

Supplementary materials

Enantioselective transesterification of allyl alcohols with (E)-4-arylbut-3-en-2-ol motif by immobilized Lecitase™ Ultra

Aleksandra Leśniarek^{1*}, Anna Chojnacka¹, Radosław Drozd², Magdalena Szymańska², Witold Gładkowski^{1*}

¹Department of Chemistry, Wrocław University of Environmental and Life Sciences, Norwida 25, 50-375 Wrocław, Poland; anna.chojnacka@upwr.edu.pl (A.C.)

²Department of Microbiology and Biotechnology, Faculty of Biotechnology
and Animal Husbandry, West Pomeranian University of Technology, Szczecin, 45 Piastów Avenue,
71-311 Szczecin, Poland; rdrozd@zut.edu.pl (R.D.); magdalena.szymanska@zut.edu.pl (M.S.)

*Correspondence: witold.gladkowski@upwr.edu.pl; aleksandrajurabio@gmail.com; tel. +48 713205154 (W.G.)

Table of Contents

Fig.S1 ¹ H NMR spectrum of (-)-(S,E)-4-phenylbut-3-en-2-ol ((S)- 1a).....	3
Fig.S2 ¹ H NMR spectrum of (+)-(R,E)-4-phenylbut-3-en-2-yl propionate ((R)- 3a).....	4
Fig.S3 ¹ H NMR spectrum of (-)-(S,E)-4-(4'-methylphenyl)but-3-en-2-ol ((S)- 1b).....	5
Fig.S4 ¹ H NMR spectrum of (+)-(R,E)-4-(4'-methylphenyl)but-3-en-2-yl propionate ((R)- 3b).....	6
Fig.S5 ¹ H NMR spectrum of (-)-(S,E)-4-(2',5'-dimethylphenyl)but-3-en-2-ol ((S)- 1c).....	7
Fig.S6 ¹ H NMR spectrum of (+)-(R,E)-4-(2',5'-dimethylphenyl)but-3-en-2-yl propionate ((R)- 3c).....	8
Fig.S7 ¹ H NMR spectrum of (-)-(S,E)-4-(4'-methoxyphenyl)but-3-en-2-ol ((S)- 1d).....	9
Fig.S8 ¹ H NMR spectrum of (+)-(R,E)-4-(4'-methoxyphenyl)but-3-en-2-yl propionate ((R)- 3d):.....	10
Fig.S9 Chromatogram from chiral GC showing traces of racemic (E)-4-phenylbut-3-en-2-ol (1a) (after derivatization into acetate) and (E)-4-phenylbut-3-en-2-yl propionate (3a).....	11
Fig.S10 Chromatogram from chiral GC after transesterification of racemic (E)-4-phenylbut-3-en-2-ol (1a) with vinyl propionate in DIPE using 0.01 U of enzyme.....	12
Fig.S11 Chromatogram from chiral GC after transesterification of racemic (E)-4-phenylbut-3-en-2-ol (1a) with vinyl propionate in DIPE using 0.02 U of enzyme.....	13
Fig.S12 Chromatogram from chiral GC after transesterification of racemic (E)-4-phenylbut-3-en-2-ol (1a) with vinyl propionate in DIPE using 0.03 U of enzyme.....	14

Figure S1. ¹H NMR spectrum of (-)-(S,E)-4-phenylbut-3-en-2-ol ((S)-1a)

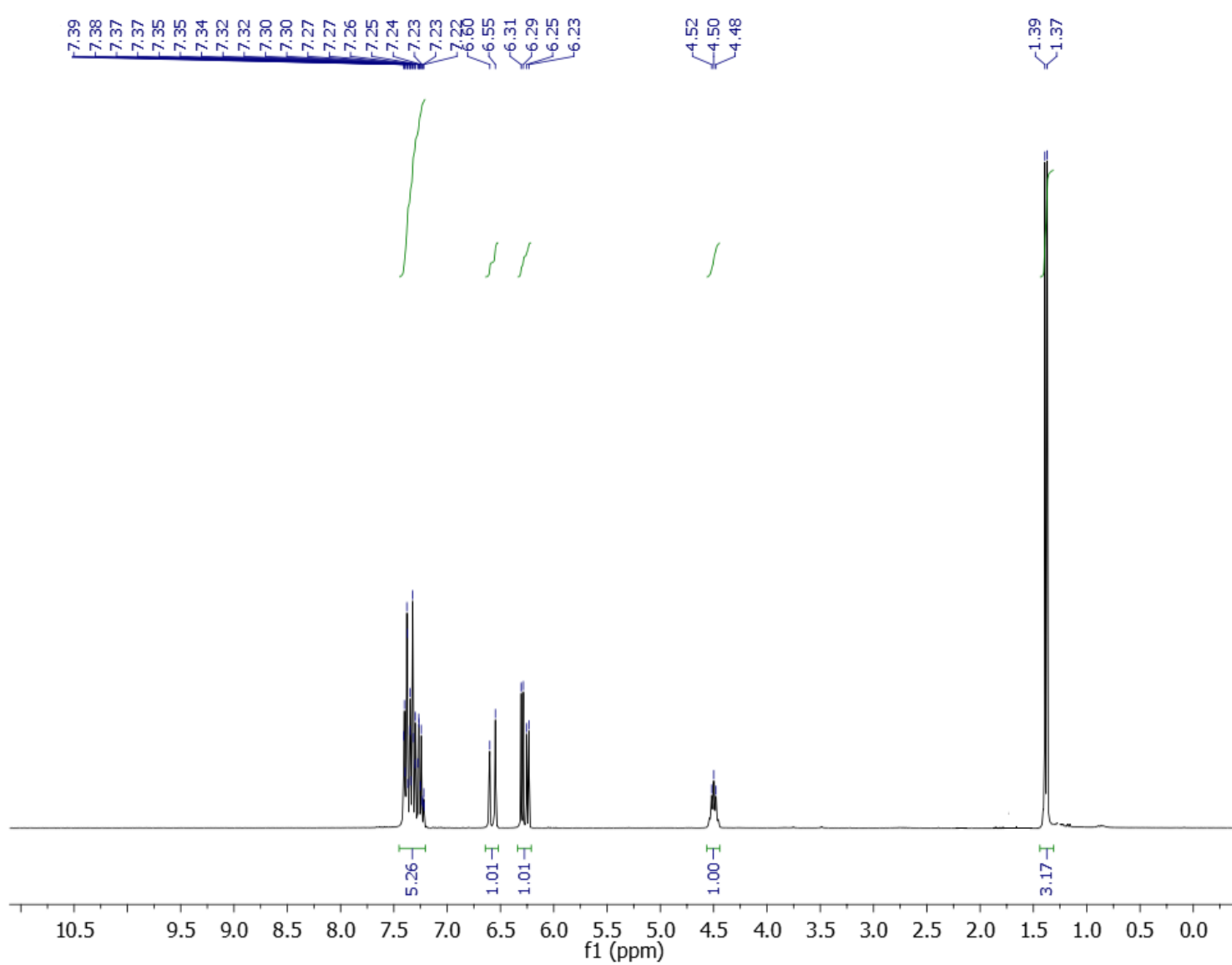


Figure S2. ^1H NMR spectrum of (+)-(*R,E*)-4-phenylbut-3-en-2-yl propionate ((*R*)-3a)

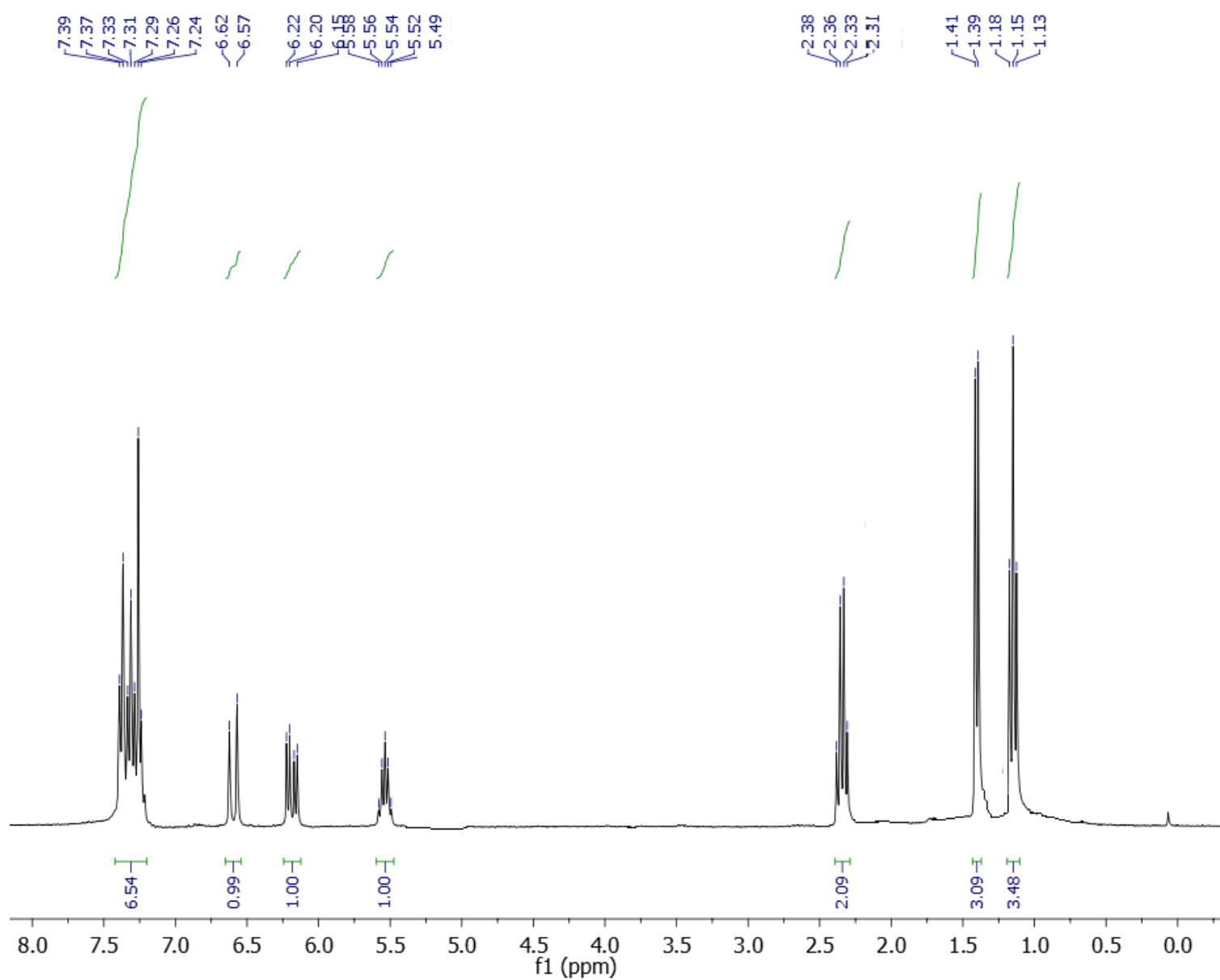


Figure S3. ^1H NMR spectrum of (-)-(*S,E*)-4-(4'-methylphenyl)but-3-en-2-ol ((*S*)-**1b**)

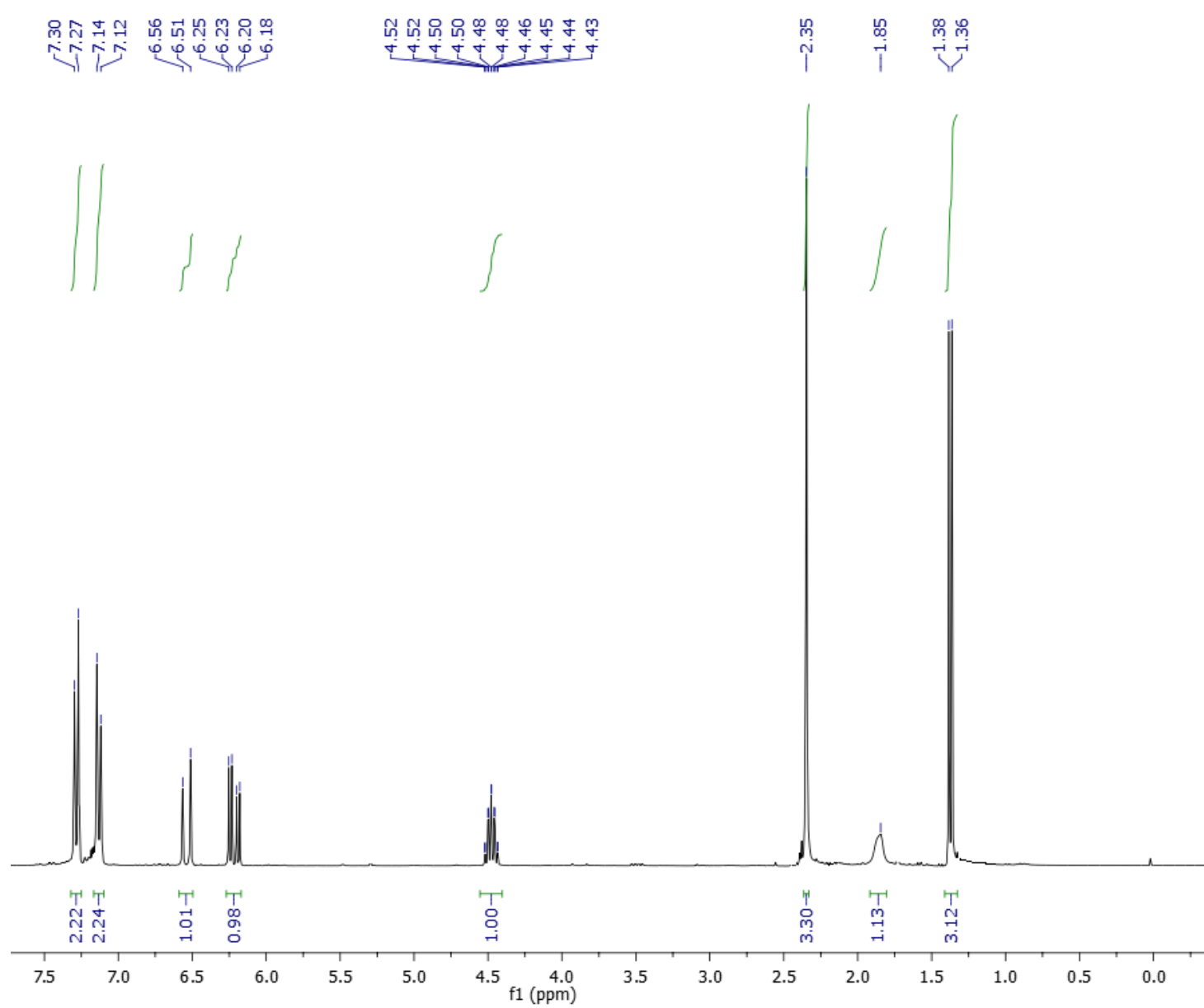


Figure S4. ¹H NMR spectrum of (+)-(R,E)-4-(4'-methylphenyl)but-3-en-2-yl propionate ((R)-3b)

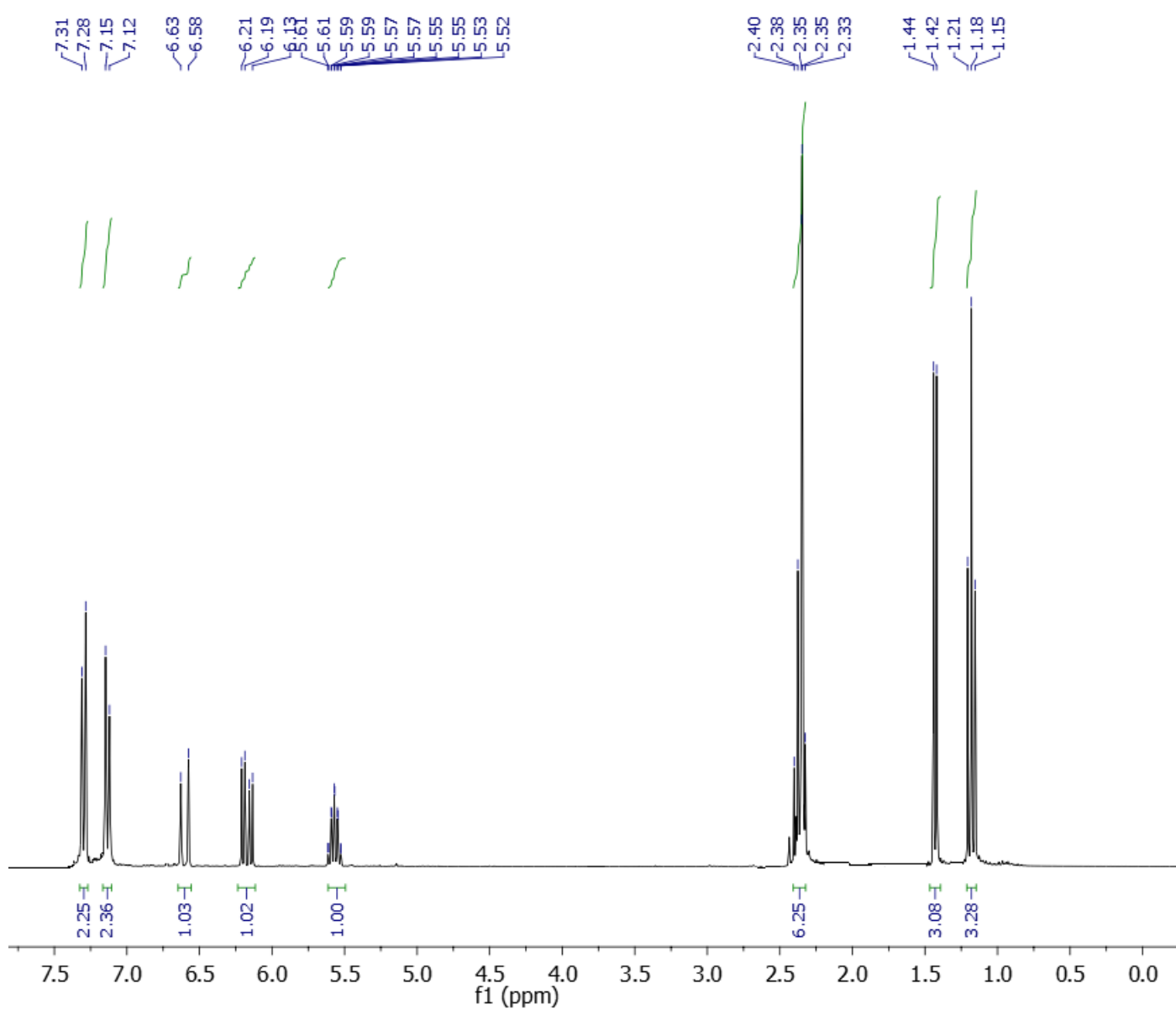


Figure S5. ¹H NMR spectrum of (-)-(S,E)-4-(2',5'-dimethylphenyl)but-3-en-2-ol ((S)-1c)

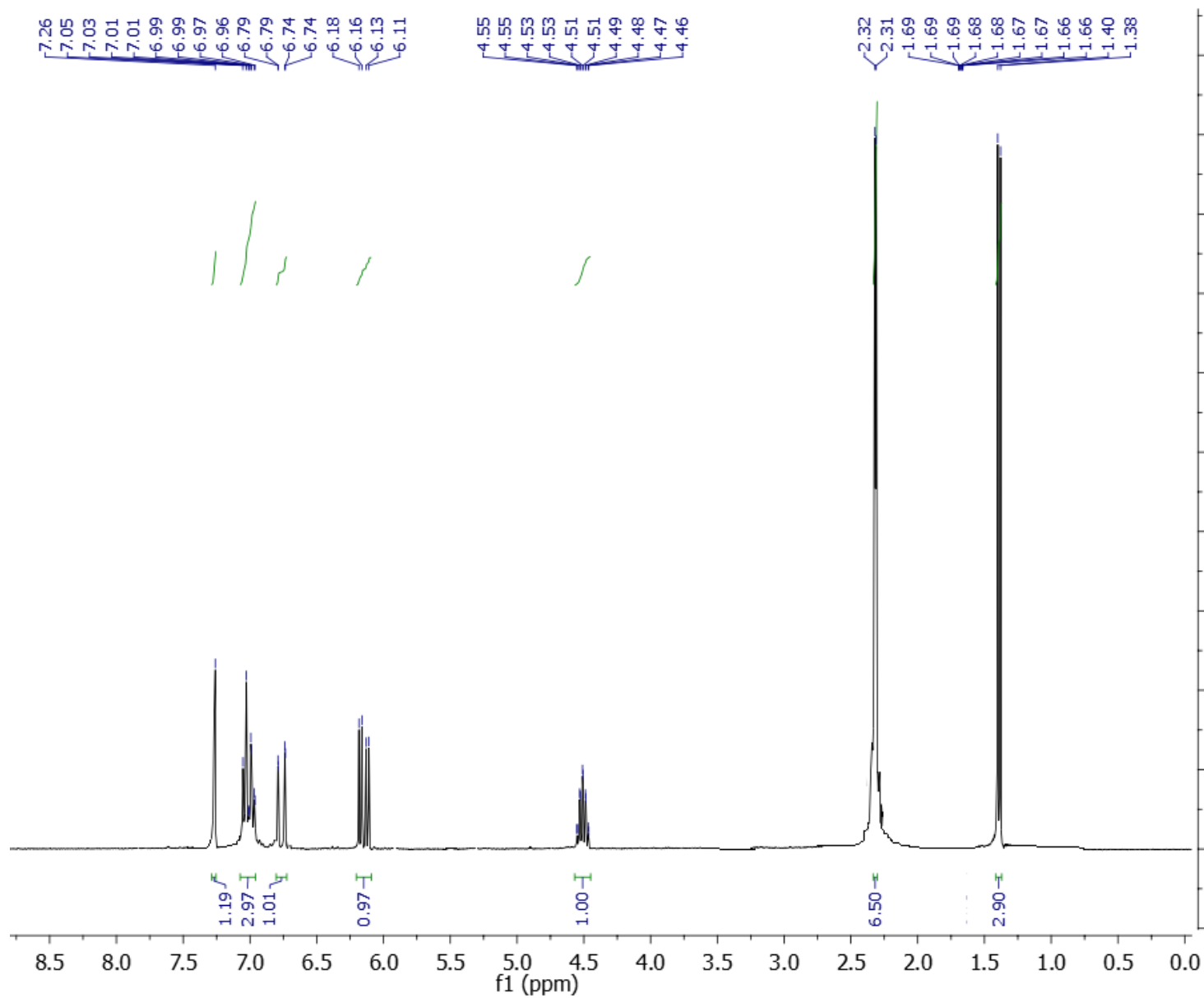


Figure S6. ¹H NMR spectrum of (+)-(R,E)-4-(2',5'-dimethylphenyl)but-3-en-2-yl propionate ((R)-3c)

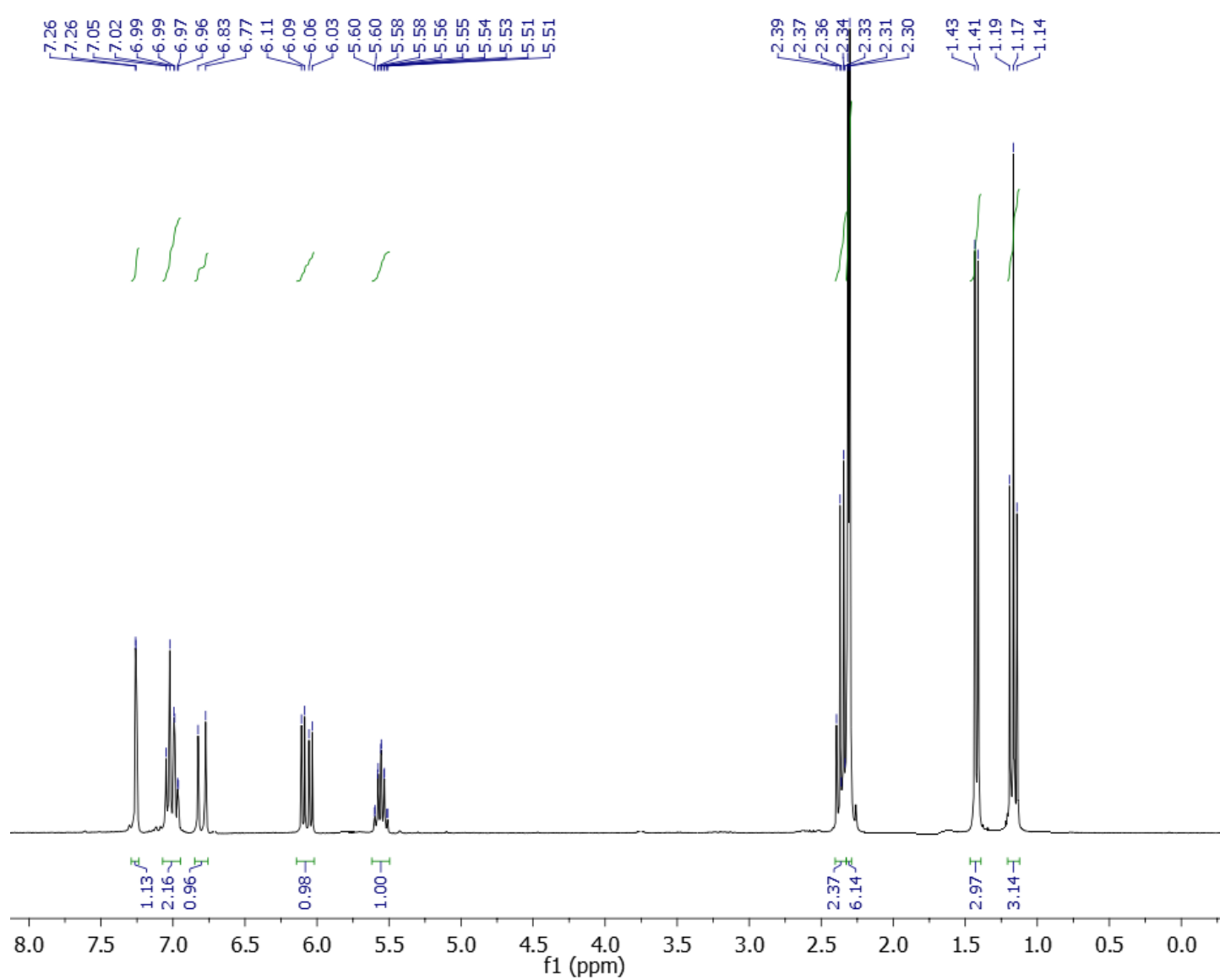


Figure S7. ^1H NMR spectrum of (-)-(S,E)-4-(4'-methoxyphenyl)but-3-en-2-ol ((S)-1d)

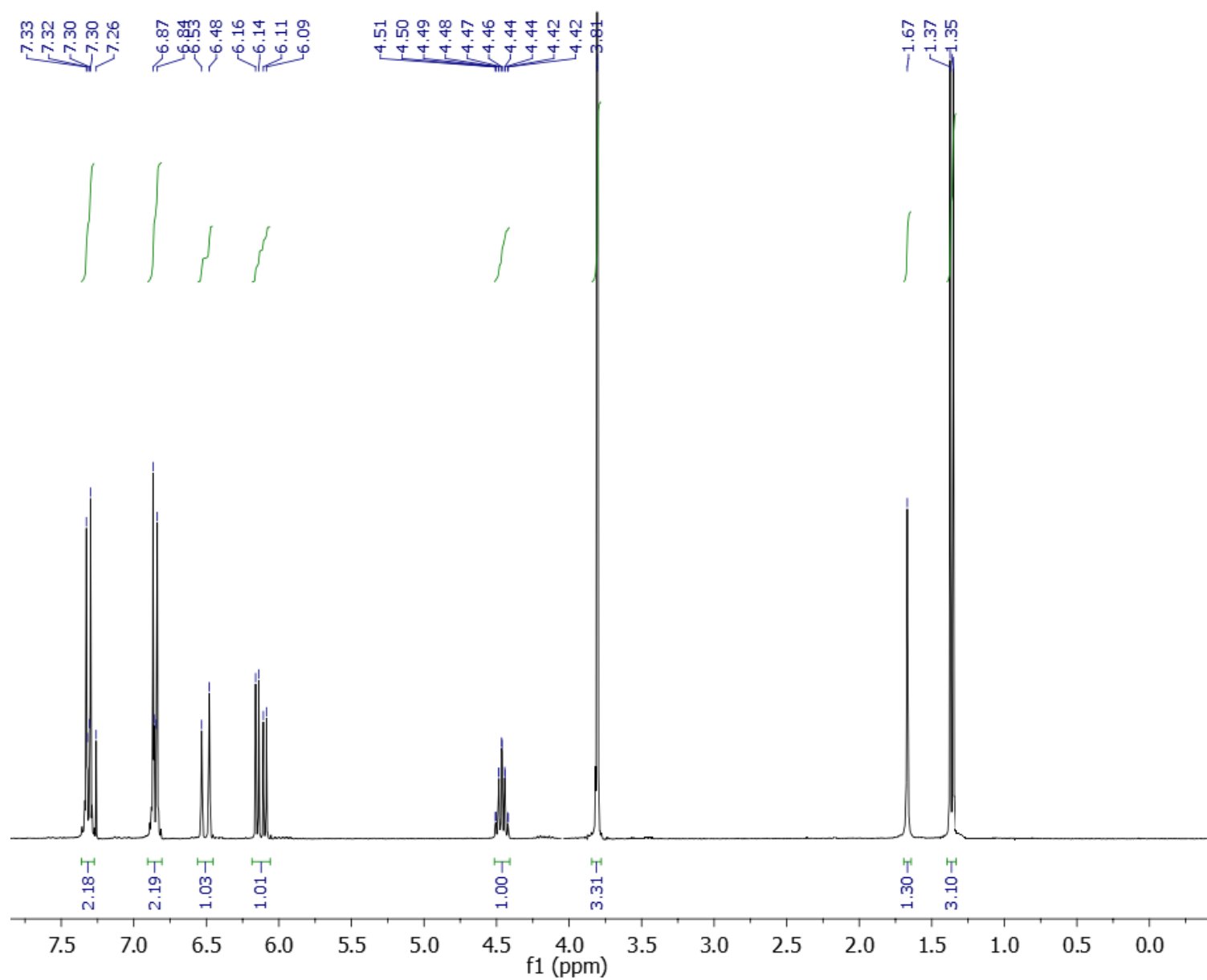


Figure S8. ¹H NMR spectrum of (+)-(R,E)-4-(4'-methoxyphenyl)but-3-en-2-yl propionate ((R)-3d)

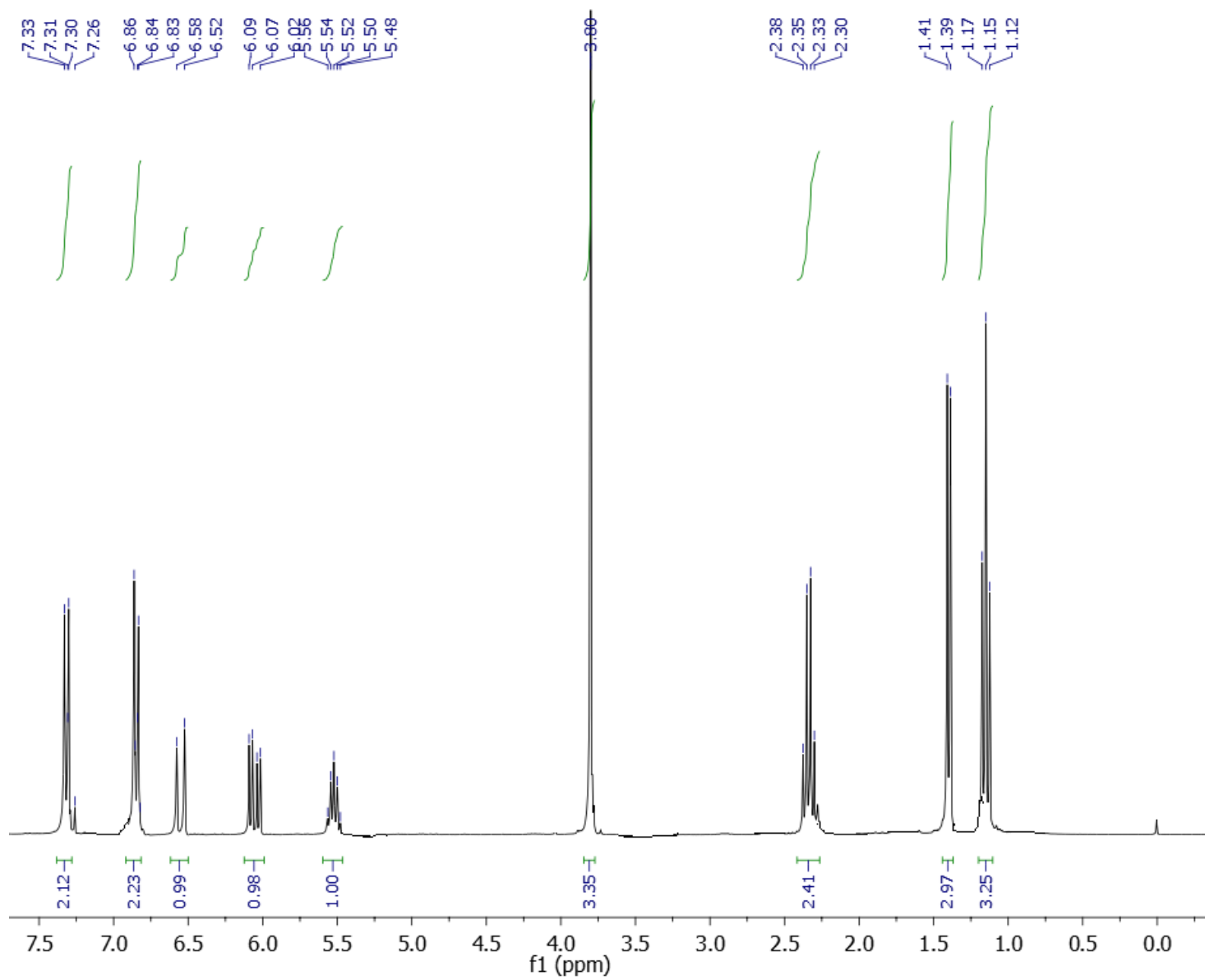
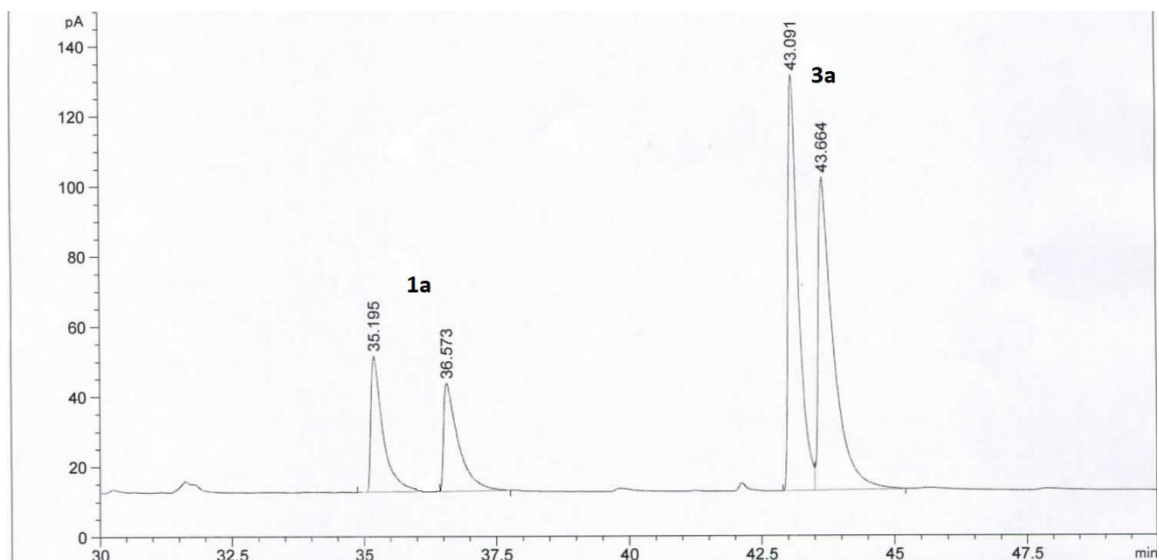


Figure S9. Chromatogram from chiral GC showing traces of racemic (*E*)-4-phenylbut-3-en-2-ol (**1a**) (after derivatization into acetate) and (*E*)-4-phenylbut-3-en-2-yl propionate (**3a**)



=====
 Area Percent Report
 =====

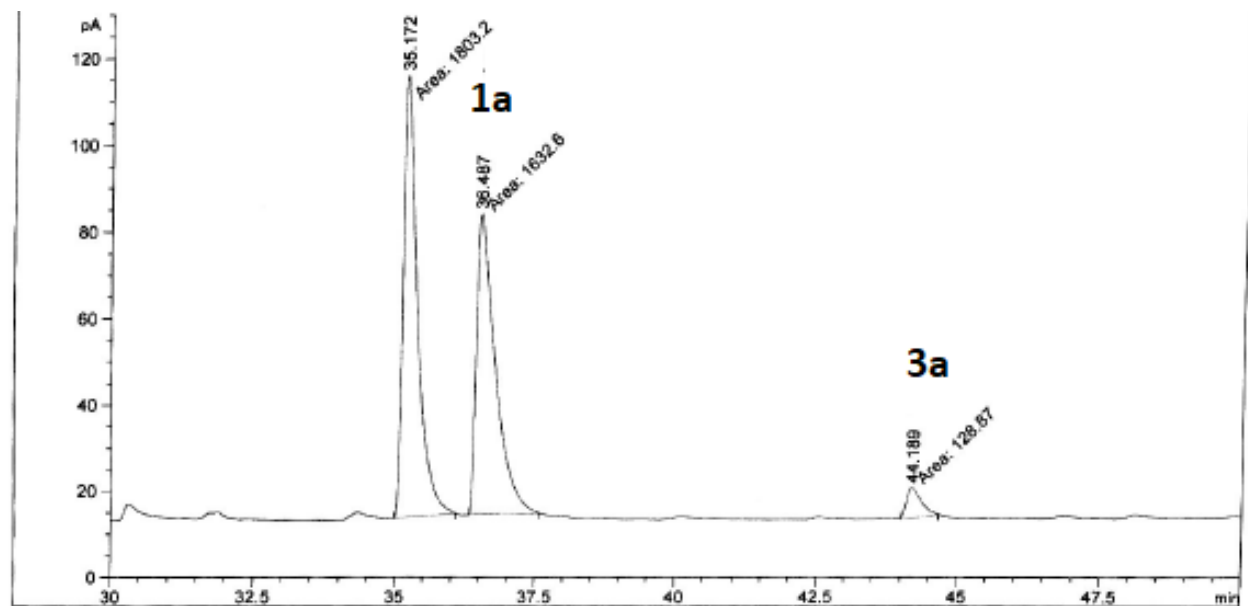
Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	35.195	BV	0.2173	616.54956	38.82421	13.48461
2	36.573	VB	0.2546	590.06738	30.78433	12.90542
3	43.091	BV	0.1937	1602.78430	118.57008	35.05464
4	43.664	VB	0.2633	1762.84485	89.28727	38.55534

Totals : 4572.24609 277.46589

Figure S10. Chromatogram from chiral GC after transesterification of racemic (*E*)-4-phenylbut-3-en-2-ol (**1a**) with vinyl propionate in DIPE using 0.01 U of enzyme



=====
 Area Percent Report
 =====

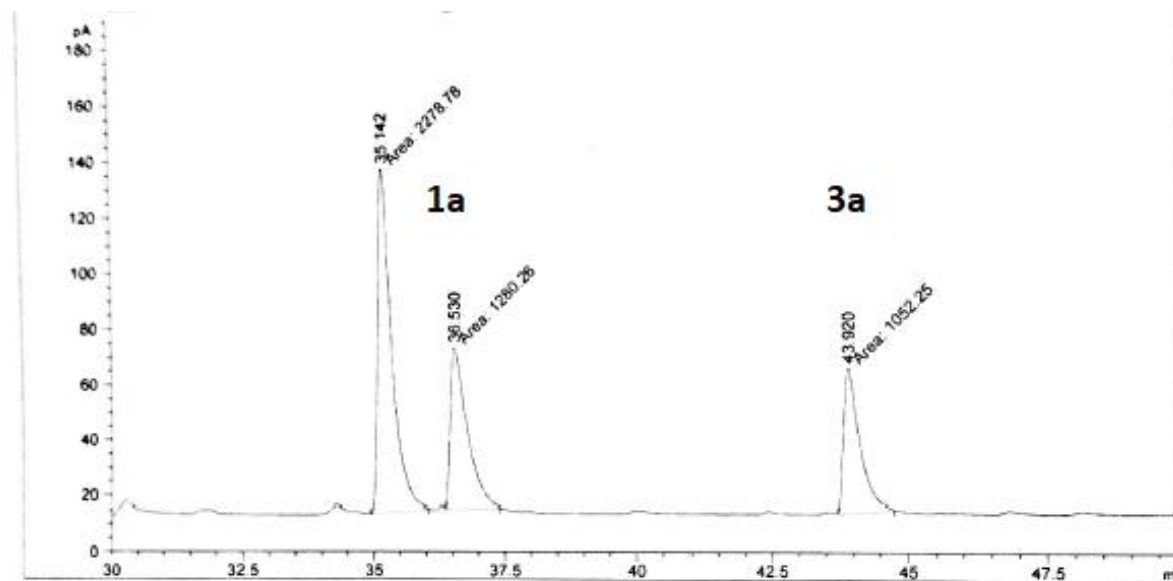
Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	35.172	MM	0.2942	1803.19727	102.14125	50.58530
2	36.487	MM	0.3902	1632.59961	69.73028	45.79951
3	44.189	MM	0.3038	128.86958	7.06896	3.61519

Totals : 3564.66646 178.94049

Figure S11. Chromatogram from chiral GC after transesterification of racemic (*E*)-4-phenylbut-3-en-2-ol (**1a**) with vinyl propionate in DIPE using 0.02 U of enzyme



=====
 Area Percent Report
 =====

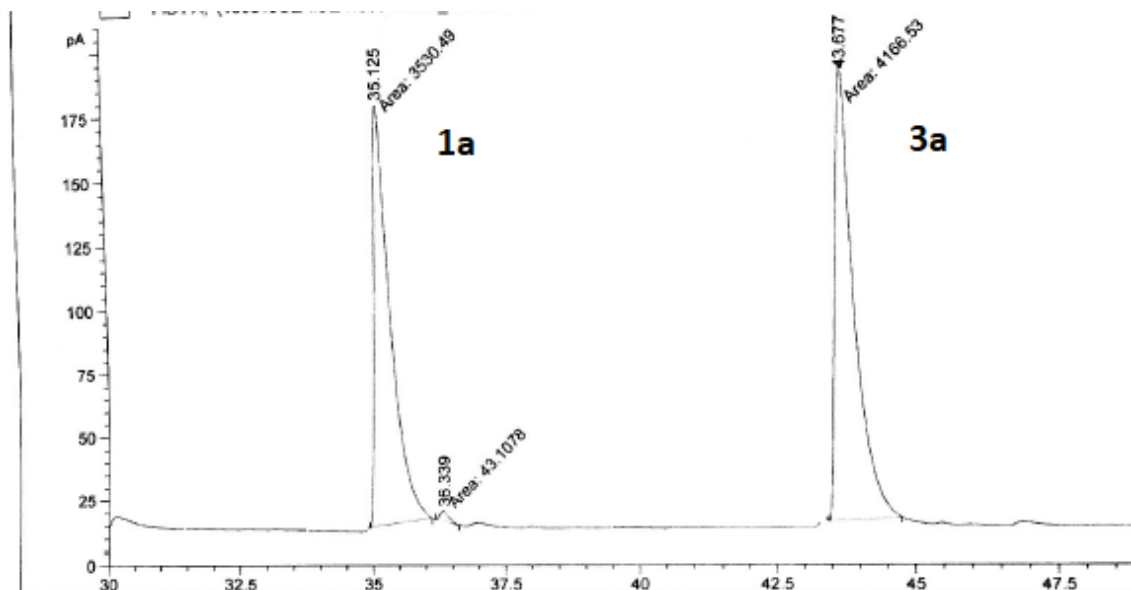
Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	35.142	MM	0.3065	2278.78320	123.92764	49.41742
2	36.530	MM	0.3687	1280.26123	57.87357	27.76359
3	43.920	MM	0.3408	1052.25049	51.46015	22.81898

Totals :
 4611.29492 233.26137

Figure S12. Chromatogram from chiral GC after transesterification of racemic (*E*)-4-phenylbut-3-en-2-ol (**1a**) with vinyl propionate in DIPE using 0.03 U of enzyme



=====
 Area Percent Report
 =====

Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	35.125	MM	0.3587	3530.48779	164.05022	45.61279
2	36.339	MM	0.1978	43.10784	3.63188	0.55694
3	43.677	MM	0.3966	4166.53174	175.10663	53.83027

Totals : 7740.12737 342.78873