

# Catalysis

## An Alternative Enzymatic Route to the Ergogenic Ketone Body Ester (*R*)-3-Hydroxybutyl (*R*)-3-Hydroxybutyrate

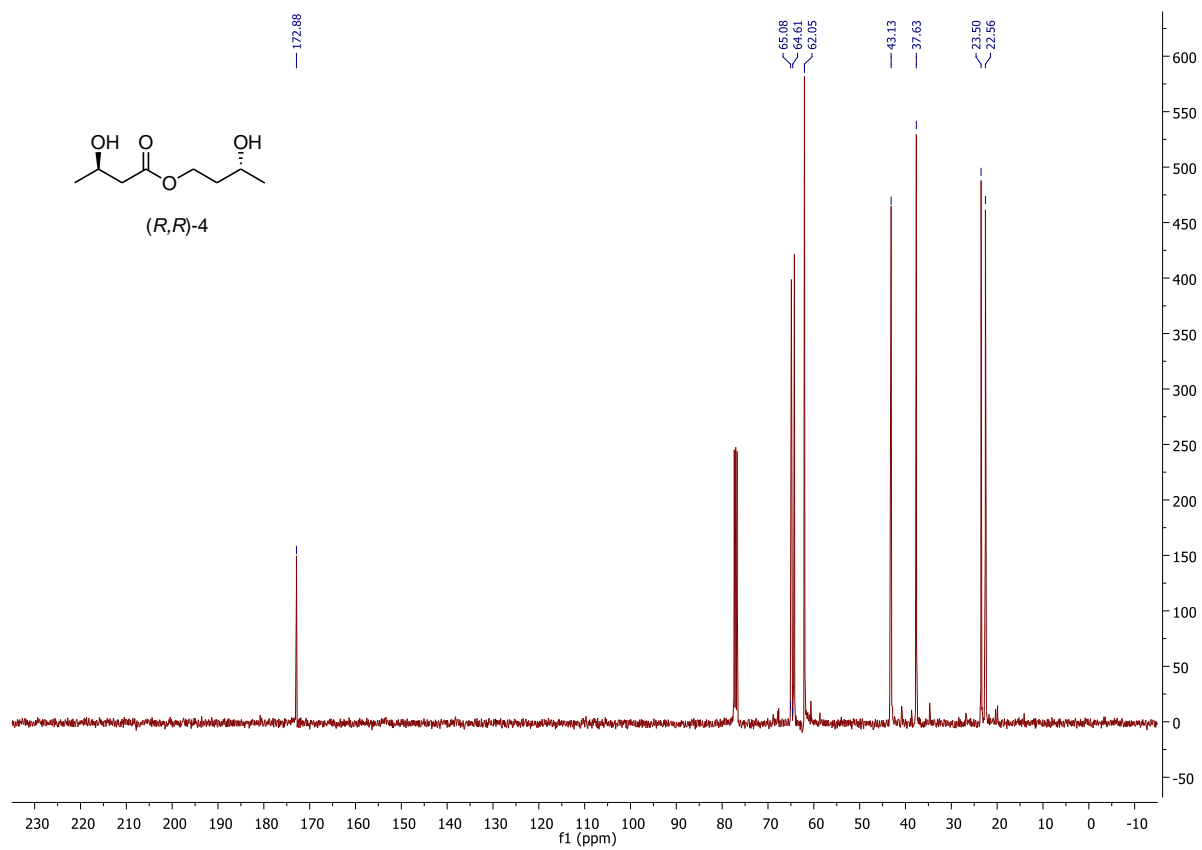
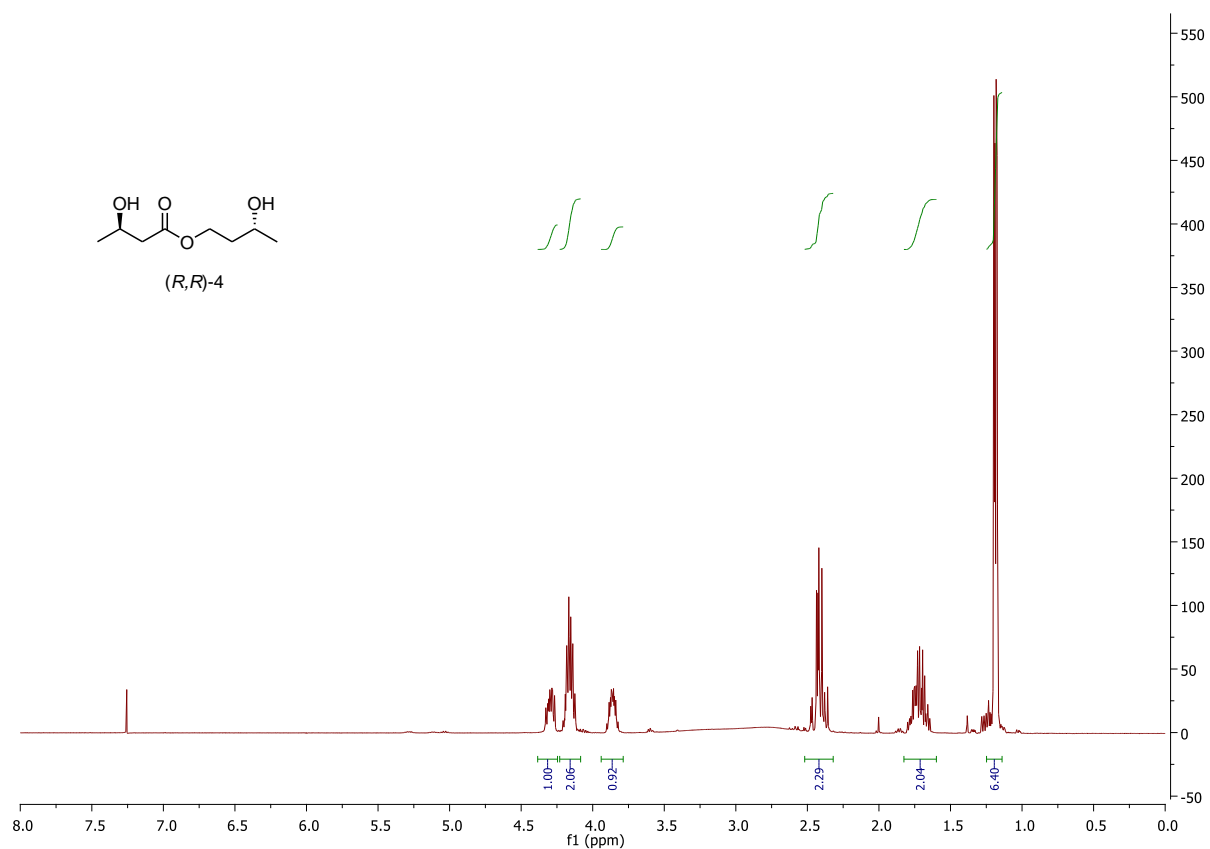
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Claudio Trapella1,..

### Supplementary Materials

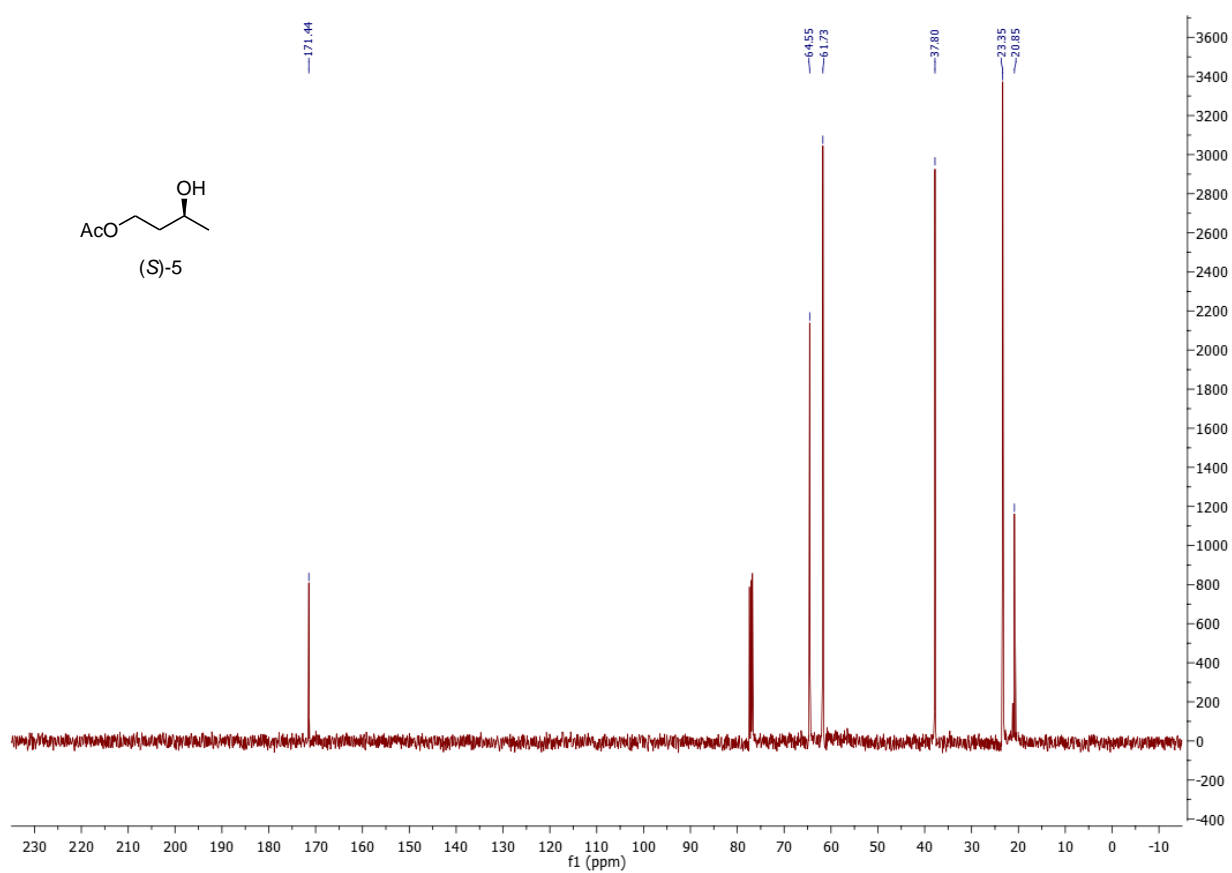
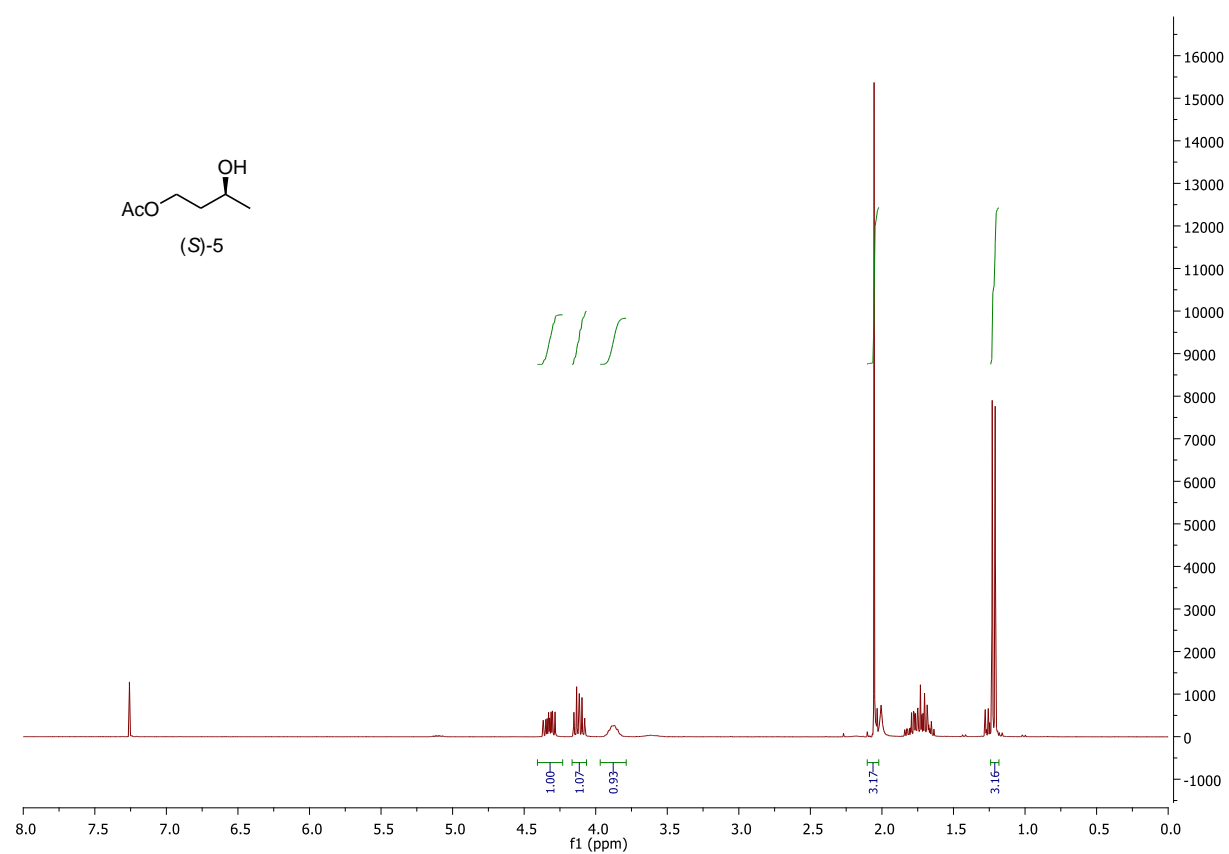
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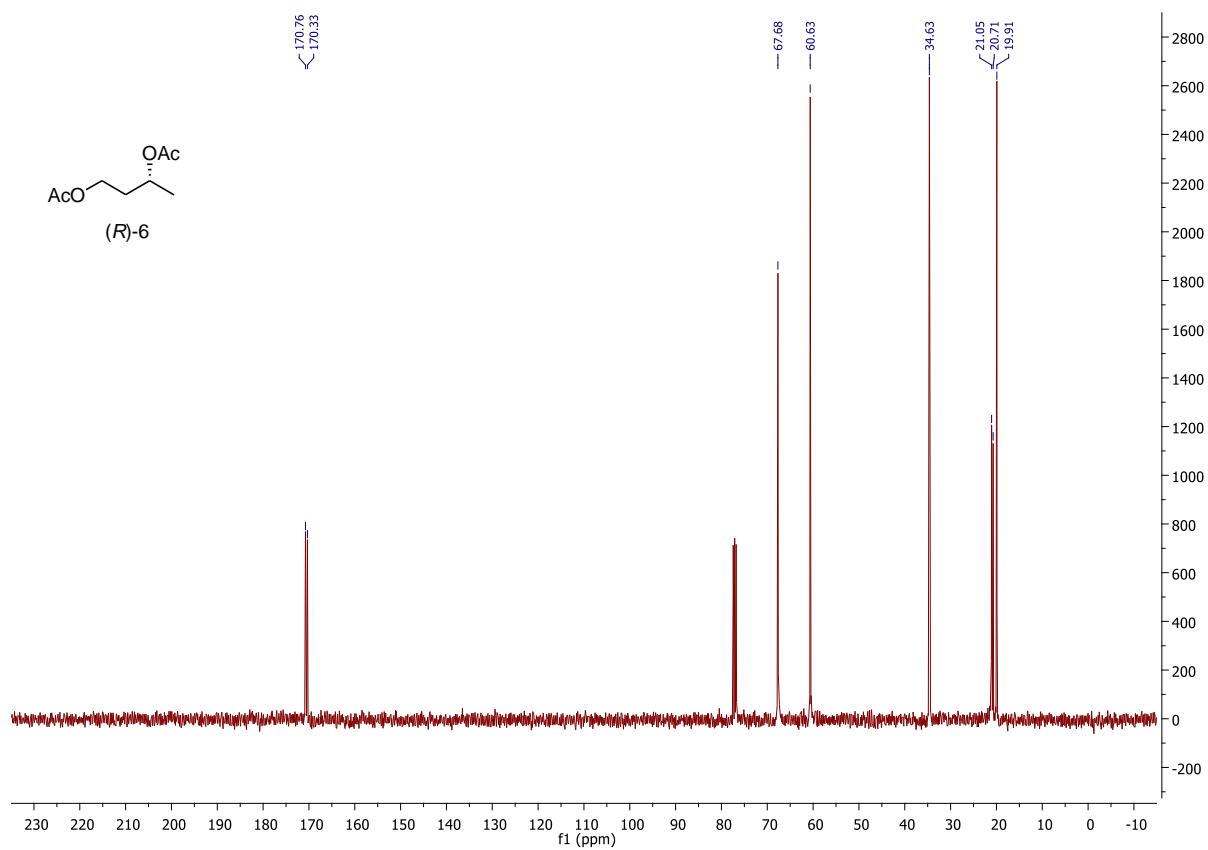
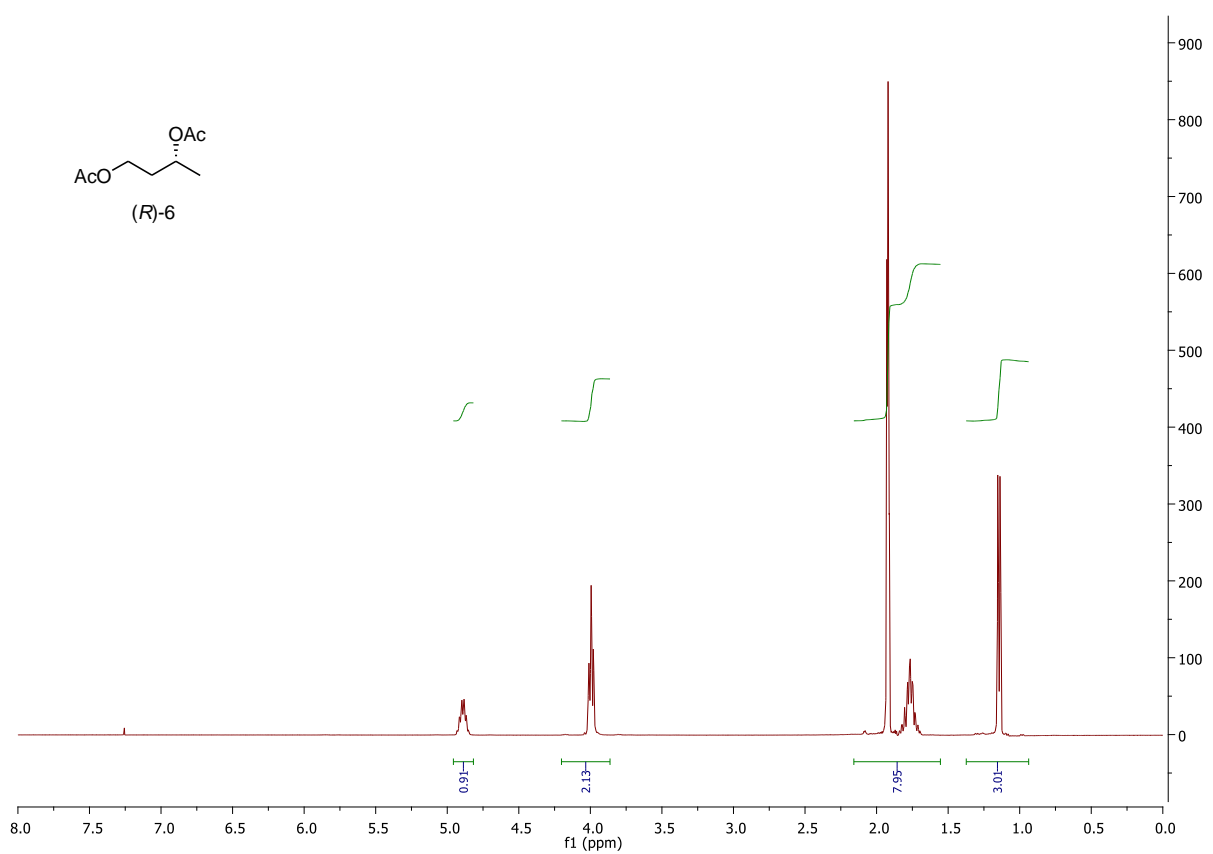
# $^1\text{H}$ - and $^{13}\text{C}$ -NMR spectra of compound **4**



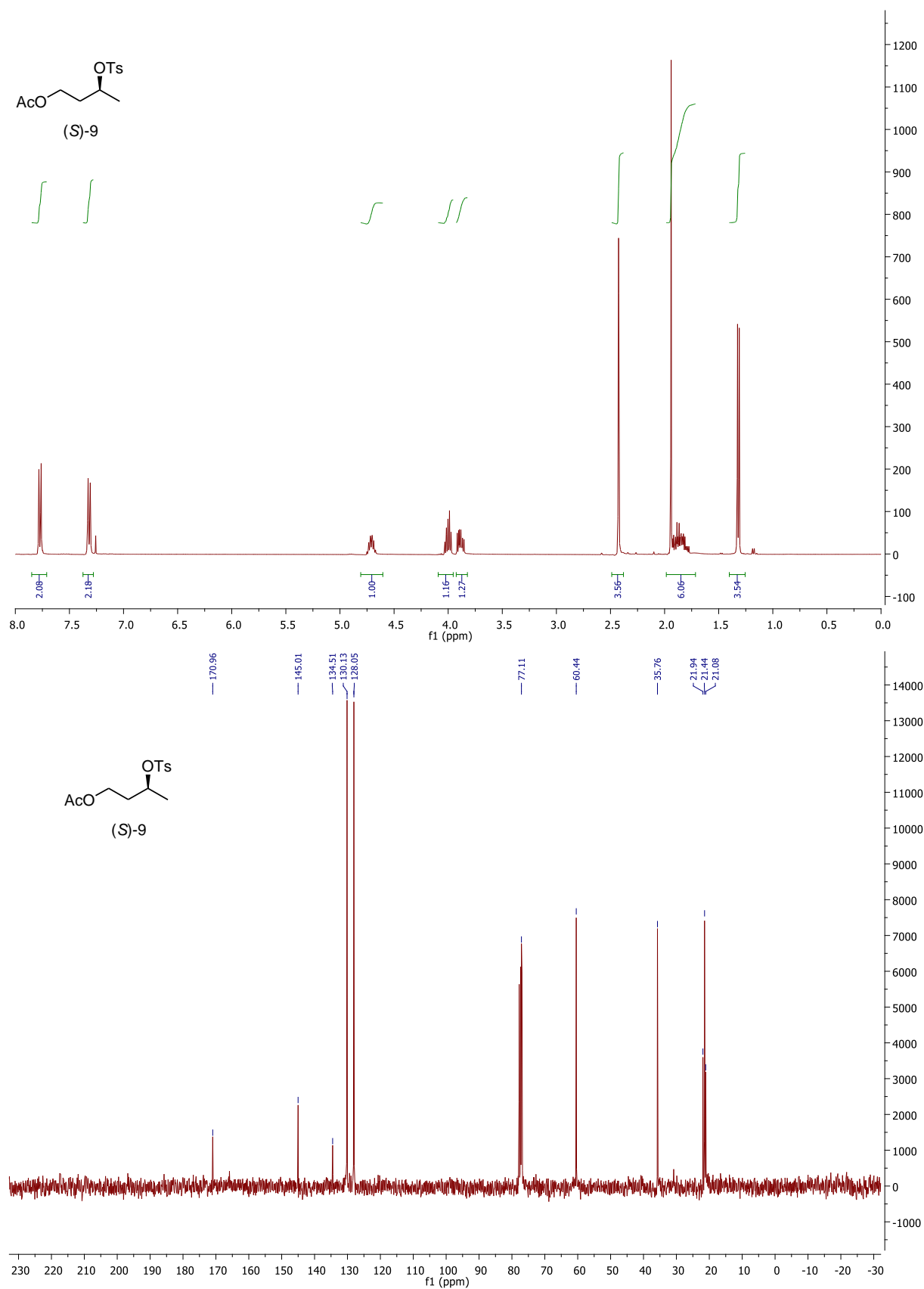
# $^1\text{H}$ - and $^{13}\text{C}$ -NMR spectra of compound 5



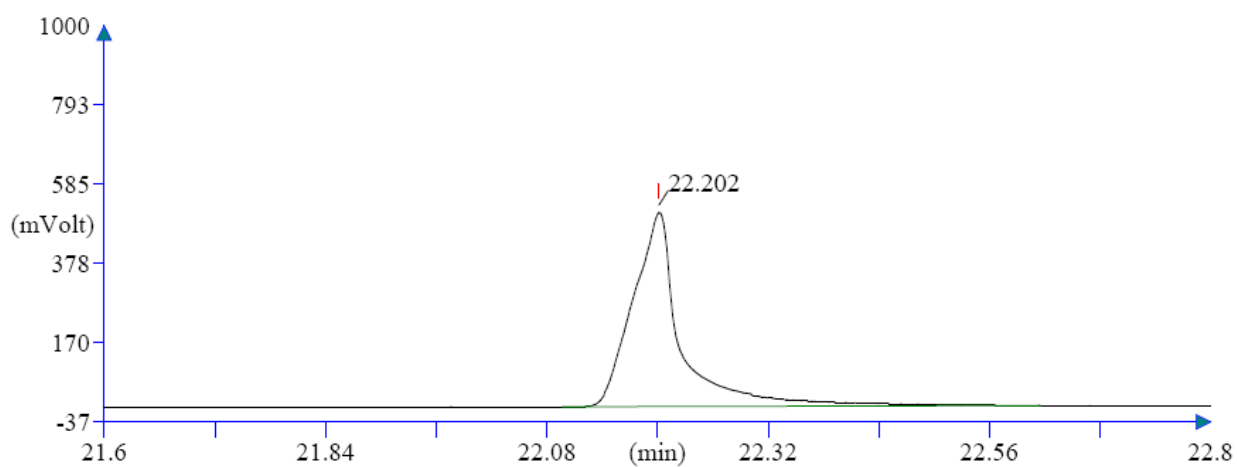
# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 6



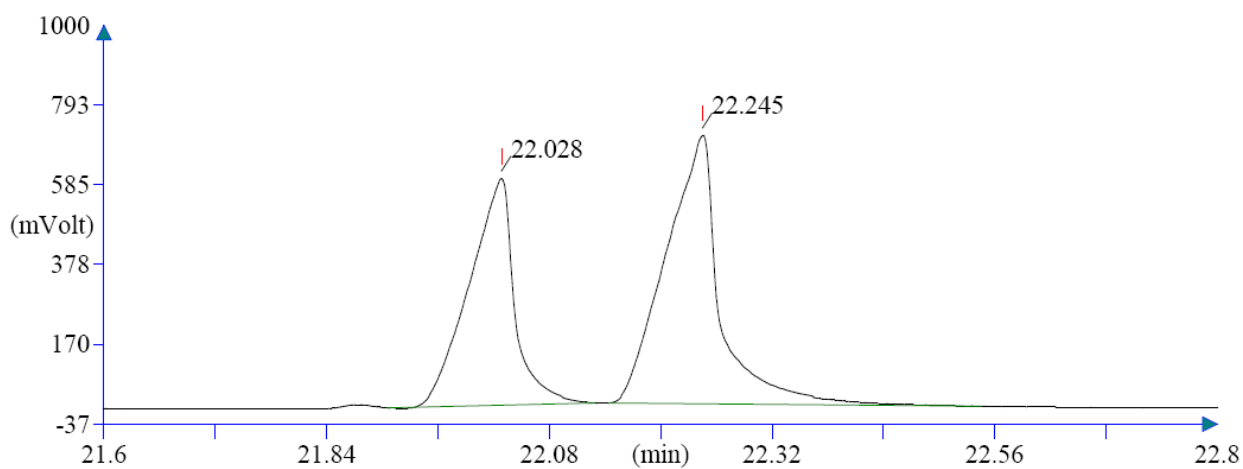
# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound **9**



# Chiral phase GC of (R,R)-**4** and (R,R)/(R,S)-**4** mixture

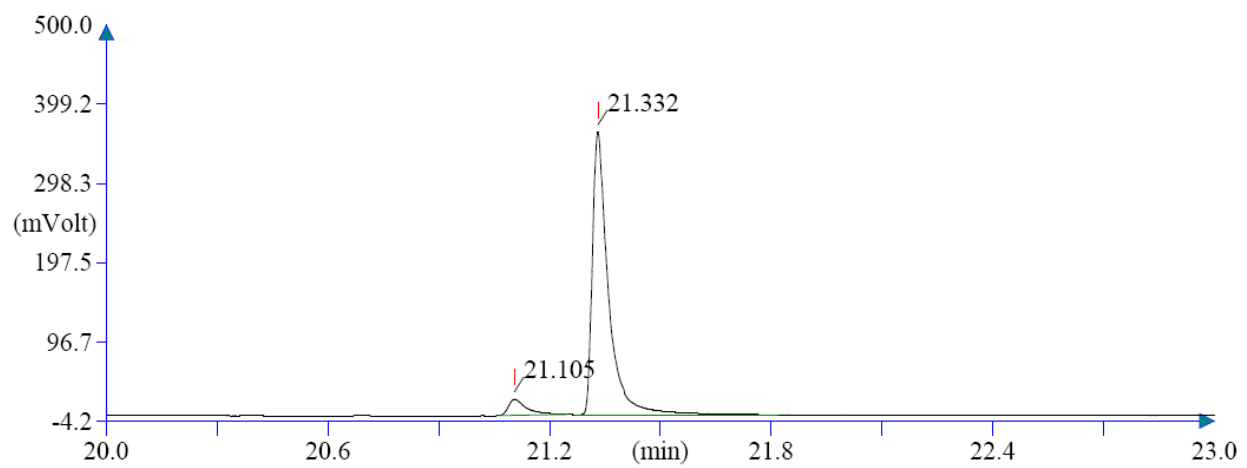


Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Co
22.202	18626870	100.000	100.000	
	18626870		100.000	

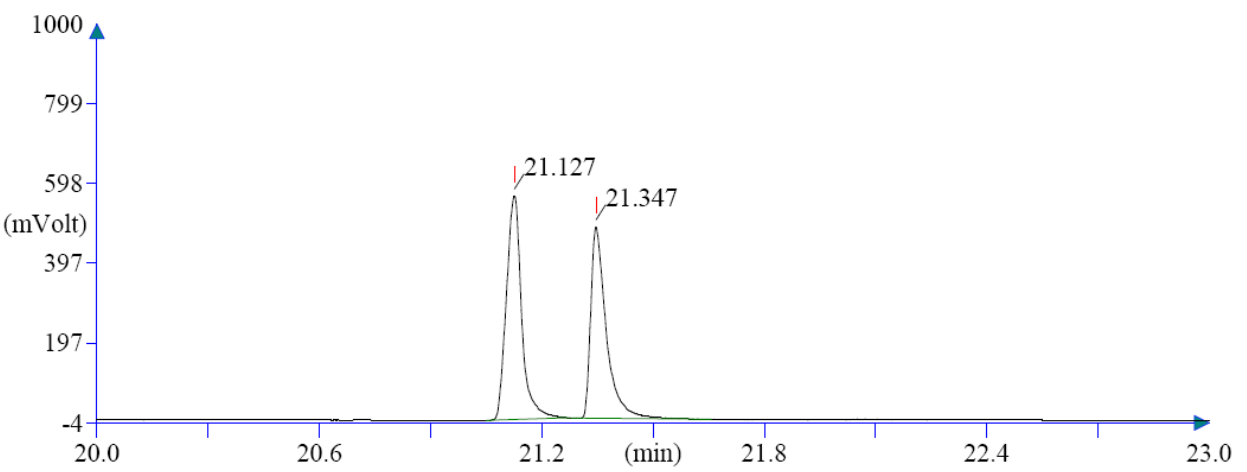


Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Co
22.028	20120600	41.202	41.202	
22.245	28713300	58.798	58.798	
	48833900		100.000	

Chiral phase GC of acetylated (*R*)-2 from (*S*)-2 inversion

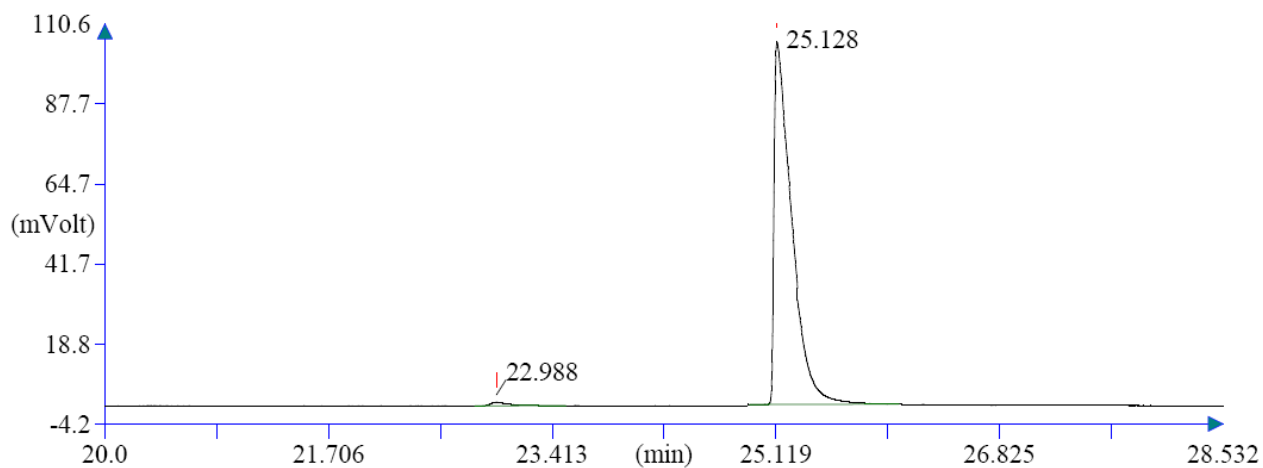


Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Con
21.105	708121	6.096	6.096	
21.332	10908030	93.904	93.904	
	11616150		100.000	

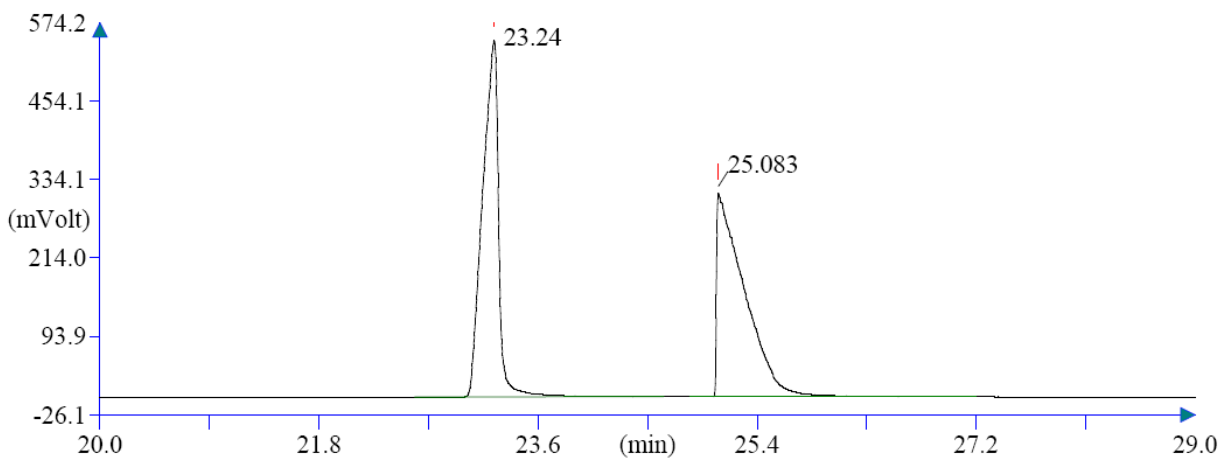


Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Con
21.127	16122260	53.444	53.444	
21.347	14044540	46.556	46.556	
	30166800		100.000	

Chiral phase GC of acetylated (*R*)-3 from kinetic resolution rac-3



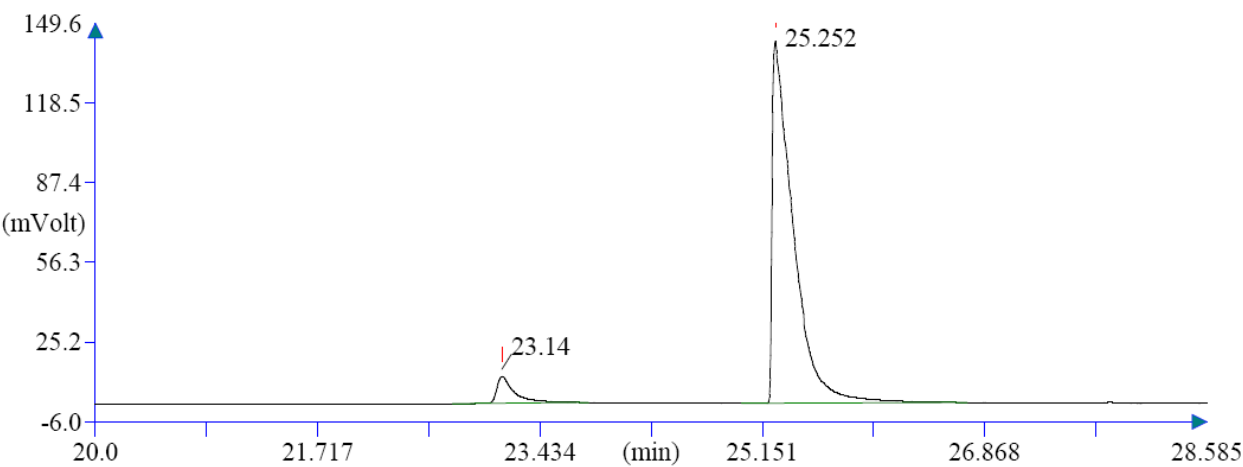
Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Cor
22.988	108327	1.103	1.103	
25.128	9713536	98.897	98.897	
	9821863		100.000	



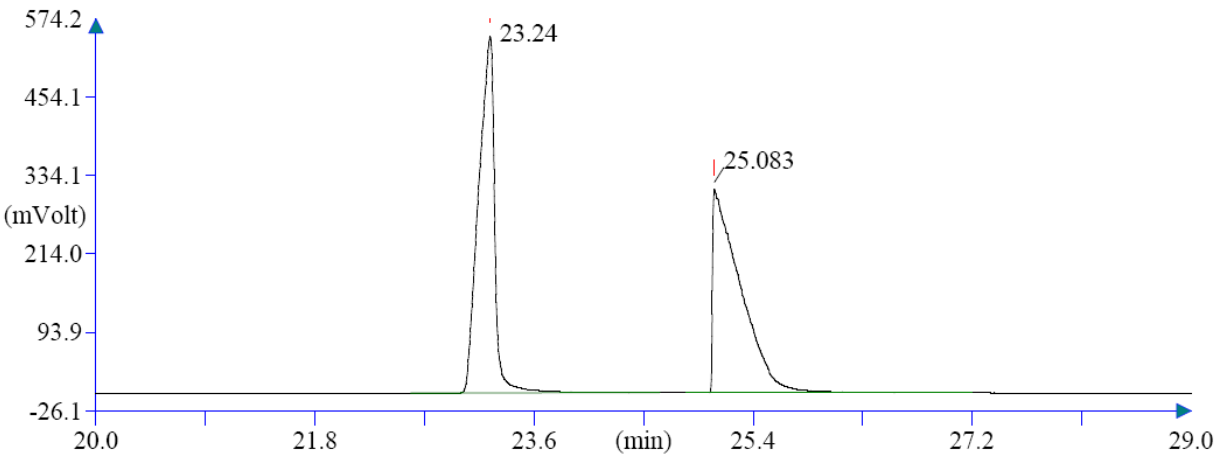
Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Con
23.240	50110000	50.339	50.339	
25.083	49436020	49.661	49.661	
	99546020		100.000	



Chiral phase GC of (R)-6 from inversion of (S)-5



Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Con
23.140	1013249	5.989	5.989	
25.252	15906180	94.011	94.011	
	16919430		100.000	



Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Con
23.240	50110000	50.339	50.339	
25.083	49436020	49.661	49.661	
	99546020		100.000	