Catalysis

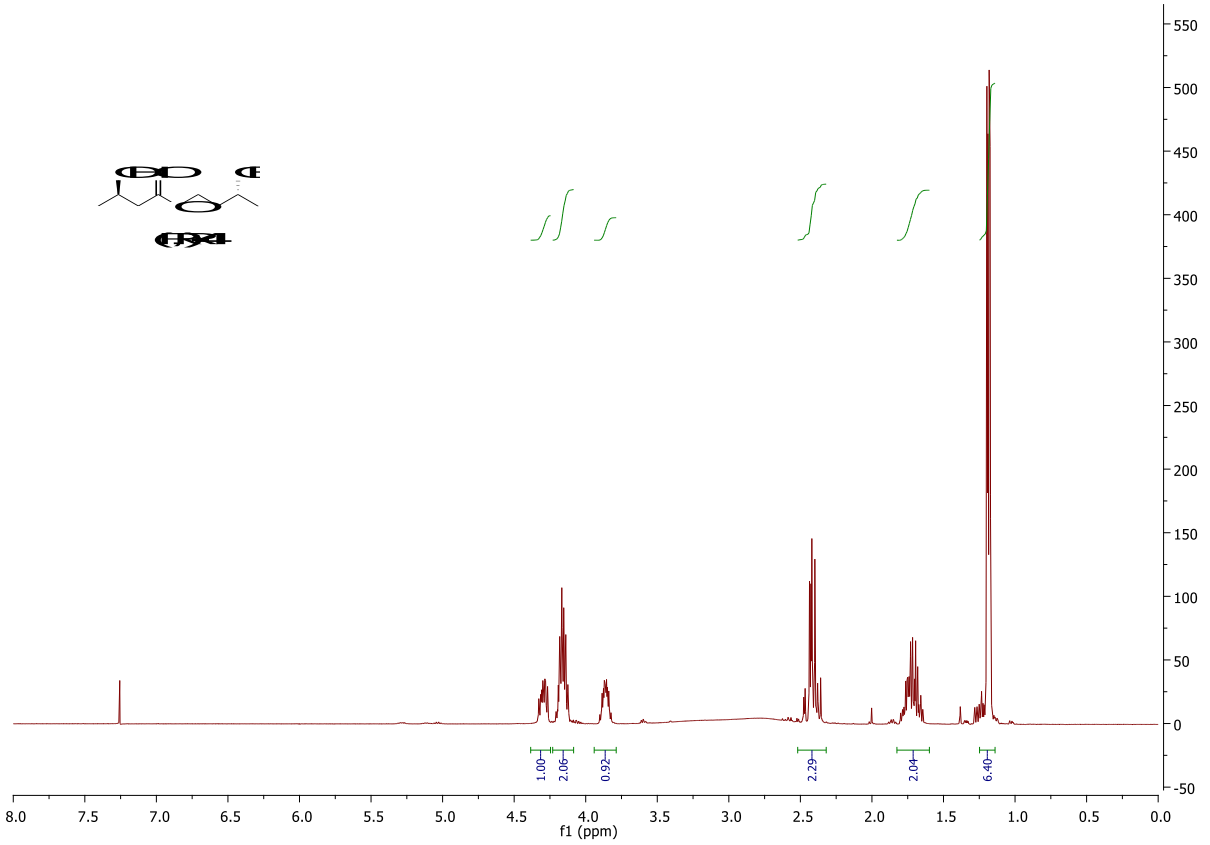
An Alternative Enzymatic Route to the Ergogenic Ketone Body Ester (R)-3-Hydroxybutyl (R)-3-Hydroxybutyrate

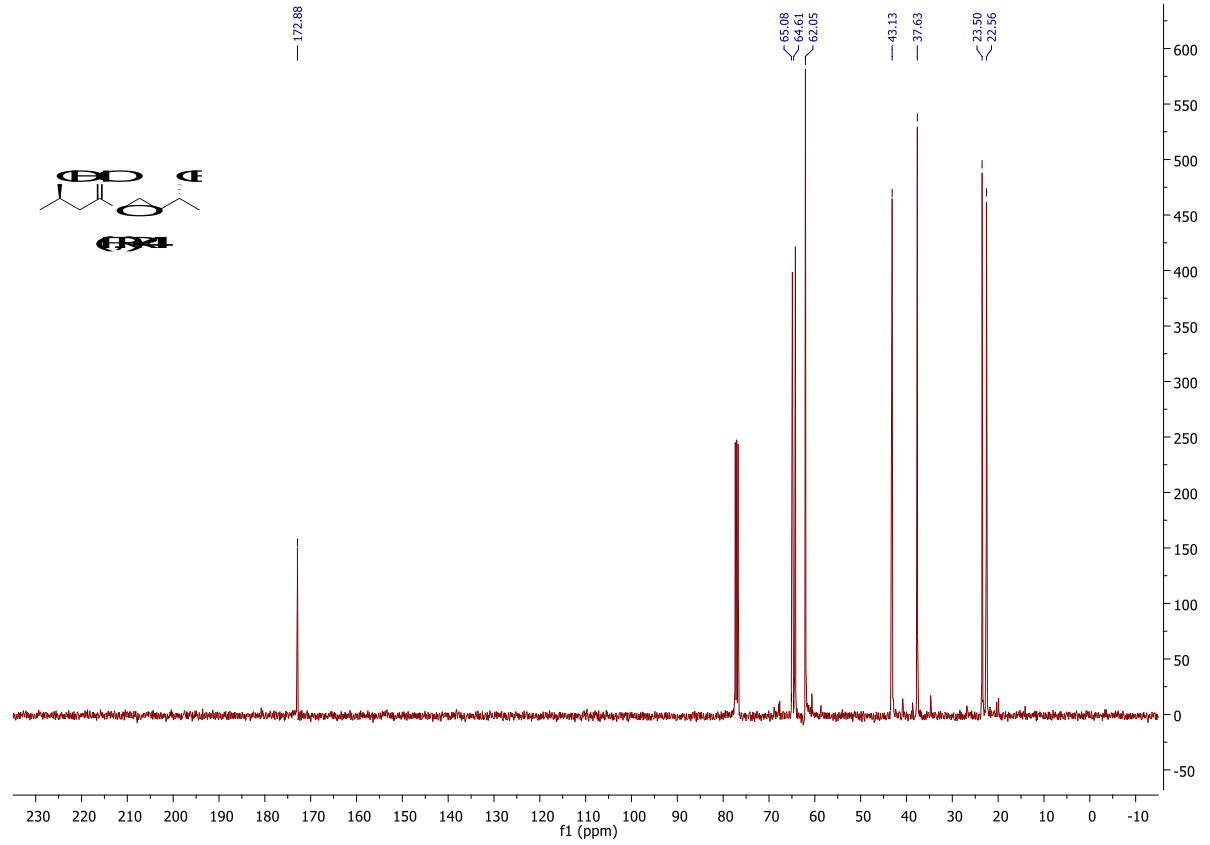
Ferdinando Zaccone 1, Valentina Venturi 1, Pier Paolo Giovannini 1,*, Claudio Trapella1,..

Supplementary Materials

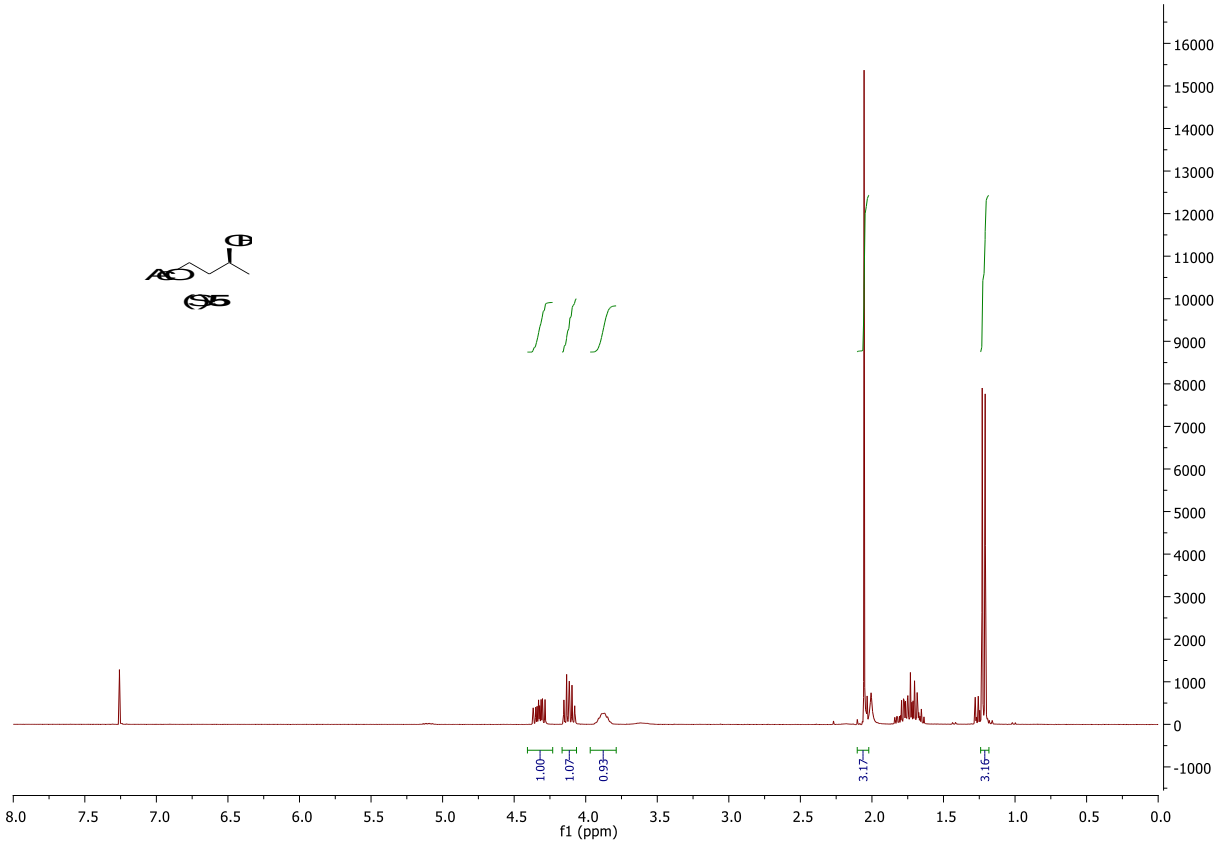
Contents

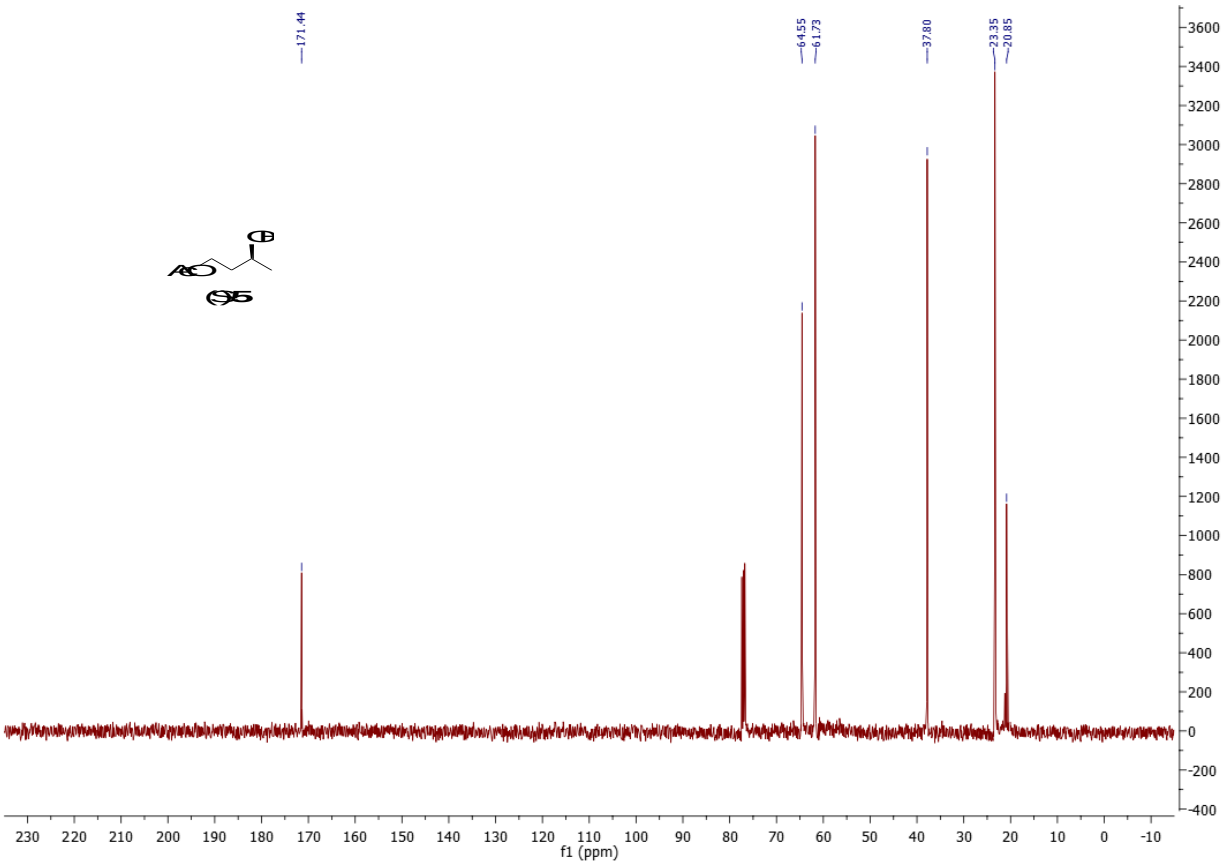
^{1}H- and ^{13}C-NMR spectra of compound **4**



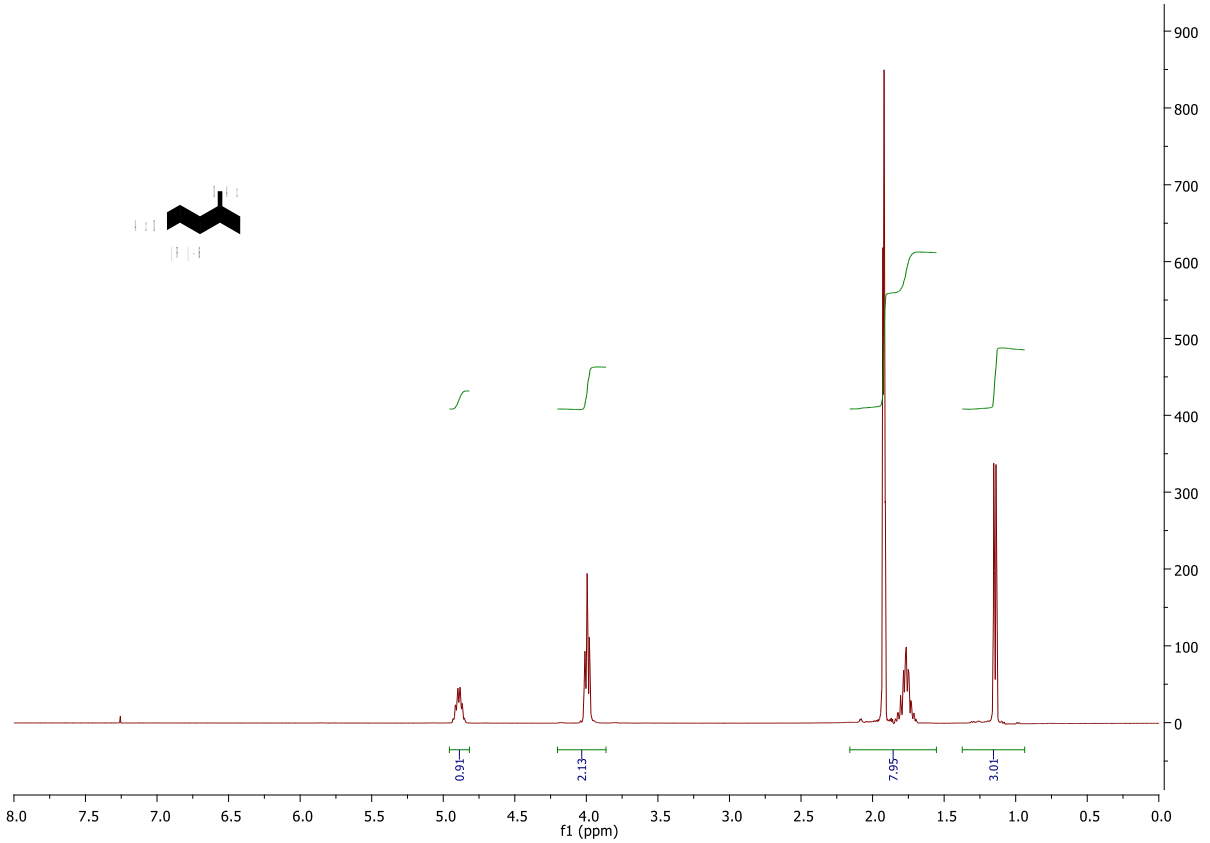


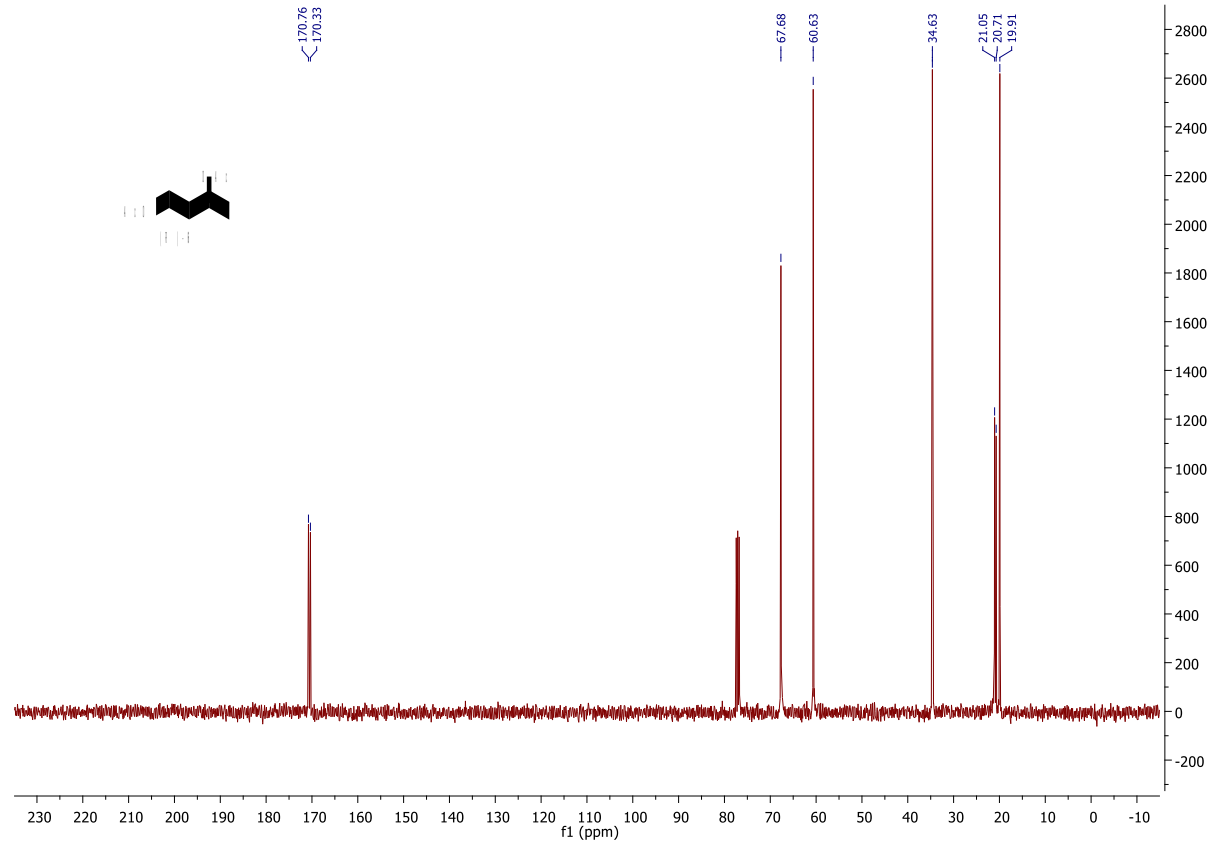
^{1}H- and ^{13}C-NMR spectra of compound **5**



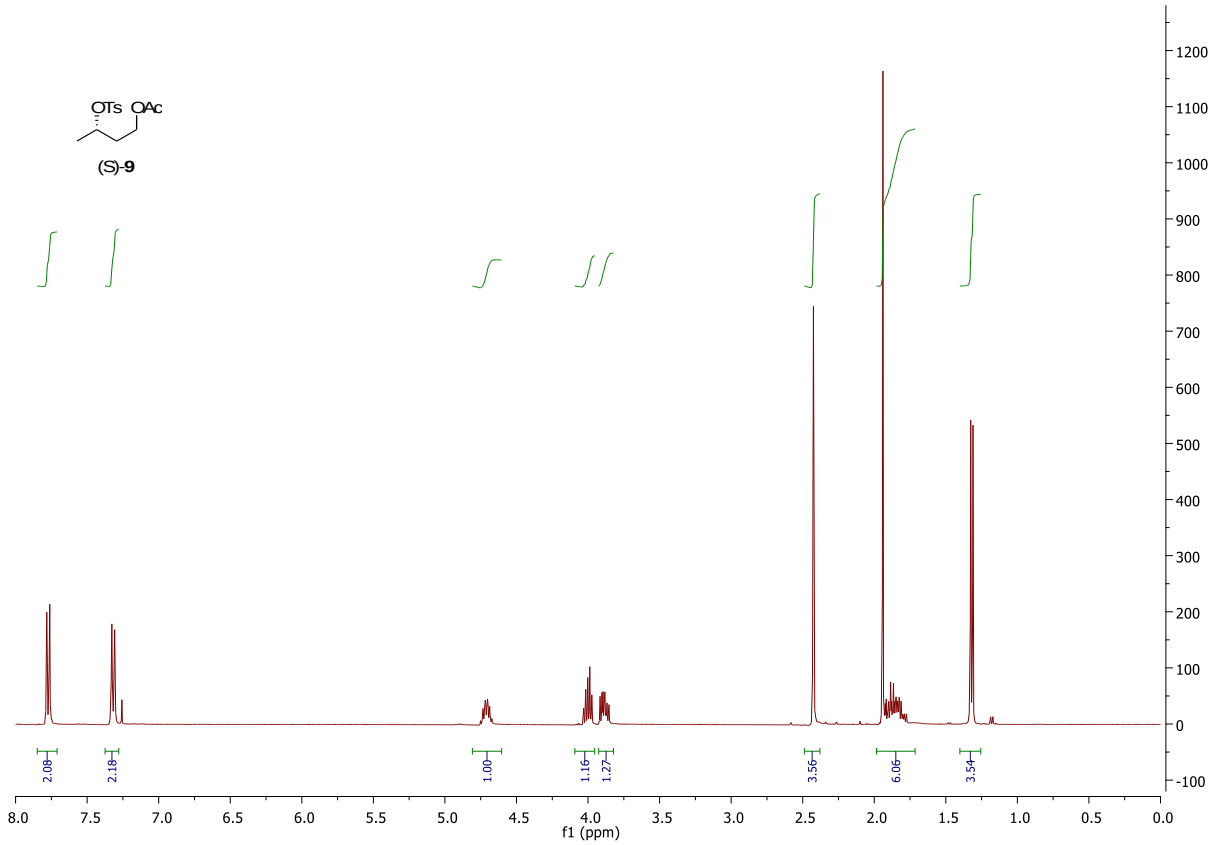


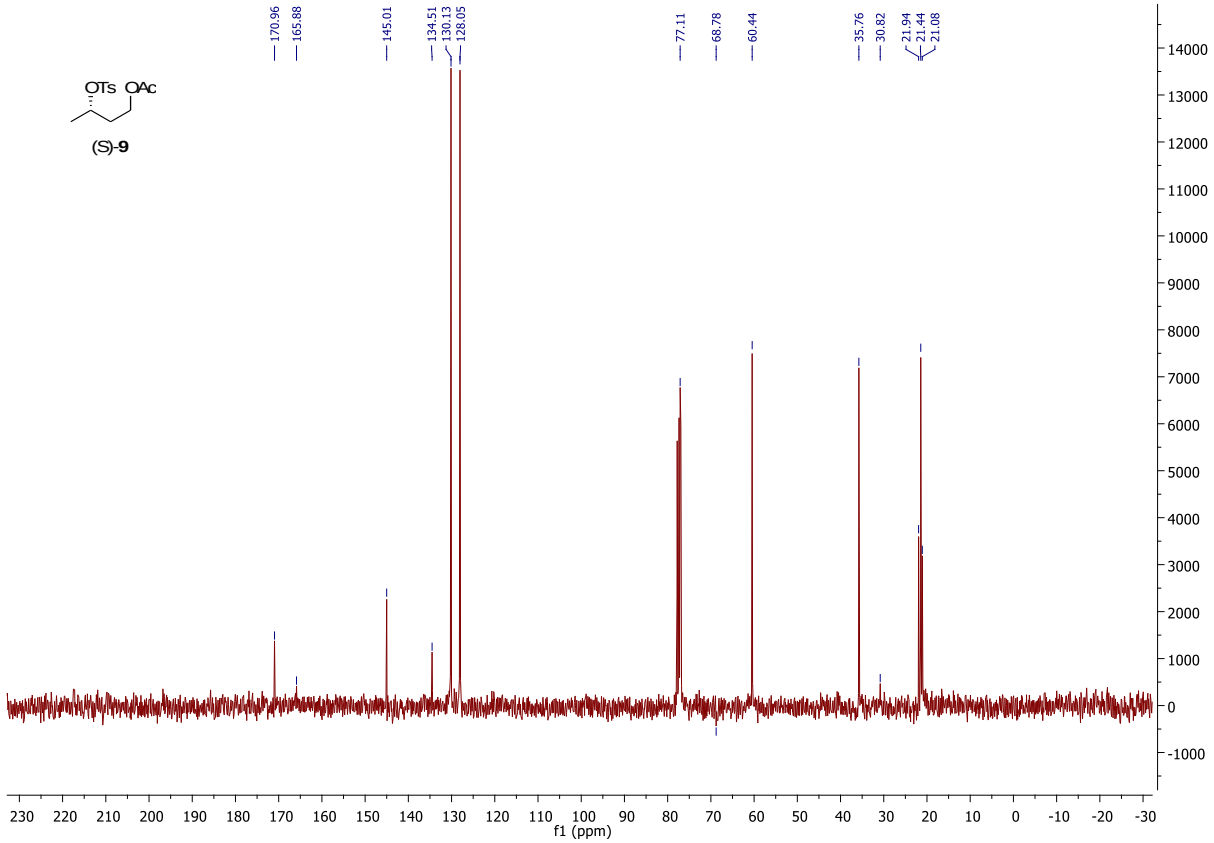
^{1}H- and ^{13}C-NMR spectra of compound **6**



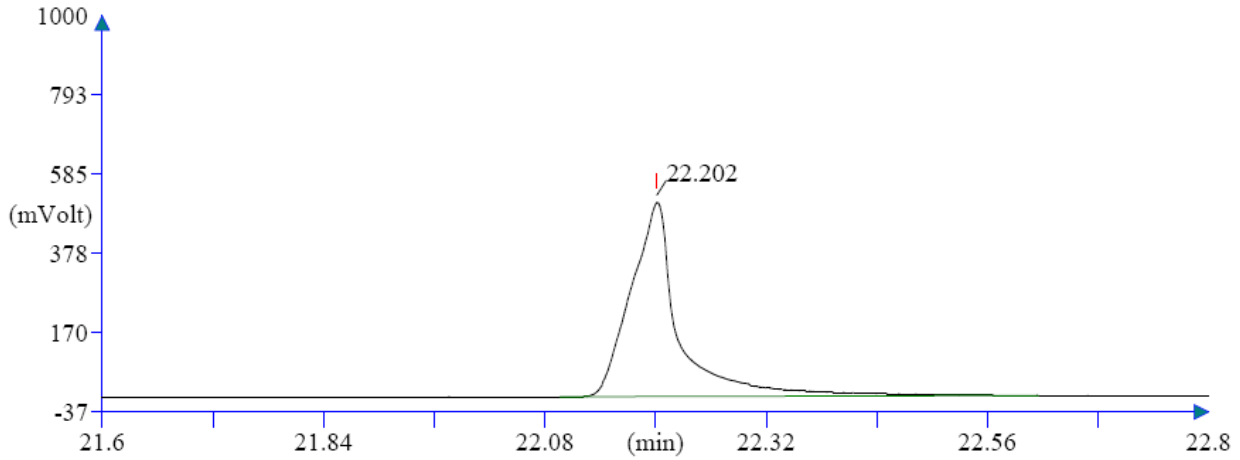


^{1}H- and ^{13}C-NMR spectra of compound **9**

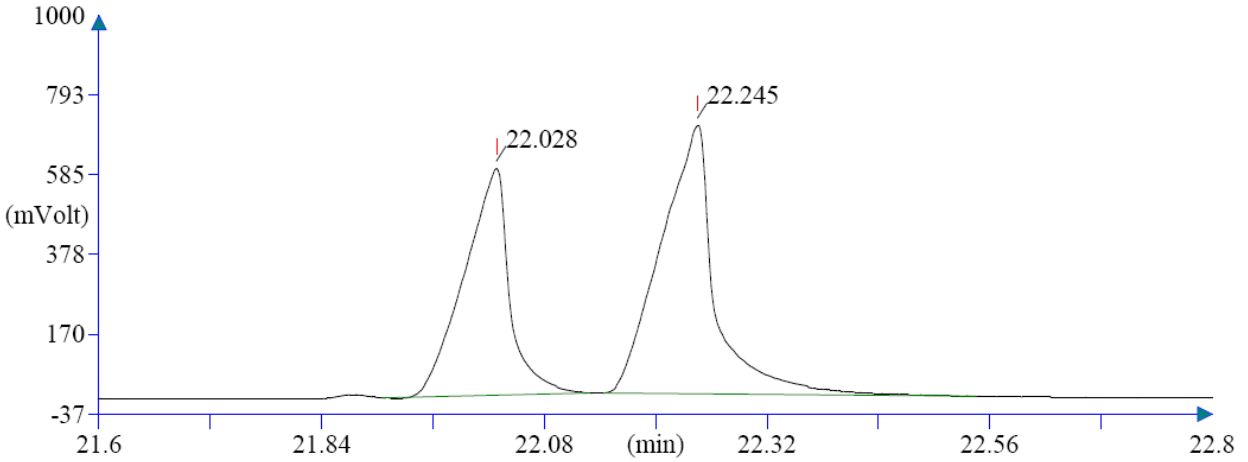




Chiral phase GC of (R,R)-**4 and** (R,R)/(R,S)-**4** mixture

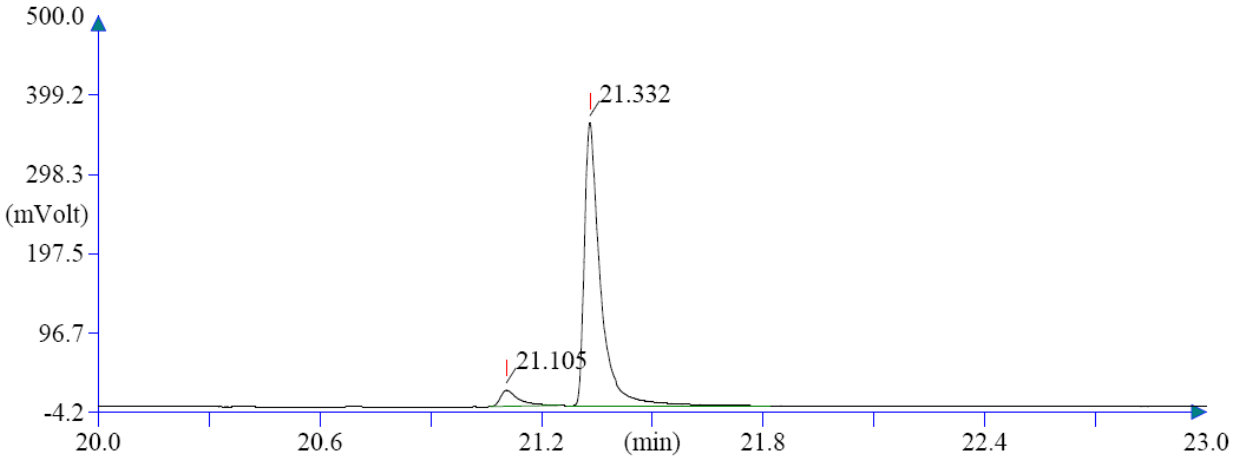


Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Co
22.202	18626870	100.000	100.000	
	18626870		100.000	

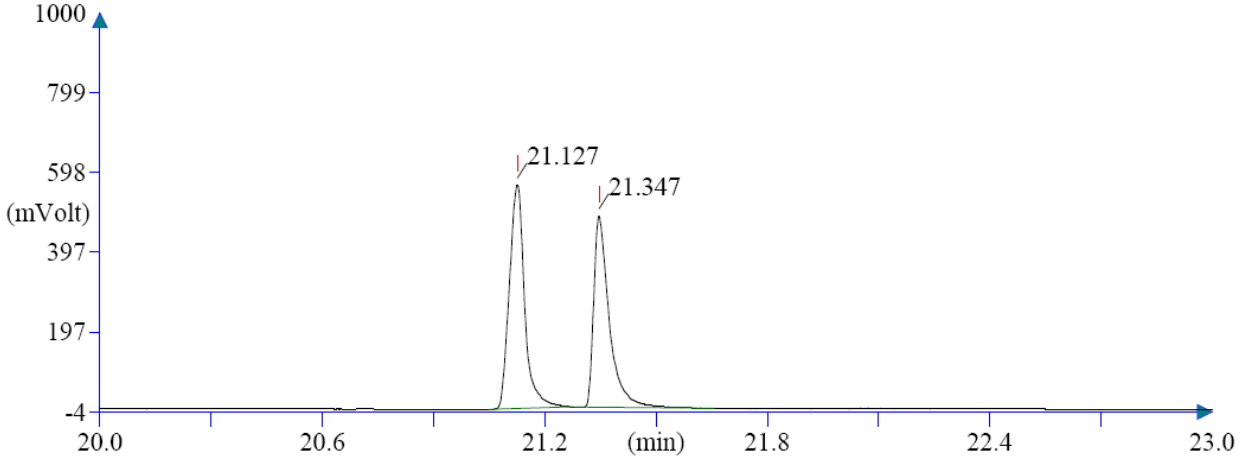


Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Co
22.028	20120600	41.202	41.202	
22.245	28713300	58.798	58.798	
	48833900		100.000	

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

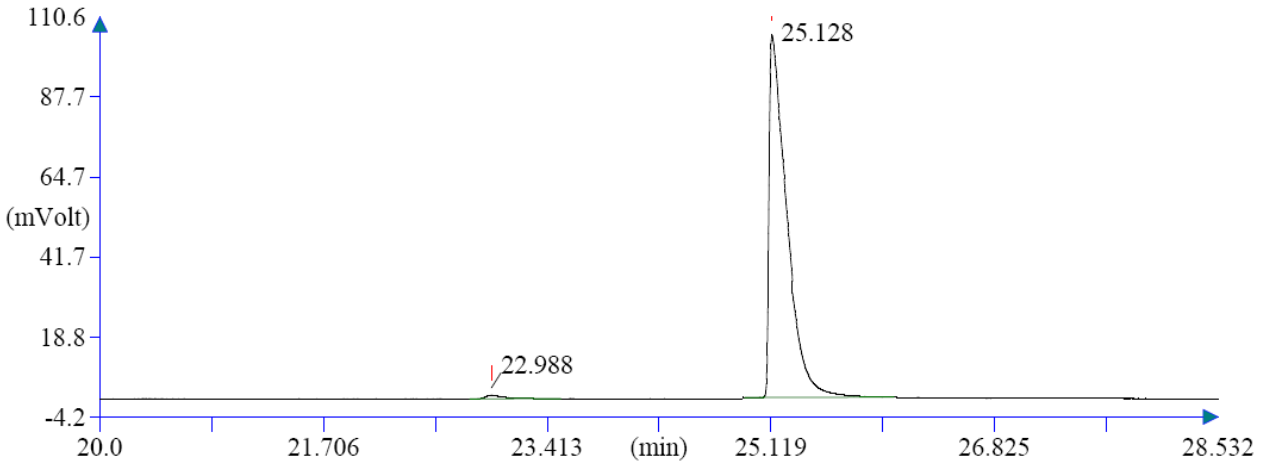


Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Con
21.105	708121	6.096	6.096	
21.332	10908030	93.904	93.904	
	11616150		100.000	

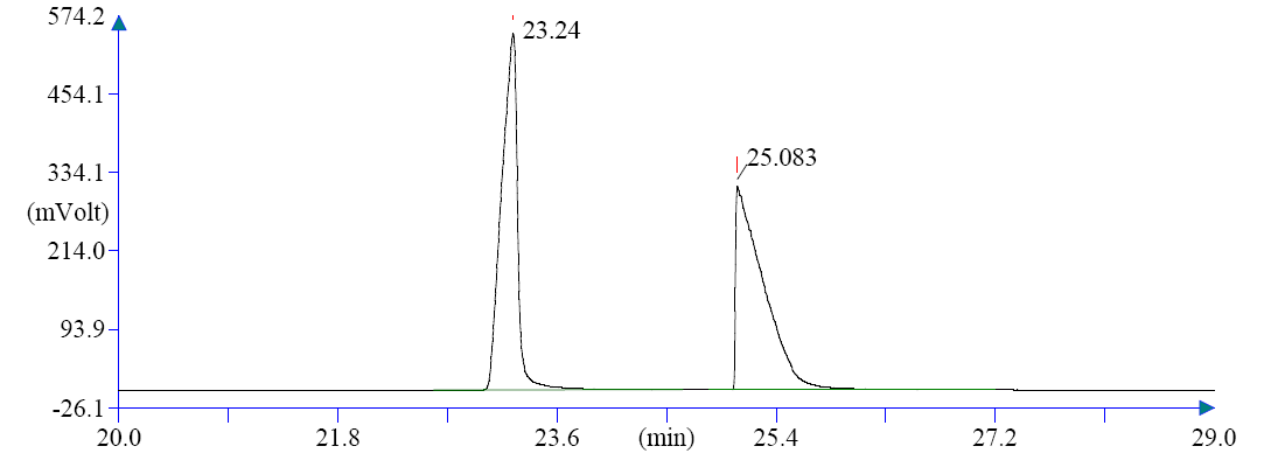


Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Con
21.127	16122260	53.444	53.444	
21.347	14044540	46.556	46.556	
	30166800		100.000	

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

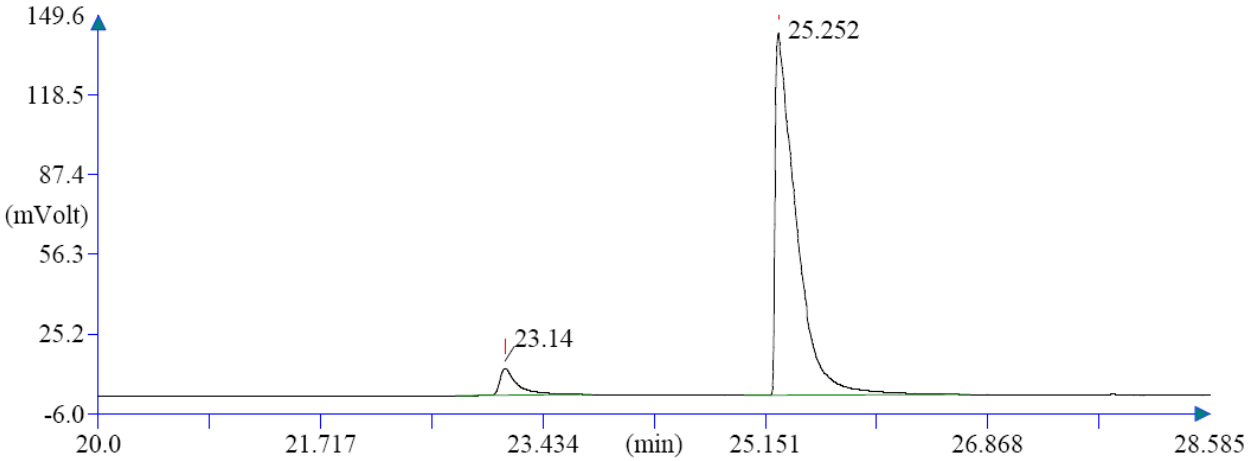


Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Cor
22.988	108327	1.103	1.103	
25.128	9713536	98.897	98.897	
	9821863		100.000	

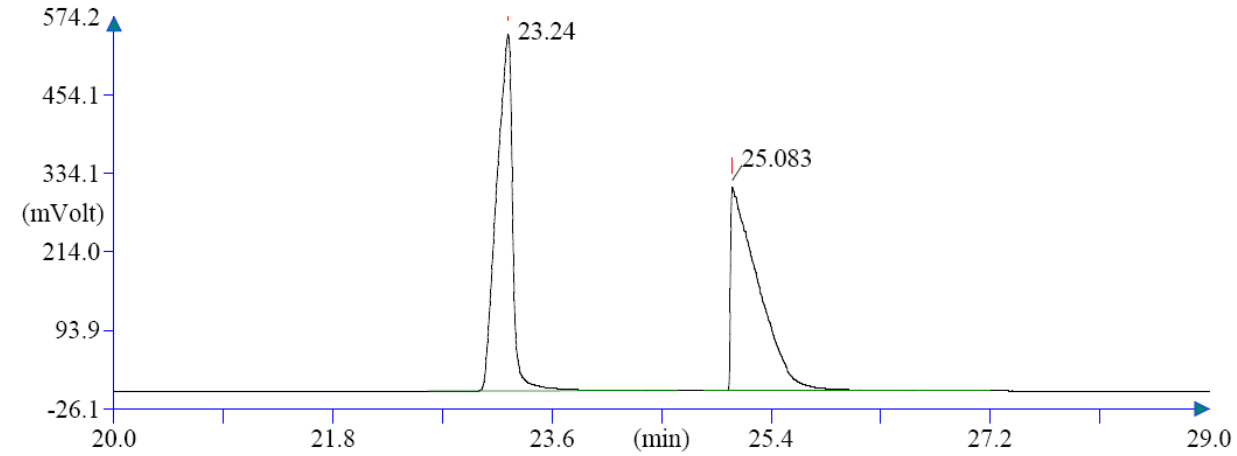


Retention Time (min)	Area (.1*uV*sec)	Area % (%)	Original Conc	Con
23.240	50110000	50.339	50.339	
25.083	49436020	49.661	49.661	
	99546020		100.000	

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	