	2.58507800	14.00618900	13.67600000
H	7.22565300	0.41648900	10.64506900	H	1.94244200	14.89966300	13.65550500
H	6.72691600	2.01346800	10.05232200	H	2.87600300	13.81072300	14.71861500
H	8.34198900	1.79783400	10.76257800	H	3.49914600	14.21641300	13.10152200
Sn	6.15194900	5.89875000	14.12552100	C	0.59887800	12.49790100	13.93490200
O	6.72233700	6.47202700	12.21452800	H	0.84497800	12.46907500	15.00656400
C	8.04303100	6.87000300	11.93435400	H	-0.15023800	13.28954300	13.77337600
H	8.41818200	7.62897000	12.64590400	H	0.16020600	11.53023900	13.66381300
H	8.74382900	6.01271900	11.94563200	C	0.47475700	11.94540800	11.10108500
H	8.08667900	7.31371900	10.92559500	H	-0.49596200	12.38719800	11.37295500
				H	0.52111200	11.84960900	10.00596600
I-8b'				H	0.54005800	10.93477900	11.53043900
Cu	4.06322100	7.18889300	10.96543100	C	1.52976000	14.21866900	10.97386100
C	1.67919400	3.68960500	8.30358800	H	1.39202400	14.14642500	9.88429500
C	2.24855500	2.70630500	7.47654800	H	0.66155900	14.75042000	11.39449000
C	3.53645400	2.93929500	7.03163100	H	2.43330400	14.81370800	11.16127200
C	4.24567900	4.08228400	7.41389300	H	-1.93259800	8.53445200	16.19056700
C	3.72662200	5.06300700	8.25230900	H	-0.03950200	9.50284800	14.88509400
C	2.37864000	4.84131500	8.65521200	H	-0.23067600	6.15176500	12.16722900
O	0.26991100	5.16328800	10.24639300	H	-2.11071100	5.22716000	13.42763300
P	4.75948900	6.40878500	8.98295100	O	-3.19218400	6.38274400	15.67684600

C	-3.80410000	5.17033300	15.33131800	C	6.42790500	5.64842200	9.12373000
H	-4.26449600	5.20570900	14.32537900	C	6.58681000	4.60436800	10.05047900
H	-4.59383000	4.98760700	16.07483000	C	7.56331100	6.18737200	8.50008300
H	-3.09301700	4.32286200	15.35141500	C	7.85783700	4.09931500	10.32578700
C	-1.55173000	8.03223200	15.29825500	H	5.71052900	4.22596200	10.58454300
C	-0.49803400	8.56624600	14.56553300	C	8.83693900	5.69435500	8.79780800
C	0.00684300	7.91518300	13.41302600	H	7.45590600	7.00388500	7.78504800
C	-0.60511400	6.69897300	13.03509600	C	8.98898000	4.64826100	9.71090800
C	-1.67477800	6.16970000	13.76029600	H	7.96884600	3.28714900	11.04430500
C	-2.15483400	6.83025600	14.89958200	H	9.71307600	6.13159400	8.31109000
C	1.08928500	8.45202900	12.66140700	H	9.98360200	4.25959700	9.94421700
C	2.07330400	8.75113700	11.98546700	C	7.39257000	7.69634200	14.96436100
C	3.21777400	9.05980600	11.20267500	H	7.40204700	8.73458500	14.59212300
C	4.20843200	10.11207000	11.79167800	H	7.18768800	7.76271200	16.04863000
H	5.01083100	10.29879000	11.05974000	C	8.74069500	7.01772000	14.72201600
H	4.68692200	9.72710900	12.70345700	H	8.71173200	5.97972300	15.10239600
H	2.90943400	9.37462600	10.19075200	H	8.92779000	6.92447900	13.63744800
C	5.62302500	2.75861900	6.20138200	C	9.93473800	7.73719300	15.35988400
C	6.10739300	2.94651200	4.77295500	H	9.76175100	7.82832000	16.44805900
C	7.52564600	3.52665700	4.74778200	H	9.97553400	8.77284500	14.97586600
C	8.49281600	2.66169800	5.56428700	C	11.27122600	7.04023700	15.10543400
C	7.99426700	2.48576000	7.00213000	H	11.47915100	6.96453700	14.02459000
C	6.57519000	1.91378900	7.04183800	H	12.11385000	7.57784000	15.57120700
H	7.87062500	3.62306600	3.70530100	H	11.26666600	6.01290100	15.50807500
H	6.08352200	1.95914200	4.28252500	C	3.86745400	7.57876200	14.82414200
H	5.38970400	3.59578900	4.24830400	H	3.35209200	6.84783600	15.46830400
H	8.59547600	1.67226600	5.07969700	H	3.22980700	7.71322300	13.94117100
H	9.49682800	3.11696500	5.56632400	C	4.10976700	8.90226300	15.54771200
H	8.67519300	1.83764800	7.57624400	H	4.70248200	9.57989600	14.90762200
H	7.99318800	3.46105200	7.50807300	H	4.71998600	8.74442100	16.45758600
H	6.54776700	0.88727100	6.63868900	C	2.81017400	9.61956900	15.92398700
H	6.19013200	1.87968900	8.07269600	H	2.24091700	9.79759400	14.99979400
H	7.49968100	4.54362900	5.17353800	H	2.19364100	8.95149500	16.55213500
C	5.01370300	7.61648900	7.61501400	C	3.04317200	10.94986000	16.63603100
C	5.12803700	8.96367300	7.98927600	H	3.59333100	11.64328200	15.98000100
C	5.09578600	7.27411200	6.25629700	H	2.09204900	11.43657600	16.91058300
C	5.32470100	9.95460100	7.02380300	H	3.62952400	10.82064500	17.56302800
H	5.03640600	9.22684100	9.04541300	C	6.06283300	4.56094200	14.71498700
C	5.28322400	8.26628900	5.29122700	H	6.63773800	4.63478700	15.65625400
H	5.02584000	6.22833800	5.95580000	H	5.07510300	4.13499700	14.94792800
C	5.39822000	9.60802800	5.67211300	C	6.78637100	3.68910800	13.69640400
H	5.40411000	11.00027700	7.33117600	H	6.18418700	3.66768700	12.77491400
H	5.34130300	7.99076700	4.23460700	H	7.75781800	4.14032700	13.42398500
H	5.54111100	10.38244300	4.91372700	C	7.01759300	2.25348900	14.17971900

H	6.04194800	1.80915100	14.44651200	C	1.23715400	12.14338300	9.97637400
H	7.60775800	2.27127600	15.11502500	O	2.35885800	11.90005300	10.85754400
C	7.71719400	1.36676500	13.14941000	O	2.51498200	10.32180300	9.21800000
H	7.86784200	0.34029000	13.52311600	C	1.06817900	13.64551500	9.79481200
H	7.12730100	1.29911400	12.22013500	H	0.27925500	13.86299200	9.05802300
H	8.70852000	1.77107200	12.88161100	H	0.77678100	14.10138300	10.75236700
Sn	5.66472300	6.61821100	14.09606200	H	2.00083300	14.12113100	9.46536800
O	5.98050100	7.12987700	12.11397500	C	0.00243400	11.54375700	10.65459500
C	7.09925600	7.82999000	11.65407900	H	-0.10021200	11.99283600	11.65279700
H	7.40341000	8.66179200	12.31904100	H	-0.91551000	11.74633000	10.08346000
H	7.97700600	7.16928500	11.50831500	H	0.10689900	10.45885800	10.79269300
H	6.86630300	8.27599700	10.67023700	C	0.51910200	10.73343800	7.90045600
Br	3.57290000	5.02660800	12.28322600	H	-0.17570400	11.50893500	7.54302400
				H	0.91207200	10.19647700	7.02429600
I-9a				H	-0.03946500	10.01965300	8.51577200
Cu	4.42176700	7.05663000	10.40717100	C	2.54145000	12.19624700	7.73392700
C	2.69640700	3.16157000	9.32971400	H	2.97251200	11.52838100	6.97318200
C	3.24742300	2.04462300	8.67652300	H	1.96104700	12.97687400	7.22100600
C	4.36254100	2.26413800	7.88753700	H	3.36860600	12.67534000	8.27751400
C	4.91694000	3.54372200	7.74038300	H	-3.30224300	9.07849000	13.71887300
C	4.40173800	4.66721800	8.37013500	H	-1.01294500	10.01772200	13.34851700
C	3.24907800	4.42902700	9.17196500	H	0.56818100	6.01751200	13.10526300
O	1.70039000	5.05250300	11.25166700	H	-1.67710900	5.08888800	13.49343800
P	5.24835000	6.29828300	8.41950700	O	-3.92241700	6.62305000	13.83495400
B	2.97676500	10.75321300	10.44601300	C	-4.18905300	5.24297100	13.90939200
S	2.49439500	5.75481700	10.16960000	H	-3.92842600	4.72175300	12.97011800
O	5.99290400	3.47086000	6.91733800	H	-5.26813600	5.13977400	14.08606300
O	5.09060100	1.37088700	7.17145800	H	-3.64185100	4.76258400	14.74057000
H	2.83361800	1.04405100	8.80483600	C	-2.43883600	8.42361500	13.58709700
H	1.85051600	3.05006300	10.00939000	C	-1.16581100	8.93753300	13.38188800
C	1.18093000	6.45888100	8.97804500	C	-0.05181500	8.08370800	13.21475100
C	0.41126700	7.45188100	9.84494600	C	-0.27173100	6.69426200	13.26479600
H	-0.05470500	6.95454300	10.70296700	C	-1.54971400	6.17082200	13.46816400
H	-0.38609200	7.90478700	9.23533400	C	-2.64380800	7.03381800	13.63248100
H	1.06138300	8.25540000	10.21462200	C	1.25398700	8.61422400	12.98657000
C	0.28706600	5.30614400	8.53967600	C	2.36561800	9.08445700	12.80426500
H	0.80299100	4.61640100	7.85703900	C	3.71768400	9.57633700	12.66543500
H	-0.58634600	5.72086800	8.01121000	C	4.09126300	9.98311100	11.22594500
H	-0.07787500	4.74655400	9.41304700	H	4.35143300	9.10000200	10.61524000
C	1.88075800	7.14430500	7.81639300	H	5.01666000	10.58192500	11.24763300
H	2.51396100	7.97359800	8.15795100	H	3.83456200	10.45328800	13.32190200
H	1.11433500	7.57468200	7.15172300	C	6.28807500	2.05718200	6.74034300
H	2.47699100	6.44389300	7.21609000	C	6.55356900	1.79064200	5.27230800
C	1.66684200	11.36451200	8.67549900	C	7.84535600	2.48069300	4.81711400

C	9.03287100	2.08259200	5.70126200	C	10.16251000	5.92377900	13.92339600
C	8.74538600	2.37039600	7.17845400	H	9.99409000	5.58442200	12.88731000
C	7.45792000	1.68265400	7.64166200	H	11.24608100	6.07902100	14.05215300
H	8.04295900	2.23364100	3.76213800	H	9.86129900	5.09946400	14.59189500
H	6.63342900	0.69863200	5.14649800	C	3.94839000	8.40732900	15.74619500
H	5.68051800	2.12809500	4.69307500	H	4.49070000	7.78569800	16.48339200
H	9.24269700	1.00549800	5.56695800	H	2.91647700	8.01854800	15.70572700
H	9.93907200	2.62074500	5.38013500	C	3.94584000	9.86759200	16.19197800
H	9.58645300	2.04756000	7.81126600	H	3.35947400	10.47410700	15.47723400
H	8.64025600	3.45495700	7.32851200	H	4.97319300	10.28089400	16.15917300
H	7.56023100	0.58547400	7.60679200	C	3.37398400	10.10226200	17.59558100
H	7.20619800	1.96000400	8.67747300	H	2.34785500	9.69387500	17.63373900
H	7.70299200	3.57343500	4.86783700	H	3.95857900	9.51215200	18.32488200
C	5.09682000	7.07038100	6.77207800	C	3.36083800	11.57242200	18.01321000
C	4.91329600	8.46225000	6.74405600	H	2.75427200	12.17758800	17.31810300
C	5.15306800	6.35291700	5.56629900	H	2.94504000	11.71023800	19.02477600
C	4.79295000	9.13049800	5.52341300	H	4.37951400	11.99651600	18.01100900
H	4.84411300	9.02023000	7.68125600	C	4.16897300	5.93004100	13.56514700
C	5.02209000	7.02503900	4.34914700	H	4.08615100	5.58896000	14.61176000
H	5.31028300	5.27381700	5.58140900	H	3.13510300	6.00865300	13.19292200
C	4.84307300	8.41239300	4.32553300	C	4.95073000	4.91051900	12.74237700
H	4.65106000	10.21366400	5.51070200	H	4.98626000	5.23922400	11.68958300
H	5.06285500	6.46306900	3.41291200	H	6.00820900	4.88682100	13.05610500
H	4.74115500	8.93371900	3.37071600	C	4.37844300	3.49129200	12.77009800
C	7.01541400	5.85738600	8.59282500	H	3.32849900	3.53015300	12.43711900
C	7.39932700	5.16283800	9.75199300	H	4.36183800	3.12110700	13.81117000
C	7.99666600	6.30449800	7.69825400	C	5.17158200	2.52512900	11.88907000
C	8.74736400	4.91073700	10.00324200	H	4.74673200	1.50830600	11.90019000
H	6.64911300	4.84580000	10.47580400	H	5.17925000	2.86405900	10.84003000
C	9.34774700	6.05978400	7.96168300	H	6.22239900	2.45254500	12.21845200
H	7.70894900	6.85069600	6.79852600	Sn	4.91033600	7.98838600	13.78083600
C	9.72651400	5.36460400	9.11293600	O	5.89485400	7.54559400	11.55069800
H	9.03402400	4.37520000	10.91089400	C	6.91405000	8.31511200	11.00564800
H	10.10728800	6.41674200	7.26201100	H	6.94339700	9.34557800	11.41764200
H	10.78299800	5.17885400	9.31943400	H	7.91245000	7.86890200	11.19434000
C	7.03130400	8.27435300	14.27145600	H	6.83050000	8.43073000	9.90198100
H	7.42540700	9.09878200	13.65679700				
H	7.08443900	8.60311700	15.32282200	**I-9a'**			
C	7.85163000	7.00346800	14.04475200	Cu	4.18325100	5.90380600	11.19584100
H	7.51199200	6.20961600	14.73630900	C	1.52540000	2.78828500	7.62182000
H	7.65050300	6.62041300	13.03113000	C	2.19580600	1.97360100	6.69616100
C	9.36229300	7.19300800	14.21440900	C	3.49025900	2.33661300	6.37560900
H	9.57787500	7.54642300	15.23917500	C	4.11129400	3.43785000	6.97375900
H	9.69624800	8.00253800	13.54004600	C	3.48747500	4.25669900	7.91219800

C	2.13551100	3.90747400	8.18451700	H	1.51493000	5.75094100	12.57580100
O	-0.09684200	3.89229400	9.60934100	H	-0.36430300	4.27705500	12.14620900
P	4.40860200	5.54030700	8.88345400	O	-2.94891200	5.13693700	11.82845900
B	3.23854100	10.91388900	10.84036700	C	-2.76502100	3.75801400	11.55868600
S	1.06841500	4.84198600	9.34241900	H	-2.00978000	3.60017900	10.77163800
O	5.37438200	3.55496900	6.46620600	H	-3.74222600	3.37525100	11.23132800
O	4.34444600	1.74155200	5.49456300	H	-2.45454300	3.20902700	12.46680600
H	1.72533800	1.09638000	6.24974700	C	-2.04231600	7.25829600	12.28523500
H	0.50862700	2.56162400	7.94717900	C	-0.95733000	8.09841600	12.51447900
C	0.29957000	6.11217200	8.12769800	C	0.35215500	7.57871000	12.61263700
C	-0.75454900	6.80386400	8.99408600	C	0.51644700	6.18438500	12.51365400
H	-1.51011200	6.08863700	9.34374800	C	-0.56277800	5.33738800	12.28451100
H	-1.25883700	7.58460800	8.40111500	C	-1.84961900	5.87393100	12.13968300
H	-0.30457100	7.28257600	9.87489500	C	1.50328500	8.40828200	12.76588500
C	-0.35102900	5.38307000	6.96152500	C	2.55235500	9.02250500	12.87087200
H	0.39347700	4.96227100	6.27057600	C	3.80649900	9.72693500	12.98698800
H	-0.98474900	6.08797600	6.39655500	C	4.39127400	10.22083900	11.63274900
H	-0.99019700	4.56904900	7.33511900	H	4.78888700	9.34806200	11.10121200
C	1.38284800	7.08334800	7.68812900	H	5.22706600	10.90959000	11.83799100
H	1.87162700	7.57015800	8.54445200	H	3.66654100	10.58846100	13.66016100
H	0.93278300	7.87884600	7.07021300	C	5.62057200	2.39501100	5.64053100
H	2.15015000	6.59445800	7.07410800	C	6.12664600	2.86123500	4.28451300
C	1.48250000	11.19461100	9.39221500	C	7.51020800	3.50844300	4.40753000
C	1.43866600	12.28242400	10.53888600	C	8.50549600	2.56071700	5.08666500
O	2.74947100	12.16872300	11.12913300	C	7.98710100	2.10631500	6.45478700
O	2.50877300	10.29414200	9.85453400	C	6.60028300	1.46756500	6.35066800
C	1.23787000	13.71384000	10.05509000	H	7.87164200	3.80742800	3.41011900
H	0.27361600	13.81895800	9.53333700	H	6.16985500	1.97764900	3.62621100
H	1.23639500	14.39556500	10.91882100	H	5.38507100	3.55547000	3.86001500
H	2.04182600	14.02958200	9.37755400	H	8.67155400	1.68014600	4.43763200
C	0.42900500	11.95019900	11.64198700	H	9.48322100	3.05718600	5.19956400
H	0.59009900	12.63964600	12.48392500	H	8.68937000	1.39948400	6.92446100
H	-0.60908600	12.05910600	11.29413200	H	7.92368900	2.97368200	7.12616400
H	0.57980100	10.92710500	12.01374500	H	6.63730300	0.52817800	5.77337400
C	0.18662500	10.41161700	9.21813900	H	6.19546400	1.23338800	7.34719400
H	-0.65013600	11.08609600	8.97716900	H	7.41972600	4.43058700	5.00573700
H	0.29762100	9.69470100	8.39402200	C	4.69511400	6.92397300	7.70478500
H	-0.06147200	9.84219000	10.12188500	C	4.59205100	8.21272800	8.24803500
C	1.94715900	11.74863800	8.04274300	C	4.97904400	6.77421600	6.33704900
H	2.14262600	10.90577500	7.36417600	C	4.77748100	9.33830800	7.44180800
H	1.18644800	12.39859400	7.58467400	H	4.34274600	8.33110200	9.30359800
H	2.88012300	12.32184300	8.14814700	C	5.15681000	7.90097800	5.53135400
H	-3.05455300	7.65448500	12.17979200	H	5.07233800	5.77611800	5.90880800
H	-1.11279300	9.17580700	12.60409800	C	5.05858500	9.18455200	6.08232200

H	4.68345600	10.33148300	7.88328000	H	5.98081900	5.30810700	13.20757900
H	5.37569400	7.77749400	4.46711200	H	6.75268500	5.59621500	14.76586000
H	5.19685300	10.06418600	5.44783100	C	5.47299900	3.86111800	14.72718100
C	6.07616000	4.75985400	9.03063600	H	4.46905900	3.60269400	14.35538800
C	6.18656000	3.58594800	9.79594300	H	5.43203100	3.80965100	15.83197100
C	7.24291200	5.38260400	8.56580800	C	6.47733500	2.84394600	14.18796100
C	7.44404800	3.05653200	10.09422200	H	6.24985800	1.81891900	14.52626400
H	5.28637500	3.11421200	10.19829800	H	6.45768500	2.84539600	13.08592200
C	8.49876200	4.85555400	8.87650200	H	7.50872200	3.08218700	14.50407000
H	7.17348200	6.29517800	7.97316700	Sn	5.16587300	8.37808600	14.14736300
C	8.60519600	3.69421200	9.64673900	O	5.39147300	7.31739300	11.84316400
H	7.51329100	2.15233100	10.70393500	C	6.59447600	7.38609600	11.15628900
H	9.39933100	5.36134500	8.51838300	H	7.21555500	8.24178600	11.48775400
H	9.58837300	3.28805600	9.89764100	H	7.22414600	6.47575400	11.27244500
C	7.25586700	9.04247000	13.97523700	H	6.46439400	7.53062100	10.06249200
H	7.37430400	9.54258400	13.00090900	Br	3.19291100	3.78084300	11.82552600
H	7.37819200	9.82423000	14.74379600				
C	8.31720300	7.95763300	14.15065300	**I-9b**			
H	8.22925600	7.50612700	15.15616300	Cu	5.19561600	7.15644700	9.95787900
H	8.13705000	7.13274600	13.44246300	C	2.92820800	3.46168300	8.72403000
C	9.75287700	8.45868100	13.95907200	C	3.31234200	2.29596800	8.03806900
H	9.95072300	9.28223700	14.67011200	C	4.50560400	2.34246200	7.34025500
H	9.84128900	8.90436000	12.95126800	C	5.30647500	3.49433800	7.31968400
C	10.80431800	7.36223800	14.12905500	C	4.94607400	4.66936400	7.96433500
H	10.64050300	6.54392500	13.40782800	C	3.70836400	4.61272500	8.66802600
H	11.82831000	7.74311200	13.97804500	O	2.27948300	5.39855100	10.78397200
H	10.75765500	6.91943000	15.13860300	P	5.98665300	6.18105300	8.07813100
C	4.67106800	9.25852700	16.15717500	B	4.08646600	10.83722100	13.36525400
H	5.24092300	8.67985800	16.90873000	S	3.16387600	5.99865300	9.71330900
H	3.60379000	9.04019000	16.34636400	O	6.42108800	3.24863100	6.58753300
C	4.94209500	10.75056200	16.32887400	O	5.09634300	1.36615500	6.60875700
H	4.38427900	11.32791800	15.56682400	H	2.71202000	1.38625700	8.07001000
H	6.00934300	10.96781300	16.13058700	H	2.03305400	3.47337600	9.34773900
C	4.58587300	11.31658300	17.70994100	C	1.99027000	6.98590200	8.58975200
H	3.51801400	11.11666500	17.91350300	C	1.58320500	8.17220500	9.46823700
H	5.14633500	10.75772200	18.48195700	H	1.12117100	7.84096900	10.40895400
C	4.86612100	12.81298400	17.85145300	H	0.85452300	8.79063200	8.92065300
H	4.29284300	13.39585900	17.11033200	H	2.44942000	8.80410000	9.71463400
H	4.60029200	13.19264900	18.85240600	C	0.79963600	6.09334400	8.26832400
H	5.93396400	13.03526900	17.68301800	H	1.07707800	5.26921600	7.59495000
C	4.69423700	6.29850100	14.60866300	H	0.02337200	6.69533800	7.76932500
H	4.43191300	6.28424300	15.68057800	H	0.37411100	5.67545000	9.19185900
H	3.78460100	6.03725600	14.04559100	C	2.74567200	7.43778000	7.34864300
C	5.80033500	5.29338300	14.29402300	H	3.63181100	8.03640500	7.60573000

H	2.08324600	8.07114400	6.73663600	C	6.43028600	1.82242300	6.29127800
H	3.06536400	6.59111700	6.72590800	C	6.71931100	1.63373300	4.81491800
C	3.66388300	12.43883400	14.94054600	C	8.15680600	2.05155800	4.48349600
C	5.21138300	12.13401500	14.87976500	C	9.17043500	1.30769300	5.36091400
O	5.32192800	11.35162400	13.66813600	C	8.87400500	1.50989200	6.85090900
O	3.10304600	11.34304900	14.18054300	C	7.43465200	1.11922700	7.19574300
C	6.10330000	13.36245900	14.75011000	H	8.35719000	1.86976100	3.41595900
H	5.98108200	14.02733100	15.61922500	H	6.56295400	0.56775900	4.58263200
H	7.15634900	13.04752600	14.70508400	H	5.98097400	2.21174000	4.23848100
H	5.88166300	13.93007200	13.83740400	H	9.13687700	0.22932700	5.12007800
C	5.69411200	11.25268400	16.03237700	H	10.19257200	1.64761600	5.12846800
H	6.71577100	10.91001700	15.81718800	H	9.57279700	0.92501900	7.46932500
H	5.70173600	11.80240400	16.98491700	H	9.02733200	2.56591500	7.11767000
H	5.05849200	10.36528500	16.14659600	H	7.27976800	0.03583300	7.06176700
C	3.06789500	12.43073200	16.34163000	H	7.19097500	1.35995100	8.24192800
H	3.53835800	13.20454800	16.96786900	H	8.25670100	3.13811500	4.64514600
H	1.99001200	12.64489900	16.28942500	C	6.02750100	6.87669900	6.38877100
H	3.19228900	11.45811500	16.82986800	C	6.58900900	8.15749700	6.24987500
C	3.27340600	13.72580600	14.20908100	C	5.52143500	6.22196900	5.25747300
H	2.17815200	13.76120900	14.11594000	C	6.65468400	8.76600000	4.99626700
H	3.60564800	14.62145500	14.75432200	H	6.97564000	8.67755600	7.13103700
H	3.70059500	13.75403100	13.19603600	C	5.57975700	6.83882600	4.00454000
H	-1.39766200	11.41453100	16.69308700	H	5.08378900	5.22779600	5.35076400
H	0.45700100	10.93620200	15.06557700	C	6.14715800	8.10840400	3.87053000
H	-1.05845100	6.94442000	14.54261800	H	7.09558400	9.76074600	4.89868800
H	-2.88059600	7.40407000	16.14047700	H	5.18138800	6.32156900	3.12838200
O	-3.21235100	9.80179500	17.42257200	H	6.19145300	8.58802900	2.88998900
C	-4.17325300	8.84588200	17.79762300	C	7.71102400	5.63187000	8.36619300
H	-4.78038800	8.51077200	16.93658000	C	8.16458100	5.61138000	9.69578500
H	-4.83286600	9.33137900	18.52956100	C	8.59544200	5.31764200	7.32361500
H	-3.71024000	7.95825300	18.26648200	C	9.47944800	5.23522800	9.97859100
C	-1.30949200	10.44187100	16.20506300	H	7.49792100	5.92729300	10.50212600
C	-0.28987700	10.17692400	15.30322000	C	9.91493900	4.96604000	7.61172000
C	-0.17561200	8.90868400	14.68503400	H	8.25156000	5.34942800	6.28907200
C	-1.13280600	7.93058900	15.00504000	C	10.35558700	4.91260000	8.93889500
C	-2.16220600	8.19142500	15.91328000	H	9.82186200	5.21872400	11.01557200
C	-2.25483100	9.45093600	16.52298200	H	10.60324800	4.73018800	6.79643800
C	0.92631700	8.65346800	13.82002000	H	11.38854700	4.63356400	9.16045900
C	1.96645200	8.52269900	13.19832700	C	6.50278900	8.01991900	14.53130400
C	3.27521700	8.44474300	12.60495300	H	6.60268200	8.98895900	14.02174900
C	3.85311500	9.81800500	12.19642000	H	6.48750900	8.21522500	15.61656300
H	3.16118700	10.29350000	11.47258700	C	7.64831900	7.08367000	14.15109900
H	4.80498200	9.63297900	11.68376600	H	7.53119500	6.10573900	14.65490200
H	3.25821900	7.77874100	11.73179200	H	7.58639900	6.88067200	13.07039100

C	9.03568700	7.64314300	14.48262400	C	3.67754500	3.23378000	6.30005300
H	9.12666300	7.78090600	15.57561400	C	4.24058900	4.26488700	7.05982300
H	9.12680300	8.65240400	14.04281400	C	3.61926600	4.82445600	8.17307600
C	10.17438700	6.76054600	13.97297000	C	2.32369000	4.30041100	8.44253800
H	10.13660400	6.67257400	12.87390900	O	0.19547300	3.87423100	9.97914900
H	11.16386100	7.16569100	14.24003400	P	4.49892000	5.95045200	9.35479500
H	10.10730700	5.74064800	14.38859600	B	3.09264500	11.56590700	12.87268000
C	3.31260400	7.04138000	15.79540200	S	1.26211200	4.94731000	9.78122500
H	3.77465400	6.27407300	16.44183100	O	5.44408200	4.60568500	6.51135400
H	2.35688400	6.62044800	15.44149700	O	4.51281600	2.90397500	5.27357800
C	3.05266400	8.32508500	16.58444000	H	2.03162100	1.85728000	6.04486600
H	2.74284800	9.13316400	15.90118500	H	0.80735600	2.86460100	8.04608900
H	3.99195400	8.66767600	17.05814500	C	0.31850100	6.30320500	8.79586400
C	1.98079500	8.16584900	17.66925100	C	-0.68730800	6.83622800	9.81732300
H	1.04377500	7.83424400	17.18950200	H	-1.36039000	6.04242500	10.16638600
H	2.27961700	7.35139500	18.35473200	H	-1.29527700	7.62701200	9.34668200
C	1.71431000	9.44241700	18.46481300	H	-0.18492600	7.26956500	10.69275000
H	1.34363900	10.24304700	17.80639200	C	-0.39603900	5.66720400	7.61307200
H	0.95414000	9.28406800	19.24683100	H	0.30268400	5.37383000	6.81673700
H	2.63099300	9.80892900	18.95855000	H	-1.11621900	6.38805900	7.18986800
C	4.50698300	5.15024000	13.28124600	H	-0.95176000	4.77734800	7.94492700
H	4.59788400	4.54054500	14.19726300	C	1.30140300	7.38698300	8.38798000
H	3.47850100	5.01817700	12.90903800	H	1.86548700	7.76012100	9.25358800
C	5.49600200	4.66236000	12.22867900	H	0.75151200	8.24254700	7.96081900
H	5.43860000	5.30871900	11.33519600	H	2.01635700	7.03917600	7.63088400
H	6.53341000	4.77409300	12.58710600	C	1.84567300	11.92142500	10.98534300
C	5.25391100	3.21229300	11.79933500	C	1.11741900	12.53818900	12.24521800
H	4.24255800	3.14167300	11.36390700	O	1.88219200	12.00566800	13.34396000
H	5.24371100	2.56840300	12.69726900	O	3.17336600	11.66078500	11.49853400
C	6.28798800	2.68716900	10.80407400	C	1.22911700	14.06369100	12.32394900
H	6.06883500	1.65081800	10.49863100	H	0.61399600	14.55998800	11.55840600
H	6.31472000	3.30575500	9.89507600	H	0.88467600	14.39168800	13.31584800
H	7.30368000	2.70467800	11.23274100	H	2.27193300	14.39119400	12.20284500
Sn	4.54570800	7.22188100	13.98738400	C	-0.33576100	12.10874400	12.41080900
O	6.19618800	7.87450900	11.36757100	H	-0.75091900	12.55966800	13.32466400
C	7.22043400	8.77382700	11.11198000	H	-0.94397300	12.44044000	11.55463700
H	6.87643200	9.83311700	11.11144400	H	-0.42042100	11.01898000	12.50094500
H	8.01504500	8.71451700	11.88564700	C	1.25259400	10.58170400	10.54112600
H	7.73233300	8.60812100	10.13437800	H	0.24914400	10.70836400	10.10836100
				H	1.90304900	10.14049300	9.77491200
I-9b'				H	1.19829500	9.87078600	11.37610300
Cu	4.56372100	5.71828300	11.71596600	C	1.95632500	12.86222100	9.79008600
C	1.77597700	3.24527200	7.71709200	H	2.46090400	12.34568200	8.96031300
C	2.45038400	2.68375400	6.62080000	H	0.95688000	13.16629600	9.44148100

H	2.53457100	13.76305000	10.03375700	C	4.84014200	9.08511900	6.63221300
H	-2.51691700	7.37849700	13.36835100	H	4.90852300	6.92880700	6.49156300
H	-0.54441100	8.90585800	13.59165200	C	4.71020000	10.19111200	7.48146400
H	2.06670700	5.55444800	12.82249500	H	4.39804900	10.84665200	9.53258000
H	0.16373100	4.07868500	12.60190200	H	4.99435200	9.23379600	5.55986400
O	-2.44667400	4.90057200	12.76807100	H	4.76260500	11.20354900	7.07166600
C	-2.28636300	3.56641300	12.31926500	C	6.23724300	5.33184800	9.23221200
H	-1.65627500	3.51680000	11.41526200	C	6.50739300	4.04666300	9.73621400
H	-3.29581200	3.19080300	12.09926300	C	7.30821000	6.14848300	8.84331100
H	-1.83263000	2.92984600	13.10091500	C	7.82505600	3.60182200	9.86010200
C	-1.49811600	6.99905900	13.26452000	H	5.68425300	3.41334400	10.07697800
C	-0.39835000	7.84481200	13.37733200	C	8.62556900	5.70354900	8.98143600
C	0.91308900	7.35173600	13.19899300	H	7.11626700	7.14663800	8.44900800
C	1.07023900	5.97279100	12.96178300	C	8.89038600	4.43232100	9.49739800
C	-0.02264100	5.12103600	12.85130300	H	8.01808800	2.60737800	10.27015000
C	-1.32034400	5.63726300	12.96603100	H	9.44953200	6.36022600	8.69025000
C	2.06970400	8.18372300	13.22512300	H	9.92131900	4.09055600	9.61786700
C	3.13914400	8.77269500	13.22318200	C	7.70379400	7.78645300	14.77760900
C	4.39949900	9.45976300	13.36083800	H	8.13715100	8.54102800	14.10139100
C	4.21121900	10.94014000	13.77768800	H	8.04459400	8.04820500	15.79353400
H	5.17073300	11.47314300	13.67007000	C	8.16229000	6.38143500	14.37626200
H	3.91183300	11.01583500	14.83393800	H	7.98973000	5.68211600	15.21285000
H	4.95987400	9.40331200	12.41979800	H	7.53188800	6.01200000	13.55357100
C	5.73468100	3.64222100	5.47391600	C	9.63071000	6.29438600	13.94877500
C	6.10656600	4.39109800	4.20420900	H	10.28657700	6.59860000	14.78647300
C	7.43541000	5.13501700	4.37481800	H	9.80836500	7.03038600	13.14327100
C	8.55124400	4.18040800	4.81482100	C	10.02146400	4.90160200	13.45347300
C	8.16704300	3.44036000	6.09994200	H	9.40259100	4.61007700	12.58863500
C	6.83562100	2.70106400	5.95017500	H	11.07936900	4.85285100	13.14397300
H	7.70187900	5.64230700	3.43327500	H	9.86617400	4.14122100	14.23780600
H	6.18031200	3.64857000	3.39234500	C	5.25616400	9.22324300	16.65183300
H	5.28182300	5.07613600	3.95417700	H	5.40136400	8.50044200	17.47655800
H	8.74680200	3.45078300	4.00635800	H	4.20187600	9.54897400	16.71216400
H	9.48881000	4.73974800	4.96736300	C	6.19524800	10.41475200	16.82932500
H	8.95679200	2.73143500	6.39483900	H	6.07001600	11.12400500	15.99075800
H	8.07568100	4.16299600	6.92237000	H	7.24713300	10.07723700	16.76897700
H	6.91311800	1.88837000	5.20814400	C	6.00889200	11.18611900	18.14235400
H	6.52046300	2.25420900	6.90558900	H	4.96256900	11.53713500	18.20526100
H	7.30747700	5.92103300	5.13785900	H	6.14113200	10.48893000	18.99019700
C	4.58319200	7.59006700	8.52625100	C	6.95994100	12.37317300	18.29746000
C	4.43653400	8.70414700	9.36736600	H	6.82435400	13.09977100	17.47802600
C	4.78347600	7.78915600	7.15063100	H	6.80301300	12.90990500	19.24822700
C	4.51109900	10.00112300	8.85150800	H	8.01330200	12.04515700	18.26929700
H	4.25219600	8.55029000	10.43336400	C	4.31952300	6.27733600	15.18830200

H	3.76805700	6.49107800	16.12017100
H	3.57135800	6.21605600	14.38642000
C	5.07090600	4.95206900	15.28820300
H	5.55129700	4.73789700	14.31999200
H	5.88769000	5.01619100	16.03193000
C	4.16207500	3.77330300	15.64971300
H	3.31789400	3.75475200	14.94121600
H	3.73143200	3.93878300	16.65569500
C	4.88226900	2.42756600	15.59527500
H	4.22121000	1.59591300	15.89236000
H	5.22746400	2.22804200	14.56806400
H	5.76305800	2.41127700	16.26198000
Sn	5.51068300	8.05007800	14.75614300
O	5.74178000	7.06138100	12.49064200
C	6.73403100	7.65192800	11.72665200
H	7.07122100	8.61909400	12.16165600
H	7.64524600	7.02420900	11.62480200
H	6.41474800	7.89421000	10.69580200
Br	3.65266000	3.50905800	11.96023100

$TS_{2a\text{-}3a}$

Cu	3.84632200	9.43170700	9.41319500
C	0.73296700	7.23123100	6.88827100
C	0.66965100	5.88180000	6.50281200
C	1.84954300	5.16454100	6.55221100
C	3.05424400	5.75260300	6.96108400
C	3.14639800	7.07319200	7.37920500
C	1.92953700	7.80654900	7.30345300
O	0.36781700	9.77198400	8.25300600
P	4.62434200	7.74376400	8.24462300
B	4.64147600	11.31202400	9.81150900
S	1.82129300	9.50559900	7.93154700
O	4.04301700	4.81651200	6.90889900
O	2.06229500	3.85116700	6.27535300
H	-0.27017000	5.40512600	6.22719500
H	-0.17088300	7.83800800	6.93264000
C	2.15528500	10.53626700	6.36694900
C	1.96247900	11.97286500	6.86141600
H	0.94298000	12.11264800	7.24728300
H	2.11562300	12.66626000	6.01810200
H	2.67761700	12.22930300	7.65613500
C	1.11315400	10.17049400	5.31823800
H	1.27532200	9.16188800	4.91194300
H	1.17225500	10.88913000	4.48450100
H	0.10256200	10.22455100	5.74881600
C	3.58036800	10.28072500	5.89985100
H	4.30376800	10.47336000	6.70370900
H	3.81547100	10.95726000	5.06182300
H	3.72098500	9.24969900	5.54578600
C	5.43790200	13.32430600	9.05445000
C	6.51794600	12.62924600	9.96412800
O	6.00232300	11.27703400	10.06330700
O	4.24856200	12.55346100	9.35663400
C	7.91996700	12.57706800	9.37277400
H	8.31366200	13.59240600	9.20961800
H	8.59497000	12.05517600	10.06702000
H	7.93545300	12.03852300	8.41655200
C	6.56010100	13.19582000	11.38463600
H	7.16732900	12.52946200	12.01446100
H	7.00556200	14.20127300	11.41070400
H	5.55222300	13.25208300	11.82139200
C	5.16757300	14.78726500	9.37829200
H	6.07926500	15.39114300	9.24837800
H	4.39748200	15.18013200	8.69801100
H	4.80437200	14.91281000	10.40602800
C	5.72017800	13.15581800	7.55871100
H	4.83226600	13.46629000	6.98979500
H	6.57109000	13.77336900	7.23568700
H	5.93186500	12.10725600	7.30670000
H	-0.14535600	3.39130400	9.40209100
H	1.38527500	4.97423300	10.56759100
H	-1.27727900	8.22630000	9.61619300
H	-2.81065300	6.65531500	8.49732800
O	-2.31994300	3.96841700	8.21878200
C	-3.54073700	4.36238800	7.64679200
H	-4.23733300	4.77415300	8.40034900
H	-3.98856900	3.46297600	7.20206500
H	-3.40291300	5.12045100	6.85262000
C	-0.38534200	4.45473200	9.46868700
C	0.46269900	5.34331300	10.11530500
C	0.16836700	6.73043500	10.18551600
C	-1.04082700	7.16245900	9.59818500
C	-1.89617300	6.27014100	8.94922800
C	-1.56997600	4.90930200	8.86768100
C	1.08296800	7.64142900	10.76961700
C	2.02636200	8.37642900	11.07090800
C	3.17651600	9.11490400	11.38232000
C	3.39664100	10.54041600	11.05658700

H	2.48924000	11.12095400	10.85057000	C	3.56064600	4.70269800	8.87644300
H	4.02725400	11.05063600	11.80068400	C	4.48564700	3.85307300	8.24376800
H	3.93860200	8.61971600	11.99342300	C	5.66236100	4.42959500	7.79756800
C	3.37649000	3.53880000	6.80762900	C	5.91751700	5.79644200	7.96613100
C	4.11411500	2.63701500	5.84058000	C	5.04526400	6.65515600	8.62150900
C	3.22449500	2.93301700	8.19864300	C	3.82617200	6.06013400	9.04466100
C	3.45807700	1.25230300	5.77636400	O	1.86195100	5.96233800	10.82007800
H	5.15355200	2.55726500	6.19864600	P	5.50963300	8.34377200	9.17745100
H	4.13439800	3.12487800	4.85428500	B	4.16063600	7.95531000	12.70608100
C	2.56617100	1.55292600	8.12677100	S	2.59979300	7.00282600	9.99967100
H	4.23059300	2.87082200	8.64283700	O	7.12373000	6.09265600	7.40870700
H	2.64100000	3.62909300	8.81963900	O	6.71943900	3.84464300	7.17667700
C	3.32574600	0.62669600	7.17004800	H	4.29622300	2.78592300	8.12282400
H	4.04139900	0.59781300	5.10949500	H	2.63320200	4.30674600	9.29270400
H	2.45714000	1.35660000	5.32512100	C	1.36996700	7.58340000	8.67644400
H	2.51375000	1.11298200	9.13515700	C	0.27474500	8.23195200	9.52774500
H	1.52712600	1.67255800	7.77684700	H	-0.19063000	7.49117700	10.19268300
H	2.81907900	-0.34923800	7.09929200	H	-0.49322500	8.65937800	8.86533500
H	4.33403100	0.42884900	7.57806800	H	0.68216700	9.05293500	10.13486700
C	5.19210100	6.30516100	9.23000500	C	0.84030000	6.38267200	7.90705700
C	6.39635800	5.63497500	8.98486200	H	1.60551200	5.94391200	7.25065500
C	4.35862100	5.88361900	10.27878900	H	-0.00557800	6.70493200	7.27784800
C	6.75983500	4.54157300	9.77638500	H	0.47537100	5.61059200	8.60077100
H	7.04632300	5.95665500	8.16976500	C	2.08751000	8.59982500	7.80050600
C	4.72146100	4.78451900	11.05747800	H	2.51490500	9.41399700	8.40207400
H	3.42617300	6.41488500	10.48137300	H	1.36306100	9.06006500	7.11033100
C	5.92244600	4.11091100	10.80911800	H	2.88382400	8.13756100	7.19958700
H	7.70160300	4.02254300	9.58156500	C	3.46021200	6.39587600	14.23893500
H	4.06448100	4.45864200	11.86755600	C	4.92838900	6.08537100	13.76462700
H	6.20821500	3.25442700	11.42471300	O	5.32130600	7.34450600	13.14936800
C	5.93525700	8.02039000	7.00219600	O	3.05199000	7.41567300	13.29656700
C	6.82301900	9.07927400	7.25272700	C	5.91525900	5.75474600	14.87415600
C	6.08013700	7.24901000	5.83960900	H	5.59668500	4.85460800	15.42272500
C	7.84844200	9.36110100	6.34752800	H	6.90735100	5.55597100	14.44093200
H	6.69537000	9.68623200	8.15358700	H	6.01647100	6.58405800	15.58571500
C	7.10014200	7.54452400	4.93152000	C	4.97577700	5.01935400	12.66464600
H	5.40522400	6.41297700	5.65045800	H	5.97500800	5.01972700	12.20416500
C	7.98396500	8.59885600	5.18313200	H	4.78264000	4.01524100	13.06983200
H	8.53812700	10.18478600	6.54801000	H	4.23216100	5.22268900	11.88287700
H	7.20663400	6.94672400	4.02307100	C	2.49086900	5.22609200	14.12652100
H	8.77937700	8.82662600	4.46939200	H	2.85136200	4.35875600	14.70201600
				H	1.51136100	5.52182900	14.53096500
TS_{2b-3b}				H	2.34248400	4.94724500	13.07635700
Cu	4.17038200	8.88889600	10.86444200	C	3.40006800	7.02506500	15.63149700

H	2.38563400	7.41525500	15.79903400	C	9.65455400	8.42201800	9.06030700
H	3.62361700	6.29015600	16.41942200	H	8.06833000	9.08323600	7.75498200
H	4.10664700	7.86317100	15.72251900	C	8.96431700	7.38538700	11.13467200
H	-2.79182200	11.66005500	8.77719800	H	6.83502100	7.30439300	11.49472600
H	-0.95931100	11.37043500	10.39296400	C	9.98140500	7.79926700	10.26896800
H	1.92795300	12.20859700	7.30557200	H	10.44561500	8.76181000	8.38717000
H	0.06920500	12.54071600	5.67529200	H	9.21219300	6.92053600	12.09207700
O	-2.41610700	12.30510900	6.13749400	H	11.02902900	7.65063200	10.54239900
C	-3.77297500	12.15945700	6.47464200	C	5.42453500	9.39845100	7.67949100
H	-4.00185800	11.13975400	6.83631300	C	4.97025500	10.71558400	7.84058900
H	-4.34901100	12.34872500	5.55863100	C	5.75053100	8.93051400	6.39571200
H	-4.08628600	12.88313600	7.24961500	C	4.85458800	11.55977500	6.73375800
C	-1.76347700	11.78802100	8.43915800	H	4.67468300	11.06313800	8.83183500
C	-0.72423000	11.62503900	9.35780200	C	5.62485200	9.77591700	5.29128900
C	0.62783000	11.76713300	8.98205000	H	6.10838200	7.90955700	6.25816800
C	0.89106900	12.10536200	7.62998800	C	5.17768600	11.09094000	5.45784700
C	-0.13747000	12.28266700	6.71599500	H	4.49718800	12.58294400	6.87121400
C	-1.47791900	12.12106400	7.10716000	H	5.87506800	9.40506200	4.29430200
C	1.68783100	11.53423900	9.89682700	H	5.07546700	11.74757000	4.59045600
C	2.64347100	11.23496100	10.61180600				
C	3.77925300	10.88478200	11.36268800	**$TS_{3a\text{-}4a}$**			
C	3.74047400	9.98354200	12.52250700	Cu	6.18154600	8.47849600	10.37468700
H	2.74992000	9.81357100	12.95531000	C	4.18632800	4.16630700	8.35901100
H	4.49829100	10.19201500	13.28855300	C	4.75269900	3.34079900	7.37115500
H	4.67848700	11.49463200	11.22445700	C	5.84707500	3.83976700	6.68598800
C	7.78371600	4.83673200	7.15472400	C	6.36597000	5.10969700	6.96558000
C	8.42798300	4.85694700	5.78295000	C	5.83289100	5.95312800	7.93288100
C	8.77409300	4.54804400	8.27732100	C	4.69729500	5.43701700	8.61848400
C	9.20988500	3.56448400	5.52202800	O	3.18630000	5.25298100	10.80197600
H	9.10147700	5.72911300	5.75451700	P	6.64722000	7.51524900	8.45095600
H	7.64069100	5.01694200	5.03082800	B	5.30082600	9.13674200	13.19099700
C	9.55244000	3.25651400	8.01062900	S	3.97448500	6.31417300	10.03725400
H	9.45354000	5.41314200	8.34102600	O	7.42466700	5.34874900	6.15229200
H	8.22385300	4.50643800	9.23035000	O	6.57822300	3.25515400	5.70119000
C	10.22811500	3.29088800	6.63499200	H	4.36140300	2.34435600	7.16216100
H	9.71024700	3.62678300	4.54286900	H	3.35750300	3.81703700	8.97774600
H	8.49685700	2.72507600	5.46221000	C	2.62974400	7.38993400	9.21371400
H	10.29767800	3.10024300	8.80642500	C	2.07926200	8.17382500	10.40894300
H	8.85506600	2.40306400	8.05485400	H	1.70761400	7.49107200	11.18657700
H	10.75250900	2.34101000	6.44336500	H	1.24663000	8.81491400	10.07774600
H	10.99924700	4.08290400	6.62698800	H	2.86055600	8.81699800	10.84160000
C	7.29647600	8.18011000	9.56409800	C	1.58852600	6.45559900	8.61512900
C	8.31686100	8.61078800	8.70597500	H	1.97548600	5.93738900	7.72498100
C	7.62469000	7.58519500	10.79350100	H	0.70458600	7.04048200	8.31255300

H	1.27666300	5.70493600	9.35553000	H	3.59169300	10.28530500	12.48016000
C	3.24922400	8.32228800	8.18259300	H	4.80537200	11.29378700	13.27353200
H	4.01914100	8.96529400	8.63210800	H	4.70764500	11.26412800	10.46840300
H	2.46093200	8.97748900	7.77599600	C	8.42268300	7.03963000	8.45473700
H	3.69225300	7.77484200	7.33893600	C	9.40133500	7.84223200	7.85482100
C	5.91631900	6.91375600	13.27750200	C	8.81386300	5.90629400	9.18413000
C	6.54743600	7.71977500	14.47092100	C	10.75231100	7.50928000	7.97634500
O	5.77569300	8.95144200	14.45327400	H	9.11342600	8.73721700	7.30298900
O	5.48040700	8.00264000	12.40614600	C	10.16462700	5.57259500	9.29604200
C	6.39748700	7.06432400	15.83536300	H	8.05853300	5.27814800	9.66287500
H	6.90063800	6.08514800	15.85128700	C	11.13795600	6.37508700	8.69309100
H	6.86244700	7.70097700	16.60234800	H	11.50918700	8.15187700	7.52323900
H	5.34313200	6.92279900	16.10357000	H	10.45817700	4.68517800	9.86229500
C	8.00221900	8.11576800	14.21537600	H	12.19631000	6.12429900	8.79231500
H	8.31308800	8.84586200	14.97626700	C	6.48968800	8.68386200	7.04443600
H	8.67515200	7.24749000	14.26989800	C	6.60069600	10.05365500	7.33624600
H	8.11047500	8.59026700	13.23077900	C	6.26279400	8.28028200	5.71992500
C	6.88723900	6.03708600	12.49966500	C	6.50332200	11.00145600	6.31524500
H	7.36599900	5.30329500	13.16575900	H	6.76459900	10.37379800	8.36709400
H	6.34014900	5.48175400	11.72353600	C	6.15221700	9.23330700	4.70463100
H	7.66774000	6.63597800	12.01149000	H	6.18241400	7.22323100	5.47397800
C	4.67158200	6.12380800	13.67618000	C	6.27590700	10.59450100	4.99783500
H	4.15728400	5.75102700	12.77888000	H	6.59566600	12.06325700	6.55550100
H	4.94171900	5.26064400	14.30238600	H	5.97093700	8.90829800	3.67715400
H	3.96977400	6.75387700	14.24249800	H	6.19116200	11.33681600	4.20048200
H	12.12301400	8.44185100	11.17239900	C	7.70904900	4.11686700	5.43873000
H	9.70242300	8.34638600	11.72082800	C	8.98381300	3.50678300	6.00616600
H	9.00453800	11.73388800	9.15183000	C	7.80615000	4.42350300	3.95525600
H	11.38997800	11.78317600	8.55229900	C	10.19206400	4.40020100	5.70705300
O	13.25602300	10.03095600	9.54705600	H	9.10499400	2.51026800	5.55007400
C	13.80897900	10.97200400	8.66302400	H	8.85137300	3.36496100	7.08996200
H	13.35708900	10.91013800	7.65495600	C	9.01703800	5.31732800	3.66228500
H	13.69041400	12.00727300	9.03304100	H	7.89531800	3.46151400	3.42450400
H	14.88079800	10.74356000	8.58471900	H	6.86334900	4.89240700	3.63392100
C	11.42577600	9.16502700	10.74559200	C	10.30964900	4.70025500	4.20897000
C	10.07550000	9.12463000	11.05426500	H	11.10953500	3.92113900	6.08293200
C	9.15937900	10.04974600	10.49720000	H	10.08056500	5.34221900	6.26457500
C	9.68304600	11.00601700	9.60158200	H	9.09519300	5.48990600	2.57722000
C	11.03887200	11.03330700	9.26157400	H	8.85310400	6.30164100	4.13203400
C	11.92282900	10.10906100	9.83239500	H	11.15859300	5.37806500	4.02487100
C	7.75040500	9.94821300	10.73515600	H	10.52850200	3.76586500	3.65983100
C	6.61821500	10.48068200	10.97228400				
C	5.28372700	10.68885900	11.20141900	**$TS_{3b\text{-}4b}$**			
C	4.68229900	10.44041900	12.57978700	Cu	4.65676200	6.91892900	9.45470900

C	0.87947500	5.02463600	7.84935100	H	9.21954900	12.72266900	12.60186800
C	0.55355600	3.68377600	7.57068600	H	9.81741200	11.84747200	14.03456600
C	1.60749500	2.80076300	7.41276700	H	10.57477000	11.58509300	12.43724600
C	2.93979200	3.22430800	7.51434100	H	6.44133300	5.25587900	15.49706700
C	3.29727500	4.52982800	7.81503000	H	6.72120100	6.59712300	13.39515200
C	2.20666200	5.43116200	7.95532200	H	2.55963500	6.01087100	12.48603400
O	1.19281000	7.61228700	9.12575200	H	2.26352900	4.71980400	14.57149100
P	4.99256100	5.03586000	8.33006300	O	4.29596900	4.18796700	16.33395300
B	8.23446100	9.16695800	10.99719700	C	3.06717700	3.63724700	16.73612000
S	2.48737800	7.14583100	8.49910200	H	2.29784600	4.41498900	16.89629500
O	3.76039300	2.15910600	7.30516600	H	3.24905200	3.11653300	17.68618700
O	1.57642300	1.46291400	7.17715400	H	2.67862300	2.90974500	15.99913800
H	-0.48158000	3.34603600	7.50817500	C	5.59719300	5.44077300	14.82929500
H	0.09924500	5.76319200	8.04258000	C	5.74688400	6.18771800	13.66874800
C	2.61862800	8.09473400	6.85393600	C	4.65224200	6.41716900	12.80101900
C	2.86870700	9.52843800	7.33000700	C	3.41093400	5.86099200	13.15460800
H	2.04012700	9.88030900	7.96092100	C	3.24717200	5.12295700	14.33072700
H	2.95794600	10.19549600	6.45781900	C	4.34500800	4.90360700	15.17579500
H	3.80307200	9.58712300	7.91048900	C	4.84553700	7.11103600	11.55442700
C	1.28968200	7.96291600	6.12429800	C	5.44739400	8.06142600	10.95754900
H	1.13878900	6.94522100	5.73513800	C	6.05098400	8.78893800	9.95531500
H	1.27011600	8.66082200	5.27140900	C	7.55754600	8.61295600	9.69823000
H	0.45769000	8.21456800	6.79817800	H	7.85272100	9.16028700	8.78992400
C	3.79992400	7.55800900	6.05956100	H	7.80471300	7.54806200	9.56291600
H	4.73008400	7.61989800	6.64245000	H	5.63755600	9.77640000	9.71591600
H	3.93007500	8.16670900	5.14978900	C	5.50952300	3.61564700	9.37017000
H	3.65197900	6.51452100	5.74605200	C	6.41022300	2.62532600	8.95927800
C	8.61824300	10.65262200	12.67380600	C	4.96050800	3.56411100	10.66176400
C	9.07474800	9.21131000	13.12097800	C	6.74621600	1.58514400	9.83025600
O	8.49550300	8.37704300	12.09185300	H	6.84486800	2.66142800	7.95920000
O	8.47577200	10.49621400	11.24168900	C	5.29111300	2.51976200	11.52546700
C	10.59113600	9.01344700	13.05570200	H	4.29278800	4.35894200	10.99883300
H	11.10852000	9.55745200	13.85978700	C	6.18507300	1.52708900	11.11003500
H	10.81181300	7.94125900	13.16246100	H	7.45341500	0.81691800	9.50737200
H	10.99486900	9.34910300	12.08934700	H	4.86578400	2.50178500	12.53157100
C	8.54399700	8.76798500	14.47866900	H	6.45620100	0.71510300	11.78933600
H	8.91183500	7.75674100	14.70869800	C	6.05303500	4.98550500	6.84067700
H	8.89264300	9.44635100	15.27298000	C	7.07269100	5.94892200	6.77245300
H	7.44767700	8.73815100	14.49536800	C	5.89205800	4.07446600	5.78455200
C	7.23670200	11.03196700	13.21429100	C	7.92939800	5.99261100	5.67068500
H	7.26223100	11.23428600	14.29505300	H	7.17917400	6.67512100	7.58196100
H	6.89316600	11.93979400	12.69719500	C	6.74427900	4.12989500	4.67880700
H	6.50286000	10.23591100	13.02094800	H	5.11058200	3.31586200	5.82997000
C	9.62281000	11.76160200	12.95415200	C	7.76403300	5.08497700	4.62074800

H	8.72034700	6.74500400	5.62854500
H	6.61147300	3.42125600	3.85758200
H	8.42771800	5.12419400	3.75357900
C	2.93335700	0.97950200	7.38147500
C	3.29821800	0.01514900	6.27089200
C	3.05500200	0.36648200	8.77214800
C	2.49201600	-1.28402600	6.38291000
H	4.37731900	-0.19070700	6.36162300
H	3.13223900	0.51665500	5.30542600
C	2.24858600	-0.93103000	8.87739100
H	4.12611800	0.18178900	8.95338100
H	2.73321100	1.11173000	9.51620800
C	2.63941400	-1.91772800	7.77114700
H	2.81307000	-1.98654000	5.59777000
H	1.42911900	-1.05866400	6.19305700
H	2.39767900	-1.38151500	9.87126200
H	1.17489400	-0.69277800	8.79316300
H	2.02466800	-2.82965600	7.83803800
H	3.68828000	-2.23425200	7.91842600

$TS_{4'a\text{-}4'b}$

Cu	4.74840700	5.82754200	11.33922100
C	1.42432200	3.54442800	8.69261700
C	1.67343600	2.55447900	7.72655000
C	2.79679900	2.72490700	6.93987300
C	3.64002500	3.83058400	7.09901600
C	3.44485200	4.81339700	8.06054000
C	2.26786100	4.64134900	8.84224600
O	0.86971300	4.94094400	11.10153100
P	4.71325100	6.09914200	8.47349200
B	6.03926400	10.77532900	10.64291400
S	1.87611300	5.71914600	10.27045500
O	4.64053500	3.75150400	6.16775800
O	3.27789000	1.92399100	5.94204800
H	1.03039100	1.67992900	7.61714800
H	0.59629300	3.45142700	9.39811200
C	0.79436400	7.06013400	9.43640800
C	0.40063100	7.95441100	10.61492100
H	-0.14750900	7.38111600	11.37399100
H	-0.24153500	8.77441300	10.25199100
H	1.28184700	8.39266900	11.10331000
C	-0.42751100	6.39053600	8.82445400
H	-0.16678700	5.80496500	7.93048200
H	-1.16242500	7.15970100	8.53100700
H	-0.89567300	5.72176800	9.56211500
C	1.62875800	7.81725600	8.41839500
H	2.57070500	8.17325000	8.85692900
H	1.07275000	8.70323700	8.06729400
H	1.86506700	7.20284700	7.54037200
C	4.81249200	12.33177100	9.49875100
C	4.01589600	11.81149000	10.74839000
O	5.06781300	11.20609100	11.52623100
O	5.87006500	11.35544500	9.39060500
C	3.33878700	12.88851700	11.58545700
H	2.60130100	13.44506800	10.98526000
H	2.80778900	12.41617400	12.42528900
H	4.06859800	13.59758200	11.99864500
C	3.01752700	10.71047500	10.38458700
H	2.64879000	10.24233800	11.30572600
H	2.15879400	11.10413600	9.82086300
H	3.50652900	9.92566900	9.79179300
C	4.00606400	12.36697100	8.20718200
H	3.14171200	13.04182100	8.31273900
H	4.63206500	12.74334800	7.38323700
H	3.64220600	11.37098200	7.93040800
C	5.47591300	13.69192000	9.73997600
H	6.19630900	13.88266800	8.93031400
H	4.73932500	14.50976900	9.75328400
H	6.02396600	13.69793100	10.69335500
H	1.72844600	10.54150300	14.53165500
H	3.86526600	9.94622500	13.37469500
H	2.50911100	5.86416300	13.05446100
H	0.39989200	6.45650700	14.11613900
O	-0.23459400	8.98719600	15.01620200
C	-1.26891500	8.06083300	15.19297000
H	-1.62138900	7.63895900	14.23193600
H	-2.10220200	8.59647600	15.67188100
H	-0.97016600	7.21612200	15.84346700
C	1.91550300	9.51959600	14.19073200
C	3.10373400	9.18457000	13.55109600
C	3.35015300	7.86137300	13.09485600
C	2.35130900	6.89895300	13.36174000
C	1.14755000	7.23836700	13.98201200
C	0.91624100	8.55508100	14.39900300
C	4.58411000	7.51748300	12.44058000
C	5.34639000	7.92238100	11.47956900
C	6.28788200	8.42898100	10.65082100
C	7.09411300	9.68485400	10.99415200

H	8.00505400	9.74308300	10.37803300	Cu	3.87372900	6.61672900	10.49525100
H	7.38379200	9.70139000	12.05859600	C	1.34309400	3.37429500	8.57407800
H	6.48656100	7.95090600	9.69046500	C	1.60695000	2.40156700	7.59203200
C	4.61468600	2.41436800	5.65759700	C	2.73098500	2.58900300	6.80728000
C	4.83847100	2.43028400	4.15709800	C	3.57363100	3.69705500	6.98104500
C	5.63837600	1.55936200	6.40052000	C	3.35545900	4.66599600	7.94968800
C	4.89714100	1.00762900	3.59096700	C	2.18153900	4.47382000	8.73333400
H	5.78822100	2.96019000	3.97813500	O	0.90606800	4.80929000	11.06086600
H	4.03353500	3.02096000	3.69407700	P	4.55526800	5.97927500	8.41383300
C	5.68981400	0.13922400	5.83200200	B	6.11262400	10.64320400	10.79469100
H	6.61425100	2.06083100	6.30392500	S	1.78566700	5.59031800	10.11403400
H	5.38597000	1.56408800	7.47200500	O	4.57870000	3.63762300	6.07020700
C	5.94350000	0.15611300	4.32001400	O	3.21086600	1.80809700	5.80834300
H	5.11017900	1.04464300	2.51003700	H	0.96665000	1.52830800	7.46311700
H	3.90364400	0.54156400	3.70494300	H	0.50033300	3.26454700	9.25869400
H	6.46892800	-0.44326500	6.34957100	C	0.66408700	6.90422200	9.31694000
H	4.72841500	-0.36216500	6.03527800	C	0.35956700	7.84648900	10.48350600
H	5.94344100	-0.87099700	3.91839500	H	-0.13979000	7.31752500	11.30548500
H	6.94966400	0.57099400	4.12476800	H	-0.29986300	8.65425400	10.12843800
C	4.56119200	7.30237900	7.06808400	H	1.27677600	8.30021800	10.88375600
C	5.03417200	8.60730900	7.27842900	C	-0.58751400	6.19670900	8.81722300
C	4.04036500	6.96691700	5.80758200	H	-0.37906600	5.56303900	7.94271100
C	5.02048600	9.54466300	6.24162200	H	-1.33270200	6.95265400	8.52167600
H	5.41658400	8.89834800	8.25910600	H	-1.02191800	5.57687700	9.61488100
C	4.00101800	7.91331500	4.78105300	C	1.43109800	7.61352000	8.21031800
H	3.68043300	5.95611300	5.61795500	H	2.35062500	8.08347100	8.58752900
C	4.49904400	9.20346300	4.99148200	H	0.79898500	8.41751700	7.80014600
H	5.41776700	10.54344100	6.42873400	H	1.69187600	6.94037000	7.38217200
H	3.58890300	7.63653600	3.80662300	C	4.97166800	12.17446400	9.53685400
H	4.47878100	9.93914600	4.18278300	C	4.08585600	11.67951900	10.73666700
C	6.29873700	5.26374800	7.98988000	O	5.07552700	11.07813400	11.59577400
C	6.74002300	4.17434000	8.75966800	O	6.03441500	11.19289400	9.52319700
C	7.10785400	5.71806000	6.93645800	C	3.35973300	12.77448300	11.50577500
C	7.94749100	3.54059100	8.46119300	H	2.66988300	13.32480200	10.84674300
H	6.13041600	3.81410900	9.59270700	H	2.76982400	12.32239100	12.31692700
C	8.31953800	5.08570600	6.64664400	H	4.06485500	13.48639300	11.95391100
H	6.78903100	6.56265200	6.32590700	C	3.10168500	10.57763000	10.32733300
C	8.74317100	3.98942800	7.40294900	H	2.66792700	10.13758700	11.23473600
H	8.26677700	2.69016500	9.06959800	H	2.28683400	10.97050600	9.70147100
H	8.93431000	5.45379200	5.82039500	H	3.61976300	9.77606300	9.78190600
H	9.69138100	3.49488200	7.17443400	C	4.26075000	12.18238900	8.19031800
Br	4.37865500	3.51228200	11.38976900	H	3.39548900	12.86313500	8.21733100
				H	4.94592500	12.53850500	7.40586100
TS_{4a-4b}				H	3.91034500	11.18238900	7.90942700

C	5.61819200	13.53790400	9.79728500
H	6.39281400	13.71365600	9.03621800
H	4.88370200	14.35525300	9.74320300
H	6.09930200	13.56418100	10.78562700
H	2.00336800	10.63283500	14.91817900
H	3.89470300	9.95103400	13.43862100
H	2.05885100	6.07074000	12.95701900
H	0.19353700	6.75798200	14.36447600
O	-0.03139000	9.23563700	15.53974400
C	-1.10720700	8.38773200	15.84284800
H	-1.65944000	8.07582400	14.93585300
H	-1.78731000	8.95516900	16.49343800
H	-0.78021100	7.47610400	16.37746800
C	2.03119900	9.63621700	14.47125800
C	3.08605500	9.25155900	13.65520900
C	3.13030900	7.95573400	13.06780800
C	2.06657000	7.07923600	13.37331200
C	0.99483600	7.47334000	14.17761500
C	0.96600200	8.75834500	14.73621700
C	4.23937500	7.58524900	12.23923200
C	5.19862400	7.90709500	11.43740700
C	6.31728800	8.31788300	10.78294000
C	7.11564400	9.53774500	11.24797400
H	8.08944100	9.57589500	10.73787300
H	7.28535700	9.53443700	12.33762300
H	6.59776900	7.86765000	9.83069000
C	4.52233600	2.33040300	5.45701300
C	4.62567900	2.46126100	3.94982700
C	5.60181100	1.43840800	6.05734700
C	4.65059000	1.08355100	3.27768600
H	5.55489700	3.01372800	3.73436000
H	3.78329200	3.07403600	3.59455400
C	5.62161600	0.06407200	5.38088700
H	6.56487500	1.95699200	5.92234600
H	5.42995700	1.35893600	7.14225500
C	5.75706600	0.19645700	3.85972800
H	4.77988900	1.20579100	2.19094100
H	3.67210100	0.59765700	3.42912300
H	6.44356600	-0.54098700	5.79425400
H	4.68439300	-0.46535100	5.62116200
H	5.73253000	-0.79832900	3.38710100
H	6.74239700	0.63496200	3.61737900
C	4.63231000	7.16611000	7.02907400
C	5.20281300	8.42159300	7.30280100
C	4.17805100	6.87774700	5.73317600
C	5.34985700	9.35944200	6.27947800
H	5.53352300	8.67495200	8.31350300
C	4.30827200	7.83057900	4.71955100
H	3.73389700	5.90835500	5.50807100
C	4.90202100	9.06758700	4.98791200
H	5.81119600	10.32082700	6.50892700
H	3.95078900	7.60064100	3.71288400
H	5.01192000	9.80561300	4.18967100
C	6.19009900	5.16077900	8.43121100
C	6.67679500	4.73916700	9.67890800
C	6.97477900	4.98615100	7.28155400
C	7.91863700	4.10647300	9.76795500
H	6.09286100	4.93071900	10.58338200
C	8.21891500	4.36164300	7.37734800
H	6.61080900	5.33833000	6.31627600
C	8.68769800	3.91337800	8.61763200
H	8.29289700	3.78425300	10.74204500
H	8.83004600	4.22972600	6.48104100
H	9.66434600	3.42852300	8.68904200

TS5'$_{a\text{-}6'a}$

Cu	4.95904700	6.51572400	11.52376400
C	1.44559300	3.50558000	9.32578700
C	1.77785900	2.48129400	8.42306200
C	2.96093300	2.63145000	7.72559800
C	3.80545600	3.72704800	7.94058000
C	3.52373700	4.74685000	8.84256900
C	2.26769600	4.61402700	9.50180700
O	0.56902100	5.14500600	11.50468800
P	4.77245500	6.02961100	9.31649200
B	4.81183400	11.96443600	10.01935200
S	1.64401400	5.85371700	10.69361100
O	4.88561400	3.61494300	7.11050400
O	3.49839300	1.81466200	6.77208300
H	1.14010500	1.60819200	8.27762400
H	0.54501000	3.45087900	9.94017000
C	0.60129100	6.93167300	9.49051800
C	0.02512400	8.00132900	10.41867800
H	-0.61975200	7.55497200	11.18647900
H	-0.57438800	8.71679300	9.83102500
H	0.81963100	8.55844900	10.93276800
C	-0.50902200	6.08847300	8.88220300
H	-0.12624000	5.38634500	8.12767500

H	-1.24782500	6.74799300	8.39491700	C	6.11236700	11.34205800	10.63985100
H	-1.01808400	5.51773700	9.67333900	H	6.50961100	10.60320200	9.91805900
C	1.51665400	7.54686400	8.44729400	H	6.89248000	12.12219800	10.69164800
H	2.36762100	8.06069800	8.91358400	H	6.30323000	11.25466000	12.86916200
H	0.96121300	8.29625600	7.85812900	C	4.83455000	2.29516500	6.52640500
H	1.90889100	6.79594500	7.74961700	C	5.08550900	2.41571500	5.03304900
C	3.43354800	13.07462500	8.56723900	C	6.52009100	2.87951100	4.75729300
C	2.58983900	12.34522800	9.68218800	C	7.54103000	1.95216600	5.42653400
O	3.60240100	12.01453800	10.65609300	C	7.27916400	1.83924300	6.93163500
O	4.74633500	12.49212800	8.74755800	C	5.84594700	1.39156400	7.22512100
C	1.52334100	13.19928100	10.35520900	H	6.69227900	2.93231200	3.66974300
H	0.77718300	13.54272500	9.62158100	H	4.90534600	1.42432600	4.58509600
H	1.00468200	12.59712200	11.11575900	H	4.34213700	3.11102300	4.61371700
H	1.95908000	14.07406700	10.85502500	H	7.48525700	0.95043600	4.95969100
C	1.98750100	11.02127800	9.21148900	H	8.56283300	2.32619400	5.24973400
H	1.63133000	10.46609300	10.08878400	H	7.99234400	1.14358500	7.40152600
H	1.14097200	11.17554900	8.52607700	H	7.44383400	2.81784200	7.40155600
H	2.73797600	10.39962500	8.70530800	H	5.66776100	0.36361300	6.86635800
C	2.96681700	12.81059100	7.14090800	H	5.63785000	1.40864700	8.30624900
H	1.93698900	13.17331300	6.99716700	H	6.64396500	3.90109600	5.15362800
H	3.62010600	13.34257400	6.43256900	C	4.73755800	7.23646800	7.92707400
H	2.99923300	11.74168000	6.89680600	C	5.05243100	8.56493800	8.24452900
C	3.57660800	14.57893900	8.80940000	C	4.43216300	6.90240600	6.59846600
H	4.34219900	14.97770800	8.12739500	C	5.07188100	9.54889800	7.25117200
H	2.63195500	15.11213700	8.62545900	H	5.26795600	8.81993900	9.28543300
H	3.89887900	14.78449600	9.84051800	C	4.43419600	7.88697300	5.60819300
H	0.44435600	10.70852000	13.29124200	H	4.20464100	5.86792900	6.33824400
H	2.86479900	10.69669300	12.65783600	C	4.75507400	9.21000200	5.93242100
H	3.01748800	6.46972900	13.45354500	H	5.30852600	10.58146400	7.51205400
H	0.65591800	6.45915000	14.02440600	H	4.18880500	7.61940100	4.57677500
O	-0.95483900	8.68130000	13.95600700	H	4.75703100	9.97987900	5.15607400
C	-1.64269300	7.48578300	14.23993700	C	6.41089900	5.21567900	9.03849300
H	-1.51818000	6.73854200	13.43579600	C	6.84235400	4.26952500	9.98400900
H	-2.70639700	7.74792100	14.33307400	C	7.30810000	5.65126600	8.05161200
H	-1.30227000	7.03047300	15.18837600	C	8.15216300	3.78915700	9.94831400
C	1.03249100	9.78838600	13.33257800	H	6.15814900	3.94357300	10.77227500
C	2.37875800	9.77440400	12.98211300	C	8.61839700	5.16620800	8.02023900
C	3.13114400	8.57871600	13.01156900	H	6.99361000	6.38725500	7.31188500
C	2.47280900	7.41514400	13.43049500	C	9.04887800	4.24269700	8.97615400
C	1.12099500	7.41110500	13.77727800	H	8.47875100	3.07599300	10.70790600
C	0.38713700	8.59895300	13.71326000	H	9.30806700	5.52501300	7.25143300
C	4.56658800	8.53234400	12.62710500	H	10.07873500	3.87644600	8.96368800
C	5.20371100	9.61914300	12.24963500	C	8.02088100	8.77115700	14.33974300
C	5.89831800	10.71456600	12.00246600	H	8.08919700	9.44464400	13.47051500

H	7.85640200	9.40731500	15.22610900
C	9.29681300	7.94325500	14.48910800
H	9.22767200	7.30170800	15.38757500
H	9.38558700	7.24264300	13.64052100
C	10.58000300	8.77705400	14.57653300
H	10.50022300	9.47926900	15.42708200
H	10.65562700	9.40892300	13.67261500
C	11.84575300	7.93203000	14.72048100
H	11.95966300	7.24348000	13.86615400
H	12.75581300	8.55301000	14.77447600
H	11.80866100	7.31289000	15.63313600
C	4.92094700	8.27367400	15.73011600
H	5.40607400	7.92932400	16.66169700
H	3.96738800	7.73014500	15.64768000
C	4.68409400	9.78096200	15.75404800
H	4.57365900	10.17087100	14.72776400
H	5.57353100	10.29471200	16.16600000
C	3.44084700	10.21043000	16.54189800
H	2.56872800	9.67396000	16.12914100
H	3.53547300	9.88193200	17.59384400
C	3.17885500	11.71475200	16.48346600
H	3.03635300	12.04232300	15.43992600
H	2.27566100	11.99998100	17.04891900
H	4.02759600	12.28832900	16.89561200
C	6.51385100	5.47604800	14.83627300
H	6.87960400	5.60584200	15.87243000
H	5.49635200	5.06120900	14.89971000
C	7.41000300	4.53778400	14.03660000
H	7.12144600	4.58668000	12.97810800
H	8.45934200	4.88481400	14.07517100
C	7.33263000	3.08435700	14.51354500
H	6.27326700	2.77494800	14.50131200
H	7.66631800	3.01638800	15.56679800
C	8.14602700	2.12126800	13.64907700
H	8.11246100	1.08733300	14.03286000
H	7.75312800	2.10423100	12.61906000
H	9.20643300	2.42439800	13.59388700
Sn	6.23879000	7.51261000	14.08118000
O	6.95608900	6.84475100	12.07537500
C	7.76223000	7.56159400	11.20495500
H	8.63757200	8.02032200	11.71025200
H	8.16724300	6.90451700	10.41019700
H	7.23096800	8.39629900	10.69579500
Br	4.12183200	4.31542000	12.40393100

$TS_{5a\text{-}6a}$

Cu	4.69315600	6.61019400	10.42807300
C	1.39416600	3.89419900	8.83944200
C	1.50748200	2.78681600	7.98254400
C	2.64405500	2.71883300	7.19634100
C	3.63053900	3.71287500	7.24501800
C	3.54496400	4.82658800	8.06956400
C	2.36944800	4.88881900	8.87136000
O	1.30159700	5.43821000	11.24660700
P	4.87983800	6.08947300	8.23067500
B	5.95962300	10.68151500	9.54559200
S	2.19708700	6.10745200	10.21709100
O	4.61711700	3.39889300	6.36378100
O	3.00033900	1.76441000	6.30025900
H	0.75081500	2.00214000	7.95327600
H	0.56577900	3.96549300	9.54555900
C	1.11587300	7.47999900	9.48417000
C	0.87945700	8.39075200	10.69278600
H	0.36076600	7.85010700	11.49485700
H	0.25983300	9.24704800	10.38249700
H	1.82502000	8.77709300	11.10008300
C	-0.18553100	6.86962600	8.98424300
H	-0.02999200	6.25242400	8.08761300
H	-0.88766500	7.67889800	8.72493100
H	-0.64704400	6.25324800	9.76948600
C	1.90646400	8.18217100	8.39293000
H	2.85109300	8.59021800	8.77808200
H	1.31498700	9.02747800	8.00389700
H	2.11999400	7.51606500	7.54575000
C	3.93585500	11.75153700	9.43179900
C	5.02817600	12.69272700	10.07507300
O	6.25893100	12.00017900	9.76029000
O	4.60417600	10.46691300	9.42057300
C	5.08930400	14.09702200	9.48907200
H	4.13379900	14.62348400	9.63733500
H	5.87856800	14.67234000	9.99492700
H	5.32016100	14.07958100	8.41631900
C	4.93555800	12.75762200	11.60084700
H	5.83800100	13.25085900	11.98969100
H	4.05512500	13.32586900	11.93363700
H	4.88600600	11.74973600	12.03352900
C	2.64953700	11.63328900	10.23851900
H	2.18719800	12.62240000	10.37901400

H	1.93250400	10.99687400	9.70257900	C	4.68256000	7.10127000	6.70857300
H	2.82923900	11.18166600	11.22217100	C	4.44280100	6.50496700	5.45730100
C	3.61829500	12.10233800	7.97683600	C	4.77983600	8.49619100	6.79370900
H	3.01910200	11.29183500	7.53743700	C	4.30982100	7.29587100	4.31520300
H	3.04532100	13.03781300	7.90078700	H	4.37801900	5.42079600	5.37124400
H	4.53824200	12.20885600	7.38351600	C	4.65170400	9.28395900	5.64616800
H	2.74828700	10.76259300	14.47649200	H	4.92123400	8.97773300	7.75896200
H	4.75594700	9.98752600	13.19980700	C	4.41691100	8.68774800	4.40589800
H	3.07550300	6.03967100	12.98756900	H	4.12413300	6.82178200	3.34830400
H	1.10332600	6.77885400	14.22437000	H	4.72673600	10.36983200	5.72966600
O	0.73777200	9.35045700	15.12427400	H	4.31342500	9.30508600	3.51023900
C	-0.33037900	8.49692500	15.45708500	C	6.44991500	5.17786400	7.94963900
H	-0.81338700	8.07199900	14.55814300	C	6.85164100	4.25203800	8.92744000
H	-1.06382500	9.10645600	16.00210300	C	7.30368400	5.45695300	6.87292300
H	-0.00436800	7.66293900	16.10479100	C	8.07917100	3.59946200	8.81144300
C	2.83610200	9.72876400	14.13600900	H	6.21579300	4.07754000	9.79726800
C	3.94550100	9.29115200	13.42496600	C	8.53911000	4.81076200	6.77106800
C	4.06356700	7.95460000	12.98666200	H	7.01113400	6.18115100	6.11232400
C	3.02369500	7.07577300	13.31946900	C	8.92873500	3.87992500	7.73675500
C	1.89530600	7.49965500	14.02605700	H	8.37653500	2.87994500	9.57541400
C	1.79284900	8.83423400	14.43882100	H	9.19948500	5.04016500	5.93123700
C	5.24084400	7.47956200	12.22208900	H	9.89419700	3.37520600	7.65496400
C	6.04124700	8.29063100	11.56164500	C	8.14598100	5.81621800	11.97232000
C	6.97586600	9.05996300	11.02262000	H	8.73438100	4.91261700	11.74719100
C	7.01138100	9.52284900	9.57340200	H	7.85409500	6.25917500	11.00783300
H	6.75275700	8.69036200	8.90245800	C	8.96392200	6.81514600	12.78892500
H	8.01871000	9.87820800	9.31180100	H	8.31968200	7.64585400	13.11969400
H	7.75162600	9.45575200	11.68960600	H	9.33088400	6.33925000	13.71743800
C	4.35957100	2.04762500	5.89849800	C	10.15395300	7.39469600	12.01784100
C	4.48180300	2.01964200	4.38689900	H	9.77874100	7.84113700	11.07983800
C	5.92954200	2.27751000	3.95220700	H	10.82554900	6.57135700	11.71367900
C	6.89508800	1.29326100	4.62215200	C	10.93719900	8.44062900	12.80925700
C	6.76248600	1.33989600	6.14768200	H	11.33781000	8.01721000	13.74579700
C	5.31915400	1.09086400	6.59489500	H	11.78727200	8.84043300	12.23310200
H	6.00289900	2.21212100	2.85514000	H	10.29215000	9.29176200	13.08612200
H	4.14703500	1.02577400	4.04769300	C	6.65130900	3.03723600	13.34169700
H	3.78736300	2.76381400	3.96757200	H	5.73683500	2.56094300	13.73536000
H	6.68290200	0.27012200	4.26085500	H	7.37052200	3.04648900	14.18130200
H	7.93166600	1.52178500	4.32677300	C	7.22022600	2.24377000	12.16891700
H	7.42941400	0.60244700	6.62117000	H	8.17196600	2.70255900	11.84512500
H	7.07927200	2.32765700	6.51156400	H	6.54737700	2.31854700	11.29644600
H	4.99827000	0.06598900	6.34534700	C	7.46907700	0.75756600	12.44736900
H	5.21001600	1.21647400	7.68385500	H	8.15133100	0.65752800	13.31069700
H	6.20809700	3.30773900	4.23124500	H	6.51916500	0.28662500	12.75904700

C	8.04348100	0.01216800	11.24259100
H	9.01485900	0.43778600	10.93751600
H	8.20200400	-1.05754700	11.45420900
H	7.36825300	0.08408400	10.37257100
C	5.78605400	5.86410300	14.97329200
H	4.68639200	5.83460600	15.01995500
H	6.15519000	5.07894500	15.65356300
C	6.29973500	7.24782300	15.37179200
H	7.36548700	7.18255100	15.65635500
H	6.26831700	7.93258300	14.50963900
C	5.50149900	7.89135200	16.51021000
H	5.54386400	7.24357700	17.40489100
H	4.43999600	7.93241300	16.20941200
C	5.98282600	9.29827000	16.85863500
H	5.39086100	9.74339100	17.67461700
H	7.04020100	9.29641800	17.17369300
H	5.89940600	9.96571100	15.98464800
Sn	6.28591800	5.19524000	12.93612300
O	4.83675400	4.72281400	11.41874900
C	4.09186500	3.53259200	11.32988500
H	3.01512400	3.72887200	11.46312700
H	4.22875300	3.05074700	10.34052400
H	4.39490300	2.79800500	12.09359800

$TS_{5'b\text{-}6'b}$

Cu	5.02060500	6.59407300	11.70059600
C	1.86078000	3.98278600	8.81449500
C	2.20065400	3.19603900	7.70018400
C	3.40733400	3.47603800	7.08732100
C	4.25648400	4.47558300	7.57193700
C	3.96698400	5.25477700	8.68623400
C	2.69777800	4.99594200	9.27369600
O	0.98461800	4.99260200	11.31665300
P	5.20826900	6.40194400	9.43049100
B	6.59354500	11.30534300	11.96161700
S	2.09673700	5.87141900	10.76590800
O	5.35840100	4.54614500	6.76992500
O	3.96524900	2.88747500	5.98820200
H	1.55121500	2.39832300	7.33661800
H	0.94337200	3.80270900	9.37846900
C	1.14332500	7.32129400	9.95200500
C	0.64260200	8.10866200	11.16659800
H	0.07404500	7.46247200	11.85040800
H	-0.01484100	8.92616500	10.82584700
H	1.47747300	8.54984600	11.72763800
C	-0.01406500	6.75553100	9.14315100
H	0.33420500	6.25259100	8.22875500
H	-0.69402500	7.57302400	8.84838100
H	-0.57630000	6.03188500	9.75209500
C	2.10332100	8.15412900	9.11936200
H	2.98908600	8.43954300	9.70300100
H	1.60553100	9.08590000	8.80108100
H	2.43411400	7.62595900	8.21541800
C	8.82891200	11.13134400	12.46930800
C	8.56995700	10.71399500	10.96441900
O	7.21306500	11.17575400	10.73915100
O	7.49176700	11.25139100	12.99478600
C	9.48002800	11.38957900	9.94556800
H	10.53212200	11.11641800	10.12189000
H	9.20496700	11.05258900	8.93493000
H	9.38918600	12.48335300	9.97618300
C	8.58097700	9.19923400	10.76247100
H	8.31206600	8.96919500	9.72384900
H	9.57868900	8.77694000	10.94847600
H	7.85935400	8.69589900	11.42367700
C	9.57279800	10.08859500	13.29662800
H	10.57775200	9.90452300	12.88603000
H	9.68187900	10.44682600	14.33074300
H	9.02147300	9.14133600	13.32564600
C	9.48926900	12.50336600	12.62163000
H	9.46589200	12.79239700	13.68270000
H	10.53783200	12.48897300	12.28857400
H	8.94921500	13.27110400	12.04838900
H	0.32831100	9.31281000	15.53803700
H	2.53998900	9.73464600	14.45079800
H	2.83030400	5.55575100	13.46886600
H	0.64077000	5.14549400	14.45722000
O	-0.89646400	7.08371600	15.66616000
C	-1.50877900	5.82100200	15.64397800
H	-1.66244400	5.45222800	14.61280300
H	-2.48737600	5.93314200	16.13325800
H	-0.92016200	5.06299700	16.19433100
C	0.89468300	8.49877100	15.07960200
C	2.13017900	8.72214400	14.48188700
C	2.86202700	7.67310000	13.88313100
C	2.30091700	6.38825500	13.93338300
C	1.04867900	6.15396100	14.50590300
C	0.33624400	7.21035800	15.08379600

C	4.14020900	7.91764700	13.17792700	H	10.36016800	3.93029700	8.81971200
C	4.29703300	8.98179800	12.42863400	C	8.24595700	6.93195500	15.54954600
C	4.45337700	10.07718500	11.69590200	H	8.69737500	6.01634200	15.13517000
C	5.04307900	11.39737100	12.18246800	H	8.88147100	7.77400300	15.22630700
H	4.83062500	11.56046500	13.25073400	C	8.20992000	6.84601900	17.07490200
H	4.60051900	12.23682800	11.61853600	H	7.73879500	7.75079800	17.50039800
H	4.24400700	10.02505300	10.62281900	H	7.56256300	6.00627300	17.38918700
C	5.27124400	3.47127200	5.81119500	C	9.58556600	6.66676200	17.72907200
C	5.39621000	4.05823800	4.41255900	H	10.23763500	7.50686700	17.42663100
C	6.78926800	4.65862500	4.19581100	H	10.06098800	5.75663900	17.31996100
C	7.88663300	3.62587800	4.47823300	C	9.53083100	6.57949300	19.25430300
C	7.74754200	3.04285400	5.88840700	H	8.90906600	5.72846600	19.58066000
C	6.35607100	2.44587600	6.11868800	H	10.53209800	6.45138900	19.69882300
H	6.87297700	5.04726000	3.16771000	H	9.08667300	7.49158600	19.68840900
H	5.20556700	3.24541700	3.69202900	C	5.61008900	8.96741600	15.84941900
H	4.60274500	4.81038800	4.28218800	H	5.35294900	8.59425500	16.85726600
H	7.82346300	2.81281800	3.73035900	H	4.68732200	9.36201400	15.40608000
H	8.88031300	4.08781400	4.35751200	C	6.69128000	10.03938400	15.91152500
H	8.51778400	2.27696800	6.07232200	H	7.01936600	10.29500000	14.89531800
H	7.91454200	3.83725000	6.62974100	H	7.58612900	9.65189900	16.43101500
H	6.18391500	1.57374000	5.46541800	C	6.24886000	11.33659400	16.59768200
H	6.23311800	2.11553700	7.16140700	H	5.34178300	11.71434400	16.09148600
H	6.91218000	5.51798900	4.87577600	H	5.94629400	11.12534100	17.64042300
C	5.28467600	7.80763100	8.23863000	C	7.33145300	12.41619400	16.57075200
C	5.76951700	9.02020400	8.74462100	H	7.60869000	12.65326400	15.53067000
C	4.91994600	7.73356500	6.88495100	H	7.00213200	13.34931700	17.05804700
C	5.90628400	10.13989400	7.91916100	H	8.24579200	12.07489700	17.08670100
H	6.03143800	9.09644900	9.79777800	C	5.27037500	5.33783300	15.45197200
C	5.04211800	8.85475800	6.06127500	H	4.99086100	5.54224200	16.50116600
H	4.54815100	6.79824000	6.46940200	H	4.34529500	5.17120100	14.89089100
C	5.53858600	10.05919800	6.57411400	C	6.17905900	4.11498000	15.34618500
H	6.29210100	11.06410600	8.35358300	H	6.53477000	4.01711900	14.30807300
H	4.75015600	8.78627800	5.00968000	H	7.07601400	4.23750700	15.98085500
H	5.63290400	10.93331200	5.92403500	C	5.47015900	2.80949900	15.71738800
C	6.81905400	5.56505300	9.07650000	H	4.58119300	2.71028500	15.07182700
C	7.04688300	4.27496400	9.58482800	H	5.10013900	2.87112600	16.75839200
C	7.87524900	6.24453800	8.45072900	C	6.35942500	1.57844400	15.54869100
C	8.31098000	3.69278300	9.48394600	H	5.83371600	0.64790600	15.82183900
H	6.24233800	3.75163000	10.10684500	H	6.68697600	1.48209100	14.50015400
C	9.14224700	5.66052700	8.36136800	H	7.26665700	1.64651800	16.17472200
H	7.71486900	7.23940400	8.03509900	Sn	6.19028700	7.16962900	14.70355200
C	9.36816200	4.38494200	8.88437200	O	6.91316400	7.06162200	12.69747100
H	8.47288100	2.69408900	9.89786800	C	8.01216800	6.23816300	12.39354400
H	9.95583800	6.21048400	7.88069800	H	8.92682400	6.53306100	12.94185600

H	7.80993700	5.17142200	12.60538200	H	4.82011200	12.34182500	11.69833000
H	8.23758500	6.31307600	11.31637800	C	6.40656800	14.76362900	11.22067700
Br	4.66850700	4.10044000	12.10552500	H	5.84819200	15.59957100	11.66990200
				H	7.19267200	15.18400300	10.57585800
TS_{5b-6b}				H	5.72389600	14.18349300	10.58707100
Cu	4.81817900	6.85272200	11.40196300	C	8.15443300	14.66194700	13.01393500
C	1.49869200	5.70840900	8.50795100	H	8.94219800	14.90443100	12.28576600
C	1.48119500	4.87252800	7.37512700	H	7.78441000	15.60025700	13.45283400
C	2.70187000	4.57035900	6.79760700	H	8.60379600	14.05536500	13.81353600
C	3.90340400	5.07132200	7.31896500	H	3.37274700	11.25335500	15.88272300
C	3.96152600	5.86450700	8.45569500	H	5.19773400	10.38258000	14.41823400
C	2.69748900	6.19854100	9.01784700	H	2.84536100	6.87409500	13.61230200
O	1.26643000	6.83597800	11.19142600	H	1.02743300	7.74022700	15.00839400
P	5.52696200	6.21396100	9.36053500	O	1.14054600	10.13465900	16.34883700
B	7.48007600	11.66662200	12.50323900	C	-0.06620500	9.44505400	16.56327900
S	2.59477300	7.17827600	10.54802900	H	-0.62197500	9.28252300	15.62147600
O	4.93696100	4.63379900	6.55548200	H	-0.67352900	10.07054100	17.23165500
O	2.97020200	3.78488900	5.72350800	H	0.09950900	8.46353200	17.04414100
H	0.55112000	4.46442600	6.97781200	C	3.27228200	10.29356700	15.37078600
H	0.57628700	5.95419400	9.03719700	C	4.28753000	9.79940600	14.56085500
C	2.41363900	8.95441500	9.88714800	C	4.16046500	8.55569200	13.90586400
C	2.38622700	9.80160400	11.16220200	C	2.97570700	7.83293100	14.11006400
H	1.59837500	9.46302000	11.84944800	C	1.93829000	8.32911000	14.90491800
H	2.18730500	10.85054100	10.89011000	C	2.08246900	9.56657200	15.54712000
H	3.34666000	9.76061900	11.69247000	C	5.24896200	8.02229000	13.06212100
C	1.09679500	9.03670900	9.12841100	C	5.96942500	8.75756200	12.24387100
H	1.13156800	8.47289000	8.18477000	C	6.83398900	9.49497600	11.55786700
H	0.88295300	10.09080400	8.88865000	C	8.00604300	10.22100600	12.20800200
H	0.27494700	8.64740900	9.74694500	H	8.87659200	10.23070900	11.53228900
C	3.62548600	9.28400200	9.02699000	H	8.29193800	9.71088500	13.14099000
H	4.56417000	9.12022600	9.57552000	H	6.68208600	9.66673300	10.48752800
H	3.58796600	10.34936700	8.74762300	C	4.41395800	3.59662500	5.69975600
H	3.64895500	8.69538400	8.09994300	C	4.75865100	2.23245800	6.28559900
C	7.03929100	13.89532800	12.29980100	C	4.28154700	1.10119700	5.37027700
C	6.02031000	13.22334400	13.29612600	C	4.82306500	1.27555200	3.94671400
O	6.67673600	11.96397100	13.57958200	C	4.44956000	2.64740700	3.37308100
O	7.65046200	12.74186700	11.67087900	C	4.92399900	3.78471300	4.28504100
C	5.80163600	13.96890400	14.60473700	H	4.59019100	0.13008000	5.78806100
H	5.38590000	14.97131500	14.41847500	H	5.85235100	2.20075600	6.41402600
H	5.08602600	13.41309100	15.22867900	H	4.31988700	2.15972600	7.29311400
H	6.73484800	14.07228500	15.17273600	H	5.92364300	1.17286400	3.95990200
C	4.67654500	12.89728500	12.63665900	H	4.44169400	0.47521800	3.29254400
H	4.08395300	12.26320400	13.30935300	H	4.87715500	2.77838000	2.36661400
H	4.10235200	13.81064800	12.42308300	H	3.35393900	2.71399100	3.26452300

H	6.02478200	3.80562900	4.33771600	C	6.24832700	1.15225400	14.48221700
H	4.58878500	4.76792600	3.92175600	H	7.08564400	1.05770500	15.19707200
H	3.17883900	1.10162100	5.34560200	H	5.32701700	1.06532100	15.08644200
C	6.52243700	7.30481200	8.28642500	C	6.30697600	0.01149300	13.46634100
C	7.72572100	7.79240500	8.82548100	H	7.23109900	0.06116700	12.86565600
C	6.14208800	7.68982300	6.99366300	H	6.27929500	-0.97700900	13.95241900
C	8.53774200	8.64506000	8.07701600	H	5.45550000	0.05950900	12.76581600
H	8.01978600	7.51346600	9.83896700	C	6.20284000	6.91328100	15.88763500
C	6.95195100	8.55405300	6.25183500	H	5.15730100	7.19635900	16.08317200
H	5.21570500	7.31122900	6.56057200	H	6.51222800	6.21792600	16.68592500
C	8.14975300	9.03197500	6.79026100	C	7.09882300	8.14849600	15.83057800
H	9.46935600	9.01895100	8.50755700	H	8.16129100	7.84235700	15.79759800
H	6.64554000	8.85248100	5.24637100	H	6.92137100	8.69331500	14.88961200
H	8.78041100	9.70828100	6.20846600	C	6.89474700	9.12937500	16.99030400
C	6.39486900	4.59810200	9.27186700	H	7.13975200	8.63056300	17.94570200
C	6.00709400	3.61470700	10.19538200	H	5.82259600	9.38648300	17.04491700
C	7.39947200	4.31532400	8.33584400	C	7.71835700	10.40825700	16.83568200
C	6.58989600	2.34596100	10.15142800	H	7.56213800	11.09836600	17.68100700
H	5.28386100	3.86679600	10.97241200	H	8.79798100	10.18447800	16.78592100
C	7.99467200	3.05276600	8.31117100	H	7.44766700	10.94192900	15.90967700
H	7.70782400	5.07793700	7.61993500	Sn	6.21327400	5.75981200	14.00892200
C	7.58231100	2.06242600	9.20911100	O	4.61315700	5.21766400	12.65458800
H	6.28785600	1.58803500	10.87583900	C	3.49650700	4.39582300	12.85742400
H	8.78315900	2.84023100	7.58509700	H	2.55226900	4.96208700	12.75068100
H	8.04805900	1.07425800	9.18587200	H	3.46391300	3.57391700	12.11156900
C	7.95806800	6.05500000	12.72036000	H	3.50135800	3.92486700	13.85721800
H	7.55091100	6.55036700	11.82677400				
H	8.58761000	6.81014800	13.22108400	**$TS_{8'a\text{-}9'a}$**			
C	8.76754700	4.82267100	12.33042600	Cu	4.38746000	6.73225600	10.95554600
H	9.20275300	4.34771300	13.22884800	C	1.47053800	3.18164000	8.64431000
H	8.10452200	4.06617000	11.88231600	C	2.02589000	2.12499300	7.90753800
C	9.88795500	5.12594500	11.32924400	C	3.27630100	2.34347800	7.36299300
H	10.55483900	5.90059300	11.74976800	C	3.96502400	3.54340700	7.56681000
H	9.43881700	5.57004300	10.42287200	C	3.45410000	4.60840200	8.30708700
C	10.69988100	3.89205900	10.93957900	C	2.14140500	4.39093600	8.81092600
H	10.05075100	3.12390000	10.48959600	O	0.09470600	4.77965900	10.45161500
H	11.48846500	4.13461800	10.20886700	P	4.48144900	6.09145500	8.74552800
H	11.18766700	3.44098100	11.82006800	B	3.96886000	10.70425000	10.30641000
C	6.22743500	3.69922700	14.82419600	S	1.20813100	5.60669000	9.82259600
H	5.33824400	3.60449800	15.47313400	O	5.16190400	3.47381400	6.90916800
H	7.09728900	3.67862300	15.50604700	O	4.02139200	1.50091800	6.59054700
C	6.29378700	2.54028800	13.83388600	H	1.50501800	1.17609500	7.77167000
H	7.21282000	2.61637700	13.22947800	H	0.50138400	3.08459600	9.13738800
H	5.46327200	2.61517800	13.11253800	C	0.27794400	6.55909200	8.43840200

C	-0.67471600	7.45297000	9.23453700	C	0.13944700	6.66720400	12.78503700
H	-1.31916100	6.85741000	9.89572400	C	-1.13415300	6.19074700	13.09352600
H	-1.30943400	8.02344300	8.53553800	C	-2.22453100	7.06867700	13.11589900
H	-0.11933900	8.16737000	9.85472900	C	1.66836900	8.48024900	12.14750000
C	-0.49555900	5.57769100	7.57096300	C	2.86277900	8.66730600	11.93064500
H	0.16947500	4.98501300	6.92646900	C	4.27034600	8.89933100	11.97169200
H	-1.19823000	6.13117100	6.92437300	C	4.98602900	9.63052000	10.79446900
H	-1.07706400	4.89308800	8.20669500	H	5.29974100	8.93823200	10.00169700
C	1.28017700	7.38995700	7.65659300	H	5.90713700	10.08354700	11.18773700
H	1.88840400	8.01964800	8.32245900	H	4.46755100	9.48638200	12.88237500
H	0.74452200	8.06316200	6.96477300	C	5.28850900	2.14440600	6.36019800
H	1.94724300	6.76462700	7.04964200	C	5.55058800	2.26002800	4.86502400
C	2.14142400	11.58416200	9.22609600	C	6.91897900	2.89426400	4.59480200
C	2.50902500	12.44888000	10.50267800	C	8.03546300	2.11960500	5.30415000
O	3.81956800	11.95834600	10.85200200	C	7.76358200	2.01768300	6.80825600
O	3.00007500	10.43834200	9.36376200	C	6.39414900	1.39805500	7.09694900
C	2.60185200	13.94976900	10.24956500	H	7.10173000	2.93942900	3.50865700
H	1.63274200	14.35143100	9.91407200	H	5.50442800	1.24305300	4.44102600
H	2.87923500	14.46026700	11.18392600	H	4.73190400	2.84349100	4.41573900
H	3.36340900	14.18894800	9.49579700	H	8.11096200	1.10599400	4.86679400
C	1.59861800	12.17176200	11.70278200	H	9.00654800	2.61128200	5.12935900
H	2.02635700	12.66485700	12.58829100	H	8.55107600	1.43249100	7.30936300
H	0.58215000	12.56265400	11.54329300	H	7.79337100	3.02254200	7.25123100
H	1.54499000	11.09412600	11.91297700	H	6.35555800	0.34622100	6.76633600
C	0.69600800	11.09998700	9.18514100	H	6.16694600	1.42052800	8.17372000
H	-0.00506400	11.94912900	9.16085700	H	6.90838300	3.93396000	4.96267000
H	0.53636900	10.49319700	8.28184100	C	4.51381300	7.06029300	7.16787700
H	0.46841900	10.46986500	10.05263700	C	4.41859100	8.45475700	7.25029000
C	2.50910700	12.25919400	7.90181400	C	4.62210500	6.46042100	5.90075700
H	2.38666300	11.52752200	7.08966900	C	4.43815400	9.24013400	6.09367600
H	1.86445600	13.12515800	7.68906700	H	4.28789500	8.93553600	8.21657800
H	3.55714300	12.59306800	7.90476700	C	4.63505400	7.24483400	4.74614700
H	-2.88457800	9.10147000	12.87171700	H	4.71345400	5.37832400	5.81885000
H	-0.60001100	9.95815000	12.31610500	C	4.54476500	8.63847200	4.83851700
H	0.97810100	5.97070900	12.74095400	H	4.35510000	10.32564100	6.18372200
H	-1.25725200	5.12382400	13.27247900	H	4.71827100	6.76434600	3.76741100
O	-3.50874200	6.69352400	13.39129800	H	4.55349200	9.25061200	3.93264200
C	-3.76800900	5.33202300	13.62209600	C	6.19358500	5.39881300	8.78022300
H	-3.48960100	4.70551700	12.75498000	C	6.50294600	4.46146800	9.77931600
H	-4.84953300	5.24079800	13.79777900	C	7.22060300	5.89308500	7.96378000
H	-3.22906800	4.95169400	14.50973400	C	7.81729100	4.02773500	9.94884200
C	-2.02247200	8.43178100	12.84075900	H	5.71566500	4.10240200	10.44704000
C	-0.75156000	8.89863800	12.53159900	C	8.53835300	5.46141100	8.14333100
C	0.35904200	8.02433700	12.48266500	H	6.99905500	6.62865000	7.19015600

C	8.84116800	4.53258000	9.14098100	O	6.39670600	6.75029200	11.69581800
H	8.04709600	3.31507500	10.74163400	C	7.53466100	7.39205700	11.22530200
H	9.33000600	5.86343400	7.50532500	H	7.62883000	8.44236700	11.56907200
H	9.87193700	4.20089000	9.29053300	H	8.46520700	6.86811100	11.53652000
C	6.86708500	8.88808800	14.23576600	H	7.54090000	7.42205400	10.11965400
H	6.92848600	9.60680200	13.40182400	Br	3.55458900	4.71754600	12.11123300
H	6.36235900	9.41730700	15.06318200				
C	8.26567700	8.44127100	14.65734700	**TS_{8a-9a}**			
H	8.19691600	7.74453500	15.51256600	Cu	4.52924600	7.49618600	10.56088200
H	8.73472600	7.85677800	13.84554700	C	2.96487200	3.33440100	9.96059700
C	9.20473100	9.59253200	15.03576600	C	3.58840300	2.21237800	9.38652000
H	8.74500600	10.18034100	15.85161500	C	4.59177400	2.45438600	8.46620500
H	9.28559000	10.28506200	14.17794500	C	4.98441600	3.75810000	8.13497600
C	10.59957400	9.12891500	15.45583400	C	4.41415600	4.88917800	8.70481900
H	11.09028000	8.56433600	14.64483100	C	3.35174300	4.62559400	9.61726600
H	11.25599200	9.97532200	15.71884100	O	1.74643100	5.31456700	11.63708800
H	10.54903700	8.46020200	16.33209300	P	5.13021000	6.57818600	8.54194100
C	3.66273300	7.35352300	14.81461000	B	3.26501300	10.74545400	10.02876000
H	3.86670900	6.69763500	15.67946800	S	2.46450800	5.97065900	10.46862900
H	2.90278100	6.84811700	14.20348200	O	5.98514300	3.70372400	7.22169700
C	3.17626300	8.72349200	15.27285100	O	5.35490200	1.56074400	7.78787500
H	3.09589300	9.40704200	14.41257100	H	3.30993300	1.19554400	9.66452300
H	3.90738900	9.18570800	15.96392400	H	2.18183900	3.21974100	10.71192700
C	1.80061900	8.68103900	15.95165700	C	1.07465300	6.31903400	9.18659200
H	1.09643100	8.16398500	15.27858200	C	0.17011100	7.32557500	9.89053500
H	1.85982000	8.06287500	16.86680800	H	-0.26679200	6.90294000	10.80230900
C	1.25092100	10.06612800	16.28989500	H	-0.65139000	7.59539900	9.20776700
H	1.13721100	10.67230200	15.37518500	H	0.71871700	8.23723500	10.15768400
H	0.26255500	10.00996800	16.77601400	C	0.33823700	5.01248200	8.92498000
H	1.92797800	10.61593100	16.96720200	H	0.93735900	4.30813900	8.33145500
C	6.36142500	5.39458000	14.51801400	H	-0.58402600	5.23430300	8.36350700
H	6.93089800	5.70767800	15.41392700	H	0.05298000	4.53337900	9.87301400
H	5.47996000	4.83742400	14.87510700	C	1.69476800	6.91473800	7.93473500
C	7.20684800	4.50630800	13.61578100	H	2.25316000	7.83326800	8.15872000
H	6.59537800	4.20892900	12.75008100	H	0.88521700	7.18327000	7.23587600
H	8.05539700	5.07519000	13.19504800	H	2.34762700	6.20266300	7.41441900
C	7.74319100	3.25366500	14.31862400	C	1.68159200	11.20303400	8.44086400
H	6.89434900	2.69898200	14.75839900	C	1.57881900	12.23009400	9.63505900
H	8.37756500	3.55695400	15.17300300	O	2.81497500	11.99428100	10.34909700
C	8.53555700	2.32266400	13.40010700	O	2.56484000	10.18618800	8.98263700
H	8.94136200	1.45072600	13.94082400	C	1.53011400	13.69377100	9.21606700
H	7.89968700	1.93890000	12.58452700	H	0.64426200	13.89232200	8.59311000
H	9.38480000	2.85115900	12.93358700	H	1.46685500	14.32885200	10.11180100
Sn	5.53151800	7.23789600	13.62472700	H	2.42843000	13.98713000	8.65789000

C	0.43483900	11.91553900	10.60002800	H	9.48966600	3.04414800	4.78890500
H	0.55949500	12.52967600	11.50360800	H	9.79313400	2.62123100	7.25595600
H	-0.54518700	12.14298800	10.15572600	H	8.63232100	3.91454200	6.95603800
H	0.45510600	10.86313200	10.91005400	H	7.92076900	0.99719500	7.63682900
C	0.36081800	10.56177600	8.03872900	H	7.71839600	2.41314000	8.69315000
H	-0.34273100	11.32755000	7.67754200	H	7.12074300	3.79267800	4.80544900
H	0.53036700	9.84146700	7.22498400	C	4.77382500	7.16182400	6.84020100
H	-0.10219400	10.02699500	8.87470000	C	4.55430400	8.53435600	6.65515100
C	2.37633900	11.78005100	7.20611600	C	4.77848700	6.30642100	5.72621300
H	2.55507500	10.96615700	6.49036900	C	4.36286800	9.04737900	5.36864100
H	1.75704700	12.54235500	6.71198300	H	4.50896400	9.20029600	7.51889900
H	3.34508000	12.23133900	7.46610000	C	4.56506000	6.82064000	4.44635700
H	-2.67316200	10.28839000	14.32543400	H	4.96829500	5.24160900	5.85784700
H	-0.44826100	10.78233900	13.29617700	C	4.36371500	8.19284100	4.26388700
H	0.36808600	6.55942800	13.06159900	H	4.20729600	10.11932900	5.23120600
H	-1.81677100	6.06646300	14.10512700	H	4.56578200	6.14755700	3.58548300
O	-3.61393700	7.99481800	14.85039700	H	4.20681800	8.59507900	3.26017000
C	-4.06004200	6.69196700	15.14323700	C	6.93967200	6.26299000	8.47177500
H	-4.15348300	6.07409900	14.23163300	C	7.53949300	5.50691900	9.49126100
H	-5.05055600	6.79525500	15.60624700	C	7.74861600	6.86032200	7.49448400
H	-3.38546100	6.17589200	15.85003800	C	8.92389100	5.34919800	9.52653000
C	-1.99412600	9.48357100	14.03781400	H	6.92939700	5.06784600	10.27514800
C	-0.75993000	9.74981900	13.46089500	C	9.13777400	6.70606700	7.53932000
C	0.11641000	8.70262100	13.09788900	H	7.29948900	7.45066600	6.69483200
C	-0.29813000	7.37820700	13.34263900	C	9.72966700	5.95318400	8.55575900
C	-1.53530900	7.10408400	13.92717200	H	9.37541300	4.76105200	10.32900900
C	-2.39368400	8.15766000	14.27855200	H	9.75753600	7.17885500	6.77359000
C	1.41383500	8.96029200	12.56392200	H	10.81524200	5.83491600	8.59080700
C	2.57228100	9.10997500	12.20547900	C	6.76215700	7.83533900	14.56716200
C	3.98708600	9.21006900	11.99787600	H	7.15677600	8.78138600	14.16291000
C	4.46618000	10.04212600	10.75086200	H	6.44342400	8.03979200	15.60287500
H	5.04233800	9.46155300	10.00190600	C	7.83196100	6.74286300	14.52117900
H	5.17396000	10.80976200	11.10003800	H	7.44793900	5.82332500	15.00082100
H	4.40999300	9.71321600	12.88235600	H	8.02934800	6.46389800	13.47179500
C	6.34842300	2.30711300	7.04895300	C	9.15556000	7.13147100	15.18740700
C	6.27013200	1.96148000	5.57180400	H	8.96764600	7.40369000	16.24185900
C	7.34224700	2.71242300	4.77367600	H	9.54148800	8.04786800	14.70473000
C	8.74021400	2.46469900	5.35153800	C	10.21138800	6.02893300	15.11660000
C	8.79687500	2.83297100	6.83764600	H	10.43520300	5.76284900	14.06952800
C	7.73109300	2.08326700	7.64360100	H	11.15710400	6.33265800	15.59387500
H	7.29625500	2.40835800	3.71597600	H	9.86318100	5.11095000	15.61957400
H	6.41267700	0.87219900	5.48183800	C	3.33194300	7.60452500	14.85903200
H	5.25472600	2.19206000	5.21378100	H	3.58403600	6.86288900	15.64066500
H	9.00474900	1.39903300	5.22259800	H	2.40222300	7.25837700	14.38689000

C	3.15370600	8.98548600	15.47904500	H	1.46401100	1.93676000	7.25568100
H	3.01201000	9.74103100	14.68871900	H	0.64111500	3.50508000	9.09247500
H	4.06950900	9.28076900	16.02522500	C	0.53287400	7.02318600	9.06952900
C	1.95193800	9.07323600	16.42902000	C	-0.24954000	7.88740000	10.06283200
H	1.05144900	8.73643300	15.88723500	H	-0.96264900	7.27884000	10.63975900
H	2.09194600	8.35901500	17.26108800	H	-0.81182200	8.66416300	9.51089900
C	1.71712400	10.47794400	16.98146900	H	0.42209800	8.38609200	10.78031400
H	1.52693200	11.19400600	16.16412500	C	-0.41861500	6.21631600	8.19678100
H	0.85011000	10.51155500	17.66110900	H	0.11336200	5.66762300	7.40205400
H	2.59540800	10.84332400	17.54074900	H	-1.14667100	6.89848100	7.71693800
C	4.73216700	5.07721200	13.30090900	H	-0.97642300	5.49419500	8.81671600
H	4.86286300	4.77812300	14.35747100	C	1.51281400	7.85608300	8.26017300
H	3.67586600	4.89323900	13.05242400	H	2.26219800	8.33696200	8.90781800
C	5.65905600	4.27426700	12.39994800	H	0.97242900	8.66074200	7.72657400
H	5.43601100	4.52199900	11.35165100	H	2.04404800	7.25190400	7.50857700
H	6.70763300	4.57538500	12.55923100	C	2.78798800	12.06394100	10.69883600
C	5.54271400	2.75757500	12.57563400	C	2.30939100	12.50676400	12.13853000
H	4.49968200	2.44986600	12.38359100	O	2.95687000	11.54833200	12.99179000
H	5.74467700	2.49830400	13.63073600	O	4.02360100	11.37182100	10.98130200
C	6.48901000	1.97656400	11.66475900	C	2.82261800	13.89183000	12.54830800
H	6.40138600	0.88790000	11.81159600	H	2.32447100	14.69929800	11.98427000
H	6.27666600	2.18320400	10.60424800	H	2.62132900	14.03855100	13.62296200
H	7.54024200	2.25522100	11.85074300	H	3.91168000	13.97287800	12.39463900
Sn	4.98246400	7.25613700	13.42195300	C	0.80221000	12.41469700	12.36392600
O	6.29503200	7.18606300	11.58407300	H	0.56547300	12.73076400	13.39440700
C	7.25670800	8.16963700	11.35587400	H	0.25499500	13.07324500	11.66565500
H	6.97506500	9.16392400	11.76154600	H	0.44300200	11.38226400	12.24232200
H	8.22966200	7.90314100	11.81492400	C	1.85369400	11.04316300	10.04532800
H	7.44453900	8.30851000	10.27175800	H	0.88469400	11.48927300	9.76385100
				H	2.33689900	10.65315000	9.13531000
$TS_{8'b-9'b}$				H	1.66931400	10.19350300	10.72144900
Cu	4.60825200	6.40571400	11.47015500	C	3.06779600	13.21249900	9.73459000
C	1.58070500	3.68785300	8.56570000	H	3.38329400	12.80654100	8.75825100
C	2.03624900	2.81494700	7.56255300	H	2.15833100	13.81822400	9.57368400
C	3.25155400	3.12051600	6.97869800	H	3.86923700	13.86939200	10.10589700
C	4.01000500	4.21862600	7.39835500	H	-2.12200200	9.70844800	15.52238400
C	3.60589500	5.08763500	8.40606200	H	0.18335200	10.02057100	14.59099200
C	2.31993300	4.80324700	8.94828800	H	-0.02545900	6.09112300	12.81431000
O	0.43368500	4.98940500	10.83293300	H	-2.28618900	5.78851500	13.72043100
P	4.74355100	6.32168200	9.17782300	O	-3.61036800	7.66565100	15.23319900
B	3.96599700	10.93361300	12.29307700	C	-4.35340100	6.49292200	15.04092600
S	1.52812800	5.85259200	10.22363500	H	-4.55383100	6.29872500	13.96742500
O	5.14999800	4.27729300	6.64665200	H	-5.31360000	6.63860600	15.56274400
O	3.90156700	2.46944100	5.96947400	H	-3.84425500	5.60423900	15.46589200

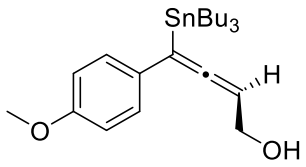
C	-1.64548200	8.92680900	14.92425500	H	5.98990100	4.04493000	10.41892000
C	-0.36713200	9.09445600	14.40579100	C	8.73623100	5.72799200	8.23548300
C	0.25437100	8.07725200	13.64050300	H	7.17827800	7.05622700	7.55827100
C	-0.47232600	6.88918000	13.41397500	C	9.06599500	4.64654700	9.05718500
C	-1.76208300	6.72383100	13.92527600	H	8.31993900	3.19290300	10.47841900
C	-2.35709300	7.73949300	14.68760100	H	9.50762500	6.21755900	7.63208200
C	1.57055200	8.24721100	13.13649100	H	10.09817800	4.28523600	9.10507000
C	2.73413800	8.34620700	12.76515800	C	7.05692500	8.21671600	14.91754100
C	4.09902800	8.45780400	12.39850900	H	7.16017500	9.07230600	14.22996800
C	4.81912800	9.75903000	12.86338500	H	6.62251500	8.61571600	15.85309500
H	5.84889400	9.76155700	12.47353200	C	8.42467700	7.58418100	15.18233100
H	4.87602300	9.81044000	13.96210100	H	8.32846300	6.76949700	15.92576400
H	4.18967900	8.40251400	11.29632300	H	8.79761000	7.09598400	14.26133200
C	5.21603500	3.05312800	5.88241500	C	9.48601400	8.57696300	15.67588100
C	5.54444700	3.39788400	4.43843700	H	9.12232800	9.06822000	16.59989700
C	6.96271100	3.97113200	4.32178300	H	9.59734600	9.38525000	14.92668100
C	7.99938900	3.01257700	4.92253000	C	10.84792200	7.92960700	15.93793500
C	7.65989200	2.67683800	6.37955400	H	11.24390000	7.45544900	15.02031100
C	6.24146900	2.11532500	6.51444600	H	11.59579600	8.66638100	16.28639500
H	7.19262200	4.18187600	3.26193900	H	10.77075300	7.13863200	16.70760800
H	5.45195300	2.47089800	3.84427400	C	3.80852500	6.75783800	15.34032500
H	4.78527000	4.10869500	4.07064900	H	4.02590600	5.95549300	16.07165900
H	8.02941500	2.08237000	4.32009300	H	2.98429300	6.40477600	14.70075400
H	9.00692100	3.46201800	4.86455000	C	3.44162000	8.05635700	16.05088900
H	8.38720300	1.95715600	6.79390100	H	3.30057700	8.86319500	15.31150100
H	7.73829900	3.58853400	6.99099100	H	4.27019000	8.38261100	16.71272700
H	6.15094000	1.13799900	6.00574200	C	2.15463100	7.94834700	16.88252800
H	5.97296800	1.96882300	7.57440000	H	1.33910700	7.59584900	16.22610600
H	7.00281600	4.93488900	4.86065800	H	2.28497900	7.17068800	17.66127100
C	4.78748300	7.74341700	8.00800600	C	1.74418400	9.27044000	17.53361200
C	4.94086100	9.02557400	8.55579900	H	1.58319000	10.04983800	16.76611000
C	4.66650700	7.60775000	6.61489800	H	0.80524100	9.17001200	18.10928000
C	4.97017100	10.15474600	7.73198600	H	2.52763400	9.64106600	18.22267300
H	5.01035800	9.15979500	9.63728300	C	6.38015500	4.76749300	14.61756300
C	4.69091200	8.73583300	5.79153600	H	6.87407300	4.89636500	15.60294800
H	4.56172300	6.61347700	6.17446900	H	5.47100100	4.16446200	14.78459300
C	4.84228900	10.01243800	6.34782500	C	7.30213500	4.05330500	13.63684300
H	5.08061000	11.14102600	8.19054500	H	6.76812500	3.93451900	12.68001100
H	4.59149600	8.61875600	4.70746300	H	8.18747500	4.67640400	13.40885800
H	4.85662500	10.89464600	5.69967000	C	7.76424100	2.67641500	14.13348700
C	6.42261000	5.59347400	8.96650300	H	6.87386500	2.07191600	14.39382900
C	6.75612200	4.49860400	9.78181800	H	8.33686300	2.79775800	15.07525400
C	7.42065800	6.19949500	8.19001300	C	8.61316300	1.91087900	13.11515600
C	8.06926100	4.02777800	9.81956100	H	8.97333800	0.94461400	13.51671300

H	8.02925900	1.69465800	12.20118500	H	6.76994900	13.55226500	15.83059600
H	9.49859000	2.50040200	12.80977000	H	7.94442600	12.33129000	15.27838000
Sn	5.62426400	6.76298300	14.06949700	H	7.15107500	13.38990400	14.09229700
O	6.62899700	6.62196300	12.13030800	C	5.85883400	10.90695000	16.13630300
C	7.43565000	7.58341200	11.54316200	H	6.82047300	10.38433200	16.23045500
H	6.86499400	8.34001600	10.95555300	H	5.69409000	11.49950200	17.04788500
H	8.04371300	8.15055800	12.28251000	H	5.06791900	10.15003100	16.06285600
H	8.14716600	7.10441500	10.83720900	C	3.51885800	12.53813400	15.69613800
Br	3.75689700	4.23870500	12.13111100	H	3.93946400	13.22264700	16.44883000
				H	2.56439400	12.96156600	15.35031800
TS_{8b-9b}				H	3.30617800	11.57576300	16.17484800
Cu	4.67447200	6.75303800	10.82382200	C	4.55164100	13.69525200	13.73220300
C	3.47433400	2.51003900	9.39120300	H	3.55286000	13.92905200	13.33584700
C	4.05693500	1.63374400	8.45863700	H	4.88020500	14.53250200	14.36525100
C	4.95272300	2.18051900	7.55688400	H	5.24204700	13.60865900	12.88050700
C	5.26926900	3.54595700	7.57267600	H	-0.74292100	12.27364500	15.20622700
C	4.71854000	4.43794800	8.48319100	H	1.27881600	11.52948100	13.91275400
C	3.78511600	3.86673800	9.38927900	H	-0.77976400	7.91416600	12.81983300
O	2.58024500	3.85991400	11.76453100	H	-2.76720900	8.63961200	14.07500600
P	5.31115700	6.16129300	8.71537300	O	-2.92047700	10.99893000	15.46017400
B	5.01595500	10.69170400	13.08457500	C	-4.08799800	10.22363900	15.57441000
S	3.04456800	4.85692500	10.72205100	H	-4.56350800	10.04576500	14.59220500
O	6.16796800	3.80637800	6.59041300	H	-4.78344700	10.79082800	16.20779500
O	5.65616700	1.56285900	6.57413100	H	-3.88827500	9.24537200	16.04910000
H	3.83423200	0.56633300	8.45751000	C	-0.73285800	11.32326500	14.66870800
H	2.79800600	2.13901800	10.16269000	C	0.38052400	10.91284000	13.95177100
C	1.43077900	5.47525400	9.91670600	C	0.39401800	9.67264700	13.26801000
C	0.68770900	6.10302300	11.09629000	C	-0.76603500	8.87860100	13.32926800
H	0.49745900	5.35666600	11.87950600	C	-1.89229000	9.28875800	14.04725800
H	-0.27689200	6.49783600	10.73883900	C	-1.88148100	10.51472400	14.72789700
H	1.25060600	6.94032000	11.53146500	C	1.57708200	9.26131300	12.59643300
C	0.67570000	4.27166400	9.36753700	C	2.66432100	8.96166800	12.12531400
H	1.16039200	3.84829700	8.47644400	C	3.96548800	8.66446600	11.63897300
H	-0.34082200	4.59018200	9.08521200	C	4.97815400	9.82626000	11.77164900
H	0.58586000	3.48957800	10.13538900	H	4.75973200	10.58082700	10.98371600
C	1.76365400	6.49843000	8.84099500	H	5.99429800	9.47167800	11.56485200
H	2.32773200	7.34958500	9.24613900	H	3.85429900	8.46205200	10.54317700
H	0.82355300	6.89426800	8.42380700	C	6.61223000	2.52247200	6.07071300
H	2.33273000	6.05806700	8.01016400	C	6.56980800	2.56522200	4.55541800
C	4.47388100	12.38464200	14.51994000	C	7.60881900	3.55035400	4.00666000
C	5.89067600	11.79835500	14.89497500	C	9.01190000	3.23344100	4.53692000
O	6.18486100	10.95591300	13.75419300	C	9.03209500	3.20625000	6.06872200
O	3.95455200	11.38690300	13.60962900	C	7.99888300	2.22189700	6.62474200
C	6.99957600	12.83545900	15.02708200	H	7.59261400	3.52834500	2.90558600

H	6.77453200	1.54472400	4.19282100	C	3.09296000	7.05340000	14.66713800
H	5.54778200	2.82867300	4.24264600	H	3.06920000	6.12201600	15.26196800
H	9.33763800	2.25275800	4.14397300	H	2.27870000	6.98685300	13.93253700
H	9.73372100	3.97660100	4.16182900	C	2.92752000	8.27139800	15.56693300
H	10.03362700	2.94326000	6.44286800	H	2.97890000	9.19313500	14.96561200
H	8.80721200	4.21025600	6.45784700	H	3.76569300	8.32443500	16.28674700
H	8.24744200	1.18544700	6.34272600	C	1.61267200	8.26356500	16.35803800
H	7.95474800	2.26651400	7.72423600	H	0.77046900	8.20123100	15.64957100
H	7.32562800	4.57244400	4.30997000	H	1.56854200	7.34374700	16.96962400
C	4.79919900	7.12953900	7.25077400	C	1.43268300	9.48926700	17.25161300
C	4.56706600	8.49965500	7.45268200	H	1.39165500	10.40882500	16.64830300
C	4.63075500	6.58376500	5.96830800	H	0.49630400	9.43784700	17.83013400
C	4.17639600	9.31508400	6.38805900	H	2.26546700	9.59097800	17.96893100
H	4.68738300	8.92756400	8.45132700	C	5.09097000	4.59763500	13.62862400
C	4.22842100	7.40000900	4.90904900	H	5.46953000	4.33889300	14.63439300
H	4.82775600	5.52639800	5.79457100	H	4.04332700	4.26768700	13.58035000
C	4.00141200	8.76460100	5.11572300	C	5.91028600	3.90604400	12.54456300
H	3.99821400	10.37947200	6.55692900	H	5.61852700	4.30345800	11.55966700
H	4.09425100	6.96792000	3.91440100	H	6.97496900	4.17661200	12.64207200
H	3.68584000	9.39882100	4.28392000	C	5.75537000	2.38496800	12.50289500
C	7.12398000	5.97388000	8.54469100	H	4.68505000	2.14741000	12.38061500
C	7.77214700	5.07107100	9.40257500	H	6.06073400	1.95265000	13.47313900
C	7.88203600	6.77467300	7.68082600	C	6.56173100	1.74633000	11.37133300
C	9.16208200	4.96518100	9.38451000	H	6.43858200	0.65153300	11.33955800
H	7.19271500	4.47028300	10.10299400	H	6.24457300	2.14075800	10.39177800
C	9.27652300	6.67462200	7.67763000	H	7.63963800	1.95781400	11.47884900
H	7.38592500	7.47929500	7.01107600	Sn	5.02270700	6.79840800	13.61083500
C	9.91934000	5.77125600	8.52768600	O	6.43344700	6.70254300	11.88836400
H	9.65644900	4.26102600	10.05773400	C	7.52961900	7.51836700	11.60987900
H	9.86169700	7.30498000	7.00377300	H	7.66595600	8.32954600	12.35036400
H	11.00906900	5.69450300	8.52299700	H	8.46863900	6.92889000	11.60061700
C	6.58320100	7.67295100	14.86627300	H	7.45372700	8.00134100	10.61404600
H	6.87040900	8.64514200	14.44103500				
H	6.13066100	7.87983200	15.84893400				
C	7.79272800	6.74929900	15.00319300				
H	7.49967000	5.81584500	15.51764100				
H	8.14348400	6.43407400	14.00601900				
C	8.96324200	7.38778400	15.75888200				
H	8.62045900	7.70105000	16.76198900				
H	9.25676400	8.31723600	15.23790300				
C	10.17425000	6.46536000	15.89053700				
H	10.55120800	6.16332000	14.89882400				
H	11.00382500	6.95022600	16.43014300				
H	9.91473500	5.54262900	16.43642300				

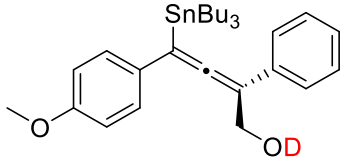
11.Characterization Data for allene products.

(S)-4-(4-methoxyphenyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2a**)

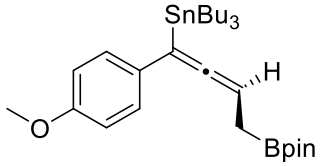


Colorless oil (71 mg, 76 % yield, 97 % *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.17 (d, *J* = 8.7 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 5.24 (tt, *J* = 6.6, 6.6Hz, 1H), 4.26-4.19 (m, 2H), 3.82 (s, 3H), 1.56-1.46 (m, 6H), 1.38-1.29 (m, 7H), 1.16-0.99 (m, 6H), 0.90 (t, *J* = 7.2 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 202.2, 158.4, 130.2, 128.9, 114.1, 98.4, 84.9, 61.7, 55.3, 28.9, 27.2, 13.7, 11.1; **HRMS (M/Z, ESI)** Calcd. for $C_{23}H_{38}O_2Sn$ [M+Na]: 489.1791, Found: 489.1794; **HPLC analysis:** Daicel Chiralpak IC, hexane/iso-propanol = 50: 1, 0.5 ml/min, λ= 254 nm, retention time: 16.63 min (minor) and 17.99 min (major). Optical Rotation: $[\alpha]_D^{25}$ -19.6 (c 0.915, $CHCl_3$).

(*S*)-4-(4-methoxyphenyl)-2-phenyl-4-(tributylstannyl)buta-2,3-dien-1-ol-d (**2a**-d)



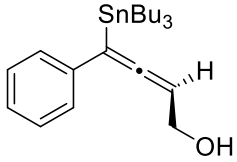
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.17 (d, *J* = 8.7 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 5.24 (tt, *J* = 6.6, 6.6Hz, 1H), 4.24-4.16 (m, 2H), 3.82 (s, 3H), 1.62-1.48 (m, 6H), 1.38-1.31 (m, 6H), 1.16-0.99 (m, 6H), 0.90 (t, *J* = 7.2 Hz, 9H).



2a'

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.21 (d, *J* = 8.4 Hz, 2H), 6.83 (d, *J* = 8.4 Hz, 2H), 5.06 (tt, *J* = 7.6, 7.6 Hz, 1H); 3.81 (s, 3H), 1.74-1.61 (m, 2H), 1.58-1.50 (m, 6H), 1,36-1,31 (m, 6H), 1.28-1.27 (m, 12H), 1.13-0.99 (m, 6H), 0.90 (t, *J* = 7.2 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 205.3, 157.9, 131.9, 128.9, 113.8, 95.9, 83.3, 79.7, 55.2, 29.0, 27.3, 24.9, 24.8, 13.7, 10.9; **HRMS (M/Z, ESI)** Calcd. for $C_{29}H_{49}BO_3Sn$ [M+Na]: 599.2694, Found: 599.2702; Optical Rotation: $[\alpha]_D^{25}$ -23.9 (c 0.935, $CHCl_3$).

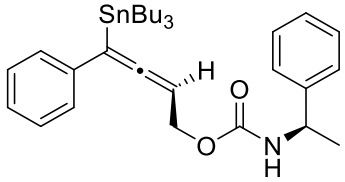
(S)-4-phenyl-4-(tributylstannyl)buta-2,3-dien-1-ol (**2b**)



Colorless oil (75 mg, 86% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.33-7.28 (m, 2H), 7.25-7.18 (m, 3H), 5.26 (tt, *J* = 6.8, 6.4 Hz, 1H), 4.28-4.18 (m, 2H), 1.59-1.44 (m, 6H), 1.38-1.28 (m, 7H), 1.17-1.02 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 202.8, 138.2, 128.6, 127.8, 126.3, 99.0, 84.7, 61.6, 28.9, 27.2, 13.6, 11.1; **HRMS (M/Z, ESI)** Calcd. for

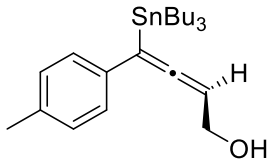
$C_{23}H_{38}O_2Sn$ [M+Na]: 459.1686, Found: 459.1682; Optical Rotation: $[\alpha]_D^{25}$ -28.2 (c 1.315, $CHCl_3$); The *ee* value of **2b** was determined by chiral HPLC analysis after derivatization to **2b'**.

(*S*)-4-phenyl-4-(tributylstannyl)buta-2,3-dien-1-yl ((*R*)-1-phenylethyl)carbamate (**2b'**)



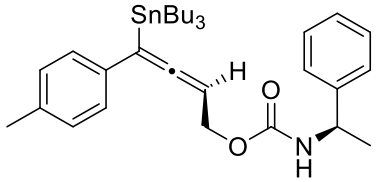
Colorless oil (93% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.37-7.30 (m, 7H), 7.26-7.17 (m, 3H), 5.17 (t, *J* = 7.3 Hz, 1H), 4.94-4.88 (m, 2H), 4.64-4.63 (m, 2H), 1.57-1.43 (m, 9H), 1.37-1.28 (m, 6H), 1.16-1.01 (m, 6H), 0.89 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 204.0, 155.6, 143.6, 137.9, 128.6, 128.5, 128.0, 127.3, 126.4, 126.0, 98.1, 80.4, 64.0, 50.6, 28.9, 27.2, 22.5, 13.7, 11.1; **HRMS (M/Z, ESI)** Calcd. for $C_{31}H_{45}NO_2Sn$ [M+Na]: 606.2370, Found: 606.2362; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 50: 1, 0.5 ml/min, λ= 254 nm, retention time: 8.59 min (major) and14.74 min (minor).

(S)-4-(*p*-tolyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2c**)



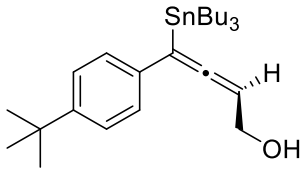
Colorless oil (72 mg, 80% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.16-7.11 (m, 4H), 5.24 (tt, *J* = 6.6, 6.6 Hz, 1H), 4.27-4.17 (m, 2H), 2.35 (s, 3H), 1.59-1.46 (m, 6H), 1.40-1.29 (m, 7H), 1.17-1.00 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 202.6, 136.1, 135.0, 129.3, 127.7, 98.7, 84.8, 61.7, 28.9, 27.2, 21.1, 13.7, 11.1; **HRMS (M/Z, ESI)** Calcd. for $C_{23}H_{38}OSn$ [M+Na]: 473.1842, Found: 473.1851; Optical Rotation: $[\alpha]_D^{25}$ -26.9 (c 1.105, $CHCl_3$). The *ee* value of **2c** was determined by chiral HPLCanalysisafter a derivatization to **2c'**.

(*S*)-4-(*p*-tolyl)-4-(tributylstannyl) buta-2,3-dien-1-yl ((*R*)-1-phenylethyl)carbamate (**2c'**)



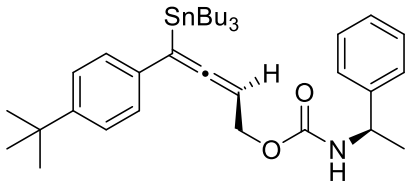
Colorless oil (94% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.39-7.35 (m, 5H), 7.16-7.11 (m, 4H), 5.18 (t, *J* = 7.2 Hz, 1H), 4.98-4.90 (m, 2H), 4.66-4.64 (m, 2H), 2.36 (s, 3H), 1.59-1.50 (m, 9H), 1.39-1.30 (m, 6H), 1.18-1.03 (m, 6H), 0.91 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 203.8, 155.6, 143.6, 136.1, 134.7, 129.3, 128.6, 127.9, 127.3, 126.0, 97.8, 80.4, 64.1, 50.6, 28.9, 27.2, 22.5, 21.1, 13.7, 11.1; **HRMS (M/Z, ESI)** Calcd. for $C_{32}H_{47}NO_2Sn$ [M+Na]: 620.2526, Found: 620.2535; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 8.16 min (major) and11.60 min (minor).

(*S*)-4-(4-(tert-butyl)phenyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2d**)



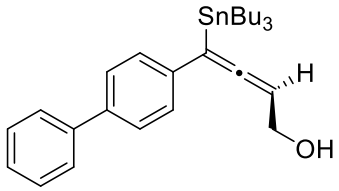
Colorless oil (62 mg, 63% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.36 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 5.26 (tt, *J* = 6.4, 6.8 Hz, 1H), 4.26-4.21 (m, 2H), 1.61-1.51 (m, 7H), 1.39-1.34 (m, 15H), 1.20-1.03 (m, 6H), 0.92 (t, *J* = 7.2 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 202.7, 149.4, 134.9, 127.5, 125.5, 98.6, 84.8, 61.7, 34.5, 31.3, 28.9, 27.2, 13.7, 11.1; **HRMS (M/Z, ESI)** Calcd. for $C_{26}H_{44}OSn$ [M+Na]: 515.2312, Found: 515.2323; Optical Rotation: $[\alpha]_D^{25}$ -19.7 (c 0.75, $CHCl_3$).The *ee* value of **2d** was determined by chiral HPLCanalysis after derivatization to **2d'**.

(*S*)-4-(4-(tert-butyl)phenyl)-4-(tributylstannyl)buta-2,3-dien-1-yl ((*R*)-1-phenylethyl)carbamate (**2d'**)



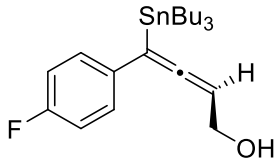
Colorless oil (94% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.36-7.30 (m, 7H), 7.22-7.20 (m, 2H), 5.20 (t, *J* = 7.3 Hz, 1H), 5.02-4.91 (m, 2H), 4.67-4.65 (m, 2H), 1.62-1.51 (m, 9H), 1.41-1.32 (m, 15H), 1.19-1.06 (m, 6H), 0.93 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 204.0, 155.7, 149.4, 143.7, 134.7, 128.6, 127.7, 127.3, 126.0, 125.5, 97.7, 80.5, 64.1, 50.6, 34.5, 31.4, 29.0, 27.2, 22.5, 13.7, 11.1; **HRMS (M/Z, ESI)** Calcd. for $C_{35}H_{53}NO_2Sn$ [M+H]: 640.3171, Found: 640.3180. **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 7.22 min (major) and 9.78 min (minor).

(*S*)-4-([1,1'-biphenyl]-4-yl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2e**)



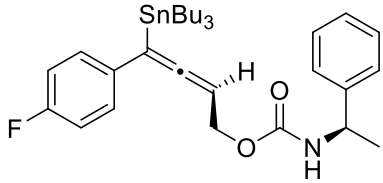
Colorless oil (96 mg, 94% yield, 94% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.64-7.62 (m, 2H), 7.57 (d, *J* = 8.3 Hz, 2H), 7.46 (t, *J* = 7.3 Hz, 2H), 7.38-7.32 (m, 3H), 5.30 (tt, *J* = 6.8, 6.8 Hz, 1H), 4.31-4.21 (m, 2H), 1.62-1.50 (m, 6H), 1.47-1.44 (t, *J* = 6.0 Hz, 1H, OH), 1.41-1.30 (m, 6H), 1.22-1.05 (m, 6H), 0.93 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 203.1, 140.8, 139.2, 137.2, 128.7, 128.3, 127.3, 127.2, 126.9, 98.7, 84.9, 61.6, 28.9, 27.2, 13.7, 11.2; **HRMS (M/Z, ESI)** Calcd. for $C_{28}H_{40}OSn$ [M+Na]: 535.1999, Found: 535.1997; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 100: 1, 1.0 ml/min, λ= 254 nm, retention time: 8.56 min (minor) and 10.17 min (major); Optical Rotation: $[\alpha]_D^{25}$ -0.33 (c 1.90, $CHCl_3$).

(*S*)-4-(4-fluorophenyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2f**)



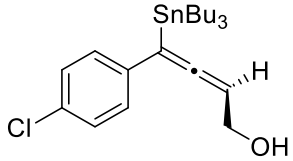
Colorless oil (74 mg, 81% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.21-7.18 (m, 2H), 7.00 (t, *J* = 8.6 Hz, 2H), 5.25 (tt, *J* = 6.6, 6.6Hz, 1H), 4.24-4.20 (m, 2H), 1.58-1.48 (m, 7H), 1.38-1.29 (m, 6H), 1.17-1.02 (m, 6H), 0.90 (t, *J* = 7.3Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 202.7, 161.6 (d, *J* = 243.9Hz), 134.17 (d, *J* = 3.2 Hz), 129.15 (d, *J* = 7.8 Hz), 115.4 (d, *J* = 21.6 Hz), 97.98, 84.9, 61.5,28.9, 27.2, 13.6, 11.1; **^{19}F NMR (376 MHz, $CDCl_3$):** δ = -116.5; **HRMS (M/Z, ESI)** Calcd. for $C_{22}H_{35}FOSn$ [M+Na]: 477.1592, Found: 477.1598; Optical Rotation: $[\alpha]_D^{25}$ -38.2 (c 3.86, $CHCl_3$).The *ee* value of **2f** was determined by chiral HPLC analysis after derivatization to **2f'**.

(*S*)-4-(4-fluorophenyl)-4-(tributylstannyl)buta-2,3-dien-1-yl ((*R*)-1-phenylethyl)carbamate (**2f'**)



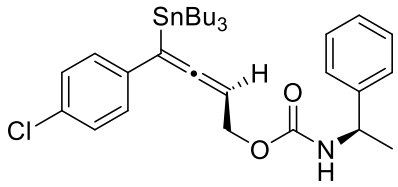
Colorless oil (94% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.37-7.26 (m, 5H), 7.20-7.16 (m, 2H), 7.01-6.97 (m, 2H), 5.17 (t, *J* = 7.2 Hz, 1H), 4.95-4.88 (m, 2H), 4.64-4.62 (m, 2H), 1.56-1.49 (m, 9H), 1.35-1.28 (m, 6H), 1.14-1.01 (m, 6H), 0.89 (t, *J* = 7.3 Hz, 9H); **^{13}NMR (101 MHz, $CDCl_3$):** δ = 203.9, 161.6 (d, *J* = 246.5 Hz), 155.6, 143.5, 133.8 (d, *J* = 3.2 Hz), 129.3 (d, *J* = 8.1 Hz), 128.6, 127.3, 125.9, 115.4 (d, *J* = 21.5 Hz), 91.2, 80.7, 63.8, 50.6, 28.9, 27.2, 22.5, 13.7, 11.1; **HRMS (M/Z, ESI)** Calcd. for $C_{31}H_{44}FNO_2Sn$ [M+Na]: 624.2270, Found: 624.2274; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 50: 1, 0.5 ml/min, λ= 254 nm, retention time: 13.27 min (major) and 15.05 min (minor).

(*S*)-4-(4-chlorophenyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2g**)



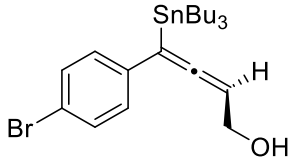
Colorless oil (80 mg, 85% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.27 (m, 2H), 7.16 (m, 2H), 5.26 (tt, *J* = 6.8, 6.8 Hz, 1H), 4.27-4.17 (m, 2H), 1.62-1.45 (m, 6H), 1.41-1.38 (t, *J* = 6 Hz, 1H, OH), 1.36-1.29 (m, 6H), 1.16-1.00 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 203.0, 136.9, 131.99, 128.99, 128.68, 98.1, 85.1, 61.4, 28.9, 27.2, 13.7, 11.2; **HRMS (M/Z, ESI)** Calcd. for $C_{22}H_{35}ClOSn$ [M+Na]: 493.1296, Found: 493.1284; Optical Rotation: $[\alpha]_D^{25}$ -16.8 (c 2.10, $CHCl_3$). The *ee* value of **2g** was determined by chiral HPLCanalysis after derivatization to **2g'**.

(*S*)-4-(4-chlorophenyl)-4-(tributylstannyl)buta-2,3-dien-1-yl ((*R*)-1-phenylethyl)carbamate (**2g')**



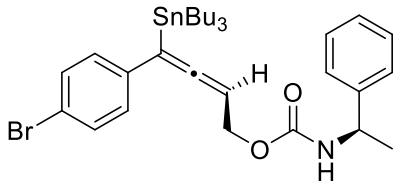
Colorless oil (89% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.36-7.25 (m, 7H), 7.17-7.15 (m, 2H), 5.19 (t, *J* = 7.2 Hz, 1H), 4.98-4.89 (m, 2H), 4.65-4.63 (m, 2H), 1.58-1.49 (m, 9H), 1.38-1.29 (m, 6H), 1.17-1.01(m, 6H), 0.91(t, *J* = 7.3 Hz, 9H); **^{13}NMR (101 MHz, $CDCl_3$):** δ = 204.2, 155.5, 143.6, 136.6, 132.8, 132.0, 129.1, 128.7, 127.3, 126.0, 97.3, 80.8, 63.7, 50.7, 28.9, 27.2, 22.5, 13.7, 11.2; **HRMS (M/Z, ESI)** Calcd. for $C_{31}H_{44}ClNO_2Sn$ [M+Na]: 640.1980, Found: 640.1984; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 8.67 min (major) and11.44 min (minor).

(*S*)-4-(4-bromophenyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2h**)



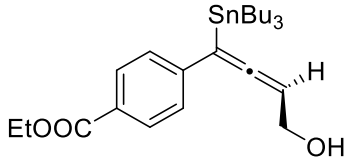
Colorless oil (86 mg, 86% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.43-7.41(d, *J* = 8.4 Hz, 2H), 7.11-7.10 (d, *J* = 8.4 Hz, 2H), 5.25 (tt, *J* = 6.4, 6.4 Hz, 1H), 4.27-4.17 (m, 2H), 1.60-1.50 (m, 6H), 1.43 (t, *J* = 6.0 Hz, 1H, OH), 1.38-1.29 (m, 6H), 1.18-1.00 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 203.0, 137.4, 131.6, 129.4, 120.0, 98.2, 61.4, 28.9, 27.2, 13.7, 11.2; **HRMS (M/Z, ESI)** Calcd. for $C_{22}H_{35}BrOSn$ [M+Na]: 537.0791, Found: 537.0780; Optical Rotation: $[\alpha]_D^{25}$ -11.6 (c 2.53, $CHCl_3$). The *ee* value of **2h** was determined by chiral HPLCanalysis after derivatization to **2h'**.

(*S*)-4-(4-bromophenyl)-4-(tributylstannyl)buta-2,3-dien-1-yl ((*R*)-1-phenylethyl)carbamate (**2h'**)



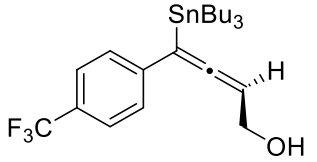
Colorless oil (90% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.43-7.29 (m, 7H), 7.11-7.09 (m, 2H), 5.18 (t, *J* = 7.2 Hz, 1H), 4.98-4.88 (m, 2H), 4.65-4.63 (m, 2H), 1.60-1.45 (m, 9H), 1.38-1.29 (m, 6H), 1.17-1.02 (m, 6H), 0.90 (t,*J* = 7.3 Hz, 9H); **^{13}NMR (101 MHz, $CDCl_3$):** δ = 204.2, 155.5, 143.5, 137.1, 131.6, 129.5, 128.6, 127.3, 125.9, 120.1, 97.4, 80.9, 63.6, 50.7, 28.9, 27.2, 22.5, 13.7, 11.2; **HRMS (M/Z, ESI)** Calcd. for $C_{31}H_{44}BrNO_2Sn$ [M+Na]: 684.1475, Found: 684.1455; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 9.06 min (major) and 12.37 min (minor).

ethyl (S)-4-(4-hydroxy-1-(tributylstannyl)buta-1,2-dien-1-yl)benzoate (**2i**)



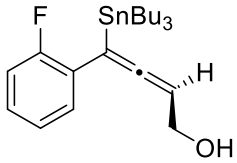
Colorless oil (79 mg, 78% yield, 68% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.98 (d, *J* = 8.3 Hz, 2H), 7.29-7.27 (m, 2H), 5.29 (tt, *J* = 6.7, 6.7 Hz, 1H), 4.39 (q,*J* = 7.1, 7.1 Hz, 2H), 4.29-4.19 (m, 2H), 1.58-1.50 (m, 6H), 1.43-1.39 (m, 4H), 1.36-1.26 (m, 6H), 1.18-1.01 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 203.8, 166.5, 143.5, 129.9, 128.2, 127.7, 98.7, 85.0, 61.4, 60.1, 28.9, 27.2, 14.4, 13.7, 11.2; **HRMS (M/Z, ESI)** Calcd. for $C_{25}H_{40}O_3Sn$ [M+Na]: 531.1897, Found: 531.1904; **HPLC analysis:** Daicel Chiralpak IC, hexane/iso-propanol = 50: 1, 1.0 ml/min,λ= 254 nm, retention time: 26.66 min (minor) and 32.94 min (major); Optical Rotation: $[\alpha]_D^{25}$ -4.27 (c 4.05, $CHCl_3$).

(*S*)-4-(tributylstannyl)-4-(4-(trifluoromethyl)phenyl)buta-2,3-dien-1-ol (**2j**)



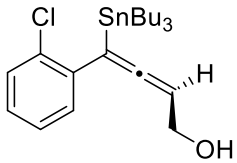
Colorless oil(74mg, 74% yield, 80% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.55 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1Hz, 2H), 5.29 (tt, *J* = 6.7, 6.7 Hz, 1H), 4.29-4.19 (m, 2H), 1.58-1.45 (m, 6H), 1.39-1.31 (m, 7H), 1.18-1.01 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 203.8, 142.6, 131.9, 128.2 (d, *J* = 30 Hz), 127.9 (t, *J* = 8 Hz), 126.3 (d, *J* = 130 Hz),125.4 (q, *J* = 3.7 Hz), 98.3, 85.1, 61.3, 28.9, 27.2, 13.6, 11.2; **^{19}F NMR (376 MHz, $CDCl_3$):** δ = -62.3; **HRMS (M/Z, ESI)** Calcd. for $C_{23}H_{35}F_3OSn$ [M+Na]: 527.1560, Found: 527.1553; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 500: 1, 1.0 ml/min, λ= 254 nm, retention time: 15.90 min (minor) and 19.04 min (major); Optical Rotation: $[\alpha]_D^{25}$ -19.7 (c 0.76, $CHCl_3$)

(*S*)-4-(2-fluorophenyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2k**)



Colorless oil(85mg, 94% yield, 90% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.28-7.23 (m, 1H), 7.20-7.14 (m, 1H), 7.11-7.07 (m, 1H), 7.05-7.00 (m, 1H), 5.21 (tt, *J* = 6.7, 6.6 Hz, 1H), 4.29-4.18 (m, 2H), 1.59-1.46 (m, 7H), 1.37-1.28 (m, 6H), 1.13-0.97 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 203.5, 159.6 (d, *J* = 244.1 Hz), 130.06 (d, *J* = 3.3 Hz), 127.7 (d, *J* = 8.1 Hz), 124.24 (d, *J* = 3.5 Hz), 115.47 (d, *J* = 22.0 Hz), 92.35 (d, *J* = 5.0 Hz), 61.5, 28.8, 27.2, 13.7, 11.3 (d, *J* = 3.2 Hz); **^{19}F NMR (376 MHz, $CDCl_3$):** δ = -115.0; **HRMS (M/Z, ESI)** Calcd. for $C_{22}H_{35}FOSn$ [M+Na]: 477.1592, Found: 477.1606; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 500: 1, 1.0 ml/min, λ= 254 nm, retention time: 17.75 min (minor) and 29.35 min (major); Optical Rotation: $[\alpha]_D^{25}$ -27.8 (c 0.89, $CHCl_3$).

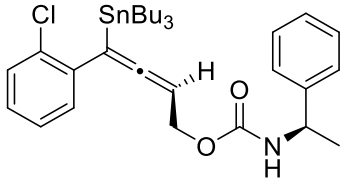
(*S*)-4-(2-chlorophenyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2l**)



Colorless oil (45 mg, 48% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.37-7.35 (m, 1H), 7.22-7.10

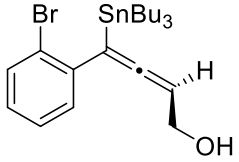
(m, 3H),5.10 (tt, *J* = 6.6, 6.4 Hz, 1H), 4.25-4.19 (m, 2H), 1.54-1.47 (m, 6H), 1.42 (t, *J* = 6.2 Hz, 1H, OH), 1.34-1.25 (m, 6H), 1.09-0.96 (m, 6H), 0.88 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 201.7, 138.1, 132.0, 129.7, 129.4, 127.1, 126.9, 97.4, 88.8, 61.4, 28.8, 27.2, 13.7, 11.8; **HRMS (M/Z, ESI)** Calcd. for $C_{22}H_{35}ClOSn$ [M+Na]: 493.1296, Found: 493.1286; Optical Rotation: $[\alpha]_D^{25}$ -34.6 (c 1.12, $CHCl_3$); The *ee* value of **2l** was determined by chiral HPLC analysis after derivatization to **2l'**.

(*S*)-4-(2-chlorophenyl)-4-(tributylstannyl)buta-2,3-dien-1-yl ((*R*)-1-phenylethyl)carbamate (**2l'**)



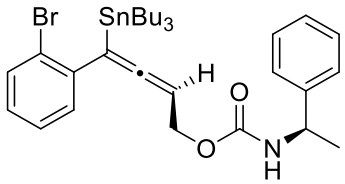
Colorless oil (83% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.37-7.27 (m, 6H), 7.23-7.11 (m, 3H), 5.09-4.89 (m, 3H), 4.68-4.66 (br, 2H), 1.60-1.45 (m, 9H), 1.36-1.27 (m, 6H),1.14-1.00 (m, 6H), 0.90 (t, *J* = 7.2 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 202.8, 155.6, 143.6, 137.7, 132.0, 129.9, 129.4, 128.6, 127.3, 127.1, 126.9, 126.0, 96.5, 78.5, 69.3, 50.6, 28.8, 27.2, 22.5, 13.7, 11.9; **HRMS (M/Z, ESI)** Calcd. for $C_{31}H_{44}ClNO_2Sn$ [M+Na]: 640.1980, Found: 640.1976; **HPLC analysis:** Daicel Chiralpak ODH-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 9.217 min (major) and 18.923 min (minor).

(*S*)-4-(2-bromophenyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2m**)



Colorless oil (93 mg, 90% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.55 (d, *J* = 7.3 Hz, 1H), 7.27-7.23 (m, 1H), 7.13-7.11 (m, 1H), 7.06-7.02 (m, 1H), 5.09 (tt, *J* = 6.6, 6.6 Hz, 1H), 4.27-4.19 (m, 2H), 1.57-1.42 (m, 7H), 1.36-1.25 (m, 6H), 1.12-0.97 (m, 6H), 0.88 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 201.3, 140.1, 132.6, 129.4, 127.4, 127.2, 122.5, 99.6, 88.9, 61.3, 28.8, 27.2, 13.7, 11.9; **HRMS (M/Z, ESI)** Calcd. for $C_{22}H_{35}BrOSn$ [M+Na]: 537.0791, Found: 537.0776; Optical Rotation: $[\alpha]_D^{25}$ -44.7 (c 0.93, $CHCl_3$); The *ee* value of **2m** was determined by chiral HPLC analysis after derivatization to **2m'**.

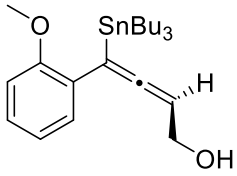
(*S*)-4-(2-bromophenyl)-4-(tributylstannyl)buta-2,3-dien-1-yl ((*R*)-1-phenylethyl)carbamate (**2m'**)



Colorless oil (82% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.57-7.55 (m, 1H), 7.36-7.23 (m, 6H), 7.16-7.14 (m, 1H), 7.06-7.02 (m, 1H), 5.05-4.89 (m, 3H), 4.69-4.67 (m, 2H), 1.57-1.46 (m, 9H), 1.36-1.27 (m, 6H), 1.13-1.00 (m, 6H), 0.90 (t, *J* = 7.2 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 202.3, 155.6, 143.6, 139.8, 132.5, 129.6, 128.6, 127.5, 127.3, 127.2, 126.0, 122.5, 98.7, 78.5, 68.3, 50.6, 28.8, 27.2, 22.5, 13.7, 12.0; **HRMS (M/Z, ESI)** Calcd. for $C_{31}H_{44}BrNO_2Sn$ [M+Na]: 684.1475, Found: 684.1480; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 50:

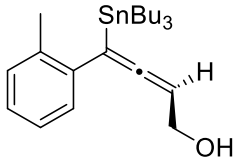
1, 1.0 ml/min, λ= 254 nm, retention time: 9.18 min (major) and 19.23 min (minor).

(*S*)-4-(2-methoxyphenyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2n**)



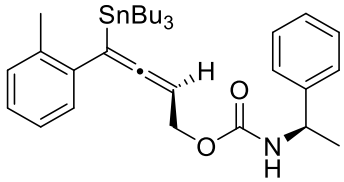
Colorless oil (69 mg, 74% yield, 97% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.25-7.23 (m, 1H), 7.20-7.16 (m, 1H), 6.95-6.91 (m, 1H), 6.84 (d, *J* = 8.2 Hz, 1H), 5.17 (tt, *J* = 6.5, 6.4 Hz, 1H), 4.22-4.21 (m, 2H), 3.82 (s, 3H), 1.54-1.40 (m, 7H), 1.33-1.28 (m, 6H), 1.13-0.95 (m, 6H), 0.88 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 202.5, 155.4, 129.4, 127.5, 127.0, 121.0, 110.1, 95.3, 83.5, 61.5, 54.95, 28.9, 27.3, 13.7, 11.5; **HRMS (M/Z, ESI)** Calcd. for $C_{23}H_{38}O_2Sn$ [M+Na]: 489.1791, Found: 489.1791; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 50: 1, 0.5 ml/min, λ= 254 nm, retention time: 10.26 min (minor) and 13.41 min (major); Optical Rotation: $[\alpha]_D^{25}$ -40.6 (c 0.34, $CHCl_3$)

(*S*)-4-(o-tolyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2o**)



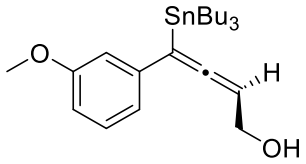
Colorless oil (55 mg, 62% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.16-7.06 (m, 3H), 6.99-6.97 (m, 1H), 4.99 (tt, *J* = 6.8, 6.8 Hz, 1H), 4.19 (t, *J* = 5.6 Hz, 2H), 2.35 (s, 3H), 1.57-1.44 (m, 6H), 1.33-1.28 (m, 7H), 1.05-0.99 (m, 6H), 0.91 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 200.6, 137.9, 134.8, 130.2, 127.96, 125.8, 97.2, 81.6, 61.9, 28.8, 27.2, 20.8, 13.7, 11.3; **HRMS (M/Z, ESI)** Calcd. for $C_{23}H_{38}OSn$ [M+Na]: 473.1842, Found: 473.1840; Optical Rotation: $[\alpha]_D^{25}$ -52.3 (c 1.25, $CHCl_3$); The *ee* value of **2o** was determined by chiral HPLC analysis after derivatization to **2o'**.

(*S*)-4-(o-tolyl)-4-(tributylstannyl)buta-2,3-dien-1-yl ((*R*)-1-phenylethyl)carbamate (**2o'**)



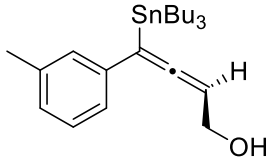
Colorless oil (91 % *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.39-7.28 (m, 5H), 7.19-7.09 (m, 3H), 7.01-6.99 (m, 1H), 4.99-4.89 (m, 3H), 4.69-4.63 (m, 2H), 2.36 (s, 3H), 1.59-1.42 (m, 9H), 1.37-1.28 (m, 6H), 1.12-0.97 (m, 6H), 0.93-0.89 (m, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 201.6, 155.7, 143.6, 137.5, 135.0, 130.3, 128.6, 128.0, 127.3, 126.0, 125.8, 96.4, 77.2, 64.3, 50.6, 28.8, 27.2, 22.5, 20.8, 13.7, 11.3; **HRMS (M/Z, ESI)** Calcd. for $C_{32}H_{47}NO_2Sn$ [M+Na]: 620.2526, Found: 620.2533; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 5.79 min (major) and 7.28 min (minor).

(*S*)-4-(3-methoxyphenyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2p**)



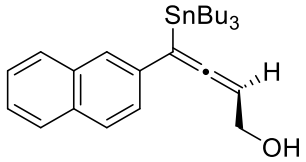
Colorless oil (84.5 mg, 91% yield, 95% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.23 (t, *J* = 8.0 Hz, 1H), 6.84-6.81 (m, 2H), 6.77-6.75 (m, 1H), 5.25 (tt, *J* = 6.7,6.6 Hz, 1H), 4.27-4.17 (m, 2H), 3.82 (s, 3H), 1.59-1.42 (m, 7H), 1.39-1.29 (m, 6H), 1.17-1.00 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ =202.8, 159.8, 139.7, 129.4, 120.4, 113.3, 111.96, 98.97, 84.8, 65.6, 55.2, 28.9, 27.2, 13.7, 11.2; **HRMS (M/Z, ESI)** Calcd. for $C_{23}H_{38}O_2Sn$ [M+Na]: 489.1791, Found: 489.1793; **HPLC analysis:** Daicel Chiralpak IC, hexane/iso-propanol = 50: 1, 0.5 ml/min, λ= 254 nm, retention time: 13.56 min (minor) and 15.25 min (major); Optical Rotation: $[\alpha]_D^{25}$ -24.9 (c 1.53, $CHCl_3$)

(*S*)-4-(m-tolyl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2q**)



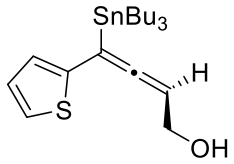
Colorless oil (66mg, 73% yield, 94% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.22-7.18 (m, 1H), 7.07 (s, 1H), 7.03-7.01 (m, 2H), 5.24 (tt, *J* = 6.6, 6.6 Hz, 1H), 4.27-4.18 (m, 2H), 2.35 (s, 3H), 1.61-1.45 (m, 6H), 1.40-1.28 (m, 7H), 1.17-1.00 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 202.6, 138.1, 138.0, 128.5, 128.4, 127.2, 124.9, 99.0, 84.7, 61.7, 28.9, 27.2, 21.4, 13.7, 11.2; **HRMS (M/Z, ESI)** Calcd. for $C_{23}H_{38}OSn$ [M+Na]: 473.1842, Found: 473.1841; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 500: 1, 0.5 ml/min, λ= 254 nm, retention time: 16.22 min (minor) and 23.57 min (major); Optical Rotation: $[\alpha]_D^{25}$ -30.7 (c 0.60, $CHCl_3$)

(*S*)-4-(naphthalen-2-yl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2r**)



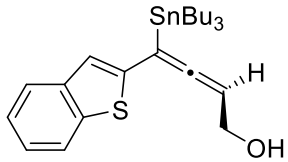
Colorless oil (87mg, 94% yield, 90% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.83-7.78 (m, 3H), 7.56 (br s, 1H), 7.52-7.43 (m, 3H), 5.34 (tt, *J* = 6.8, 6.8 Hz, 1H), 4.33-4.23 (m, 2H), 1.65-1.56 (m, 6H), 1.46 (t, *J* = 6.0 Hz, 1H, OH), 1.41-1.32 (m, 6H), 1.22-1.08 (m, 6H), 0.92 (t, *J* = 7.2 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 203.4, 135.6, 133.7, 133.2, 128.1, 127.7, 127.6, 126.4, 126.3, 126.1, 125.5, 99.3, 85.2, 61.6, 28.98, 27.2, 13.7, 11.3; **HRMS (M/Z, ESI)** Calcd. for $C_{26}H_{38}OSn$ [M+Na]: 509.1842, Found: 509.1852; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 100: 1, 1.0 ml/min, λ= 254 nm, retention time: 7.80 min (minor) and 9.21 min (major); Optical Rotation: $[\alpha]_D^{25}$ -9.1 (c 3.55, $CHCl_3$)

(S)-4-(thiophen-3-yl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2s**)



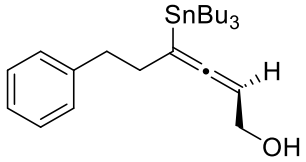
Colorless oil (75mg, 85% yield, 94% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.28-7.26 (m, 1H), 7.09-7.08 (m, 1H), 6.95 (d, *J* = 2.0 Hz, 1H), 5.22 (tt, *J* = 6.6, 6.6 Hz, 1H), 4.26-4.16 (m, 2H), 1.65-1.46 (m, 7H), 1.40-1.29 (m, 6H), 1.20-1.02 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ =203.2, 138.9, 127.5, 125.4, 120.7, 92.8, 84.6, 61.6, 28.9, 27.2, 13.7, 11.0; **HRMS (M/Z, ESI)** Calcd. for $C_{20}H_{34}SOSn$ [M+Na]: 465.1250, Found: 465.1244; **HPLC analysis:** Daicel Chiralpak IC, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 23.17 min (minor) and 25.82 min (major); Optical Rotation: $[\alpha]_D^{25}$ -35.3 (c 2.38, $CHCl_3$)

(*S*)-4-(benzo[b]thiophen-2-yl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2t**)



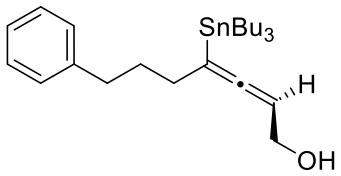
Colorless oil (90 mg, 91% yield, 92% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ =8.21-8.19 (m, 1H), 7.87-7.85 (m, 1H), 7.47-7.36 (m, 2H), 7.06 (s, 1H), 5.24 (tt, *J* = 6.6, 6.5 Hz, 1H), 4.34-4.25 (m, 2H), 1.60-1.48 (m, 6H), 1.43 (t, *J* = 6.0 Hz, 1H, OH), 1.39-1.30 (m, 6H), 1.20-1.03 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 202.4, 140.3, 138.2, 132.5, 124.5, 124.1, 123.3, 122.8, 122.4, 91.6, 83.4, 61.9, 28.9, 27.2, 13.7, 11.3; **HRMS (M/Z, ESI)** Calcd. for $C_{24}H_{36}SOSn$ [M+Na]: 515.1407, Found: 515.1413; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 5.58 min (minor) and 6.10 min (major); Optical Rotation: $[\alpha]_D^{25}$ -8.6 (c 5.20, $CHCl_3$)

(*S*)-6-phenyl-4-(tributylstannyl)hexa-2,3-dien-1-ol (**2u**)



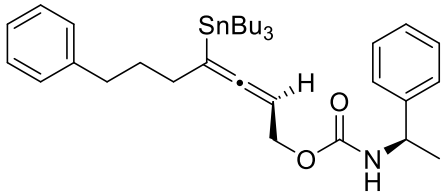
Colorless oil (74 mg, 79% yield, 94% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.34-7.28 (m, 2H), 7.23-7.21 (m, 3H), 4.95-4.84 (m, 1H), 4.08-3.92 (m, 2H), 2.87-2.74 (m, 2H), 2.50-2.39 (m, 2H), 1.61-1.46 (m, 6H), 1.39-1.30 (m, 6H), 1.07 (t, *J* = 6.0 Hz, 1H, OH), 1.01-0.91 (m, 15H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 200.8, 142.0, 128.5, 128.3, 125.9, 94.8, 83.3, 62.0, 35.9, 33.9, 29.0, 27.3, 13.7, 10.3; **HRMS (M/Z, ESI)** Calcd. for $C_{24}H_{40}OSn$ [M+Na]: 487.1999, Found: 487.1996; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 500: 1, 1.0 ml/min, λ= 254 nm, retention time: 11.65 min (minor) and 13.61 min (major); Optical Rotation: $[\alpha]_D^{25}$ -66.1 (c 1.76, $CHCl_3$)

(*S*)-7-phenyl-4-(tributylstannyl)hepta-2,3-dien-1-ol (**2v**)



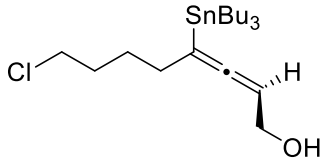
Colorless oil (78 mg, 82% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.32-7.28 (m, 2H), 7.22-7.19 (m, 2H), 4.97-4.88 (m, 1H), 4.12 (brs, 2H), 2.68 (d, J = 8 Hz, 2H), 2.19-2.15 (m, 2H), 1.84-1.77 (m, 2H), 1.60-1.45 (m, 6H), 1.39-1.30 (m, 7H), 1.04-0.91 (m, 15H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 200.4, 142.3, 128.5, 128.3, 125.7, 95.2, 82.9, 62.1, 35.4, 33.9, 33.5, 29.0, 27.3, 13.7, 10.3; **HRMS (M/Z, ESI)** Calcd. for $C_{25}H_{42}OSn$ [M+Na]: 501.2155, Found: 501.2142; Optical Rotation: $[\alpha]_D^{25}$ -57.2 (c 4.57, $CHCl_3$). The *ee* value of **2v** was determined by chiral HPLC analysis after derivatization to **2v'**.

(*S*)-7-phenyl-4-(tributylstannyl)hepta-2,3-dien-1-yl ((*R*)-1-phenylethyl)carbamate (**2v'**)



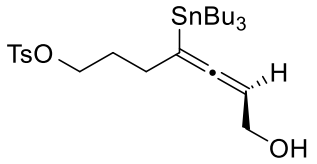
Colorless oil (96% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.38-7.26 (m, 7H), 7.22-7.18 (m, 3H), 4.90-4.82 (m, 3H), 4.56-4.54 (m, 2H), 2.68 (t, *J* = 7.6 Hz, 2H), 2.18-2.14 (m, 2H), 1.84-1.77 (m, 2H), 1.57-1.42 (m, 9H), 1.38-1.29 (m, 6H), 1.06-0.90 (m, 15H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 201.8, 155.7, 143.7, 142.4, 128.6, 128.5, 128.3, 127.3, 125.9, 125.7, 94.1, 78.3, 65.0, 50.6, 35.4, 31.6, 31.4, 29.0, 27.3, 22.5, 13.7, 10.3; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 250: 1, 1.0 ml/min, λ= 254 nm, retention time: 17.475 min (major) and 19.222 min (minor).

(*S*)-8-chloro-4-(tributylstannyl)octa-2,3-dien-1-ol (**2w**)



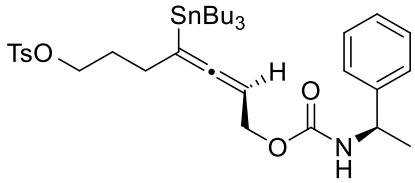
Colorless oil (75 mg, 83% yield, 88% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 4.96-4.84 (m, 1H), 4.14-4.04 (m, 2H), 3.56 (t, *J* = 6.8 Hz, 2H); 2.19-2.10 (m, 2H), 1.90-1.80 (m, 2H), 1.65-1.60 (m, 2H), 1.57-1.46 (m, 6H), 1.38-1.27 (m, 7H), 0.99-0.90 (m, 15H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 200.5, 94.9, 83.0, 62.1, 44.9, 32.1, 31.6, 29.0, 27.3, 26.9, 13.7, 10.3; **HRMS (M/Z, ESI)** Calcd. for $C_{20}H_{39}ClOSn$ [M+Na]: 473.1609, Found: 473.1607; **HPLC analysis:** Daicel Chiralpak IC, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 28.05 min (minor) and 29.35 min (major); Optical Rotation: $[\alpha]_D^{25}$ -67.2 (c 1.89, $CHCl_3$.

(*S*)-7-hydroxy-4-(tributylstannyl)hepta-4,5-dien-1-yl 4-methylbenzenesulfonate (**2x**)



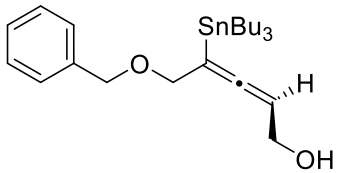
Colorless oil (103 mg, 90% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.81 (d, *J* = 8.2 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 4.89-4.86 (m, 1H), 4.10-4.03 (m, 4H), 2.47 (s, 3H), 2.13-2.10 (m, 2H), 1.89-1.80 (m, 2H), 1.58-1.41 (m, 7H), 1.36-1.28 (m, 6H), 1.08-0.86 (m, 15H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 200.4, 144.7, 133.2, 129.8, 127.9, 93.8, 83.7, 69.9, 61.9, 28.9, 28.6, 27.8, 27.3, 21.6, 13.7, 10.2; **HRMS (M/Z, ESI)** Calcd. for $C_{26}H_{44}O_4Sn$ [M+Na]: 595.1880, Found: 595.1919; Optical Rotation: $[\alpha]_D^{25}$ -54.9 (c 6.29, $CHCl_3$); The *ee* value of **2x** was determined by chiral HPLC analysis after derivatization to **2x'**.

(*S*)-7-((((R)-1-phenylethyl)carbamoyl)oxy)-4-(tributylstannyl)hepta-4,5-dien-1-yl-4-methylbenzen esulfonate (**2x'**)



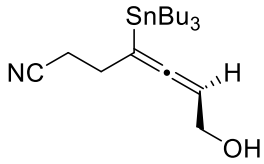
Colorless oil (92% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.81-7.78 (m, 2H), 7.36-7.26 (m, 7H), 5.11 (s, 1H), 4.85-4.78 (m, 2H), 4.49-4.41 (m, 2H), 4.11-4.08 (m, 2H), 2.46 (s, 3H), 2.12-2.08 (m, 2H), 1.84-1.82 (m, 2H), 1.56-1.41 (m, 9H), 1.35-1.26 (m, 6H), 1.01-0.86 (m, 15H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 201.5, 155.7, 144.7, 143.8, 133.2, 129.8, 128.6, 127.9, 127.2, 125.9, 93.1, 79.2, 70.0, 64.4, 50.7, 28.9, 28.5, 27.5, 27.2, 22.5, 21.6, 13.7, 10.2; **HRMS (M/Z, ESI)** Calcd. for $C_{35}H_{53}NO_5SSn$ [M+Na]: 742.2564, Found: 742.2584; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 20: 1, 1.0 ml/min, λ= 254 nm, retention time: 8.62 min (major) and 12.89 min (minor).

(*S*)-5-(benzyloxy)-4-(tributylstannyl)penta-2,3-dien-1-ol (**2y**)



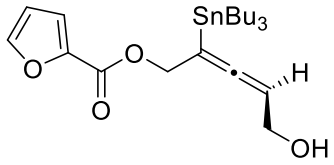
Colorless oil (75 mg, 78% yield, 95% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.38-7.30 (m, 5H), 5.06-4.95 (m, 1H), 4.53 (s, 2H), 4.19-4.11 (m, 4H), 1.61-1.48 (m, 6H), 1.43 (t, *J* = 6.2 Hz, 1H, OH), 1.38-1.27 (m, 6H), 1.07-0.97 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 200.1, 138.2, 128.3, 127.8, 127.6, 95.1, 83.6,72.1, 70.9, 61.7, 29.0, 27.3, 13.7, 10.6; **HRMS (M/Z, ESI)** Calcd. for $C_{24}H_{40}O_2Sn$ [M+Na]: 503.1948, Found: 503.1948; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 100: 1, 1.0 ml/min, λ= 254 nm, retention time: 8.75 min (minor) and 11.89 min (major); Optical Rotation: $[\alpha]_D^{25}$ -50.9 (c 2.12, $CHCl_3$).

(*S*)-7-hydroxy-4-(tributylstannyl)hepta-4,5-dienenitrile (**2z**)



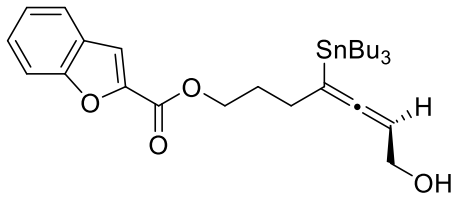
Colorless oil (80 mg, 71% yield, 85% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 5.13-5.04 (m, 1H), 4.18-4.12 (m, 2H), 2.60-2.52 (m, 2H), 2.49-2.33 (m, 2H), 1.59-1.44 (m, 6H), 1.38-1.27 (m, 6H), 1.08-1.00 (m, 6H), 0.92 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 200.8, 120.1, 92.5, 85.8, 61.7, 28.9, 27.5, 27.3, 17.0, 16.7, 10.3; **HRMS (M/Z, ESI)** Calcd. for $C_{19}H_{35}NOSn$ [M+Na]: 436.1638, Found: 436.1638; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 20: 1, 1.0 ml/min, λ= 254 nm, retention time: 13.70 min (minor) and 14.83 min (major); Optical Rotation: $[\alpha]_D^{25}$ -100.4 (c 1.14, $CHCl_3$).

(*S*)-5-hydroxy-2-(tributylstannyl)penta-2,3-dien-1-yl furan-2-carboxylate (**2aa**)



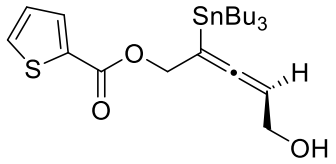
Colorless oil (54 mg, 53% yield, 90% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.60-7.59 (m, 1H), 7.21-7.20 (m, 1H), 6.54-6.53 (m, 1H), 5.12-5.01(m, 1H), 4.96-4.89 (m, 2H), 4.10 (t, *J* = 5.7 Hz, 2H), 1.62-1.45 (m, 7H), 1.36-1.27 (m, 6H), 1.11-0.96 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 201.5, 158.5, 146.4, 144.6, 118.1, 111.9, 92.7, 85.2, 65.7, 61.1, 28.9, 27.2, 13.6, 10.5; **HRMS (M/Z, ESI)** Calcd. for $C_{22}H_{36}O_4Sn$ [M+H]: 485.1708, Found: 535.1722; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 17.91 min (minor) and 20.87 min (major); Optical Rotation: $[\alpha]_D^{25}$ -91.8 (c 2.35, $CHCl_3$).

(*S*)-7-hydroxy-4-(tributylstannyl)hepta-4,5-dien-1-yl benzofuran-2-carboxylate (**2ab**)



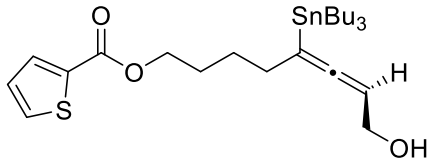
Colorless oil (80mg, 71% yield, 91% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.70 (d, *J* = 7.8 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.55 (s, 1H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.32 (t, *J* = 7.4 Hz, 1H), 5.00-4.90 (m, 1H), 4.52-4.39 (m, 2H), 4.13 (brs, 2H), 2.32-2.21 (m, 2H), 2.05-1.97 (m, 2H), 1.65 (brs, 1H, OH), 1.57-1.44 (m, 6H), 1.39-1.27 (m, 6H), 1.07-0.97(m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 200.6, 159.7, 155.7, 145.6, 127.6, 127.0, 123.8, 122.8, 113.9, 112.4, 94.1, 83.7, 64.8, 62.1, 29.0, 28.5, 28.4, 27.3, 13.7, 10.3; **HRMS (M/Z, ESI)** Calcd. for $C_{28}H_{42}O_2Sn$ [M+Na]: 585.2003, Found: 585.2007; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 20: 1, 1.0 ml/min, λ= 254 nm, retention time: 13.70 min (minor) and 14.83 min (major); Optical Rotation: $[\alpha]_D^{25}$ -53.6 (c 2.44, $CHCl_3$).

(*S*)-5-hydroxy-2-(tributylstannyl)penta-2,3-dien-1-yl thiophene-2-carboxylate (**2ac**)



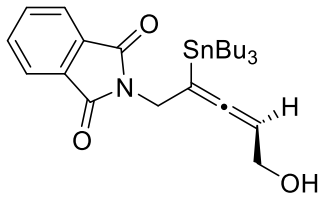
Colorless oil (60 mg, 60% yield, 88% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ =7.84-7.83 (m, 1H), 7.59-7.58 (m, 1H), 7.14-7.12 (m, 1H), 5.11-5.02 (m, 1H), 4.96-4.89 (m, 2H), 4.13-4.07 (m, 2H), 1.67 (brs, 1H, OH), 1.60-1.45 (m, 6H), 1.41-1.27 (m, 6H), 1.12-0.96 (m, 6H), 0.90 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 201.5, 162.0, 133.6, 132.5, 127.8, 92.8, 85.2, 65.96, 61.0, 28.9, 27.2, 13.7, 10.6; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 12.68 min (minor) and 15.89 min (major); Optical Rotation: $[\alpha]_D^{25}$ -63.1 (c 1.33, $CHCl_3$).

(*S*)-8-hydroxy-5-(tributylstannyl)octa-5,6-dien-1-yl thiophene-2-carboxylate (**2ad**)



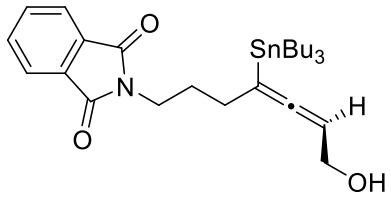
Colorless oil (76 mg, 70% yield, 91% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.83-7.81 (m, 1H), 7.57-7.56 (m, 1H), 7.13-7.11 (m, 1H), 4.95-4.86 (m, 1H), 4.34-4.31 (m, 2H), 4.11-4.08 (m, 2H), 2.22-2.16 (m, 2H), 1.84-1.77 (m, 2H), 1.64-1.59 (m, 2H), 1.54-1.48 (m, 6H), 1.43-1.40 (m, 1H, OH), 1.37-1.28 (m, 6H), 1.05-0.89 (m, 15H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 200.5, 162.4, 134.0, 133.3, 132.2, 127.7, 95.0, 83.0, 65.1, 62.1, 32.0, 29.0, 28.2, 27.3, 26.1, 13.7, 10.3; **HRMS (M/Z, ESI)** Calcd. for $C_{25}H_{42}O_3SSn$ [M+Na]: 565.1774, Found: 565.1778; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 12.81 min (minor) and 13.94 min (major); Optical Rotation: $[\alpha]_D^{25}$ -51.5 (c 1.93, $CHCl_3$).

(*S*)-2-(5-hydroxy-2-(tributylstannyl)penta-2,3-dien-1-yl)isoindoline-1,3-dione (**2ae**)



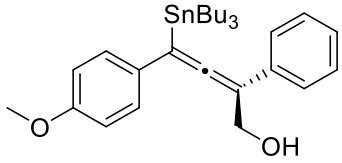
Colorless oil (68 mg, 66% yield, 92% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.87-7.85 (m, 2H), 7.74-7.72 (m, 2H), 4.96-4.91 (m, 1H), 4.40-4.33 (m, 2H), 3.94 (t, *J* = 6.4 Hz, 2H), 1.81 (t, *J* = 5.6Hz, 1H, OH), 1.60-1.47 (m, 6H), 1.36-1.25 (m, 6H), 1.11-0.98 (m, 6H), 0.89 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 201.2, 168.2, 134.0, 132.0, 123.3, 92.9, 86.7, 60.5, 40.1, 28.9, 27.2, 13.6, 10.4; **HRMS (M/Z, ESI)** Calcd. for $C_{27}H_{41}O_3NSn$ [M+Na]: 542.1693, Found: 542.1702; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 25.06 min (minor) and 36.44 min (major); Optical Rotation: $[\alpha]_D^{25}$ -153.1 (c 2.05, $CHCl_3$).

(*S*)-2-(7-hydroxy-4-(tributylstannyl)hepta-4,5-dien-1-yl)isoindoline-1,3-dione (**2af**)



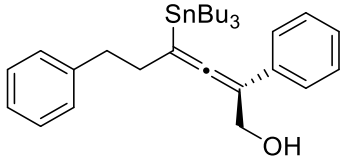
Colorless oil (83 mg, 73% yield, 92% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.87-7.85 (m, 2H), 7.75-7.72(m, 2H), 5.99-4.97 (m, 1H), 4.17-4.13 (m, 2H), 3.88-3.67 (m, 2H), 2.42-2.39 (m, 2H), 2.00-1.83 (m, 2H), 1.56-1.43 (m, 6H), 1.37-1.28 (m, 6H), 1.06-0.89 (m, 15H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 200.3, 168.5, 134.0, 132.1, 123.3, 93.6, 84.1, 62.3, 37.5, 29.2, 29.0, 28.0, 27.3, 13.7, 10.2; **HRMS (M/Z, ESI)** Calcd. for $C_{27}H_{41}O_3NSn$ [M+Na]: 570.2006, Found: 570.2009; **HPLC analysis:** Daicel Chiralpak OD-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 11.80 min (minor) and 12.81 min (major); Optical Rotation: $[\alpha]_D^{25}$ -67.1 (c 2.50, $CHCl_3$).

(*S*)-4-(4-methoxyphenyl)-2-phenyl-4-(tributylstannyl)buta-2,3-dien-1-ol (**2ag**)



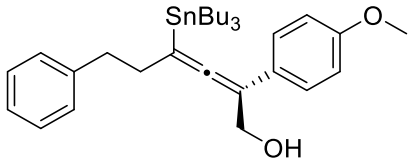
Colorless oil (61 mg, 56% yield, 84% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.49-7.47 (m, 2H), 7.37-7.33 (m, 2H), 7.28-7.19 (m, 3H), 6.90 (d, *J* = 8.6 Hz, 2H), 4.75-4.61 (m, 2H), 3.84 (s, 3H), 1.64-1.61 (t, *J* = 6 Hz, 1H, OH), 1.59-1.52 (m, 6H), 1.37-1.28 (m, 6H), 1.18-1.04 (m, 6H), 0.88 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 201.7, 158.7, 135.8, 129.4, 129.2, 128.6, 126.1, 125.5, 114.2, 101.9, 100.3, 62.4, 55.4, 29.0, 27.3, 13.7, 11.5; **HRMS (M/Z, ESI)** Calcd. for $C_{29}H_{42}O_2Sn$ [M+H]: 543.2280, Found: 543.2289; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 7.33 min (major) and 9.74 min (minor); Optical Rotation: $[\alpha]_D^{25}$ -57.6 (c 1.15, $CHCl_3$).

(*S*)-2,6-diphenyl-4-(tributylstannyl)hexa-2,3-dien-1-ol (**2ah**)



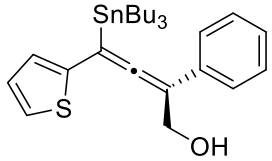
Colorless oil (58 mg, 54% yield, 91% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.42-7.40 (m, 2H), 7.37-7.33 (m, 4H), 7.28-7.26 (m, 2H), 7.22-7.18 (m, 2H), 4.55-4.38 (m, 2H), 2.97-2.88 (m, 2H), 2.69-2.65 (m, 2H), 1.65-1.50 (m, 6H), 1.41-1.31 (m, 6H), 1.25 (t, *J* = 6 Hz, 1H, OH), 1.13-1.00 (m, 6H), 0.94 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 198.9, 141.7, 136.6, 128.5, 128.4, 128.4, 126.0, 125.6, 125.4, 98.5, 98.3, 62.7, 36.1, 34.0, 29.1, 27.4, 13.7, 10.8; **HRMS (M/Z, ESI)** Calcd. for $C_{30}H_{44}OSn$ [M+Na]: 563.2312, Found: 563.2315; **HPLC analysis:** Daicel Chiralpak IC, hexane/iso-propanol = 500: 1, 1.0 ml/min, λ= 254 nm, retention time: 18.26 min (major) and 22.43 min (minor); Optical Rotation: $[\alpha]_D^{25}$ -7.7 (c 1.00, $CHCl_3$).

(*S*)-2-(4-methoxyphenyl)-6-phenyl-4-(tributylstannyl)hexa-2,3-dien-1-ol (2**ai**)



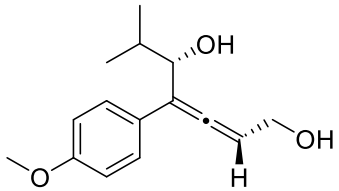
Colorless oil (57 mg, 50% yield, 89% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.33-7.27 (m, 4H), 7.24-7.21 (m, 3H), 6.87 (d, J = 8.8 Hz, 2H), 4.48-4.32 (m, 2H), 3.83 (s, 3H), 2.90-2.84 (m, 2H), 2.62-2.59 (m, 2H), 1.57-1.49 (m, 6H), 1.36-1.27 (m, 6H), 1.16 (t, *J* = 6 Hz, 1H, OH), 1.07-0.93 (m, 6H), 0.89 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 198.9, 157.8, 141.8, 128.7, 128.5, 128.3, 126.4, 125.9, 114.0, 98.4, 98.2, 62.9, 55.3, 36.0, 34.1, 29.1, 27.4, 13.7, 10.7; **HRMS (M/Z, ESI)** Calcd. for $C_{31}H_{46}O_2Sn$ [M+Na]: 593.2417, Found: 593.2413; **HPLC analysis:** Daicel Chiralpak IC, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 8.84 min (major) and 10.13 min (minor); Optical Rotation: $[\alpha]_D^{25}$ -108.3 (c 2.89, $CHCl_3$).

(*S*)-2-phenyl-4-(thiophen-3-yl)-4-(tributylstannyl)buta-2,3-dien-1-ol (**2aj**)



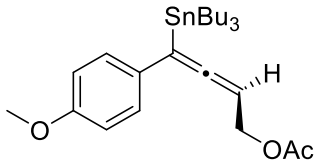
Colorless oil (64 mg, 62% yield, 82% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.46-7.44 (m, 2H), 7.36-7.28 (m, 3H), 7.21-7.18 (m, 1H), 7.11-7.10 (m, 1H), 7.00 (brs, 1H), 4.72-4.58 (m, 2H), 1.58-1.50 (m, 6H), 1.35-1.26 (m, 7H), 1.19-1.03 (m, 6H), 0.86 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 202.6, 138.1, 135.6, 128.6, 127.7, 126.2, 125.7, 125.6 121.4, 99.8, 96.3, 62.3, 29.0, 27.3, 13.6, 11.4; **HPLC analysis:** Daicel Chiralpak OZ-H, hexane/iso-propanol = 50: 1, 1.0 ml/min, λ= 254 nm, retention time: 5.30 min (major) and 7.50 min (minor); Optical Rotation: $[\alpha]_D^{25}$ -108.7 (c 0.54, $CHCl_3$).

(*3R,5S*)-4-(4-methoxyphenyl)-6-methylhepta-2,3-diene-1,5-diol (**3a**)



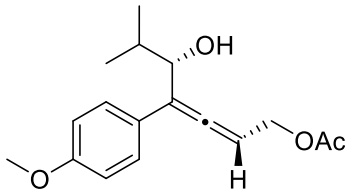
Colorless oil (47 mg, 63% yield, 96% *ee*, 4:1 dr). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.35 (d, *J* = 8.8 Hz, 2H), 6.89 (d, *J* = 8.8 Hz, 2H), 5.88-5.85 (m, 1H), 4.41-4.39 (m, 1H), 4.29-4.22 (m, 2H), 3.82 (s, 3H), 2.03 (brs, OH, 1H), 1.97-1.88 (m, 1H), 1.00 (d, *J* = 6.4 Hz, 3H), 0.95 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 201.4, 159.0, 128.3, 127.0, 114.0, 112,4, 97.2, 75.4, 60.7, 55.3, 31.9, 19.8, 16.5; **HRMS (M/Z, ESI)** Calcd. for $C_{15}H_{20}O_3$ [M+Na]: 271.1310, Found: 271.1308; **HPLC analysis:** Daicel Chiralpak IC, hexane/iso-propanol = 95: 5, 1.0 ml/min, λ= 254 nm, retention time: 21.66 min (major) and 37.38 min (minor).

(*S*)-4-(4-methoxyphenyl)-4-(tributylstannyl)buta-2,3-dien-1-yl acetate (**4aa**)



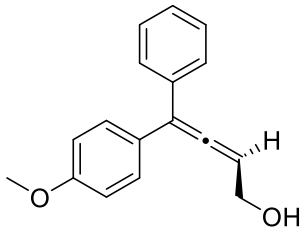
Colorless oil (99% yield). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.17 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 5.17 (tt, *J* = 6.8, 8.0 Hz, 1H), 4.67-4.62 (m, 2H), 3.82 (s, 3H), 2.09 (s, 3H), 1.64-1.45 (m, 6H), 1.39-1.30 (m, 6H), 1.18-1.01 (m, 6H), 0.91 (t, J = 7.6 Hz, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 203.5, 170.9, 158.4, 129.7, 129.0 (t, *J* = 9 Hz), 114.0, 97.6, 80.0, 63.8, 55.3, 28.9, 27.2, 21.1, 13.7, 11.1.

(*3R*, *5S*)-5-hydroxy-4-(4-methoxyphenyl)-6-methylhepta-2,3-dien-1-yl acetate (**4a**)



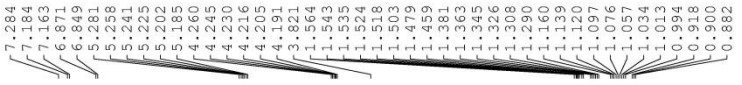
Colorless oil (56 mg, 55% yield, 96% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.32 (d, *J* = 8.8 Hz, 2H), 6.89 (d, *J* = 8.8 Hz, 2H), 5.81-5.77 (m, 1H), 4.76-4.66 (m, 2H), 4.42-4.39 (m, 1H), 3.82 (s, 3H), 2.11 (s, 3H), 1.96 (d, *J* = 7.2 Hz, OH, 1H), 1.93-1.87 (m, 1H), 1.01 (d, *J* = 6.8 Hz, 3H), 0.93 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 203.1, 171.1, 159.1, 128.3, 126.7, 114.1, 112,4, 92.7, 75.1, 62.4, 55.3, 31.8, 21.0, 19.8, 16.1; **HRMS (M/Z, ESI)** Calcd. for $C_{17}H_{22}O_4$ [M+Na]: 313.1416, Found: 313.1412; **HPLC analysis:** Daicel Chiralpak AS-H, hexane/iso-propanol = 95: 5, 1.0 ml/min, λ= 254 nm, retention time: 10.77 min (minor) and 11.62 min (major); Optical Rotation: $[\alpha]_D^{25}$ -62.7 (c 2.17, $CHCl_3$).

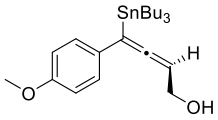
(*R*)-4-(4-methoxyphenyl)-4-phenylbuta-2,3-dien-1-ol (**5a**)



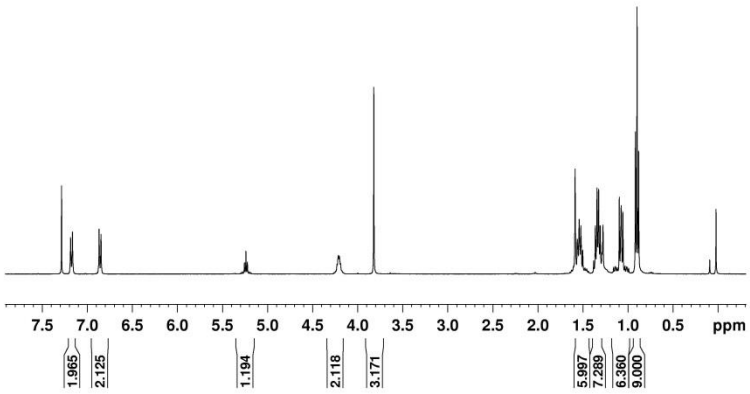
Colorless oil (47 mg, 53% yield, 60% *ee*). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.38-7.36 (m, 4H), 7.32-7.28 (m, 3H), 6.92-6.90 (m, 2H), 5.90 (t, *J* = 6 Hz, 1H), 4.32 (t, J = 6.0 Hz, 2H), 3.85 (s, 3H), 1.67 (t, *J* = 6.4 Hz, OH, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ = 204.0, 159.2, 136.6, 129.7, 128.5, 128.4, 127.5, 113.9, 112.2, 94.9, 60.8, 55.3; **HPLC analysis:** Daicel Chiralpak OJ-H, hexane/iso-propanol = 90: 10, 1.0 ml/min, λ= 254 nm, retention time: 18.53 min (major) and 23.84 min (minor).

11.NMR Spectra and HPLC chromatograms

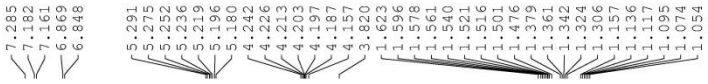


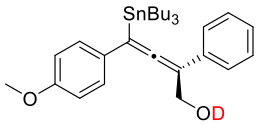


2a

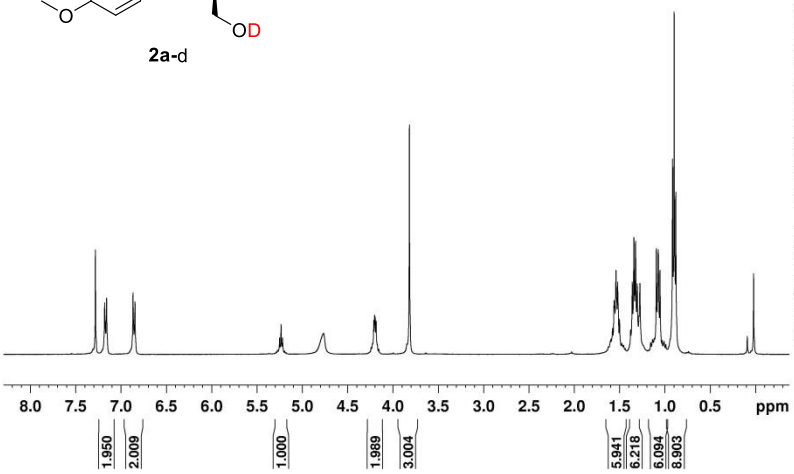



```
NAME          yjl-hk-259-1
EXPNO                   10
PROCNO                   1
Date_             20200902
Time                 17.15
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                       4
DS                       0
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                   78.29
DW                  62.400 usec
DE                    6.50 usec
TE                     0.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                   1H
P1                   9.99 usec
SI                  65536
SF             400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

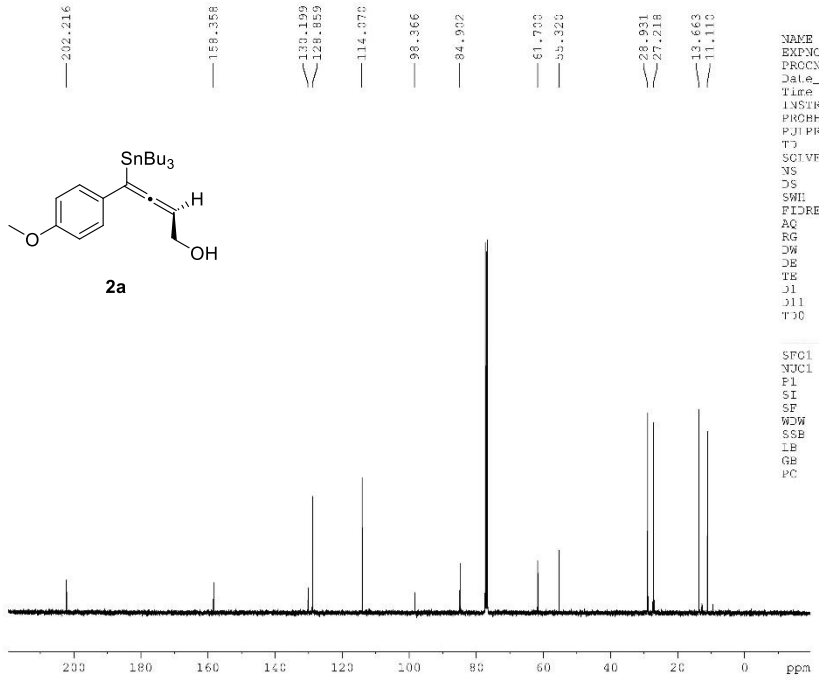




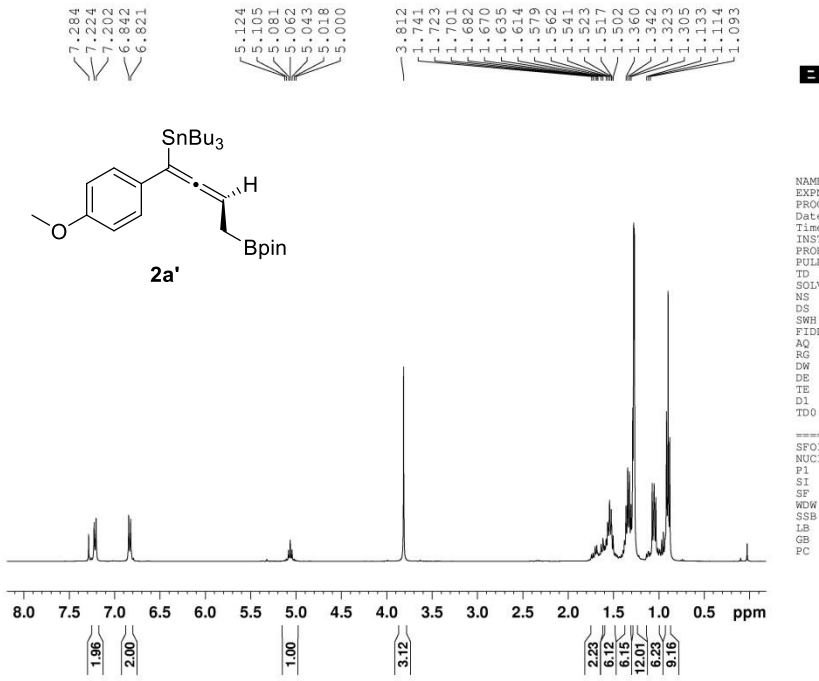
2a-d



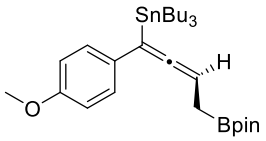

```
NAME          yjl-hk-259-1-d
EXPNO                   10
PROCNO                   1
Date_             20200902
Time                 17.19
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      16
DS                       0
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                   78.29
DW                  62.400 usec
DE                    6.50 usec
TE                     0.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                   1H
P1                   9.99 usec
SI                  65536
SF             400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME          yjl-hk-259-c
EXPNO                   11
PROCNO                   1
Date_             20181012
Time                 19.38
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      400
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631988 sec
RG                   197.54
DW                   20.800 usec
DE                    6.50 usec
TE                  298.9 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                   13C
P1                    9.31 usec
SI                   32768
SF            100.6127685 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

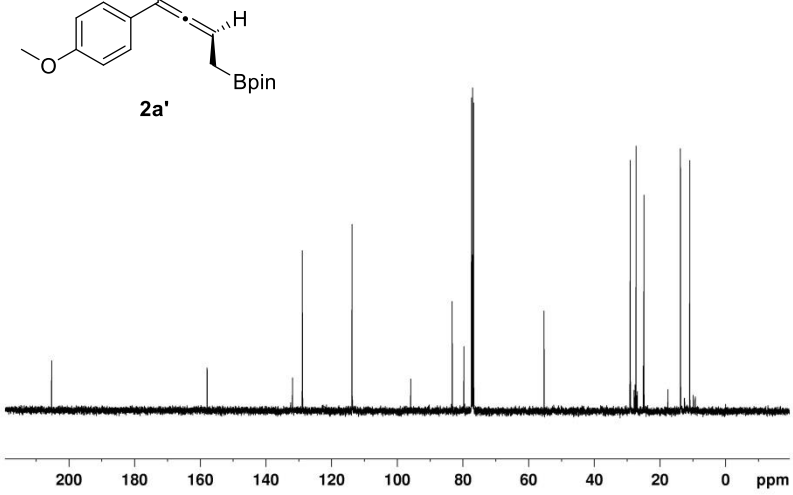



```
NAME          yjl-hk-529-h
EXPNO                   10
PROCNO                   1
Date_             20181204
Time                 12.58
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        4
DS                        0
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894966 sec
RG                   30.81
DW                   62.400 usec
DE                    6.50 usec
TE                  295.1 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                    9.99 usec
SI                   65536
SF            400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



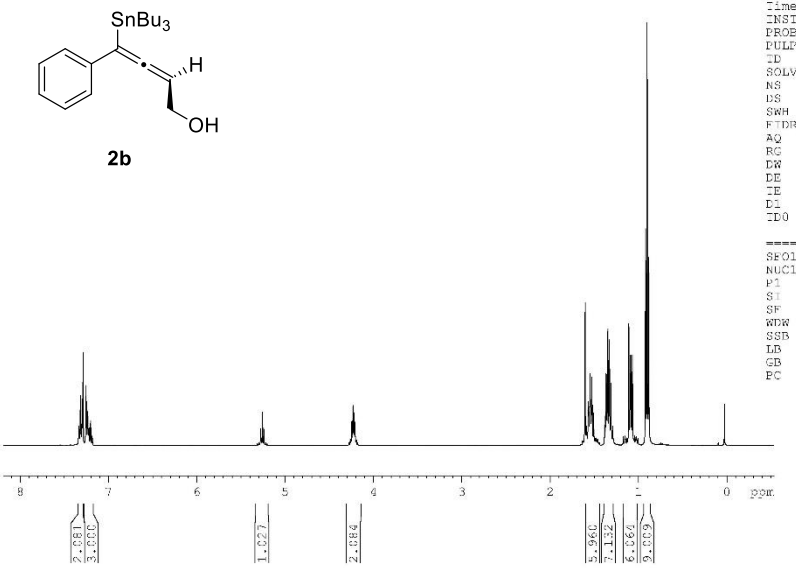
2a'

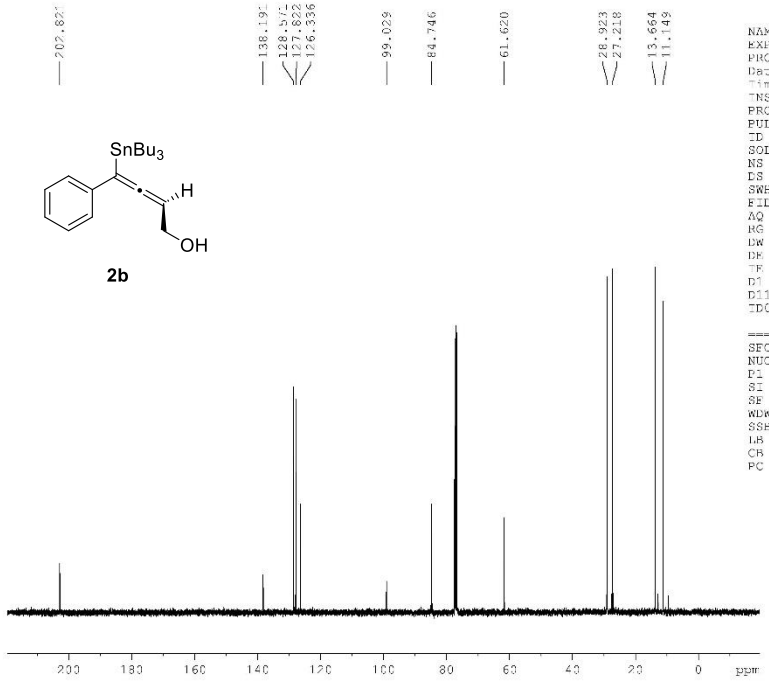
```
NAME          yjl-hk-529-c
EXPNO                   11
PROCNO                   1
Date_             20181204
Time                 13.12
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                    65536
SOLVENT             CDCl3
NS                      218
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                   197.54
DW                  20.800 use
DE                   6.50 use
TE                  295.7 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 =======
SFO1            100.6228293 MHz
NUC1                    13C
P1                   9.31 use
SI                     32768
SF              100.6127685 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



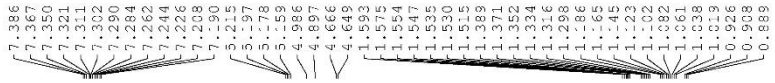
2b

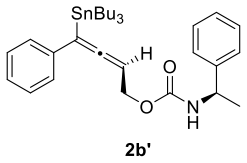
```
NAME          yjl-hk-199-h
EXPNO                   10
PROCNO                   1
Date_             20180918
Time                 17.51
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG          zg30
TD                    65536
SOLVENT             CDCl3
NS                        4
DS                        0
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894966 sec
RG                   63.21
DW                  62.400 usec
DE                   6.50 usec
TE                  297.2 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 =======
SFO1            400.1324710 MHz
NUC1                    1H
P1                   9.99 usec
SI                     65536
SF              400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



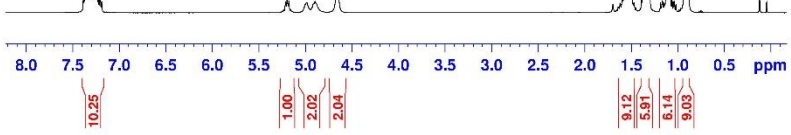


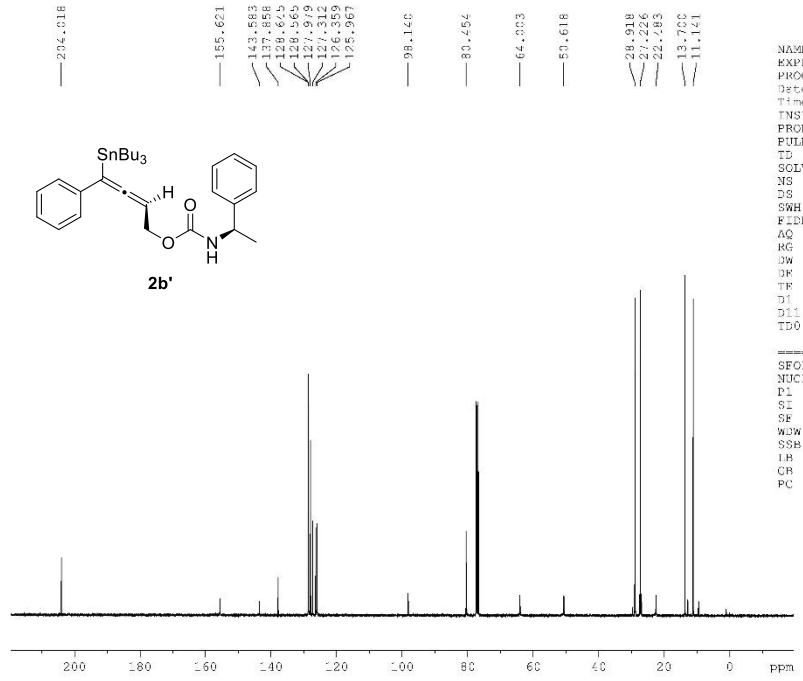

```
NAME          yjl-hk-199-c
EXPNO                   21
PROCNO                   1
Date_             20180921
Time                 18.31
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     256
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                  197.54
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                   13C
P1                   9.31 usec
SI                  32768
SF           100.6127685 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```



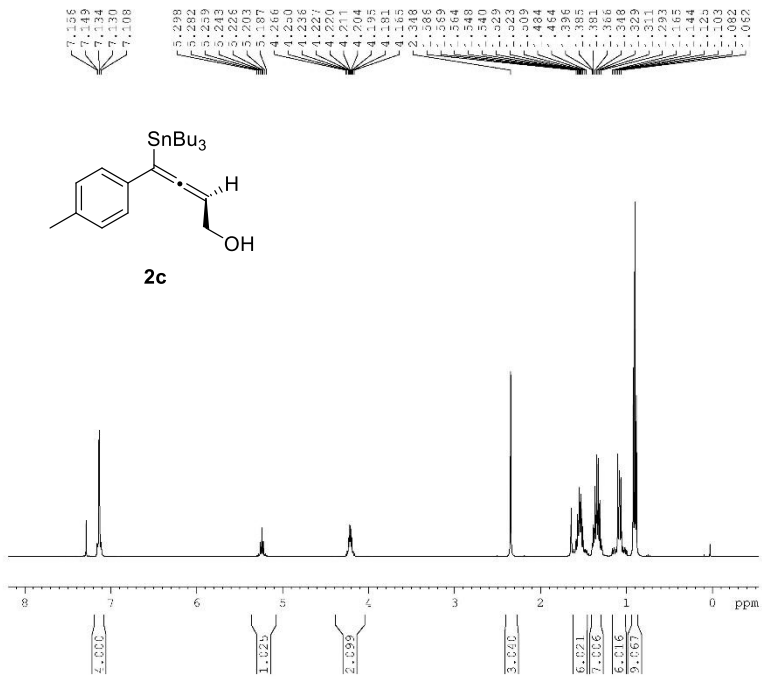



```
NAME          yjl-hk-502-c-1
EXPNO                   10
PROCNO                   1
Date_             20181119
Time                 20.59
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                   65536
SOLVENT              CDCl3
NS                       4
DS                       0
SWH               8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                   19.81
DW                62.400 usec
DE                 6.50 usec
TE                295.0 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                    1H
P1                   9.99 usec
SI                  65536
SF           400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

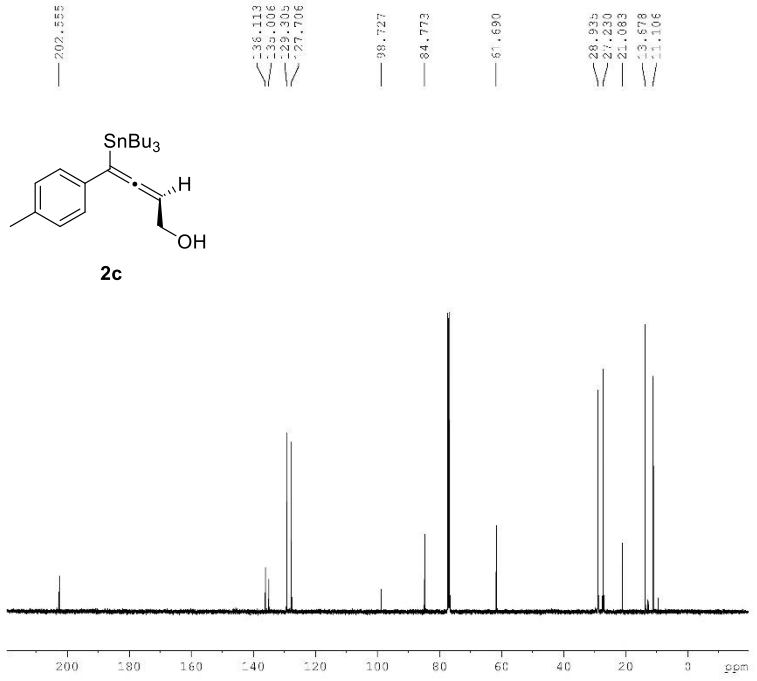




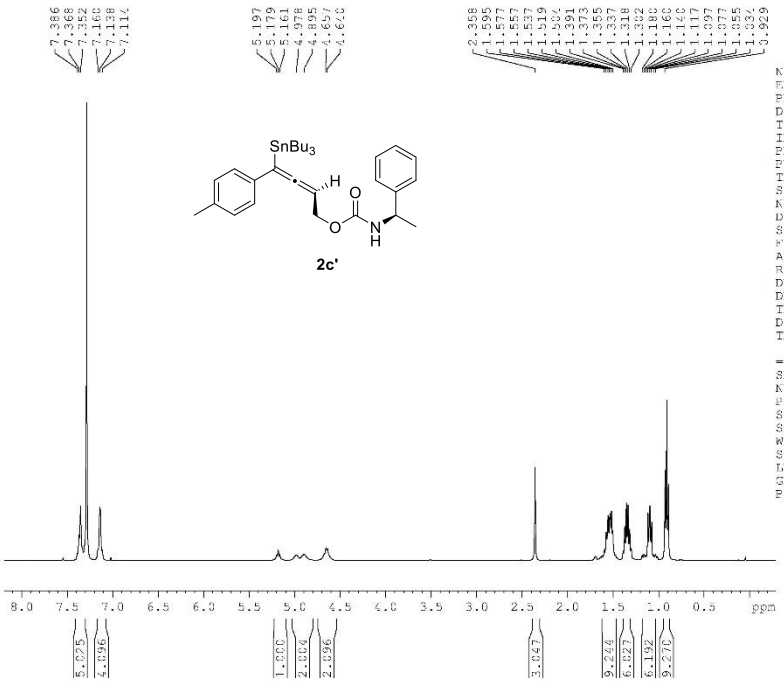

```
NAME        yjl-hk-502-c-1
EXPNO               11
PROCNO               1
Date_         20181119
Time             21.17
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 714
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG               197.54
DW               20.800 usec
DE                6.50 usec
TE               295.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1               13C
P1                9.31 usec
SI               32768
SF          100.6127685 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```



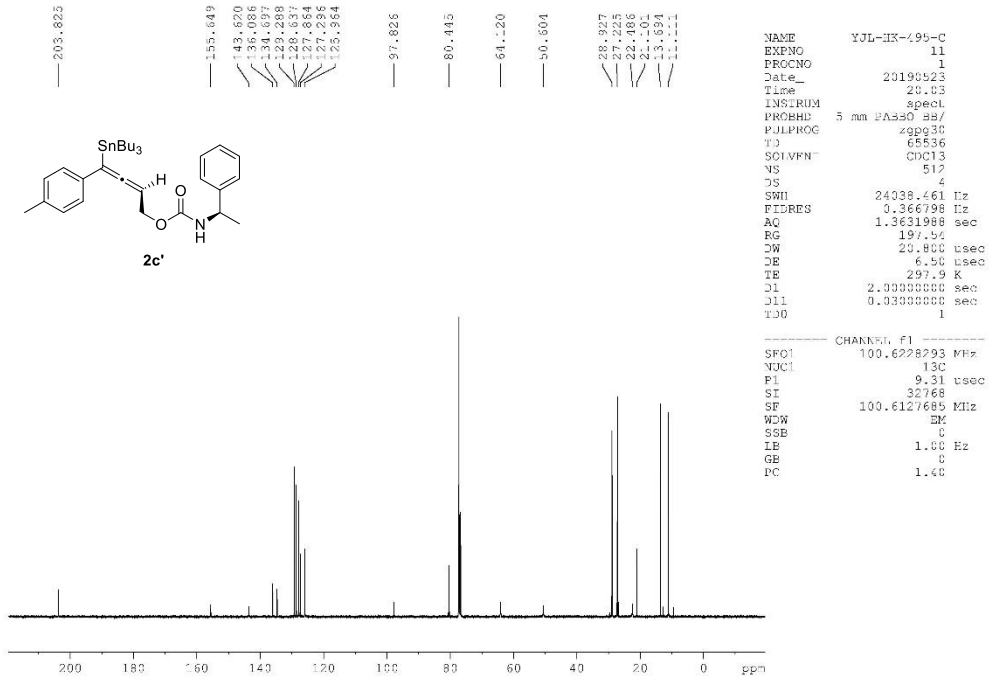

```
NAME        yjl-hk-183-h
EXPNO               10
PROCNO               1
Date_         20180914
Time             23.58
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zg30
TD               65536
SOLVENT          CDCl3
NS                   4
DS                   0
SWH          8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG               30.81
DW               62.400 usec
DE                6.50 usec
TE               296.6 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1               1H
P1                9.99 usec
SI               65536
SF          400.1300000 MHz
WDW                EM
SSB                 0
LB                0.30 Hz
GB                  0
PC                1.00
```

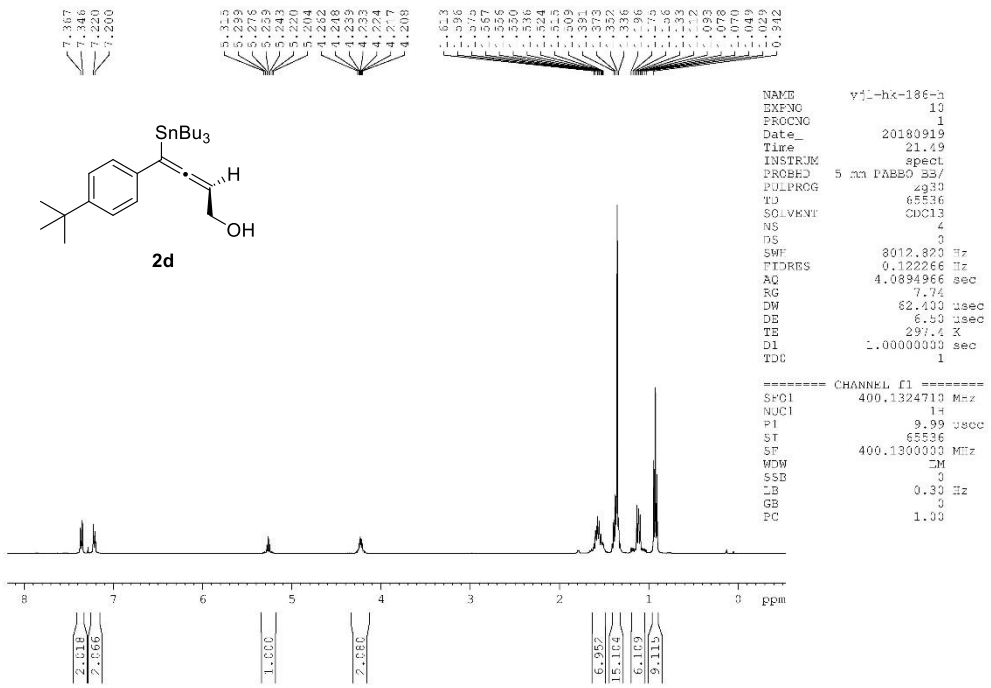


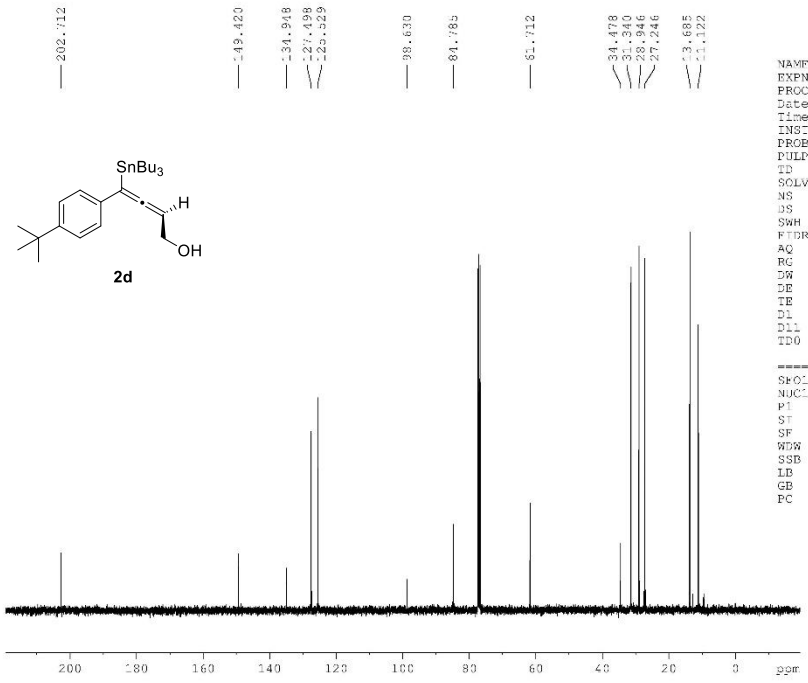

```
NAME          yjl-hk-183-c
EXPNO                   11
PROCNO                   1
Date_          20180915
Time                 0.28
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     512
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                  197.54
DW                  20.800 usec
DE                   6.50 usec
TE                  297.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                  13C
P1                   9.31 usec
SI                  32768
SF           100.6127685 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```



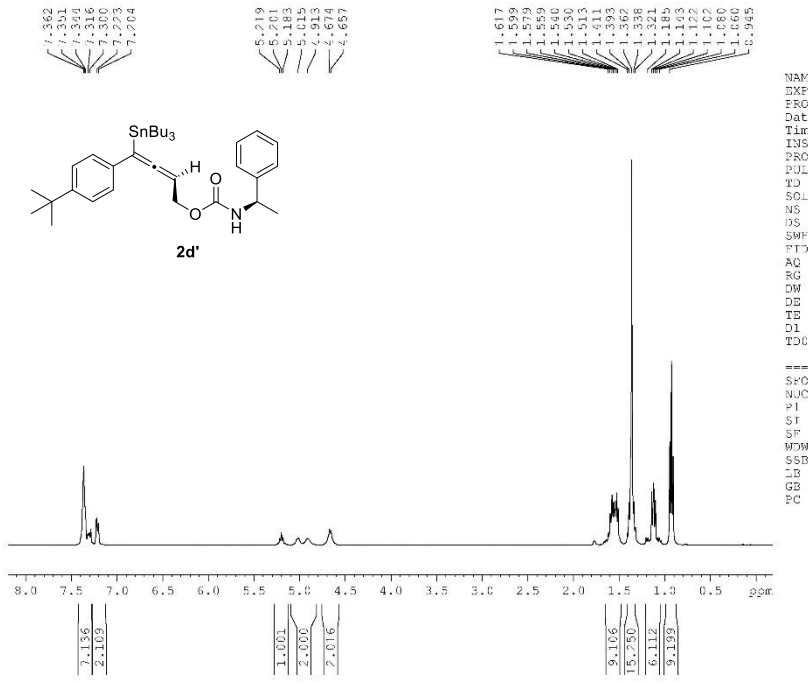

```
NAME          YJL-HK-495-H
EXPNO                   10
PROCNO                   1
Date           20190523
Time                19.32
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                  65536
SOLVENT             CDCl3
NS                      4
DS                      0
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894965 sec
RG                  17.39
DW                  62.400 usec
DE                   6.50 usec
TE                  297.2 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                   9.99 usec
SI                  65536
SF           400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```


203.823
155.649
143.620
136.086
134.697
129.288
128.637
127.854
127.296
125.954
97.826
80.443
64.520
50.604
28.927
27.225
22.486
21.101
13.694
SnBu3
H
O
O
N
H
2c'
NAME YJL-HK-495-C
EXPNO 11
PROCNO 1
Date_ 20190523
Time 20.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.56
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

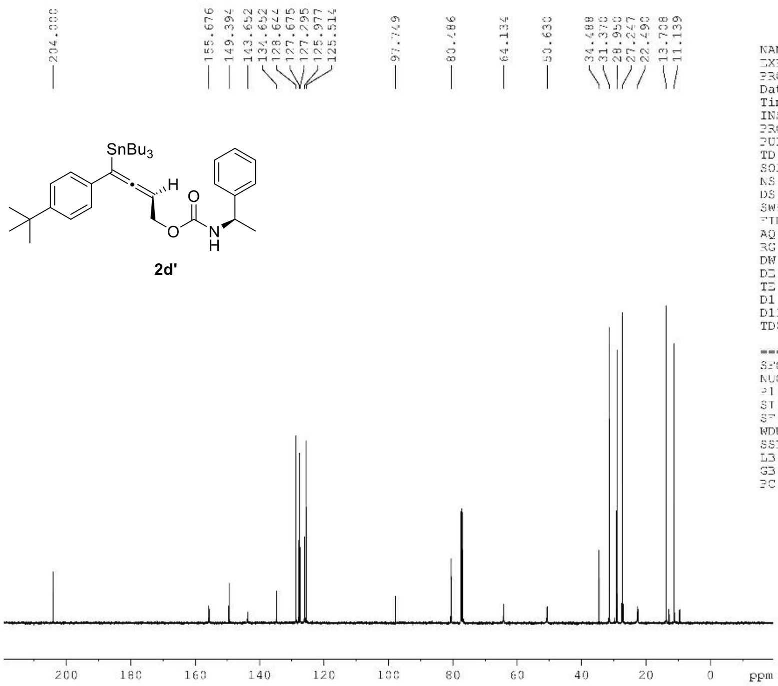

7.367
7.346
7.220
7.200
5.315
5.299
5.276
5.259
5.243
5.220
5.204
4.262
4.248
4.239
4.233
4.224
4.217
4.208
SnBu3
H
OH
2d
NAME yjl-hk-186-h
EXPNO 10
PROCNO 1
Date_ 20180919
Time 21.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 7.74
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8
7
6
5
4
3
2
1
0
ppm
2.618
2.866
1.000
2.660
6.965
15.164
6.169
9.115




```
NAME          yjl-hk-186-c
EXPNO                   10
PROCNO                   1
Date_             20180327
Time                 20.41
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    200
DS                      4
SWH             24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                 197.56
DW                 20.800 use
DE                  6.50 use
TE                296.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1

======== CHANNEL f1 =======
SFO1         100.6228293 MHz
NUC1                  13C
P1                   9.31 use
SI                  32768
SF           100.6127685 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

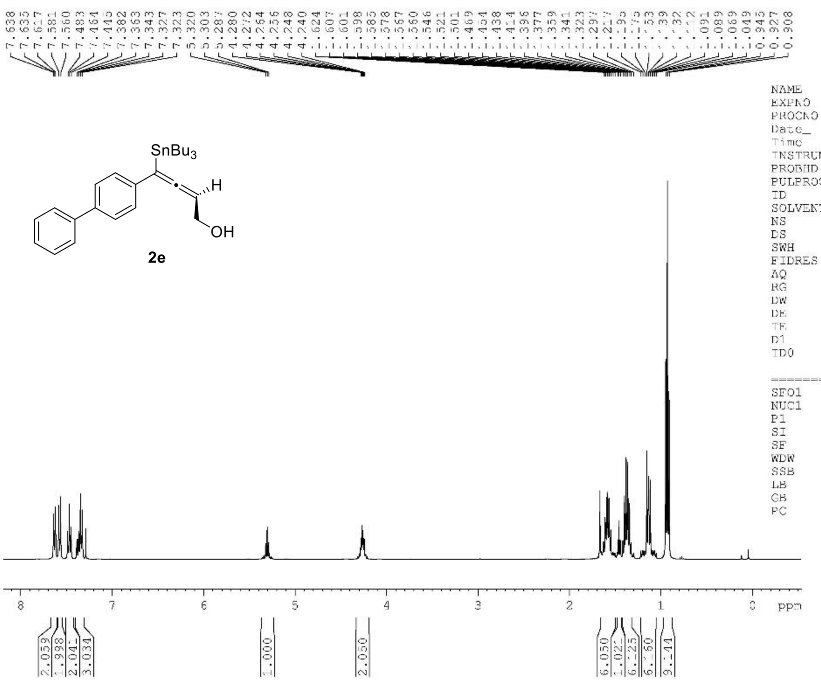



```
NAME          YJL-HK-499-H
EXPNO                   20
PROCNO                   1
Date_             20190612
Time                 16.56
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                  65536
SOLVENT             CDCl3
NS                      4
DS                      0
SWH              8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894966 sec
RG                   8.85
DW                 62.400 use
DE                  6.50 use
TE                297.9 K
D1           1.00000000 sec
TD0                     1

======== CHANNEL f1 =======
SFO1         400.1324710 MHz
NUC1                   1H
P1                   9.99 use
SI                  65536
SF           400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



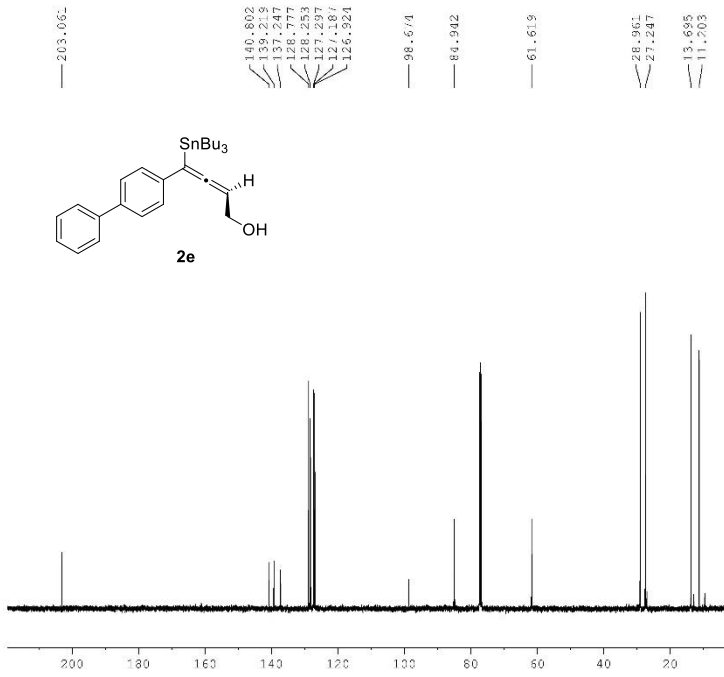
2d'

NAME	YCL-HK-499-C	
EXPNO	21	
PROCNO	1	
Date_	20190612	
Time	17.19	
INSTRUM	spect	
PROBHD	5 mm PABBO BB/	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	398	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	197.54	
DW	20.800	usec
DE	6.50	usec
TE	298.6	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
SFO1	100.6228293	MHz
NUC1	13C	
P1	9.31	usec
SI	32768	
SF	100.6127685	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

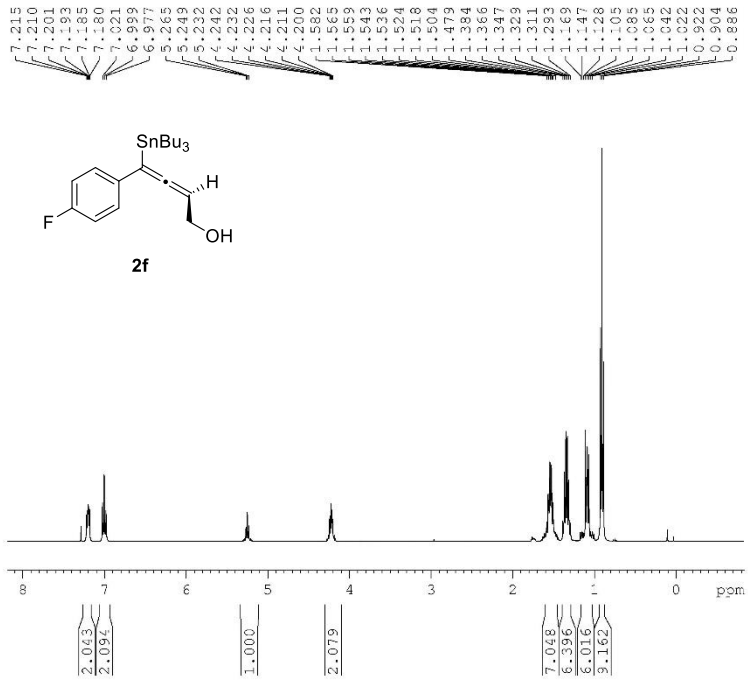


2e

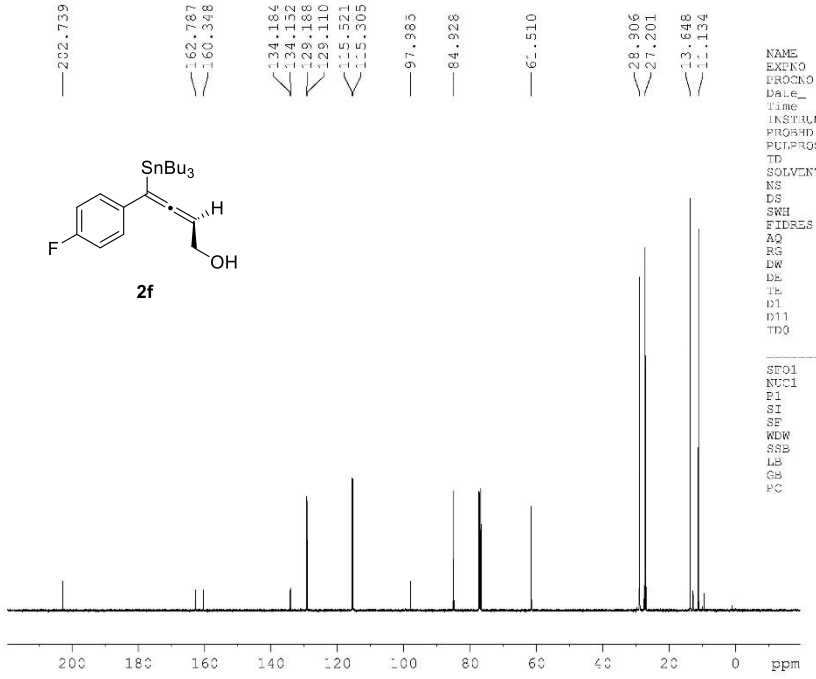
NAME	yjl-hk-253-h	
EXPNO	10	
PROCNO	1	
Date_	20180920	
Time	18.27	
INSTRUM	spect	
PROBHD	5 mm PABBO BB/	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	4	
DS	0	
SWH	8012.820	Hz
FIDRES	0.122266	Hz
AQ	4.0894966	sec
RG	30.81	
DW	62.400	usec
DE	6.50	usec
TE	297.5	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
SFO1	400.1324710	MHz
NUC1	1H	
P1	9.99	usec
SI	65536	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	




```
NAME          yjl-hk-253-c
EXPNO                   11
PROCNO                   1
Date_         20180920
Time                 18.39
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT              CDCl3
NS                     200
DS                       4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  197.54
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                 13C
P1                  9.31 usec
SI                 32768
SF           100.6127686 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

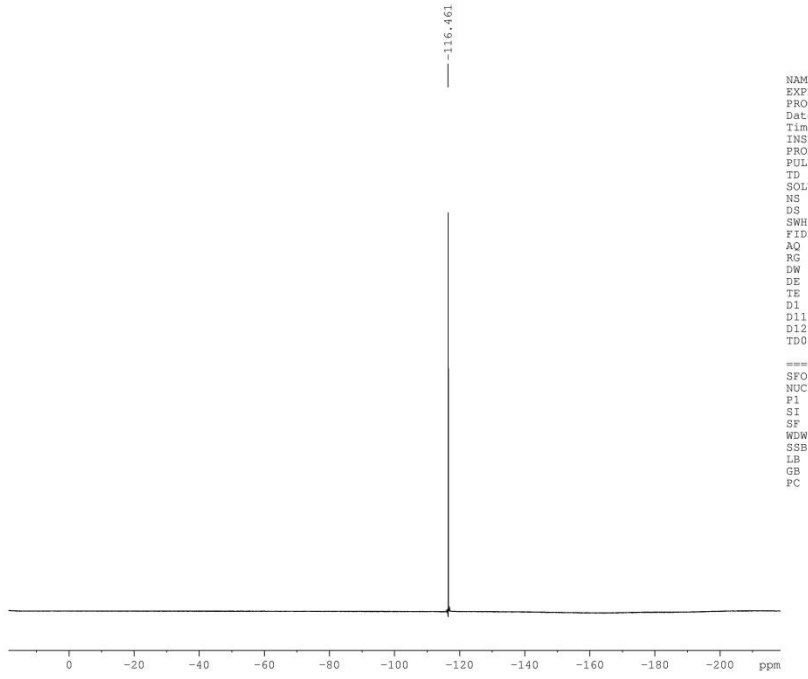



```
NAME          YJL HK 185 H
EXPNO                   10
PROCNO                   1
Date_         20180919
Time                 21.15
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                    65536
SOLVENT              CDCl3
NS                       4
DS                       0
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG                  75.46
DW                62.400 usec
DE                 6.50 usec
TE                297.5 K
D1            1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                  9.99 usec
SI                 65536
SF           400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

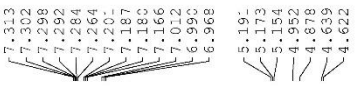


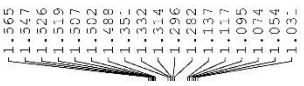
2f

```
NAME          yjl-hk-185-c
EXPNO                   11
PROCNO                   1
Date_           20180919
Time                 21.45
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    522
DS                      4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                197.54
DW                20.800 usec
DE                 6.50 usec
TE                297.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1               13C
P1                9.30 usec
SI                32768
SF          100.6127685 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

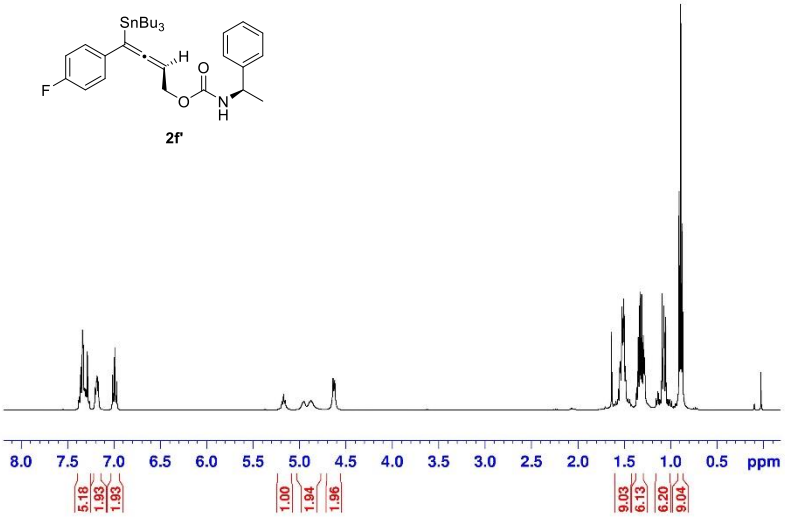



```
NAME          yjl-hk-185-f
EXPNO                   10
PROCNO                   1
Date_           20200916
Time                 18.55
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG       zgfhigqn.2
TD                 131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH           89285.711 Hz
FIDRES         0.681196 Hz
AQ            0.7340532 sec
RG                197.54
DW                 5.600 usec
DE                 6.50 usec
TE                297.5 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1        376.4607164 MHz
NUC1               19F
P1                14.00 usec
SI                65536
SF          376.4983662 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



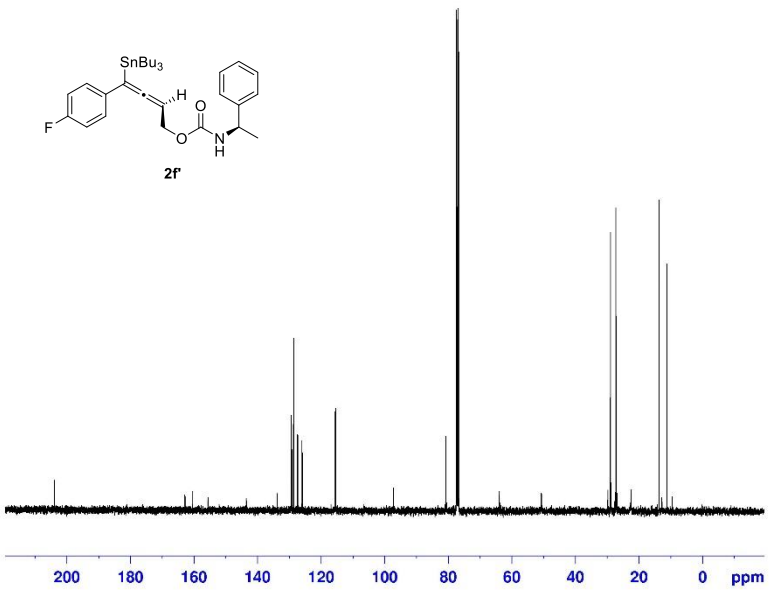


2f'

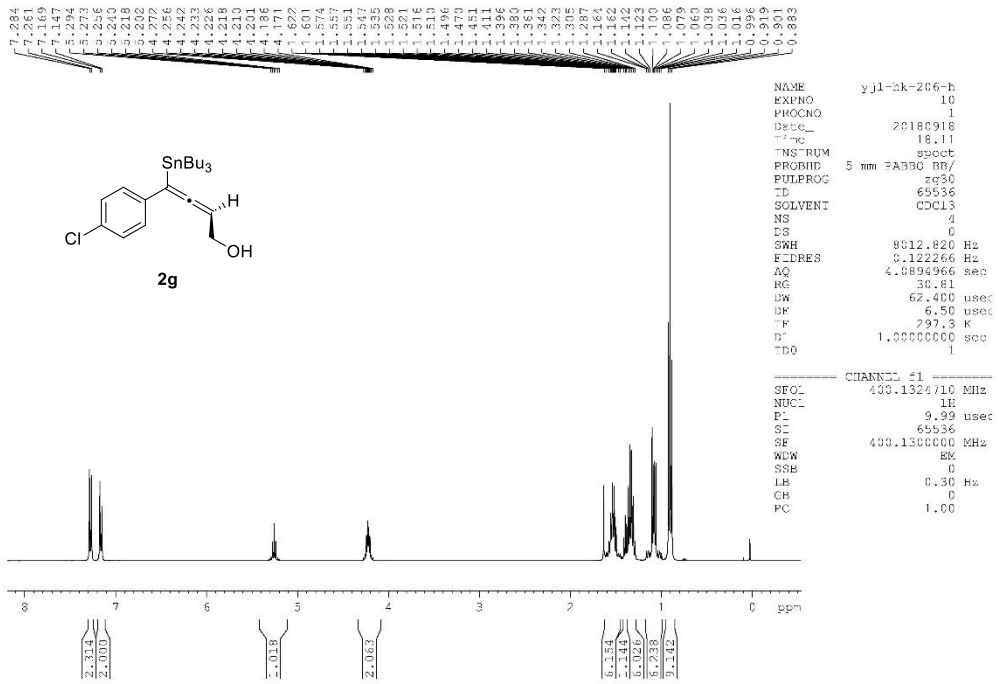


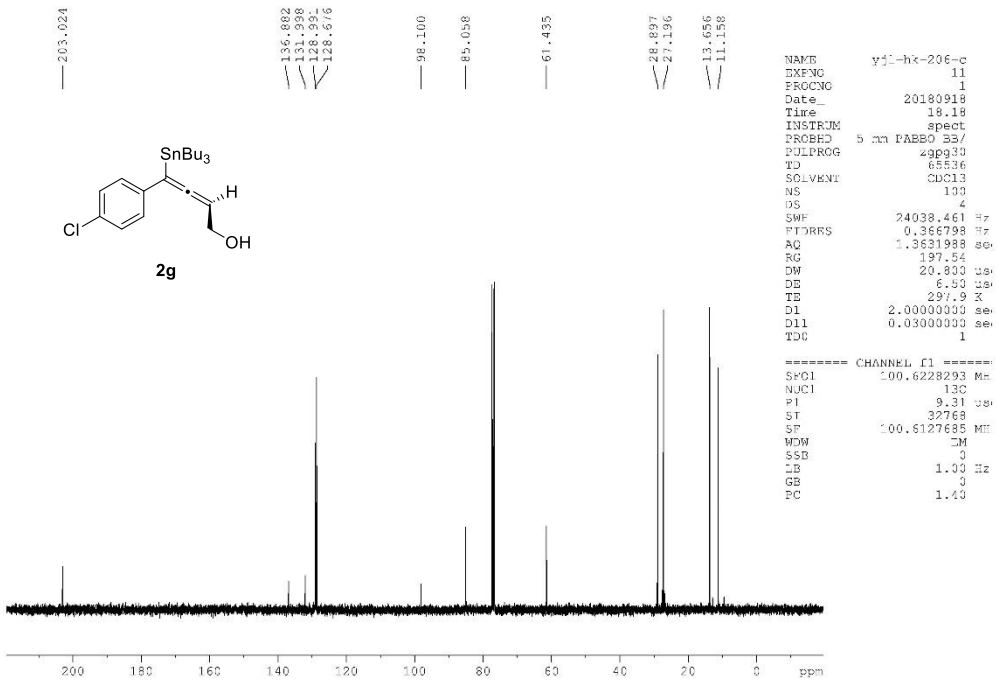

```
NAME          yjl-hk-498-h
EXPNO                    10
PROCNO                    1
Date_          20181115
Time                19.42
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      16
DS                       2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                   30.81
DW                 62.400 usec
DE                  6.50 usec
TE                 295.4 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                     1H
P1                   9.99 usec
SI                  65536
SF            400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

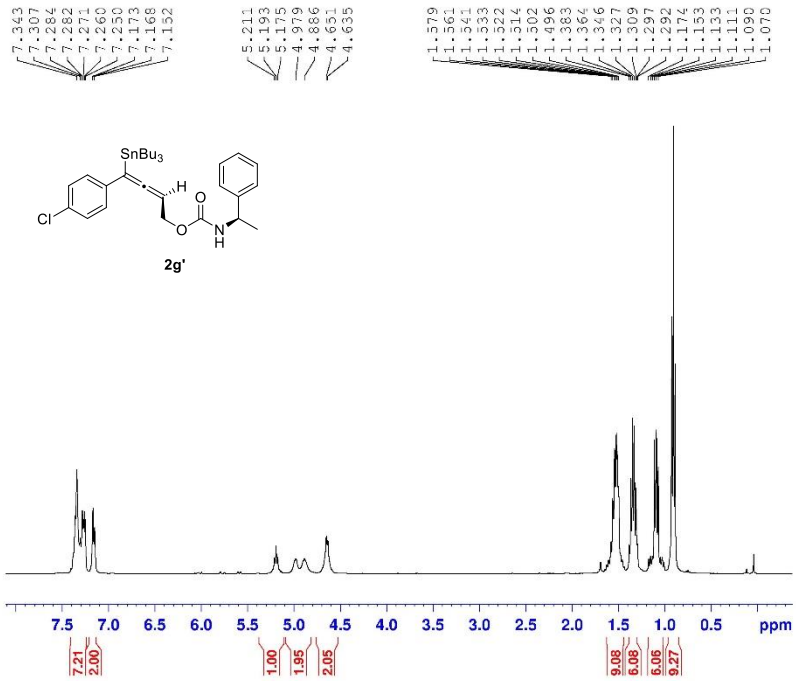
2f'

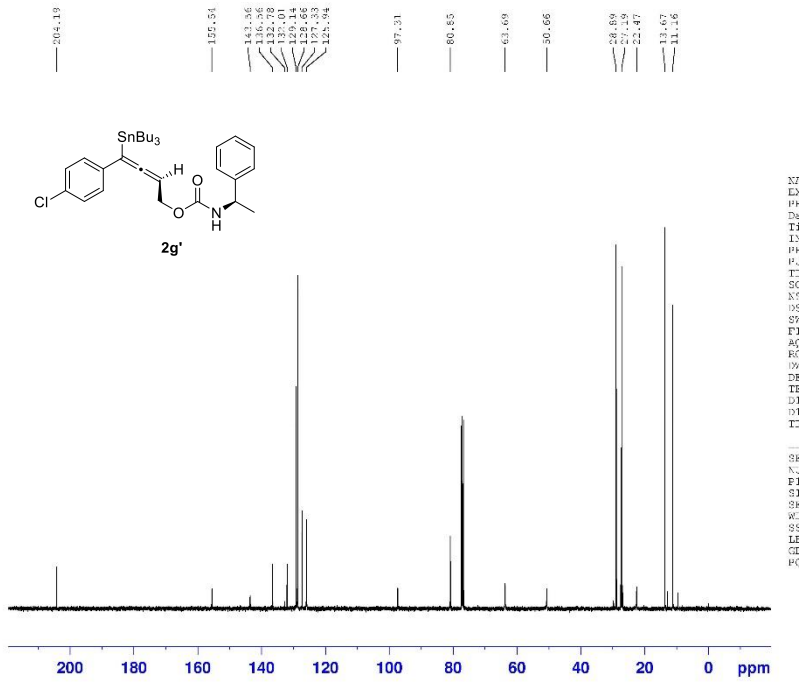


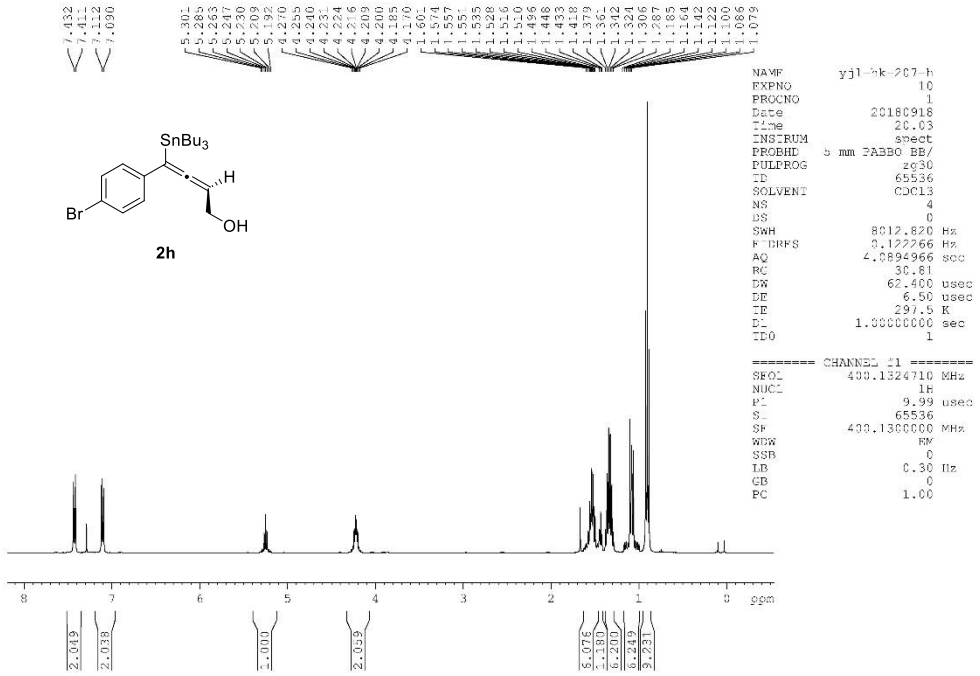

```
NAME          yjl-hk-498-c
EXPNO                    12
PROCNO                    1
Date_          20181115
Time                20.08
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     924
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                  197.54
DW                 20.800 usec
DE                  6.50 usec
TE                 296.3 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                     13C
P1                   9.31 usec
SI                  32768
SF            100.6127685 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

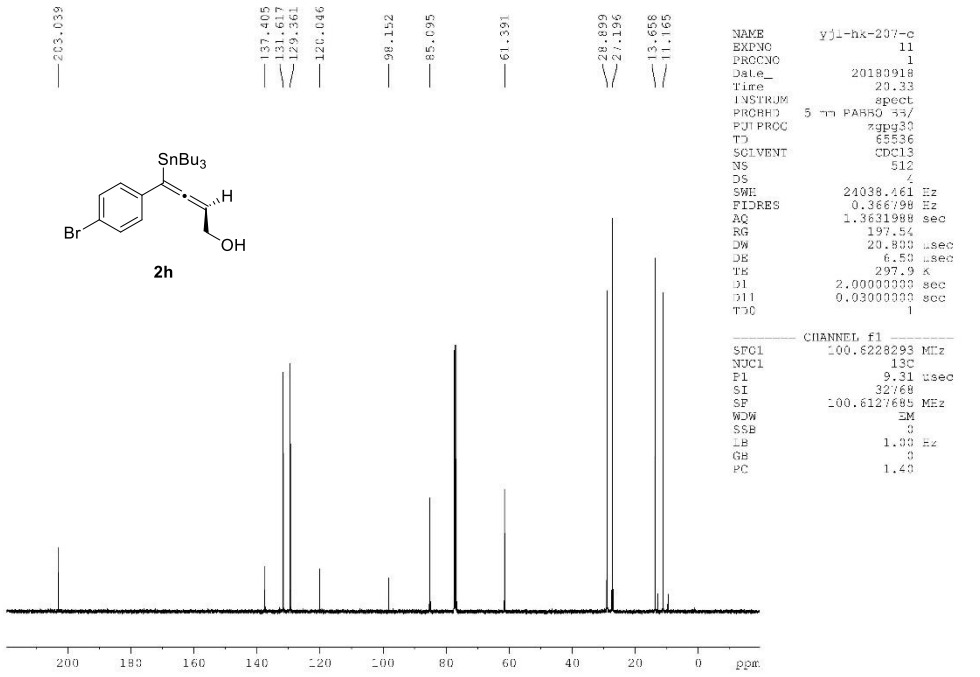

7.284
7.261
7.169
7.147
5.294
5.273
5.256
5.240
5.218
5.202
4.272
4.256
4.242
4.233
4.226
4.218
4.210
4.201
4.186
4.171
1.622
1.601
1.574
1.557
1.551
1.547
1.535
1.528
1.521
1.516
1.510
1.496
1.470
1.451
1.411
1.396
1.380
1.361
1.342
1.323
1.305
1.287
1.164
1.162
1.142
1.123
1.100
1.086
1.079
1.060
1.038
1.036
1.016
0.996
0.919
0.891
0.883
SnBu3
H
Cl
OH
2g
NAME yjl-hk-206-h
EXPNO 10
PROCNO 1
Date_ 20180918
Time 18.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 30.81
DW 62.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8 7 6 5 4 3 2 1 0 ppm
2.314
2.000
1.018
2.063
6.154
4.144
4.026
6.238
9.142

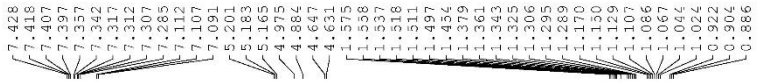

203.024
136.882
131.938
128.991
128.676
98.100
85.058
61.435
28.897
27.196
13.656
11.158
SnBu3
H
Cl
OH
2g
NAME yjl-hk-206-c
EXPNO 11
PROCNO 1
Date_ 20180918
Time 18.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

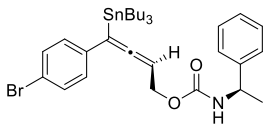

7.343
7.307
7.284
7.282
7.271
7.260
7.250
7.173
7.168
7.152
5.211
5.193
5.175
4.979
4.886
4.651
4.635
1.579
1.561
1.541
1.533
1.522
1.514
1.502
1.496
1.383
1.364
1.346
1.327
1.309
1.297
1.292
1.174
1.153
1.133
1.111
1.090
1.070
BRUKER
SnBu3
H
Cl
O
O
N
H
2g'
NAME yjl hk 505 h
EXPNO 10
PROCNO 1
Date_ 20190603
Time 20.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 17.39
DW 62.400 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.98 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
7.21
2.00
1.00
1.95
2.05
9.08
6.08
6.06
9.27


204.19
155.54
143.56
135.66
132.78
131.01
129.14
128.66
127.33
125.94
97.31
80.85
63.69
30.66
28.89
27.19
22.47
13.67
11.16
BRUKER
SnBu3
H
Cl
O
O
N
H
2g'
NAME yjl hk 505 c
EXPNO 11
PROCNO
Date_ 20190603
Time 21.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 348
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

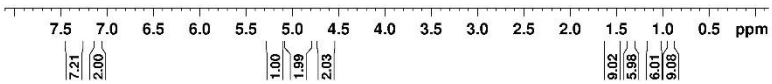

7.432
7.411
7.112
7.090
5.302
5.285
5.263
5.247
5.230
5.209
5.192
4.270
4.255
4.240
4.231
4.224
4.216
4.209
4.200
4.185
4.170
1.602
1.574
1.557
1.551
1.535
1.528
1.516
1.510
1.496
1.448
1.433
1.418
1.379
1.362
1.342
1.324
1.306
1.287
1.185
1.164
1.142
1.122
1.100
1.086
1.079
SnBu3
H
Br
OH
2h
NAME yjl-hk-207-h
EXPNO 10
PROCNO 1
Date 20180918
Time 20.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 30.81
DW 62.400 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8 7 6 5 4 3 2 1 0 ppm
2.049
2.038
3.000
2.059
5.076
5.180
6.200
6.249
9.231


203.039
137.405
131.617
129.361
120.046
98.152
85.095
61.391
28.899
27.196
13.658
11.165
SnBu3
H
Br
OH
2h
NAME yjl-hk-207-c
EXPNO 11
PROCNO 1
Date_ 20180918
Time 20.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631989 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

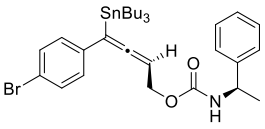




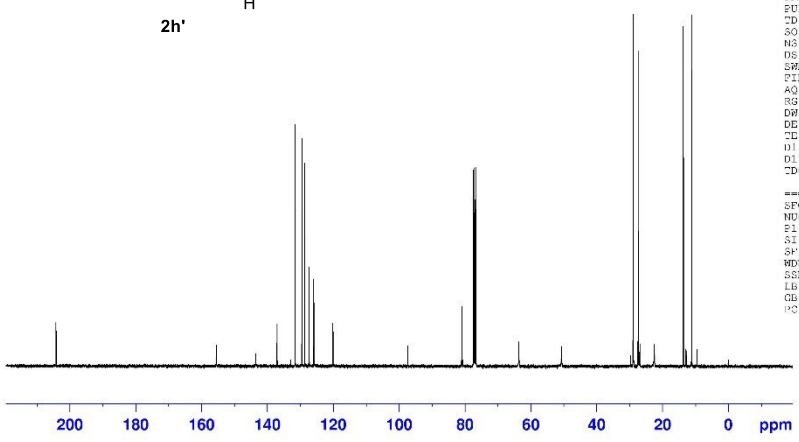
2h'



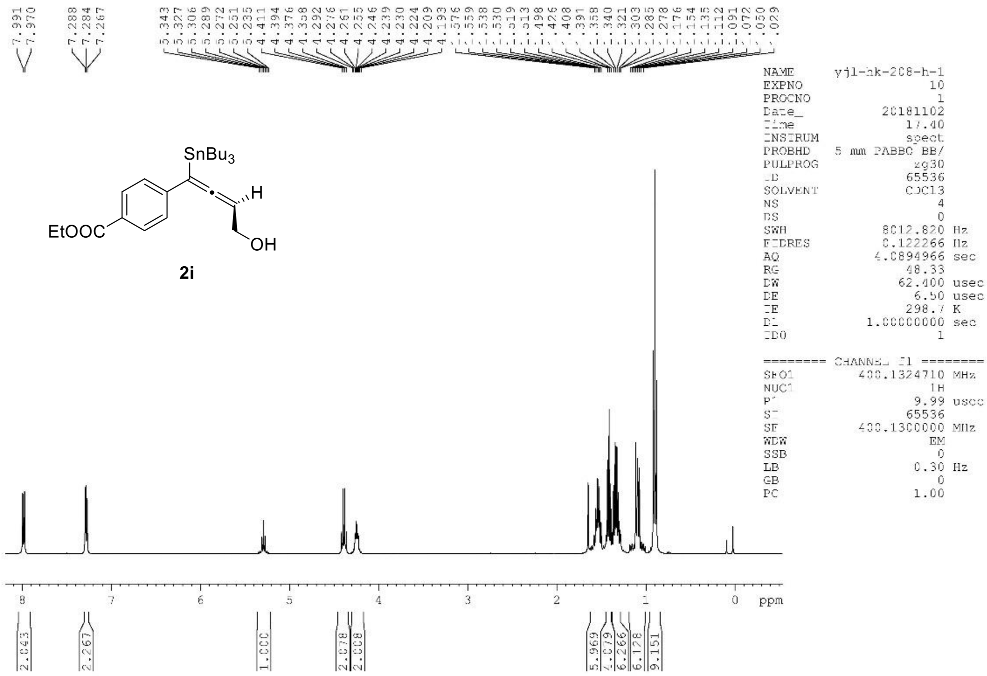

```
NAME          yjl-hk-503-h
EXPNO              10
PROCNO              1
Date_          20190603
Time              19.48
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zg30
TD                65536
SOLVENT           CDCl3
NS                   4
DS                   0
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG                9.81
DW               62.400 usec
DE                6.50 usec
TE              297.7 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1              1H
P1                9.99 usec
SI               65536
SF          400.1300000 MHz
WDW               EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

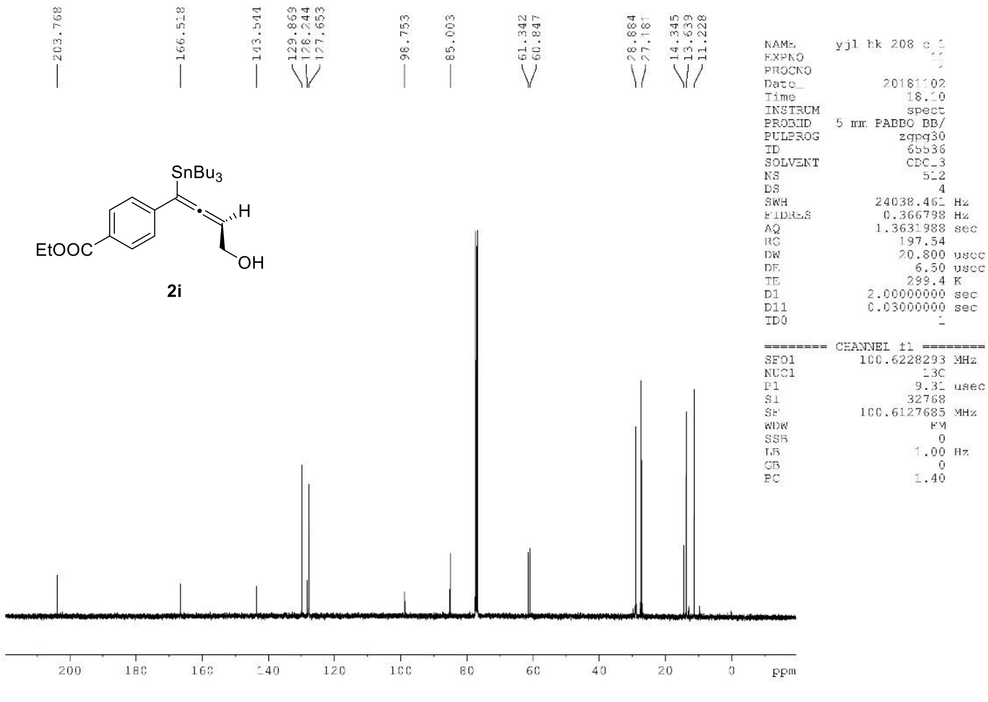


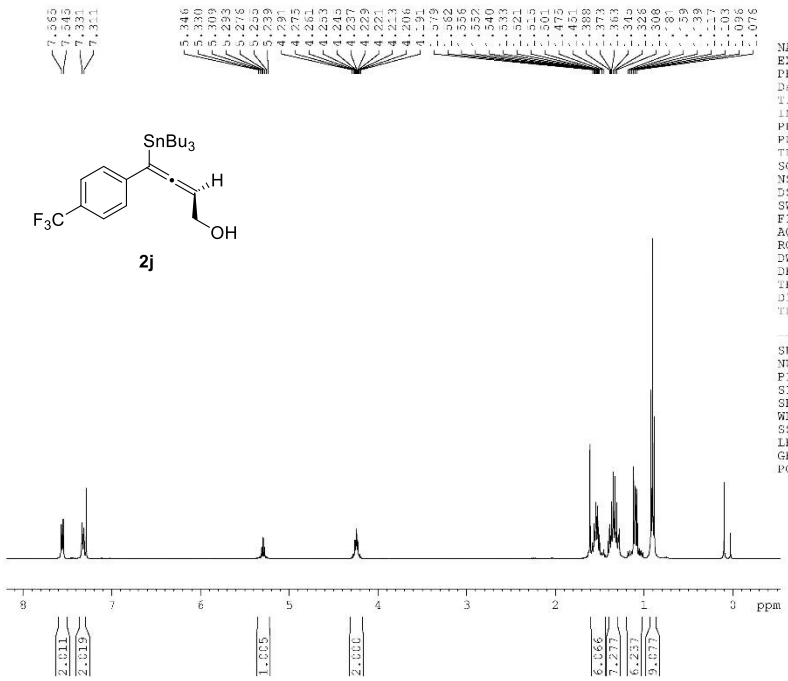
2h'

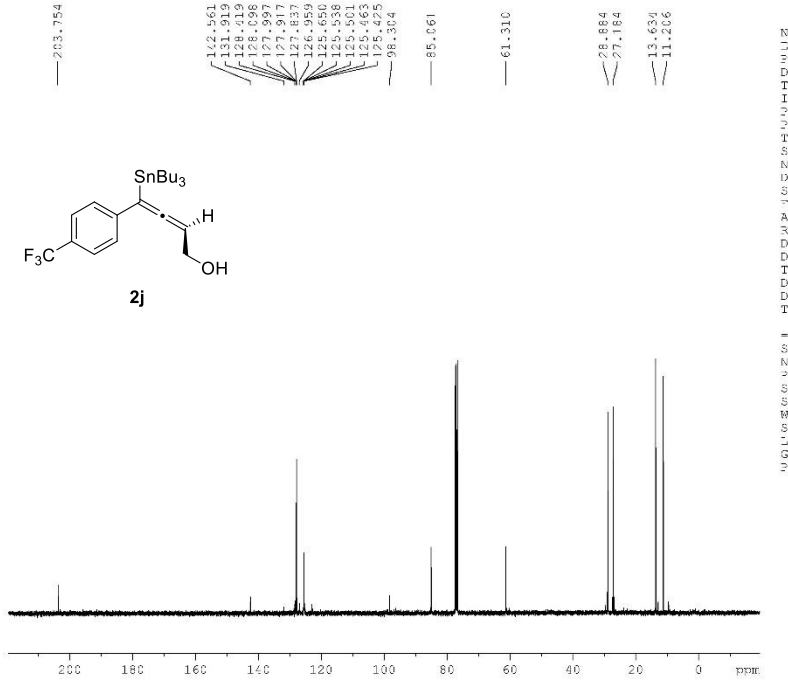


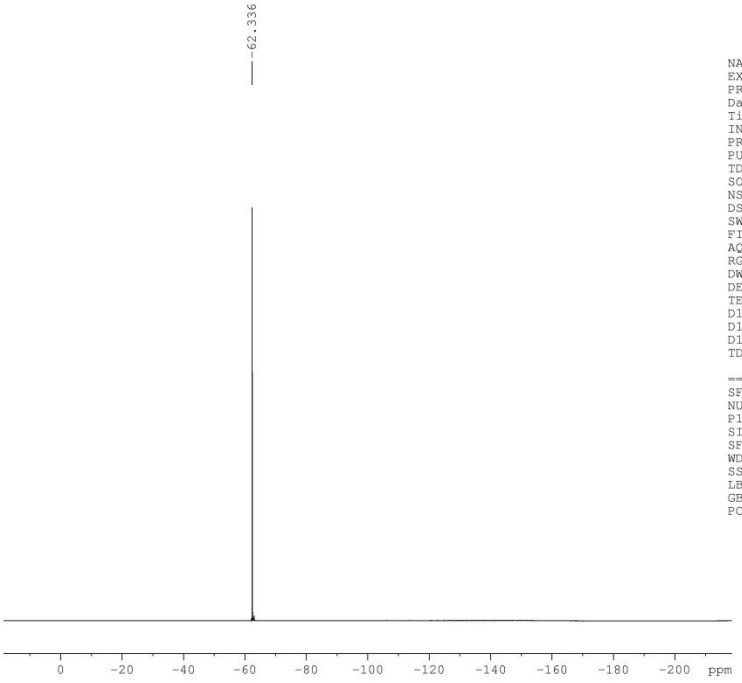

```
NAME          yjl-hk-503-c
EXPNO              11
PROCNO              1
Date_          20190603
Time              20.34
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 800
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG              197.54
DW               20.800 usec
DE                6.50 usec
TE              298.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1              13C
P1                9.31 usec
SI               32768
SF          100.6127685 MHz
WDW               EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```


7.991
7.970
7.288
7.284
7.267
5.343
5.327
5.306
5.289
5.272
5.251
5.235
4.411
4.394
4.376
4.358
4.292
4.276
4.261
4.255
4.246
4.239
4.230
4.224
4.209
4.193
SnBu3
H
EtOOC
OH
2i
NAME yjl-hk-208-h-1
EXPNO 10
PROCNO 1
Date_ 20181102
Time 17.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 48.33
DW 62.400 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8
7
6
5
4
3
2
1
0
ppm
2.043
2.267
1.000
2.078
2.008
5.969
4.079
6.266
6.128
9.151

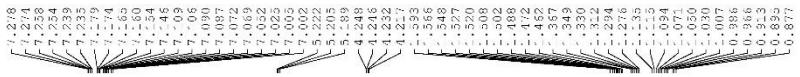

203.768
166.518
143.544
129.863
128.244
127.653
98.753
85.003
61.342
60.847
28.884
27.181
14.345
13.639
11.228
SnBu3
H
EtOOC
OH
2i
NAME yjl hk 208 c 1
PROCNO
Date_ 20181102
Time 18.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

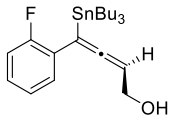

7.365
7.345
7.331
7.321
5.346
5.330
5.309
5.293
5.276
5.255
5.239
4.291
4.275
4.261
4.253
4.245
4.237
4.229
4.221
4.213
4.206
1.579
1.562
1.556
1.552
1.540
1.533
1.521
1.515
1.501
1.475
1.451
1.388
1.373
1.363
1.345
1.328
1.308
1.087
1.059
1.039
1.027
1.003
0.996
0.976
SnBu3
H
F3C
OH
2j
NAME yjl-ak-184-1-h
EXPNO 10
PROCNO 1
Date_ 20180919
Time 17.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 63.21
DW 62.400 use
DE 6.50 use
TE 297.3 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 use
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm
2.011
2.019
1.005
2.000
6.666
7.273
6.237
9.077


203.754
142.561
131.919
128.419
128.098
127.997
127.917
127.837
126.959
125.650
125.538
125.561
125.463
125.425
98.304
85.061
61.310
28.884
27.184
13.634
11.206
SnBu3
H
F3C
OH
2j
NAME yjl-hk-184-c
EXPNO 21
PROCNO 1
Date_ 20180926
Time 19.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 use
DE 6.50 use
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 use
ST 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm



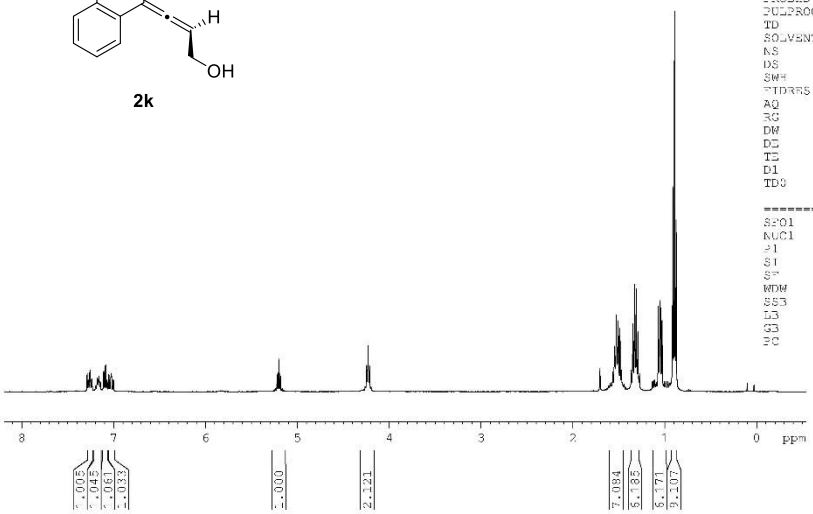

```
NAME        yjl-hk-184-f
EXPNO                 32
PROCNO                 1
Date_           20180928
Time               16.48
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                    16
DS                     4
SWH           89285.711 H
FIDRES         0.681196 H
AQ             0.7340532 s
RG                197.54
DW                 5.600 u
DE                 6.50 u
TE                297.0 K
D1           1.00000000 s
D11          0.03000000 s
D12          0.00002000 s
TD0                    1

======== CHANNEL f1 ======
SFO1         376.4607164 M
NUC1                19F
P1                14.00 u
SI                65536
SF           376.4983662 M
WDW                  EM
SSB                   0
LB                 0.30 H
GB                    0
PC                 1.00
```

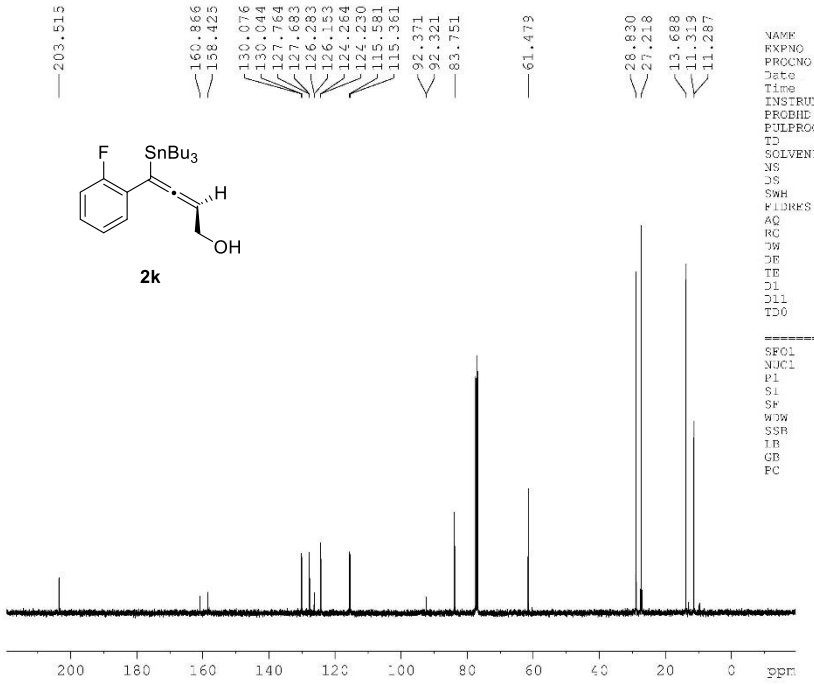




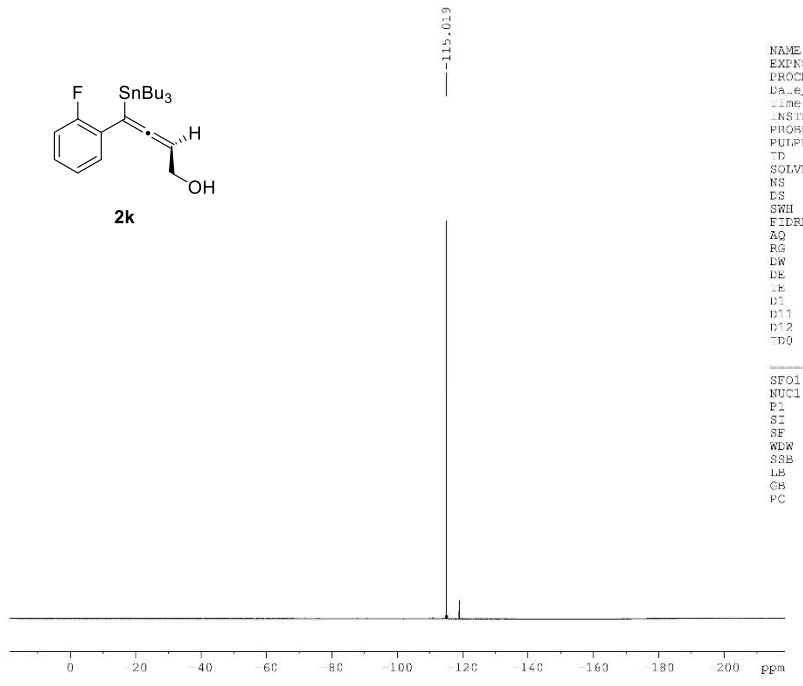
2k

```
NAME        yjl-hk-212-h
EXPNO                 10
PROCNO                 1
Date_           20180320
Time               16.40
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             CDCl3
NS                     4
DS                     0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894366 sec
RG                30.81
DW                82.400 usec
DE                 6.50 usec
TE                294.8 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                 9.99 usec
SI                65536
SF           400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

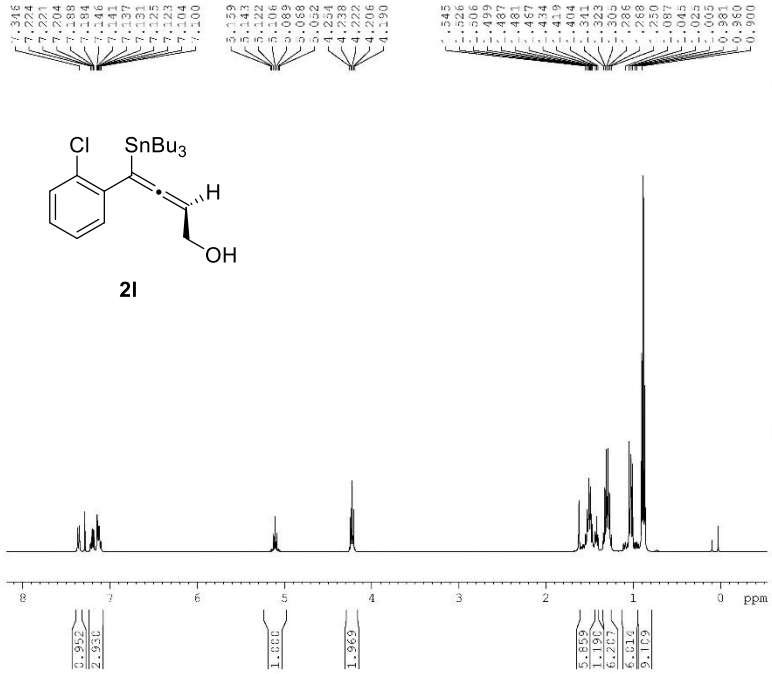


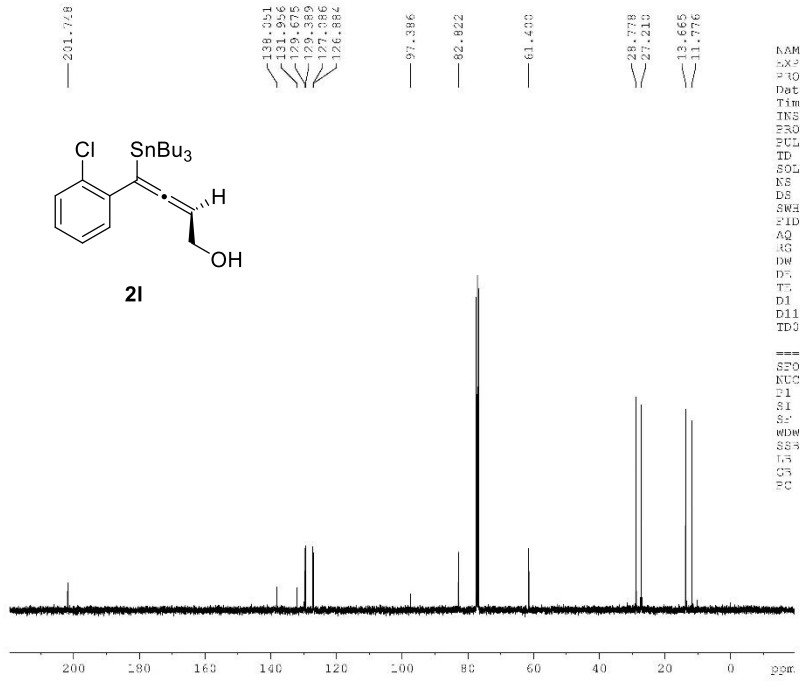


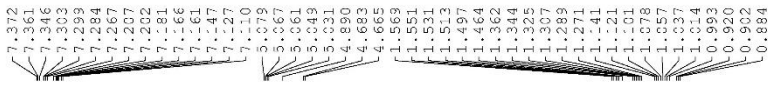

```
NAME          yjl-hk-212-c
EXPNO                   11
PROCNO                   1
Date_          20180320
Time                16.51
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  180
DS                    4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                197.54
DW               20.800 usec
DE                6.50 usec
TE                295.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1                13C
P1                9.31 usec
SI                32768
SF          100.6127685 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

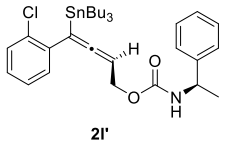



```
NAME          yjl-hk-212-f
EXPNO                   10
PROCNO                   1
Date_          20180321
Time                18.12
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG       zgfhigqn.2
TD                131072
SOLVENT           CDCl3
NS                   16
DS                    4
SWH           89285.711 Hz
FIDRES        0.681196 Hz
AQ            0.7340532 sec
RG                197.54
DW                5.600 usec
DE                6.50 usec
TE                295.1 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        376.4607164 MHz
NUC1                19F
P1                14.00 usec
SI                65536
SF          376.4983662 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

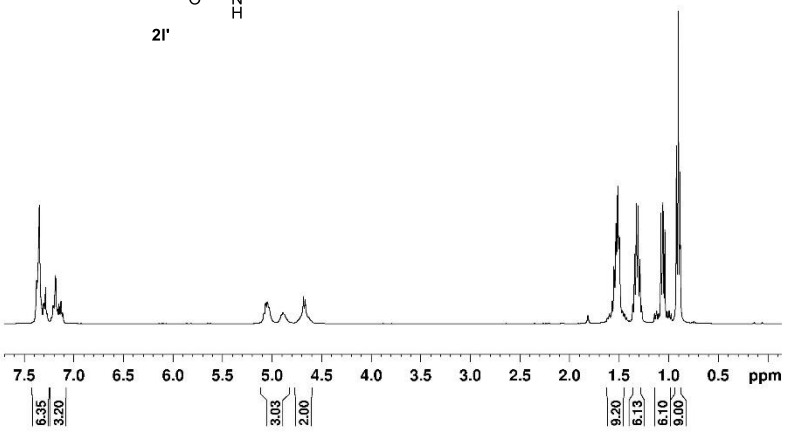

7.346
7.224
7.221
7.204
7.188
7.184
7.146
7.141
7.137
7.131
7.125
7.123
7.104
7.100
5.159
5.143
5.122
5.106
5.089
5.088
5.052
4.234
4.238
4.222
4.206
4.190
1.545
1.526
1.506
1.499
1.487
1.481
1.457
1.434
1.419
1.404
1.341
1.323
1.306
1.286
1.268
1.250
1.097
1.045
1.025
1.005
0.981
0.960
0.900
Cl
SnBu3
H
OH
2l
NAME yjl-hk-241-h
EXPNO 10
PROCNO 1
Date_ 20180926
Time 17.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 53.87
DW 62.400 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8
7
6
5
4
3
2
1
0
ppm
2.952
2.936
1.000
1.969
5.859
1.190
1.207
6.612
9.169


201.748
138.351
131.956
129.675
129.389
127.386
126.884
97.386
82.822
61.433
28.778
27.218
13.665
11.776
Cl
SnBu3
H
OH
2l
NAME yjl-hk-241-c
EXPNO 11
PROCNO 1
Date_ 20180926
Time 17.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 180
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

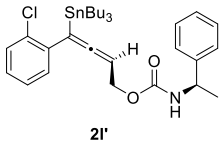




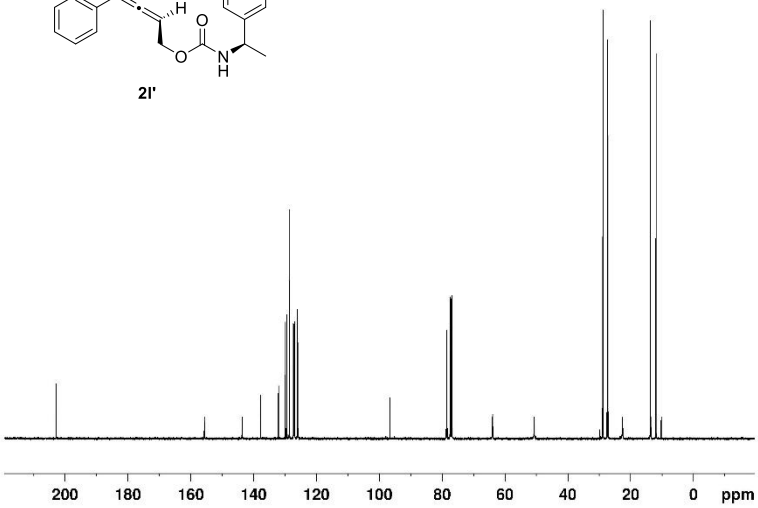
2l'



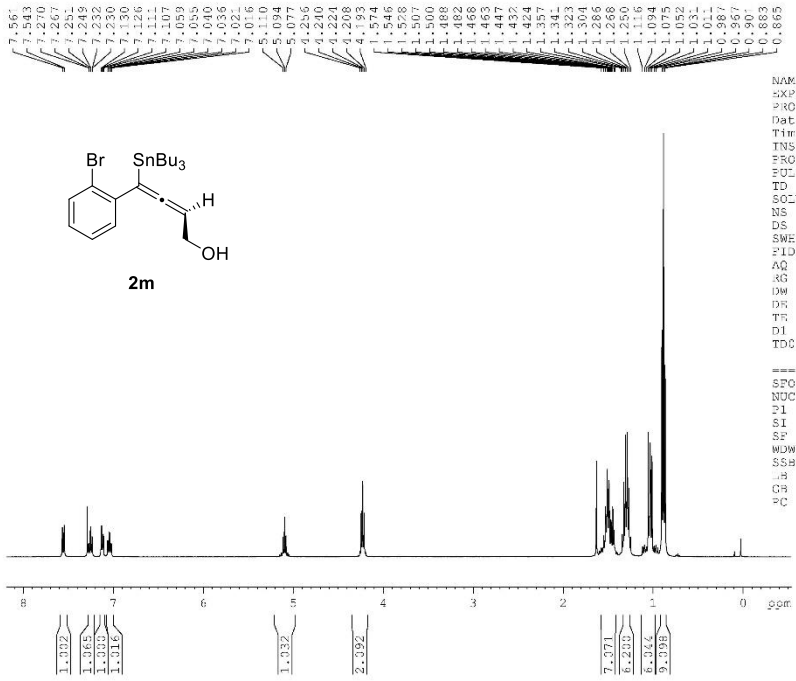

```
NAME          yjl-hk-507-h
EXPNO                   10
PROCNO                   1
Date_         20190611
Time               17.41
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     0
SWH           8012.820 Hz
FIDRES        0.122256 Hz
AQ            4.0896966 sec
RG                  7.76
DW              62.400 use
DE               6.50 use
TE              297.7 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1              1H
P1               9.99 use
SI                65536
SF          400.1300000 MHz
WDW                EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```

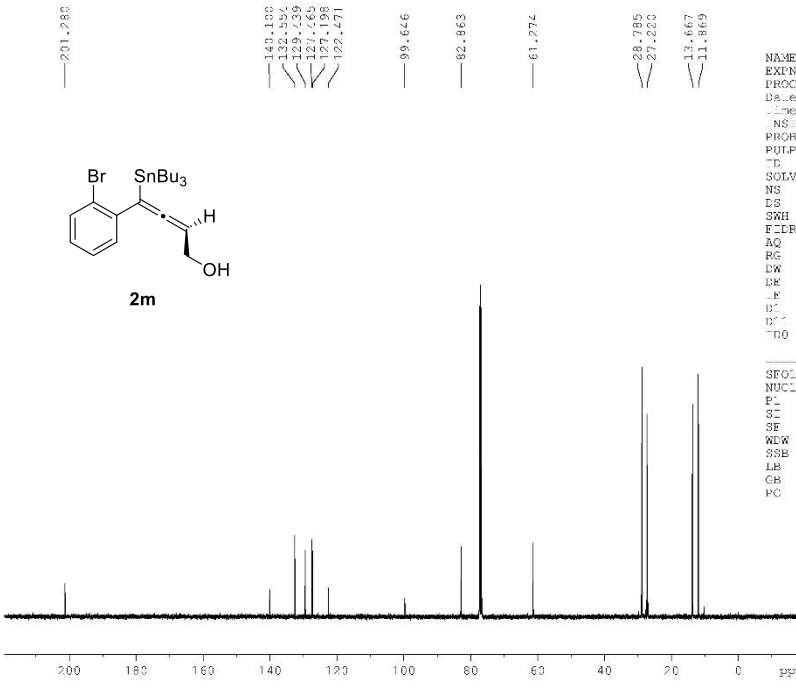


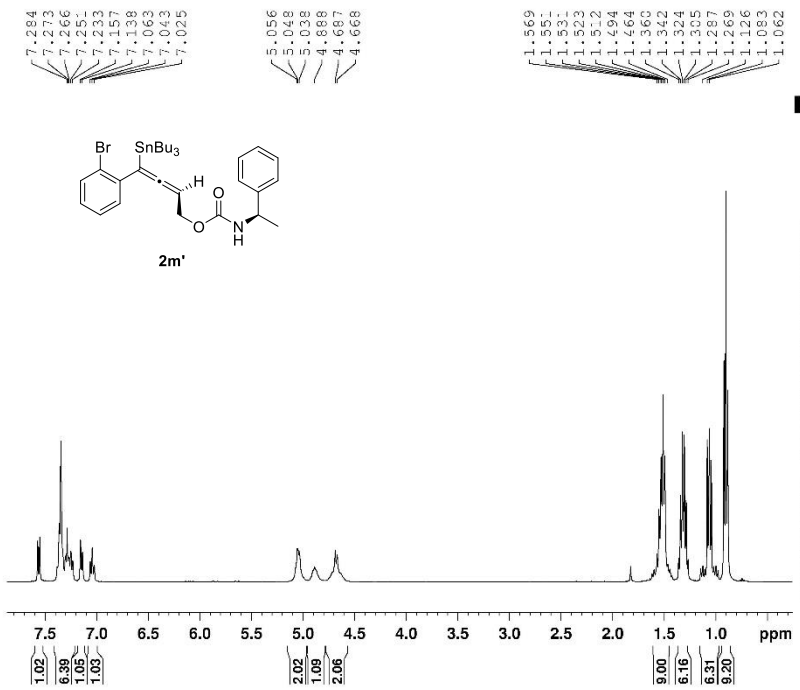
2l'

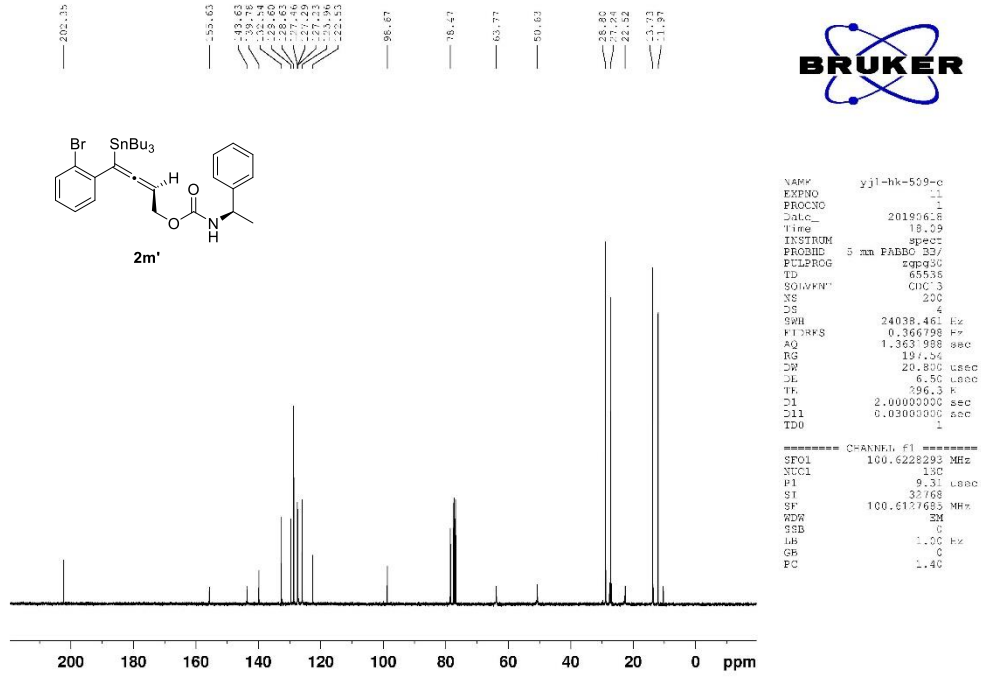


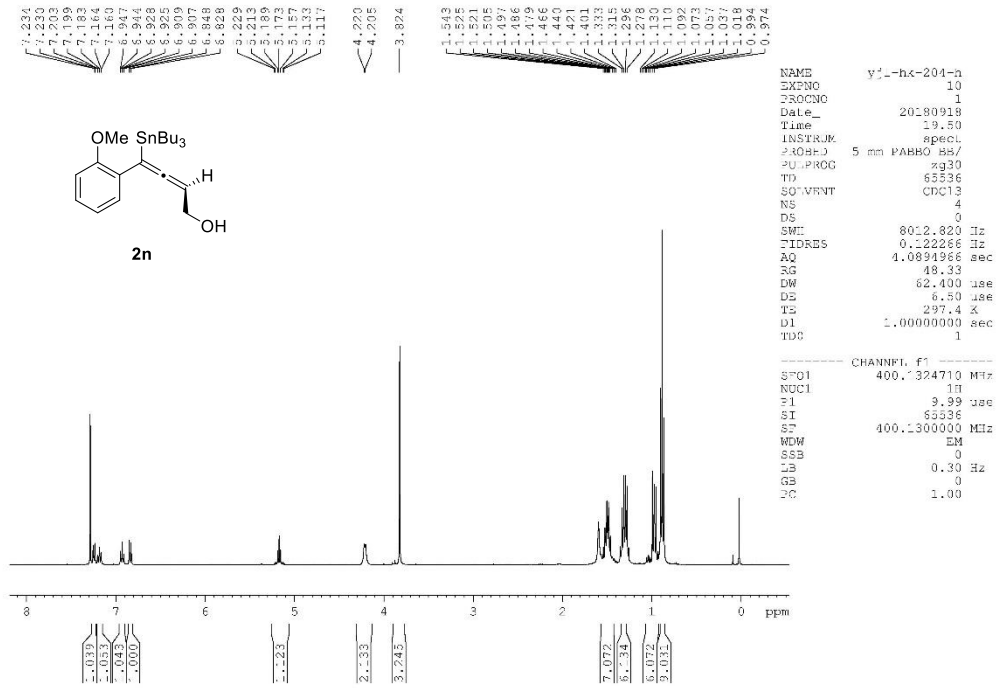

```
NAME          yjl-hk-507-c
EXPNO                   11
PROCNO                   1
Date_         20190611
Time               18.11
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                197.54
DW              20.800 usec
DE               6.50 usec
TE              298.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1              13C
P1               9.31 usec
SI                32768
SF          100.6127685 MHz
WDW                EM
SSB                0
LB              1.00 Hz
GB                 0
PC              1.40
```

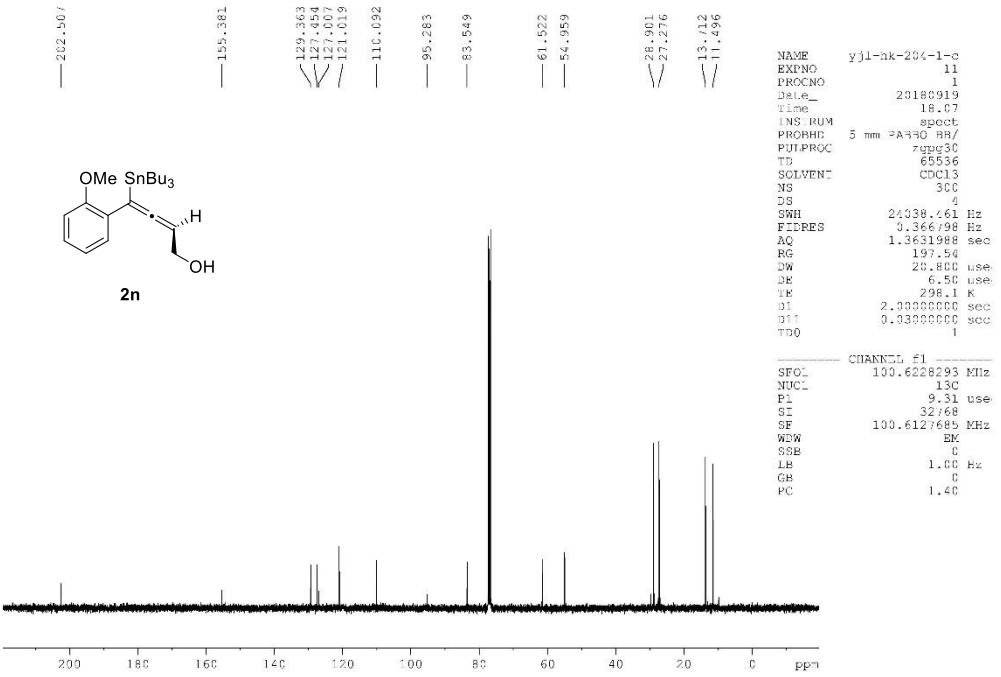

7.567
7.543
7.270
7.267
7.251
7.249
7.232
7.230
7.130
7.126
7.111
7.107
7.053
7.055
7.040
7.036
7.022
7.016
5.110
5.094
5.077
4.256
4.240
4.221
4.208
4.193
1.574
1.546
1.528
1.507
1.500
1.488
1.482
1.468
1.463
1.447
1.432
1.424
1.357
1.341
1.323
1.304
1.286
1.268
1.250
1.116
1.094
1.075
1.052
1.031
0.987
0.967
0.883
0.865
Br
SnBu3
H
OH
2m
NAME yjl-hk-251-h
EXPNO 10
PROCNO 1
Date_ 20180918
Time 20.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 30.81
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8
7
6
5
4
3
2
1
0
ppm
1.032
1.065
1.033
1.016
1.032
2.392
7.371
6.238
6.044
9.098

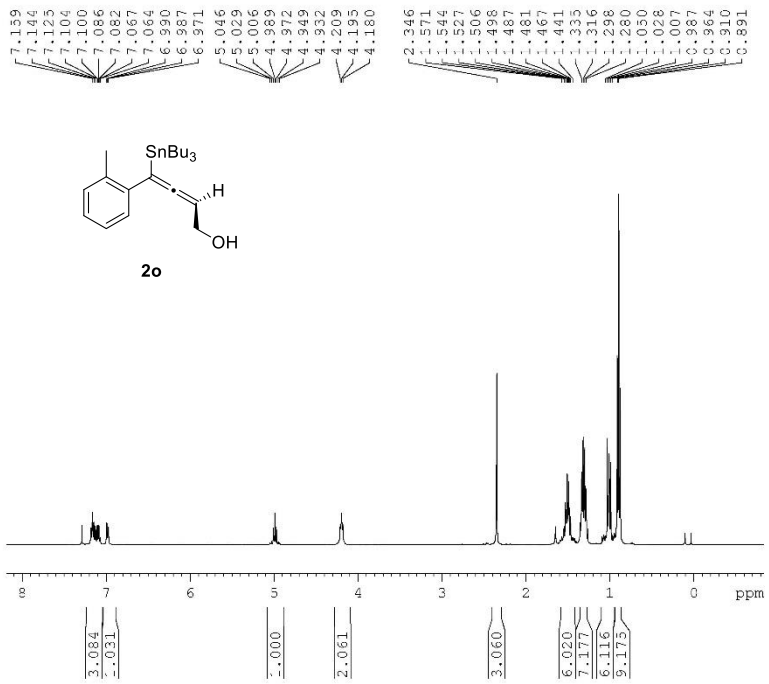

201.288
140.188
132.554
129.439
127.465
127.198
122.471
99.646
82.863
61.274
28.785
27.223
13.667
11.869
Br
SnBu3
H
OH
2m
NAME yjl-hk-251-c
EXPNO 11
PROCNO 1
Date_ 20180918
Time 21.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

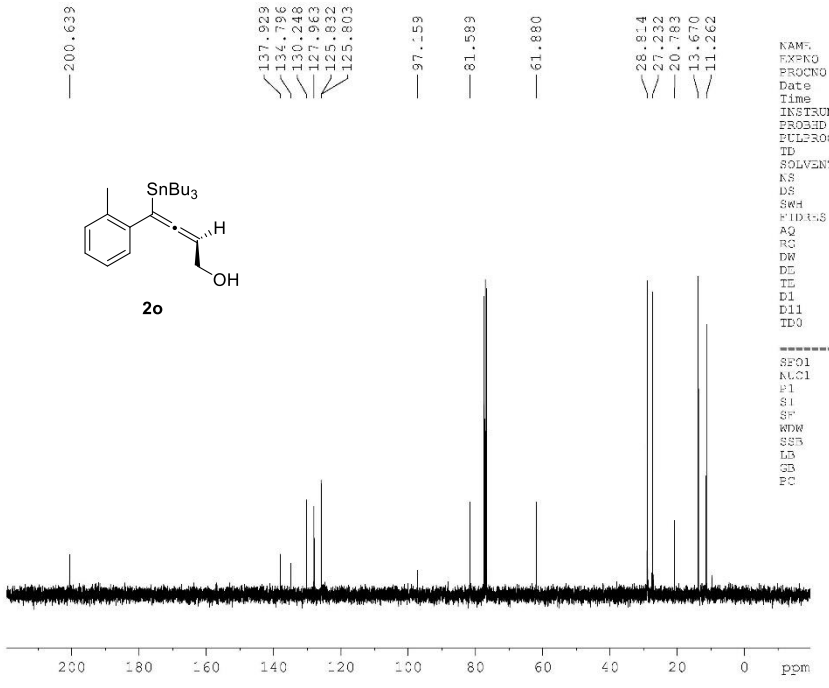

7.284
7.273
7.266
7.251
7.233
7.157
7.138
7.063
7.043
7.025
5.056
5.048
5.038
4.888
4.687
4.668
1.569
1.551
1.531
1.523
1.512
1.494
1.464
1.360
1.342
1.324
1.305
1.287
1.269
1.126
1.083
1.062
Br
SnBu3
H
O
N
H
2m'
NAME yjl-hk-509-h
EXPNO 10
PROCNO 1
Date_ 20190618
Time 18.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 6012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 7.74
DW 62.400 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.02 6.39 1.05 1.03 2.02 1.09 2.06 9.00 6.16 6.31 9.20

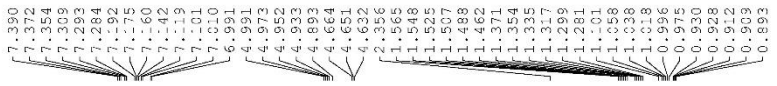

202.35
155.63
143.63
139.76
139.34
128.60
128.63
127.46
127.29
127.23
125.96
122.53
96.67
78.47
63.77
59.63
28.80
27.24
22.52
13.73
11.97
Br
SnBu3
H
O
N
H
2m'
NAME yjl-hk-509-c
EXPNO 11
PROCNO 1
Date_ 20190618
Time 18.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.56
DW 20.800 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

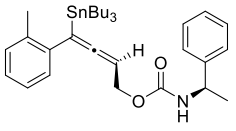

7.234
7.230
7.203
7.199
7.183
7.164
7.160
6.947
6.944
6.928
6.925
6.909
6.907
6.848
6.828
5.229
5.213
5.189
5.173
5.157
5.133
5.117
4.220
4.205
3.824
1.543
1.525
1.521
1.505
1.497
1.486
1.479
1.466
1.440
1.421
1.401
1.333
1.315
1.296
1.278
1.130
1.110
1.092
1.073
1.057
1.037
1.018
0.994
0.974
OMe SnBu3
H
OH
2n
NAME yjl-hk-204-n
EXPNO 10
PROCNO 1
Date_ 20180918
Time 19.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 48.33
DW 62.400 use
DE 6.50 use
TE 297.4 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 use
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8 7 6 5 4 3 2 1 0 ppm
1.039
1.053
1.043
1.000
1.123
2.133
3.245
7.072
6.734
6.072
3.031


202.907
159.381
129.363
127.454
127.007
121.019
110.092
95.283
83.549
61.522
54.959
28.901
27.276
13.712
11.496
OMe SnBu3
H
OH
2n
NAME yjl-hk-204-1-c
EXPNO 11
PROCNO 1
Date_ 20180919
Time 18.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.56
DW 20.800 use
DE 6.50 use
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 use
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

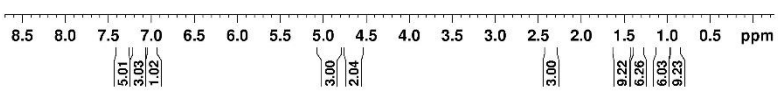

7.159
7.144
7.125
7.104
7.100
7.086
7.082
7.067
7.064
6.990
6.987
6.971
5.046
5.029
5.006
4.989
4.972
4.949
4.932
4.209
4.195
4.180
2.346
1.571
1.544
1.527
1.506
1.498
1.487
1.481
1.467
1.441
1.335
1.316
1.298
1.280
1.030
1.028
1.007
0.987
0.964
0.910
0.891
SnBu3
H
OH
2o
NAME yjl-hk-196-n
EXPNO 20
PROCNO 1
Date_ 20180928
Time 16.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 30.81
DW 62.400 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8 7 6 5 4 3 2 1 0 ppm
3.084
2.031
2.000
2.061
3.060
6.020
7.177
6.116
9.175


200.639
137.929
134.796
130.248
127.863
125.832
125.803
97.159
81.589
61.880
28.814
27.232
20.783
13.670
11.262
SnBu3
H
OH
2o
NAME yjl-hk-196-c
EXPNO 21
PROCNO 1
Date 20180928
Time 16.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

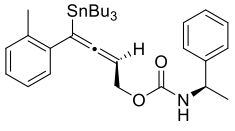




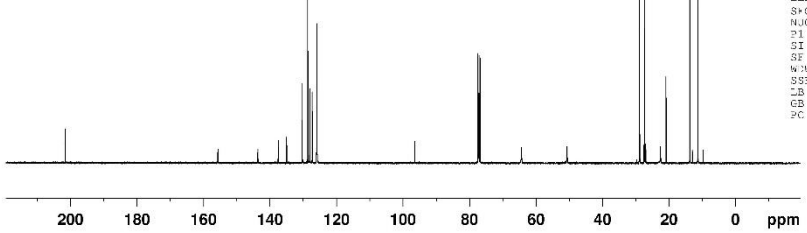
2o'



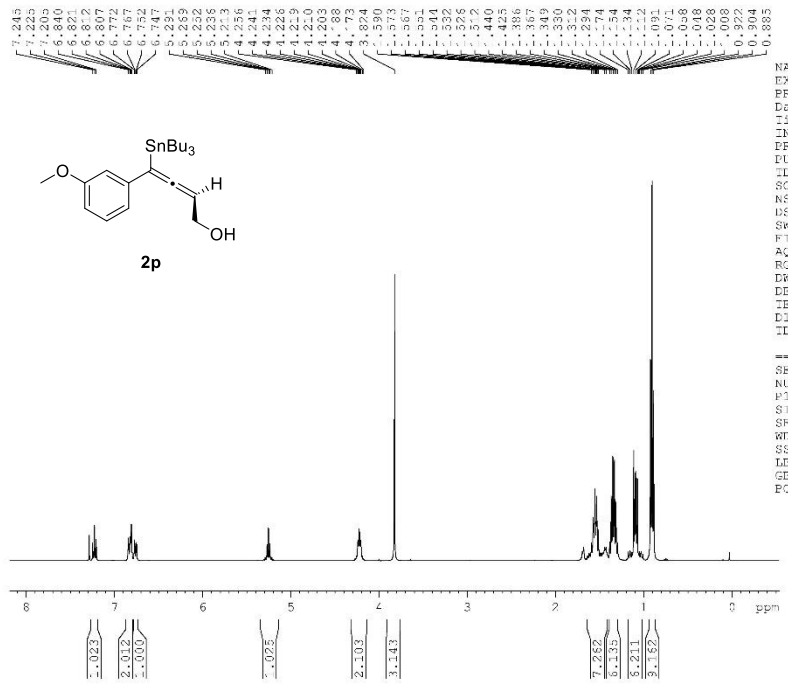

```
NAME          yjl-hk-493-h
EXPNO                   20
PROCNO                   1
Date_         20190624
Time                 17.31
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                       4
DS                       0
SWH             8012.820 Hz
FIDRES          0.122256 Hz
AQ              4.0894966 sec
RG                    8.85
DW                 62.400 usec
DE                  6.50 usec
TE                295.5 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1               1H
P1                 9.99 usec
SI                65536
SF            400.1300000 MHz
WDW                EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

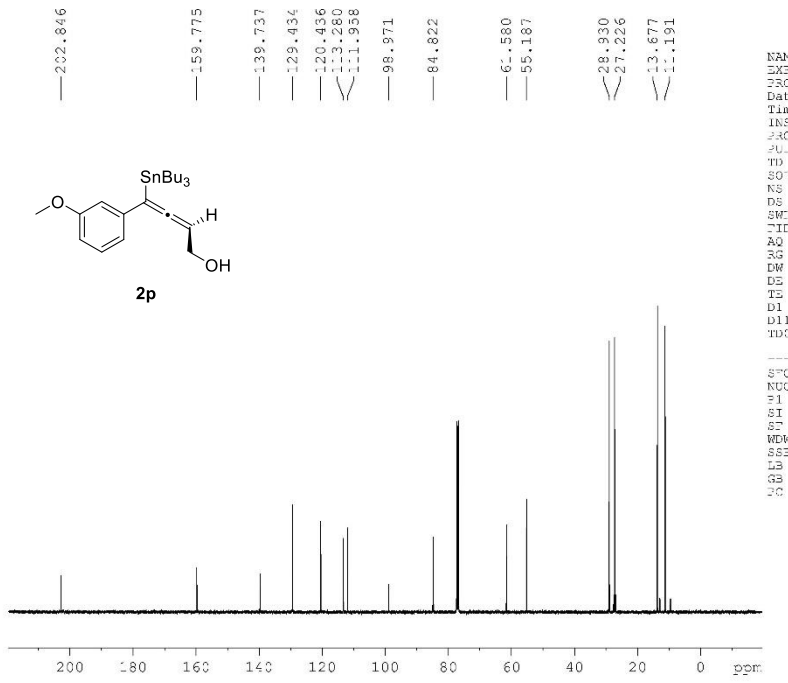


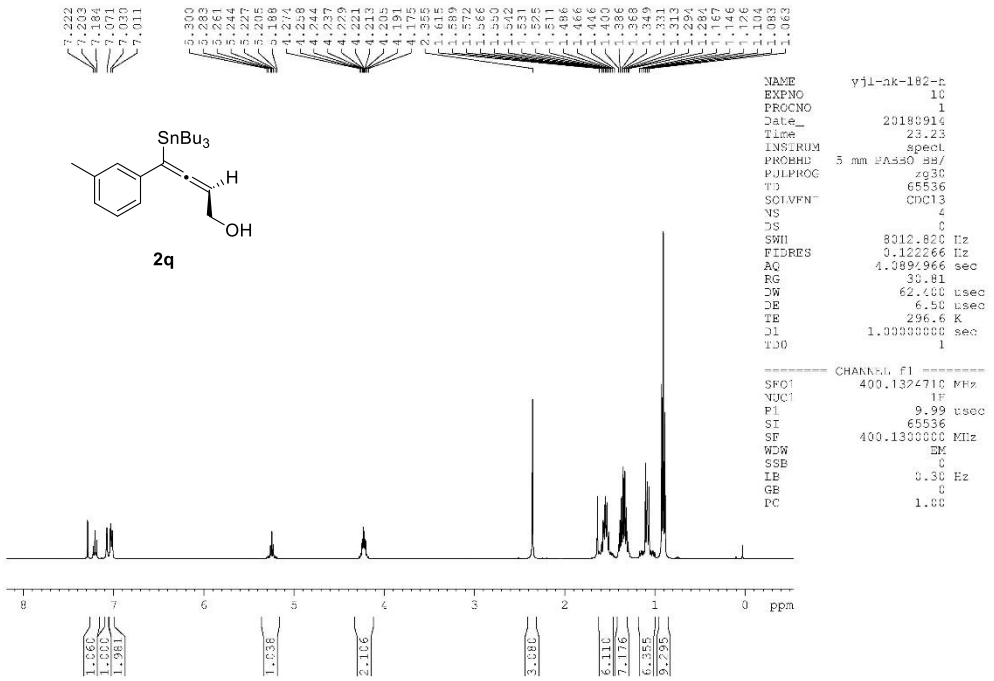
2o'

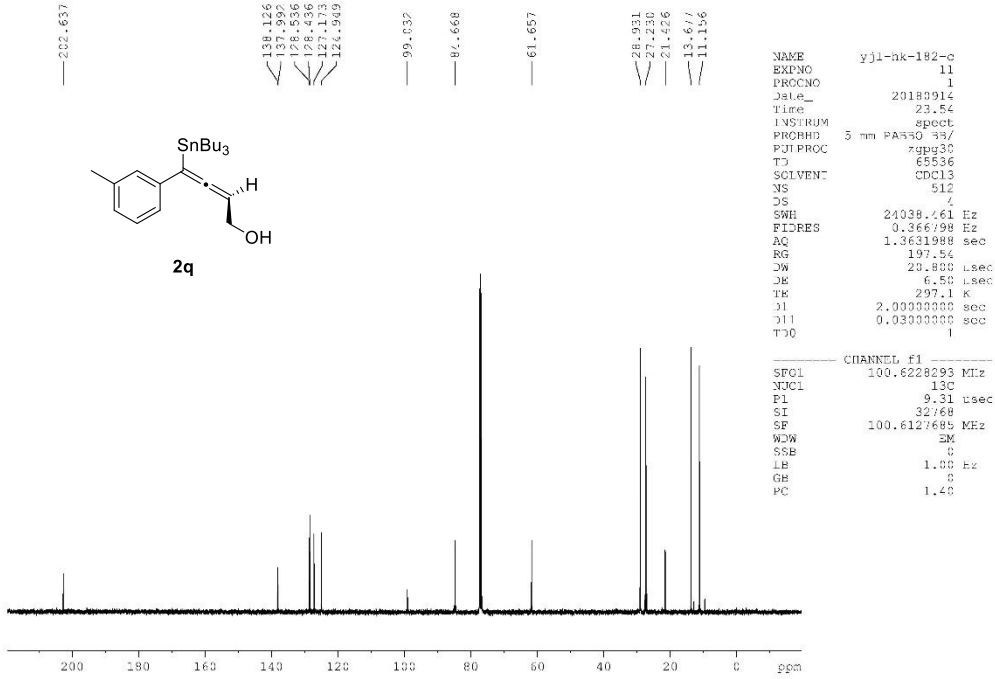


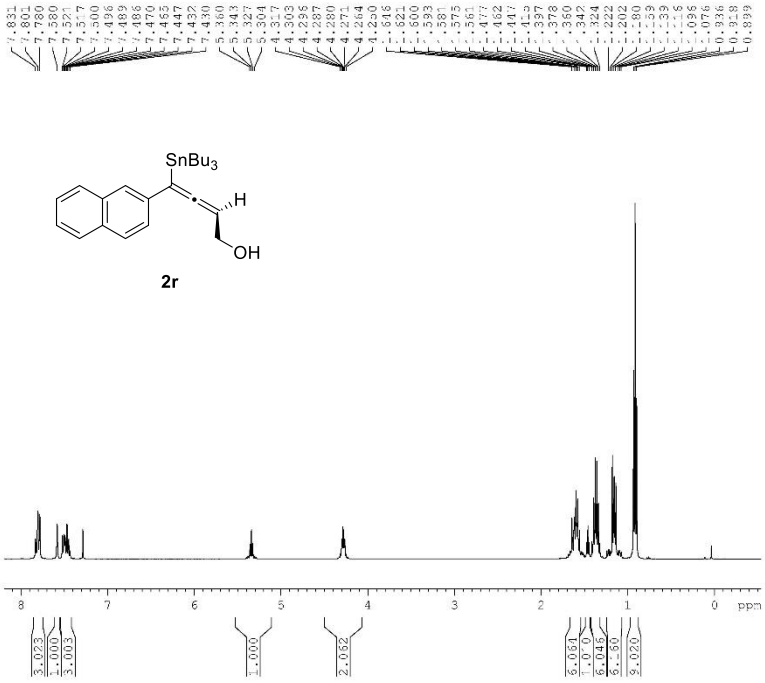

```
NAME          yjl-hk-493-c
EXPNO                   21
PROCNO                   1
Date_         20190624
Time                 18.01
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     512
DS                       4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                  197.54
DW                 20.800 usec
DE                  6.50 usec
TE                296.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6278293 MHz
NUC1               13C
P1                 9.31 usec
SI                32768
SF            100.6127685 MHz
WDW                EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.40
```

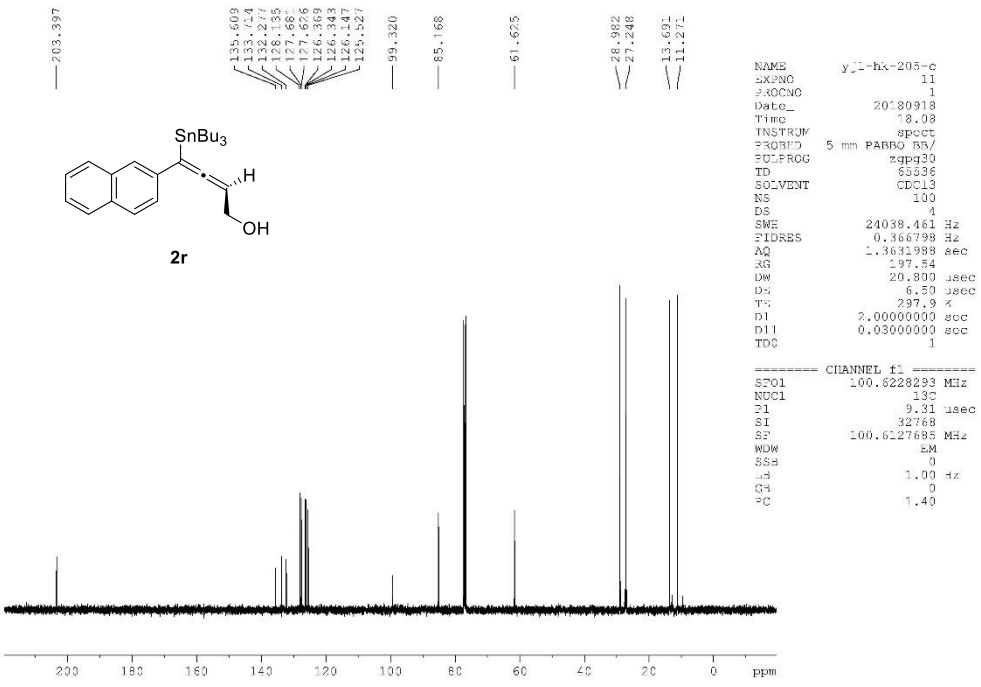

SnBu3
H
OH
2p
ppm

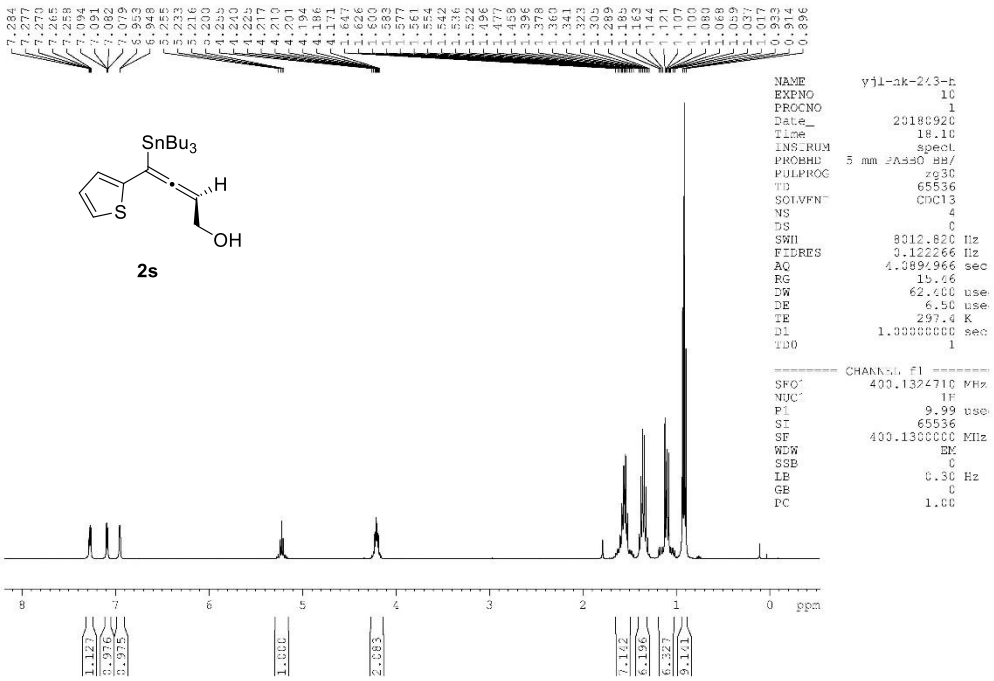

SnBu3
H
OH
2p
ppm

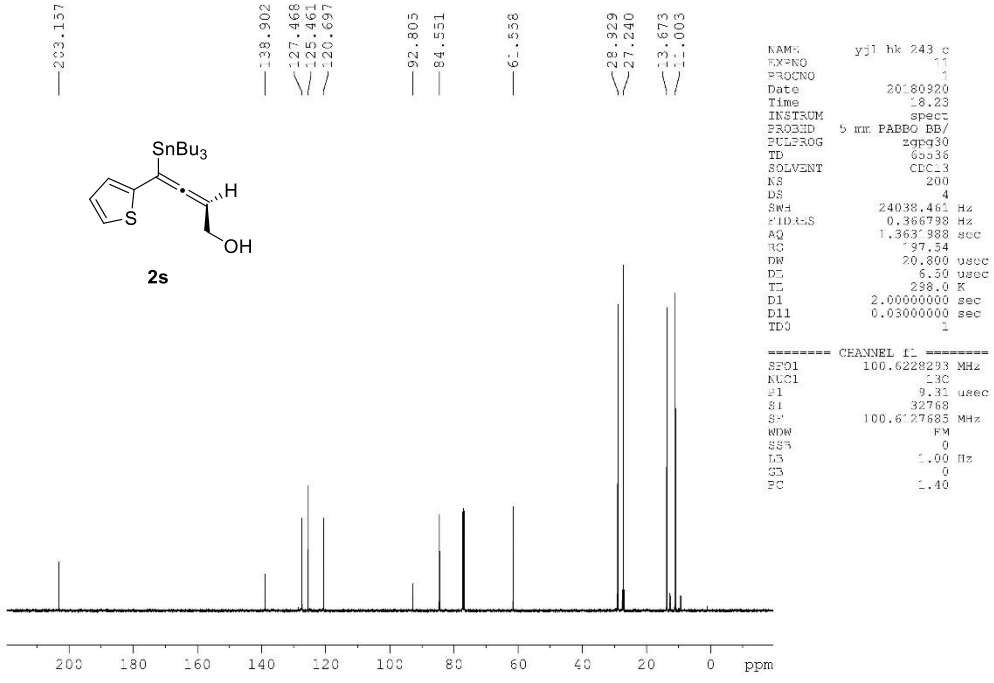

7.222
7.203
7.184
7.071
7.030
7.011
5.300
5.283
5.261
5.244
5.227
5.205
5.188
4.274
4.258
4.244
4.237
4.229
4.221
4.213
4.205
4.191
4.175
2.355
1.615
1.589
1.572
1.566
1.550
1.542
1.531
1.525
1.511
1.486
1.466
1.446
1.400
1.386
1.368
1.349
1.331
1.313
1.294
1.284
1.167
1.146
1.126
1.104
1.083
1.063
SnBu3
H
OH
2q
NAME yjl-nk-182-h
EXPNO 10
PROCNO 1
Date_ 20180914
Time 23.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0899966 sec
RG 30.81
DW 62.400 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 ppm
1.660
1.605
1.981
1.638
2.106
3.080
6.110
7.176
6.355
9.295

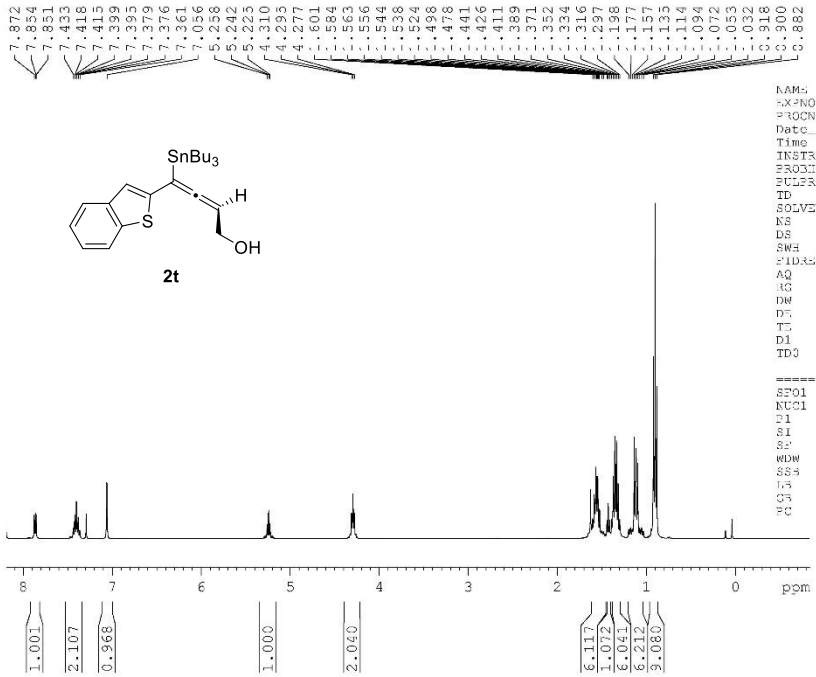

202.637
138.126
137.992
128.536
128.436
127.173
124.949
99.632
87.668
61.657
28.931
27.230
21.426
13.677
11.156
SnBu3
H
OH
2q
NAME yjl-nk-182-c
EXPNO 11
PROCNO 1
Date_ 20180914
Time 23.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

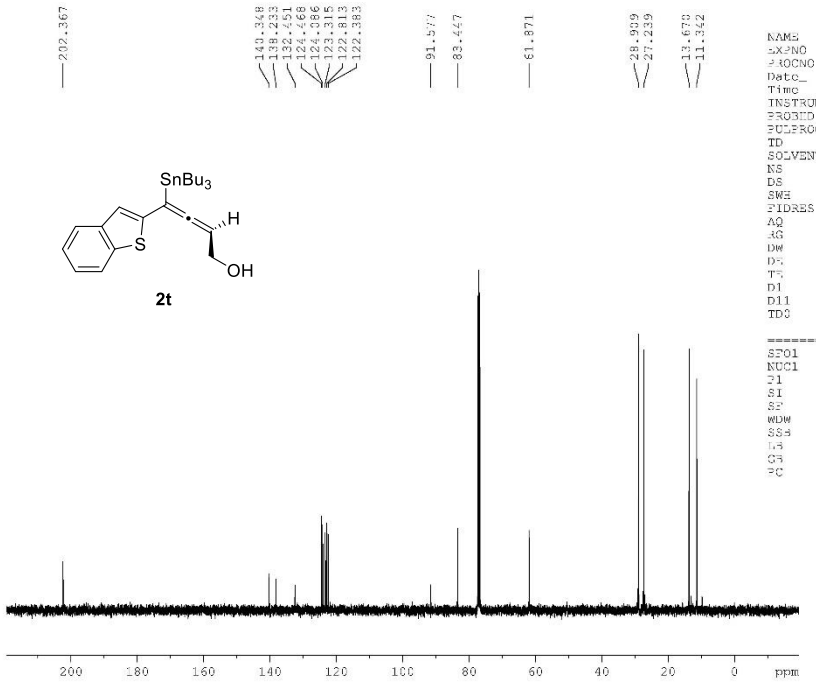

SnBu3
H
OH
2r
NAME yjl-hk-205-h
EXPNO 10
PROCNO 1
Date_ 20180918
Time 18.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 38.81
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8 7 6 5 4 3 2 1 0 ppm
3.023
1.000
3.003
1.000
2.062
6.061
6.045
9.020

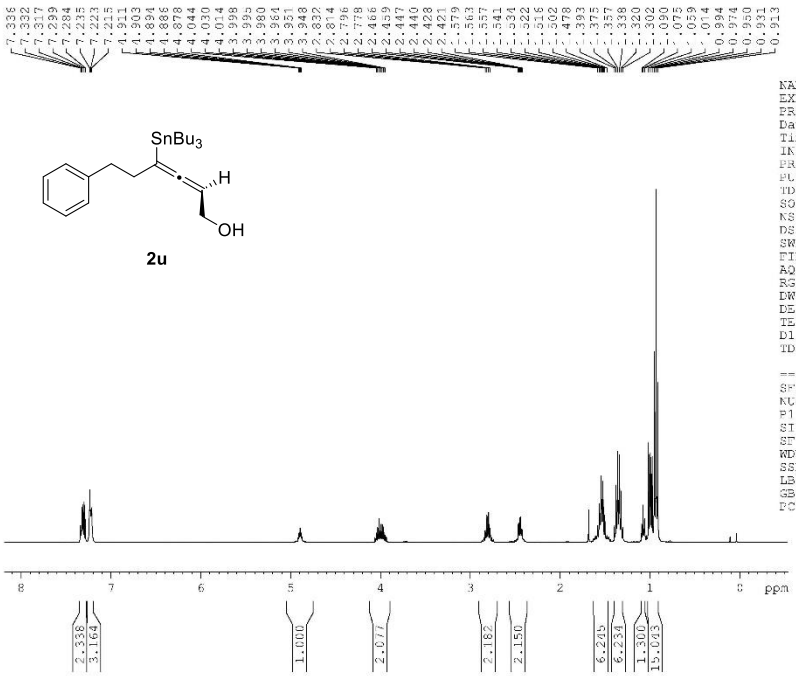

203.397
135.609
133.214
132.277
128.135
127.681
127.626
126.369
126.343
126.147
125.527
99.320
85.168
61.625
28.982
27.248
13.691
11.271
SnBu3
H
OH
2r
NAME yjl-hk-205-c
EXPNO 11
PROCNO 1
Date_ 20180918
Time 18.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

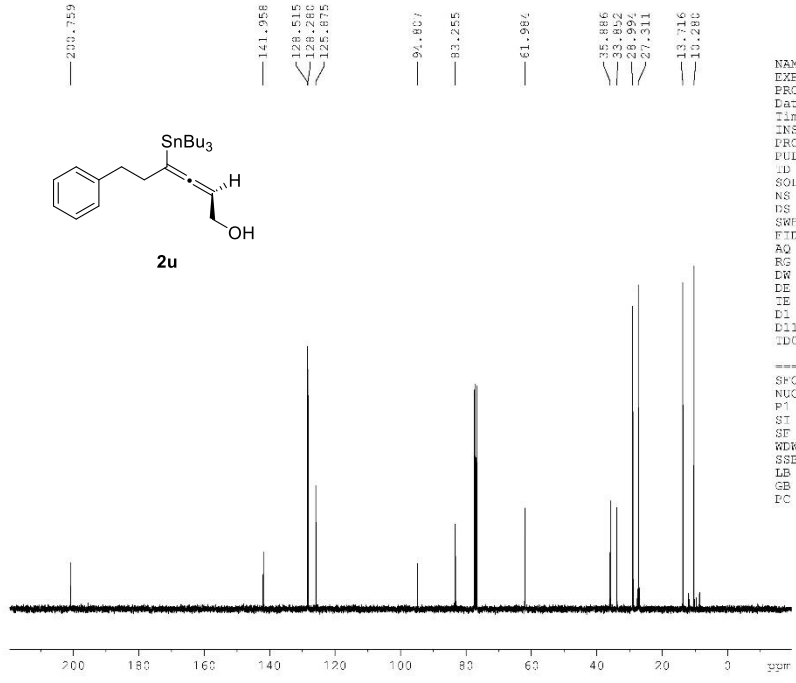

7.284
7.277
7.270
7.265
7.258
7.094
7.091
7.082
7.079
6.953
6.948
5.255
5.233
5.216
5.200
4.255
4.240
4.225
4.217
4.210
4.201
4.194
4.186
4.171
1.647
1.626
1.600
1.583
1.577
1.561
1.554
1.542
1.536
1.522
1.496
1.477
1.458
1.396
1.378
1.360
1.341
1.323
1.305
1.289
1.185
1.163
1.144
1.121
1.107
1.100
1.080
1.068
1.059
1.037
1.017
0.933
0.914
0.896
SnBu3
H
S
OH
2s
NAME yjl-nk-243-h
EXPNO 10
PROCNO 1
Date_ 20180920
Time 18.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 15.66
DW 62.400 use
DE 6.50 use
TE 297.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 use
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8 7 6 5 4 3 2 1 0 ppm
1.127
3.976
3.975
1.000
2.083
7.142
6.196
6.327
9.141

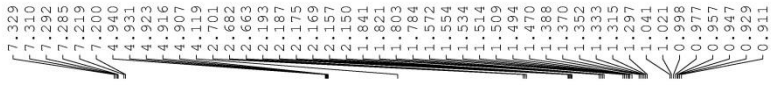

203.157
138.902
127.468
125.461
120.697
92.805
84.551
61.538
28.929
27.240
13.673
11.003
SnBu3
H
S
OH
2s
NAME yjl hk 243 c
EXPNO 11
PROCNO 1
Date 20180920
Time 18.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm


7.872
7.854
7.851
7.433
7.418
7.415
7.399
7.395
7.379
7.376
7.361
7.056
5.258
5.242
5.225
4.310
4.293
4.277
4.601
4.584
4.563
4.556
4.544
4.538
4.524
4.498
4.478
4.441
4.426
4.411
4.389
4.371
4.352
4.334
4.316
4.297
4.198
4.177
4.157
4.135
4.114
4.094
4.072
4.053
4.032
3.918
3.900
3.882
SnBu3
H
S
OH
2t
NAME yjl-hk-252-h
EXPNO 10
PROCNO 1
Date_ 20180412
Time 13.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 30.81
DW 62.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8
7
6
5
4
3
2
1
0
ppm
1.001
2.107
0.968
1.000
2.040
6.117
1.072
6.041
6.212
9.080

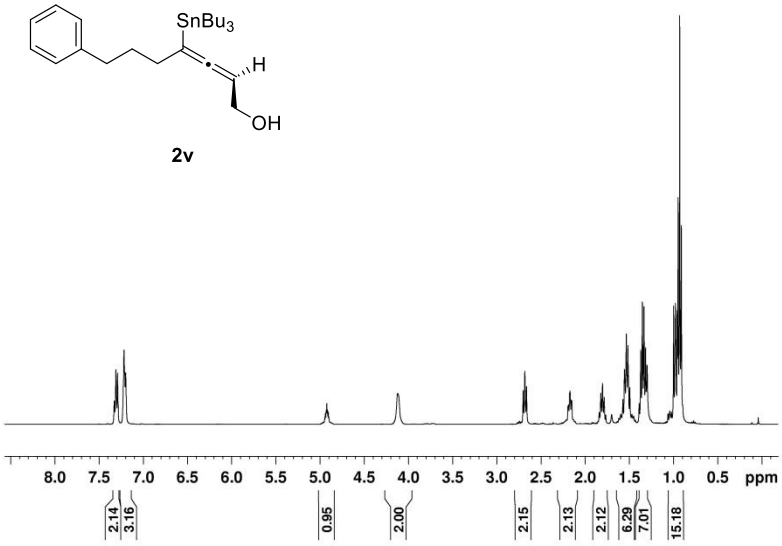

202.367
140.348
138.233
132.761
124.768
124.386
123.315
122.813
122.383
91.577
83.447
61.871
28.939
27.239
13.678
11.342
SnBu3
H
S
OH
2t
NAME yjl-hk-252-c
EXPNO 11
PROCNO 1
Date_ 20180412
Time 19.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm


7.336
7.332
7.317
7.299
7.284
7.235
7.223
7.215
4.911
4.903
4.894
4.886
4.878
4.044
4.030
4.014
3.998
3.995
3.980
3.964
3.951
3.948
2.832
2.814
2.796
2.778
2.466
2.459
2.447
2.440
2.428
2.421
2.379
2.363
2.357
2.341
2.334
2.322
2.315
2.302
2.478
2.393
2.375
2.357
2.338
2.320
2.302
2.090
2.075
2.059
2.014
0.994
0.974
0.960
0.931
0.913
SnBu3
H
OH
2u
NAME yjl-hk-476-h
EXPNO 10
PROCNO 1
Date_ 20180920
Time 18.43
INSTRUM spec
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 0
SWH 8012.820 Hz
FIDRES 0.122265 Hz
AQ 4.0894966 sec
RG 2.43
DW 62.400 use
DE 6.50 use
TE 297.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.33 use
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8
7
6
5
4
3
2
1
0
ppm
2.338
3.164
1.000
2.077
2.182
2.150
6.245
6.234
1.300
15.003

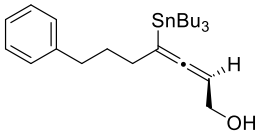

200.759
141.958
128.515
128.280
125.875
94.807
83.255
61.984
35.886
33.852
28.994
27.311
13.716
10.280
SnBu3
H
OH
2u
NAME yjl-hk-476-c
EXPNO 11
PROCNO 1
Date_ 20180920
Time 18.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 4
SWH 24038.46
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 use
DE 6.50 use
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 100.6228293 MHz
NUC1 13C
P1 9.3 use
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm



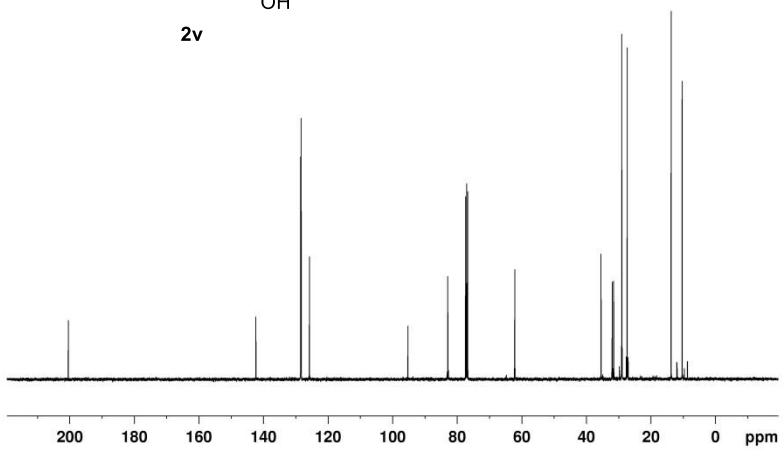
2v




```
NAME          yjl-hk-396-h
EXPNO                   10
PROCNO                   1
Date_             20200916
Time                 19.04
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       4
DS                       2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894966 sec
RG                    12.35
DW                  62.400 usec
DE                   6.50 usec
TE                  297.4 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                    1H
P1                    9.99 usec
SI                   65536
SF              400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

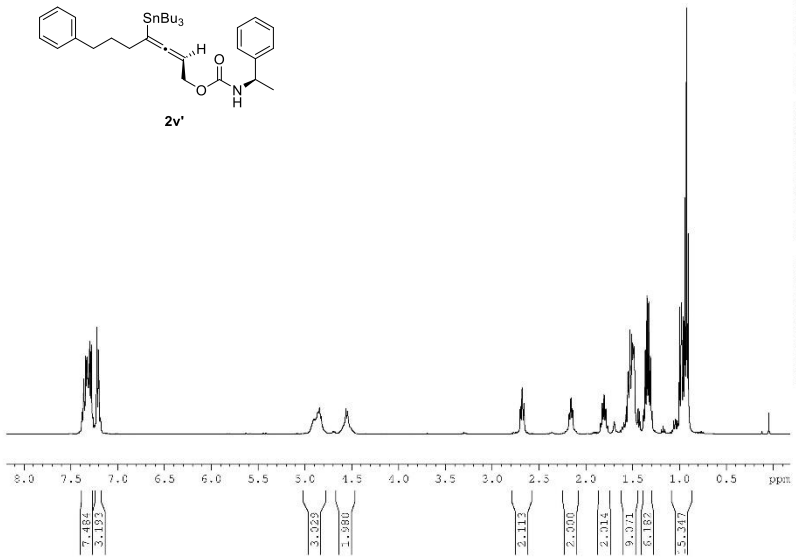


2v

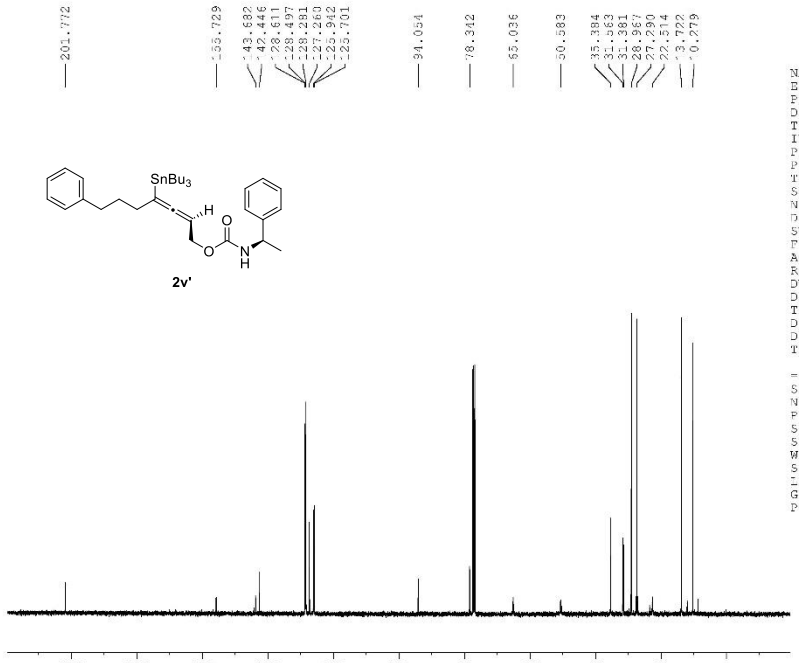



```
NAME          yjl-hk-396-c
EXPNO                   11
PROCNO                   1
Date_             20200916
Time                 19.35
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     512
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                   197.54
DW                  20.800 usec
DE                   6.50 usec
TE                  298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            100.6228293 MHz
NUC1                    13C
P1                    9.31 usec
SI                   32768
SF              100.6127685 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

2v'

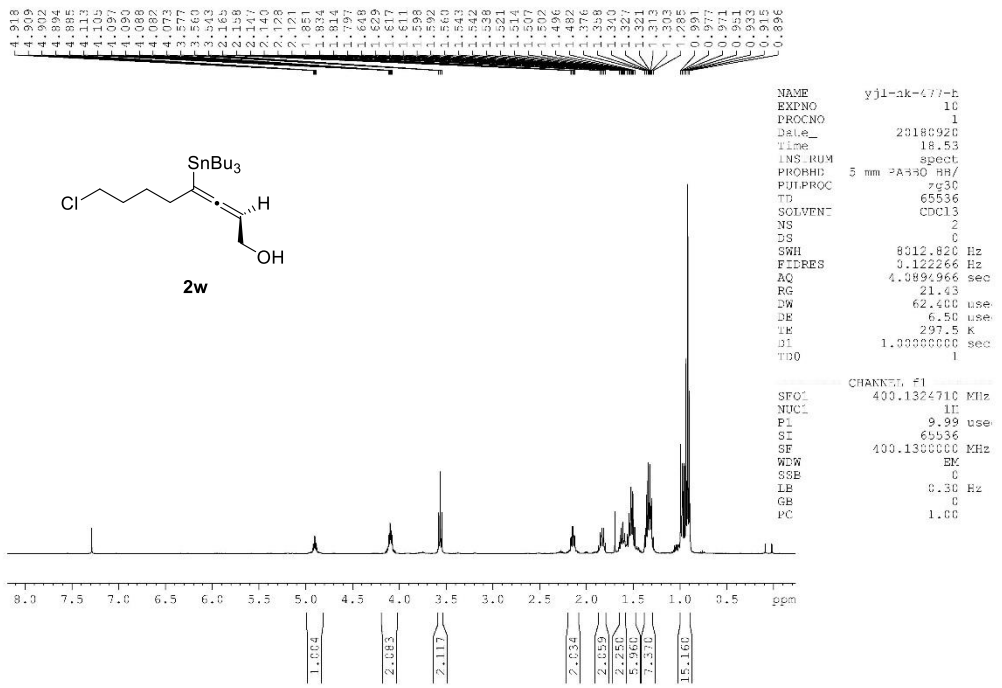


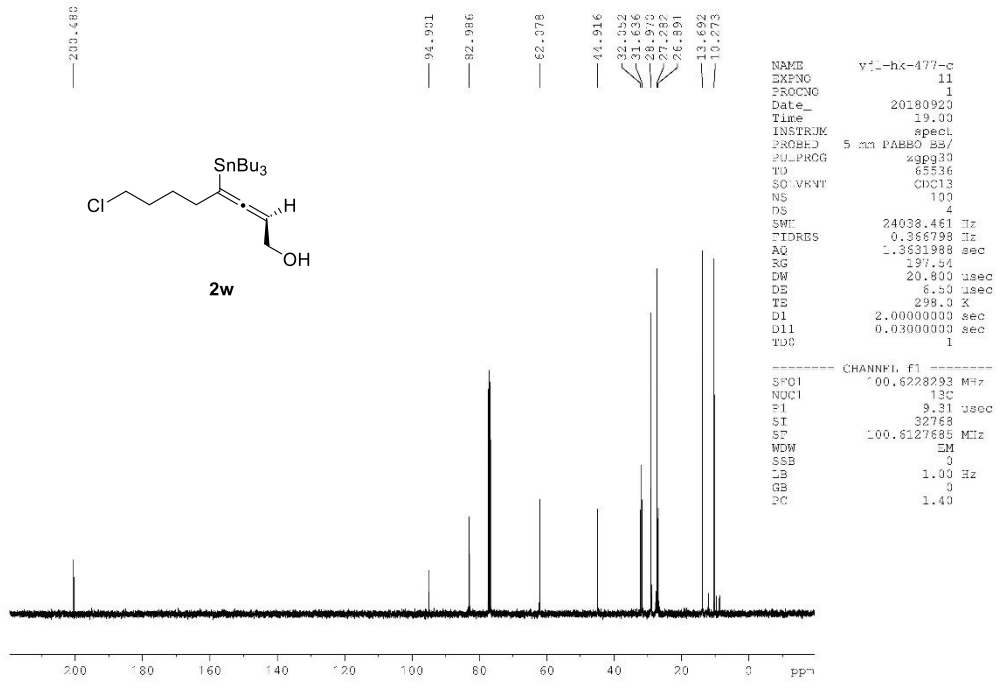
```
NAME        yjl-hk-474-h-3
EXPNO               10
PROCNO               1
Date_         20181016
Time             13.45
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG          zg30
TD              65536
SOLVENT          CDCl3
NS                   4
DS                   0
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG                30.81
DW               62.400 use
DE                6.50 use
TE              297.8 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                9.99 use
SI                65536
SF          400.1300000 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

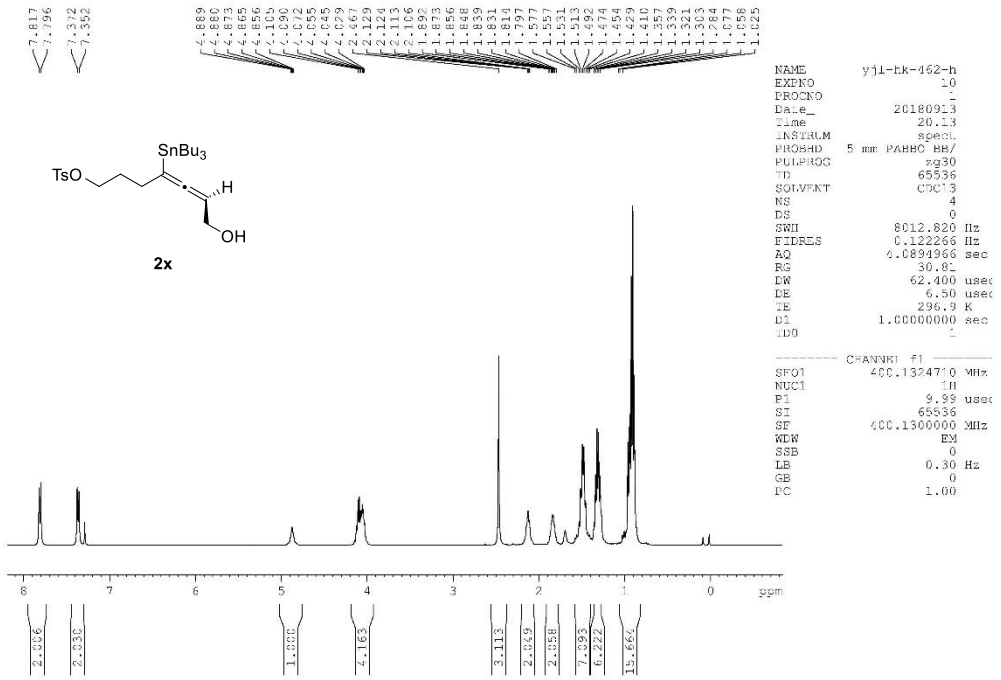


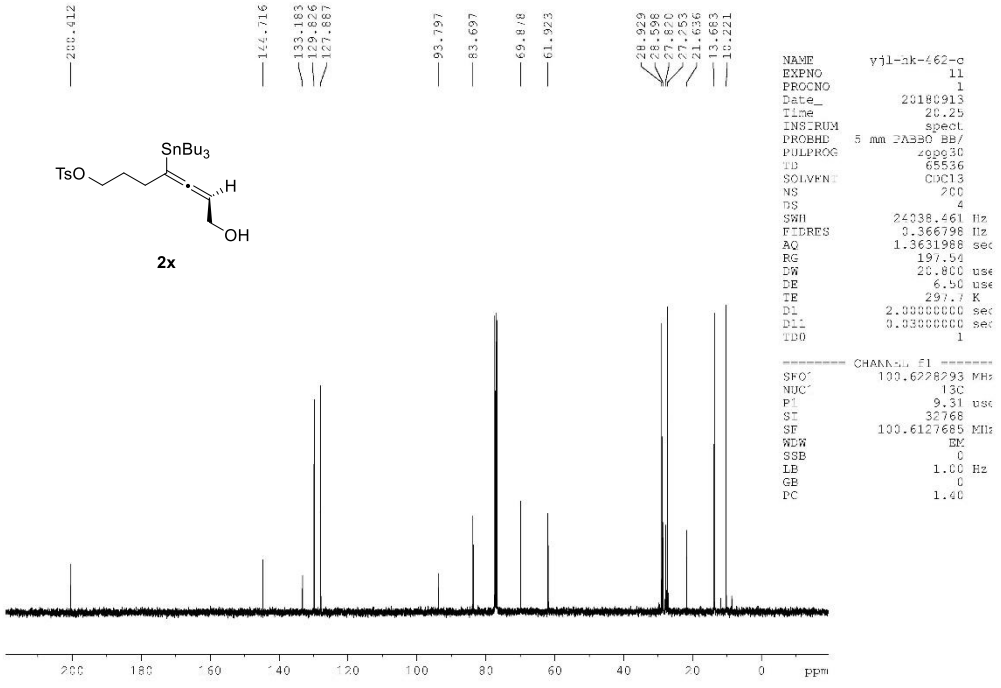
2v'

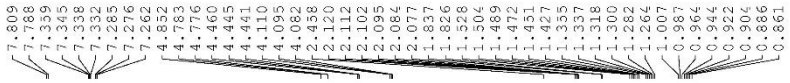

```
NAME        YCL-HK-474-C-3
EXPNO               10
PROCNO               1
Date_         20181016
Time             17.50
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD              65536
SOLVENT          CDCl3
NS                 328
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 se
RG               197.54
DW               20.800 us
DE                6.50 us
TE              298.5 K
D1            2.00000000 se
D11           0.03000000 se
TD0                  1

======== CHANNEL f1 ======
SFO1        100.6228293 MH
NUC1                13C
P1                9.31 us
SI                32768
SF          100.6127685 MH
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

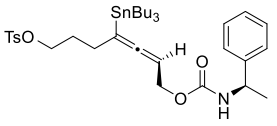

4.918
4.909
4.902
4.894
4.885
4.113
4.105
4.097
4.090
4.088
4.082
4.073
3.577
3.560
3.543
2.165
2.158
2.147
2.140
2.128
2.121
1.851
1.834
1.814
1.797
1.648
1.629
1.617
1.611
1.598
1.592
1.560
1.543
1.538
1.521
1.514
1.507
1.502
1.496
1.482
1.376
1.358
1.340
1.327
1.321
1.313
1.303
1.285
0.991
0.977
0.971
0.951
0.933
0.915
0.896
SnBu3
Cl
H
OH
2w
NAME yji-nk-477-h
EXPNO 10
PROCNO 1
Date_ 20180920
Time 18.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 21.43
DW 62.400 use
DE 6.50 use
TE 297.5 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 use
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.000
2.083
2.117
2.034
2.059
2.250
5.960
7.370
15.160


200.488
94.931
82.986
62.078
44.916
32.052
31.636
28.978
27.282
26.891
13.692
10.273
SnBu3
Cl
H
OH
2w
NAME yji-hk-477-c
EXPNO 11
PROCNO 1
Date_ 20180920
Time 19.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

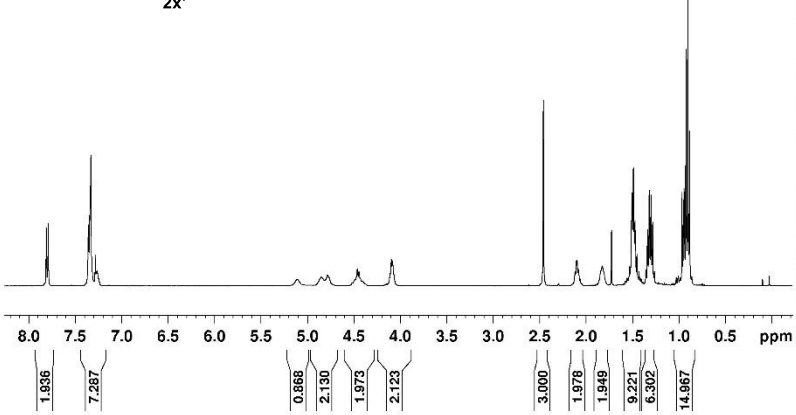

7.817
7.796
7.372
7.352
4.889
4.880
4.873
4.865
4.856
4.105
4.090
4.072
4.055
4.045
4.029
2.467
2.129
2.124
2.113
2.106
1.892
1.873
1.856
1.848
1.839
1.831
1.814
1.797
1.577
1.557
1.531
1.513
1.492
1.474
1.454
1.429
1.410
1.357
1.339
1.321
1.303
1.284
1.077
1.058
1.025
SnBu3
TsO
H
OH
2x
NAME yjl-hk-462-h
EXPNO 10
PROCNO 1
Date_ 20180913
Time 20.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 30.81
DW 62.400 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8
7
6
5
4
3
2
1
0
ppm
2.026
2.036
1.000
4.163
3.113
2.049
2.058
7.093
6.222
15.662


208.412
144.716
133.183
129.826
127.867
93.797
83.697
69.878
61.923
28.929
28.598
27.820
27.253
21.636
13.683
10.221
SnBu3
TsO
H
OH
2x
NAME yjl-hk-462-c
EXPNO 11
PROCNO 1
Date_ 20180913
Time 20.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 use
DE 6.50 use
TE 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 use
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

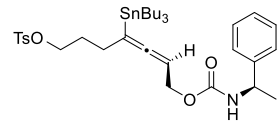




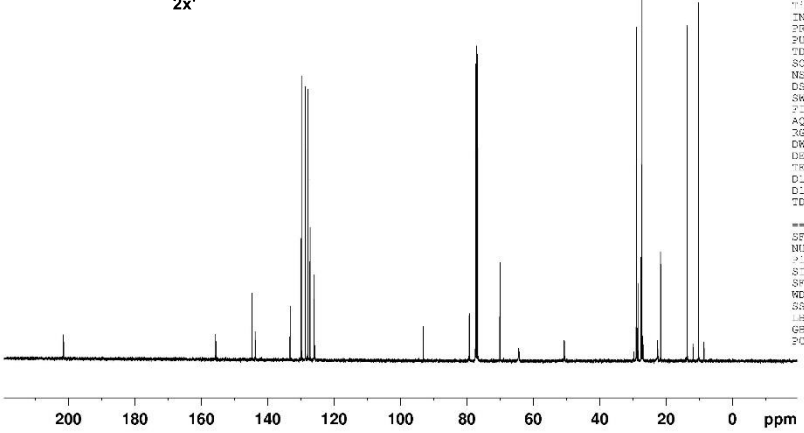
2x'



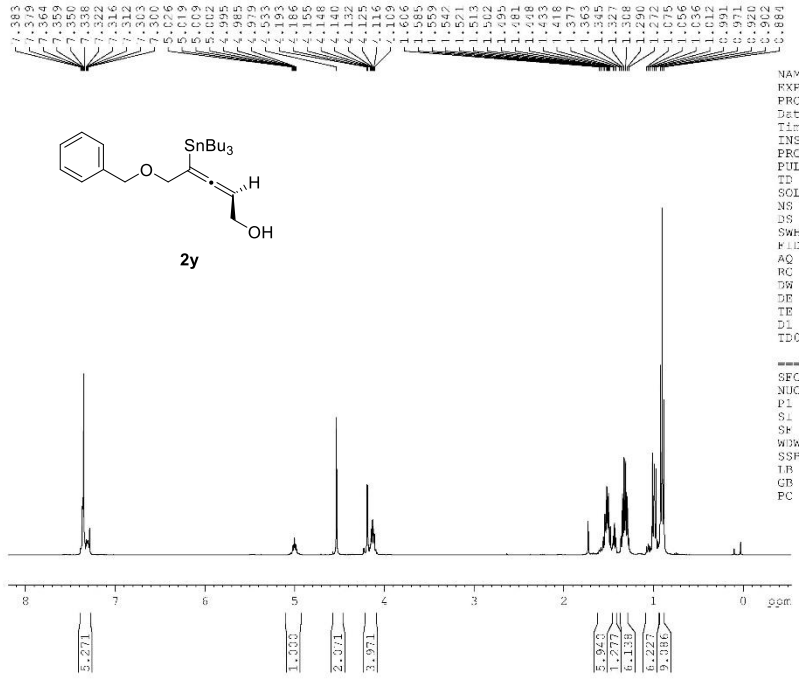

```
NAME        yjl-hk-446-h
EXPNO              10
PROCNO              1
Date_        20180824
Time            17.50
INSTRUM         spect
PROBHD   5 mm PABBO BB/
PULPROG         zg30
TD              65536
SOLVENT         CDCl3
NS                  4
DS                  0
SWH          8012.820 Hz
FIDRES       0.122256 Hz
AQ           4.0894966 sec
RG               21.23
DW              62.400 use
DE               6.50 use
TE             298.8 K
D1          1.00000000 sec
TD0                 1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1               1H
P1                9.99 use
SI              65536
SF        400.1300000 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```

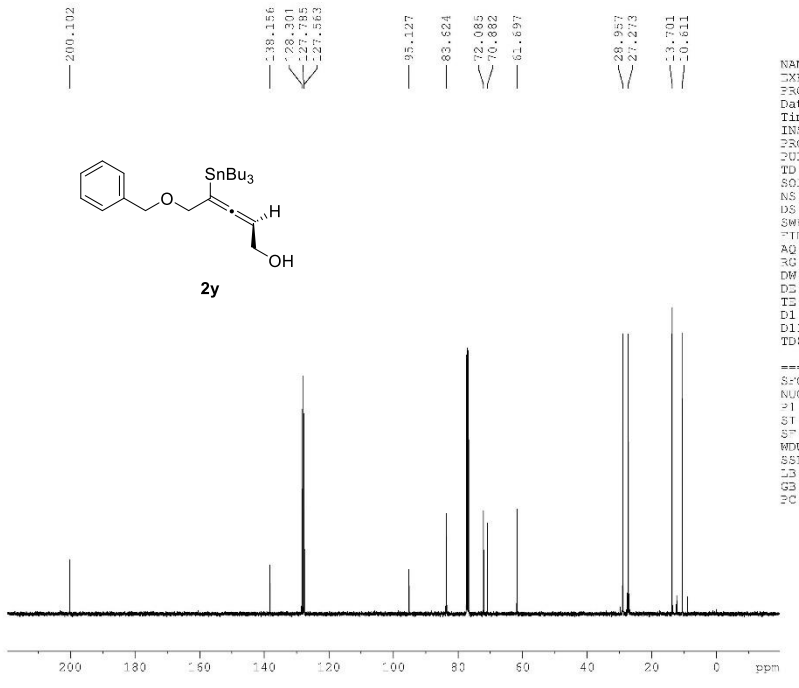


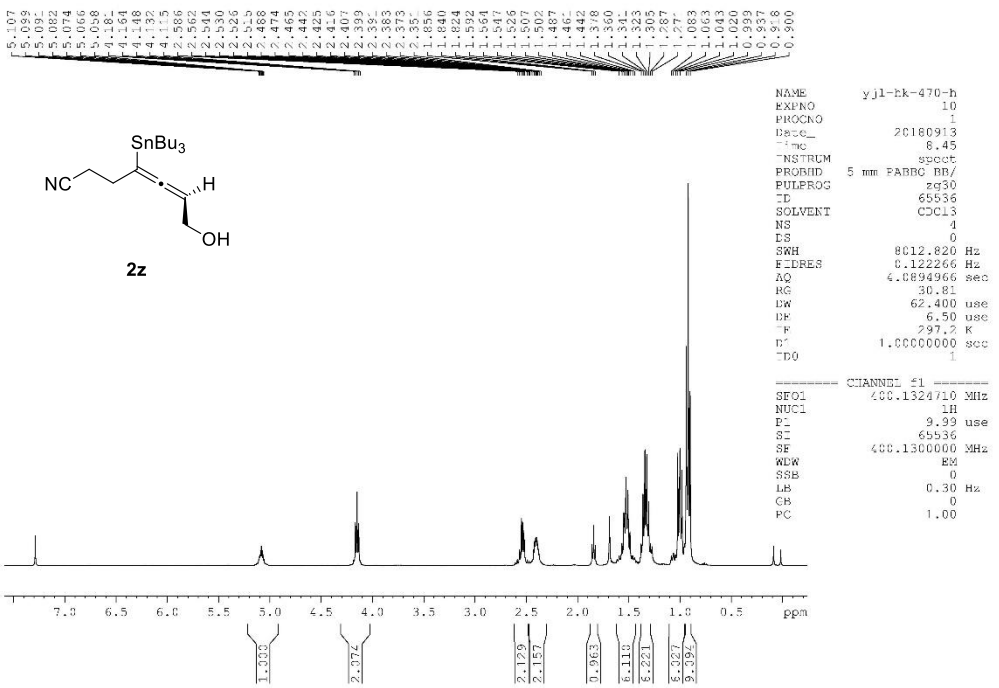
2x'

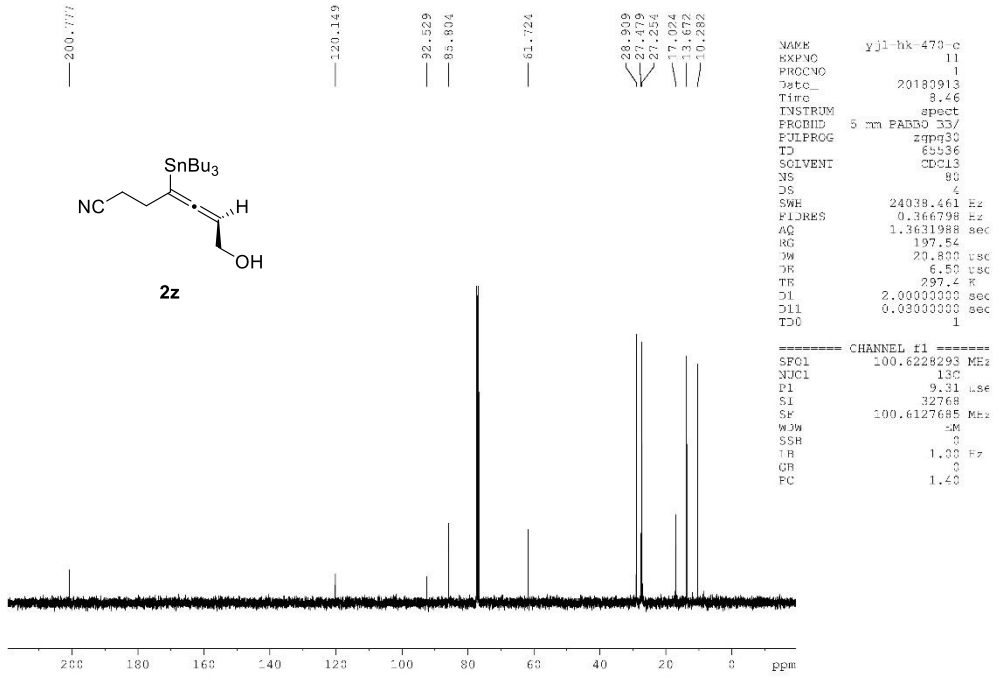


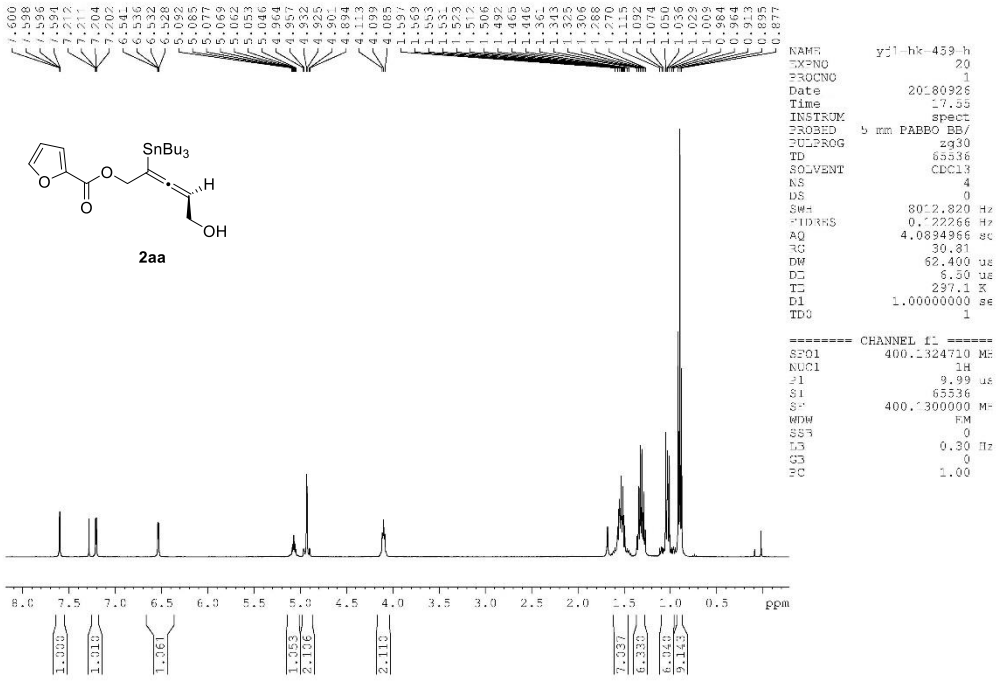

```
NAME        yjl-hk-446-h
EXPNO              11
PROCNO              1
Date_        20180824
Time            18.49
INSTRUM         spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              65536
SOLVENT         CDCl3
NS               1024
DS                  4
SWH         24038.461 Hz
FIDRES       0.366798 Hz
AQ           1.3631988 sec
RG              197.24
DW             20.800 usec
DE              6.50 usec
TE             299.5 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                 1

======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1               13C
P1                9.31 usec
SI              32768
SF        100.6127685 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

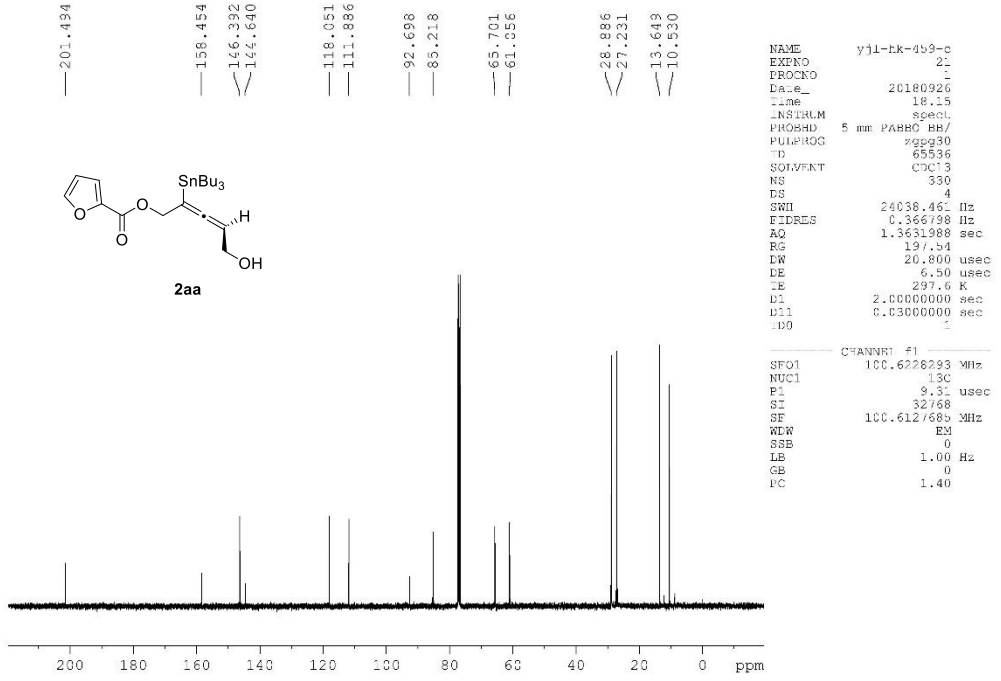

7.383
7.379
7.364
7.359
7.350
7.338
7.322
7.316
7.312
7.303
7.300
5.026
5.019
5.009
5.002
4.995
4.985
4.979
4.533
4.193
4.186
4.155
4.148
4.140
4.132
4.125
4.116
4.109
1.606
1.585
1.559
1.542
1.521
1.513
1.502
1.495
1.481
1.448
1.433
1.418
1.377
1.363
1.345
1.327
1.308
1.290
1.272
1.075
1.056
1.036
1.012
0.991
0.971
0.920
0.902
0.884
SnBu3
O
H
OH
2y
NAME yjl hk 461 h
EXPNO 10
PROCNO 1
Date 20180912
Time 21.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 30.81
DW 62.400 use
DE 6.50 use
TE 297.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 use
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8
7
6
5
4
3
2
1
0
ppm
5.271
1.000
2.071
3.971
5.943
1.277
6.138
6.227
9.086

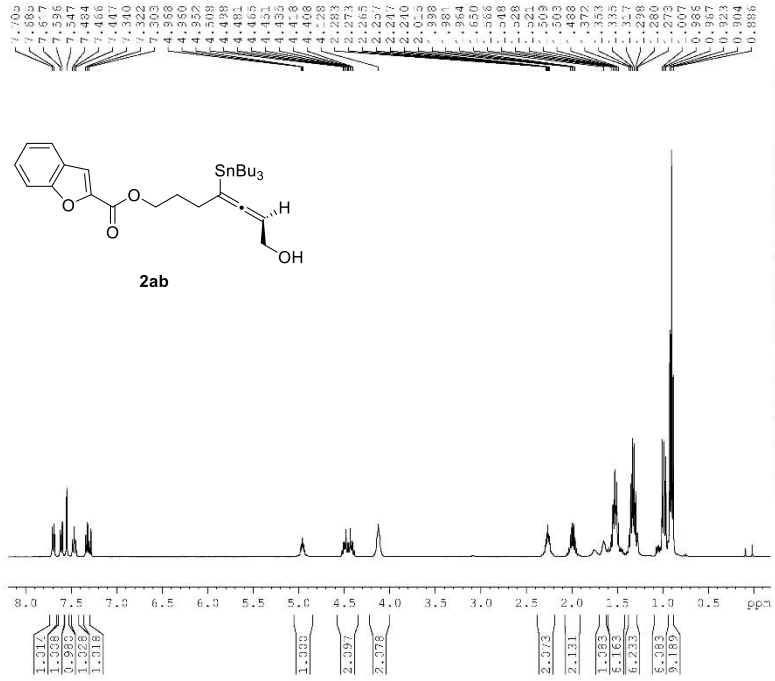

200.102
138.156
128.391
127.785
127.563
95.127
83.624
72.085
70.882
61.697
28.957
27.273
13.701
10.611
SnBu3
O
H
OH
2y
NAME yjl-hk-461-c
EXPNO 11
PROCNO 1
Date 20180912
Time 21.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 use
DE 6.50 use
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 use
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

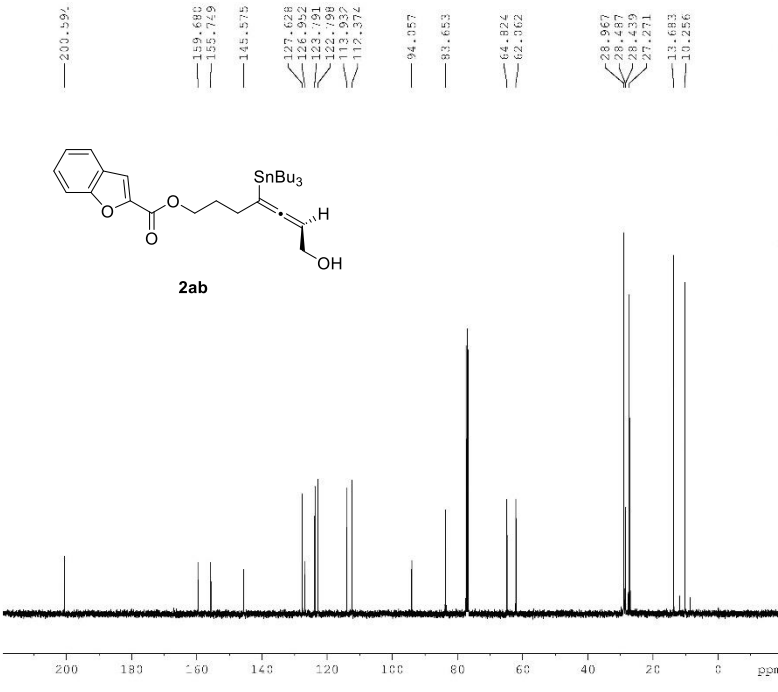

SnBu3
NC
H
OH
2z
NAME yjl-hk-470-h
EXPNO 10
PROCNO 1
Date_ 20180913
Time 8.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 30.81
DW 62.400 use
DE 6.50 use
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 use
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.000
2.072
2.129
2.157
0.963
6.118
6.221
6.327
9.395

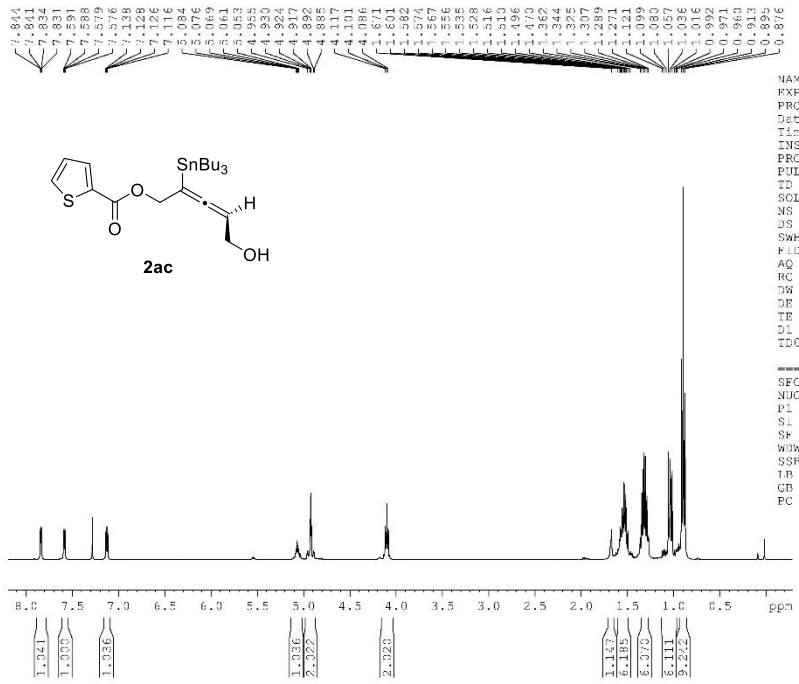

200.777
120.149
92.529
85.804
61.724
28.999
27.479
27.254
17.024
13.672
10.282
SnBu3
NC
H
OH
2z
NAME yjl-hk-470-c
EXPNO 11
PROCNO 1
Date_ 20180913
Time 8.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 88
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 use
DE 6.50 use
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 use
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

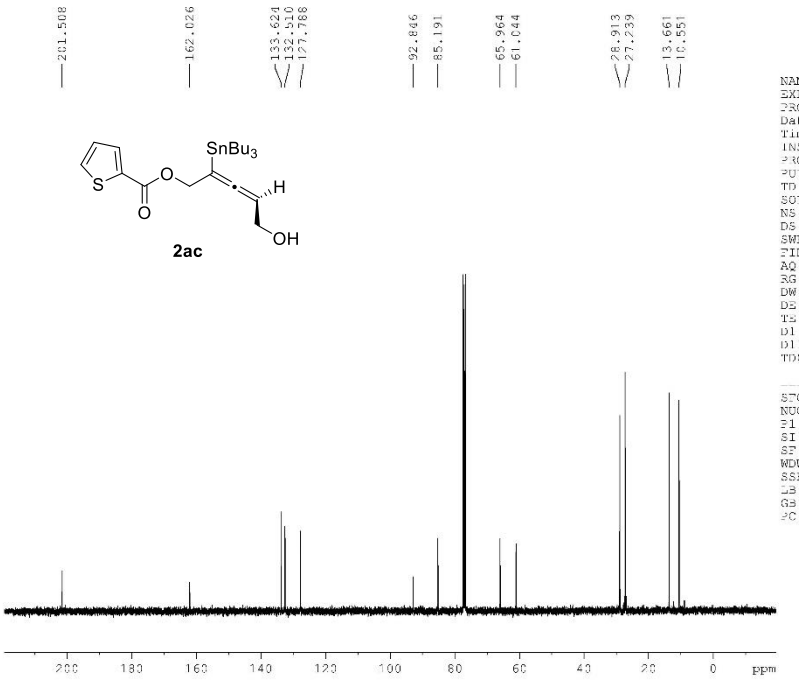

7.600
7.598
7.596
7.594
7.212
7.211
7.204
7.202
6.541
6.536
6.532
6.528
5.092
5.085
5.077
5.069
5.062
5.053
5.046
4.964
4.957
4.932
4.925
4.901
4.894
4.113
4.099
4.085
1.597
1.563
1.553
1.531
1.523
1.506
1.492
1.465
1.446
1.361
1.343
1.325
1.286
1.276
1.215
1.092
1.074
1.050
1.036
1.029
1.009
0.984
0.964
0.913
0.895
0.877
SnBu3
O
O
O
H
OH
2aa
NAME yjl-hk-459-h
EXPNO 20
PROCNO 1
Date 20180926
Time 17.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 30.81
DW 62.400 us
DE 6.50 us
TE 297.1 K
D1 1.00000000 se
TD0 1
======== CHANNEL f1 ======
SFO1 400.1324710 MH
NUC1 1H
P1 9.99 us
SI 65536
SF 400.1300000 MH
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.000
1.010
1.261
1.953
2.136
2.116
7.037
6.338
6.046
9.143

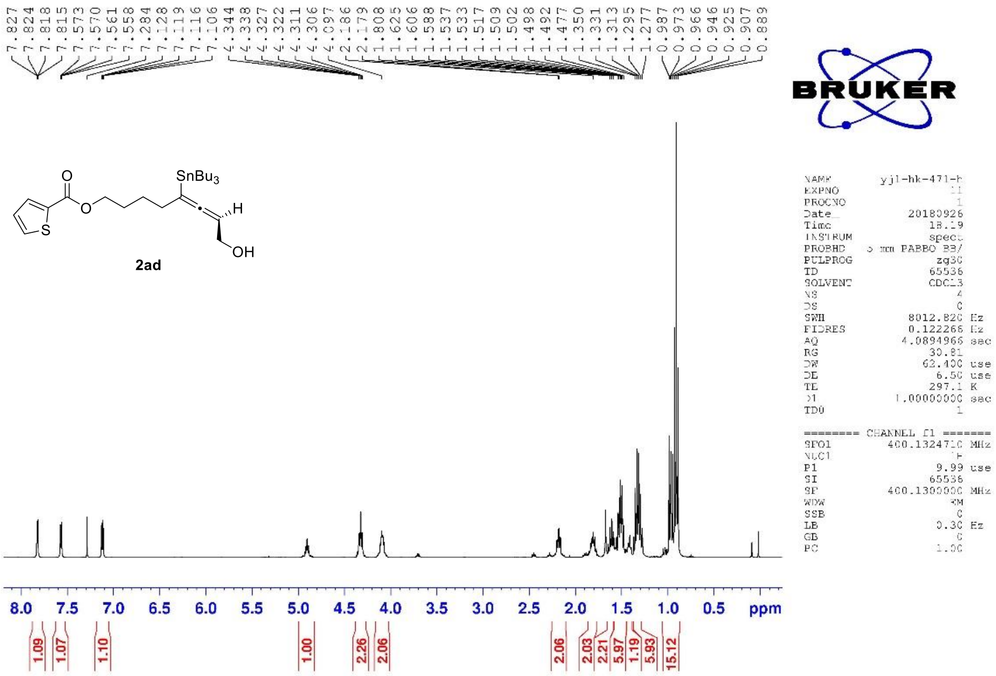

201.494
158.454
146.392
142.640
118.051
111.886
92.698
85.218
65.701
61.956
28.886
27.231
13.649
10.530
SnBu3
O
O
O
H
OH
2aa
NAME yjl-hk-459-c
EXPNO 2
PROCNO 1
Date_ 20180926
Time 18.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 330
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127680 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

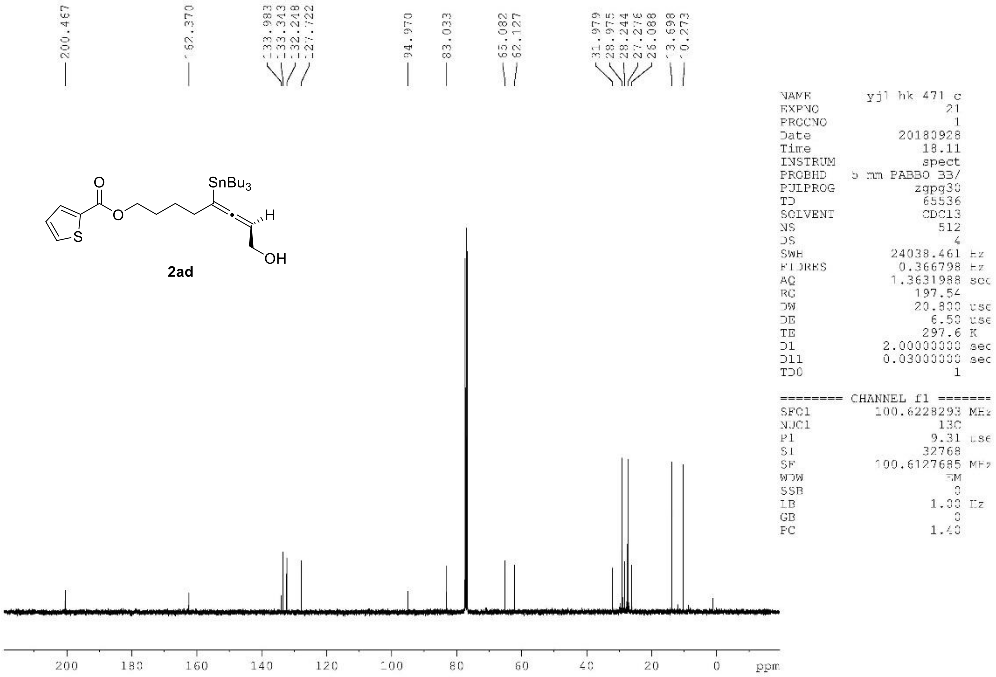

SnBu3
H
O
O
OH
2ab

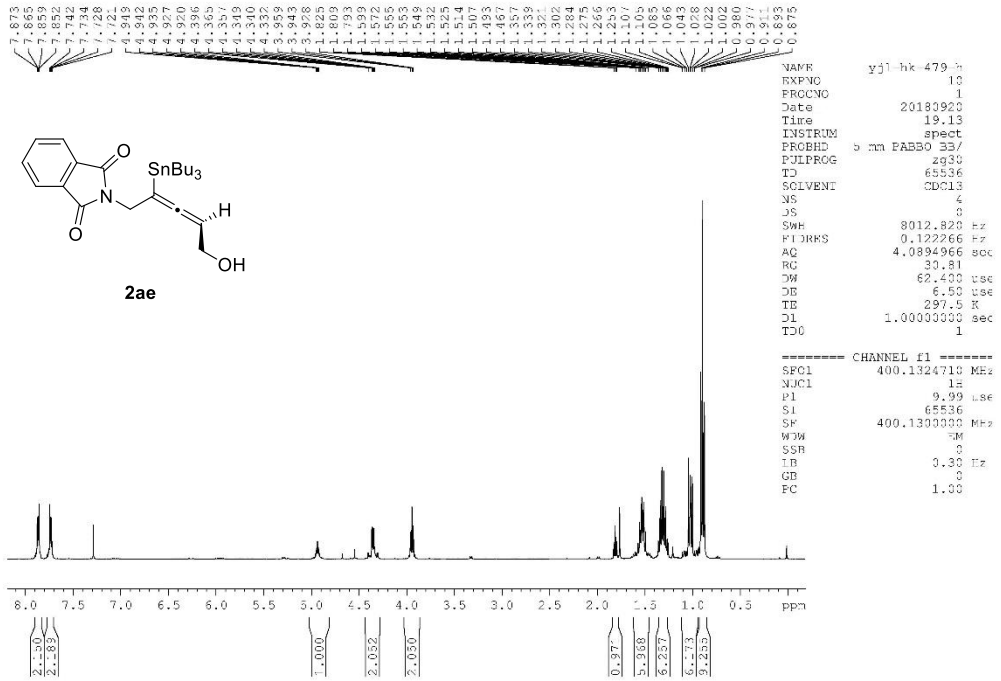

SnBu3
H
O
O
OH
2ab

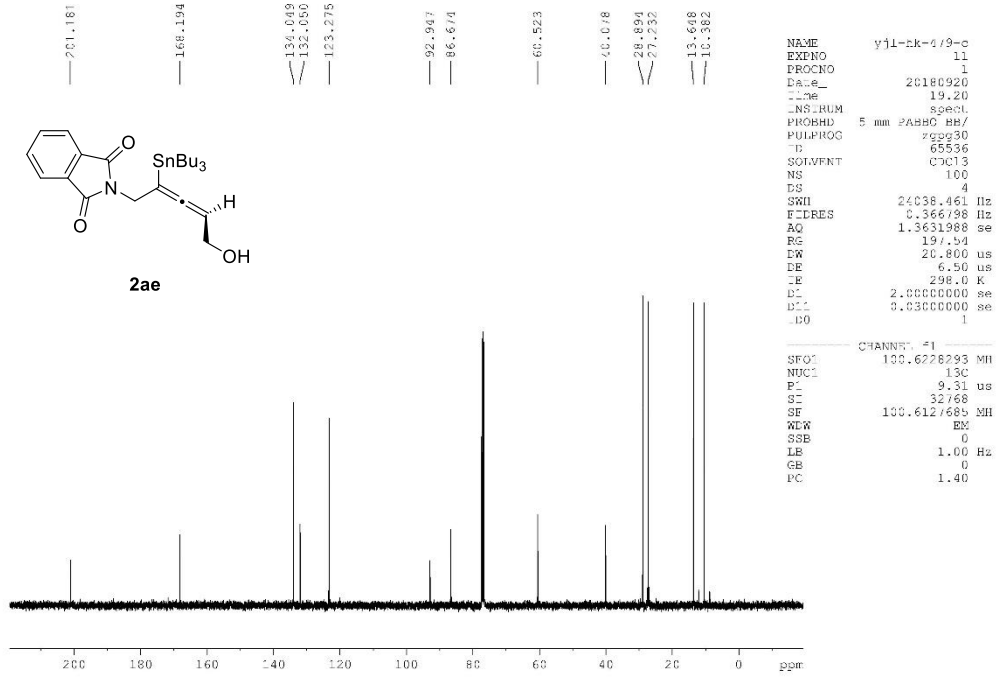

7.844
7.841
7.834
7.831
7.591
7.588
7.579
7.576
7.138
7.128
7.116
5.084
5.076
5.069
5.061
5.053
4.955
4.930
4.924
4.917
4.892
4.885
4.117
4.101
4.086
1.671
1.601
1.582
1.574
1.567
1.556
1.535
1.528
1.516
1.510
1.496
1.470
1.362
1.344
1.335
1.307
1.289
1.271
1.121
1.099
1.080
1.057
1.036
1.016
0.992
0.971
0.960
0.913
0.895
0.876
SnBu3
S
O
O
H
OH
2ac
NAME yjl hk 460 h 1
EXPNO 10
PROCNO 1
Date 20180913
Time 20.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 30.81
DW 62.400 use
DE 6.50 use
TE 297.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 use
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.941
1.936
1.936
1.036
2.322
2.028
1.147
6.185
6.379
6.111
9.222

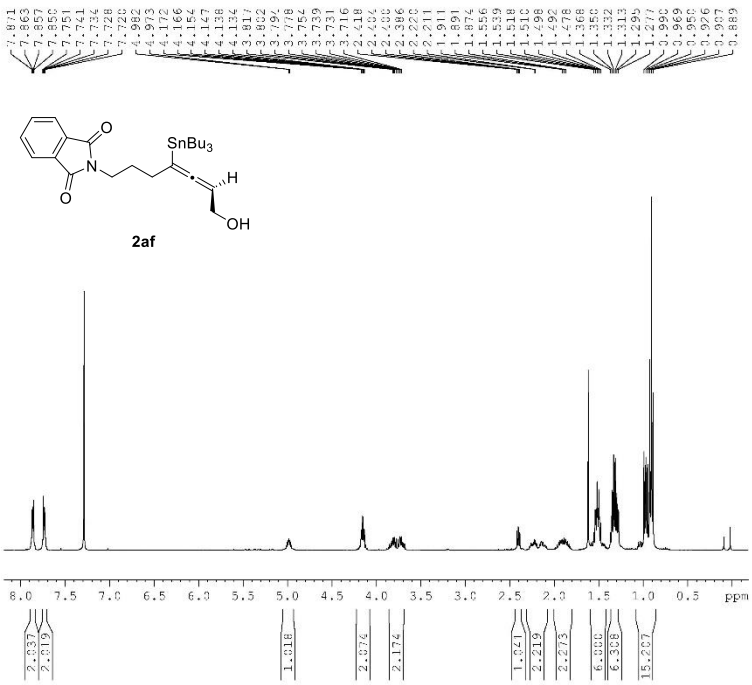

201.508
162.026
133.624
132.510
127.788
92.866
85.191
65.964
61.044
28.913
27.239
13.661
10.551
SnBu3
S
O
O
H
OH
2ac
NAME yjl-hk-460-c-1
EXPNO 11
PROCNO 1
Date_ 20180913
Time 20.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 use
DE 6.50 use
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 use
SI 32768
SF 100.6127689 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm


SnBu3
OH
S
2ad
BRUKER
NAME yjl-hk-471-h
EXPNO 11
PROCNO 1
Date_ 20180926
Time 18.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 30.81
DW 62.400 use
DE 6.50 use
TE 297.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 use
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.09 1.07 1.10 1.00 2.26 2.06 2.06 2.03 2.21 5.97 1.19 5.93 15.12

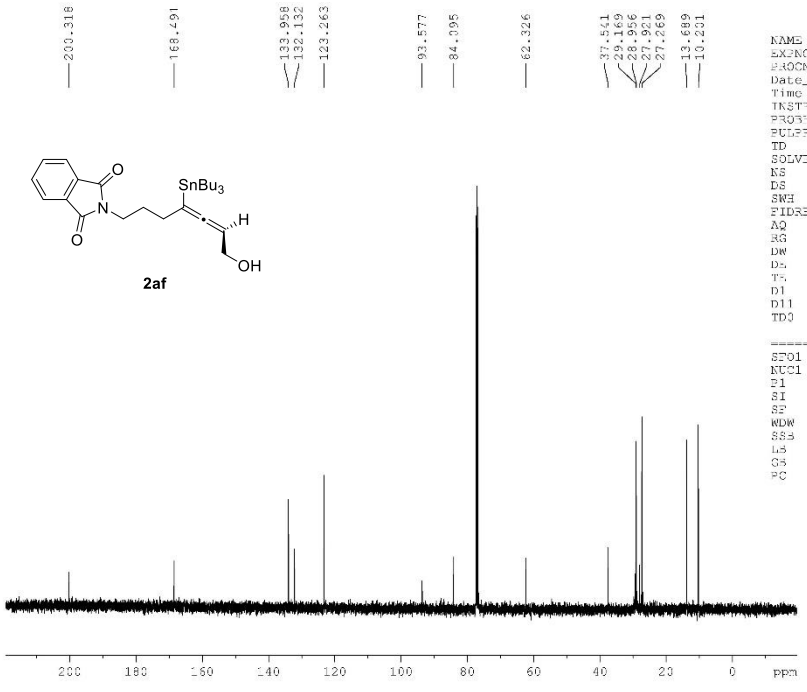

200.467
162.370
133.983
133.343
132.248
127.722
94.970
83.033
65.082
62.127
31.979
28.975
28.244
27.276
26.088
13.698
10.273
SnBu3
OH
S
2ad
NAME yjl hk 471 c
EXPNO 21
PROCNO 1
Date_ 20180928
Time 18.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 use
DE 6.50 use
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 use
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm


SnBu3
H
OH
2ae

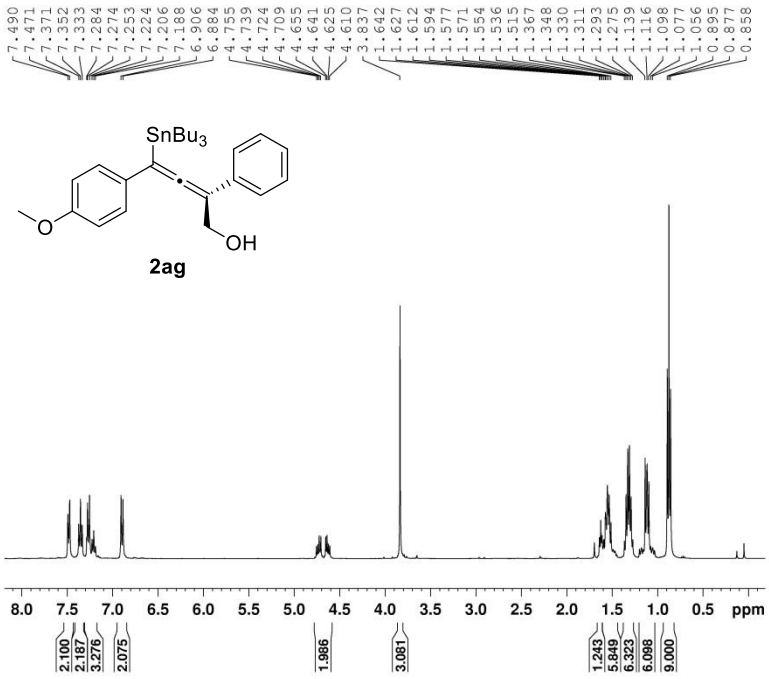

SnBu3
H
OH
2ae




```
NAME          yjl-hk-478-h-1
EXPNO                    10
PROCNO                    1
Date_              20181011
Time                  17.16
INSTRUM               spect
PROBHD     5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       4
DS                       0
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894966 sec
RG                   71.18
DW                   62.400 usec
DE                    6.50 usec
TE                   298.5 K
D1                 1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                    1H
P1                    9.99 usec
SI                   65536
SF              400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

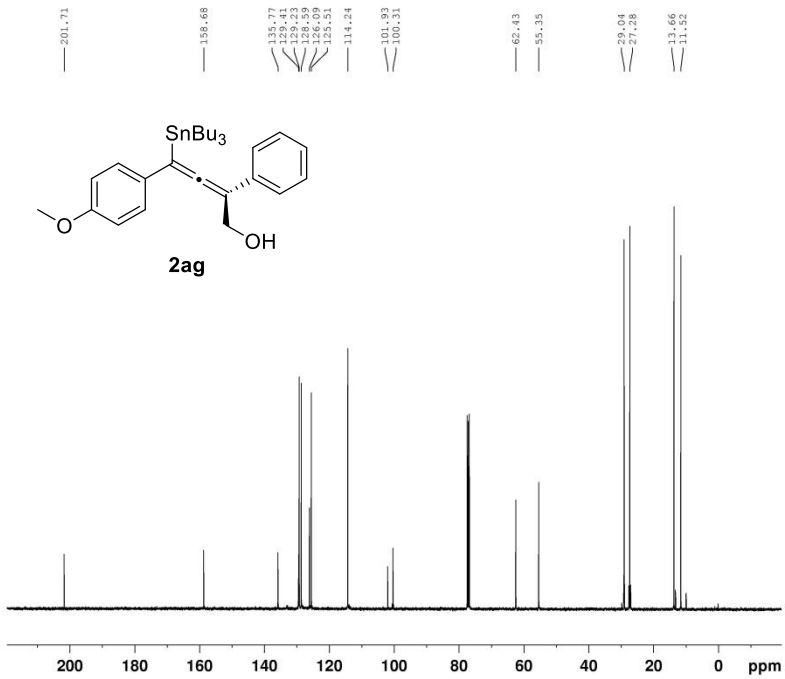



```
NAME          YJL-HK-478-C-3
EXPNO                    10
PROCNO                    1
Date_              20181016
Time                  17.18
INSTRUM               spect
PROBHD     5 mm PABBO BB/
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     200
DS                       4
SWH              24038.461 Hz
FIDRES               0.366798 Hz
AQ                1.3631988 sec
RG                   197.54
DW                   20.800 usec
DE                    6.50 usec
TE                   298.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            100.6228293 MHz
NUC1                    13C
P1                   9.31 usec
SI                   32768
SF              100.6127695 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



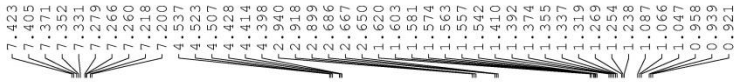
BRUKER

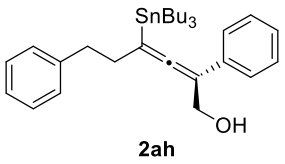
```
NAME          yjl-hk-718-h
EXPNO                   10
PROCNO                   1
Date_             20191203
Time                 21.07
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894966 sec
RG                     11.08
DW                    62.400 usec
DE                     6.50 usec
TE                   295.1 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                     1H
P1                     9.99 usec
SI                    65536
SF               400.1300000 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



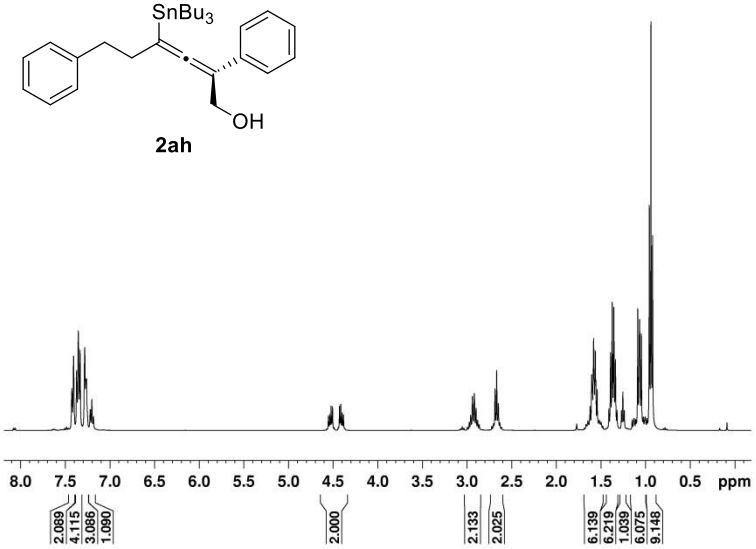
BRUKER

```
NAME          yjl-hk-718-c
EXPNO                   11
PROCNO                   1
Date_             20191203
Time                 21.37
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      512
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                    197.54
DW                    20.800 usec
DE                     6.50 usec
TE                   295.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             100.6228293 MHz
NUC1                     13C
P1                     9.31 usec
SI                    32768
SF               100.6127685 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

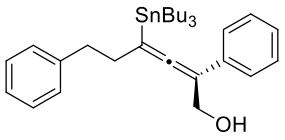




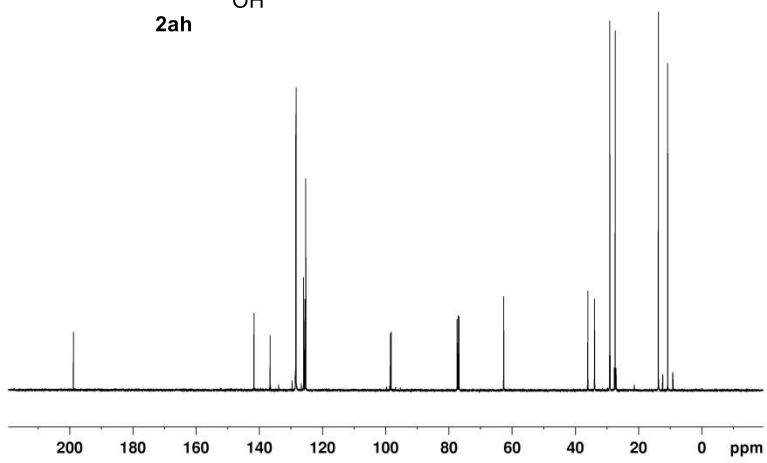
2ah



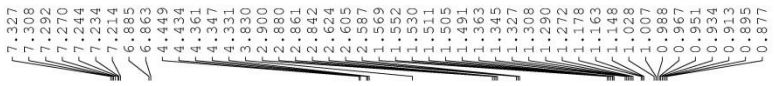

```
NAME          yjl-hk-719-h
EXPNO                   10
PROCNO                   1
Date_             20191211
Time                 20.05
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894966 sec
RG                   7.74
DW                62.400 usec
DE                 6.50 usec
TE                294.8 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                   1H
P1                   9.99 usec
SI                  65536
SF             400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

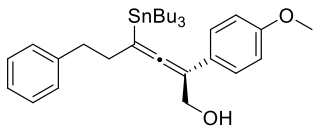


2ah

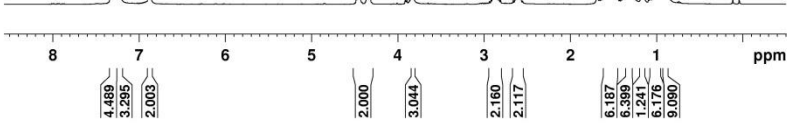



```
NAME          yjl-hk-719-c
EXPNO                   11
PROCNO                   1
Date_             20191211
Time                 20.19
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    218
DS                      4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631988 sec
RG                 197.54
DW                20.800 usec
DE                 6.50 usec
TE                295.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1           100.6228293 MHz
NUC1                   13C
P1                   9.31 usec
SI                  32768
SF             100.6127685 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

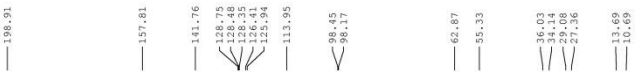


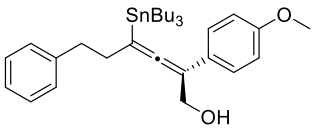


2ai

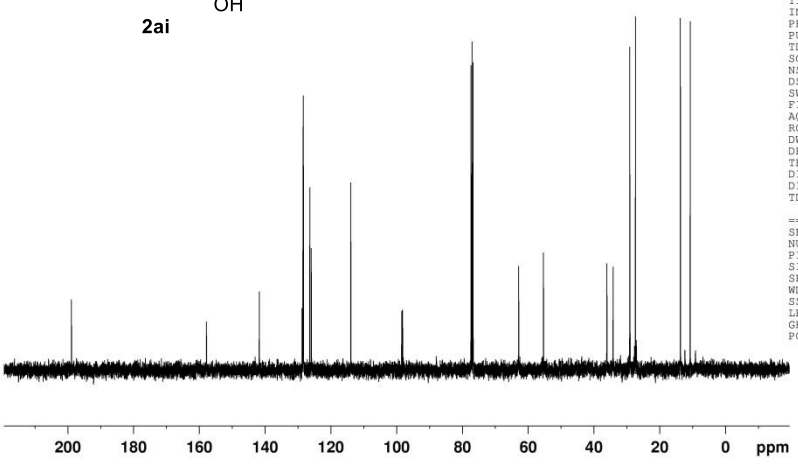



```
NAME          yjl-hk-770-h
EXPNO                   10
PROCNO                   1
Date_             20200824
Time                 14.44
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                       4
DS                       0
SWH              8012.820 Hz
FIDRES              0.122266 Hz
AQ                4.0894966 sec
RG                   19.81
DW                  62.400 usec
DE                   6.50 usec
TE                    0.0 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                   9.99 usec
SI                  65536
SF           400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

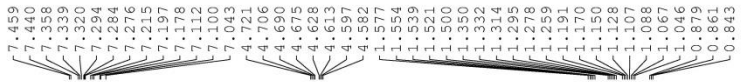


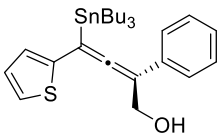


2ai



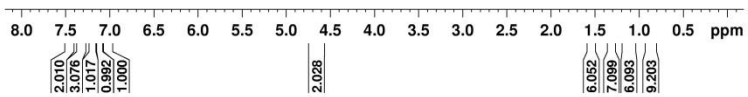

```
NAME          yjl-hk-770-c
EXPNO                   11
PROCNO                   1
Date_             20200824
Time                 14.47
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                      43
DS                       4
SWH             24038.461 Hz
FIDRES              0.366798 Hz
AQ                1.3631988 sec
RG                   197.54
DW                  20.800 usec
DE                   6.50 usec
TE                    0.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                   13C
P1                   9.31 usec
SI                  32768
SF           100.6127685 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

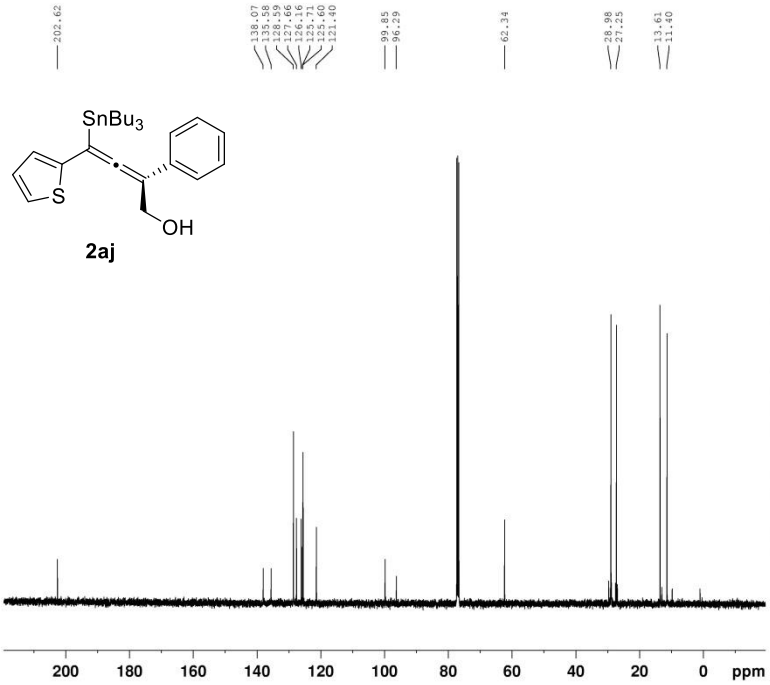




2aj

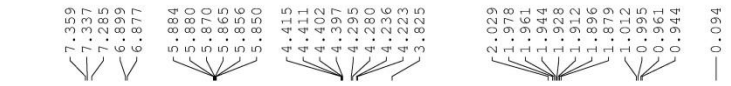
```
NAME          yjl-hk-722-race-h
EXPNO                        10
PROCNO                        1
Date_                  20200825
Time                      19.07
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894966 sec
RG                        30.81
DW                       62.400 usec
DE                        6.50 usec
TE                         0.0 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               400.1324710 MHz
NUC1                         1H
P1                         9.99 usec
SI                        65536
SF                 400.1300000 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

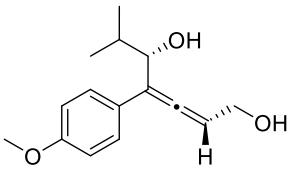




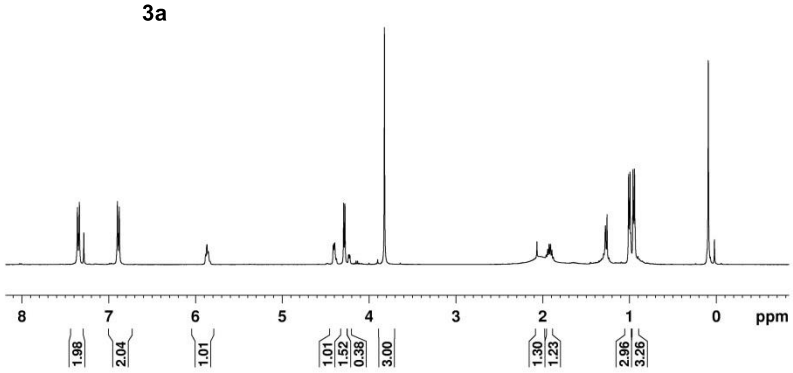
2aj

```
NAME          yjl-hk-722-race-c
EXPNO                        11
PROCNO                        1
Date_                  20200825
Time                      19.37
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         512
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                       197.54
DW                       20.800 usec
DE                        6.50 usec
TE                         0.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               100.6228293 MHz
NUC1                        13C
P1                         9.31 usec
SI                        32768
SF                 100.6127685 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```



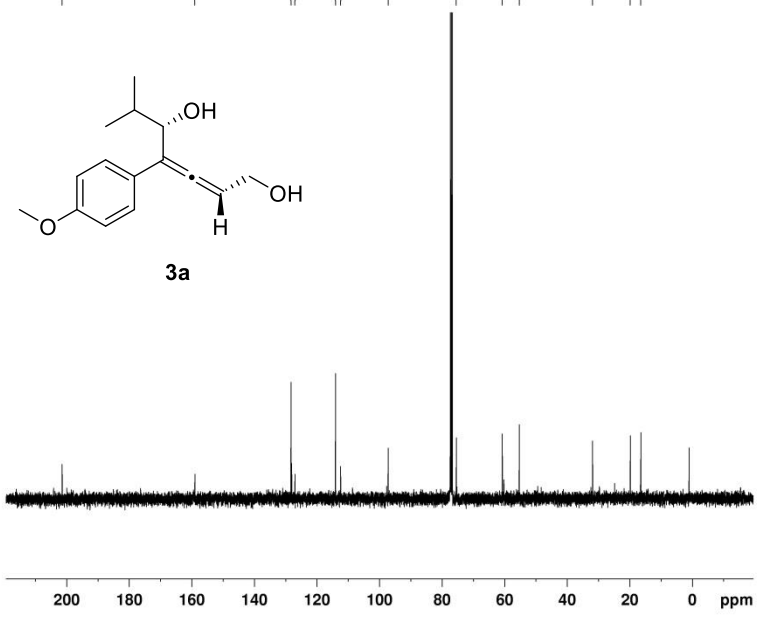


3a

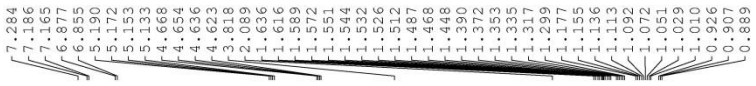


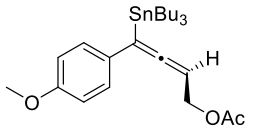

```
NAME            wm-15-80-3
EXPNO                   10
PROCNO                   1
Date_             20201110
Time                 14.45
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                       4
DS                       2
SWH              8012.820 Hz
FIDRES              0.122266 Hz
AQ                4.0894966 sec
RG                   63.21
DW                  62.400 usec
DE                    6.50 usec
TE                     0.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                    1H
P1                    9.99 usec
SI                   65536
SF              400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

3a



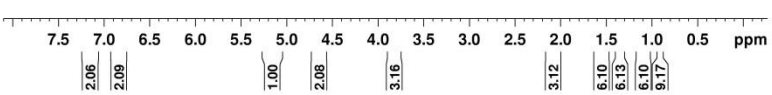

```
NAME            wm-15-80-3
EXPNO                   11
PROCNO                   1
Date_             20201110
Time                 14.51
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     140
DS                       4
SWH             24038.461 Hz
FIDRES              0.366798 Hz
AQ                1.3631988 sec
RG                  197.54
DW                  20.800 usec
DE                    6.50 usec
TE                     0.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            100.6228293 MHz
NUC1                    13C
P1                    9.31 usec
SI                   32768
SF              100.6127685 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

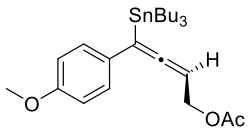




4aa

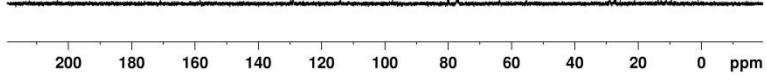
```
NAME        yjl-hk-807-2-h
EXPNO                   10
PROCNO                   1
Date_             20200917
Time                 23.52
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                       4
DS                       2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894966 sec
RG                    11.08
DW                  62.400 usec
DE                    6.50 usec
TE                  297.4 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                    1H
P1                    9.99 usec
SI                   65536
SF              400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

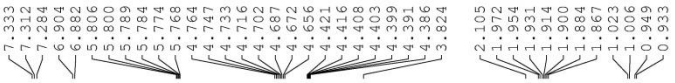


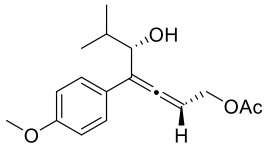


4aa

```
NAME        yjl-hk-807-2-h
EXPNO                   11
PROCNO                   1
Date_             20200918
Time                  0.00
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     128
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                   197.54
DW                  20.800 usec
DE                    6.50 usec
TE                  297.9 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            100.6228293 MHz
NUC1                    13C
P1                    9.31 usec
SI                   32768
SF              100.6127685 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

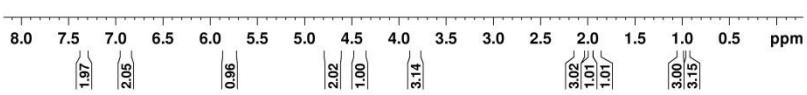


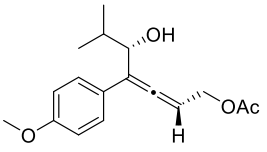




4a

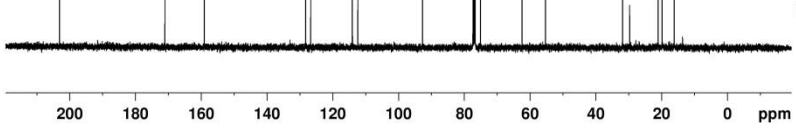
```
NAME          yjl-hk-772-race-h
EXPNO                        10
PROCNO                        1
Date_                  20200825
Time                      19.41
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894966 sec
RG                        30.81
DW                       62.400 usec
DE                        6.50 usec
TE                           0.0 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                400.1324710 MHz
NUC1                        1H
P1                        9.99 usec
SI                       65536
SF                  400.1300000 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

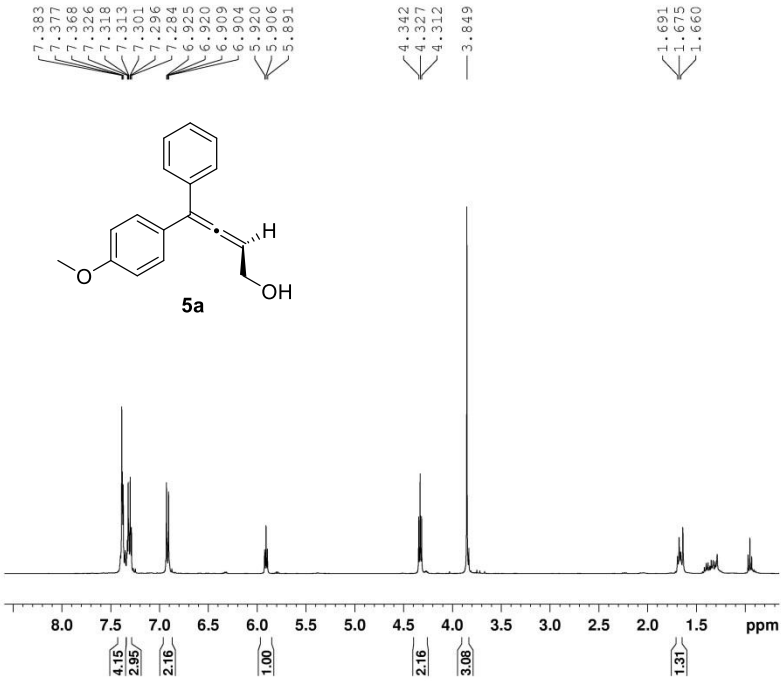




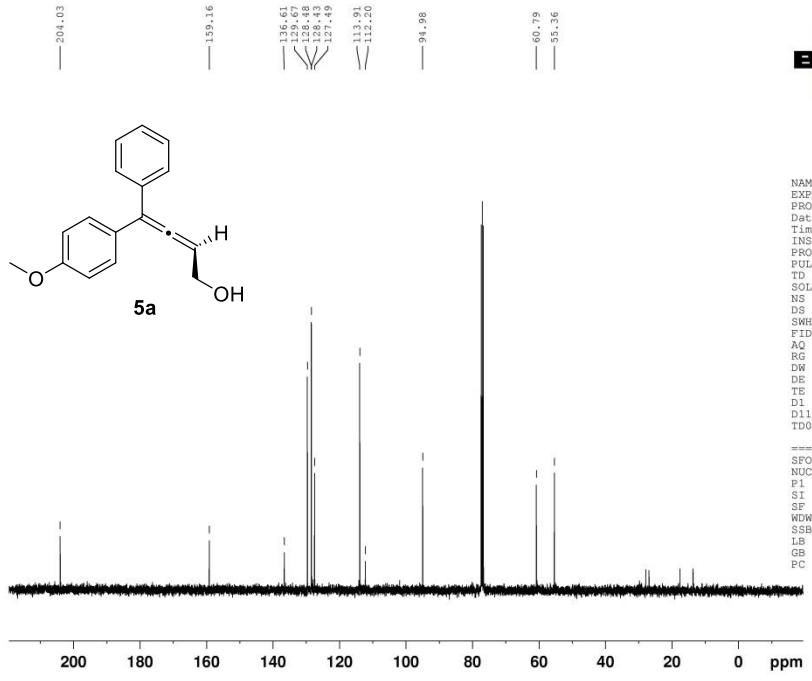
4a

```
NAME          yjl-hk-772-race-c
EXPNO                        11
PROCNO                        1
Date_                  20200825
Time                      19.55
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         218
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                       197.54
DW                       20.800 usec
DE                        6.50 usec
TE                           0.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                100.6228293 MHz
NUC1                        13C
P1                        9.31 usec
SI                       32768
SF                  100.6127685 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

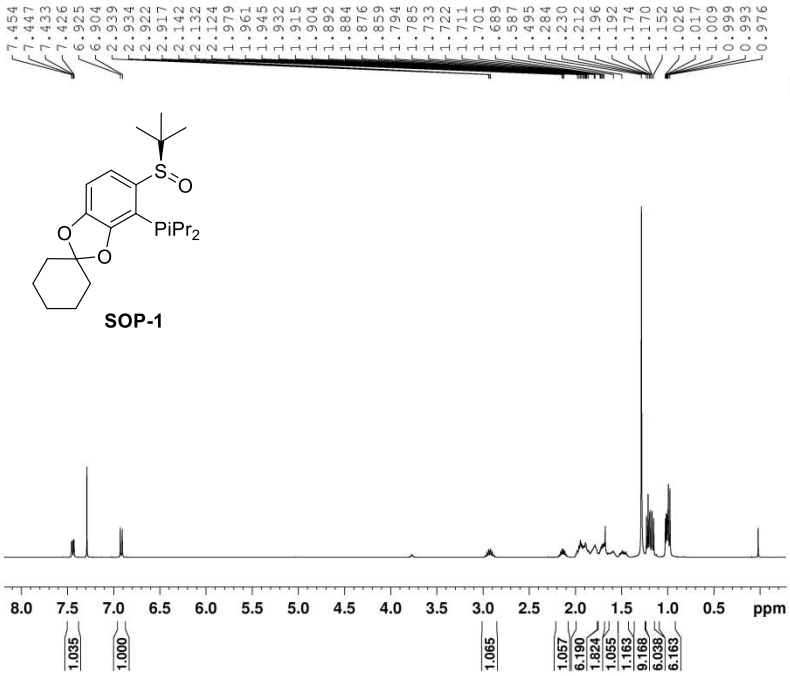



7.383
7.377
7.368
7.326
7.318
7.313
7.301
7.296
7.284
6.925
6.920
6.909
6.904
5.920
5.906
5.891
4.342
4.327
4.312
3.849
1.691
1.675
1.660
H
O
OH
5a
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
4.15
2.95
2.16
1.00
2.16
3.08
1.31

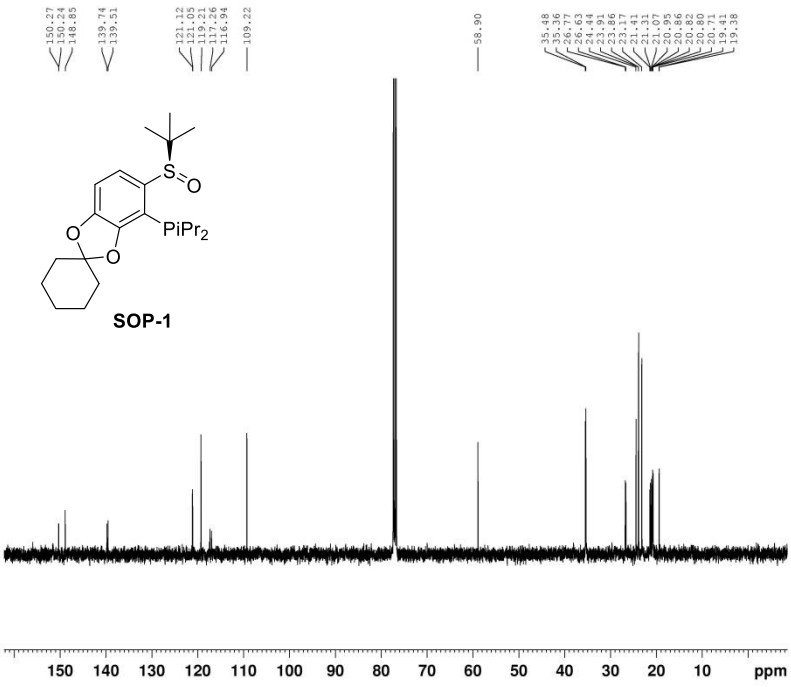

NAME yjl-hk-556-h
EXPNO 10
PROCNO 1
Date_ 20181220
Time 17.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 63.21
DW 62.400 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.99 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


204.03
159.16
136.61
129.67
128.48
128.43
127.49
113.91
112.20
94.98
60.79
55.36
H
O
OH
5a
200
180
160
140
120
100
80
60
40
20
0
ppm


NAME yjl-hk-556-c
EXPNO 11
PROCNO 1
Date_ 20181220
Time 17.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 197.54
DW 20.800 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.31 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

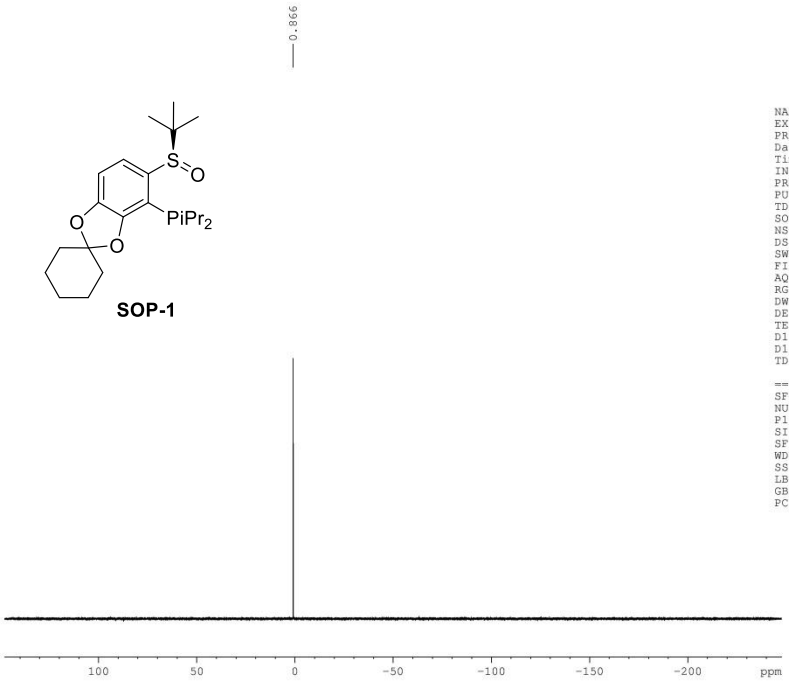



```
NAME        yjl-hk-108-1-h
EXPNO                   10
PROCNO                   1
Date_             20171129
Time                 17.50
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                       4
DS                       0
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894966 sec
RG                   71.18
DW                   62.400 usec
DE                    6.50 usec
TE                     0.0 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                    1H
P1                    9.99 usec
SI                   65536
SF              400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

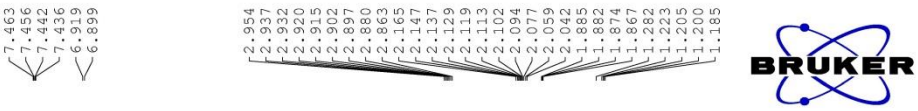


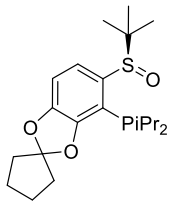

```
NAME        yjl-hk-108-c
EXPNO                   10
PROCNO                   1
Date_             20200903
Time                 19.49
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     350
DS                       0
SWH              24038.461 Hz
FIDRES               0.366798 Hz
AQ                1.3631988 sec
RG                   197.54
DW                   20.800 use
DE                    6.50 use
TE                   298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            100.6228293 MHz
NUC1                    13C
P1                    9.31 use
SI                   32768
SF              100.6127685 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

SOP-1

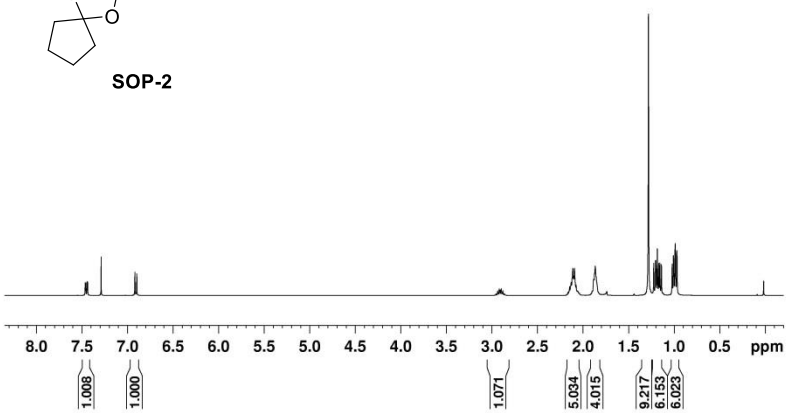



```
NAME      yjl-hk-108-1-p
EXPNO                 11
PROCNO                 1
Date_           20171129
Time               17.51
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    4
SWH           64102.563 Hz
FIDRES         0.978127 Hz
AQ            0.5112308 sec
RG               197.54
DW                7.800 usec
DE                6.50 usec
TE                 0.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1       161.9674942 MHz
NUC1              31P
P1                8.00 usec
SI               32768
SF         161.9755930 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

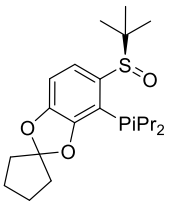




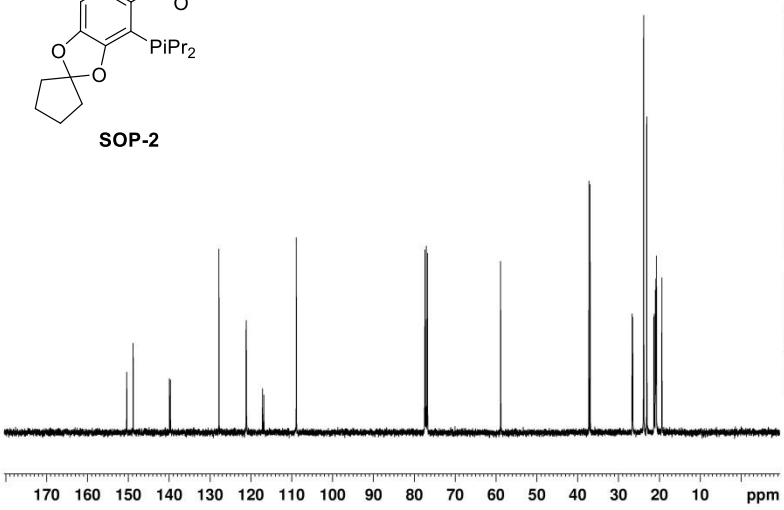
SOP-2



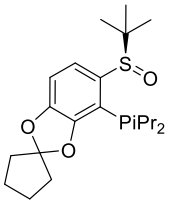

```
NAME       yjl-hk-101-h
EXPNO                10
PROCNO                1
Date_          20171121
Time              21.02
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894966 sec
RG                53.87
DW                62.400 usec
DE                 6.50 usec
TE                  0.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1       400.1324710 MHz
NUC1               1H
P1                 9.99 usec
SI                65536
SF         400.1300000 MHz
WDW                EM
SSB                 0
LB                0.30 Hz
GB                  0
PC                1.00
```



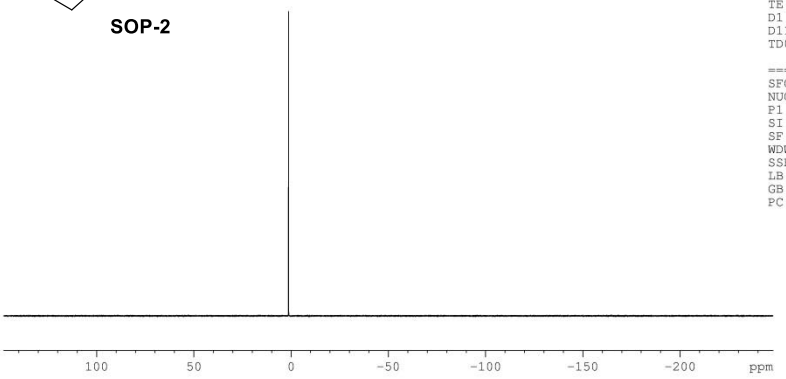
SOP-2



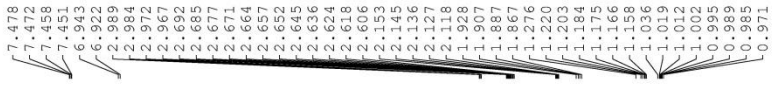

```
NAME          yjl-hk-101-c-1
EXPNO                    10
PROCNO                    1
Date_              20200911
Time                   1.20
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631988 sec
RG                    197.54
DW                  20.800 usec
DE                   6.50 usec
TE                   298.4 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             100.6228293 MHz
NUC1                     13C
P1                    9.31 usec
SI                   32768
SF               100.6127685 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

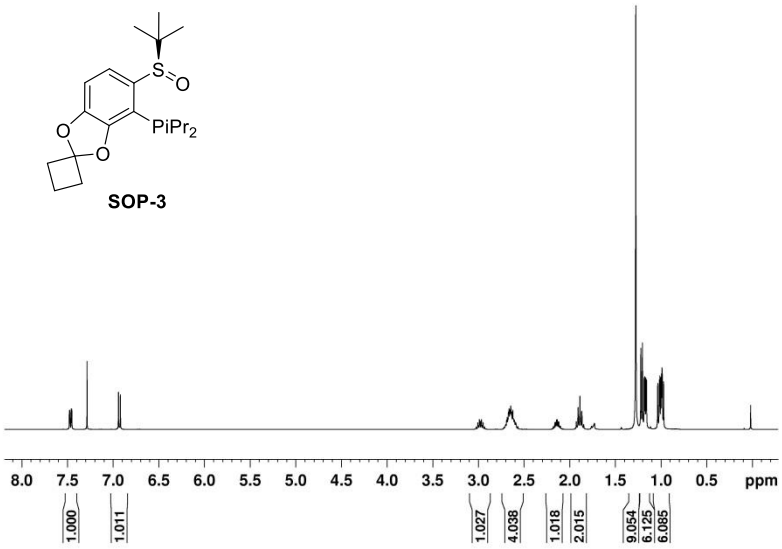
SOP-2



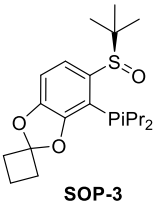

```
NAME          yjl-hk-101-p
EXPNO                    11
PROCNO                    1
Date_              20171121
Time                  21.04
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        4
SWH               64102.563 Hz
FIDRES             0.978127 Hz
AQ                0.5112308 sec
RG                    197.54
DW                   7.800 usec
DE                   6.50 usec
TE                     0.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             161.9674942 MHz
NUC1                     31P
P1                    8.00 usec
SI                   32768
SF               161.9755930 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



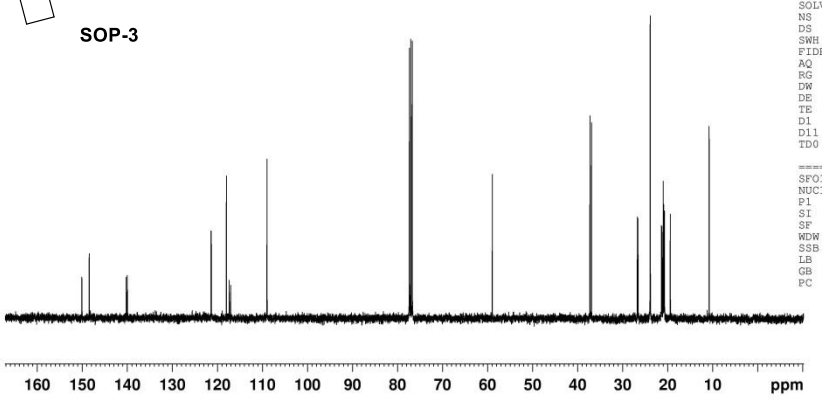
SOP-3




```
NAME        yjl-hk-102-h
EXPNO                 10
PROCNO                 1
Date_           20171121
Time              21.07
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     0
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894966 sec
RG                 53.87
DW                 62.400 usec
DE                  6.50 usec
TE                   0.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                   1H
P1                   9.99 usec
SI                 65536
SF              400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

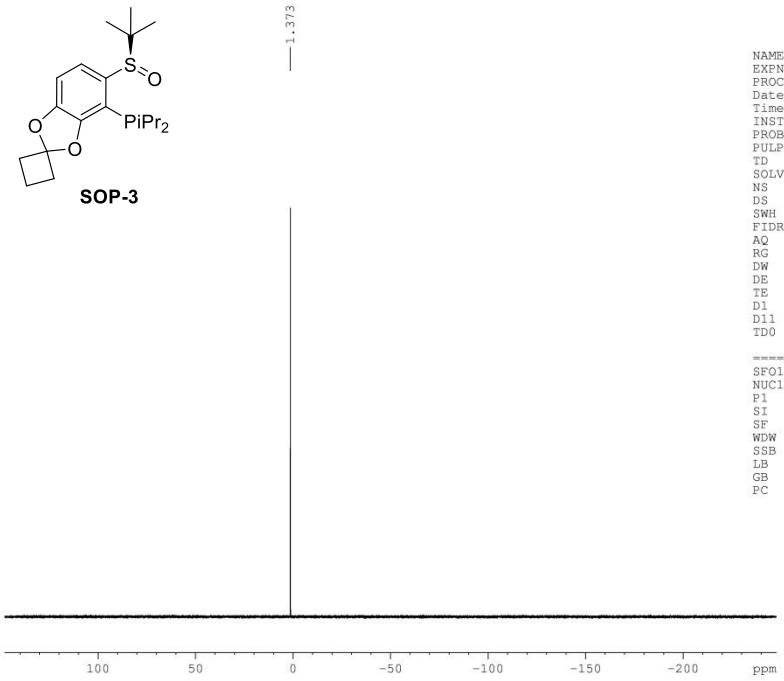


SOP-3

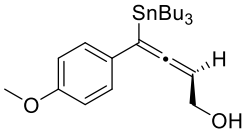



```
NAME      yjl-hk-102-c-1
EXPNO                 10
PROCNO                 1
Date_           20200911
Time               1.38
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631988 sec
RG                197.54
DW                 20.800 use
DE                  6.50 use
TE                298.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1            100.6228293 MHz
NUC1                   13C
P1                   9.31 use
SI                 32768
SF              100.6127685 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

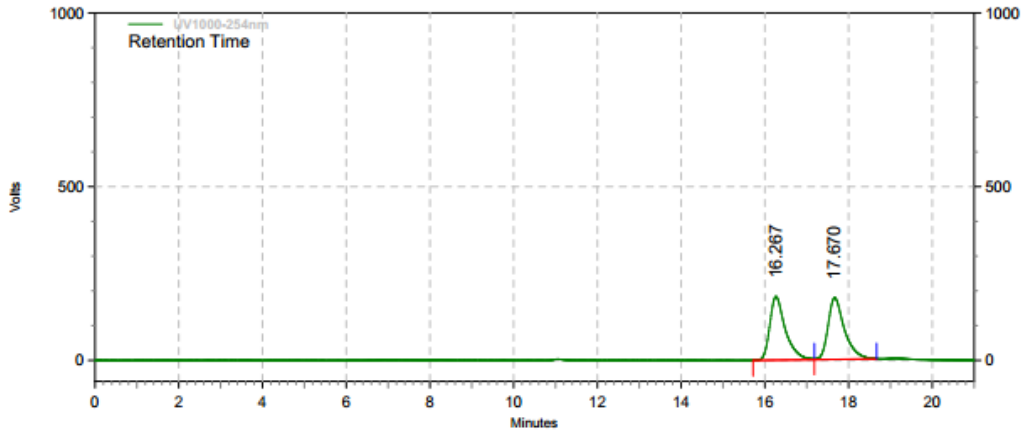
SOP-3



NAME	yjl-hk-102-p
EXPNO	10
PROCNO	1
Date_	20200921
Time	13.57
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	4
SWH	64102.563 Hz
FIDRES	0.978127 Hz
AQ	0.5112308 sec
RG	197.54
DW	7.800 usec
DE	6.50 usec
TE	297.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	161.9674942 MHz
NUC1	31P
P1	8.00 usec
SI	32768
SF	161.9755930 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

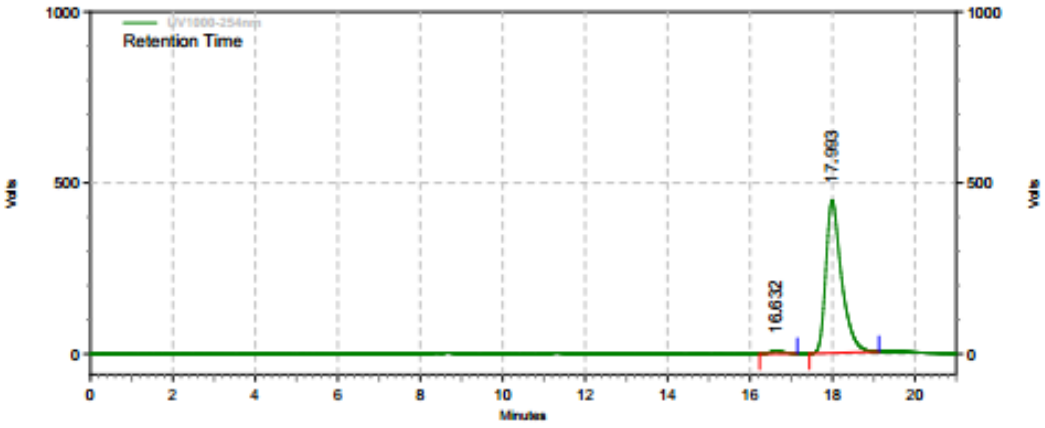


2a



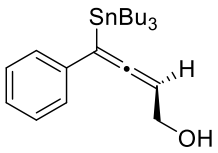
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
16.267	4749735	49.56	183140	50.80
17.670	4834268	50.44	177339	49.20
Totals	9584003	100.00	360479	100.00

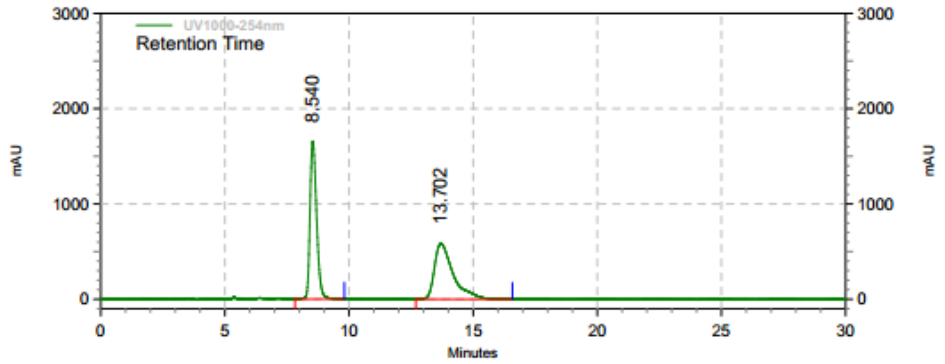


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
16.632	186956	1.56	8303	1.83
17.993	11800744	98.44	446442	98.17
Totals	11987700	100.00	454745	100.00

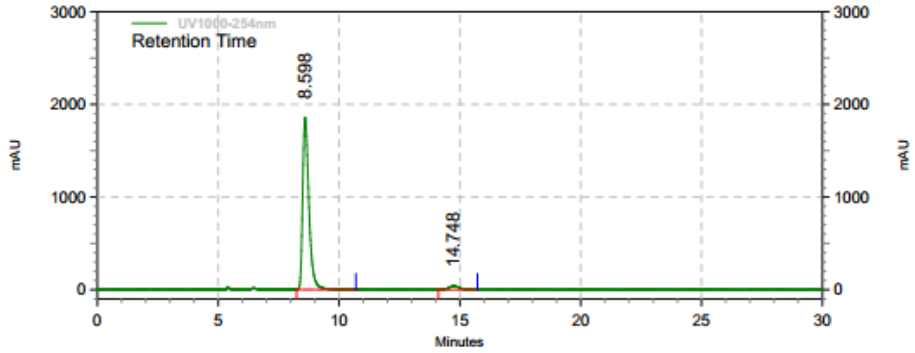


2b



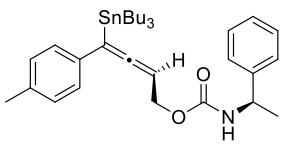
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.540	30502178	50.03	1657782	73.98
13.702	30469555	49.97	583023	26.02
Totals	60971733	100.00	2240805	100.00

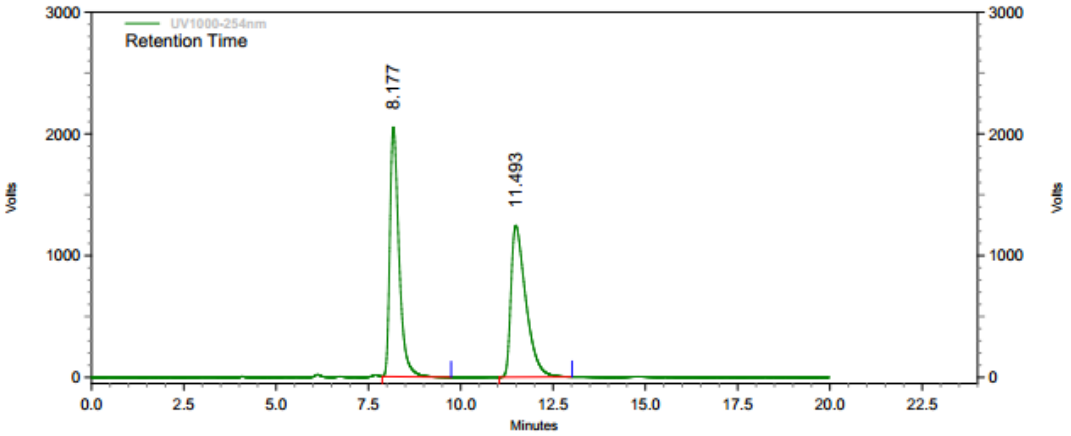


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.598	33442047	96.51	1855238	97.94
14.748	1210809	3.49	39039	2.06
Totals	34652856	100.00	1894277	100.00

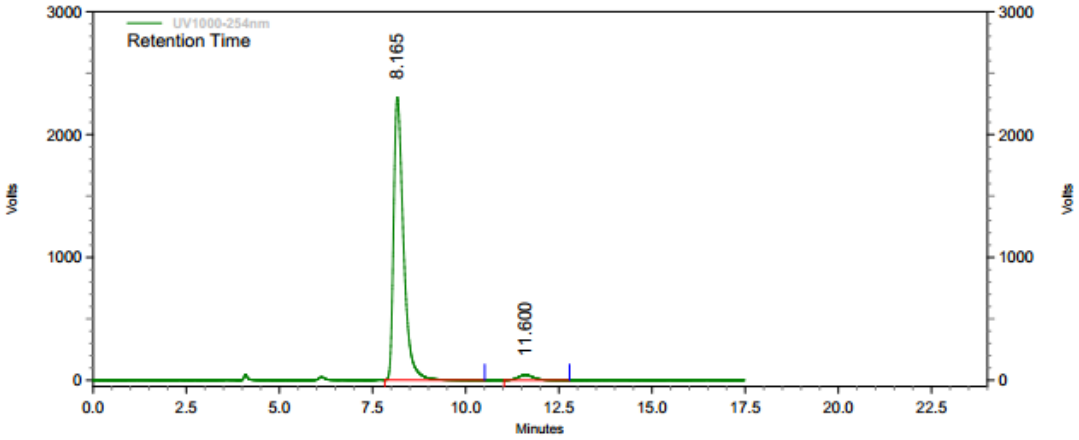


2c'



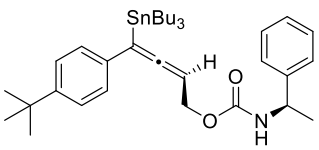
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.177	35380102	50.35	2049160	62.20
11.493	34890882	49.65	1245407	37.80
Totals	70270984	100.00	3294567	100.00

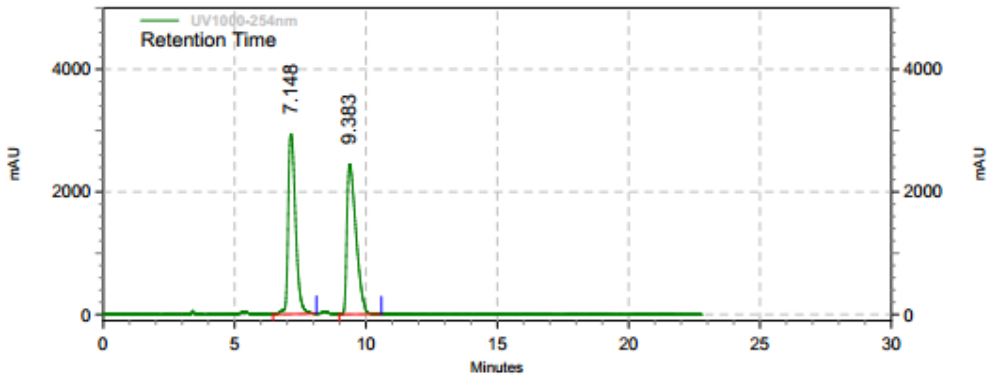


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.165	42367376	97.20	2301824	98.18
11.600	1219681	2.80	42554	1.82
Totals	43587057	100.00	2344378	100.00

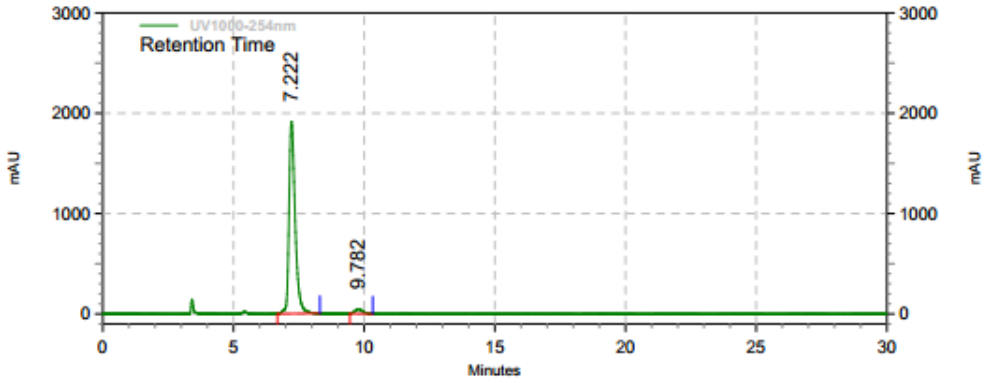


2d'



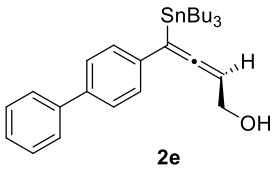
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
7.148	57386033	49.32	2934618	54.51
9.383	58974185	50.68	2448658	45.49
Totals	116360218	100.00	5383276	100.00

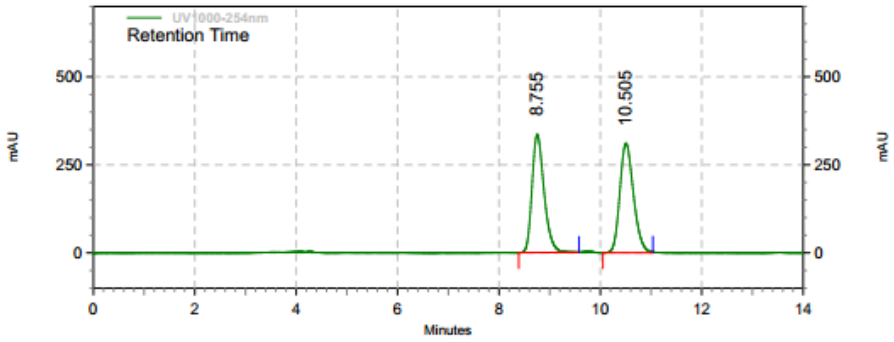


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
7.222	31425552	97.01	1914879	97.70
9.782	967739	2.99	45029	2.30
Totals	32393291	100.00	1959908	100.00

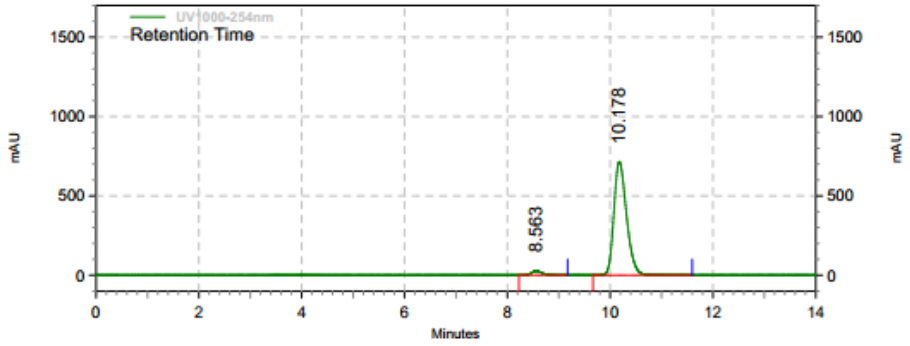


2e



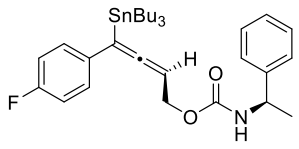
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.755	5536904	48.74	335051	51.90
10.505	5823060	51.26	310545	48.10
Totals	11359964	100.00	645596	100.00

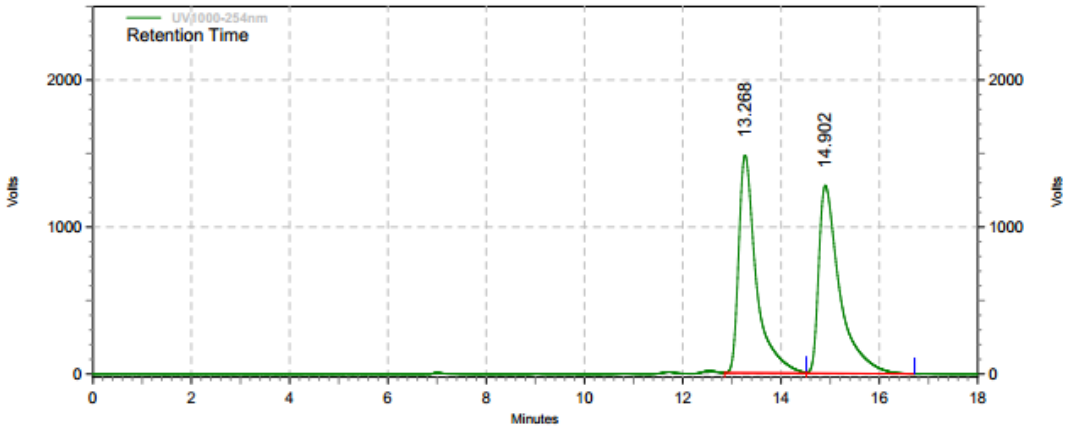


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.563	381094	3.03	26666	3.60
10.178	12213851	96.97	714944	96.40
Totals	12594945	100.00	741610	100.00

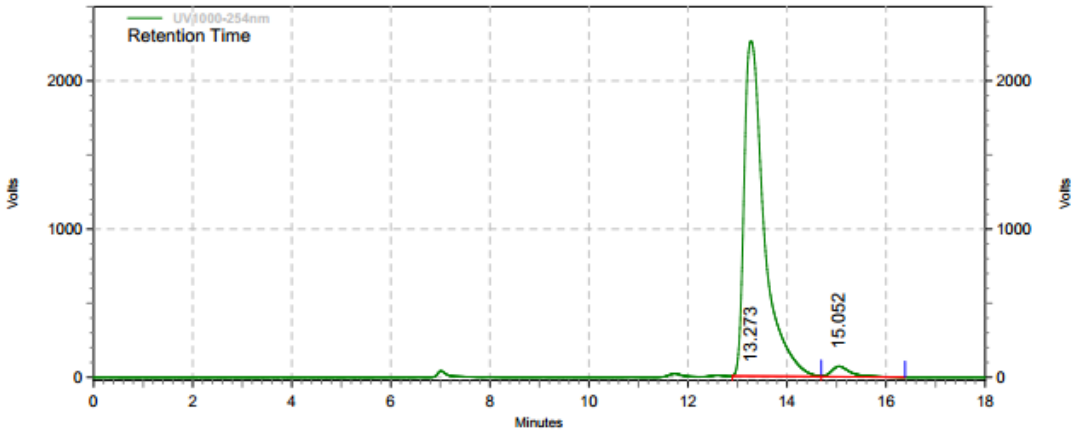


2f'



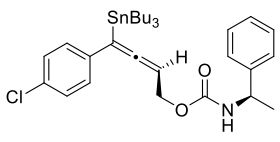
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
13.268	36821922	49.31	1480527	53.67
14.902	37856385	50.69	1277883	46.33
Totals	74678307	100.00	2758410	100.00

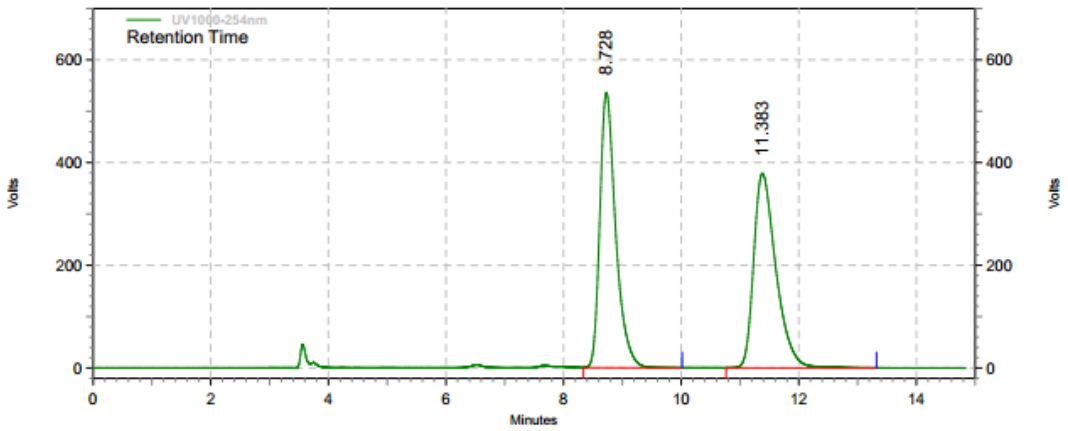


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
13.273	63558864	97.11	2260347	96.99
15.052	1888678	2.89	70077	3.01
Totals	65447542	100.00	2330424	100.00

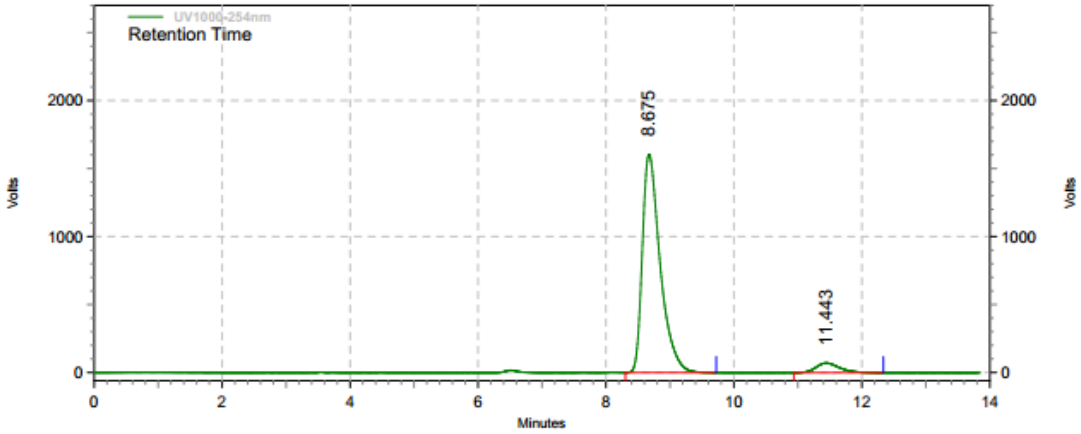


2g'



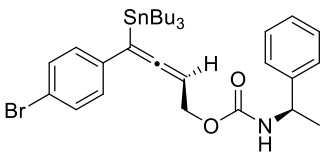
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.728	10017603	50.16	535893	58.60
11.383	9952522	49.84	378652	41.40
Totals	19970125	100.00	914545	100.00

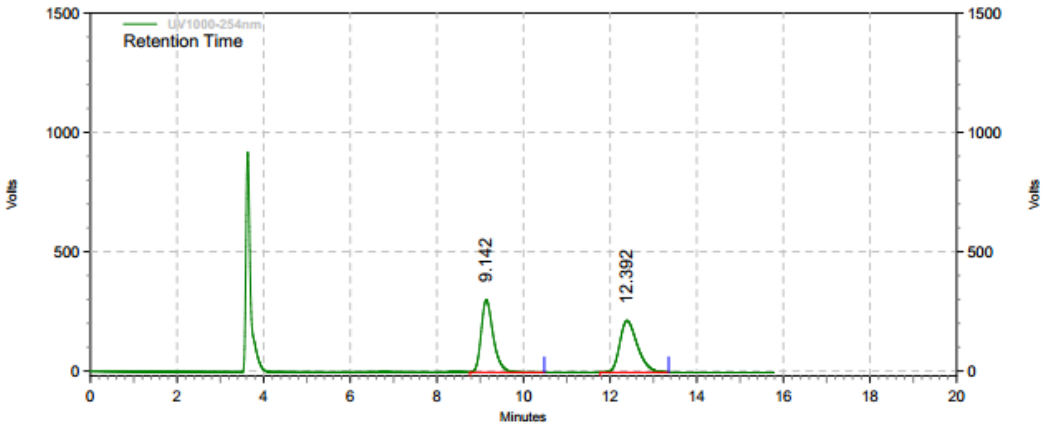


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.675	31025568	94.58	1604243	95.81
11.443	1779370	5.42	70101	4.19
Totals	32804938	100.00	1674344	100.00

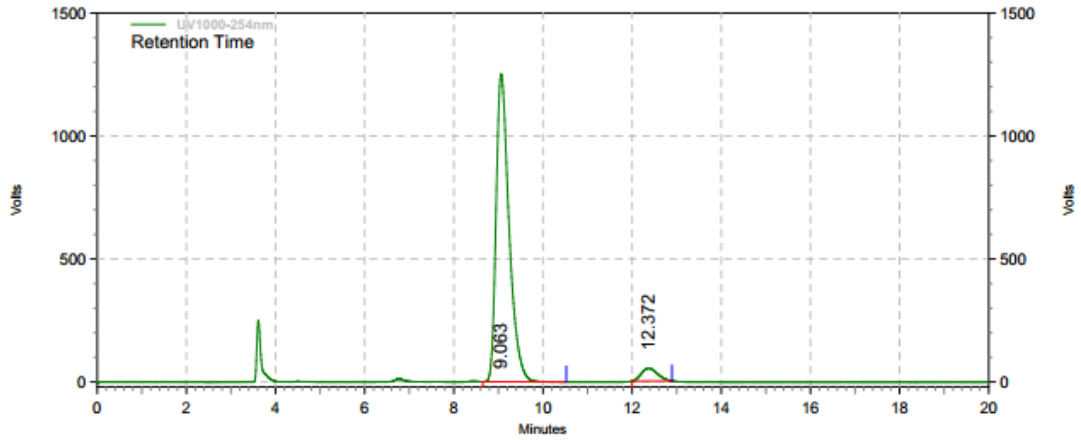


2h'



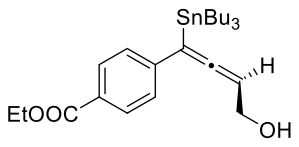
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
9.142	5861582	48.96	303055	58.36
12.392	6111253	51.04	216208	41.64
Totals	11972835	100.00	519263	100.00

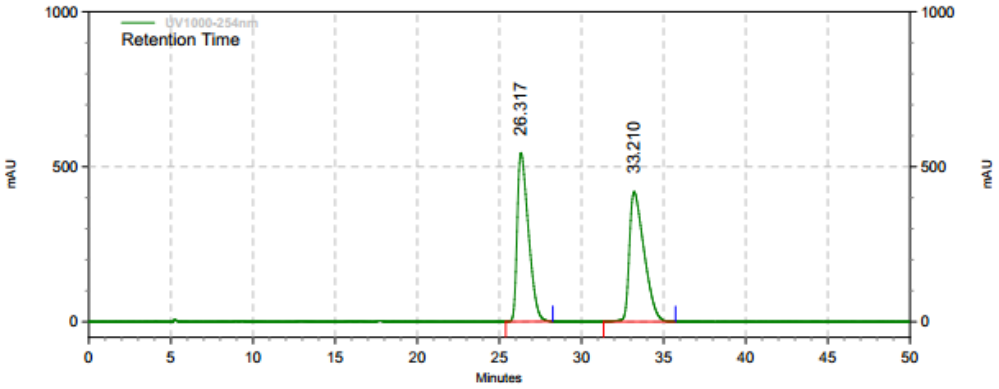


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
9.063	25200193	95.02	1251543	95.99
12.372	1322089	4.98	52254	4.01
Totals	26522282	100.00	1303797	100.00

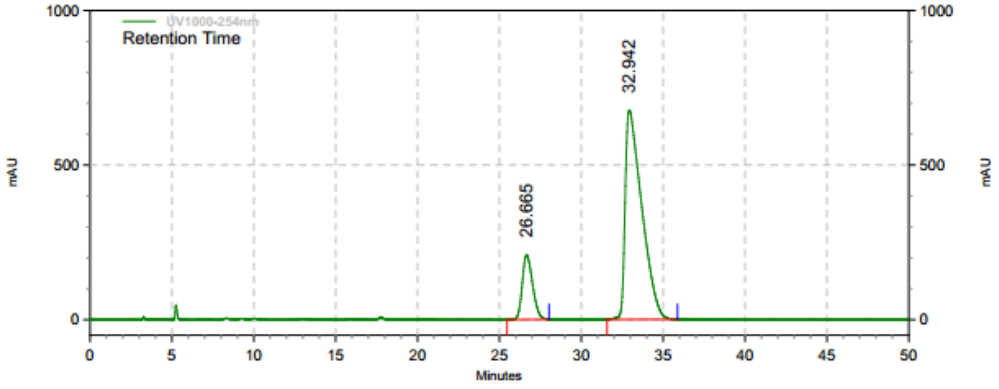


2i



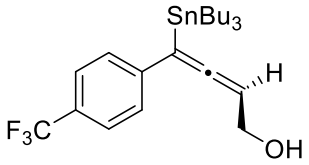
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
26.317	25915772	49.76	544574	56.52
33.210	26167581	50.24	418912	43.48
Totals	52083353	100.00	963486	100.00

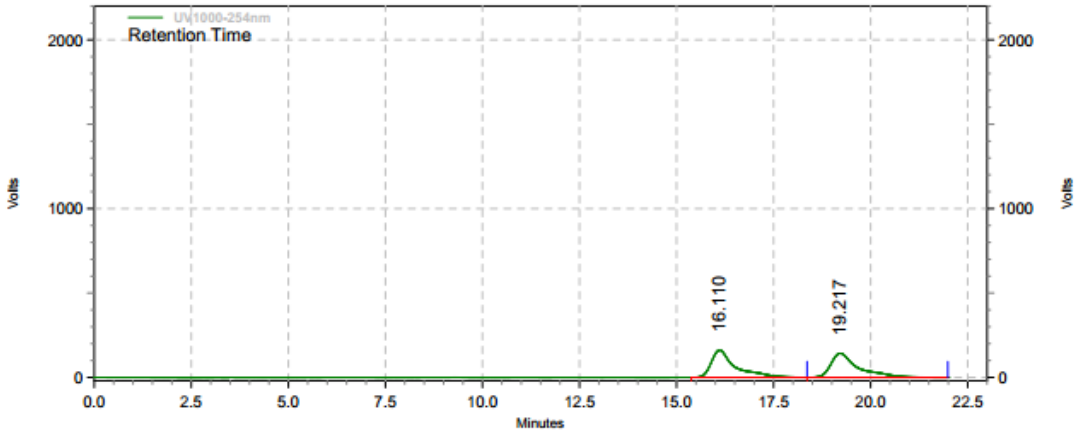


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
26.665	9158729	16.10	208639	23.56
32.942	47719602	83.90	676870	76.44
Totals	56878331	100.00	885509	100.00

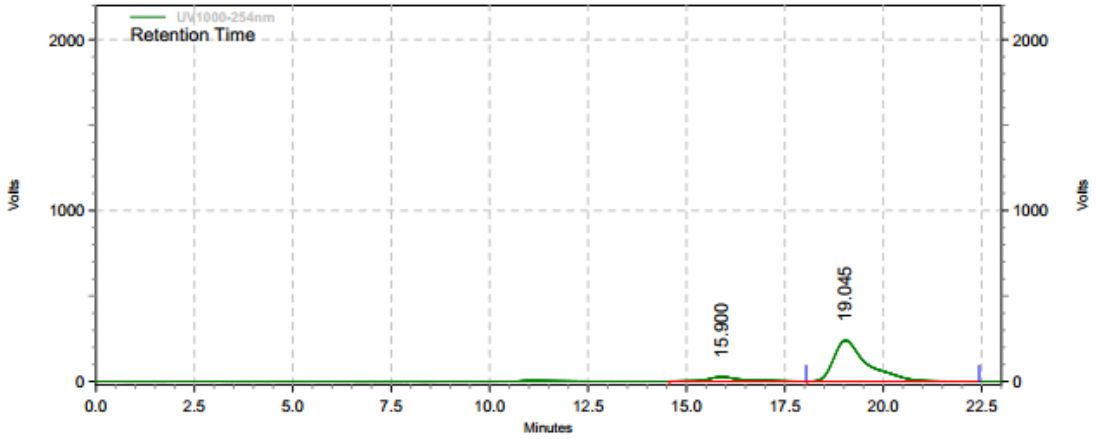


2j



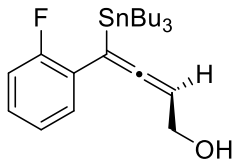
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
16.110	6928406	49.98	161714	53.13
19.217	6933098	50.02	142648	46.87
Totals	13861504	100.00	304362	100.00

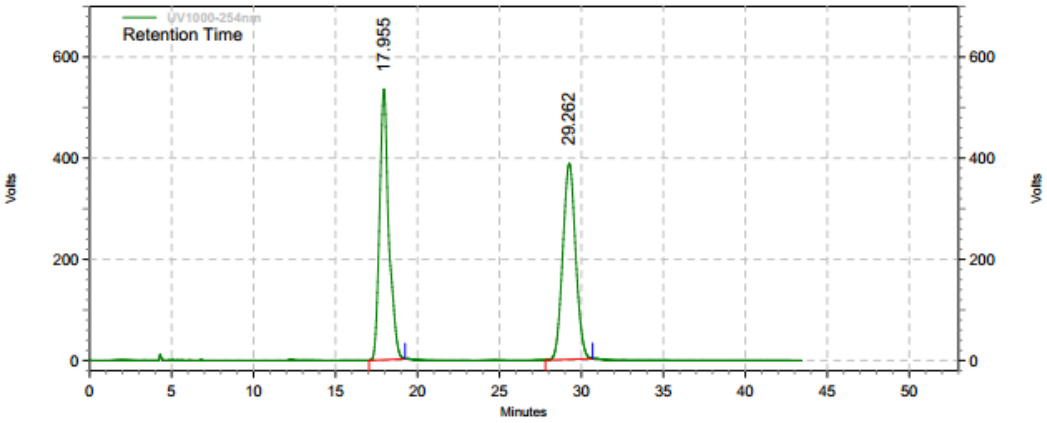


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
15.900	1580384	10.04	26536	9.95
19.045	14153097	89.96	240229	90.05
Totals	15733481	100.00	266765	100.00

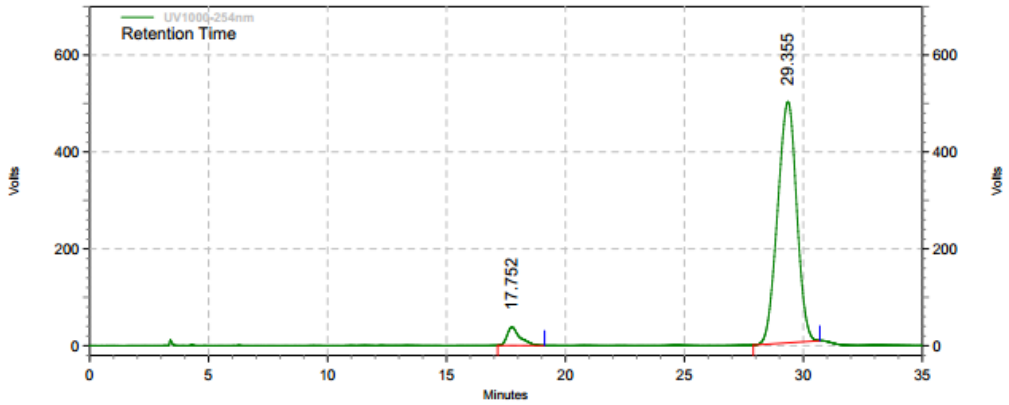


2k



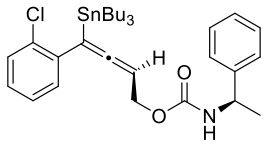
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
17.955	20901670	49.84	534971	58.02
29.262	21038792	50.16	387071	41.98
Totals	41940462	100.00	922042	100.00

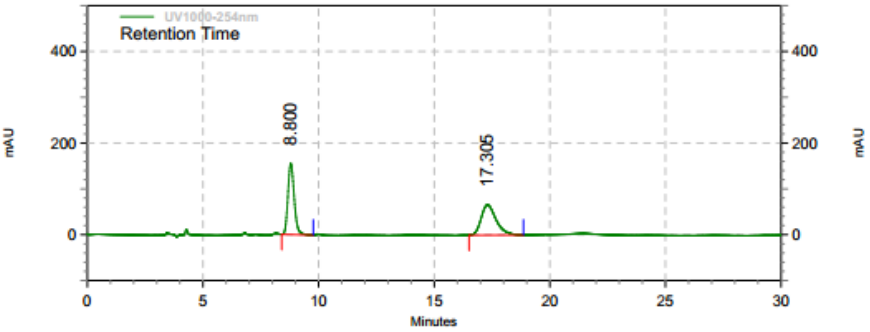


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
17.752	1414723	4.85	38358	7.16
29.355	27743782	95.15	497563	92.84
Totals	29158505	100.00	535921	100.00

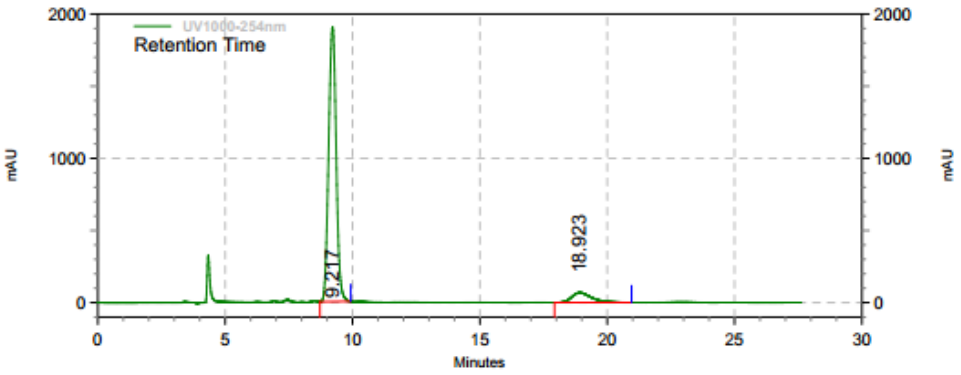


2l'



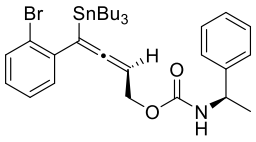
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.800	2920447	49.63	155044	70.12
17.305	2963411	50.37	66077	29.88
Totals	5883858	100.00	221121	100.00

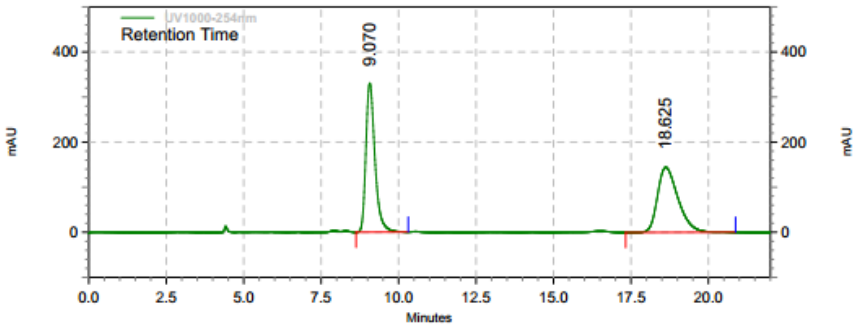


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
9.217	39195824	91.31	1902846	96.54
18.923	3729577	8.69	68208	3.46
Totals	42925401	100.00	1971054	100.00

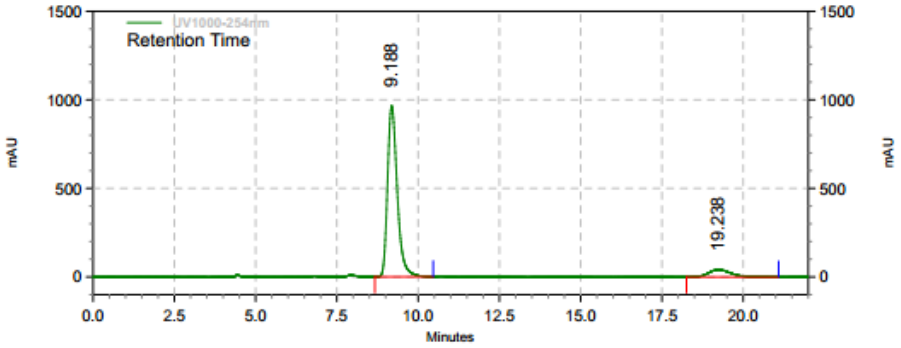


2m'



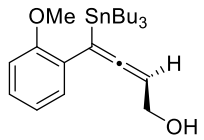
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
9.070	6711166	50.19	330661	69.59
18.625	6661070	49.81	144461	30.41
Totals	13372236	100.00	475122	100.00

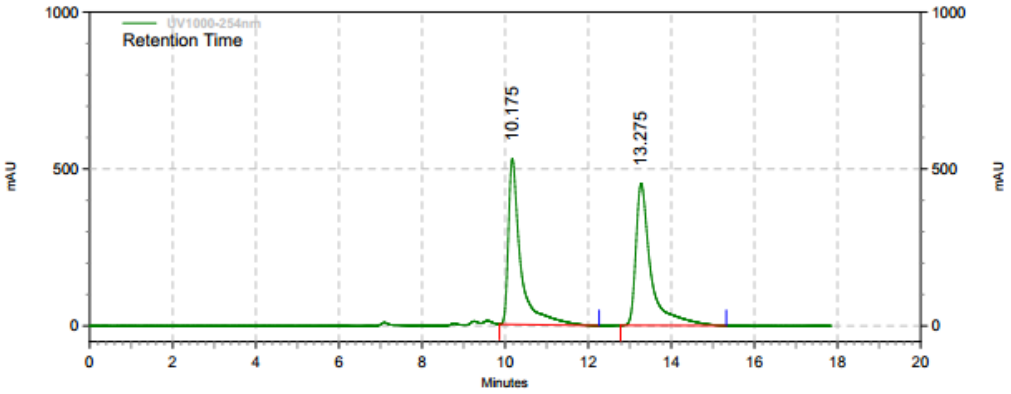


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
9.188	20065969	91.08	965298	95.89
19.238	1964046	8.92	41420	4.11
Totals	22030015	100.00	1006718	100.00

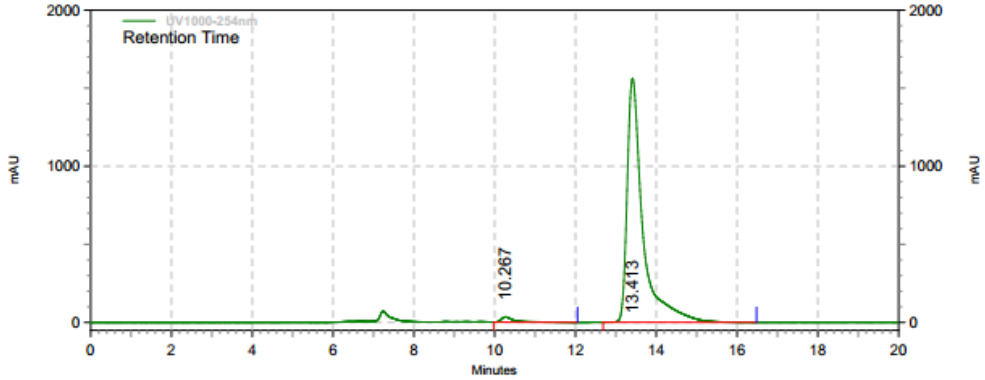


2n



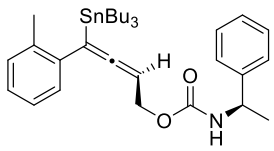
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
10.175	10844388	48.85	527729	53.86
13.275	11356625	51.15	452163	46.14
Totals	22201013	100.00	979892	100.00

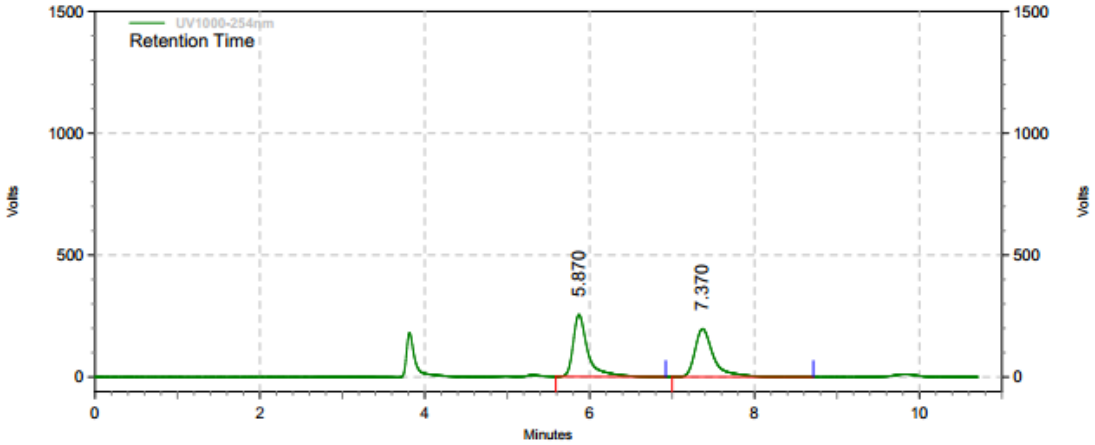


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
10.267	705654	1.66	33306	2.09
13.413	41917060	98.34	1559407	97.91
Totals	42622714	100.00	1592713	100.00

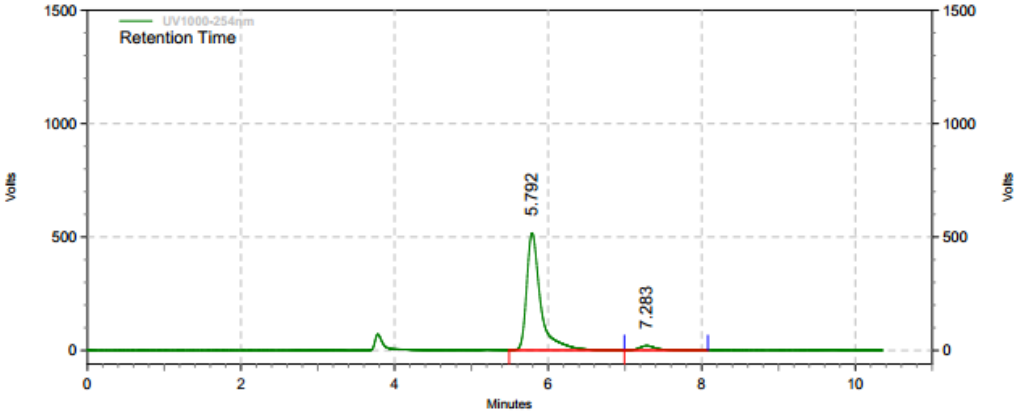


2o'



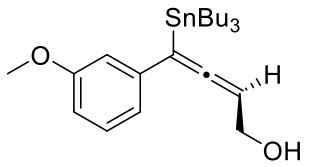
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
5.870	3149906	50.62	254609	56.36
7.370	3072420	49.38	197177	43.64
Totals	6222326	100.00	451786	100.00

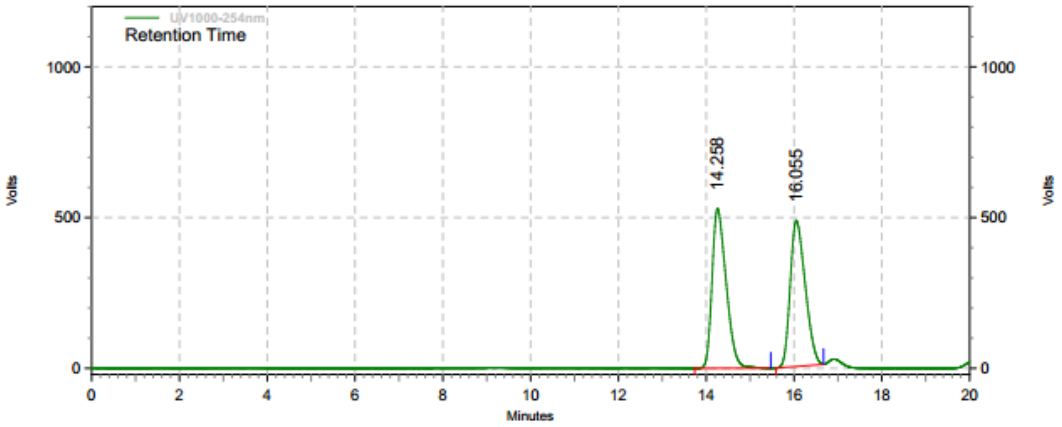


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
5.792	6512573	95.58	517103	96.32
7.283	301306	4.42	19757	3.68
Totals	6813879	100.00	536860	100.00

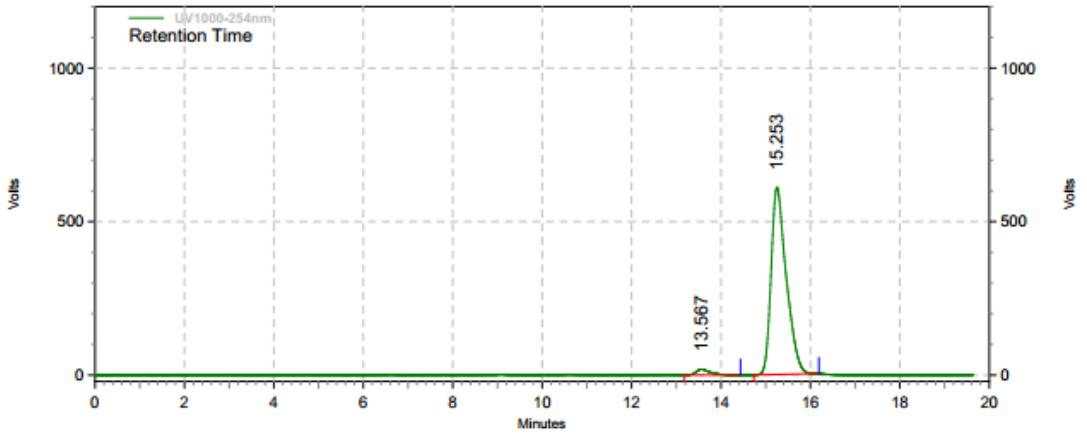


2p



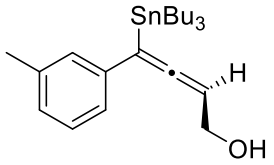
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
14.258	11782291	50.59	529562	52.29
16.055	11505393	49.41	483188	47.71
Totals	23287684	100.00	1012750	100.00

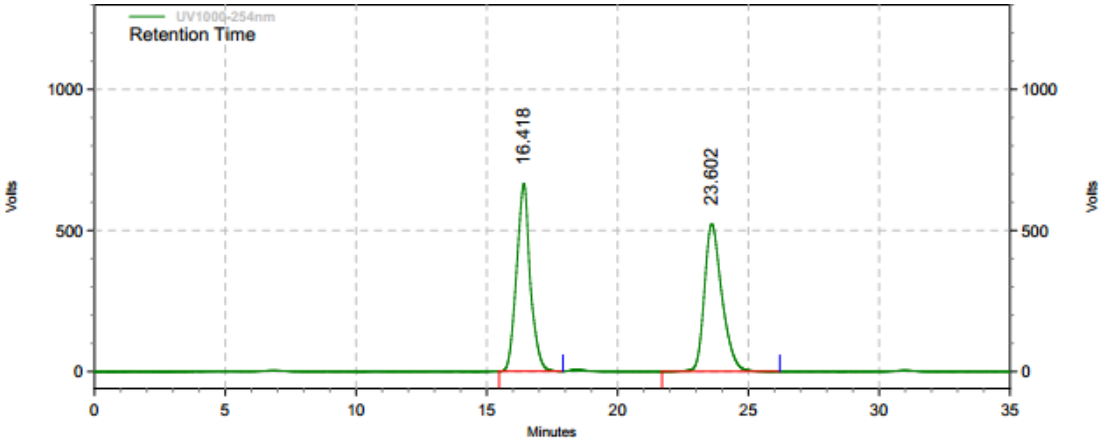


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
13.567	404733	2.75	18775	2.99
15.253	14321329	97.25	608949	97.01
Totals	14726062	100.00	627724	100.00

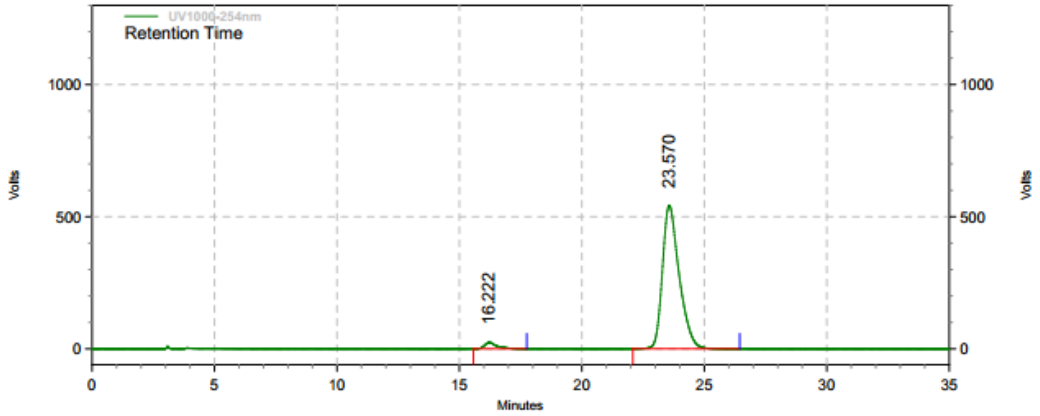


2q



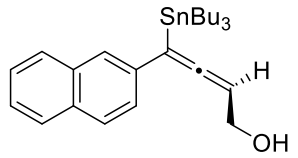
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
16.418	24108190	49.74	664329	55.96
23.602	24356052	50.26	522762	44.04
Totals	48464242	100.00	1187091	100.00

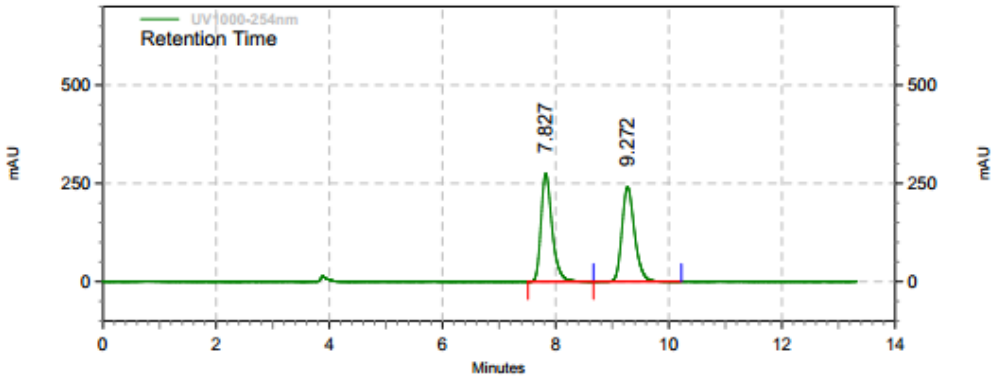


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
16.222	832903	3.13	24079	4.25
23.570	25785143	96.87	542884	95.75
Totals	26618046	100.00	566963	100.00

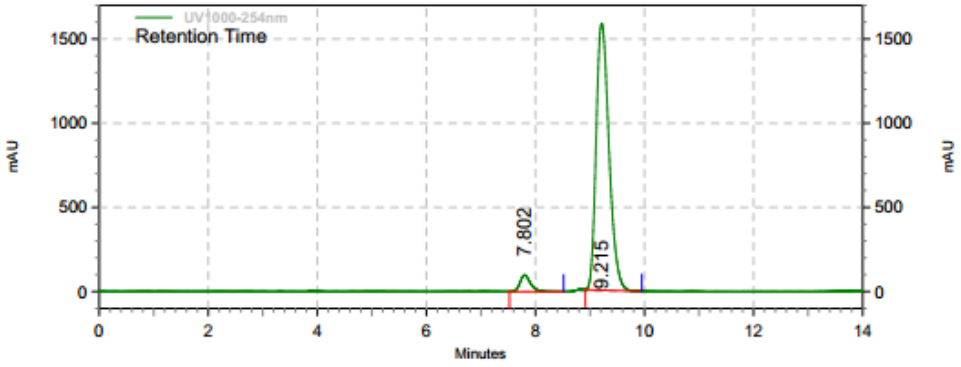


2r



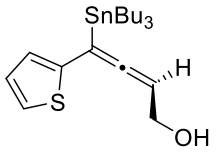
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
7.827	3741900	50.00	274154	53.29
9.272	3741186	50.00	240325	46.71
Totals	7483086	100.00	514479	100.00

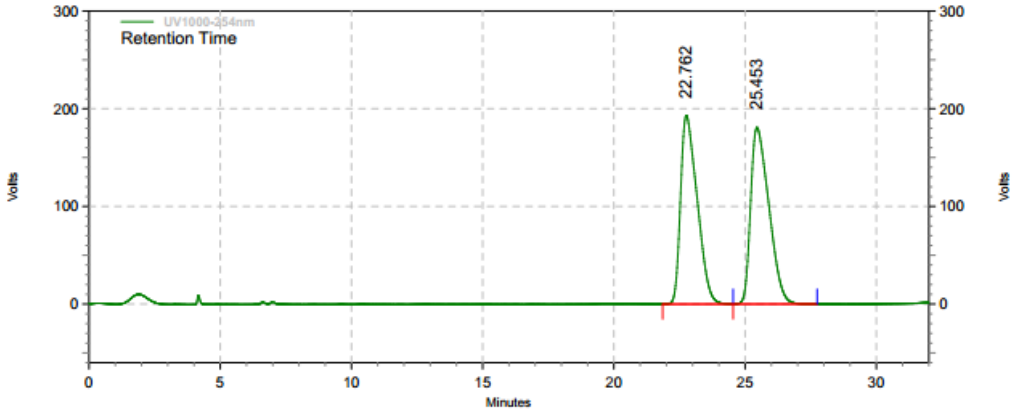


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
7.802	1317446	4.82	98463	5.86
9.215	25987926	95.18	1582456	94.14
Totals	27305372	100.00	1680919	100.00

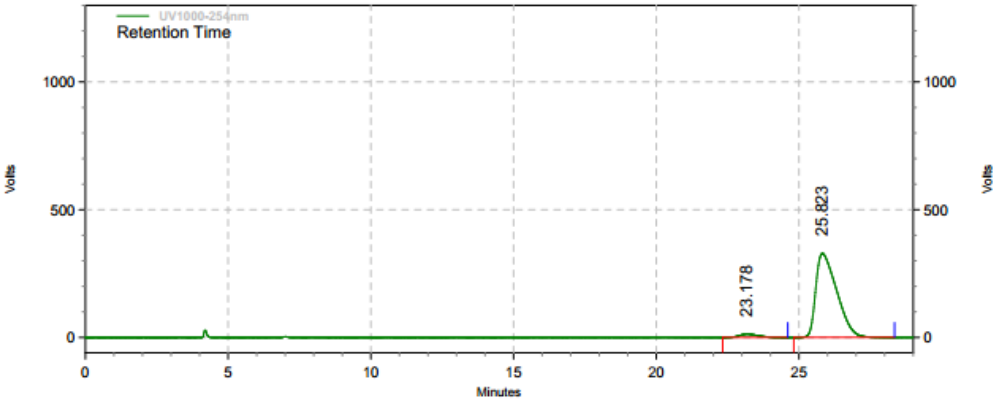


2s



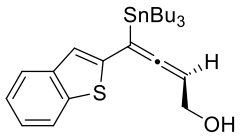
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
22.762	8509280	49.32	193223	51.67
25.453	8743402	50.68	180762	48.33
Totals	17252682	100.00	373985	100.00

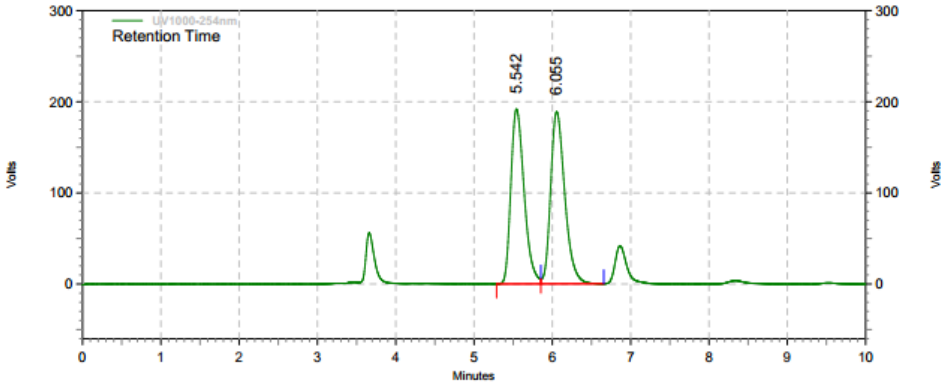


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
23.178	560511	3.25	12935	3.79
25.823	16704709	96.75	328469	96.21
Totals	17265220	100.00	341404	100.00

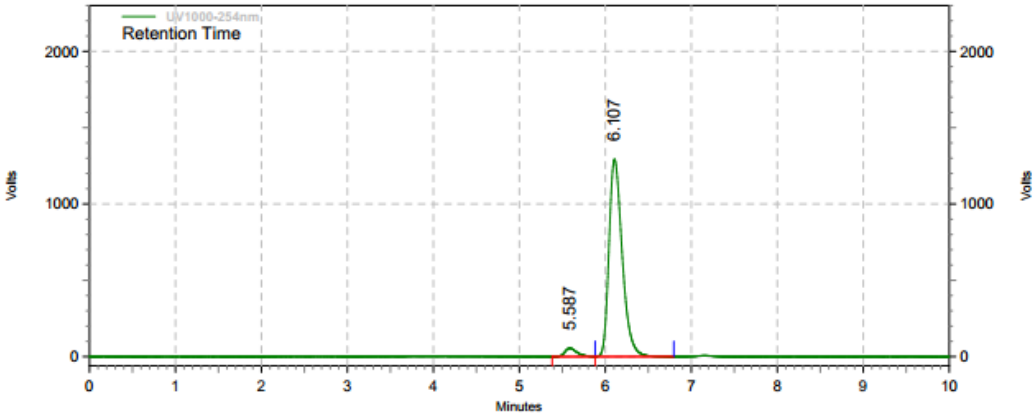


2t



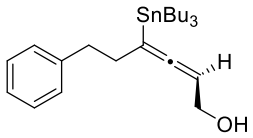
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
5.542	2258230	48.77	191842	50.40
6.055	2372048	51.23	188768	49.60
Totals	4630278	100.00	380610	100.00

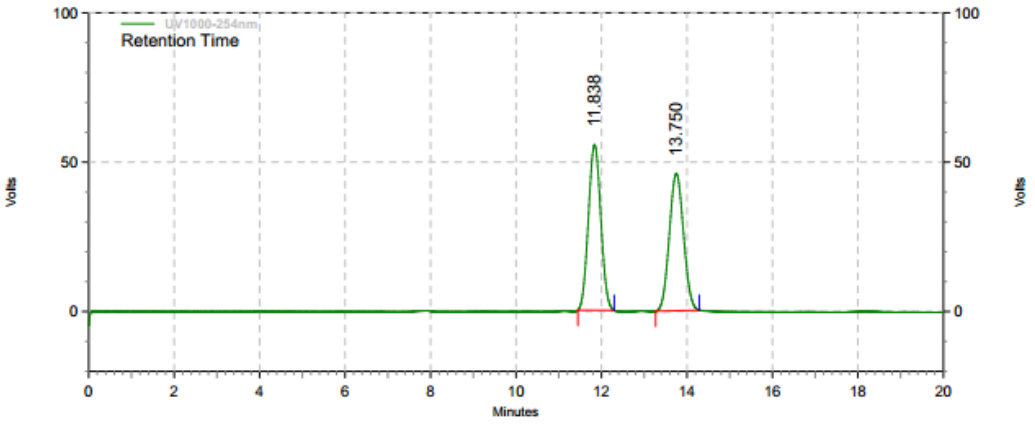


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
5.587	545013	3.79	55554	4.12
6.107	13825041	96.21	1292092	95.88
Totals	14370054	100.00	1347646	100.00

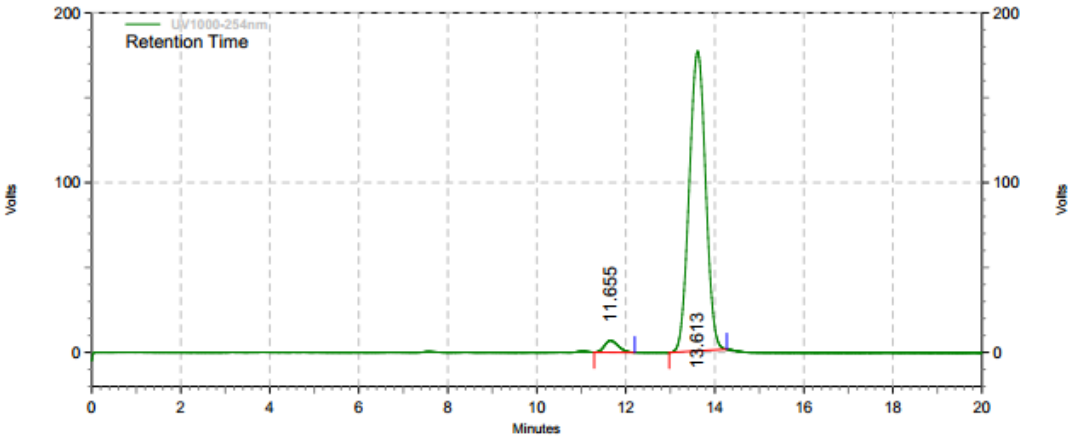


2u



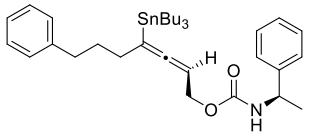
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
11.838	1114971	51.25	55384	54.66
13.750	1060426	48.75	45937	45.34
Totals	2175397	100.00	101321	100.00

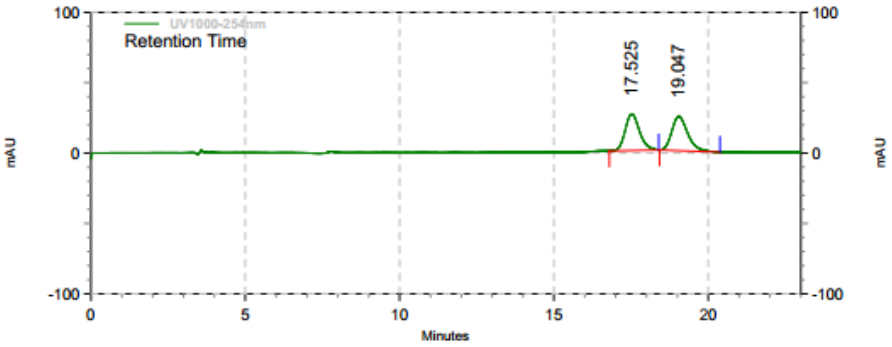


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
11.655	147857	3.17	6960	3.79
13.613	4511255	96.83	176448	96.21
Totals	4659112	100.00	183408	100.00

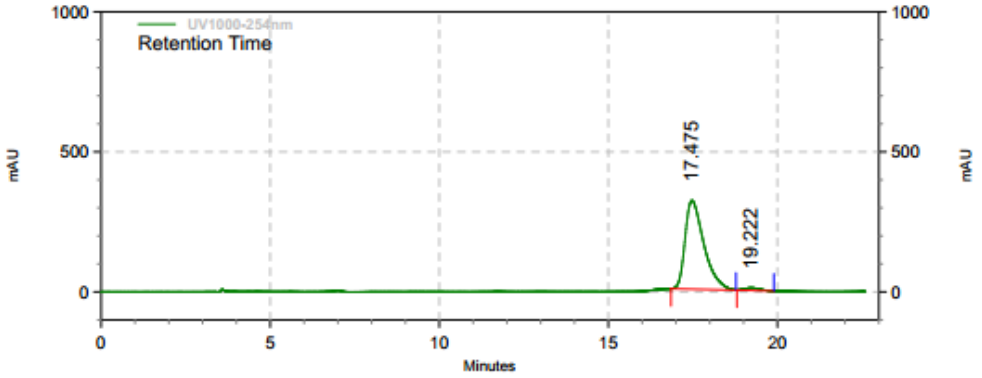


2v'



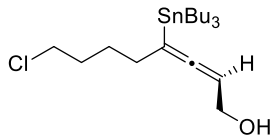
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
17.525	836650	49.04	25985	51.75
19.047	869380	50.96	24231	48.25
Totals	1706030	100.00	50216	100.00

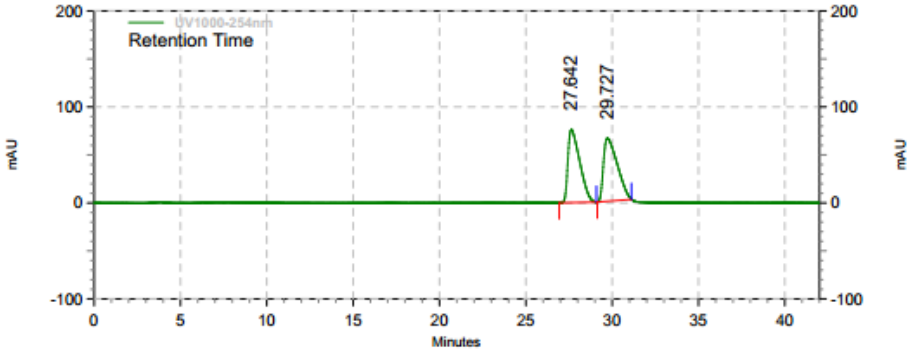


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
17.475	12233166	97.79	316406	97.26
19.222	276753	2.21	8913	2.74
Totals	12509919	100.00	325319	100.00

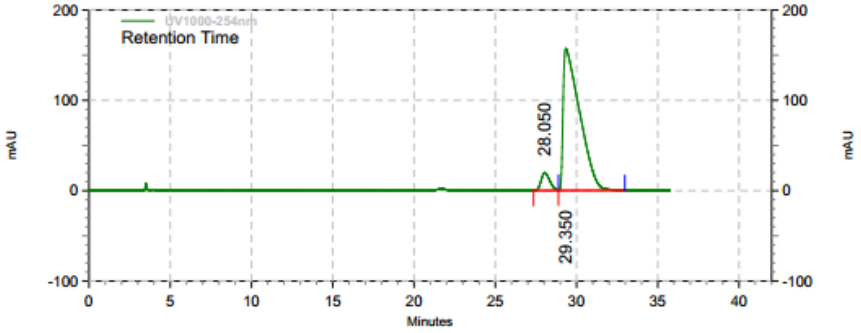


2w



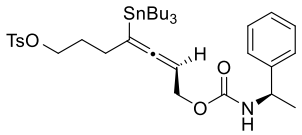
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
27.642	3623932	49.86	75982	53.69
29.727	3644994	50.14	65540	46.31
Totals	7268926	100.00	141522	100.00

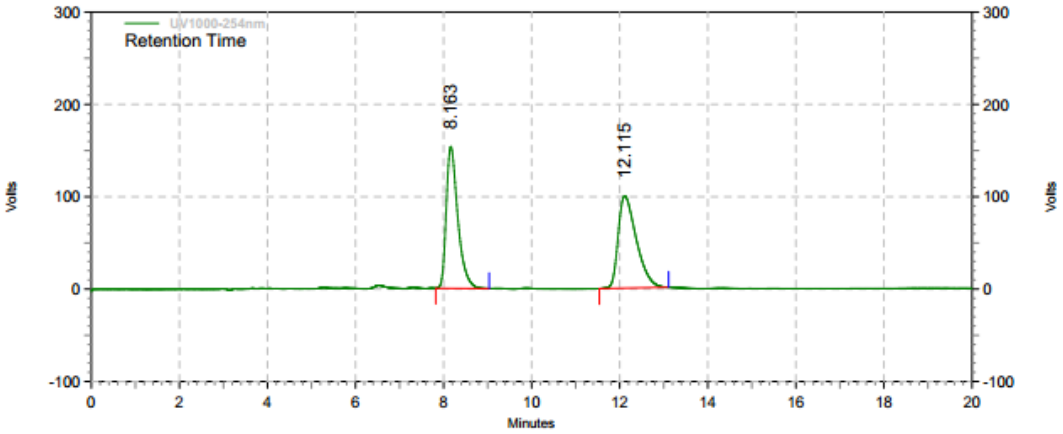


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
28.050	725059	6.14	19498	11.05
29.350	11082558	93.86	156948	88.95
Totals	11807617	100.00	176446	100.00



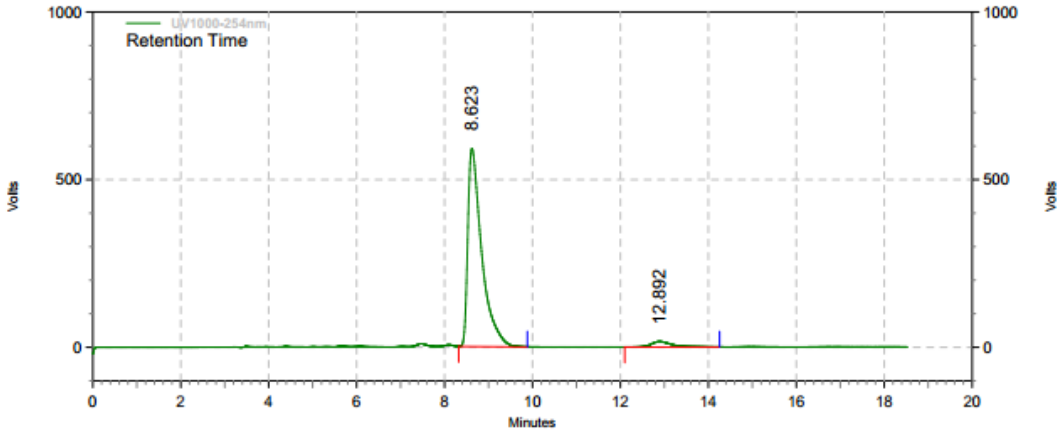
2x'



UV1000-254nm

Results

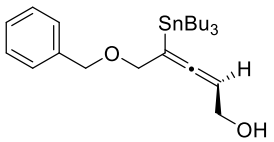
Retention Time	Area	Area %	Height	Height %
8.163	2798842	49.43	153548	60.59
12.115	2862978	50.57	99883	39.41
Totals	5661820	100.00	253431	100.00



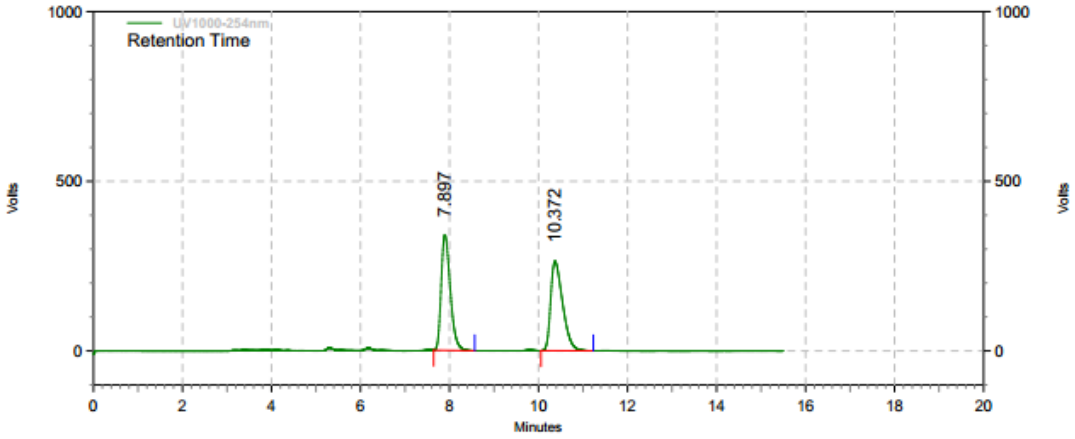
UV1000-254nm

Results

Retention Time	Area	Area %	Height	Height %
8.623	12951588	96.11	589935	97.31
12.892	523754	3.89	16279	2.69
Totals	13475342	100.00	606214	100.00

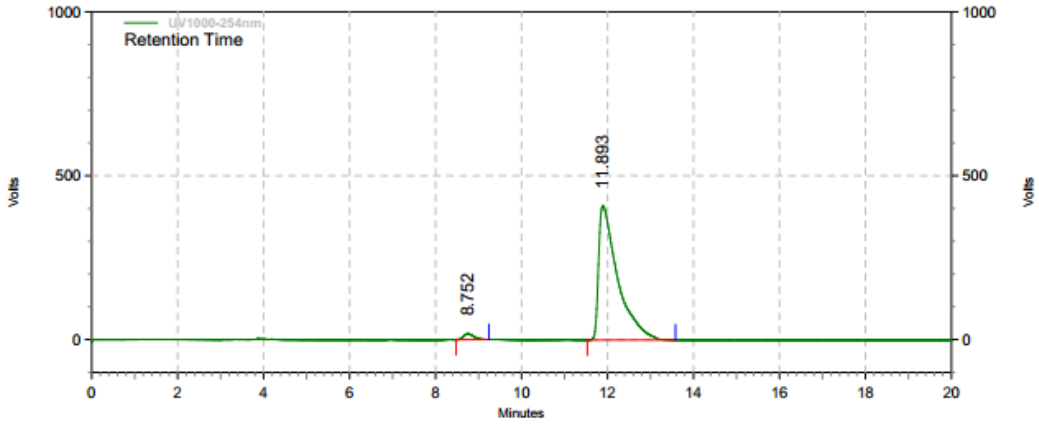


2y



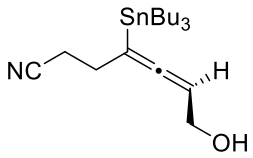
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
7.897	4842603	49.58	340715	56.38
10.372	4925472	50.42	263625	43.62
Totals	9768075	100.00	604340	100.00

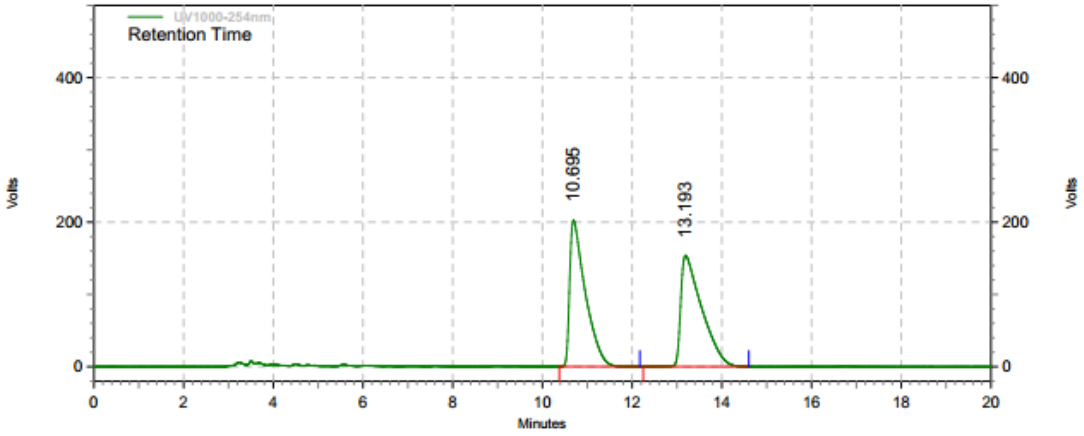


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.752	296004	2.30	17606	4.12
11.893	12589565	97.70	410009	95.88
Totals	12885569	100.00	427615	100.00

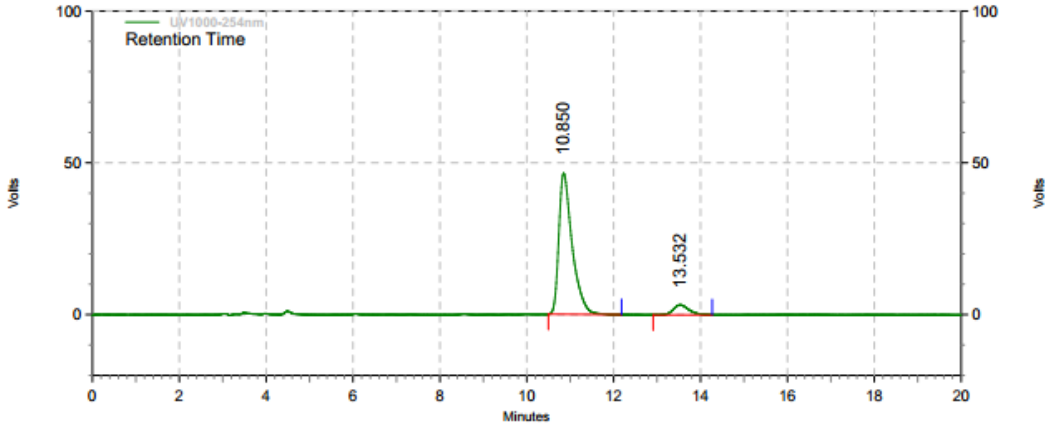


2z



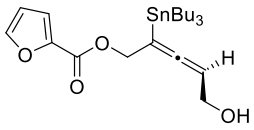
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
10.695	4910706	49.57	202331	56.81
13.193	4995353	50.43	153793	43.19
Totals	9906059	100.00	356124	100.00

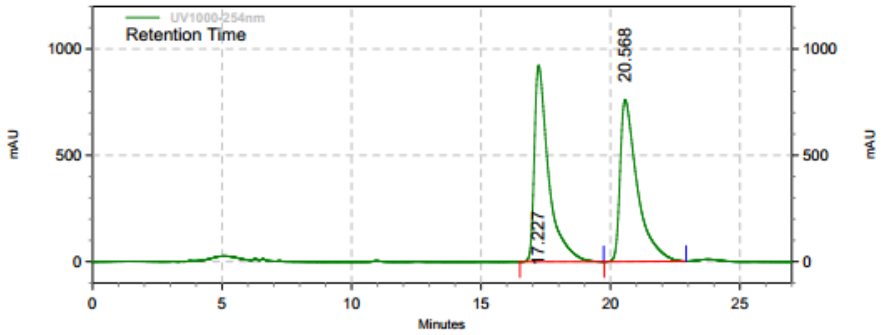


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
10.850	992279	92.36	46452	93.41
13.532	82090	7.64	3278	6.59
Totals	1074369	100.00	49730	100.00

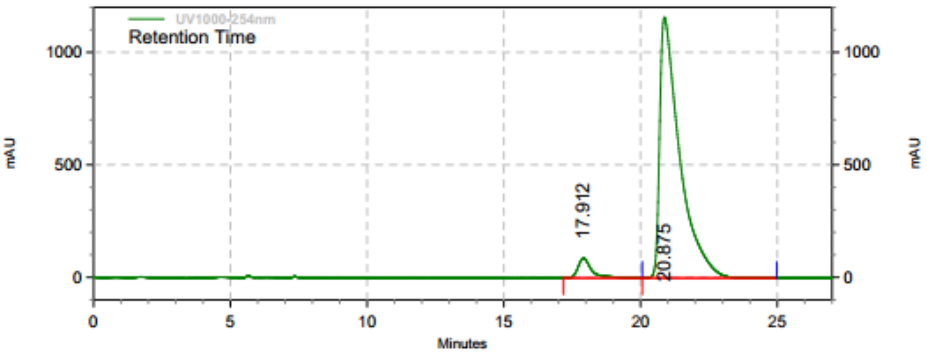


2aa



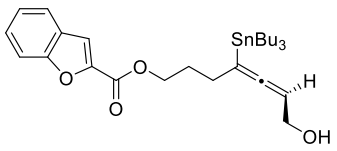
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
17.227	35317177	50.14	921959	54.80
20.568	35126439	49.86	760343	45.20
Totals	70443616	100.00	1682302	100.00

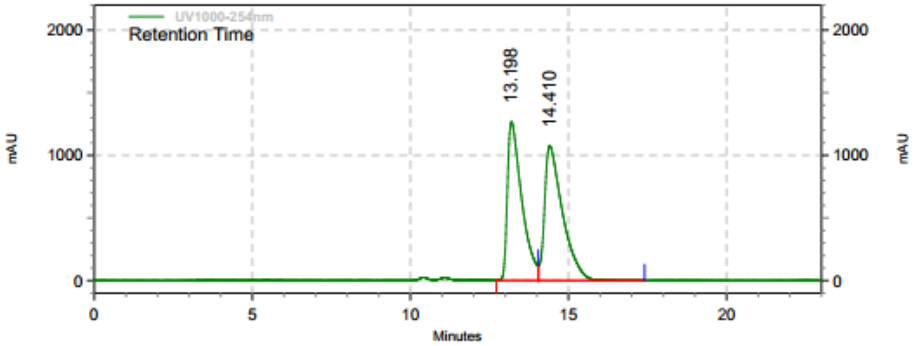


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
17.912	3082889	4.98	88105	7.07
20.875	58817876	95.02	1158034	92.93
Totals	61900765	100.00	1246139	100.00

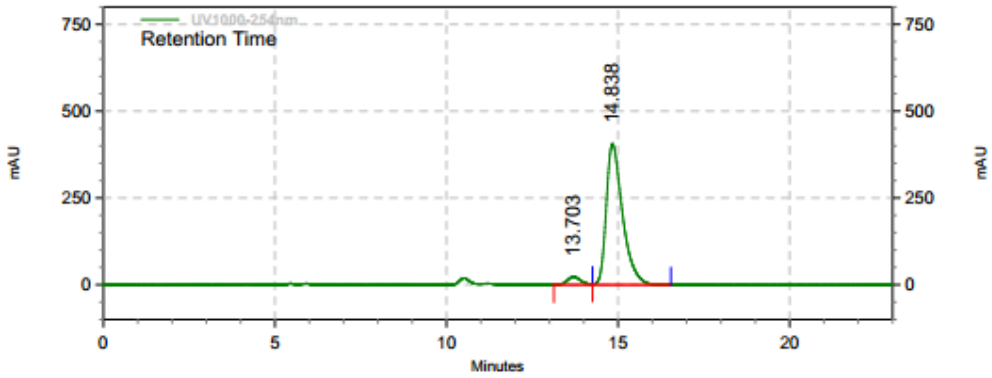


2ab



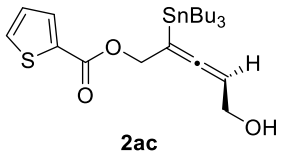
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
13.198	39933441	48.39	1264960	54.07
14.410	42583373	51.61	1074578	45.93
Totals	82516814	100.00	2339538	100.00

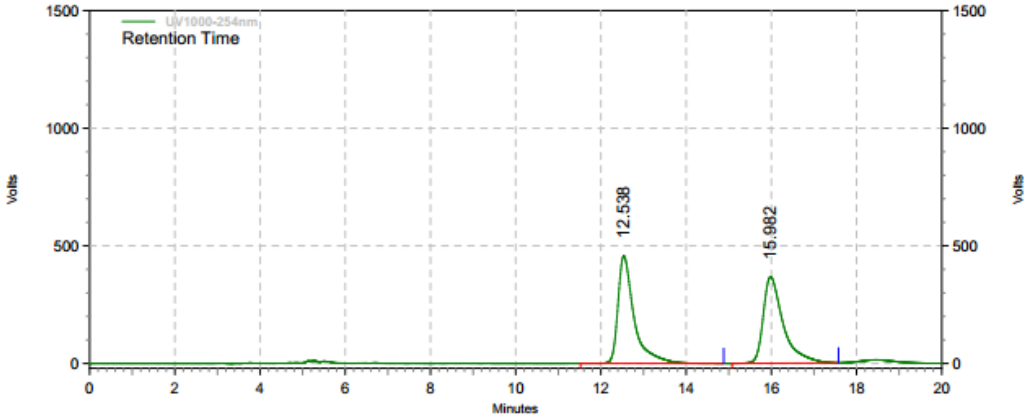


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
13.703	628752	4.50	23294	5.43
14.838	13358766	95.50	406017	94.57
Totals	13987518	100.00	429311	100.00



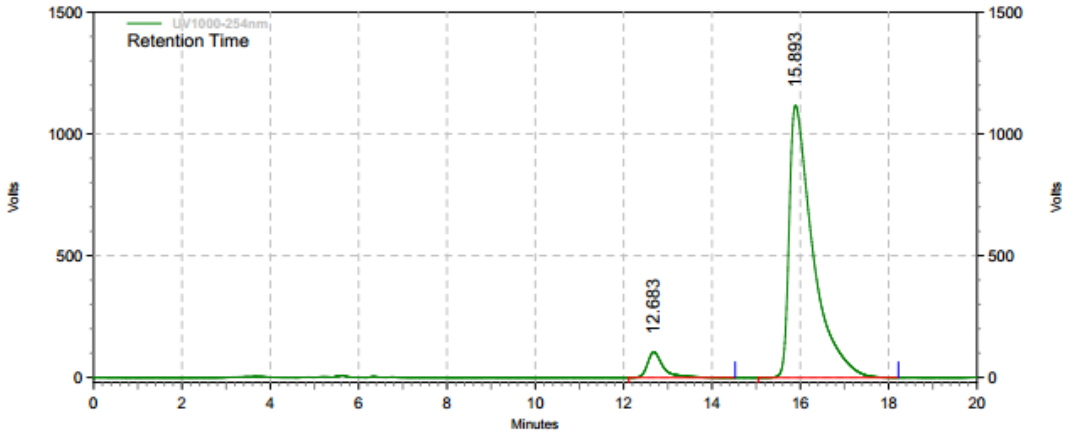
2ac



UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
12.538	12028007	50.12	456769	55.40
15.982	11970327	49.88	367674	44.60

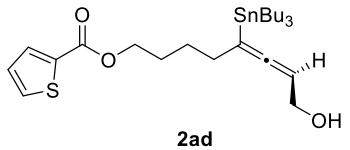
Totals				
	23998334	100.00	824443	100.00



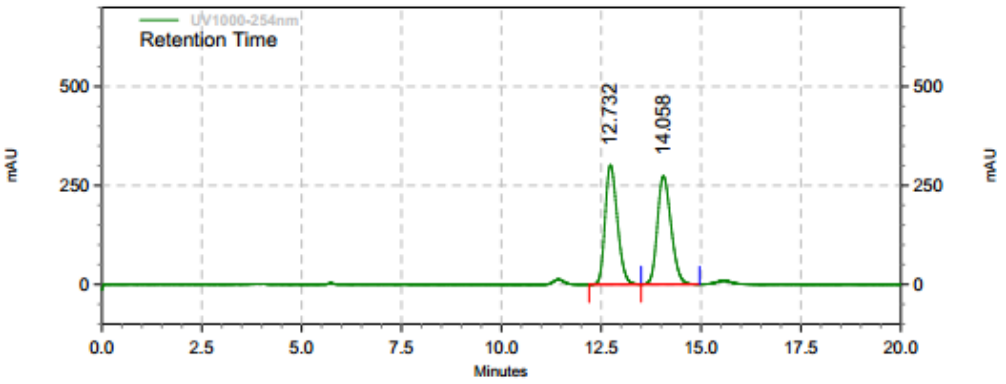
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
12.683	2608054	5.91	104852	8.58
15.893	41550259	94.09	1117216	91.42

Totals				
	44158313	100.00	1222068	100.00

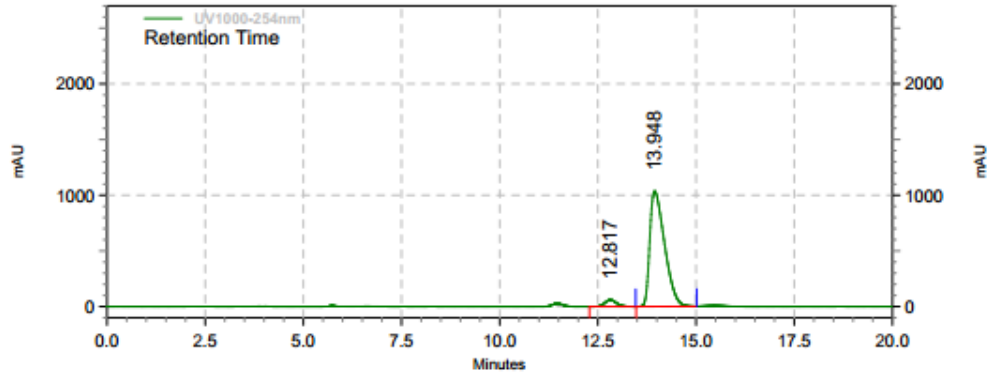


2ad



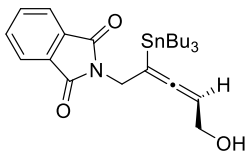
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
12.732	6423444	49.60	301396	52.46
14.058	6526947	50.40	273180	47.54
Totals	12950391	100.00	574576	100.00

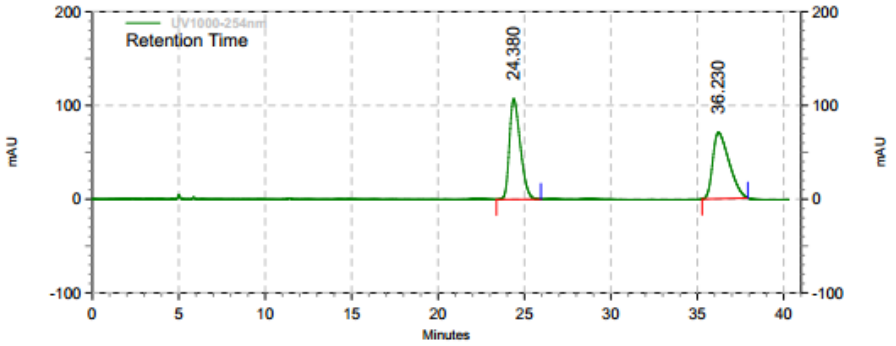


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
12.817	1230299	4.35	60218	5.50
13.948	27077664	95.65	1035498	94.50
Totals	28307963	100.00	1095716	100.00

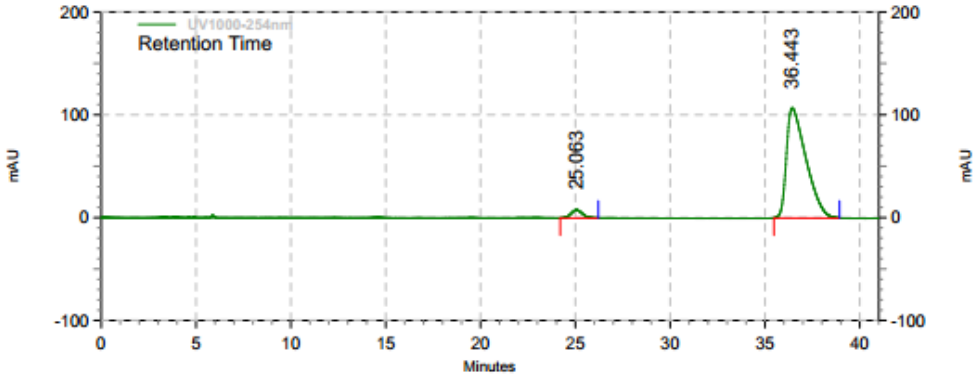


2ae



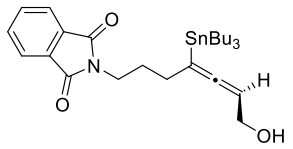
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
24.380	4704299	50.28	107129	60.30
36.230	4651237	49.72	70529	39.70
Totals	9355536	100.00	177658	100.00

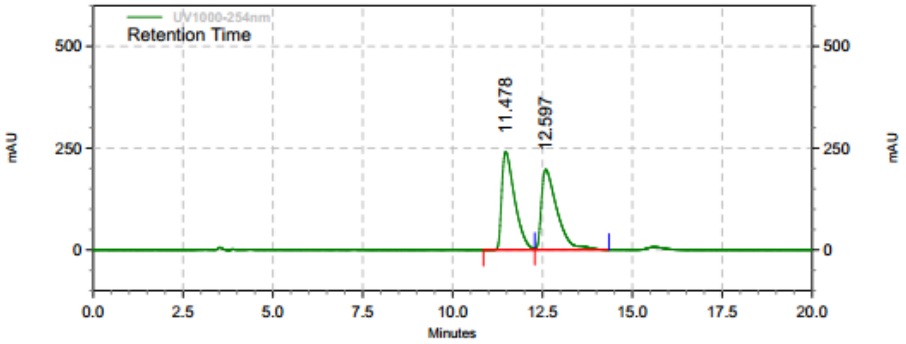


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
25.063	324730	4.06	7832	6.82
36.443	7680507	95.94	106968	93.18
Totals	8005237	100.00	114800	100.00

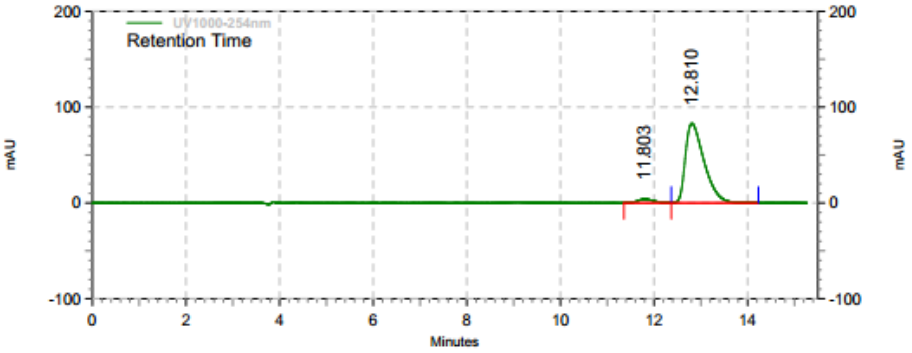


2af



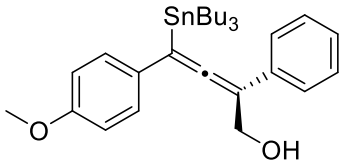
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
11.478	5992610	49.99	240729	55.02
12.597	5994237	50.01	196832	44.98
Totals	11986847	100.00	437561	100.00

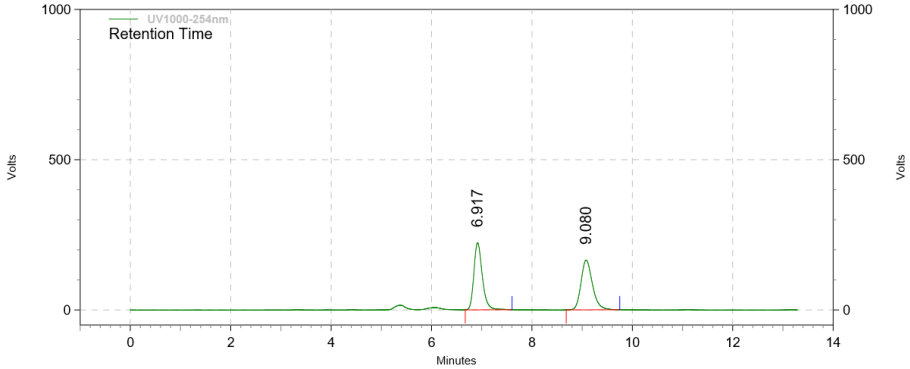


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
11.803	92215	3.84	3920	4.51
12.810	2309293	96.16	83012	95.49
Totals	2401508	100.00	86932	100.00

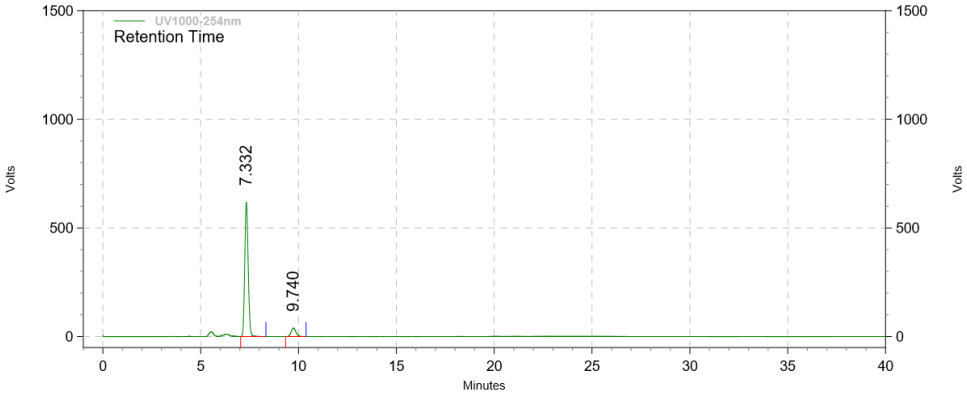


2ag



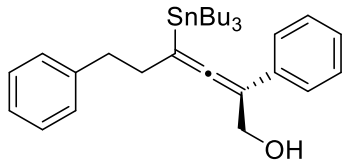
UV1000-254nm
Results

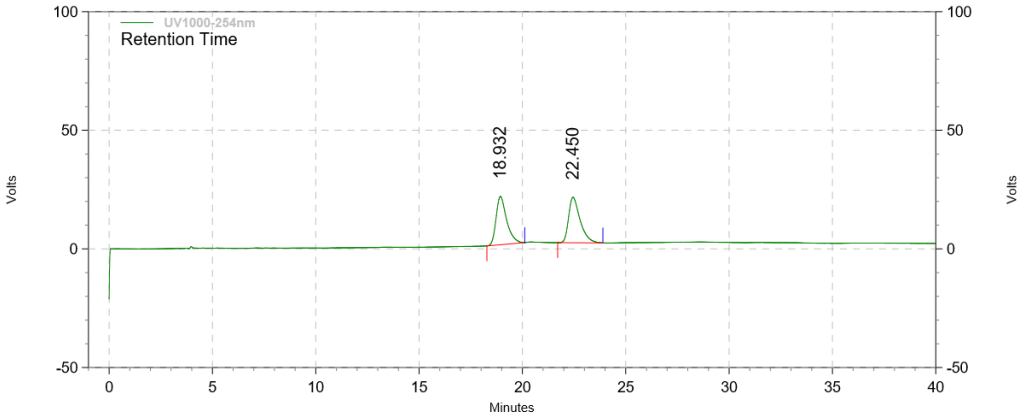
Retention Time	Area	Area %	Height	Height %
6.917	2612069	49.93	223598	57.42
9.080	2619395	50.07	165794	42.58
Totals	5231464	100.00	389392	100.00



UV1000-254nm
Results

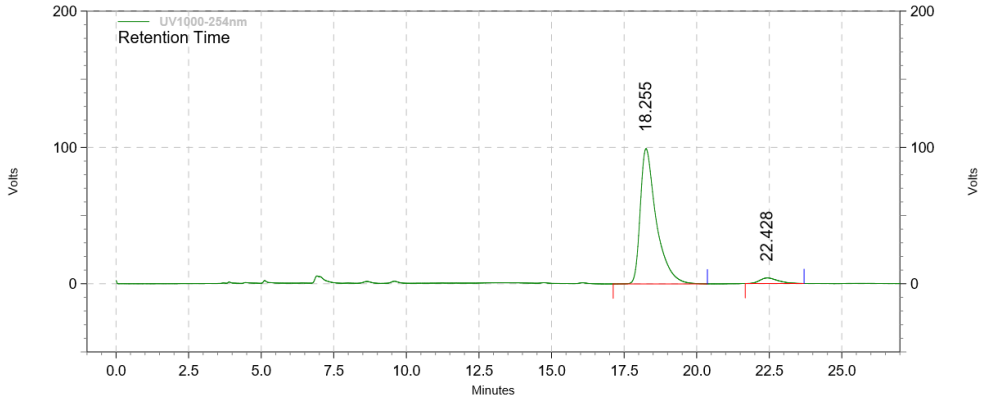
Retention Time	Area	Area %	Height	Height %
7.332	7537754	91.81	618313	94.03
9.740	672393	8.19	39291	5.97
Totals	8210147	100.00	657604	100.00





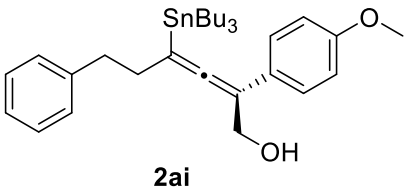
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
18.932	726575	49.48	20372	51.51
22.450	741870	50.52	19174	48.49
Totals	1468445	100.00	39546	100.00

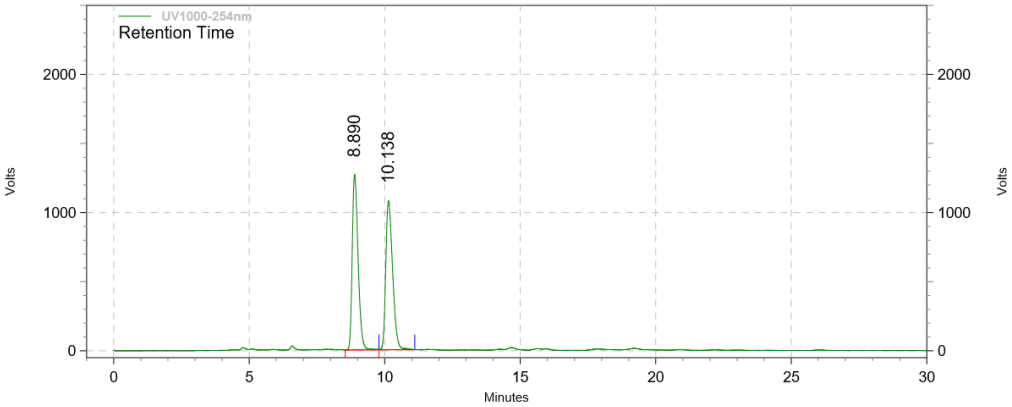


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
18.255	3801100	95.46	99227	96.03
22.428	180975	4.54	4104	3.97
Totals	3982075	100.00	103331	100.00

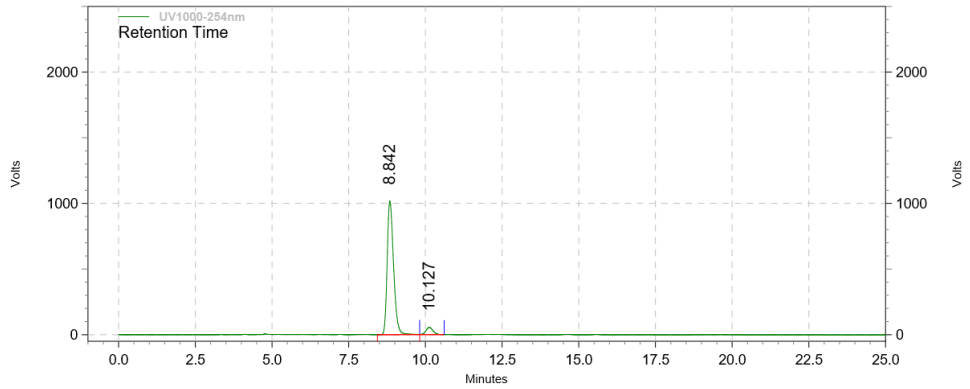


2ai



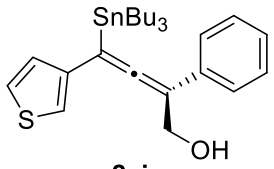
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.890	19033021	50.16	1270003	54.05
10.138	18909384	49.84	1079744	45.95
Totals	37942405	100.00	2349747	100.00

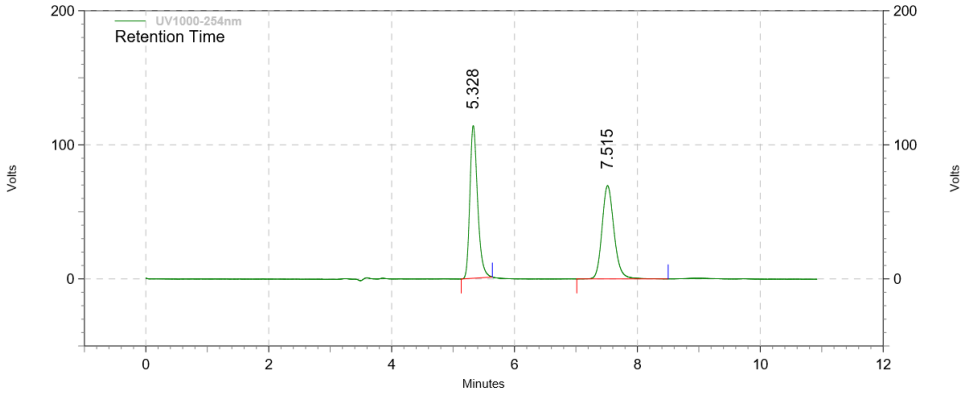


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
8.842	14699364	94.31	1018496	94.86
10.127	886320	5.69	55166	5.14
Totals	15585684	100.00	1073662	100.00

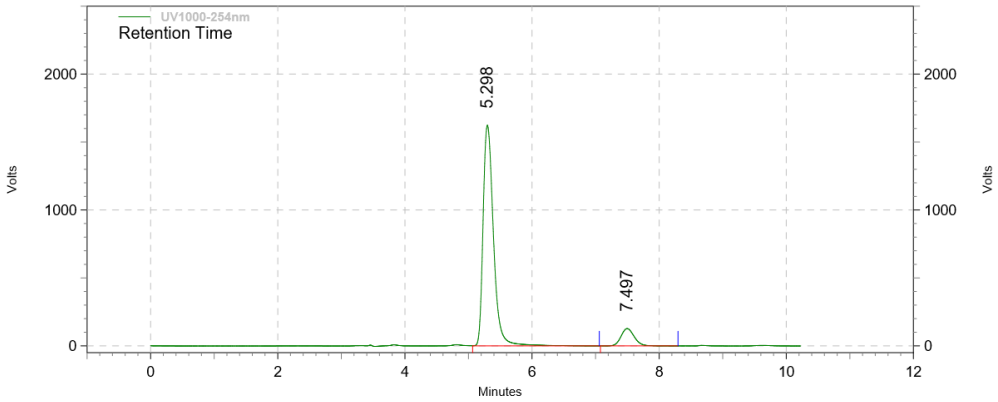


2aj



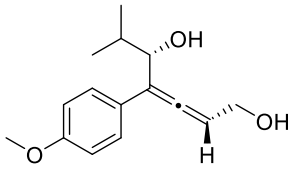
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
5.328	991252	51.28	113900	62.09
7.515	941865	48.72	69550	37.91
Totals	1933117	100.00	183450	100.00

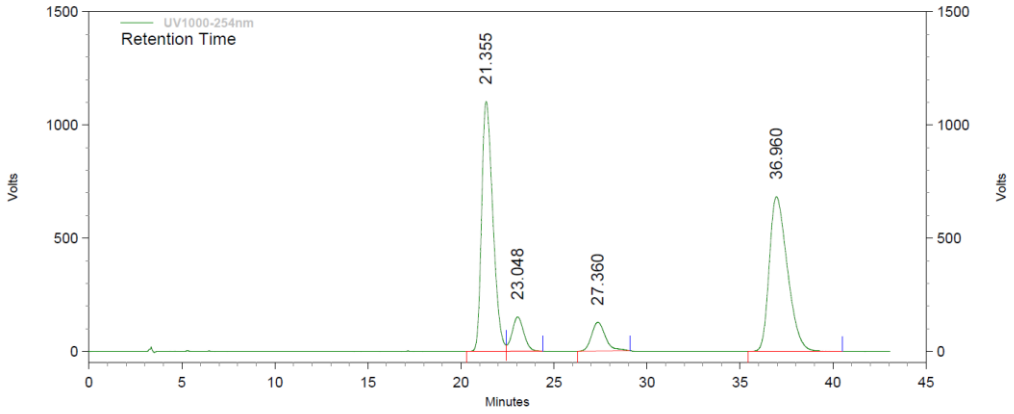


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
5.298	18390385	90.94	1623431	92.72
7.497	1832770	9.06	127420	7.28
Totals	20223155	100.00	1750851	100.00

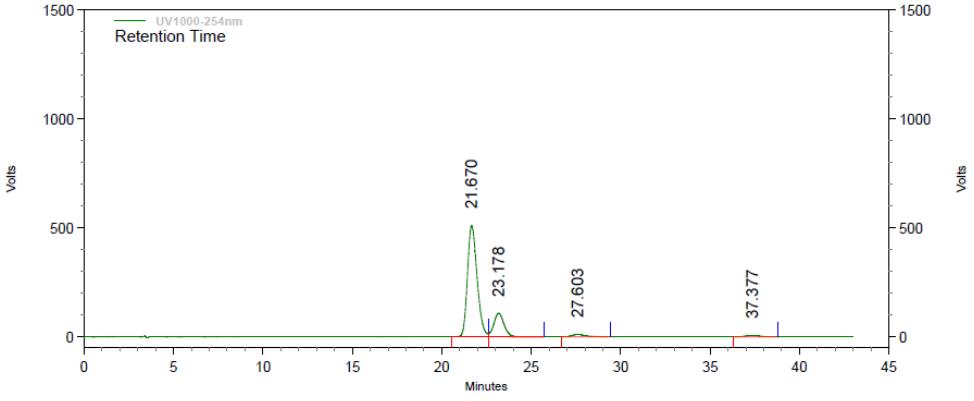


3a



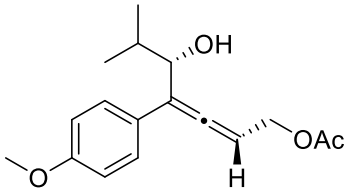
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
21.355	46222430	43.73	1103210	53.44
23.048	6617047	6.26	151186	7.32
27.360	6594937	6.24	126932	6.15
36.960	46262220	43.77	682884	33.08
Totals	105696634	100.00	2064212	100.00

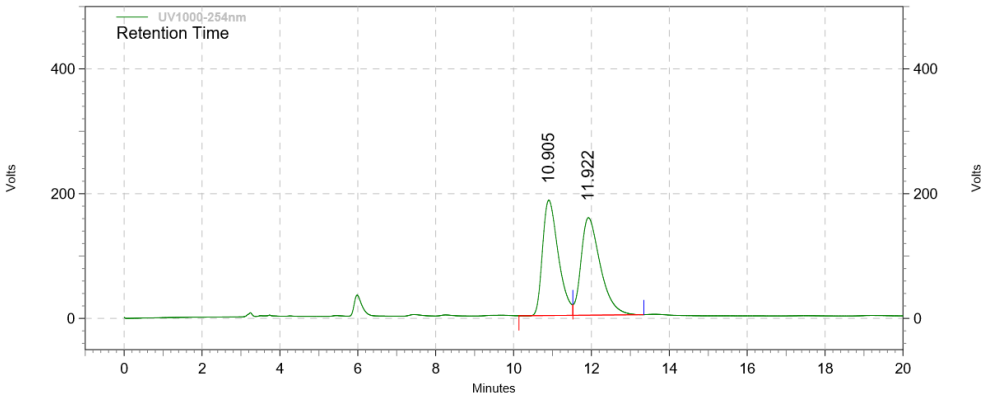


UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
21.670	18975917	78.39	510025	80.33
23.178	4246404	17.54	107746	16.97
27.603	609883	2.52	10992	1.73
37.377	375258	1.55	6181	0.97
Totals	24207462	100.00	634944	100.00

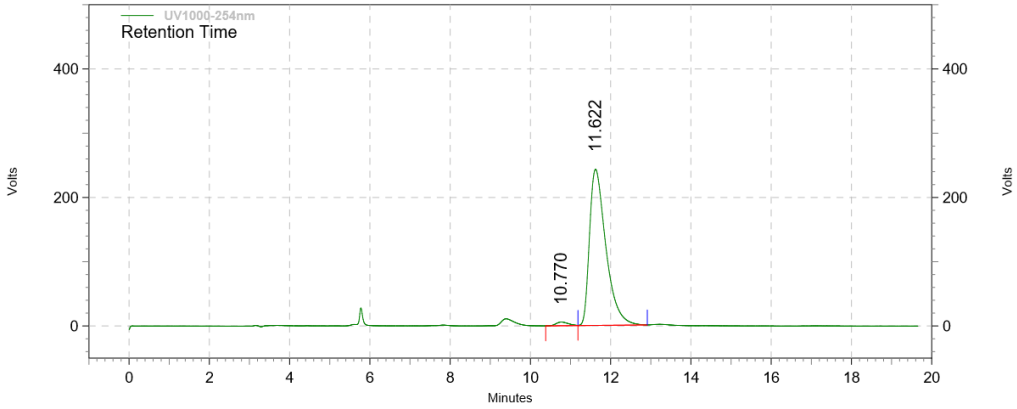


4a



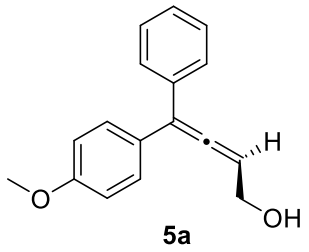
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
10.905	5199514	49.12	185008	54.21
11.922	5385943	50.88	156249	45.79
Totals	10585457	100.00	341257	100.00



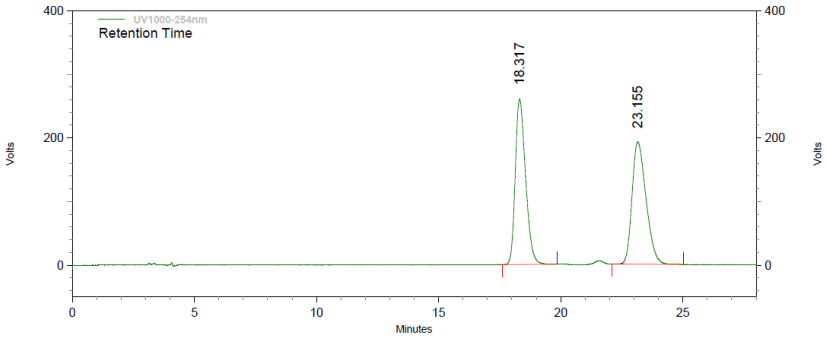
UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
10.770	123312	1.76	5788	2.33
11.622	6877369	98.24	243078	97.67
Totals	7000681	100.00	248866	100.00



5a

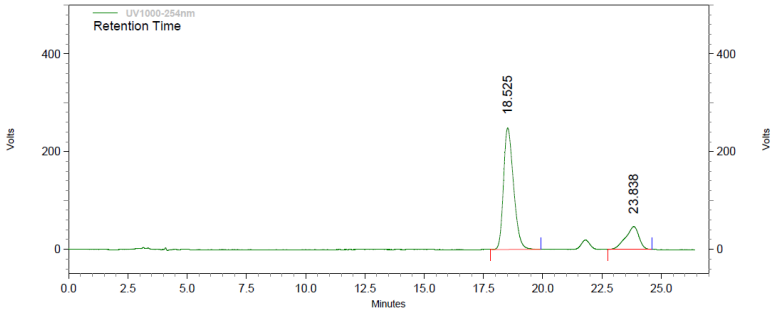
Data File: D:\HPLC\yjl\race\stille\race 20201121
Method: C:\EZChrom Elite\Enterprise\Projects\Default\Method\zyl-BN.met
Acquired: 2020-11-21 上午 09:18:24
Printed: 2020-11-25 14:15:55



UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
18.317	7631697	49.91	260229	57.52
23.155	7659184	50.09	192185	42.48
Totals	15290881	100.00	452414	100.00

Data File: D:\HPLC\yjl\race\stille\cu sop 20201121
Method: C:\EZChrom Elite\Enterprise\Projects\Default\Method\zyl-BN.met
Acquired: 2020-11-21 上午 09:50:08
Printed: 2020-11-25 14:17:47



UV1000-254nm
Results

Retention Time	Area	Area %	Height	Height %
18.525	7312734	79.87	248700	84.17
23.838	1843128	20.13	46757	15.83
Totals	9155862	100.00	295457	100.00