

Supplementary Information

BINAP-CuH-Catalysed Enantioselective Allylation Using Alkoxyallenes to Access 1,2-*syn-tert,sec*-Diols

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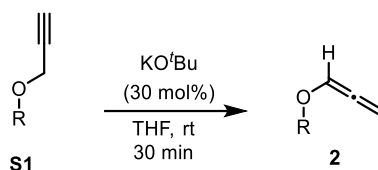
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1. General details

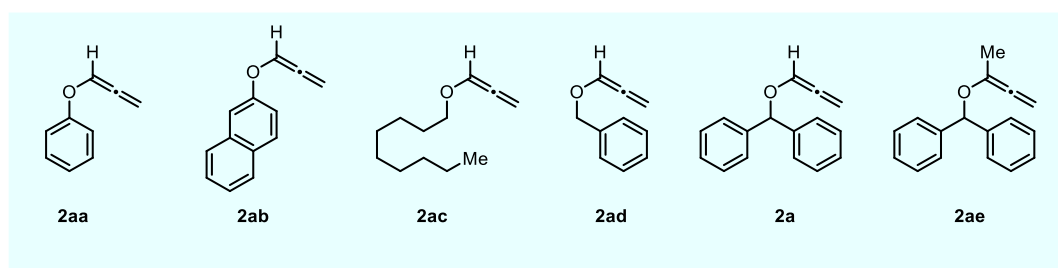
General information: Unless otherwise noted, all reagents, catalysts and ligands were purchased from commercial suppliers and used without further purification. All the acetophenones, indanones, tetralones and symmetrical ketones were purchased from commercial suppliers and used without further purification. All reactions were performed under nitrogen atmosphere and in a flame-dried or oven-dried glassware with magnetic stirring. All solvents were dried before use following the standard procedures. Reactions were monitored using thin-layer chromatography (SiO₂). TLC plates were visualized with UV light (254 nm), iodine treatment or using *p*-anisaldehyde stain or β -naphthol stain. Column chromatography was carried out using 100-200 mesh silica gel packed in glass columns. NMR spectra were recorded at 300, 400, 500 MHz (H) and at 75, 101, 126 MHz (C), respectively. Chemical shifts (δ) are reported in ppm, using the residual solvent peak in CDCl₃ (H: δ = 7.26 and C: δ = 77.16 ppm) as internal standard. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, dd = doublet of doublets, m = multiplet), coupling constants (Hz) and integration. HRMS were recorded using ESI-TOF techniques. Enantiomeric ratio (*er*) values were determined by chiral HPLC (Shimadzu LC-20AD) of the purified product and diastereomer ratio (*dr*) values were determined by ¹H NMR analysis. HRMS were recorded using ESI-TOF techniques. Optical rotations of all chiral compounds were measured on Horiba SEPA-300.

2. Experimental Procedures and Analytical Data

2a. General procedure for synthesis of allene ethers **2**:¹



An oven-dried round-bottomed flask equipped with a magnetic stir bar under an argon atmosphere was charged with alkyl propargyl ether **S1** (500 mg), and dissolved in dry THF (10 mL). To this was added K^tOBu (30 mol%) and the reaction mixture was allowed to stir for 30 mins. The reaction mixture was diluted with hexanes (50 mL), filtered through a pad of silica gel with the aid of hexanes. The filtrate was concentrated *in vacuo* and the residue was subjected to flash column chromatography (neat hexanes) to furnish the mono-substituted alkoxyallenes **2** as a colourless oil.



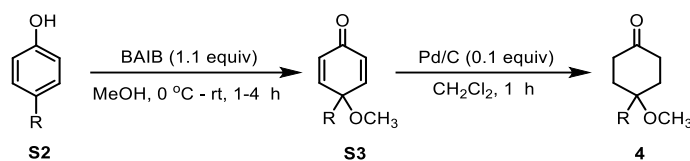
Compound **2aa** was prepared according to a previously reported procedure.²

Compounds **2ab** was prepared according to a previously reported procedure.³

Compounds **2ac** was prepared according to a previously reported procedure.⁴

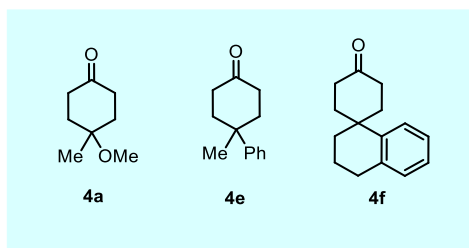
Compounds **2ad**, **2ae** and **2a** were prepared according to a previously reported procedure.¹

2b. Preparation of 4,4-disubstituted cyclohexanone substrates⁴:



The general experimental procedures for the preparation of *p*-quinol methyl ether were followed as reported in literature.⁵ (Diacetoxiiodo)benzene (BAIB, 1.1 equiv) was added portion wise to a stirred solution of 4-substituted phenol **S2** (2.0-10 mmol) in methanol (5 mL/mmol) at 0 °C. The solution was allowed to warm to room temperature for 1-4 h. Reaction was quenched with saturated aqueous NaHCO₃ solution to neutralize the acidic reaction mixture and extracted with EtOAc three times. The combined organic phase was washed with brine, dried over Na₂SO₄, filtered and concentrated under reduced pressure. The residue was purified by column chromatography (5-10% EtOAc in hexane) to give pure *p*-quinol **S3** and used in the next step.

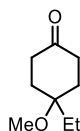
The obtained *p*-quinol **S3** was dissolved in CH₂Cl₂ under nitrogen atmosphere and 10% Pd/C (0.1 equiv) was added to it. The reaction mixture was then stirred under hydrogen atmosphere for 1 h. Then, the reaction mixture was filtered on celite, concentrated under reduced pressure. The crude product was purified using flash column chromatography (5% EtOAc/Hexanes) to obtain the 4,4-disubstituted cyclohexanone substrate **4** as colourless oil.



Compounds **4a** was prepared according to a previously reported procedure.⁵

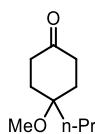
Compounds **4e** and **4f** were prepared according to a previously reported procedure.⁶

4-Ethyl-4-methoxycyclohexan-1-one (**4b**):



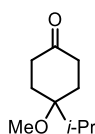
Prepared according to the general procedure as described above in 85% yield (174 mg): It was purified by flash chromatography (10% EtOAc/hexanes; *R_f* = 0.3) to afford a colourless oil; ¹H NMR (400 MHz, CDCl₃) δ 3.23 (s, 3H), 2.58 (td, *J* = 14.3, 6.2 Hz, 2H), 2.28 – 2.07 (m, 3H), 1.64 – 1.55 (m, 5H), 0.90 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 213.0, 74.0, 49.0, 37.0, 33.2, 28.3, 7.5; HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₉H₁₇O₂⁺, 157.1228; found: 157.1225.

4-Methoxy-4-propylcyclohexan-1-one (4c):



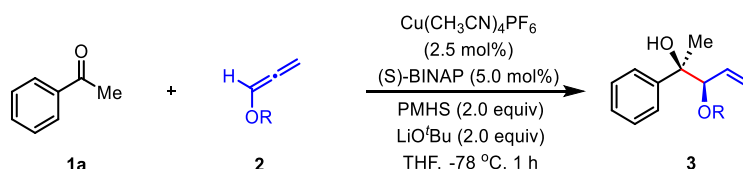
Prepared according to the general procedure as described above in 80 % yield (164 mg): It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 3.22 (s, 3H), 2.56 (td, J = 14.2, 6.1 Hz, 2H), 2.19 – 2.09 (m, 4H), 1.61 (td, J = 13.7, 4.7 Hz, 2H), 1.51 – 1.42 (m, 2H), 1.39 – 1.30 (m, 2H), 0.93 (t, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 212.5, 74.0, 49.0, 38.3, 37.0, 33.6, 16.4, 14.7; HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{10}\text{H}_{19}\text{O}_2^+$, 171.1385; found: 171.1378.

4-iso-Propyl-4-methoxycyclohexan-1-one (4d):



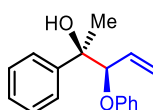
Prepared according to the general procedure as described above in 86% yield (176 mg): It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 3.23 (s, 3H), 2.58 (td, J = 14.3, 6.4 Hz, 2H), 2.26 – 2.17 (m, 2H), 2.12 – 1.93 (m, 3H), 1.79 (dt, J = 13.7, 6.9 Hz, 2H), 0.91 (d, J = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, CDCl_3) δ 212.6, 76.3, 48.1, 36.7, 31.1, 29.2, 17.1; HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{10}\text{H}_{19}\text{O}_2^+$, 171.1385; found: 171.1379.

2c. CuH-Catalysed coupling of alkoxyallenes with acetophenone:



A solution of $\text{Cu}(\text{CH}_3\text{CN})_4\text{PF}_6$ (6.2 mg, 2.5 mol%), (*S*)-BINAP (21.0 mg, 5 mol%), PMHS (178 μL , 1.33 mmol) and LiO^tBu (1.3 mL, 1.33 mmol, 1 M in THF) in dry THF (2.0 mL) was stirred at room temperature for 10 min and then maintained at the temperature of $-78\text{ }^\circ\text{C}$ under inert atmosphere. A solution of acetophenone **1a** (80 mg, 0.67 mmol) and corresponding allene ether **2** (0.67 mmol, 1.0 equiv) in dry THF (1.0 mL) was added *via* syringe and the resulting mixture was stirred at $-78\text{ }^\circ\text{C}$ for 1 h. The reaction mixture was quenched with saturated NH_4Cl (10 mL) solution and extracted with EtOAc (3 $\times$ 15 mL) and dried over anhydrous Na_2SO_4 , filtered and concentrated *in vacuo*. The resultant crude product was purified by column chromatography (hexanes/EtOAc).

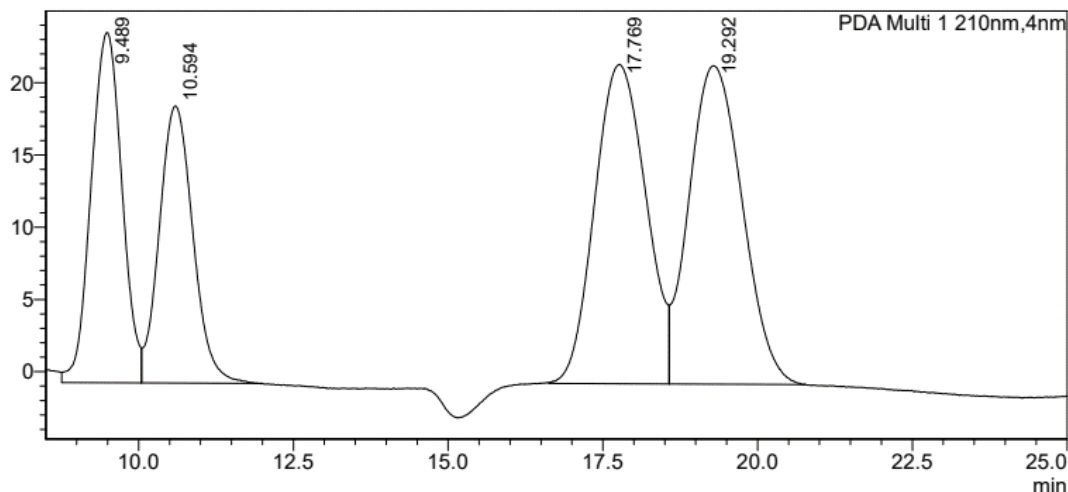
(2*R*,3*R*)-3-Phenoxy-2-phenylpent-4-en-2-ol (3aa):



Prepared according to the general procedure as described above in 85% combined yield (143 mg) with 2:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; Major

isomer: ^1H NMR (400 MHz, CDCl_3) δ 7.61 – 7.56 (m, 2H), 7.41 (t, J = 7.2 Hz, 2H), 7.31 – 7.27 (m, 2H), 7.01 – 6.96 (m, 2H), 6.95 – 6.89 (m, 2H), 5.81 (ddd, J = 17.3, 10.7, 6.3 Hz, 1H), 5.33 (d, J = 10.7 Hz, 1H), 5.28 (dd, J = 8.5, 1.0 Hz, 1H), 4.76 (dd, J = 6.3, 0.8 Hz, 1H), 1.69 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 158.1, 144.5, 133.5, 129.4, 128.1, 127.3, 126.0, 121.6, 119.9, 116.6, 86.4, 76.3, 24.3; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{17}\text{H}_{18}\text{O}_2\text{Na}^+$, 277.1204; found: 277.1196; $[\alpha]^{20}_{\text{D}}$ = -18.80° (c 1.0, CHCl_3); major/minor isomers: 74:26/73:27 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5μ column; hexane/2-propanol = 99/01, detected at 210 nm, Flow rate = 1 mL/min, Retention times: 9.499 min (minor), 10.581 min (major); 17.760 min (minor), 19.278 min (major).

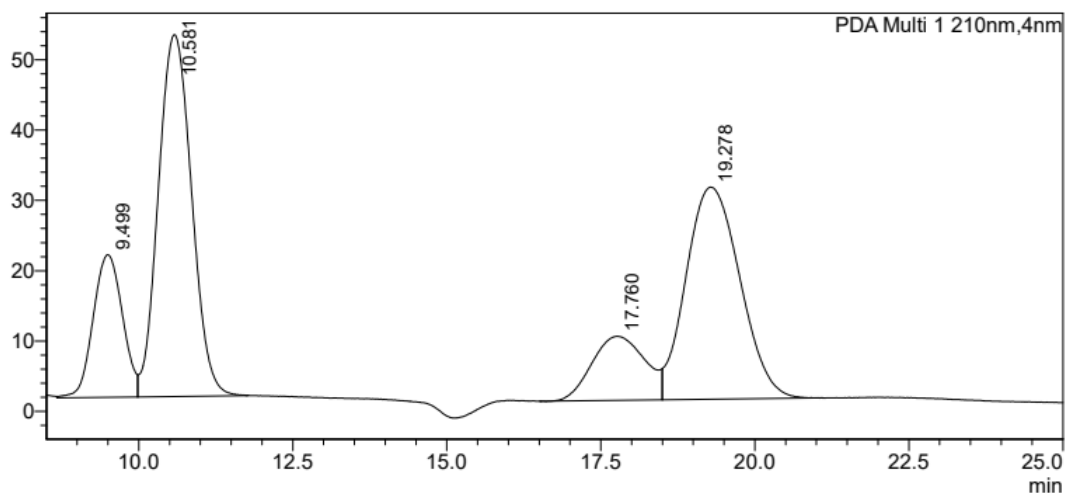
mAU



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PDA Ch1 210nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.489	841060	24246	20.179	27.680
2	10.594	726085	19187	17.421	21.904
3	17.769	1276330	22110	30.622	25.242
4	19.292	1324497	22050	31.778	25.173
Total		4167973	87594	100.000	100.000

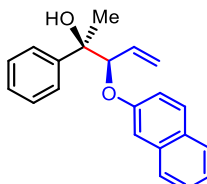
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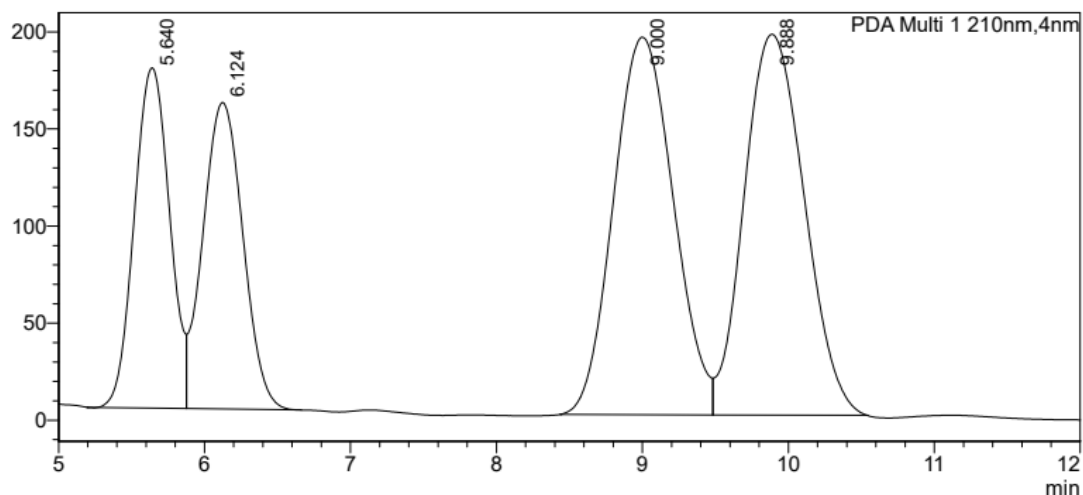
PDA Ch1 210nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.499	671321	20271	13.449	18.266
2	10.581	1932953	51454	38.724	46.366
3	17.760	547558	9099	10.969	8.199
4	19.278	1839812	30150	36.858	27.169
Total		4991644	110974	100.000	100.000

(2R,3R)-3-(Naphthalen-2-yloxy)-2-phenylpent-4-en-2-ol (3ab):



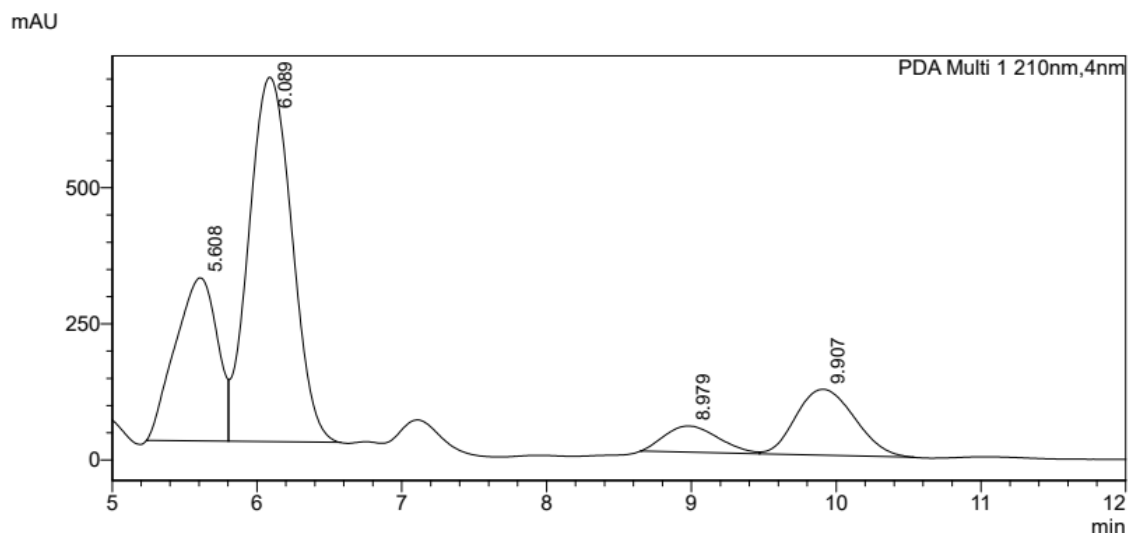
Prepared according to the general procedure as described above in 73% combined yield (148 mg) with 2:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; major isomer; ^1H NMR (500 MHz, CDCl_3) δ 7.81 – 7.70 (m, 3H), 7.64 – 7.58 (m, 2H), 7.49 – 7.10 (m, 7H), 5.87 (ddd, J = 17.1, 11.5, 7.5 Hz, 1H), 5.36 (d, J = 11.2 Hz, 1H), 4.93 (s, 2H), 2.70 (s, 1H), 1.73 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 156.0, 145.0, 134.4, 133.3, 130.1, 129.4, 128.2, 128.0, 127.4, 127.1, 127.0, 126.1, 126.0, 124.1, 120.0, 119.4, 110.2, 86.4, 76.3, 24.4; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{21}\text{H}_{20}\text{O}_2\text{Na}^+$, 327.1361; found: 327.1361; $[\alpha]_D^{20}$ = -27.76° (c 1.0, CHCl_3); major/minor isomers: 69:31/73:27 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 99/01, detected at 210 nm, Flow rate = 1 mL/min, Retention times: 5.608 min (minor), 6.089 min (major); 8.979 min (minor), 9.907 min (major).

mAU



<Peak Table>

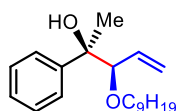
PDA Ch1 210nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.640	2959066	175265	17.256	24.220
2	6.124	3005650	157906	17.528	21.821
3	9.000	5564918	194365	32.452	26.860
4	9.888	5618286	196100	32.764	27.099
Total		17147920	723635	100.000	100.000



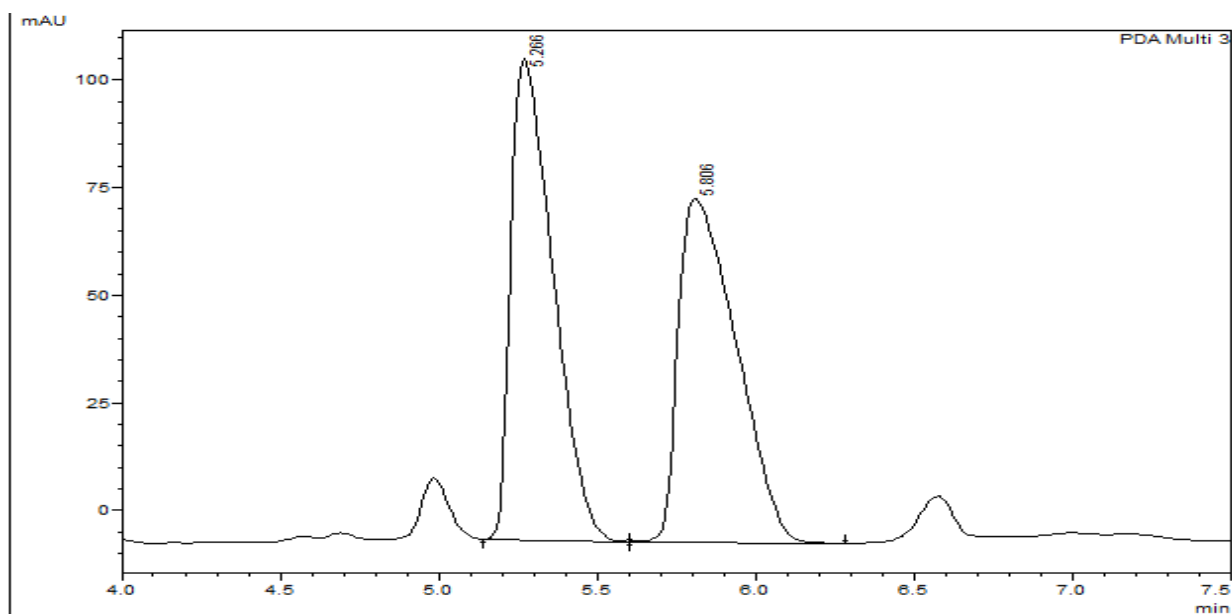
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PDA Ch1 210nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.608	6085647	299654	24.753	26.329
2	6.089	13855257	669439	56.355	58.820
3	8.979	1240206	47987	5.044	4.216
4	9.907	3404498	121038	13.848	10.635
Total		24585607	1138118	100.000	100.000

(2*R*,3*R*)-3-(Nonyloxy)-2-phenylpent-4-en-2-ol (3ac):

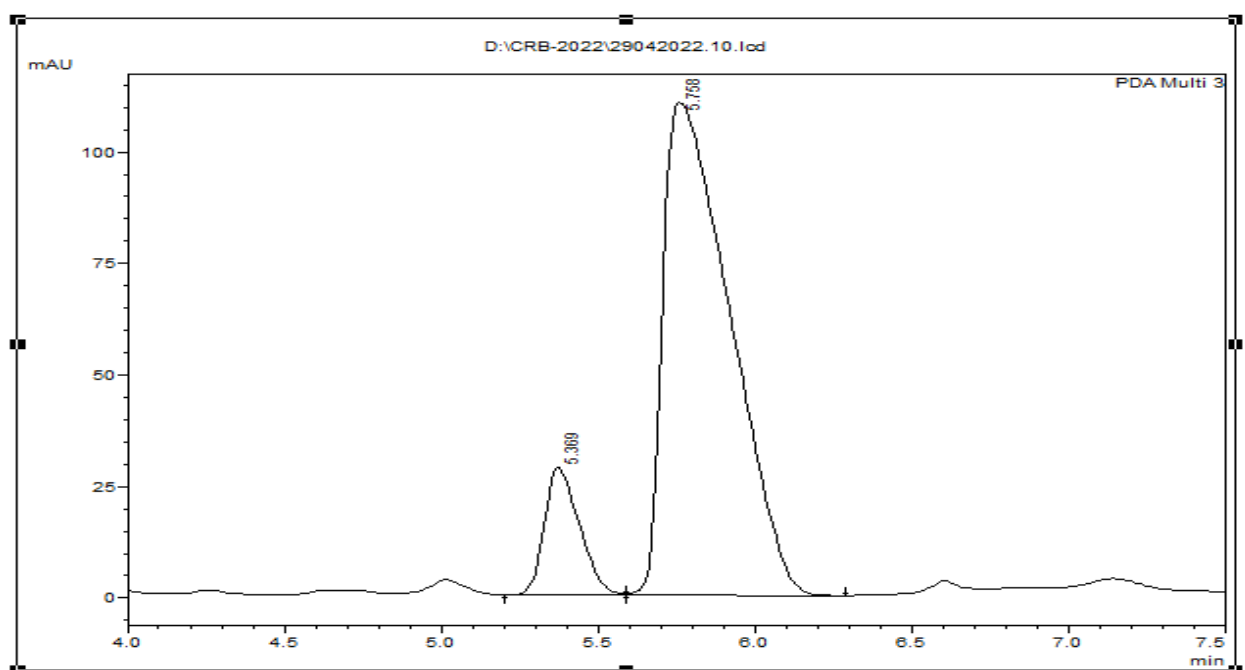


Prepared according to the general procedure as described above in 86% yield (173 mg) with >20:1 *dr*. It was purified by flash chromatography (5% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.41 – 7.36 (m, 2H), 7.30 – 7.21 (m, 2H), 7.21 – 7.13 (m, 1H), 5.62 (ddd, J = 17.4, 10.4, 7.6 Hz, 1H), 5.07 (dd, J = 1.8, 0.9 Hz, 1H), 5.03 (dd, J = 1.8, 0.9 Hz, 1H), 3.66 (d, J = 7.6 Hz, 1H), 3.42 (dt, J = 9.3, 6.5 Hz, 1H), 3.11 (dt, J = 9.3, 6.5 Hz, 1H), 1.38 (s, 3H), 1.27 – 1.09 (m, 14H), 0.81 (t, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 145.7, 134.7, 128.0, 127.1, 126.0, 119.6, 88.1, 76.1, 69.4, 32.0, 29.8, 29.7, 29.5, 29.4, 26.2, 24.4, 22.8, 14.3; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{20}\text{H}_{32}\text{O}_2\text{Na}^+$, 327.2272; found: 327.2300; $[\alpha]^{20}_{\text{D}}$ = -11.65° (c 1.0, CHCl_3); 88:12 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IC 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 5.758 min (major), 5.369 min (minor).



PDA Ch3 254nm 1nm

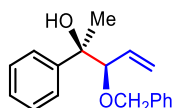
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.266	1036733	111853	50.544	58.366
2	5.806	1014423	79787	49.456	41.634
Total		2051156	191640	100.000	100.000



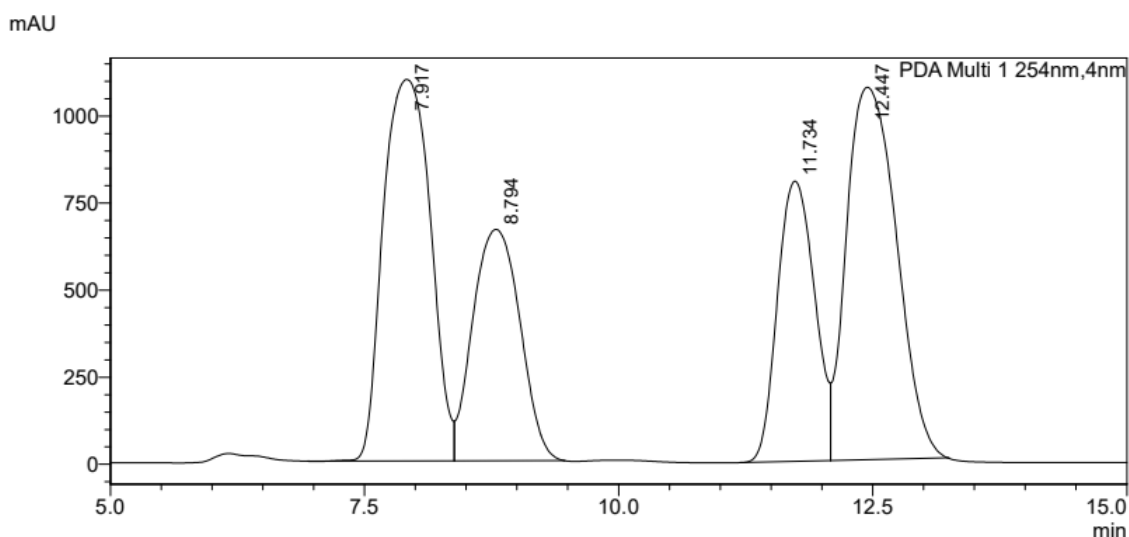
PDA Ch3 254nm 1nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.369	223854	28658	12.010	20.593
2	5.758	1640065	110507	87.990	79.407
Total		1863919	139165	100.000	100.000

(2*R*,3*R*)-3-(Benzyloxy)-2-phenylpent-4-en-2-ol (3ad):

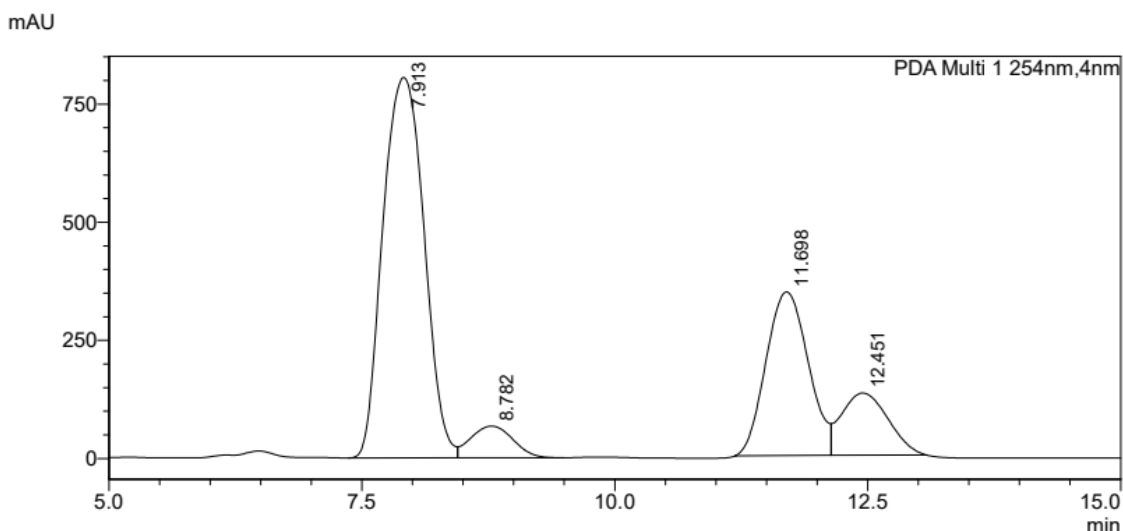


Prepared according to the general procedure as described above in 91% combined yield (163 mg) with 4:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; Major isomer; ^1H NMR (500 MHz, CDCl_3) δ 7.35 – 7.30 (m, 2H), 7.25 – 7.14 (m, 6H), 7.00 – 6.97 (m, 2H), 5.71 (ddd, J = 17.4, 10.4, 8.0 Hz, 1H), 5.27 (ddd, J = 10.5, 1.7, 0.6 Hz, 1H), 5.11 (ddd, J = 17.3, 1.7, 0.8 Hz, 1H), 4.48 (d, J = 11.9 Hz, 1H), 4.19 (d, J = 11.9 Hz, 1H), 3.79 (d, J = 8.0 Hz, 1H), 2.85 (s, 1H), 1.37 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 145.8, 138.0, 134.2, 128.4, 128.0, 127.8, 127.6, 126.8, 125.7, 120.6, 87.1, 76.0, 70.6, 25.0; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{18}\text{H}_{20}\text{O}_2\text{Na}^+$, 291.1361; found: 291.1365; $[\alpha]^{20}_{\text{D}}$ = -3.20° (c 1.0, CHCl_3); major/minor isomers: 83:17/84:16 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5μ column connected; hexane/2-propanol = 99/01, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 7.913 min (major), 12.451 min (minor); 8.782 min (minor); 11.698 min (major).



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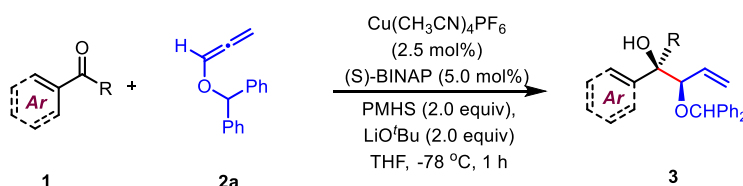
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.917	35502972	1095639	31.071	30.150
2	8.794	21501738	664060	18.818	18.274
3	11.734	20559026	804774	17.993	22.146
4	12.447	36700014	1069492	32.119	29.430
Total		114263751	3633965	100.000	100.000



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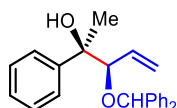
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.913	22832809	805091	58.398	59.621
2	8.782	1946263	67121	4.978	4.971
3	11.698	10118149	346539	25.879	25.663
4	12.451	4201287	131586	10.745	9.745
Total		39098509	1350338	100.000	100.000

2d. Enantioselective CuH-catalysed reductive coupling allene ether **2a**:



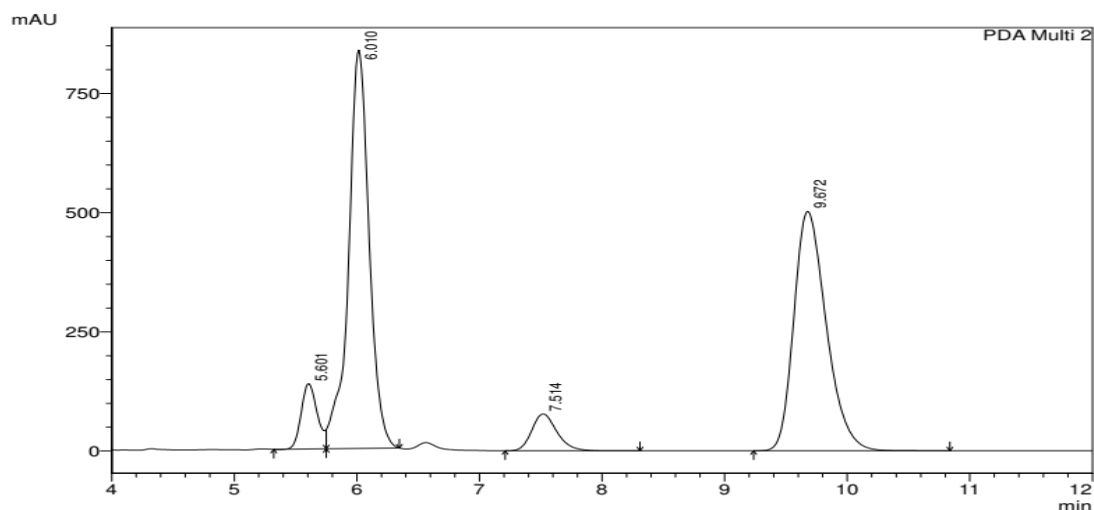
A solution of $\text{Cu}(\text{CH}_3\text{CN})_4\text{PF}_6$ (3.4 mg, 2.5 mol%), (*S*)-BINAP (11.2 mg, 5 mol%), PMHS (97 μL , 0.72 mmol) and LiO'Bu (0.7 ml, 0.72 mmol, 1 M in THF) in dry THF (2.0 mL) was stirred at room temperature for 10 min and then maintained at the temperature of -78°C under inert atmosphere. A solution of corresponding acetophenone **1** (0.36 mmol, 1.0 equiv) and *O*-benzhydryl allene **2a** (80 mg, 0.36 mmol) in dry THF (1.0 mL) was added *via* syringe and the resulting mixture was stirred at -78°C for 1 h. The reaction mixture was quenched with saturated NH_4Cl (10 mL) solution and extracted with EtOAc (3 $\times$ 15 mL) and dried over anhydrous Na_2SO_4 , filtered and concentrated *in vacuo*. The resultant crude product was purified by column chromatography (hexanes/EtOAc).

(2*R*,3*R*)-3-(Benzhydryloxy)-2-phenylpent-4-en-2-ol (**3a**):



Prepared according to the general procedure as described above in 93% yield (115 mg) with 11:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.30 – 7.14 (m, 8H), 7.13 – 7.07 (m, 5H), 6.83 – 6.79 (m, 2H), 5.78 (ddd, J = 17.4, 10.3, 8.5 Hz, 1H), 5.33 (dd, J = 10.3, 1.7 Hz, 1H), 5.33 (s, 1H), 5.08 (ddd, J = 17.3, 1.7, 0.6 Hz, 1H), 3.77 (d, J = 8.5 Hz, 1H), 1.37

(s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 146.4, 142.9, 140.8, 134.2, 128.5, 128.3, 128.0, 127.8, 127.3, 126.8, 126.6, 125.7, 121.5, 84.9, 80.0, 76.1, 25.5; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{24}\text{H}_{24}\text{O}_2\text{Na}^+$, 367.1674; found: 367.1666; $[\alpha]^{20}_{\text{D}} = -41.99^\circ$ (c 1.0, CHCl_3); 98:2 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak EUROCEL-01 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 225 nm, Flow rate = 1 mL/min, Retention times: 5.975 min (major), 9.694 min (minor).

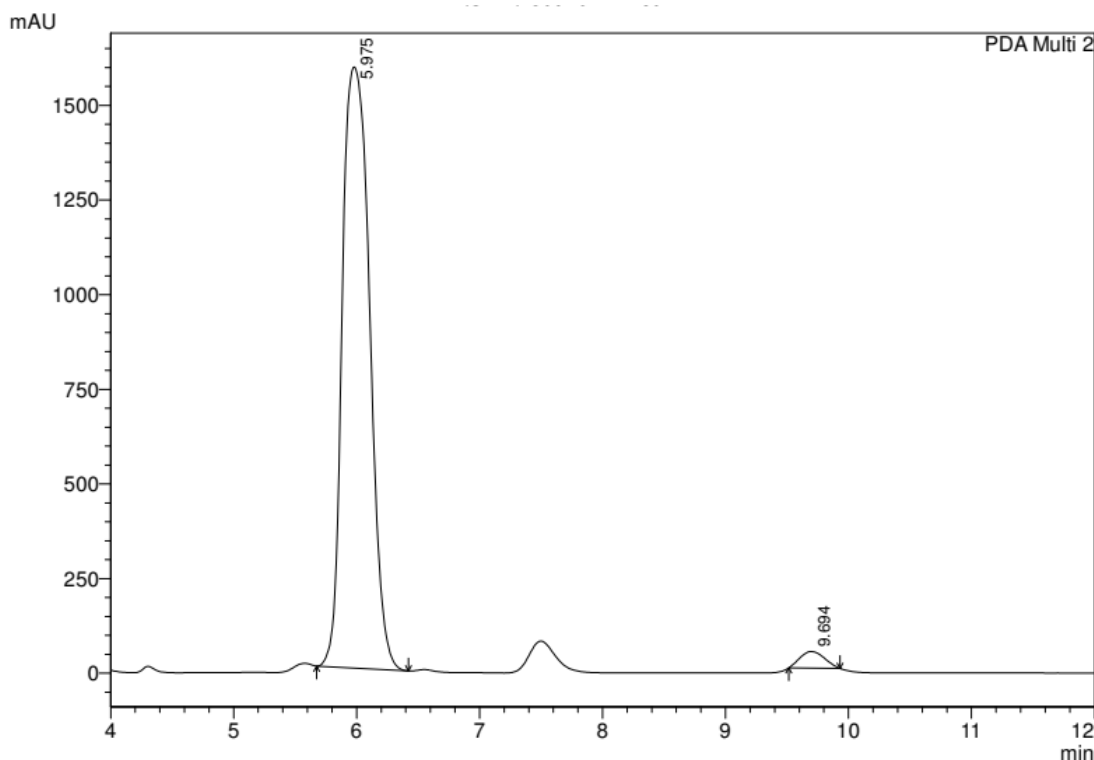


1 PDA Multi 2/225nm 4nm

PeakTable

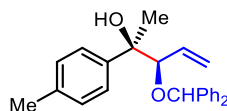
PDA Ch2 225nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.601	1268455	137158	5.929	8.834
2	6.010	9796900	836005	45.795	53.843
3	7.514	1102237	77367	5.152	4.983
4	9.672	9225196	502133	43.123	32.340
Total		21392788	1552663	100.000	100.000

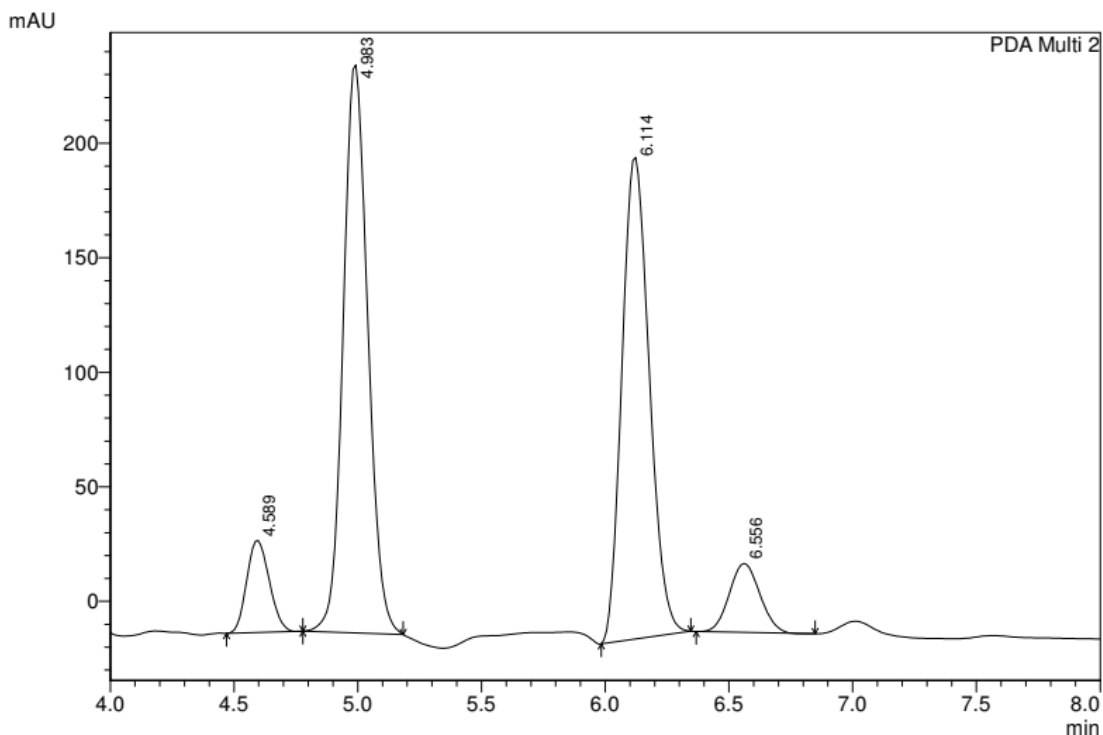


PDA Ch2 225nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.975	24577670	1587953	97.594	97.308
2	9.694	605858	43925	2.406	2.692
Total		25183528	1631878	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(*p*-tolyl)pent-4-en-2-ol (3b):

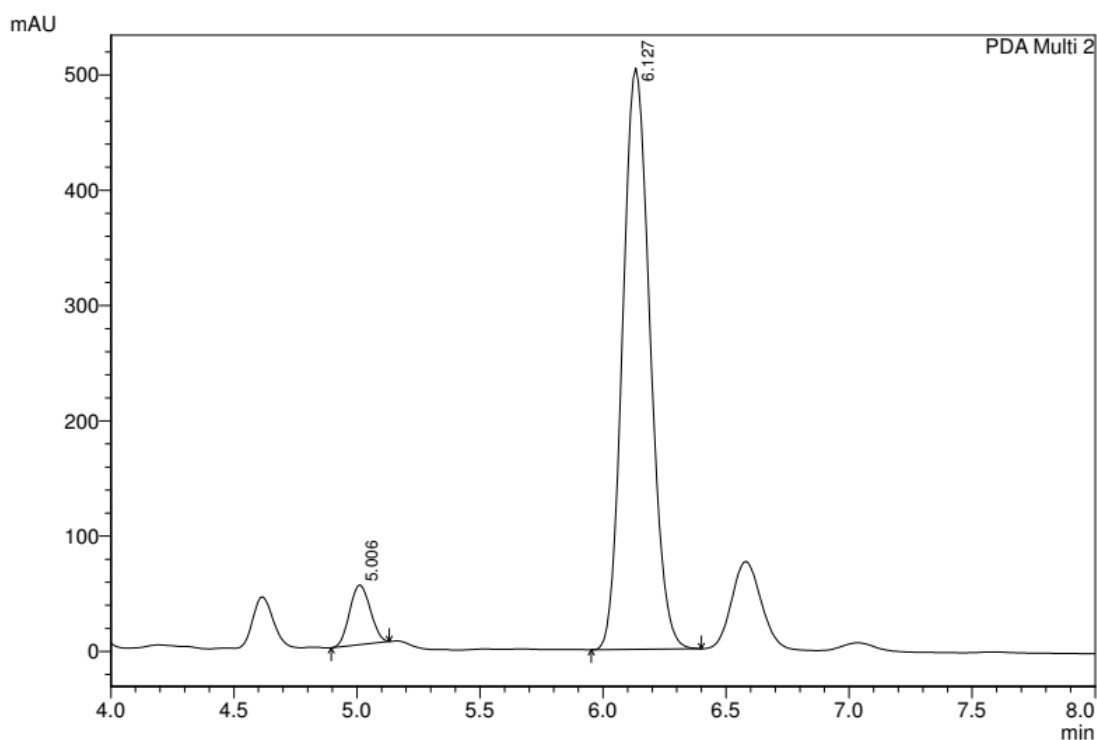
Prepared according to the general procedure as described above in 72% yield (93 mg) with 9:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.28 – 7.22 (m, 5H), 7.22 – 7.10 (m, 7H), 6.95 – 6.88 (m, 2H), 5.83 (ddd, J = 17.4, 10.3, 8.5 Hz, 1H), 5.41 (s, 1H), 5.38 (dd, J = 10.4, 1.7 Hz, 1H), 5.14 (dd, J = 17.3, 1.6 Hz, 1H), 3.82 (d, J = 8.5 Hz, 1H), 3.06 (s, 1H), 2.36 (s, 3H), 1.43 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 143.3, 142.9, 140.9, 136.2, 134.3, 128.6, 128.5, 128.3, 127.8, 127.7, 127.2, 126.6, 125.6, 121.3, 84.9, 80.0, 76.0, 25.5, 21.2; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{25}\text{H}_{26}\text{O}_2\text{Na}^+$, 381.1830; found: 381.1823; $[\alpha]_D^{20}$ = -32.77° (c 1.0, CHCl_3); 93:7 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IC-3 250X4.6 mm 5μ column; hexane/2-propanol = 98/02, detected at 225 nm, Flow rate = 1 mL/min, Retention times: 5.006 min (minor), 6.127 min (major).



PeakTable

PDA Ch2 225nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.589	255053	40257	6.623	7.614
2	4.983	1719519	247920	44.653	46.889
3	6.114	1618521	210463	42.030	39.805
4	6.556	257752	30099	6.693	5.693
Total		3850846	528739	100.000	100.000

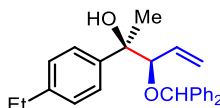


1 PDA Multi 2/225nm 4nm

PeakTable

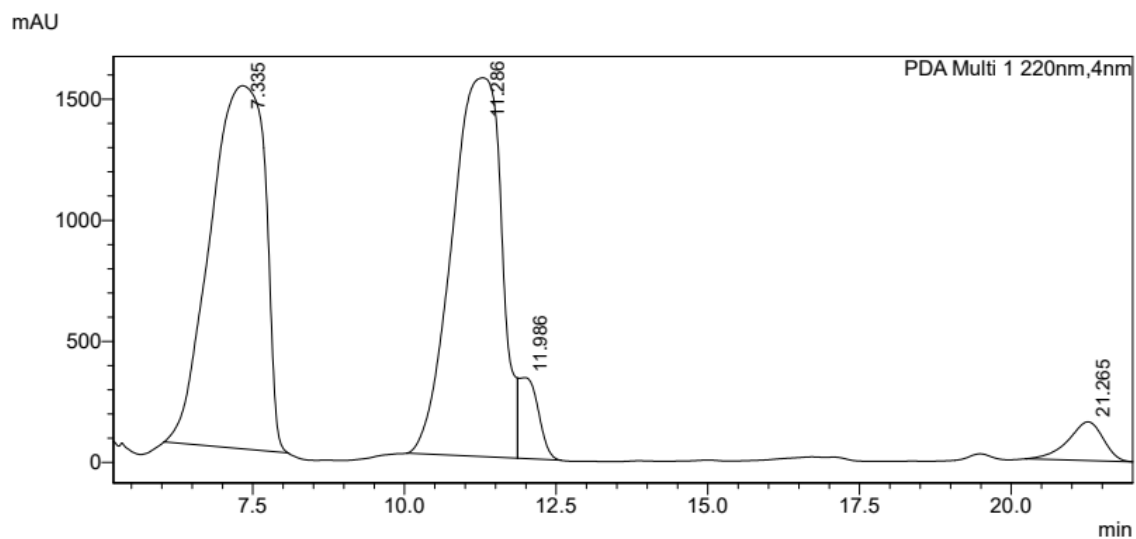
PDA Ch2 225nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.006	302730	51923	7.214	9.334
2	6.127	3893538	504327	92.786	90.666
Total		4196269	556250	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-ethylphenyl)pent-4-en-2-ol (3c):

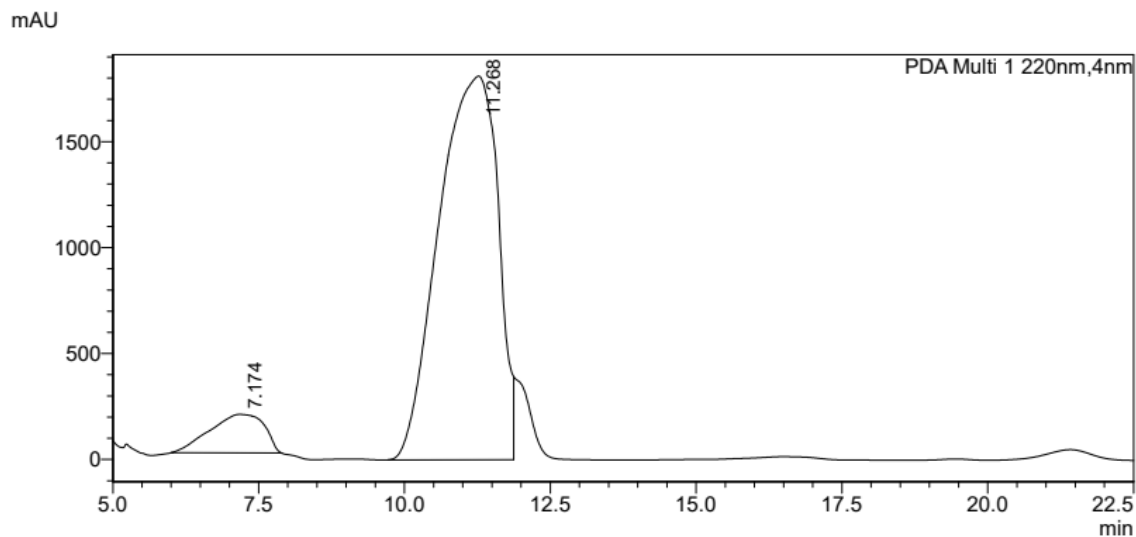
Prepared according to the general procedure as described above in 82% yield (110 mg) with 11:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.25) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.24 – 7.03 (m, 12H), 6.81 (d, J = 7.4 Hz, 2H), 5.82 (ddd, J = 17.4, 10.3, 8.5 Hz, 1H), 5.36 (s, 1H), 5.29 (dd, J = 10.3, 1.7 Hz, 1H), 5.07 (d, J = 17.3 Hz, 1H), 3.74 (d, J = 8.5 Hz, 1H), 2.58 (q, J = 7.7 Hz, 2H), 1.36 (s, 3H), 1.18 (t, J = 7.6 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 143.5, 143.0, 142.6, 141.0, 134.3, 128.5, 128.3, 127.7, 127.7, 127.4, 127.2, 126.6, 125.6, 121.3, 85.0, 80.0, 76.0, 28.6, 25.5, 15.8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{26}\text{H}_{28}\text{O}_2\text{Na}^+$, 395.1987; found: 395.1982; $[\alpha]_D^{20}$ = -29.25° (c 1.0, CHCl_3); 92:8 *er*; Chiral HPLC analysis

of the product: Daicel Chiralpak IC 250X4.6 mm 5 μ column; hexane/2-propanol = 99/01, detected at 220 nm, Flow rate = 1 mL/min, Retention times: 7.174 min (minor), 11.268 min (major).



<Peak Table>

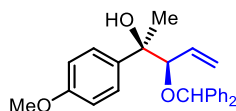
PDA Ch1 220nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.335	94516816	1500367	47.897	42.161
2	11.286	88838869	1564321	45.019	43.958
3	11.986	7514671	334018	3.808	9.386
4	21.265	6464397	159993	3.276	4.496
Total		197334753	3558699	100.000	100.000



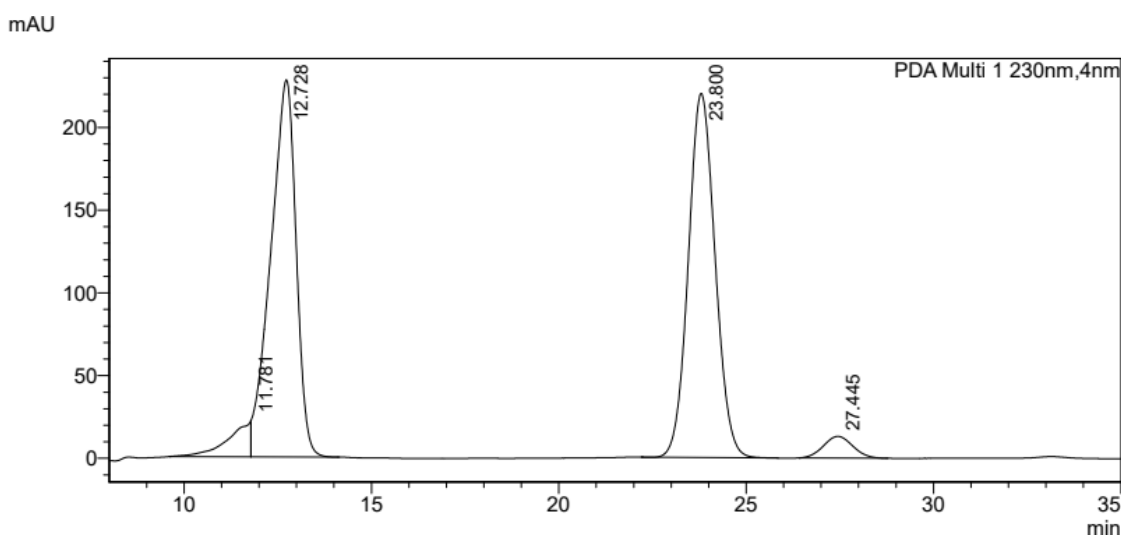
<Peak Table>

PDA Ch1 220nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.174	11740988	181220	8.409	9.099
2	11.268	127887488	1810325	91.591	90.901
Total		139628476	1991545	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-methoxyphenyl)pent-4-en-2-ol (3d):

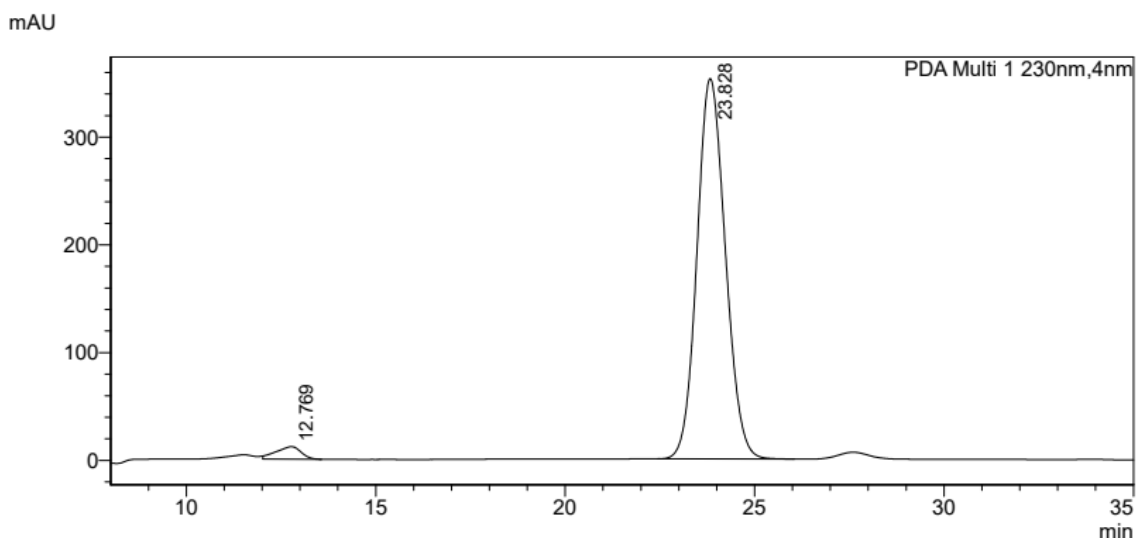


Prepared according to the general procedure as described above in 91% yield (124 mg) with 13:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.4) to afford a brown solid; mp = 200-202 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.34 – 7.16 (m, 10H), 7.00 – 6.94 (m, 2H), 6.88 – 6.81 (m, 2H), 5.81 (ddd, J = 17.4, 10.3, 8.4 Hz, 1H), 5.42 (s, 1H), 5.37 (dd, J = 10.4, 1.7 Hz, 1H), 5.12 (dd, J = 17.3, 1.1 Hz, 1H), 3.82 (s, 3H), 3.05 (s, 1H), 1.44 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 158.5, 143.0, 141.0, 138.3, 134.3, 128.5, 128.3, 127.8, 127.6, 127.2, 127.0, 126.6, 121.3, 113.3, 85.1, 80.1, 75.8, 55.4, 25.4; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{25}\text{H}_{26}\text{O}_3\text{Na}^+$, 397.1780; found: 397.1772; $[\alpha]^{20}_{\text{D}}$ = -21.70° (c 1.0, CHCl_3); 97:3 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IC 250X4.6 mm 5 μ column; hexane/2-propanol = 99/01, detected at 230 nm, Flow rate = 1 mL/min, Retention times: 12.769 min (minor), 23.828 min (major).



<Peak Table>

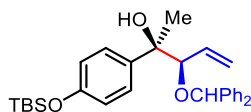
PDA Ch1 230nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.781	896441	21432	3.841	4.441
2	12.728	10778097	227950	46.180	47.233
3	23.800	10948751	220103	46.911	45.607
4	27.445	716208	13123	3.069	2.719
Total		23339498	482608	100.000	100.000



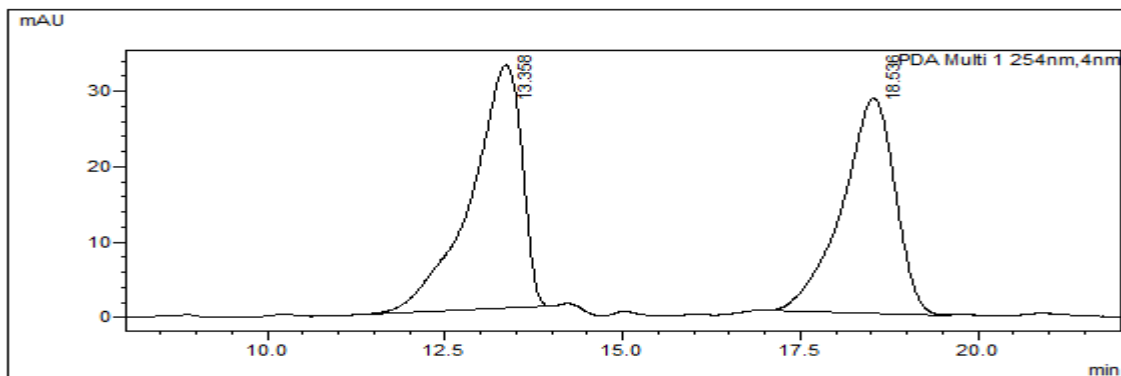
<Peak Table>

PDA Ch1 230nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.769	534039	11593	2.823	3.180
2	23.828	18384382	353021	97.177	96.820
Total		18918421	364614	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-((*tert*-butyldimethylsilyl)oxy)phenyl)pent-4-en-2-ol (3e):

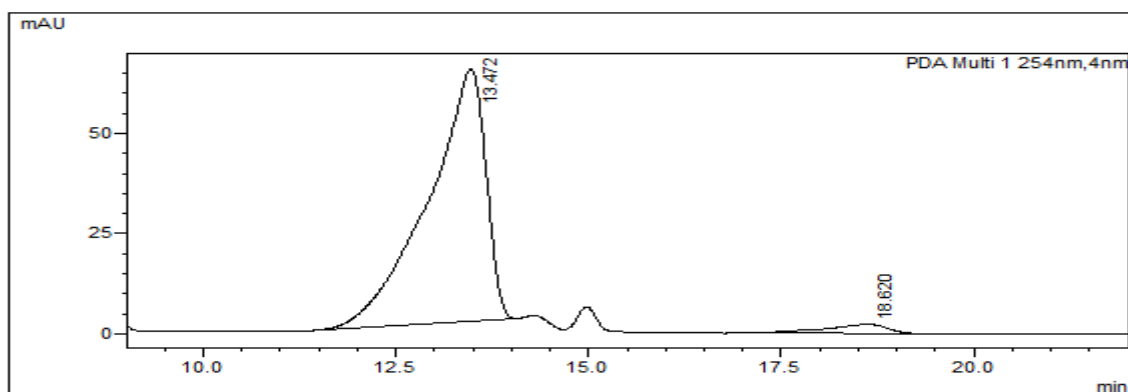


Prepared according to the general procedure as described above in 95% yield (162 mg) with >20:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.4) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.34 – 7.19 (m, 10H), 7.06 – 6.99 (m, 2H), 6.85 – 6.81 (m, 2H), 5.84 (ddd, J = 17.4, 10.3, 8.4 Hz, 1H), 5.46 (s, 1H), 5.40 (dd, J = 10.4, 1.8 Hz, 1H), 5.14 (ddd, J = 17.3, 2.1, 0.6 Hz, 1H), 3.85 (d, J = 8.4 Hz, 1H), 1.47 (s, 3H), 1.04 (s, 9H), 0.25 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.5, 143.0, 141.0, 139.0, 134.3, 128.5, 128.3, 127.8, 127.2, 126.8, 126.58, 121.3, 119.4, 85.0, 80.0, 76.0, 26.0, 25.3, 18.4, -4.2; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{30}\text{H}_{38}\text{O}_3\text{SiNa}^+$, 497.2487; found: 497.2481; $[\alpha]^{20}_{\text{D}}$ = -17.83° (c 1.0, CHCl_3); 97:3 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5 μ column connected to Daicel Chiralpak IA 250X4.6 mm 5 μ column in tandem; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 13.472 min (major), 18.620 min (minor).



<Peak Table>

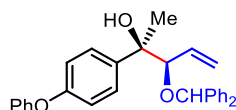
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.358	1464303	31531	49.767	52.547
2	18.536	1478015	28474	50.233	47.453
Total		2942318	60006	100.000	100.000



<Peak Table>

PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.472	3271758	62960	96.663	96.582
2	18.620	112937	2228	3.337	3.418
Total		3384695	65188	100.000	100.000

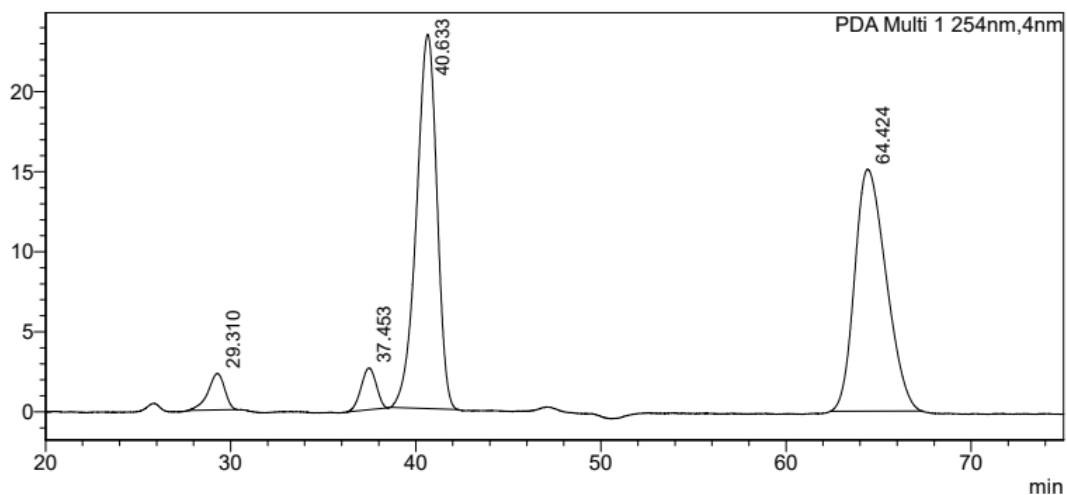
(2R,3R)-3-(Benzhydryloxy)-2-(4-phenoxyphenyl)pent-4-en-2-ol (3f):



Prepared according to the general procedure as described above in 81% yield (127 mg) with 12:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.25) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.28 – 7.10 (m, 13H), 7.05 – 6.99 (m, 1H), 6.98 – 6.85 (m, 5H), 5.77 (ddd, J = 17.4, 10.3, 8.6 Hz, 1H), 5.36 (s, 1H), 5.33 (d, J = 10.4 Hz, 1H), 5.08 (d, J = 17.3 Hz, 1H), 3.76 (d, J = 8.5 Hz, 1H), 1.38 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 157.7, 155.9, 142.8, 141.3, 141.0, 134.1, 130.0, 128.6, 128.3, 128.0, 127.8, 127.3, 127.2, 126.6, 123.2, 121.6, 118.7, 118.5, 85.0, 80.0, 76.0, 25.5; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{30}\text{H}_{28}\text{O}_3\text{Na}^+$,

459.1936; found: 459.1930; $[\alpha]^{20}_D = -50.59^\circ$ (c 1.0, CHCl_3); 97:3 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 0.6 mL/min, Retention times: 40.613 min (major), 64.149 min (minor).

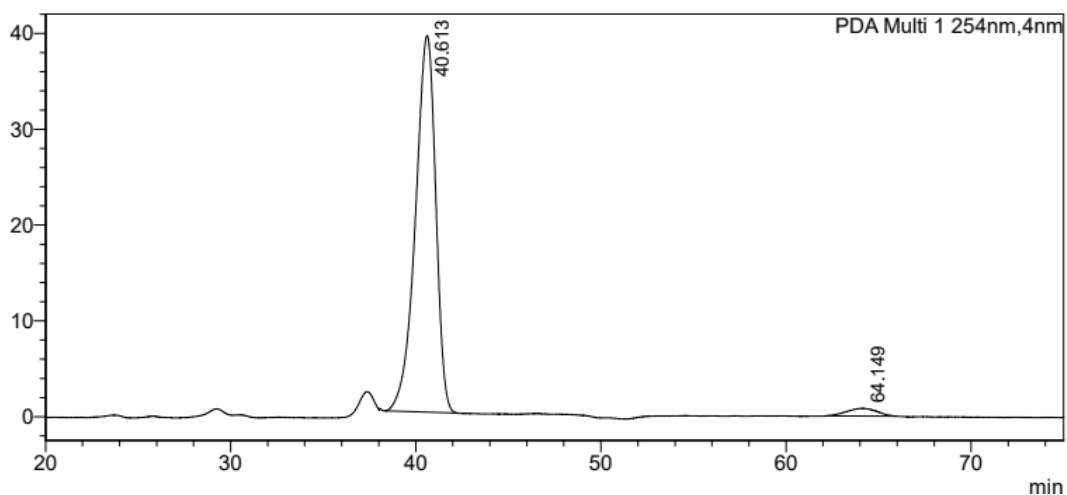
mAU



<Peak Table>

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	29.310	142002	2275	3.666	5.243
2	37.453	147383	2600	3.805	5.993
3	40.633	1798475	23389	46.426	53.909
4	64.424	1785973	15122	46.104	34.855
Total		3873833	43386	100.000	100.000

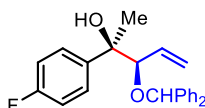
mAU



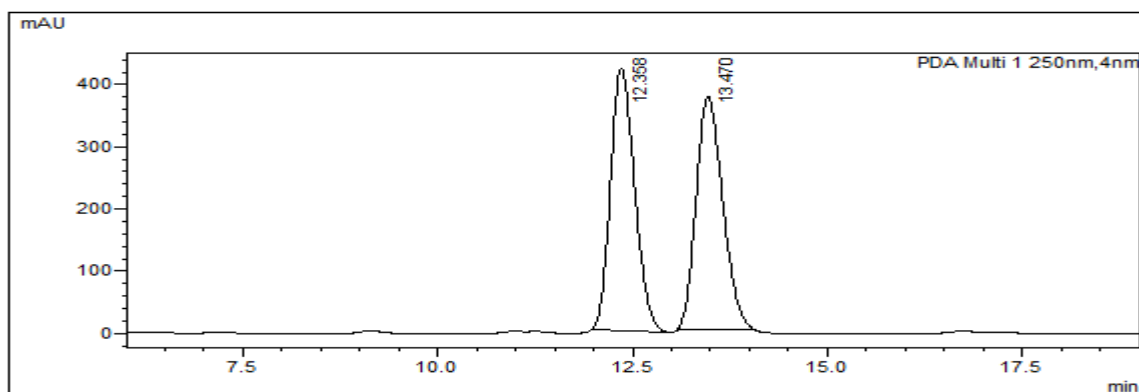
<Peak Table>

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	40.613	2998828	39307	97.103	97.985
2	64.149	89464	808	2.897	2.015
Total		3088292	40115	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-fluorophenyl)pent-4-en-2-ol (3g):

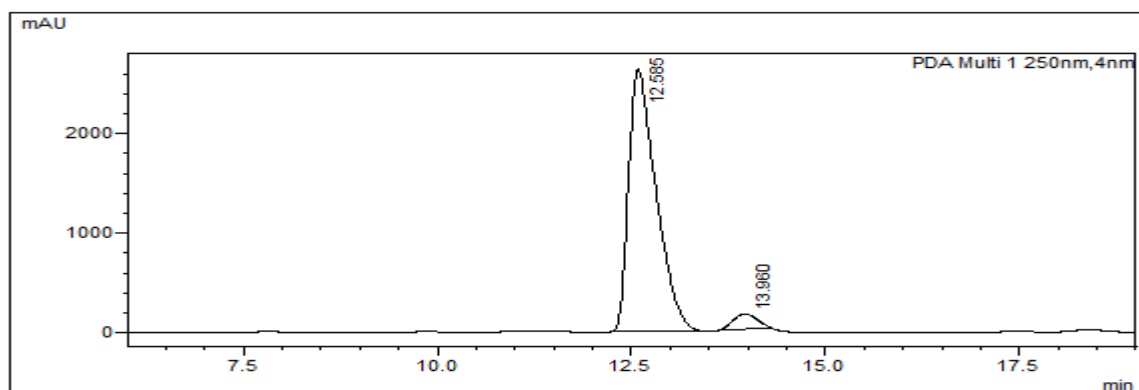


Prepared according to the general procedure as described above in 85% yield (111 mg) with >20:1. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a white semi solid; ^1H NMR (400 MHz, CDCl_3) δ 7.27 – 7.09 (m, 10H), 6.96 – 6.83 (m, 4H), 5.75 (ddd, J = 17.3, 10.3, 8.5 Hz, 1H), 5.34 (s, 1H), 5.32 (d, J = 1.7 Hz, 1H), 5.07 (ddd, J = 17.3, 1.1, 0.5 Hz, 1H), 3.72 (d, J = 8.5 Hz, 1H), 1.35 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 161.9 (d, J_{CF} = 244.5 Hz), 142.7, 142.0 (d, J_{CF} = 2.7 Hz), 140.7, 134.0, 128.6, 128.3, 127.9, 127.8, 127.4, 127.3, 126.5, 121.8, 114.6 (d, J_{CF} = 21.1 Hz), 84.8, 79.9, 75.9, 25.6; ^{19}F NMR (376 MHz, CDCl_3) δ -116.98 (s); HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{24}\text{H}_{23}\text{FO}_2\text{Na}^+$, 385.1580; found: 385.1564; $[\alpha]^{20}_{\text{D}}$ = -32.83° (c 1.0, CHCl_3); 95:5 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IC 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 250 nm, Flow rate = 1 mL/min, Retention times: 12.585 min (major), 13.960 min (minor).



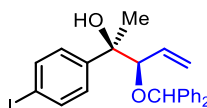
<Peak Table>

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.358	9093507	421008	50.552	52.946
2	13.470	8894843	374153	49.448	47.054
Total		17988351	795162	100.000	100.000



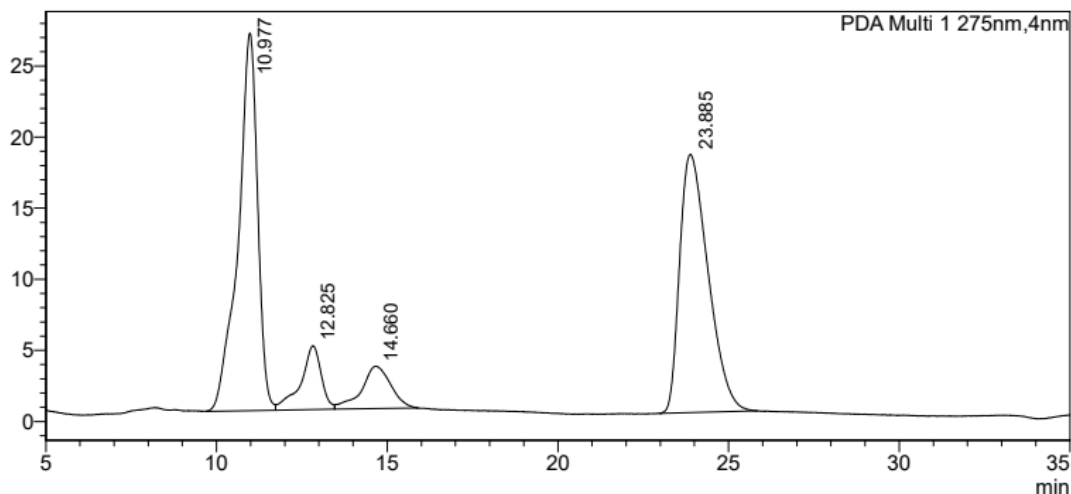
<Peak Table>

PDA Ch1 250nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.585	65072544	2638244	95.081	94.502
2	13.960	3366238	153485	4.919	5.498
Total		68438782	2791729	100.000	100.000

(2R,3R)-3-(Benzhydryloxy)-2-(4-iodophenyl)pent-4-en-2-ol (3h):

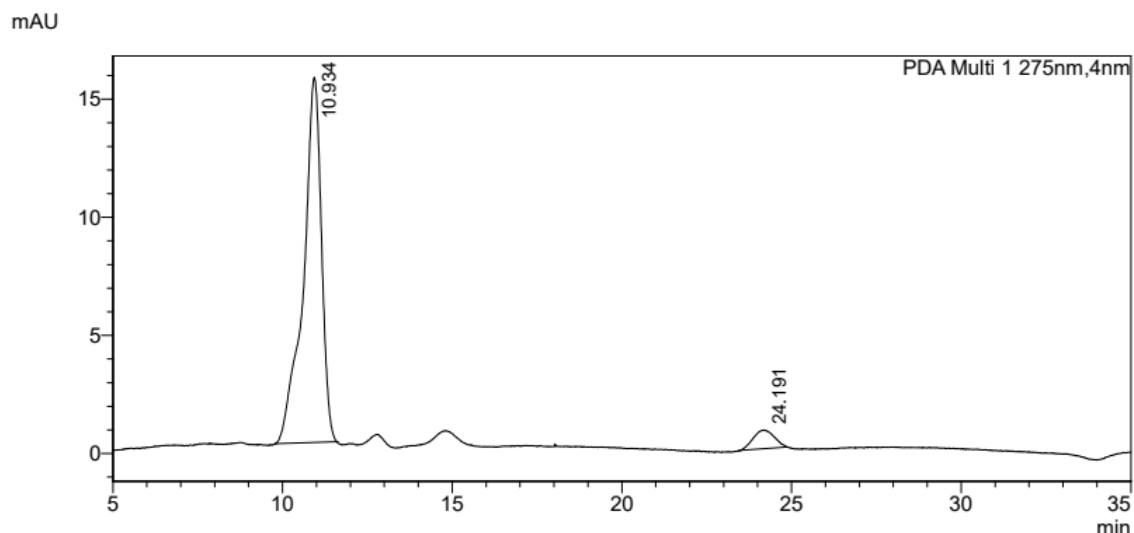
Prepared according to the general procedure as described above in 81% yield (137 mg) with 10:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.64 – 7.58 (m, 2H), 7.32 – 7.14 (m, 8H), 7.11 – 7.06 (m, 2H), 6.91 – 6.85 (m, 2H), 5.84 (ddd, J = 17.4, 10.3, 8.6 Hz, 1H) 5.43 (dd, J = 10.3, 1.6 Hz, 1H), 5.40 (s, 1H), 5.18 (dd, J = 17.3, 1.5 Hz, 1H), 3.78 (d, J = 8.6 Hz, 1H), 3.07 (s, 1H), 1.39 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 146.3, 142.6, 140.6, 137.0, 133.8, 128.6, 128.3, 128.0, 127.8, 127.8, 127.3, 126.5, 122.0, 92.3, 84.6, 80.0, 76.0, 25.6; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{24}\text{H}_{23}\text{IO}_2\text{Na}^+$, 493.0640; found: 493.0638; $[\alpha]^{20}_{\text{D}}$ = -109.96° (c 2.0, CHCl_3); 94:6 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 99/01, detected at 275 nm, Flow rate = 1 mL/min, Retention times: 10.934 min (major), 24.191 min (minor).

mAU



<Peak Table>

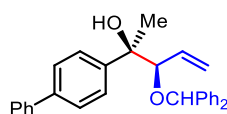
PDA Ch1 275nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.977	1052825	26548	42.599	50.884
2	12.825	187866	4494	7.601	8.612
3	14.660	177584	2980	7.185	5.711
4	23.885	1053226	18153	42.615	34.792
Total		2471502	52175	100.000	100.000



<Peak Table>

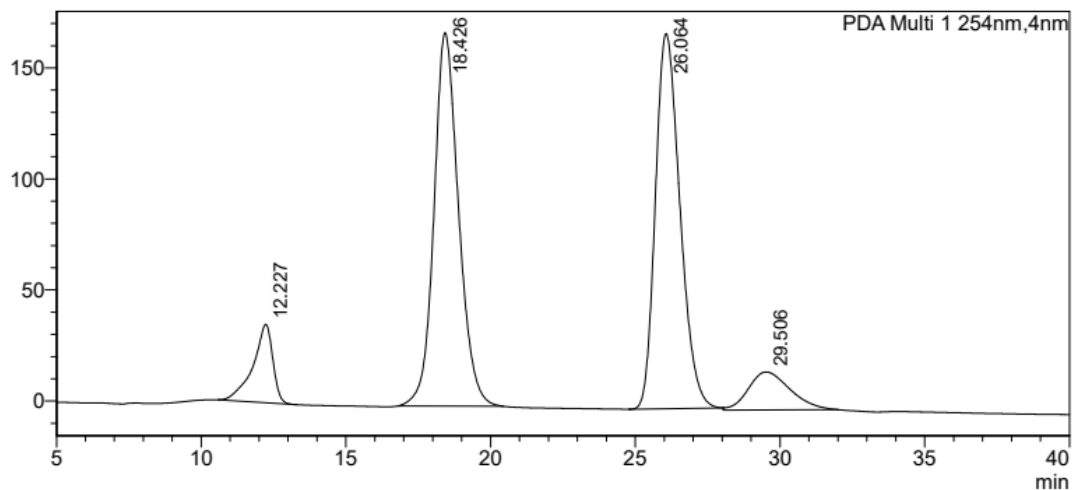
PDA Ch1 275nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.934	571254	15454	94.345	95.131
2	24.191	34240	791	5.655	4.869
Total		605494	16245	100.000	100.000

(2*R*,3*R*)-2-([1,1'-Biphenyl]-4-yl)-3-(benzhydryloxy)pent-4-en-2-ol (3i):



Prepared according to the general procedure as described above in 86% yield (130 mg) with 15:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.5) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.59 – 7.46 (m, 3H), 7.42 – 7.05 (m, 14H), 6.85 – 6.82 (m, 2H), 5.82 (ddd, J = 17.4, 10.3, 8.5 Hz, 1H), 5.38 (d, J = 1.7 Hz, 1H), 5.36 (s, 1H), 5.13 (dd, J = 17.4, 1.2 Hz, 1H), 3.80 (d, J = 8.5 Hz, 1H), 1.40 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 145.6, 142.8, 141.1, 140.8, 139.6, 134.2, 129.0, 128.5, 128.3, 127.8, 127.3, 127.2, 126.7, 126.6, 126.1, 121.6, 85.0, 80.0, 76.1, 25.6; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{30}\text{H}_{28}\text{O}_2\text{Na}^+$, 443.1987; found: 443.1980; $[\alpha]^{20}_{\text{D}}$ = -24.60° (c 1.0, CHCl_3); 98:2 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 99/01, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 18.108 min (major), 26.158 min (minor).

mAU

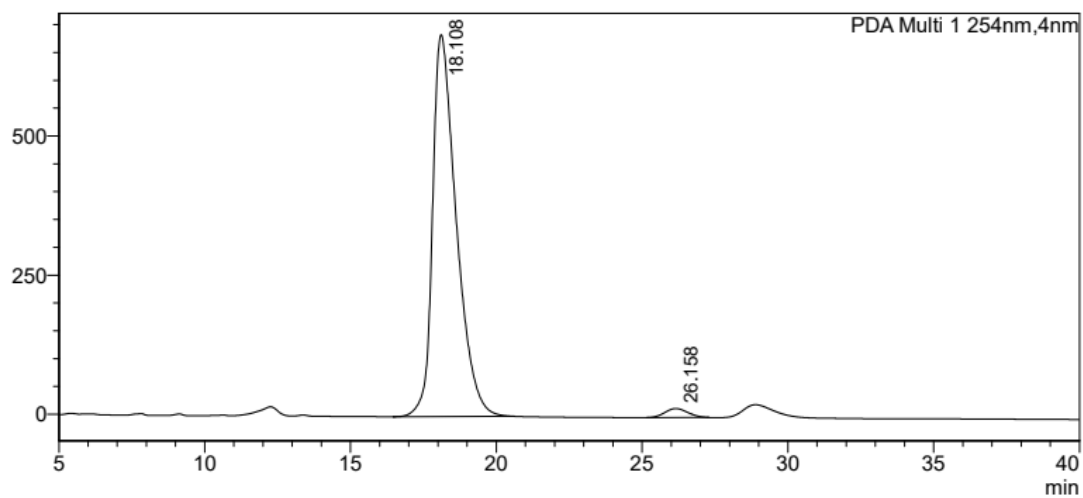


<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.227	1682443	35336	7.217	9.074
2	18.426	9947222	168079	42.668	43.160
3	26.064	9960790	168883	42.726	43.366
4	29.506	1722657	17136	7.389	4.400
Total		23313113	389434	100.000	100.000

mAU

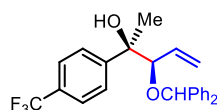


<Peak Table>

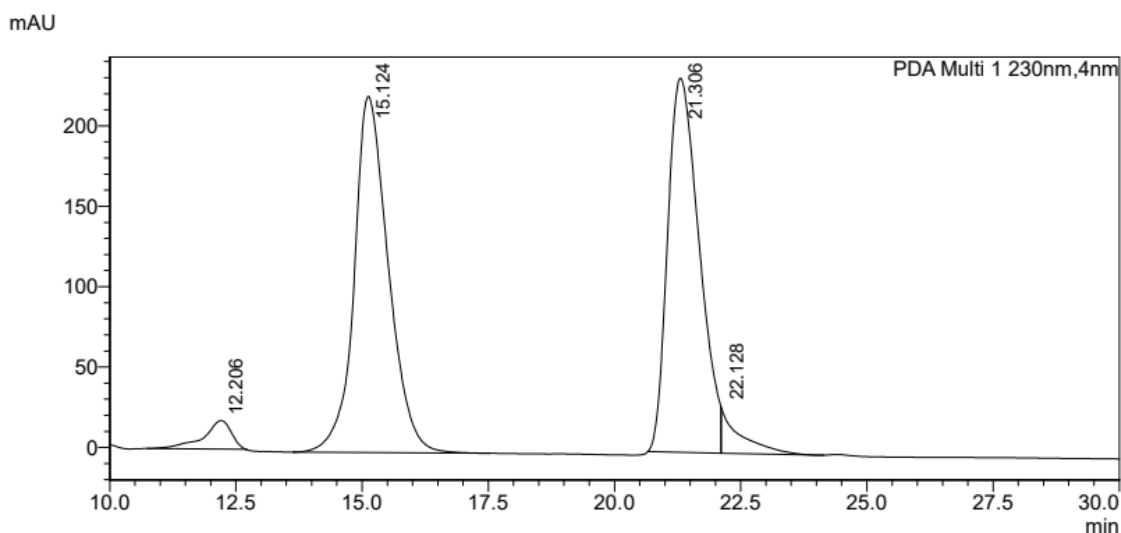
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	18.108	38788653	685745	97.795	97.707
2	26.158	874494	16093	2.205	2.293
Total		39663147	701839	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-(trifluoromethyl)phenyl)pent-4-en-2-ol (3j):

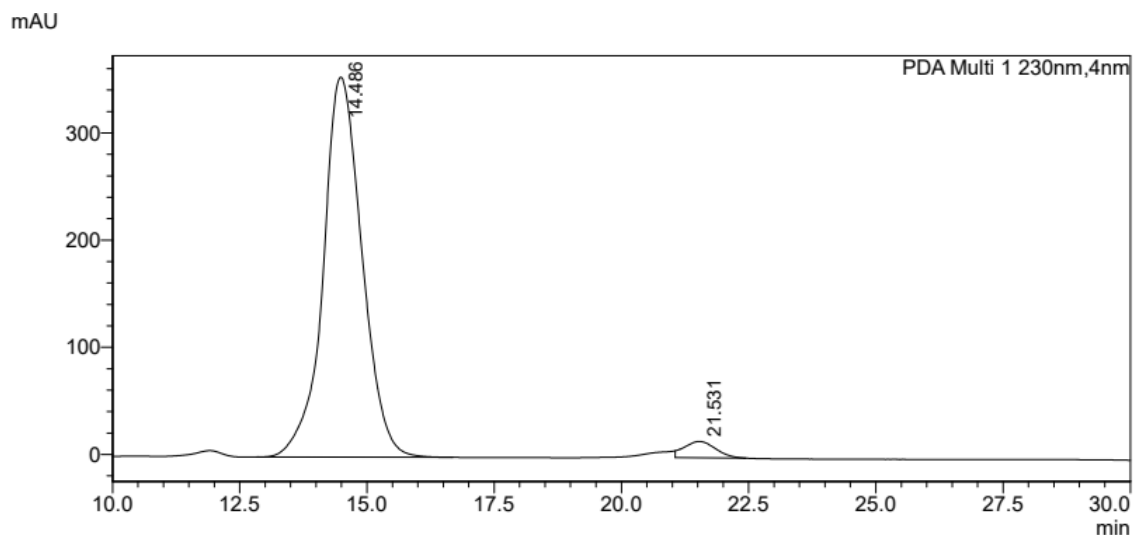


Prepared according to the general procedure as described above in 98% yield (146 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a white semi solid; ^1H NMR (400 MHz, CDCl_3) δ 7.47 (d, J = 8.2 Hz, 2H), 7.38 (d, J = 8.2 Hz, 2H), 7.23 – 6.98 (m, 8H), 6.82 – 6.65 (m, 2H), 5.81 (ddd, J = 17.3, 10.3, 8.6 Hz, 1H), 5.40 (dd, J = 10.3, 1.6 Hz, 1H), 5.33 (s, 1H), 5.15 (ddd, J = 17.3, 1.6, 0.6 Hz, 1H), 3.76 (d, J = 8.6 Hz, 1H), 3.07 (s, 1H), 1.35 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 150.7, 142.5, 140.4, 133.7, 129.0 (q, J_{CF} = 32.1 Hz), 128.6, 128.3, 127.9, 127.8, 127.4, 126.5, 126.0, 124.9 (q, J_{CF} = 3.5 Hz), 124.5 (d, J_{CF} = 271.9 Hz), 122.2, 84.6, 79.9, 76.2, 25.7; ^{19}F NMR (376 MHz, CDCl_3) δ -62.24 (s); HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{25}\text{H}_{23}\text{F}_3\text{O}_2\text{Na}^+$, 435.1547; found: 435.1542; $[\alpha]^{20}_{\text{D}}$ = -46.00° (c 1.0, CHCl_3); 97:3 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5 μ column in tandem; hexane/2-propanol = 99/01, detected at 230 nm, Flow rate = 1 mL/min, Retention times: 14.486 min (major), 21.531 min (minor).



<Peak Table>

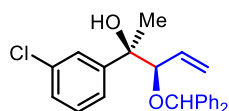
PDA Ch1 230nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.206	683773	17793	3.110	3.561
2	15.124	10469220	221592	47.620	44.349
3	21.306	10115016	232635	46.009	46.559
4	22.128	717008	27635	3.261	5.531
Total		21985017	499656	100.000	100.000



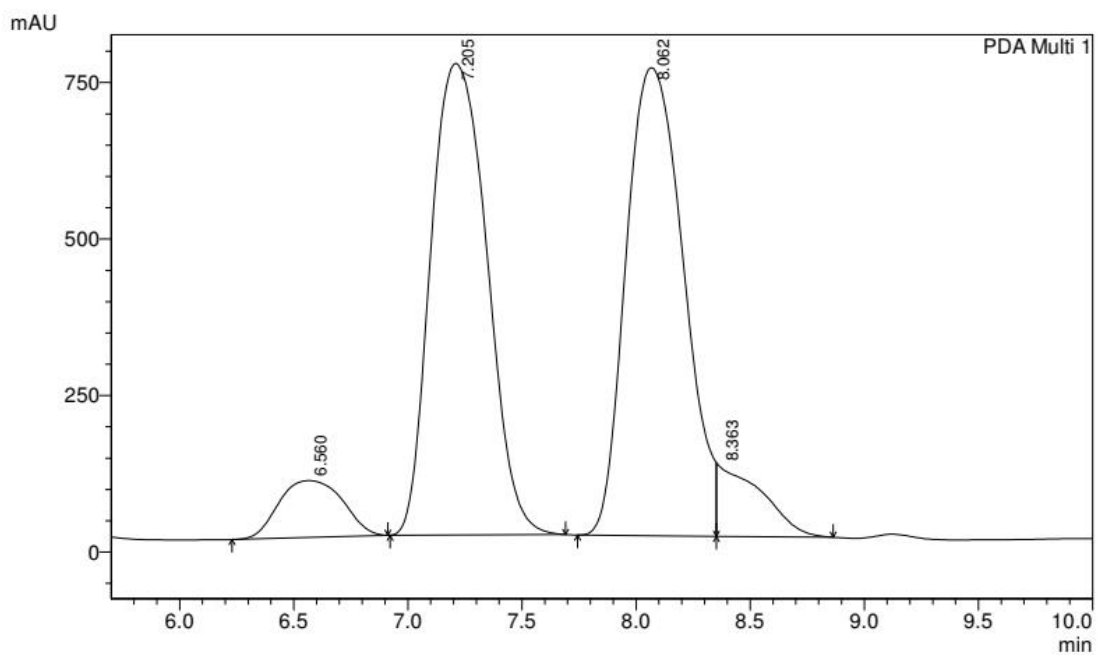
<Peak Table>

PDA Ch1 230nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	14.486	18854966	354657	96.654	95.895
2	21.531	652650	15180	3.346	4.105
Total		19507616	369837	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(3-chlorophenyl)pent-4-en-2-ol (3k):



Prepared according to the general procedure as described above in 89% yield (122 mg) with 13:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.24 – 7.23 (m, 1H), 7.20 – 7.068 (m, 11H), 6.84 – 6.78 (m, 2H), 5.78 (ddd, J = 17.3, 10.3, 8.6 Hz, 1H), 5.37 (dd, J = 10.3, 1.6 Hz, 1H), 5.33 (s, 1H), 5.11 (dd, J = 17.3, 1.1 Hz, 1H), 3.72 (d, J = 8.6 Hz, 1H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 148.8, 142.6, 140.5, 134.1, 133.8, 129.3, 128.6, 128.3, 128.0, 127.8, 127.3, 127.0, 126.5, 126.0, 124.0, 122.1, 84.5, 80.0, 76.0, 25.8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{24}\text{H}_{23}\text{ClO}_2\text{Na}^+$, 401.1284; found: 401.1275; $[\alpha]^{20}_{\text{D}}$ = -36.33° (c 1.0, CHCl_3); 93:7 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IC-3 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 210 nm, Flow rate = 0.7 mL/min, Retention times: 7.319 min (minor), 8.224 min (major).

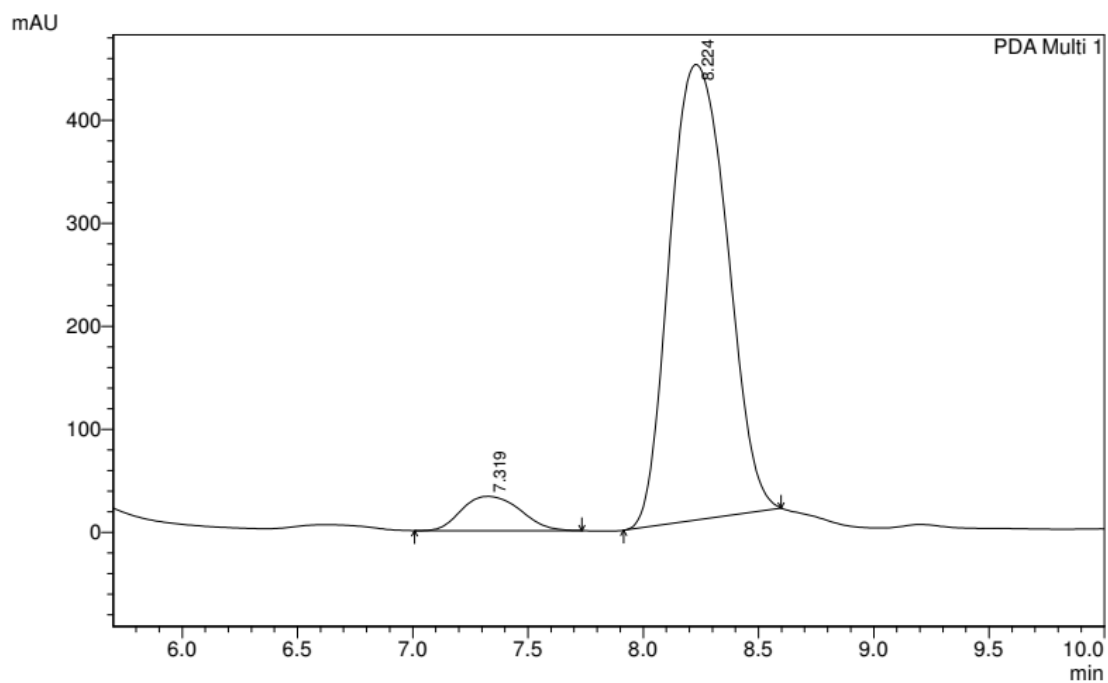


1 PDA Multi 1/210nm 4nm

PeakTable

PDA Ch1 210nm 4nm

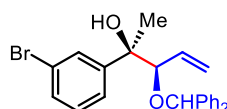
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.560	1765424	90881	6.024	5.329
2	7.205	12902590	753921	44.026	44.205
3	8.062	13124754	747885	44.784	43.851
4	8.363	1514092	112839	5.166	6.616
Total		29306859	1705526	100.000	100.000



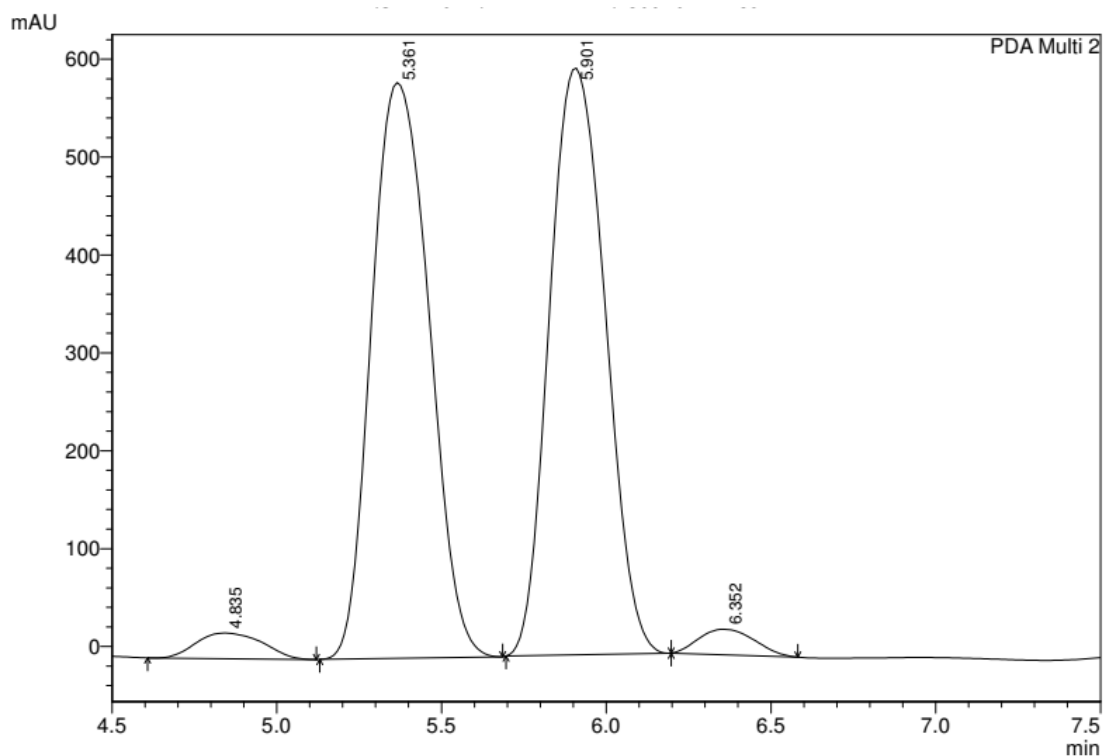
PeakTable

PDA Ch1 210nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.319	588048	33249	7.086	6.991
2	8.224	7710953	442358	92.914	93.009
Total		8299001	475607	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(3-bromophenyl)pent-4-en-2-ol (3l):

Prepared according to the general procedure as described above in 85% yield (129 mg) with 12:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.41 (t, J = 1.8 Hz, 1H), 7.35 – 7.32 (m, 1H), 7.26 – 7.24 (m, 1H), 7.21 – 7.08 (m, 9H), 6.84 – 6.81 (m, 2H), 5.79 (ddd, J = 17.3, 10.3, 8.7 Hz, 1H), 5.39 (dd, J = 10.4, 1.7 Hz, 1H), 5.34 (s, 1H), 5.13 (dd, J = 17.3, 1.1 Hz, 1H), 3.73 (d, J = 8.6 Hz, 1H), 1.32 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 149.1, 142.6, 140.5, 133.8, 130.0, 129.6, 129.0, 128.6, 128.4, 128.0, 127.8, 127.3, 126.5, 124.1, 122.4, 122.1, 84.5, 79.9, 76.0, 25.8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{24}\text{H}_{23}\text{BrO}_2\text{Na}^+$, 445.0779; found: 445.0770; $[\alpha]^{20}_{\text{D}}$ = -37.83° (c 1.0, CHCl_3); 95:5 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IC-3 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 225 nm, Flow rate = 0.7 mL/min, Retention times: 5.284 min (minor), 5.793 min (major).

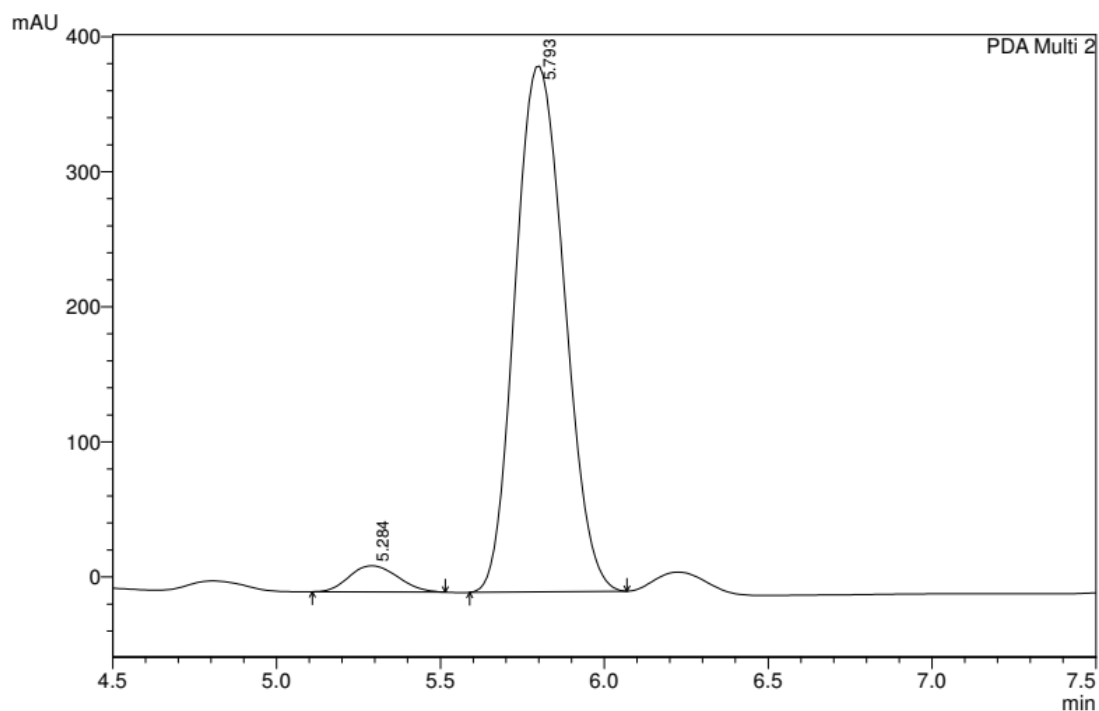


1 PDA Multi 2/225nm 4nm

PeakTable

PDA Ch2 225nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.835	364622	26103	2.453	2.105
2	5.361	7143621	588417	48.065	47.455
3	5.901	7049045	599389	47.429	48.340
4	6.352	305097	26044	2.053	2.100
Total		14862386	1239953	100.000	100.000



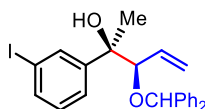
1 PDA Multi 2/225nm 4nm

PeakTable

PDA Ch2 225nm 4nm

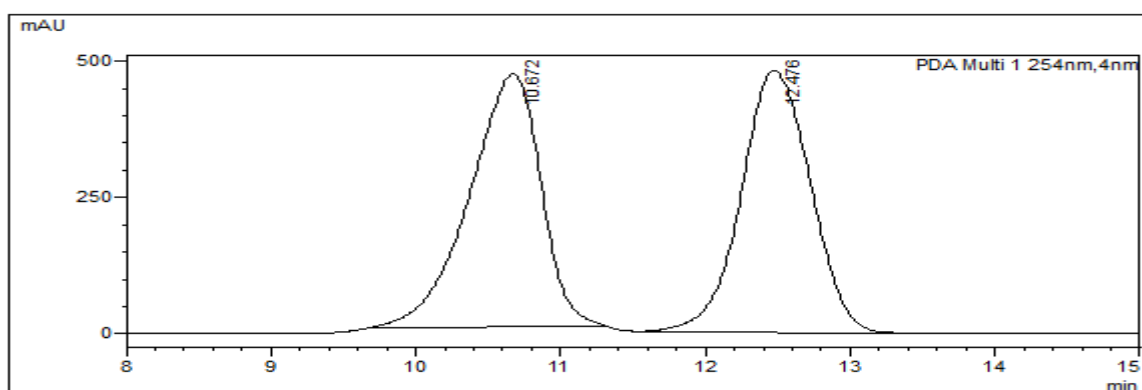
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.284	199241	19353	4.664	4.737
2	5.793	4072843	389224	95.336	95.263
Total		4272084	408578	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(3-iodophenyl)pent-4-en-2-ol (3m):



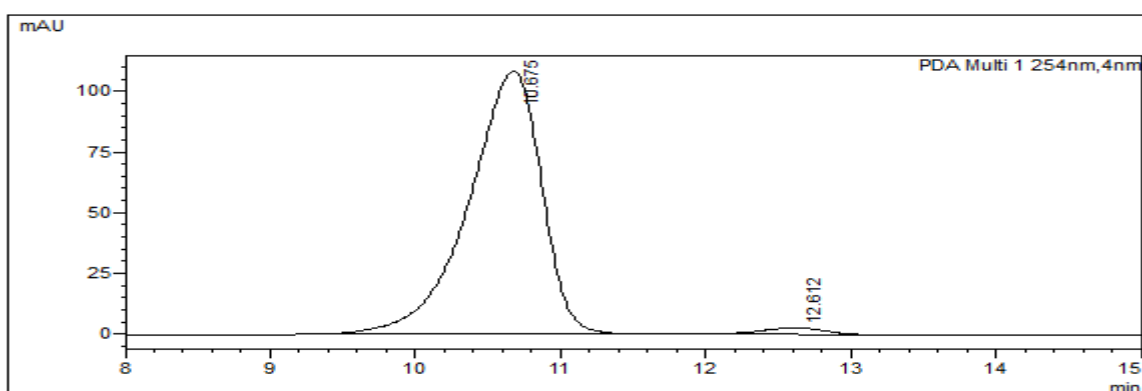
Prepared according to the general procedure as described above in 86% yield (146 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.61 – 7.53 (m, 2H), 7.31 – 7.27 (m, 1H), 7.21 – 7.05 (m, 8H), 7.00 – 6.98 (m, 1H), 6.85 – 6.74 (m, 2H), 5.78 (ddd, J = 17.4, 10.3, 8.7 Hz, 1H), 5.38 (dd, J = 10.3, 1.6 Hz, 1H), 5.33 (s, 1H), 5.12 (dd, J = 17.3, 1.0 Hz, 1H), 3.71 (d, J = 8.6 Hz, 1H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 149.2, 142.6, 140.5, 135.8, 134.8, 133.8, 129.8, 128.7, 128.4, 128.0, 127.7, 127.3, 126.5, 125.0, 122.1, 94.3, 84.4, 80.0, 75.8, 25.8; HRMS (ESI)

m/z: $[M+Na]^+$ calcd for $C_{24}H_{23}IO_2Na^+$, 493.0640; found: 493.0635; $[\alpha]^{20}_D = -41.58^\circ$ (c 1.0, $CHCl_3$); 98:2 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 10.675 min (major), 12.612 min (minor).



<Peak Table>

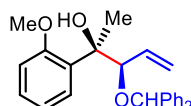
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.672	15843489	462786	49.853	49.122
2	12.476	15937037	479323	50.147	50.878
Total		31780526	942108	100.000	100.000



<Peak Table>

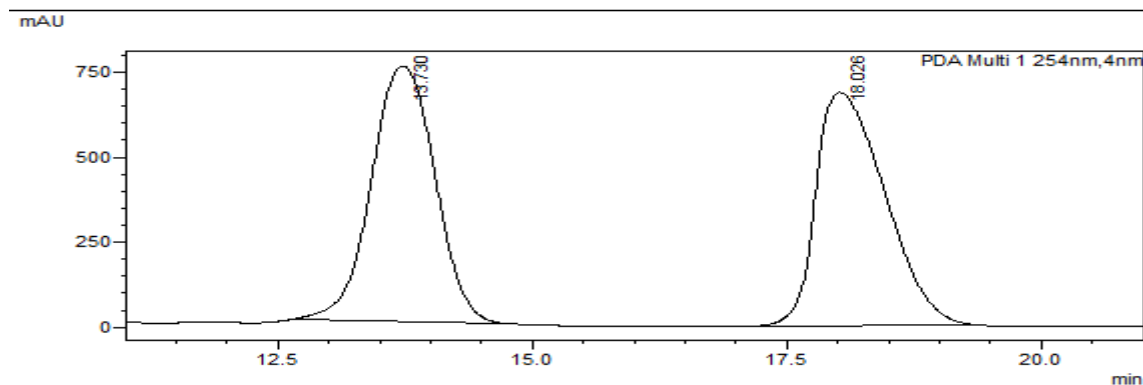
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.675	3763241	108198	98.056	97.607
2	12.612	74615	2652	1.944	2.393
Total		3837856	110851	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(2-methoxyphenyl)pent-4-en-2-ol (3n):



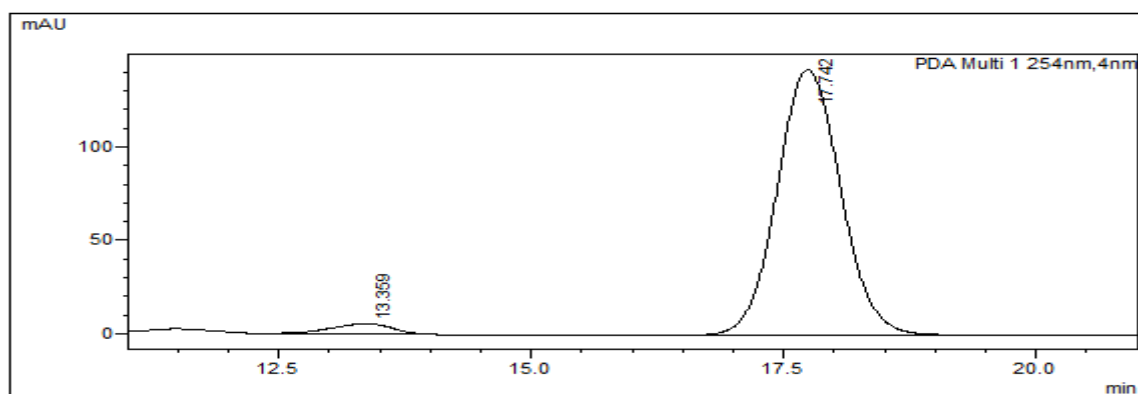
Prepared according to the general procedure as described above in 88% yield (119 mg) with >20:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; $R_f = 0.3$) to afford a white solid; mp = 160-164 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, $J = 7.7, 1.6$ Hz, 1H), 7.26 – 6.91 (m, 10H), 6.74 – 6.66 (m, 3H), 5.87 (ddd, $J = 17.6, 10.2, 8.5$ Hz, 1H), 5.32 (dd, $J = 10.3, 2.0$ Hz, 1H), 5.29 (s, 1H), 5.12 (dd, $J = 17.3, 2.0$ Hz, 1H), 4.24 (d, $J = 8.4$ Hz, 1H), 3.37 (s, 3H), 1.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.3, 143.1, 141.6, 134.8, 134.5,

128.3, 128.2, 128.1, 127.7, 127.5, 127.28, 127.1, 126.6, 120.7, 120.5, 111.2, 81.8, 79.8, 76.5, 54.5, 23.4; HRMS (ESI) m/z : $[M+Na]^+$ calcd for $C_{25}H_{26}O_3Na^+$, 397.1779; found: 397.1771; $[\alpha]^{20}_D = -52.43^\circ$ (c 1.0, $CHCl_3$); 97:3 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IA 250X4.6 mm 5μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 13.359 min (minor), 17.742 min (major).



<Peak Table>

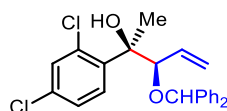
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.730	32507941	748456	50.079	52.181
2	18.026	32405593	685901	49.921	47.819
Total		64913534	1434357	100.000	100.000



<Peak Table>

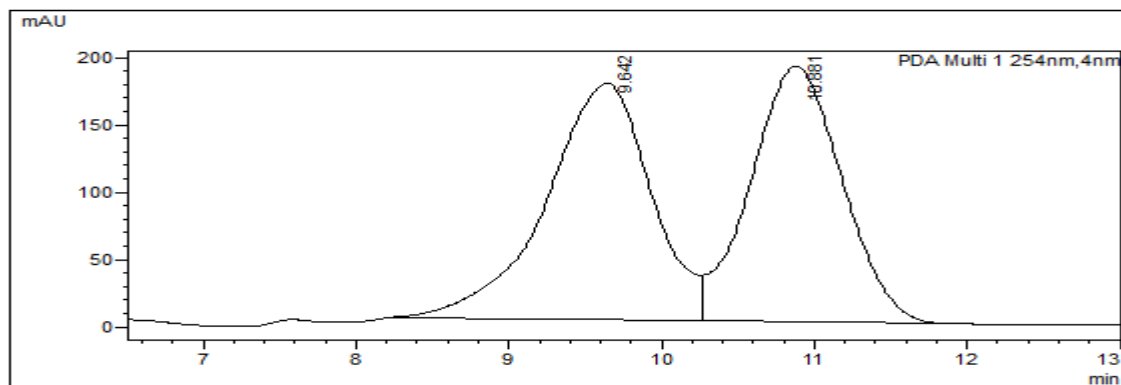
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.359	217352	5320	3.378	3.614
2	17.742	6217920	141871	96.622	96.386
Total		6435272	147191	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(2,4-dichlorophenyl)pent-4-en-2-ol (3o):



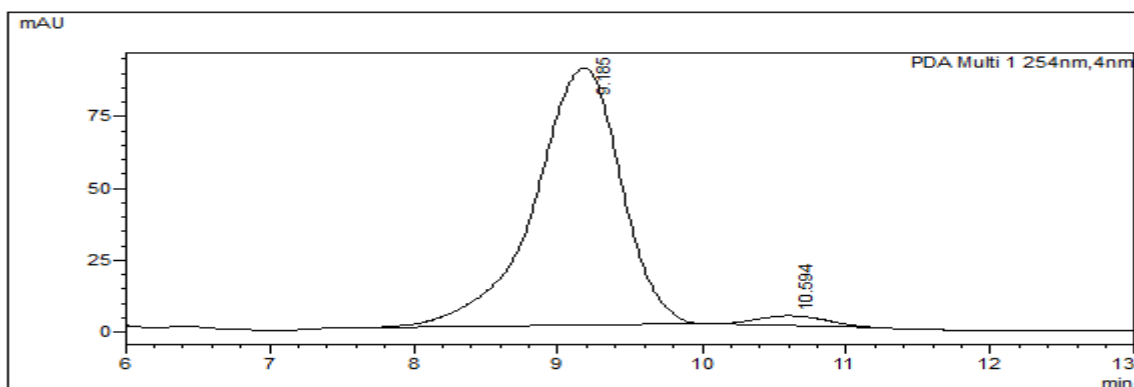
Prepared according to the general procedure as described above in 95% yield (141 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; $R_f = 0.3$) to afford a colourless oil; 1H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, $J = 8.6$ Hz, 1H), 7.31 (dd, $J = 8.6, 2.2$ Hz, 1H), 7.28 – 7.09 (m, 9H), 6.75 – 6.71 (m, 2H), 5.99

(ddd, $J = 17.4, 10.2, 8.6$ Hz, 1H), 5.50 (dd, $J = 10.3, 1.7$ Hz, 1H), 5.36 (s, 1H), 5.32 (dd, $J = 17.3, 1.6$ Hz, 1H), 4.60 (d, $J = 8.6$ Hz, 1H), 3.53 (s, 1H), 1.52 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 142.6, 142.5, 140.6, 133.6, 133.3, 131.6, 131.0, 129.8, 128.5, 128.3, 127.8, 127.5, 127.4, 127.0, 126.5, 122.0, 80.2, 80.0, 76.5, 23.2; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{24}\text{H}_{22}\text{Cl}_2\text{O}_2\text{Na}^+$, 435.0895; found: 435.0877; $[\alpha]_D^{20} = -52.66^\circ$ (c 1.0, CHCl_3); 97:3 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5μ column; hexane/2-propanol = 99/01, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 9.189 min (major), 10.594 min (minor).



<Peak Table>

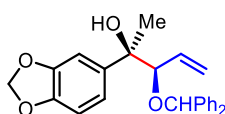
PDACH1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.642	7508212	168069	49.794	47.494
2	10.881	7570207	185804	50.206	52.506
Total		15078419	353873	100.000	100.000



<Peak Table>

PDACH1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.185	3720518	89286	96.805	96.190
2	10.594	122784	3537	3.195	3.810
Total		3843302	92823	100.000	100.000

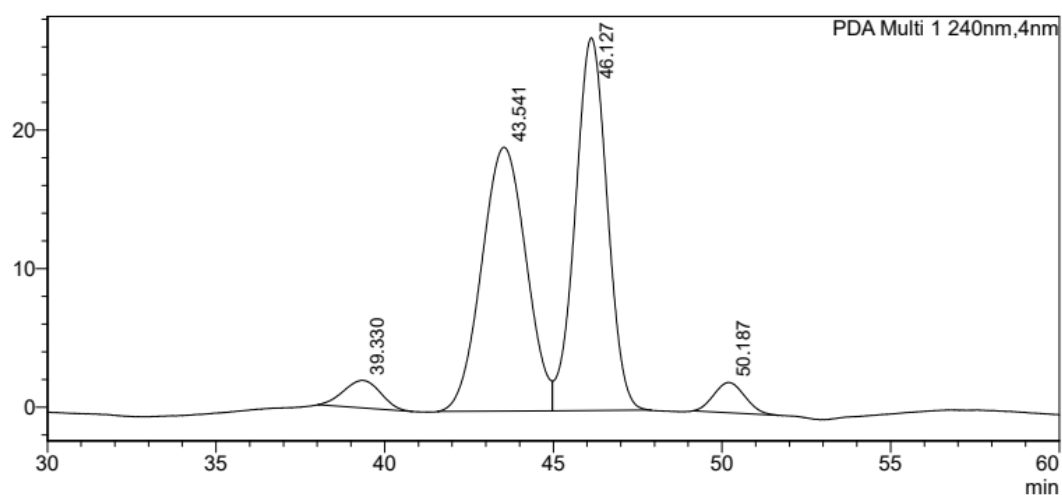
(2*R*,3*R*)-3-(benzhydryloxy)-2-(benzo[*d*][1,3]dioxol-5-yl)pent-4-en-2-ol (3p):



Prepared according to the general procedure as described above in 86% yield (120 mg) with 12:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; $R_f = 0.3$) to afford a colourless oil; ^1H NMR (500 MHz,

CDCl₃) δ 7.30 – 7.07 (m, 9H), 6.95 – 6.91 (m, 2H), 6.79 – 6.73 (m, 1H), 6.67 (d, J = 8.1 Hz, 1H), 5.88 (s, 2H), 5.74 (ddd, J = 17.4, 10.3, 8.5 Hz, 1H), 5.35 (s, 1H), 5.31 (dd, J = 10.3, 1.6 Hz, 1H), 5.07 (dd, J = 17.3, 1.0 Hz, 1H), 3.72 (d, J = 8.4 Hz, 1H), 2.96 (s, 1H), 1.34 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 147.4, 146.3, 142.8, 141.0, 140.4, 134.2, 128.5, 128.3, 128.0, 127.3, 126.7, 126.6, 121.4, 119.0, 107.6, 106.8, 101.0, 85.0, 80.020, 76.0, 25.6; HRMS (ESI) m/z : [M+Na]⁺ calcd for C₂₅H₂₄O₄Na⁺, 411.1572; found: 411.1569; [α]_D²⁰ = -68.02° (c 1.0, CHCl₃); 94:6 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 95/05, detected at 240 nm, Flow rate = 1 mL/min, Retention times: 43.492 min (major), 46.441 min (minor).

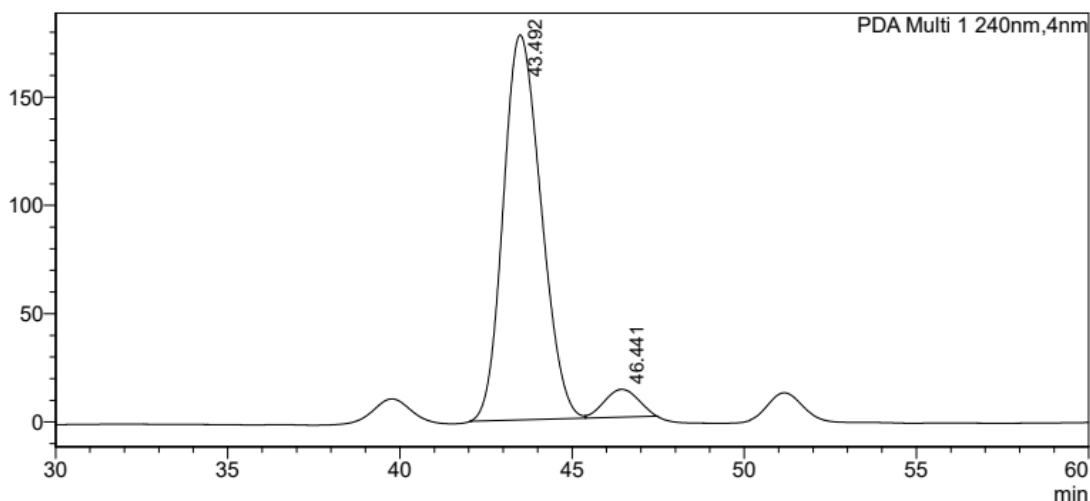
mAU



<Peak Table>

PDA Ch1 240nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	39.330	150749	1989	3.948	3.968
2	43.541	1750045	19050	45.829	37.993
3	46.127	1777670	26915	46.552	53.677
4	50.187	140201	2187	3.671	4.362
Total		3818665	50141	100.000	100.000

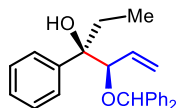
mAU



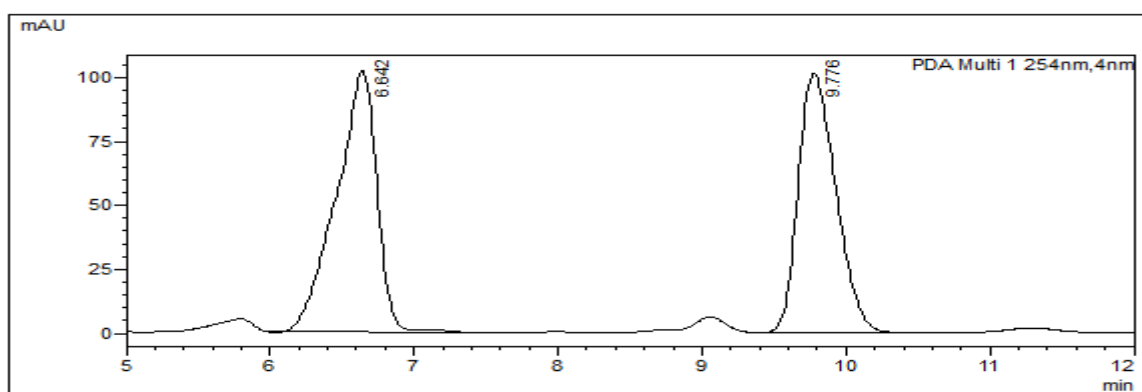
<Peak Table>

PDA Ch1 240nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	43.492	13590728	177815	93.885	93.259
2	46.441	885216	12853	6.115	6.741
Total		14475944	190668	100.000	100.000

(3*R*,4*R*)-4-(Benzhydryloxy)-3-phenylhex-5-en-3-ol (3q):

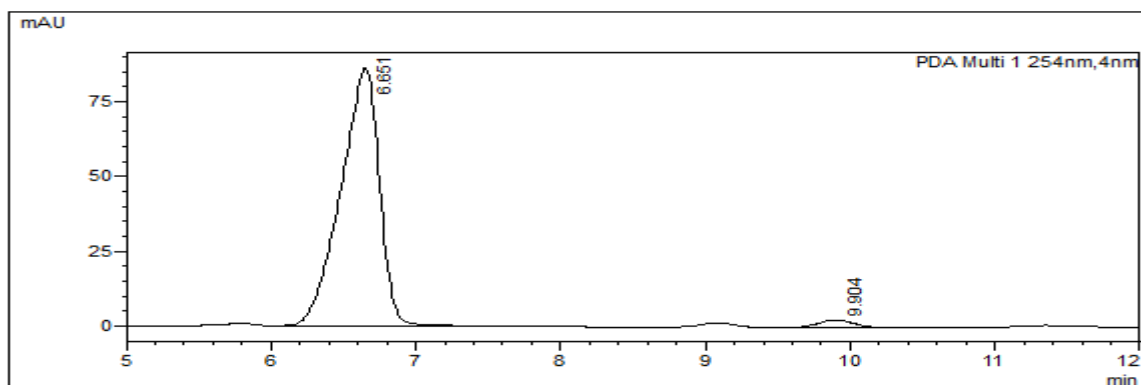


Prepared according to the general procedure as described above in 95% yield (123 mg) with >20:1 *dr*. It was purified by flash chromatography (5% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (500 MHz, CDCl_3) δ 7.27 – 7.14 (m, 7H), 7.12 – 7.05 (m, 6H), 6.78 (d, J = 7.6 Hz, 2H), 5.84 (ddd, J = 17.3, 10.3, 8.6 Hz, 1H), 5.35 (d, J = 10.3 Hz, 1H), 5.32 (s, 1H), 5.10 (d, J = 17.3 Hz, 1H), 3.77 (d, J = 8.7 Hz, 1H), 2.75 (s, 1H), 1.78 – 1.62 (m, 2H), 0.58 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 144.3, 143.0, 140.8, 134.4, 128.5, 128.3, 128.1, 128.0, 127.7, 127.2, 126.6, 126.5, 126.3, 121.5, 84.8, 79.8, 78.8, 30.5, 7.4; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{25}\text{H}_{26}\text{O}_2\text{Na}^+$, 381.1830; found: 381.1830; $[\alpha]^{20}_{\text{D}} = -22.90^\circ$ (c 1.0, CHCl_3); 97:3 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5μ column; hexane/2-propanol = 96/04, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 6.651 min (major), 9.904 min (minor).



<Peak Table>

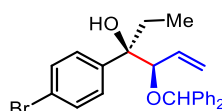
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.642	2008180	102214	52.107	50.243
2	9.776	1845763	101224	47.893	49.757
Total		3853943	203438	100.000	100.000



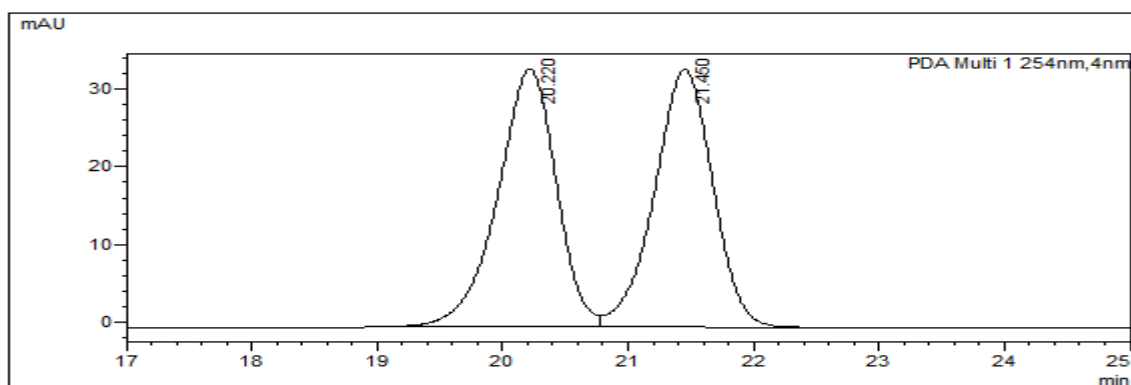
<Peak Table>

Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.651	1596274	86176	97.470	97.160
2	9.904	41438	2519	2.530	2.840
Total		1637711	88695	100.000	100.000

(3*R*,4*R*)-4-(Benzhydryloxy)-3-(4-bromophenyl)hex-5-en-3-ol (3r):

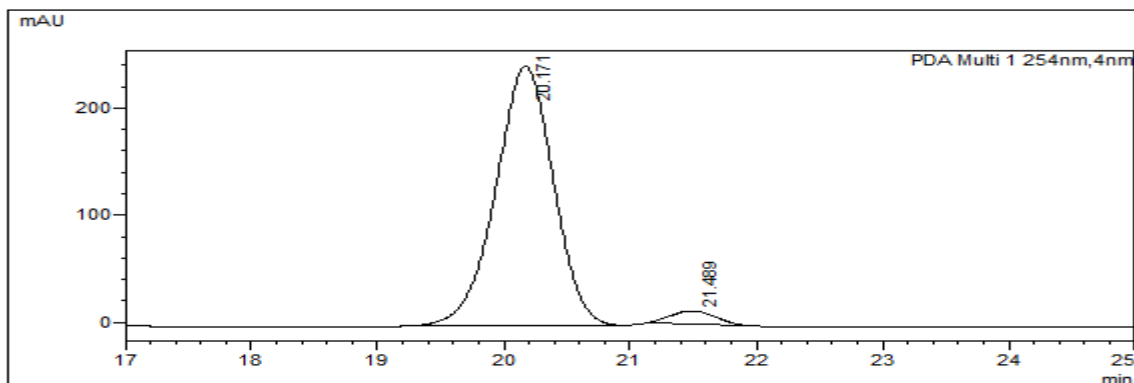


Prepared according to the general procedure as described above in 94% yield (148 mg) with >20:1 *dr*. It was purified by flash chromatography (5% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.36 – 7.32 (m, 2H), 7.21 – 7.05 (m, 10H), 6.81 (dd, J = 7.7, 1.6 Hz, 2H), 5.78 (ddd, J = 17.4, 10.2, 8.8 Hz, 1H), 5.37 (dd, J = 10.3, 1.6 Hz, 1H), 5.32 (s, 1H), 5.12 (dd, J = 17.3, 1.1 Hz, 1H), 3.72 (d, J = 8.7 Hz, 1H), 2.49 (s, 1H), 1.78 – 1.54 (m, 2H), 0.56 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 143.5, 142.7, 140.6, 134.0, 131.0, 128.5, 128.3, 128.2, 128.0, 129.0, 127.3, 126.5, 122.0, 120.5, 84.6, 79.8, 78.6, 30.5, 7.3; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{25}\text{H}_{25}\text{BrO}_2\text{Na}^+$, 459.0935; found: 459.0929; $[\alpha]_D^{20}$ = -40.59° (c 1.0, CHCl_3); 96:4 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column connected to Daicel Chiralpak AD-H 250X4.6 mm 5 μ column in tandem; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 20.171 min (major), 21.489 min (minor).



<Peak Table>

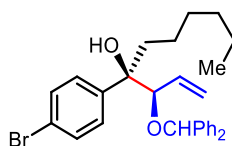
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	20.220	1073910	33064	50.097	50.011
2	21.450	1069762	33049	49.903	49.989
Total		2143671	66114	100.000	100.000



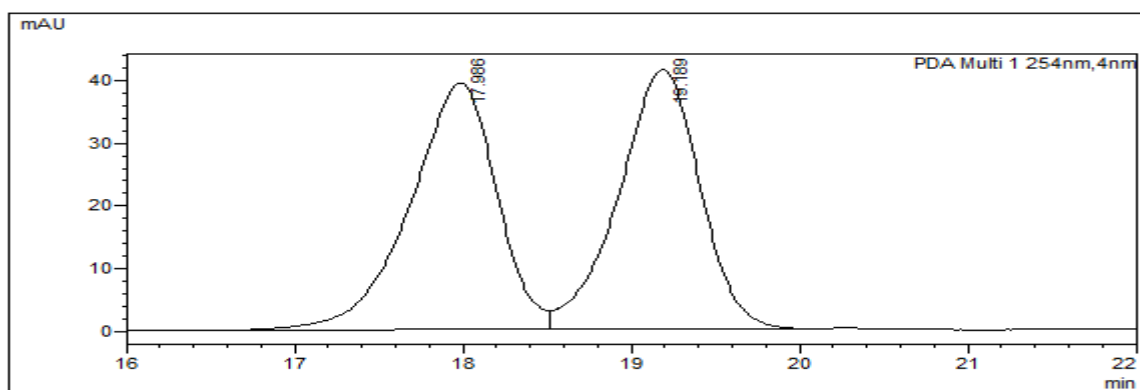
<Peak Table>

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	20.171	7707132	242542	96.206	95.144
2	21.489	303911	12379	3.794	4.856
Total		8011042	254921	100.000	100.000

(3*R*,4*R*)-3-(Benzhydryloxy)-4-(4-bromophenyl)dec-1-en-4-ol (3s):

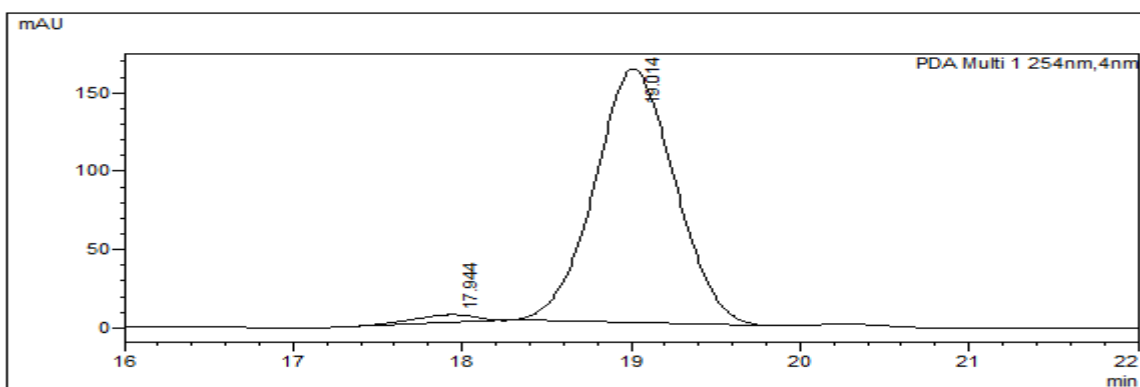


Prepared according to the general procedure as described above in 91% yield (166 mg) with >20:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.4) to afford a colourless oil; ^1H NMR (500 MHz, CDCl_3) δ 7.36 – 7.32 (m, 2H), 7.20 – 7.06 (m, 10H), 6.80 – 6.78 (m, 2H), 5.78 (ddd, J = 17.4, 10.2, 8.8 Hz, 1H), 5.38 (dd, J = 10.3, 1.6 Hz, 1H), 5.31 (s, 1H), 5.13 (dd, J = 17.3, 1.2 Hz, 1H), 3.70 (d, J = 8.8 Hz, 1H), 2.72 (s, 1H), 1.67 – 1.53 (m, 2H), 1.23 – 0.99 (m, 8H), 0.73 (t, J = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 144.0, 142.7, 140.5, 134.1, 131.0, 128.5, 128.3, 128.0, 128.1, 127.3, 126.5, 122.1, 120.4, 84.6, 79.7, 78.4, 38.4, 31.8, 29.8, 23.0, 22.7, 14.2; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{29}\text{H}_{33}\text{BrO}_2\text{Na}^+$, 515.1562; found: 515.1562; $[\alpha]_D^{20}$ = -59.59° (c 1.0, CHCl_3); 97:3 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column connected to Daicel Chiralpak AD-H 250X4.6 mm 5 μ column in tandem; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 17.944 min (minor), 19.014 min (major).



<Peak Table>

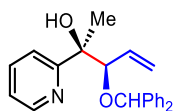
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	17.986	1402785	39281	50.306	48.695
2	19.189	1385710	41386	49.694	51.305
Total		2788495	80667	100.000	100.000



<Peak Table>

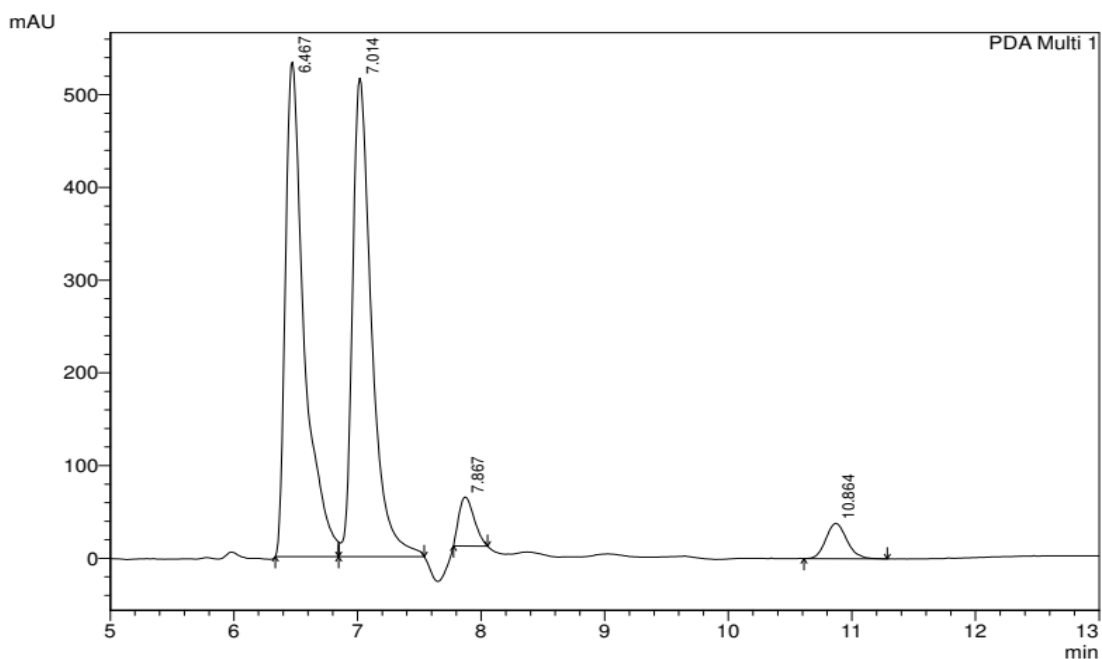
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	17.944	136698	5027	2.504	3.019
2	19.014	5321616	161464	97.496	96.981
Total		5458315	166491	100.000	100.000

(2*R*,3*R*)-3-(Benzhydryloxy)-2-(pyridin-2-yl)pent-4-en-2-ol (3u):



Prepared according to the general procedure as described above in 81% yield (101 mg) with 11:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a white solid; mp = 146-148 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.49 (ddd, J = 4.9, 1.7, 0.9 Hz, 1H), 7.71 – 7.65 (m, 1H), 7.54 – 7.51 (m, 1H), 7.28 – 7.14 (m, 9H), 6.92 – 6.89 (m, 2H), 5.73 (ddd, J = 17.3, 10.3, 8.6 Hz, 1H), 5.39 (s, 1H), 5.36 (d, J = 1.8 Hz, 1H), 5.22 (ddd, J = 17.3, 1.9, 0.6 Hz, 1H), 4.89 (s, 1H), 3.99 (d, J = 8.6 Hz, 1H), 1.46 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 163.6, 147.5, 143.1, 141.2, 136.5, 134.3, 128.4, 128.2, 127.9, 127.7, 127.1, 126.5, 122.0, 121.4, 120.7, 84.2, 79.8, 76.0, 25.6; HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{23}\text{H}_{24}\text{NO}_2^+$, 346.1807; found: 346.1805; $[\alpha]^{20}_{\text{D}}$ = -59.59° (c 1.0, CHCl_3); 95:5 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IA-3 250X4.6 mm 5 μ

column; hexane/2-propanol = 95/05, detected at 210 nm, Flow rate = 1 mL/min, Retention times: 6.460 min (major), 7.051 min (minor).

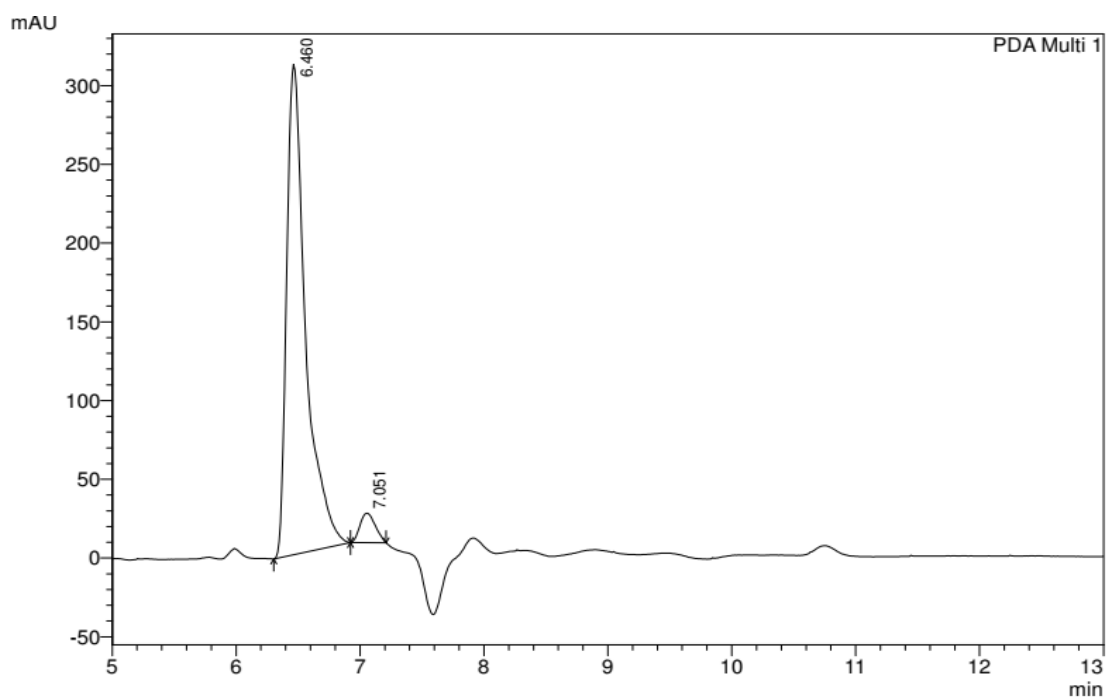


1 PDA Multi 1/210nm 4nm

PeakTable

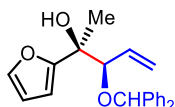
PDA Ch1 210nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.467	5674996	533857	46.729	46.779
2	7.014	5567605	516249	45.845	45.236
3	7.867	452196	53052	3.723	4.649
4	10.864	449599	38068	3.702	3.336
Total		12144397	1141226	100.000	100.000

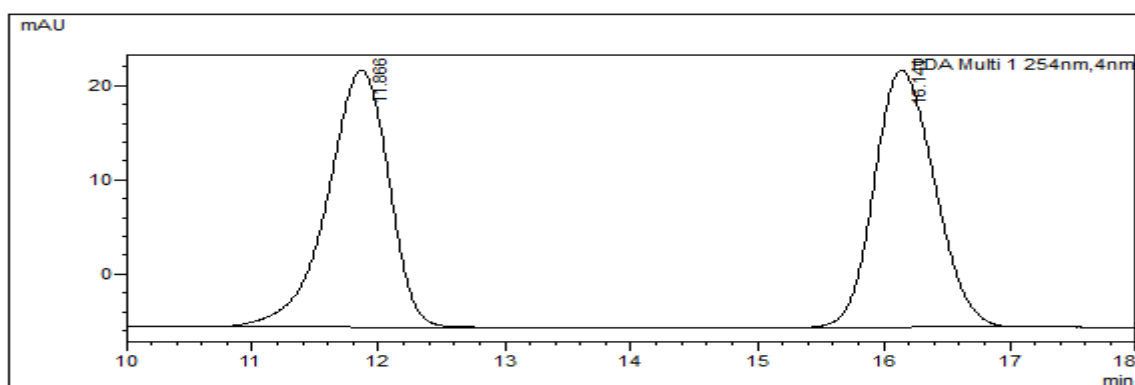


PDA Ch1 210nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.460	3325890	311362	95.392	94.340
2	7.051	160645	18682	4.608	5.660
Total		3486535	330044	100.000	100.000

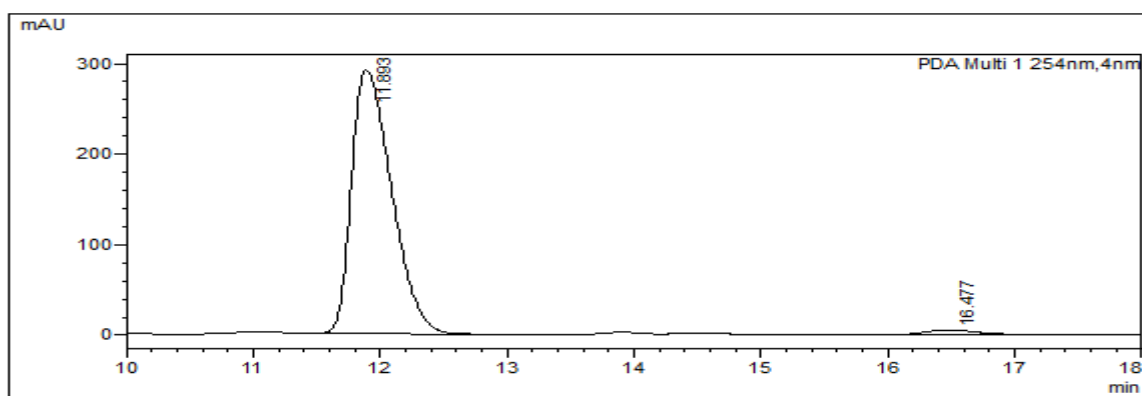
(2*S*,3*R*)-3-(Benzhydryloxy)-2-(furan-2-yl)pent-4-en-2-ol (3v):

Prepared according to the general procedure as described above in 96% yield (116 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.33 – 7.17 (m, 9H), 7.06 – 6.99 (m, 2H), 6.35 (dd, J = 3.2, 1.8 Hz, 1H), 6.28 (dd, J = 3.2, 0.8 Hz, 1H), 5.82 (ddd, J = 17.3, 10.3, 8.6 Hz, 1H), 5.43 (s, 1H), 5.38 (dd, J = 10.4, 1.7 Hz, 1H), 5.17 (dd, J = 17.3, 1.7 Hz, 1H), 3.98 (d, J = 8.6 Hz, 1H), 3.14 (s, 1H), 1.43 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 158.4, 142.8, 141.3, 141.1, 133.8, 128.6, 128.3, 127.8, 127.7, 127.3, 126.7, 121.5, 110.4, 106.0, 83.0, 80.1, 73.7, 23.1; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{22}\text{H}_{22}\text{O}_3\text{Na}^+$, 357.1466; found: 357.1463; $[\alpha]_D^{20}$ = -52.83° (c 1.0, CHCl_3); 98:2 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 11.893 min (major), 16.477 min (minor).



<Peak Table>

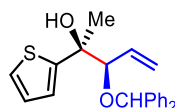
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.866	918861	27263	50.325	49.982
2	16.141	907010	27283	49.675	50.018
Total		1825870	54546	100.000	100.000



<Peak Table>

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.893	6347216	290970	98.159	98.344
2	16.477	119015	4899	1.841	1.656
Total		6466231	295869	100.000	100.000

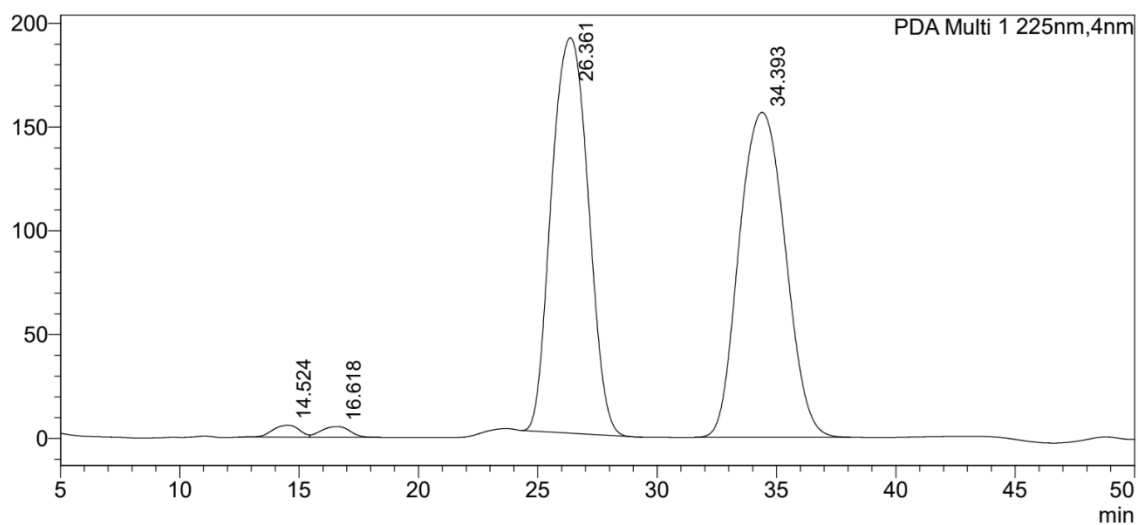
(2S,3R)-3-(Benzhydryloxy)-2-(thiophen-2-yl)pent-4-en-2-ol (3w):



Prepared according to the general procedure as described above in 81% yield (102 mg) with 11:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (500 MHz, CDCl_3) δ 7.23 – 7.11 (m, 9H), 7.04 – 7.00 (m, 2H), 6.87 (dd, J = 5.0, 3.6 Hz, 1H), 6.76 (dd, J = 3.6, 1.2 Hz, 1H), 5.71 (ddd, J = 17.3, 10.4, 8.5 Hz, 1H), 5.40 (s, 1H), 5.32 (dd, J = 10.4, 1.6 Hz, 1H), 5.09 (ddd, J = 17.3, 1.7, 0.7 Hz, 1H), 3.76 (d, J = 8.5 Hz, 1H), 1.48 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 151.0, 142.7, 141.0, 134.0, 128.6, 128.3, 128.0, 127.8, 127.3, 126.6, 124.0, 123.3, 122.0, 85.4, 80.4, 75.5, 26; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{22}\text{H}_{22}\text{O}_2\text{SNa}^+$, 373.1239; found: 373.1229; $[\alpha]^{20}_{\text{D}}$ = -48.33° (c 1.0, CHCl_3); 96:4 *er* Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 99/01, detected at 225 nm, Flow rate = 0.8 mL/min, Retention times: 26.300 min (minor), 34.234 min (major).

<Chromatogram>

mAU

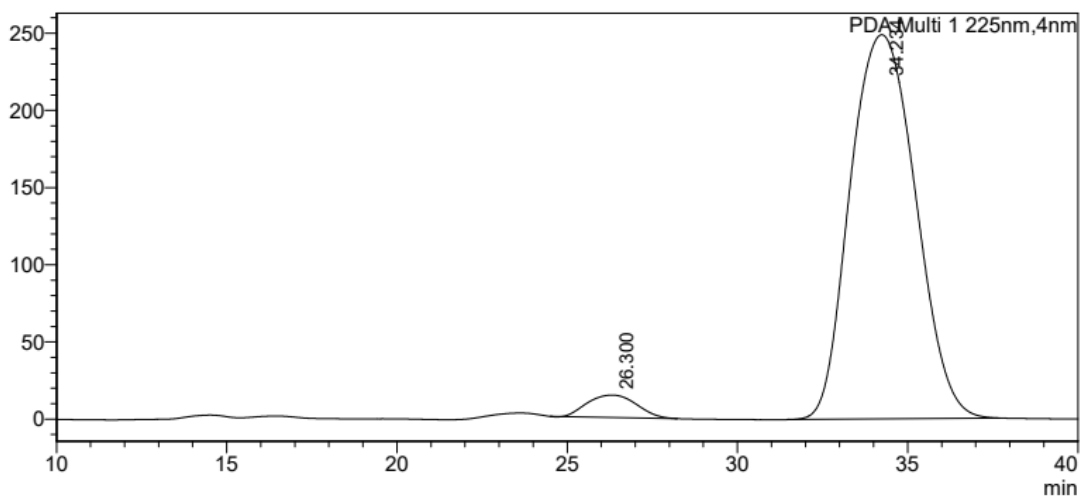


<Peak Table>

PDA Ch1 225nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	14.524	452833	5793	1.068	1.617
2	16.618	431572	5196	1.018	1.451
3	26.361	20500528	190537	48.337	53.202
4	34.393	21026683	156615	49.578	43.730
Total		42411617	358141	100.000	100.000

mAU

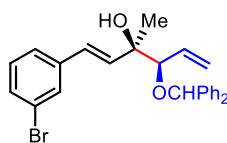


<Peak Table>

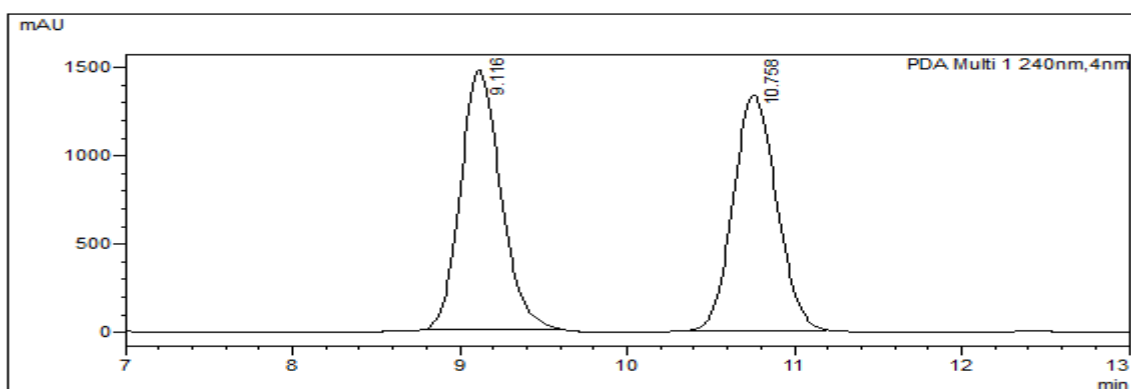
PDA Ch1 225nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	26.300	1460900	14530	4.202	5.517
2	34.234	33302052	248842	95.798	94.483
Total		34762952	263372	100.000	100.000

(3*R*,4*R*,*E*)-4-(Benzhydryloxy)-1-(3-bromophenyl)-3-methylhexa-1,5-dien-3-ol (3x):

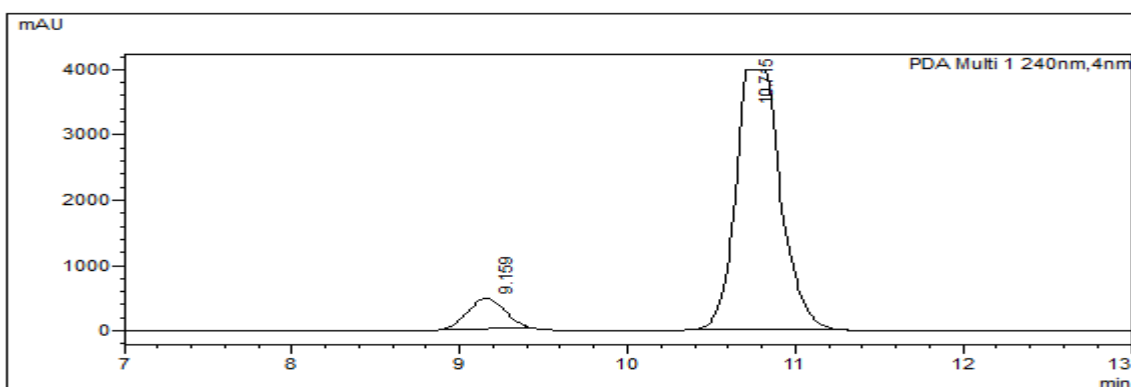


Prepared according to the general procedure as described above in 88% yield (142 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.2) to afford a semi solid; ^1H NMR (400 MHz, CDCl_3) δ 7.44 (s, 1H), 7.30 – 7.17 (m, 11H), 7.17 – 7.08 (m, 2H), 6.53 (d, J = 16.0 Hz, 1H), 6.14 (d, J = 16.0 Hz, 1H), 5.80 (ddd, J = 17.5, 10.1, 8.9 Hz, 1H), 5.43 (s, 1H), 5.38 (dd, J = 10.3, 1.6 Hz, 1H), 5.18 (dd, J = 17.3, 1.5 Hz, 1H), 3.56 (d, J = 8.7 Hz, 1H), 2.52 (s, 1H), 1.21 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 142.7, 141.1, 139.4, 137.1, 134.2, 130.3, 130.2, 129.2, 128.8, 128.3, 128.2, 128.2, 127.3, 127.0, 126.7, 125.4, 123.0, 122.0, 84.2, 80.0, 74.7, 24.3; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{26}\text{H}_{25}\text{BrO}_2\text{Na}^+$, 471.0935; found: 471.0928; $[\alpha]^{20}_{\text{D}}$ = -81.65° (c 1.0, CHCl_3); 91:9 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 95/05, detected at 240 nm, Flow rate = 1 mL/min, Retention times: 9.159 min (minor), 10.715 min (major).



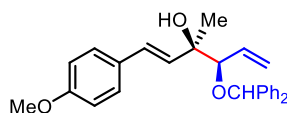
<Peak Table>

PDA Ch1 240nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.116	24638390	1469733	50.462	52.409
2	10.758	24187591	1334625	49.538	47.591
Total		48825981	2804359	100.000	100.000

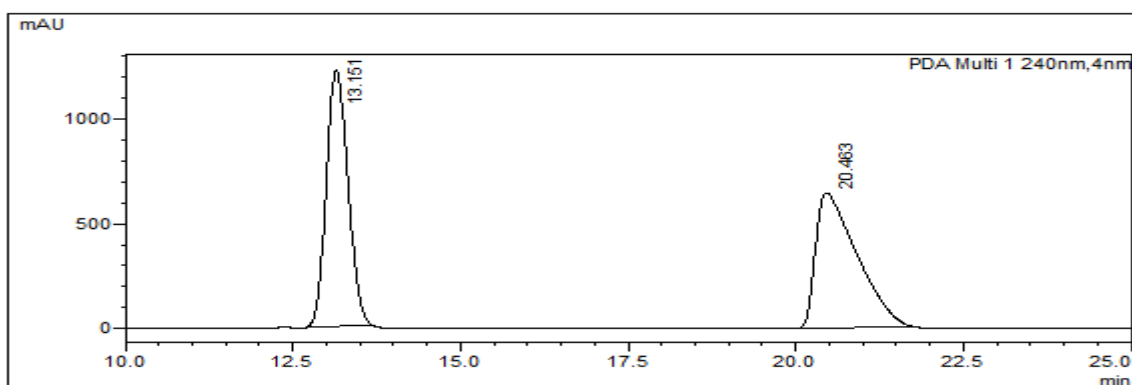


<Peak Table>

PDA Ch1 240nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.159	7303852	469637	8.976	10.564
2	10.715	74071516	3976197	91.024	89.436
Total		81375369	4445835	100.000	100.000

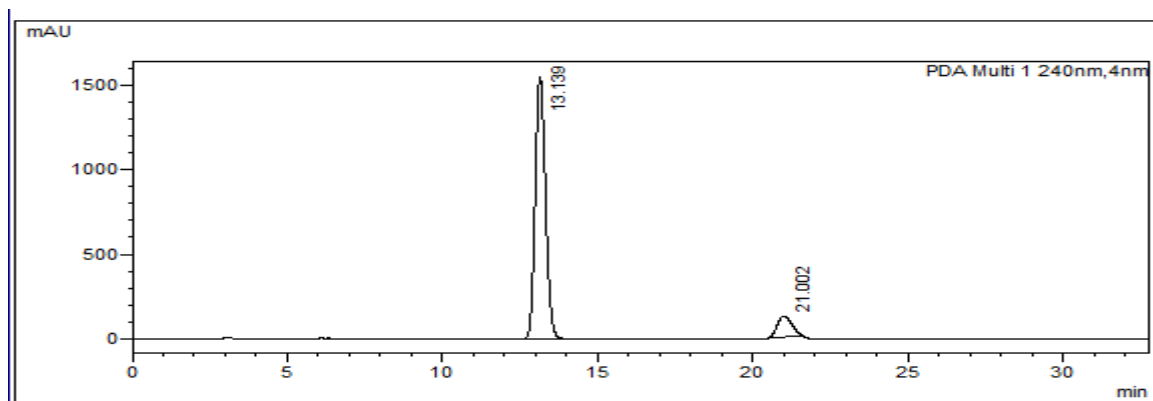
(3R,4R,E)-4-(Benzhydryloxy)-1-(4-methoxyphenyl)-3-methylhexa-1,5-dien-3-ol (3y):

Prepared according to the general procedure as described above in 83% yield (120 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.2) to afford a white solid; mp = 70-73 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.32 – 7.19 (m, 9H), 7.19 – 7.10 (m, 3H), 6.80 – 6.76 (m, 2H), 6.52 (d, J = 16.1 Hz, 1H), 6.04 (d, J = 16.1 Hz, 1H), 5.78 (ddd, J = 17.3, 10.3, 8.6 Hz, 1H), 5.43 (s, 1H), 5.34 (dd, J = 10.3, 1.8 Hz, 1H), 5.15 (dd, J = 17.3, 1.2 Hz, 1H), 3.72 (s, 3H), 3.56 (d, J = 8.6 Hz, 1H), 2.50 (s, 1H), 1.23 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 159.2, 143.0, 141.3, 134.6, 132.8, 130.0, 128.7, 128.3, 128.2, 128.0, 127.7, 127.6, 127.3, 126.7, 121.6, 114.1, 84.5, 80.1, 74.7, 55.4, 24.4; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{27}\text{H}_{28}\text{O}_3\text{Na}^+$, 423.1936; found: 423.1932; $[\alpha]_D^{20}$ = -87.23° (c 2.0, CHCl_3); 90:10 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 95/05, detected at 240 nm, Flow rate = 1 mL/min, Retention times: 13.139 min (major), 21.002 min (minor).



<Peak Table>

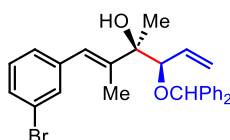
PDA Ch1 240nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.151	27668082	1228327	49.958	65.578
2	20.463	27714871	644756	50.042	34.422
Total		55382953	1873084	100.000	100.000



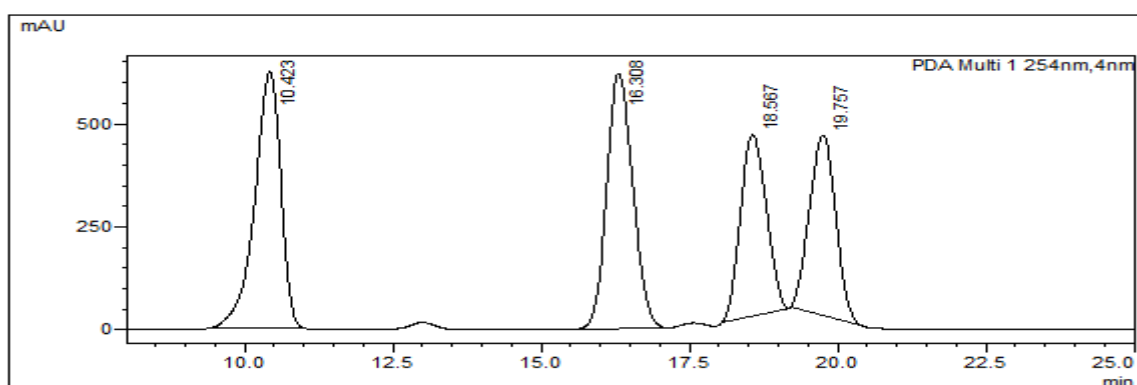
<Peak Table>

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.139	35851182	1546304	90.002	92.623
2	21.002	3982577	123162	9.998	7.377
Total		39833759	1669467	100.000	100.000

(3*R*,4*R*,*E*)-4-(Benzhydryloxy)-1-(3-bromophenyl)-2,3-dimethylhexa-1,5-dien-3-ol (3z) :

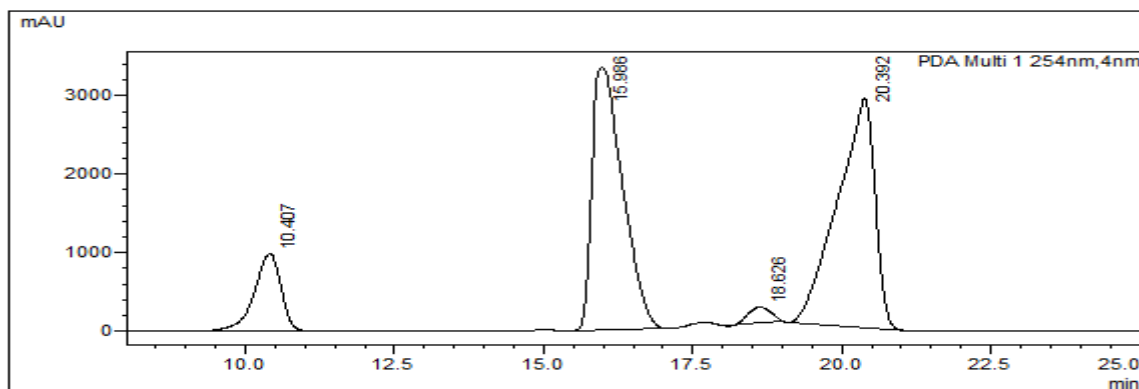


Prepared according to the general procedure as described above in 86% yield (143 mg) with 5:2 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; $R_f = 0.3$) to afford a colourless oil; Major isomer; ^1H NMR (400 MHz, CDCl_3) δ 7.29 – 7.23 (m, 5H), 7.22 – 7.18 (m, 9H), 6.60 (s, 1H), 5.86 (ddd, $J = 17.3, 10.3, 8.7$ Hz, 1H), 5.42 (s, 1H), 5.39 (dd, $J = 10.3, 1.7$ Hz, 1H), 5.18 (dd, $J = 17.4, 1.2$ Hz, 1H), 3.74 (d, $J = 8.7$ Hz, 1H), 2.38 (s, 1H), 1.48 (d, $J = 1.2$ Hz, 3H), 1.16 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 144.0, 142.8, 134.4, 129.7, 129.2, 128.7, 128.3, 128.2, 127.8, 127.3, 126.5, 123.3, 121.5, 81.9, 79.74, 23.3, 14.9; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{27}\text{H}_{27}\text{BrO}_2\text{Na}^+$, 485.1092; found: 485.1083; $[\alpha]_D^{20} = -57.76^\circ$ (c 1.0, CHCl_3); 80:20/96:4 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 10.407 min (minor), 15.986 min (major) ; 18.626 min (minor), 20.392 min (major).



<Peak Table>

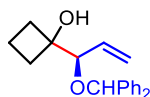
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.423	19074311	624154	29.380	29.446
2	16.308	18982808	618724	29.239	29.190
3	18.567	13369318	439052	20.593	20.714
4	19.757	13495974	437710	20.788	20.650
Total		64922411	2119639	100.000	100.000



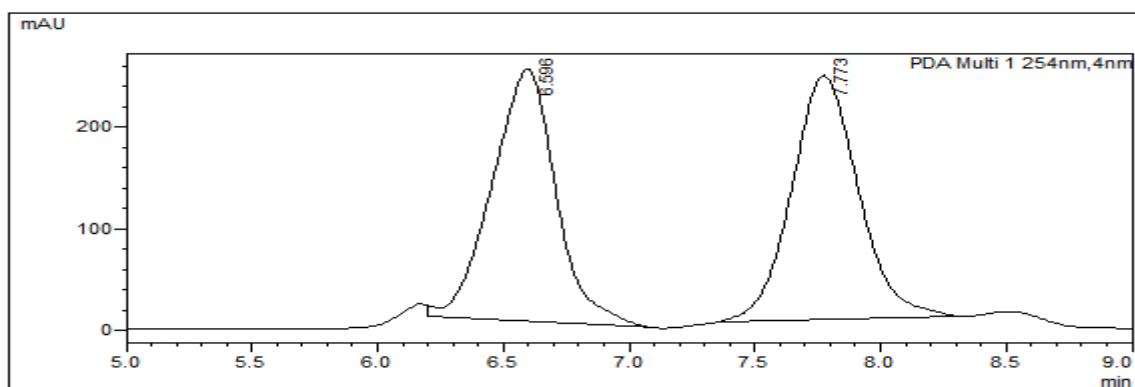
<Peak Table>

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.407	30155451	979926	10.630	13.122
2	15.986	119922145	3351693	42.272	44.882
3	18.626	5557334	206255	1.959	2.762
4	20.392	128058962	2929979	45.140	39.235
Total		283693892	7467853	100.000	100.000

(R)-1-(1-(Benzyloxy)allyl)cyclobutan-1-ol (3aa):

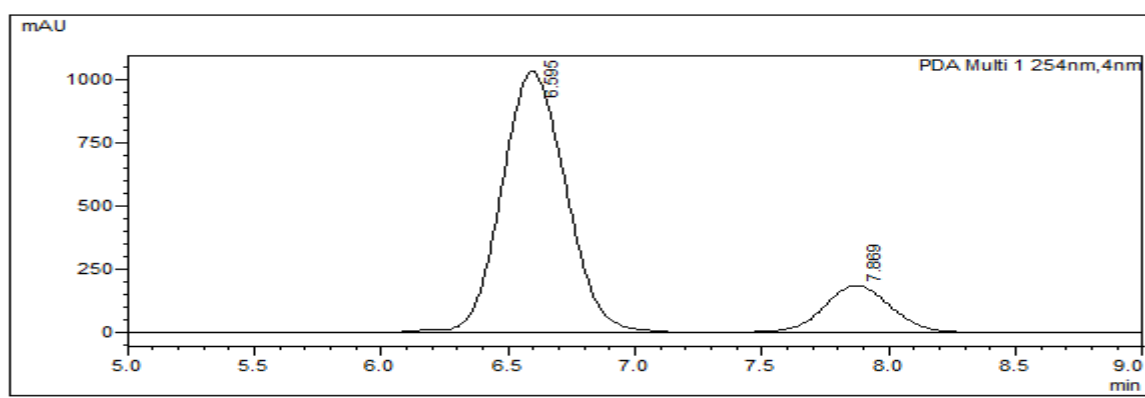


Prepared according to the general procedure as described above in 80% yield (85 mg). It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.32 – 7.17 (m, 9H), 7.17 – 7.06 (m, 1H), 5.80 (ddd, J = 17.4, 10.3, 8.6 Hz, 1H), 5.44 (s, 1H), 5.34 (dd, J = 10.3, 1.8 Hz, 1H), 5.17 (dd, J = 17.3, 1.8 Hz, 1H), 3.62 (d, J = 8.6 Hz, 1H), 2.40 (s, 1H), 2.14 – 1.85 (m, 4H), 1.73 – 1.61 (m, 1H), 1.41 – 1.27 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 142.9, 141.2, 134.1, 129.0, 128.3, 128.0, 127.2, 127.0, 121.3, 83.0, 80.0, 76.1, 33.3, 32.0, 12.3; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{20}\text{H}_{22}\text{O}_2\text{Na}^+$, 317.1517; found: 317.1513; $[\alpha]^{20}_{\text{D}}$ = -77.65° (c 2.23, CHCl_3); 85:15 er; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 6.595 min (major), 7.869 min (minor).



<Peak Table>

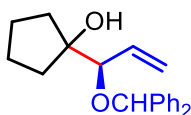
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.596	4417083	248550	49.994	50.890
2	7.773	4418149	239858	50.006	49.110
Total		8835232	488409	100.000	100.000



<Peak Table>

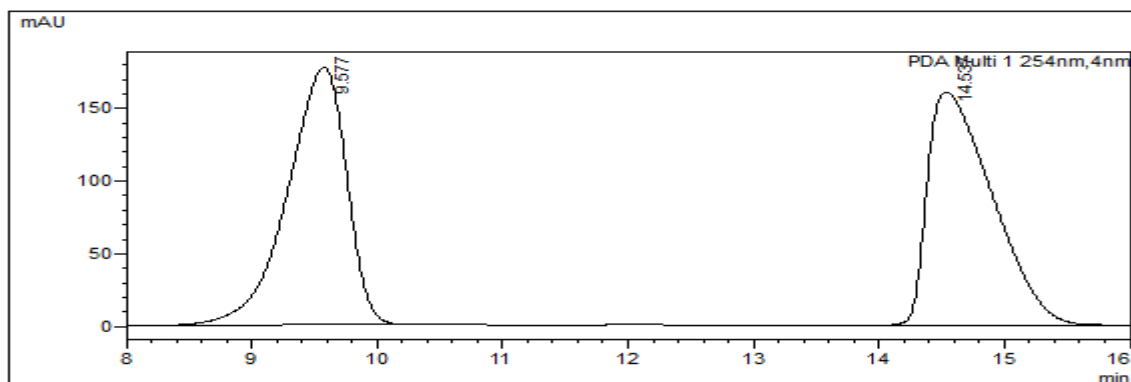
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.595	18048792	1031122	84.516	84.919
2	7.869	3306803	183114	15.484	15.081
Total		21355595	1214236	100.000	100.000

(R)-1-(1-(Benzyloxy)allyl)cyclopentan-1-ol (3ab):



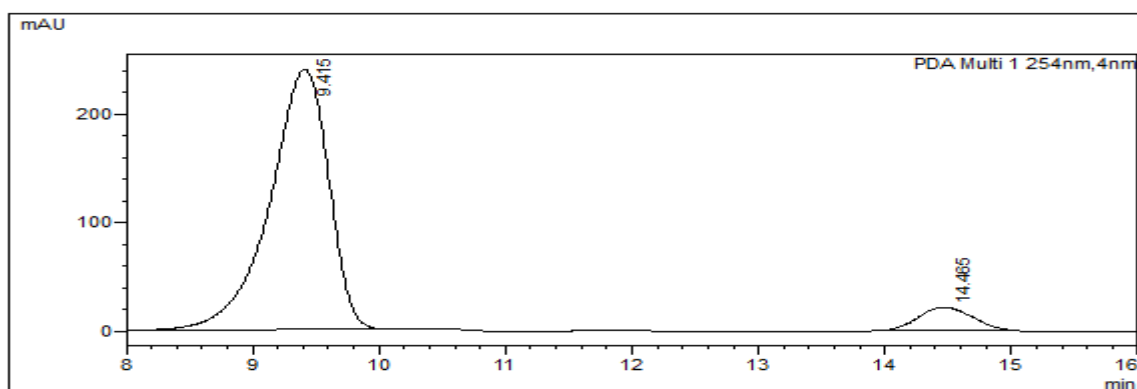
Prepared according to the general procedure as described above in 80% yield (89 mg). It was purified by flash chromatography (10% EtOAc/hexanes; $R_f = 0.4$) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.30 – 7.18 (m, 9H), 7.17 – 7.11 (m, 1H), 5.83 (ddd, $J = 17.5, 10.0, 9.0$ Hz, 1H), 5.44 (s, 1H), 5.30 (dd, $J = 10.3, 1.8$ Hz, 1H), 5.12 (dd, $J = 17.3, 1.7$ Hz, 1H), 3.54 (d, $J = 8.7$ Hz, 1H), 2.00 (s, 1H), 1.81 – 1.65 (m, 3H), 1.60 – 1.42 (m, 5H); ^{13}C NMR (101 MHz, CDCl_3) δ 143.1, 141.4, 135.2, 128.7, 128.3, 128.1, 128.1, 127.2, 126.6, 120.8, 84.1, 83.8, 79.6, 38.4, 36.1, 24.1, 24.1; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{21}\text{H}_{24}\text{O}_2\text{Na}^+$, 331.1674; found: 331.1678; $[\alpha]_D^{20} = -135.18^\circ$ (c 2.0, CHCl_3); 93:7 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-

H 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 9.415 min (major), 14.465 min (minor).



<Peak Table>

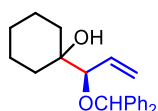
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.577	5810671	177228	50.101	52.476
2	14.537	5787234	160503	49.899	47.524
Total		11597904	337731	100.000	100.000



<Peak Table>

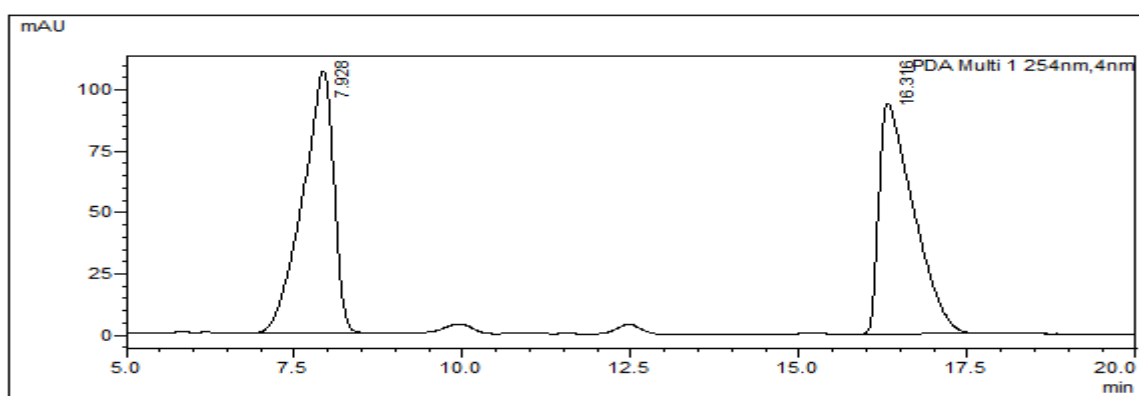
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.415	7726049	239223	92.510	91.855
2	14.465	625527	21212	7.490	8.145
Total		8351576	260434	100.000	100.000

(R)-1-(1-(Benzyloxy)allyl)cyclohexan-1-ol (3ac):



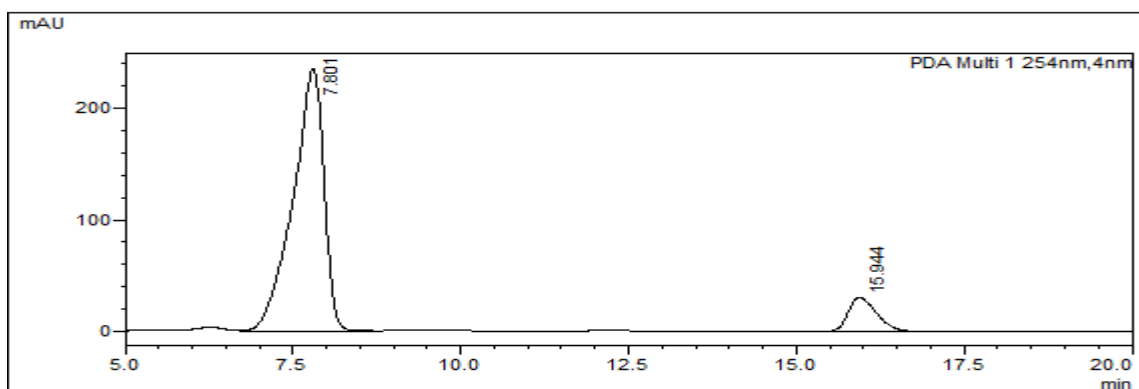
Prepared according to the general procedure as described above in 83% yield (96 mg). It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.30 – 7.02 (m, 10H), 5.83 (ddd, J = 17.5, 10.0, 9.0 Hz, 1H), 5.43 (s, 1H), 5.31 (dd, J = 10.3, 1.8 Hz, 1H), 5.08 (dd, J = 17.4, 1.7 Hz, 1H), 3.45 (d, J = 8.8 Hz, 1H), 2.03 (s, 1H), 1.70 – 1.43 (m, 5H), 1.40 – 1.16 (m, 4H), 1.15 – 1.02 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 143.1, 141.4, 134.7, 128.7, 128.3, 128.1, 128.0, 127.2, 126.6, 121.0,

84.3, 79.5, 73.0, 34.7, 33.2, 26.1, 21.8, 21.5; HRMS (ESI) m/z : $[M+Na]^+$ calcd for $C_{22}H_{26}O_2Na^+$, 345.1830; found: 345.1833; $[\alpha]^{20}_D = -101.92^\circ$ (c 2.0, $CHCl_3$); 90:10 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 7.801 min (major), 15.944 min (minor).



<Peak Table>

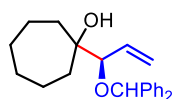
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.928	3443478	106737	50.474	53.174
2	16.316	3378829	93993	49.526	46.826
Total		6822307	200730	100.000	100.000



<Peak Table>

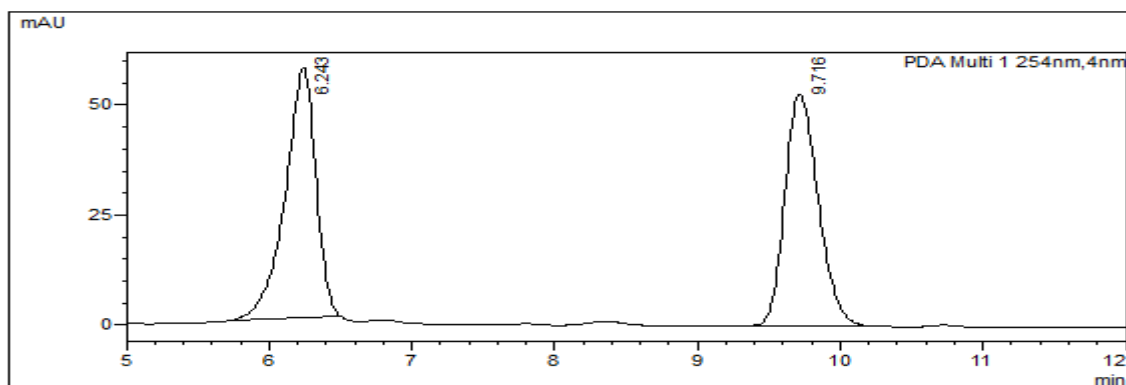
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.801	7543467	234913	89.565	88.566
2	15.944	878884	30327	10.435	11.434
Total		8422351	265239	100.000	100.000

(R)-1-(1-(Benzyloxy)allyl)cycloheptan-1-ol (3ad):



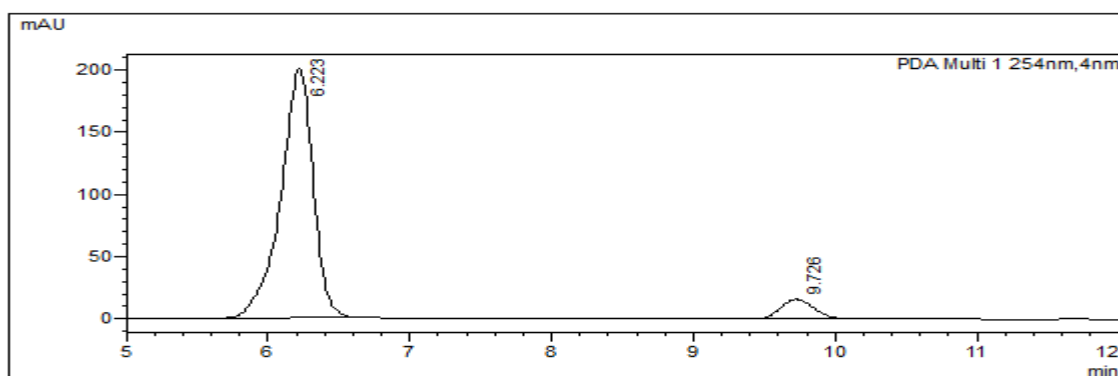
Prepared according to the general procedure as described above in 71% yield (86 mg). It was purified by flash chromatography (10% EtOAc/hexanes; $R_f = 0.3$) to afford a colourless oil; 1H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.20 (m, 8H), 7.19 – 7.10 (m, 2H), 5.76 (ddd, $J = 17.4, 10.3, 8.7$ Hz, 1H), 5.42 (s, 1H), 5.30 (dd, $J = 10.3, 1.9$

Hz, 1H), 5.10 (dd, $J = 17.3, 1.8$ Hz, 1H), 3.44 (d, $J = 8.7$ Hz, 1H), 2.12 (s, 1H), 1.79 – 1.70 (m, 1H), 1.68 – 1.26 (m, 10H), 1.24 – 1.13 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 143.1, 141.3, 134.8, 128.7, 128.3, 128.1, 128.1, 127.2, 126.6, 121.1, 85.1, 79.6, 76.7, 38.0, 37.1, 30.1, 30.0, 22.4, 22.3; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{23}\text{H}_{28}\text{O}_2\text{Na}^+$, 359.1987; found: 359.1990; $[\alpha]^{20}_{\text{D}} = -127.79^\circ$ (c 2.0, CHCl_3); 93:7 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 95/05, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 6.223 min (major), 9.726 min (minor).



<Peak Table>

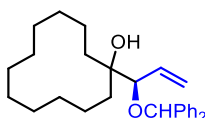
Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.243	854480	56832	49.981	51.900
2	9.716	855128	52671	50.019	48.100
Total		1709608	109503	100.000	100.000



<Peak Table>

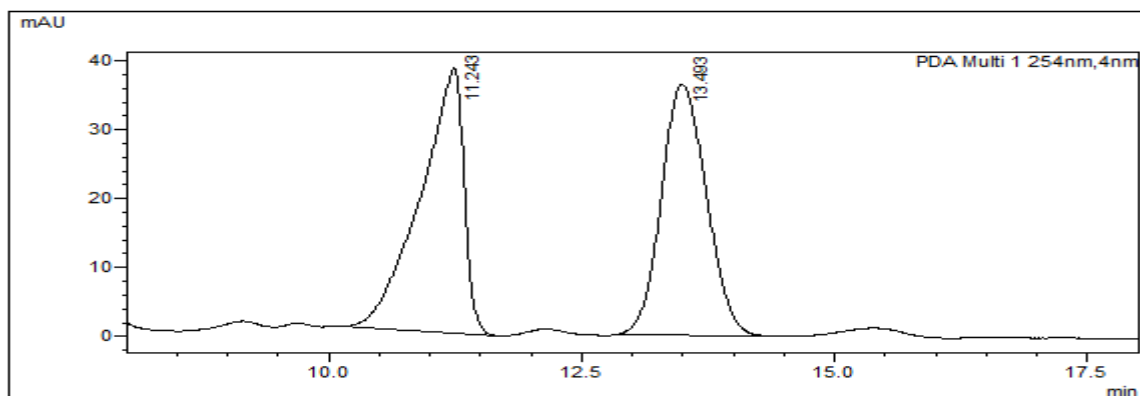
Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.223	3180898	199821	92.970	92.857
2	9.726	240510	15372	7.030	7.143
Total		3421408	215193	100.000	100.000

(*R*)-1-(1-(Benzyloxy)allyl)cyclododecan-1-ol (3ae):



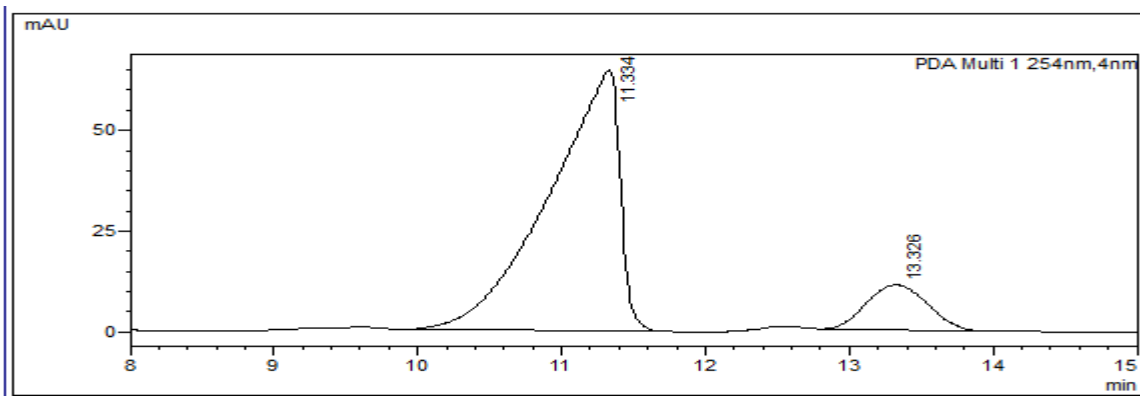
Prepared according to the general procedure as described above in 67% yield (98 mg). It was purified by flash chromatography (10% EtOAc/hexanes; $R_f = 0.3$) to afford a white semi solid; ^1H NMR (400 MHz, CDCl_3) δ 7.33

– 7.22 (m, 7H), 7.22 – 7.10 (m, 3H), 5.86 (ddd, $J = 17.4, 10.2, 9.2$ Hz, 1H), 5.44 (s, 1H), 5.34 (dd, $J = 10.3, 1.9$ Hz, 1H), 5.08 (dd, $J = 17.4, 1.8$ Hz, 1H), 3.41 (d, $J = 9.1$ Hz, 1H), 2.16 (s, 1H), 1.72 (ddd, $J = 13.8, 11.4, 4.9$ Hz, 1H), 1.49 – 1.40 (m, 2H), 1.32 – 1.07 (m, 19H); ^{13}C NMR (101 MHz, CDCl_3) δ 143.2, 141.3, 134.6, 128.6, 128.4, 128.3, 128.1, 127.2, 126.7, 121.1, 82.4, 79.2, 32.3, 31.0, 26.8, 26.8, 26.2, 23.1, 22.5, 22.4, 19.5, 18.8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{28}\text{H}_{38}\text{O}_2\text{Na}^+$, 429.2769; found: 429.2768; $[\alpha]^{20}_{\text{D}} = -123.89^\circ$ (c 2.0, CHCl_3); 92:8 er; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 11.334 min (major), 13.326 min (minor).



<Peak Table>

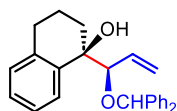
PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.243	1146869	38450	50.374	51.355
2	13.493	1129828	36420	49.626	48.645
Total		2276697	74870	100.000	100.000



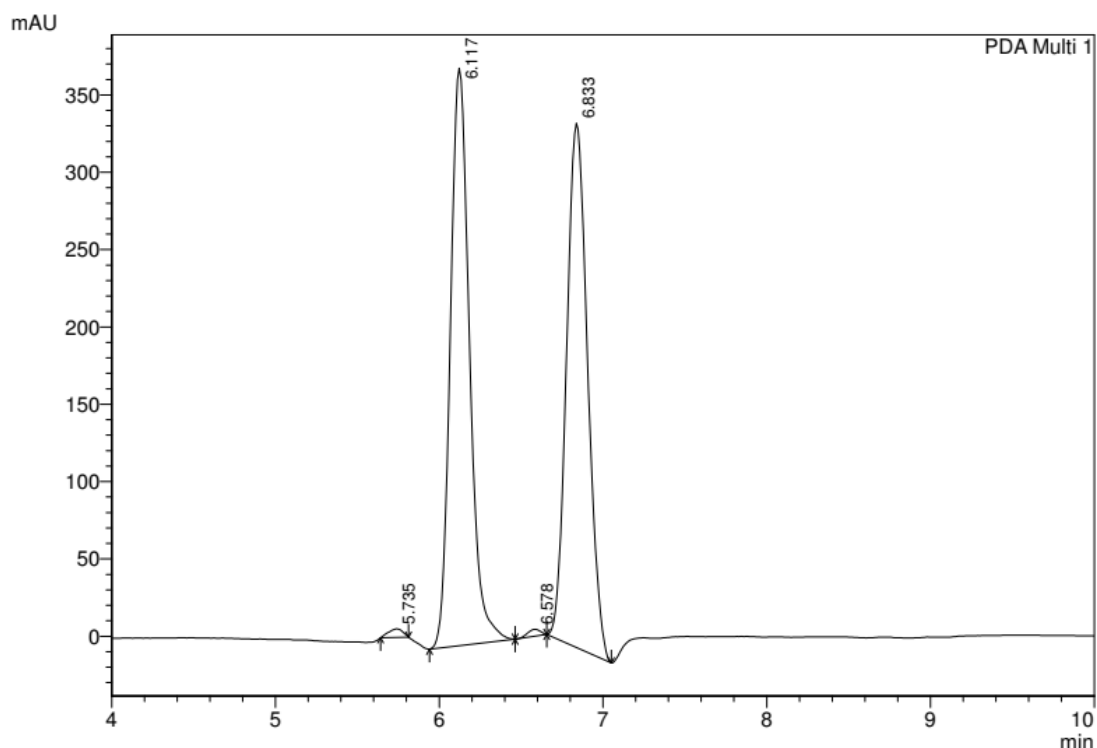
<Peak Table>

PDACh1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.334	2198702	64750	91.601	88.533
2	13.326	201593	8386	8.399	11.467
Total		2400295	73136	100.000	100.000

(*R*)-1-((*R*)-1-(Benzhydryloxy)allyl)-1,2,3,4-tetrahydronaphthalen-1-ol (3af):



Prepared according to the general procedure as described above in 81% yield (108 mg) with 9:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.2) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.43 – 7.22 (m, 9H), 7.20 – 7.02 (m, 5H), 5.64 (ddd, J = 17.7, 10.5, 7.4 Hz, 1H), 5.53 (s, 1H), 5.20 (d, J = 10.5 Hz, 1H), 5.05 (dd, J = 17.4, 0.7 Hz, 1H), 4.19 (d, J = 7.4 Hz, 1H), 2.78 – 2.72 (m, 1H), 2.63 – 2.53 (m, 1H), 2.17 – 2.08 (m, 1H), 2.04 – 1.95 (m, 1H), 1.83 – 1.73 (m, 2H); ^{13}C NMR (126 MHz, CDCl_3) δ 143.0, 141.4, 139.0, 138.0, 134.0, 129.0, 128.8, 128.4, 128.0, 127.7, 127.52, 127.3, 126.7, 125.8, 120.1, 84.2, 80.6, 74.1, 32.7, 29.7, 19.0; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{26}\text{H}_{26}\text{O}_2\text{Na}^+$, 393.1830; found: 393.1827; $[\alpha]^{20}_{\text{D}}$ = -36.91° (c 1.0, CHCl_3); 96:4 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IC-3 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 210 nm, Flow rate = 1 mL/min, Retention times: 6.230 min (minor), 6.981 min (major).

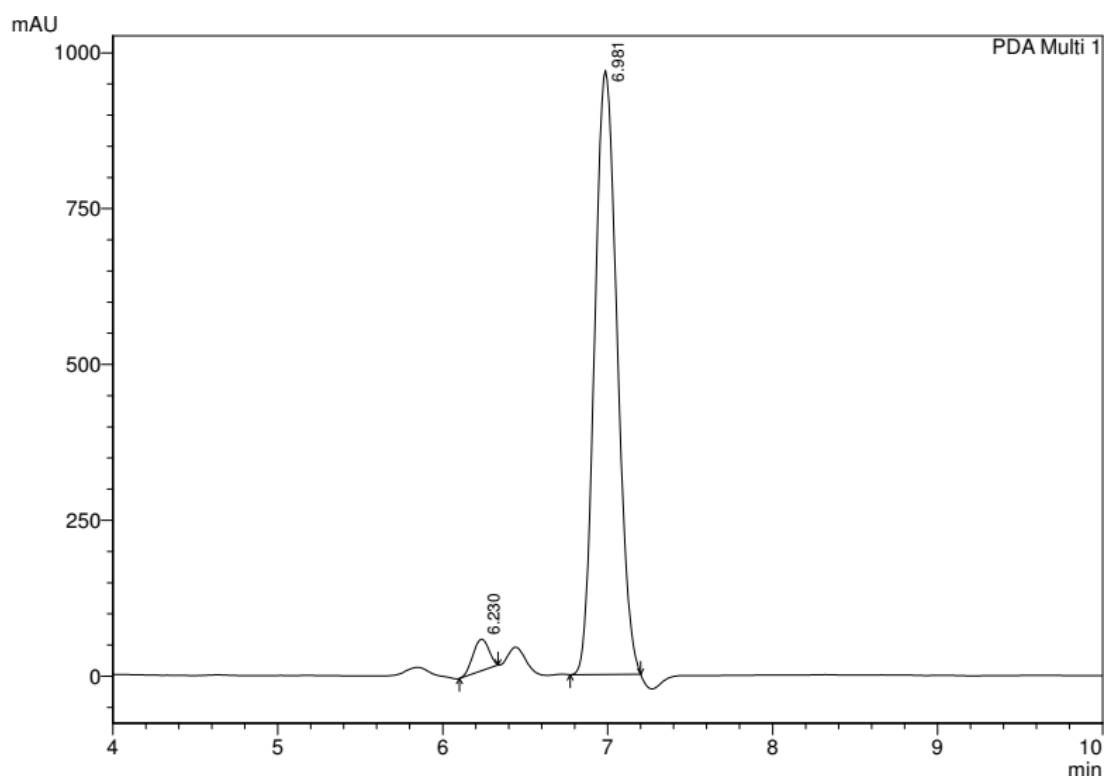


1 PDA Multi 1/210nm 4nm

PeakTable

PDA Ch1 210nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.735	34222	5511	0.560	0.763
2	6.117	3034324	373583	49.636	51.700
3	6.578	25075	4575	0.410	0.633
4	6.833	3019495	338935	49.394	46.905
Total		6113115	722604	100.000	100.000



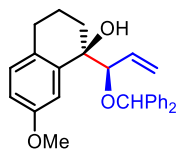
1 PDA Multi 1/210nm 4nm

PeakTable

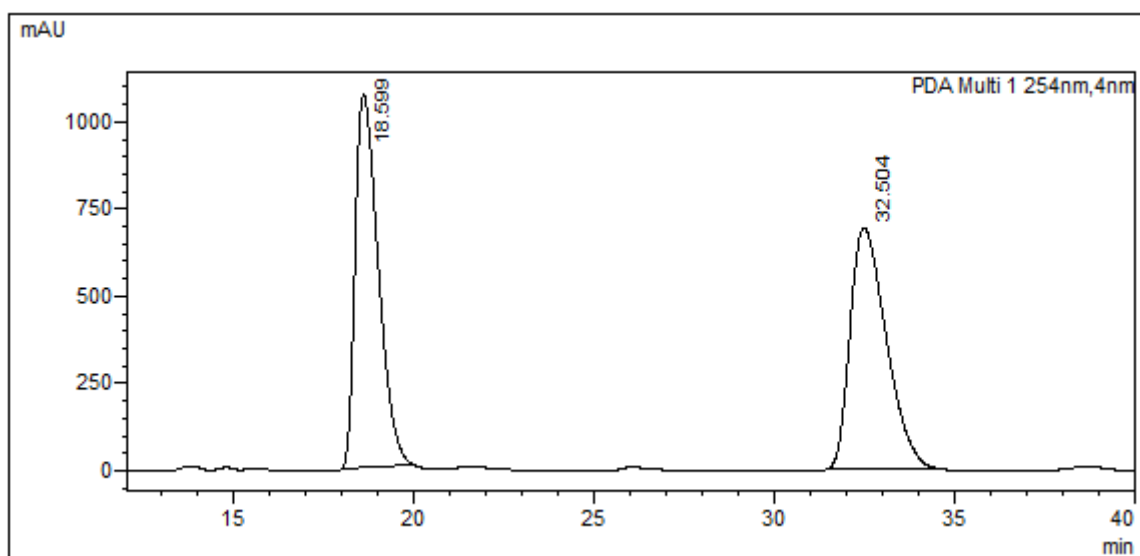
PDA Ch1 210nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.230	347143	51170	3.651	5.014
2	6.981	9160366	969317	96.349	94.986
Total		9507509	1020487	100.000	100.000

(R)-1-((R)-1-(Benzhydryloxy)allyl)-7-methoxy-1,2,3,4-tetrahydronaphthalen-1-ol (3ag):

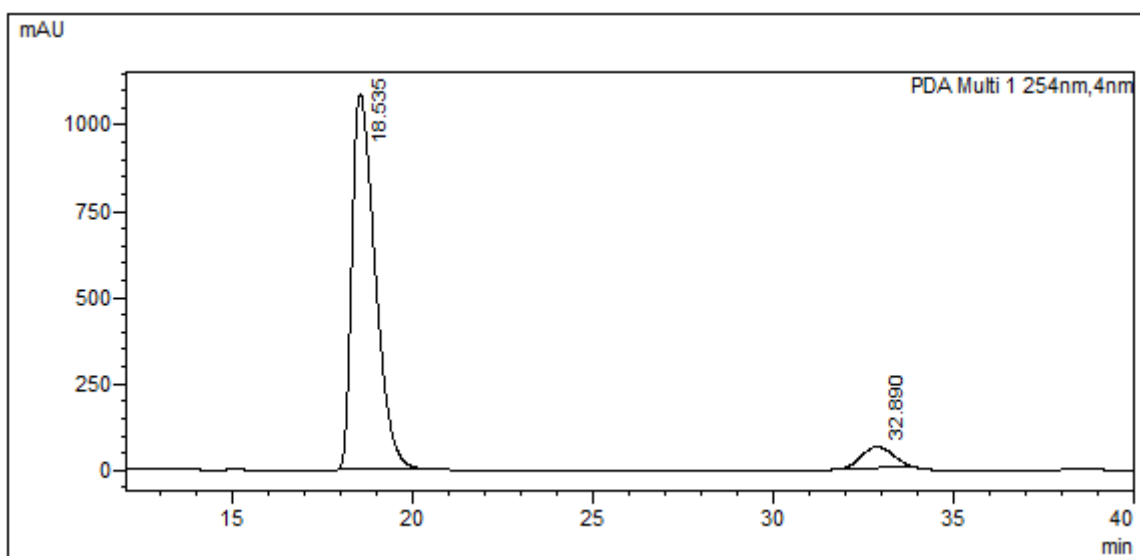


Prepared according to the general procedure as described above in 91% yield (121 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.4) to afford a colourless oil; ^1H NMR (300 MHz, CDCl_3) δ 7.33 – 7.12 (m, 8H), 7.11 – 7.03 (m, 2H), 6.93 – 6.87 (m, 2H), 6.68 (dd, J = 8.3, 2.8 Hz, 1H), 5.59 (ddd, J = 17.6, 10.5, 7.3 Hz, 1H), 5.44 (s, 1H), 5.14 (dd, J = 10.5, 0.9 Hz, 1H), 5.00 (dd, J = 17.3, 1.4 Hz, 1H), 4.08 (d, J = 7.3 Hz, 1H), 3.65 (s, 3H), 2.67 – 2.58 (m, 1H), 2.51 – 2.38 (m, 1H), 2.09 – 1.97 (m, 1H), 1.94 – 1.83 (m, 1H), 1.75 – 1.60 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 157.7, 143.0, 141.4, 140.1, 134.0, 130.2, 129.7, 128.7, 128.3, 128.0, 127.7, 127.3, 126.7, 120.0, 113.8, 112.4, 84.2, 80.8, 74.2, 55.4, 32.7, 28.8, 19.1; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{27}\text{H}_{28}\text{O}_3\text{Na}^+$, 423.1936; found: 423.1933; $[\alpha]^{20}_{\text{D}}$ = -29.25° (c 1.0, CHCl_3); 93:7 *er*; Daicel Chiralpak AD-H 250X4.6 mm 5 μ column connected to Daicel Chiralpak OD-H 250X4.6 mm 5 μ column in tandem; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 18.535 min (major), 32.890 min (minor).



<Peak Table>

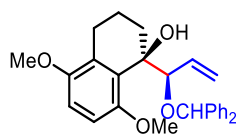
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	18.599	47878966	1072532	49.635	60.772
2	32.504	48582883	692316	50.365	39.228
Total		96461849	1764848	100.000	100.000



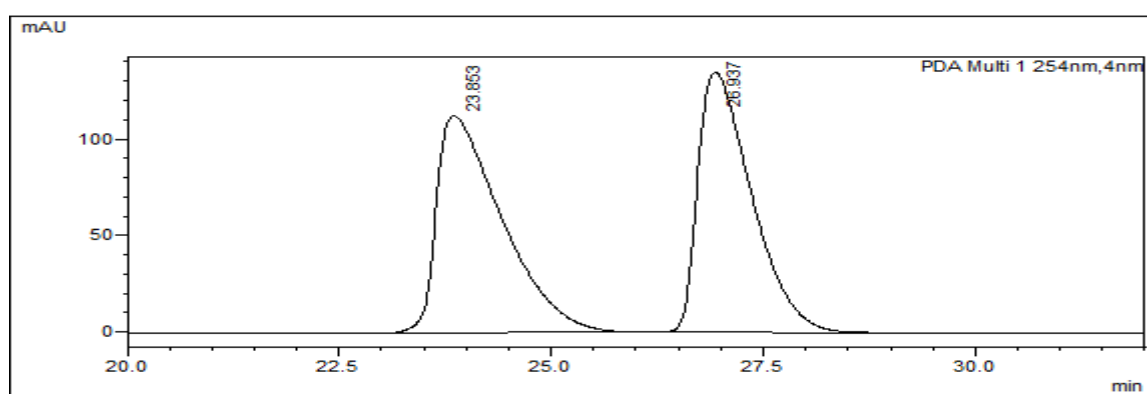
<Peak Table>

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	18.535	48693367	1086351	93.106	94.740
2	32.890	3605251	60320	6.894	5.260
Total		52298618	1146671	100.000	100.000

(R)-1-((R)-1-(Benzhydryloxy)allyl)-5,8-dimethoxy-1,2,3,4-tetrahydronaphthalen-1-ol (3ah):

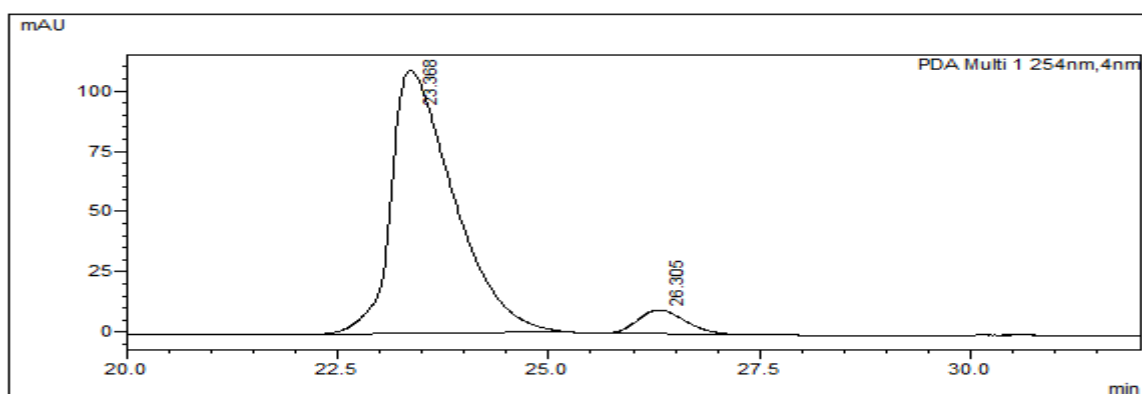


Prepared according to the general procedure as described above in 90% yield (140 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.28 – 6.93 (m, 8H), 6.67 – 6.57 (m, 3H), 6.39 (d, J = 8.9 Hz, 1H), 6.00 (ddd, J = 17.2, 10.5, 6.6 Hz, 1H), 5.32 (dd, J = 10.5, 1.0 Hz, 1H), 5.23 (ddd, J = 17.4, 3.5, 0.8 Hz, 1H), 5.13 (s, 1H), 4.37 (d, J = 6.6 Hz, 1H), 3.74 (s, 3H), 3.25 (s, 3H), 2.76 – 2.70 (m, 1H), 2.57 – 2.50 (m, 1H), 2.32 – 2.24 (m, 1H), 2.13 – 2.03 (m, 1H), 1.74 – 1.64 (m, 1H), 1.62 – 1.51 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 151.7, 151.6, 143.5, 142.2, 135.2, 130.6, 129.5, 128.3, 128.1, 127.8, 127.0, 126.8, 126.2, 119.0, 108.8, 108.2, 81.7, 80.4, 74.4, 56.1, 54.6, 32.2, 24.1, 19.0; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{28}\text{H}_{30}\text{O}_4\text{Na}^+$, 453.2041; found: 453.2036; $[\alpha]_D^{20} = -49.89^\circ$ (c 1.0, CHCl_3); 94:6 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column connected to Daicel Chiralpak OD-H 250X4.6 mm 5 μ column in tandem; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 23.368 min (major), 26.305 min (minor).



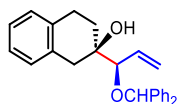
<Peak Table>

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	23.853	6050847	112453	50.470	45.497
2	26.937	5938117	134713	49.530	54.503
Total		11988964	247165	100.000	100.000

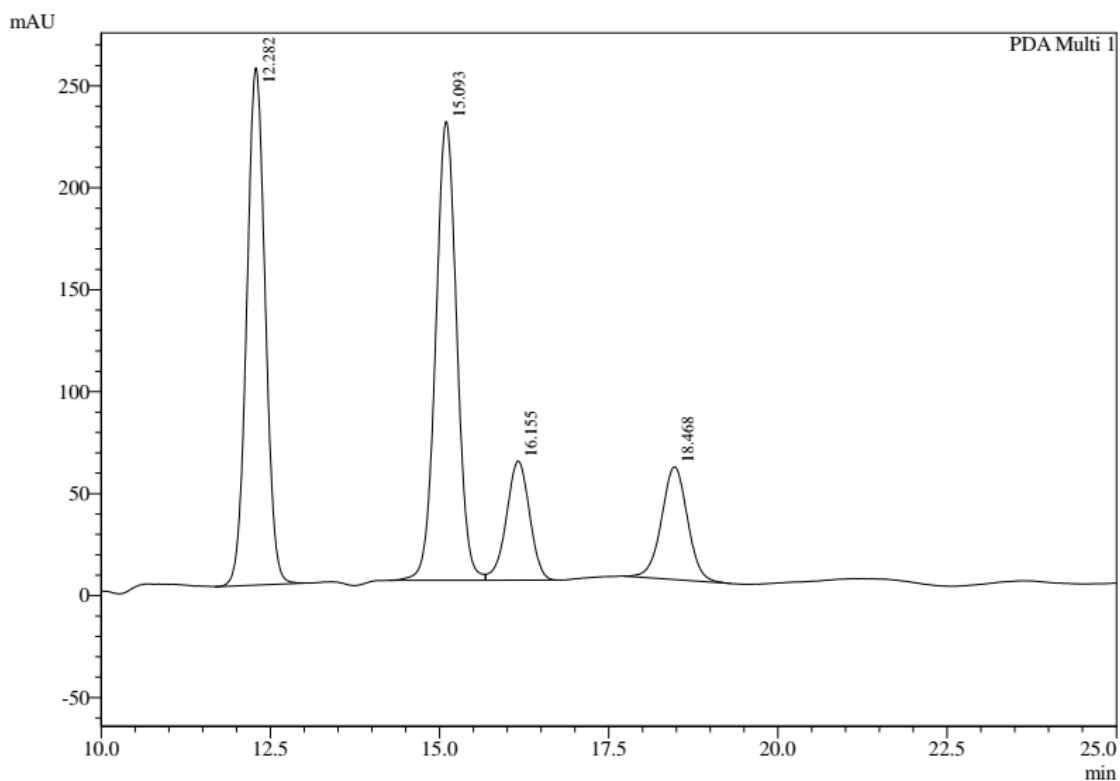


<Peak Table>					
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	23.368	5675209	109125	93.822	91.859
2	26.305	373677	9671	6.178	8.141
Total		6048886	118796	100.000	100.000

(S)-2-((R)-1-(Benzhydryloxy)allyl)-1,2,3,4-tetrahydronaphthalen-2-ol (3ai):



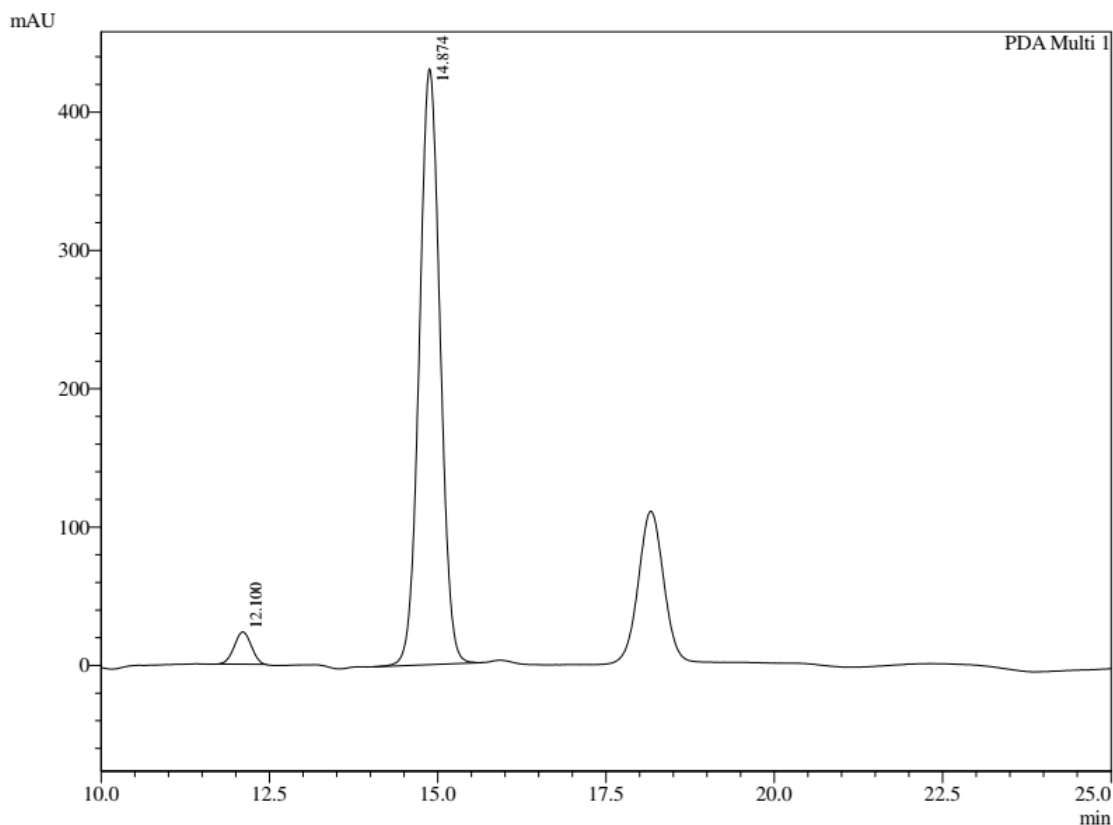
Prepared according to the general procedure as described above in 85% yield (113 mg) with 7:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.28 – 7.19 (m, 8H), 7.18 – 7.12 (m, 2H), 7.02 – 6.95 (m, 4H), 5.88 (ddd, J = 17.4, 10.3, 8.9 Hz, 1H), 5.46 (s, 1H), 5.37 (dd, J = 10.3, 1.6 Hz, 1H), 5.15 (ddd, J = 17.3, 1.6, 1.0 Hz, 1H), 3.57 (d, J = 8.8 Hz, 1H), 3.00 – 2.86 (m, 2H), 2.76 – 2.70 (m, 1H), 2.65 – 2.58 (m, 1H), 1.85 – 1.79 (m, 1H), 1.74 – 1.61 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 143.0, 141.0, 136.1, 134.4, 134.4, 129.7, 128.7, 128.6, 128.3, 128.0, 128.1, 127.3, 126.7, 125.8, 121.7, 83.6, 79.8, 72.6, 39.0, 30.1, 25.6; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{26}\text{H}_{26}\text{O}_2\text{Na}^+$, 393.1830; found: 393.1827; $[\alpha]_D^{20}$ = -75.89° (c 1.0, CHCl_3); 96:4 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column connected to Daicel Chiralpak IF 250X4.6 mm 5 μ column in tandem; hexane/2-propanol = 97/03, detected at 210 nm, Flow rate = 1 mL/min, Retention times: 12.100 min (minor), 14.874 min (major).



PeakTable

PDA Ch1 210nm 4nm

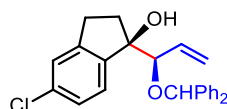
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.282	4809285	253733	38.298	42.816
2	15.093	4876349	225046	38.832	37.975
3	16.155	1390923	58463	11.076	9.865
4	18.468	1481027	55372	11.794	9.344
Total		12557584	592614	100.000	100.000



PeakTable

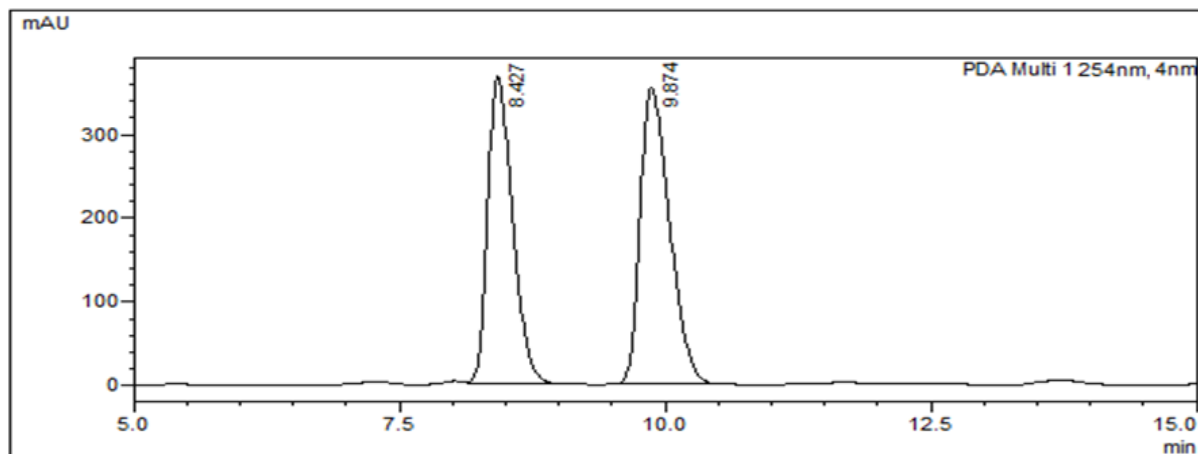
PDA Ch1 210nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.100	408927	23307	4.231	5.133
2	14.874	9257016	430750	95.769	94.867
Total		9665943	454057	100.000	100.000

(R)-1-((R)-1-(Benzhydryloxy)allyl)-5-chloro-2,3-dihydro-1H-inden-1-ol (3aj):

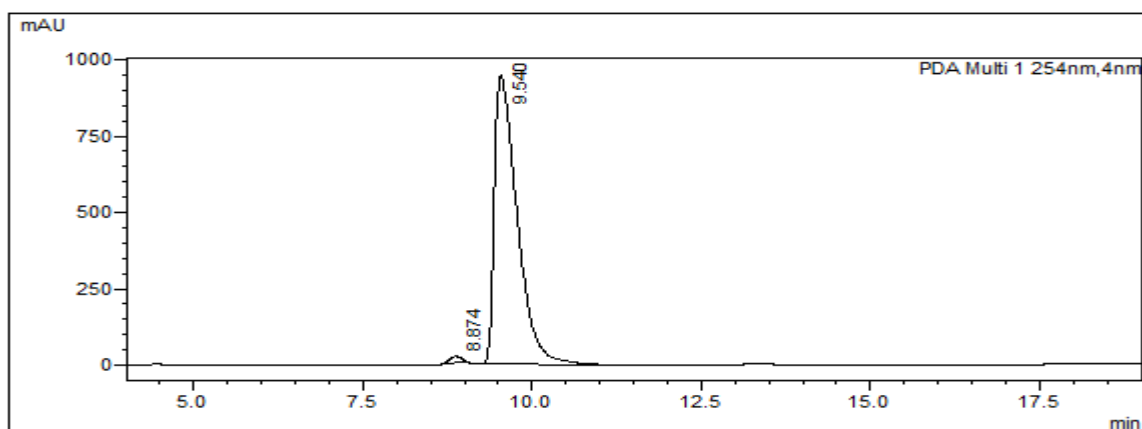
Prepared according to the general procedure as described above in 92% yield (129 mg) with >20:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.44 – 7.23 (m, 11H), 7.20 (d, J = 7.5 Hz, 2H), 5.84 – 5.72 (m, 1H), 5.57 (s, 1H), 5.31 (d, J = 10.4 Hz, 1H), 5.14 (dd, J = 17.3, 0.5 Hz, 1H), 3.96 (d, J = 8.0 Hz, 1H), 3.17 (s, 1H), 2.95 (ddd, J = 16.2, 9.2, 3.4 Hz, 1H), 2.78 – 2.70 (m, 1H), 2.56 – 2.48 (m, 1H), 2.18 – 2.05 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 146.0, 143.6, 142.7, 141.0, 134.2, 133.5, 128.8, 128.4, 128.1, 128.0, 127.3, 126.7, 126.6, 125.7, 125.0, 121.2, 84.5, 83.6, 80.3, 36.6,

30.0; HRMS (ESI) m/z : $[M+Na]^+$ calcd for $C_{25}H_{23}ClO_2Na^+$, 413.1284; found: 413.1277; $[\alpha]^{20}_D = -33.66^\circ$ (c 1.0, $CHCl_3$); 99:1 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IC 250X4.6 mm 5μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 8.874 min (minor), 9.540 min (major).



<Peak Table>

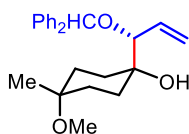
PDA Ch1 260nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	8.427	6027894	368519	47.138	50.981
2	9.874	6759851	354341	52.862	49.019
Total		12787745	722860	100.000	100.000



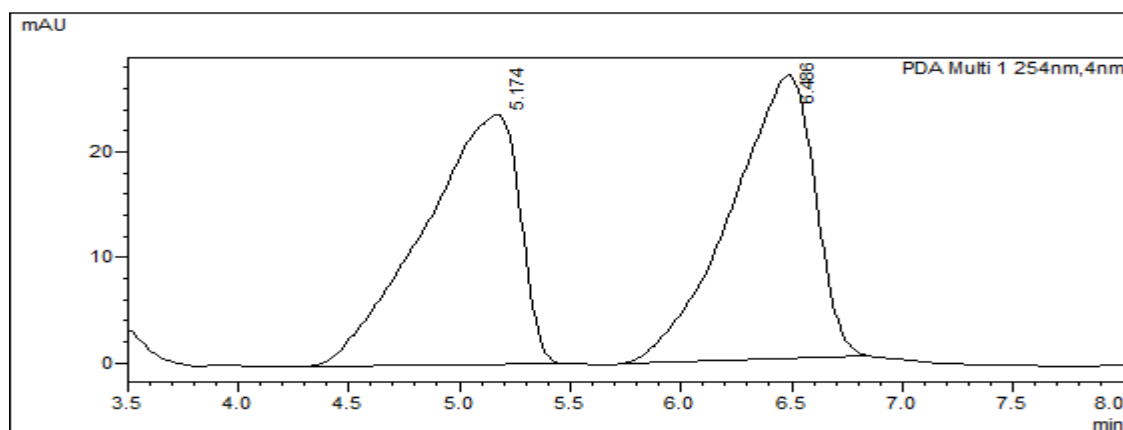
<Peak Table>

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	8.874	297381	22265	1.328	2.296
2	9.540	22101547	947268	98.672	97.704
Total		22398929	969533	100.000	100.000

(1*s*,4*S*)-1-((*R*)-1-(Benzhydryloxy)allyl)-4-methoxy-4-methylcyclohexan-1-ol (5a):

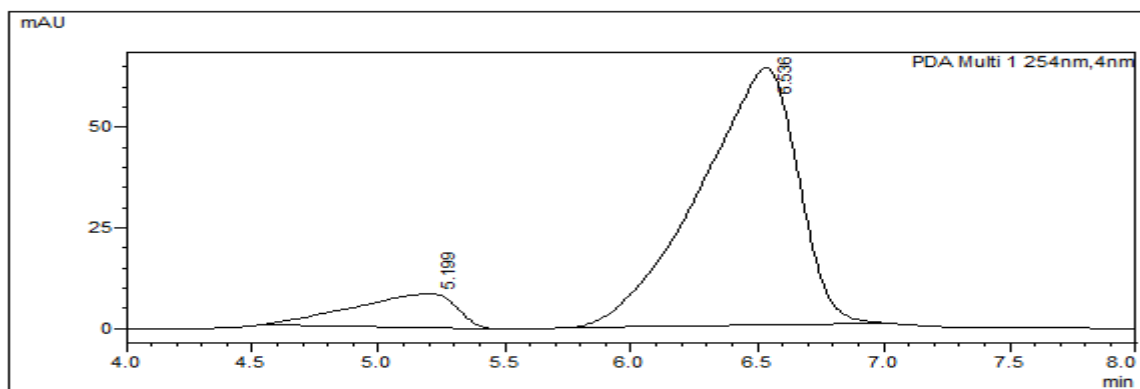


Prepared according to the general procedure as described above in 81% yield (107 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (500 MHz, CDCl_3) δ 7.33 – 7.17 (m, 9H), 7.16 – 7.11 (m, 1H), 5.83 (ddd, J = 17.5, 10.2, 8.7 Hz, 1H), 5.44 (s, 1H), 5.31 (dd, J = 10.3, 1.8 Hz, 1H), 5.08 (dd, J = 17.4, 1.5 Hz, 1H), 3.43 (d, J = 8.8 Hz, 1H), 3.04 (s, 3H), 1.58 – 1.54 (m, 5H), 1.51 – 1.34 (m, 3H), 1.04 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 143.1, 141.3, 134.6, 128.8, 128.3, 128.0, 128.0, 127.2, 126.7, 121.3, 85.1, 79.5, 72.8, 72.3, 48.8, 30.9, 30.4, 30.2, 28.3, 24.7; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{24}\text{H}_{30}\text{O}_3\text{Na}^+$, 389.2093; found: 389.2089; $[\alpha]^{20}_{\text{D}}$ = -101.87° (c 1.0, CHCl_3); 90:10 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IC 250X4.6 mm 5 μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 5.199 min (minor), 6.536 min (major).



<Peak Table>

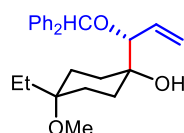
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.174	715746	23663	50.346	46.811
2	6.486	705908	26887	49.654	53.189
Total		1421654	50550	100.000	100.000



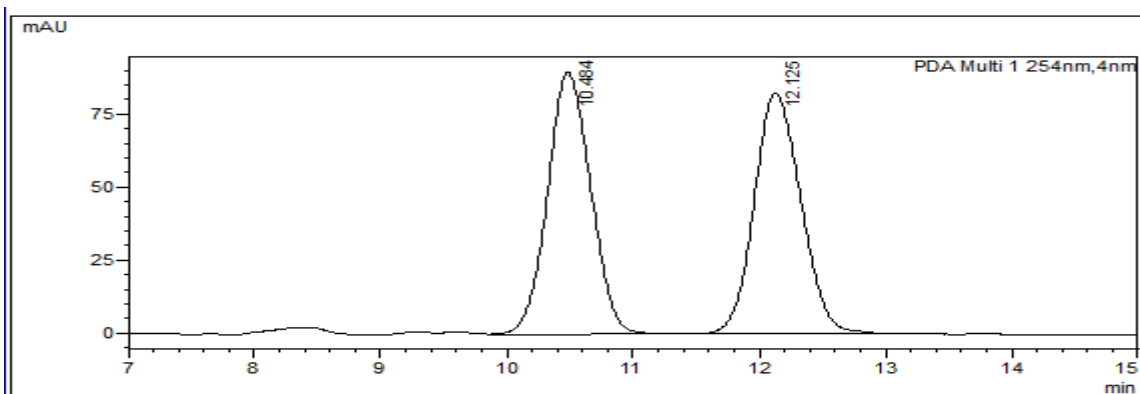
<Peak Table>

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.199	199375	7298	10.072	10.151
2	6.536	1780127	64593	89.928	89.849
Total		1979502	71891	100.000	100.000

(1*s*,4*S*)-1-((*R*)-1-(Benzhydryloxy)allyl)-4-ethyl-4-methoxycyclohexan-1-ol (5b):

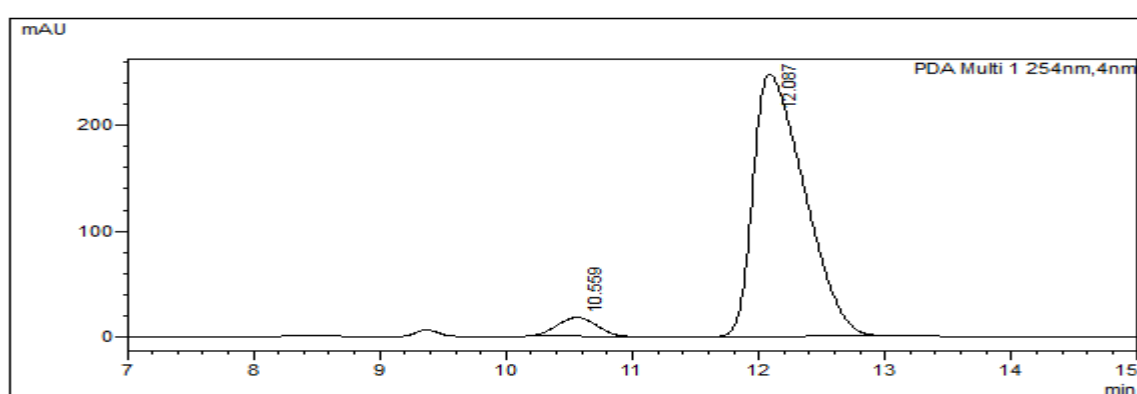


Prepared according to the general procedure as described above in 82% yield (112 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (500 MHz, CDCl_3) δ 7.16 – 7.11 (m, 9H), 6.67 – 6.60 (m, 1H), 5.82 (ddd, J = 17.4, 10.3, 8.9 Hz, 1H), 5.43 (s, 1H), 5.34 (dd, J = 10.3, 1.8 Hz, 1H), 5.10 (dd, J = 17.4, 1.5 Hz, 1H), 3.53 (d, J = 8.9 Hz, 1H), 3.05 (s, 3H), 1.69 – 1.51 (m, 5H), 1.41 – 1.26 (m, 3H), 1.24 – 1.15 (m, 1H), 1.08 – 1.00 (m, 1H), 0.68 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 143.0, 141.2, 134.5, 129.0, 128., 128.2, 1238.0, 127.2, 127.0, 121.1, 82.1, 79.5, 75.1, 73.0, 48.1, 31.1, 30.0, 29.1, 29.0, 26.0, 7.1; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{25}\text{H}_{32}\text{O}_3\text{Na}^+$, 403.2249; found: 403.2240; $[\alpha]^{20}_{\text{D}}$ = -94.12° (c 1.0, CHCl_3); 95:5 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 96/04, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 10.559 min (minor), 12.087 min (major).



<Peak Table>

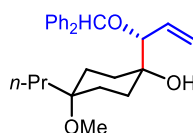
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.484	2142720	89836	50.170	52.073
2	12.125	2128170	82682	49.830	47.927
Total		4270890	172518	100.000	100.000



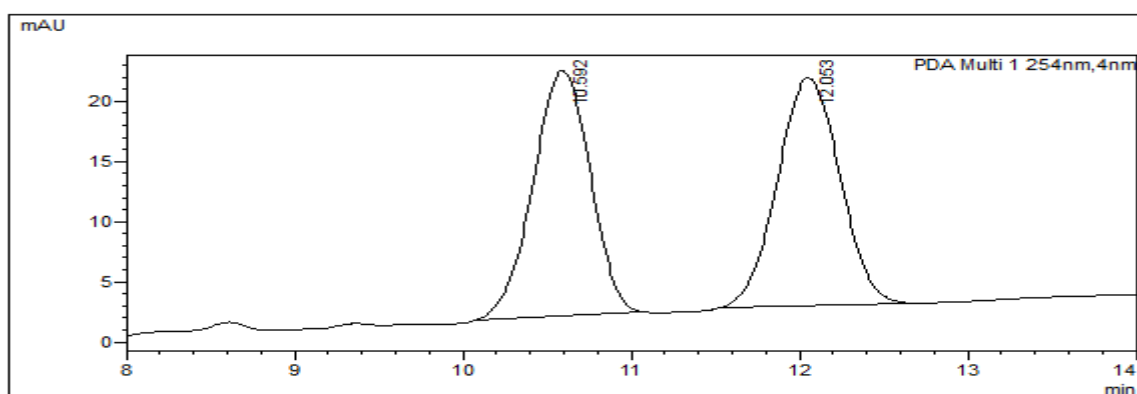
<Peak Table>

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.559	358880	17079	4.888	6.454
2	12.087	6983851	247561	95.112	93.546
Total		7342731	264641	100.000	100.000

(1*r*,4*S*)-1-((*R*)-1-(Benzhydryloxy)allyl)-4-methoxy-4-propylcyclohexan-1-ol (5c):

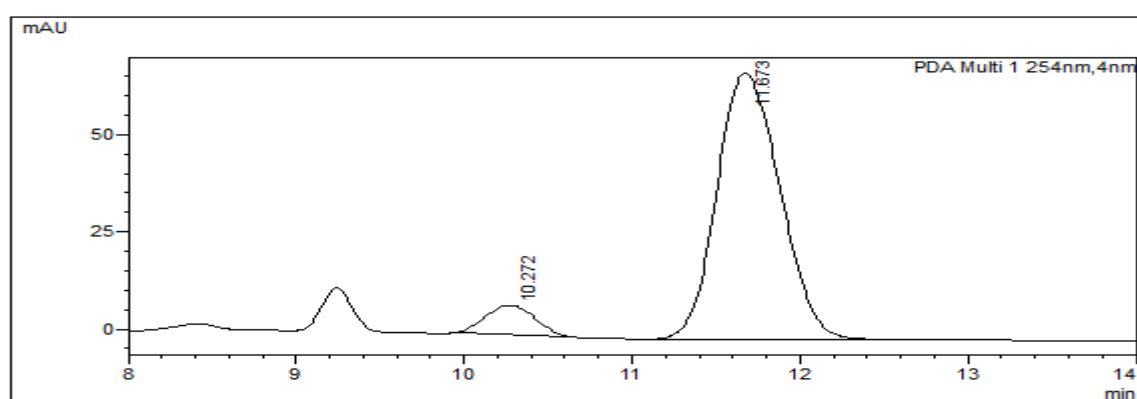


Prepared according to the general procedure as described above in 85% yield (121 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (500 MHz, CDCl_3) δ 7.17 – 7.06 (m, 9H), 7.06 – 6.98 (m, 1H), 5.68 (ddd, J = 17.4, 10.3, 8.9 Hz, 1H), 5.29 (s, 1H), 5.21 (dd, J = 10.3, 1.8 Hz, 1H), 4.96 (dd, J = 17.4, 1.5 Hz, 1H), 3.40 (d, J = 8.9 Hz, 1H), 2.92 (s, 3H), 1.55 – 1.37 (m, 6H), 1.20 (ddd, J = 13.5, 9.1, 4.0 Hz, 1H), 1.16 – 0.96 (m, 5H), 0.67 (t, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 143.0, 141.2, 134.5, 128.7, 128.3, 128.2, 128.0, 127.2, 126.6, 121.1, 82.0, 79.6, 75.0, 72.7, 48.1, 31.1, 29.7, 29.1, 29.0, 25.7, 7.1; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{26}\text{H}_{34}\text{O}_3\text{Na}^+$, 417.2406; found: 417.2397; $[\alpha]^{20}_{\text{D}}$ = -132.10° (c 1.0, CHCl_3); 93:7 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 96/04, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 10.272 min (minor), 11.673 min (major).



<Peak Table>

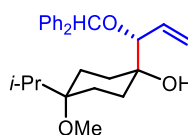
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.592	483066	20392	49.830	51.939
2	12.053	486361	18869	50.170	48.061
Total		969427	39260	100.000	100.000



<Peak Table>

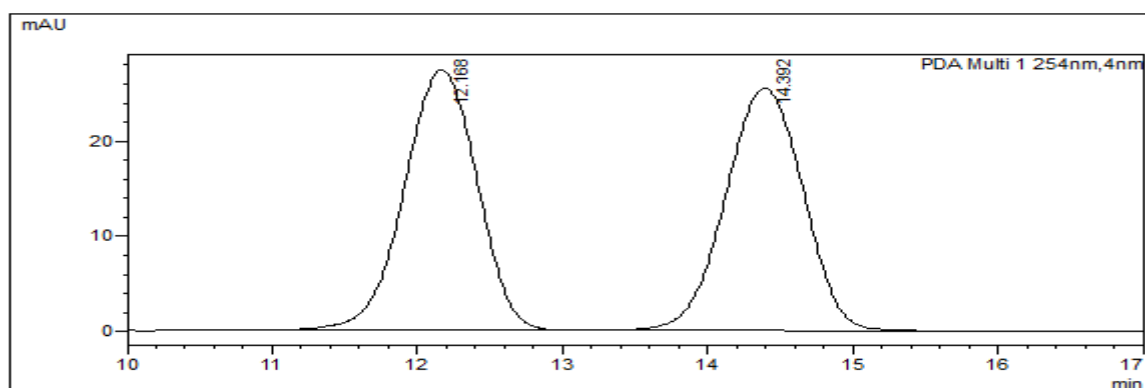
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.272	124495	6714	6.517	8.945
2	11.673	1785815	68350	93.483	91.055
Total		1910310	75064	100.000	100.000

(1*s*,4*S*)-1-((*R*)-1-(Benzhydryloxy)allyl)-4-isopropyl-4-methoxycyclohexan-1-ol (**5d**):



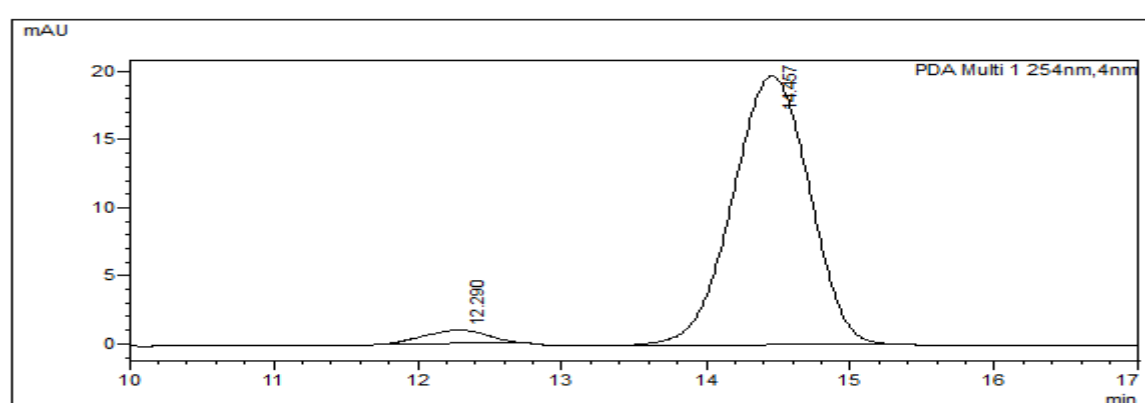
Prepared according to the general procedure as described above in 89% yield (126 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a white solid; mp= 150-152°C; ^1H MR (400 MHz, CDCl_3) δ 7.30 – 7.19 (m, 9H), 7.19 – 7.12 (m, 1H), 5.88 (ddd, J = 17.4, 10.2, 9.0 Hz, 1H), 5.42 (s, 1H), 5.36 (dd, J = 10.2, 1.9 Hz, 1H), 5.10 (dd, J = 17.4, 1.7 Hz, 1H), 3.61 (d, J = 8.9 Hz, 1H), 3.00 (s, 3H), 1.91 – 1.84 (m, 1H), 1.72-1.65 (m, 1H), 1.62 – 1.50 (m, 2H), 1.46 – 1.26 (m, 3H), 1.06 – 0.97 (m, 1H), 0.76-0.69 (m, 1H), 0.57 (t, J = 7.1 Hz, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 142.8, 141.2, 134.3, 128.7, 128.6, 128.3, 128.1, 127.2, 126.6, 120.8, 79.5, 78.6, 76.3, 73.2, 47.6, 30.7, 30.5, 29.3, 25.4, 25.0, 17.1, 17.0; HRMS (ESI) m/z :

$[M+Na]^+$ calcd for $C_{26}H_{34}O_3Na^+$, 417.2406; found: 417.2408; $[\alpha]^{20}_D = -126.43^\circ$ (c 1.0, $CHCl_3$); 96:4 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IC 250X4.6 mm 5μ column; hexane/2-propanol = 98/02, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 12.290 min (minor), 14.457 min (major).



<Peak Table>

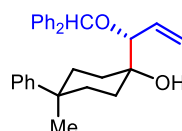
Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.168	954910	27336	50.232	51.815
2	14.392	946075	25420	49.768	48.185
Total		1900985	52756	100.000	100.000



<Peak Table>

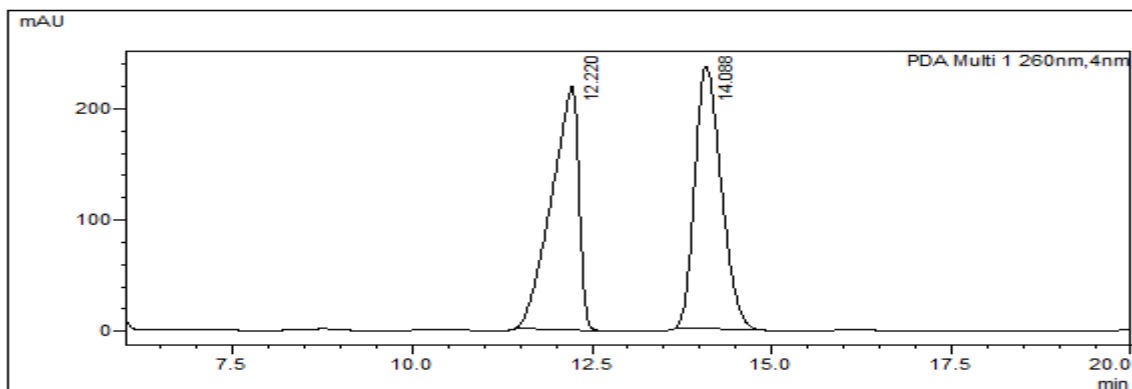
Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.290	27466	946	3.621	4.574
2	14.457	731050	19740	96.379	95.426
Total		758516	20686	100.000	100.000

(1*r*,4*R*)-1-((*R*)-1-(Benzhydryloxy)allyl)-4-methyl-4-phenylcyclohexan-1-ol (5e):



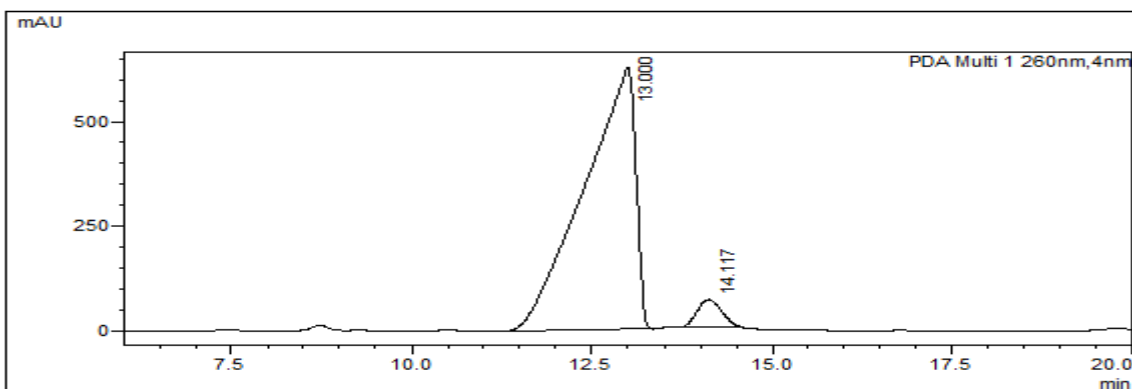
Prepared according to the general procedure as described above in 85% yield (126 mg) with >20:1 *dr*. It was purified by flash chromatography (10% EtOAc/hexanes; $R_f = 0.3$) to afford a colourless oil; 1H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.20 (m, 13H), 7.18 – 7.07 (m, 2H), 5.83 (ddd, $J = 17.4, 10.3, 8.8$ Hz, 1H), 5.46 (s, 1H), 5.36 (dd, $J = 10.3, 1.8$ Hz, 1H), 5.14 (dd, $J = 17.4, 1.5$ Hz, 1H), 3.52 (d, $J = 8.7$ Hz, 1H), 2.08 – 1.86 (m, 2H), 1.67 –

1.58 (m, 2H), 1.58 – 1.41 (m, 4H), 1.11 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 151.5, 143.1, 141.3, 135.1, 129.0, 128.3, 128.3, 128.1, 127.3, 127.0, 125.6, 126.0, 121.3, 84.5, 79.6, 72.4, 37.0, 33.0, 32.6, 31.0, 29.3, 25.0; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{29}\text{H}_{32}\text{O}_2\text{Na}^+$, 435.2300; found: 435.2292; $[\alpha]^{20}_{\text{D}} = -133.95^\circ$ (c 1.0, CHCl_3); 95:5 er; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5μ column; hexane/2-propanol = 98/02, detected at 260 nm, Flow rate = 1 mL/min, Retention times: 13.000 min (major), 14.117 min (minor).



<Peak Table>

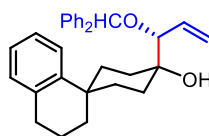
PDACH1 260nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.220	5824872	218899	49.029	48.152
2	14.088	6055543	235703	50.971	51.848
Total		11880415	454602	100.000	100.000



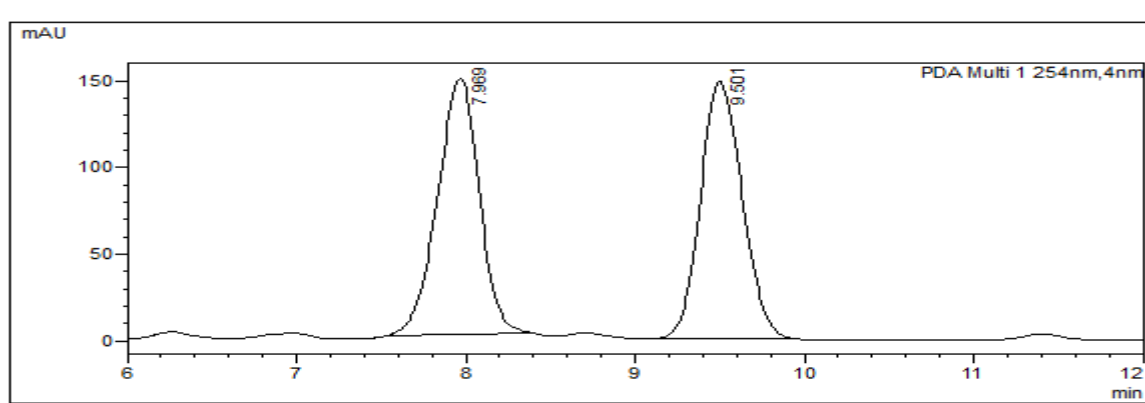
<Peak Table>

PDACH1 260nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.000	30786983	623042	95.244	90.488
2	14.117	1537176	65492	4.756	9.512
Total		32324159	688534	100.000	100.000

(1*R*,4*s*)-4-((*R*)-1-(Benzhydryloxy)allyl)-3',4'-dihydro-2'*H*-spiro[cyclohexane-1,1'-naphthalen]-4-ol (5f) :

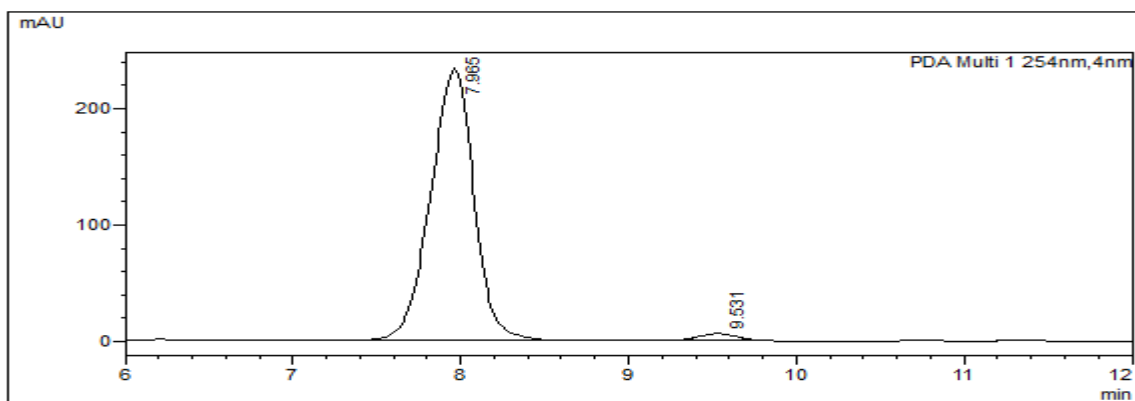


Prepared according to the general procedure as described above in 81% yield (128 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; R_f = 0.3) to afford a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.36 – 7.20 (m, 9H), 7.20 – 7.11 (m, 1H), 6.99 – 6.89 (m, 3H), 6.53 – 6.48 (m, 1H), 5.93 (ddd, J = 17.4, 10.1, 8.8 Hz, 1H), 5.52 (s, 1H), 5.42 (dd, J = 10.3, 1.7 Hz, 1H), 5.22 (dd, J = 17.4, 1.4 Hz, 1H), 4.00 (d, J = 8.9 Hz, 1H), 2.62 (t, J = 6.1 Hz, 2H), 2.46 (s, 1H), 2.13 (d, J = 13.1 Hz, 1H), 1.88 – 1.76 (m, 1H), 1.72 – 1.48 (m, 6H), 1.41 – 1.29 (m, 2H), 1.28 – 1.15 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 145.4, 143.0, 141.1, 137.5, 134.0, 129.1, 129.0, 129.1, 128.3, 127.3, 127.1, 126.5, 126.1, 125.3, 121.2, 80.0, 78.0, 73.5, 36.1, 35.3, 35.0, 32.1, 31.2, 31.1, 30.2, 19.4; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{31}\text{H}_{34}\text{O}_2\text{Na}^+$, 461.2457; found: 461.2449; $[\alpha]_D^{20}$ = -98.89° (c 1.0, CHCl_3); 98:2 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5 μ column; hexane/2-propanol = 95/05, detected at 254 nm, Flow rate = 1 mL/min, Retention times: 7.965 min (major), 9.531 min (minor).



<Peak Table>

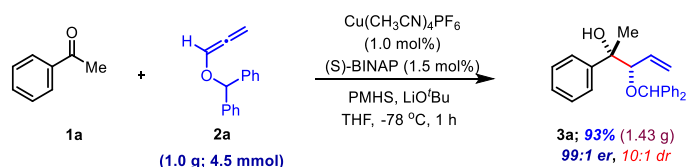
PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.969	2539523	147885	49.932	49.851
2	9.501	2546395	148772	50.068	50.149
Total		5085918	296656	100.000	100.000



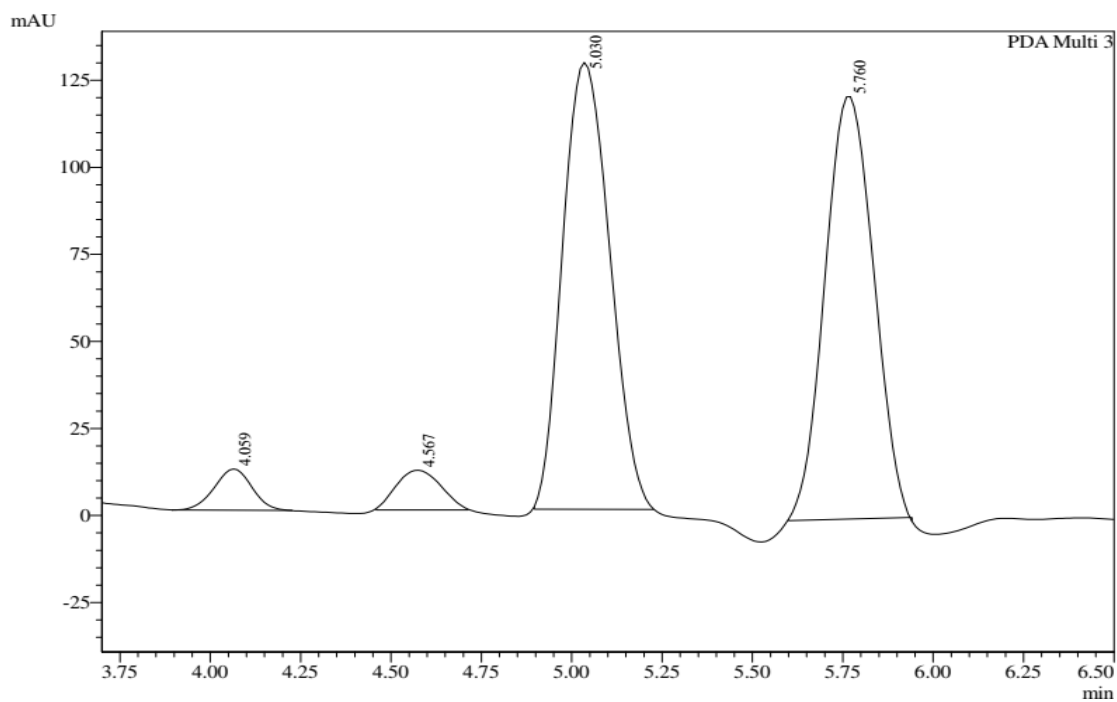
<Peak Table>

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.965	4177225	233381	97.934	97.624
2	9.531	88134	5681	2.066	2.376
Total		4265358	239061	100.000	100.000

2e. Gram-scale synthesis



A solution of $\text{Cu}(\text{CH}_3\text{CN})_4\text{PF}_6$ (16 mg, 1.0 mol%), (S)-BINAP (42 mg, 1.5 mol%), PMHS (1.2 ml, 9.0 mmol) and LiO^tBu (9 ml, 9.0 mmol, 1 M in THF) in dry THF (5.0 mL) was stirred at room temperature for 10 min and then maintained the temperature at $-78\text{ }^\circ\text{C}$. A solution of acetophenone **1a** (0.54 g, 4.5 mmol, 1.0 equiv) and allene **2a** (1.0 g, 4.5 mmol, 1.0 equiv) in dry THF (10.0 mL) was added *via* syringe and the resulting mixture was stirred at $-78\text{ }^\circ\text{C}$ for 1 h. The reaction mixture was quenched with saturated NH_4Cl (20 mL) solution and extracted with EtOAc ($3 \times 30\text{ mL}$) and dried over anhydrous Na_2SO_4 , filtered, and concentrated *in vacuo*. The resultant crude product was purified by column chromatography (10% EtOAc/hexanes; $R_f = 0.3$) to afford syn-diol product as a colourless oil in 93% yield (2.66 g) with 10:1 *dr*; 97:3 *er*; Chiral HPLC analysis of the product: Daicel Chiralpak IC-3 250X4.6 mm 5μ column connected to Daicel Chiralpak AD-H 250X4.6 mm 5μ column in tandem; hexane/2-propanol = 95/05, detected at 230 nm, Flow rate = 1 mL/min, Retention times: 5.061 min (minor), 5.779 min (major).

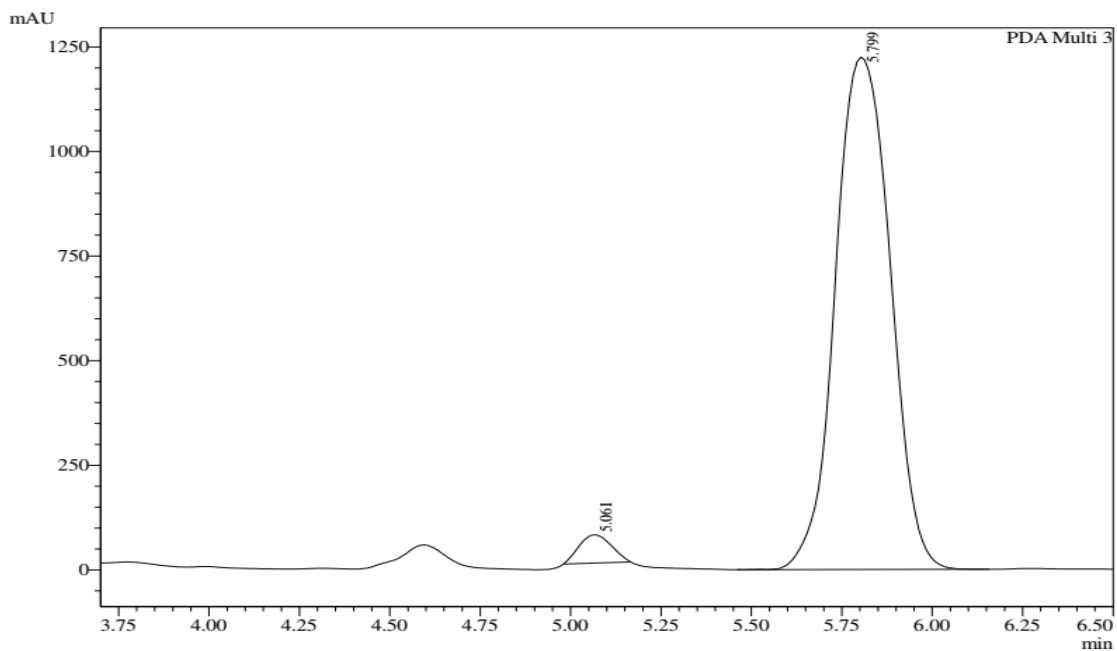


1 PDA Multi 3 / 230nm 4nm

PeakTable

PDA Ch3 230nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.059	85691	11861	3.447	4.345
2	4.567	97719	11400	3.930	4.176
3	5.030	1165568	128347	46.880	47.014
4	5.760	1137285	121387	45.743	44.465
Total		2486264	272996	100.000	100.000



1 PDA Multi 3 / 230nm 4nm

PeakTable

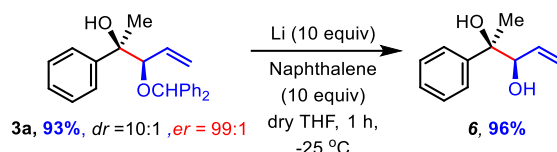
PDA Ch3 230nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.061	418435	67651	3.122	5.233
2	5.799	12984763	1225082	96.878	94.767
Total		13403198	1292733	100.000	100.000

2f. Synthetic Utility:

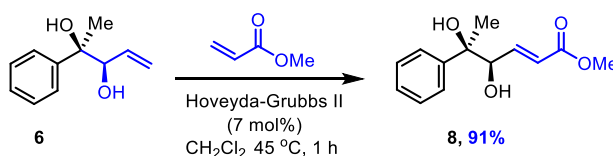
I. Synthesis of g-lactone:⁷

(2*R*,3*R*)-2-phenylpent-4-ene-2,3-diol (**6**):



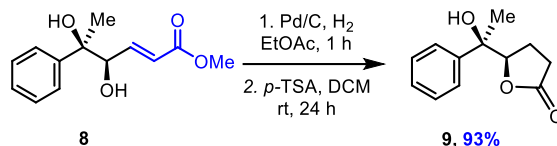
Naphthalene (1.3 g, 10.02 mmol) was dissolved in THF (8 mL), to which was added finely cut pieces of lithium metal (71.0 mg, 10.14 mmol). The reaction mixture was stirred for 1.5 h at rt under an argon atmosphere at which point the lithium metal was completely dissolved. This resulting greenish black solution was cooled to -25 °C, and a solution of **3a** (350.0 mg, 1.02 mmol) in THF (4 mL) was added to this solution dropwise. The resulting mixture was then stirred at -25 °C until the reaction mixture turned into a colourless solution, after which it was quenched with saturated aq. NH₄Cl (10 mL) and water (10 mL). The resulting solution was extracted with EtOAc (3 x 15 mL), the combined organic layer was washed with brine, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product (20% EtOAc/hexanes; *R_f* = 0.2) was purified by column chromatography using hexanes/EtOAc (4:1) to afford **6** (172 mg, 96%) as a pale liquid; ¹H NMR (400 MHz, CDCl₃) δ 7.51 – 7.45 (m, 2H), 7.37 (ddd, *J* = 7.8, 5.3, 1.2 Hz, 2H), 7.28 (ddd, *J* = 7.6, 4.0, 1.4 Hz, 1H), 5.87 (ddd, *J* = 17.0, 10.5, 6.3 Hz, 1H), 5.27 (ddt, *J* = 15.6, 10.6, 1.4 Hz, 2H), 4.28 (d, *J* = 6.2 Hz, 1H), 2.69 (s, 1H), 2.14 (s, 1H), 1.48 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.2, 135.6, 128.4, 127.4, 125.7, 118.24, 79.6, 76.4, 24.3; HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₁₁H₁₅O₂⁺, 179.1072; found: 179.1073; [α]_D²⁰ = +28.37° (c 0.12, CHCl₃).

Methyl (4*R*,5*R*, *E*)-4,5-dihydroxy-5-phenylhex-2-enoate (**8**):⁸



The diol **6** (100.0 mg, 0.56 mmol) was dissolved in dry CH₂Cl₂ (12.0 mL; degassed 10 min with Ar) in round-bottom flask, and methyl acrylate (76 μL, 73 mg, 0.84 mmol) was added followed by Hoveyda-Grubbs II catalyst (17.6 mg, 0.028 mmol). The reaction mixture was heated to 45 °C for 1h. The completion of reaction was then monitored by TLC, after which the reaction mixture was concentrated under reduced pressure and purified using flash column chromatography (20% EtOAc/hexanes *R_f* = 0.2) providing α,β-unsaturated ester **8** (120.6 mg, 91%) as a clear oil; ¹H NMR (400 MHz, CDCl₃) δ 7.47 (ddd, *J* = 4.4, 3.4, 1.9 Hz, 2H), 7.41 – 7.35 (m, 2H), 7.33 – 7.28 (m, 1H), 6.86 (dd, *J* = 15.7, 4.8 Hz, 1H), 6.09 (dd, *J* = 15.7, 1.7 Hz, 1H), 4.57 – 4.36 (m, 1H), 3.73 (s, 3H), 2.53 (d, *J* = 40.1 Hz, 2H), 1.53 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 166.7, 144.9, 144.3, 128.6, 127.7, 125.6, 122.7, 51.7, 23.6; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₃H₁₆O₄Na⁺, 259.0946; found: 259.0935; [α]_D²⁰ = +63.33° (c 0.15, CHCl₃).

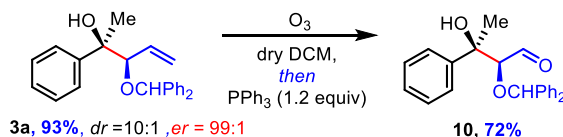
(R)-5-((R)-1-Hydroxy-1-phenylethyl)dihydrofuran-2(3H)-one (9):



The α , β -unsaturated ester **8** (75.0 mg, 0.32 mmol) was dissolved in 3 mL of ethyl acetate in a round-bottom flask and Pd/C (3.4 mg, 0.1 equiv) was added to mixture under argon atmosphere. The argon atmosphere was then replaced with hydrogen-filled bladder and the reaction mixture was stirred for 1 h. The reaction was monitored by TLC analysis, after which, the reaction mixture was filtered through a pad of celite and concentrated under reduced pressure. The crude reduction product was dissolved in 3 mL of CH₂Cl₂ and a catalytic amount of *p*-TSA was added to the reaction mixture and was left to stir for another 24 h under nitrogen atmosphere. Later, a saturated aqueous solution of NH₄Cl (10 mL) was added to the reaction mixture, combined organic layer washed with brine and concentrated under reduced pressure. The crude product was purified by column chromatography using hexanes/EtOAc (4 : 1) to afford **9** in 93% yield (61.0 mg) as a colourless oil; (20% EtOAc/hexanes, *R_f* = 0.2); ¹H NMR (500 MHz, CDCl₃) δ 7.52 – 7.44 (m, 2H), 7.40 – 7.33 (m, 2H), 7.33 – 7.27 (m, 1H), 4.71 (dd, *J* = 8.3, 6.0 Hz, 1H), 2.44 – 2.34 (m, 1H), 2.28 (s, 1H), 2.24 – 2.10 (m, 3H), 1.60 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 177.2, 143.2, 128.6, 127.8, 125.6, 85.5, 74.8, 28.6, 25.6, 22.6; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₂H₁₄O₃Na⁺, 229.0841; found: 229.0834; [α]_D²⁰ = +12.72° (c 0.12, CHCl₃).

II. Ozonolysis of product 3a:

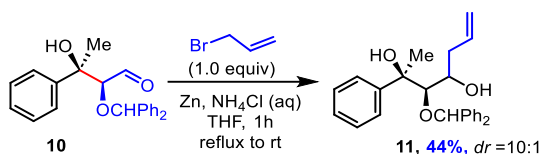
(2S,3R)-2-(Benzhydryloxy)-3-hydroxy-3-phenylbutanal (10):



The diol **3a** (100 mg, 0.29 mmol) was dissolved in 3 mL of dry CH₂Cl₂ under nitrogen atmosphere and subjected to ozone atmosphere for 5 mins. The completion of the reaction was indicated by persistent blue colour of reaction mixture after which PPh₃ (92.3 mg, 0.35 mmol) was added and stirred for 4 h. To the reaction mixture was then added 5 mL of saturated aqueous NH₄Cl solution and extracted with CH₂Cl₂ (3 x 10 mL), combined organic layer was washed with brine (10 mL) and concentrated under reduced pressure. The crude product was purified by column chromatography using hexanes/EtOAc (5 : 1) to afford compound **10** (72.4 mg, 72 %) as a colourless oil; ¹H NMR (500 MHz, CDCl₃) δ 9.66 (dd, *J* = 2.9, 0.8 Hz, 1H), 7.38 (dt, *J* = 15.1, 4.5 Hz, 4H), 7.33 – 7.27 (m, 3H), 7.27 – 7.20 (m, 6H), 6.96 (d, *J* = 7.6 Hz, 2H), 5.33 (s, 1H), 3.92 (dd, *J* = 2.8, 0.9 Hz, 1H), 3.19 (s, 1H), 1.54 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 203.1, 144.6, 141.1, 139.8, 128.5, 128.5, 128.4, 128.0, 128.0, 127.5, 127.4, 127.1, 125.2, 87.1, 83.8, 25.8; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₂₃H₂₂O₃Na⁺, 369.1467; found: 369.1450; [α]_D²⁰ = +90.91° (c 0.19, CHCl₃).

III. Barbier-allylation reaction:⁹

(2*R*,3*R*)-3-(Benzhydryloxy)-2-phenylhept-6-ene-2,4-diol (**11**):



The aldehyde **10** (50 mg, 0.15 mmol) and activated zinc powder (14 mg, 0.22 mmol) were dissolved in a saturated aqueous NH_4Cl solution (2 mL) and THF (1 mL). The reaction mixture was refluxed and allyl bromide (19 μL , 26 mg, 0.22 mmol) was added dropwise and reaction was stirred at rt for 1 h followed by quenching of the reaction using 10% aqueous HCl (5 mL). The reaction mixture was extracted with ether (3 x 10 mL), washed with brine (10 mL), dried over Na_2SO_4 , and concentrated under reduced pressure. The crude product was purified by column chromatography using hexanes/EtOAc (4 : 1) to afford **11** in 44 % yield (25 mg) as a white semi-solid; ^1H NMR (400 MHz, CDCl_3) δ 7.45 – 7.35 (m, 2H), 7.35 – 7.12 (m, 13H), 5.43 – 5.29 (m, 1H), 5.13 (s, 1H), 4.95 – 4.79 (m, 1H), 4.75 – 4.61 (m, 1H), 3.81 – 3.70 (m, 1H), 3.68 (d, J = 1.7 Hz, 1H), 3.10 (s, 1H), 2.76 (s, 1H), 2.05 – 1.67 (m, 2H), 1.65 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 146.0, 142.3, 141.7, 134.8, 128.6, 128.4, 128.4, 128.3, 128.2, 127.4, 127.3, 126.6, 125.7, 117.4, 84.3, 82.7, 70.5, 39.8, 29.9, 26.1; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{26}\text{H}_{28}\text{O}_3\text{Na}^+$, 411.1936; found: 411.1928; $[\alpha]^{20}_{\text{D}} = +48.87^\circ$ (c 0.21, CHCl_3).

2g. Determination of absolute stereochemistry via Mosher ester analysis:

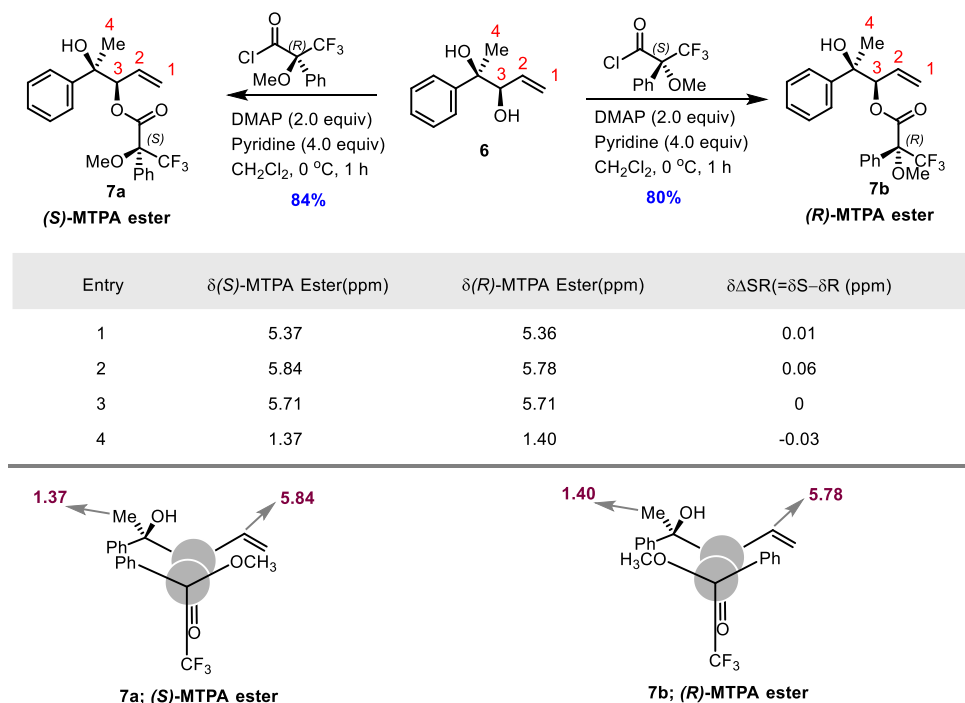
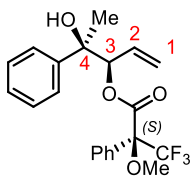


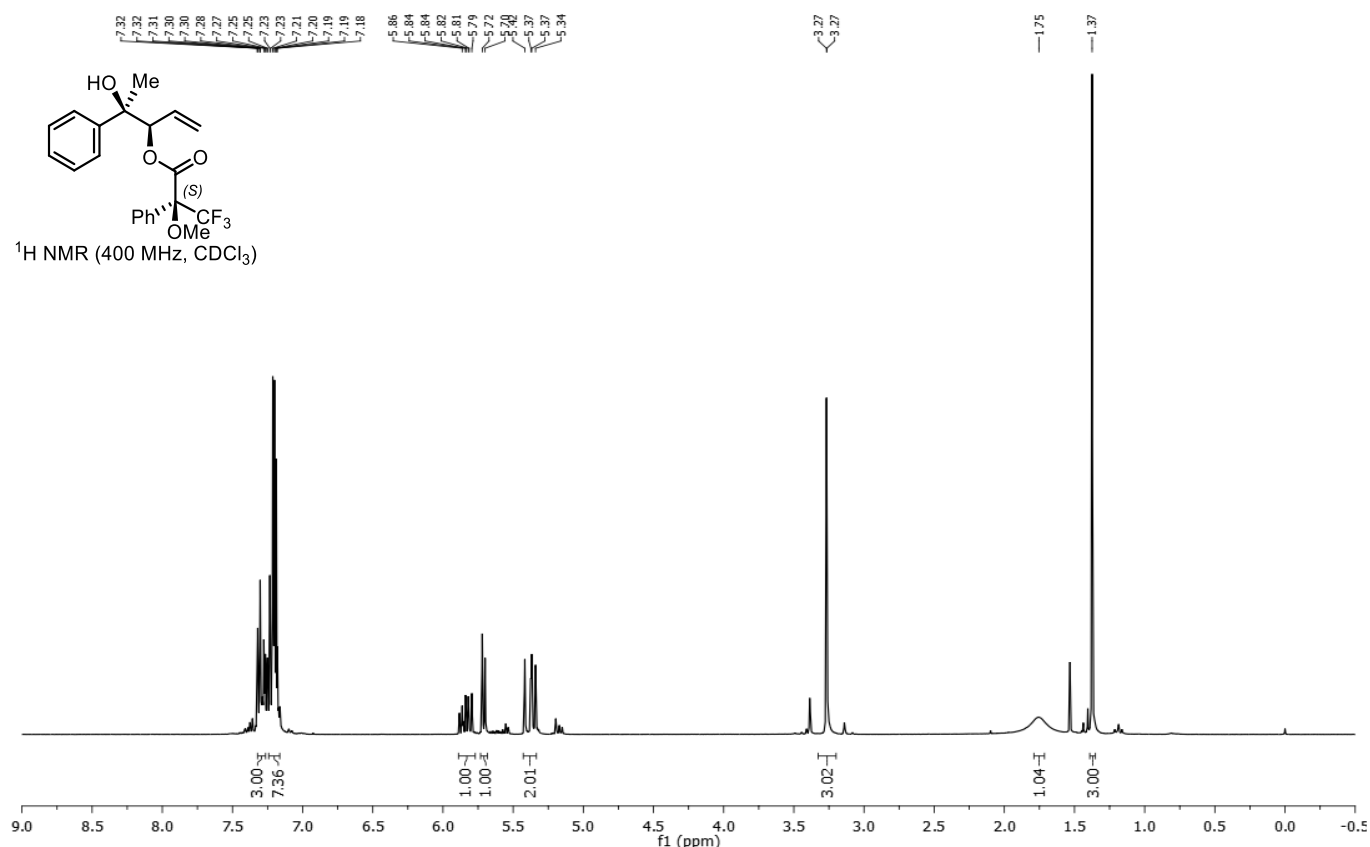
Table S_a: $\Delta\delta$ ($= \delta\text{S} - \delta\text{R}$) data (in ppm) for the (S)- and (R)-MTBA-Mosher esters **7a** and **7b**.

(3*R*,4*R*)-4-Hydroxy-4-phenylpent-1-en-3-yl (S)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate (7a):

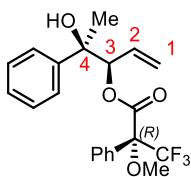


To a solution of alcohol **6** (30 mg, 0.17 mmol) in dry CH_2Cl_2 (2.0 mL) was added 4-(Dimethylamino)pyridine (41 mg, 0.33 mmol) under nitrogen atmosphere. The mixture was cooled to 0 °C, and pyridine (59 μL , 0.67 mmol) and (*R*)-(-)-MTPA-Cl (131 μL , 0.25 mmol) were added *via* syringe and the resulting mixture was stirred at ambient temperature for 1h. The mixture was diluted with EtOAc (5 mL) and washed with 1M HCl (10 mL), saturated Na_2CO_3 solution and extracted with EtOAc (3×15 mL) and dried over anhydrous Na_2SO_4 , filtered, and concentrated *in vacuo*. The resultant crude product was purified by flash chromatography (5% EtOAc/hexanes; $R_f = 0.3$) to afford ester **7a** in 84% yield (55 mg) as a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.33 – 7.25 (m, 2H), 7.24 – 7.17 (m, 3H), 5.90 – 5.78 (m, 1H), 5.71 (d, $J = 7.9$ Hz, 1H), 5.37 (dd, $J = 16.4$, 14.1 Hz, 1H), 3.27 (d, $J = 0.9$ Hz, 1H), 1.75 (s, 1H), 1.37 (s, 2H); HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{21}\text{H}_{21}\text{O}_4\text{F}_3\text{Na}^+$, 417.1289; found: 417.1290; $[\alpha]^{20}_{\text{D}} = +12.70^\circ$ (c 1.0, CHCl_3).

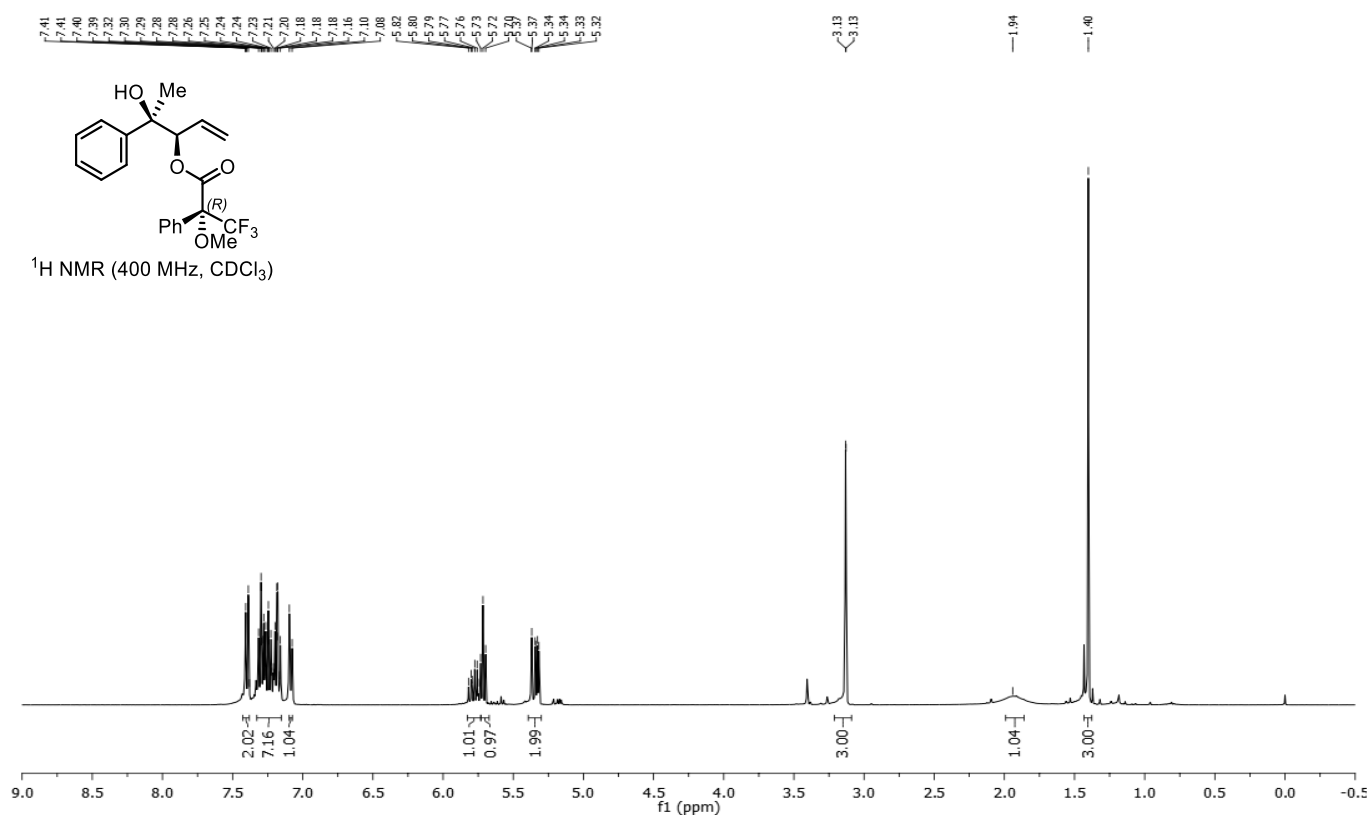
(3*R*,4*R*)-4-Hydroxy-4-phenylpent-1-en-3-yl (S)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate (7b):



(3*R*,4*R*)-4-Hydroxy-4-phenylpent-1-en-3-yl (R)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate (7b):

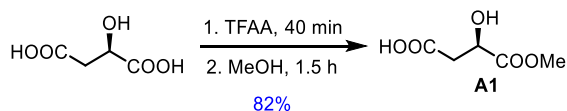


The ester **7b** was obtained with (*S*)-(-)-MTPA-Cl using above procedure in 80% yield (53 mg) as a colourless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.44 – 7.37 (m, 2H), 7.34 – 7.14 (m, 7H), 7.09 (d, J = 7.8 Hz, 1H), 5.82 – 5.73 (m, 1H), 5.71 (d, J = 7.6 Hz, 1H), 5.38 – 5.30 (m, 1H), 3.13 (d, J = 1.2 Hz, 1H), 1.94 (s, 1H), 1.40 (s, 3H); HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{21}\text{H}_{21}\text{O}_4\text{F}_3\text{Na}^+$, 417.1289; found: 417.1290; $[\alpha]^{20}_{\text{D}}$ = -20.24° (c 1.0, CHCl_3).



2h. Synthesis of Fostrecin C3-C11 fragment:¹⁰

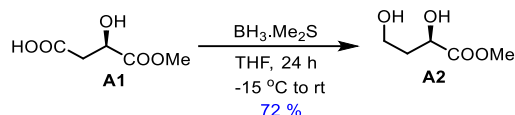
(*R*)-3-Hydroxy-4-methoxy-4-oxobutanoic acid (A1):



In a round-bottom flask, D-malic acid (2.0 g, 7.5 mmol) was dissolved in trifluoroacetic anhydride (4.3 mL) under nitrogen atmosphere and the reaction mixture was stirred for 40 min after which the trifluoroacetic anhydride was removed from the reaction mixture under reduced pressure. The crude solid obtained was dissolved in MeOH (5.7 mL) and stirred for another 1.5 h at room temperature. The volatile impurities were removed from

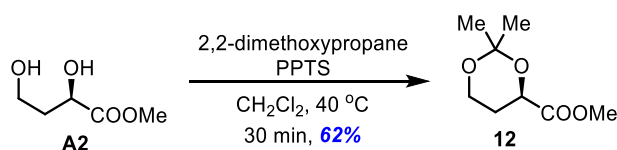
the reaction mixture under reduced pressure to provide ester **A1** in 82% yield (1.8 g) and used for next step without further purification.

Methyl (R)-2,4-Dihydroxybutanoate (**A2**):



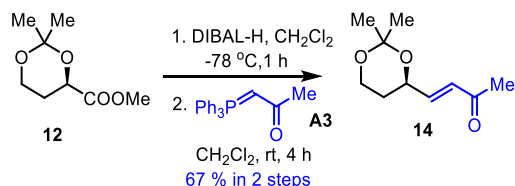
$\text{BH}_3 \cdot \text{Me}_2\text{S}$ (22.3 mmol, 23 mL) (1.0 M solution in THF) was added dropwise to a solution of ester **A1** (1.65 g, 11.15 mmol) in 50 mL of dry THF at $-15\text{ }^\circ\text{C}$ under argon atmosphere. The mixture was allowed to warm to room temperature and stirred for 24 h. The reaction was quenched by dropwise addition of 22 mL of MeOH and the reaction mixture was concentrated under reduced pressure and again co-evaporated three times with MeOH. The residue was diluted with EtOAc and filtered through a pad of Celite. Organic solution was concentrated under reduced pressure to give the crude diol **A2**, which was purified using flash column chromatography on silica gel in EtOAc/hexanes (3:2) to provide 1.08 g (72%) of pure diol **A2**.

Methyl (R)-2,2-dimethyl-1,3-dioxane-4-carboxylate (**A3**):



The diol **A2** (1.08 g, 8.1 mmol) was dissolved in 30 mL of dry CH_2Cl_2 and 30 mL of 2,2-dimethoxypropane, and PPTS (605 mg, 2.4 mmol) was added. The mixture was stirred for 30 min at $40\text{ }^\circ\text{C}$ and washed with saturated aqueous NaHCO_3 (20 mL), extracted with CH_2Cl_2 (2x15 mL), dried over Na_2SO_4 and evaporated *in vacuo* followed by chromatography on silica gel (hexane/ EtOAc 3 : 1 + 5% Et_3N) which provided 860 mg (62%) of **12** as a yellow oil.

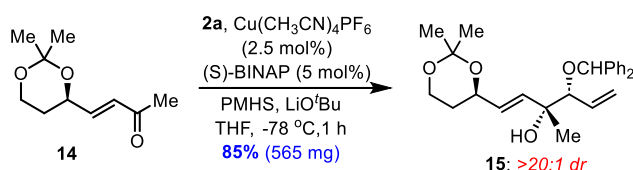
(R,E)-4-(2,2-dimethyl-1,3-dioxan-4-yl)but-3-en-2-one (**14**):



Ester **12** (0.86 g, 4.9 mmol) was dissolved in 20 mL of dry CH_2Cl_2 the reaction mixture was cooled to $-78\text{ }^\circ\text{C}$. Then a 1.0 M solution of DIBAL-H in toluene (4.9 mmol, 4.9 mL) was added dropwise and reaction was stirred at $-78\text{ }^\circ\text{C}$ for 1h. After consumption of ester (as monitored by TLC analysis), reaction was quenched by addition of 20 mL saturated aqueous solution of sodium potassium tartrate, stirred for additional 30 min and extracted with CH_2Cl_2 (2 x 20 mL). Combined organic solvent was dried over anhydrous Na_2SO_4 followed by removal of solvent under reduced pressure and immediately used for next step without further purification.

The crude aldehyde was dissolved in dry CH₂Cl₂ (20 ml) and methyl ester Wittig reagent **A3** (2.3 g, 7.2 mmol) was added to the reaction mixture under nitrogen atmosphere and reaction was stirred at rt for 4h. The solvent was removed under reduced pressure and the residue was purified using flash column chromatography on silica gel (EtOAc/hexane 1 : 5) to afford 0.6 g of ketone **14** (67% in two steps) as a yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 6.69 (dd, *J* = 16.1, 4.6 Hz, 1H), 6.27 (dd, *J* = 16.1, 1.6 Hz, 1H), 4.58 (dddd, *J* = 11.7, 4.5, 2.9, 1.7 Hz, 1H), 4.04 (td, *J* = 12.1, 2.9 Hz, 1H), 3.89 (ddd, *J* = 11.8, 5.4, 1.6 Hz, 1H), 2.28 (s, 3H), 1.71 (ddd, *J* = 17.3, 12.5, 5.4 Hz, 1H), 1.58 (dtd, *J* = 13.1, 2.9, 1.8 Hz, 1H), 1.50 (s, 3H), 1.44 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 198.7, 146.0, 129.4, 98.8, 68.3, 59.7, 30.7, 29.9, 27.5, 19.3; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₀H₁₆O₃Na⁺, 207.0997; found: 207.0992; [α]_D²⁰ = +22.85° (c 0.19, CHCl₃).

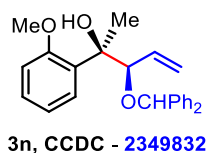
(3*R*,4*R*, *E*)-4-(benzyloxy)-1-((*R*)-2,2-dimethyl-1,3-dioxan-4-yl)-3-methylhexa-1,5-dien-3-ol (15**):**



According to the general procedure described in section 2d, compound **15** was prepared by using methyl ketone **14** (300 mg, 1.63 mmol, 1.0 equiv) and allene **2a** (1.63 mmol) in 85% yield (565 mg) with >20:1 *dr*. It was purified by flash chromatography (20% EtOAc/hexanes; *R_f* = 0.3) to afford a colourless oil; ¹H NMR (400 MHz, CDCl₃) δ 7.27 – 7.21 (m, 8H), 7.20 – 7.12 (m, 2H), 5.79 – 5.71 (m, 1H), 5.71 – 5.62 (m, 2H), 5.41 (s, 1H), 5.70 (d, 1H), 5.68 (d, *J* = 5.1 Hz, 1H), 5.33 (dd, *J* = 10.4, 1.8 Hz, 1H), 5.11 (ddd, *J* = 17.3, 1.8, 0.6 Hz, 1H), 4.35 (ddd, *J* = 11.5, 5.1, 2.7 Hz, 1H), 3.94 (td, *J* = 12.2, 2.8 Hz, 1H), 3.78 (ddd, *J* = 11.7, 5.4, 1.6 Hz, 1H), 3.49 (d, *J* = 8.7 Hz, 1H), 2.39 (s, 1H), 1.72 – 1.59 (m, 1H), 1.44 (s, 3H), 1.42 – 1.37 (m, 1H), 1.36 (s, 3H), 1.14 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 143.0, 141.3, 136.1, 134.4, 129.5, 128.7, 128.3, 128.1, 128.0, 127.3, 126.7, 121.7, 98.5, 84.0, 80.0, 74.1, 69.6, 59.9, 31.7, 30.2, 24.0, 19.4; HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₂₆H₃₃O₄⁺, 409.2378; found: 409.2369; [α]_D²⁰ = +36.50° (c 1.0, CHCl₃).

3. Single Crystal X-ray Analysis:

3a. X-ray crystallographic data for compound **3n**:



The purified compound **3n** was dissolved in a mixed solvent of CH₂Cl₂/n-hexane (1:1), and placed in a dark cabinet for slowly evaporation. Orange crystals were collected after few days for X-ray analysis.

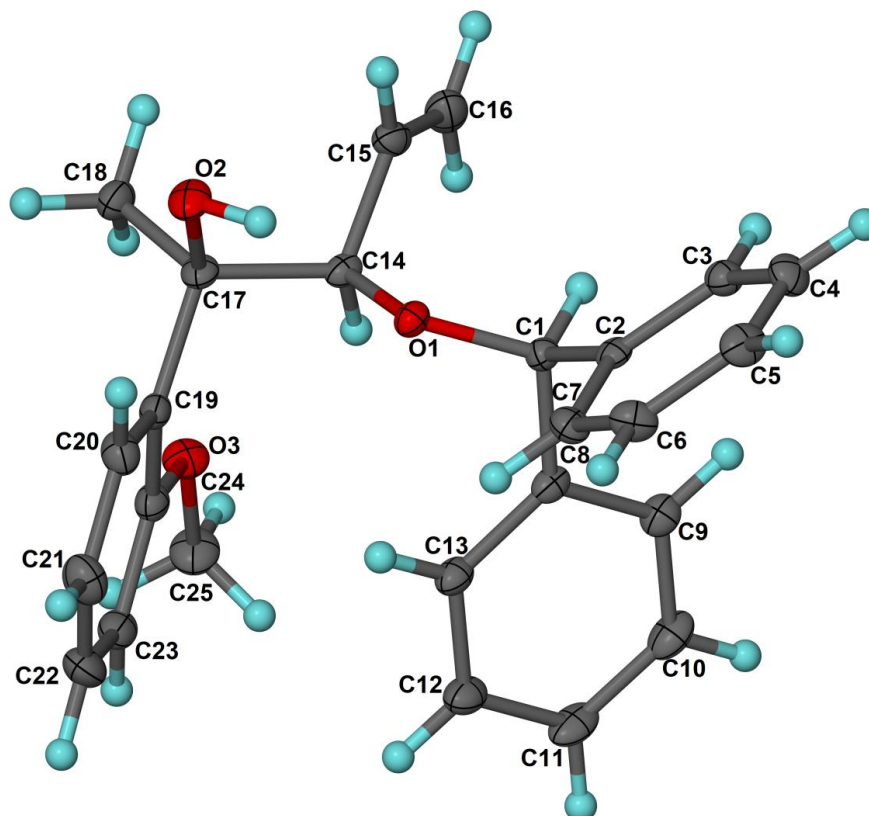
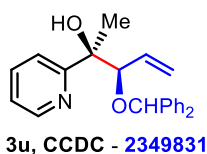


Figure caption: ORTEP diagram of compound **3n** (KB741) with the atom-numbering. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radius.

Crystal data for compound **3n (KB741):** C₂₅H₂₆O₃, *M* = 374.46, Monoclinic, space group *P*2₁ (No.4), *a* = 8.0727(18) Å, *b* = 17.381(3) Å, *c* = 8.2903(16) Å, α = 90°, β = 117.903(5)°, γ = 90°, *V* = 1028.0(4) Å³, *Z* = 2, *D_c* = 1.210 g/cm³, *F*₀₀₀ = 400, Bruker D8 QUEST PHOTON-III C7 HPAD detector, Mo-Kα radiation, λ = 0.71073 Å, *T* = 100(2) K, $2\theta_{\text{max}}$ = 55°, μ = 0.078 mm⁻¹, 14285 reflections collected, 4670 unique (*R*_{int} = 0.0457), 259 parameters, *R*1 = 0.0351, *wR*2 = 0.0820, *R* indices based on 4304 reflections with *I* > 2σ(*I*) (refinement on *F*²), Final *GooF* = 1.052, largest difference hole and peak = -0.195 and 0.214 e.Å⁻³. **CCDC deposition number 2349832** contains the supplementary crystallographic data for this paper which can be obtained free of charge at <https://www.ccdc.cam.ac.uk/structures/>

3b. X-ray crystallographic data for compound 3u:



The purified compound **3u** was dissolved in a mixed solvent of CHCl₃/n-hexane (1:1), and placed in a dark cabinet for slowly evaporation. Orange crystals were collected after few days for X-ray analysis.

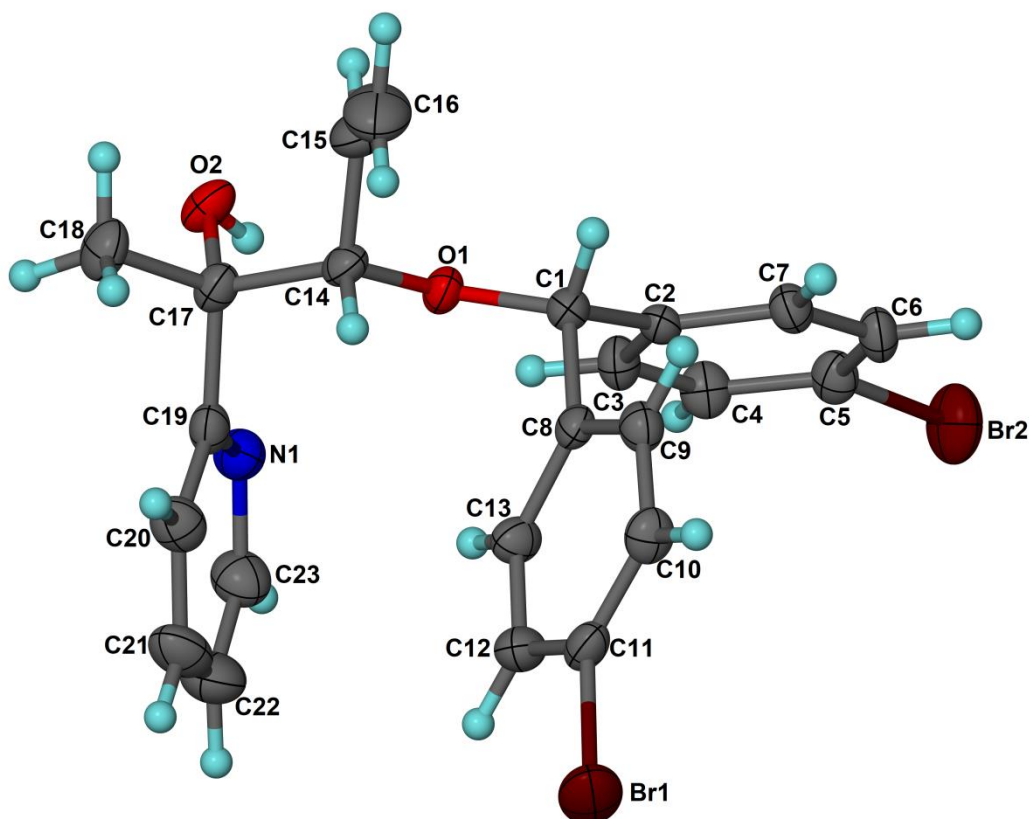
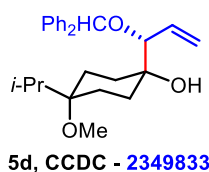


Figure caption: ORTEP diagram of compound **3u** (KB378) with the atom-numbering. Displacement ellipsoids are drawn at the 35% probability level and H atoms are shown as small spheres of arbitrary radius.

Crystal data for compound 3u (KB378): C₂₃H₂₁Br₂NO₂, *M* = 503.23, Triclinic, space group *P* $\bar{1}$ (No.2), *a* = 8.759(2)Å, *b* = 8.907(3)Å, *c* = 15.126(5)Å, α = 73.632(7)°, β = 82.000(11)°, γ = 75.587(7)°, *V* = 1093.6(6)Å³, *Z* = 2, *D*_c = 1.528 g/cm³, *F*₀₀₀ = 504, Bruker D8 QUEST PHOTON-III C7 HPAD detector, Mo-Kα radiation, λ = 0.71073 Å, *T* = 294(2)K, $2\theta_{\text{max}}$ = 55°, μ = 3.724 mm⁻¹, 18857 reflections collected, 4431 unique (*R*_{int} = 0.0725), 257 parameters, *R*1 = 0.0484, *wR*2 = 0.0940, *R* indices based on 2743 reflections with *I* > 2σ(*I*) (refinement on *F*²), Final *GooF* = 1.004, largest difference hole and peak = -0.524 and 0.722 e.Å⁻³. **CCDC deposition number 2349831** contains the supplementary crystallographic data for this paper which can be obtained free of charge at <https://www.ccdc.cam.ac.uk/structures/>.

3c. X-ray crystallographic data for compound **5d**:



The purified compound **5d** was dissolved in a mixed solvent of CHCl₃/n-hexane (1:1), and placed in a dark cabinet for slowly evaporation. Orange crystals were collected after few days for X-ray analysis.

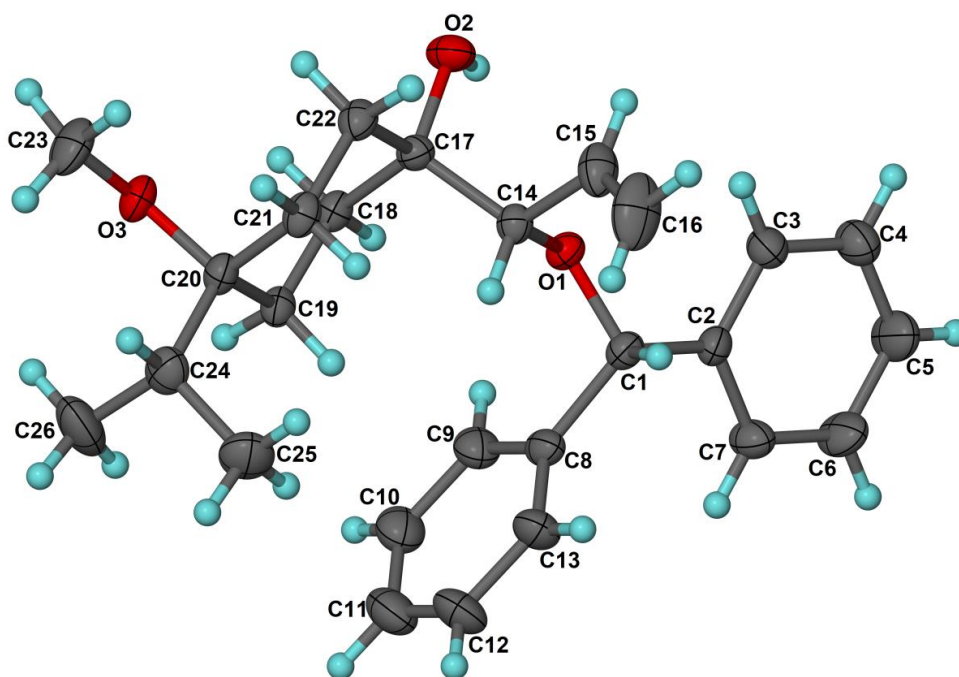


Figure caption: ORTEP diagram of compound **5d** (KB1077) with the atom-numbering. Displacement ellipsoids are drawn at the 35% probability level and H atoms are shown as small spheres of arbitrary radius.

Crystal data for compound **5d (KB1077):** C₂₆H₃₄O₃, *M* = 394.53, Monoclinic, space group *P*2₁/*n* (No.14), *a* = 12.9997(8) Å, *b* = 10.7801(6) Å, *c* = 16.7201(11) Å, α = 90°, β = 97.231(2)°, γ = 90°, *V* = 2324.5(2) Å³, *Z* = 4, *D*_c = 1.127 g/cm³, *F*₀₀₀ = 856, Bruker D8 QUEST PHOTON-III C7 HPAD detector, Mo-K α radiation, λ = 0.71073 Å, *T* = 294(2) K, $2\theta_{\text{max}}$ = 55°, μ = 0.072 mm⁻¹, 27035 reflections collected, 5306 unique (*R*_{int} = 0.0388), 330 parameters, *R*1 = 0.0506, *wR*2 = 0.1249, *R* indices based on 3734 reflections with *I* > 2 σ (*I*) (refinement on *F*²), Final *GooF* = 1.032, largest difference hole and peak = -0.142 and 0.214 e.Å⁻³. **CCDC deposition number 2349833** contains the supplementary crystallographic data for this paper which can be obtained free of charge at <https://www.ccdc.cam.ac.uk/structures/>

Data collection and Structure solution details: Single crystal X-ray data were collected at room temperature on a Bruker D8 QUEST equipped with a four-circle kappa diffractometer and PHOTON-III C7 HPAD detector. An I μ s microfocus Mo source (λ =0.71073 Å) supplied the multi-mirror monochromated incident beam. A combination of Phi and Omega scans were used to collect the necessary data. Integration and scaling of intensity data were accomplished using SAINT program.¹¹ The structures were solved by Direct Methods using SHELXS97 and refinement was carried out by full-matrix least-squares technique using SHELXL-2018/3.¹¹⁻¹³

Anisotropic displacement parameters were included for all non-hydrogen atoms. All H atoms were positioned geometrically and treated as riding on their parent C atoms, with C-H distances of 0.93--0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$ for methyl atoms. The O bound H atom was located in the difference Fourier map and its positional coordinates and isotropic displacement parameters were refined. In KB1077 compound, the two phenyl rings attached to C1 atom were disordered over two sites, with site occupancy factor of 0.650(11) for the major component of the disordered atoms (C2/C3/C4/C5/C6/C7 and C8/C9/C10/C11/C12/C13) and 0.350(11) for the minor component of the disordered atoms (C2D/C3D/C4D/C5D/C6D/C7D and C8D/C9D/C10D/C11D/C12D/C13D). PART, FVAR, DELU, and SIMU instructions were utilized for modelling the structural disorder and structural refinement.¹⁴ CCDC deposition numbers 2349831-2349833 contains the supplementary crystallographic data for this paper which can be obtained free of charge at <https://www.ccdc.cam.ac.uk/structures/>.

4. Computational studies:

4a. Computational Details: All reported calculations were performed using the ORCA 5.0.3 software.¹⁵ Images of the 3D structures were rendered using CYLView20.¹⁶ The geometry of all reactants, intermediates and transition states were optimized using the B3LYP functional in the gas phase,¹⁷ with a mixed basis set consisting of triple- ζ quality def2-TZVPP basis set on Cu and P and double- ζ split valence def2-SVP basis set for all other atoms.¹⁸ Intermediates and transition state geometries were validated by vibrational analysis at the same level of theory, showing all real normal modes for the former and one imaginary mode for the later, respectively. Single point energies were calculated at B3LYP/def2-TZVPP together with the SMD solvation model with tetrahydrofuran (dielectric constant, $\epsilon = 7.25$) as the solvent.¹⁹ Grimme's D3BJ dispersion correction was employed all through.²⁰ Further, energies were verified at M06L/ def2-TZVPP and TPSSh/ def2-TZVPP level of theory. The results are summarized in Table S1. The reported Gibbs free energies and enthalpies include zero-point and thermal corrections calculated at 298.15 K and 195.15 K temperatures. To reduce the huge computational cost associated with the linearly extended alkyl chains, PMHS was modelled by truncation of the polymeric alkoxy groups with -OMe terminals and employing Me(OMe)₂SiH during calculations. Steric plots were obtained from sambVca 2.1 web tool.²¹⁻²² Non-covalent interactions were confirmed by using Multiwfn program.²³

4b. Relative Gibbs free energy profile for complete catalytic cycle of CuH-BINAP Catalysed allylation of ketone

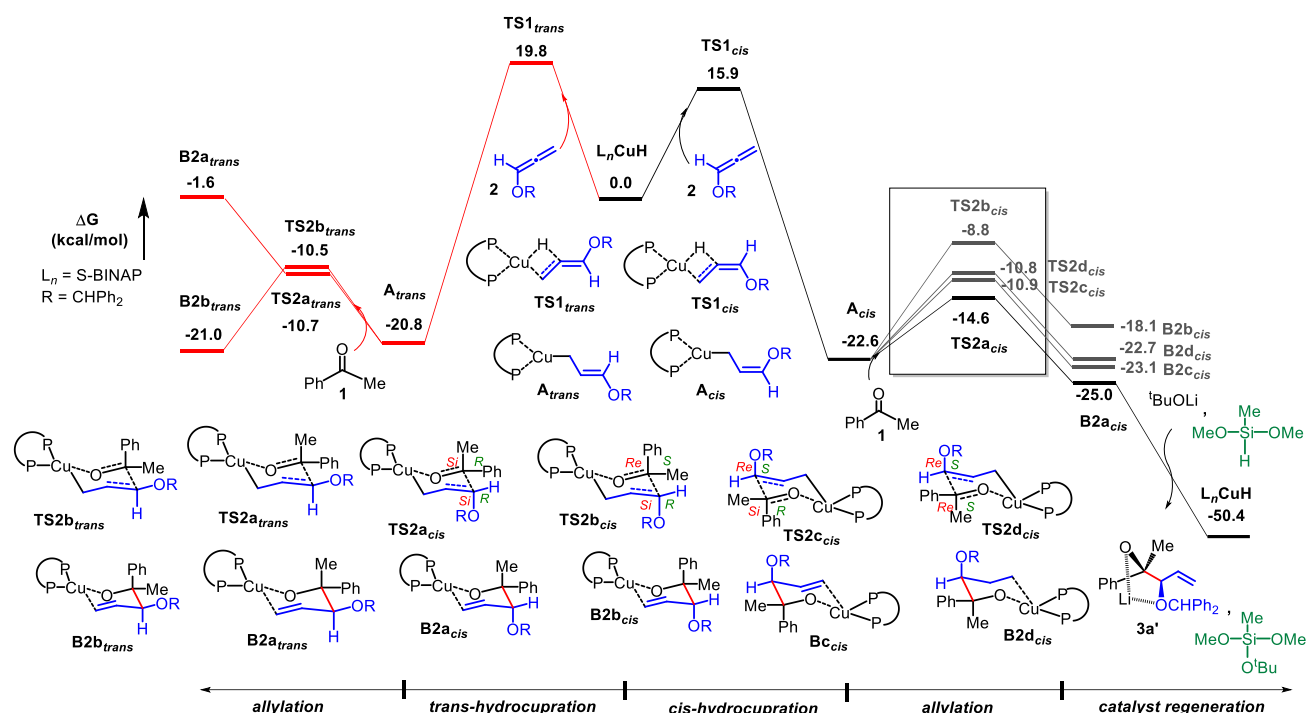


Figure S1. Relative Gibbs free energy profile for enantioselective copper catalysed reductive coupling of alkoxy allenenes to access *syn*-diols, Gibbs free energies are reported in kcal/mol at B3LYP/def2TZVPP/D3BJ/SMD level of theory.

Figure S1 depicts the complete catalytic cycle of copper catalysed allylation of acetophenone. The optimized transition state structures of the key rate determining and enantio-diastereoselectivity determining transition states are shown in Figure S4. The catalytic cycle begins with hydrocupration of alkoxy allene. Since the reaction is completed within 1 h in the experimental setup, the kinetic factors become more prominent rather than the thermodynamics. Since the activation energy barrier of $TS1_{trans}$ is 3.9 kcal higher than $TS1_{cis}$, there is high *Z*-selectivity in the hydrocupration event to proceed via $TS1_{cis}$ to reach a highly exergonic hydrocupration product A_{cis} at -22.6 kcal/mol. Thereafter, the scope of trans mode channelling of the reaction has been discarded. Subsequent ketone allylation proceeds from A_{cis} via a six membered ($TS2a_{cis}$, $\Delta G^\ddagger = 8.0$ kcal/mol) transition state affords intermediate $B2a_{cis}$ with excellent enantio- and diastereo selective control. Next, an active participation $tBuOLi$ release out lithiated product $3a'$ and PMHS transfer its hydride to generate L_nCuH . At the end, the desired product $3a$ is obtained by acidic work up. Finally, hydrosilane helps in the regeneration of the active catalyst and completes the catalytic cycle. All DFT methods are consistent with the predominance of $TS1_{cis}$ and $TS2a_{cis}$ over their competitive partners.

Table S1. Computed activation free energies ($\Delta G^\ddagger$) of the key transition states ($TS1_{trans}$, $TS1_{cis}$, $TS2a_{cis}$, and $TS2b_{cis}$) at different levels of theories.

Method for	$TS1_{trans}$	$TS1_{cis}$	$\Delta\Delta G^\ddagger$	$TS2b_{cis}$	$TS2a_{cis}$	$\Delta\Delta G^\ddagger$
Single point energy calculations	$\Delta G^\ddagger$	$\Delta G^\ddagger$	($TS1_{trans}$ - $TS1_{cis}$)	$\Delta G^\ddagger$	$\Delta G^\ddagger$	($TS2b_{cis}$ - $TS2a_{cis}$)
B3LYP/def2TZVPP/D3BJ/SMD	19.8	15.9	3.9	13.8	8.0	5.8
M06L/def2TZVPP/SMD	19.5	15.0	4.5	16.5	9.5	7.0
TPSSh/def2TZVPP/D3BJ/SMD	11.7	7.4	4.3	10.2	4.8	5.4

4c. Temperature dependence in computational studies

Figure 1 (main text) and S2 depicts the effect of temperature on free energy profile. The trend in the free energy remains unchanged at both 298.15 K and 195.15 K temperatures as Gibbs free energy is linearly dependent on temperature (Equation 1). At 195.15 K temperature $TS1_{cis}$ is favourable by 3.9 kcal/mol closer to the value at 298.15 K (Table S2). The rate determining transition state (hydrocupration step, $TS1_{cis}$) and the stereoselectivity determining transition state (allylation step, $TS2a_{cis}$) are consistent irrespective of the temperature (Figure S2, and Table S2).

$$G = H - T * S \quad \dots\dots\dots \text{(Equation 1)}$$

Where, G is the Gibbs free energy, H is the enthalpy, T is the temperature, and S is the entropy

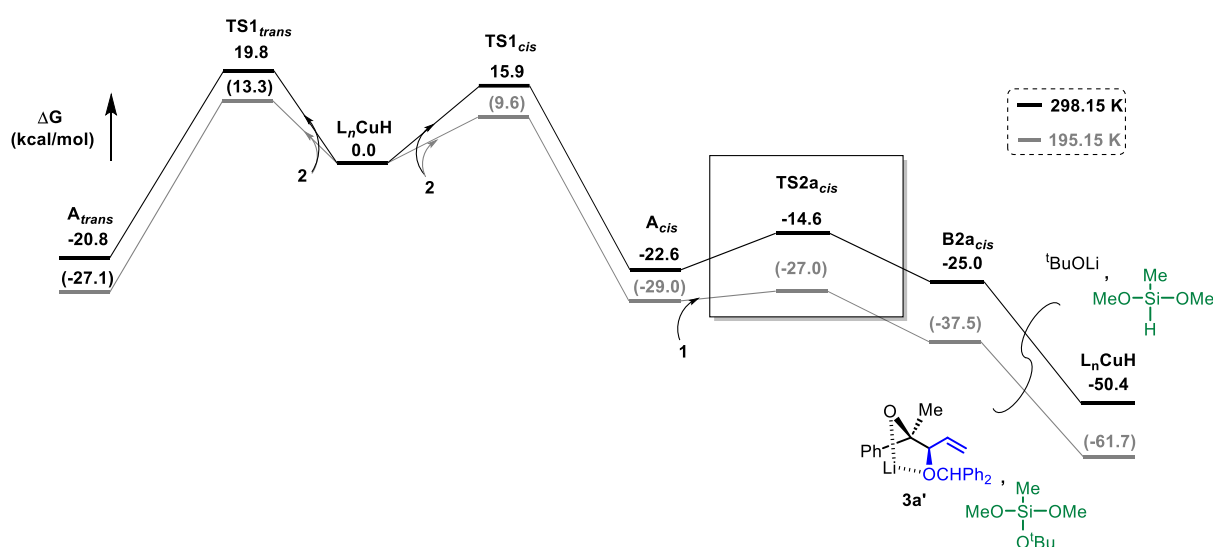


Figure S2. Relative Gibbs free energy profile for enantioselective copper catalysed reductive coupling of alkoxy allenes to access syn-diols, at different temperatures. (Black path at 298.15 K and Grey path at 195.15 K). Gibbs free energies are reported in kcal/mol at B3LYP/def2TZVPP/D3BJ/SMD level of theory.

Table S2. A comparison of effect of temperature on computed activation free energies ($\Delta G^\ddagger$) of the enantio- and diastereo-selectivity determining transition states (TS1_{trans}, TS1_{cis}, TS2a_{cis}, and TS2b_{cis}).

Temperature for calculation of thermodynamic parameters	TS1 _{trans} $\Delta G^\ddagger$	TS1 _{cis} $\Delta G^\ddagger$	$\Delta\Delta G^\ddagger$ (TS1 _{trans} - TS1 _{cis})	TS2b _{cis} $\Delta G^\ddagger$	TS2a _{cis} $\Delta G^\ddagger$	$\Delta\Delta G^\ddagger$ (TS2b _{cis} - TS2a _{cis})
298.15 K	19.8	15.9	3.9	13.8	8.0	5.8
195.15 K	13.3	9.6	3.7	7.5	2.0	5.5

4d. Hydrocupration involving transition state structures

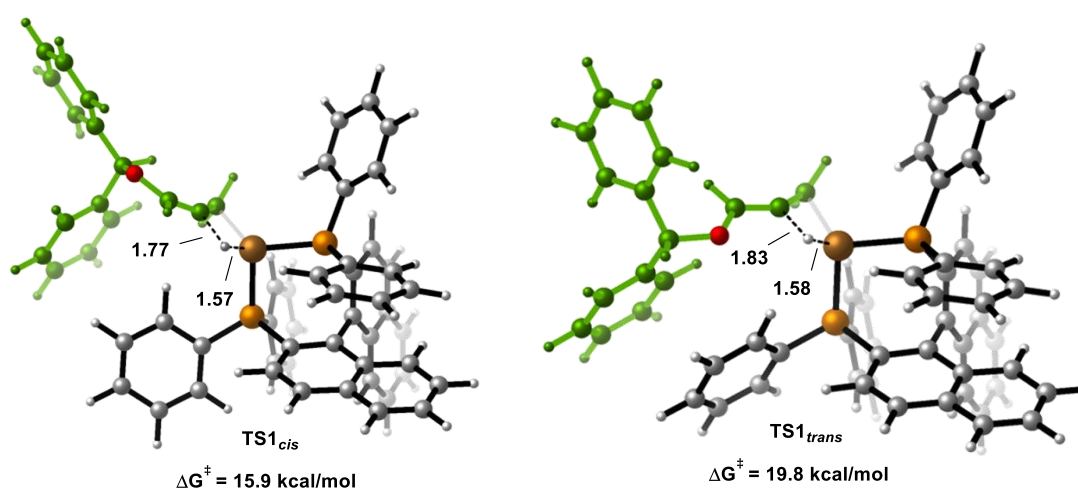


Figure S3. Activation free energies and optimized transition state structures of the hydrocupration of alkoxy allene. Bond distances are in units of Å.

4e. Ketone allylation involving transition state structures

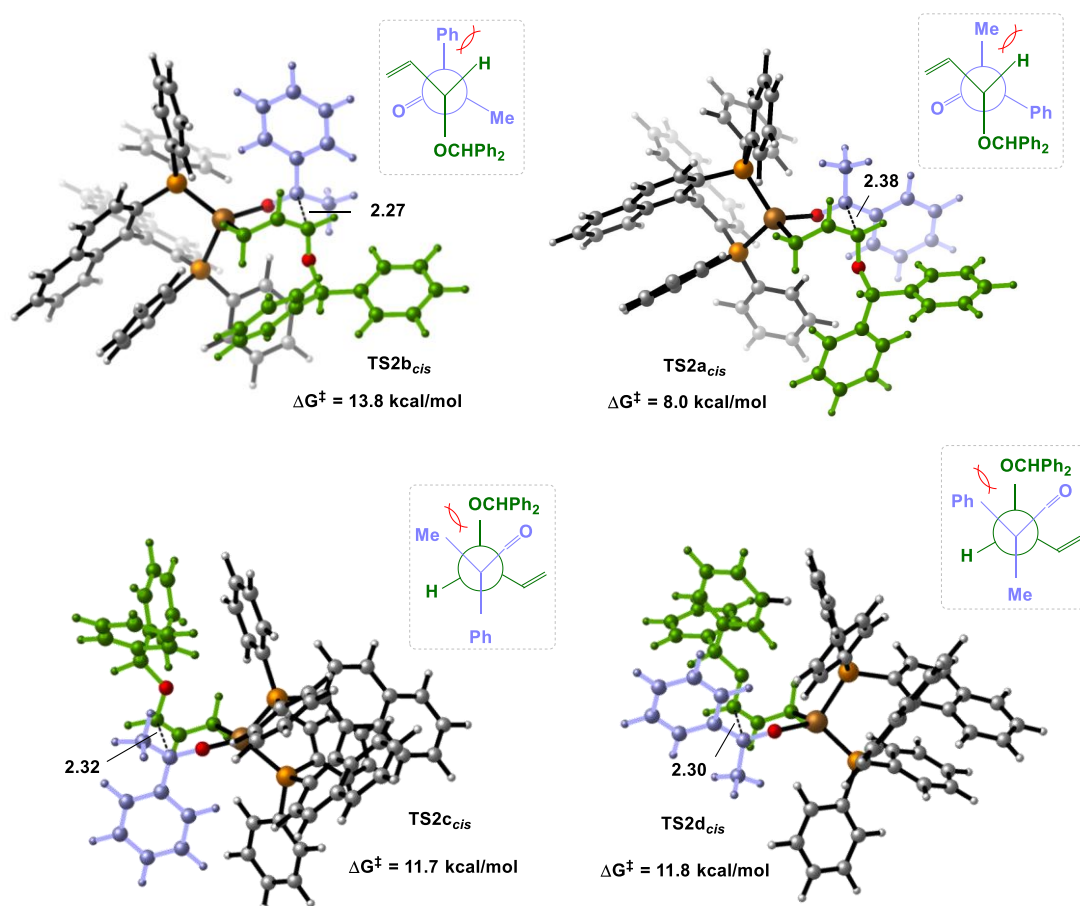


Figure S4. Activation free energies and optimized transition state structures of the allylation of ketone. Chemdraw structures highlighted in dotted lined boxes are Newman projections of the six membered transition state conformations to depict dihedral angle strain. Bond distances are in units of Å.

4f. Energy decomposition analysis

Energy decomposition analysis has been performed at B3LYP/def2TZVPP/D3BJ/SMD level of theory to examine the source of enantio- and diastereo-selectivity. The activation energy ($\Delta E^\ddagger$) required to overcome the potential barrier can be decomposed in terms of reorganization/distortion energy and interaction energy as the following equation:

$$\Delta E^\ddagger = \Delta E_{reorg} + \Delta E_{int} \quad \text{..... (Equation 2)}$$

ΔE_{reorg} is the total expenditure in energy when the reacting species gets reorganized into the transition state configuration and ΔE_{int} is the interaction energy between the reacting species in the activated complex. Table S3 and Table S4 summarise the activation energy, total reorganization energy and interaction energy for the hydrocupration and allylation transition states respectively. Figure S5 and Figure S6 depict the observation in the form of bar plot. The total demand in reorganization energy required for the separated copper hydride and alkoxy allene to overcome the activation barrier is more prominent for a *trans*-mode hydrocupration compared to *cis*-mode (Table S3 and Figure S5). Mainly, the alkoxy allene must distort at the expense of 4.4 kcal/mol energy higher than in *cis* phase attack. Hence, hydrocupration *via trans* mode is discarded. The system follows

TS1_{cis} to reach at **A_{cis}** intermediate. The decomposition of activation energy for the ketone allylation transition state is in support of the **TS2a_{cis}** transition state arrangement which undergoes minimum distortion in its configuration ultimately leading to the product (Table S4 and Figure S6).

Table S3. Decomposition of activation energy in kcal/mol for transition states participating in hydrocupration of alkoxyallene

	$\Delta E^\ddagger$	$\Delta E_{\text{reorg-LnCuH}}$	$\Delta E_{\text{reorg-2a}}$	Total ΔE_{reorg}	ΔE_{int}
TS1_{cis}	-1.8	9.8	16.8	26.6	-28.4
TS1_{trans}	1.4	11.3	19.2	30.6	-29.2

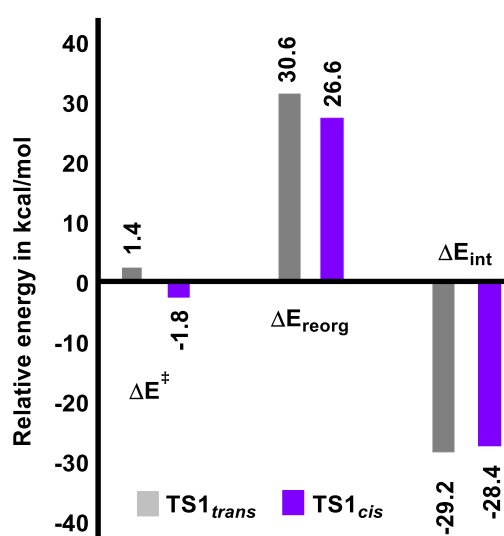


Figure S5. Energy decomposition analysis of hydrocupration transition state at B3LYP/def2TZVPP/D3BJ/SMD level of theory. Energies are reported in kcal/mol.

Table S4. Decomposition of activation energy in kcal/mol for transition states participating in allylation of ketone

	$\Delta E^\ddagger$	$\Delta E_{\text{reorg-A}}$	$\Delta E_{\text{reorg.1a}}$	Total ΔE_{reorg}	ΔE_{int}
TS2a_{cis}	-8.8	13.0	6.3	19.3	-28.1
TS2b_{cis}	-4.2	18.7	10.7	29.4	-33.6
TS2c_{cis}	-4.6	17.7	9.4	27.1	-31.7
TS2d_{cis}	-6.0	15.1	8.9	24.0	-30.0

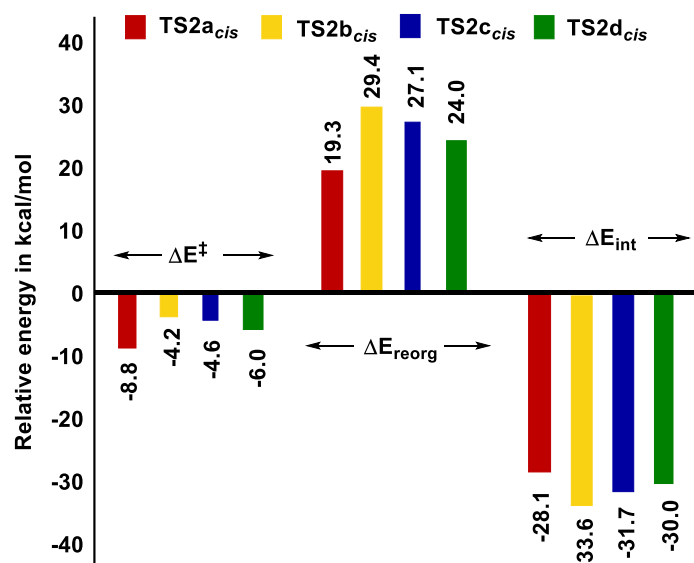


Figure S6. Energy decomposition analysis of allylation of ketone at B3LYP/def2TZVPP/D3BJ/SMD level of theory. Energies are reported in kcal/mol.

4g. Steric mapping analysis of hydrocupration of alkoxy allene.

Topographic steric maps of the transition states involved in the hydrocupration step are furnished w.r.t the % V_{Buried} . The total space of the catalytic pocket is defined by a sphere consisting of buried and free volume. The percentage buried volume of a complex gives the qualitative measure of the space occupied by the ligands coordinated to the metal centre in the first coordination sphere.⁸ On the other hand, the % V_{Free} is the free volume available for the reacting species in the catalytic pocket.

$$\%V_{Total} = \%V_{Buried} + \%V_{Free} \quad \dots\dots\dots \text{(Equation 3)}$$

In this study, copper is defined as the centre of the sphere with a radius set to 3.5 Å. The z-axis passes through the metal centre and is perpendicular to both the phosphorus atoms (which define the xy plane representing the topographic steric map) coordinated to the metal. We have adopted the bond radii scaled by 1.17 Å for the atoms, and a mesh of 0.1 Å was used to scan the sphere for buried voxels. A first coordination sphere of radius 3.5 Å is ideal for the metal complexes where the groups directly bound to the metal contribute to the steric encumbrance. In the case of our Cu-BINAP complex, the metal–phosphine ligand and metal–substrate bond distances are within 2.1–2.4 Å. A first coordination sphere of 3.5 Å is expected to also account for the van der Waals space occupied by the atoms coordinated to the metal. These insights have been put forth by Cavallo group after successfully utilizing topographic steric maps to validate many unusual regioselective and stereoselective reactions.^{22, 24-26}

The steric mapping data are shown in Table S4 and Table S5. The **TS1_{cis}** has 15.4 % of free space available as opposed to 14.1 % in **TS1_{trans}**. To have a better understanding, we have divided the coordination space into four quadrants (Figure S6a). The hydrocupration event occurs at the interface of quadrants II and III and becomes our quadrant of interest. The **TS1_{cis}** configuration in these quadrants is less sterically congested, facilitating better catalyst–substrate interaction. Further inspection of the transition state geometries for hydrocupration of alkoxy allene reveals that the -OCHPh₂ groups of allene substrate are near the hydrocupration

centre in the transition state for the trans addition, resulting in repulsive energetic contributions. The cis mode does not sterically interfere as severely as the trans transition state. This steric clash is alleviated in the transition state for cis addition making the -OCHPh₂ group to rotate away from the reacting centre, resulting in a sterically less hindered geometry as evident from the yellow-green contours at the interface of quadrant II and III in the steric map of **TS1_{cis}** (Figure S7c).

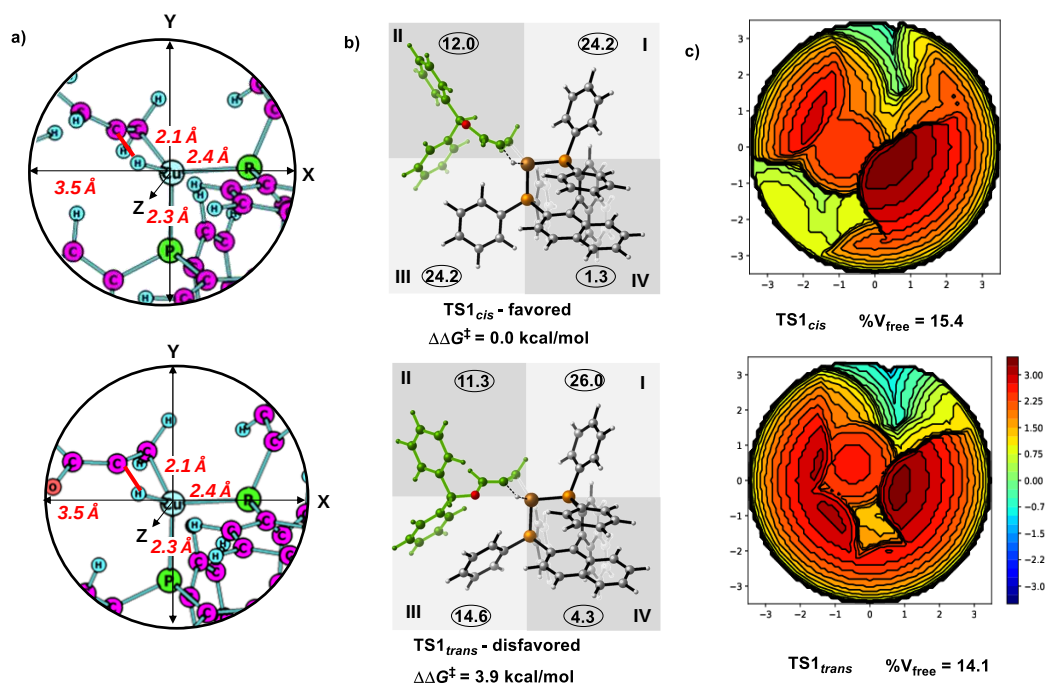


Figure S7. (a) Orientation of complex taken for topography, (b) quadrant diagram and (c) steric maps. In (b), roman numerals denote the four quadrants of the coordination space with corresponding %V_{free}; green indicates the alkoxyallene substrate. In (c), the isocontour curves of the steric maps are given in Å within a range of ±3.0 Å) along with total %V_{free} is shown within a radius of 3.5 Å from the copper centre (see Figure 1 in main text)

Table S5. Topographic steric mapping data for cis mode hydrocupration through **TS1_{cis}**

%V _{Free}	%V _{Buried}	% V _{total}			
15.4	84.6	100			
Quadrant	V _{Free} (Å ³)	V _{Buried} (Å ³)	V _{Total} (Å ³)	%V _{Free}	%V _{Buried}
SW	10.8	34	44.9	24.2	75.8
NW	5.4	39.5	44.9	12	88
NE	10.8	34	44.9	24.2	75.8
SE	0.6	44.3	44.9	1.3	98.7

Table S6. Topographic steric mapping data for trans mode hydrocupration through **TS1_{trans}**

%V _{Free}	%V _{Buried}	% V _{total}			
14.1	85.9	100			
Quadrant	V _{Free} (Å ³)	V _{Buried} (Å ³)	V _{Total} (Å ³)	%V _{Free}	%V _{Buried}
SW	6.6	38.3	44.9	14.6	85.4
NW	5.1	39.8	44.9	11.3	88.7
NE	11.7	33.2	44.9	26	74
SE	1.9	42.9	44.9	4.3	95.7

4h. Optimized geometries of possible intermediates formed after hydrocupration of alkoxy allene.

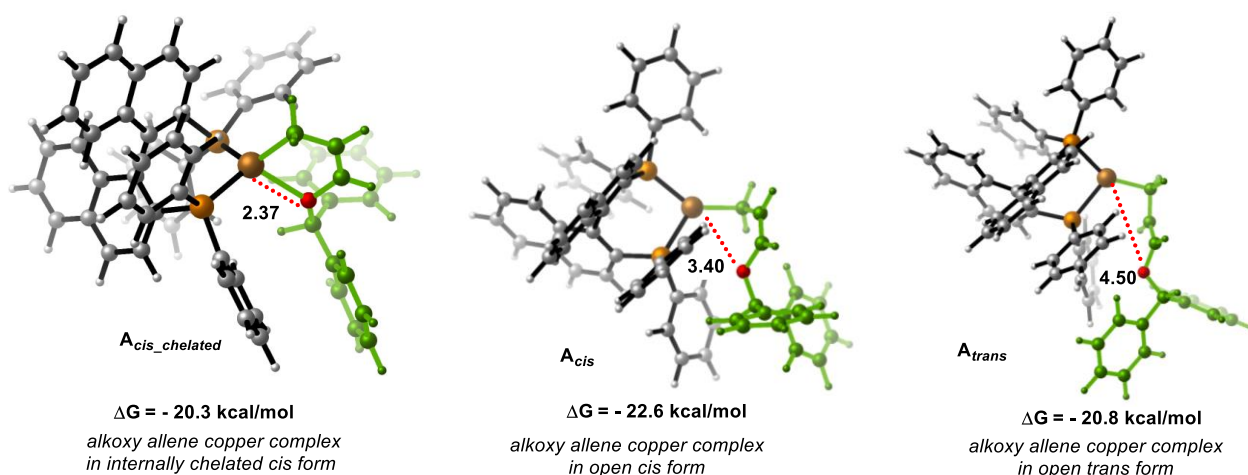


Figure S8. Gibbs free energies and optimized structures of intermediates formed after the hydrocupration of alkoxy allene. Distances from copper centre to oxygen are highlighted in red dotted lines and are in units of Å.

4i. Defining the stereochemistry of the four transition states in cis-allylation

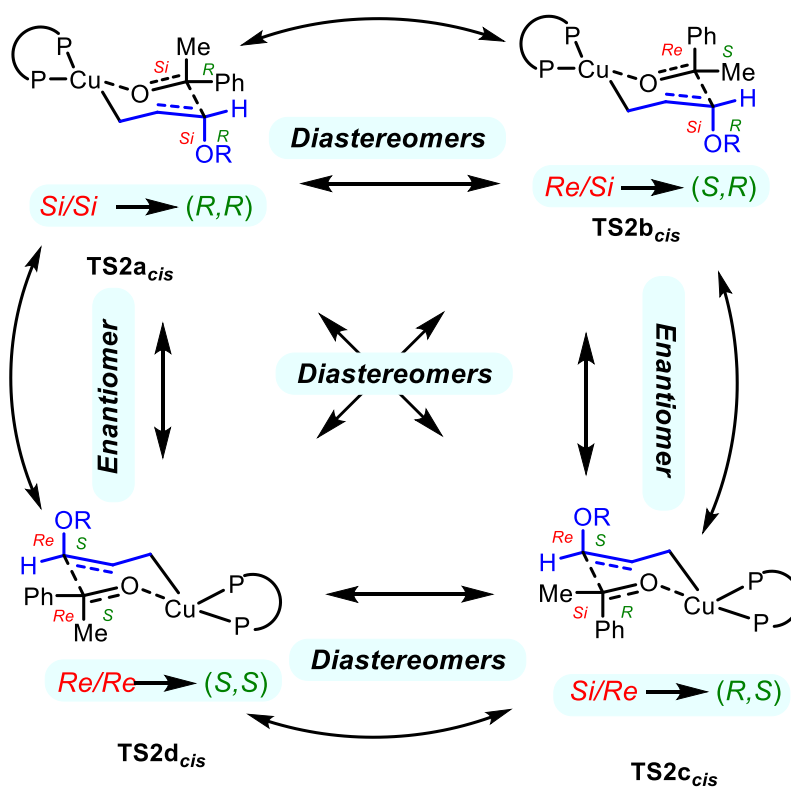


Figure S9. Model portraying absolute configuration of stereoisomers.

4j. Analysis of non-covalent interactions in TS2a_{cis}.

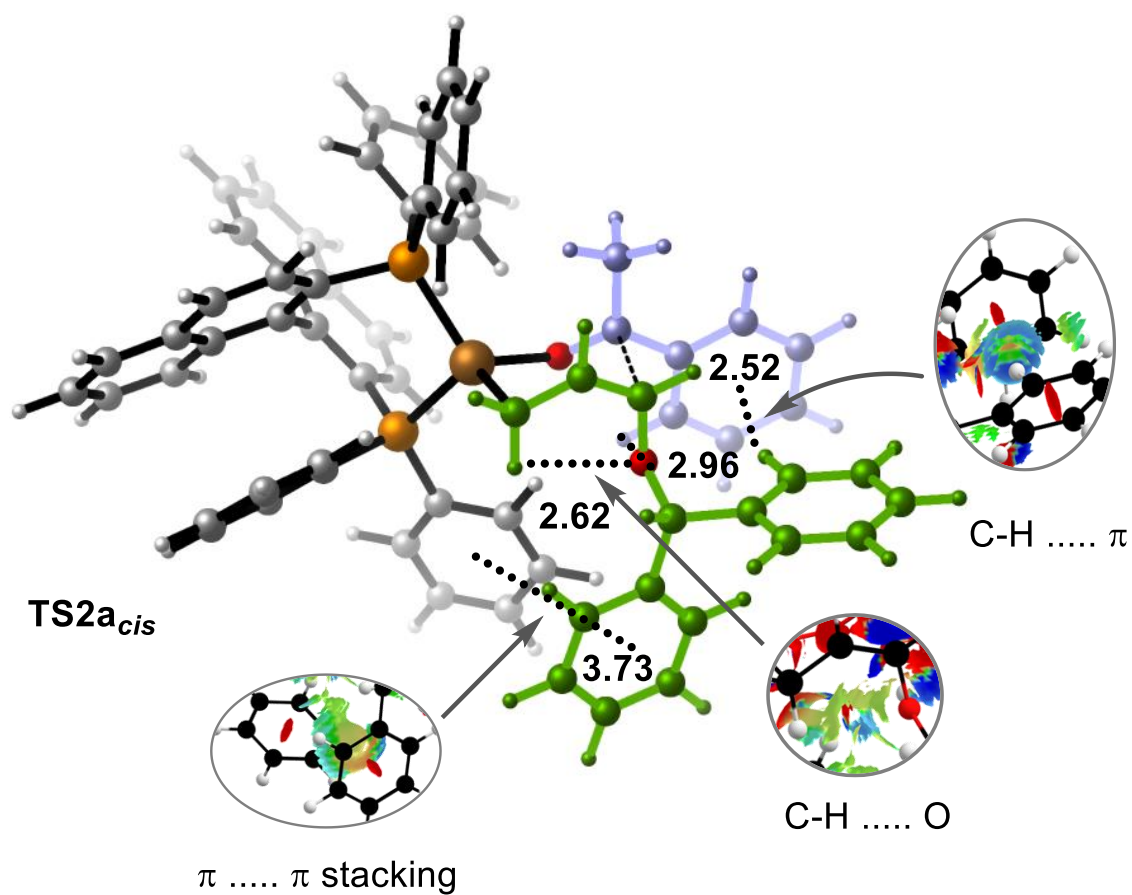


Figure S10. Non-covalent interaction analysis of stereoselective transition state **TS2a_{cis}**. Blue regions denote strongly attractive, green regions denote weakly attractive and red regions denote strongly repulsive positions.

4k. XYZ Coordinates

L_nCuH (BINAP-CuH)

1	-0.010569000	-4.249934000	-0.037463000
15	1.685909000	-1.135775000	0.234526000
15	-1.689453000	-1.124276000	-0.255586000
6	0.096376000	2.214427000	-2.970617000
6	-0.795393000	1.230716000	-3.470687000
6	-1.376066000	0.313682000	-2.629004000
6	-1.097535000	0.308247000	-1.230603000
6	-0.195695000	1.241146000	-0.708050000
6	0.390453000	2.228757000	-1.568376000
1	-1.012259000	1.208371000	-4.541852000
1	-2.050994000	-0.437969000	-3.038947000
6	-0.086725000	2.151837000	3.020111000
6	0.801266000	1.154170000	3.498794000
6	1.377646000	0.252723000	2.637535000
6	1.098364000	0.277968000	1.239486000
6	0.199697000	1.224970000	0.737319000
6	-0.381821000	2.196664000	1.618710000
1	1.018906000	1.108516000	4.569060000
1	2.050032000	-0.509958000	3.030953000
6	5.589679000	-2.700219000	2.173934000
6	5.407021000	-1.316466000	2.058335000
6	4.234138000	-0.810429000	1.498591000
6	3.226642000	-1.682736000	1.049997000
6	3.411789000	-3.067763000	1.179694000
6	4.591883000	-3.573243000	1.735536000
1	6.510543000	-3.094461000	2.611539000
1	6.183358000	-0.630295000	2.406717000
1	4.096585000	0.270025000	1.426361000
1	2.618258000	-3.741049000	0.841636000
1	4.726198000	-4.653760000	1.829282000
6	3.137924000	0.460331000	-3.861814000
6	3.599136000	1.077959000	-2.694173000
6	3.174096000	0.622751000	-1.447319000
6	2.278892000	-0.454228000	-1.351594000
6	1.825166000	-1.071454000	-2.526874000
6	2.252355000	-0.615937000	-3.776636000
1	3.465983000	0.824867000	-4.838357000
1	4.278396000	1.930974000	-2.757562000
1	3.522357000	1.126460000	-0.545185000
1	1.126224000	-1.908747000	-2.455661000
1	1.885184000	-1.100296000	-4.684609000
6	-3.137993000	0.397696000	3.870003000
6	-3.595430000	1.039940000	2.714232000
6	-3.171925000	0.606681000	1.459080000
6	-2.282008000	-0.472620000	1.343126000
6	-1.832320000	-1.114887000	2.506502000
6	-2.258122000	-0.681480000	3.764533000
1	-3.464601000	0.745183000	4.853222000

1	-4.270391000	1.895024000	2.793670000
1	-3.517317000	1.129199000	0.566568000
1	-1.137537000	-1.954149000	2.419515000
1	-1.894180000	-1.185344000	4.663152000
6	-5.595036000	-2.639184000	-2.230922000
6	-5.408565000	-1.258512000	-2.087848000
6	-4.235041000	-0.767017000	-1.516597000
6	-3.230687000	-1.650876000	-1.083678000
6	-3.419749000	-3.032515000	-1.240687000
6	-4.600495000	-3.523504000	-1.808077000
1	-6.516341000	-3.022083000	-2.677577000
1	-6.182334000	-0.563312000	-2.423833000
1	-4.094697000	0.311445000	-1.423156000
1	-4.737819000	-4.601591000	-1.923075000
6	-1.852238000	4.101874000	2.024484000
6	-1.280474000	3.198480000	1.153808000
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1	-1.519215000	3.241878000	0.091195000
6	-1.565647000	4.046834000	3.410089000
6	-0.700601000	3.088893000	3.893892000
1	-2.031868000	4.762953000	4.091277000
1	-0.472907000	3.033044000	4.961699000
6	1.870006000	4.135189000	-1.933019000
6	1.293263000	3.216465000	-1.081876000
1	2.559536000	4.884446000	-1.535989000
1	1.531040000	3.236742000	-0.018362000
6	1.584359000	4.110372000	-3.319722000
6	0.715371000	3.166686000	-3.824073000
1	2.054496000	4.838341000	-3.985478000
1	0.488510000	3.134142000	-4.893017000
1	-2.628853000	-3.714625000	-0.914355000
29	-0.006006000	-2.694733000	-0.024312000

Alkoxyallene (2a)

6	-0.744259000	4.579331000	0.607577000
1	-0.160605000	5.463319000	0.317491000
1	-1.705064000	4.770054000	1.104026000
6	-0.319944000	3.363411000	0.369407000
6	0.143905000	2.151926000	0.154268000
1	0.755671000	1.643832000	0.908938000
8	-0.057049000	1.487630000	-1.025367000
6	0.031648000	0.055989000	-1.020188000
6	-1.228794000	-0.599680000	-0.476095000
6	-1.300658000	-1.998580000	-0.375891000
6	-2.356818000	0.160457000	-0.143590000
6	-2.469014000	-2.622283000	0.063730000
6	-3.525992000	-0.464808000	0.302798000
6	-3.586770000	-1.855417000	0.410034000
1	-0.430842000	-2.604736000	-0.641466000
1	-2.320833000	1.245134000	-0.240172000

1	-2.507158000	-3.712274000	0.136828000
1	-4.396191000	0.143156000	0.563530000
1	-4.501331000	-2.342214000	0.758034000
6	1.334630000	-0.425016000	-0.394959000
6	1.412020000	-0.909272000	0.918773000
6	2.516350000	-0.307400000	-1.141708000
6	2.644255000	-1.271772000	1.470913000
6	3.747894000	-0.669697000	-0.593920000
6	3.814364000	-1.154350000	0.716400000
1	0.501192000	-1.009048000	1.512644000
1	2.465674000	0.079687000	-2.163191000
1	2.688759000	-1.647050000	2.496458000
1	4.658538000	-0.576072000	-1.190968000
1	4.776905000	-1.440734000	1.147725000
1	0.082191000	-0.177213000	-2.096208000

TS1_{cis} (BINAP-CuH + Allene Hydrocupration

TS)

$\nu = -630.0 \text{ cm}^{-1}$

15	0.032908000	-2.619266000	-0.155030000
15	0.158720000	0.480046000	-1.622903000
6	4.539186000	-1.041984000	-1.135686000
6	4.022983000	-0.611896000	-2.386700000
6	2.753909000	-0.097776000	-2.485779000
6	1.904670000	0.004066000	-1.344919000
6	2.353549000	-0.470054000	-0.109686000
6	3.698370000	-0.962473000	0.021310000
1	4.654607000	-0.693028000	-3.275292000
1	2.376904000	0.223570000	-3.456949000
6	0.834238000	0.436161000	3.299019000
6	-0.161359000	-0.568195000	3.406733000
6	-0.330190000	-1.503746000	2.414196000
6	0.469459000	-1.490894000	1.236977000
6	1.463571000	-0.514484000	1.095267000
6	1.670970000	0.451919000	2.136671000
1	-0.793127000	-0.594306000	4.298582000
1	-1.096692000	-2.269144000	2.529003000
6	-2.738697000	-5.860695000	1.676068000
6	-1.394677000	-6.170552000	1.454640000
6	-0.525018000	-5.211822000	0.925481000
6	-0.993011000	-3.928338000	0.606126000
6	-2.353808000	-3.633539000	0.811217000
6	-3.217010000	-4.586433000	1.352654000
1	-3.415420000	-6.613241000	2.088626000
1	-1.016200000	-7.168000000	1.692822000
1	0.518456000	-5.474190000	0.750567000
1	-2.730935000	-2.648784000	0.528616000
1	-4.270120000	-4.338658000	1.508024000
6	4.021847000	-4.649865000	-1.314313000

6	3.683571000	-4.531379000	0.037843000
6	2.482429000	-3.926571000	0.406085000
6	1.602957000	-3.439948000	-0.575312000
6	1.945794000	-3.565350000	-1.929090000
6	3.151703000	-4.168033000	-2.295246000
1	4.971418000	-5.108966000	-1.600036000
1	4.370984000	-4.888132000	0.807951000
1	2.237038000	-3.805956000	1.463432000
1	1.264505000	-3.163290000	-2.683618000
1	3.417002000	-4.248733000	-3.352320000
6	-1.074389000	3.185436000	1.932481000
6	0.058847000	3.523746000	1.186199000
6	0.448594000	2.731524000	0.106958000
6	-0.289243000	1.589318000	-0.239160000
6	-1.431260000	1.262506000	0.507026000
6	-1.820530000	2.055482000	1.588718000
1	-1.369354000	3.800211000	2.786365000
1	0.653851000	4.397970000	1.460087000
1	1.349064000	2.992689000	-0.449575000
1	-1.996063000	0.367044000	0.238139000
1	-2.703163000	1.781726000	2.172087000
6	0.040702000	3.273678000	-5.314079000
6	1.061478000	3.450925000	-4.372024000
6	1.135698000	2.616319000	-3.256576000
6	0.190341000	1.592079000	-3.069430000
6	-0.822739000	1.414964000	-4.025018000
6	-0.898833000	2.255319000	-5.140053000
1	-0.015520000	3.927666000	-6.188312000
1	1.804021000	4.241300000	-4.509937000
1	1.947820000	2.751095000	-2.539776000
1	-1.696377000	2.102995000	-5.868324000
6	2.846353000	2.385671000	3.051856000
6	2.677791000	1.455242000	2.048890000
1	3.626155000	3.146008000	2.961094000
1	3.318172000	1.485215000	1.167496000
6	2.008543000	2.372982000	4.193444000
6	1.022320000	1.417389000	4.309768000
1	2.146554000	3.120828000	4.978299000
1	0.368914000	1.395780000	5.186023000
6	5.520886000	-1.880614000	1.362704000
6	4.231279000	-1.401562000	1.266559000
1	5.906687000	-2.206772000	2.331866000
1	3.604554000	-1.357436000	2.156559000
6	6.343739000	-1.966255000	0.214662000
6	5.856644000	-1.557950000	-1.008772000
1	7.360884000	-2.356506000	0.300550000
1	6.480264000	-1.621444000	-1.904557000
1	-1.547890000	0.607454000	-3.903962000
29	-0.988777000	-1.483625000	-1.825808000
8	-3.956728000	-2.245390000	-4.990401000

6	-5.015374000	-1.408581000	-4.543179000
6	-6.318011000	-1.946560000	-5.118563000
6	-6.368453000	-3.173849000	-5.790098000
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1	-7.606514000	-4.617304000	-6.812431000
1	-9.629107000	-1.116509000	-5.306258000
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6	-4.438350000	0.326055000	-6.287959000
6	-4.749607000	2.412985000	-4.457685000
6	-4.273453000	1.648175000	-6.701900000
6	-4.432636000	2.696868000	-5.787285000
1	-5.162293000	0.862939000	-3.005272000
1	-4.319021000	-0.497193000	-6.995928000
1	-4.861526000	3.224847000	-3.734685000
1	-4.021781000	1.864918000	-7.743566000
1	-4.300180000	3.732412000	-6.110587000
1	-5.077138000	-1.449502000	-3.443363000
6	-3.084998000	-1.213719000	-1.961775000
1	-3.315807000	-0.144596000	-1.915560000
1	-3.652029000	-1.859060000	-1.282733000
6	-2.503662000	-1.763822000	-3.114421000
1	-0.771664000	-2.085184000	-3.260637000
6	-2.750065000	-2.213743000	-4.347898000
1	-1.972085000	-2.643027000	-4.981192000

Acis (BINAP-Cu-alkoxyallyl)

15	-0.327869000	-1.691287000	-1.450444000
15	-0.480251000	1.689430000	-1.998798000
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6	3.134832000	1.061599000	-3.765987000
6	1.879920000	1.520944000	-3.452320000
6	1.285762000	1.251629000	-2.183332000
6	1.977009000	0.472020000	-1.251989000
6	3.314074000	0.033977000	-1.543935000
1	3.565040000	1.263980000	-4.750236000
1	1.315523000	2.089326000	-4.192371000
6	1.147246000	0.319083000	2.495198000
6	0.199243000	-0.735772000	2.500501000
6	-0.147384000	-1.377849000	1.335890000
6	0.417996000	-1.003271000	0.082897000
6	1.355766000	0.036121000	0.040616000
6	1.747791000	0.698113000	1.250385000
1	-0.258069000	-1.031262000	3.448590000

1	-0.882862000	-2.181962000	1.365164000
6	-2.614673000	-5.504236000	-0.138061000
6	-1.216332000	-5.510453000	-0.088743000
6	-0.495885000	-4.370217000	-0.453568000
6	-1.166222000	-3.210039000	-0.873421000
6	-2.568964000	-3.211351000	-0.909725000
6	-3.289613000	-4.350598000	-0.545139000
1	-3.177125000	-6.403028000	0.125791000
1	-0.682620000	-6.411602000	0.224041000
1	0.593404000	-4.396878000	-0.426525000
1	-3.089624000	-2.323497000	-1.271891000
1	-4.379607000	-4.347046000	-0.612215000
6	3.212372000	-3.035335000	-4.110484000
6	3.252223000	-3.314962000	-2.741090000
6	2.197777000	-2.920546000	-1.916667000
6	1.084381000	-2.254212000	-2.453882000
6	1.052656000	-1.979123000	-3.829811000
6	2.111059000	-2.368120000	-4.651719000
1	4.043719000	-3.334151000	-4.753607000
1	4.121024000	-3.815418000	-2.307953000
1	2.262176000	-3.095519000	-0.841581000
1	0.186761000	-1.473026000	-4.260523000
1	2.068870000	-2.153784000	-5.721991000
6	-1.268794000	2.952071000	2.384825000
6	-0.279236000	3.620721000	1.656725000
6	-0.019165000	3.260979000	0.335226000
6	-0.742217000	2.223505000	-0.273508000
6	-1.739886000	1.564940000	0.460599000
6	-2.000899000	1.925349000	1.784325000
1	-1.463250000	3.229600000	3.423676000
1	0.305401000	4.414026000	2.127705000
1	0.765772000	3.779206000	-0.216093000
1	-2.301357000	0.754420000	-0.010733000
1	-2.771757000	1.395407000	2.348829000
6	-1.187600000	5.611294000	-4.356659000
6	0.010129000	5.464153000	-3.646620000
6	0.266336000	4.287811000	-2.941634000
6	-0.672262000	3.241444000	-2.941570000
6	-1.862936000	3.390612000	-3.669075000
6	-2.122541000	4.573553000	-4.367866000
1	-1.386242000	6.534295000	-4.907428000
1	0.747710000	6.270911000	-3.644289000
1	1.210514000	4.175946000	-2.404912000
1	-3.054480000	4.679186000	-4.928798000
6	3.032669000	2.406622000	2.428799000
6	2.699541000	1.757523000	1.259104000
1	3.764439000	3.218205000	2.409729000
1	3.162043000	2.058367000	0.318854000
6	2.427934000	2.035936000	3.654901000
6	1.504518000	1.012989000	3.682708000

1	2.695058000	2.561914000	4.574744000	6	2.837329000	1.559220000	-3.401216000
1	1.029571000	0.718103000	4.622275000	6	1.702368000	1.852296000	-2.685546000
6	5.363912000	-1.136542000	-0.919756000	6	1.568209000	1.464475000	-1.321314000
6	4.090675000	-0.708249000	-0.609152000	6	2.610661000	0.774952000	-0.689109000
1	5.939948000	-1.702011000	-0.182936000	6	3.798038000	0.451275000	-1.430058000
1	3.663919000	-0.941899000	0.365733000	1	2.922821000	1.866074000	-4.447098000
6	5.927400000	-0.859515000	-2.188662000	1	0.878575000	2.380628000	-3.166304000
6	5.201851000	-0.146707000	-3.119004000	6	3.201384000	0.903162000	3.100662000
1	6.934033000	-1.211927000	-2.426722000	6	2.478573000	-0.244307000	3.517557000
1	5.622546000	0.073015000	-4.103795000	6	1.844539000	-1.048072000	2.600226000
1	-2.577781000	2.563399000	-3.686256000	6	1.859984000	-0.735447000	1.212867000
29	-1.673819000	-0.141287000	-2.600016000	6	2.557552000	0.388594000	0.761649000
8	-1.864004000	-3.307900000	-3.831158000	6	3.270514000	1.205868000	1.701181000
6	-1.897394000	-4.729423000	-3.840695000	1	2.440244000	-0.487277000	4.582897000
6	-0.931640000	-5.321784000	-4.856921000	1	1.311002000	-1.935335000	2.940804000
6	-1.345820000	-5.753763000	-6.124224000	6	-1.520803000	-4.883109000	2.338788000
6	0.430556000	-5.379631000	-4.531744000	6	-0.536225000	-5.311453000	1.446031000
6	-0.415238000	-6.236367000	-7.048548000	6	0.254678000	-4.380791000	0.762869000
6	1.362262000	-5.862944000	-5.452161000	6	0.065717000	-3.005829000	0.966674000
6	0.941143000	-6.293976000	-6.713824000	6	-0.941452000	-2.586661000	1.856738000
1	-2.405563000	-5.711976000	-6.384867000	6	-1.722457000	-3.513306000	2.542962000
1	0.762455000	-5.027969000	-3.551943000	1	-2.144327000	-5.610884000	2.863526000
1	-0.750983000	-6.569390000	-8.034206000	1	-0.380127000	-6.379552000	1.273351000
1	2.420488000	-5.897516000	-5.182417000	1	1.014548000	-4.728016000	0.061483000
1	1.668595000	-6.674546000	-7.435751000	1	-1.119677000	-1.519338000	1.999965000
6	-3.311597000	-5.282086000	-3.908921000	1	-2.512954000	-3.168150000	3.212984000
6	-4.426946000	-4.442694000	-4.006275000	6	4.383527000	-3.691543000	-2.341737000
6	-3.511841000	-6.665693000	-3.786715000	6	4.321577000	-3.849457000	-0.952052000
6	-5.718909000	-4.980454000	-3.988251000	6	3.268517000	-3.284059000	-0.233200000
6	-4.800035000	-7.201991000	-3.762961000	6	2.256643000	-2.574705000	-0.901429000
6	-5.911907000	-6.358309000	-3.864967000	6	2.321648000	-2.423807000	-2.293426000
1	-4.283619000	-3.366001000	-4.089547000	6	3.387059000	-2.976555000	-3.009549000
1	-2.645363000	-7.327821000	-3.705627000	1	5.219037000	-4.118475000	-2.902381000
1	-6.580554000	-4.312326000	-4.068885000	1	5.106651000	-4.400321000	-0.427466000
1	-4.937987000	-8.282113000	-3.663480000	1	3.234800000	-3.383572000	0.854536000
1	-6.922344000	-6.775179000	-3.848428000	1	1.539858000	-1.852582000	-2.799602000
1	-1.509068000	-4.992596000	-2.846555000	1	3.442702000	-2.837588000	-4.091665000
6	-3.177980000	-0.713236000	-3.801110000	6	0.561433000	3.324002000	3.689569000
1	-3.758750000	-1.426784000	-3.192123000	6	1.204562000	3.922515000	2.601762000
1	-3.839037000	0.112812000	-4.102238000	6	1.028345000	3.410365000	1.316424000
6	-2.566879000	-1.373185000	-4.973659000	6	0.195438000	2.300334000	1.096218000
6	-2.000033000	-2.596479000	-5.007170000	6	-0.434117000	1.702203000	2.197520000
1	-1.532981000	-3.030241000	-5.894695000	6	-0.255244000	2.208750000	3.486775000
1	-2.517881000	-0.812958000	-5.915422000	1	0.711825000	3.718020000	4.697551000
Acis_chelated (BINAP-Cu-alkoxyallyl)				1	1.869130000	4.774621000	2.759843000
15	0.913830000	-1.724861000	-0.010461000	1	1.570076000	3.854516000	0.479769000
15	-0.096311000	1.576646000	-0.558038000	1	-1.051196000	0.815655000	2.038752000
6	3.909040000	0.842995000	-2.804599000	1	-0.744646000	1.722861000	4.334305000
				6	-2.586735000	4.714686000	-2.904548000
				6	-1.753085000	5.164002000	-1.875435000

6	-0.964643000	4.258104000	-1.161072000
6	-0.998870000	2.888196000	-1.468332000
6	-1.852788000	2.444798000	-2.493658000
6	-2.633465000	3.352347000	-3.211352000
1	-3.206922000	5.425140000	-3.457410000
1	-1.717321000	6.227035000	-1.622471000
1	-0.336419000	4.627193000	-0.351184000
1	-3.297028000	2.985745000	-3.998153000
6	4.665456000	3.139944000	2.223008000
6	4.028994000	2.341345000	1.296757000
1	5.241593000	4.006110000	1.887821000
1	4.096710000	2.579251000	0.235250000
6	4.574528000	2.850526000	3.606537000
6	3.857578000	1.752833000	4.031883000
1	5.077157000	3.495107000	4.331934000
1	3.784779000	1.514513000	5.096455000
6	5.990912000	-0.606547000	-1.589093000
6	4.874362000	-0.278732000	-0.850879000
1	6.795435000	-1.183276000	-1.126546000
1	4.797614000	-0.597786000	0.188177000
6	6.098620000	-0.214171000	-2.945274000
6	5.077010000	0.497316000	-3.536818000
1	6.989382000	-0.480268000	-3.519848000
1	5.145946000	0.803348000	-4.584290000
1	-1.913684000	1.376226000	-2.705251000
29	-0.550842000	-0.563754000	-1.275753000
8	-2.824751000	-0.950839000	-0.710231000
6	-3.594829000	-0.538771000	0.420058000
6	-4.378585000	-1.695226000	1.020410000
6	-5.156877000	-1.477624000	2.168012000
6	-4.270646000	-2.993170000	0.509548000
6	-5.815071000	-2.538222000	2.792410000
6	-4.941060000	-4.053952000	1.126942000
6	-5.711750000	-3.832901000	2.269776000
1	-5.245628000	-0.466232000	2.573708000
1	-3.640434000	-3.176815000	-0.360303000
1	-6.414545000	-2.354327000	3.687877000
1	-4.844550000	-5.062354000	0.716939000
1	-6.230565000	-4.663861000	2.754650000
6	-4.404596000	0.716165000	0.137686000
6	-5.722745000	0.663521000	-0.337267000
6	-3.788099000	1.966014000	0.278908000
6	-6.397903000	1.835633000	-0.685520000
6	-4.457185000	3.140141000	-0.069977000
6	-5.763836000	3.076086000	-0.559807000
1	-6.226492000	-0.301589000	-0.427801000
1	-2.767809000	2.021664000	0.658696000
1	-7.423655000	1.780063000	-1.059076000
1	-3.947429000	4.100905000	0.027155000
1	-6.290116000	3.991907000	-0.841000000

1	-2.819905000	-0.262649000	1.151778000
6	-1.215664000	-1.038119000	-3.112911000
1	-0.900480000	-0.372622000	-3.939180000
1	-0.824256000	-2.036089000	-3.396435000
6	-2.714216000	-1.115423000	-3.067976000
1	-3.305198000	-1.237614000	-3.989540000
6	-3.443461000	-1.074951000	-1.944595000
1	-4.530705000	-1.164467000	-1.920663000

TS1_{trans} (BINAP-CuH + Allene Hydrocupration TS)

$\nu = -622.1 \text{ cm}^{-1}$

15	0.062996000	-1.106375000	-0.336318000
15	0.397207000	2.295334000	-0.838386000
6	4.382843000	0.325892000	-2.320872000
6	3.689677000	1.283820000	-3.103747000
6	2.567268000	1.911684000	-2.619615000
6	2.037749000	1.606592000	-1.333547000
6	2.692616000	0.663309000	-0.533336000
6	3.892320000	0.029106000	-1.008832000
1	4.070275000	1.530593000	-4.098604000
1	2.074755000	2.661454000	-3.236260000
6	2.494876000	0.578092000	3.294627000
6	1.367934000	-0.263785000	3.476142000
6	0.715249000	-0.811794000	2.398634000
6	1.120418000	-0.532867000	1.062195000
6	2.214425000	0.310752000	0.842938000
6	2.938067000	0.853095000	1.960958000
1	1.029452000	-0.483850000	4.492213000
1	-0.136110000	-1.468522000	2.570648000
6	-2.482850000	-4.438743000	1.647697000
6	-1.391125000	-4.810252000	0.858759000
6	-0.605973000	-3.836678000	0.235289000
6	-0.912429000	-2.474408000	0.384783000
6	-2.043772000	-2.112302000	1.138681000
6	-2.807626000	-3.087127000	1.781686000
1	-3.098716000	-5.201092000	2.129560000
1	-1.146708000	-5.867292000	0.724863000
1	0.242869000	-4.144761000	-0.375075000
1	-2.335010000	-1.061763000	1.194887000
1	-3.681388000	-2.789588000	2.364760000
6	3.035542000	-2.923857000	-3.377252000
6	3.119965000	-3.313519000	-2.037027000
6	2.227841000	-2.792662000	-1.099416000
6	1.233520000	-1.884353000	-1.495514000
6	1.152478000	-1.501107000	-2.843018000
6	2.050994000	-2.016737000	-3.778963000
1	3.748391000	-3.318260000	-4.105463000
1	3.903346000	-4.004007000	-1.716675000

1	2.324372000	-3.067319000	-0.047062000
1	0.394221000	-0.770403000	-3.135037000
1	1.990304000	-1.697999000	-4.822508000
6	1.077489000	3.927576000	3.432254000
6	1.989331000	4.253807000	2.422902000
6	1.795729000	3.776521000	1.127060000
6	0.682982000	2.974360000	0.826594000
6	-0.233765000	2.659714000	1.839501000
6	-0.033832000	3.133187000	3.138380000
1	1.241099000	4.287127000	4.451096000
1	2.867854000	4.860410000	2.653613000
1	2.523916000	4.009022000	0.346780000
1	-1.090818000	2.026476000	1.594702000
1	-0.744843000	2.870657000	3.925641000
6	-0.414384000	5.945906000	-3.593929000
6	-0.119221000	6.160713000	-2.246071000
6	0.162275000	5.081611000	-1.402342000
6	0.147538000	3.767564000	-1.895588000
6	-0.178264000	3.560859000	-3.249949000
6	-0.442589000	4.639654000	-4.094047000
1	-0.633338000	6.791226000	-4.251174000
1	-0.108169000	7.176375000	-1.842135000
1	0.382897000	5.268549000	-0.351670000
1	-0.686889000	4.458078000	-5.143808000
6	4.757415000	2.195820000	2.884640000
6	4.087583000	1.678085000	1.796607000
1	5.639245000	2.822648000	2.729916000
1	4.437995000	1.903924000	0.790223000
6	4.304910000	1.933457000	4.200030000
6	3.192784000	1.143319000	4.396098000
1	4.838009000	2.357216000	5.054776000
1	2.831676000	0.931319000	5.406065000
6	5.762730000	-1.510485000	-0.700060000
6	4.620623000	-0.906552000	-0.219773000
1	6.303224000	-2.223528000	-0.072478000
1	4.260033000	-1.148481000	0.779263000
6	6.233167000	-1.225910000	-2.004712000
6	5.551856000	-0.327573000	-2.797165000
1	7.134491000	-1.718048000	-2.378619000
1	5.904883000	-0.095451000	-3.805558000
1	-0.238097000	2.541983000	-3.634803000
29	-1.179604000	0.702729000	-1.035179000
8	-4.510613000	-0.476273000	-0.145859000
6	-5.658810000	-1.299277000	0.046169000
6	-5.387319000	-2.773953000	-0.208206000
6	-6.141517000	-3.724757000	0.494781000
6	-4.410824000	-3.221293000	-1.107625000
6	-5.936115000	-5.091726000	0.297566000
6	-4.201972000	-4.588381000	-1.304088000
6	-4.964078000	-5.528650000	-0.607409000

1	-6.900343000	-3.388060000	1.207670000
1	-3.786837000	-2.502889000	-1.638131000
1	-6.533057000	-5.817468000	0.856266000
1	-3.423371000	-4.917767000	-1.996024000
1	-4.793970000	-6.597530000	-0.759419000
6	-6.881624000	-0.746737000	-0.687141000
6	-7.648794000	-1.509149000	-1.575123000
6	-7.233603000	0.594534000	-0.463408000
6	-8.751927000	-0.943478000	-2.225114000
6	-8.330574000	1.159596000	-1.112074000
6	-9.096280000	0.389501000	-1.995722000
1	-7.382666000	-2.550424000	-1.763612000
1	-6.623473000	1.198182000	0.213345000
1	-9.341030000	-1.550701000	-2.917300000
1	-8.590419000	2.205713000	-0.930438000
1	-9.956623000	0.831034000	-2.505217000
1	-5.858318000	-1.192932000	1.125056000
6	-2.210731000	0.627302000	-2.906995000
1	-2.189926000	1.620111000	-3.367082000
1	-1.926497000	-0.211559000	-3.551983000
6	-3.002488000	0.386516000	-1.781689000
6	-4.160629000	-0.164518000	-1.430851000
1	-4.914176000	-0.376007000	-2.196208000
1	-2.445324000	0.893301000	-0.112333000

A_{trans} (BINAP-Cu-alkoxyallyl)

15	0.795235000	-2.586386000	-0.256863000
15	0.398469000	0.508341000	-1.728830000
6	4.779667000	0.471703000	-0.115803000
6	4.475179000	0.958167000	-1.412915000
6	3.173275000	1.049318000	-1.845683000
6	2.087457000	0.651360000	-1.015756000
6	2.350435000	0.191068000	0.279906000
6	3.699750000	0.106459000	0.752526000
1	5.294904000	1.260040000	-2.070355000
1	2.965307000	1.424472000	-2.847602000
6	-0.292460000	0.527732000	3.034008000
6	-1.018383000	-0.678027000	2.846376000
6	-0.612201000	-1.605452000	1.919521000
6	0.533335000	-1.382276000	1.097066000
6	1.233758000	-0.179266000	1.207040000
6	0.854666000	0.776924000	2.213146000
1	-1.906727000	-0.862005000	3.456099000
1	-1.181523000	-2.527609000	1.796133000
6	-0.199112000	-6.774418000	1.453588000
6	0.416998000	-5.836566000	2.290559000
6	0.710026000	-4.558425000	1.813579000
6	0.386789000	-4.201066000	0.492868000
6	-0.248587000	-5.140892000	-0.332699000
6	-0.532586000	-6.424582000	0.142863000

1	-0.426946000	-7.775399000	1.828783000	6	6.118305000	0.334043000	0.341152000
1	0.668903000	-6.103126000	3.320258000	1	7.422470000	-0.236272000	1.949561000
1	1.175171000	-3.828001000	2.478659000	1	6.932011000	0.608216000	-0.335618000
1	-0.527447000	-4.851286000	-1.349504000	1	1.301678000	-0.324412000	-4.305352000
1	-1.024517000	-7.149069000	-0.510823000	29	-0.483251000	-1.730719000	-1.918684000
6	5.336091000	-2.889681000	-1.117171000	8	-2.823356000	1.741728000	-3.569068000
6	4.864468000	-3.216475000	0.158029000	6	-3.891678000	2.553776000	-4.016665000
6	3.501859000	-3.136318000	0.442000000	6	-4.226264000	2.286979000	-5.471165000
6	2.593342000	-2.722712000	-0.544482000	6	-3.210619000	1.915173000	-6.362184000
6	3.073425000	-2.412056000	-1.825477000	6	-5.531444000	2.443066000	-5.951273000
6	4.438053000	-2.490940000	-2.110227000	6	-3.497965000	1.709528000	-7.712816000
1	6.405769000	-2.942467000	-1.333637000	6	-5.820540000	2.242687000	-7.304556000
1	5.564320000	-3.517902000	0.940519000	6	-4.802954000	1.874764000	-8.189431000
1	3.148824000	-3.381870000	1.443550000	1	-2.197047000	1.788195000	-5.980000000
1	2.368851000	-2.090972000	-2.595827000	1	-6.329906000	2.726598000	-5.258878000
1	4.800224000	-2.231461000	-3.107795000	1	-2.698435000	1.415008000	-8.398032000
6	-2.295408000	2.974249000	1.099855000	1	-6.844159000	2.367662000	-7.667609000
6	-1.055144000	3.494597000	0.716525000	1	-5.027371000	1.711351000	-9.246789000
6	-0.230712000	2.770624000	-0.144764000	6	-3.461563000	3.989063000	-3.727695000
6	-0.640097000	1.520582000	-0.633762000	6	-3.485204000	5.004495000	-4.688823000
6	-1.884316000	1.003350000	-0.244155000	6	-2.981860000	4.282045000	-2.440481000
6	-2.708744000	1.728884000	0.617988000	6	-3.031589000	6.291426000	-4.373036000
1	-2.936518000	3.538292000	1.781552000	6	-2.527397000	5.561743000	-2.125447000
1	-0.720704000	4.458347000	1.106928000	6	-2.548104000	6.573344000	-3.093933000
1	0.747637000	3.166689000	-0.423922000	1	-3.847928000	4.787737000	-5.694914000
1	-2.194841000	0.025972000	-0.616121000	1	-2.942251000	3.488870000	-1.692553000
1	-3.673743000	1.315216000	0.920606000	1	-3.051824000	7.074042000	-5.136216000
6	0.537663000	2.621392000	-5.843392000	1	-2.149196000	5.766787000	-1.120612000
6	0.039996000	3.321899000	-4.742607000	1	-2.189346000	7.576808000	-2.849977000
6	0.020834000	2.725454000	-3.479343000	1	-4.794312000	2.337907000	-3.407605000
6	0.490860000	1.417705000	-3.304694000	6	-2.123777000	-1.908142000	-3.077775000
6	0.973862000	0.712531000	-4.422061000	1	-1.944392000	-2.675679000	-3.848395000
6	1.009598000	1.312818000	-5.680644000	1	-2.982051000	-2.220859000	-2.457893000
1	0.542456000	3.085857000	-6.832730000	6	-2.281746000	-0.559122000	-3.647145000
1	-0.362107000	4.330456000	-4.862620000	1	-1.557904000	-0.261005000	-4.414080000
1	-0.400681000	3.276721000	-2.641816000	6	-3.096012000	0.427514000	-3.231166000
1	1.385540000	0.752733000	-6.540537000	1	-3.892623000	0.297965000	-2.484904000
6	1.180848000	2.898227000	3.376578000	TS2a_{cis}			
6	1.571783000	1.990282000	2.415132000	$\nu = -118.9 \text{ cm}^{-1}$			
1	1.750960000	3.820365000	3.514403000	15	0.579046000	-1.826996000	-0.460387000
1	2.442308000	2.200373000	1.794648000	15	0.554286000	1.584916000	-1.087921000
6	0.040197000	2.651975000	4.177283000	6	5.030320000	0.257498000	-0.879076000
6	-0.681593000	1.490602000	4.003193000	6	4.536717000	1.055894000	-1.942665000
1	-0.266189000	3.383367000	4.929181000	6	3.239387000	1.509682000	-1.940473000
1	-1.566668000	1.289130000	4.612446000	6	2.336152000	1.170207000	-0.893551000
6	5.323879000	-0.482103000	2.475739000	6	2.782377000	0.370022000	0.166674000
6	4.015240000	-0.365767000	2.058331000	6	4.148763000	-0.069640000	0.201679000
1	5.542872000	-0.849992000	3.481362000	1	5.209213000	1.318058000	-2.763776000
1	3.202251000	-0.645265000	2.729130000	1	2.891729000	2.137138000	-2.760832000
6	6.389077000	-0.134514000	1.608990000				

6	1.092452000	0.382213000	3.613326000	1	0.442348000	3.236680000	-5.719678000
6	0.090042000	-0.602065000	3.409434000	6	3.103600000	2.314128000	3.976838000
6	0.012541000	-1.294524000	2.226018000	6	3.007938000	1.654056000	2.769959000
6	0.916133000	-1.034432000	1.154617000	1	3.884815000	3.064314000	4.123580000
6	1.877200000	-0.027077000	1.295334000	1	3.708153000	1.888994000	1.968706000
6	2.006068000	0.666691000	2.546523000	6	2.191255000	2.037463000	5.023080000
1	-0.621276000	-0.808001000	4.213671000	6	1.204260000	1.092741000	4.838454000
1	-0.764813000	-2.046885000	2.091188000	1	2.270834000	2.573249000	5.972196000
6	-1.901360000	-5.629939000	0.430274000	1	0.490821000	0.870308000	5.636541000
6	-0.674872000	-5.464447000	1.086743000	6	5.976441000	-1.275558000	1.281429000
6	0.100409000	-4.330704000	0.843084000	6	4.666611000	-0.846569000	1.277341000
6	-0.341313000	-3.349416000	-0.062171000	1	6.350160000	-1.869199000	2.119463000
6	-1.572255000	-3.522903000	-0.714894000	1	4.008111000	-1.104354000	2.106473000
6	-2.348010000	-4.658983000	-0.466840000	6	6.838743000	-0.964237000	0.202236000
1	-2.507208000	-6.520366000	0.617693000	6	6.370441000	-0.215128000	-0.855580000
1	-0.323867000	-6.221144000	1.793453000	1	7.872836000	-1.317584000	0.211774000
1	1.044919000	-4.203603000	1.374220000	1	7.026286000	0.033817000	-1.694122000
1	-1.933036000	-2.765240000	-1.412327000	1	0.609076000	1.524016000	-3.930493000
1	-3.296709000	-4.780781000	-0.990738000	29	-0.571216000	-0.299537000	-1.713674000
6	4.660062000	-3.119898000	-2.222823000	8	-3.553095000	-2.018532000	-3.339099000
6	4.349371000	-3.482717000	-0.908619000	6	-3.819951000	-2.896363000	-4.436660000
6	3.125818000	-3.113825000	-0.350596000	6	-5.219345000	-2.701708000	-4.991916000
6	2.194459000	-2.379801000	-1.101001000	6	-5.491893000	-2.982733000	-6.336633000
6	2.512280000	-2.024467000	-2.421235000	6	-6.261324000	-2.271318000	-4.161365000
6	3.739036000	-2.390734000	-2.978948000	6	-6.786265000	-2.842719000	-6.843710000
1	5.625947000	-3.397618000	-2.651801000	6	-7.555358000	-2.126010000	-4.666955000
1	5.075655000	-4.034035000	-0.307238000	6	-7.823159000	-2.412727000	-6.008796000
1	2.912634000	-3.368786000	0.688079000	1	-4.681667000	-3.315236000	-6.992446000
1	1.794316000	-1.438838000	-2.997836000	1	-6.047499000	-2.046000000	-3.118475000
1	3.979559000	-2.094355000	-4.002884000	1	-6.985546000	-3.063799000	-7.895710000
6	-0.765688000	3.430555000	2.937722000	1	-8.353923000	-1.783822000	-4.003643000
6	0.426202000	3.866015000	2.348982000	1	-8.835098000	-2.297005000	-6.405890000
6	0.843396000	3.323928000	1.133804000	6	-3.551279000	-4.315603000	-3.962377000
6	0.068137000	2.344411000	0.491248000	6	-4.562166000	-5.131291000	-3.436481000
6	-1.124607000	1.907357000	1.088740000	6	-2.243258000	-4.816812000	-4.024706000
6	-1.537898000	2.451654000	2.307405000	6	-4.270202000	-6.423982000	-2.989970000
1	-1.082643000	3.846692000	3.897148000	6	-1.947843000	-6.105490000	-3.577526000
1	1.045588000	4.611565000	2.852494000	6	-2.963639000	-6.915205000	-3.060904000
1	1.791347000	3.640955000	0.693985000	1	-5.585391000	-4.755455000	-3.386122000
1	-1.707696000	1.120846000	0.604843000	1	-1.448534000	-4.182265000	-4.426237000
1	-2.460742000	2.095448000	2.771816000	1	-5.069840000	-7.051013000	-2.586815000
6	0.253397000	4.890089000	-4.333285000	1	-0.921477000	-6.477206000	-3.627949000
6	0.201058000	5.263532000	-2.988185000	1	-2.736060000	-7.925695000	-2.711952000
6	0.323306000	4.301172000	-1.981006000	1	-3.095999000	-2.671443000	-5.240839000
6	0.495778000	2.947253000	-2.307584000	6	-0.913691000	-0.890751000	-3.743744000
6	0.521495000	2.579299000	-3.666389000	1	-0.019623000	-0.513695000	-4.251745000
6	0.415655000	3.541954000	-4.670594000	1	-0.945310000	-1.978525000	-3.631904000
1	0.155947000	5.644833000	-5.117736000	6	-2.128728000	-0.226331000	-4.010888000
1	0.060920000	6.312943000	-2.716167000	1	-2.076916000	0.803318000	-4.383949000
1	0.267917000	4.609517000	-0.937059000	6	-3.397695000	-0.686346000	-3.699552000

1	-4.295285000	-0.181571000	-4.068142000
6	-3.485788000	0.219336000	-1.495947000
8	-2.484948000	-0.355760000	-0.983038000
6	-4.831550000	-0.365173000	-1.236841000
6	-6.028289000	0.309282000	-1.538415000
6	-4.908820000	-1.643312000	-0.652253000
6	-7.265695000	-0.280086000	-1.270753000
1	-5.999544000	1.300820000	-1.992667000
6	-6.144019000	-2.233692000	-0.392410000
1	-3.979366000	-2.156036000	-0.412047000
6	-7.329939000	-1.555587000	-0.700232000
1	-8.185425000	0.258421000	-1.513700000
1	-6.183885000	-3.231892000	0.051856000
1	-8.298916000	-2.019225000	-0.498357000
6	-3.376558000	1.686451000	-1.859179000
1	-2.351827000	1.904845000	-2.184672000
1	-4.073890000	1.995791000	-2.648450000
1	-3.582628000	2.295326000	-0.960121000

TS2b_{cis}

$\nu = -184.9 \text{ cm}^{-1}$

15	0.387097000	-1.609238000	-0.616742000
15	0.149244000	1.849645000	-0.786745000
6	4.518556000	0.668022000	-1.942003000
6	3.737621000	1.541080000	-2.742215000
6	2.489757000	1.943857000	-2.333239000
6	1.916911000	1.471303000	-1.117575000
6	2.644650000	0.583887000	-0.314496000
6	3.976298000	0.203939000	-0.700107000
1	4.149835000	1.904221000	-3.687403000
1	1.921459000	2.633814000	-2.956421000
6	1.991386000	0.057244000	3.433157000
6	1.016200000	-0.972608000	3.380141000
6	0.623790000	-1.510512000	2.178811000
6	1.152121000	-1.031446000	0.945829000
6	2.088213000	0.009474000	0.954910000
6	2.552243000	0.539744000	2.206077000
1	0.587885000	-1.343924000	4.314958000
1	-0.116029000	-2.310997000	2.162839000
6	-1.841462000	-5.554802000	0.340594000
6	-0.516604000	-5.629542000	-0.102666000
6	0.200500000	-4.461525000	-0.373460000
6	-0.403230000	-3.204107000	-0.209041000
6	-1.741192000	-3.134938000	0.219295000
6	-2.448790000	-4.305827000	0.501692000
1	-2.402326000	-6.469947000	0.547557000
1	-0.039529000	-6.602798000	-0.244232000
1	1.225000000	-4.536768000	-0.737479000
1	-2.233357000	-2.161540000	0.289619000
1	-3.490361000	-4.239107000	0.826078000

6	3.869240000	-2.618256000	-3.492891000
6	3.933723000	-3.059076000	-2.167179000
6	2.897611000	-2.763887000	-1.281517000
6	1.778267000	-2.032164000	-1.711961000
6	1.723021000	-1.592803000	-3.043539000
6	2.762886000	-1.884930000	-3.928701000
1	4.688861000	-2.837886000	-4.181418000
1	4.807535000	-3.611792000	-1.815305000
1	2.970811000	-3.078096000	-0.238642000
1	0.864361000	-1.013229000	-3.380256000
1	2.709030000	-1.530450000	-4.960879000
6	-0.107228000	3.037330000	3.671675000
6	0.899840000	3.594731000	2.877538000
6	0.994191000	3.251616000	1.529451000
6	0.075290000	2.355722000	0.958481000
6	-0.937020000	1.801615000	1.759170000
6	-1.022594000	2.142616000	3.111484000
1	-0.169293000	3.294369000	4.731980000
1	1.631368000	4.276041000	3.317174000
1	1.806087000	3.656881000	0.922152000
1	-1.646674000	1.094930000	1.320643000
1	-1.805163000	1.697832000	3.731022000
6	-0.931607000	5.577209000	-3.334259000
6	-0.587461000	5.759237000	-1.992153000
6	-0.225410000	4.664867000	-1.200122000
6	-0.207975000	3.370515000	-1.741269000
6	-0.585025000	3.195755000	-3.085519000
6	-0.929592000	4.289410000	-3.879816000
1	-1.216889000	6.434239000	-3.949436000
1	-0.603512000	6.760185000	-1.553258000
1	0.025751000	4.823789000	-0.151623000
1	-1.220273000	4.132519000	-4.921433000
6	3.966763000	2.058689000	3.492790000
6	3.550539000	1.552952000	2.279624000
1	4.737364000	2.833241000	3.521534000
1	3.987324000	1.932889000	1.356425000
6	3.396028000	1.591570000	4.701216000
6	2.426035000	0.612652000	4.666725000
1	3.726822000	2.006182000	5.656680000
1	1.978561000	0.240598000	5.592286000
6	6.052459000	-1.016351000	-0.293864000
6	4.785950000	-0.646764000	0.105867000
1	6.653741000	-1.667768000	0.345421000
1	4.388989000	-1.011363000	1.052669000
6	6.575825000	-0.569468000	-1.531027000
6	5.818946000	0.253240000	-2.337136000
1	7.577294000	-0.876800000	-1.842253000
1	6.211010000	0.607685000	-3.294214000
1	-0.630417000	2.186287000	-3.497404000
29	-1.106248000	0.029019000	-1.329252000

8	-3.699810000	-2.365228000	-2.071440000
6	-3.784746000	-3.578590000	-2.839272000
6	-2.734374000	-3.593067000	-3.929745000
6	-1.464864000	-4.103877000	-3.623357000
6	-2.938758000	-2.988401000	-5.177548000
6	-0.409784000	-3.990788000	-4.530270000
6	-1.887465000	-2.880254000	-6.090565000
6	-0.619100000	-3.372030000	-5.766596000
1	-1.296538000	-4.564062000	-2.648049000
1	-3.919573000	-2.578594000	-5.425040000
1	0.579813000	-4.370521000	-4.265820000
1	-2.055317000	-2.395002000	-7.055604000
1	0.206345000	-3.273851000	-6.476767000
6	-5.207536000	-3.911440000	-3.267916000
6	-6.291053000	-3.472381000	-2.491636000
6	-5.468355000	-4.739681000	-4.369516000
6	-7.599919000	-3.830853000	-2.820343000
6	-6.777796000	-5.103925000	-4.697304000
6	-7.850188000	-4.646242000	-3.928074000
1	-6.099117000	-2.847849000	-1.619935000
1	-4.639894000	-5.106534000	-4.977819000
1	-8.429594000	-3.473144000	-2.204683000
1	-6.958558000	-5.748633000	-5.561575000
1	-8.874528000	-4.925989000	-4.187317000
1	-3.488101000	-4.338366000	-2.098094000
6	-1.744128000	-0.497079000	-3.322009000
1	-1.189059000	0.178529000	-3.979857000
1	-1.346099000	-1.509354000	-3.260617000
6	-3.128515000	-0.336413000	-3.270914000
1	-3.548862000	0.600376000	-3.653488000
6	-4.063831000	-1.145373000	-2.618111000
1	-5.126194000	-1.025273000	-2.851717000
6	-4.046930000	-0.006113000	-0.650630000
8	-2.842236000	-0.154003000	-0.262389000
6	-4.486921000	1.329808000	-1.170581000
6	-3.581805000	2.402177000	-1.139368000
6	-5.763231000	1.555083000	-1.719583000
6	-3.920765000	3.651680000	-1.660637000
1	-2.602125000	2.238486000	-0.698572000
6	-6.107103000	2.802568000	-2.239743000
1	-6.489030000	0.740762000	-1.765608000
6	-5.184878000	3.856847000	-2.218669000
1	-3.189687000	4.462600000	-1.632768000
1	-7.100735000	2.953462000	-2.670381000
1	-5.454183000	4.831879000	-2.633063000
6	-5.076189000	-0.873616000	0.046515000
1	-6.075705000	-0.820245000	-0.404132000
1	-4.728495000	-1.914414000	0.038190000
1	-5.155451000	-0.535724000	1.094882000

TS2c_{cis}

$\nu = -198.4 \text{ cm}^{-1}$

15	0.292281000	-2.046424000	-0.056566000
15	-0.003251000	0.989085000	-1.683361000
6	4.584234000	0.117463000	-1.427730000
6	3.978545000	0.567473000	-2.628506000
6	2.644310000	0.897227000	-2.665845000
6	1.821135000	0.790761000	-1.509770000
6	2.390668000	0.368426000	-0.301744000
6	3.783449000	0.037208000	-0.242583000
1	4.588817000	0.645387000	-3.532279000
1	2.204136000	1.236778000	-3.603151000
6	0.792162000	1.403767000	3.025040000
6	-0.199513000	0.394078000	3.154293000
6	-0.262083000	-0.645974000	2.262739000
6	0.643999000	-0.736049000	1.162294000
6	1.567363000	0.288690000	0.947350000
6	1.693700000	1.347688000	1.913196000
1	-0.912430000	0.454415000	3.980580000
1	-1.033303000	-1.408770000	2.380699000
6	-0.605016000	-5.994938000	2.189980000
6	0.113277000	-4.998924000	2.860732000
6	0.380484000	-3.780632000	2.232034000
6	-0.081178000	-3.539439000	0.927383000
6	-0.813041000	-4.539799000	0.267090000
6	-1.065118000	-5.763404000	0.890598000
1	-0.809625000	-6.948655000	2.683017000
1	0.473862000	-5.174449000	3.877656000
1	0.949137000	-3.013987000	2.761637000
1	-1.195795000	-4.346382000	-0.737326000
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6	4.106716000	-3.500335000	-0.689897000
6	2.925430000	-3.104009000	-0.064703000
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1	4.927525000	-3.905000000	-0.093511000
1	2.824441000	-3.213023000	1.016194000
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1	3.301521000	-2.729859000	-3.914893000
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6	0.046198000	4.312619000	0.763656000
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1	-2.295914000	1.292161000	0.025632000	1	-6.667994000	1.589667000	-5.440848000
1	-2.937480000	2.981205000	1.746194000	1	-3.282907000	4.326386000	-3.029257000
6	-0.611666000	2.965564000	-5.836753000	1	-7.185516000	3.948687000	-4.841214000
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6	-0.304391000	3.223913000	-3.445548000	1	-5.300182000	-0.353685000	-5.066042000
6	-0.196232000	1.832050000	-3.295782000	6	-1.685004000	-2.369034000	-3.159439000
6	-0.301610000	1.019239000	-4.438398000	1	-1.059141000	-3.256142000	-3.028231000
6	-0.500473000	1.579067000	-5.700447000	1	-1.324869000	-1.650067000	-3.901043000
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6	0.900511000	2.465734000	3.961057000	6	-6.179328000	-3.898230000	-0.038382000
1	1.954212000	4.240179000	4.559108000	1	-6.545142000	-2.277248000	-1.403145000
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1	6.186463000	-1.108467000	1.918387000	1	-7.149881000	-4.364061000	-0.229800000
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6	6.519134000	-0.693944000	-0.191495000	1	-5.561405000	-5.403622000	1.393579000
6	5.952778000	-0.261578000	-1.371358000	6	-5.260776000	0.200313000	-1.416776000
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1	-0.250851000	-0.064554000	-4.332242000	1	-5.546066000	0.664722000	-0.455142000
29	-1.185772000	-1.078611000	-1.482759000	TS2d_{cis}			
8	-3.578253000	-0.392786000	-3.929529000	$\nu = -172.4 \text{ cm}^{-1}$			
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6	-3.590796000	0.088579000	-6.282494000	15	3.205235000	0.291378000	-1.657628000
6	-3.622391000	1.099033000	-7.251414000	6	7.790094000	0.397247000	-0.712864000
6	-2.838487000	-1.068687000	-6.535987000	6	7.311875000	0.310128000	-2.044780000
6	-2.914839000	0.959491000	-8.450055000	6	5.965887000	0.361999000	-2.316181000
6	-2.130750000	-1.207898000	-7.731213000	6	4.998933000	0.472168000	-1.276252000
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1	-2.945318000	1.761786000	-9.192113000	1	5.635110000	0.319240000	-3.351975000
1	-1.545957000	-2.114141000	-7.909993000	6	3.461721000	2.277303000	2.851577000
1	-1.606255000	-0.300029000	-9.628090000	6	2.740201000	1.173439000	3.373319000
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6	-3.738334000	2.414560000	-3.908010000	6	3.763242000	-0.332567000	1.742731000
6	-5.921974000	2.195636000	-4.917843000	6	4.483273000	0.734831000	1.194705000
6	-4.028712000	3.735135000	-3.565891000	6	4.359226000	2.052195000	1.758997000
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6	3.956468000	-4.084336000	2.864528000	6	7.335896000	0.685487000	1.675602000
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1	1.644251000	-5.578845000	4.886925000	6	9.177140000	0.341223000	-0.408445000
1	4.066434000	-5.694606000	4.296213000	1	10.690921000	0.421509000	1.113440000
1	5.015255000	-4.153651000	2.616096000	1	9.886278000	0.205356000	-1.229498000
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1	0.171194000	-3.924073000	3.733775000	29	2.337725000	-1.767348000	-0.903235000
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6	5.828614000	-2.851568000	-0.637242000	6	-0.130498000	-1.465533000	-5.898015000
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1	5.063803000	-2.899713000	-1.415889000	1	0.694938000	-0.959625000	-5.395963000
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6	1.187893000	3.894982000	0.408805000	1	0.972926000	-1.806146000	-7.718498000
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6	2.904951000	3.055940000	-1.077051000	6	-1.533243000	0.417954000	-3.769931000
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6	0.705312000	2.595703000	0.587315000	6	-0.721989000	2.549963000	-2.942180000
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1	3.778084000	3.233016000	-1.708819000	1	0.169783000	0.627684000	-2.489511000
1	0.953381000	0.504731000	0.082148000	1	-3.270638000	0.519065000	-5.051611000
1	-0.150898000	2.409743000	1.240031000	1	-0.009320000	3.111339000	-2.333241000
6	2.807951000	0.725808000	-6.262960000	1	-3.462990000	2.991965000	-4.921276000
6	2.313148000	1.736914000	-5.437199000	1	-1.834681000	4.303261000	-3.553736000
6	2.465783000	1.655226000	-4.050406000	1	-2.431114000	-1.470484000	-3.371523000
6	3.100734000	0.551343000	-3.462847000	6	2.009093000	-2.997446000	-2.638401000
6	3.576577000	-0.473409000	-4.305463000	1	2.858531000	-3.688305000	-2.666457000
6	3.446476000	-0.380145000	-5.691208000	1	2.064244000	-2.151236000	-3.326904000
1	2.682943000	0.789238000	-7.346578000	6	0.732275000	-3.553049000	-2.474049000
1	1.792972000	2.595439000	-5.868438000	1	0.638580000	-4.586154000	-2.125368000
1	2.066464000	2.451649000	-3.426136000	6	-0.457626000	-2.840733000	-2.553235000
1	3.824649000	-1.186123000	-6.324913000	1	-1.421071000	-3.345504000	-2.651517000
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6	-3.227167000	0.273165000	-0.813523000
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1	-3.113589000	-3.592999000	-0.477495000
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6	4.141469000	-0.144649000	0.088006000
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6	-0.500239000	-5.856392000	1.096676000
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6	-0.299916000	-3.541191000	0.388394000
6	-1.691468000	-3.390208000	0.544448000
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6	3.177845000	-3.241221000	0.024458000
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1	-2.382699000	2.013138000	2.732617000
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6	-0.331085000	4.625317000	-3.493124000
6	-0.077445000	3.799043000	-2.393003000
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6	0.350270000	1.954441000	-3.896705000
6	0.103142000	2.779729000	-4.991998000
1	-0.453078000	4.764020000	-5.648513000
1	-0.611021000	5.669110000	-3.328400000
1	-0.175491000	4.203291000	-1.385431000
1	0.141400000	2.369111000	-6.002962000
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1	3.935755000	3.421706000	3.597110000
1	3.673068000	2.015401000	1.594591000
6	2.374623000	2.411535000	4.726495000
6	1.435158000	1.402849000	4.717714000
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1	0.796827000	1.229785000	5.588265000
6	6.058696000	-1.140453000	1.226796000
6	4.732430000	-0.764834000	1.226014000
1	6.488057000	-1.611422000	2.114648000
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6	6.866197000	-0.933409000	0.082363000
6	6.326954000	-0.337352000	-1.037129000
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6	-2.134983000	1.664907000	-8.084434000

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6	-2.262080000	2.995788000	-7.681872000
1	-2.777466000	-0.376690000	-7.757284000
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1	-1.453950000	1.399835000	-8.897468000
1	-3.226811000	4.362080000	-6.306665000
1	-1.682070000	3.777655000	-8.179477000
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TS2b_{trans}

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6	-0.577410000	-3.375985000	0.476875000
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6	5.880321000	-0.733331000	1.289745000
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1	4.953454000	-2.386821000	-2.008651000	6	-1.724556000	-0.841053000	0.152112000
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6	3.811818000	2.942264000	3.411418000	6	-4.159353000	-0.837354000	0.057784000
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1	6.734670000	0.711536000	3.173785000	6	-2.245932000	-6.960034000	-2.110825000
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6	5.799293000	0.900540000	-1.056599000
6	5.138683000	0.440592000	0.119021000
6	5.783429000	-0.479870000	0.955708000
6	7.123644000	-0.900183000	0.651278000
1	7.542518000	0.819006000	-2.301695000
1	5.290135000	1.612736000	-1.706630000
6	4.877906000	-0.963252000	4.655188000
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6	3.529014000	-2.483034000	3.324894000
6	4.152139000	-2.033319000	2.126759000
6	5.128633000	-1.032397000	2.187938000
6	5.534250000	-0.512571000	3.464010000
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1	2.758855000	-3.252054000	3.266390000
6	0.937546000	-6.377797000	1.384571000
6	2.278020000	-6.551363000	1.022301000
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6	2.563375000	-4.141875000	0.895803000
6	1.210818000	-3.970118000	1.246196000
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1	0.303643000	-7.249226000	1.568812000
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1	4.125327000	-5.589875000	0.479529000
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6	5.964612000	-3.923567000	0.119986000
6	4.944793000	-3.130534000	-0.430556000
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1	5.902517000	-4.239544000	1.163213000
1	4.295379000	-2.050943000	-2.180495000
1	6.272478000	-2.673005000	-3.546273000
6	2.824696000	2.043070000	4.775033000
6	3.908926000	2.566275000	4.063377000
6	4.091382000	2.225543000	2.723760000
6	3.185550000	1.365979000	2.080332000

6	2.096304000	0.841043000	2.797905000
6	1.923453000	1.183139000	4.142108000
1	2.690923000	2.299546000	5.828964000
1	4.629901000	3.217914000	4.561659000
1	4.961795000	2.601461000	2.182312000
1	1.390007000	0.164641000	2.302740000
1	1.080198000	0.765661000	4.697760000
6	2.440388000	4.602655000	-2.244611000
6	2.825941000	4.787565000	-0.914182000
6	3.152049000	3.688780000	-0.113882000
6	3.092749000	2.387746000	-0.635003000
6	2.687220000	2.212839000	-1.970083000
6	2.374699000	3.309800000	-2.772935000
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1	2.867099000	5.794459000	-0.490756000
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6	6.920435000	0.962608000	4.830068000
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1	9.538656000	-0.531031000	-1.781743000
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6	-3.153597000	-1.599420000	-1.002624000
6	-2.907108000	0.599809000	0.683020000
1	-0.896395000	-0.148259000	1.050312000
6	-4.225718000	-0.716332000	-0.847412000
1	-3.280158000	-2.474248000	-1.645670000
6	-4.103247000	0.396314000	-0.009793000
1	-2.807080000	1.454371000	1.358699000
1	-5.161810000	-0.898929000	-1.382360000
1	-4.938132000	1.091818000	0.108671000
6	-1.106495000	-3.645929000	0.223455000
1	-2.001578000	-4.119527000	-0.212081000
1	-0.277270000	-4.367737000	0.204612000
1	-1.324795000	-3.415772000	1.276963000

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15	3.545372000	-2.856310000	0.499841000
15	3.288371000	0.564938000	-0.067914000
6	7.829791000	-0.470835000	-0.387394000
6	7.182706000	0.319713000	-1.371952000

6	5.866566000	0.688788000	-1.226708000	6	2.915506000	1.847399000	-1.306419000
6	5.096993000	0.265131000	-0.106628000	6	2.978052000	1.489268000	-2.668454000
6	5.695836000	-0.529057000	0.879783000	6	2.504871000	2.349564000	-3.657317000
6	7.084052000	-0.879608000	0.765872000	1	1.536429000	4.238559000	-4.076736000
1	7.753522000	0.652060000	-2.243294000	1	1.410590000	4.894769000	-1.671855000
1	5.404454000	1.323319000	-1.982474000	1	2.263220000	3.371367000	0.084162000
6	4.470466000	-0.648290000	4.512630000	1	2.549453000	2.048774000	-4.705716000
6	3.531998000	-1.709223000	4.438336000	6	6.361980000	1.429516000	4.620816000
6	3.330541000	-2.392243000	3.263570000	6	6.143985000	0.772840000	3.428661000
6	4.035416000	-2.045948000	2.076543000	1	7.096104000	2.237812000	4.667558000
6	4.945837000	-0.982819000	2.098882000	1	6.700469000	1.069813000	2.540513000
6	5.197586000	-0.287427000	3.332088000	6	5.632690000	1.075731000	5.781344000
1	2.970201000	-1.983786000	5.334923000	6	4.703290000	0.060034000	5.722549000
1	2.607077000	-3.206236000	3.234201000	1	5.806924000	1.609566000	6.718846000
6	1.175442000	-6.651748000	1.680801000	1	4.129531000	-0.221658000	6.609462000
6	2.527281000	-6.787508000	1.350898000	6	9.092486000	-1.964742000	1.632843000
6	3.283853000	-5.664301000	1.003470000	6	7.760916000	-1.634547000	1.766175000
6	2.688977000	-4.393477000	0.979408000	1	9.589105000	-2.541163000	2.417395000
6	1.319223000	-4.261624000	1.288769000	1	7.208683000	-1.954968000	2.649024000
6	0.575616000	-5.388294000	1.647608000	6	9.819274000	-1.574839000	0.482019000
1	0.588396000	-7.532520000	1.954373000	6	9.195591000	-0.845551000	-0.507423000
1	2.998523000	-7.773878000	1.361886000	1	10.872292000	-1.850012000	0.383474000
1	4.334291000	-5.787639000	0.738060000	1	9.745835000	-0.532617000	-1.398926000
1	0.836788000	-3.275472000	1.224345000	1	3.377058000	0.512429000	-2.950997000
1	-0.483929000	-5.270623000	1.889925000	29	2.126810000	-1.380099000	-0.463527000
6	7.548527000	-3.944377000	-1.536617000	6	1.673584000	-2.044593000	-2.603598000
6	7.339907000	-4.315568000	-0.205010000	1	2.520487000	-1.723939000	-3.216185000
6	6.133708000	-4.011090000	0.426187000	1	1.530803000	-3.122180000	-2.482008000
6	5.115934000	-3.343137000	-0.273089000	6	0.735810000	-1.154519000	-2.174052000
6	5.331672000	-2.979707000	-1.611078000	1	0.848810000	-0.102049000	-2.440967000
6	6.542532000	-3.275113000	-2.239174000	6	-0.558697000	-1.582221000	-1.500522000
1	8.502356000	-4.165227000	-2.021453000	6	-0.666687000	-0.915452000	-0.079680000
1	8.132973000	-4.817949000	0.353040000	8	0.451901000	-1.394822000	0.607896000
1	5.993133000	-4.262398000	1.479363000	6	-1.905602000	-1.420346000	0.676916000
1	4.549356000	-2.436129000	-2.143033000	6	-2.237903000	-2.786217000	0.640884000
1	6.706764000	-2.968709000	-3.275089000	6	-2.665219000	-0.591553000	1.511764000
6	2.443164000	2.370869000	4.087783000	6	-3.290008000	-3.299566000	1.398695000
6	3.470863000	2.911380000	3.307028000	1	-1.662839000	-3.467699000	0.013009000
6	3.730692000	2.388861000	2.040668000	6	-3.714825000	-1.101019000	2.282495000
6	2.960749000	1.323180000	1.546748000	1	-2.450438000	0.475219000	1.562363000
6	1.924321000	0.784314000	2.327368000	6	-4.036087000	-2.457170000	2.230458000
6	1.672555000	1.314068000	3.595949000	1	-3.528107000	-4.365762000	1.342329000
1	2.251612000	2.771917000	5.086313000	1	-4.292151000	-0.424695000	2.918754000
1	4.085037000	3.726365000	3.697014000	1	-4.859820000	-2.856176000	2.828415000
1	4.549796000	2.791834000	1.440323000	6	-0.595806000	0.618086000	-0.159951000
1	1.328040000	-0.049228000	1.934734000	1	-1.442186000	1.068153000	-0.683572000
1	0.873878000	0.885308000	4.206508000	1	-0.544695000	1.043335000	0.851004000
6	1.935972000	3.578161000	-3.303865000	1	0.324915000	0.921298000	-0.672637000
6	1.861363000	3.940923000	-1.957788000	8	-1.669368000	-1.641364000	-2.412416000
6	2.348247000	3.084951000	-0.964449000	6	-2.498594000	-0.600516000	-2.933805000

6	-1.775209000	0.380585000	-3.858347000
6	-2.230615000	1.675575000	-4.151765000
6	-0.695412000	-0.114243000	-4.611935000
6	-0.048375000	0.674392000	-5.562054000
1	-0.376963000	-1.142602000	-4.451951000
1	0.790540000	0.258202000	-6.126614000
6	-3.527118000	-0.096300000	-1.916915000
6	-4.448184000	-1.059126000	-1.467908000
6	-3.643309000	1.203829000	-1.409550000
6	-5.453844000	-0.737425000	-0.560718000
6	-4.655380000	1.535291000	-0.501543000
6	-5.567327000	0.569846000	-0.078088000
1	-4.353133000	-2.085134000	-1.830409000
1	-2.937435000	1.978032000	-1.702880000
1	-6.144025000	-1.511673000	-0.218981000
1	-4.721419000	2.558307000	-0.121977000
1	-6.354566000	0.828551000	0.634453000
1	-3.115135000	-1.188018000	-3.638115000
6	-1.581837000	2.471331000	-5.103425000
6	-0.478775000	1.982661000	-5.803209000
1	-3.118198000	2.070857000	-3.662923000
1	0.027470000	2.606104000	-6.544822000
1	-1.954902000	3.479732000	-5.301128000
1	-0.427761000	-2.647614000	-1.271723000

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15	3.218046000	-2.049492000	0.089618000
15	2.940142000	1.254672000	1.177065000
6	7.253418000	0.749692000	-0.540930000
6	6.415723000	1.829488000	-0.922841000
6	5.181133000	2.001962000	-0.344836000
6	4.685203000	1.091915000	0.632110000
6	5.467760000	-0.006630000	1.011032000
6	6.781013000	-0.171010000	0.450249000
1	6.774014000	2.537812000	-1.674738000
1	4.565469000	2.852134000	-0.639649000
6	5.072690000	-1.820307000	4.370138000
6	4.102727000	-2.796464000	4.026952000
6	3.627625000	-2.896587000	2.742051000
6	4.064637000	-2.006919000	1.720951000
6	4.997257000	-1.008185000	2.026053000
6	5.543529000	-0.928089000	3.352948000
1	3.741783000	-3.479442000	4.800350000
1	2.891509000	-3.662331000	2.501244000
6	1.040232000	-6.133652000	-0.023913000
6	2.258225000	-6.011988000	-0.697652000
6	2.950557000	-4.797584000	-0.687736000
6	2.425245000	-3.690657000	-0.003470000
6	1.175090000	-3.804525000	0.638950000

6	0.498816000	-5.025875000	0.635820000
1	0.504834000	-7.086800000	-0.028850000
1	2.677017000	-6.867923000	-1.233746000
1	3.897112000	-4.716806000	-1.222451000
1	0.730702000	-2.920863000	1.117564000
1	-0.467348000	-5.104382000	1.140966000
6	6.686718000	-1.953005000	-2.967461000
6	6.719789000	-2.885585000	-1.926347000
6	5.676413000	-2.940496000	-1.002145000
6	4.579572000	-2.070911000	-1.116061000
6	4.554863000	-1.139190000	-2.164577000
6	5.602421000	-1.079667000	-3.085047000
1	7.515279000	-1.897343000	-3.677343000
1	7.577726000	-3.552634000	-1.816540000
1	5.727843000	-3.640827000	-0.166003000
1	3.724240000	-0.436577000	-2.230811000
1	5.580460000	-0.335860000	-3.885138000
6	2.981788000	0.806325000	5.772045000
6	3.915732000	1.651354000	5.163984000
6	3.916604000	1.803985000	3.778037000
6	2.976735000	1.120509000	2.988774000
6	2.037483000	0.272412000	3.601873000
6	2.047431000	0.121181000	4.991234000
1	2.992004000	0.675391000	6.857023000
1	4.662986000	2.169723000	5.768825000
1	4.673579000	2.431170000	3.302478000
1	1.303951000	-0.266430000	2.990294000
1	1.321410000	-0.545658000	5.462733000
6	1.497803000	5.535509000	0.136332000
6	2.004354000	5.290521000	1.415276000
6	2.484984000	4.022310000	1.754472000
6	2.462842000	2.980585000	0.815509000
6	1.937547000	3.235134000	-0.464037000
6	1.468010000	4.503052000	-0.806308000
1	1.114995000	6.525851000	-0.122415000
1	2.019479000	6.090095000	2.160412000
1	2.855687000	3.841538000	2.763260000
1	1.057735000	4.679695000	-1.803566000
6	7.030218000	0.099156000	4.996079000
6	6.535249000	0.029609000	3.711483000
1	7.793059000	0.841810000	5.243186000
1	6.903061000	0.720100000	2.953359000
6	6.549154000	-0.774276000	6.001036000
6	5.587148000	-1.710820000	5.690453000
1	6.941700000	-0.703238000	7.018435000
1	5.206447000	-2.392465000	6.455686000
6	8.902634000	-1.370343000	0.289619000
6	7.646863000	-1.232235000	0.841388000
1	9.548338000	-2.191396000	0.611088000
1	7.304308000	-1.944649000	1.591288000

6	9.357950000	-0.466281000	-0.699888000
6	8.544409000	0.569141000	-1.106921000
1	10.351866000	-0.590818000	-1.136823000
1	8.883094000	1.276280000	-1.868948000
1	1.881388000	2.420504000	-1.188383000
29	1.673405000	-0.371720000	0.228540000
6	1.012999000	-0.246396000	-2.115277000
1	1.631321000	0.523499000	-2.585742000
1	1.244901000	-1.284901000	-2.356736000
6	-0.072434000	0.080672000	-1.380803000
1	-0.320077000	1.135263000	-1.228832000
6	-1.031918000	-0.918149000	-0.767792000
6	-1.146952000	-0.678899000	0.778522000
8	0.111573000	-0.910569000	1.306962000
6	-1.635132000	0.766751000	1.028672000
6	-2.895774000	1.223198000	0.603811000
6	-0.782093000	1.686072000	1.651243000
6	-3.268840000	2.560323000	0.768496000
1	-3.580976000	0.530763000	0.116137000
6	-1.147348000	3.025275000	1.815561000
1	0.181113000	1.329288000	2.003917000
6	-2.392303000	3.471659000	1.367534000
1	-4.251641000	2.892973000	0.422099000
1	-0.448976000	3.720469000	2.287805000
1	-2.681439000	4.519339000	1.487922000
6	-2.141774000	-1.687289000	1.378022000
1	-2.110242000	-1.594659000	2.473954000
1	-3.173680000	-1.532969000	1.032840000
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8	-2.329797000	-0.870618000	-1.356102000
6	-2.535781000	-1.338176000	-2.688620000
6	-1.697573000	-2.575250000	-2.988856000
6	-0.563210000	-2.563289000	-3.809128000
6	-2.022570000	-3.760888000	-2.311626000
6	-1.225056000	-4.898449000	-2.433563000
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1	-1.483466000	-5.806521000	-1.884690000
6	-2.469815000	-0.207987000	-3.709478000
6	-2.540537000	-0.477631000	-5.085458000
6	-2.449665000	1.128342000	-3.288461000
6	-2.547915000	0.561503000	-6.018711000
6	-2.454268000	2.169079000	-4.221609000
6	-2.495456000	1.891494000	-5.590163000
1	-2.589138000	-1.512489000	-5.432335000
1	-2.446999000	1.349618000	-2.221598000
1	-2.596309000	0.330247000	-7.086164000
1	-2.434066000	3.204844000	-3.872034000
1	-2.498462000	2.705767000	-6.319483000
1	-3.589021000	-1.672074000	-2.671712000
6	0.237311000	-3.702989000	-3.936833000

6	-0.086266000	-4.871217000	-3.244211000
1	-0.291651000	-1.649997000	-4.338960000
1	0.550139000	-5.754731000	-3.326518000
1	1.126532000	-3.671453000	-4.571911000
1	-0.609590000	-1.929279000	-0.877722000

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6	1.872038000	-2.032578000	-2.649678000
1	2.878962000	-1.940318000	-3.064545000
1	1.593083000	-3.011781000	-2.248464000
6	1.023877000	-0.999023000	-2.640604000
1	1.346107000	-0.041753000	-3.064062000
6	-0.354925000	-0.990364000	-2.058626000
1	-1.042785000	-0.485675000	-2.756366000
6	-0.438223000	-0.314710000	-0.601685000
6	-1.937759000	0.013516000	-0.375481000
6	-2.666345000	0.861594000	-1.223783000
6	-2.605470000	-0.570196000	0.707233000
6	-4.028091000	1.092757000	-1.016701000
1	-2.172760000	1.343677000	-2.072221000
6	-3.970753000	-0.349441000	0.917598000
1	-2.013815000	-1.193972000	1.379714000
6	-4.690723000	0.478754000	0.051644000
1	-4.577471000	1.747777000	-1.698346000
1	-4.474755000	-0.820973000	1.766387000
1	-5.757991000	0.653217000	0.212377000
6	0.364968000	1.004524000	-0.592555000
1	0.071190000	1.710147000	-1.387982000
1	0.208092000	1.491143000	0.381293000
1	1.435891000	0.774152000	-0.688246000
8	-0.832985000	-2.330720000	-1.828846000
6	-1.243925000	-3.111974000	-2.949303000
6	-2.608321000	-2.698327000	-3.470875000
6	-2.917609000	-2.906517000	-4.821974000
6	-3.578206000	-2.148001000	-2.623119000
6	-4.840718000	-1.816370000	-3.121906000
1	-3.339158000	-1.948916000	-1.578494000
1	-5.578672000	-1.372938000	-2.449922000
6	-1.200238000	-4.548448000	-2.457671000
6	-0.334060000	-5.482106000	-3.038151000
6	-1.987895000	-4.938644000	-1.360190000
6	-0.253781000	-6.786014000	-2.536931000
6	-1.897768000	-6.236261000	-0.850675000
6	-1.030938000	-7.164439000	-1.439680000
1	0.288135000	-5.183236000	-3.885990000
1	-2.691665000	-4.227545000	-0.919652000
1	0.424661000	-7.505604000	-3.002030000
1	-2.517075000	-6.529406000	0.000875000
1	-0.966601000	-8.181398000	-1.045142000
1	-0.507770000	-2.999503000	-3.761538000

6	-4.181170000	-2.581069000	-5.319102000
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1	-6.134517000	-1.771903000	-4.856070000
1	-4.409767000	-2.746020000	-6.375137000
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8	2.667602000	0.464490000	1.057861000
6	1.505856000	-1.718016000	2.589246000
1	2.064543000	-2.515185000	2.072887000
1	2.080226000	-1.421053000	3.481571000
1	0.544299000	-2.141131000	2.919741000
6	0.805494000	1.877252000	3.111289000
1	0.067312000	2.689044000	3.211370000
1	0.936428000	1.412808000	4.107104000
1	1.771241000	2.314642000	2.803778000
6	3.735757000	-0.164065000	0.394056000
1	3.429414000	-0.567621000	-0.589199000
1	4.537067000	0.573629000	0.226610000
1	4.160791000	-0.997950000	0.985154000
14	1.223695000	-0.263888000	1.462524000
6	0.343256000	1.153369000	-1.276513000
6	-0.342307000	-0.158175000	-0.875618000
1	1.372093000	0.964810000	-1.619098000
1	0.383369000	1.847313000	-0.424005000
1	-0.210019000	1.641977000	-2.093890000
6	-1.748317000	0.108591000	-0.327523000
6	-0.389973000	-1.125890000	-2.058769000
1	-2.220461000	-0.839268000	-0.025770000
1	-2.383616000	0.588042000	-1.089195000
1	-1.690544000	0.763609000	0.554016000
1	-0.988389000	-0.710497000	-2.884699000
1	-0.835899000	-2.082443000	-1.746360000
1	0.627737000	-1.326338000	-2.428454000
8	0.414815000	-0.830991000	0.144775000

(MeO)₂MeSiH

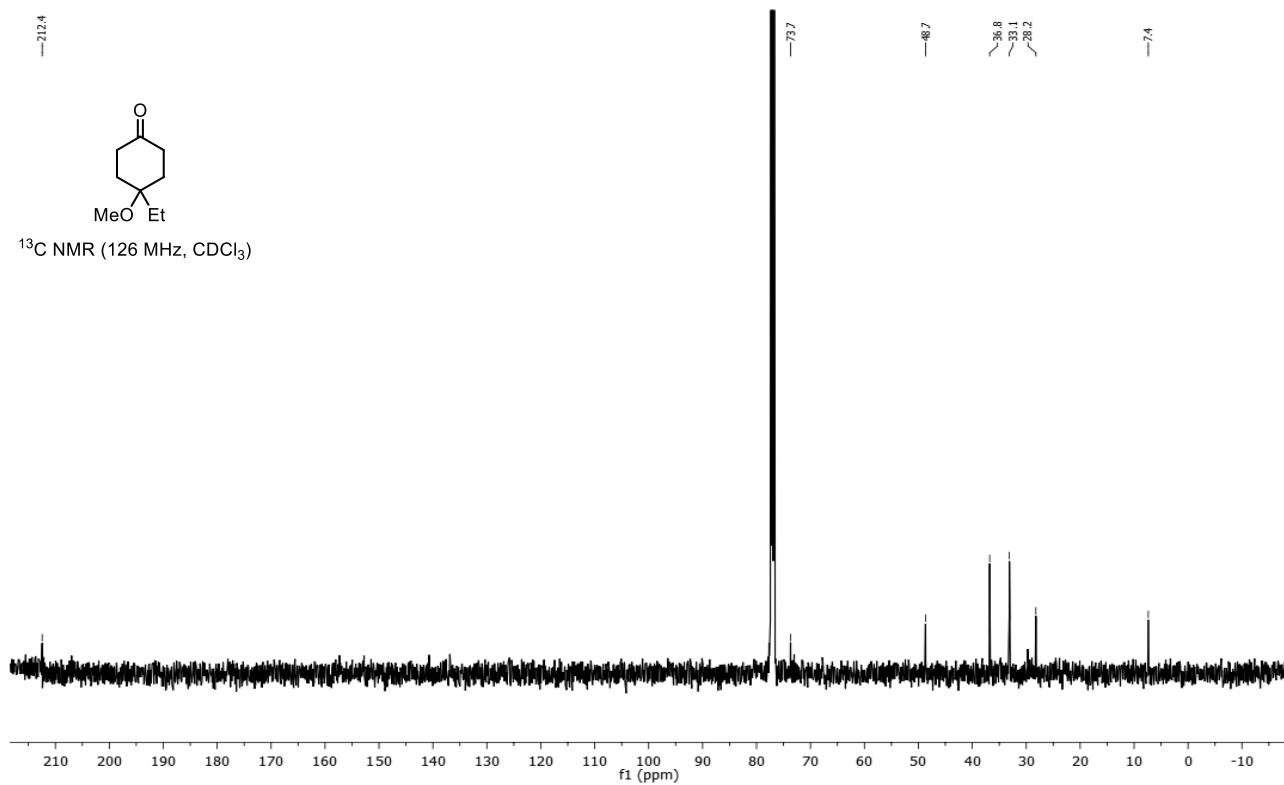
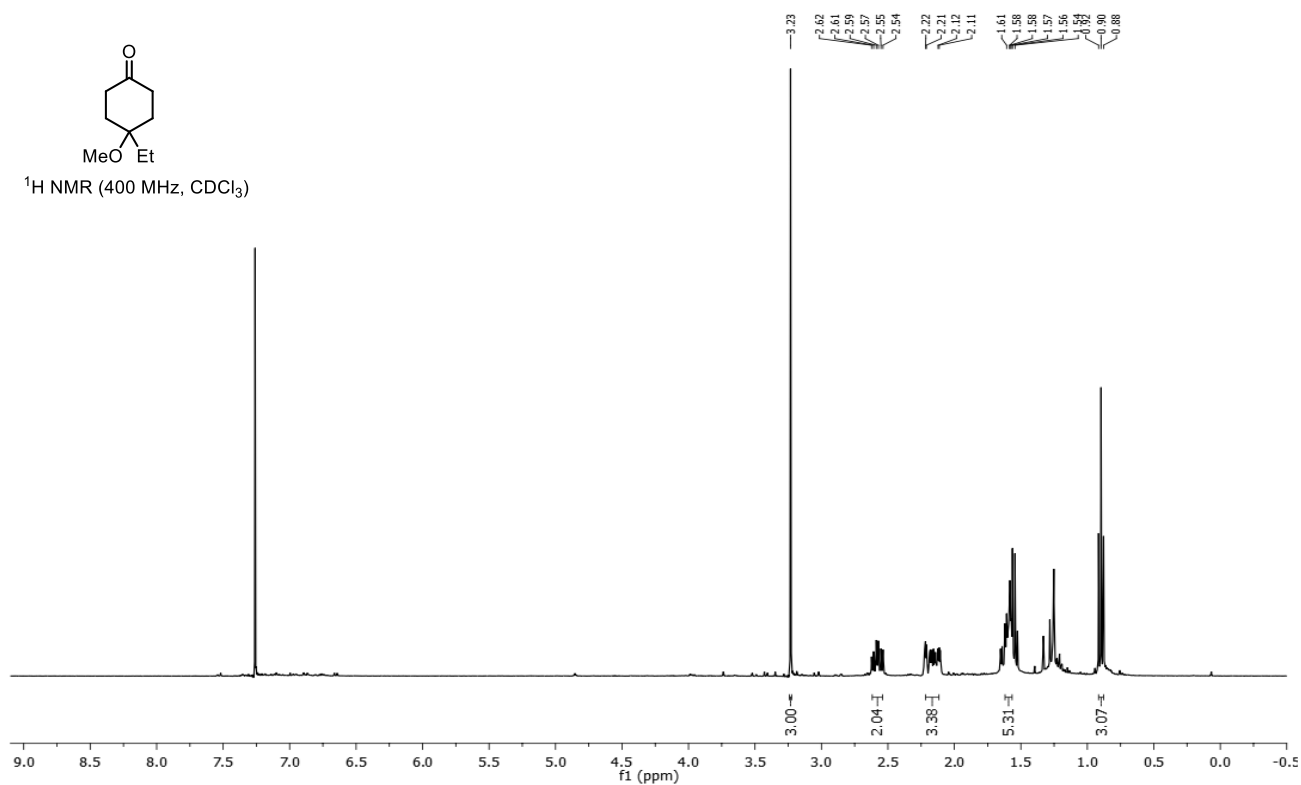
6	-0.957695000	1.921224000	-0.350552000
1	-1.902477000	2.137244000	0.174298000
1	-0.349196000	2.839680000	-0.359164000
1	-1.192915000	1.664053000	-1.395977000
8	-0.969748000	-0.850923000	0.607432000
8	1.316262000	0.245257000	-0.438357000
6	-1.621259000	-1.480443000	-0.471102000
1	-2.048413000	-2.434000000	-0.121312000
1	-2.449376000	-0.863804000	-0.869416000
1	-0.928582000	-1.699643000	-1.304953000
6	2.327062000	-0.676861000	-0.099277000
1	3.099974000	-0.661981000	-0.884256000
1	2.811218000	-0.421706000	0.862735000
1	1.935451000	-1.707740000	-0.018499000
14	-0.041500000	0.529168000	0.486996000
1	0.342203000	0.828511000	1.892124000

^tBuOLi

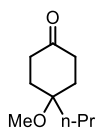
6	-1.666323000	-2.611871000	4.210269000
6	-0.720156000	-1.462936000	4.617979000
1	-1.168080000	-3.580326000	4.380607000
1	-1.900959000	-2.535714000	3.135753000
1	-2.613573000	-2.602132000	4.775761000
6	-1.418668000	-0.111858000	4.354186000
6	-0.392129000	-1.580085000	6.121342000
1	-0.747597000	0.716338000	4.635122000
1	-2.358657000	-0.007090000	4.922222000
1	-1.647855000	-0.013968000	3.280310000
1	-1.292143000	-1.522284000	6.756634000
1	0.294755000	-0.769434000	6.414716000
1	0.112628000	-2.540232000	6.317685000
8	0.444135000	-1.540399000	3.882409000
3	1.765668000	-1.668236000	3.038149000

5. ^1H NMR, ^{13}C NMR spectra:

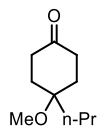
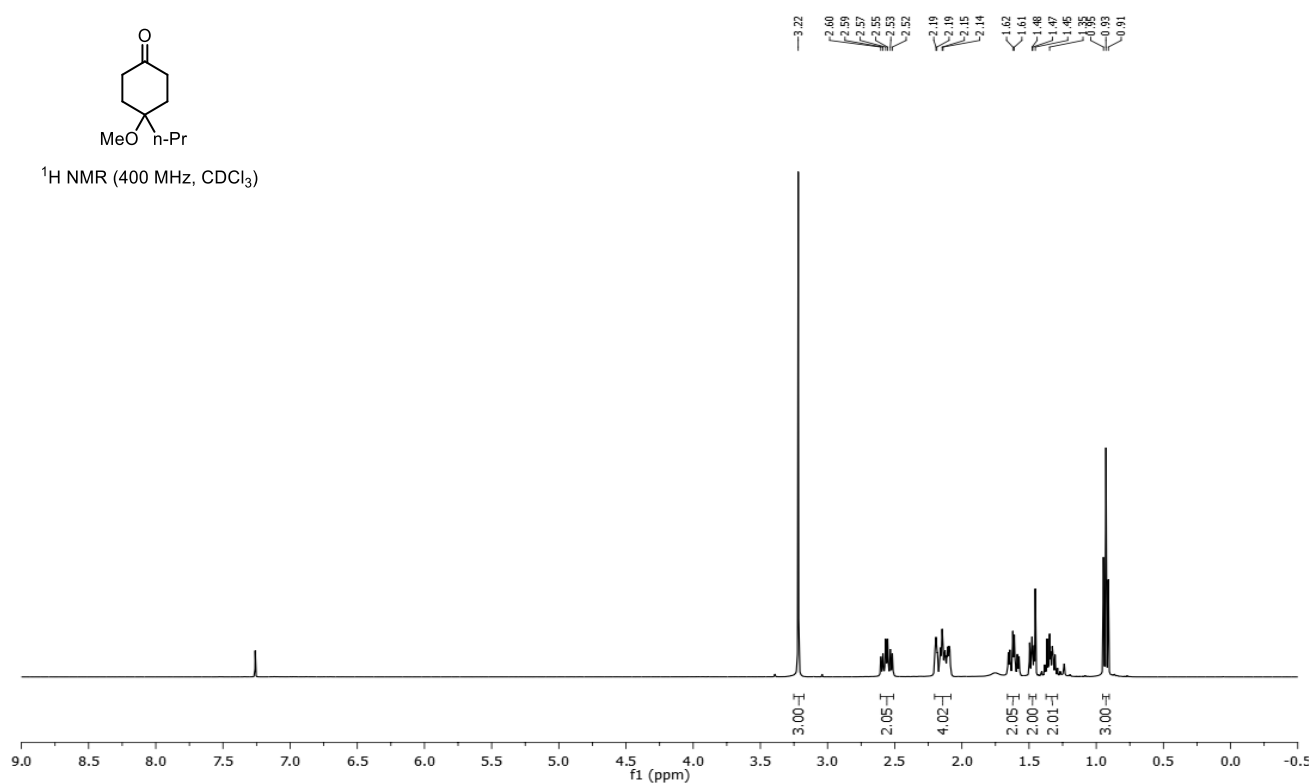
4-Ethyl-4-methoxycyclohexan-1-one (4b):



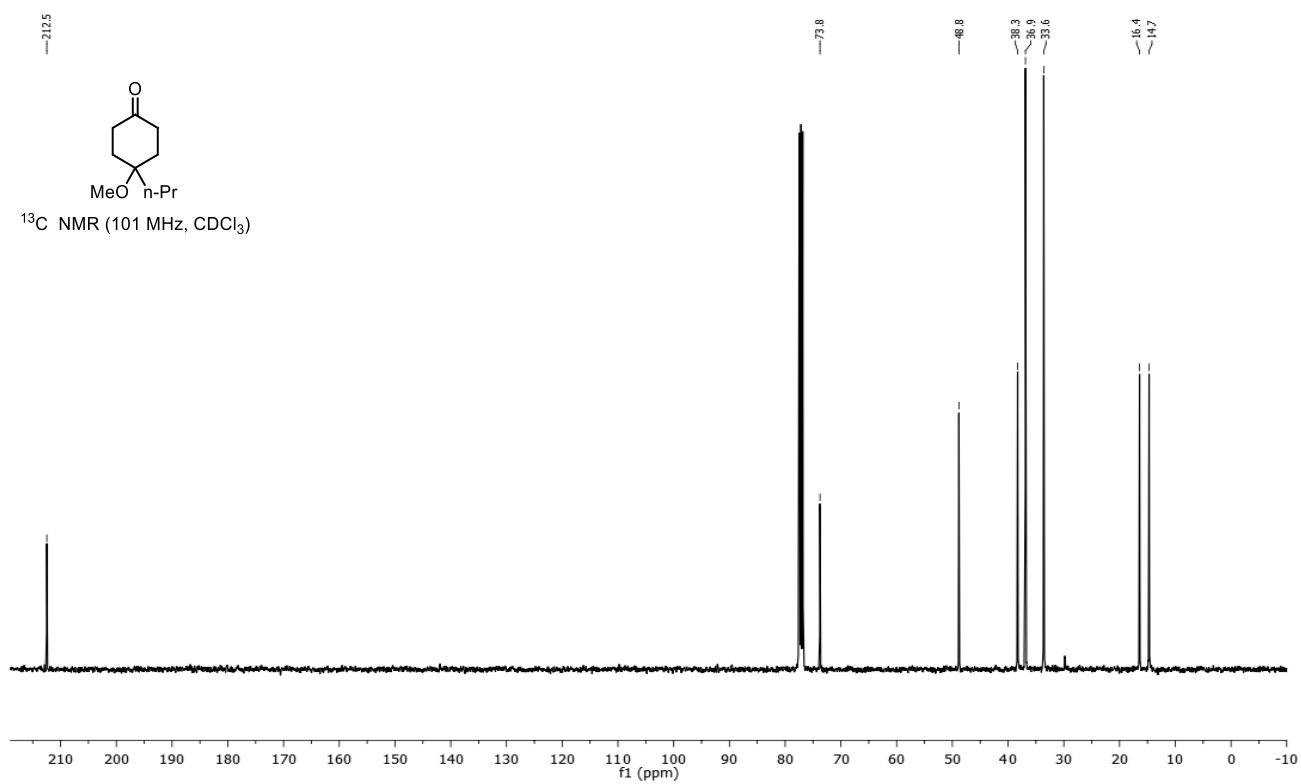
4-Methoxy-4-propylcyclohexan-1-one (4c):



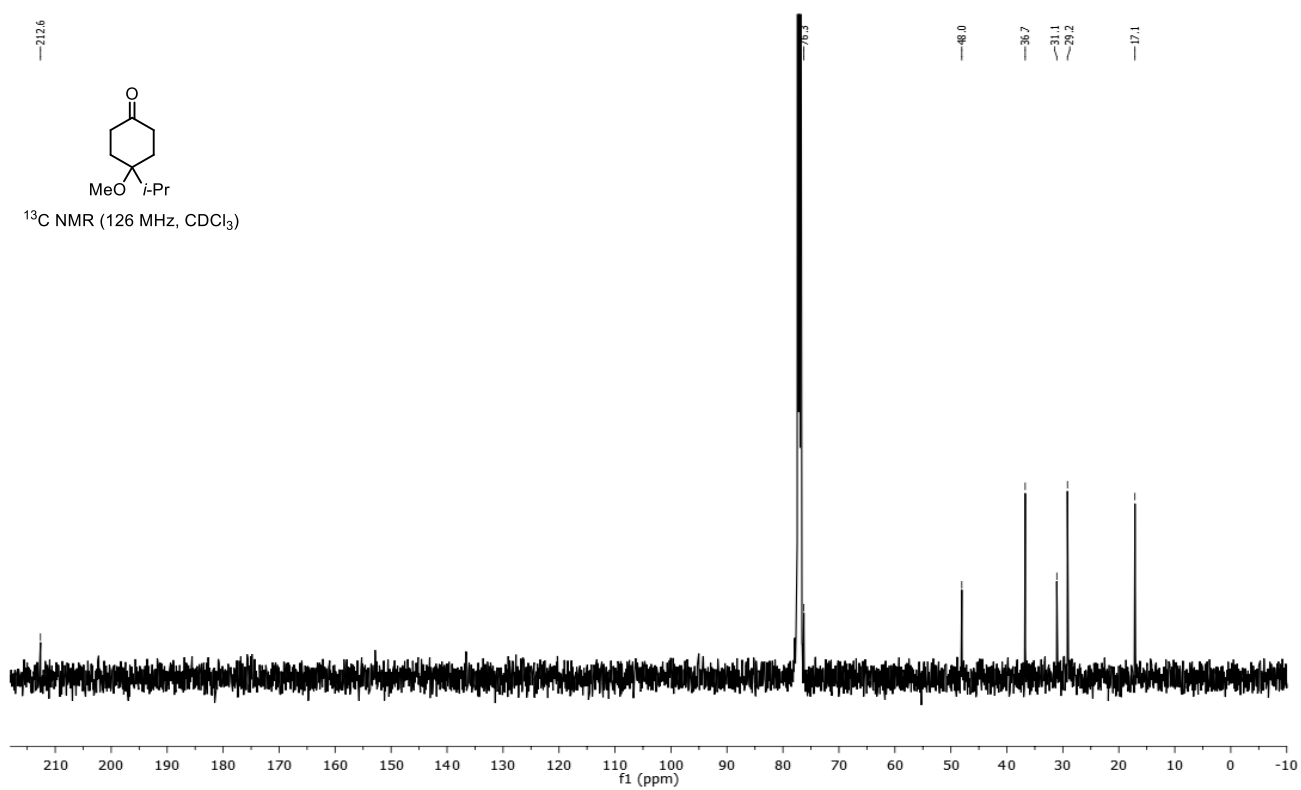
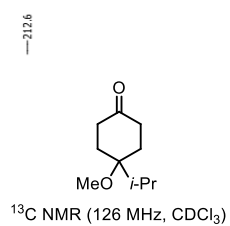
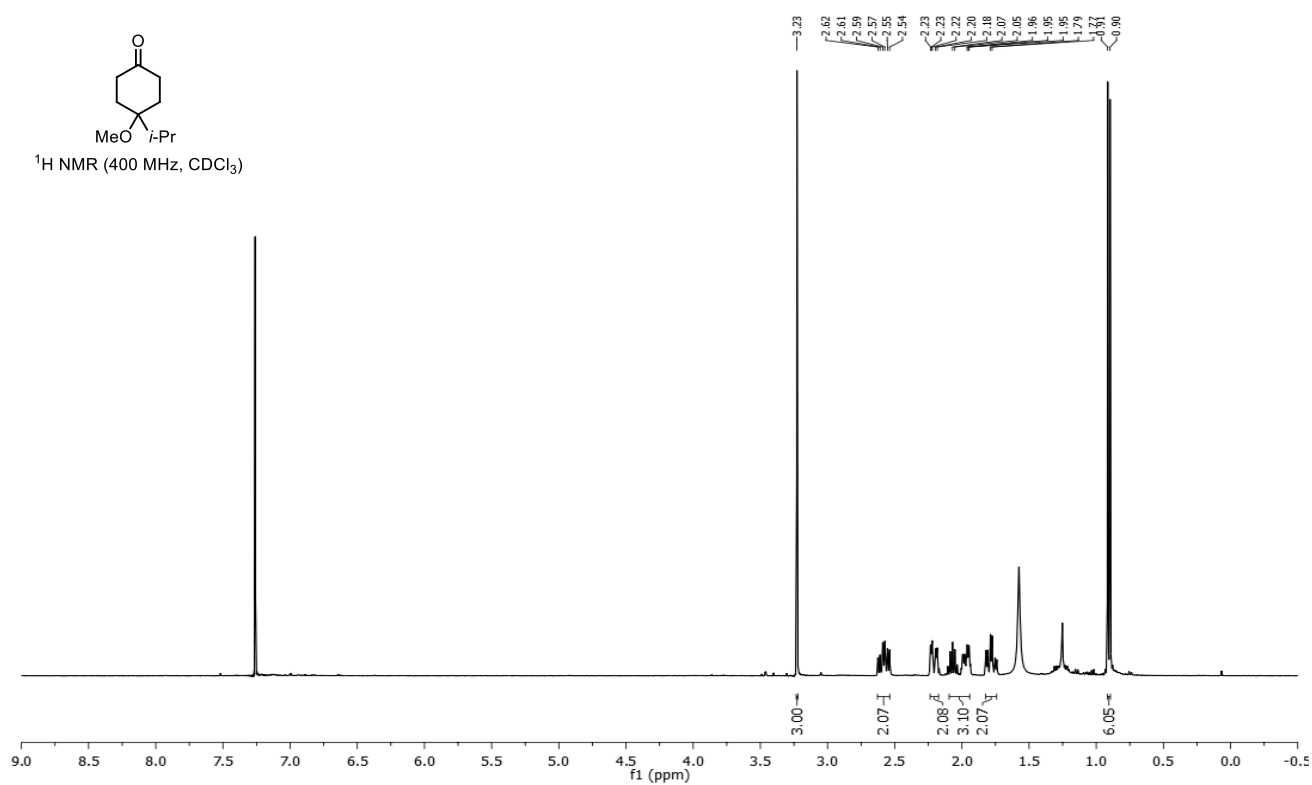
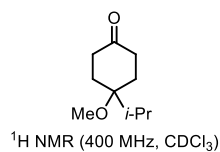
^1H NMR (400 MHz, CDCl_3)



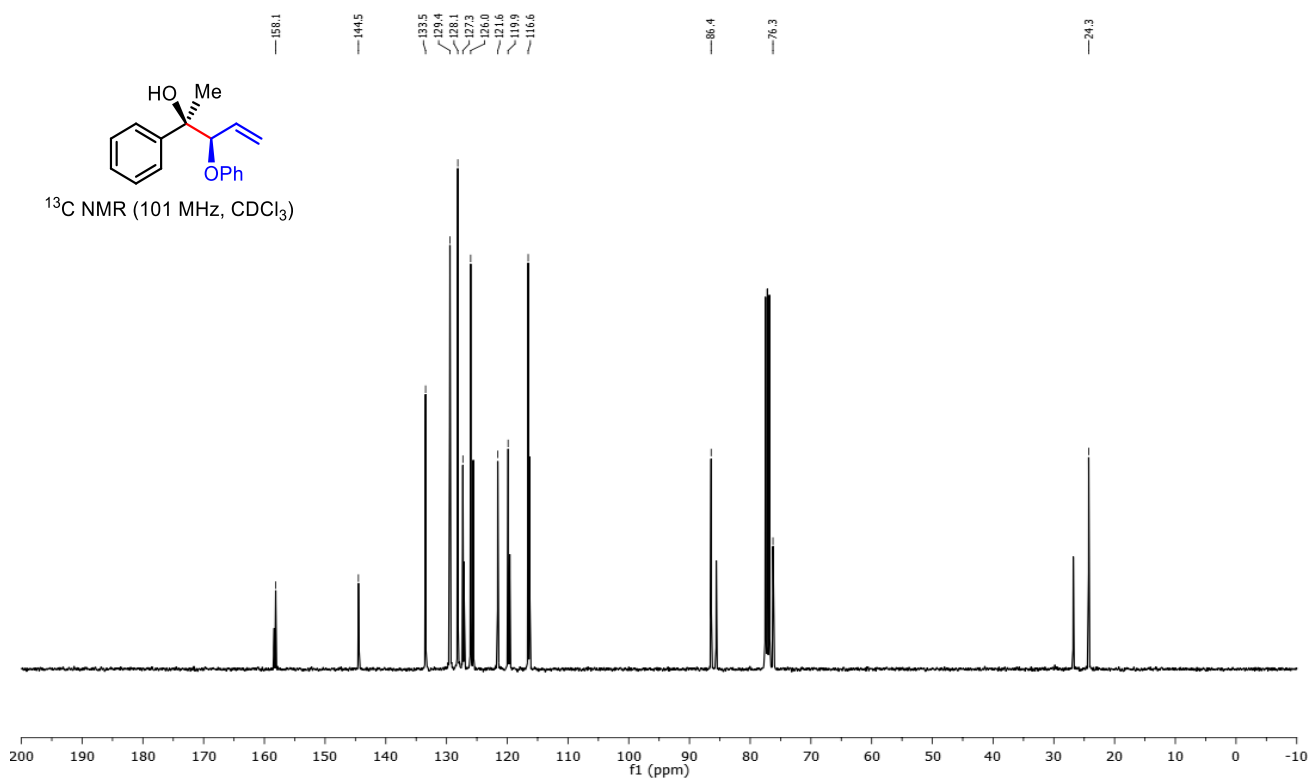
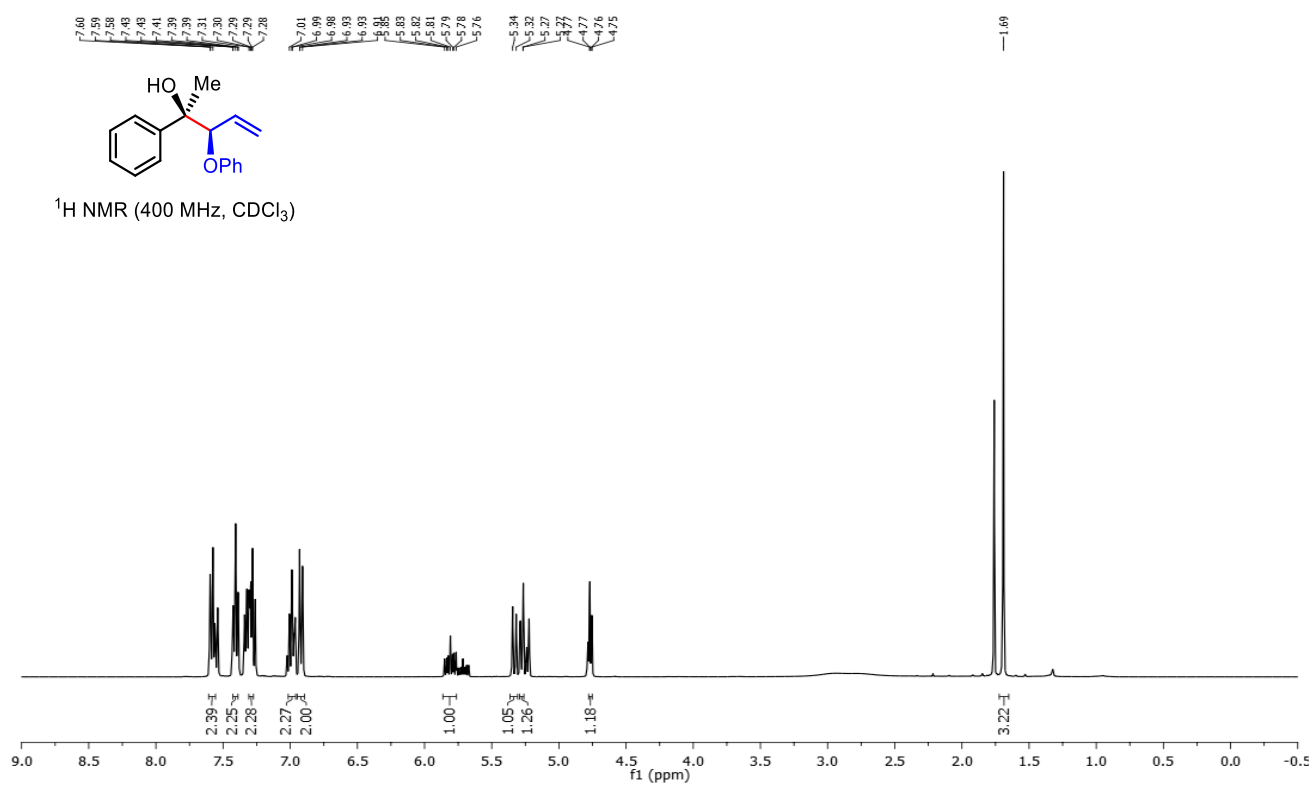
^{13}C NMR (101 MHz, CDCl_3)



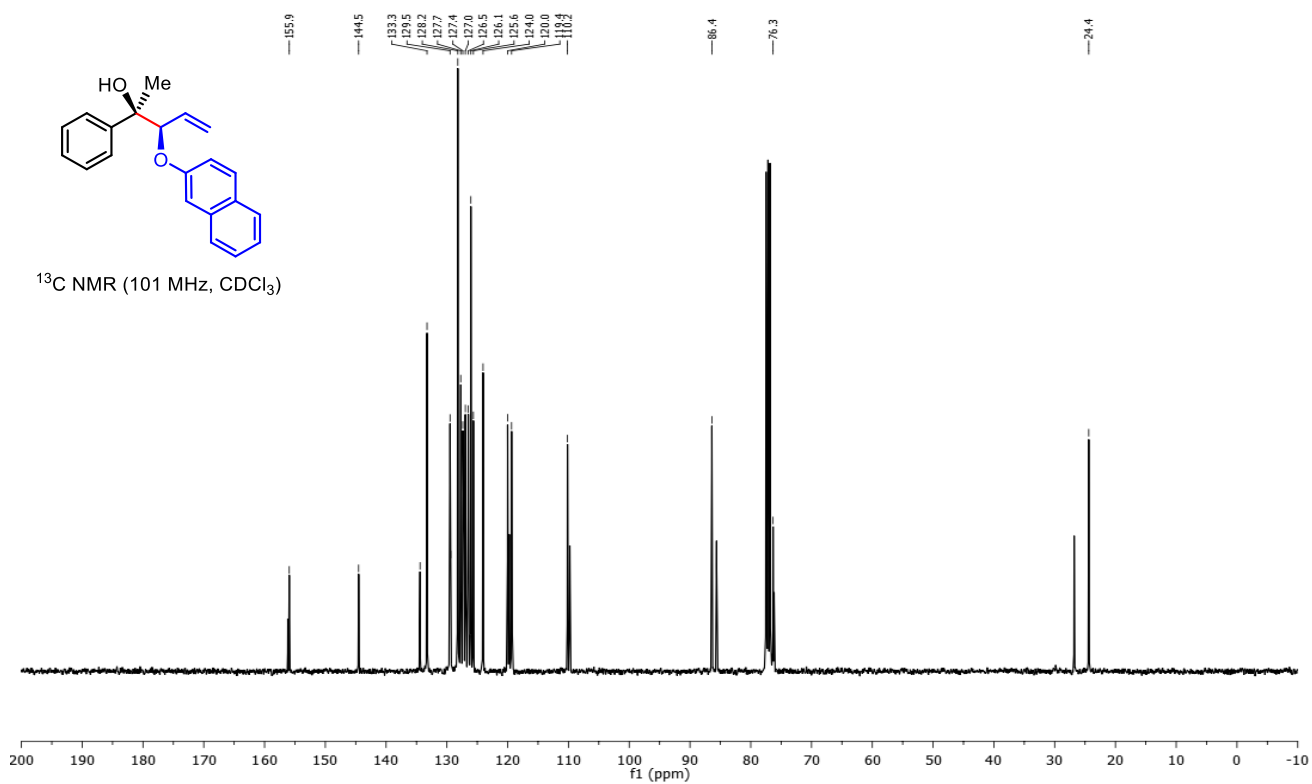
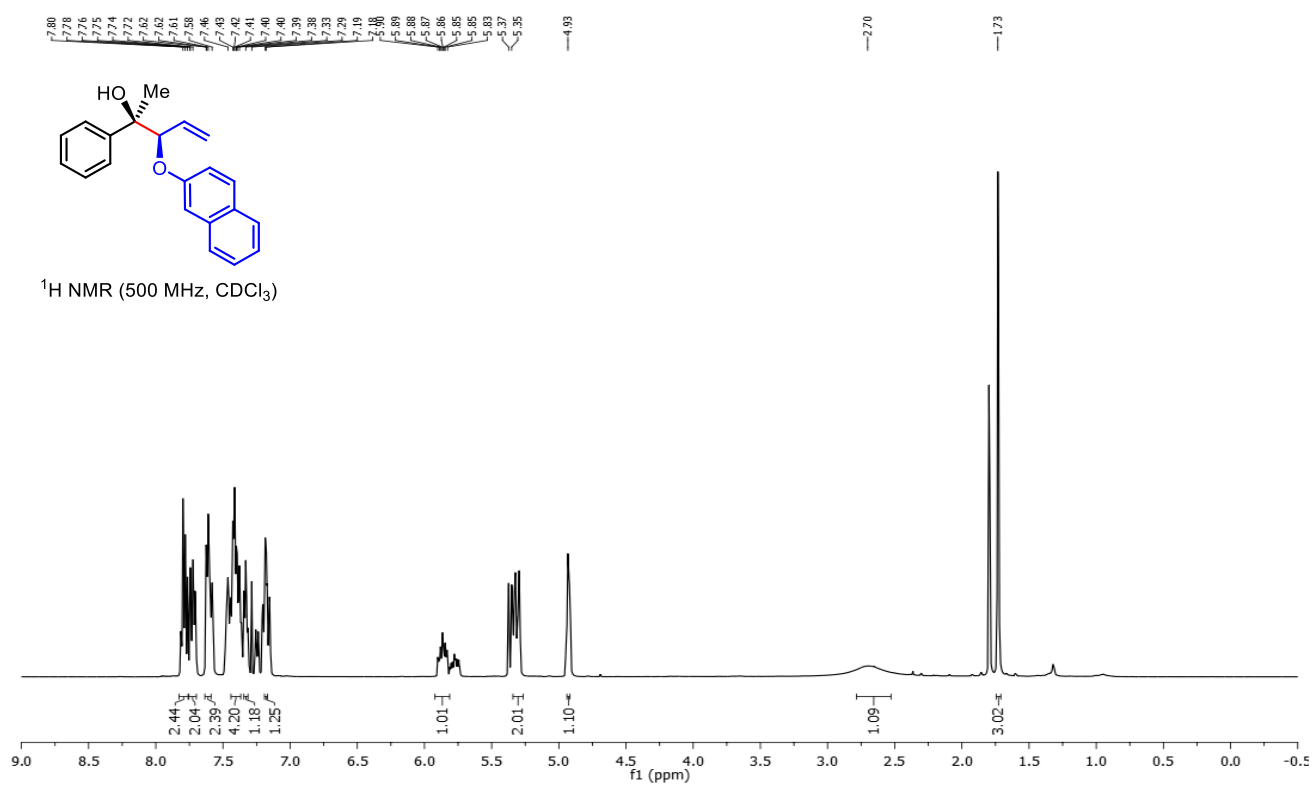
4-iso-Propyl-4-methoxycyclohexan-1-one (4d):



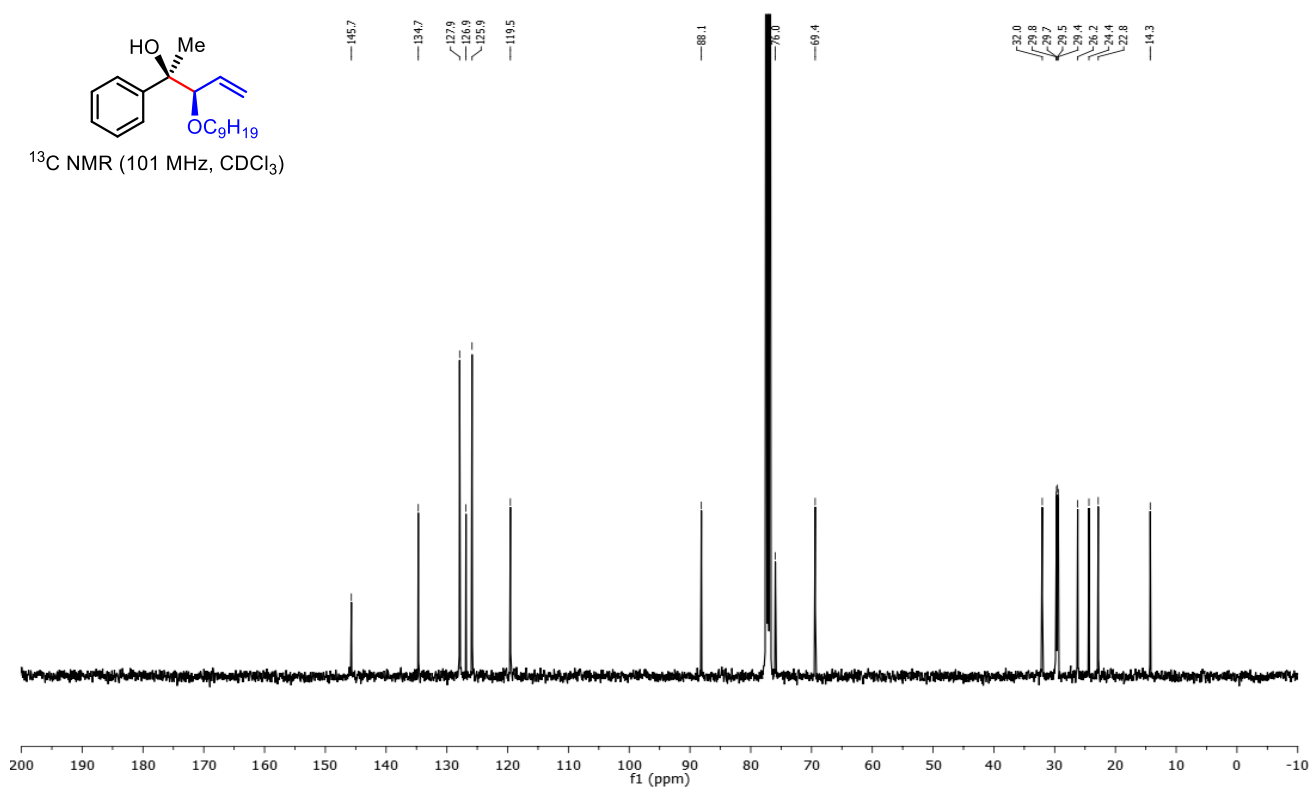
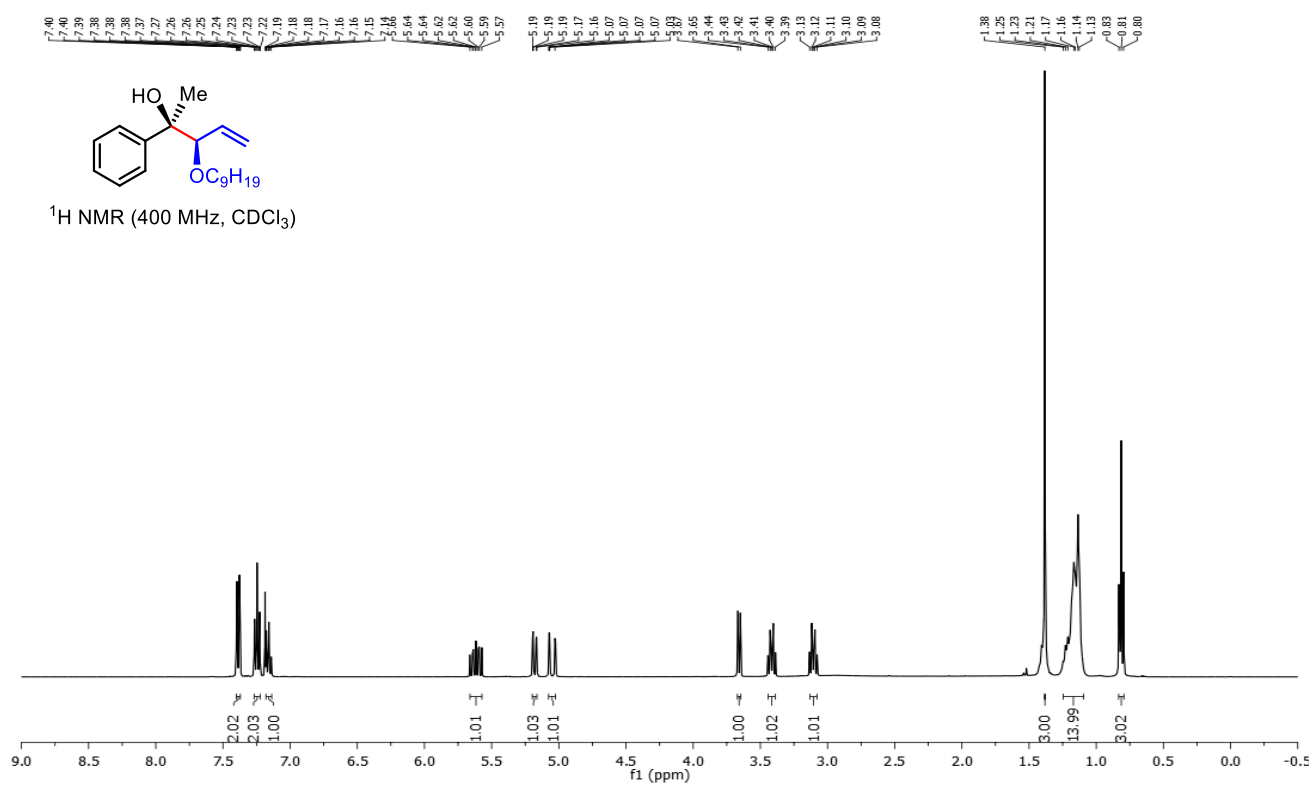
(2*R*,3*R*)-3-Phenoxy-2-phenylpent-4-en-2-ol (3aa):



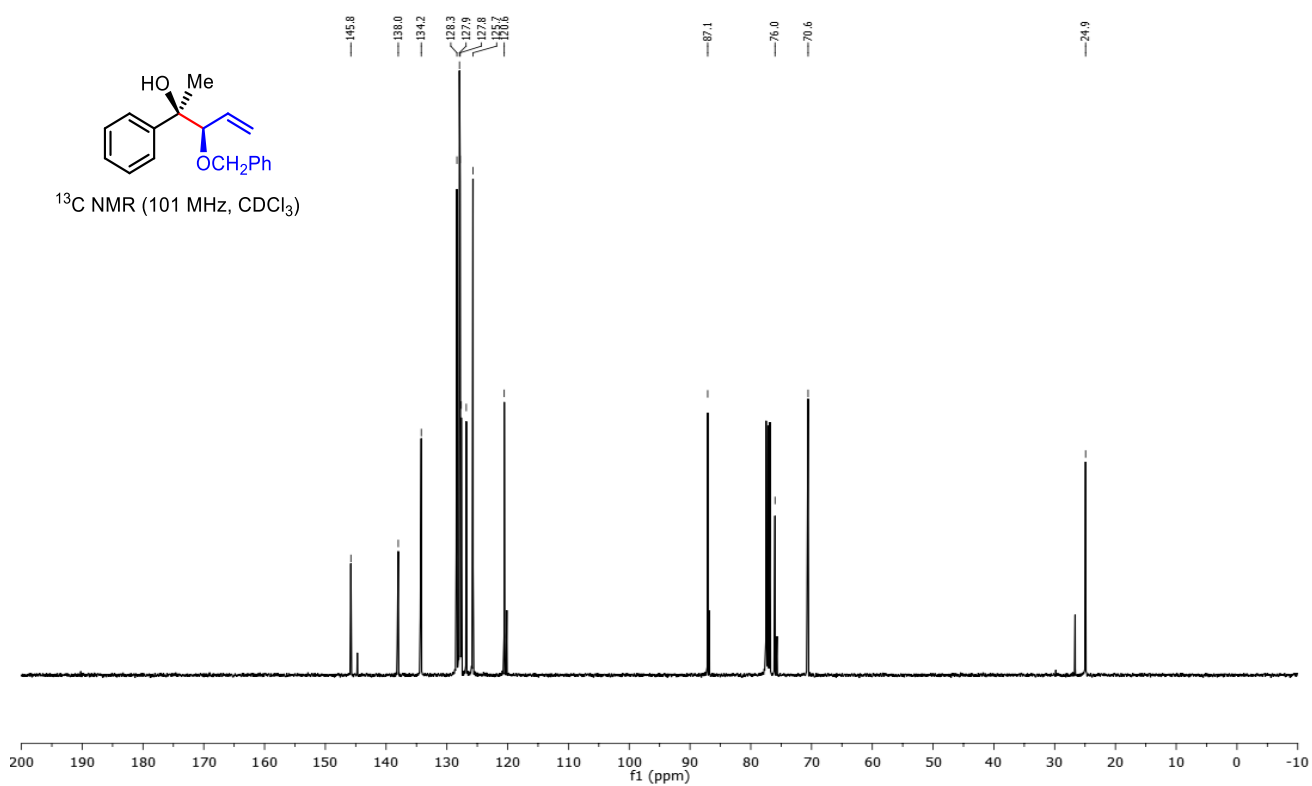
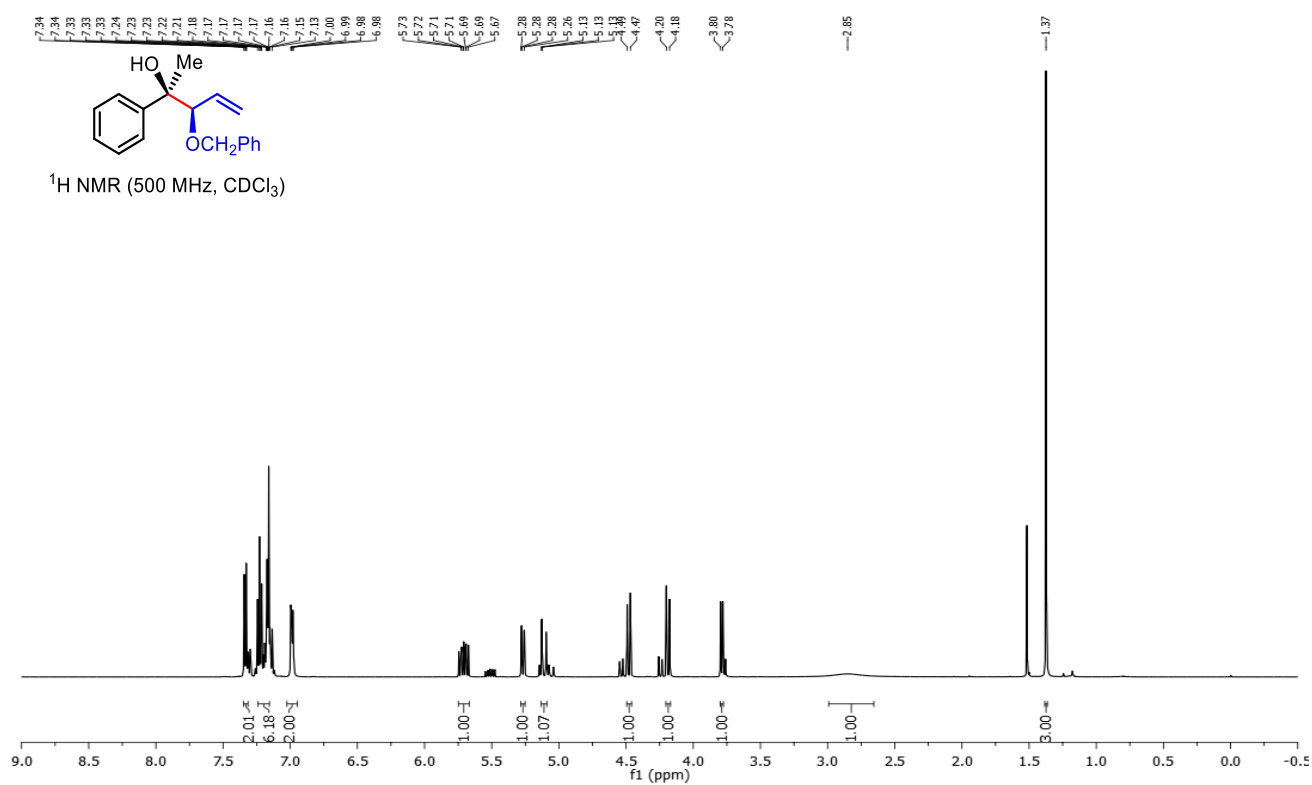
(2*R*,3*R*)-3-(Naphthalen-2-yloxy)-2-phenylpent-4-en-2-ol (3ab):



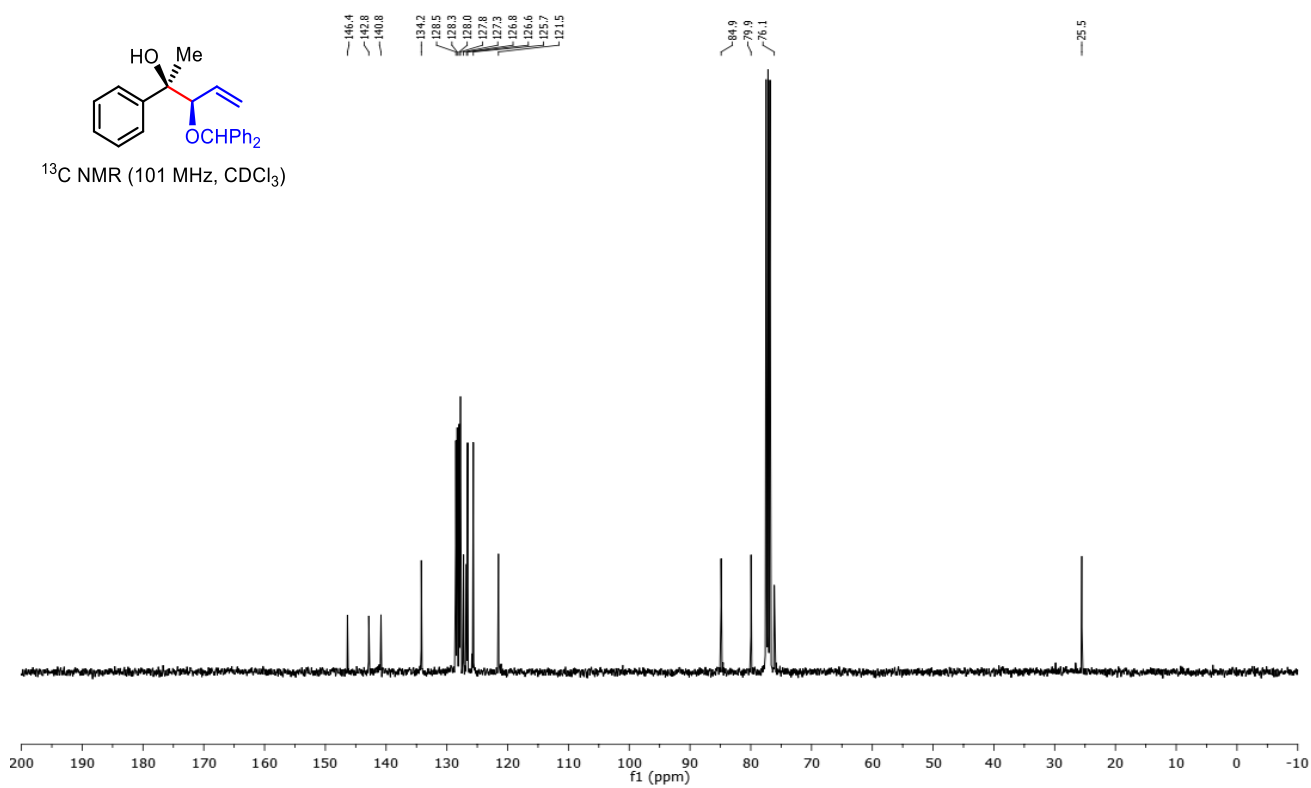
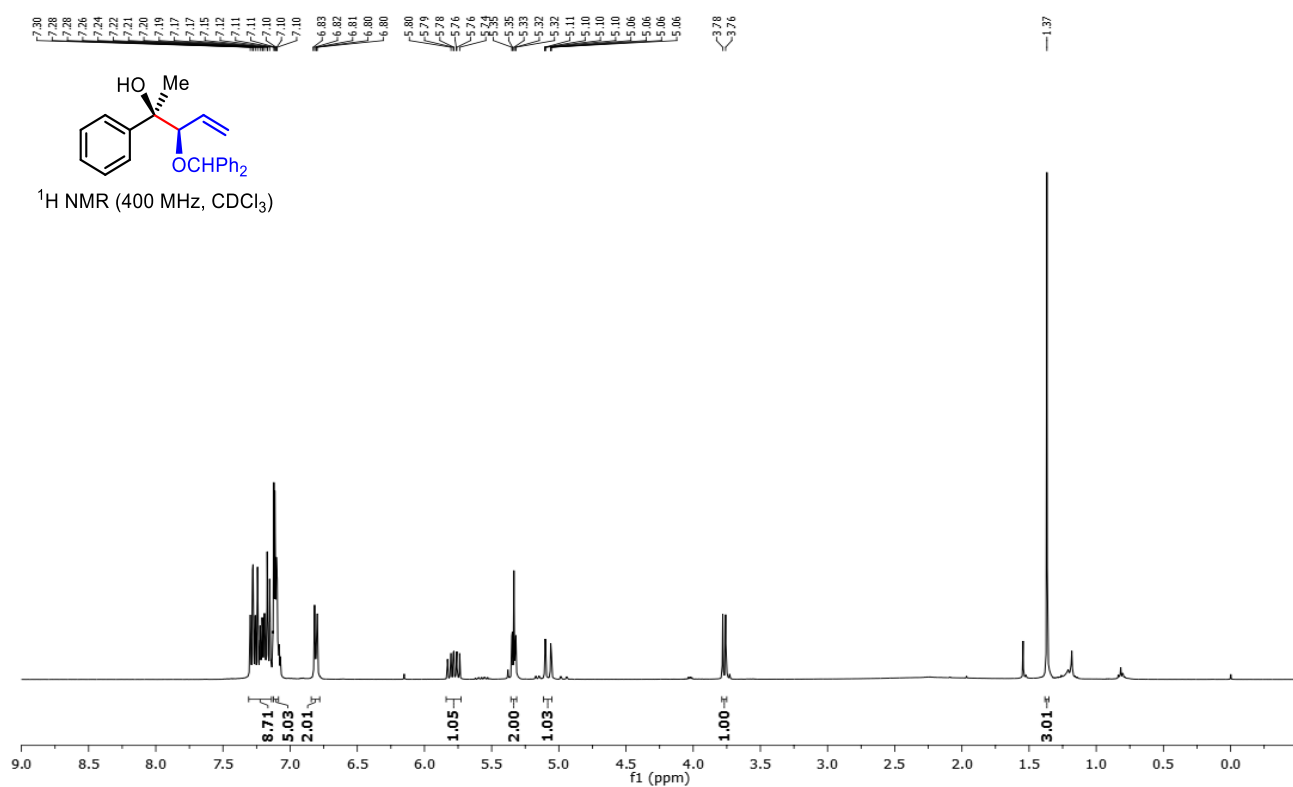
(2*R*,3*R*)-3-(Nonyloxy)-2-phenylpent-4-en-2-ol (3ac):



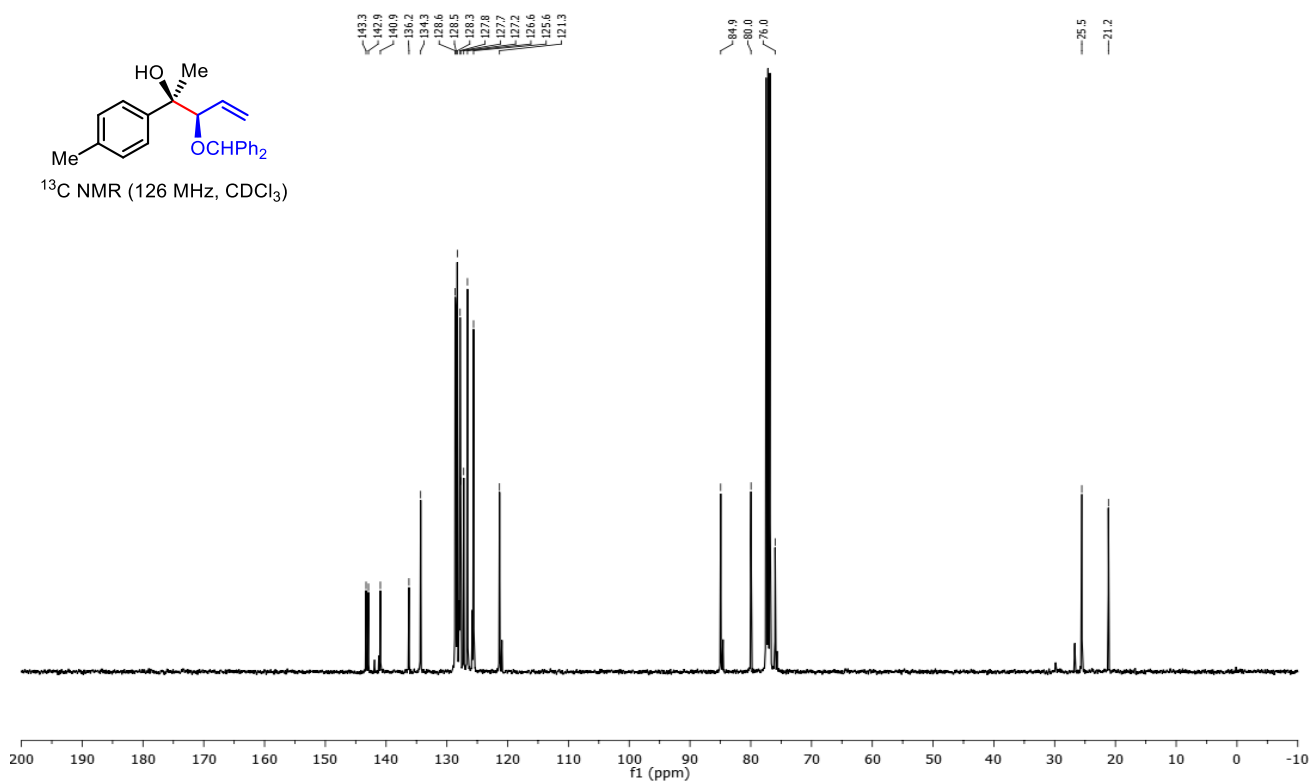
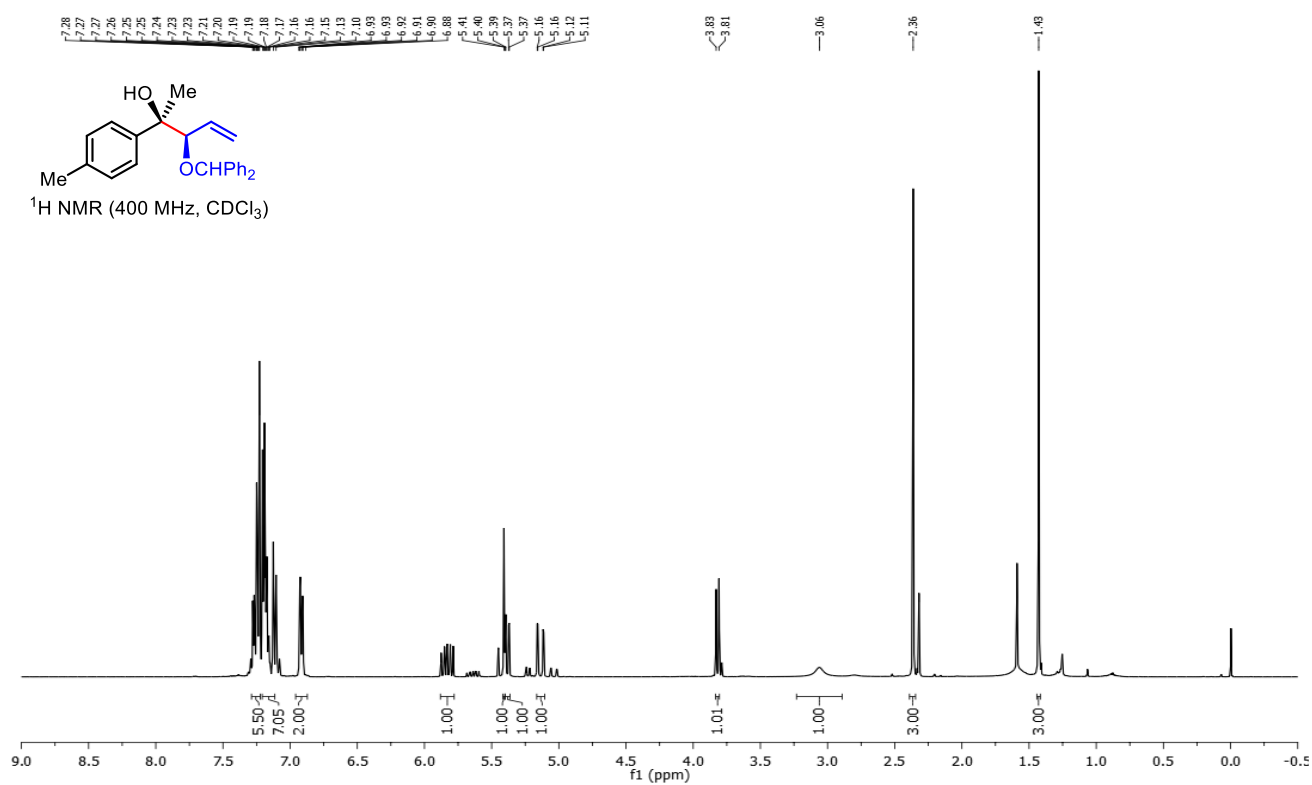
(2*R*,3*R*)-3-(Benzyloxy)-2-phenylpent-4-en-2-ol (3ad):



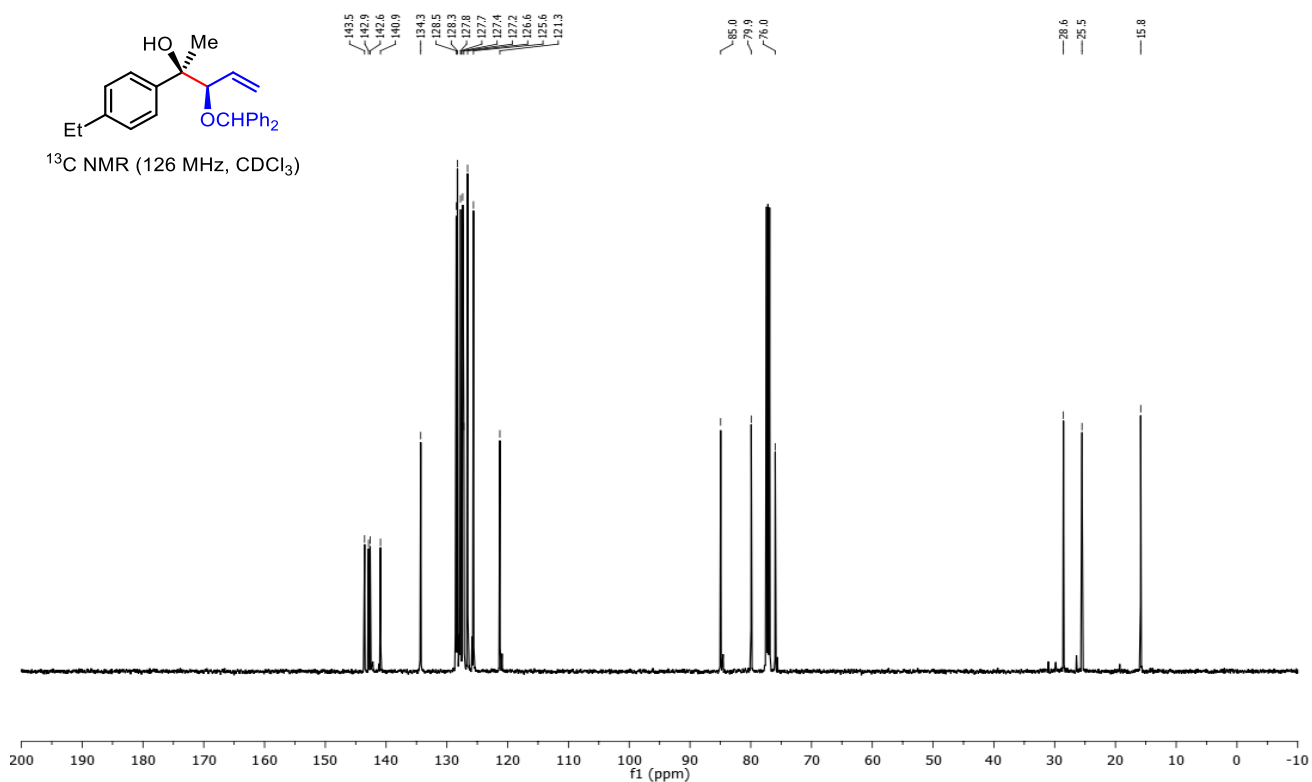
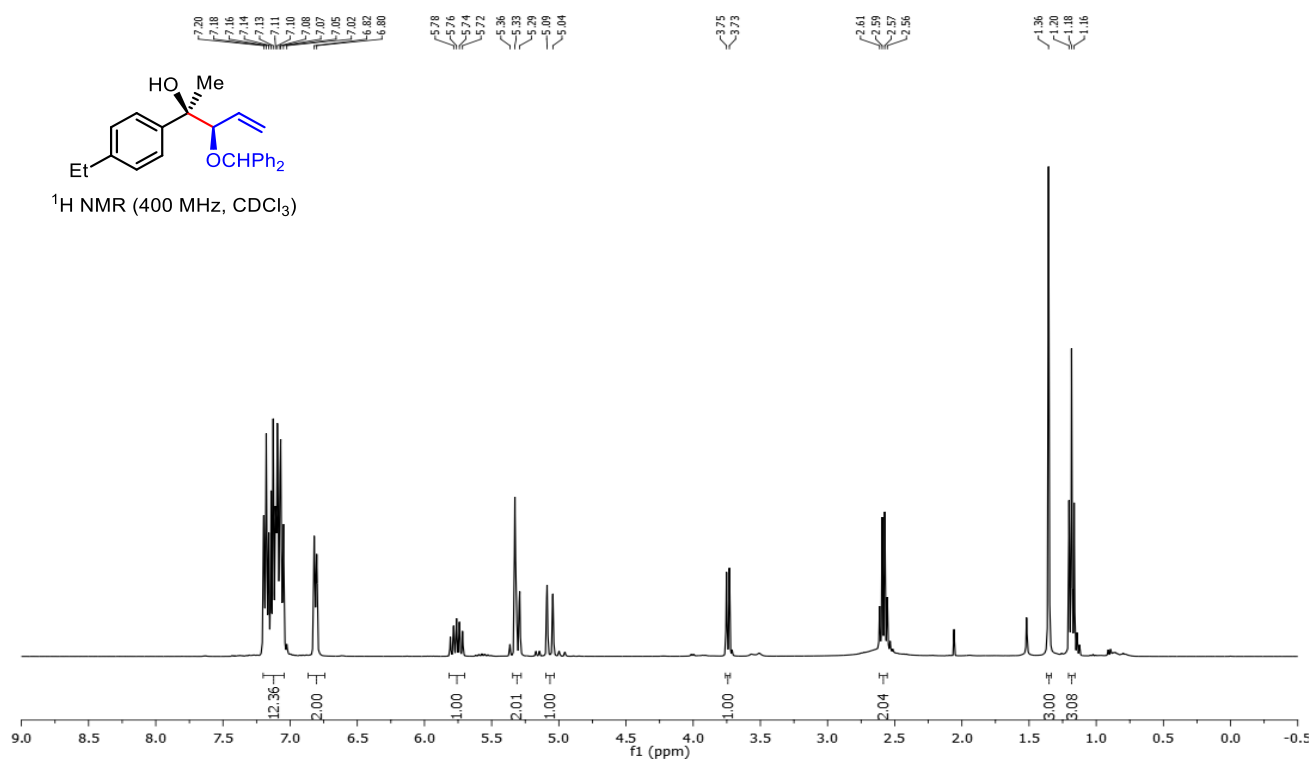
(2*R*,3*R*)-3-(Benzhydryloxy)-2-phenylpent-4-en-2-ol (3a):



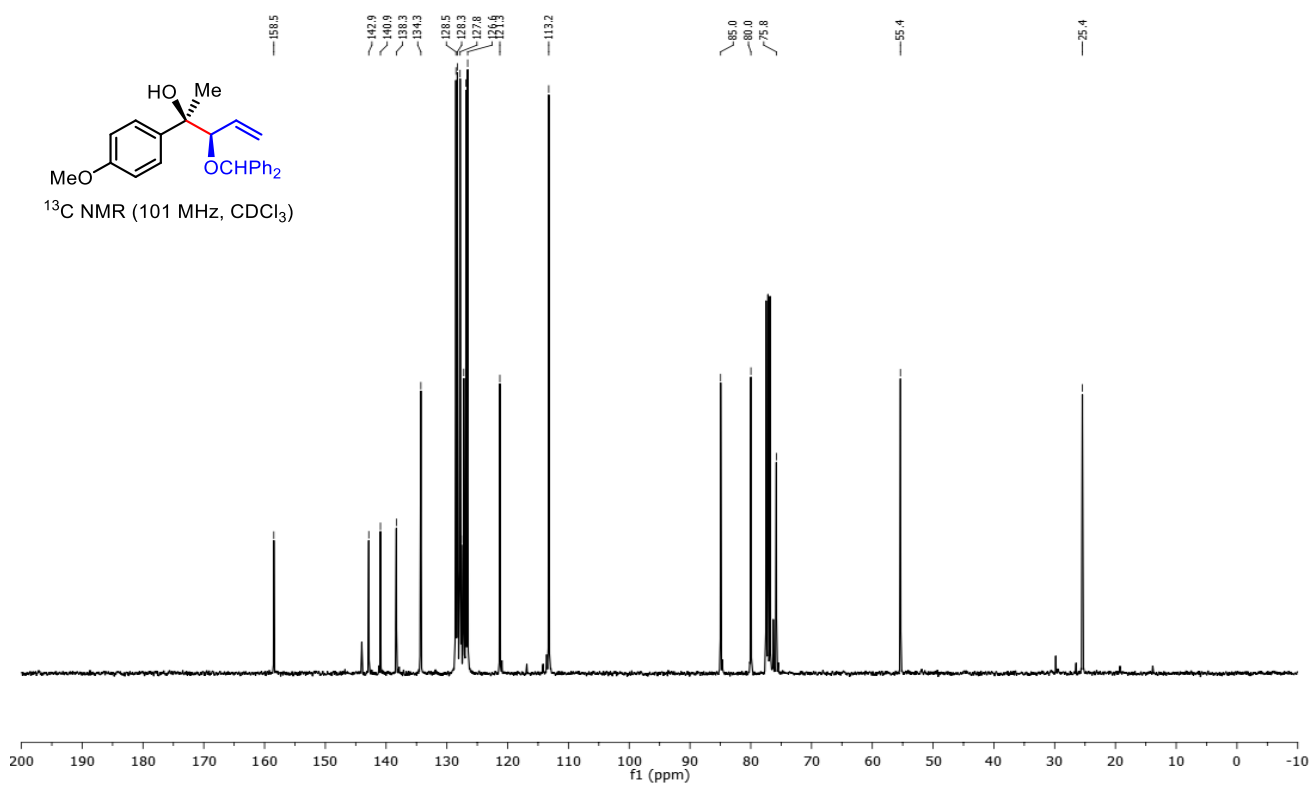
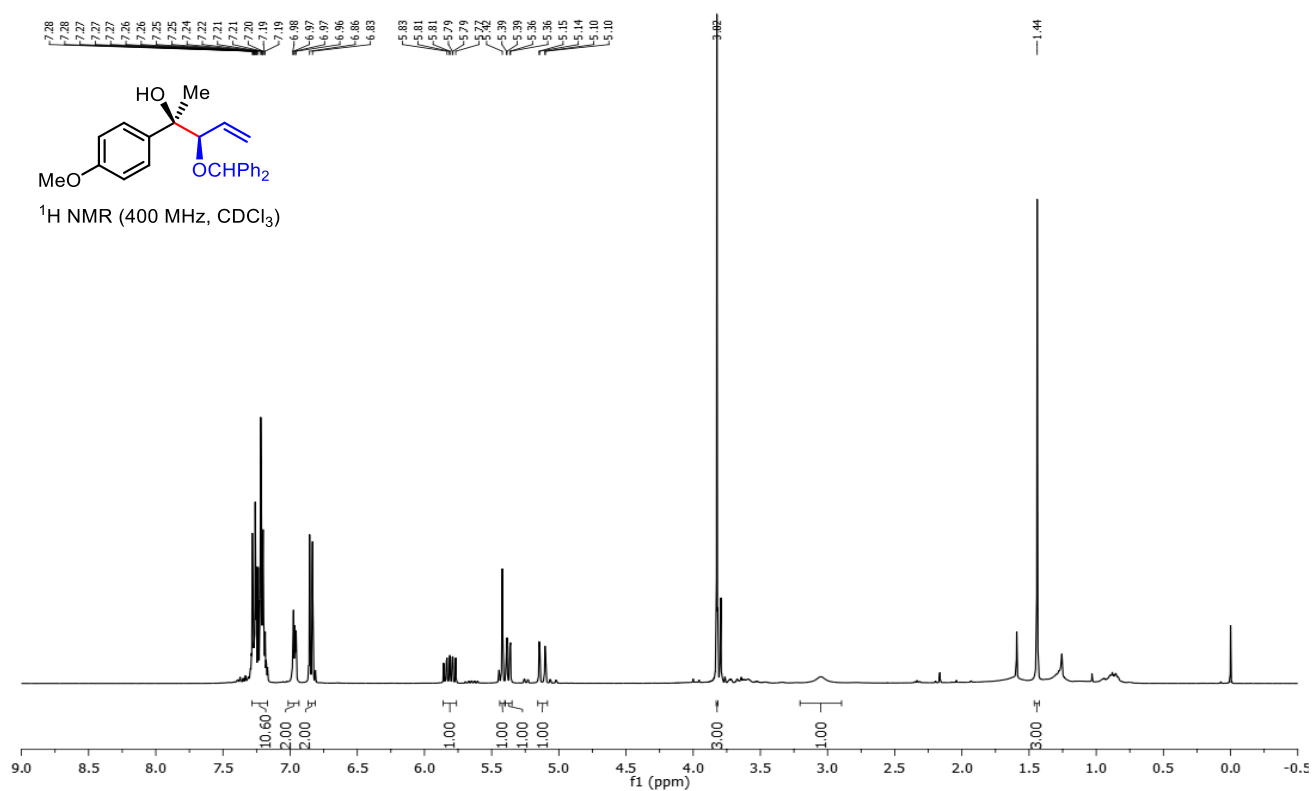
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(*p*-tolyl)pent-4-en-2-ol (3b):



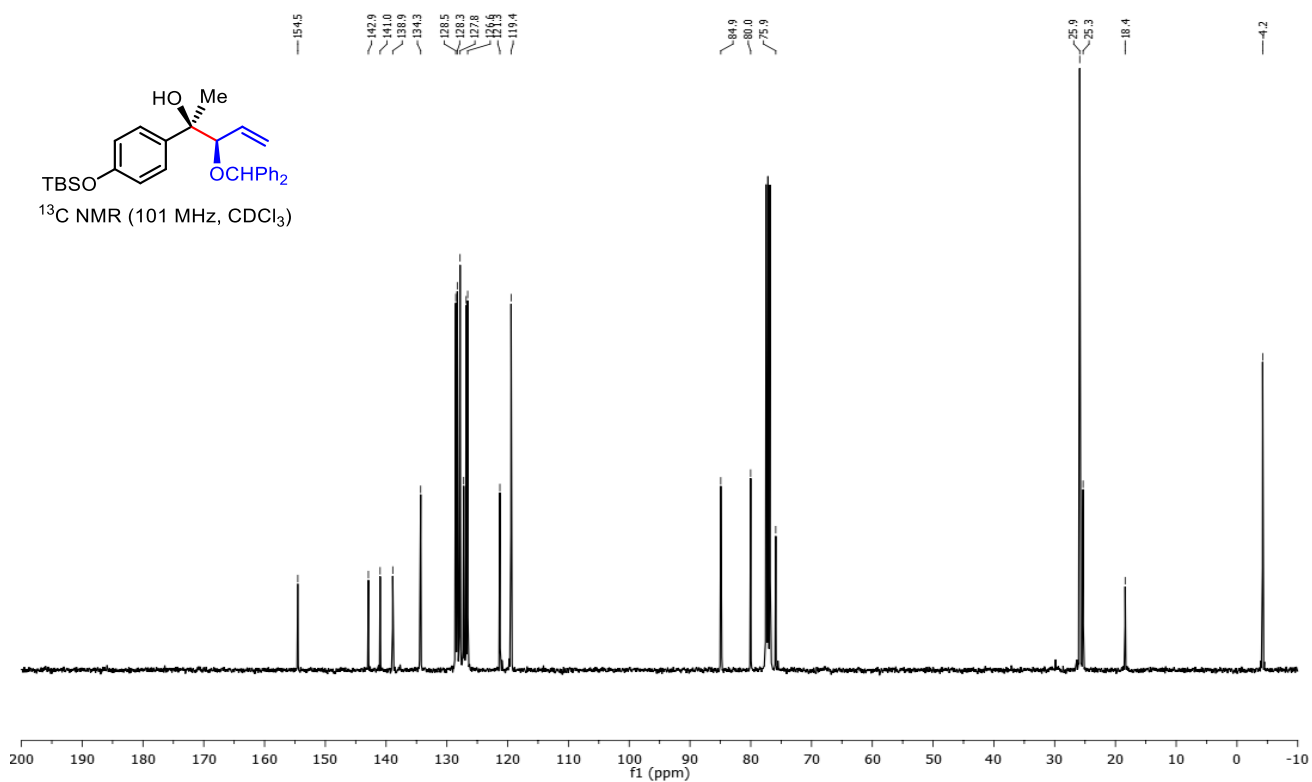
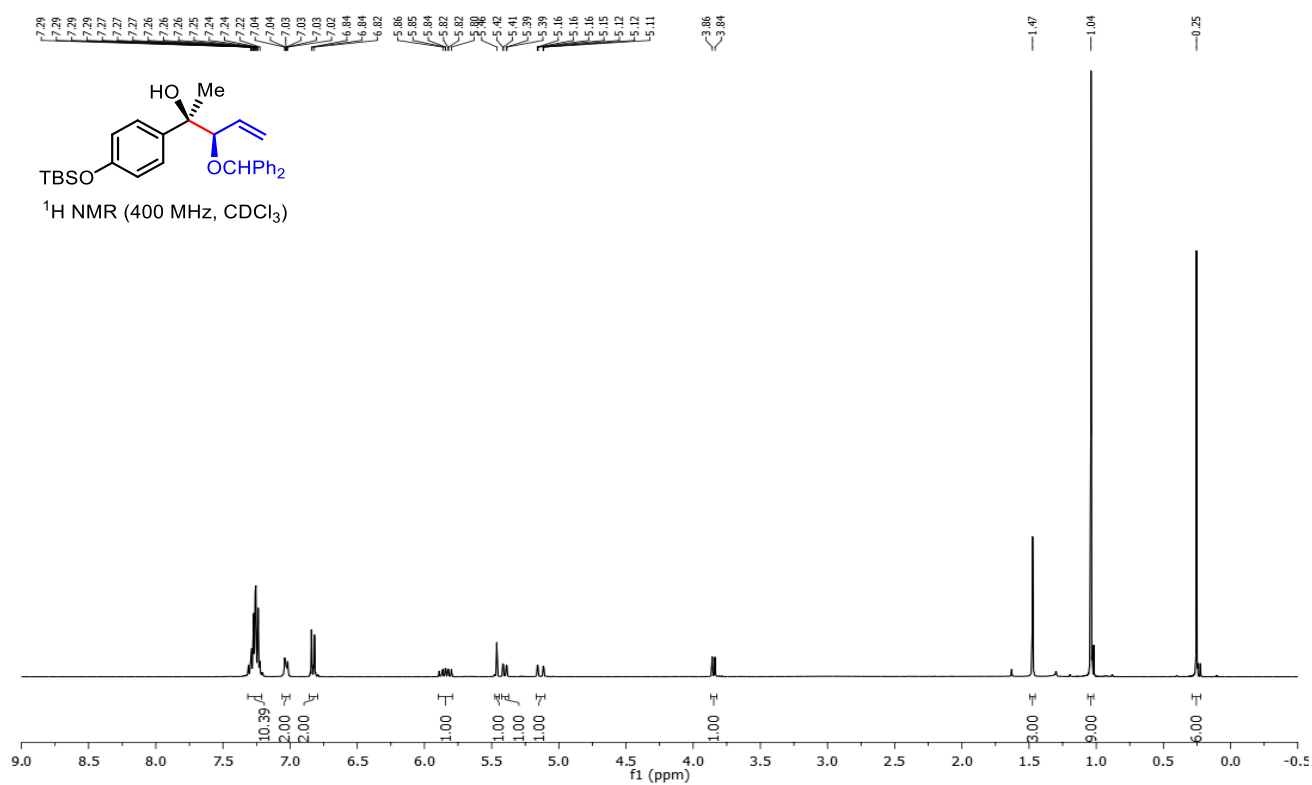
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-ethylphenyl)pent-4-en-2-ol (3c):



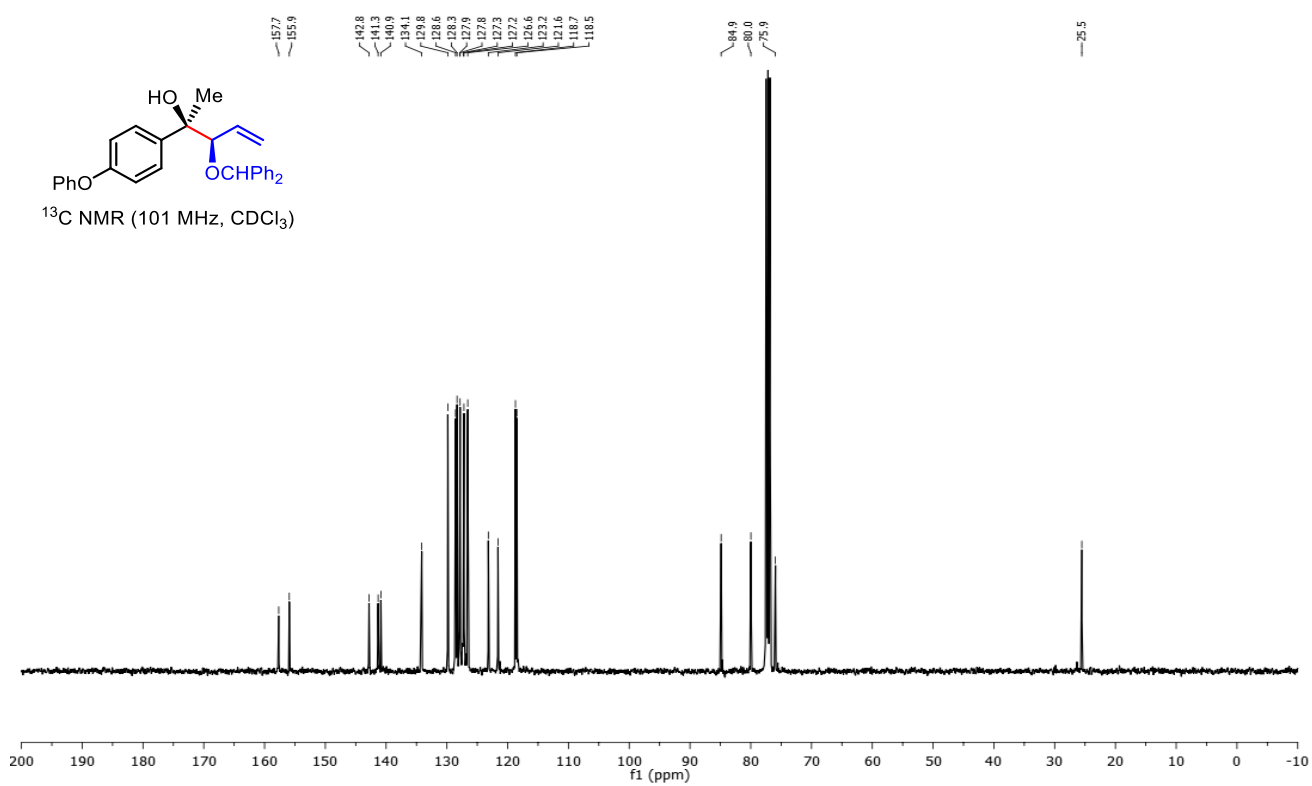
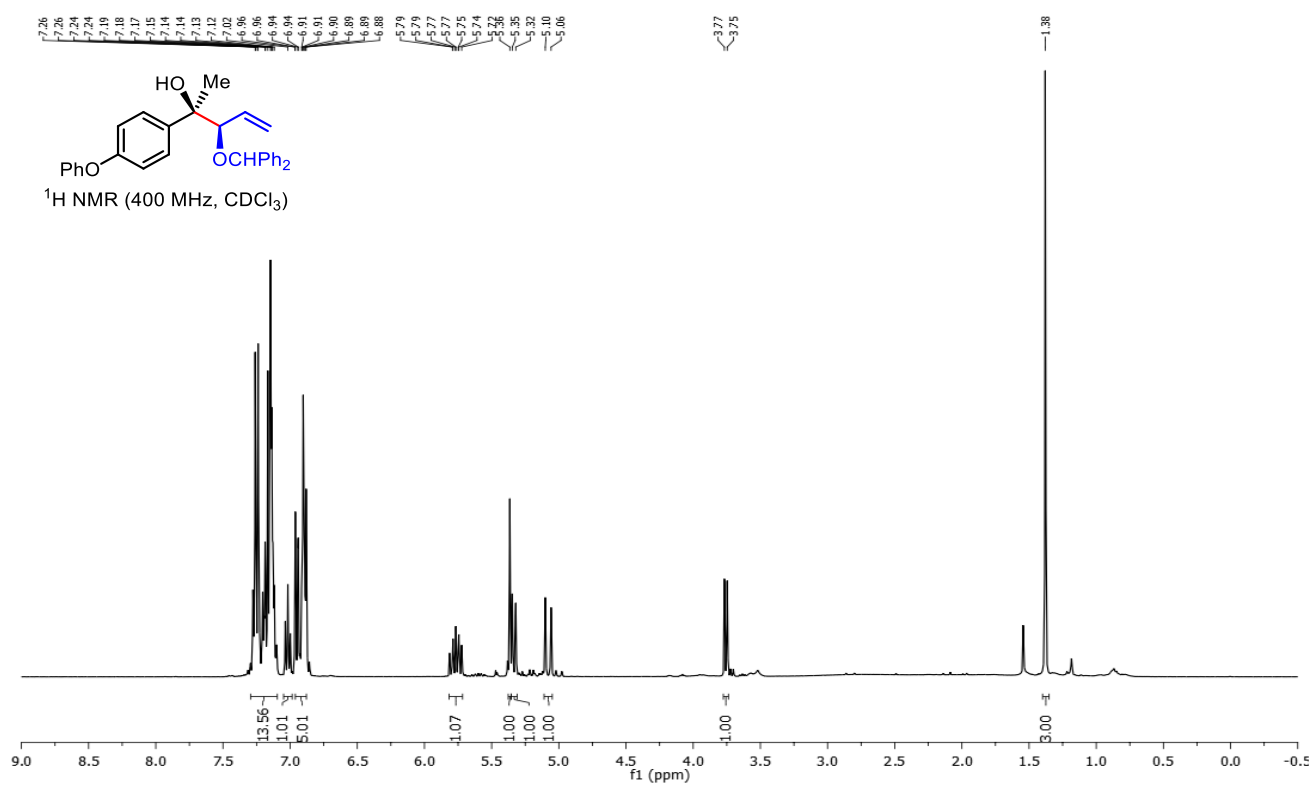
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-methoxyphenyl)pent-4-en-2-ol (3d):



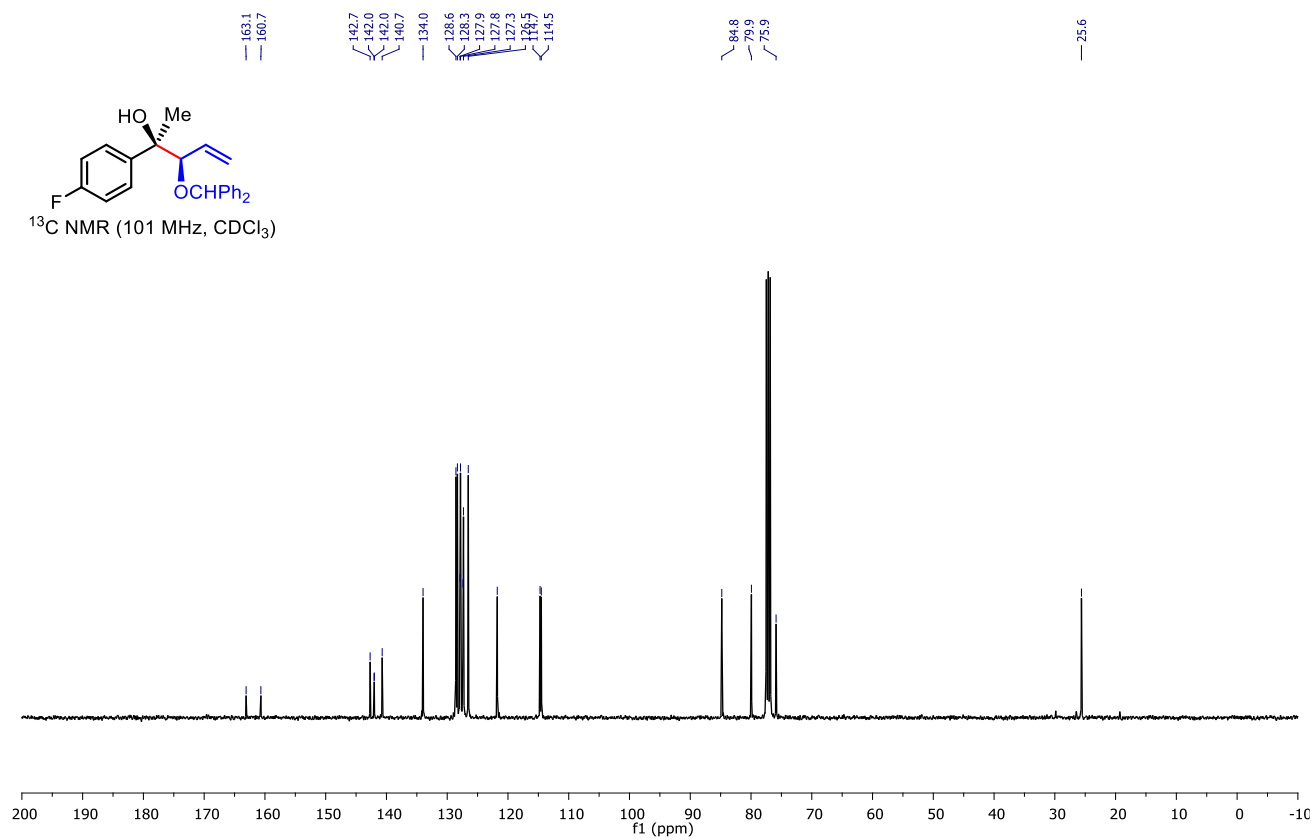
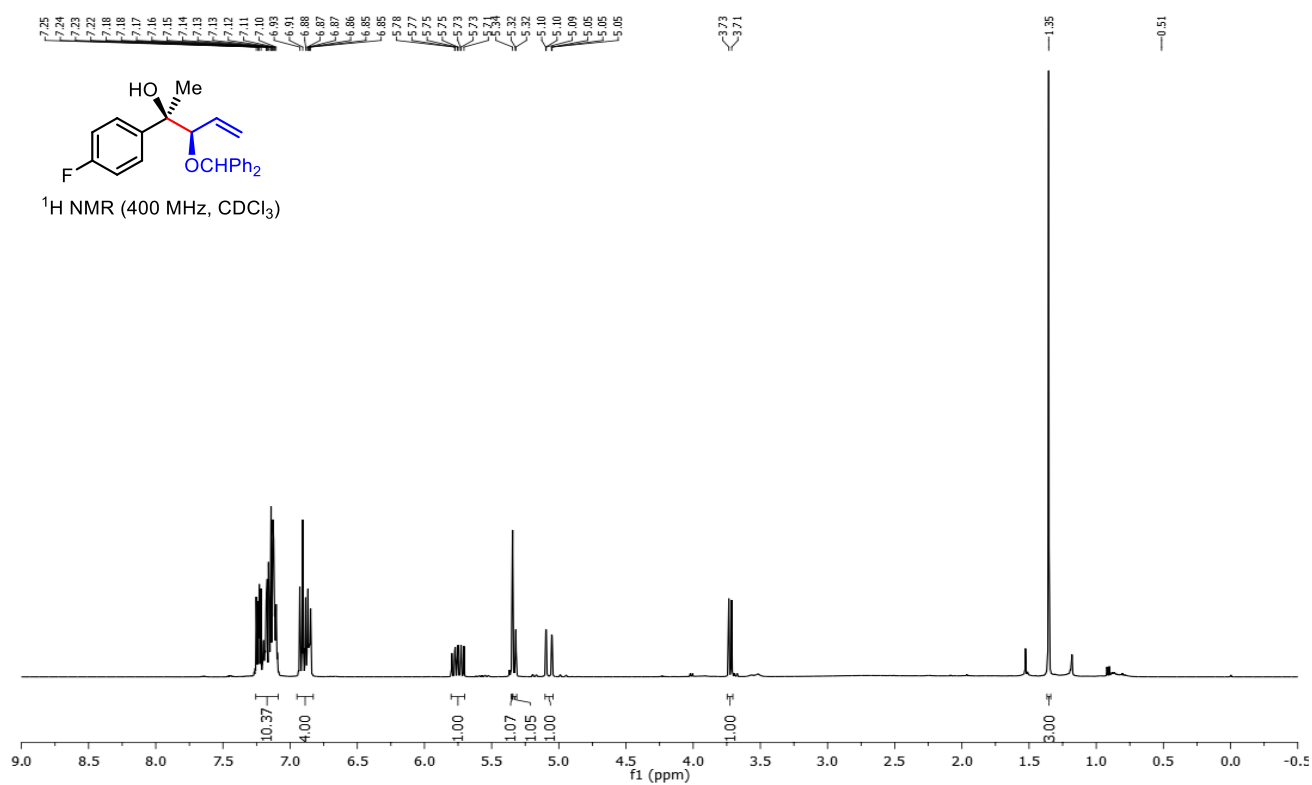
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-((tert-butyldimethylsilyl)oxy)phenyl)pent-4-en-2-ol (3e):

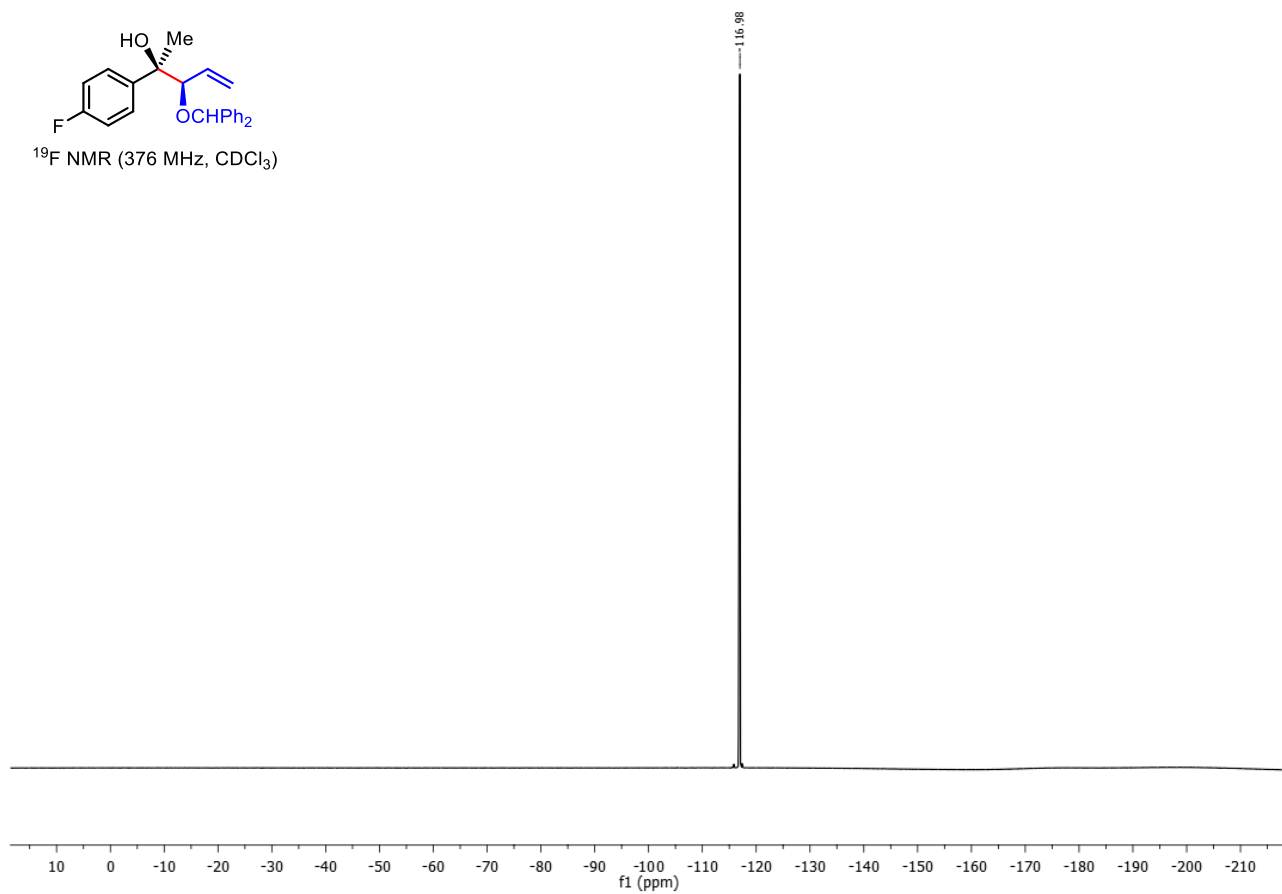
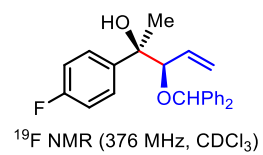


(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-phenoxyphenyl)pent-4-en-2-ol (3f):

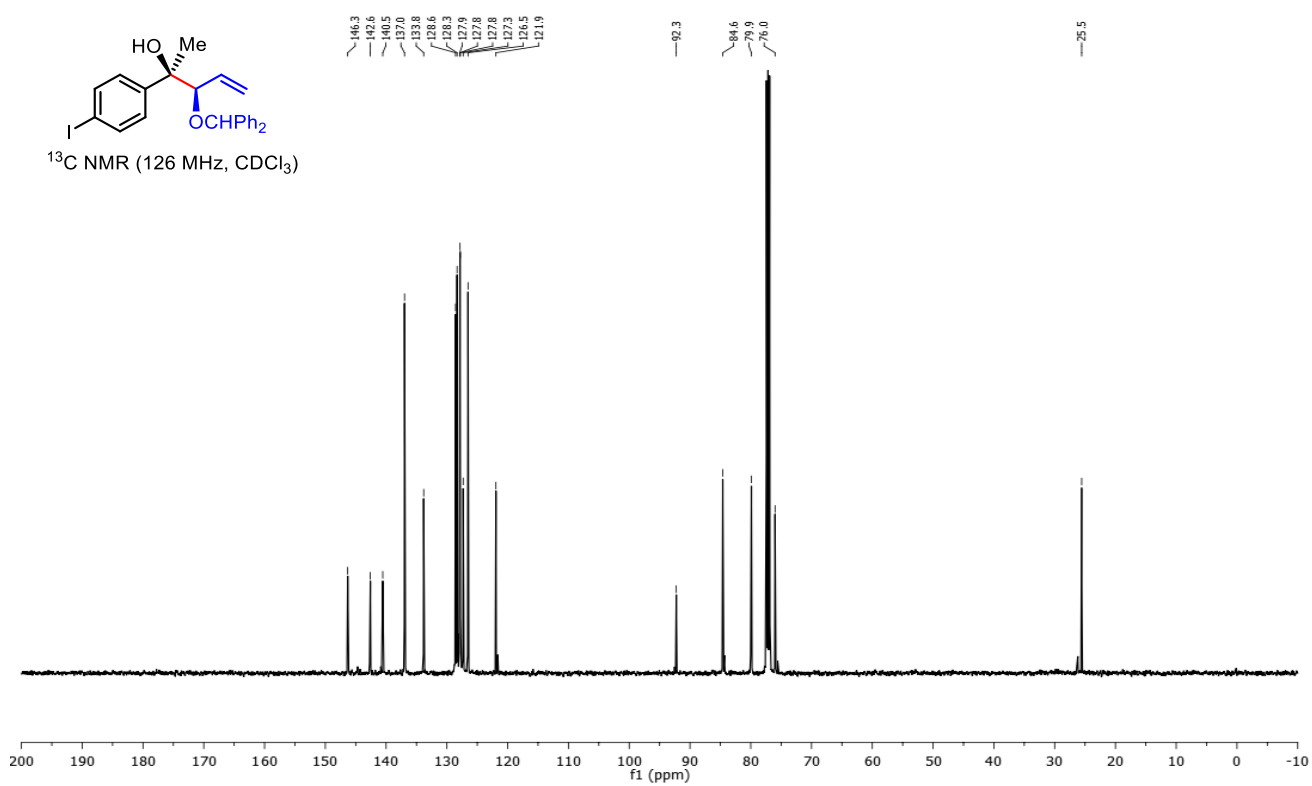
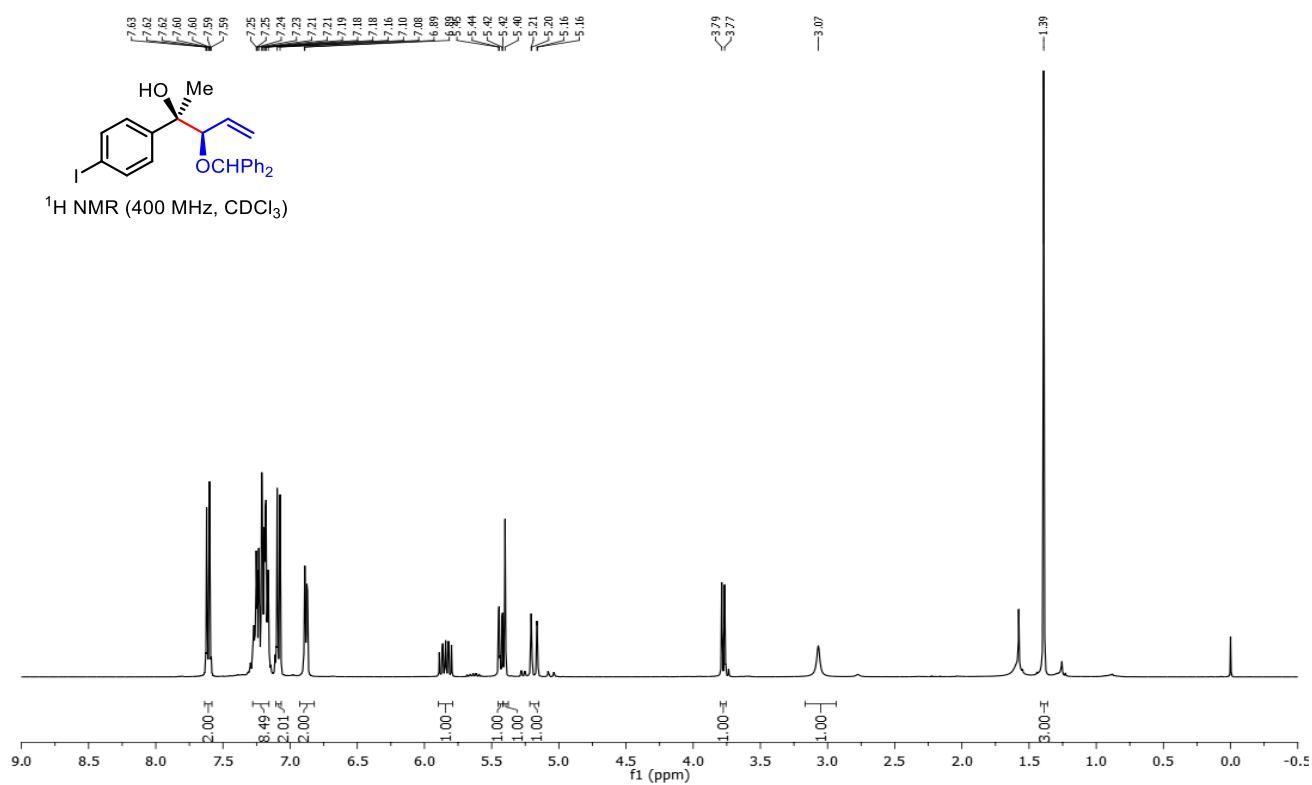


(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-fluorophenyl)pent-4-en-2-ol (3g):

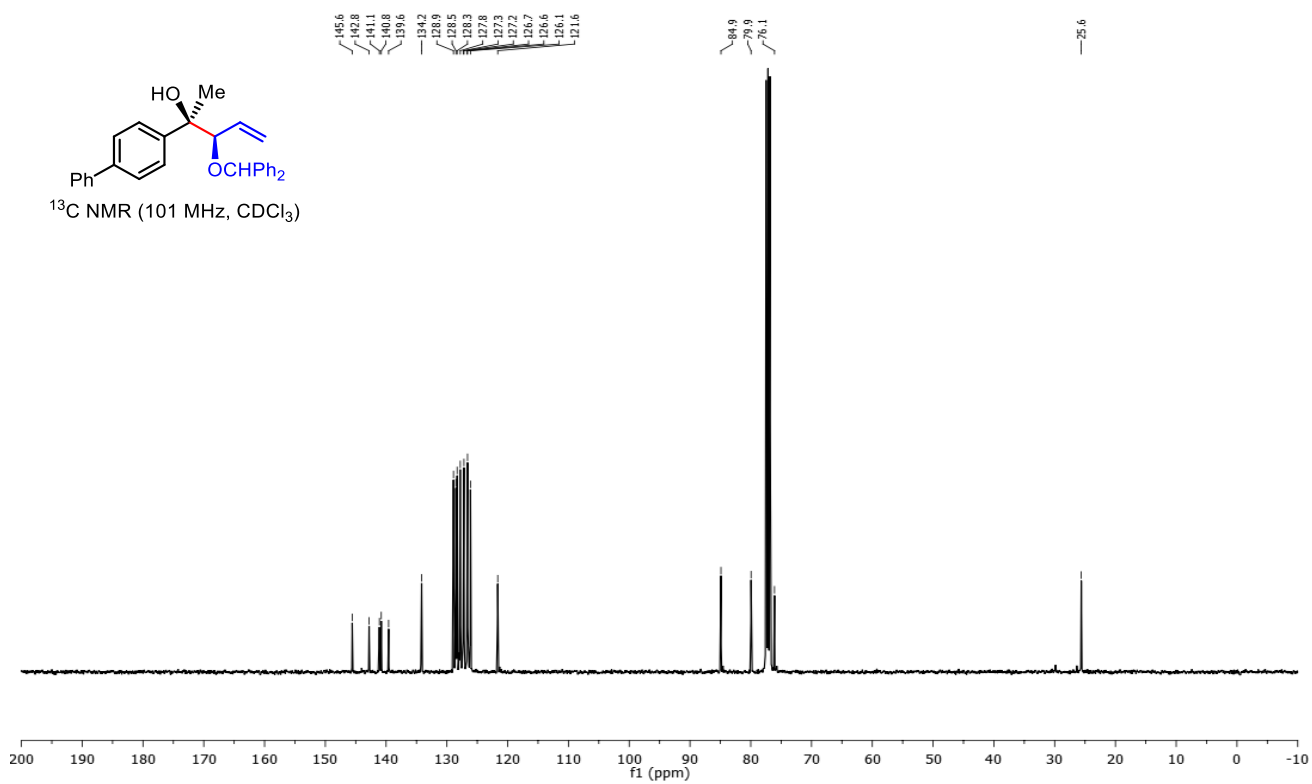
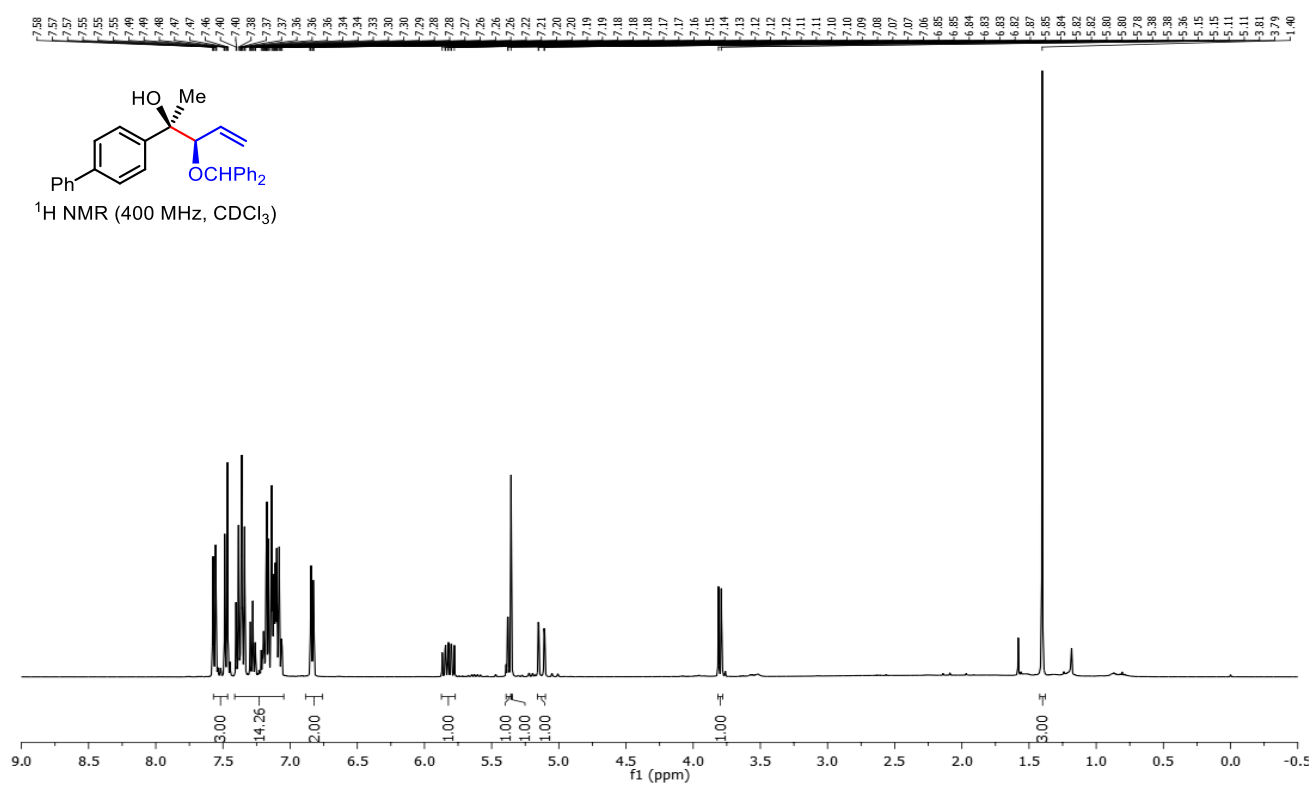




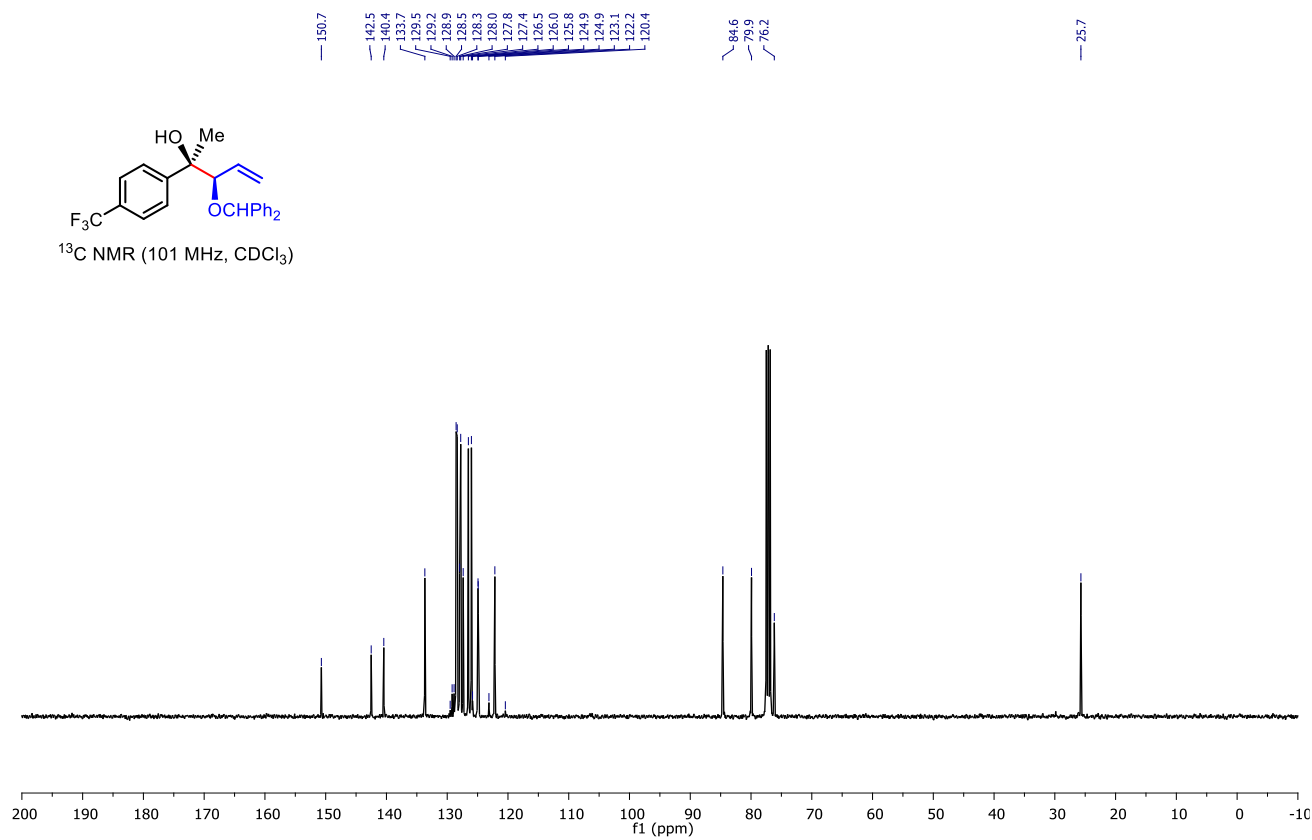
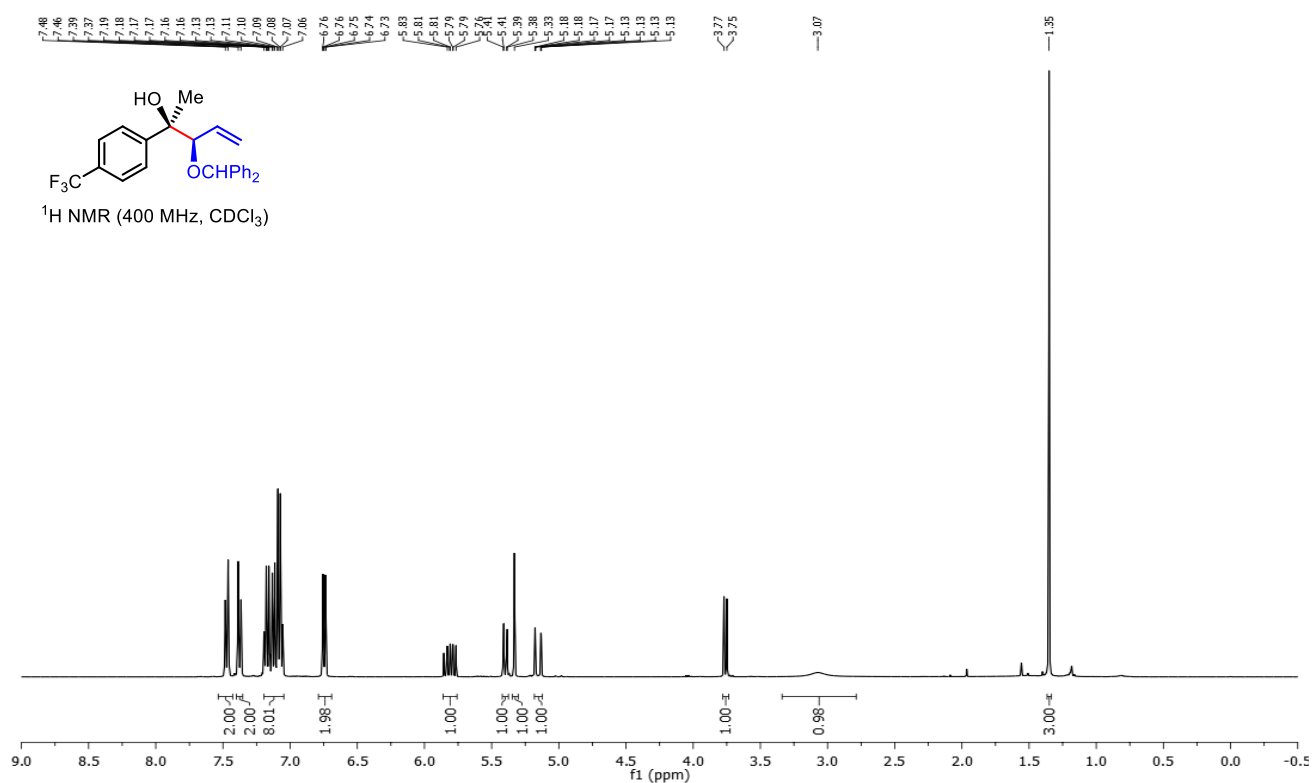
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-iodophenyl)pent-4-en-2-ol (3h):

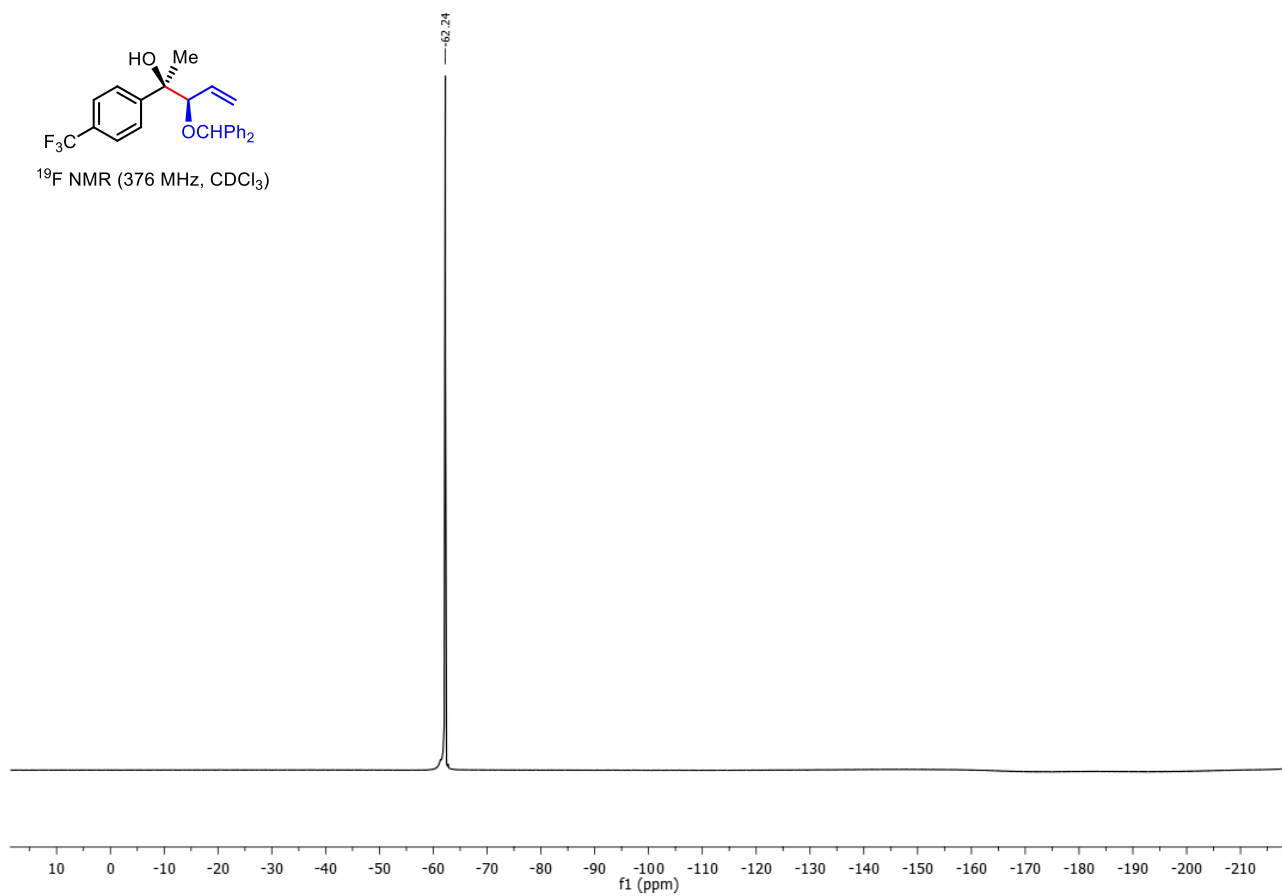
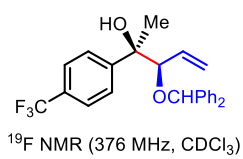


(2*R*,3*R*)-2-([1,1'-Biphenyl]-4-yl)-3-(benzhydryloxy)pent-4-en-2-ol (3i):

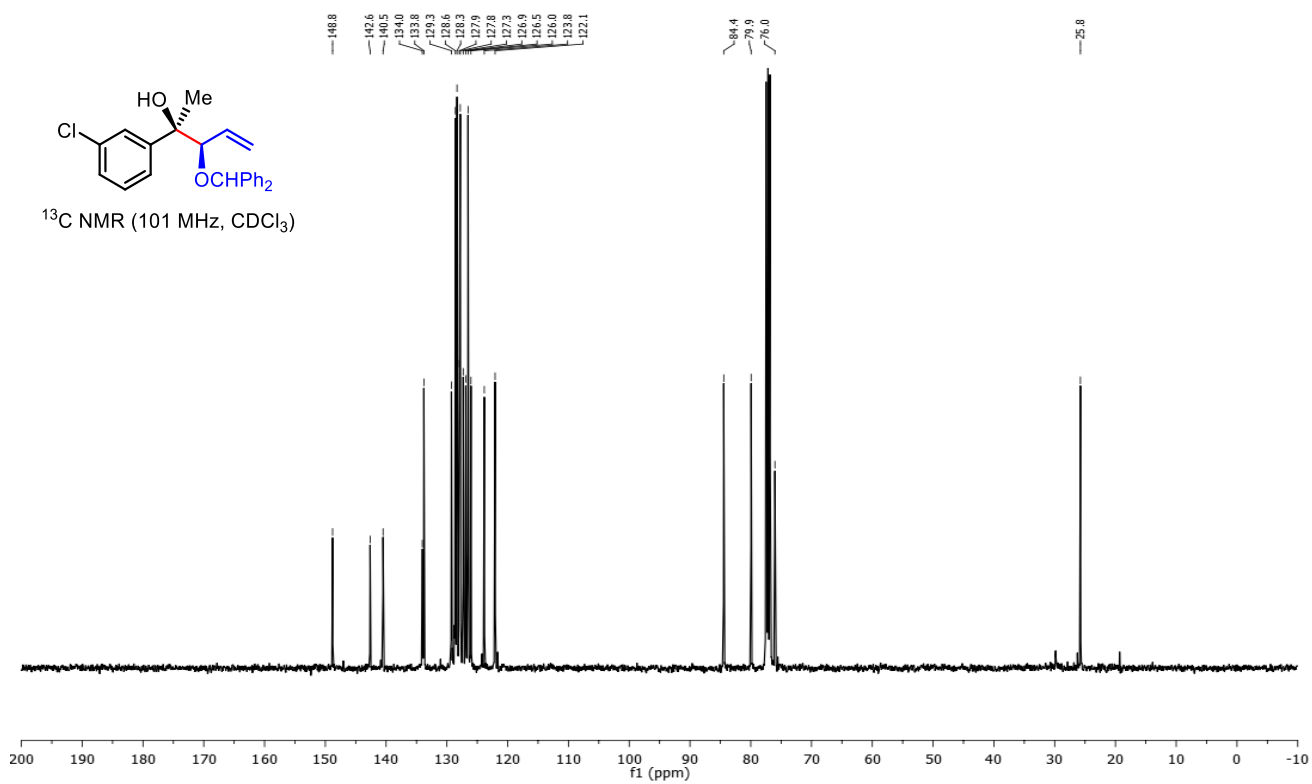
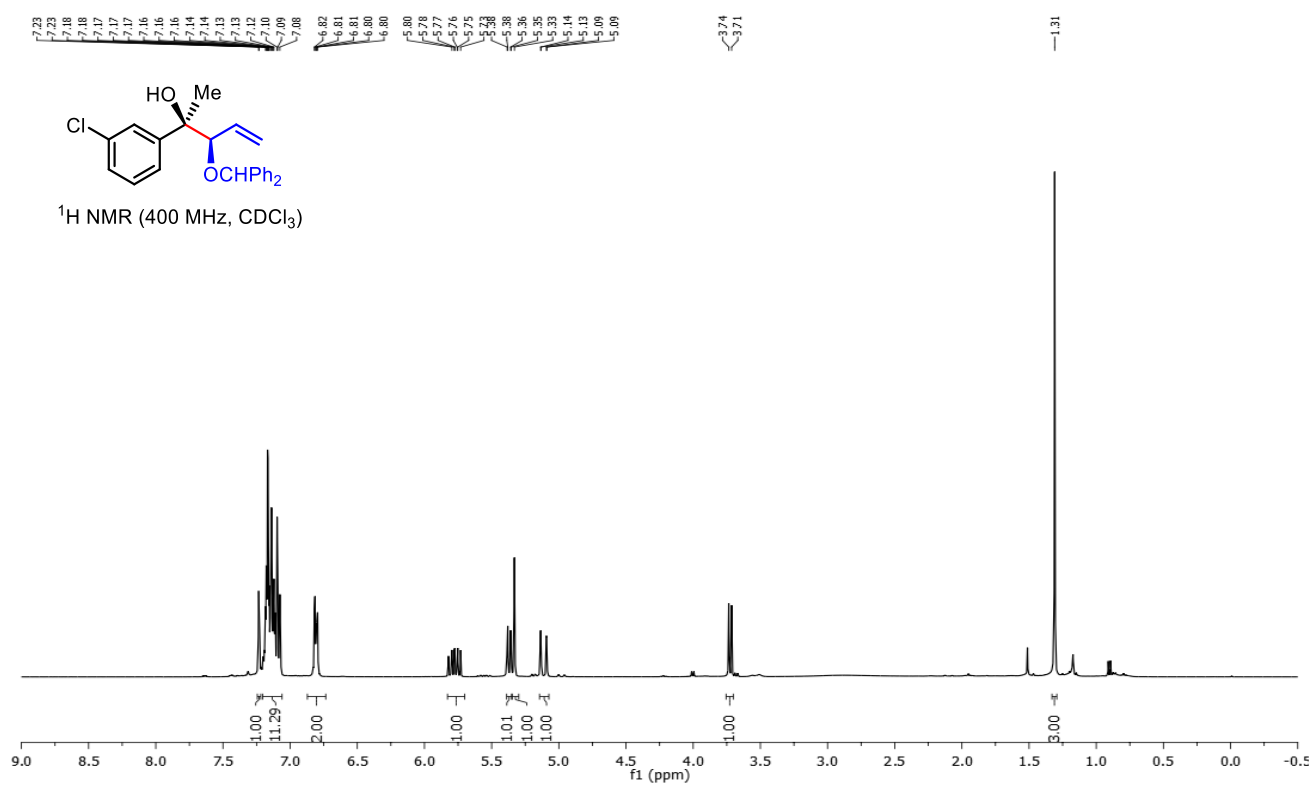


(2*R*,3*R*)-3-(Benzhydryloxy)-2-(4-(trifluoromethyl)phenyl)pent-4-en-2-ol (3j):

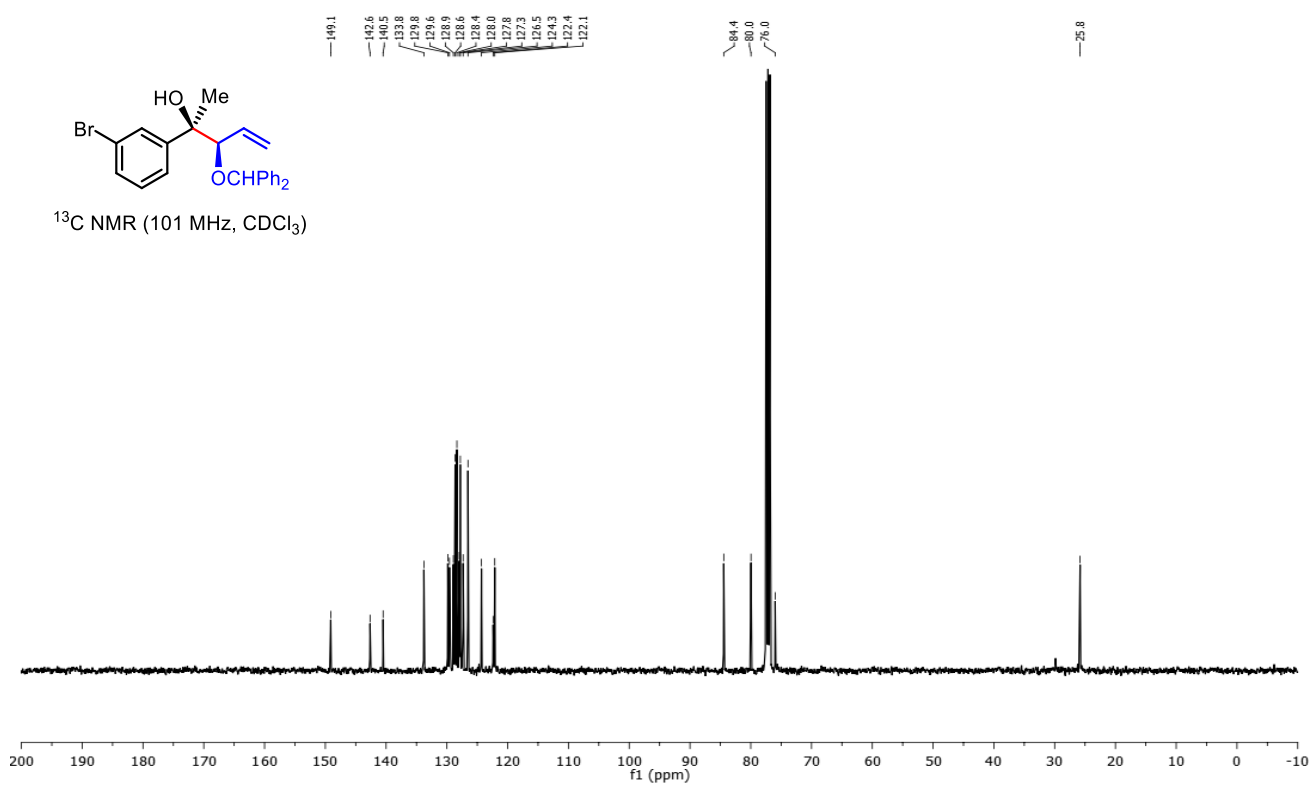
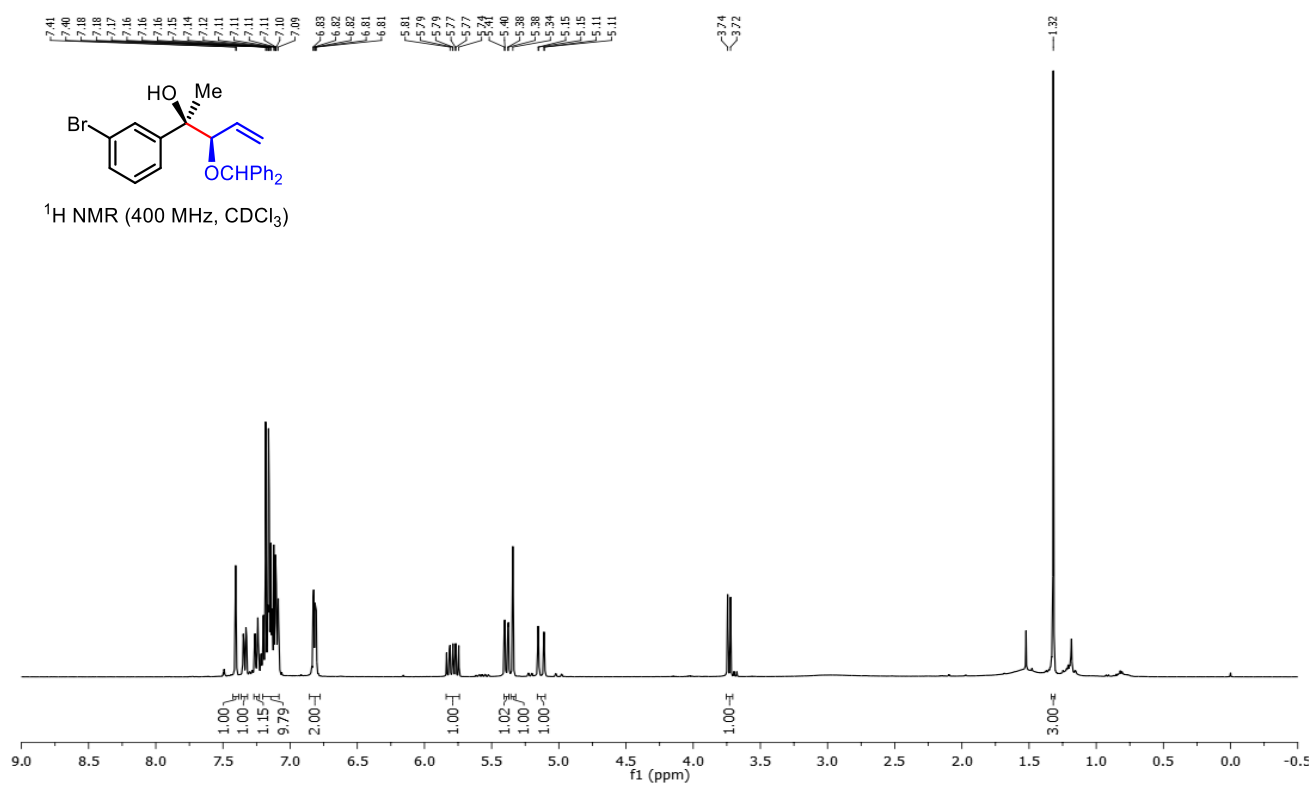




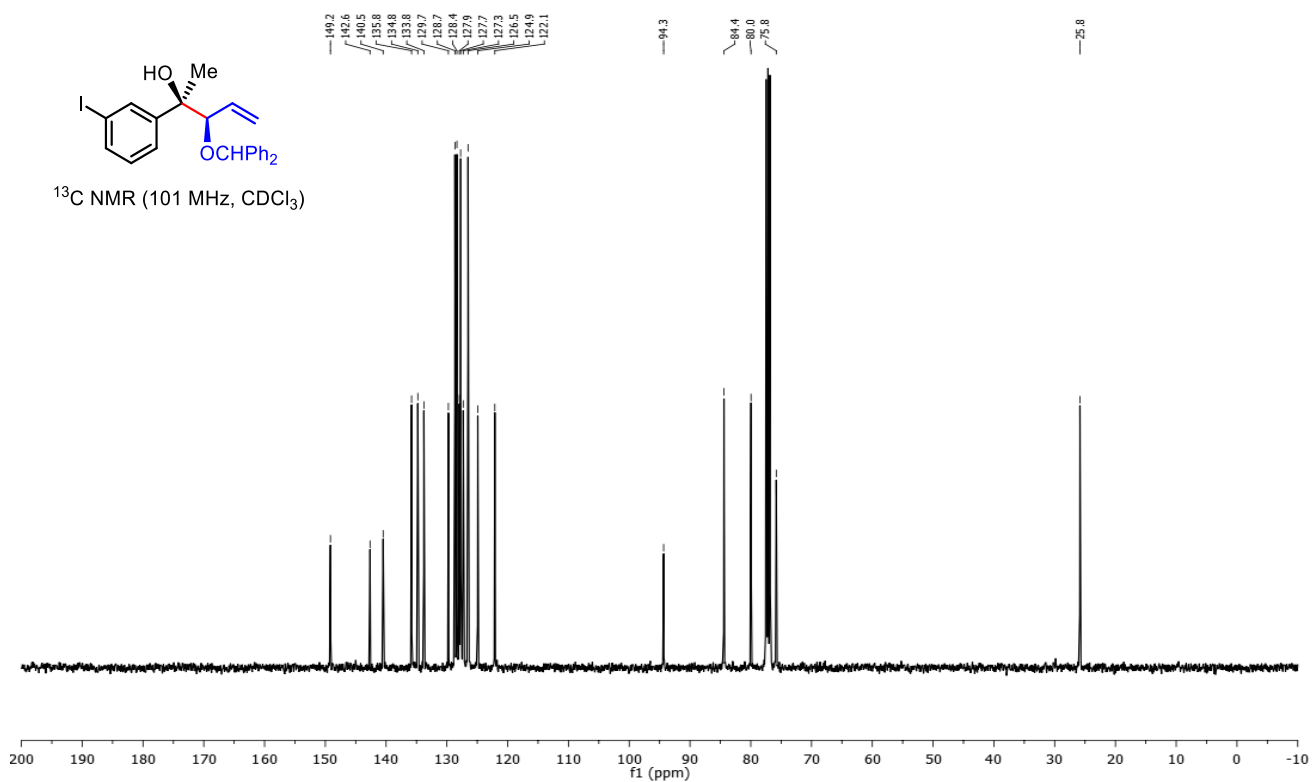
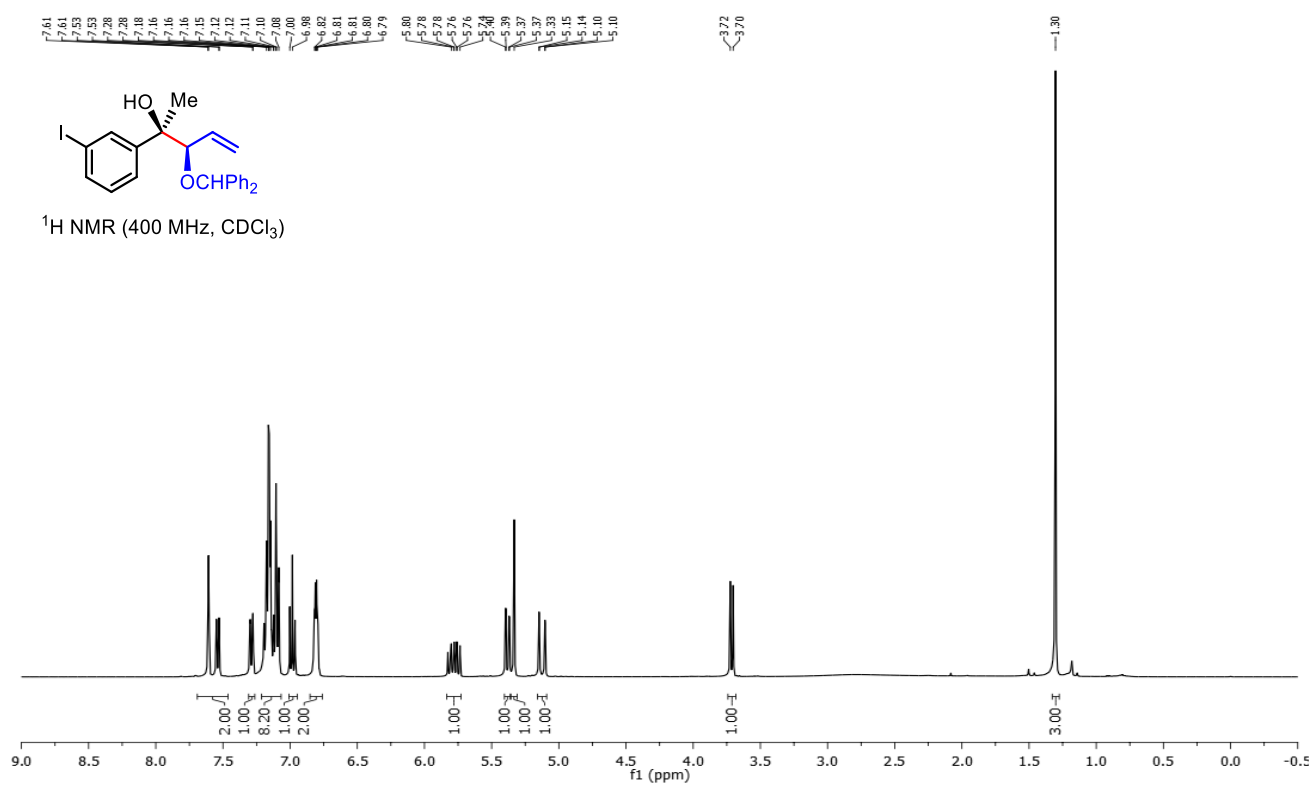
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(3-chlorophenyl)pent-4-en-2-ol (3k):



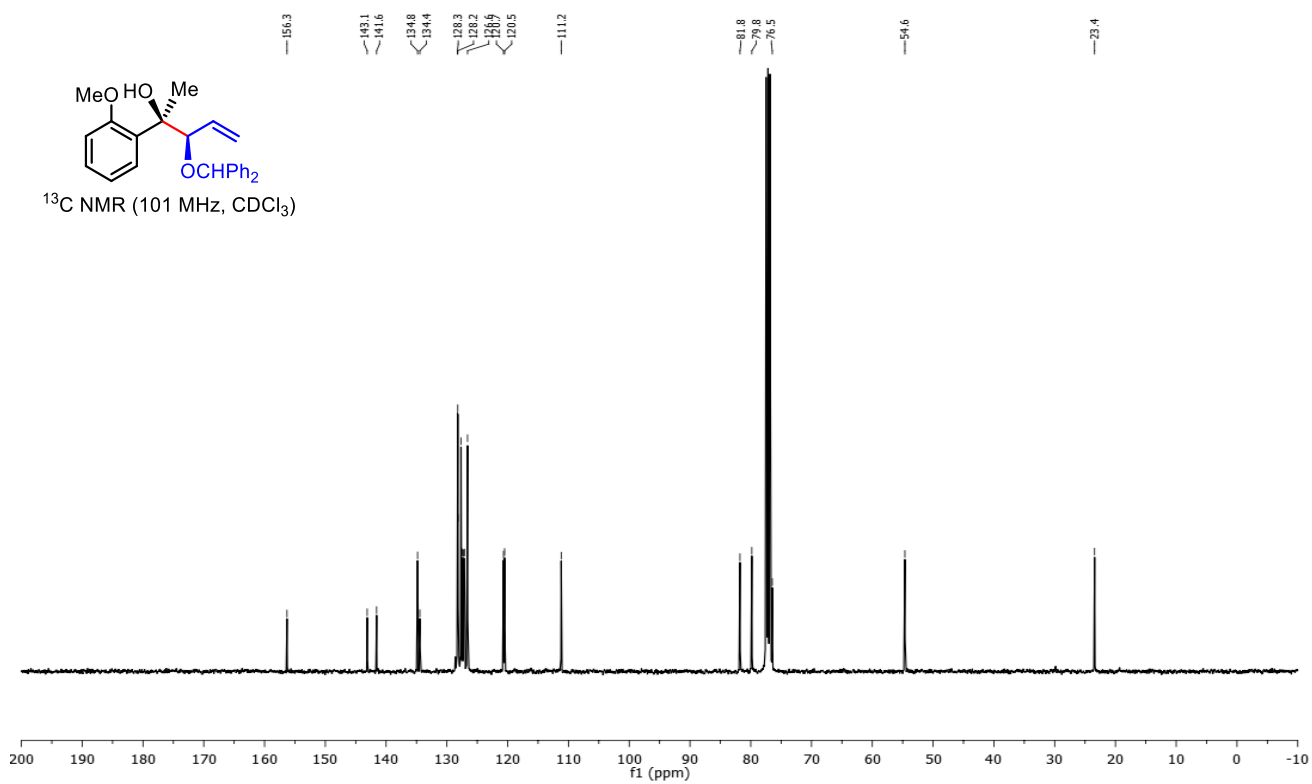
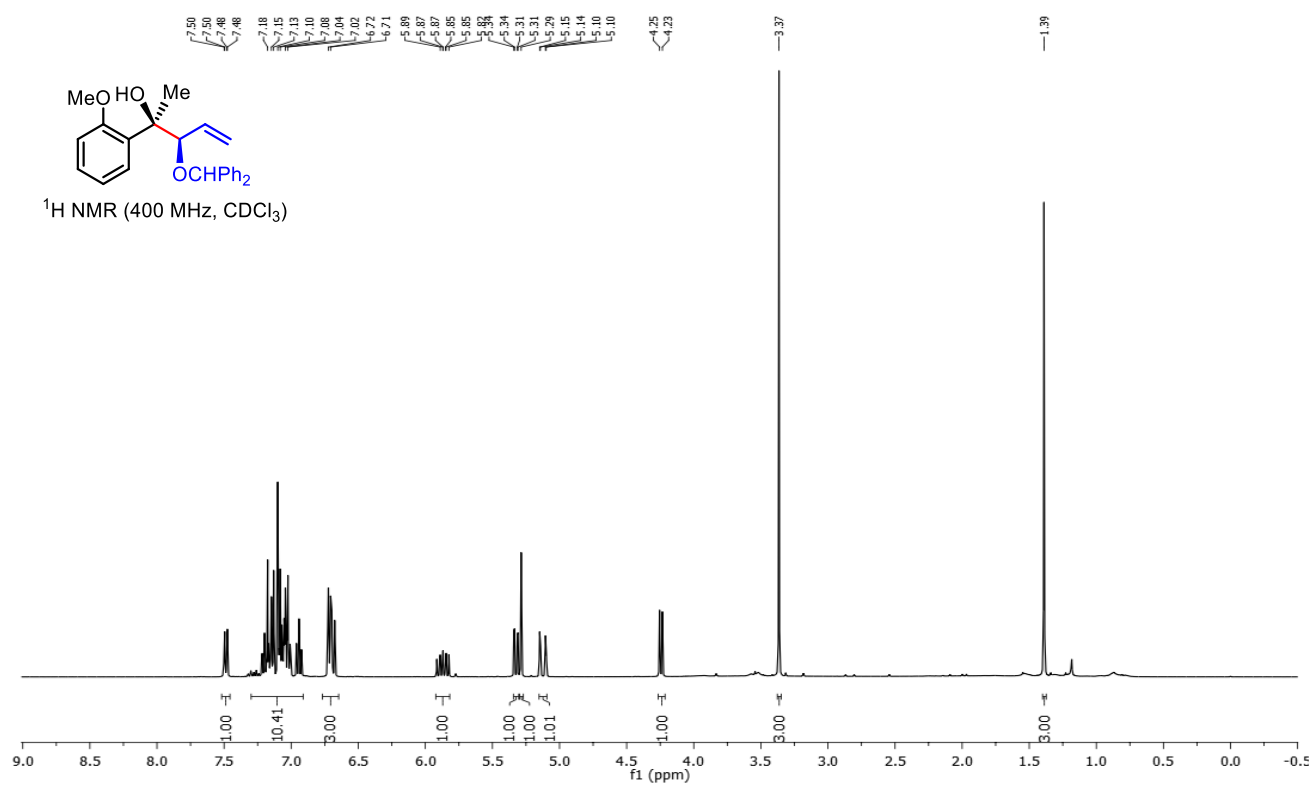
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(3-bromophenyl)pent-4-en-2-ol (3l):



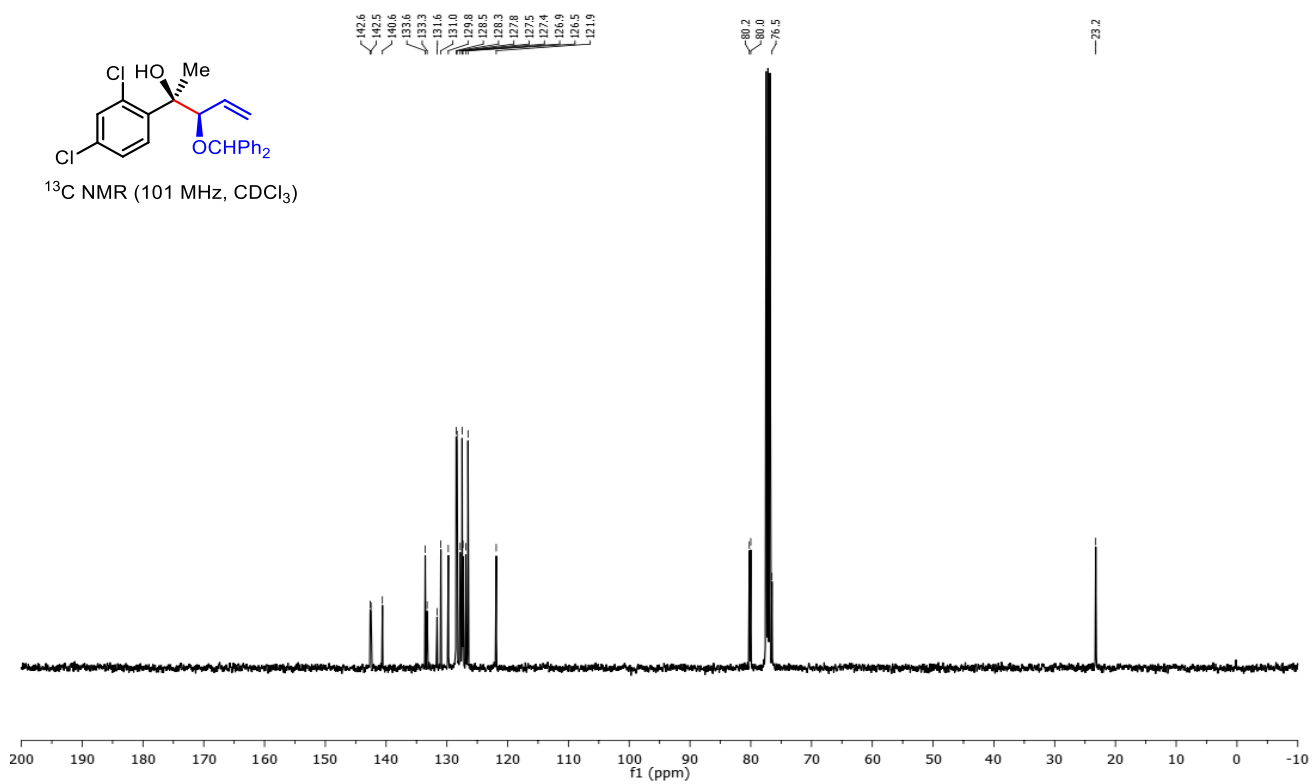
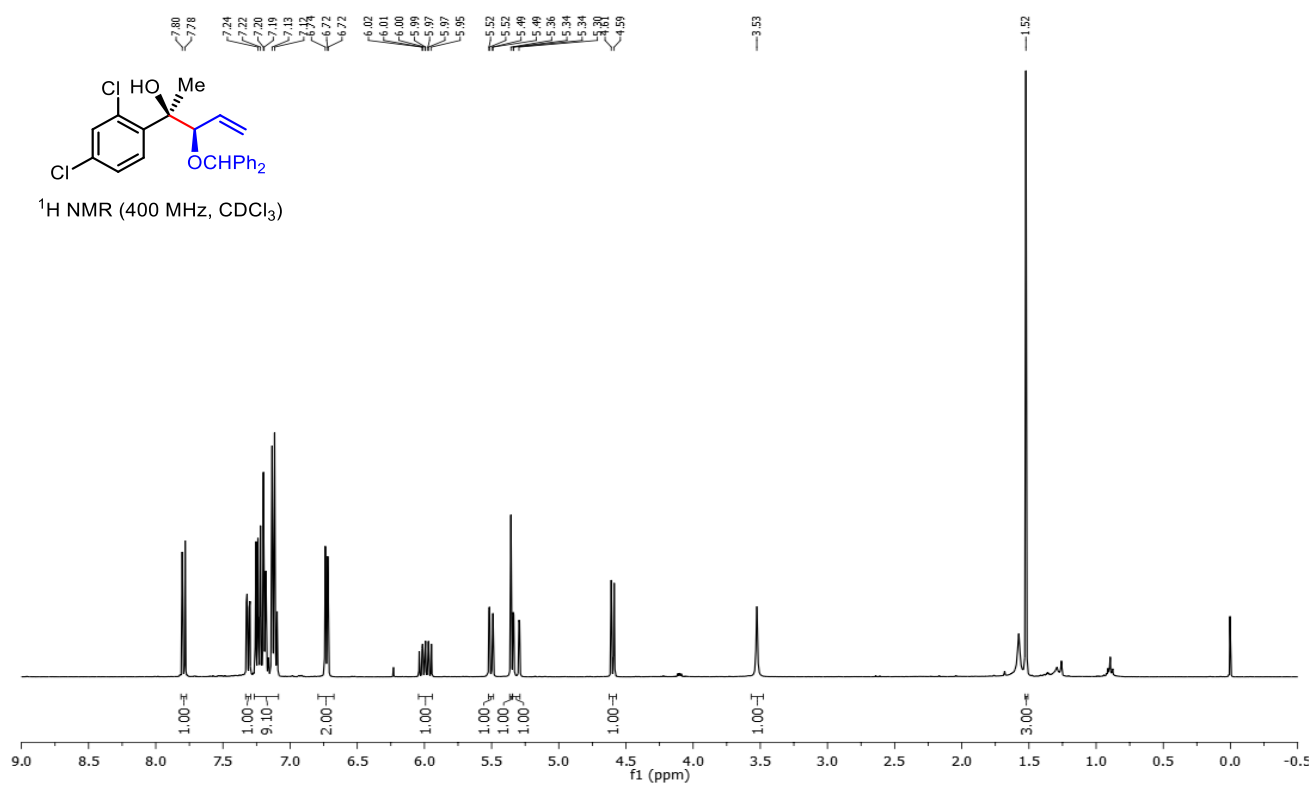
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(3-iodophenyl)pent-4-en-2-ol (3m):



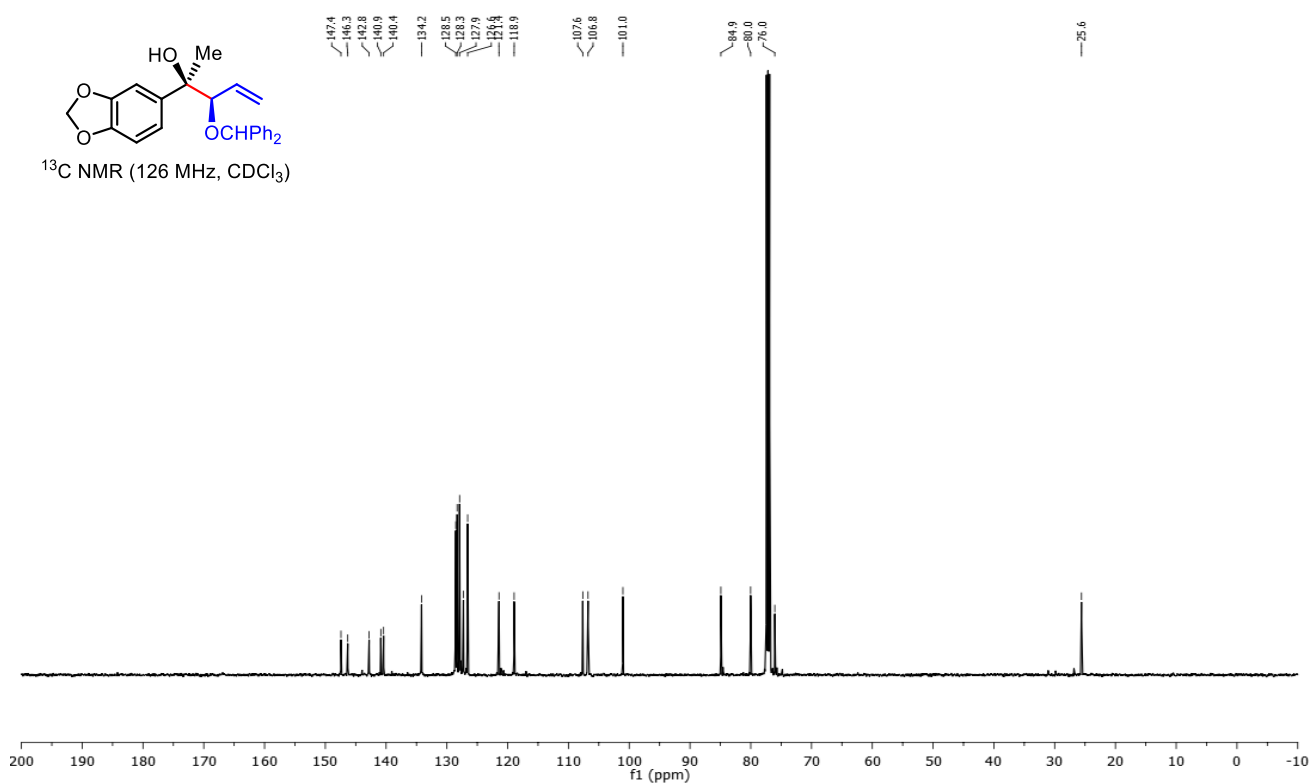
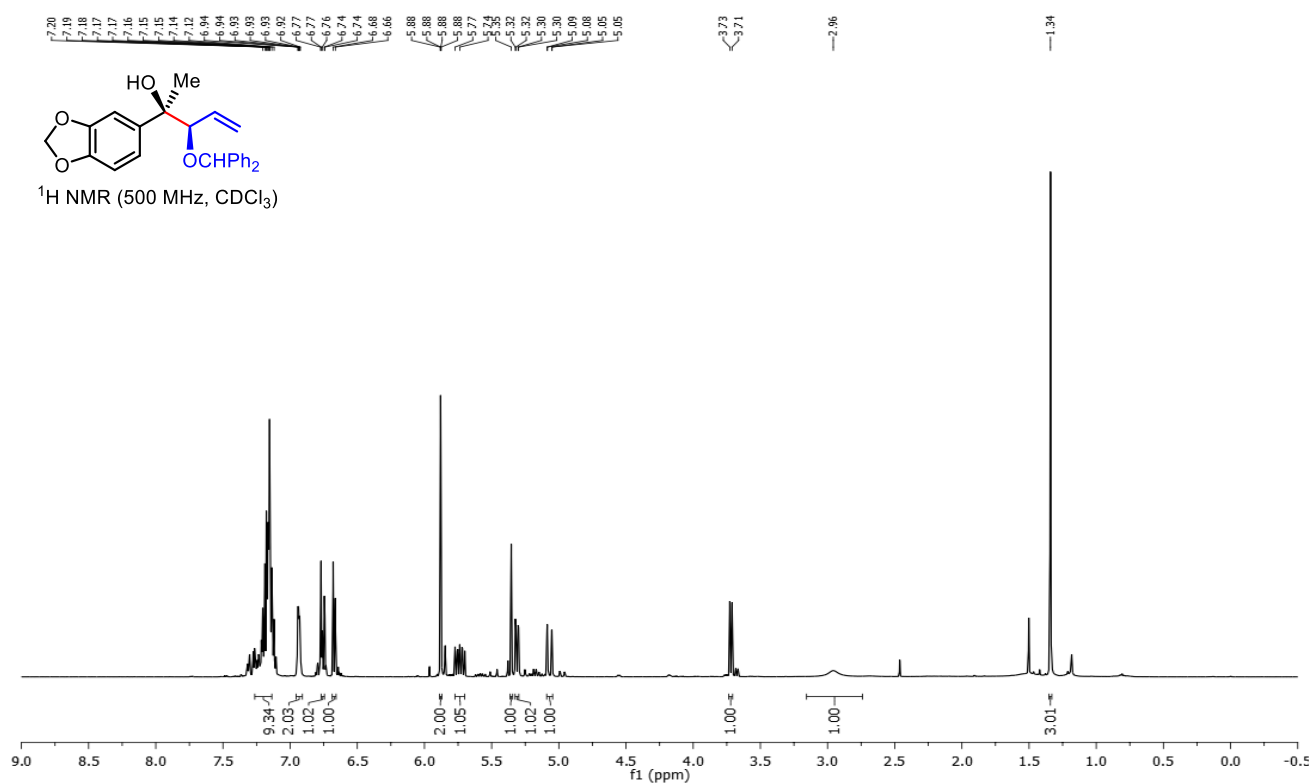
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(2-methoxyphenyl)pent-4-en-2-ol (3n):



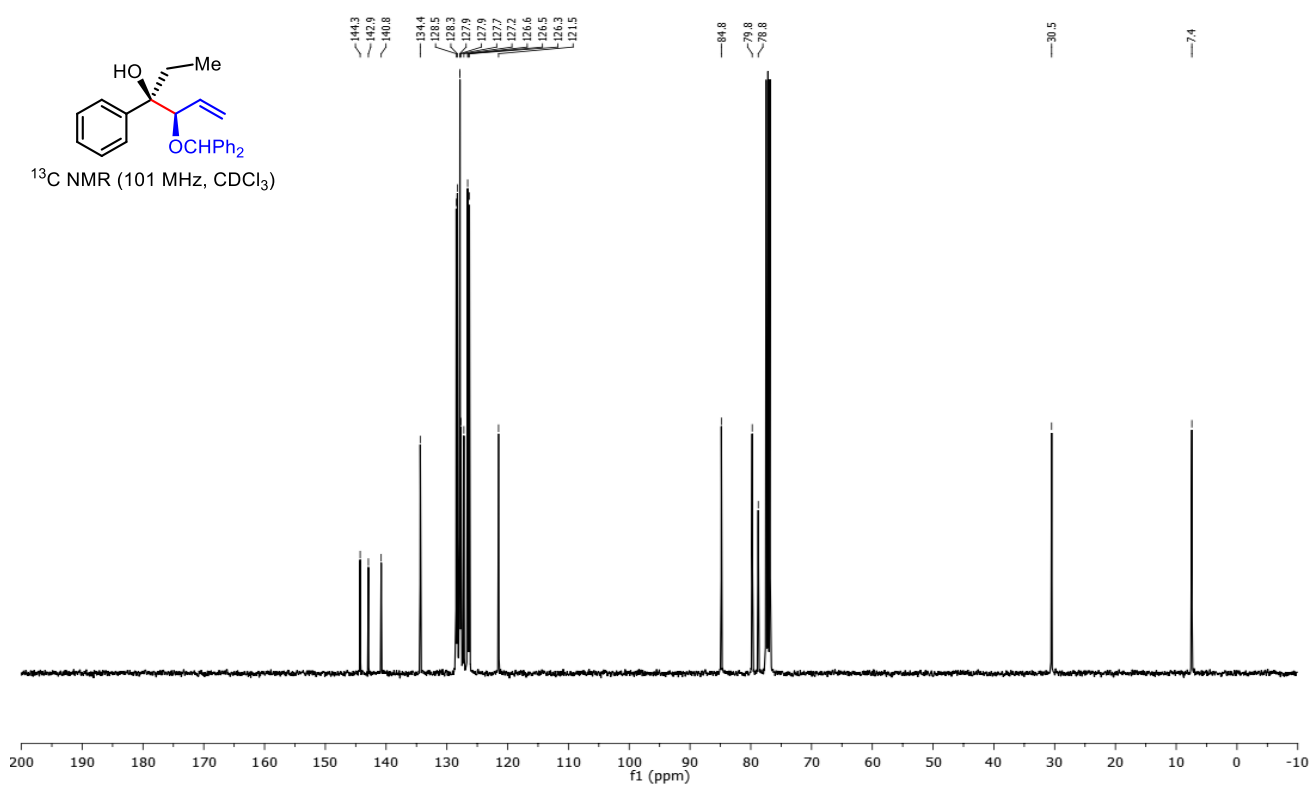
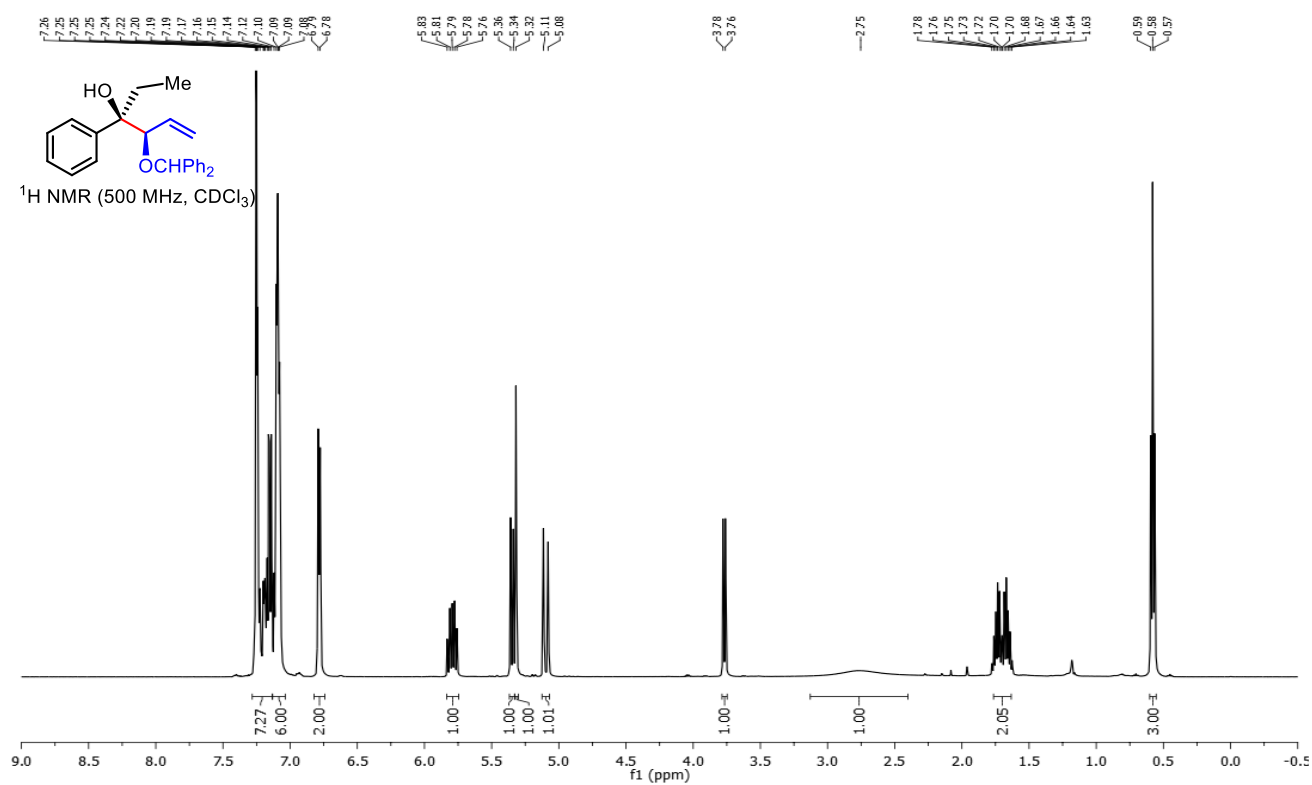
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(2,4-dichlorophenyl)pent-4-en-2-ol (3o):



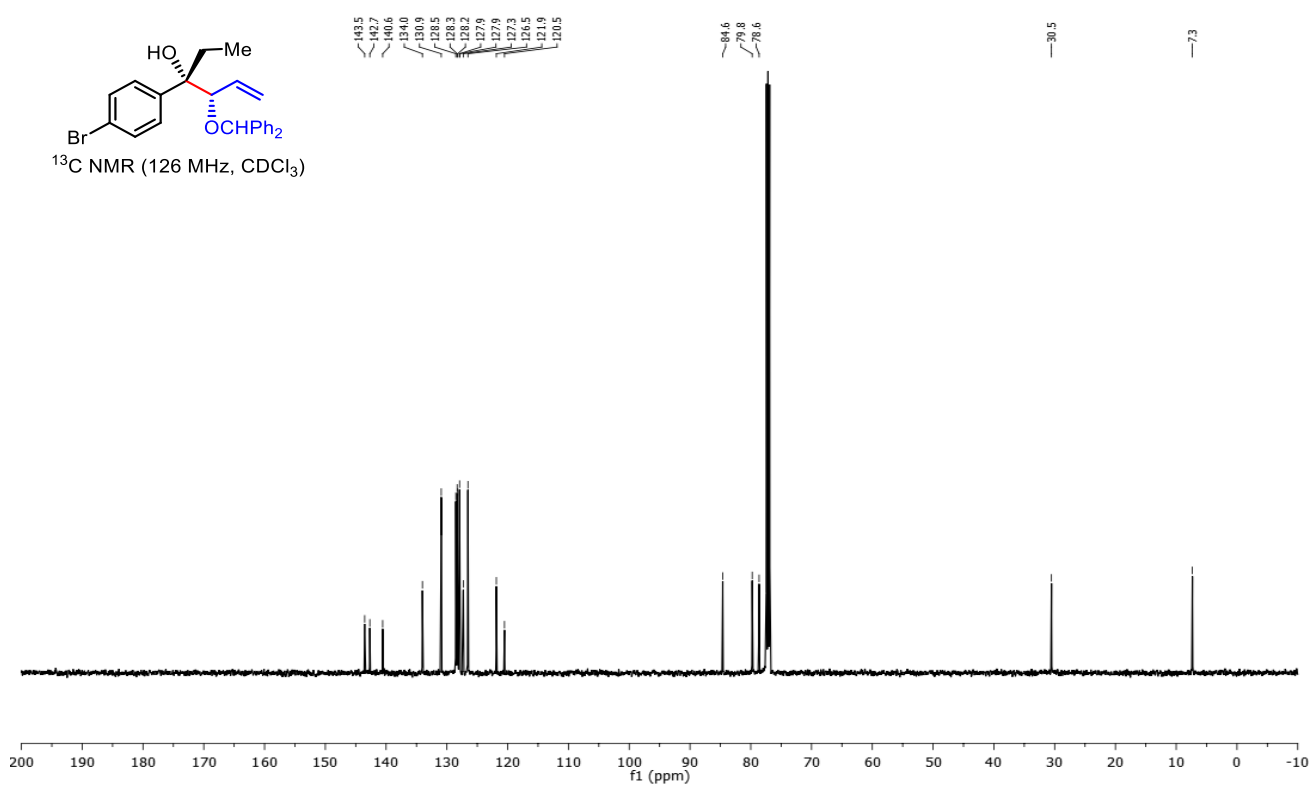
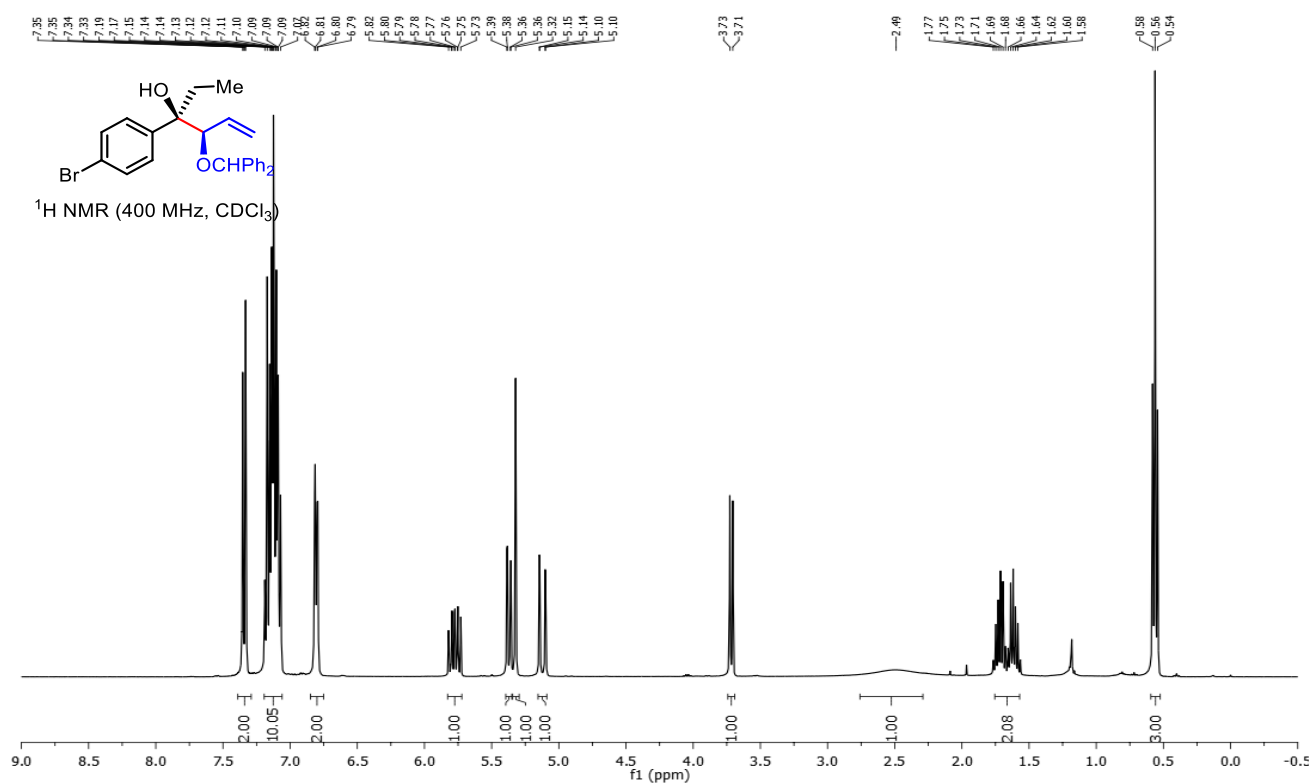
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(benzo[d][1,3]dioxol-5-yl)pent-4-en-2-ol (3p):



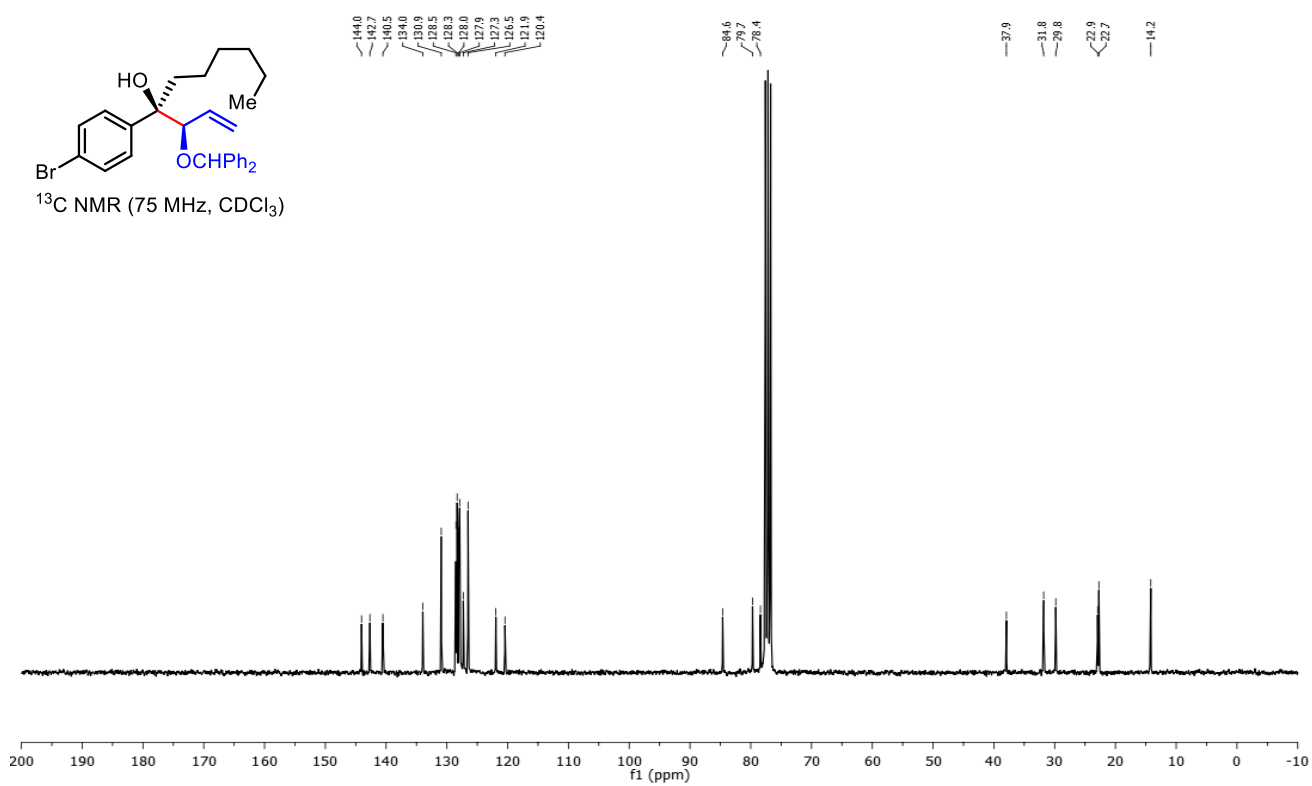
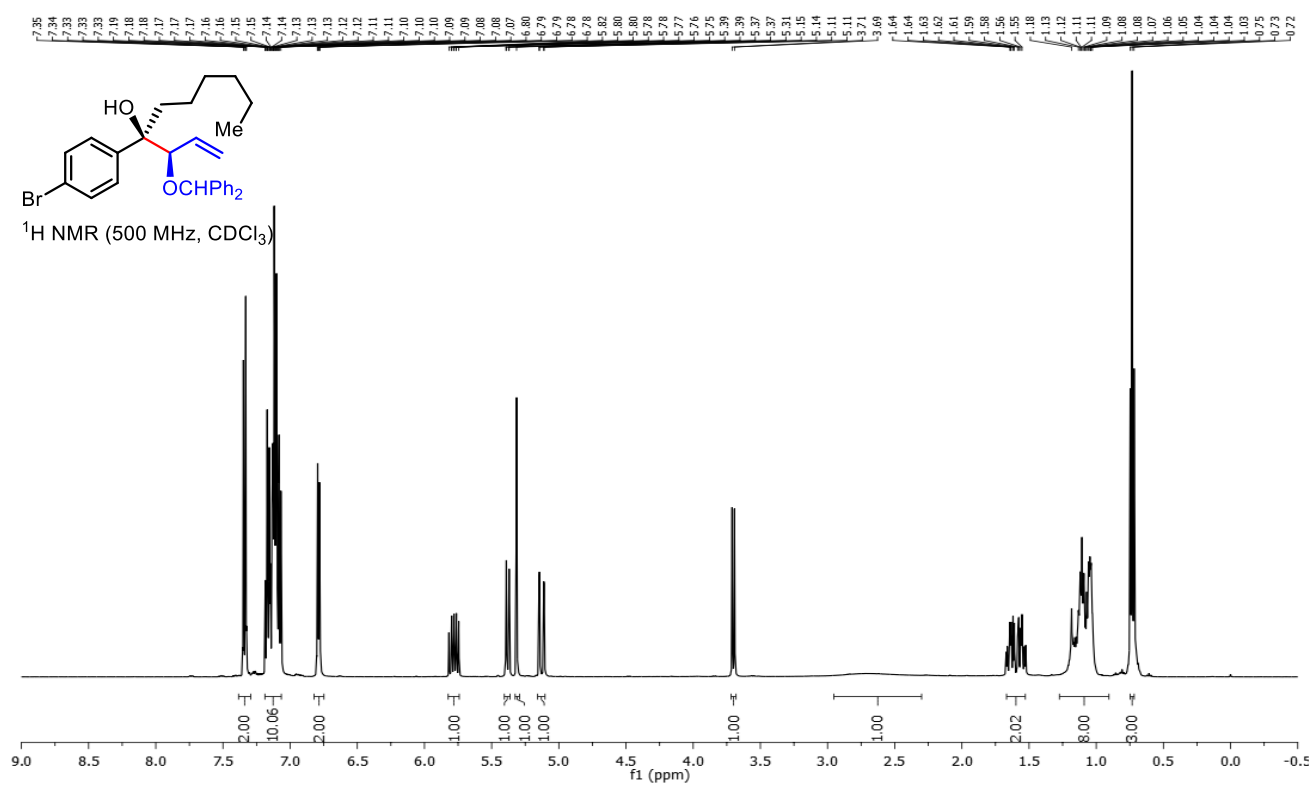
(3*R*,4*R*)-4-(Benzhydryloxy)-3-phenylhex-5-en-3-ol (3q):



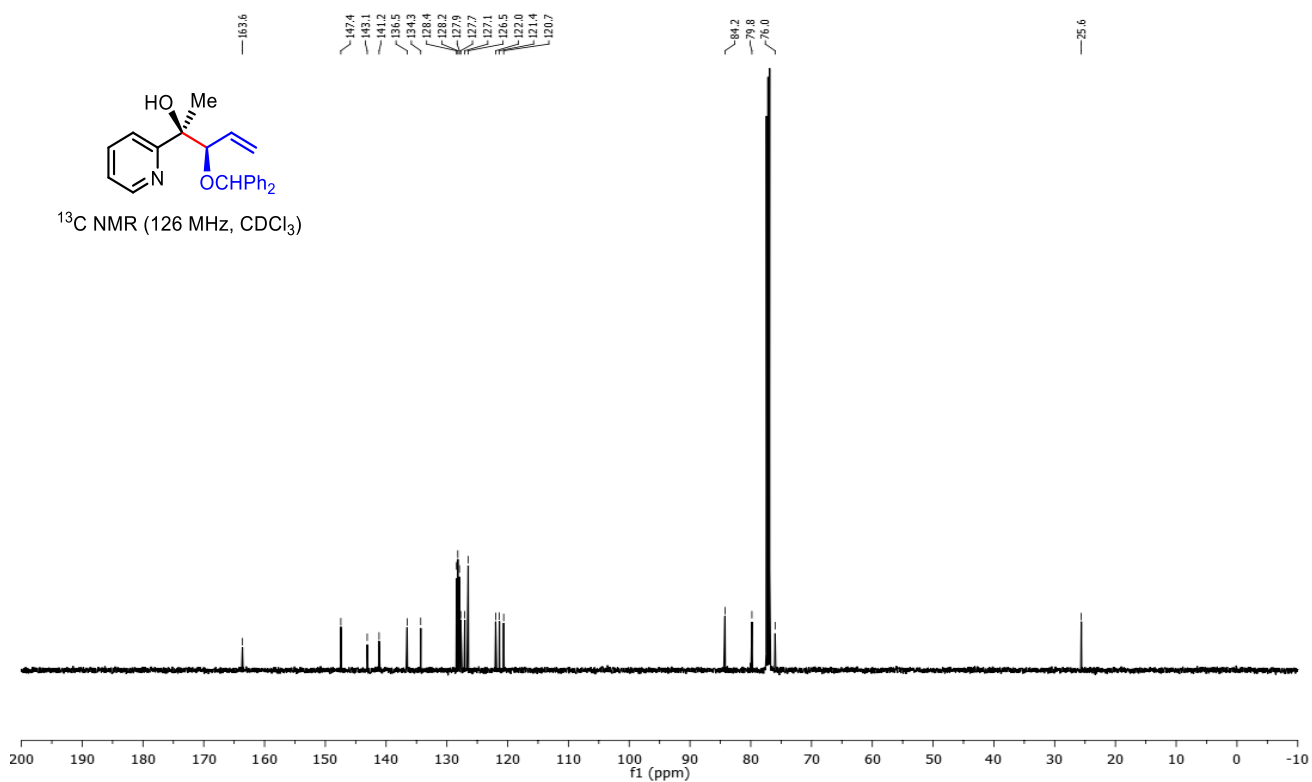
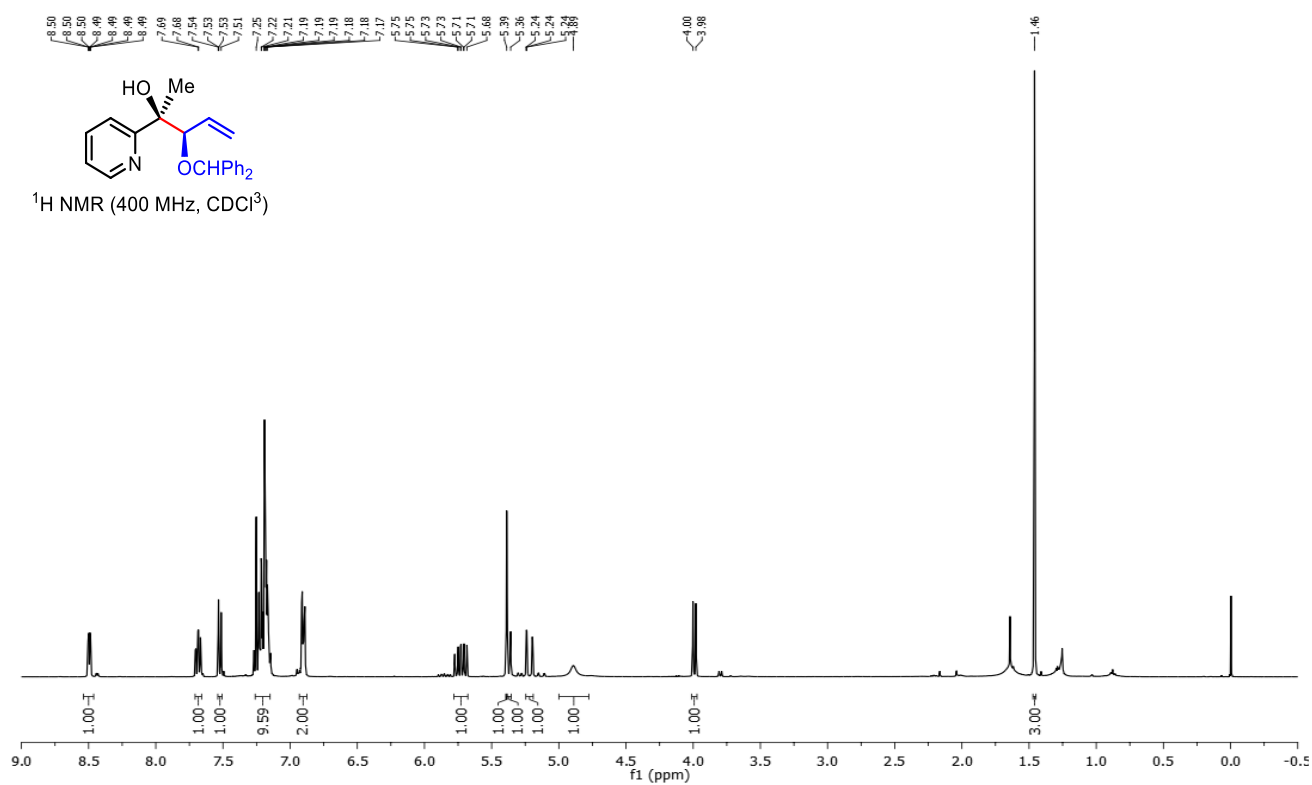
(3*R*,4*R*)-4-(Benzhydryloxy)-3-(4-bromophenyl)hex-5-en-3-ol (3r):



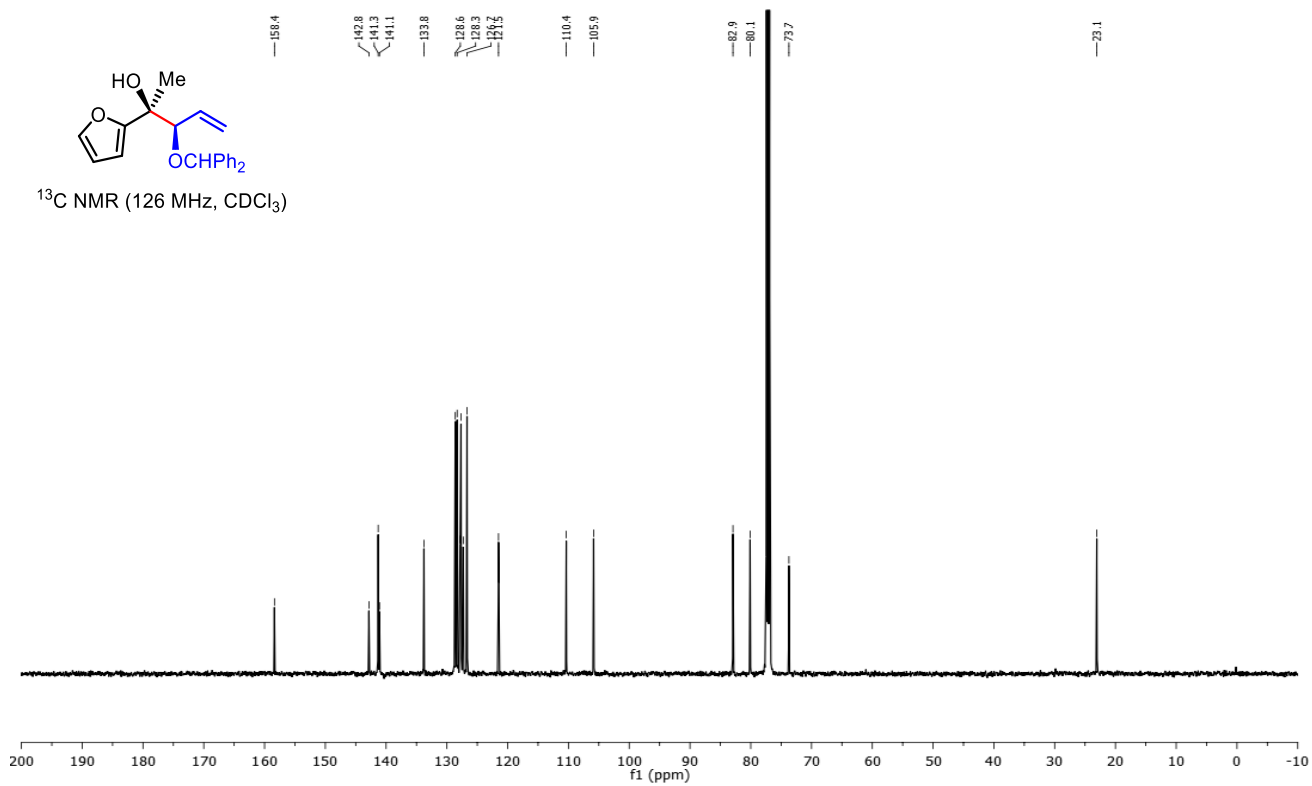
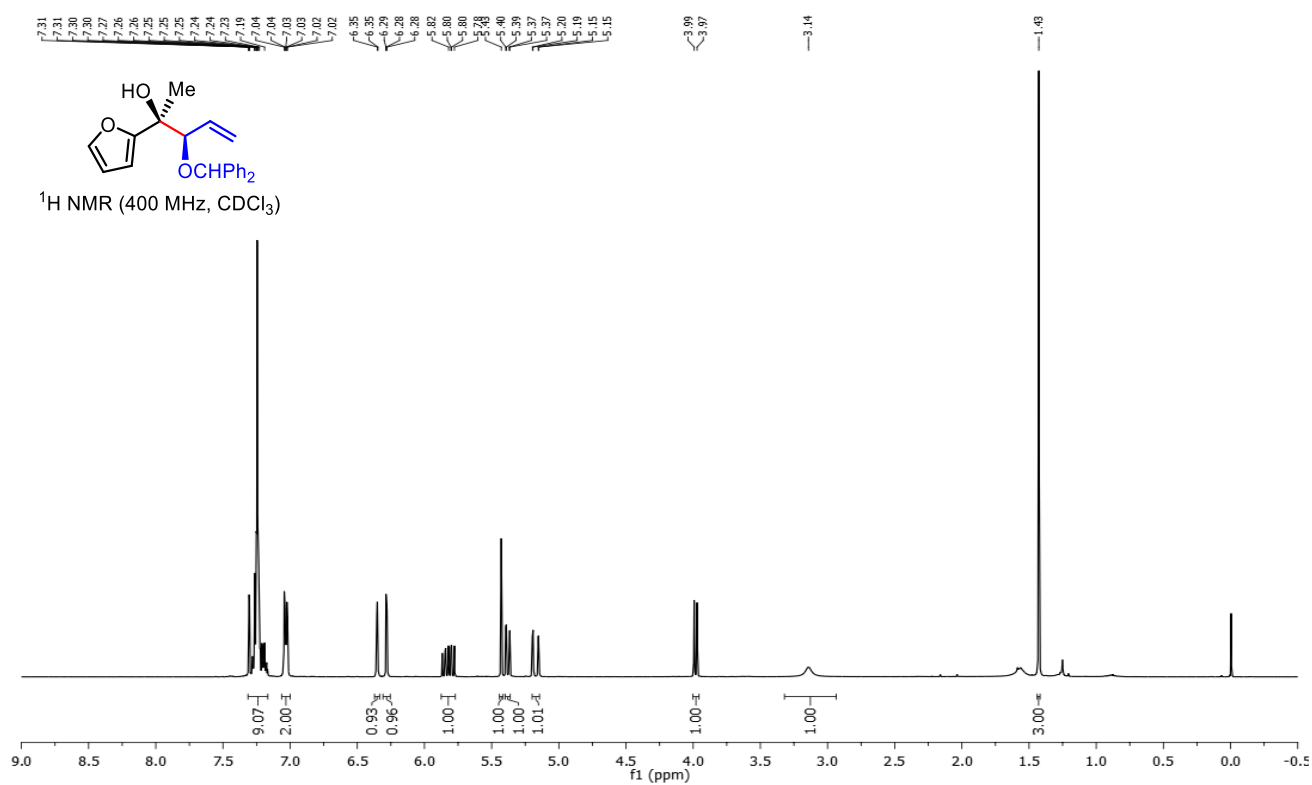
(3*R*,4*R*)-3-(Benzhydryloxy)-4-(4-bromophenyl)dec-1-en-4-ol (3s):



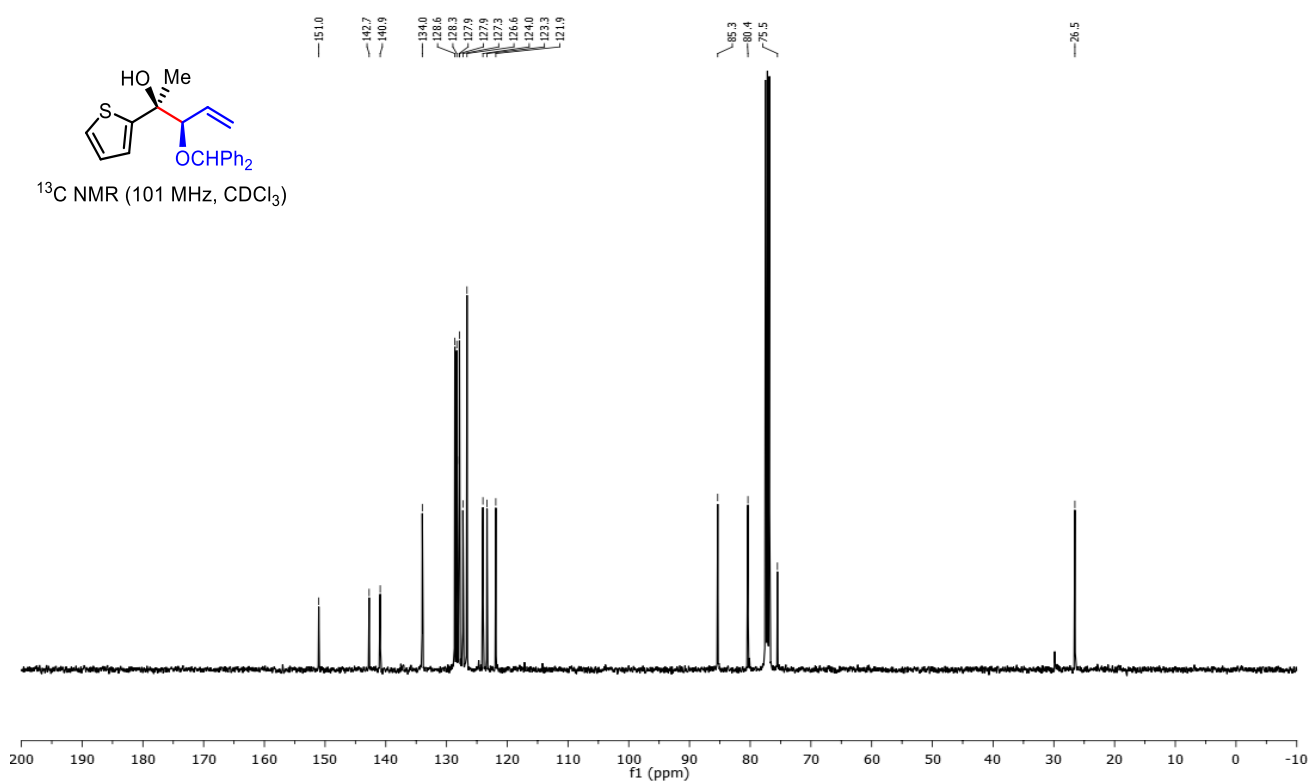
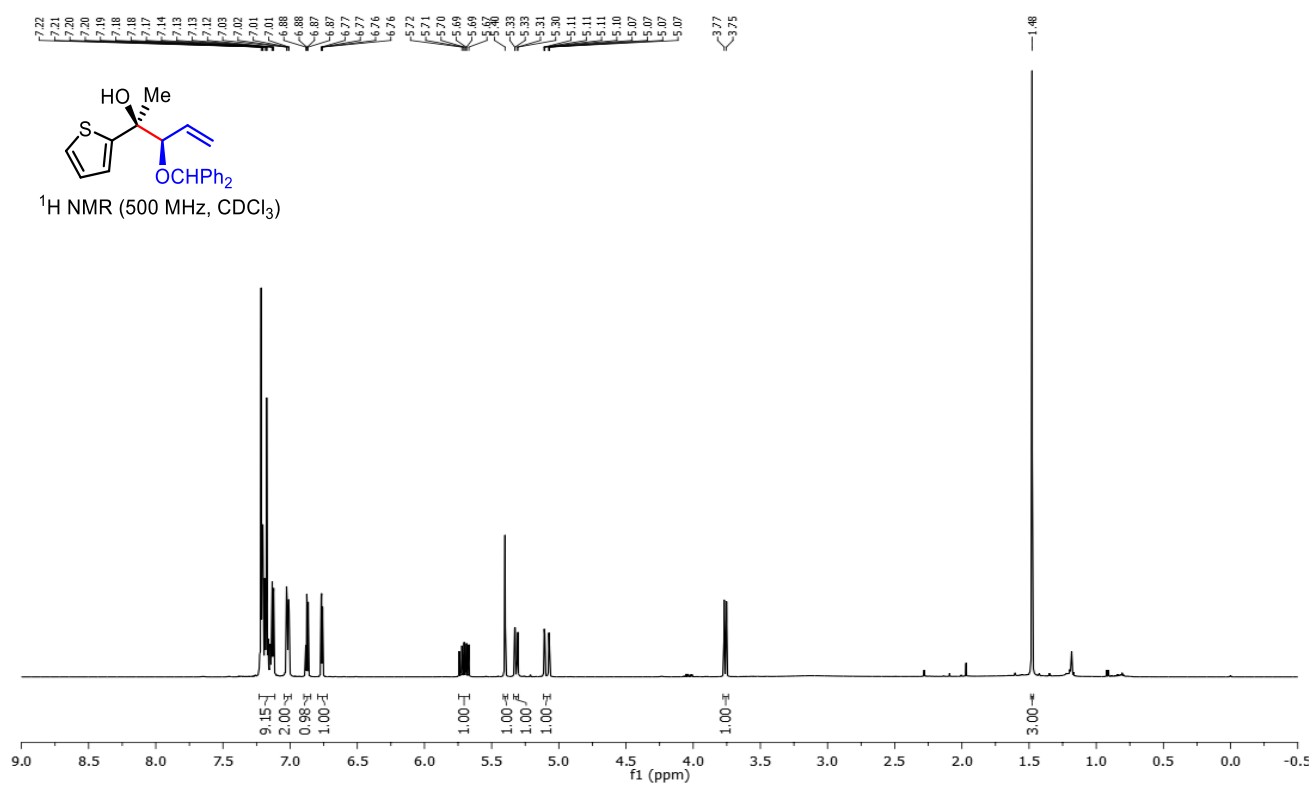
(2*R*,3*R*)-3-(Benzhydryloxy)-2-(pyridin-2-yl)pent-4-en-2-ol (3u):



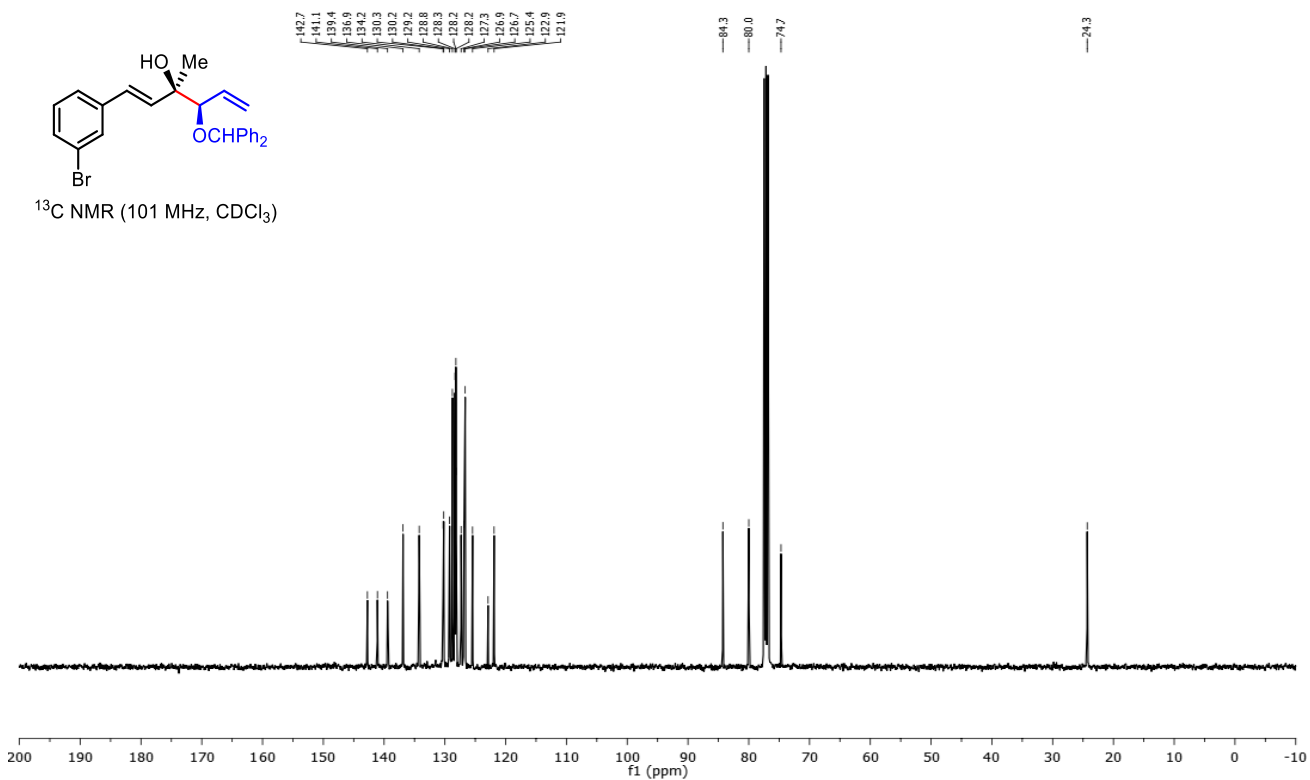
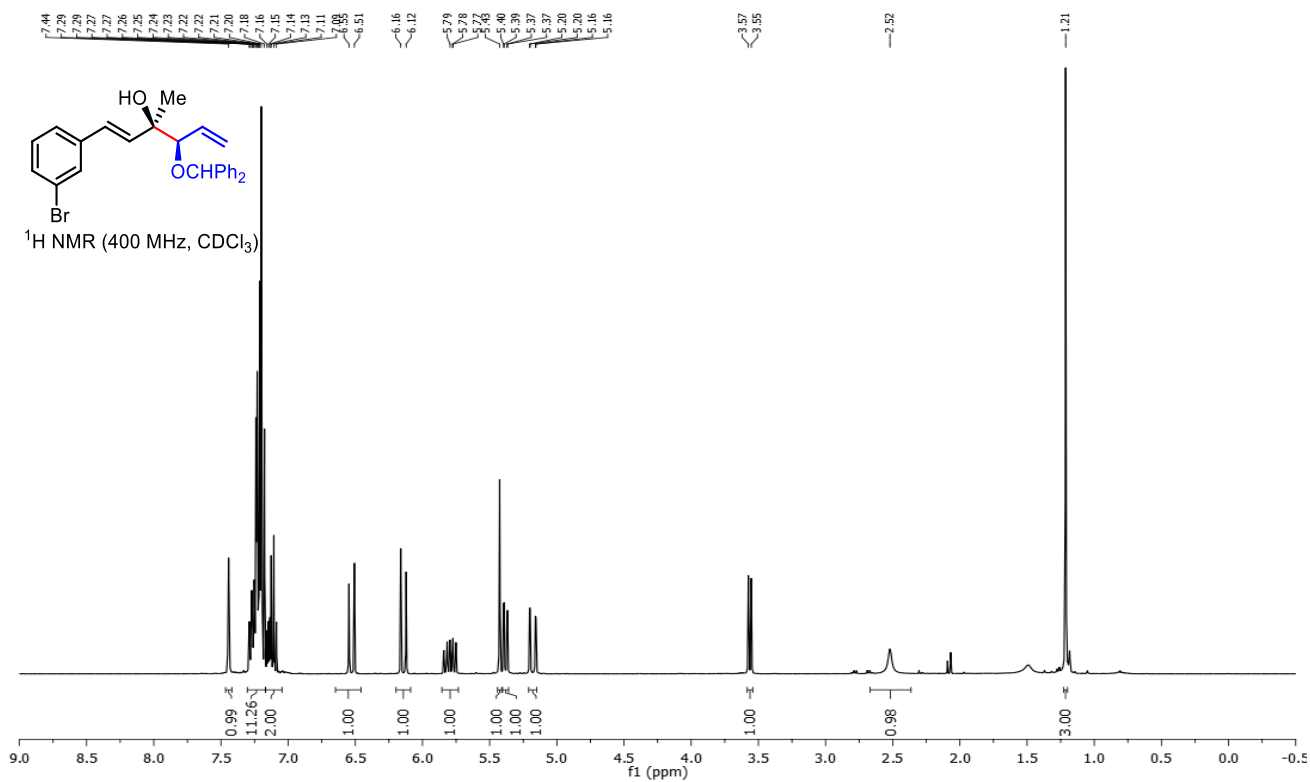
(2*S*,3*R*)-3-(Benzhydryloxy)-2-(furan-2-yl)pent-4-en-2-ol (3v):



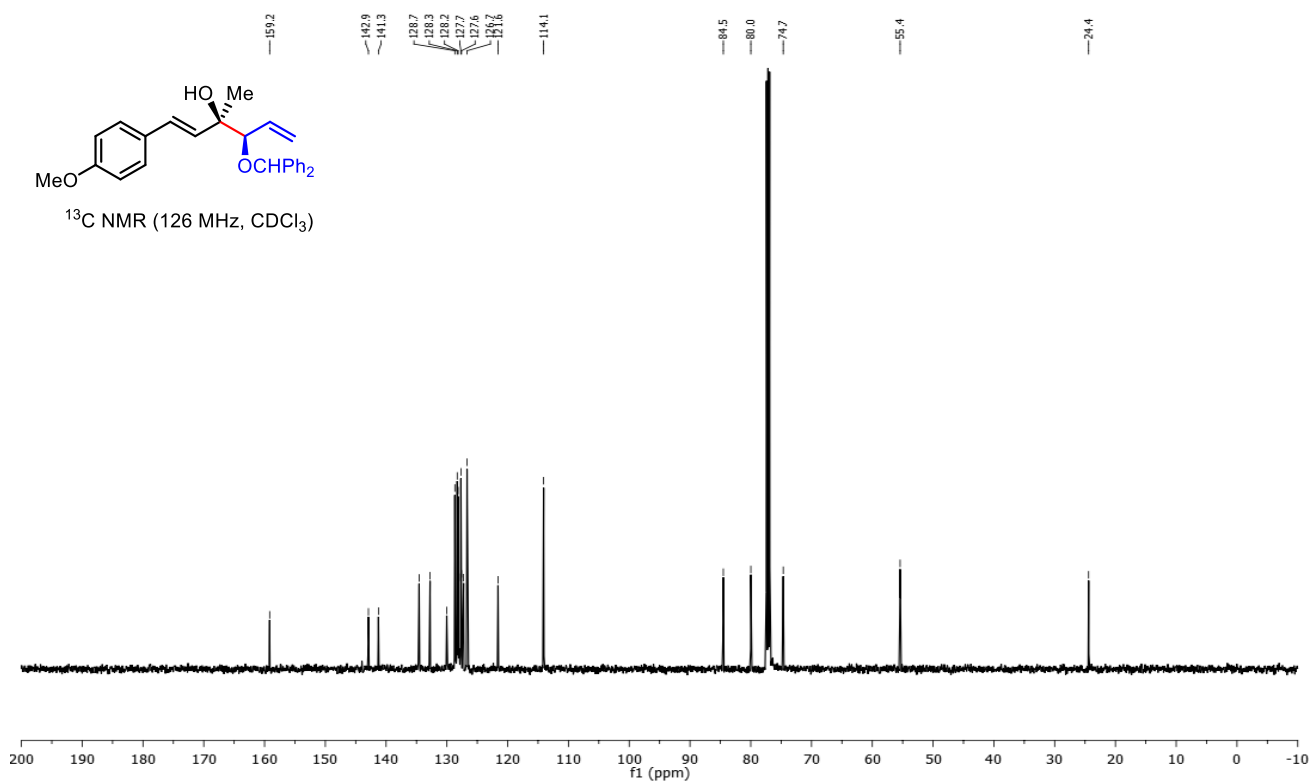
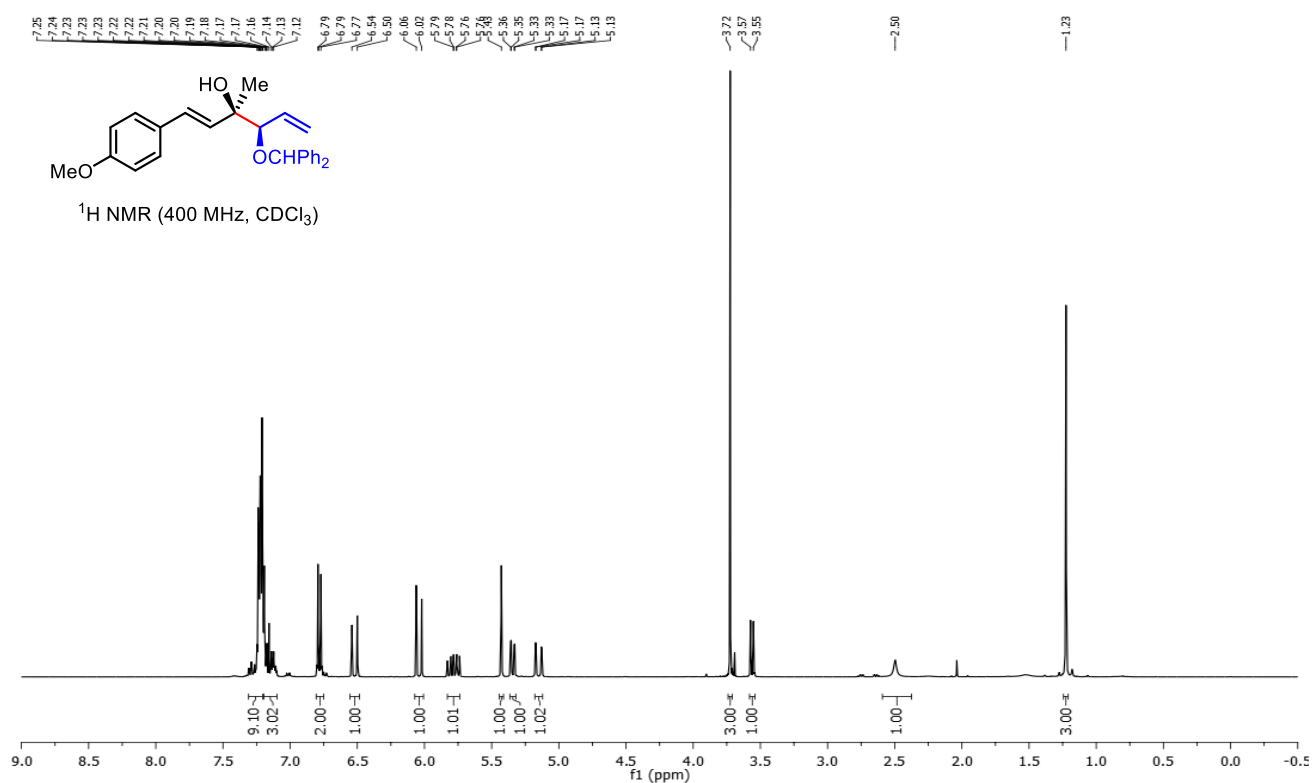
(2*S*,3*R*)-3-(Benzhydryloxy)-2-(thiophen-2-yl)pent-4-en-2-ol (3w):



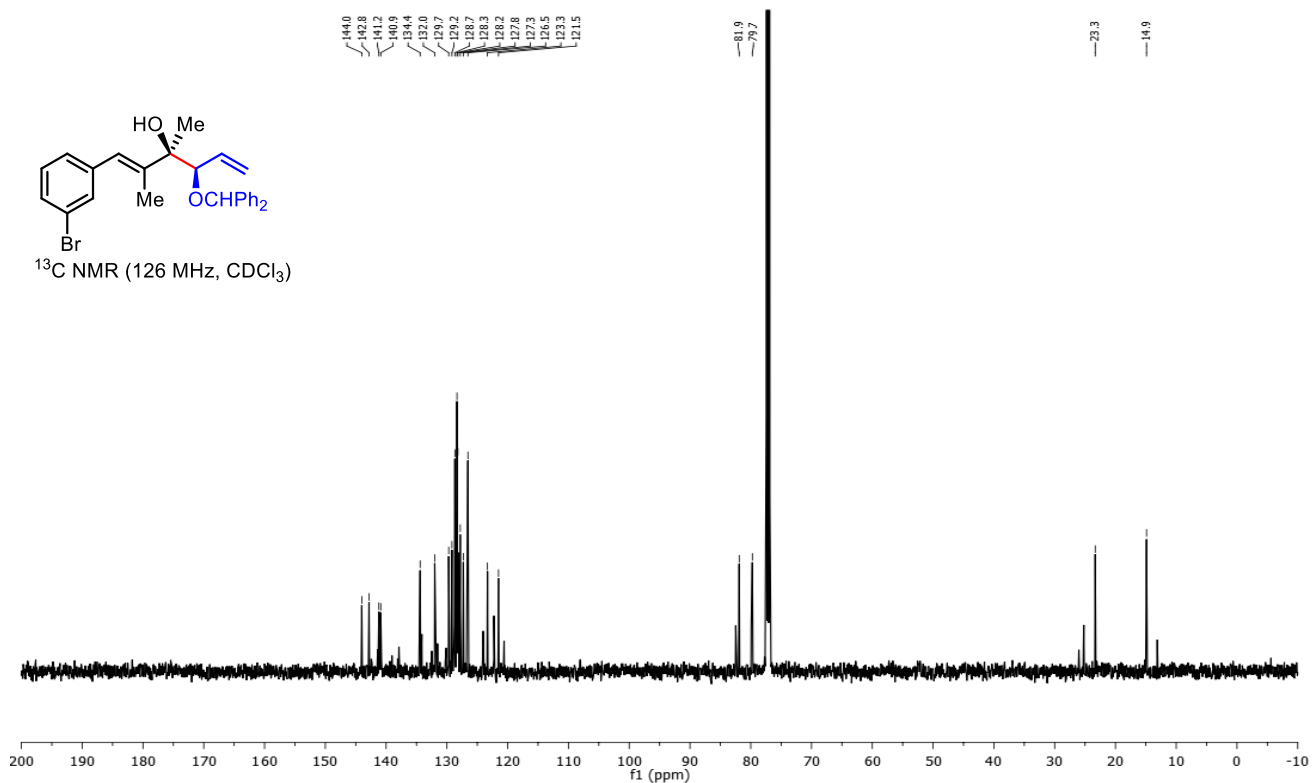
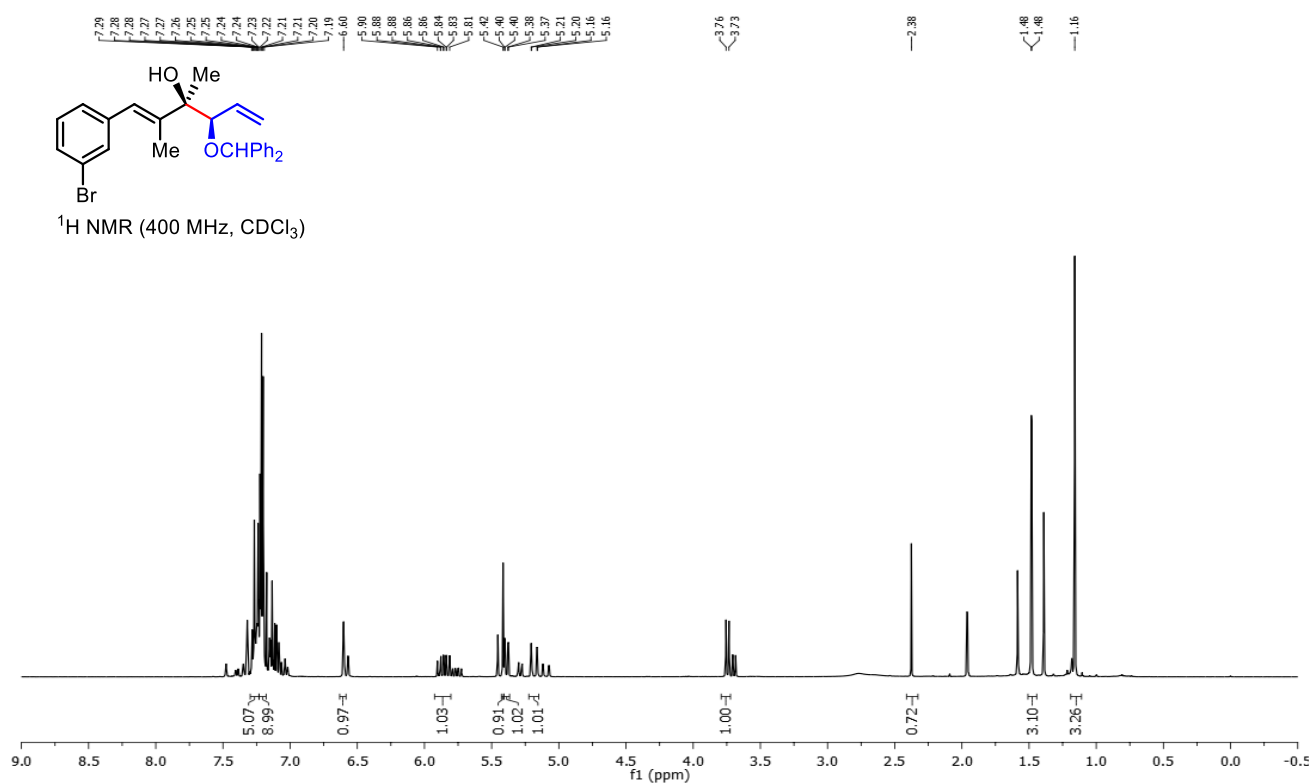
(3*R*,4*R*, *E*)-4-(Benzhydryloxy)-1-(3-bromophenyl)-3-methylhexa-1,5-dien-3-ol (3x):



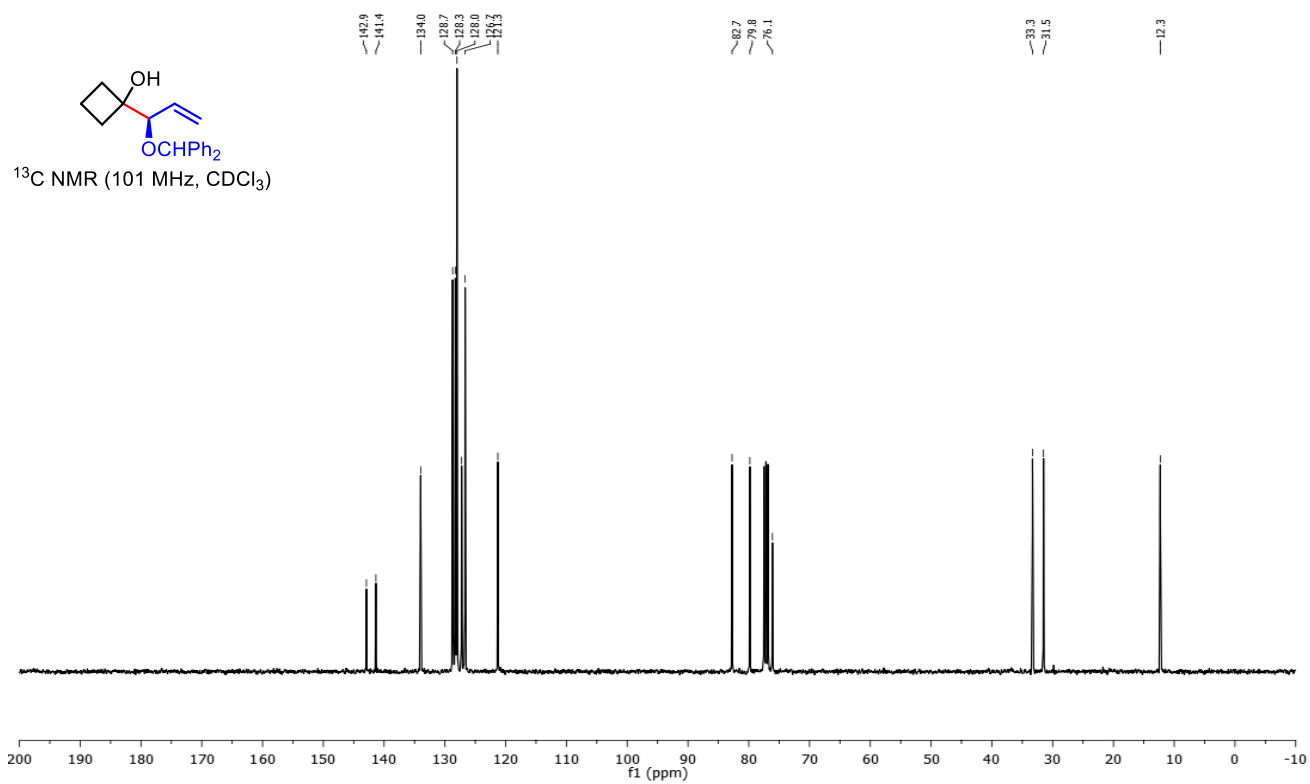
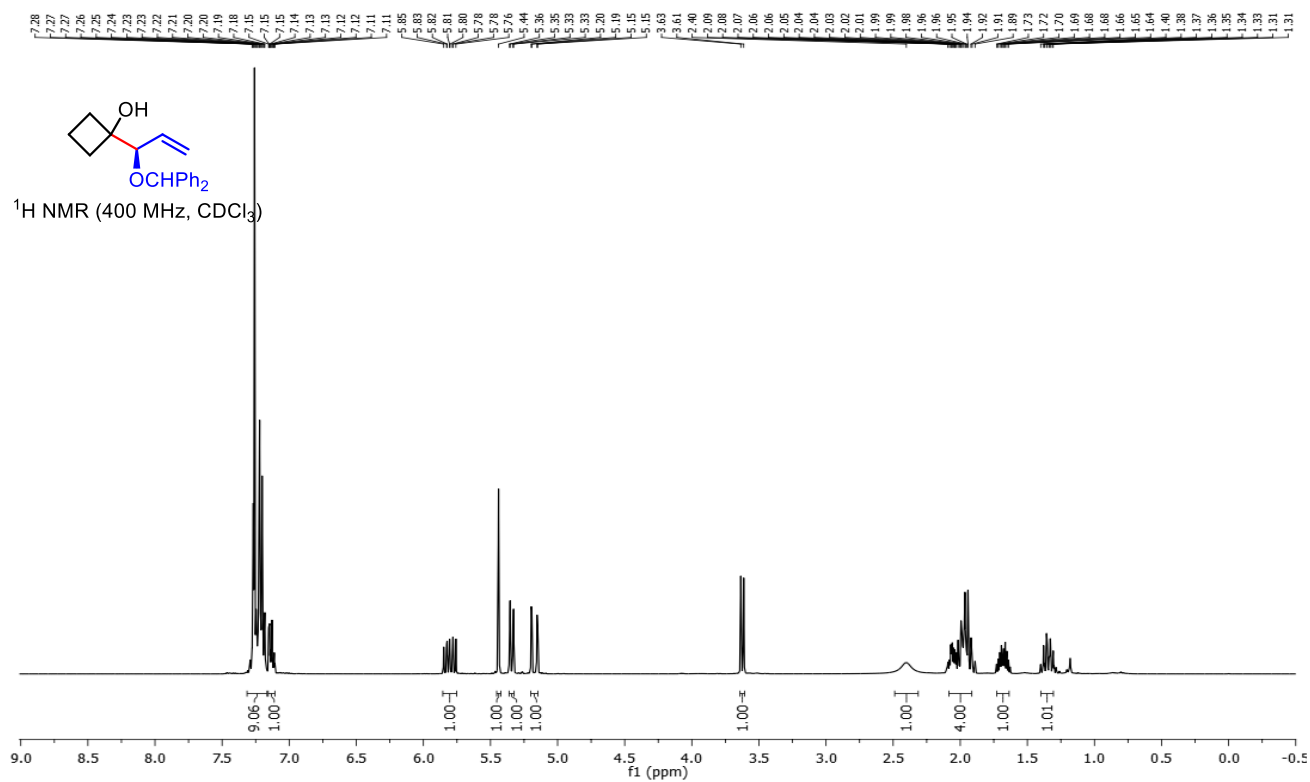
(3*R*,4*R*, *E*)-4-(Benzhydryloxy)-1-(4-methoxyphenyl)-3-methylhexa-1,5-dien-3-ol (3y):



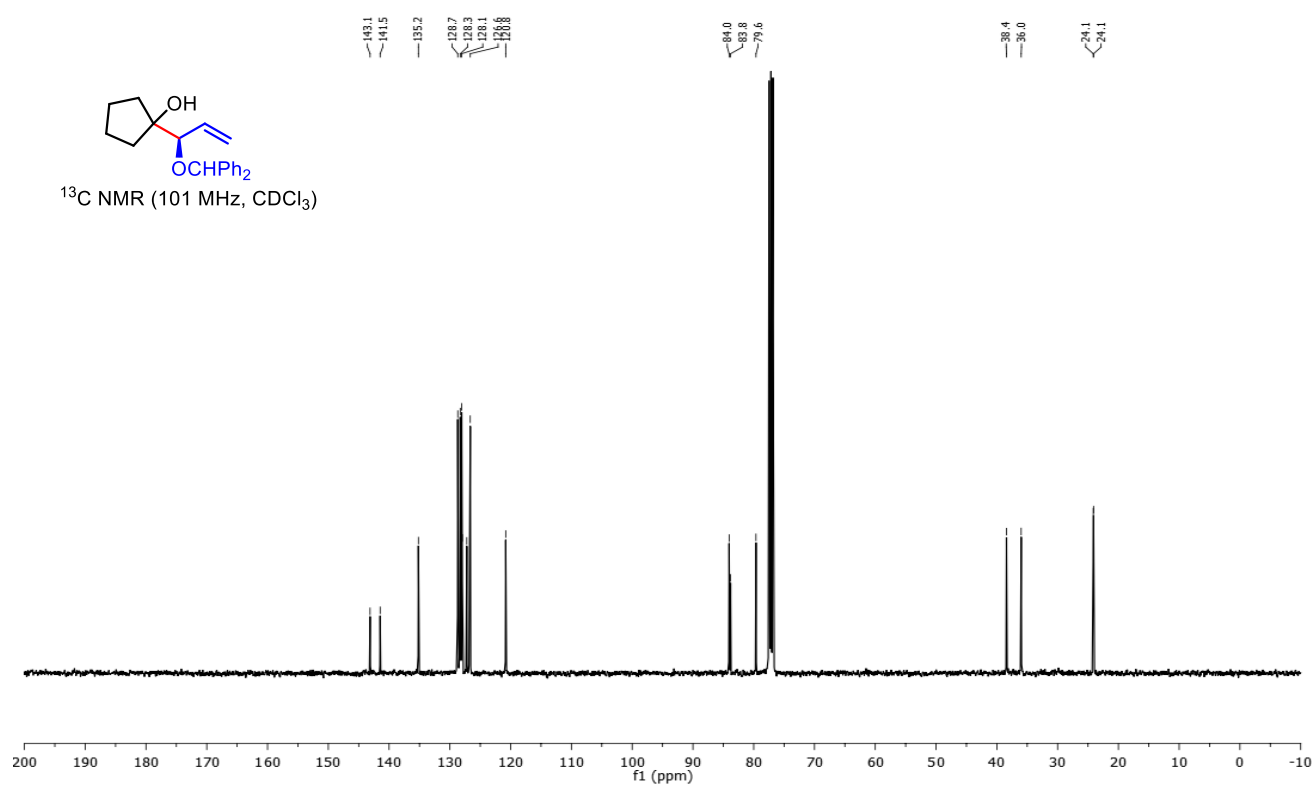
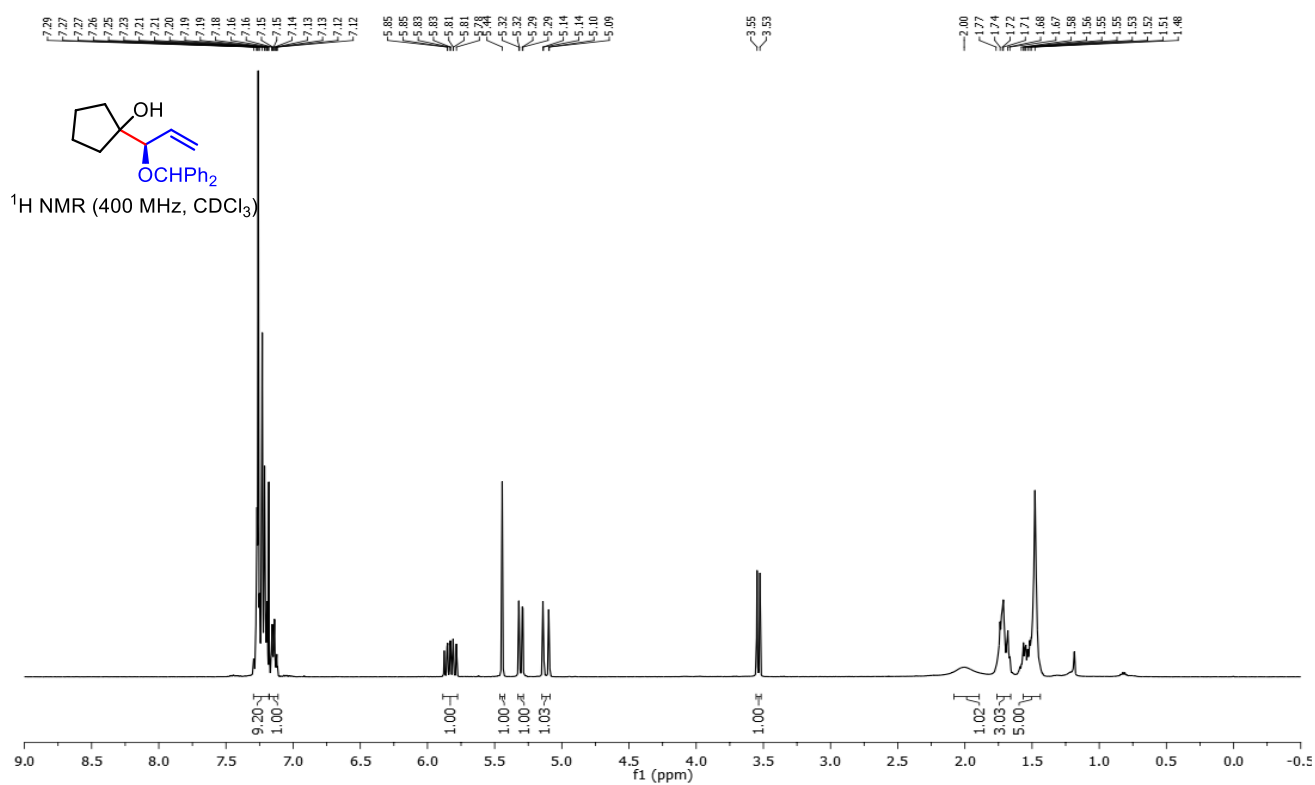
(3*R*,4*R*, *E*)-4-(Benzhydryloxy)-1-(3-bromophenyl)-3-methylhexa-1,5-dien-3-ol (3z):



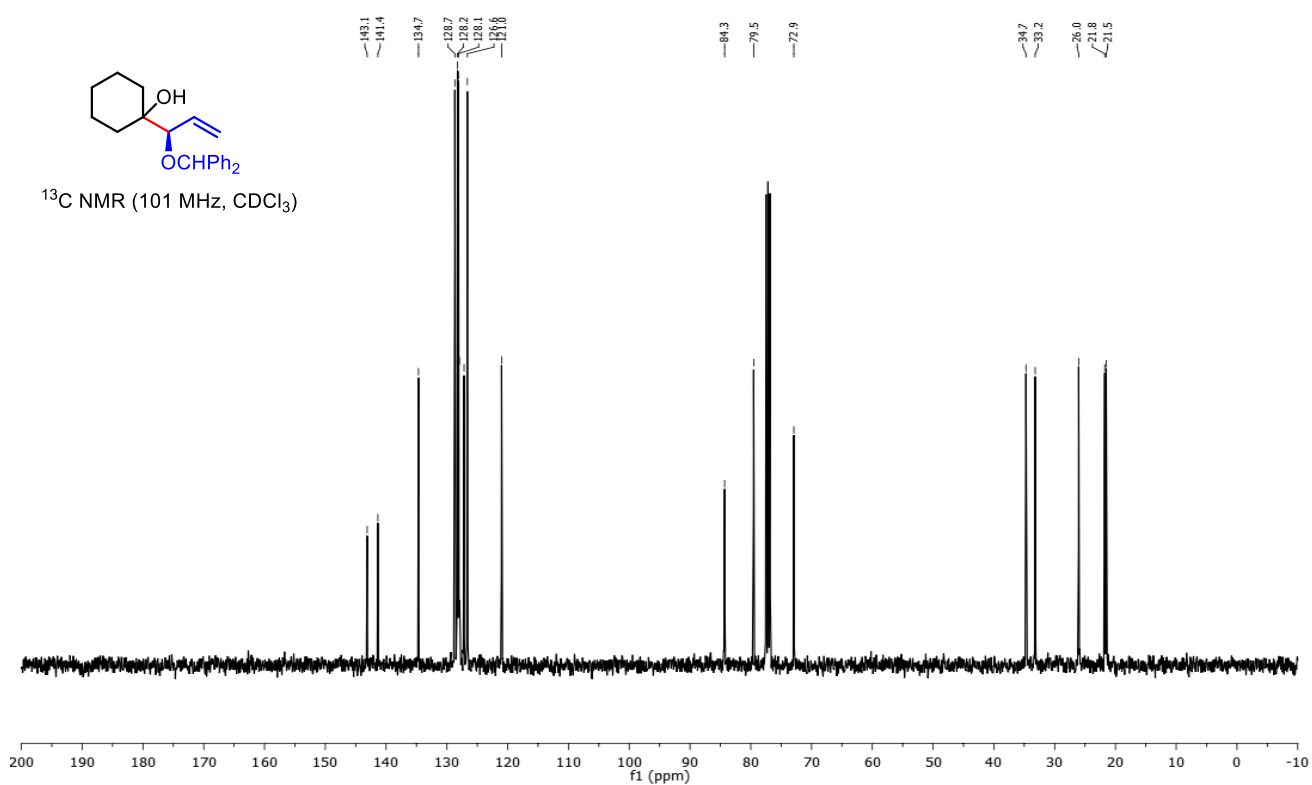
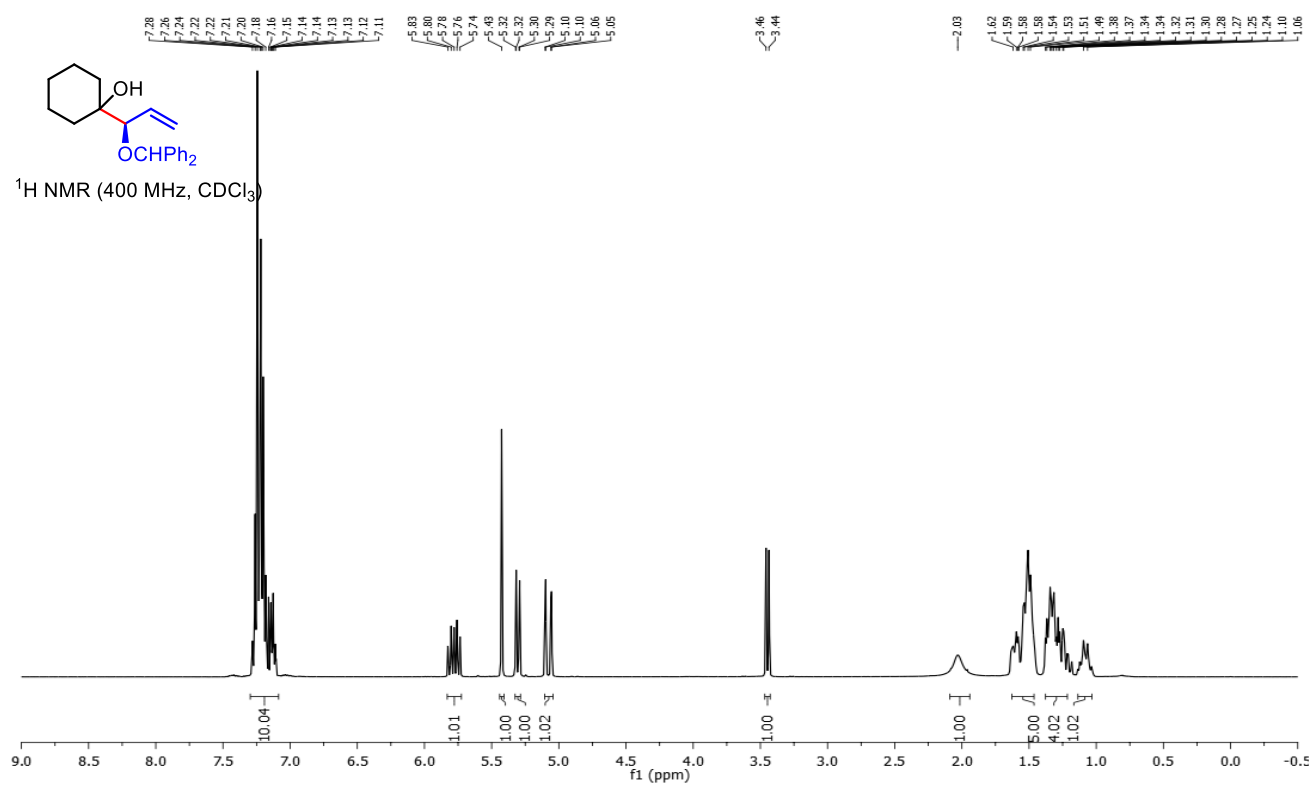
(R)-1-(1-(Benzyloxy)allyl)cyclobutan-1-ol (3aa):



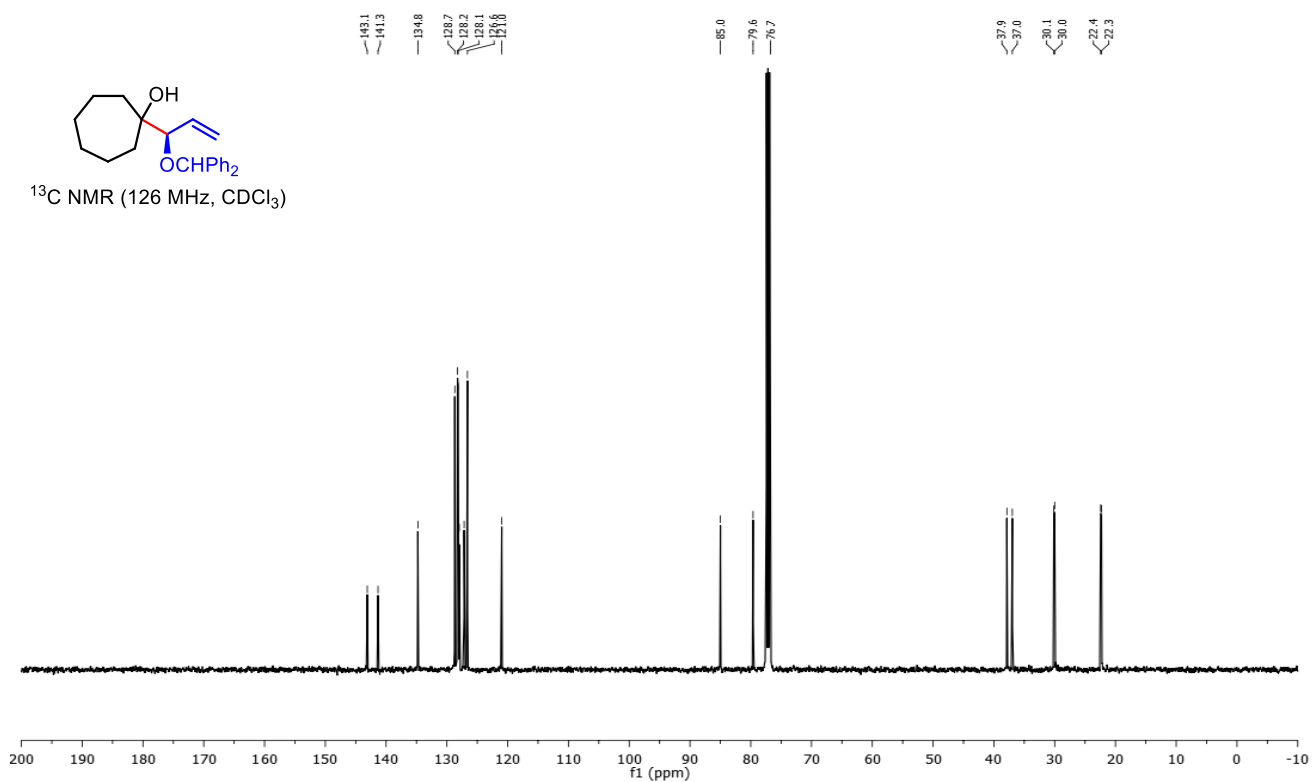
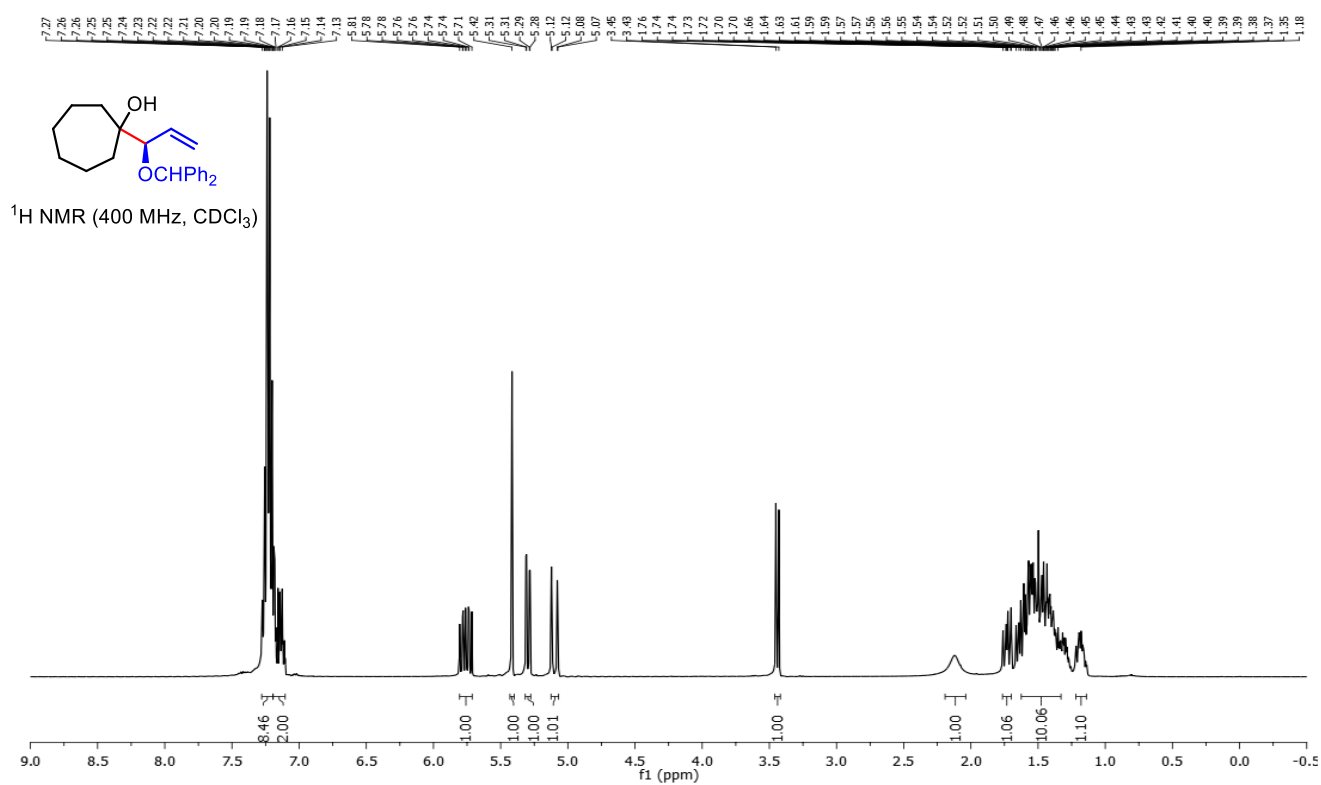
(R)-1-(1-(Benzyloxy)allyl)cyclopentan-1-ol (3ab):



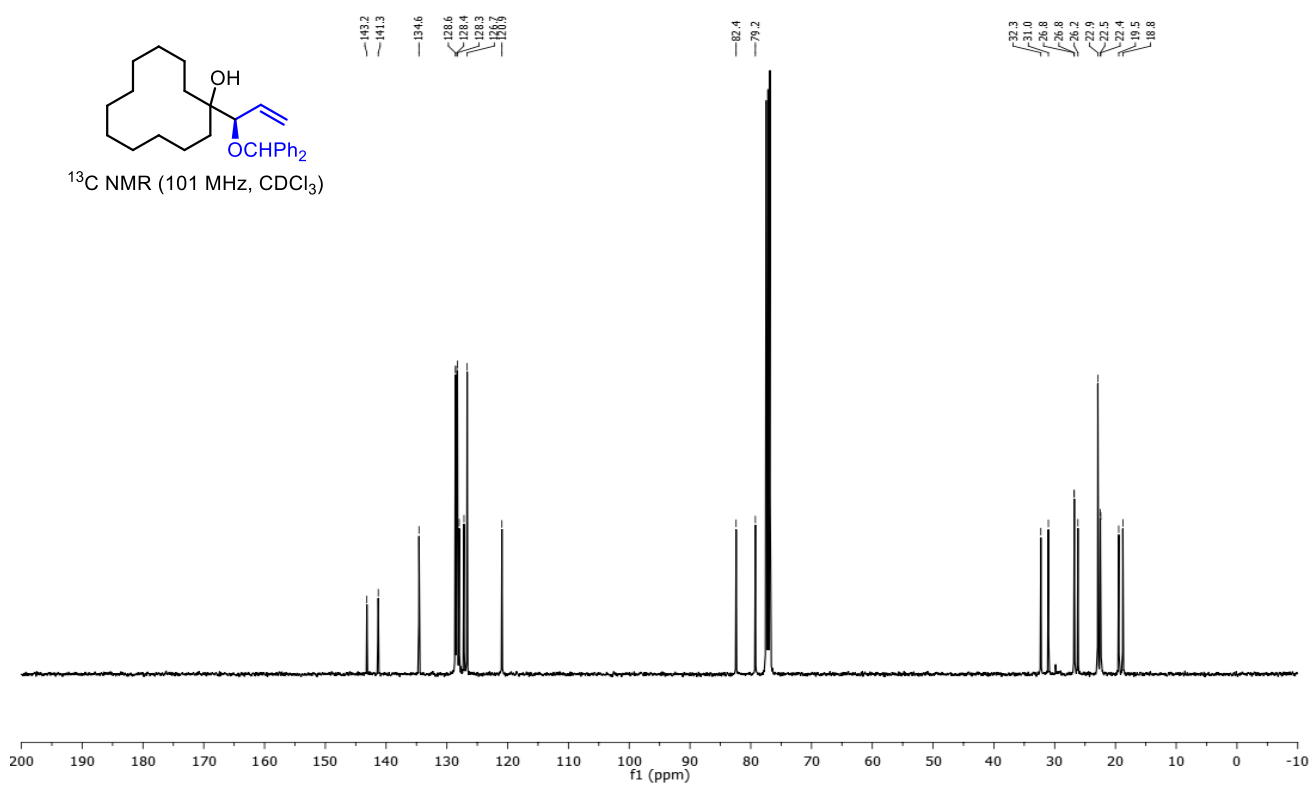
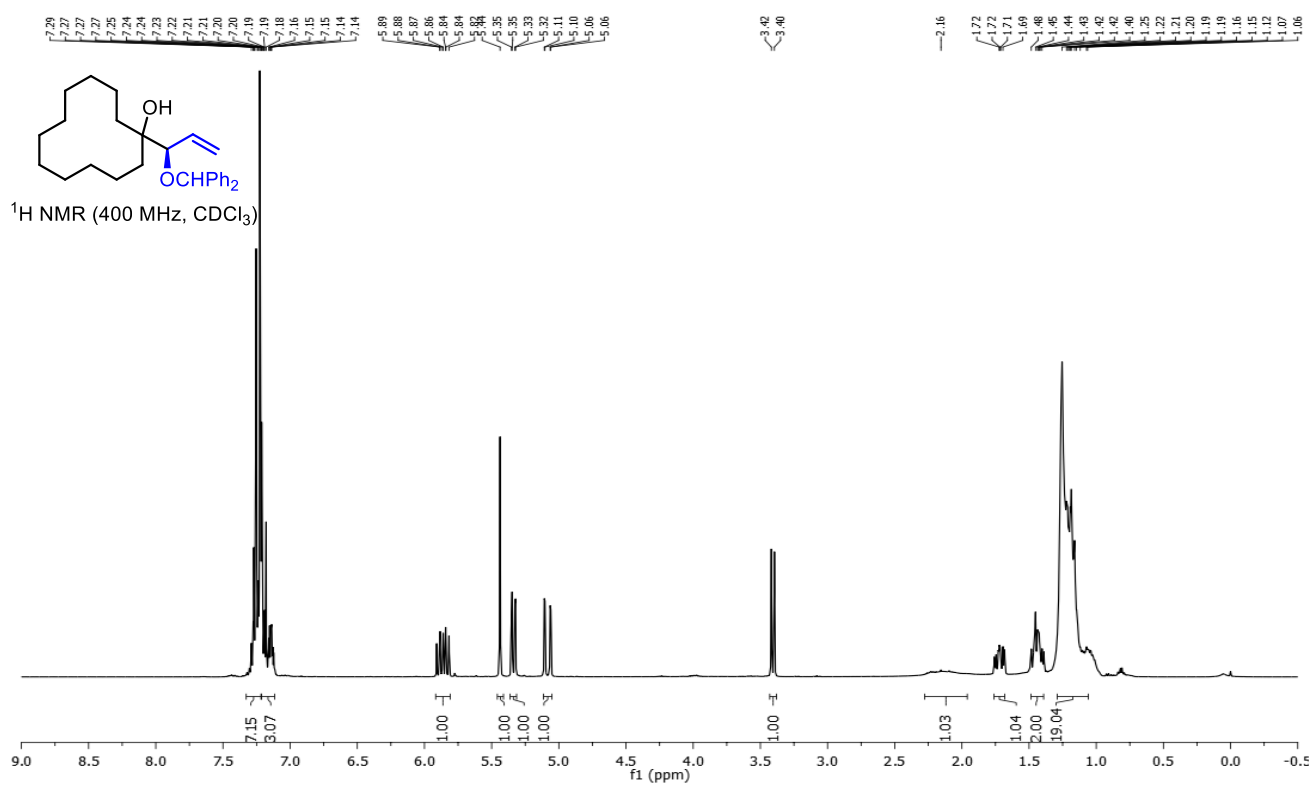
(R)-1-(1-(Benzyloxy)allyl)cyclohexan-1-ol (3ac):



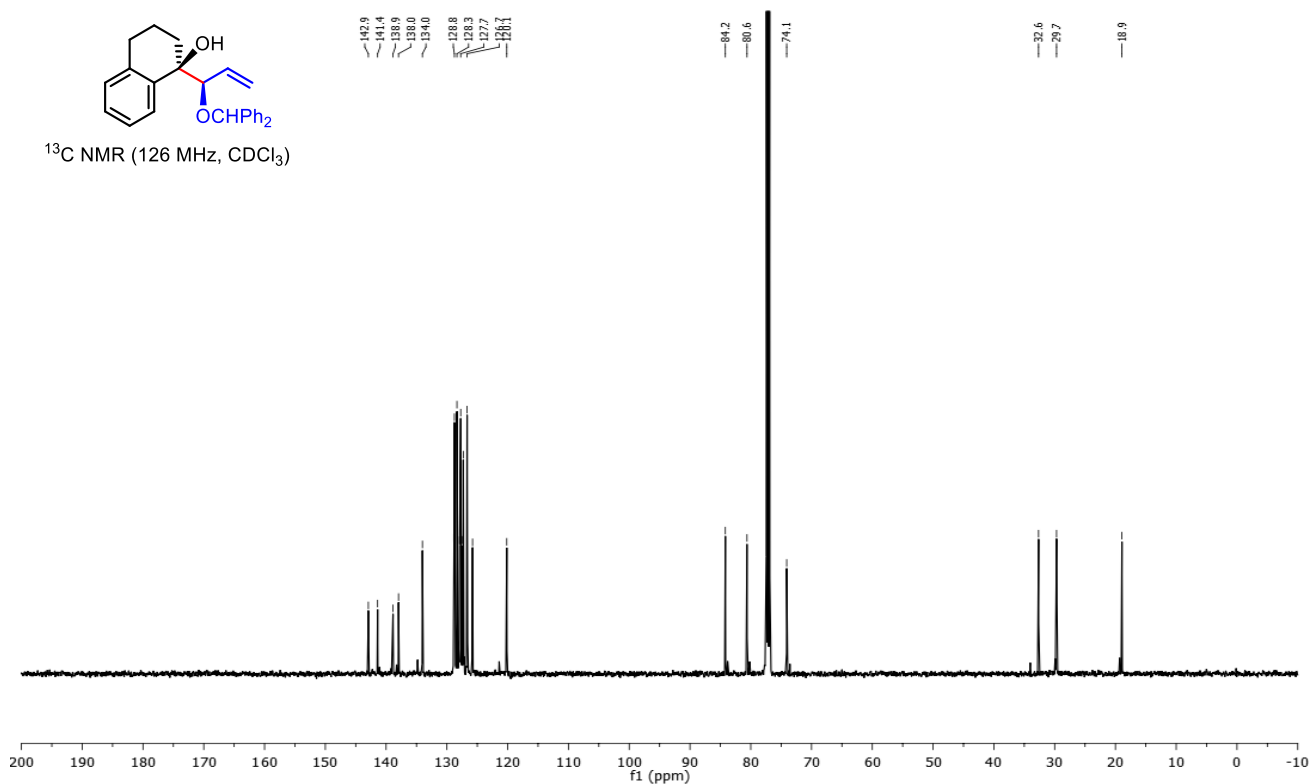
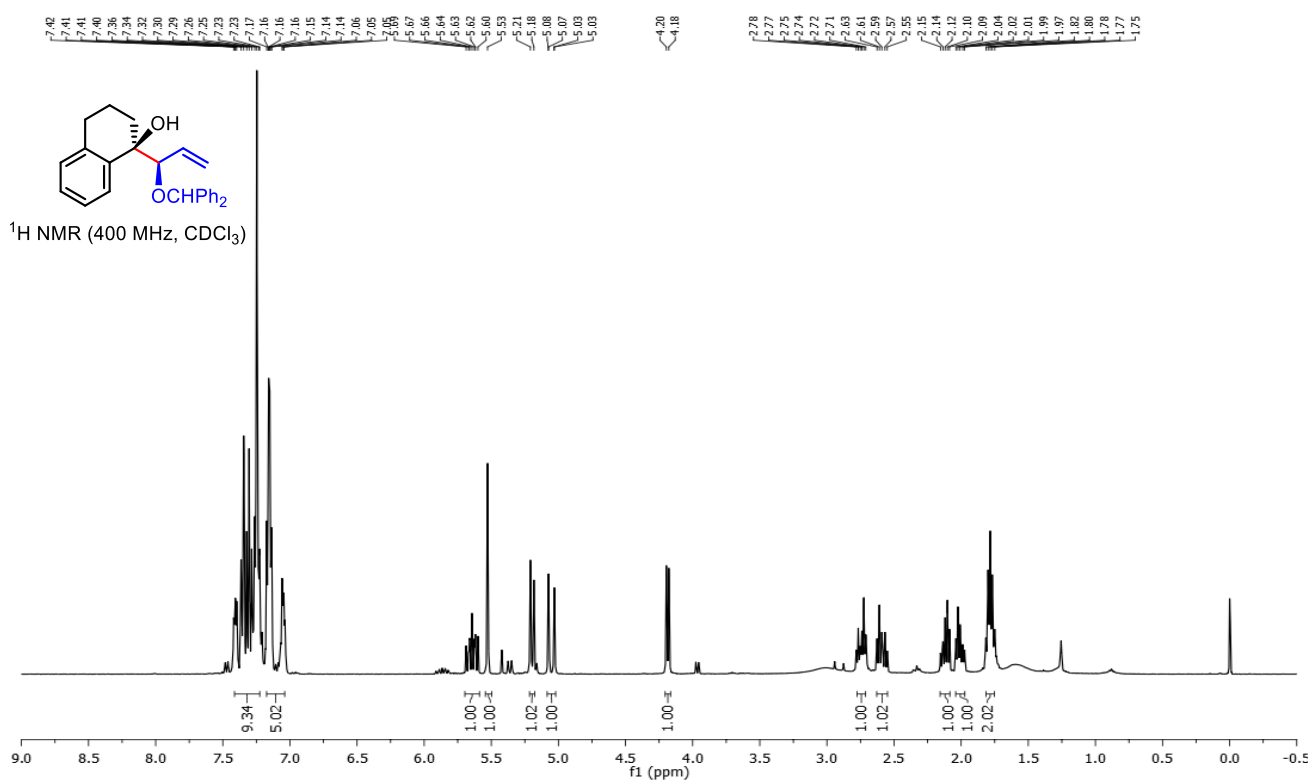
(R)-1-(1-(Benzyloxy)allyl)cycloheptan-1-ol (3ad):



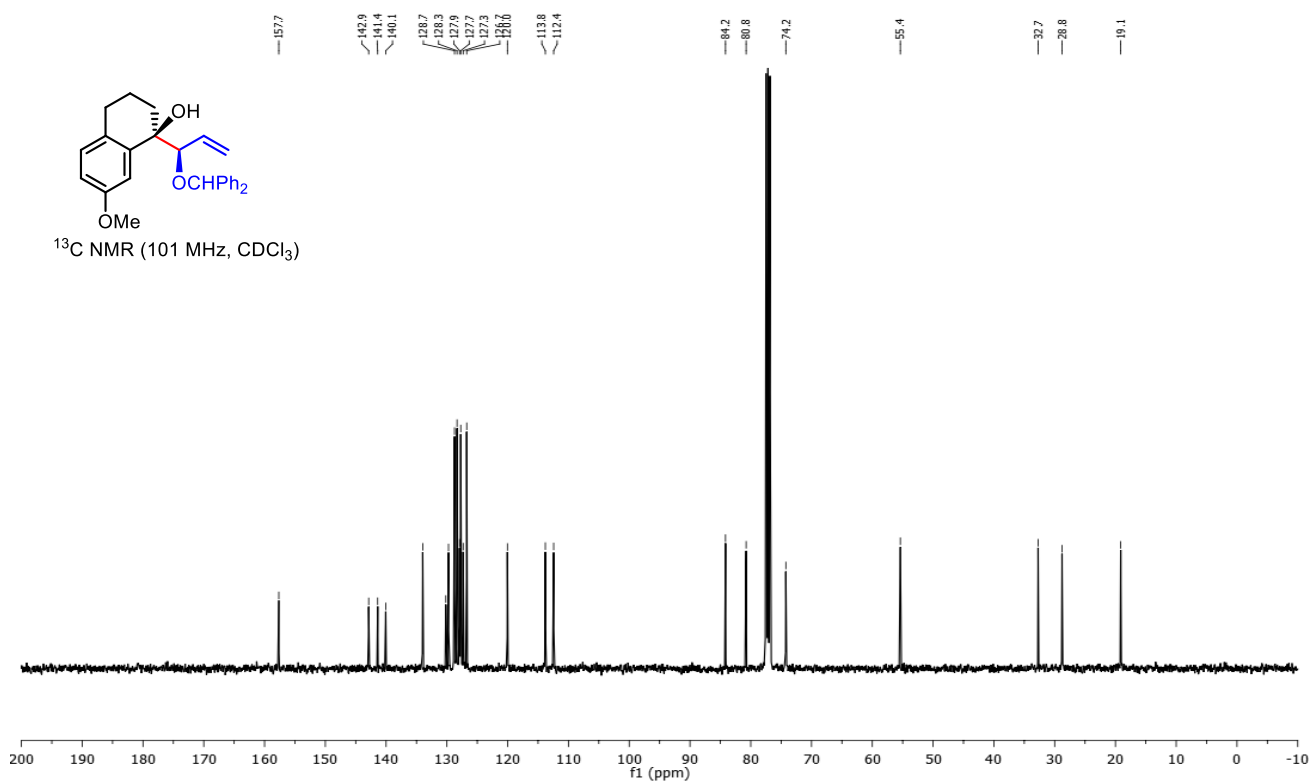
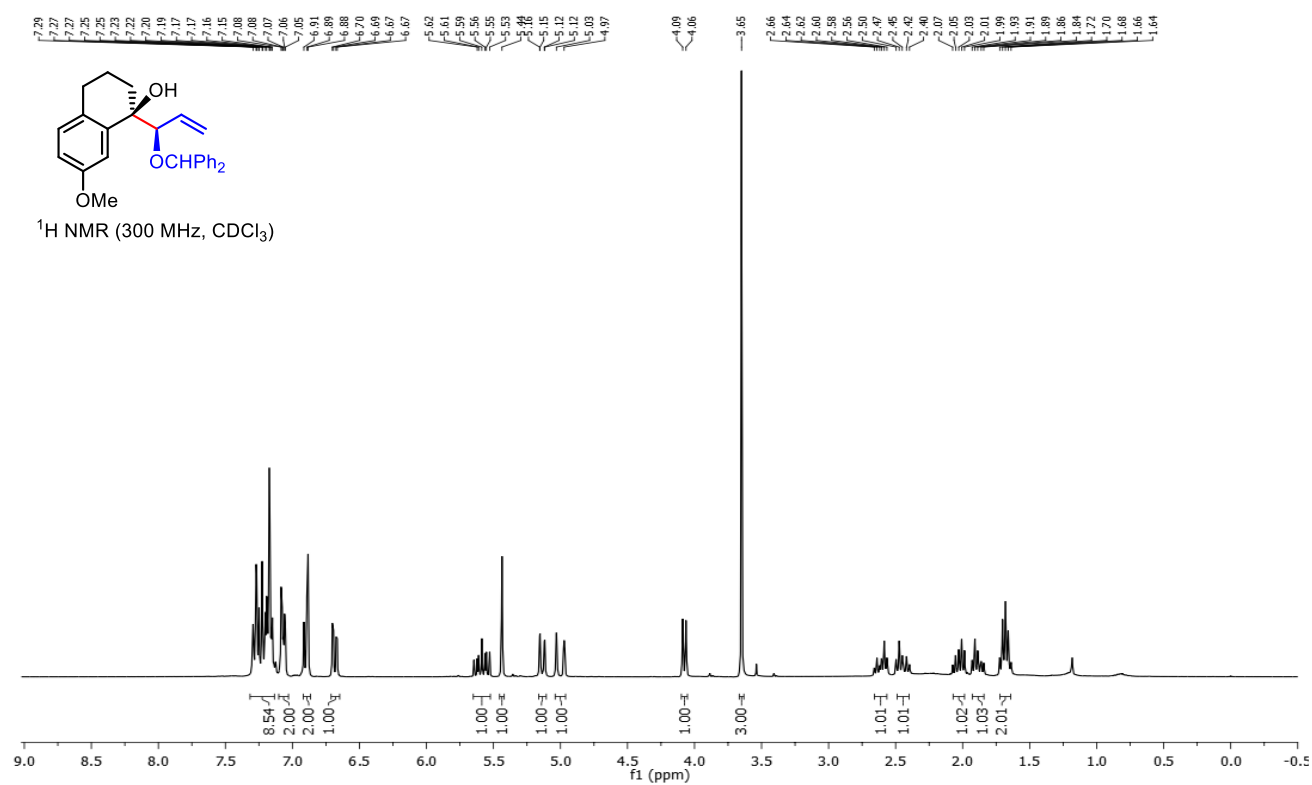
(R)-1-(1-(Benzyloxy)allyl)cyclododecan-1-ol (3ae):



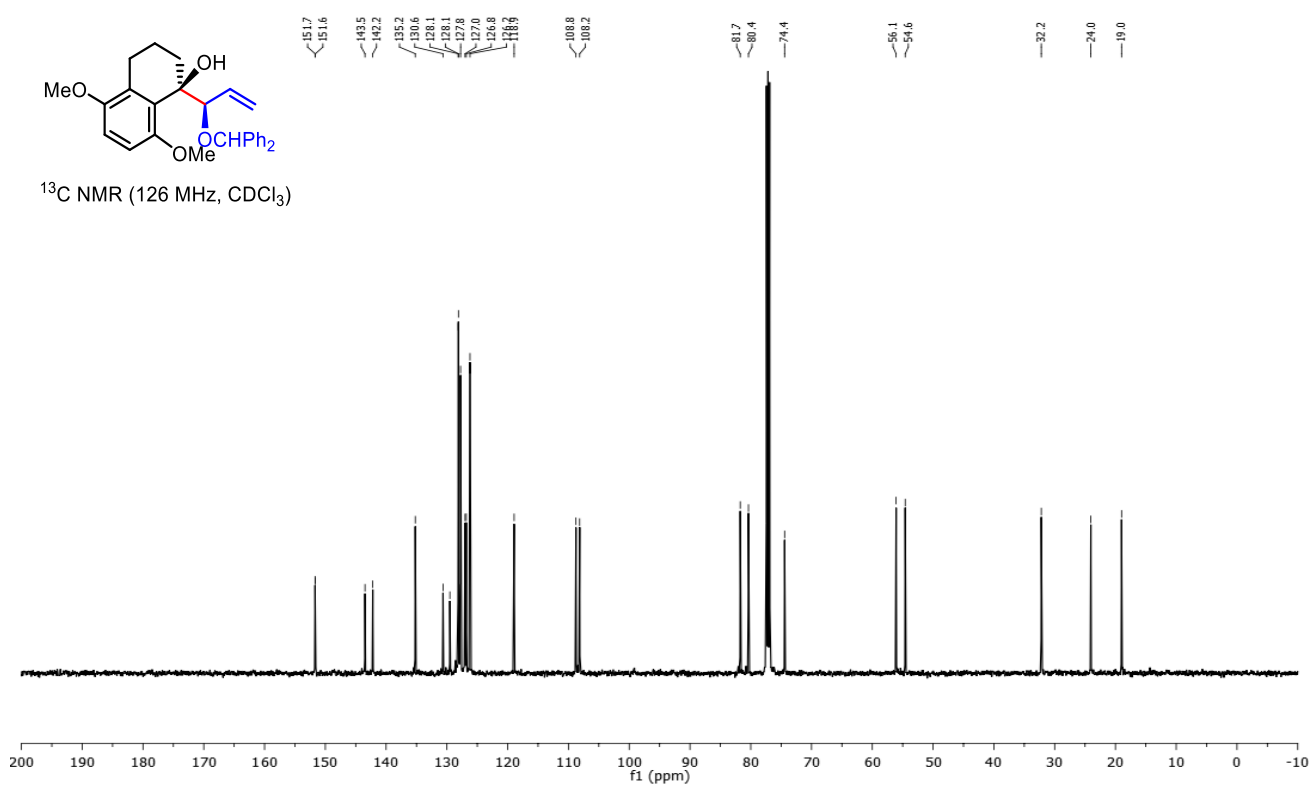
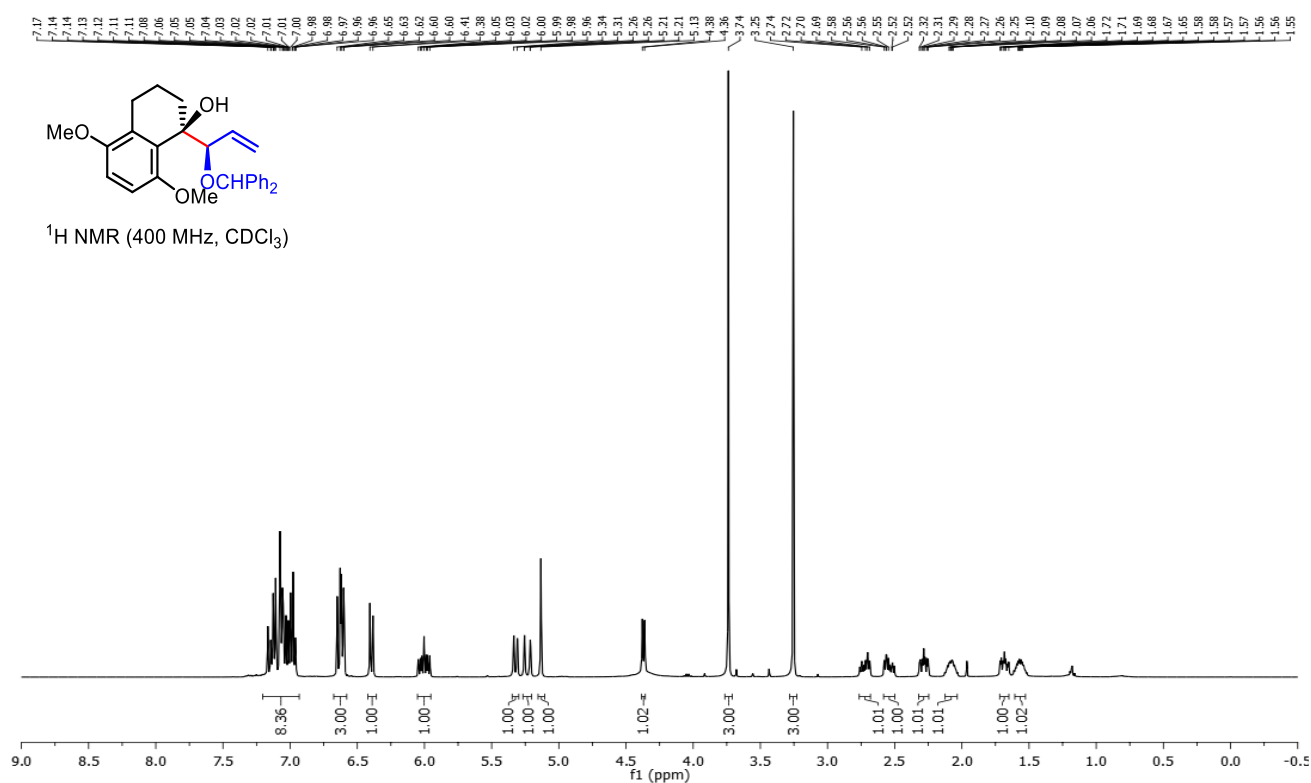
(R)-1-((R)-1-(Benzhydryloxy)allyl)-1,2,3,4-tetrahydronaphthalen-1-ol (3af):



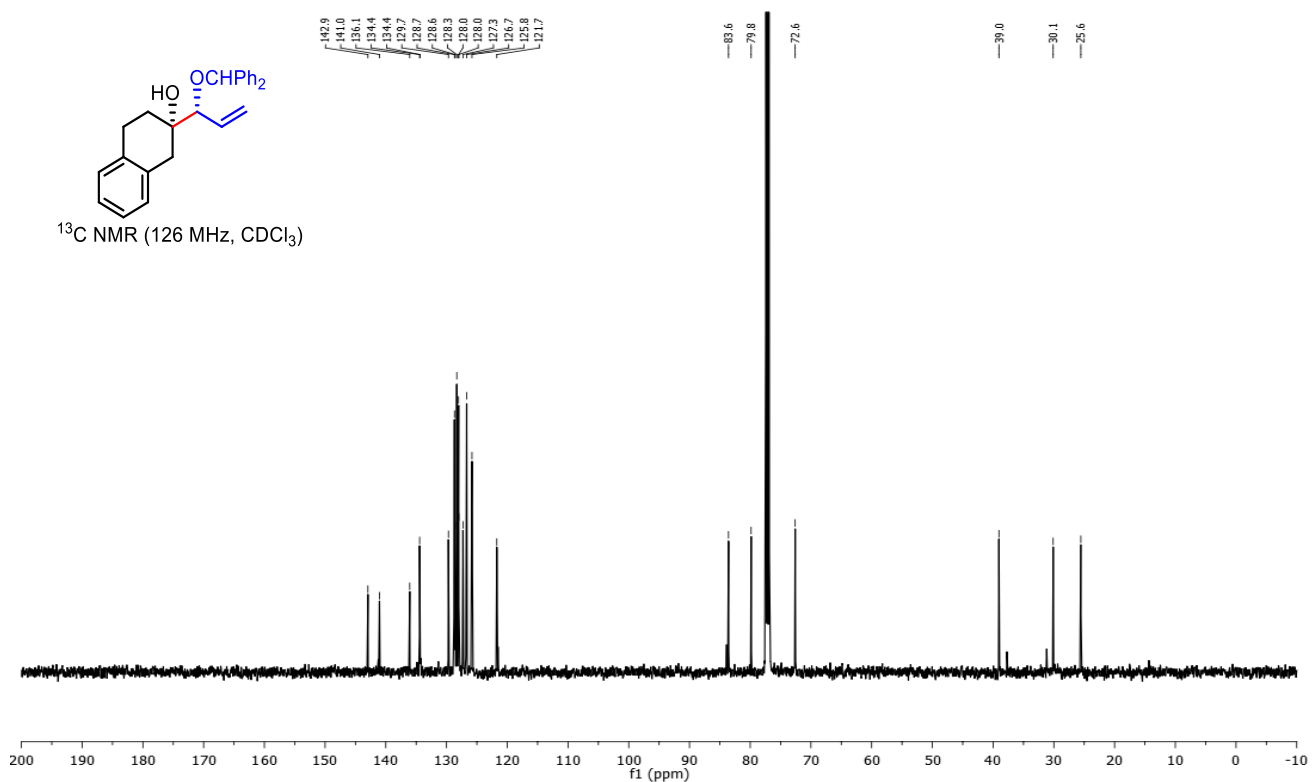
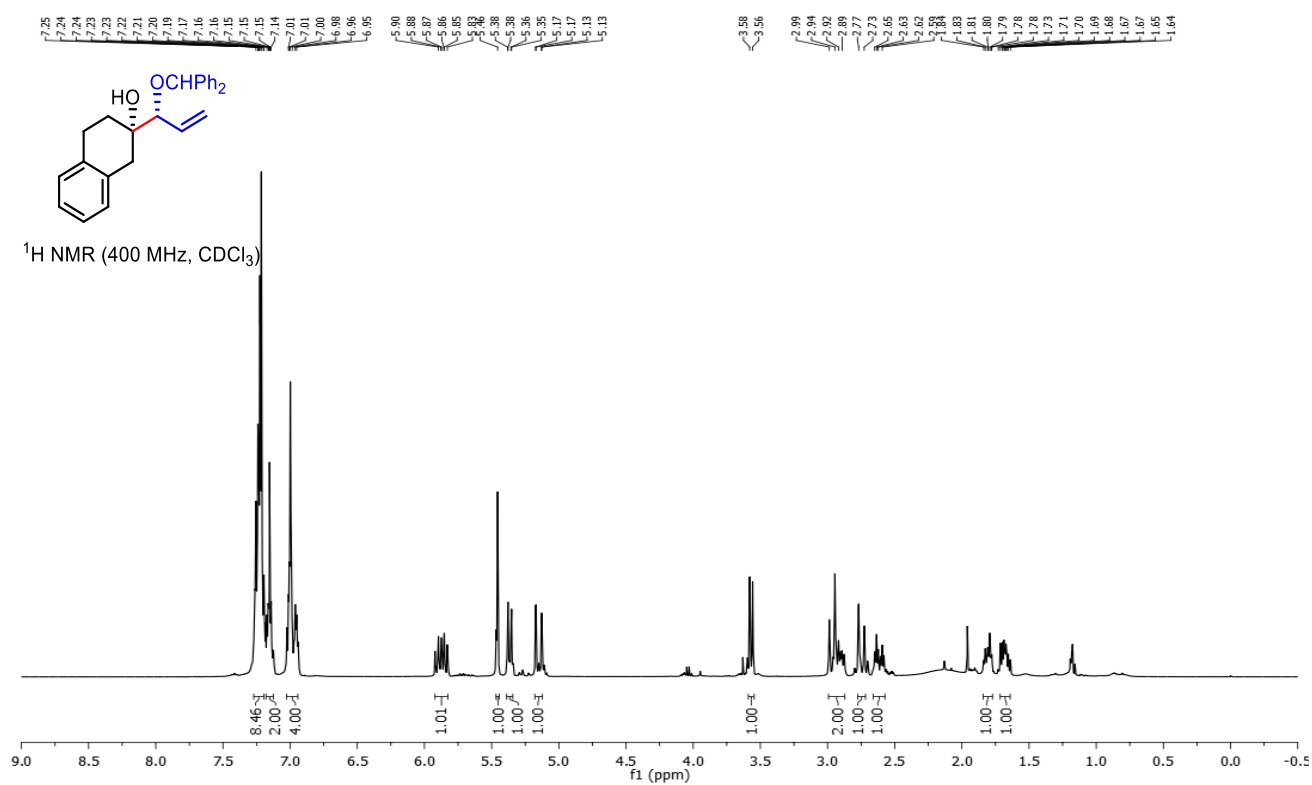
(R)-1-((R)-1-(Benzhydryloxy)allyl)-7-methoxy-1,2,3,4-tetrahydronaphthalen-1-ol (3ag):



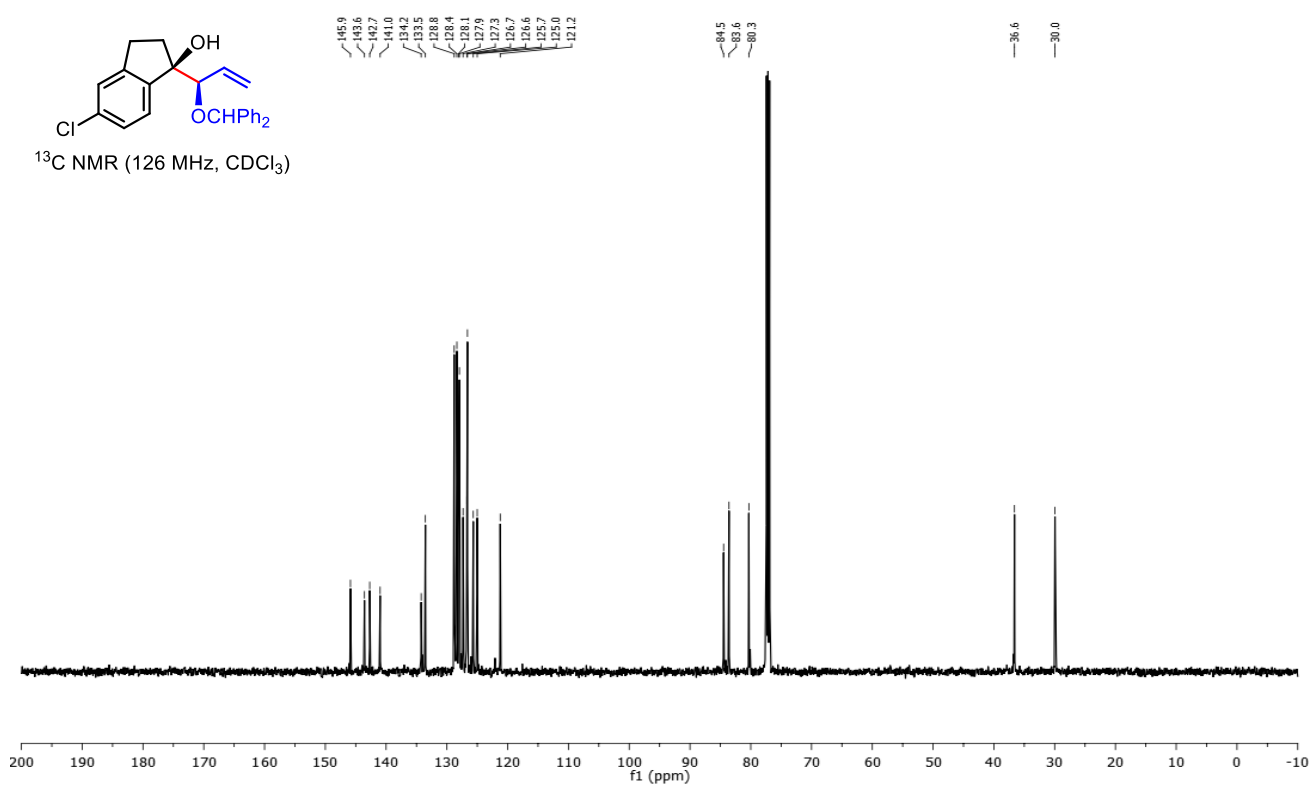
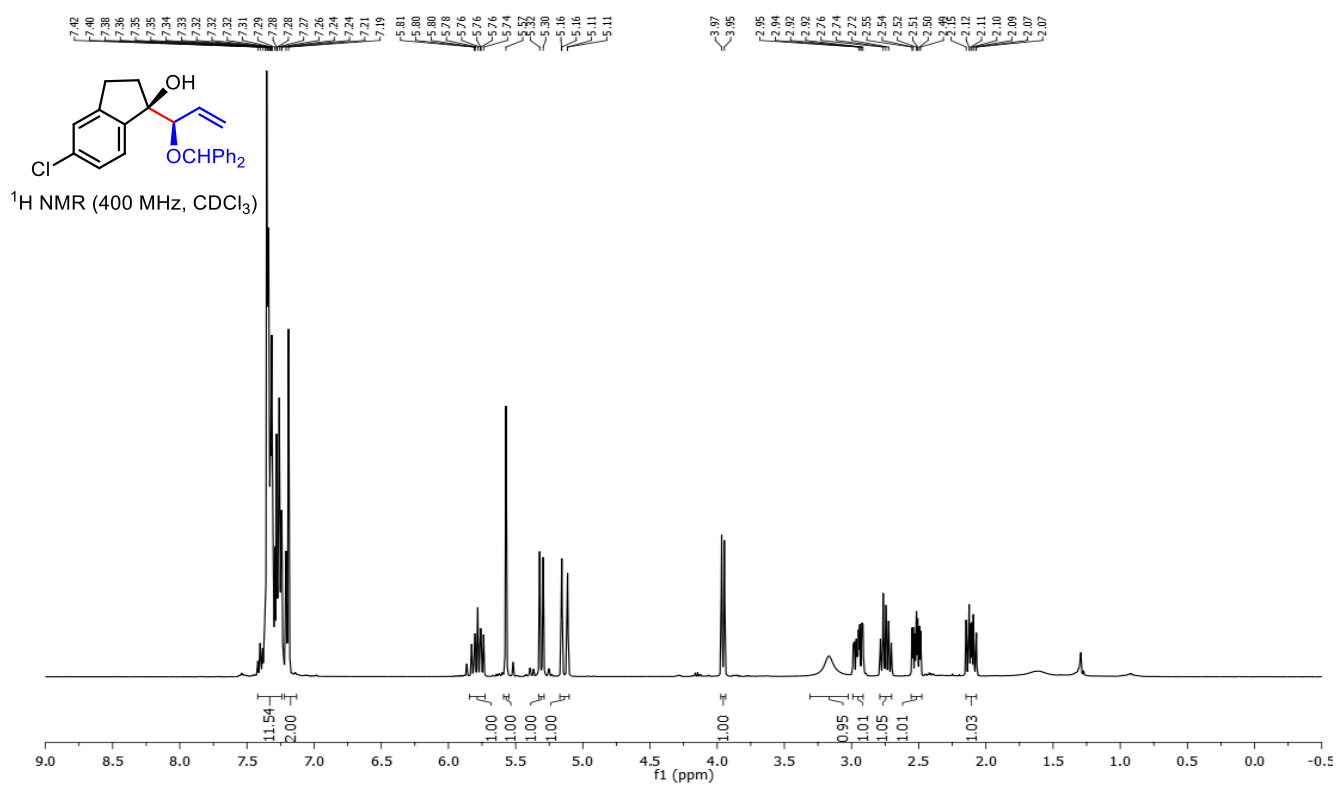
(R)-1-((R)-1-(Benzhydryloxy)allyl)-5,8-dimethoxy-1,2,3,4-tetrahydronaphthalen-1-ol (3ah):



(S)-2-((R)-1-Benzhydryloxy)allyl)-1,2,3,4-tetrahydronaphthalen-2-ol (3ai):



(R)-1-((R)-1-(Benzhydryloxy)allyl)-5-chloro-2,3-dihydro-1H-inden-1-ol (3aj):



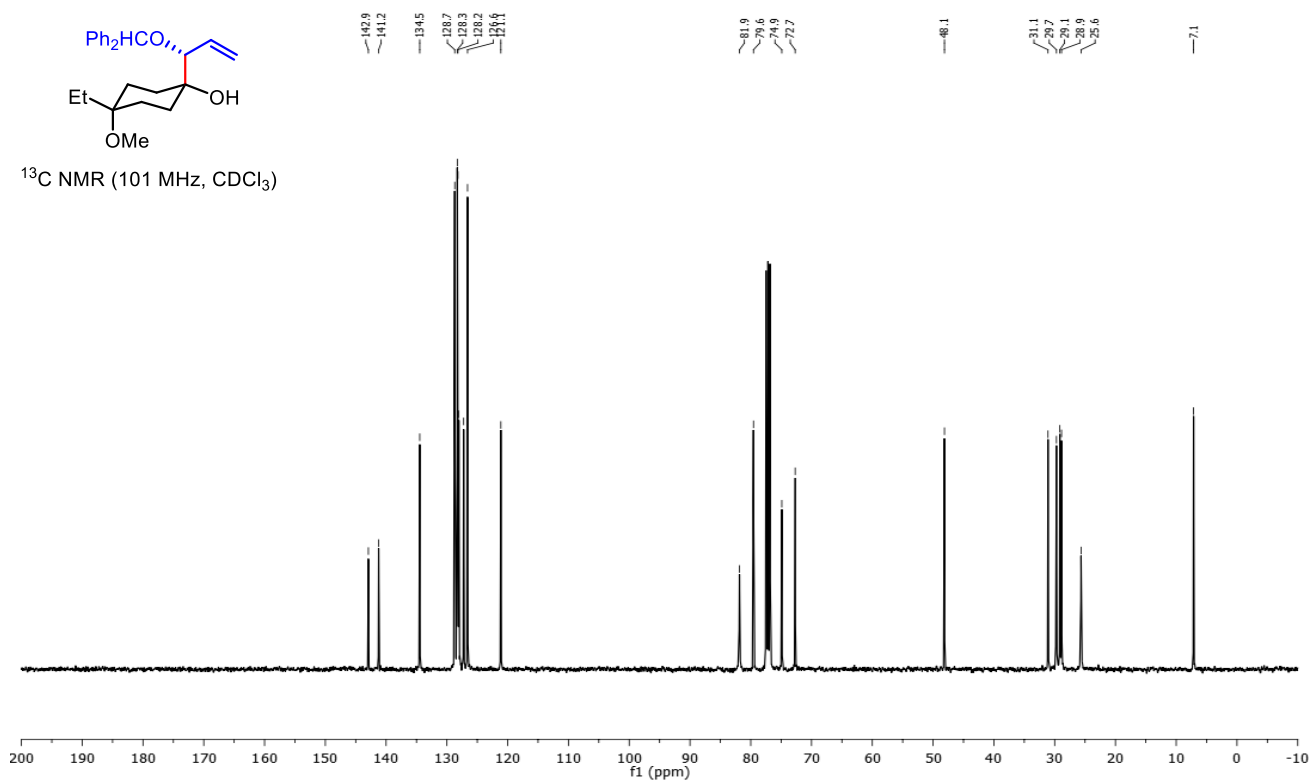
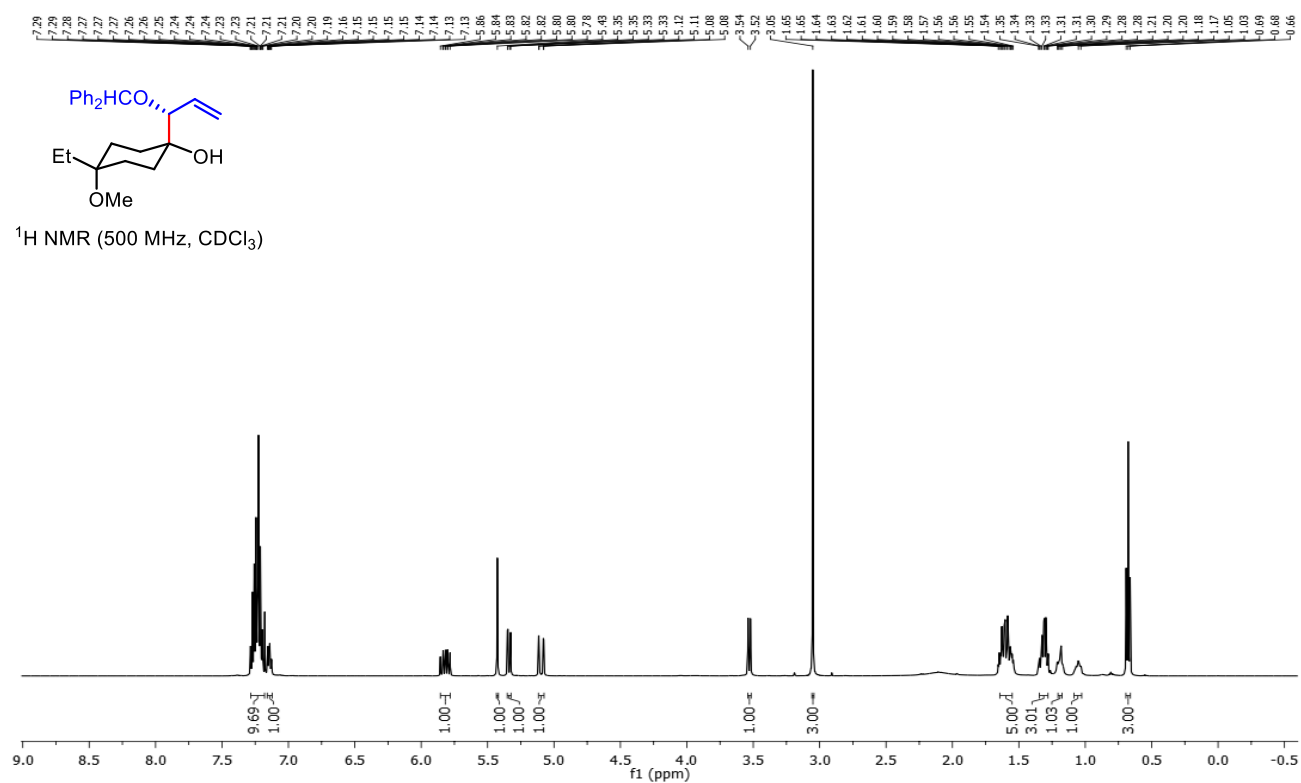
¹H NMR (500 MHz, CDCl₃)

Chemical structure: COC1C(C)CC(C1C(=O)C2=CC=CC=C2)O

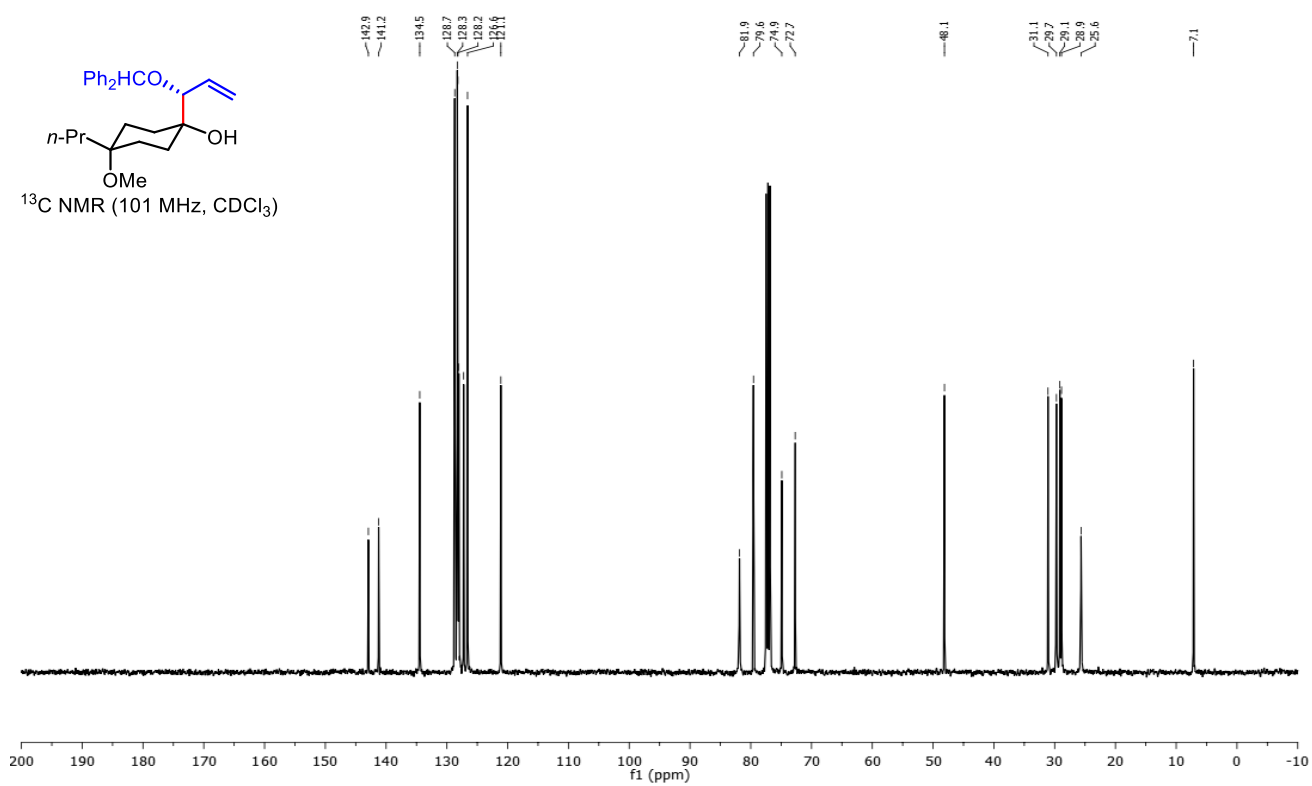
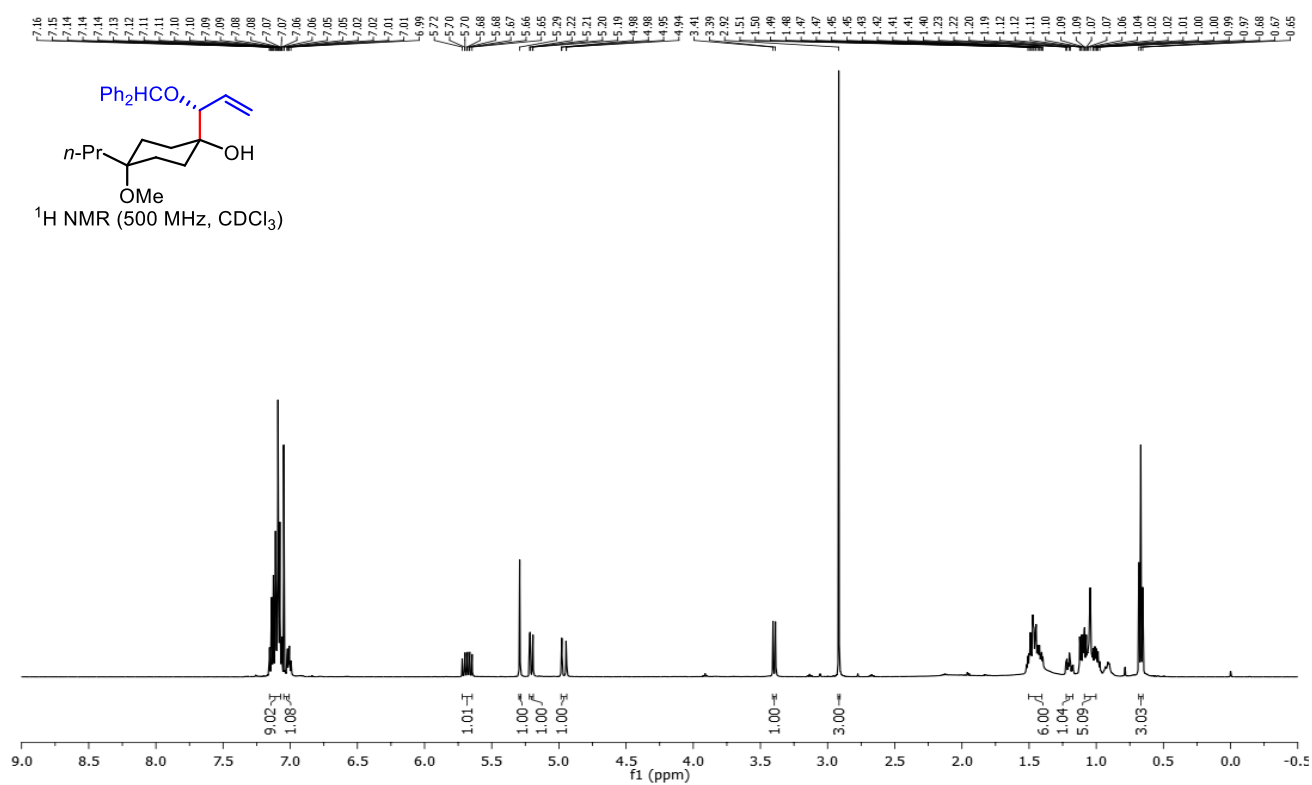
Peak list (ppm): 7.27, 7.26, 7.26, 7.26, 7.25, 7.24, 7.24, 7.24, 7.23, 7.23, 7.22, 7.22, 7.21, 7.21, 7.20, 7.20, 7.19, 7.19, 7.18, 7.18, 7.14, 5.80, 5.79, 5.78, 5.78, 5.76, 5.76, 5.74, 5.74, 5.33, 5.33, 5.32, 5.32, 5.31, 5.31, 5.30, 5.30, 5.10, 5.10, 5.06, 5.06, 3.44, 3.42, 3.04, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.48, 1.48, 1.47, 1.47, 1.46, 1.43, 1.41, 1.39, 1.38, 1.37, 1.36, 1.36.



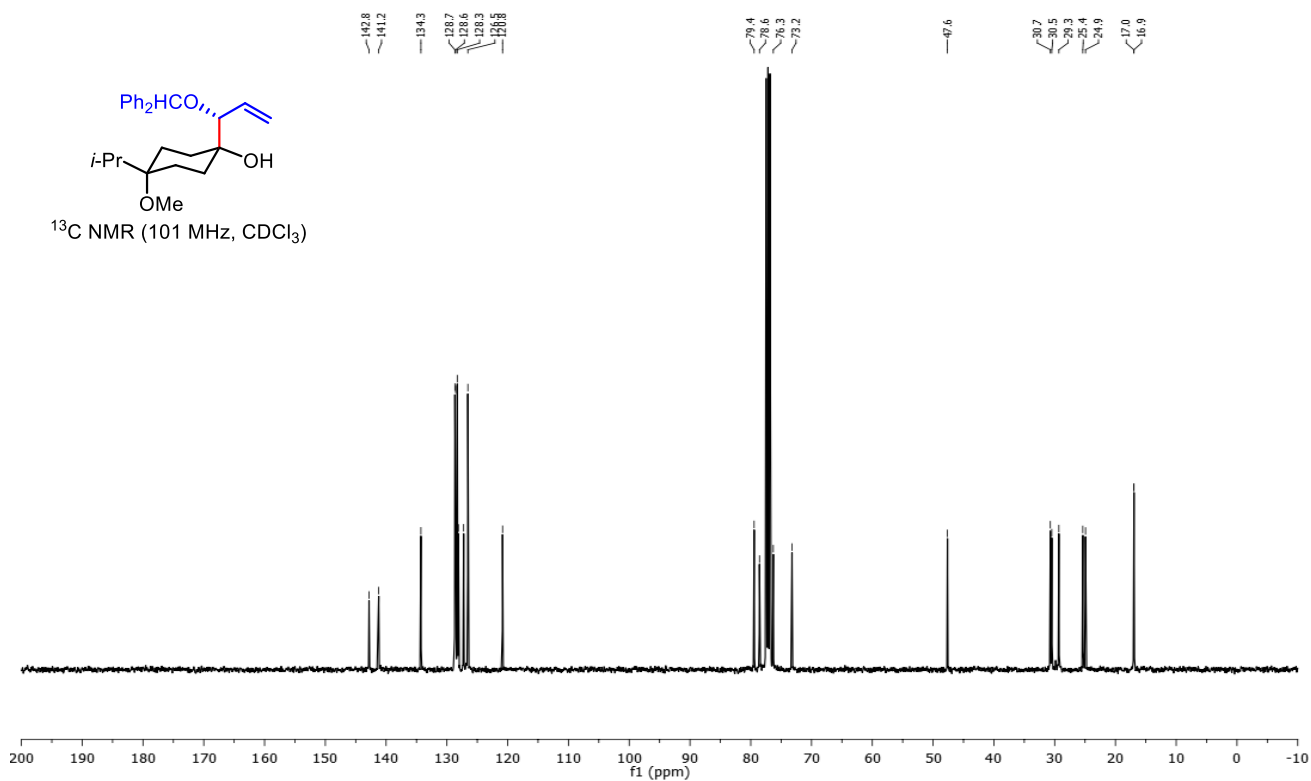
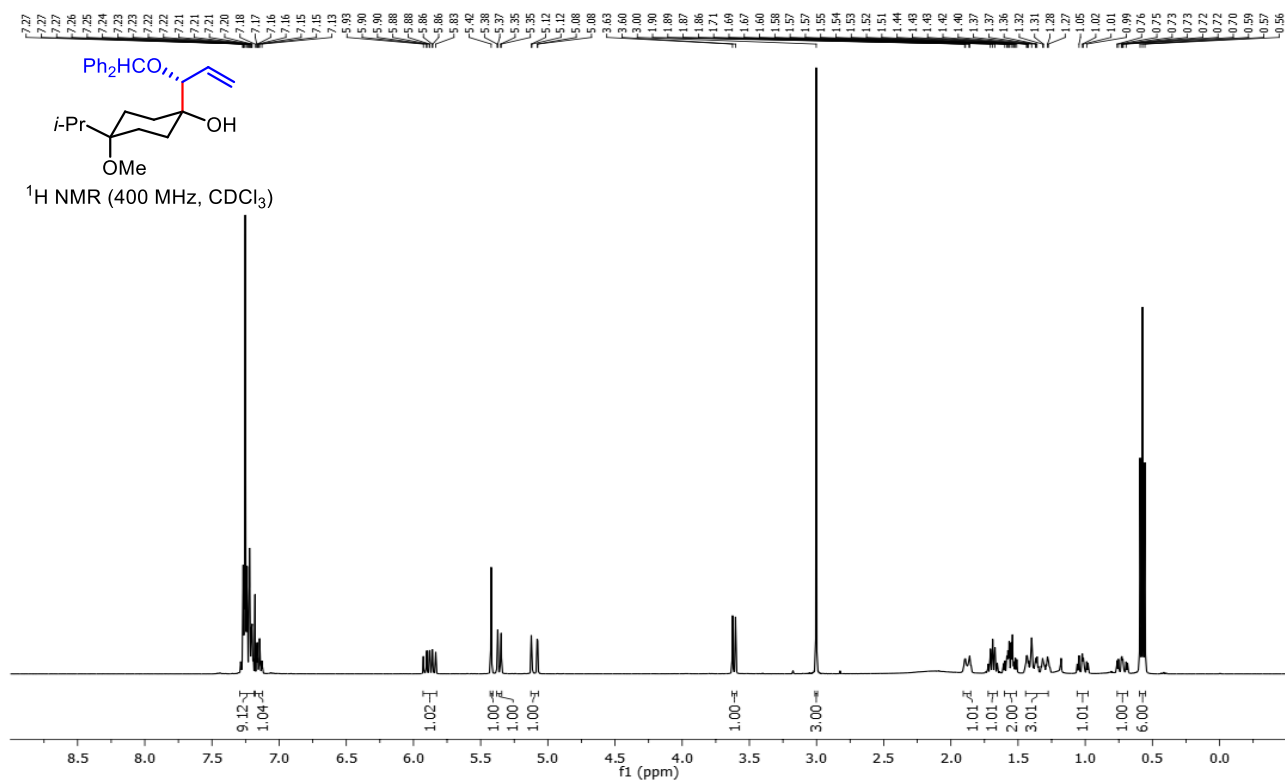
(1*S*,4*S*)-1-((*R*)-1-(Benzhydryloxy)allyl)-4-ethyl-4-methoxycyclohexan-1-ol (5b):



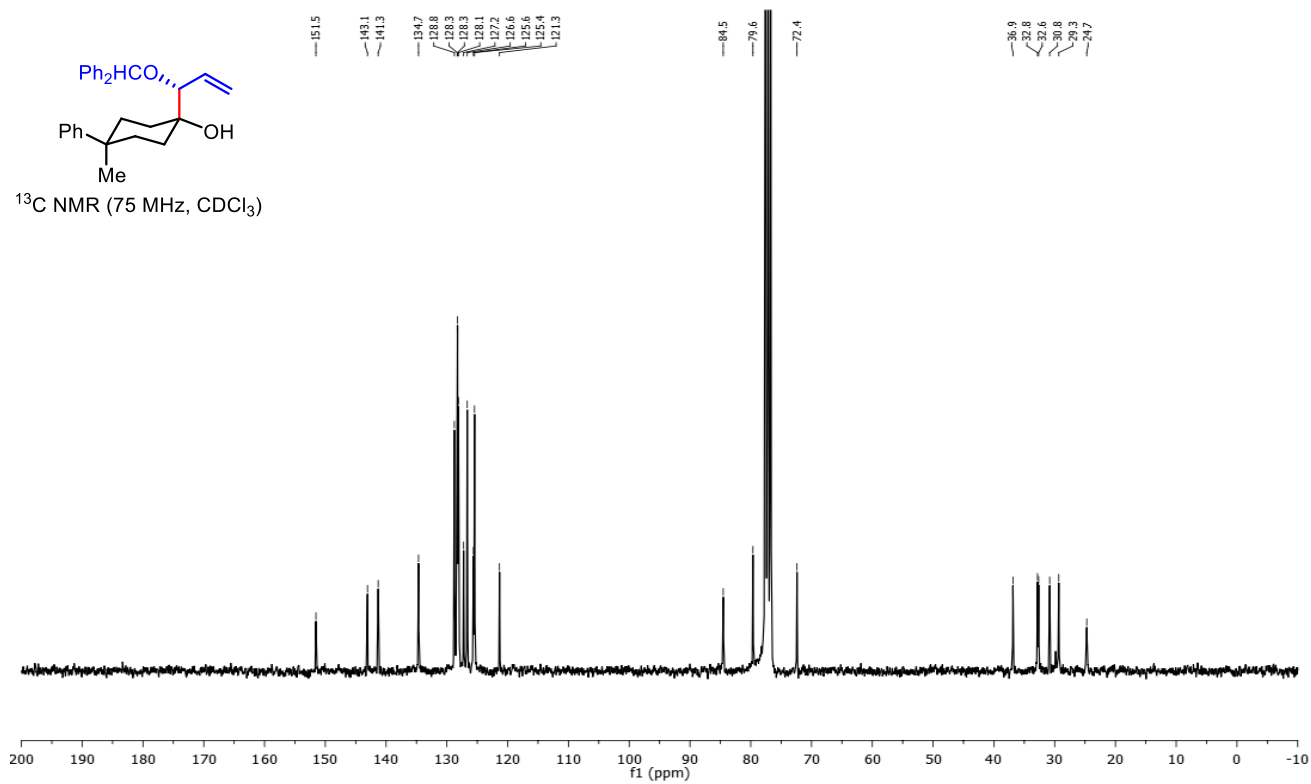
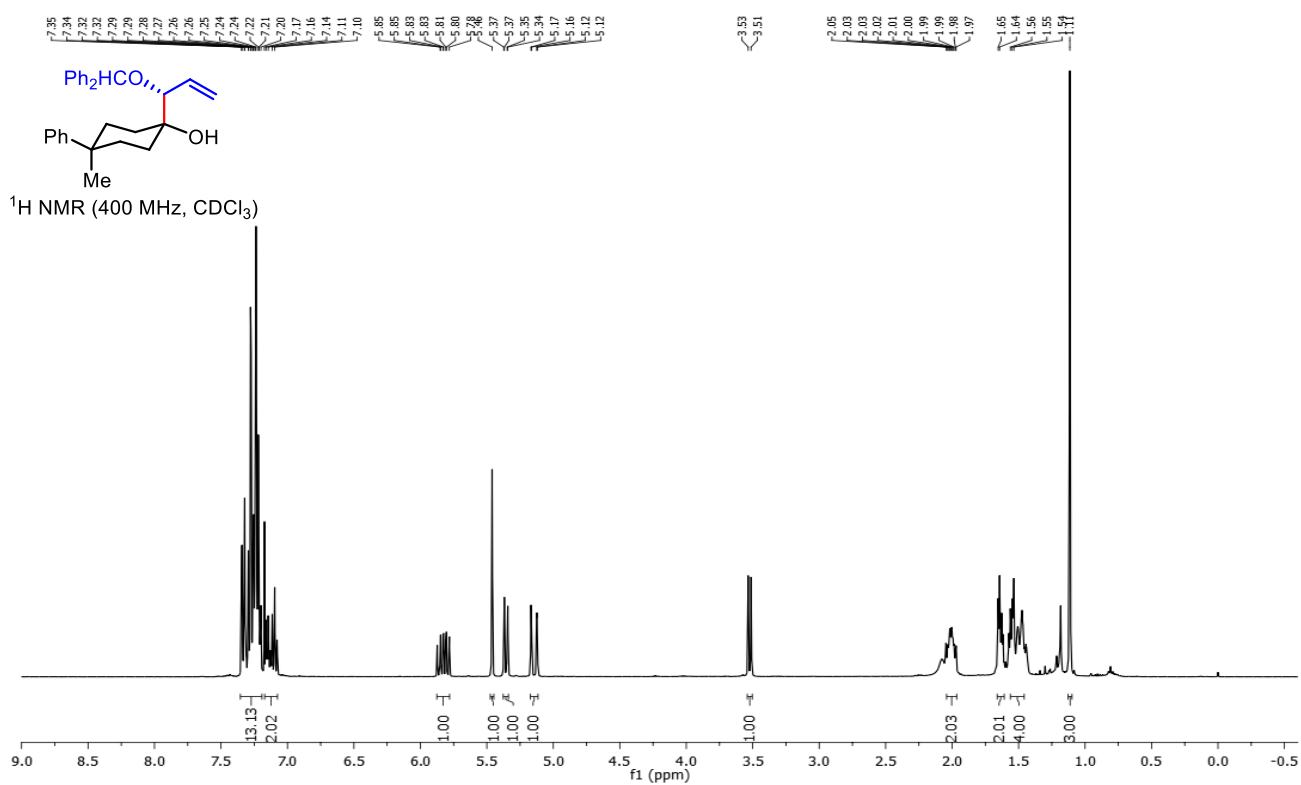
(1*r*,4*S*)-1-((*R*)-1-(Benzhydryloxy)allyl)-4-methoxy-4-propylcyclohexan-1-ol (5c):



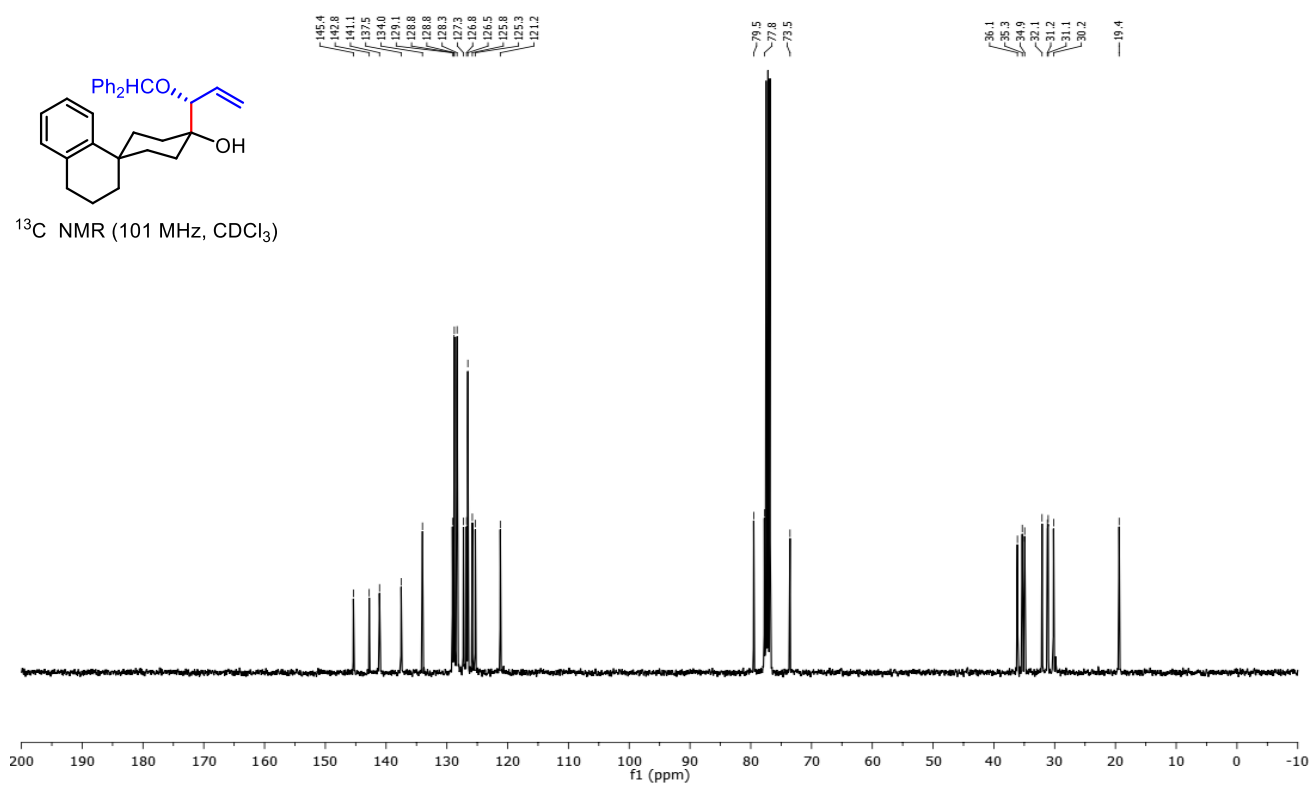
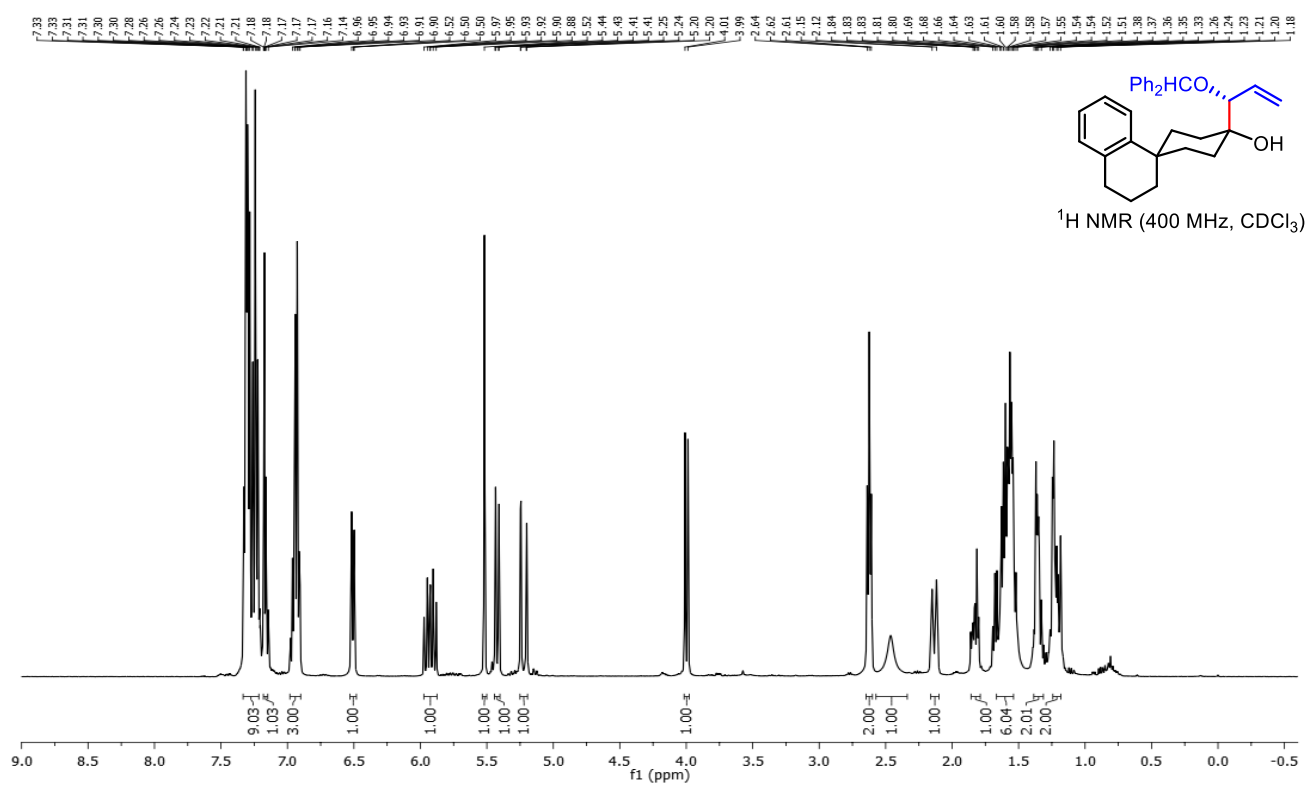
(1*s*,4*S*)-1-((*R*)-1-(Benzhydryloxy)allyl)-4-isopropyl-4-methoxycyclohexan-1-ol (5d):



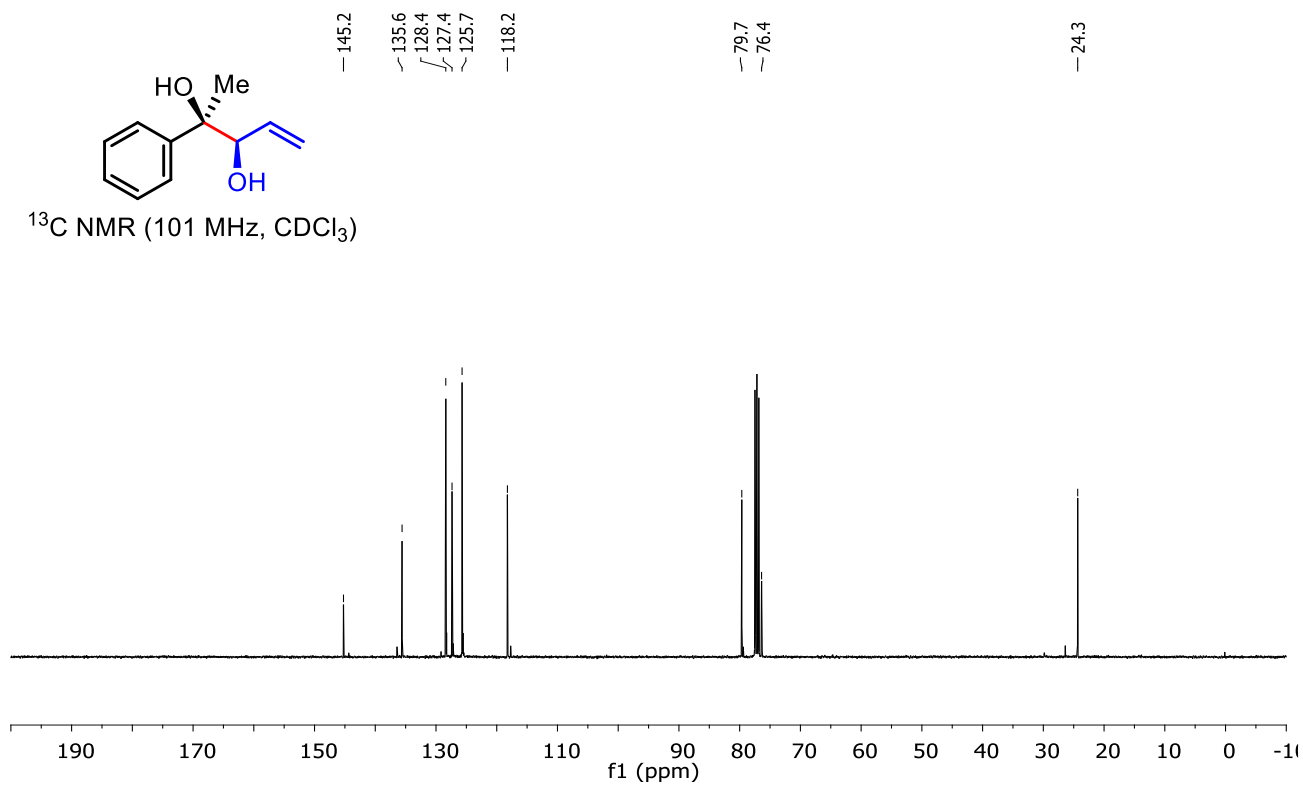
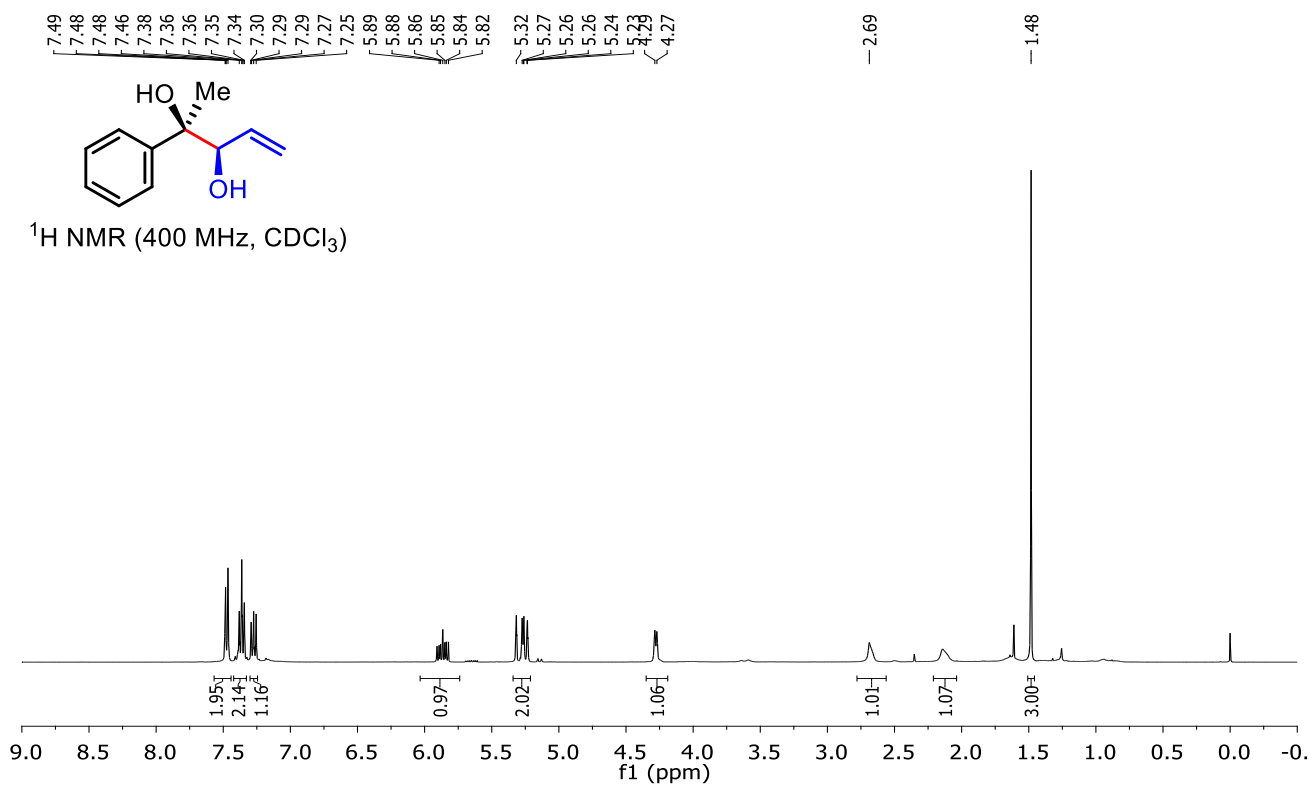
(1*r*,4*R*)-1-((*R*)-1-(Benzhydryloxy)allyl)-4-methyl-4-phenylcyclohexan-1-ol (5e):



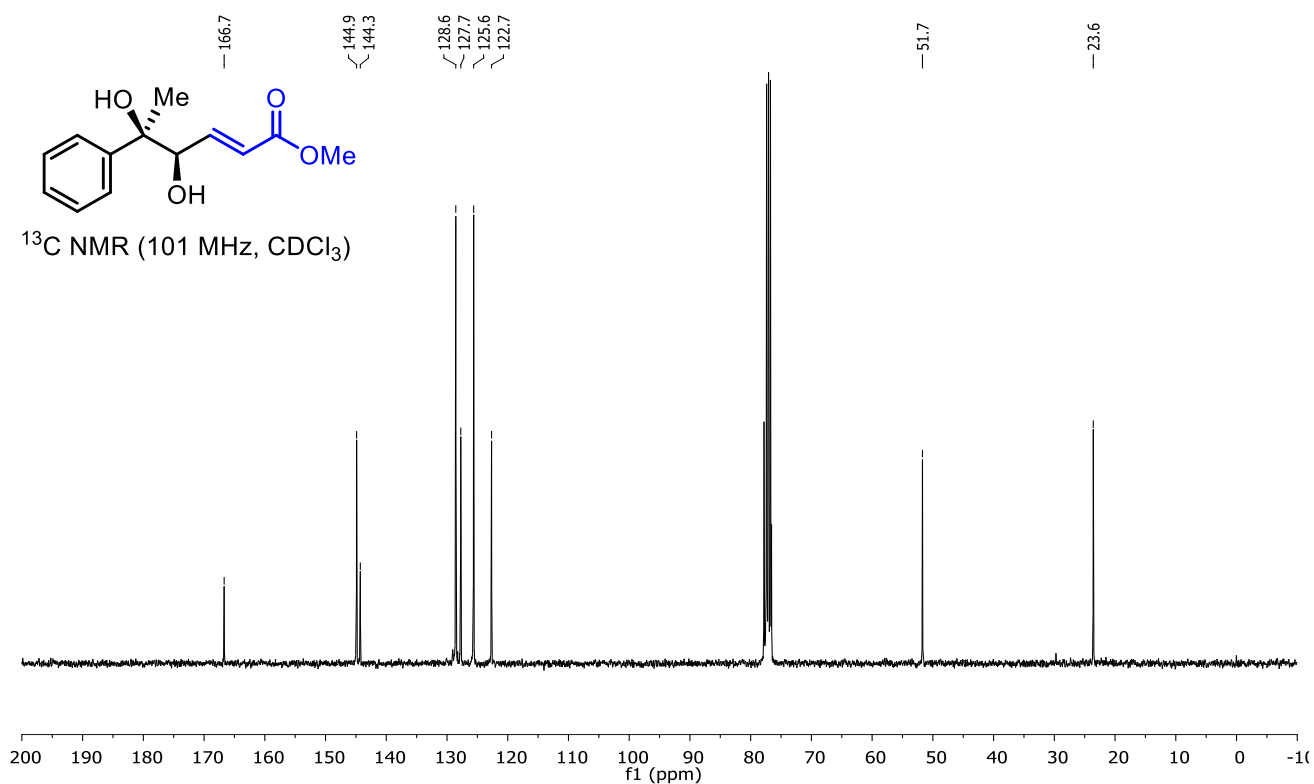
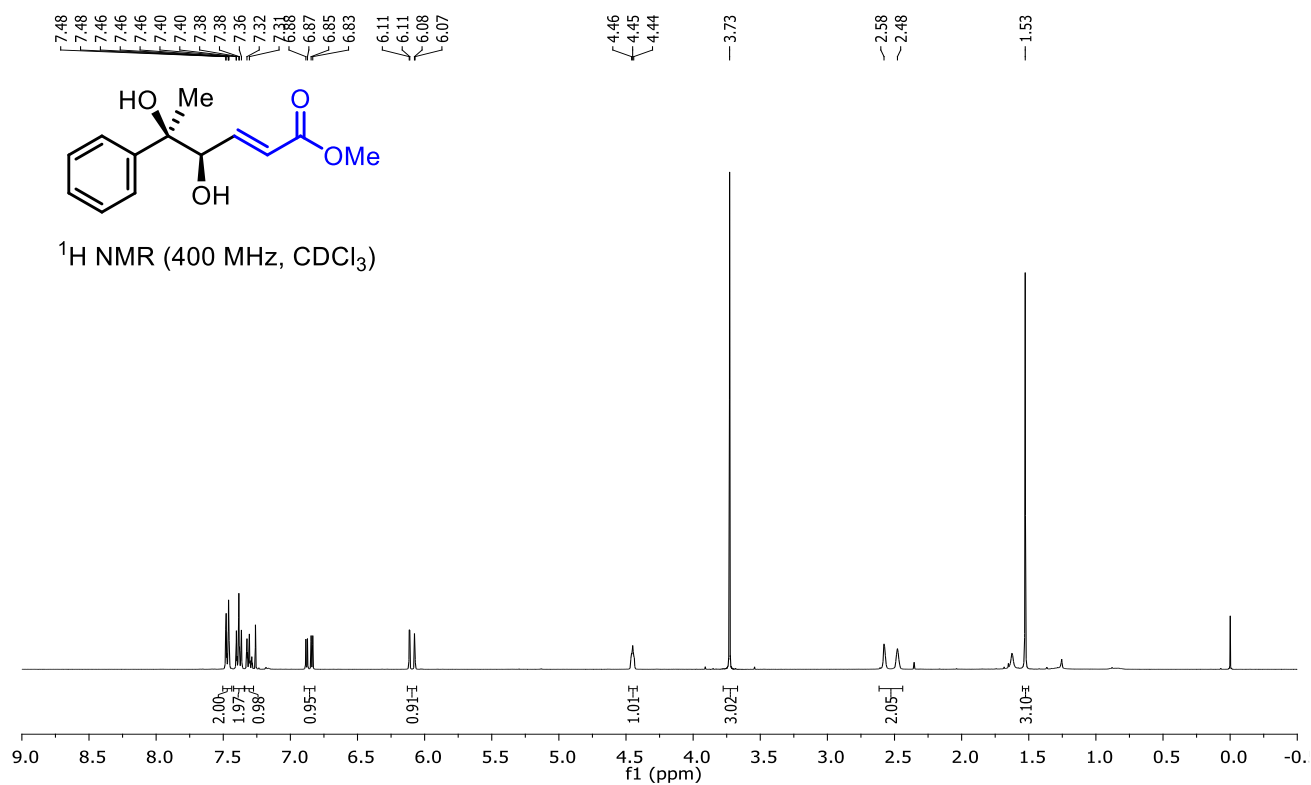
(1*R*,4*s*)-4-((*R*)-1-(Benzhydryloxy)allyl)-3',4'-dihydro-2'*H*-spiro[cyclohexane-1,1'-naphthalen]-4-ol (5f):



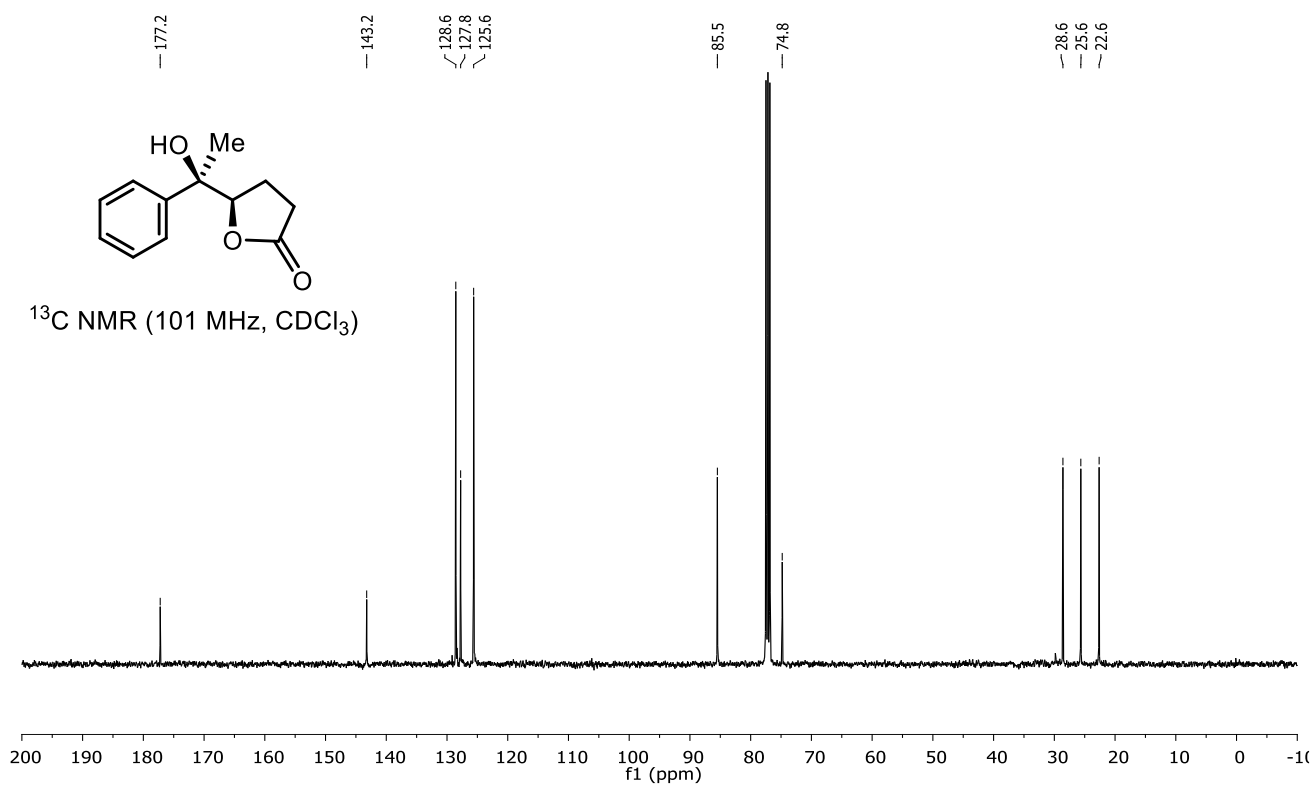
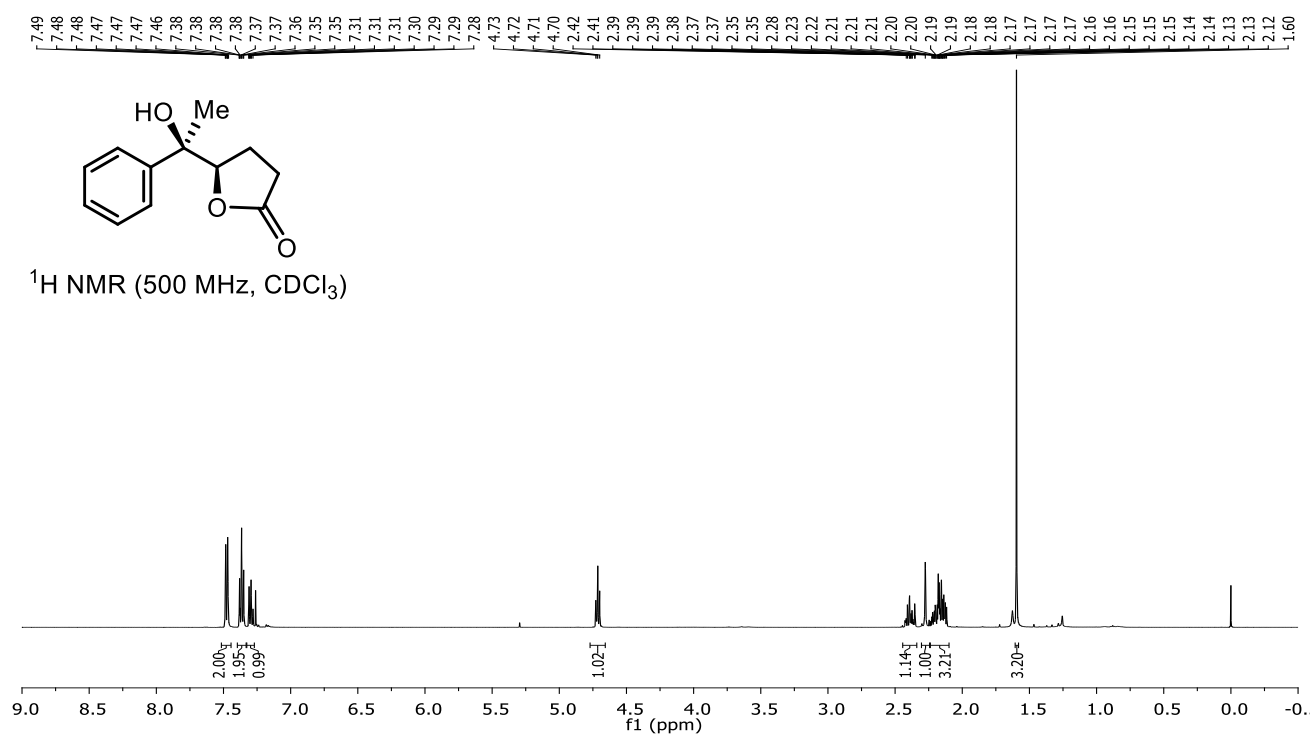
(2*R*,3*R*)-2-Phenylpent-4-ene-2,3-diol (6):



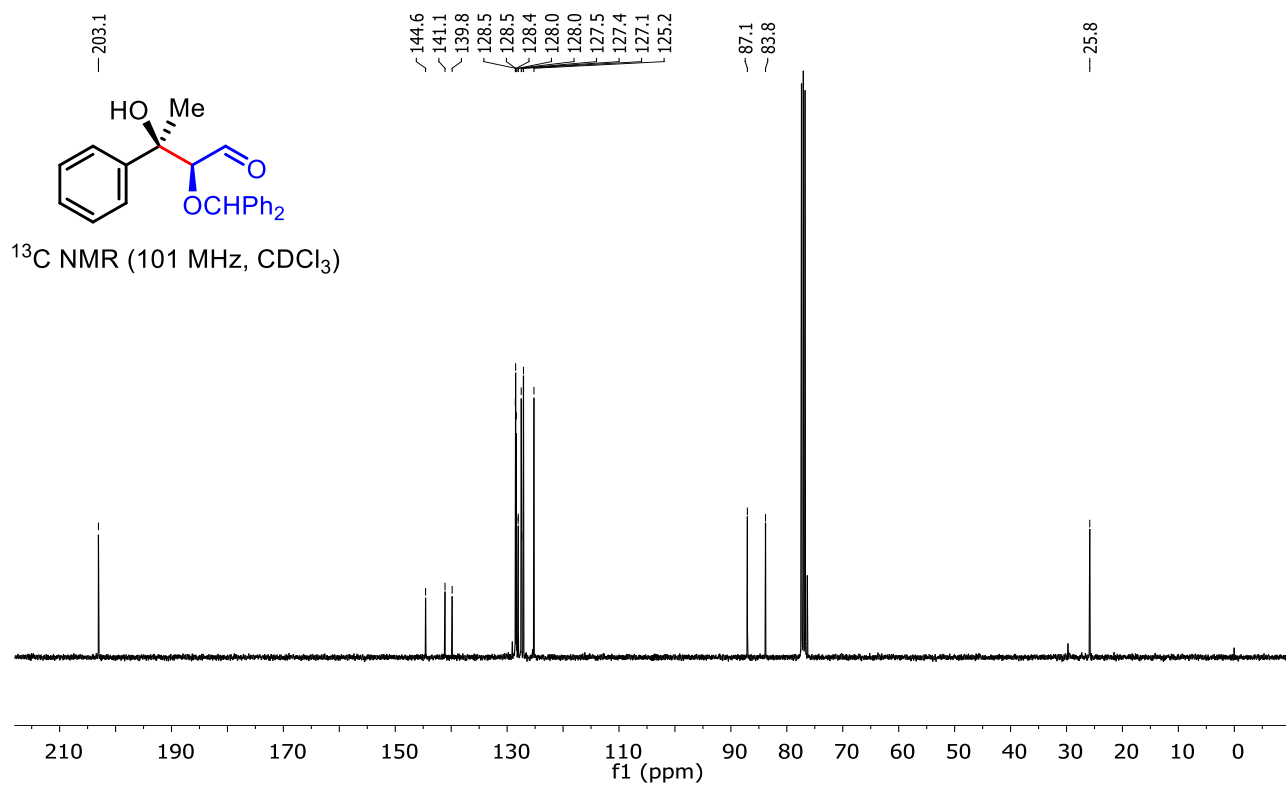
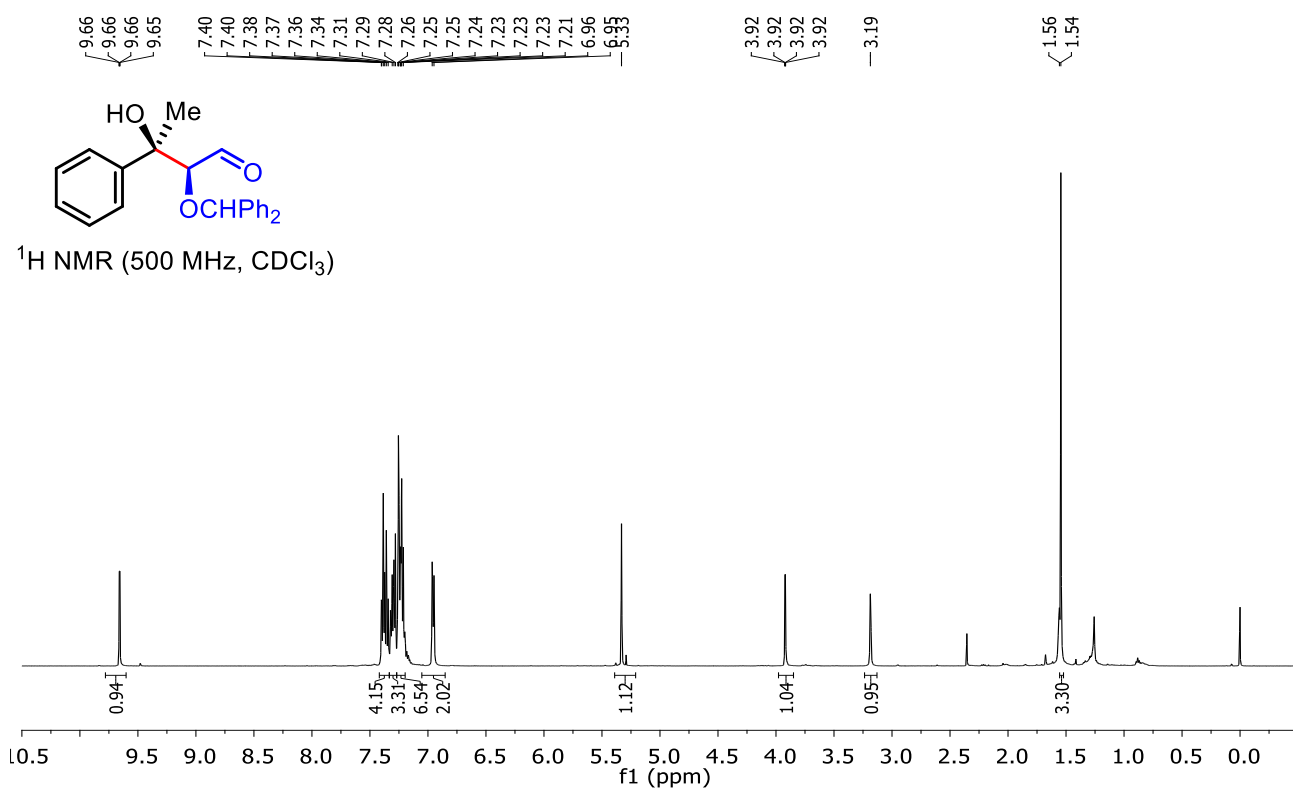
Methyl (4*R*,5*R*, *E*)-4,5-Dihydroxy-5-phenylhex-2-enoate (8):



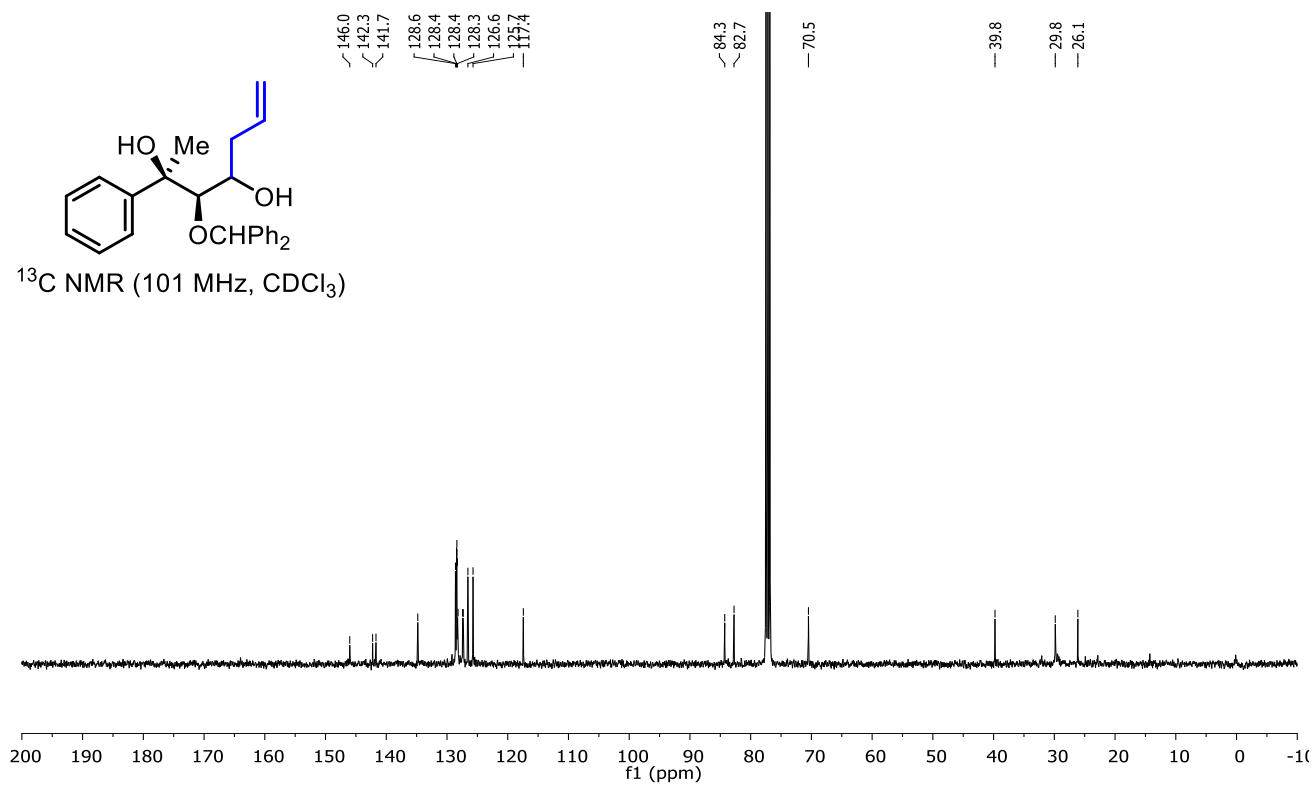
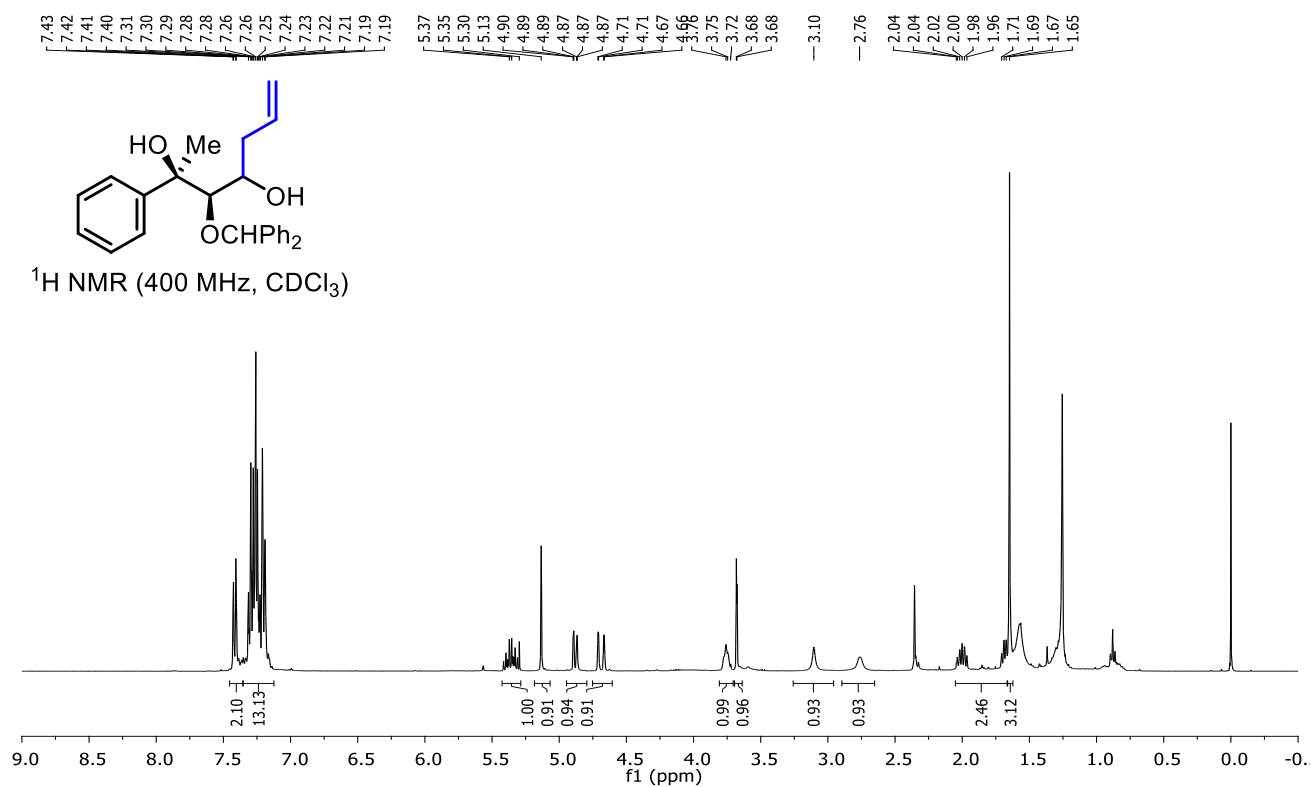
(R)-5-((R)-1-Hydroxy-1-phenylethyl)dihydrofuran-2(3H)-one (9):



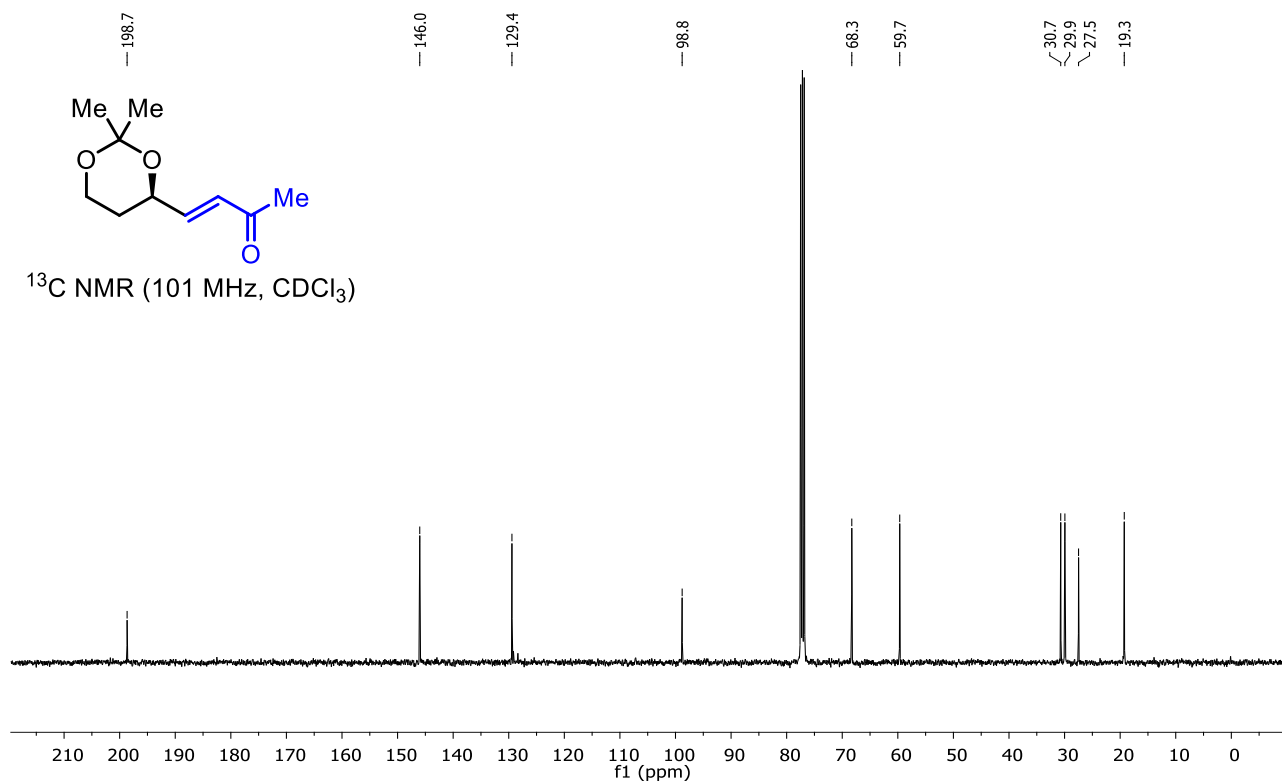
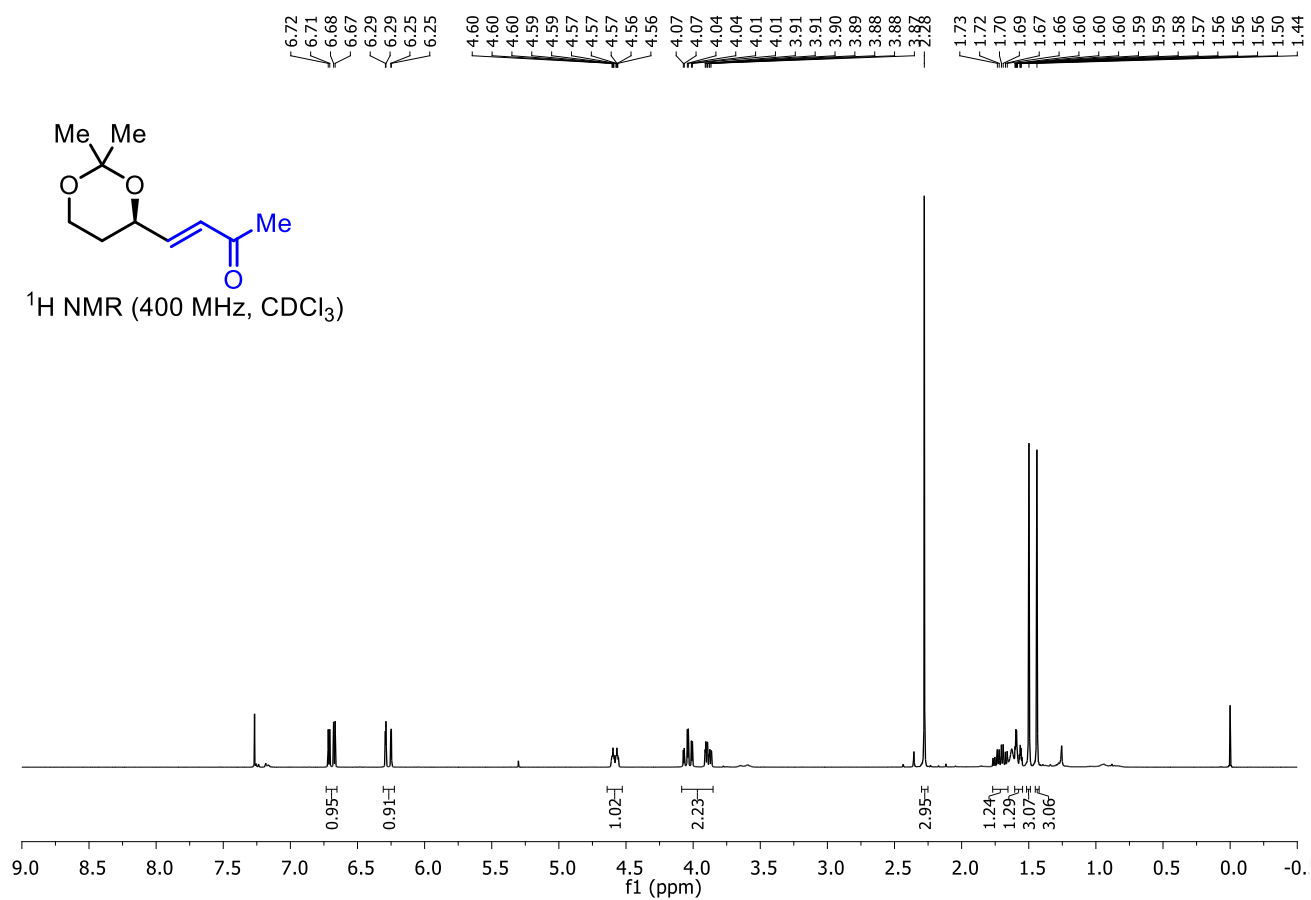
(2*S*,3*R*)-2-(Benzhydryloxy)-3-hydroxy-3-phenylbutanal (10):



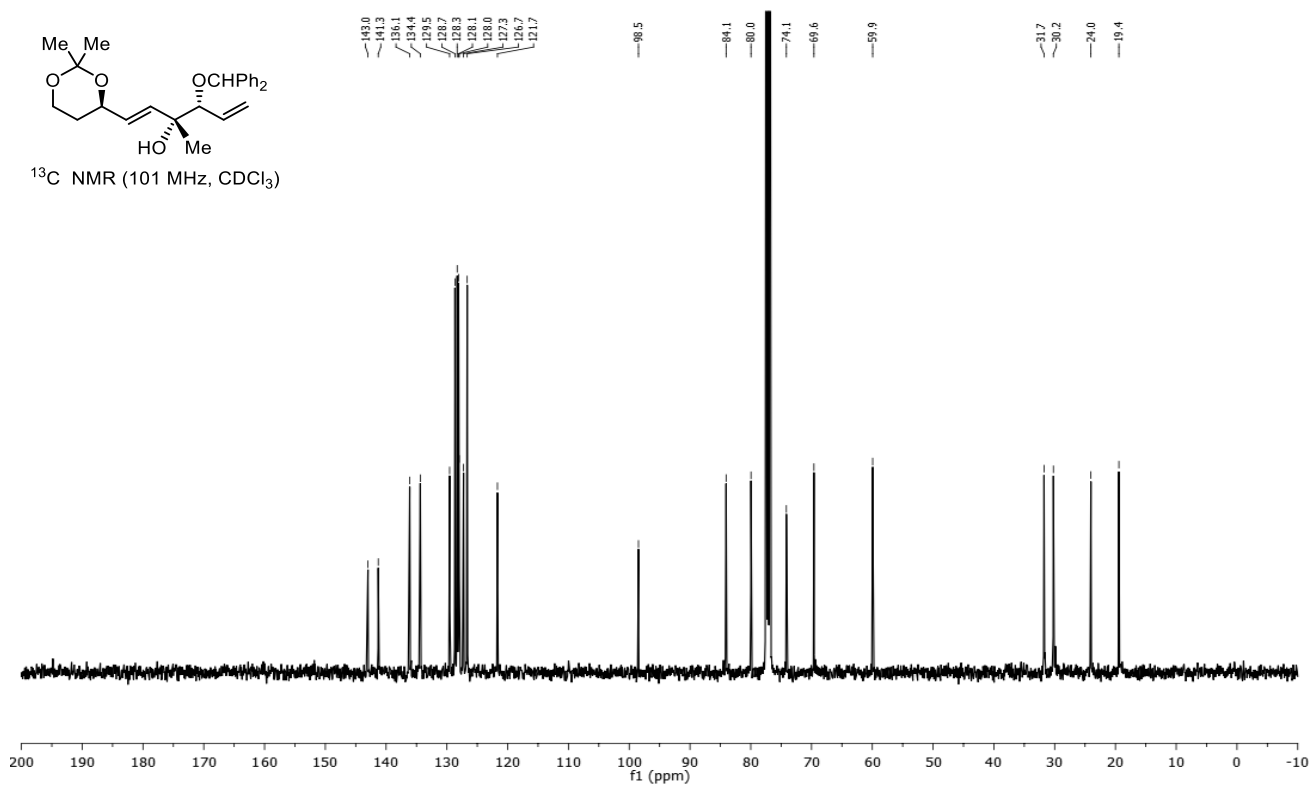
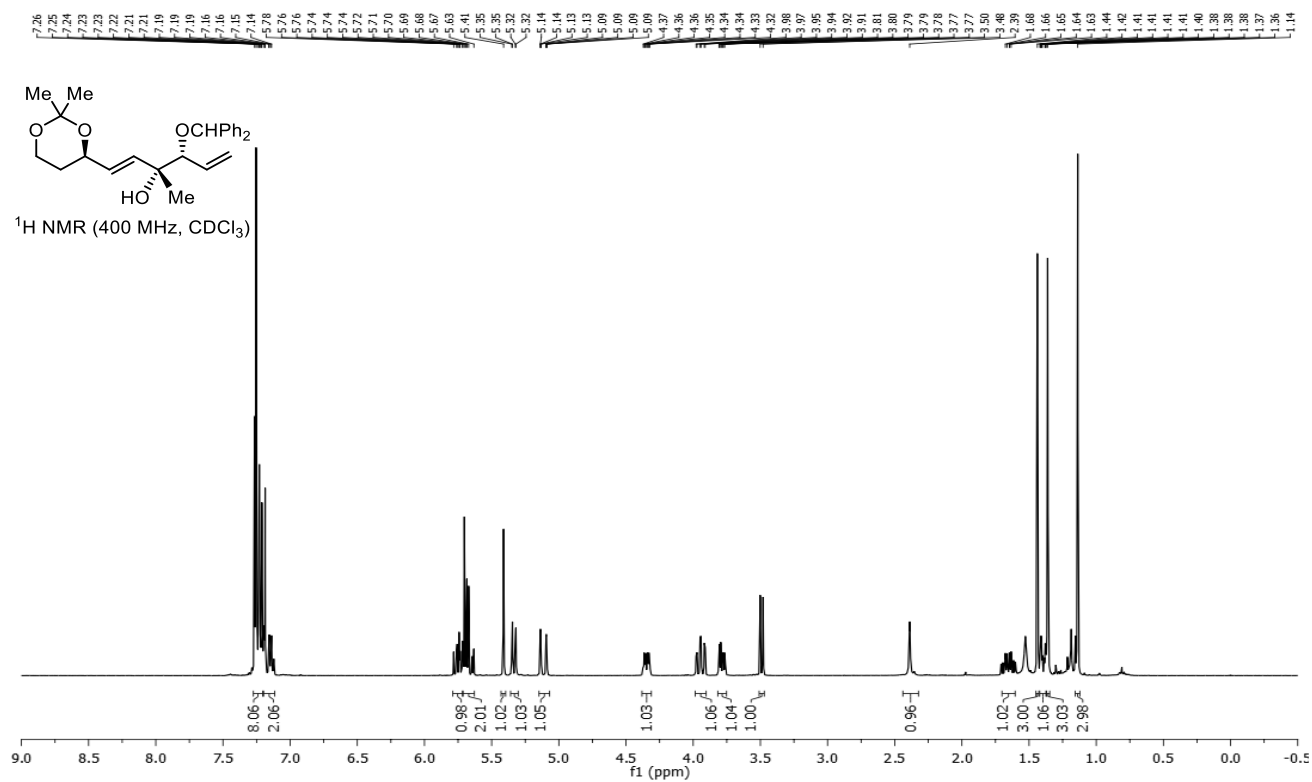
(2*R*,3*R*)-3-(Benzhydryloxy)-2-phenylhept-6-ene-2,4-diol (11):



(R, E)-4-(2,2-Dimethyl-1,3-dioxan-4-yl)but-3-en-2-one (14):



(3*R*,4*R*, *E*)-4-(Benzyloxy)-1-((*R*)-2,2-dimethyl-1,3-dioxan-4-yl)-3-methylhexa-1,5-dien-3-ol (15):



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