

Supplementary Material

The Conversion of Levoglucosenone into Isolevoglucosenone

*Xinghua Ma,^A Natasha Anderson,^A Lorenzo V. White,^A Song Bae,^A Warwick Raverty,^B
Anthony C. Willis,^A and Martin G. Banwell^{A,C}*

^AResearch School of Chemistry, Institute of Advanced Studies, The Australian National University, Canberra ACT 2601, Australia.

^BCirca Group Pty Ltd, 34 Norfolk Court, Coburg North VIC 3058, Australia

^CCorresponding author. Email: Martin.Banwell@anu.edu.au

Contents	Page
– Anisotropic Displacement Ellipsoid Plots for Compounds 5, 9, 10 and 14	S2
– ¹ H and ¹³ C NMR Spectra of Compounds 2–16	S5

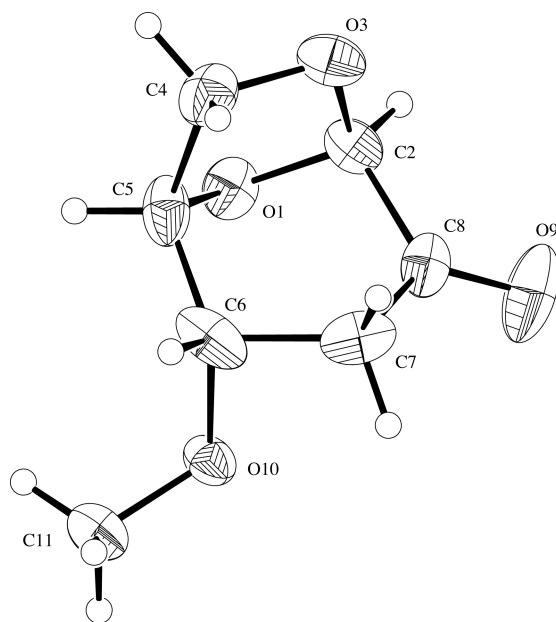


Figure S1: Structure of compound **5** (CCDC 1023960) with labelling of selected atoms, showing one location of the disordered atoms (O10: occupancy 0.5). Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

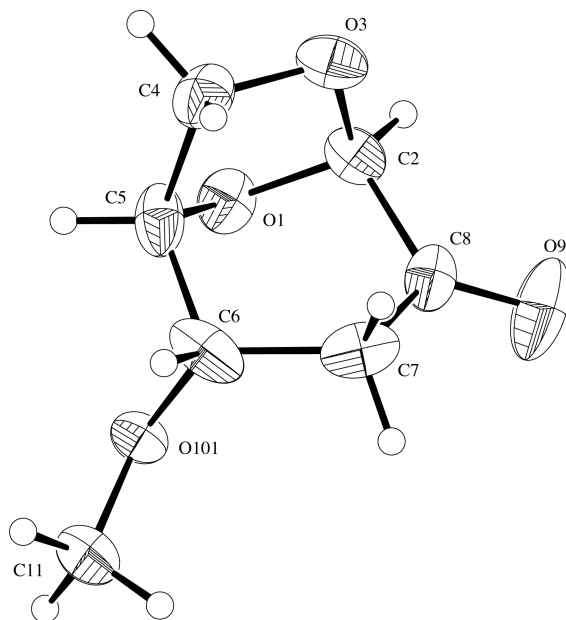


Figure S2: Structure of compound **5** (CCDC 1023960) with labelling of selected atoms, showing the alternative location of the disordered atoms (O101: occupancy 0.5). Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

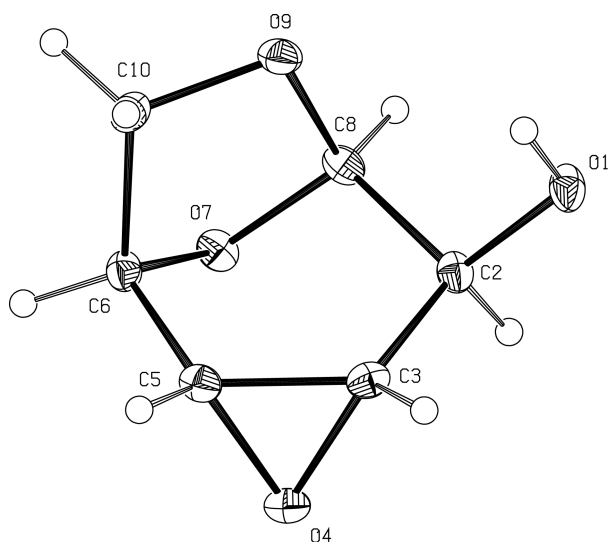


Figure S3: Structure of compound **9** (CCDC 1023961) with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

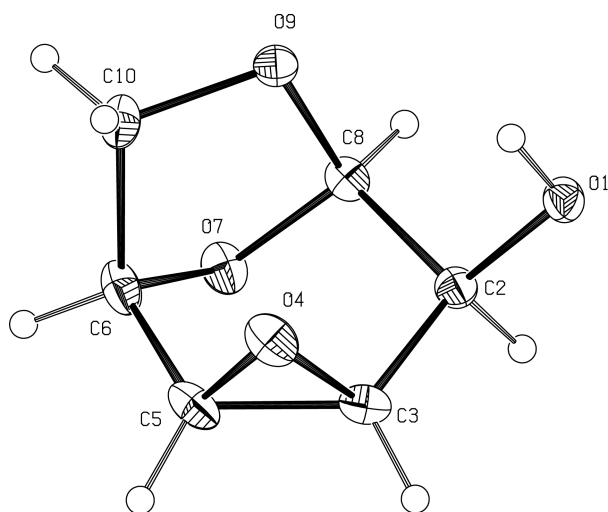


Figure S4: Structure of compound **10** (CCDC 1023962) with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

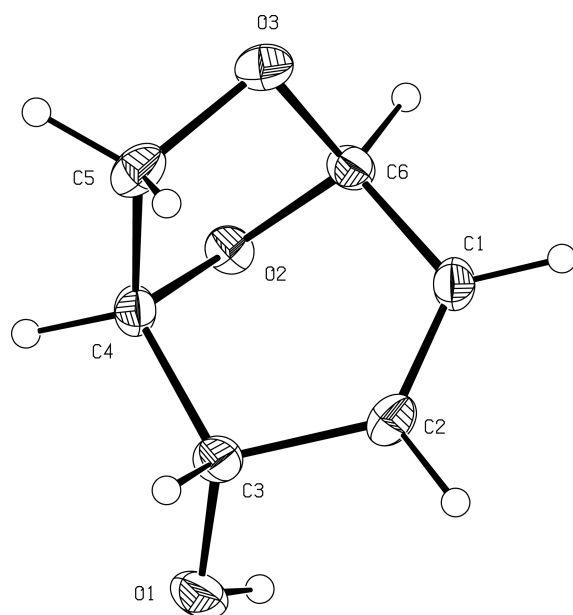
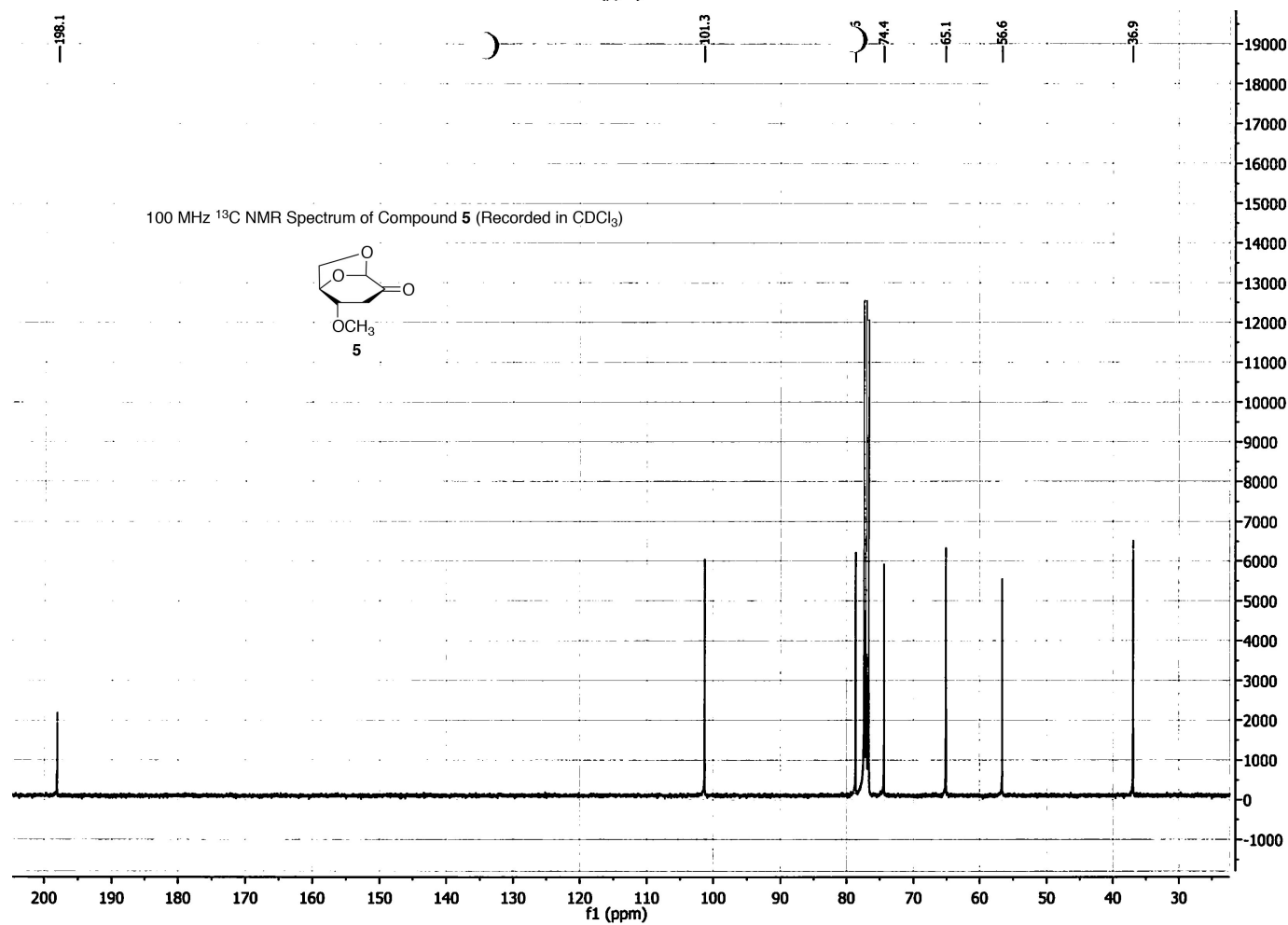
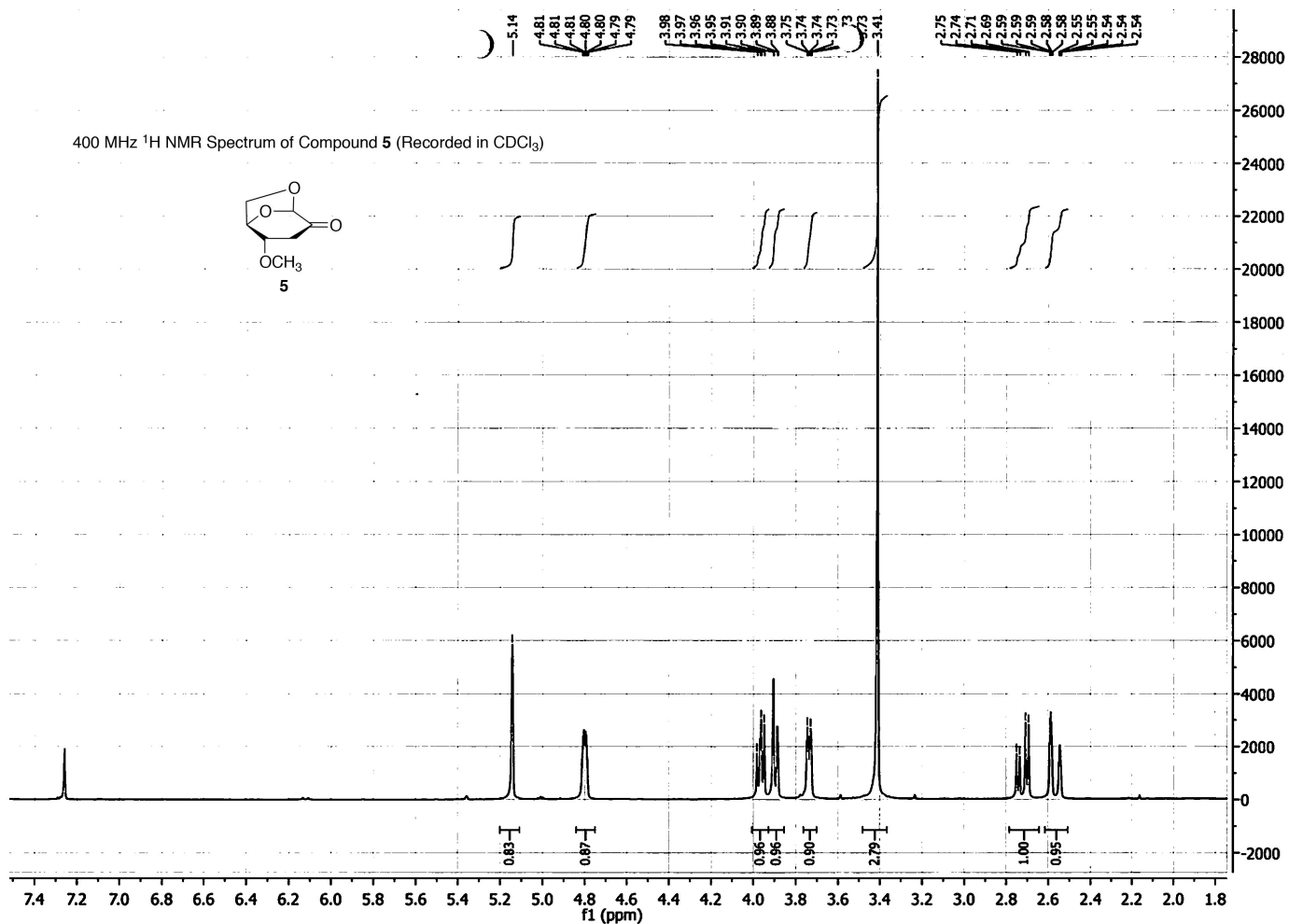
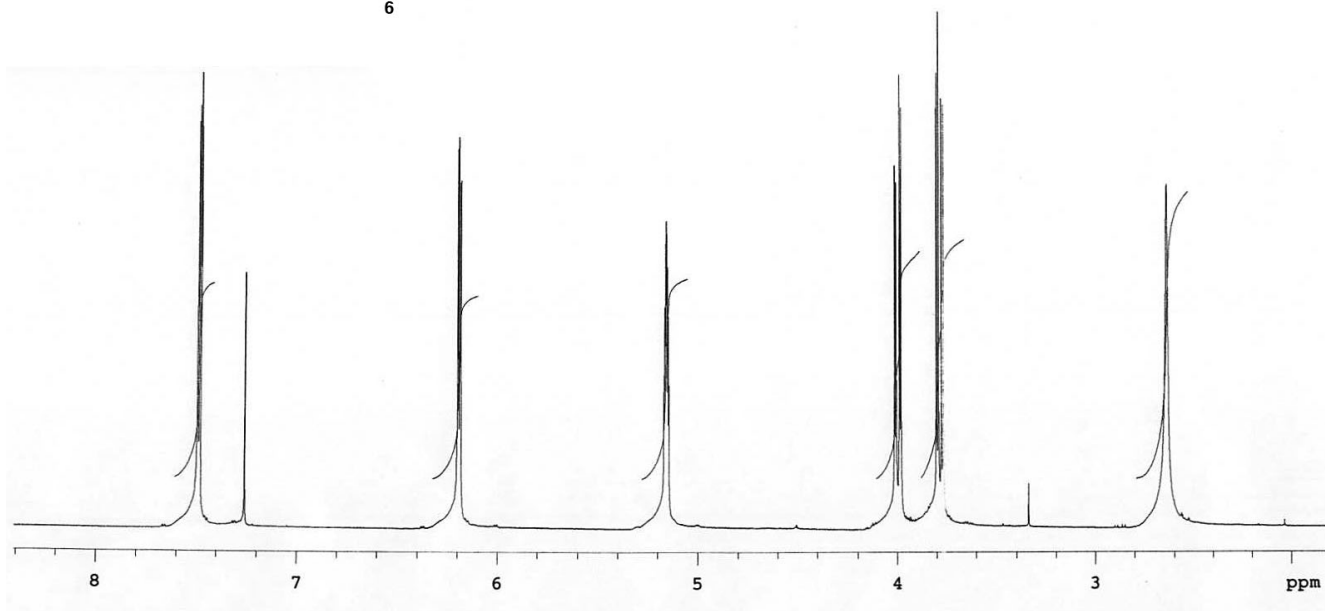
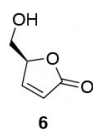


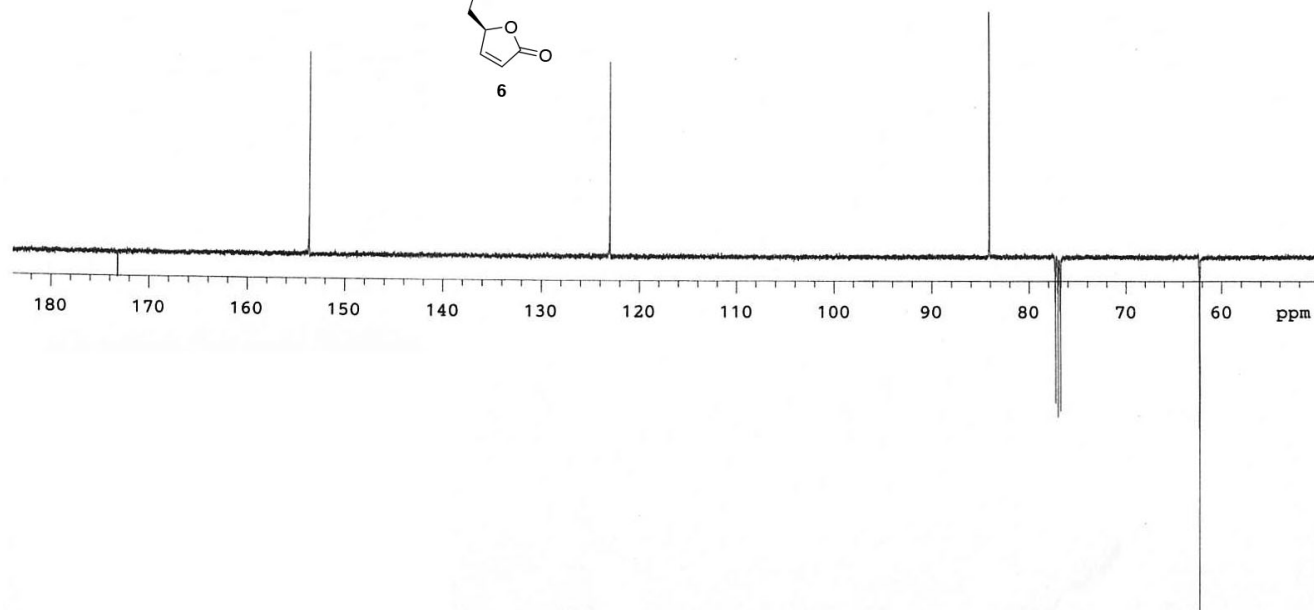
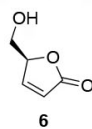
Figure S5: Structure of compound **14** (CCDC 1023963) with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.



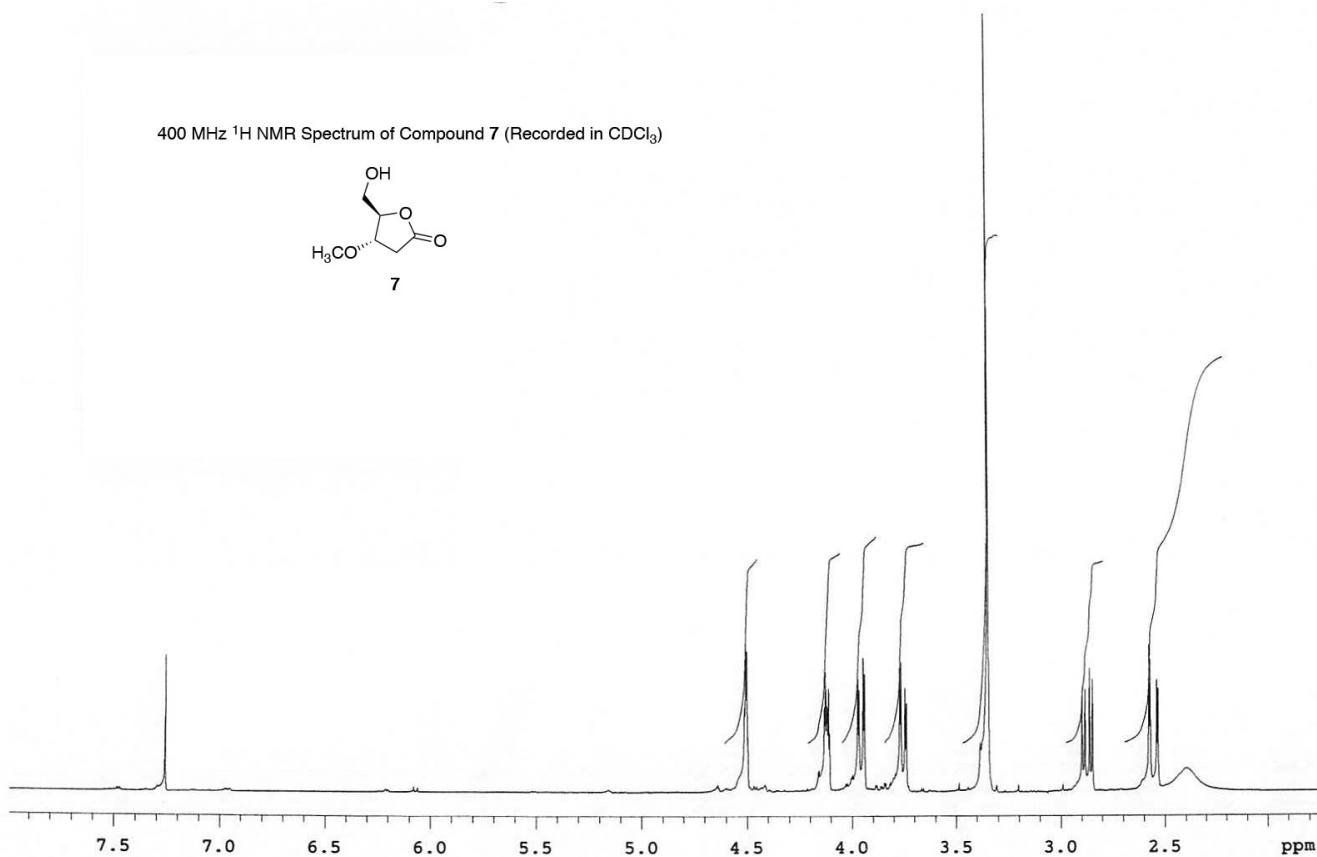
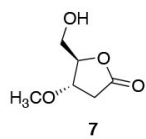
500 MHz ^1H NMR Spectrum of Compound 6 (Recorded in CDCl_3)



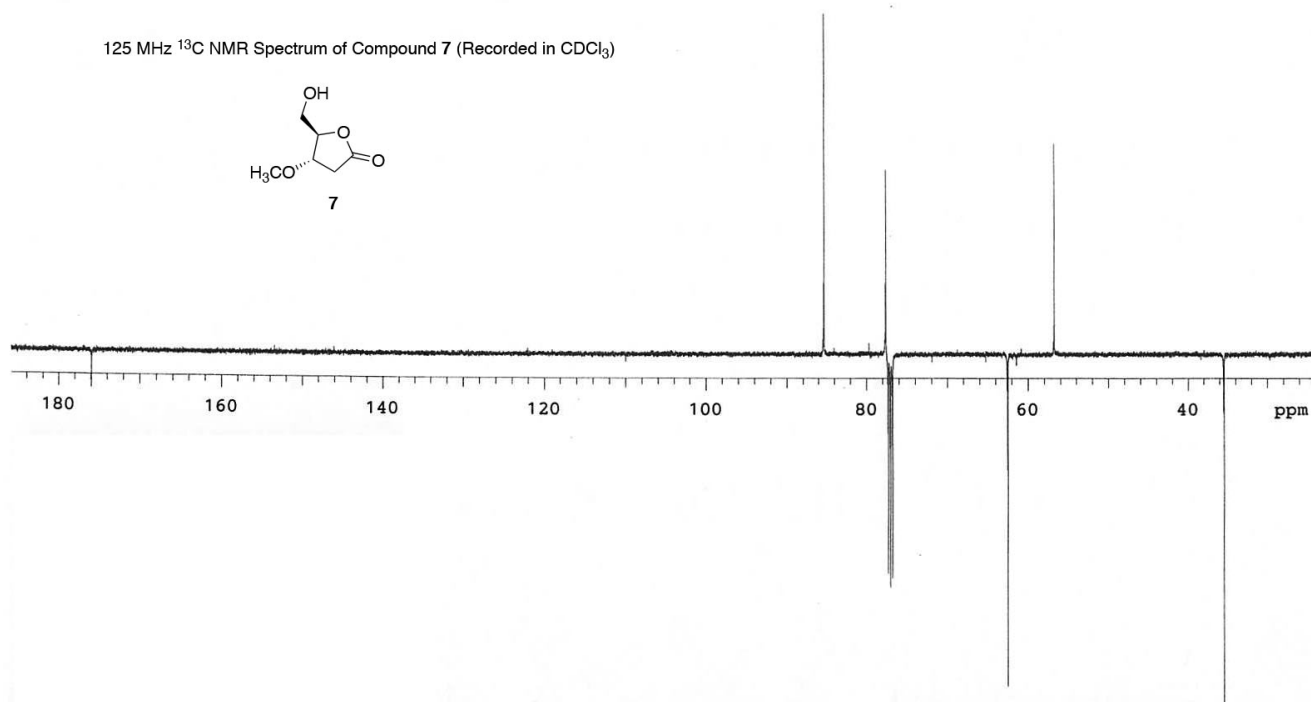
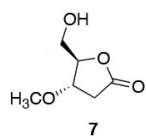
75 MHz ^{13}C NMR Spectrum of Compound 6 (Recorded in CDCl_3)



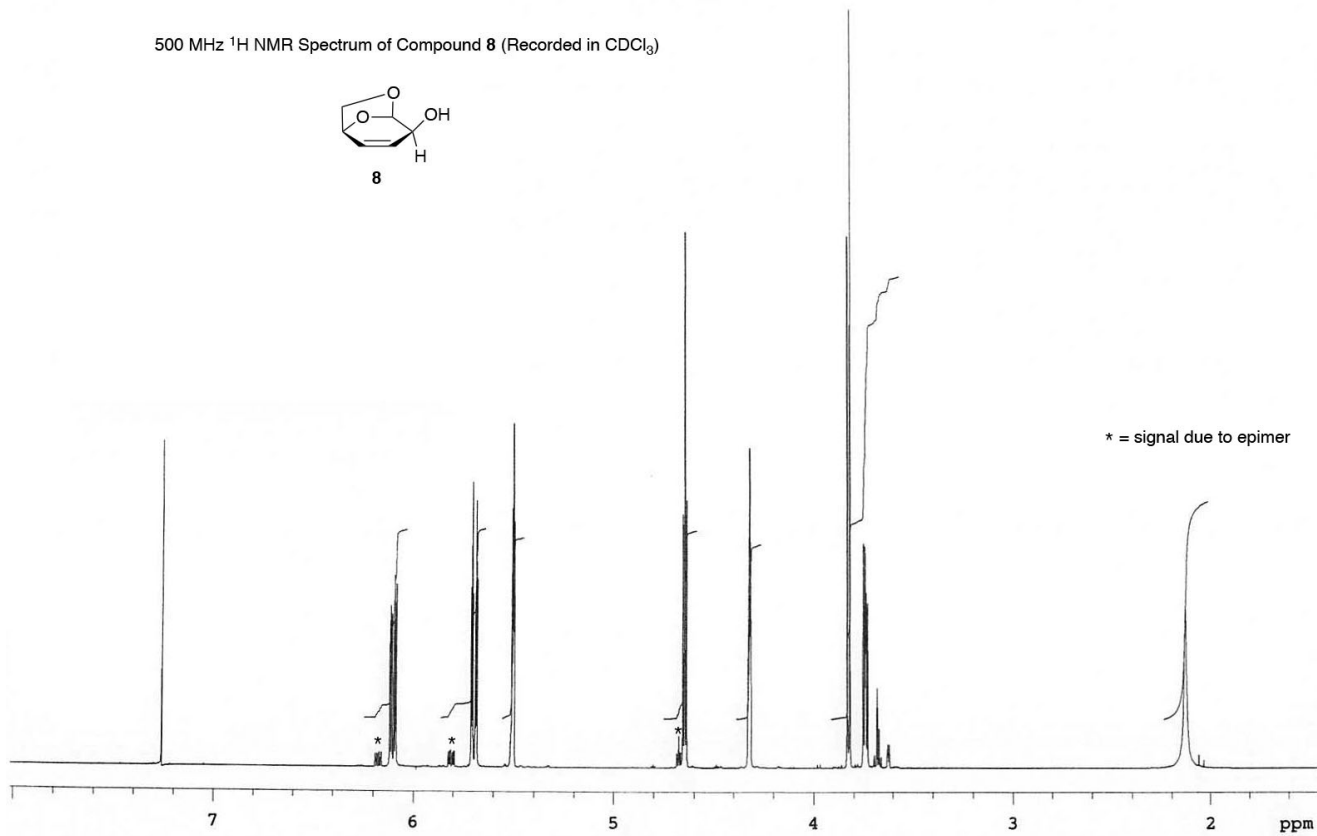
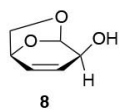
400 MHz ¹H NMR Spectrum of Compound 7 (Recorded in CDCl₃)



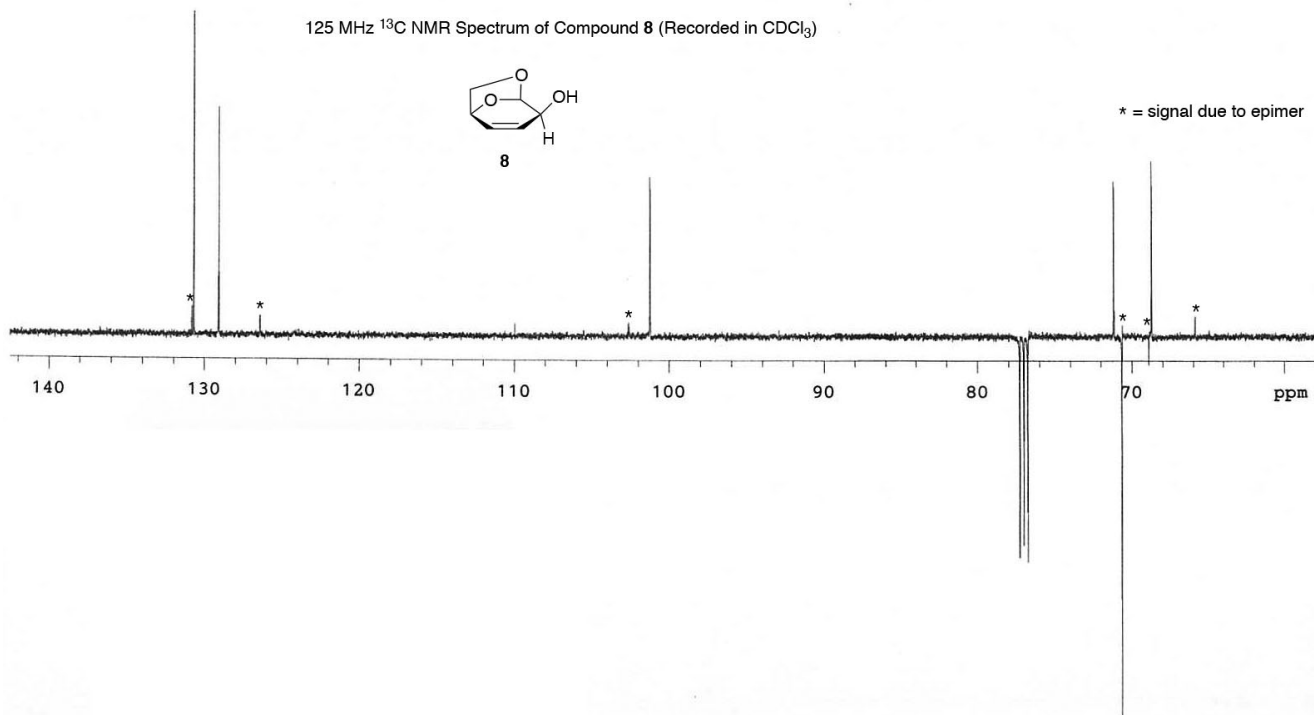
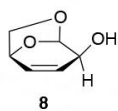
125 MHz ¹³C NMR Spectrum of Compound 7 (Recorded in CDCl₃)



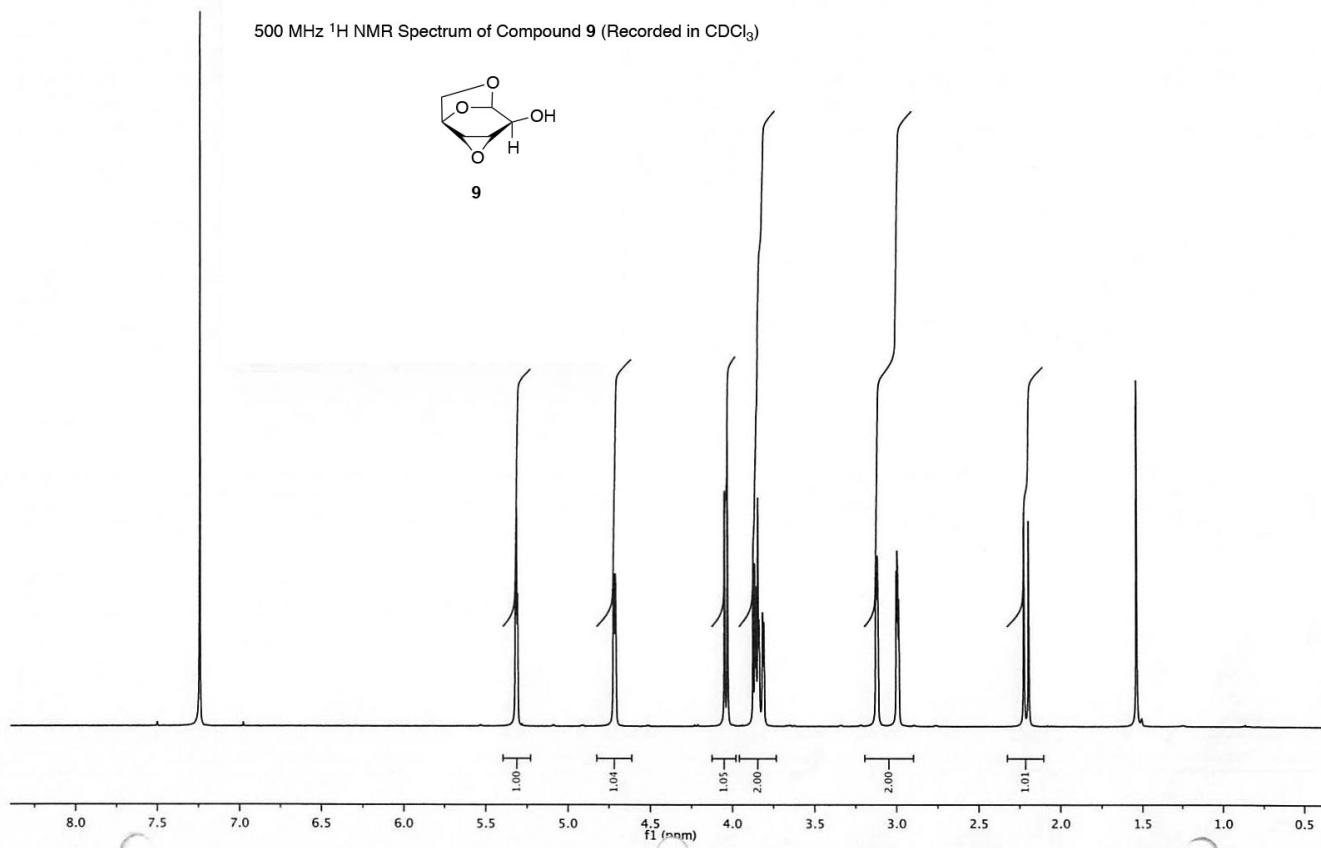
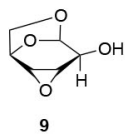
500 MHz ^1H NMR Spectrum of Compound 8 (Recorded in CDCl_3)



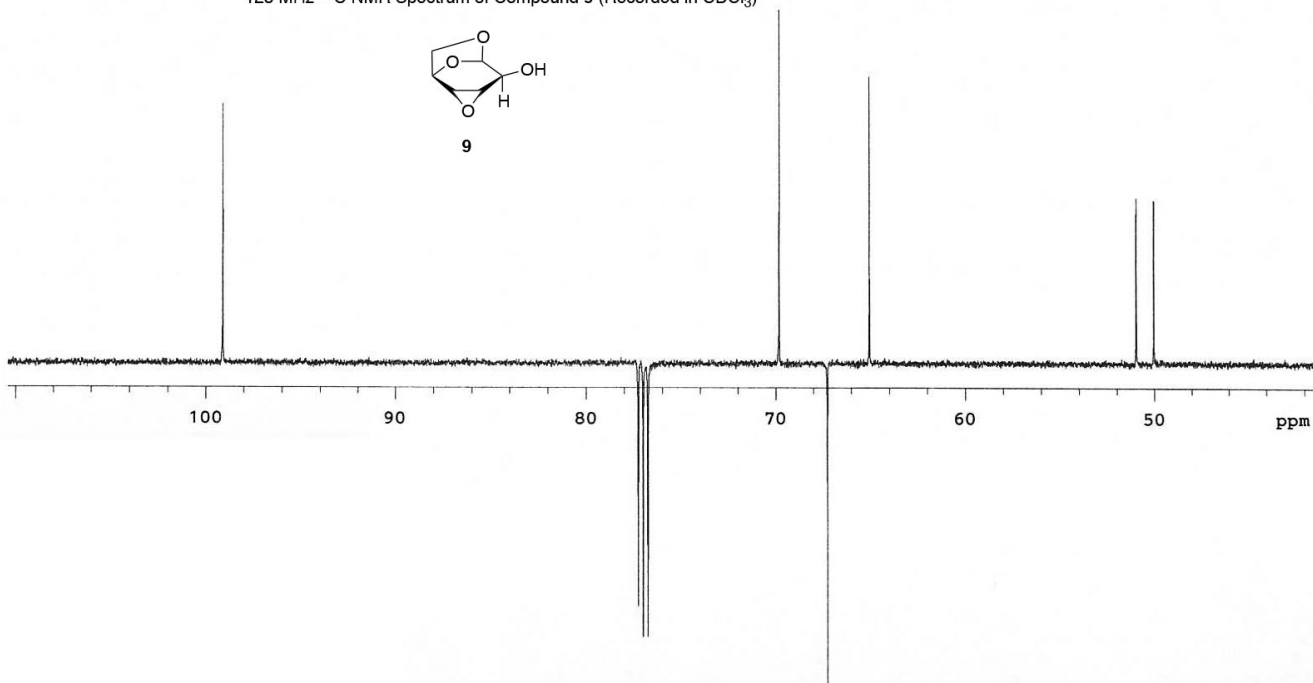
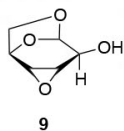
125 MHz ^{13}C NMR Spectrum of Compound 8 (Recorded in CDCl_3)



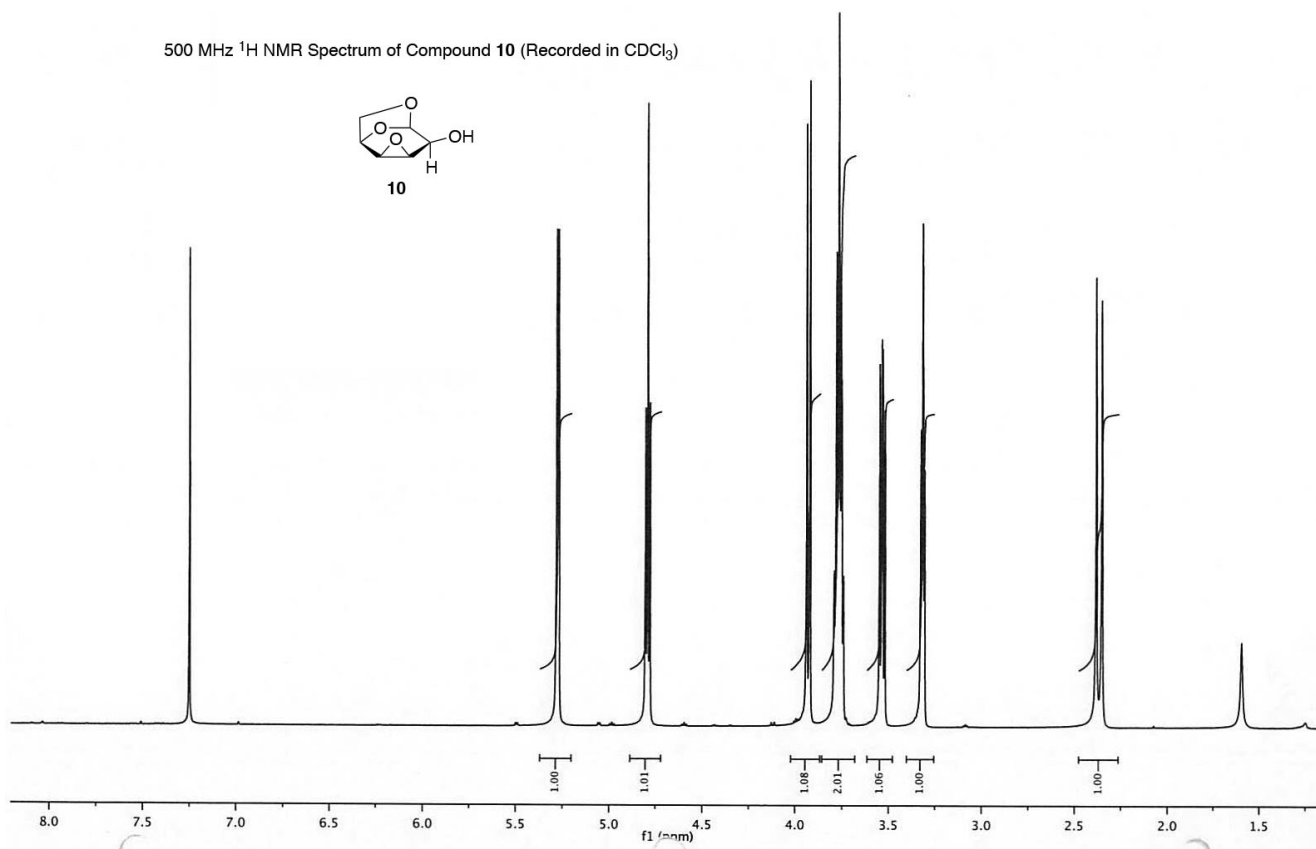
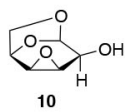
500 MHz ^1H NMR Spectrum of Compound 9 (Recorded in CDCl_3)



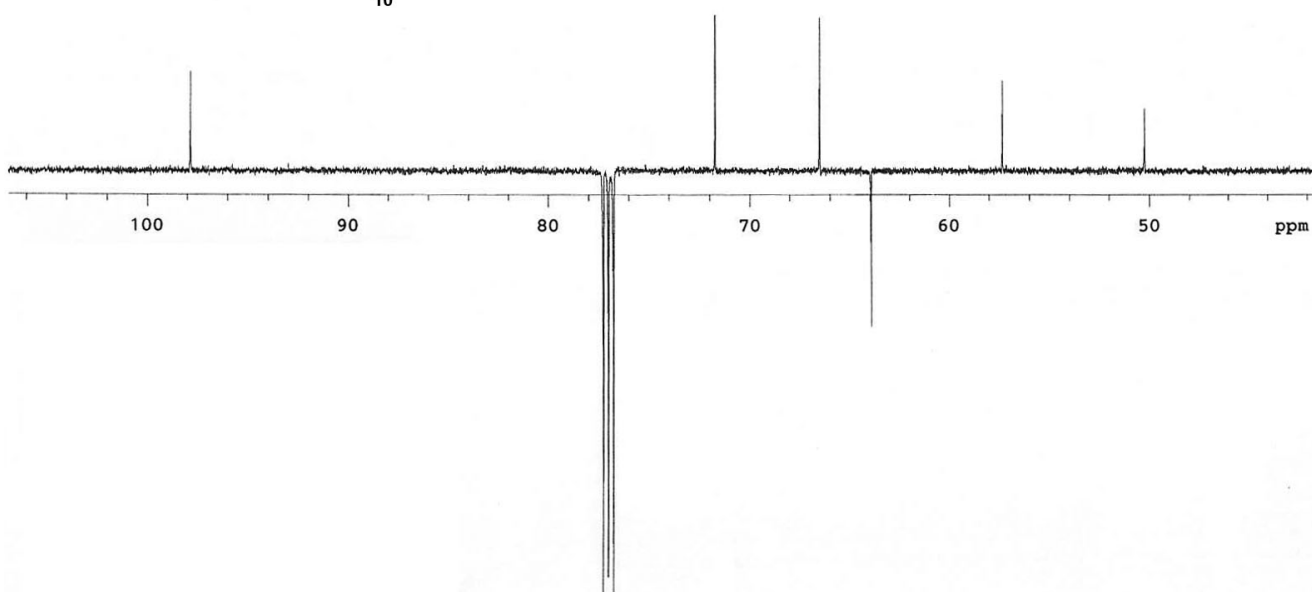
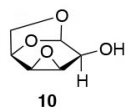
125 MHz ^{13}C NMR Spectrum of Compound 9 (Recorded in CDCl_3)



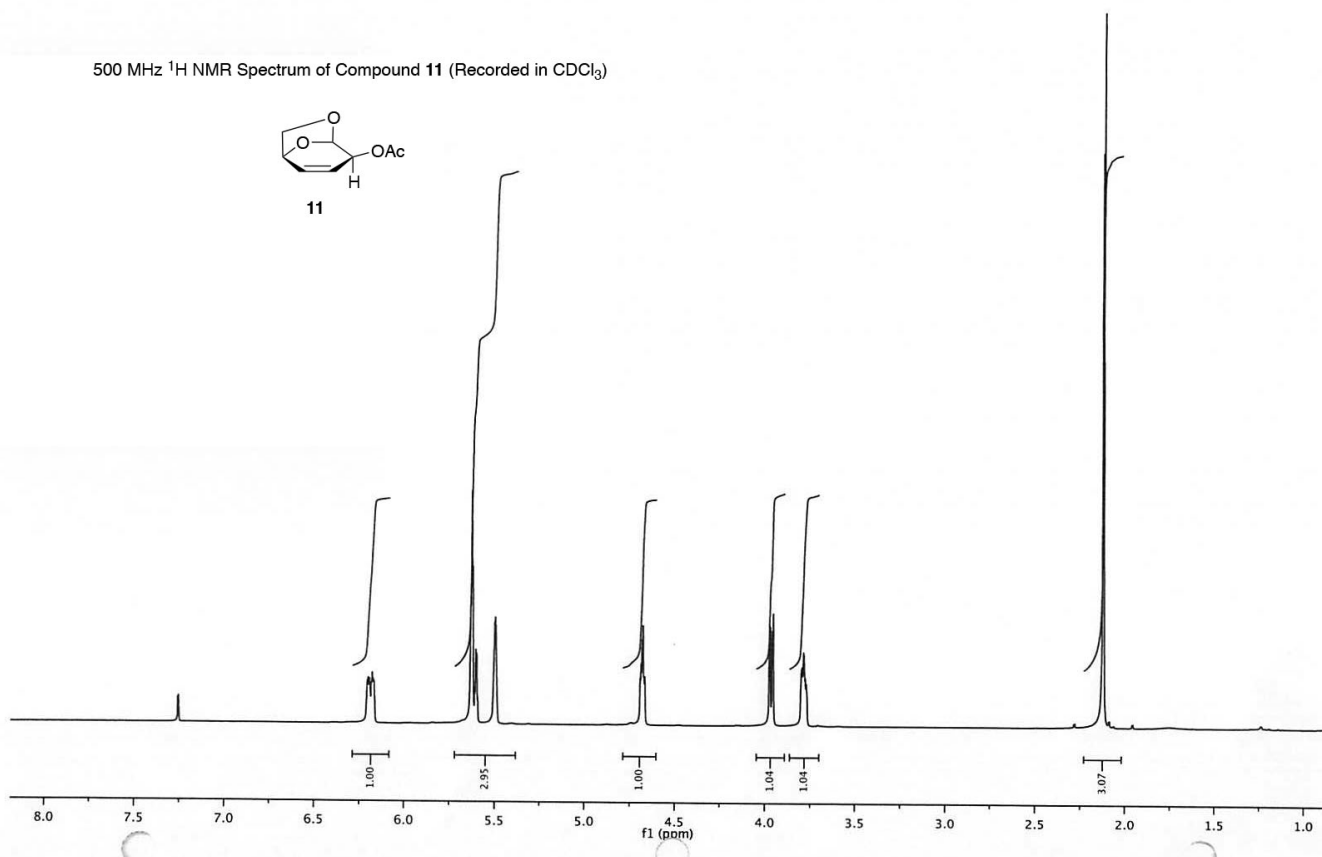
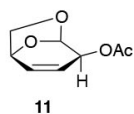
500 MHz ^1H NMR Spectrum of Compound **10** (Recorded in CDCl_3)



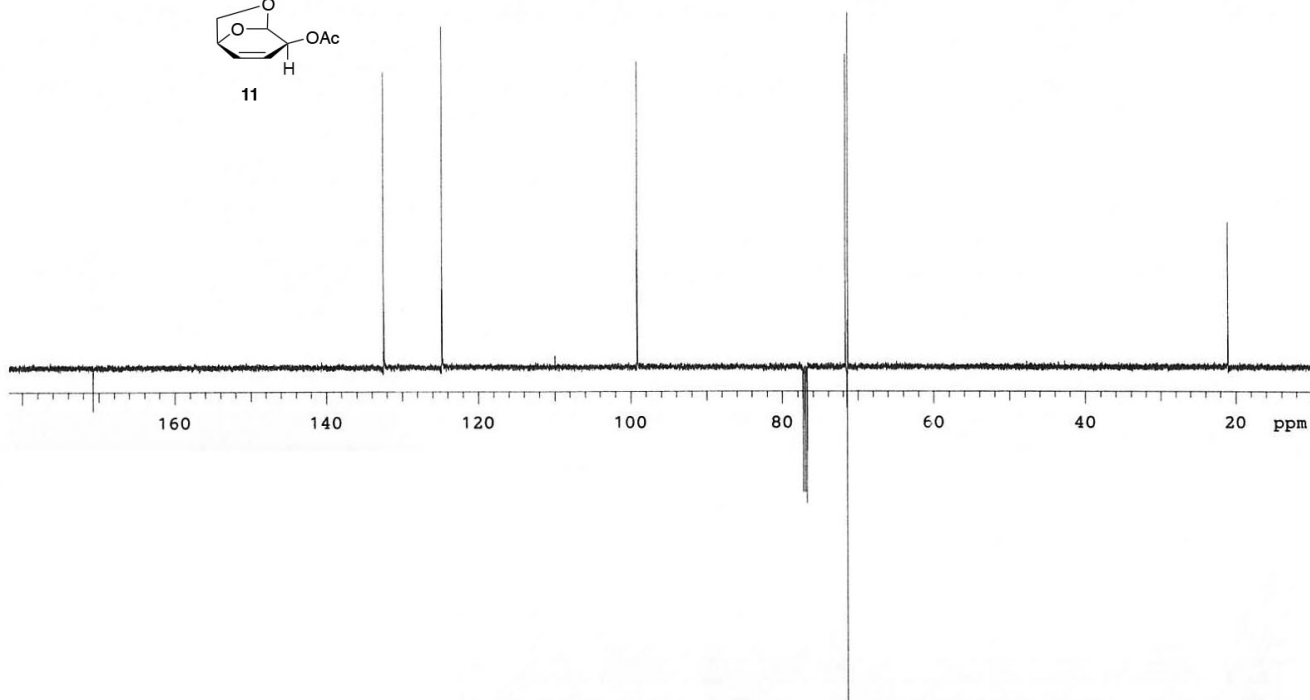
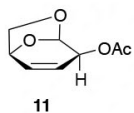
125 MHz ^{13}C NMR Spectrum of Compound **10** (Recorded in CDCl_3)



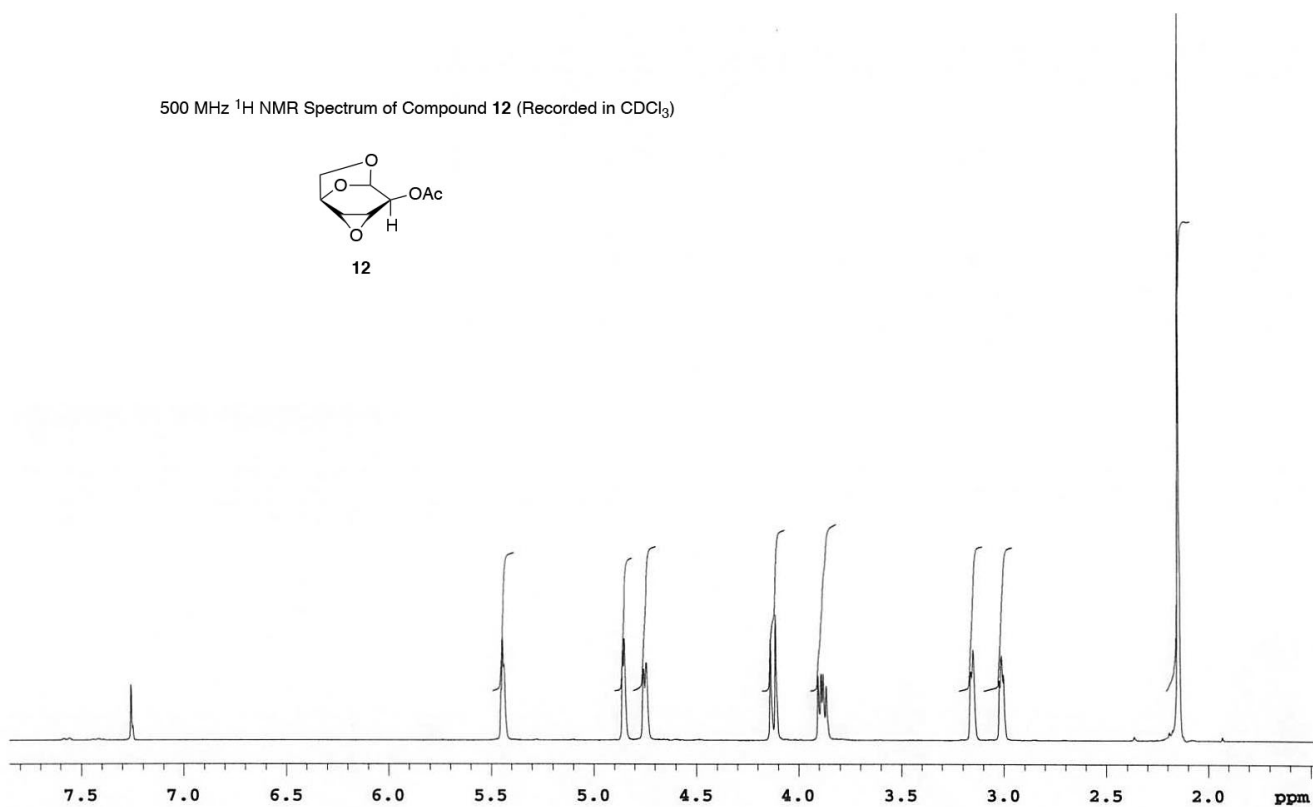
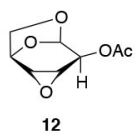
500 MHz ^1H NMR Spectrum of Compound **11** (Recorded in CDCl_3)



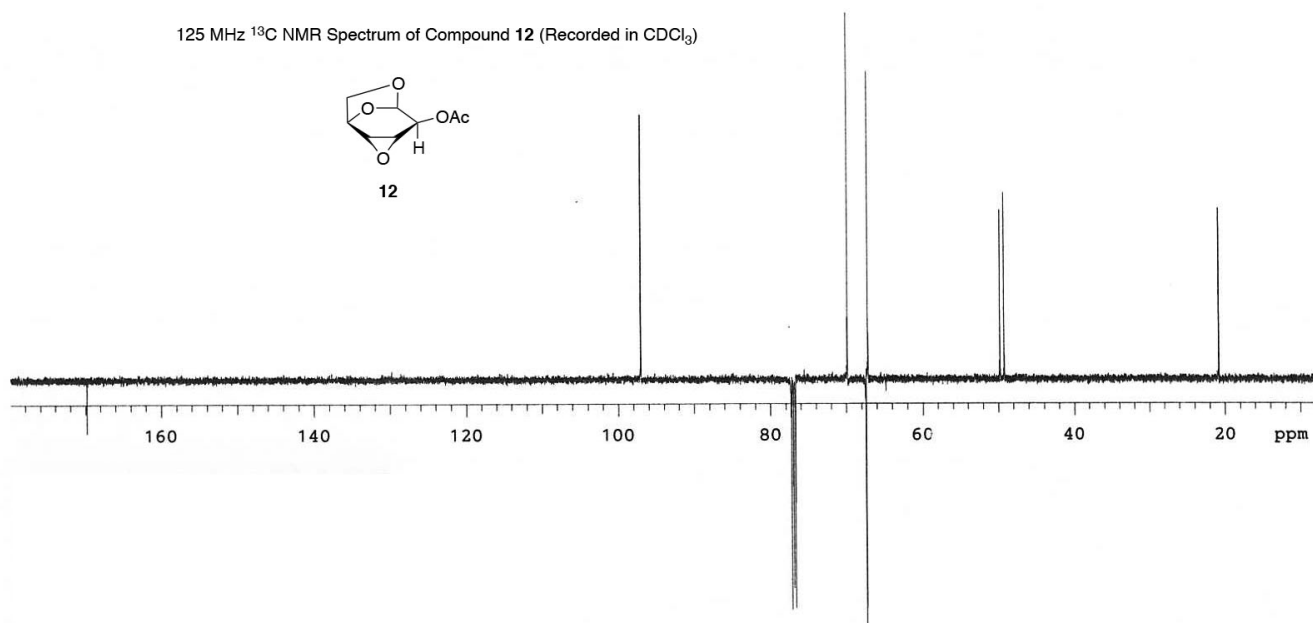
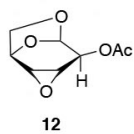
125 MHz ^{13}C NMR Spectrum of Compound **11** (Recorded in CDCl_3)



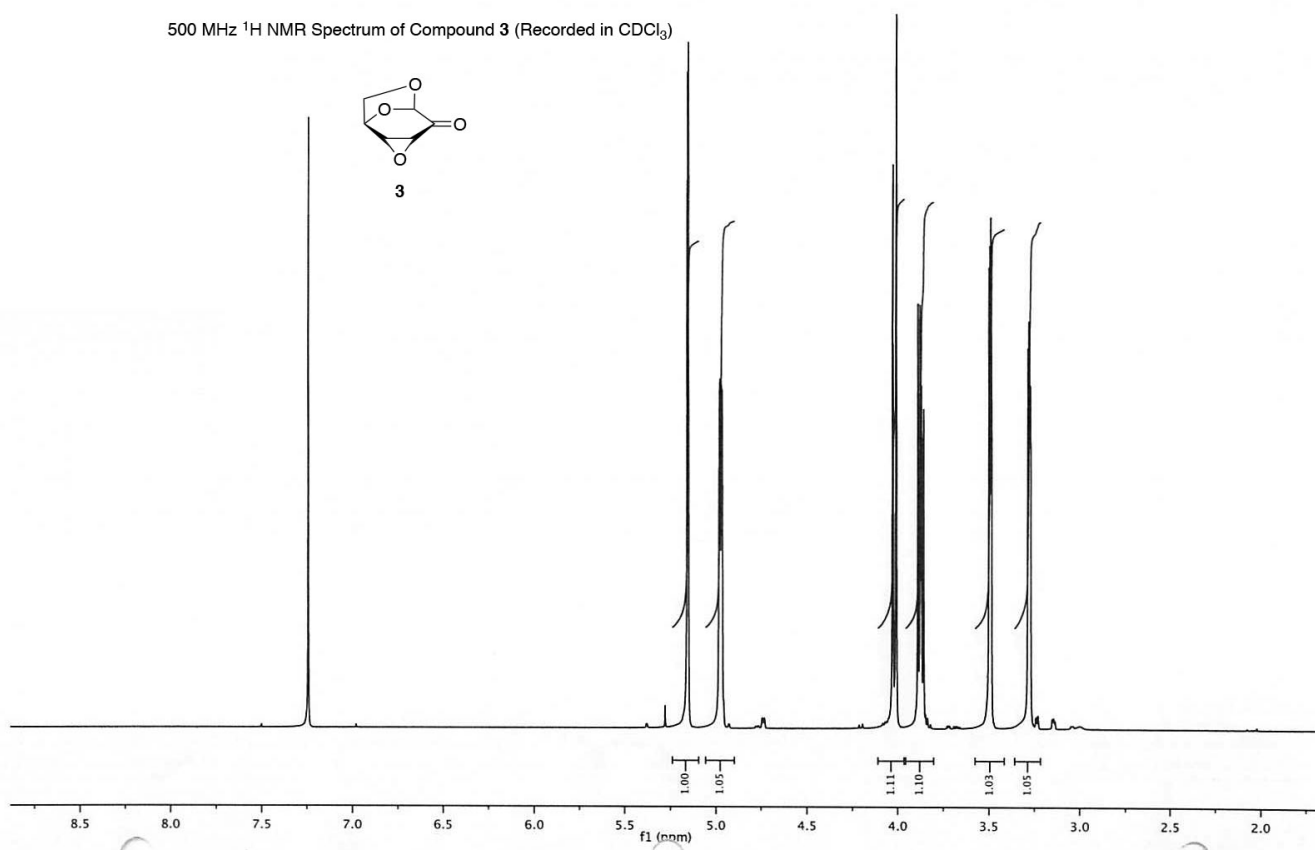
500 MHz ^1H NMR Spectrum of Compound 12 (Recorded in CDCl_3)



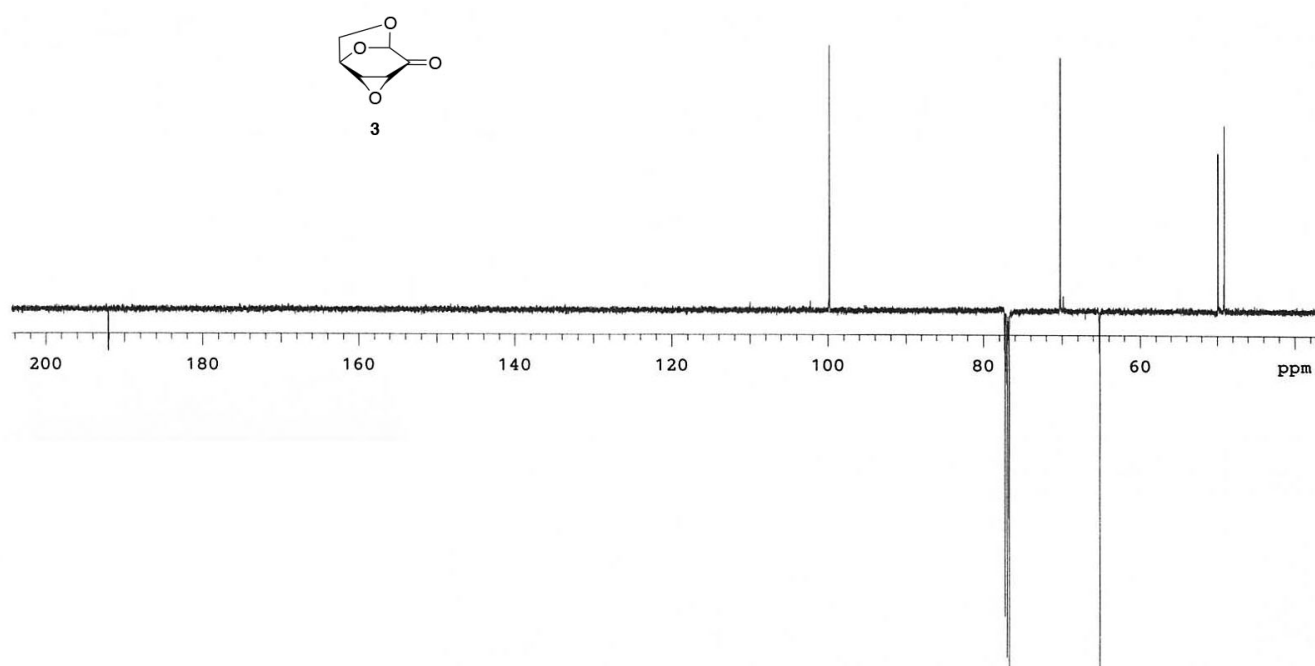
125 MHz ^{13}C NMR Spectrum of Compound 12 (Recorded in CDCl_3)



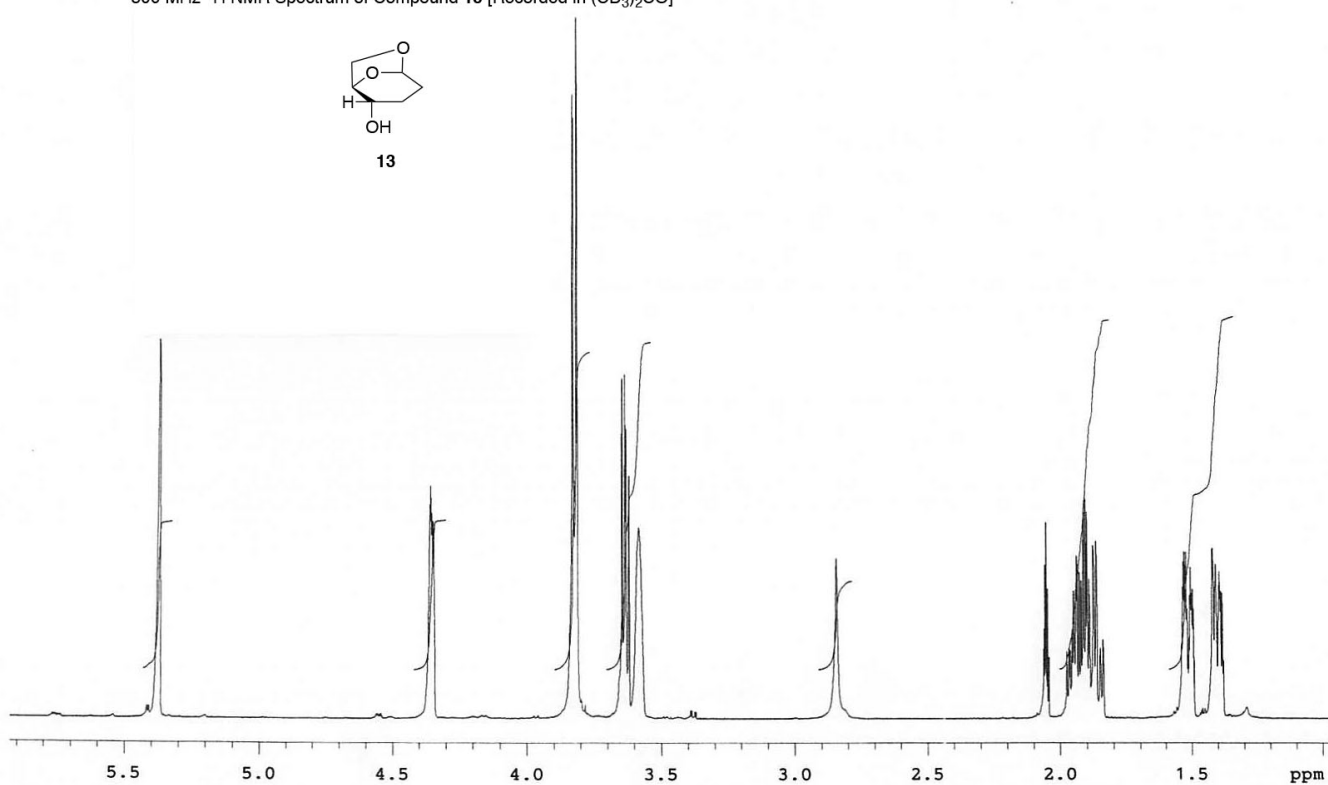
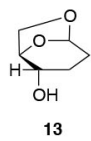
500 MHz ^1H NMR Spectrum of Compound **3** (Recorded in CDCl_3)



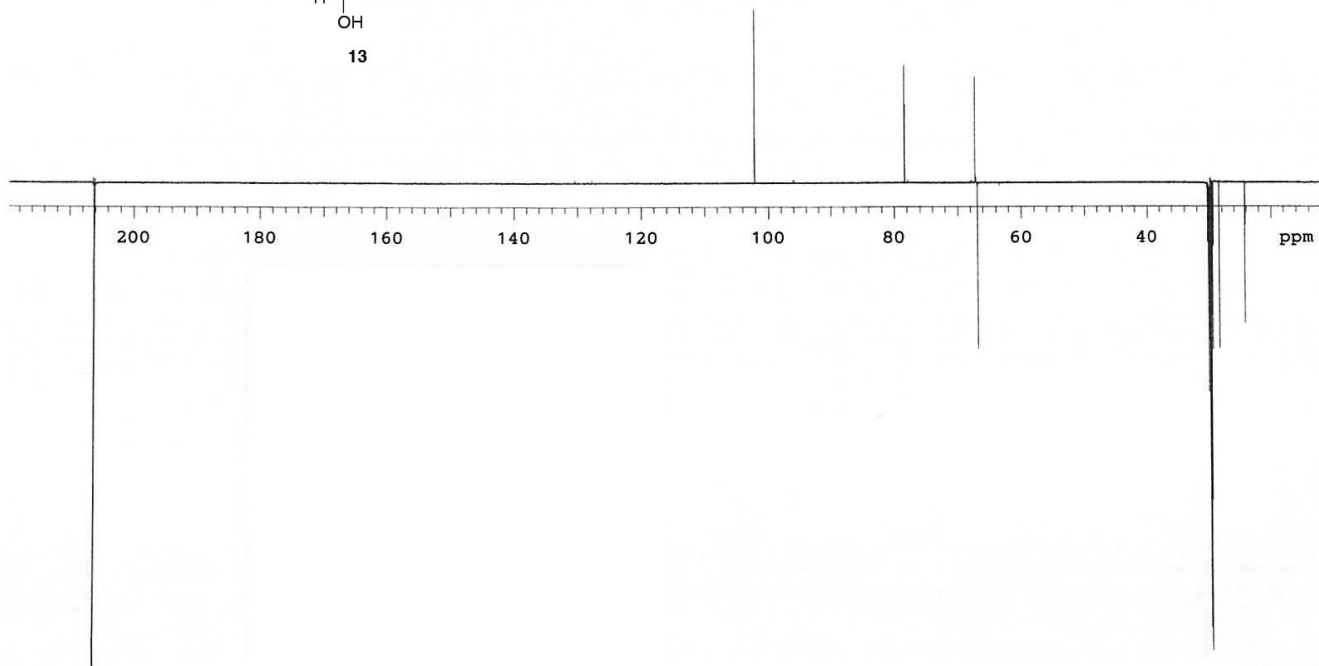
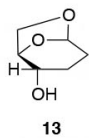
125 MHz ^{13}C NMR Spectrum of Compound **3** (Recorded in CDCl_3)



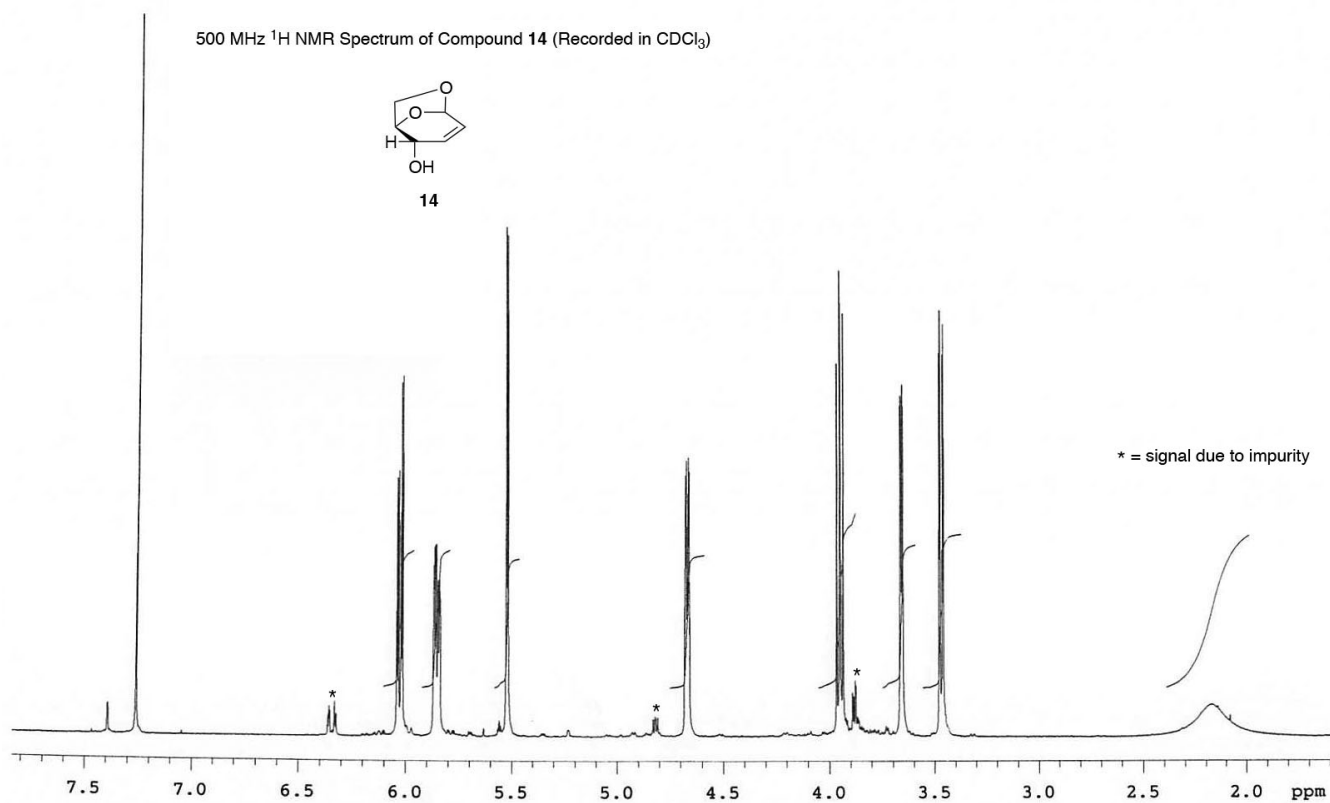
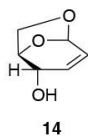
500 MHz ^1H NMR Spectrum of Compound **13** [Recorded in $(\text{CD}_3)_2\text{CO}$]



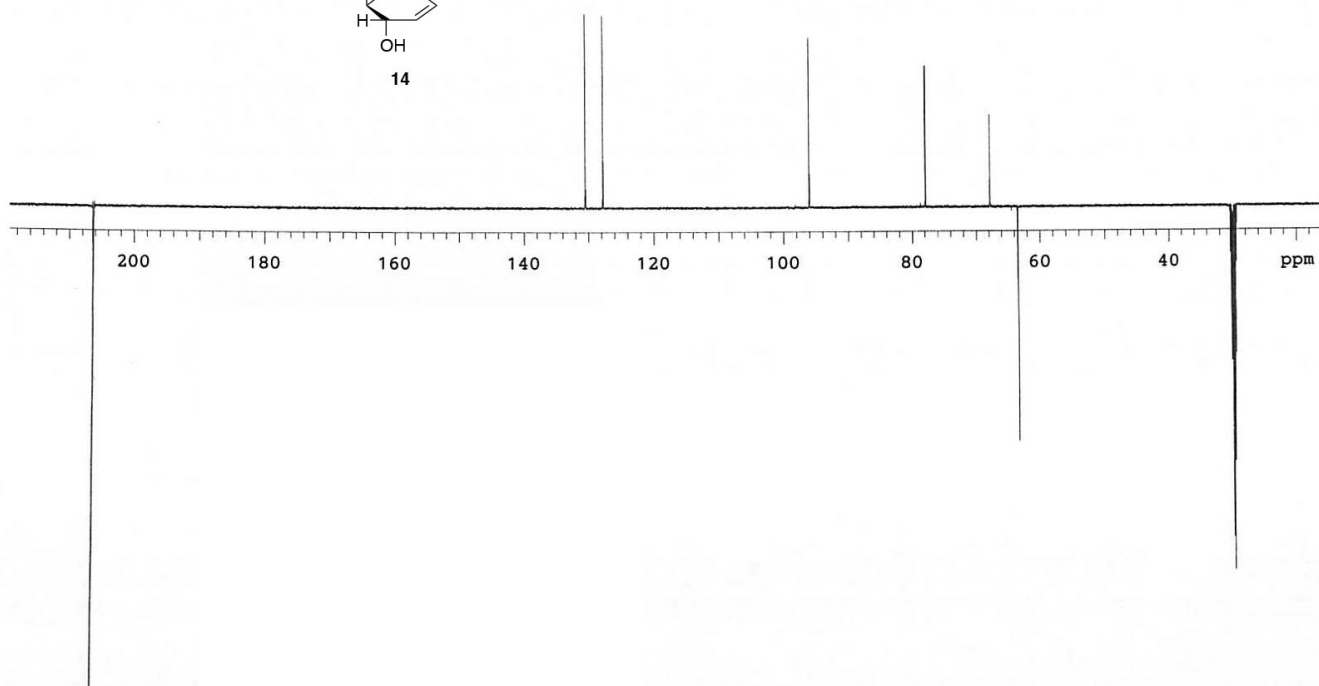
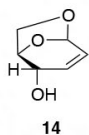
125 MHz ^{13}C NMR Spectrum of Compound **13** [Recorded in $(\text{CD}_3)_2\text{CO}$]



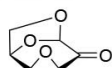
500 MHz ^1H NMR Spectrum of Compound 14 (Recorded in CDCl_3)



125 MHz ^{13}C NMR Spectrum of Compound 14 [Recorded in $(\text{CD}_3)_2\text{CO}$]

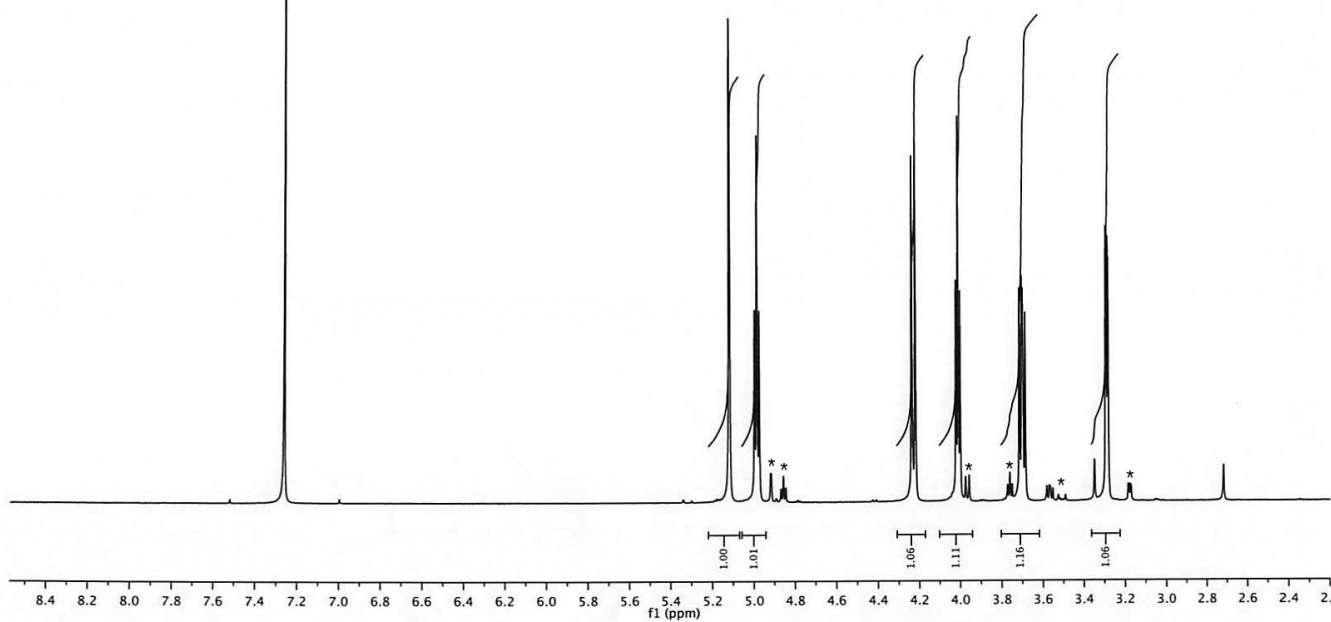


500 MHz ^1H NMR Spectrum of Compound 4 (Recorded in CDCl_3)

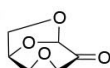


4

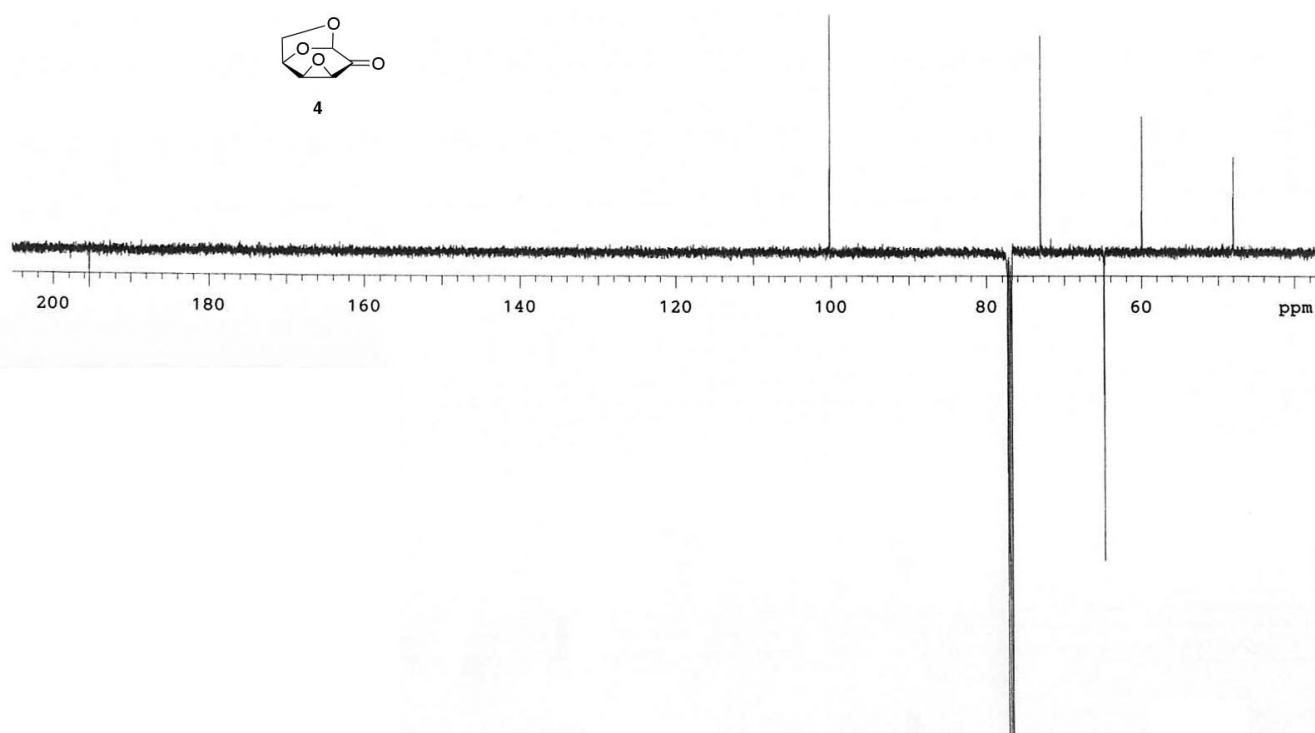
* = signal due to impurity



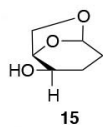
125 MHz ^{13}C NMR Spectrum of Compound 4 (Recorded in CDCl_3)



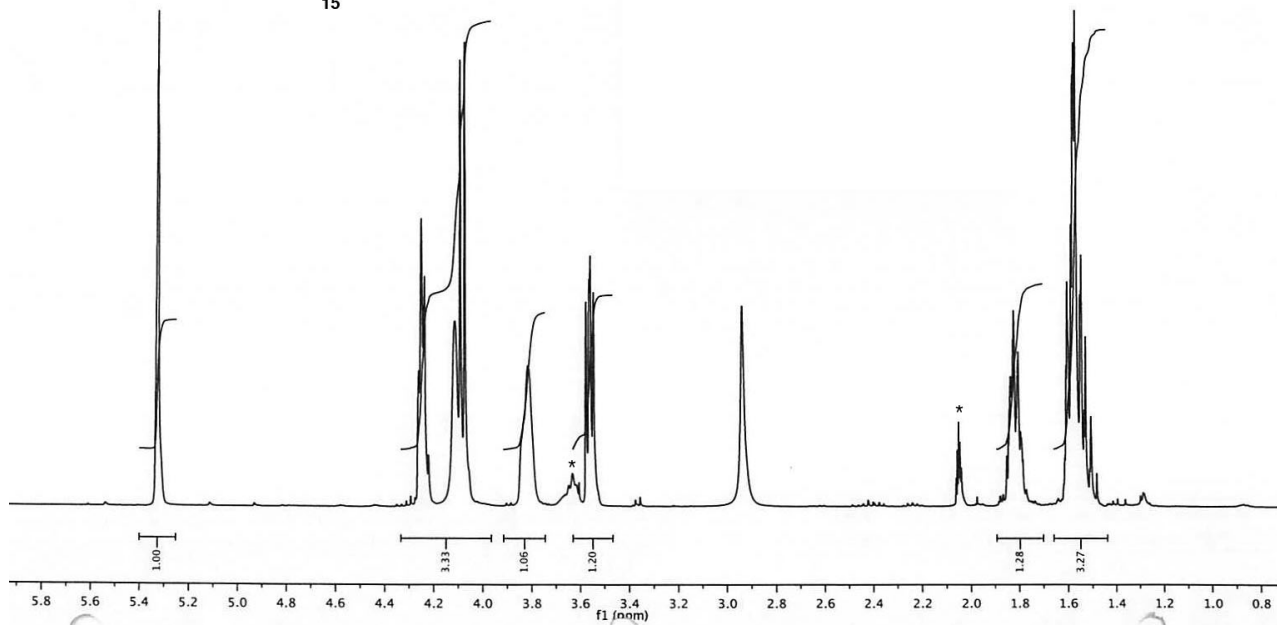
4



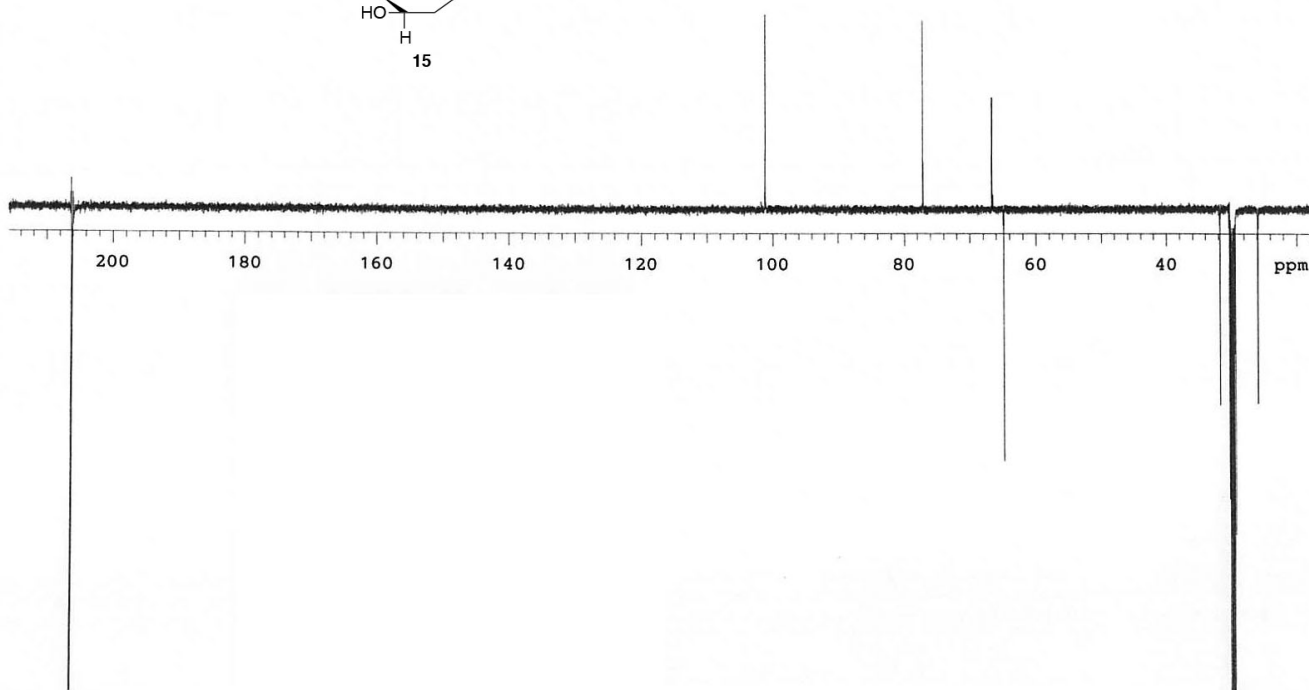
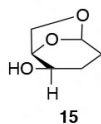
500 MHz ^1H NMR Spectrum of Compound 15 [Recorded in $(\text{CD}_3)_2\text{CO}$]



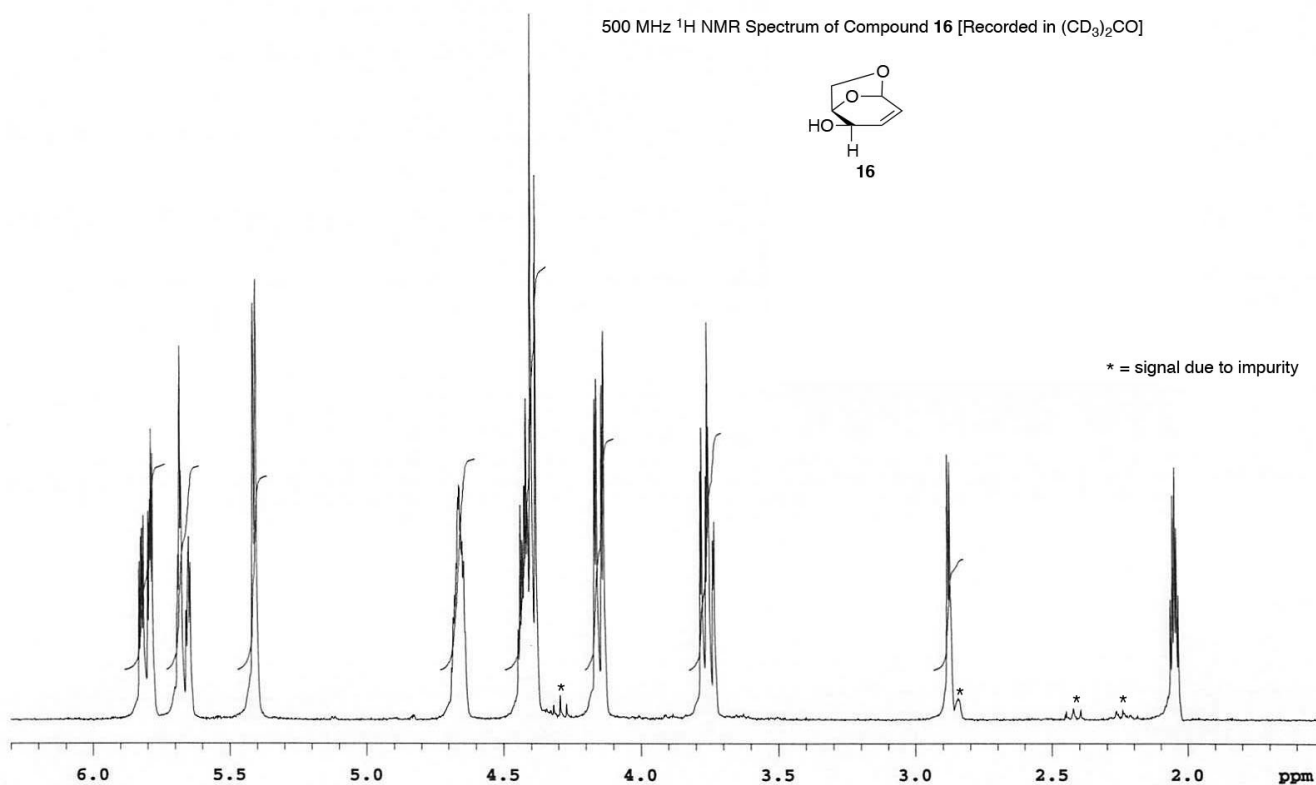
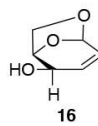
* = signal due to impurity



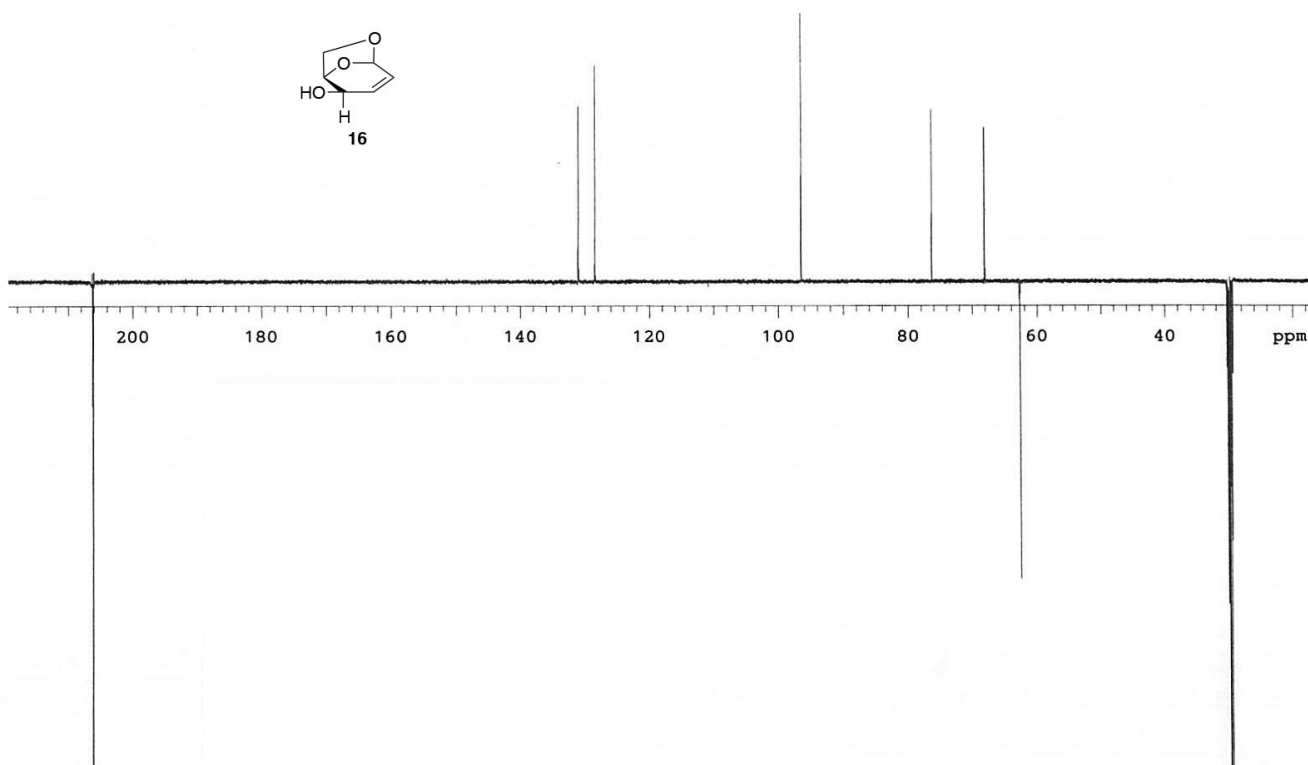
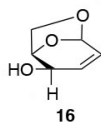
125 MHz ^{13}C NMR Spectrum of Compound 15 [Recorded in $(\text{CD}_3)_2\text{CO}$]



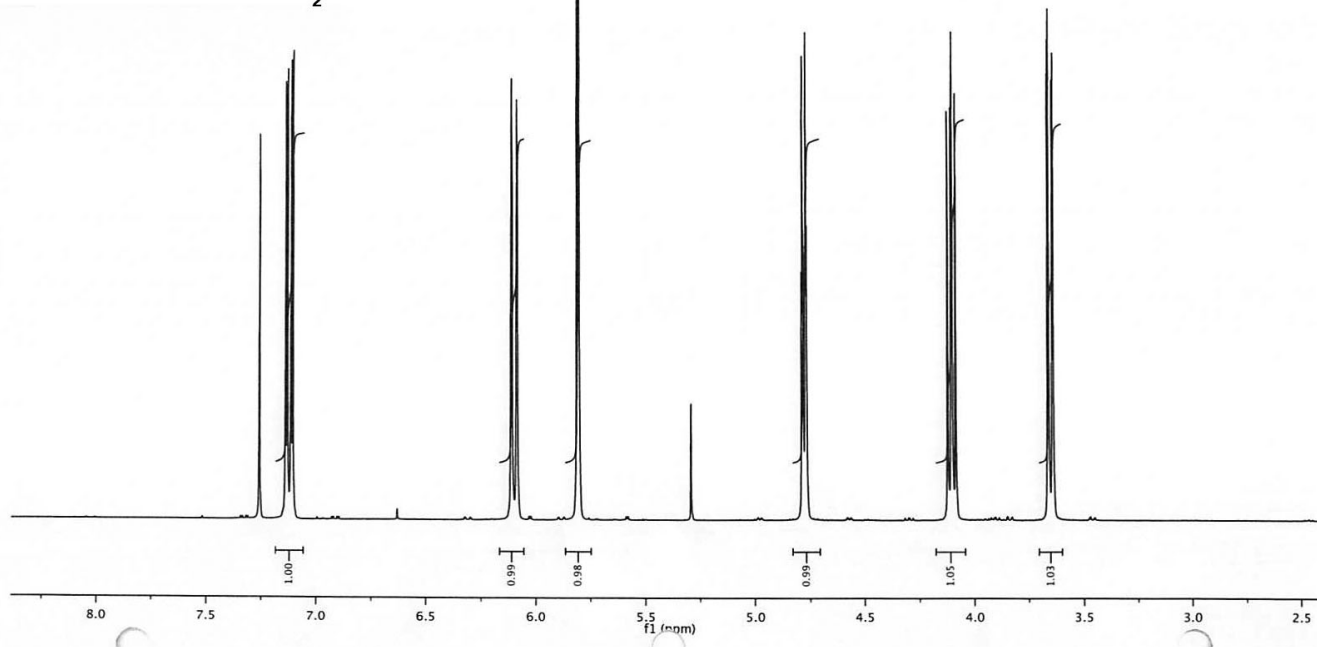
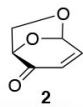
500 MHz ^1H NMR Spectrum of Compound 16 [Recorded in $(\text{CD}_3)_2\text{CO}$]



125 MHz ^{13}C NMR Spectrum of Compound 16 [Recorded in $(\text{CD}_3)_2\text{CO}$]



500 MHz ^1H NMR Spectrum of Compound 2 (Recorded in CDCl_3)



125 MHz ^{13}C NMR Spectrum of Compound 2 (Recorded in CDCl_3)

