

Structure Elucidation of Hypocreolide A by Enantioselective Total Synthesis

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Hamburg, Germany

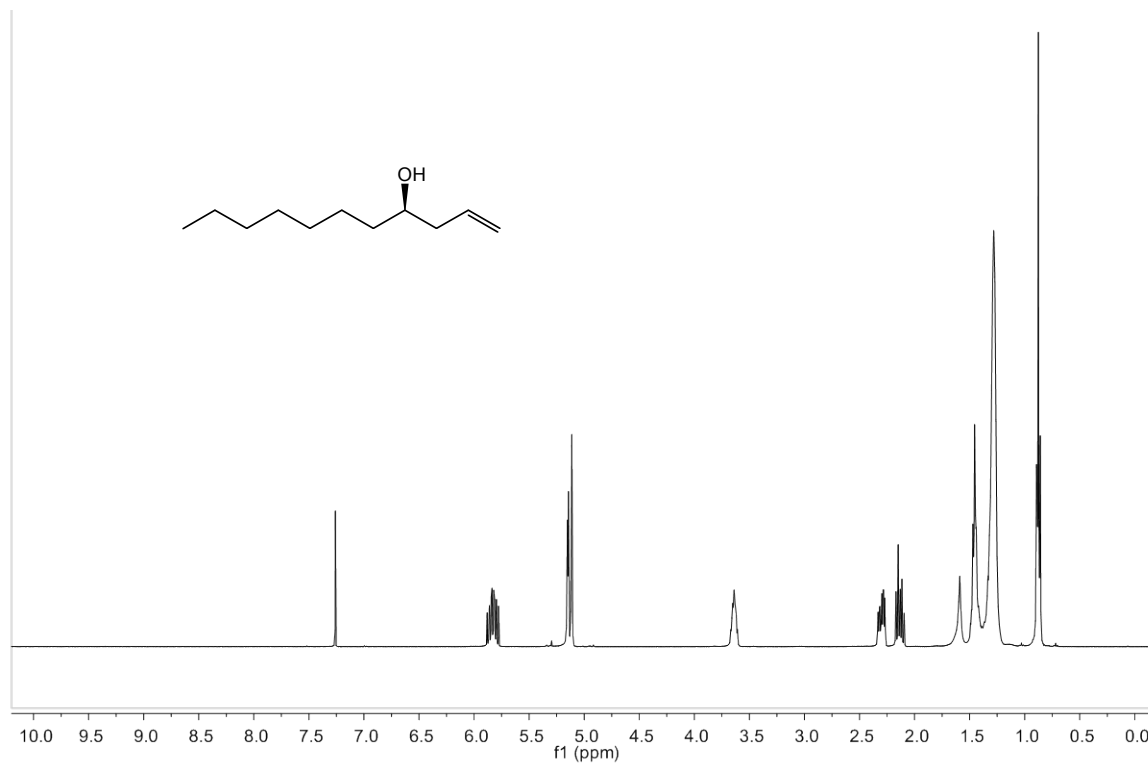
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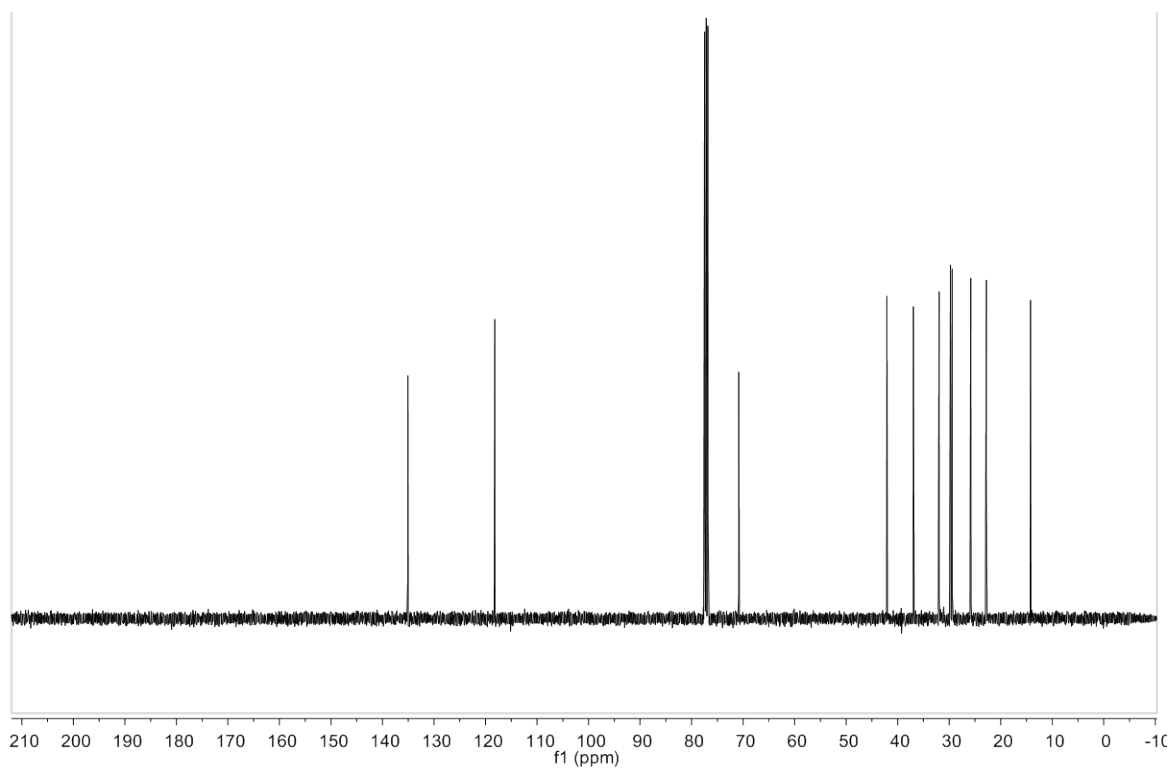
Electronic Supplementary Information

NMR spectra.....	S2
Gas Chromatography	S17

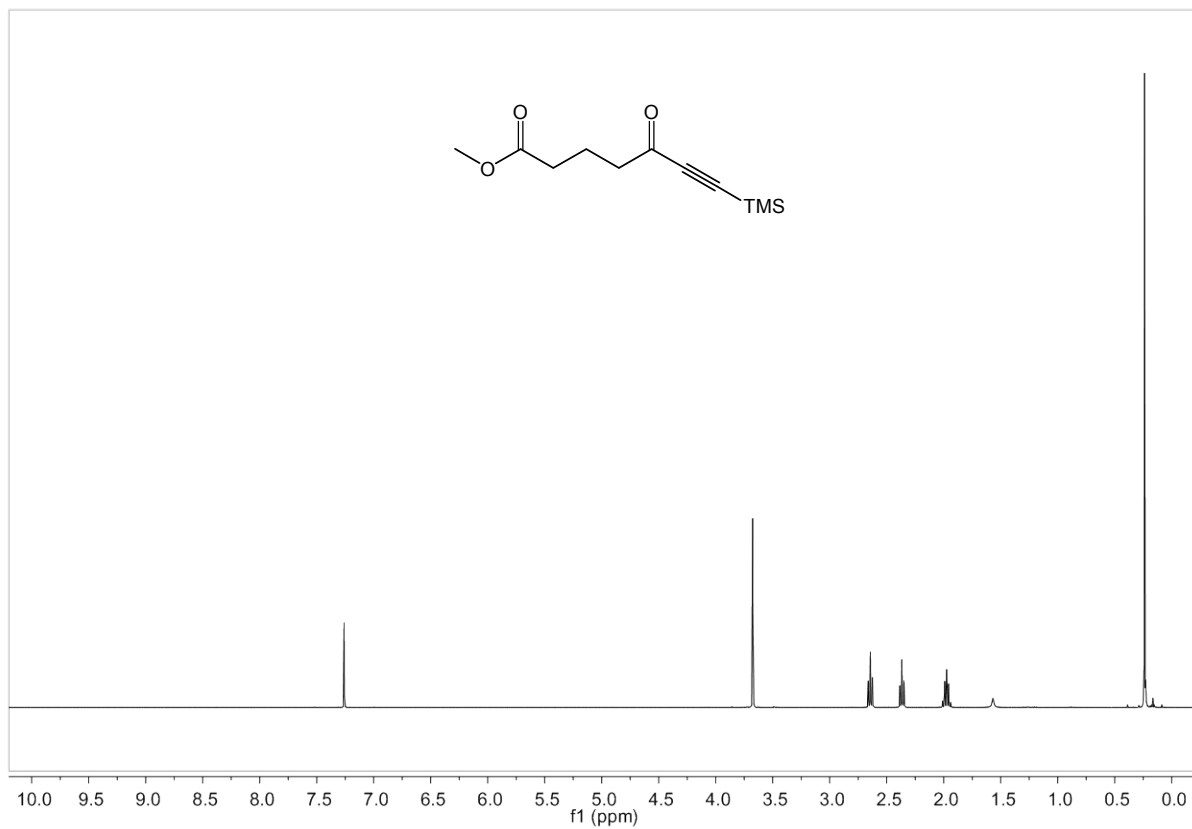
NMR spectra



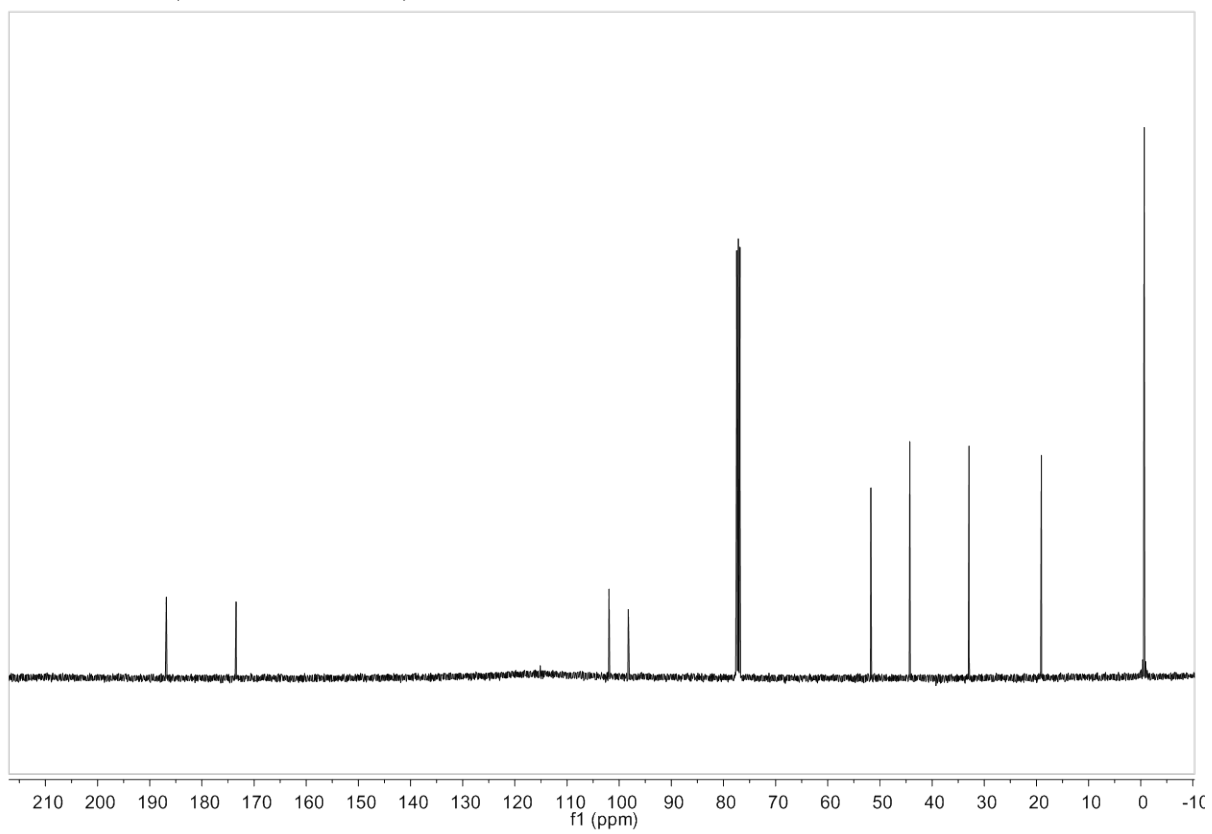
10: ¹H NMR (400 MHz, CDCl₃)



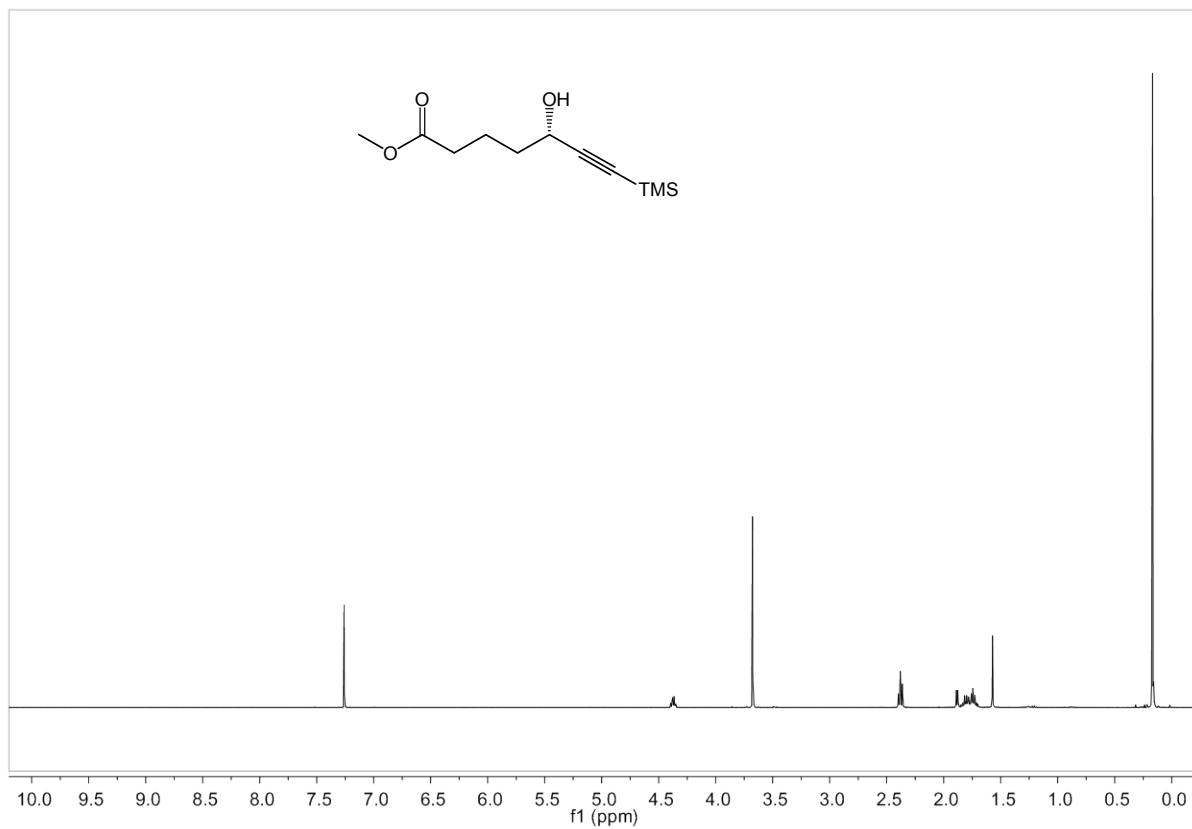
10: ¹³C NMR (101 MHz, CDCl₃)



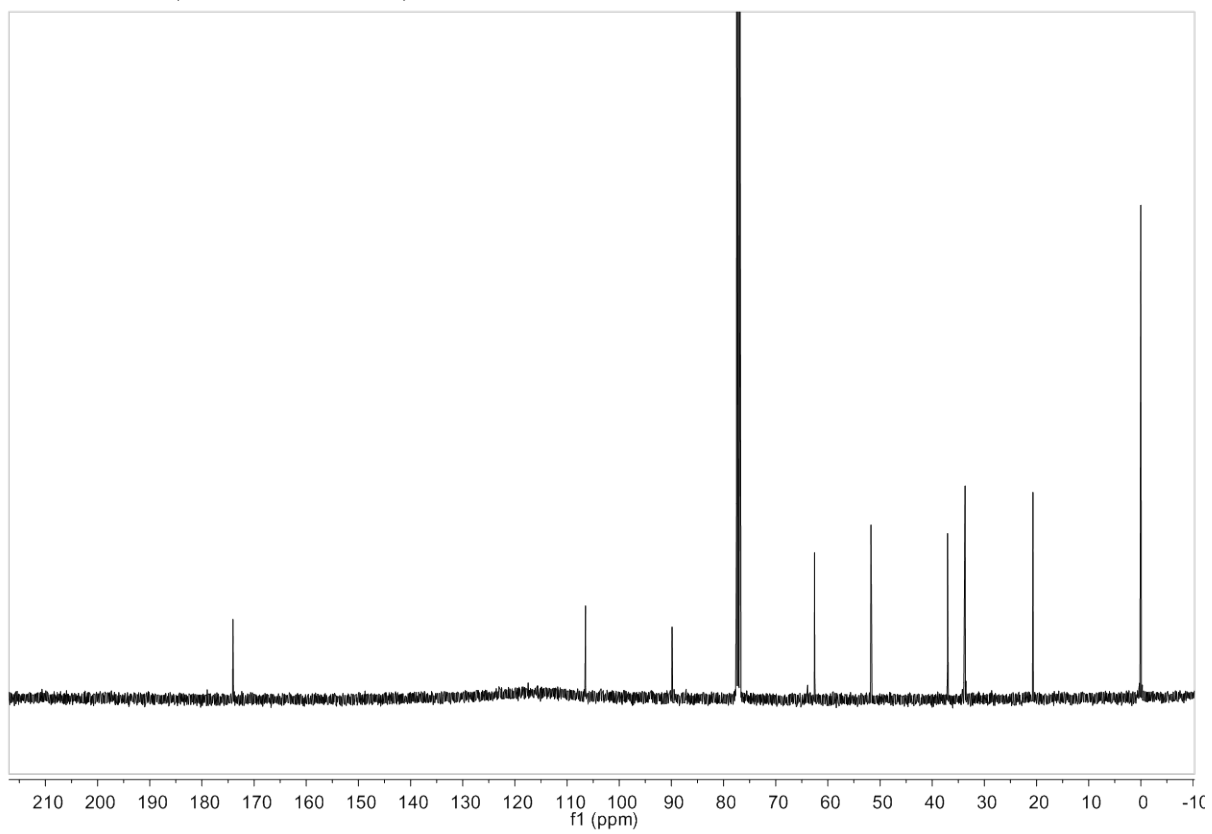
12: ¹H NMR (400 MHz, CDCl₃)



12: ¹³C NMR (101 MHz, CDCl₃)

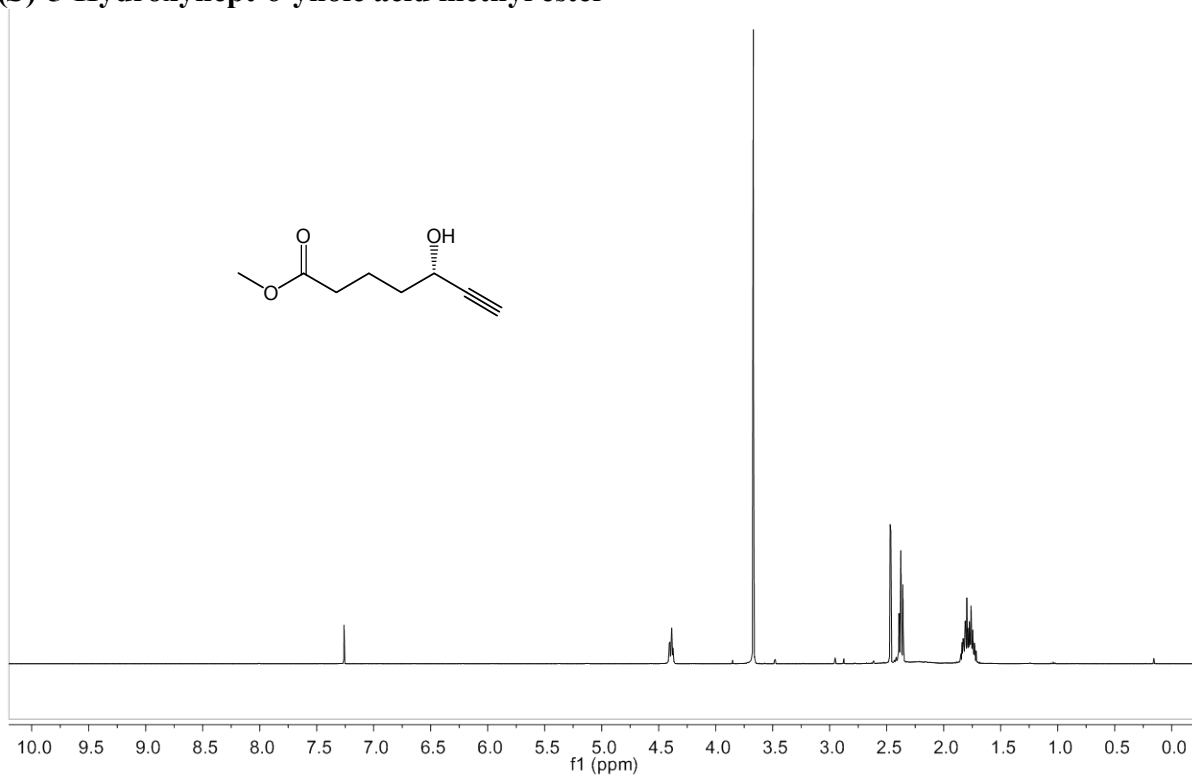


13: ¹H NMR (400 MHz, CDCl₃)

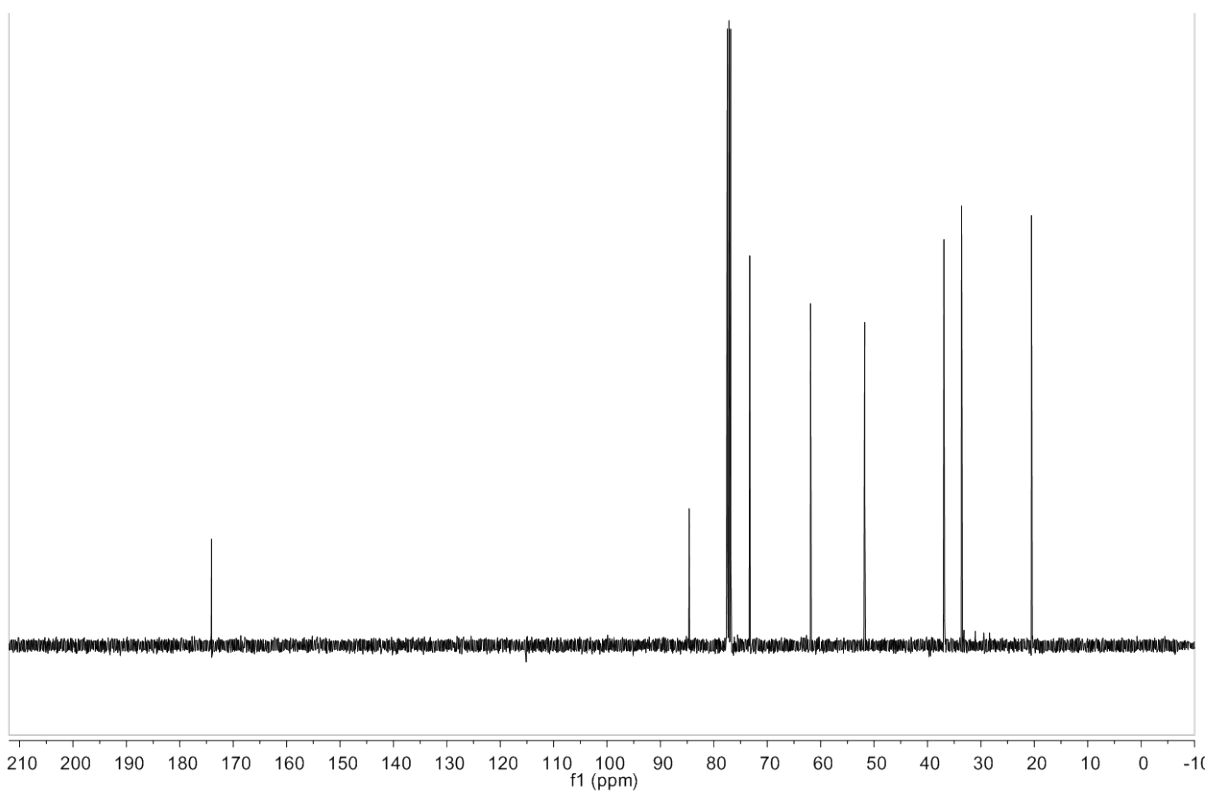


13: ¹³C NMR (101 MHz, CDCl₃)

(S)-5-Hydroxyhept-6-ynoic acid methyl ester

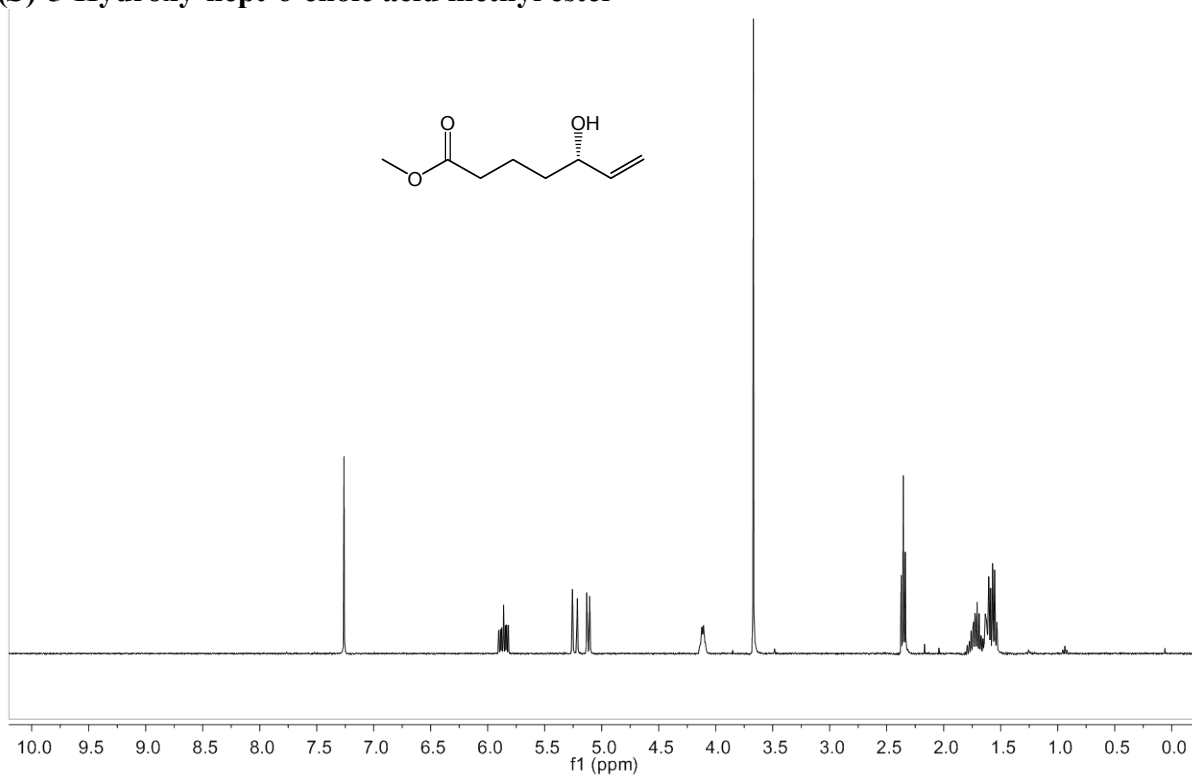


^1H NMR (400 MHz, CDCl_3)

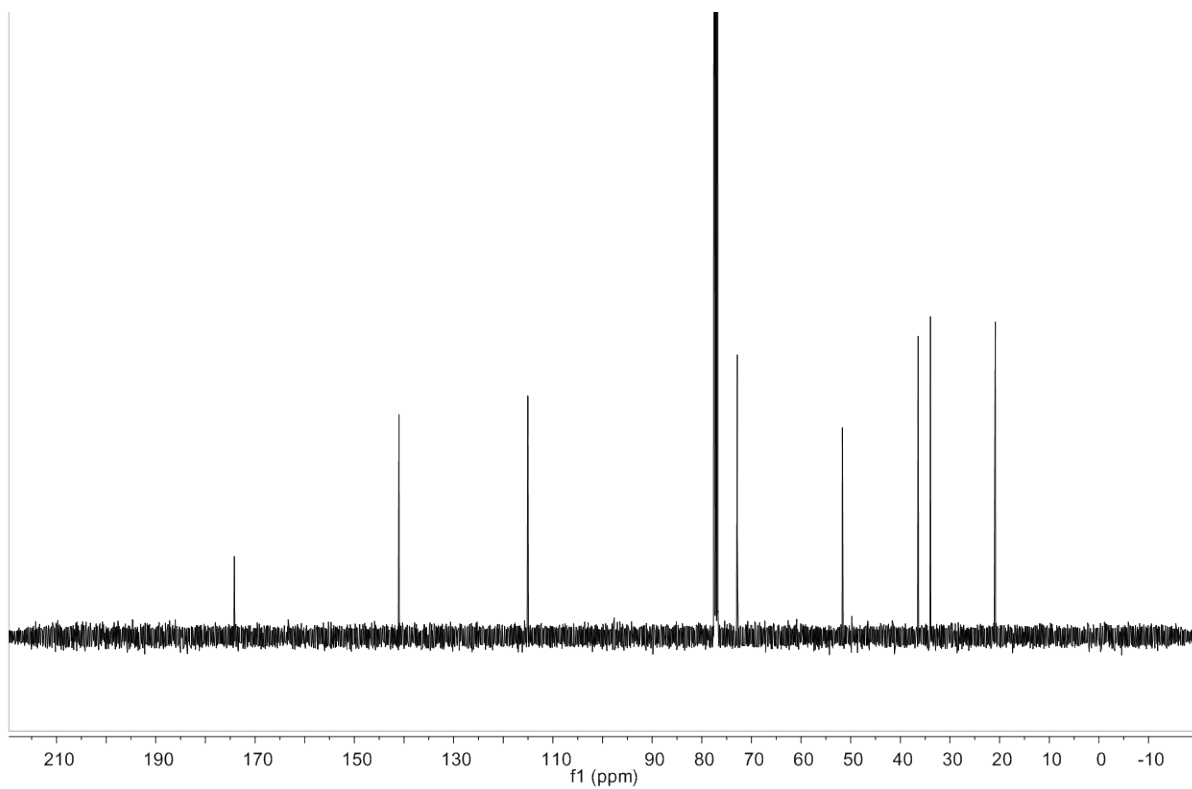


^{13}C NMR (101 MHz, CDCl_3)

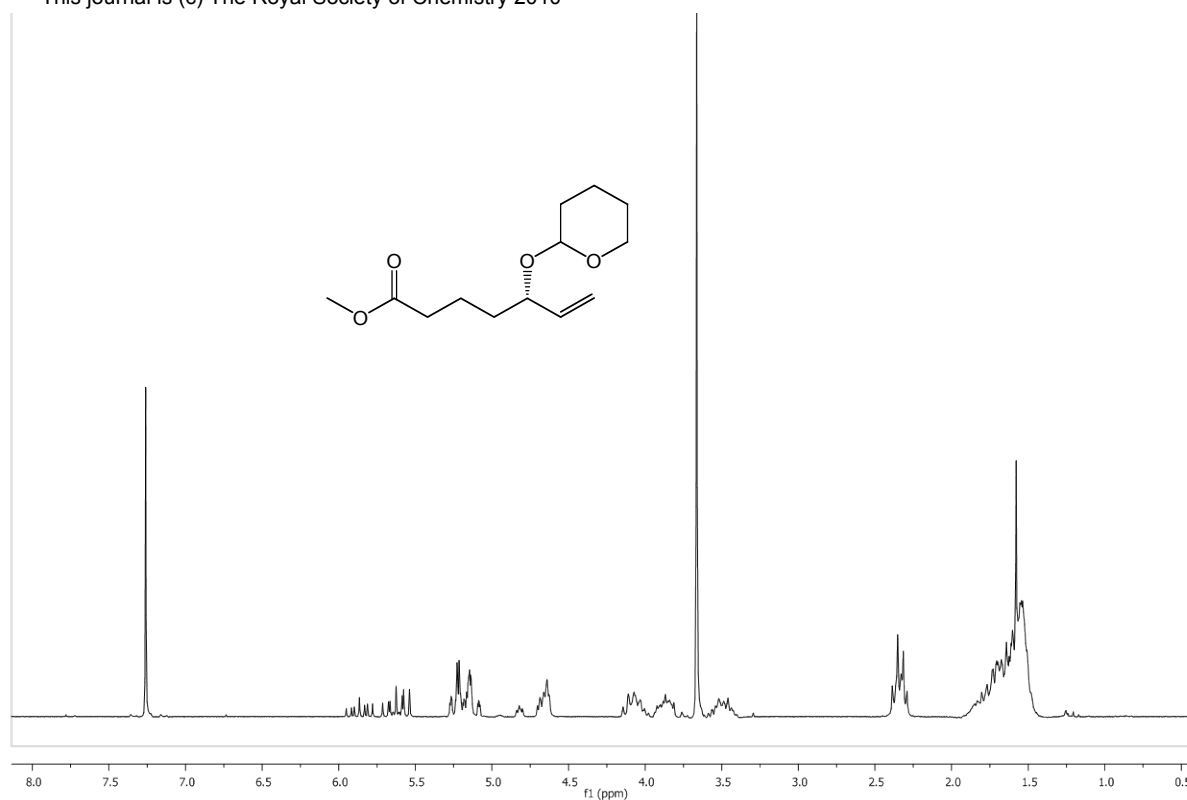
(S)-5-Hydroxy-hept-6-enoic acid methyl ester



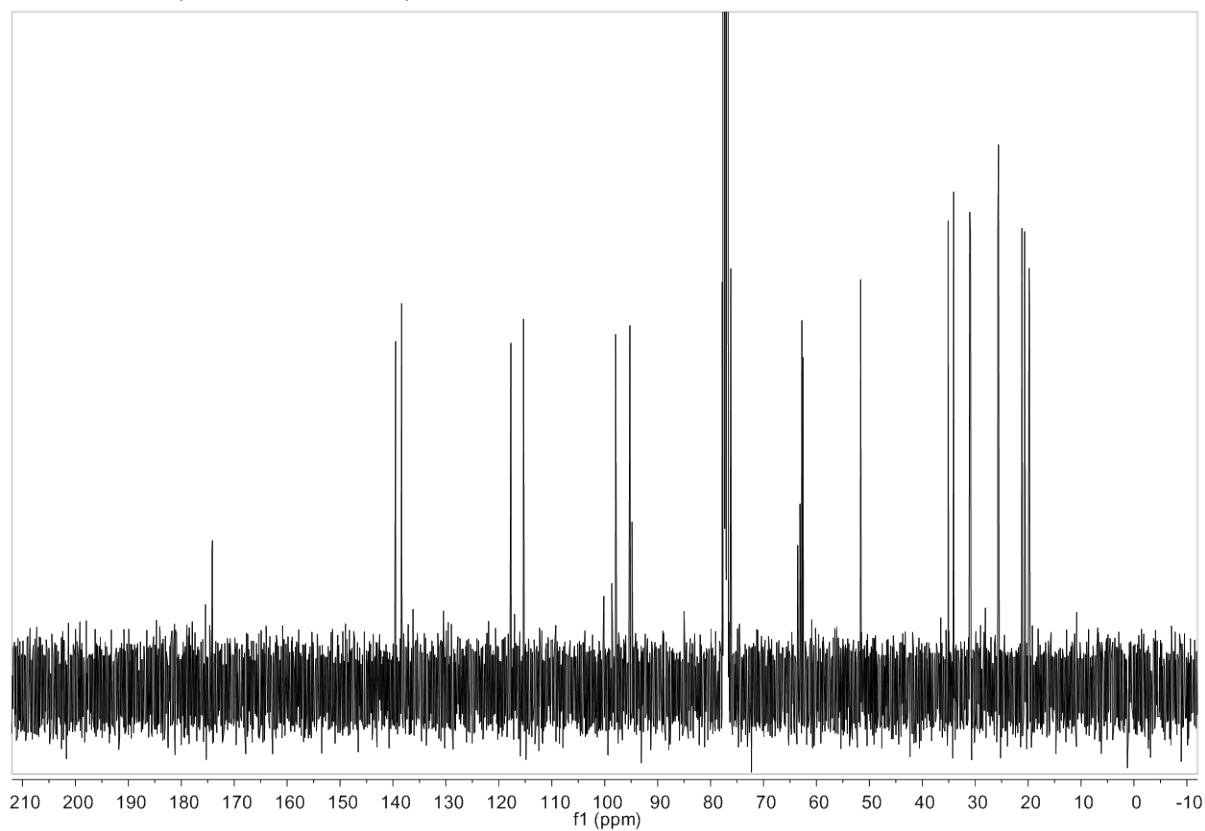
$^1\text{H NMR}$ (400 MHz, CDCl_3)



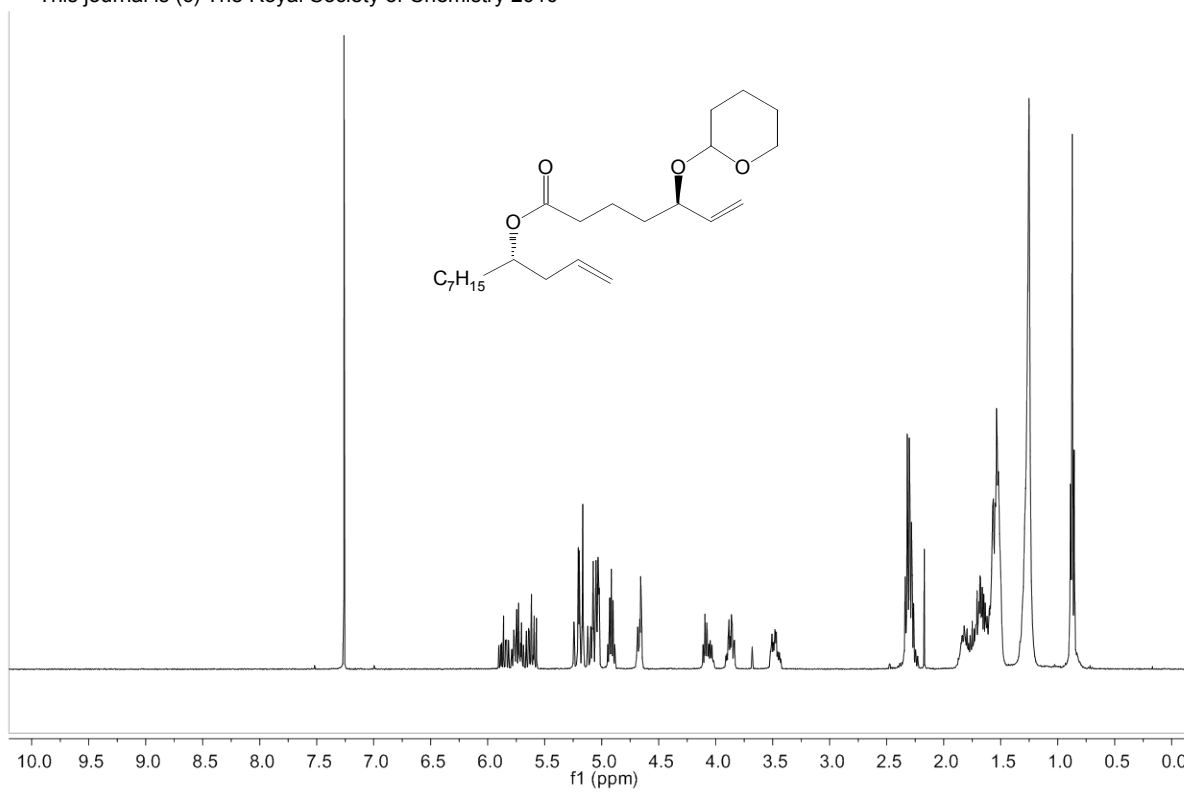
$^{13}\text{C NMR}$ (101 MHz, CDCl_3)



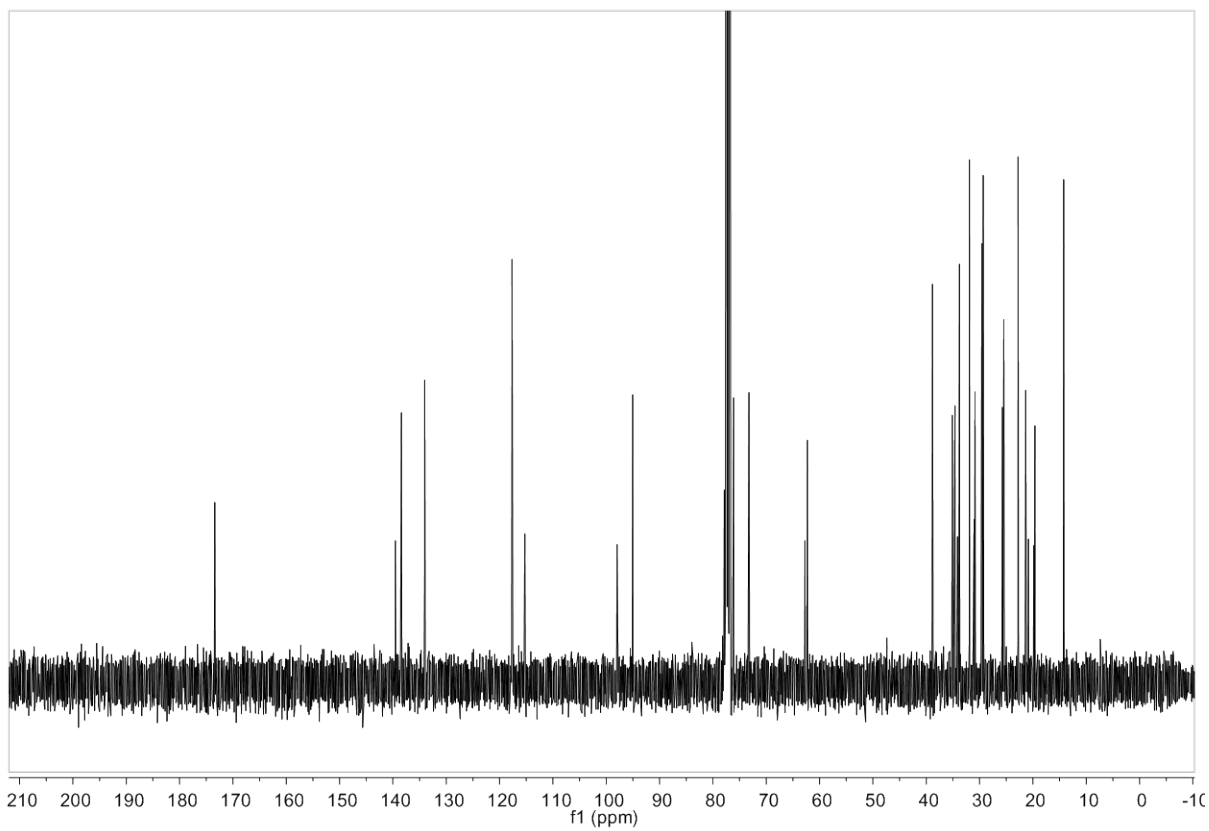
14: ¹H NMR (200 MHz, CDCl₃)



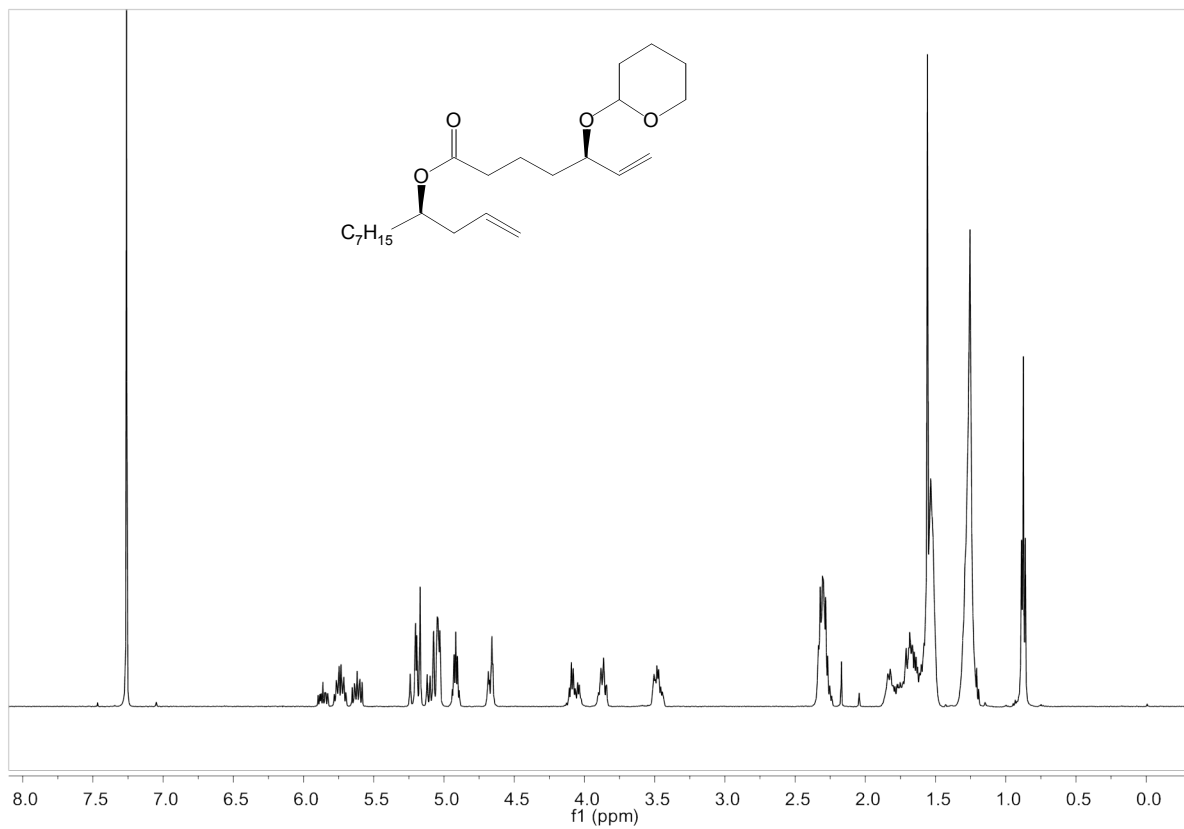
14: ¹³C NMR (101 MHz, CDCl₃)



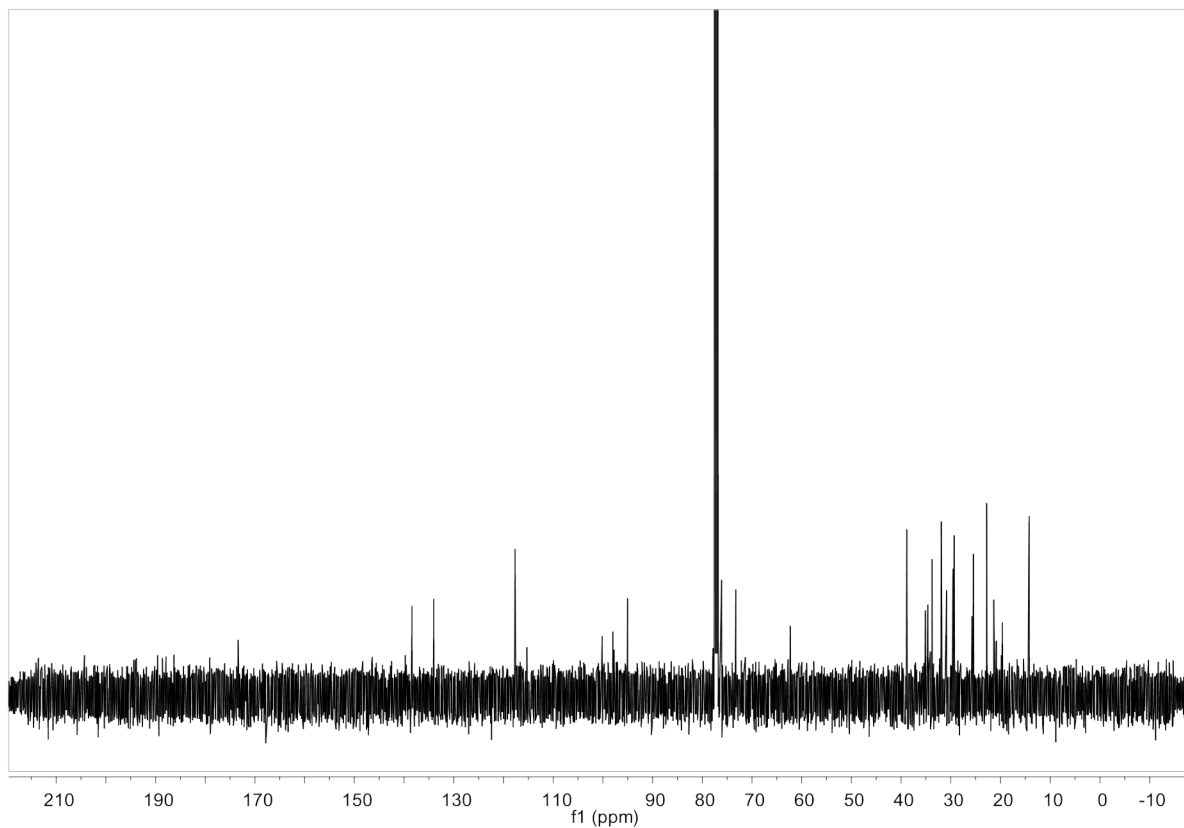
15: ¹H NMR (400 MHz, CDCl₃)



15: ¹³C NMR (101 MHz, CDCl₃)

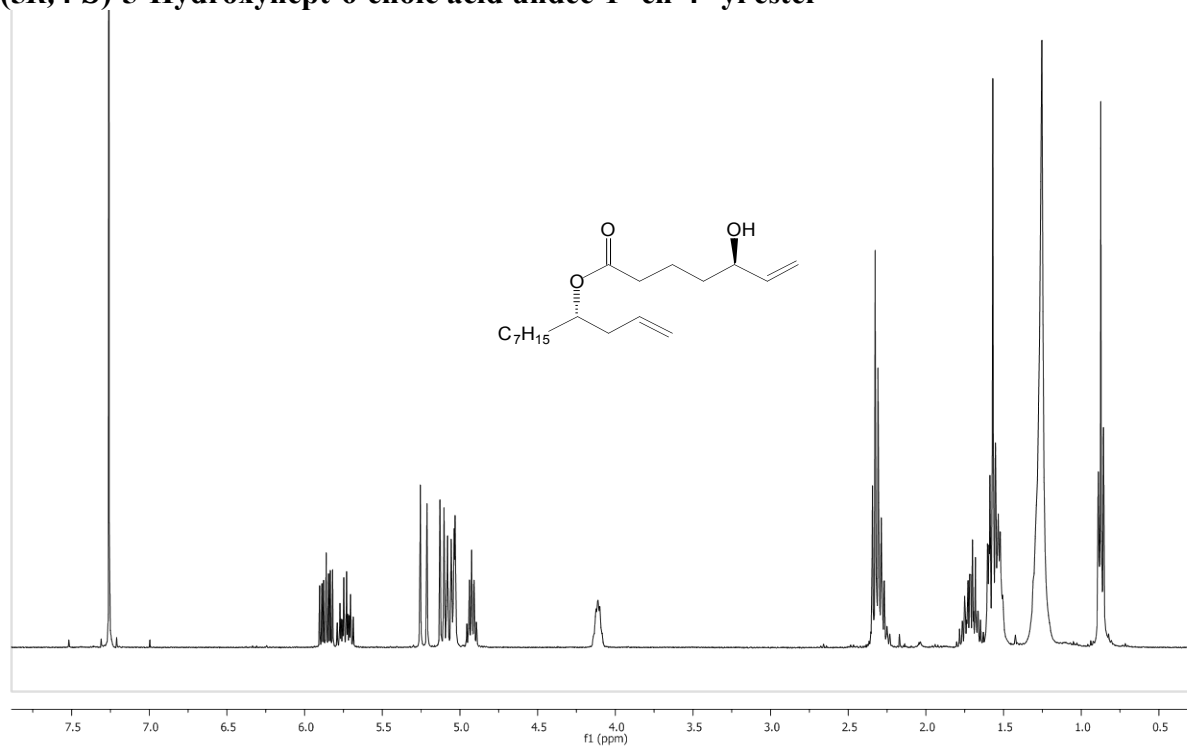


epi-15: ¹H NMR (500 MHz, CDCl₃)

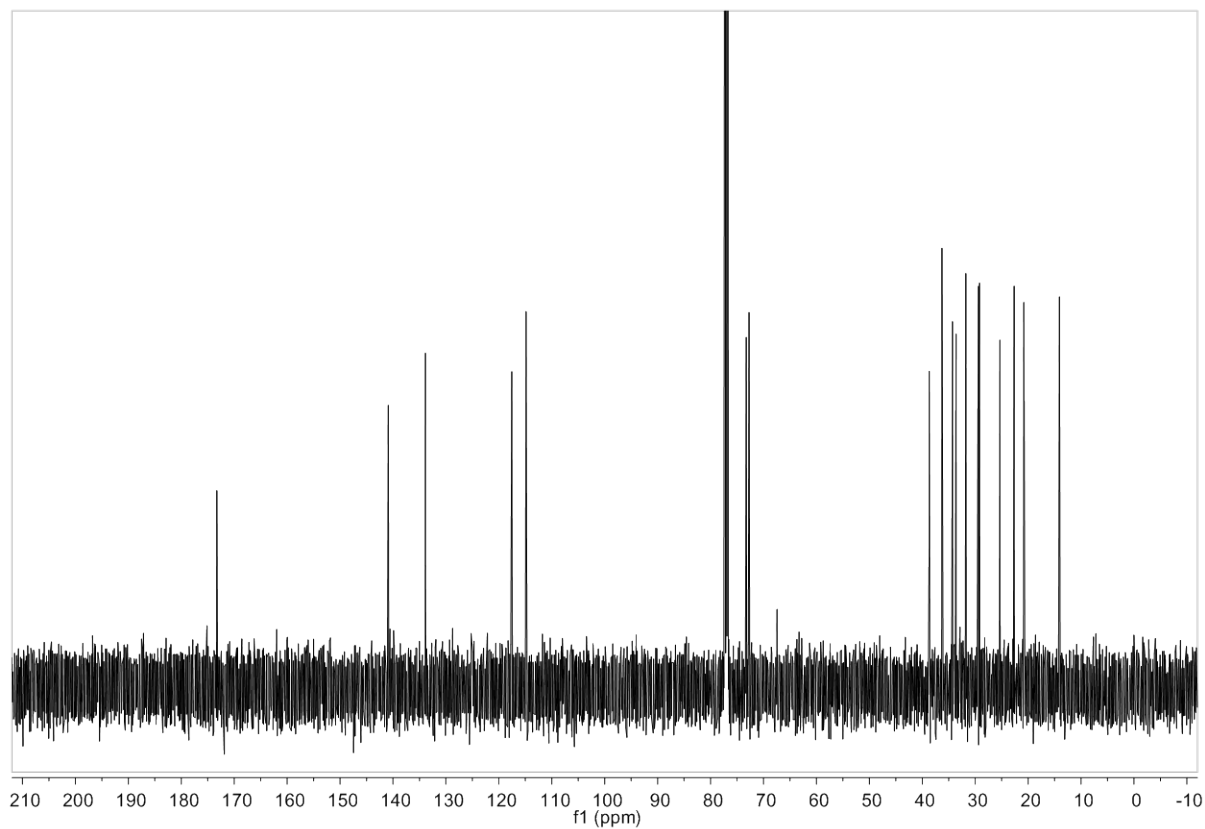


epi-15: ¹³C NMR (126 MHz, CDCl₃)

(5*R*,4'*S*)-5-Hydroxyhept-6-enoic acid undec-1'-en-4'-yl ester

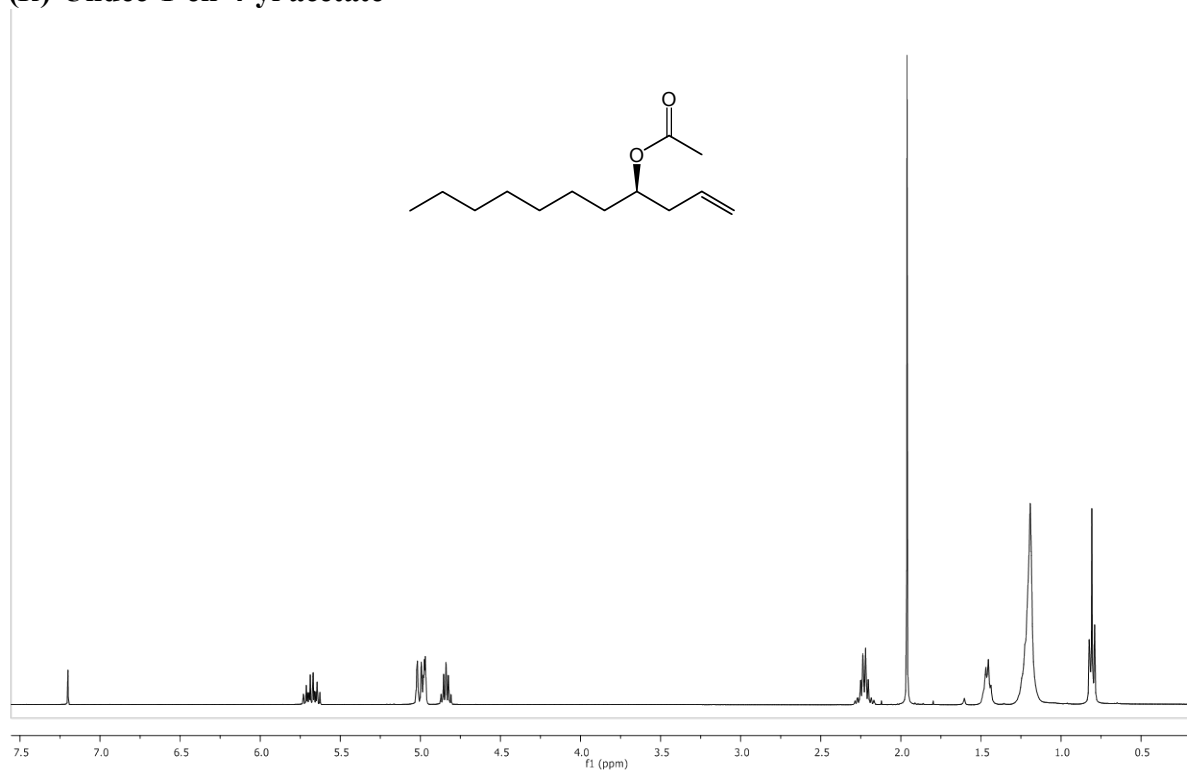


¹H NMR (400 MHz, CDCl₃)

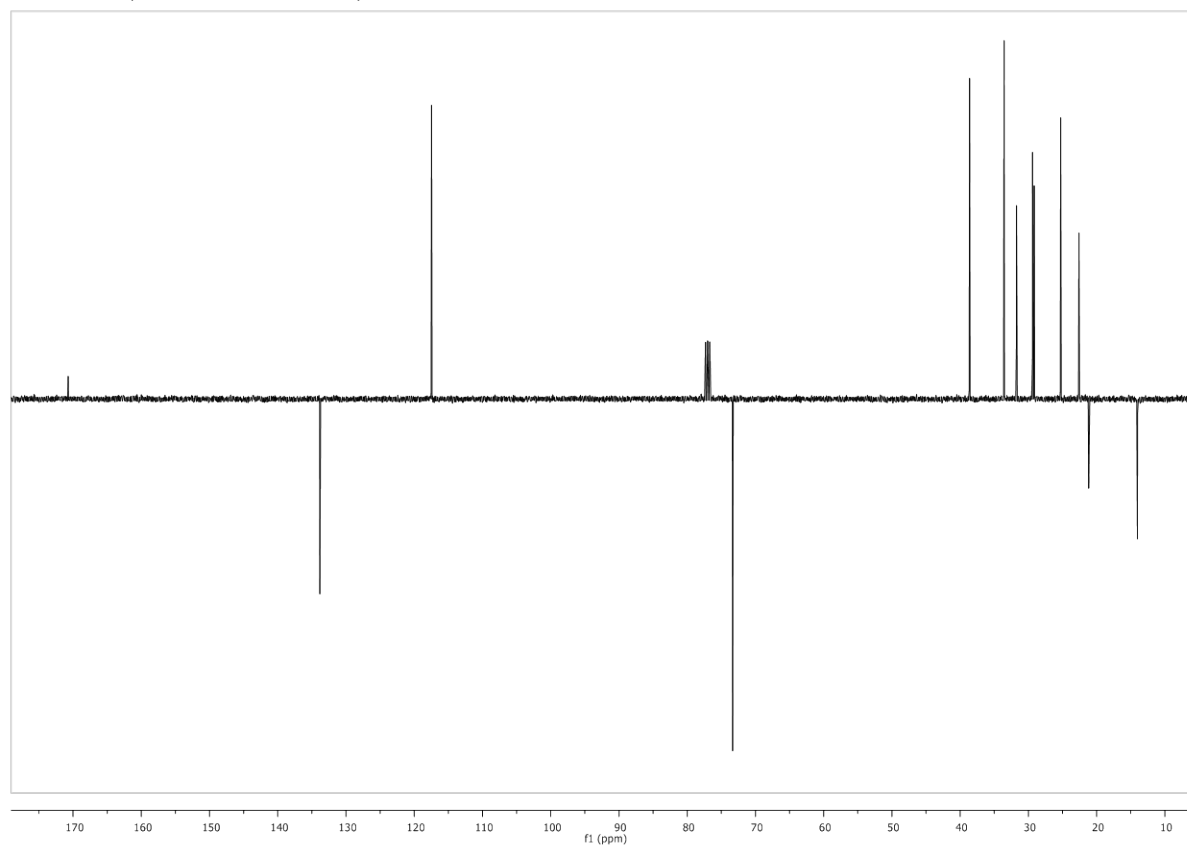


¹³C NMR (101 MHz, CDCl₃)

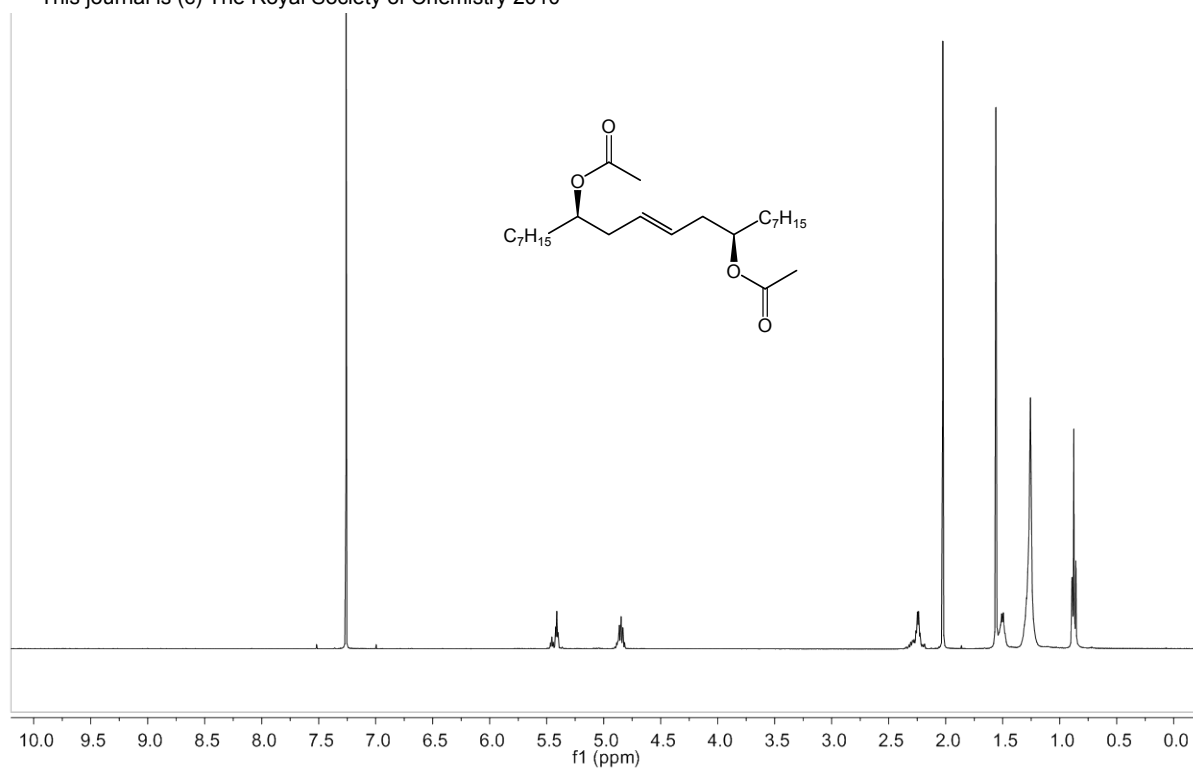
(R)-Undec-1-en-4-yl acetate



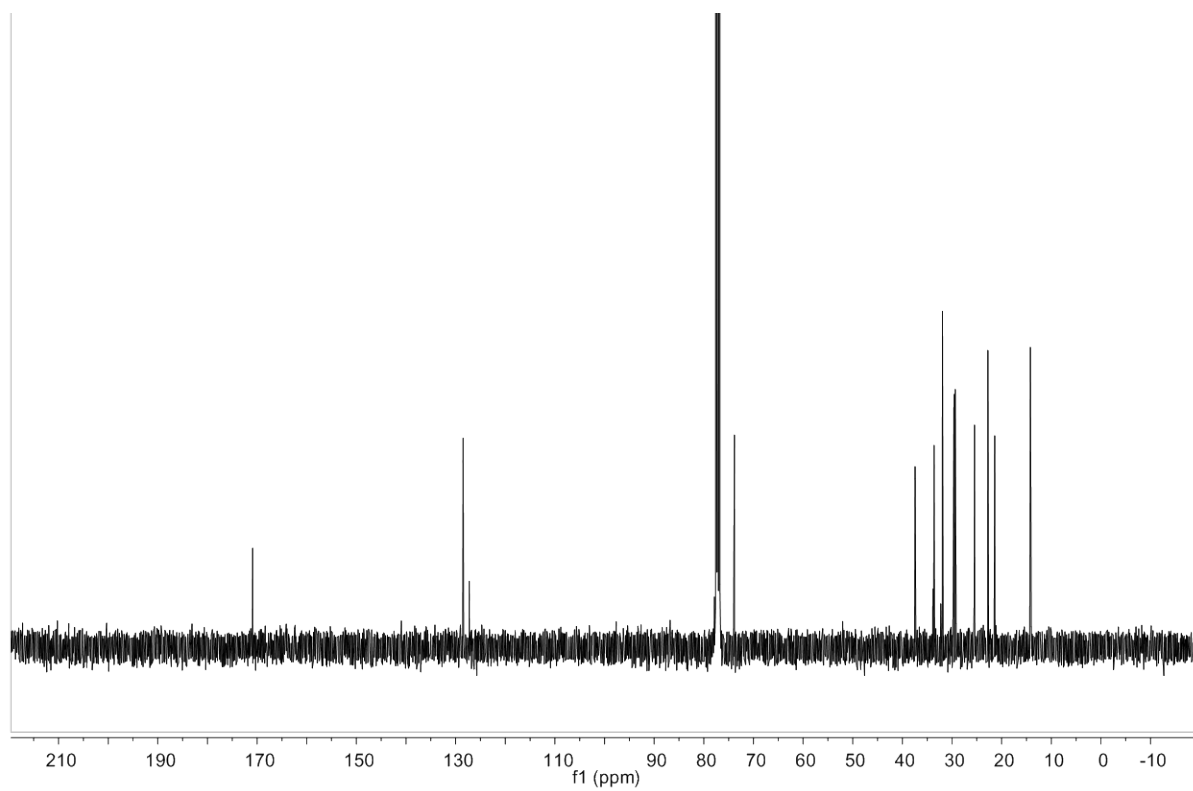
¹H NMR (400 MHz, CDCl₃)



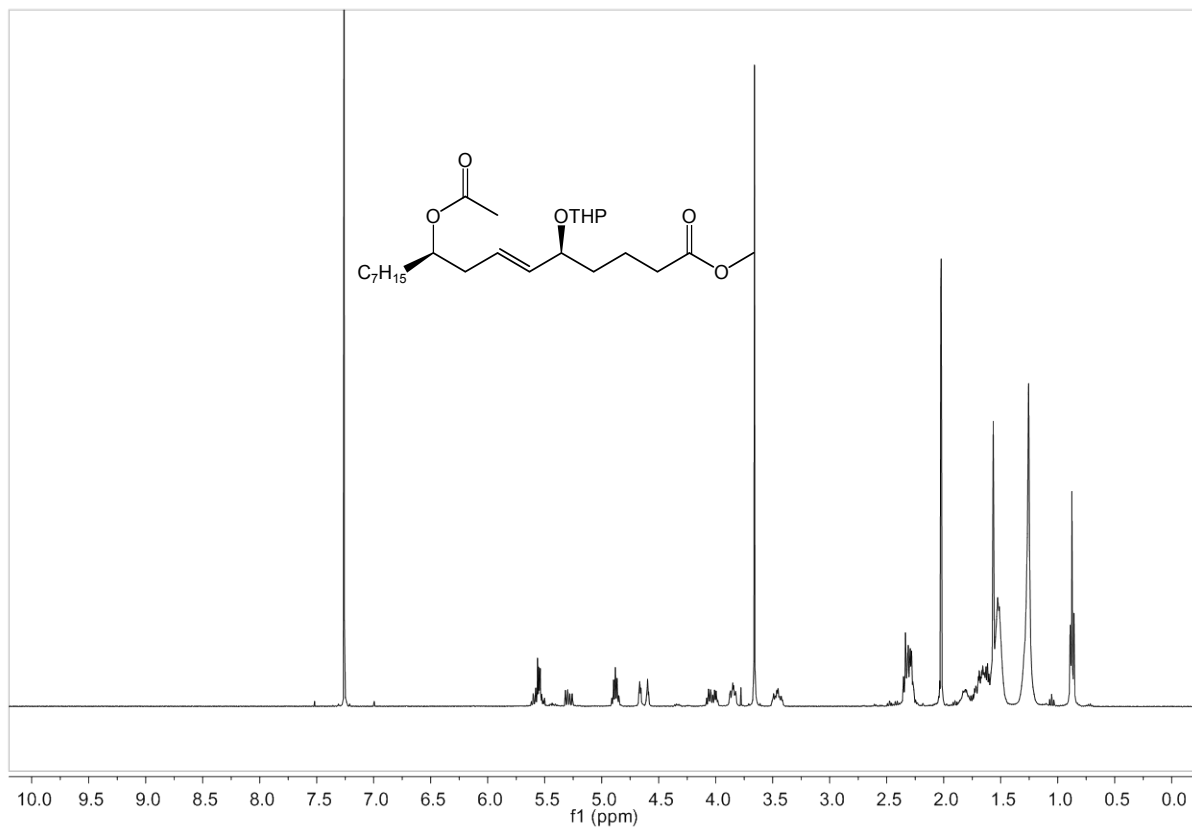
APT (101 MHz, CDCl₃)



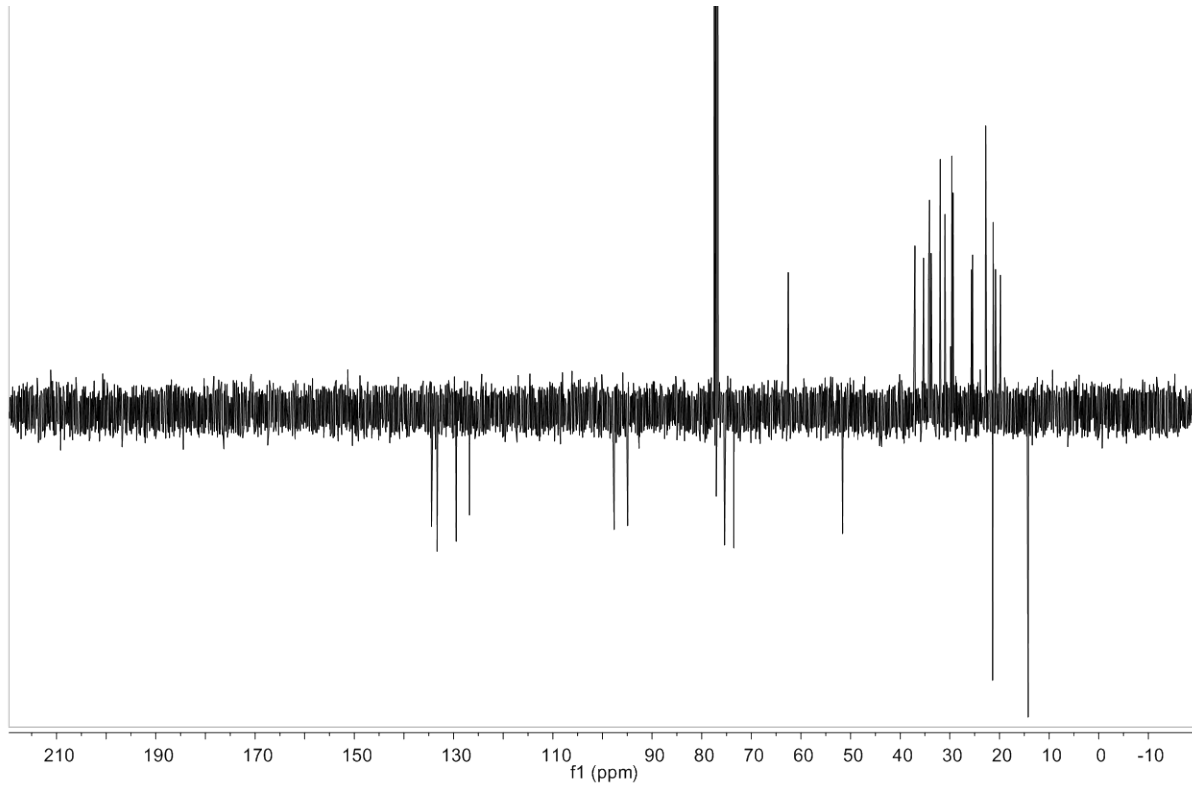
16: ¹H NMR (400 MHz, CDCl₃)



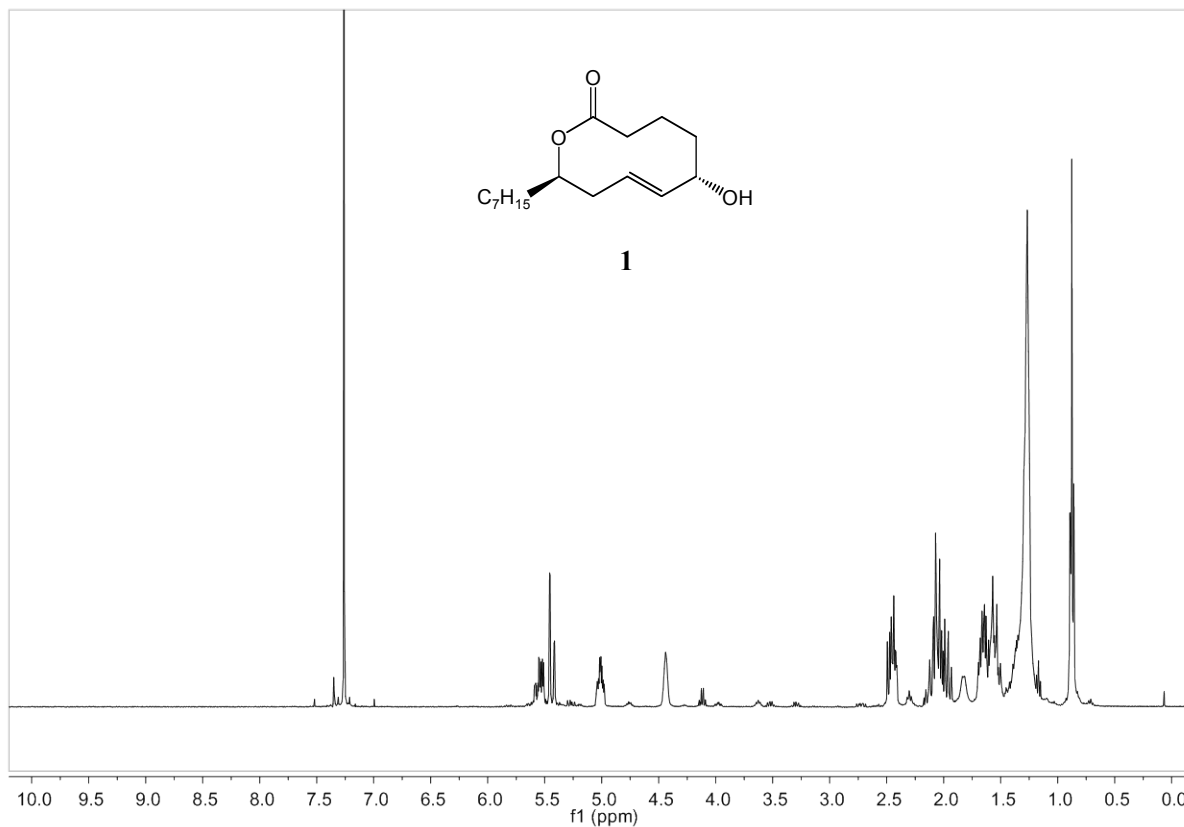
16: ¹³C NMR (101 MHz, CDCl₃)



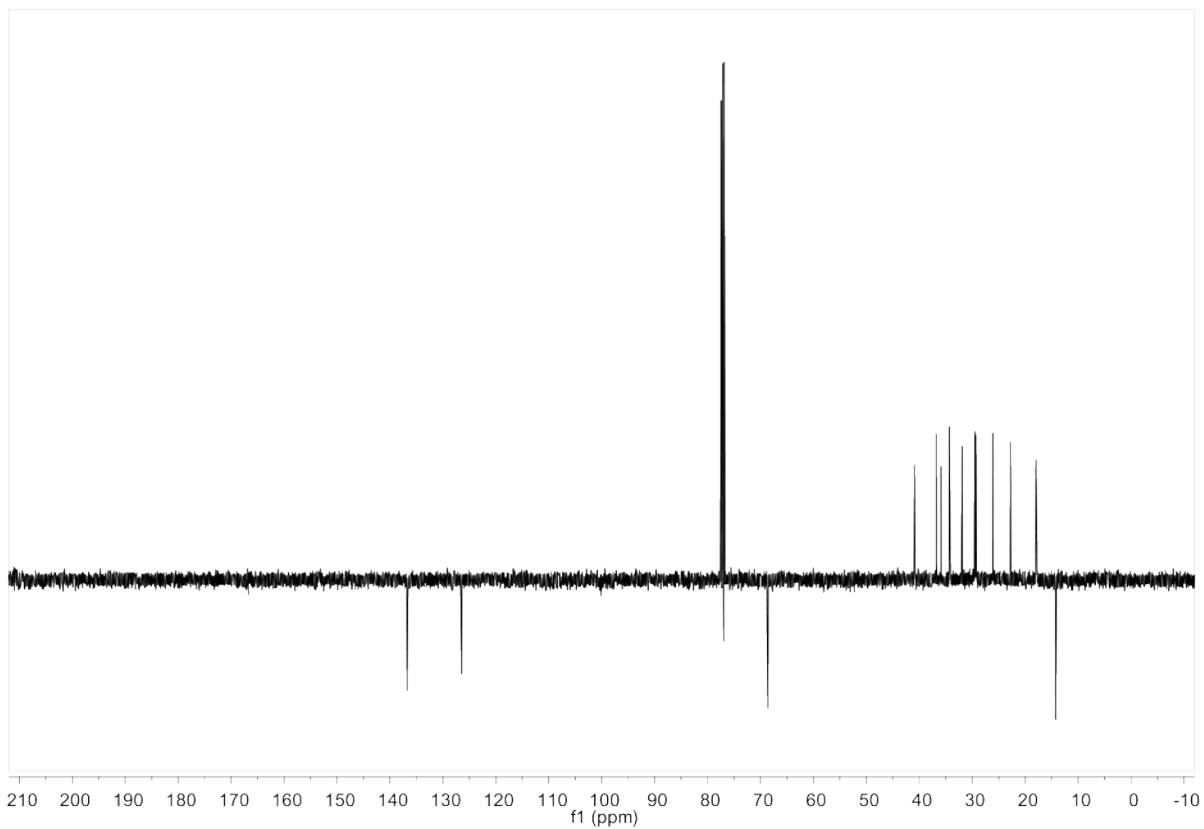
17: ¹H NMR (400 MHz, CDCl₃)



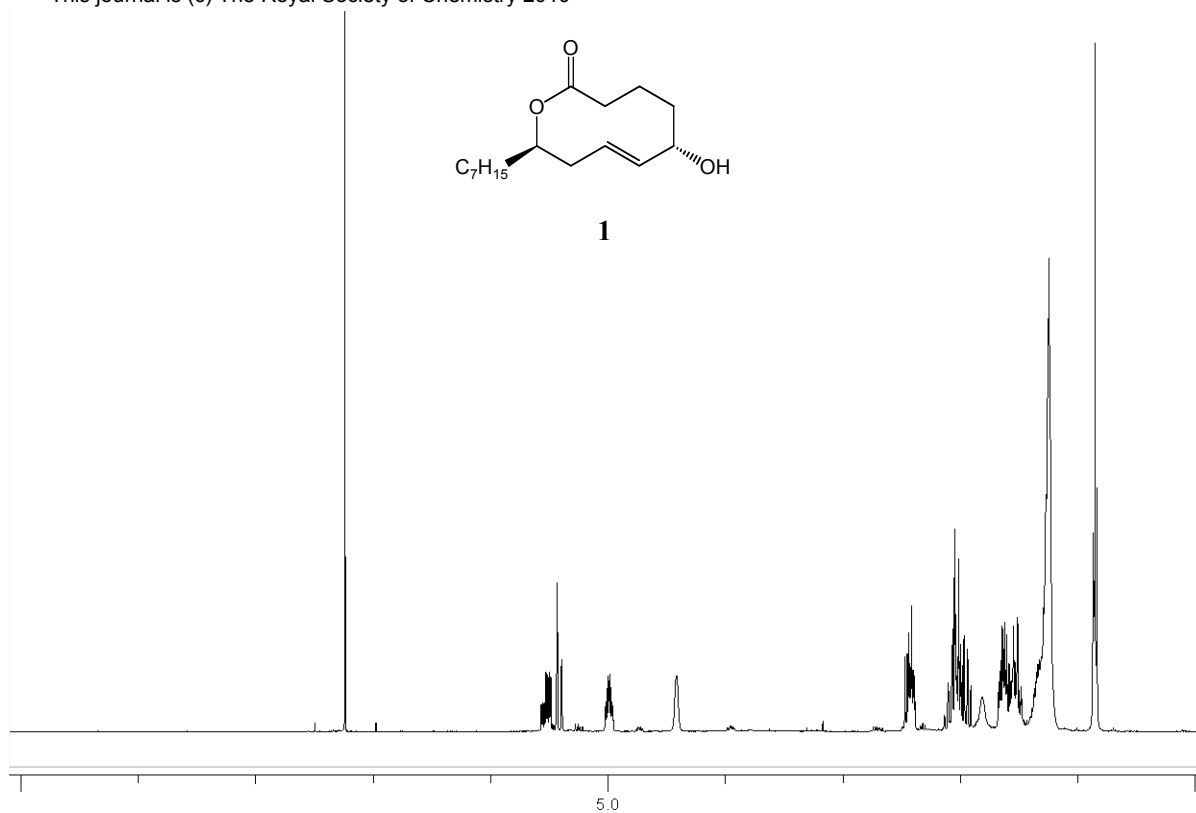
17: DEPTQ (101 MHz, CDCl₃)



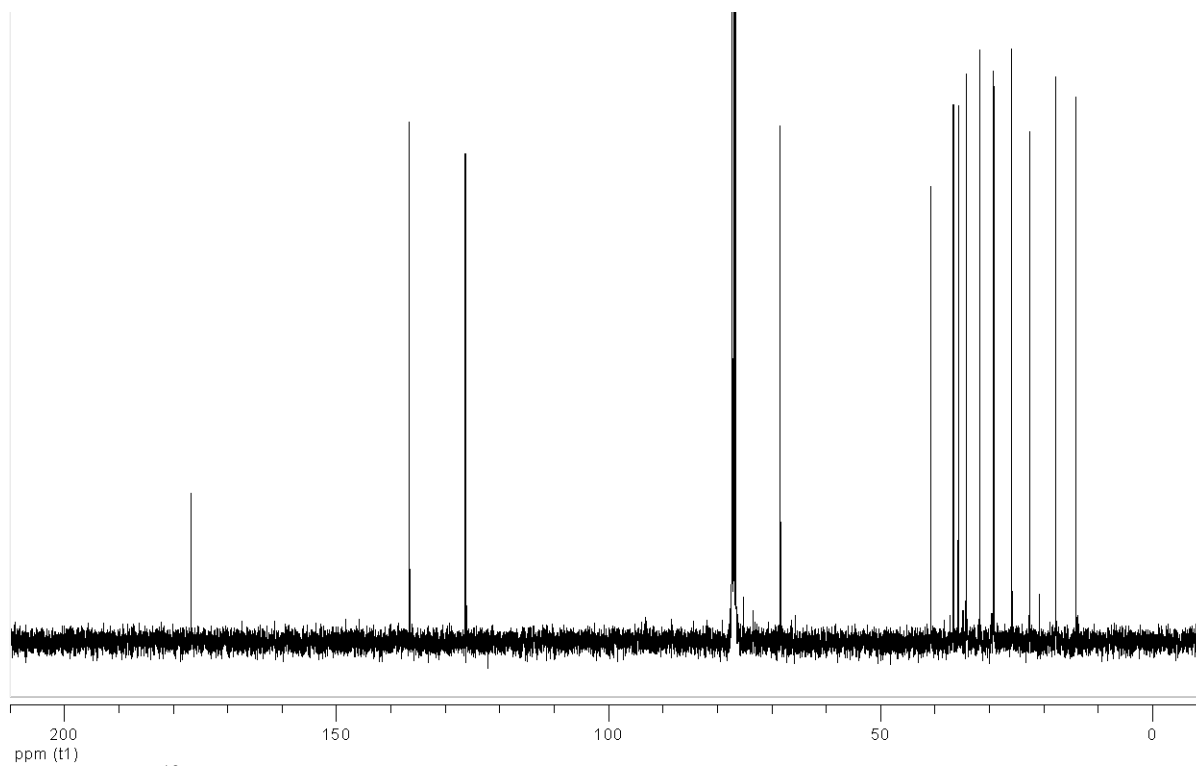
1 (synthetic): ¹H NMR (400 MHz, CDCl₃).



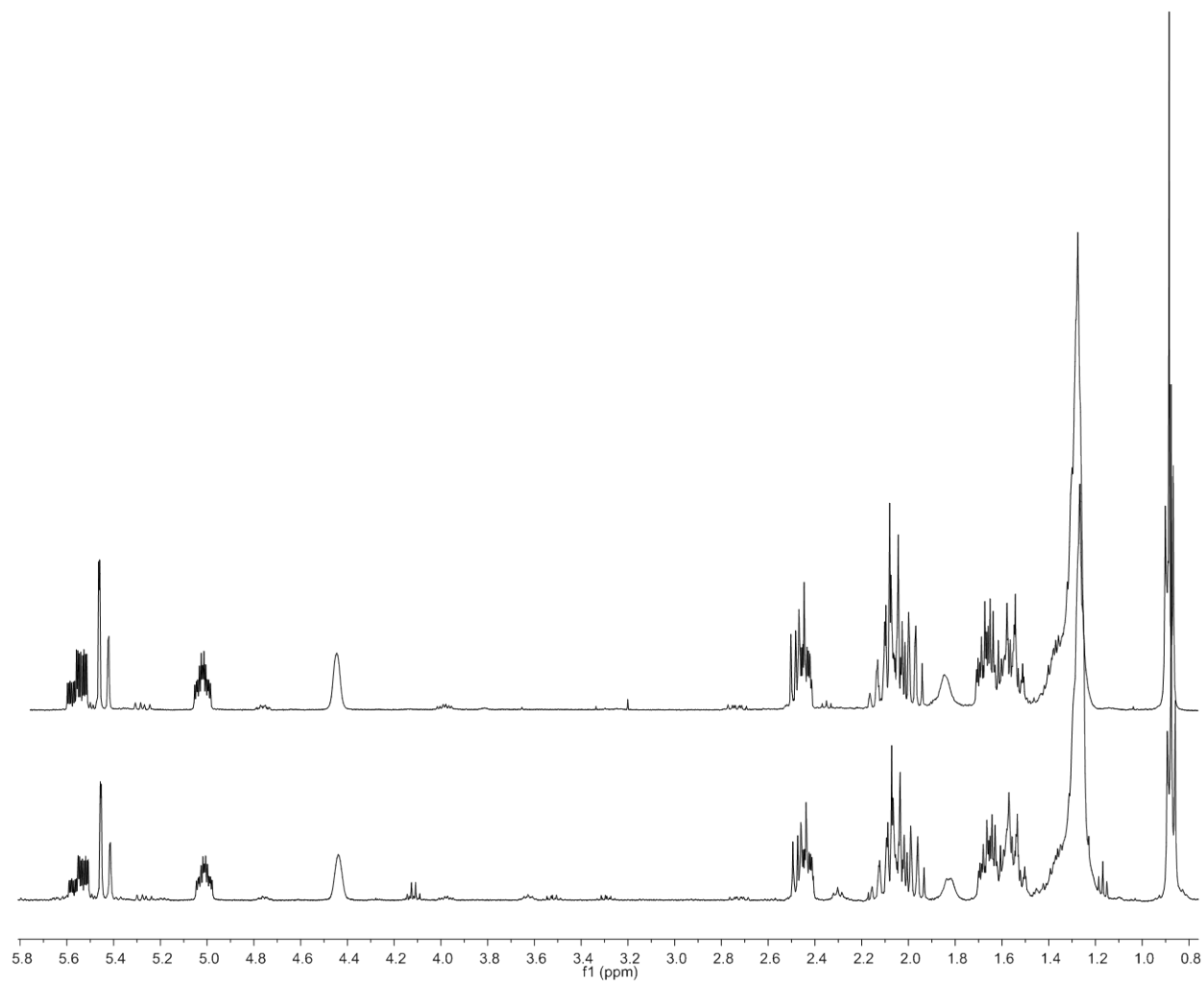
1 (synthetic): DEPTQ (101 MHz, CDCl₃).



1 (natural): ¹H NMR (400 MHz, CDCl₃). The spectrum shows the presence of a minor conformer also present in the synthetic material



1 (natural): ¹³C NMR (101 MHz, CDCl₃)



Overlay of ¹H NMR spectra of natural (top) and synthetic (bottom) **1**.

Gas Chromatography

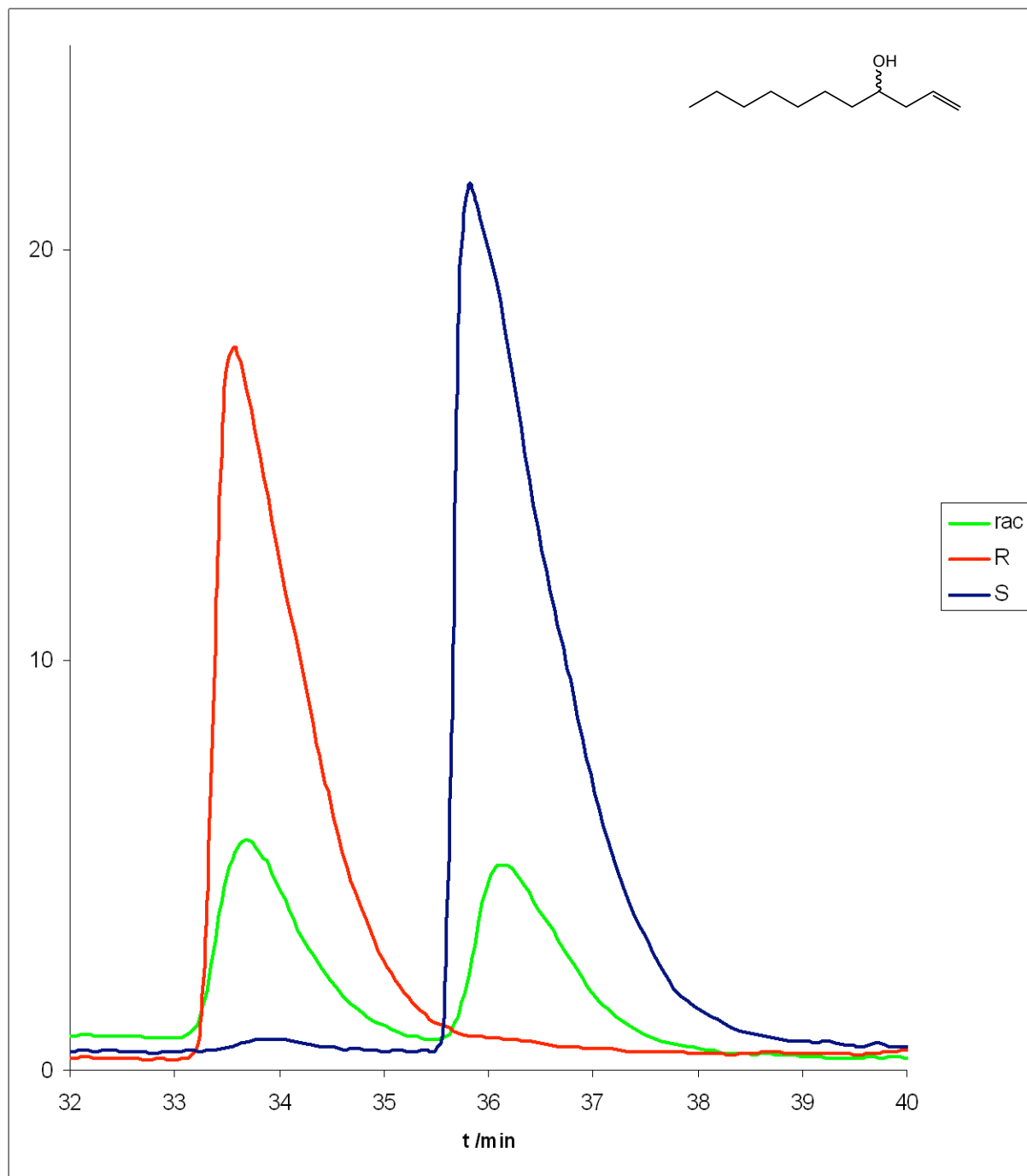


Fig. S1: Chiral GC of **10**, ent-**10** and rac-**10**.

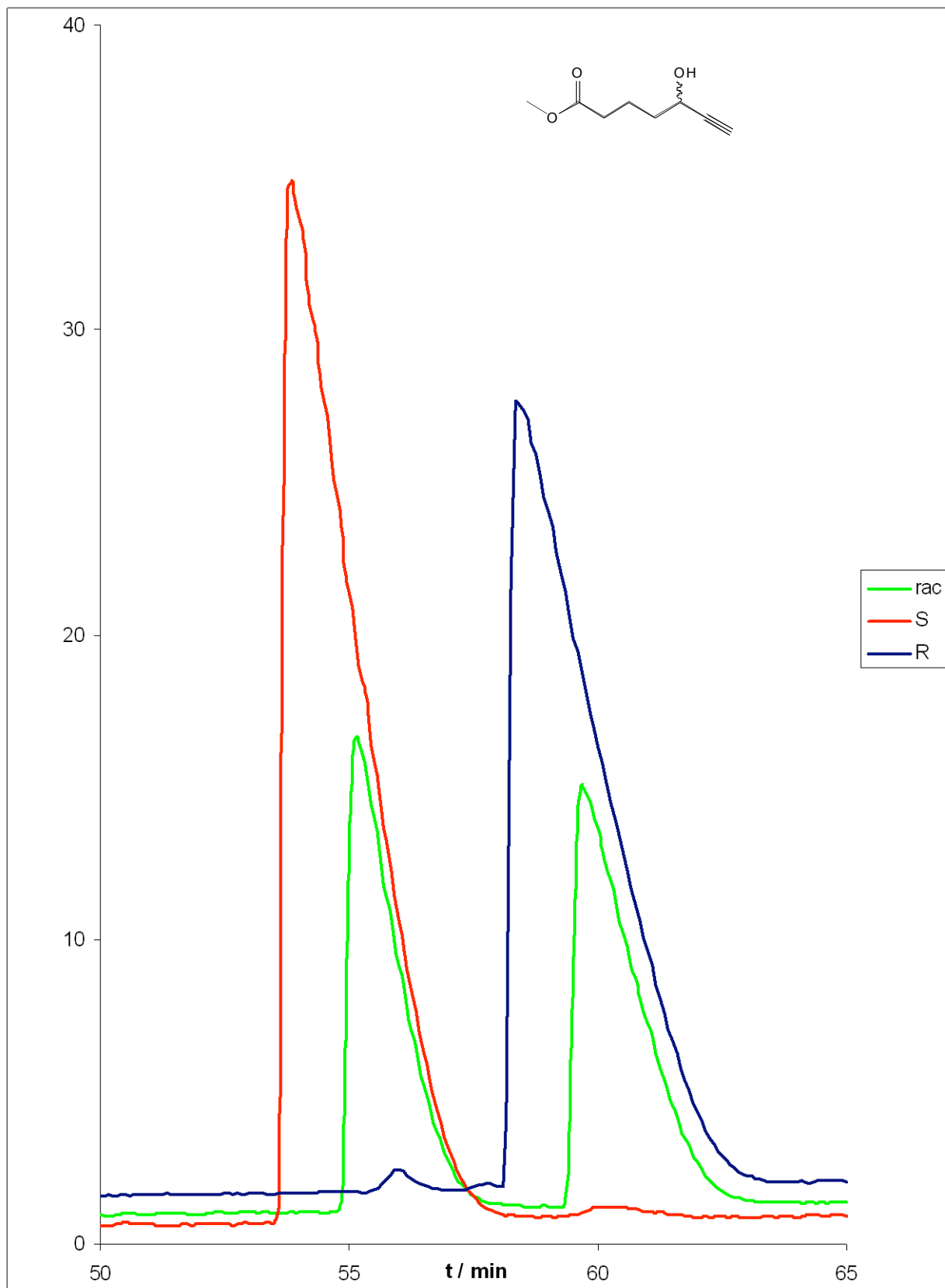


Fig. S2: Chiral GC of 5-Hydroxyhept-6-ynoic acid methyl ester

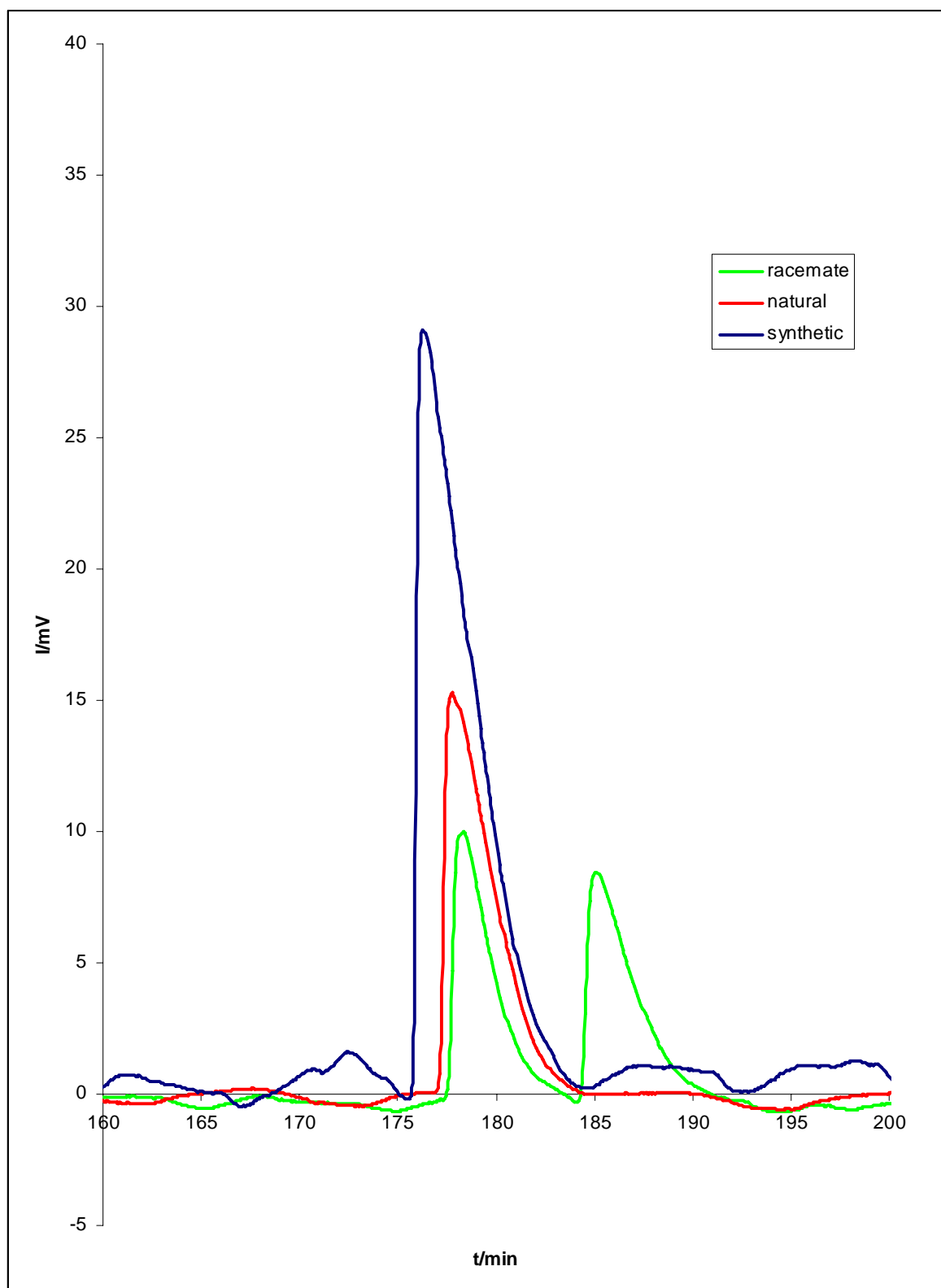


Fig. S3: Chiral GC of hypocreolide A (**1**) and ent-hypocreolide A (*ent-1*).