An Expeditious Synthesis of DPD and Boron Binding Studies

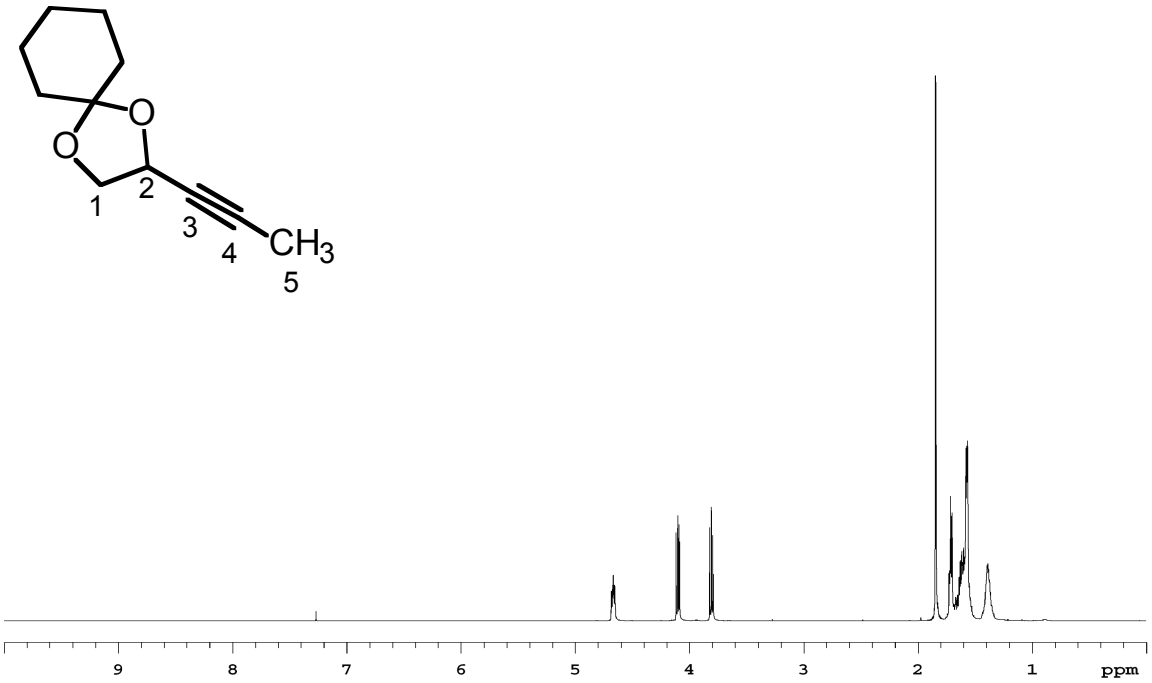
Martin F. Semmelhack,[a*] Shawn R. Campagna,[a] Michael J. Federle,[b] Bonnie L. Bassler[b]

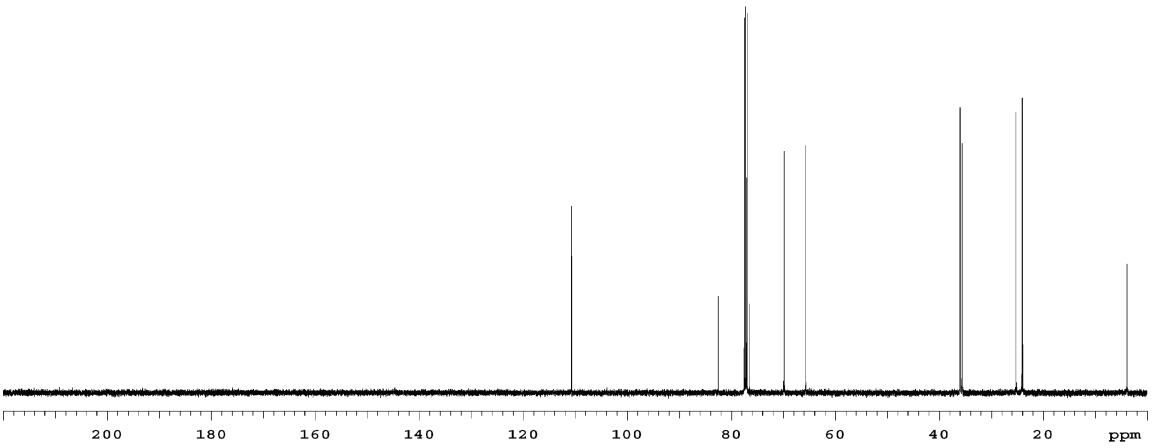
Departments of Chemistry[a] and Molecular Biology, [b] Princeton University, Princeton, NJ 08544

Table of Contents:

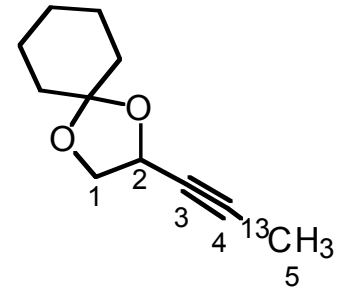
page	content
1	Cover page
2	NMR spectra for **10**
3	NMR spectra for **10**-($^{13}C_5$)
4	NMR spectra for **11**
5	NMR spectra for **13**
6	^{1}HNMR for **13** extracted into $CDCl_3$ from D_2O and ^{13}CNMR spectrum of a mixture of **13** and **11** in $CDCl_3$
7	^{1}HNMR monitoring of conversion of **13** to **11** in $CDCl_3$
8	NMR spectra for **11-($^{13}C_1$)** in $CDCl_3$
9	NMR spectra for **13-($^{13}C_1$)** in D_2O
10	^{1}HNMR spectrum of **1 (DPD)** in D_2O, pD 1.5
11	^{1}H-^{1}H DQCOSY spectrum of **1** in D_2O, pD 1.5
12	^{13}CNMR spectrum of **1** in 95:5 H2O:D2O, pH 1.5
13	^{1}HNMR of (S)-1-(3-methylquinoxalin-2-yl)-ethane-1,2-diol in D_2O, pD 1.5
14	^{11}B NMR spectrum of 0.1 mM DPD in 0.4 nM $B(OH)_3$, pH 7.5

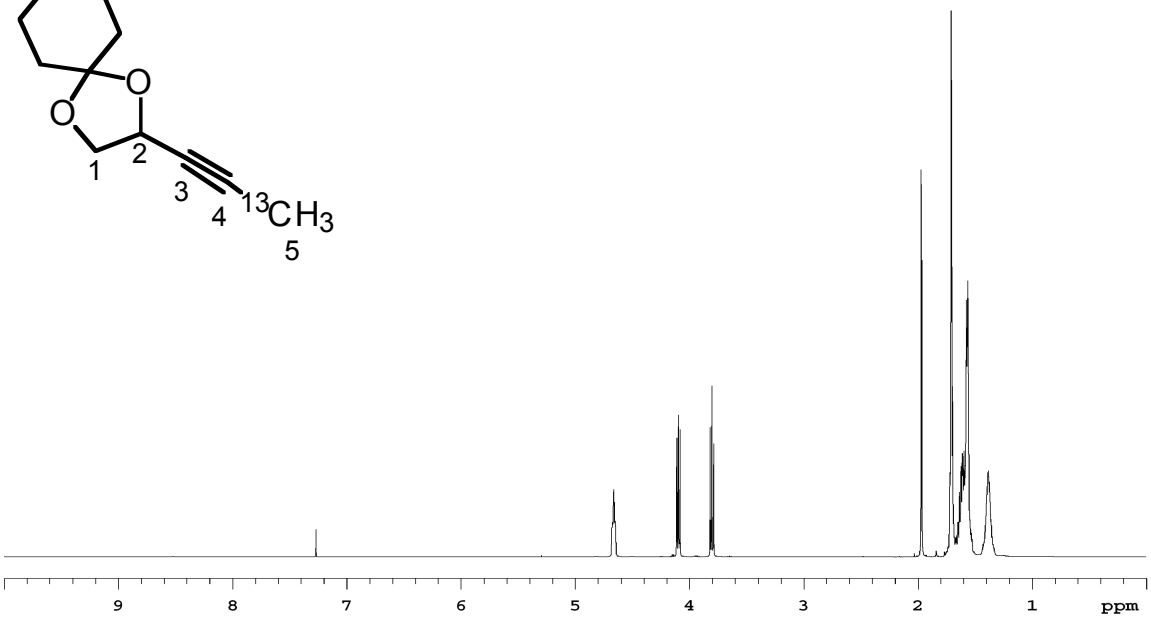
^{1}H and ^{13}C NMR spectra of **10** in $CDCl_3$

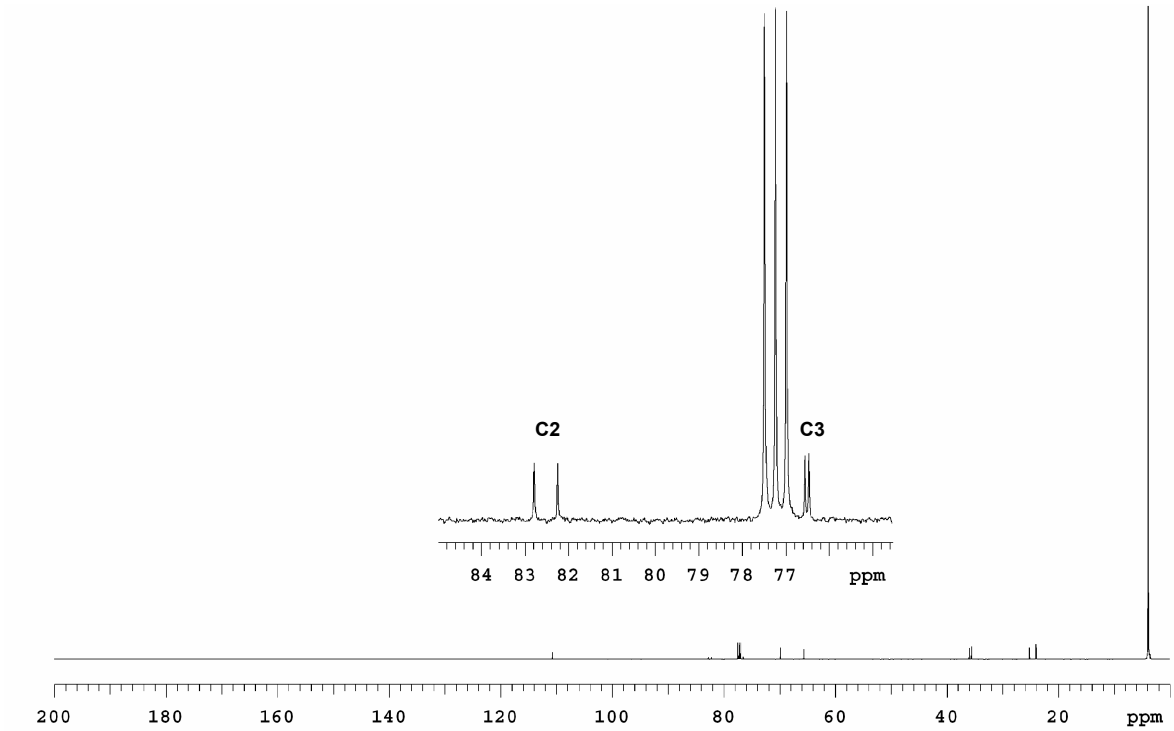




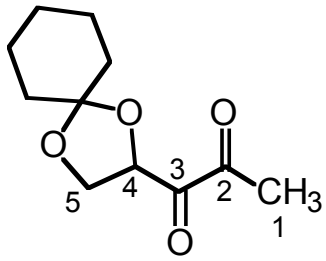
^{1}H and ^{13}C NMR spectra of **10-($^{13}C_5$)** in $CDCl_3$

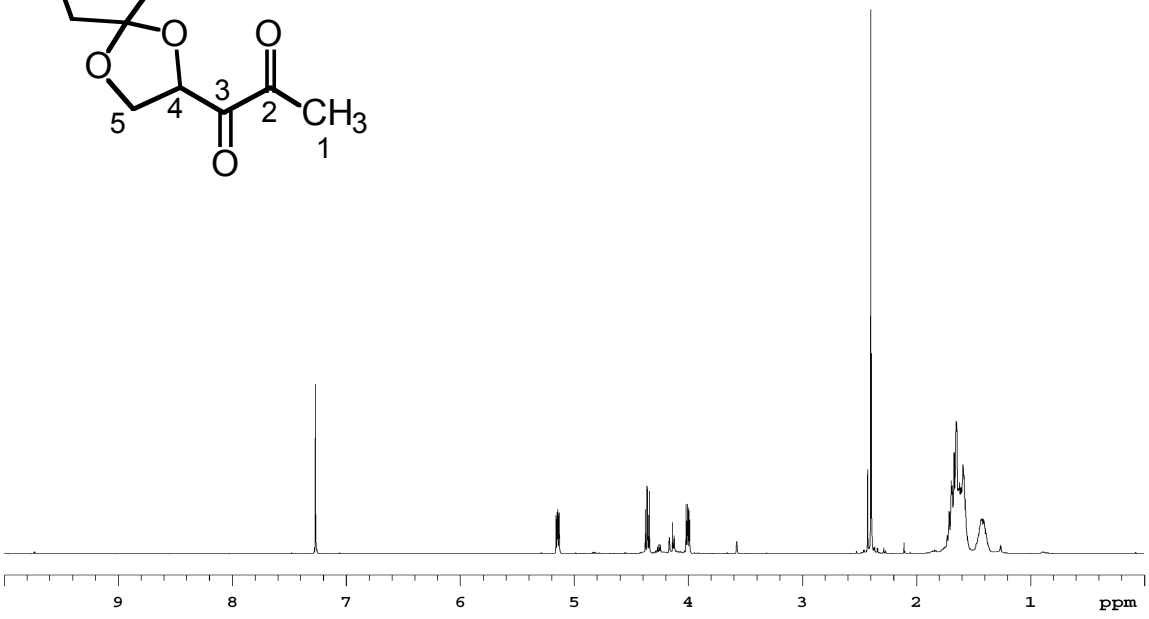


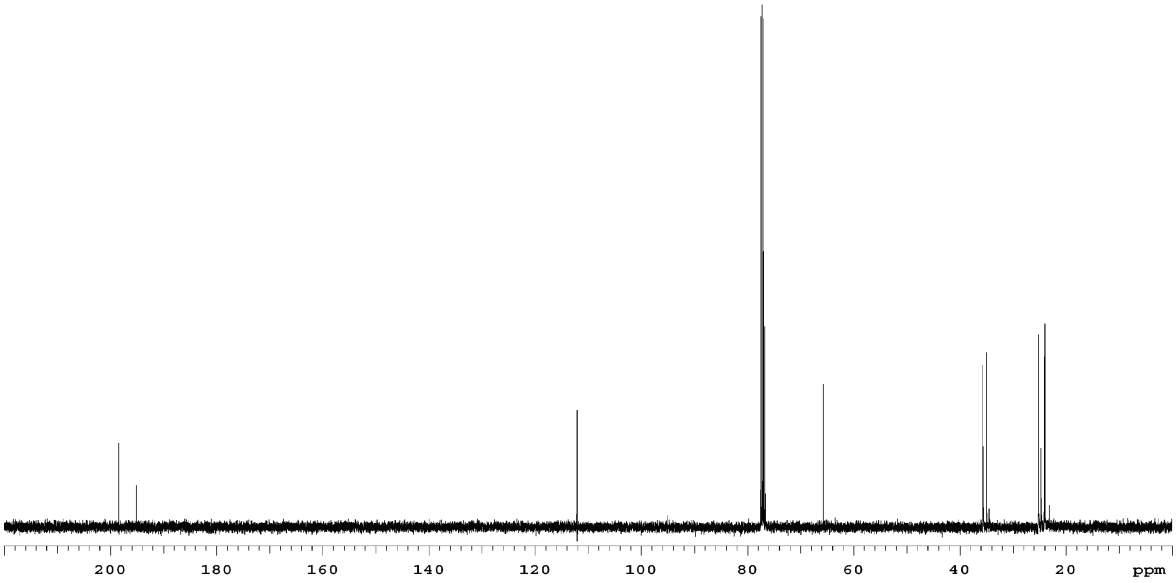




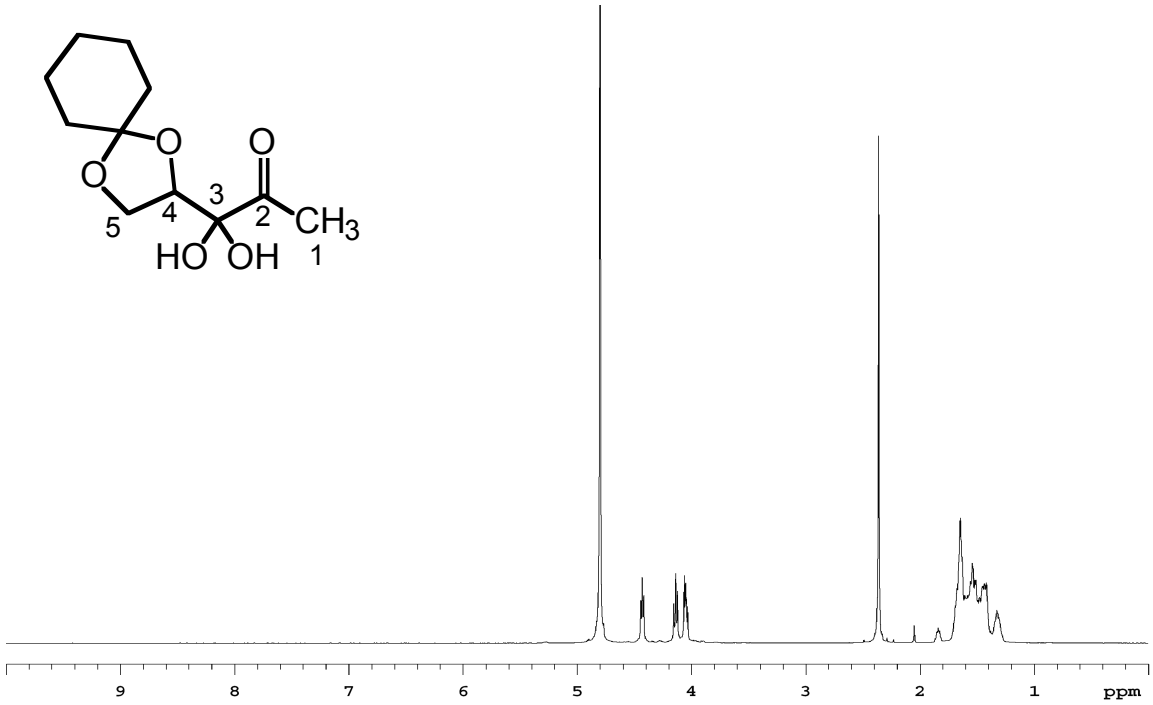
^{1}H and ^{13}C NMR spectra of **11** in $CDCl_3$

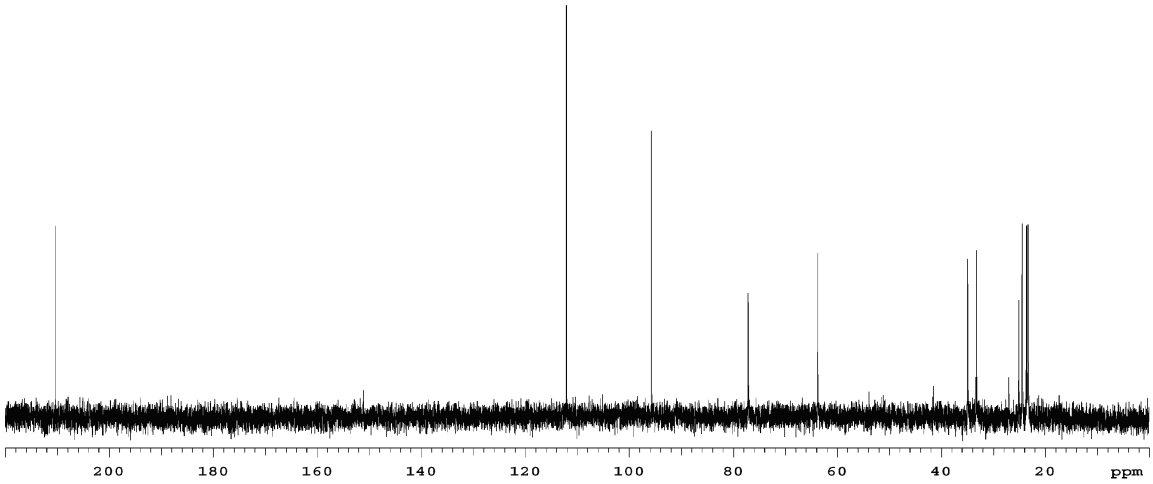




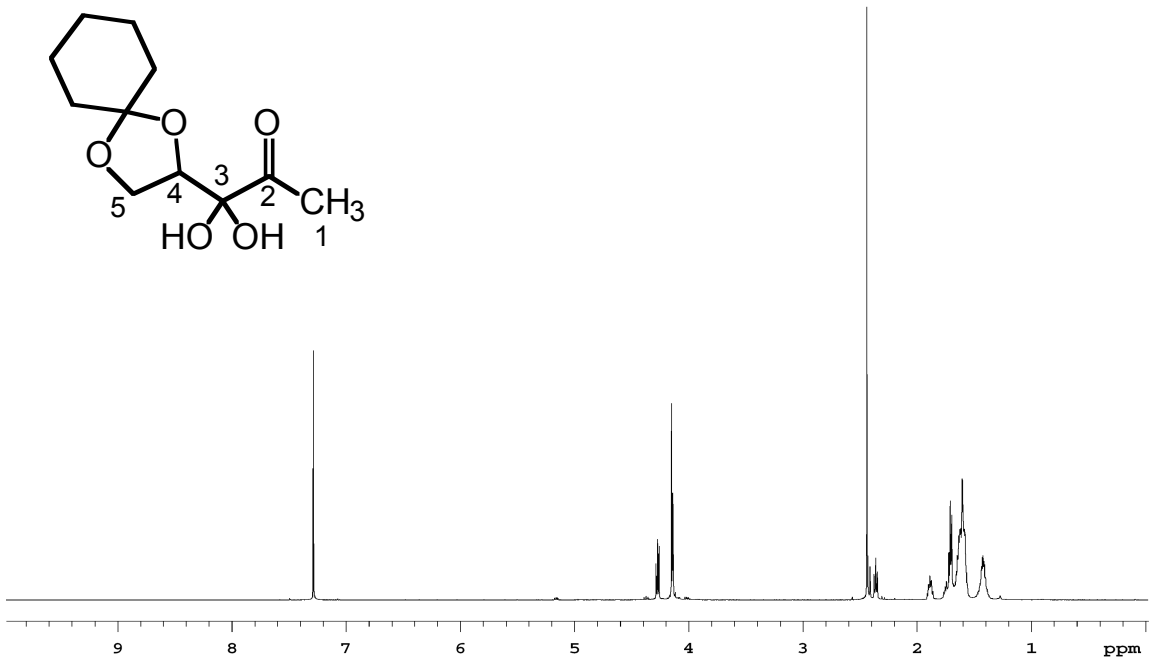


^{1}H and ^{13}C NMR spectra of **13** in D_2O

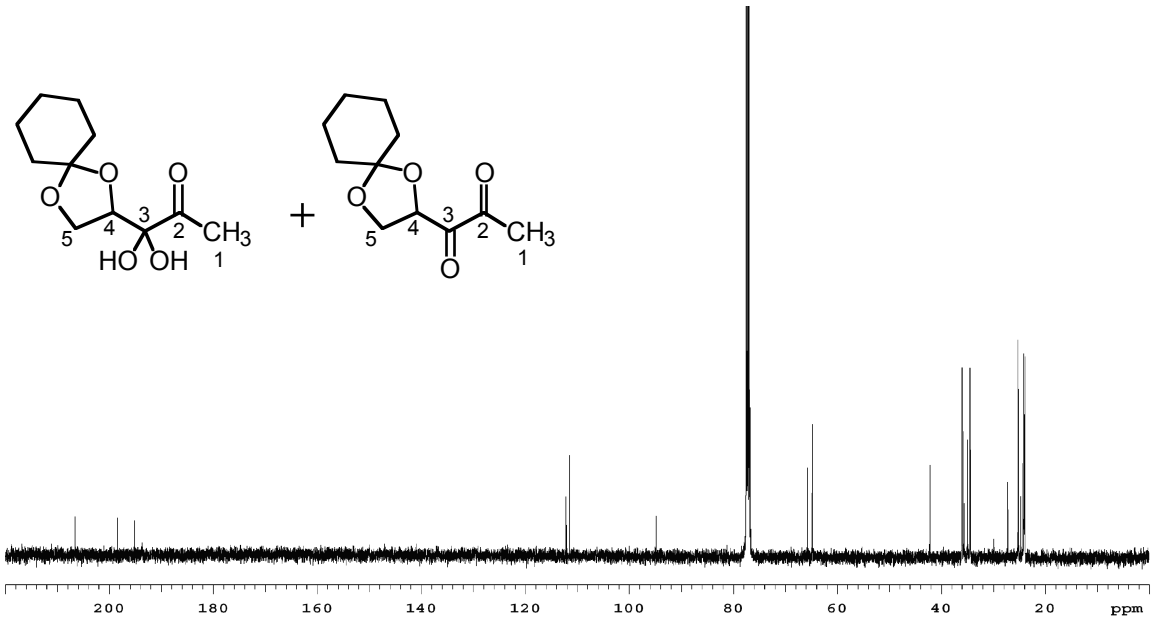




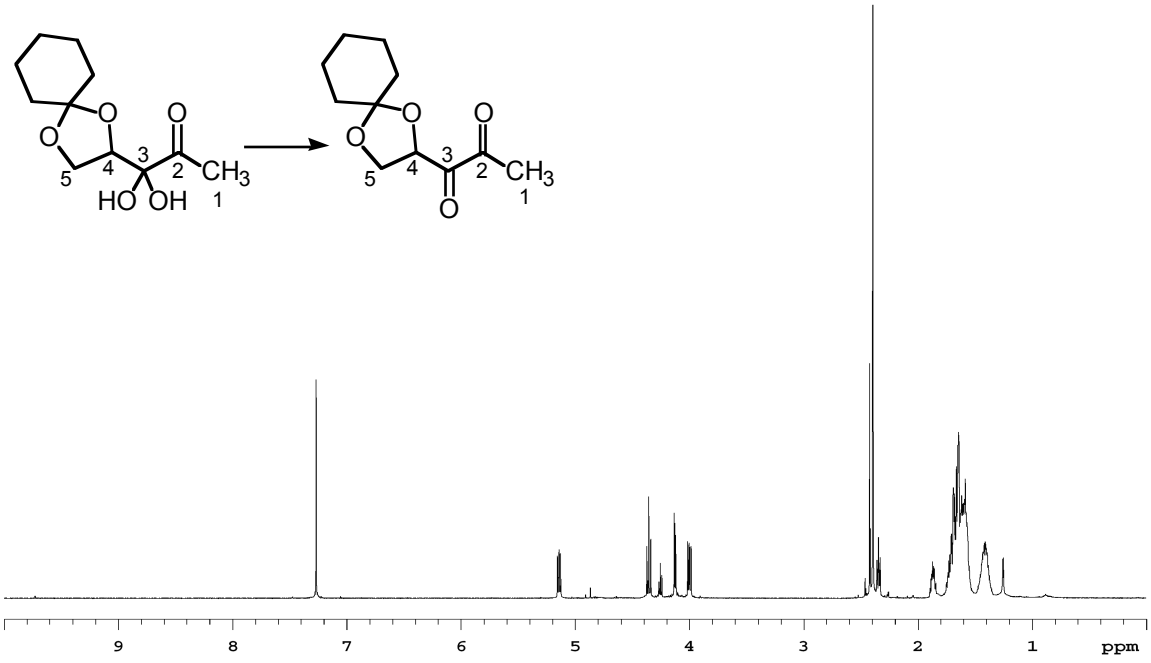
^{1}H NMR spectrum of **13** extracted into $CDCl_3$ from D_2O



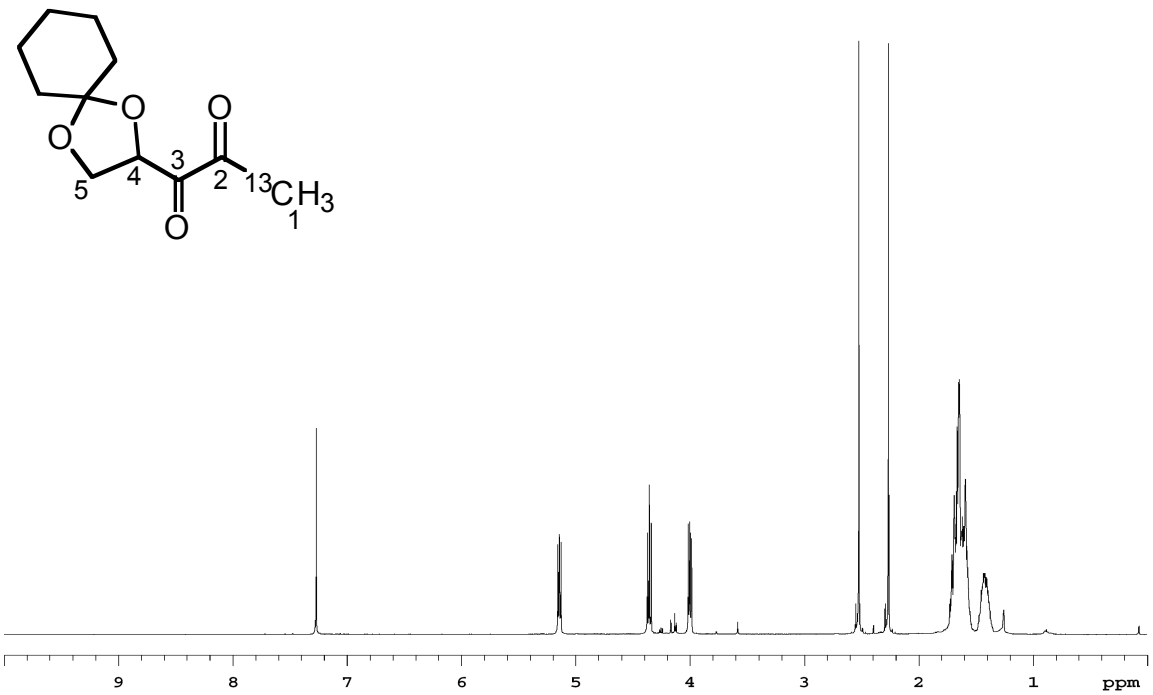
^{13}C NMR spectrum of a mixture of **13** and **11** in $CDCl_3$

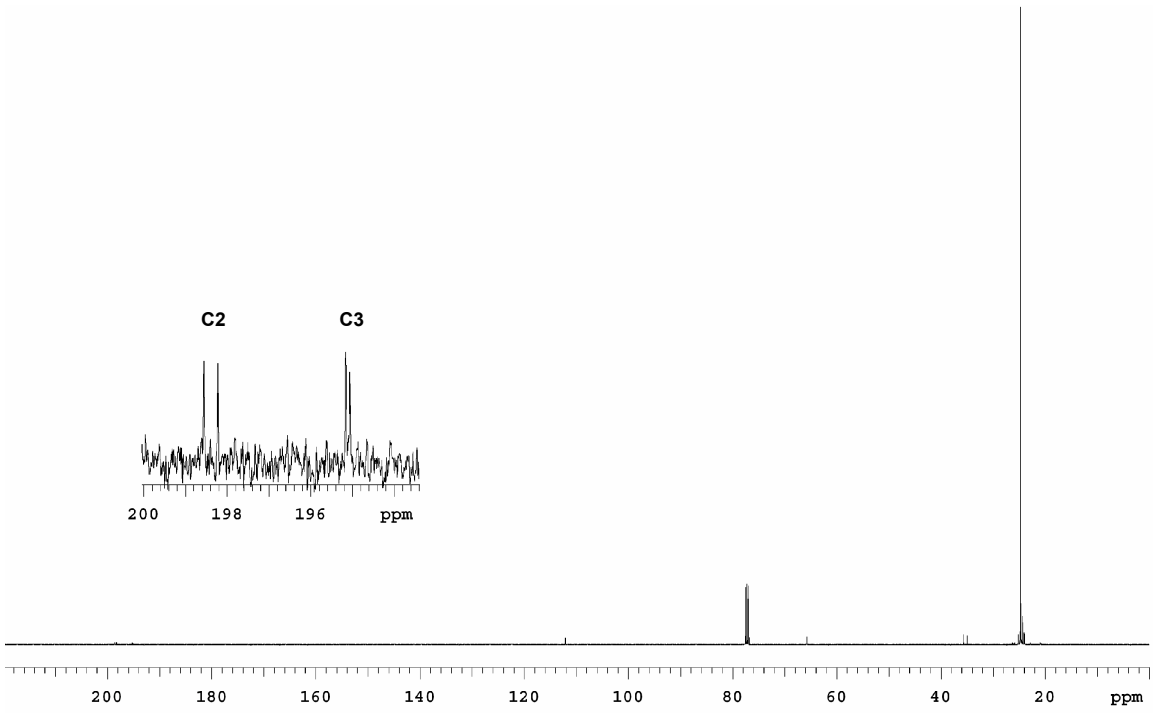


^{1}H NMR monitoring of conversion of **13** to **11** after 26 h in $CDCl_3$

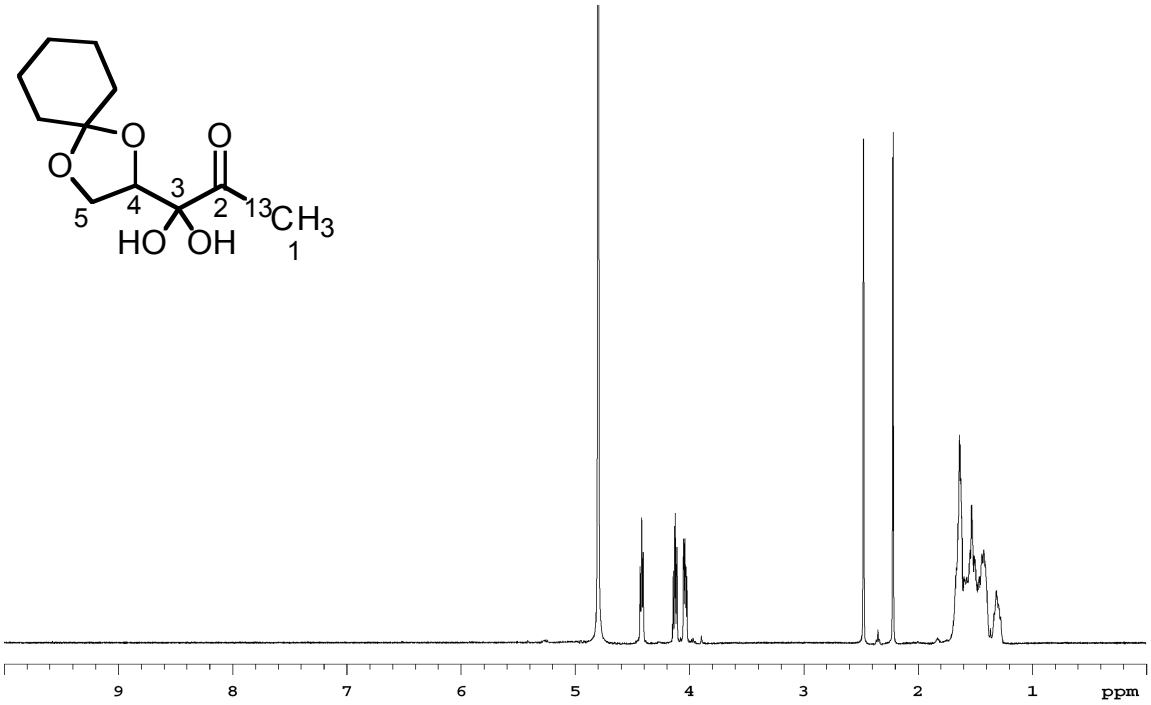


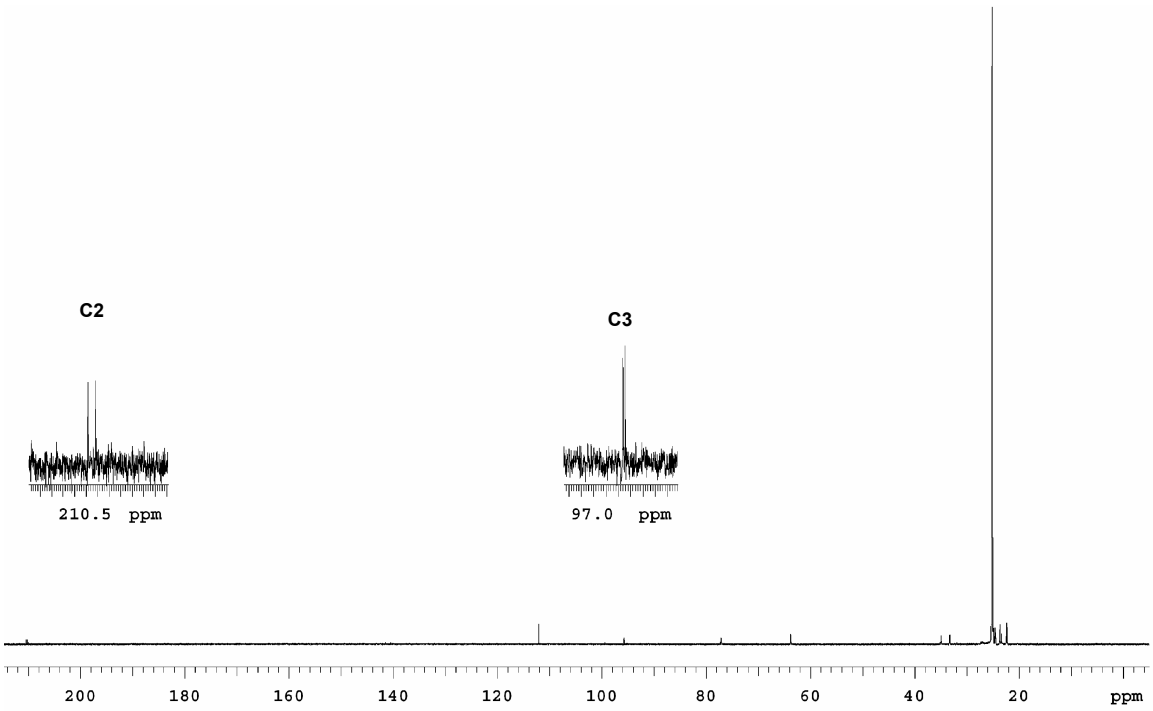
^{1}H and ^{13}C NMR spectrum of **11-($^{13}C_1$)** in $CDCl_3$



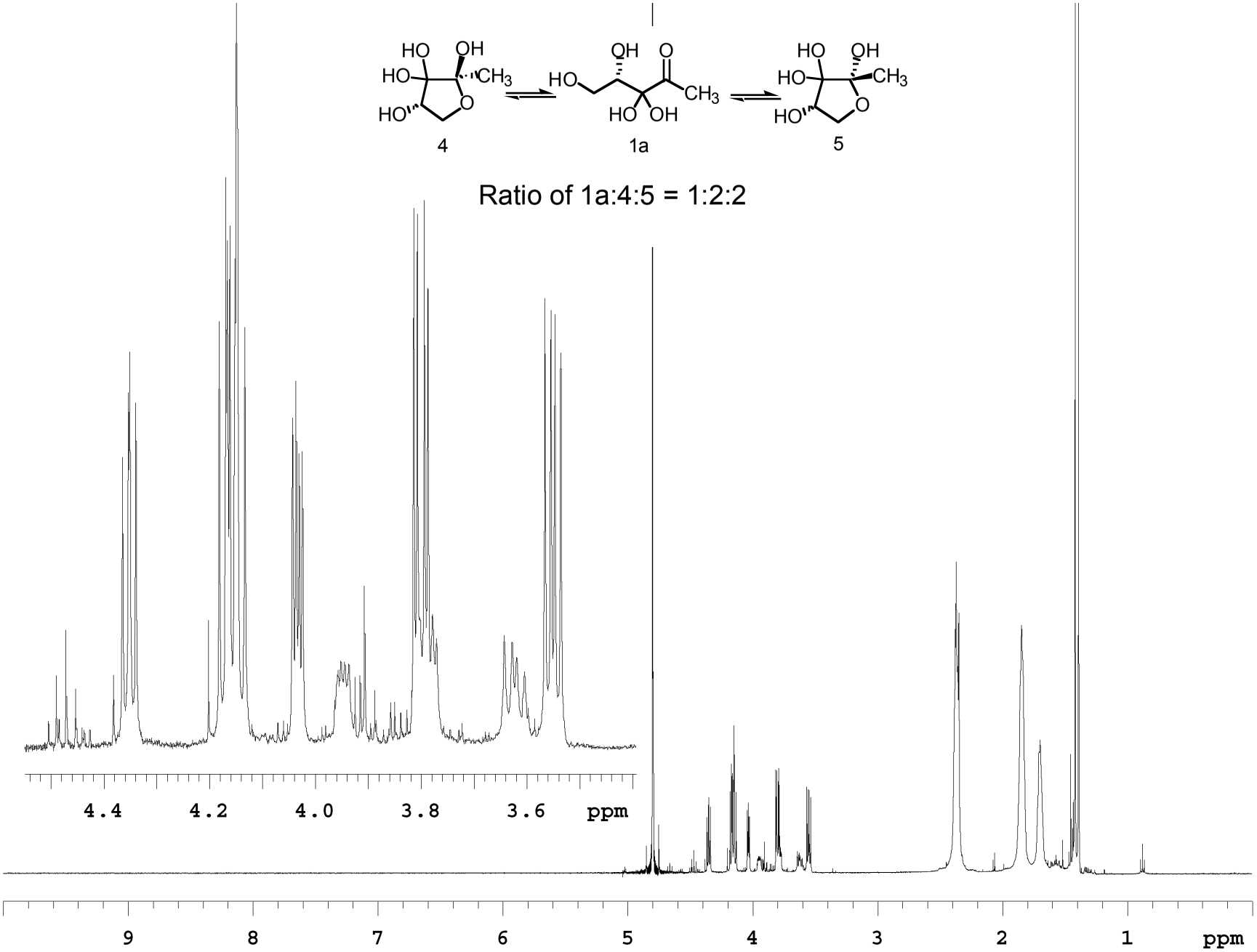


^{1}H and ^{13}C NMR spectrum of **13-($^{13}C_1$)** in D_2O

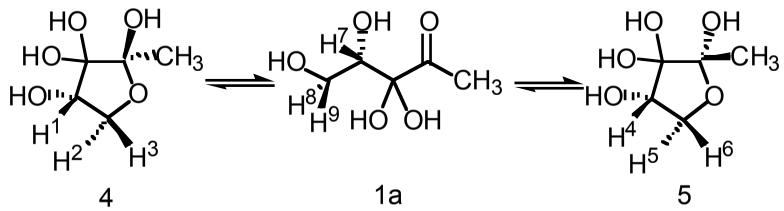




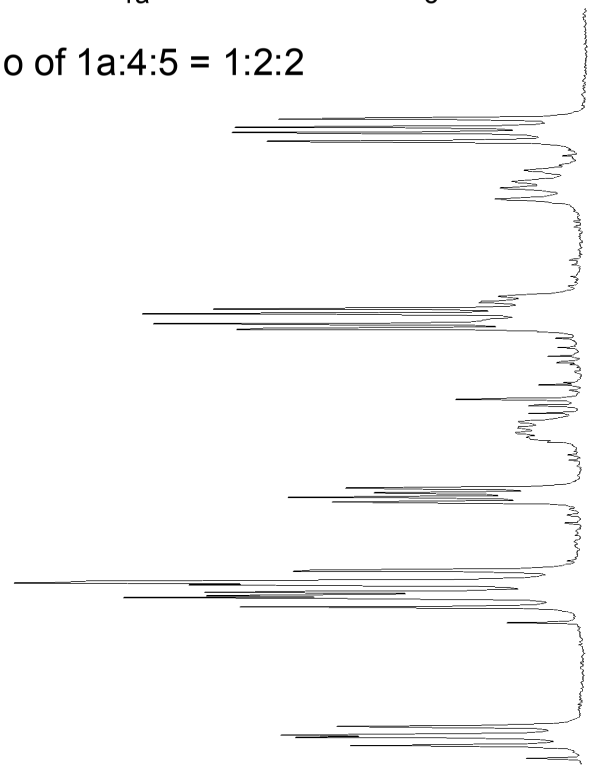
^{1}H NMR spectrum of **1**, DPD, in D_2O, pD 1.5

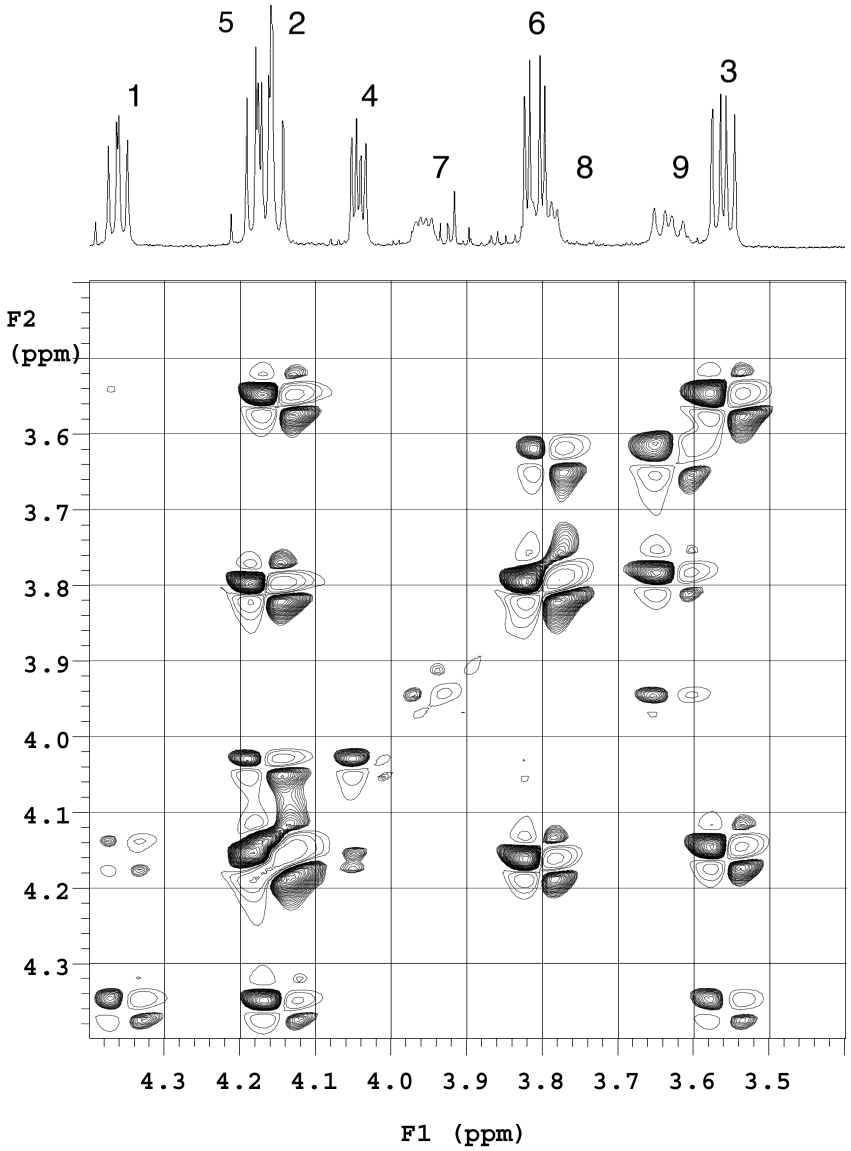


^{1}H-^{1}H DQCOSY spectrum of **1**, DPD, in D_2O, pD 1.5

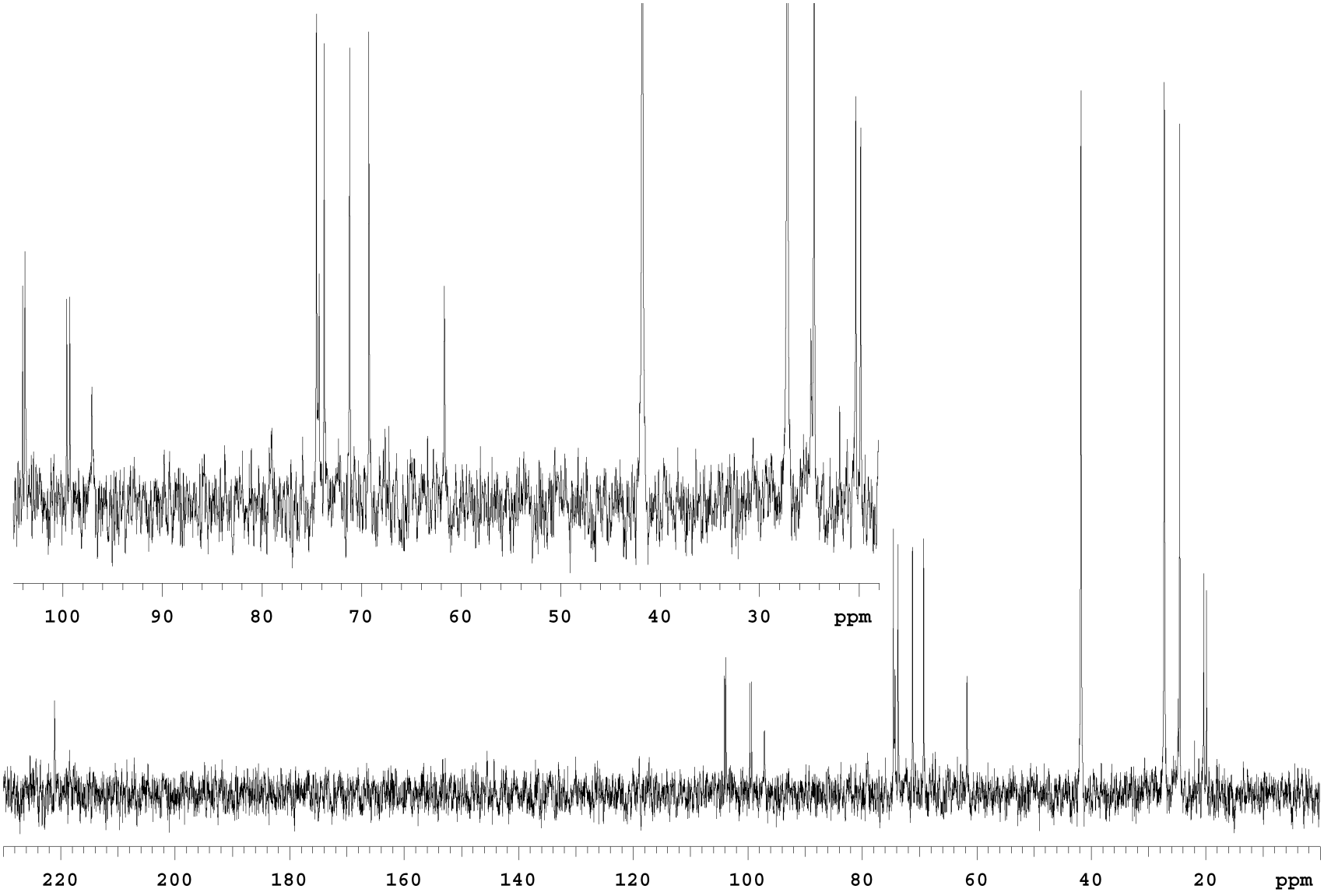


Ratio of 1a:4:5 = 1:2:2



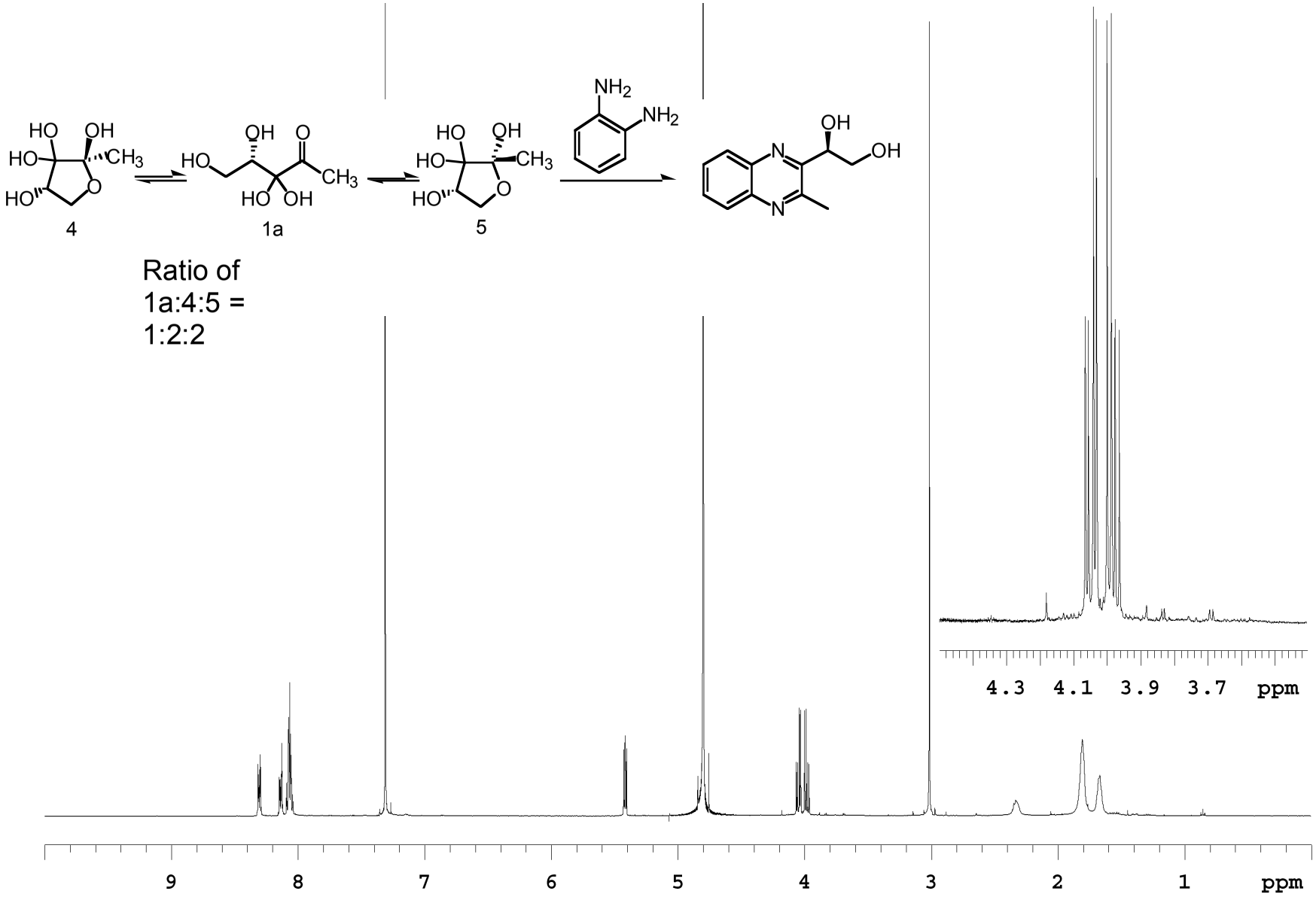
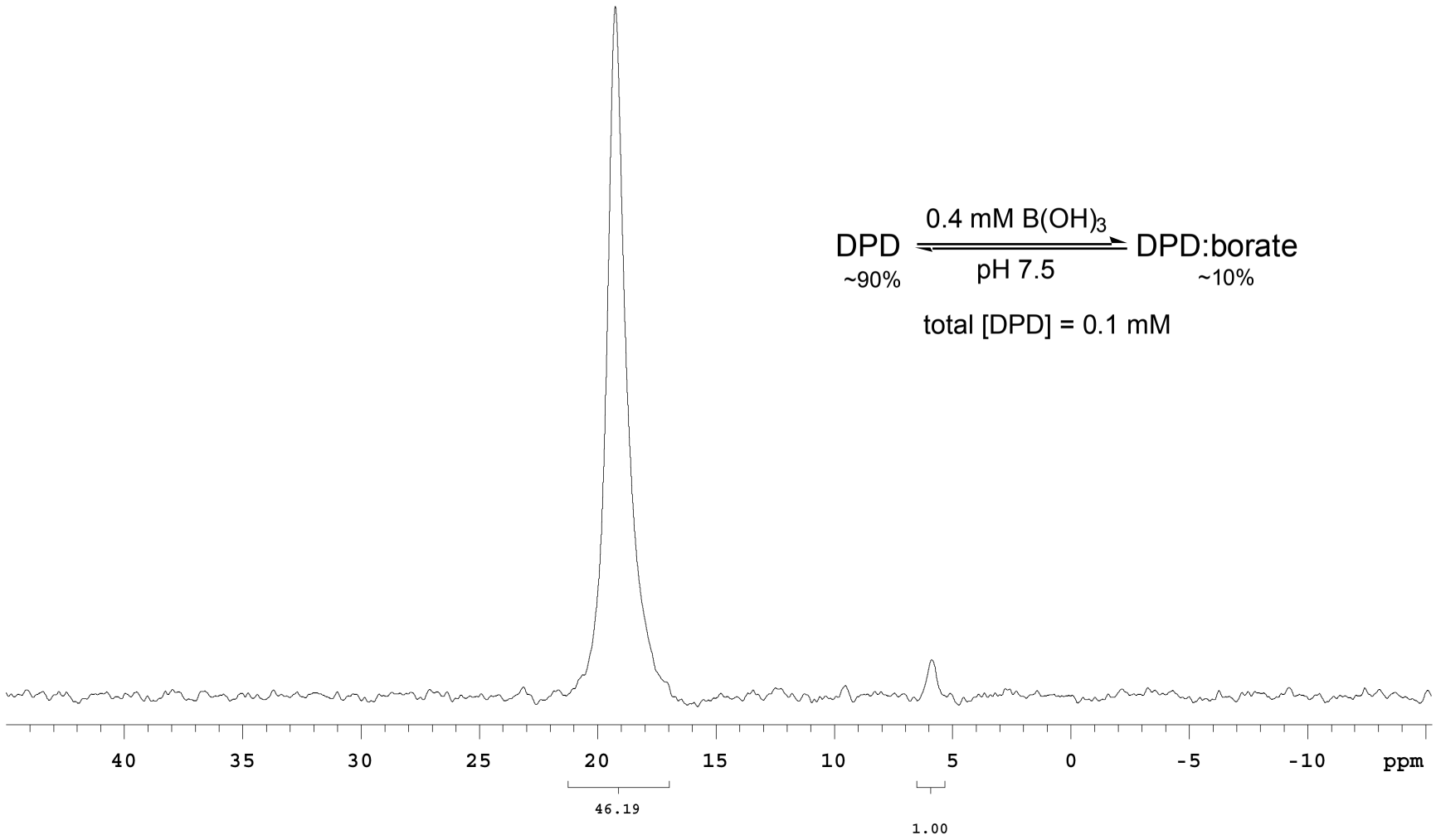


^{13}C NMR spectrum of **1**, DPD, in 95:5 H_2O:D_2O, pH 1.5



^{1}H NMR spectrum of

(S)-1-(3-Methylquinoxalin-2-yl)-ethane-1,2-diol in D_2O, pD 1.5



^{11}B NMR spectrum of 0.1 mM DPD in 0.4 mM $B(OH)_3$, pH 7.5