# Tailoring the AIE Chromogen 2-(2-Hydroxyphenyl)benzothiazole for Use in Enzyme-Triggered Molecular Brachytherapy

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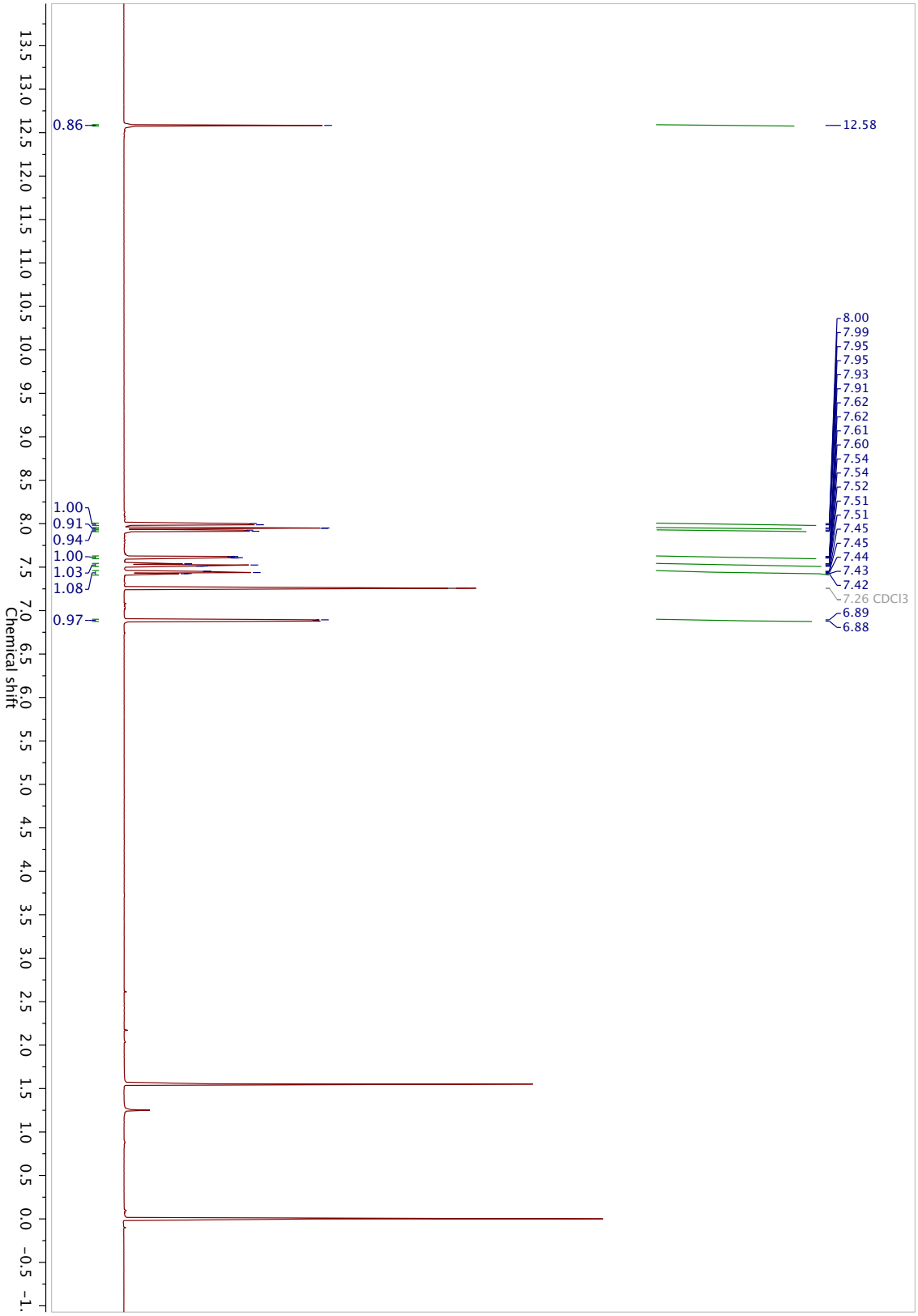
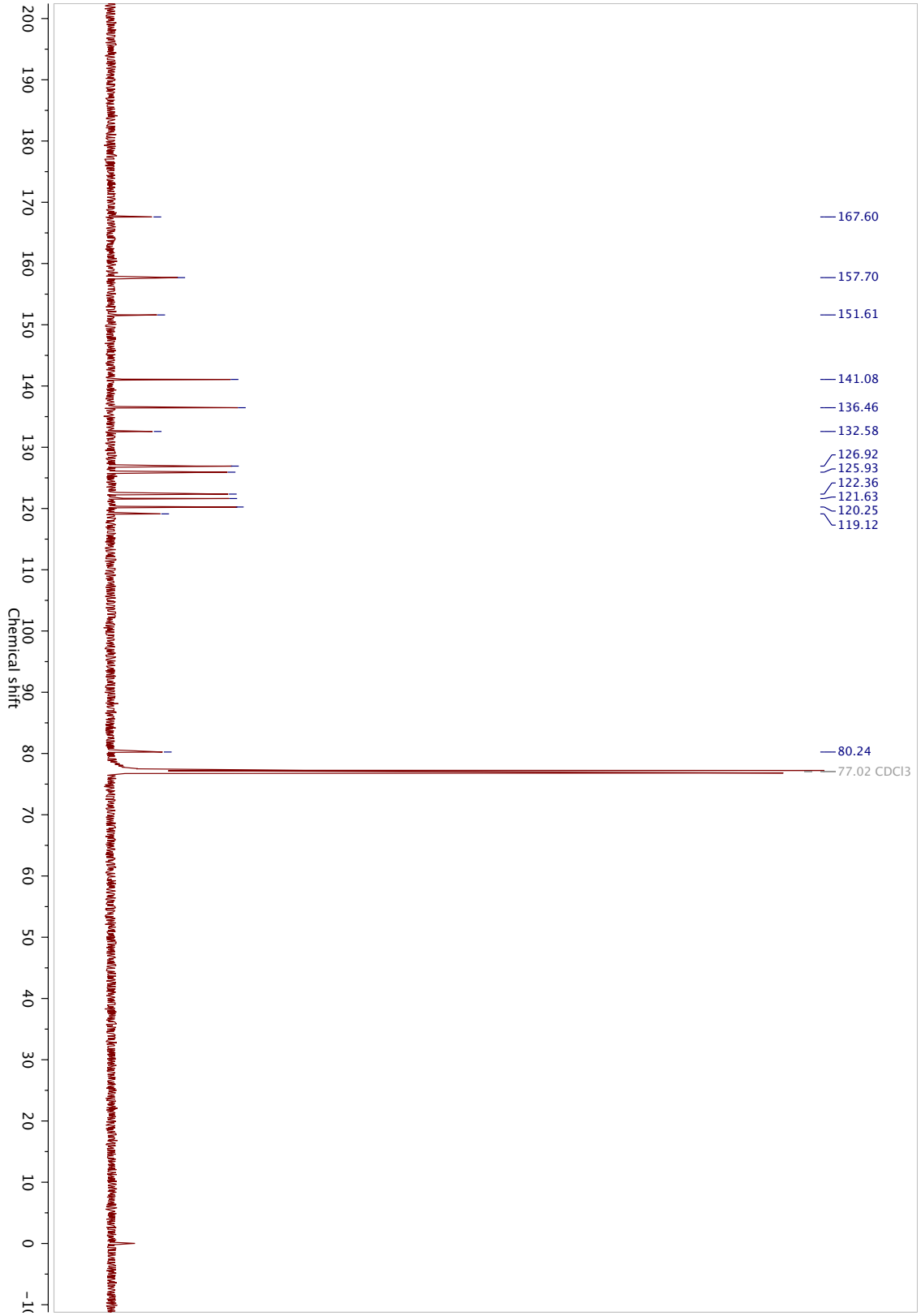
$^{1}$H, $^{13}$C, and $^{31}$P NMR spectra S2–S52

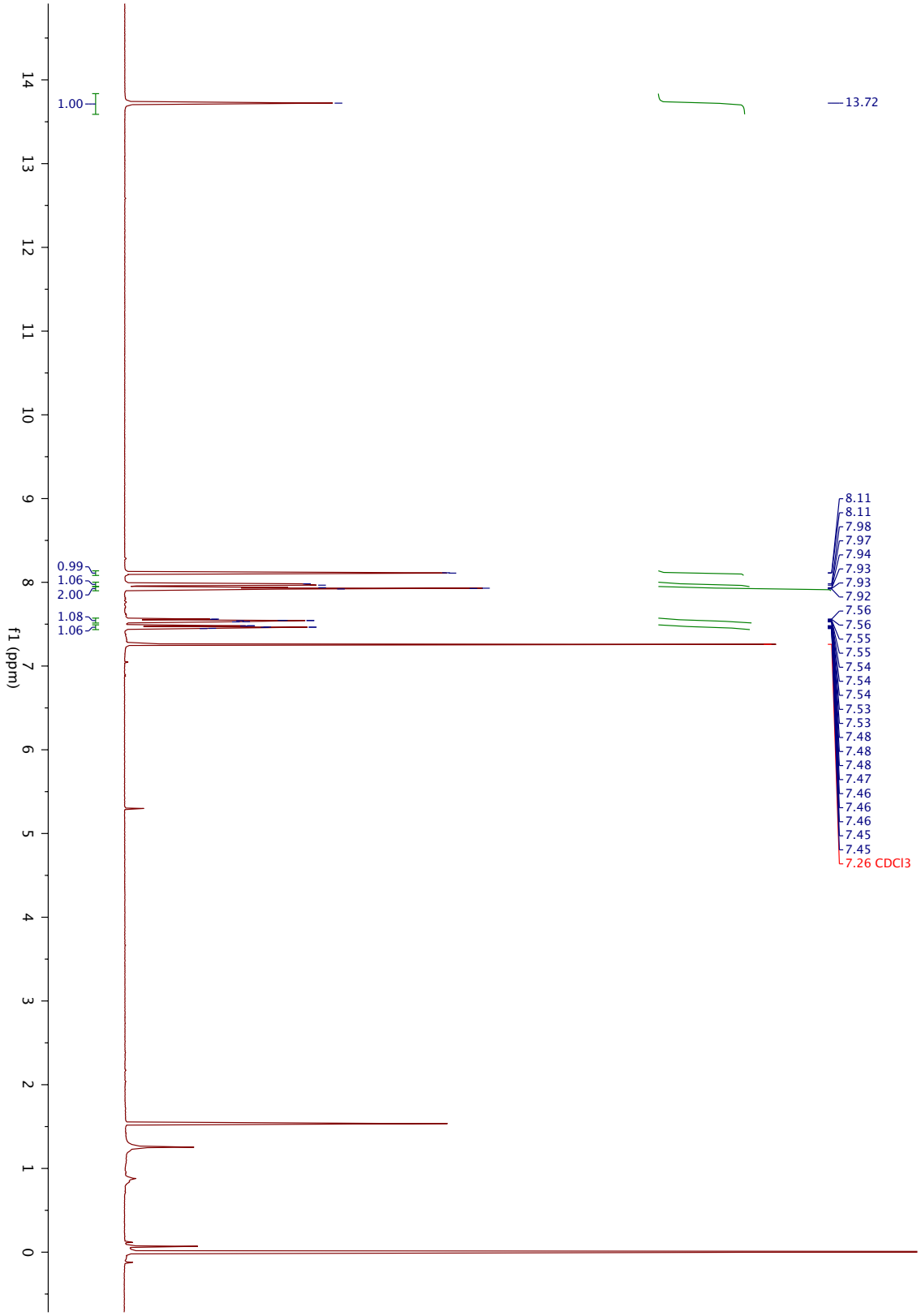
**1-I**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



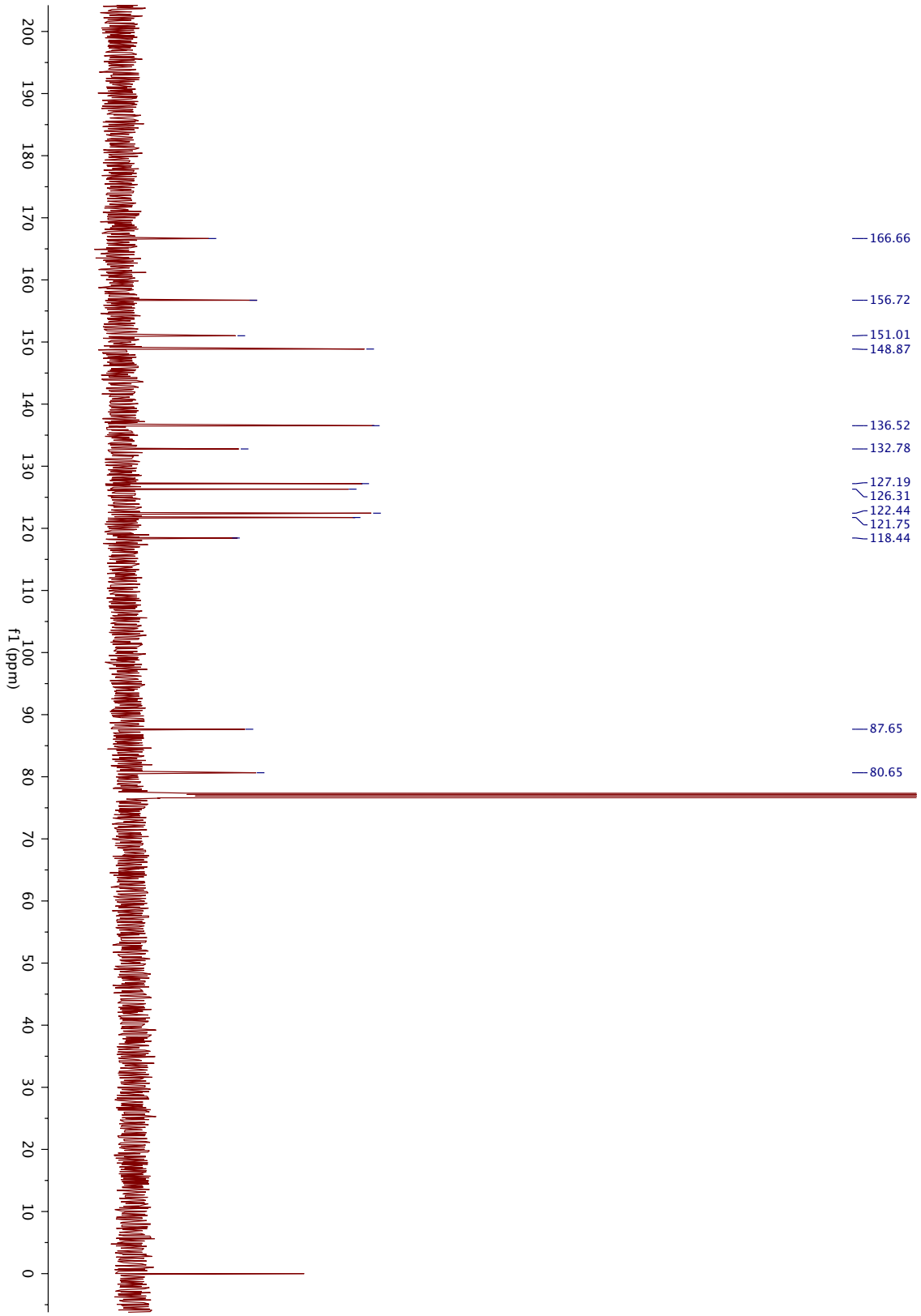
**1-I**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



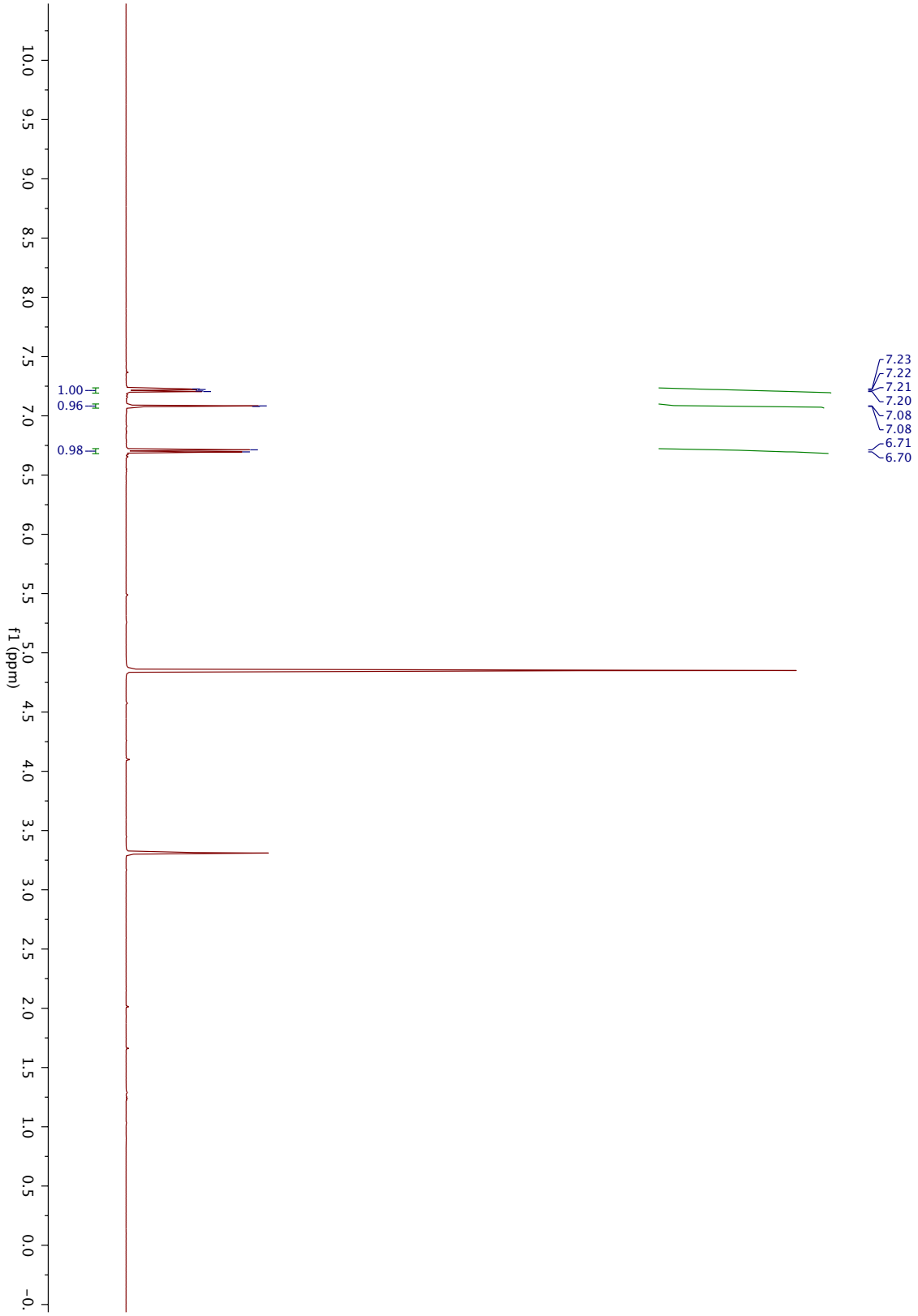
**1-I$_2$**: $^1$H NMR ($CDCl_3$, 500 MHz)



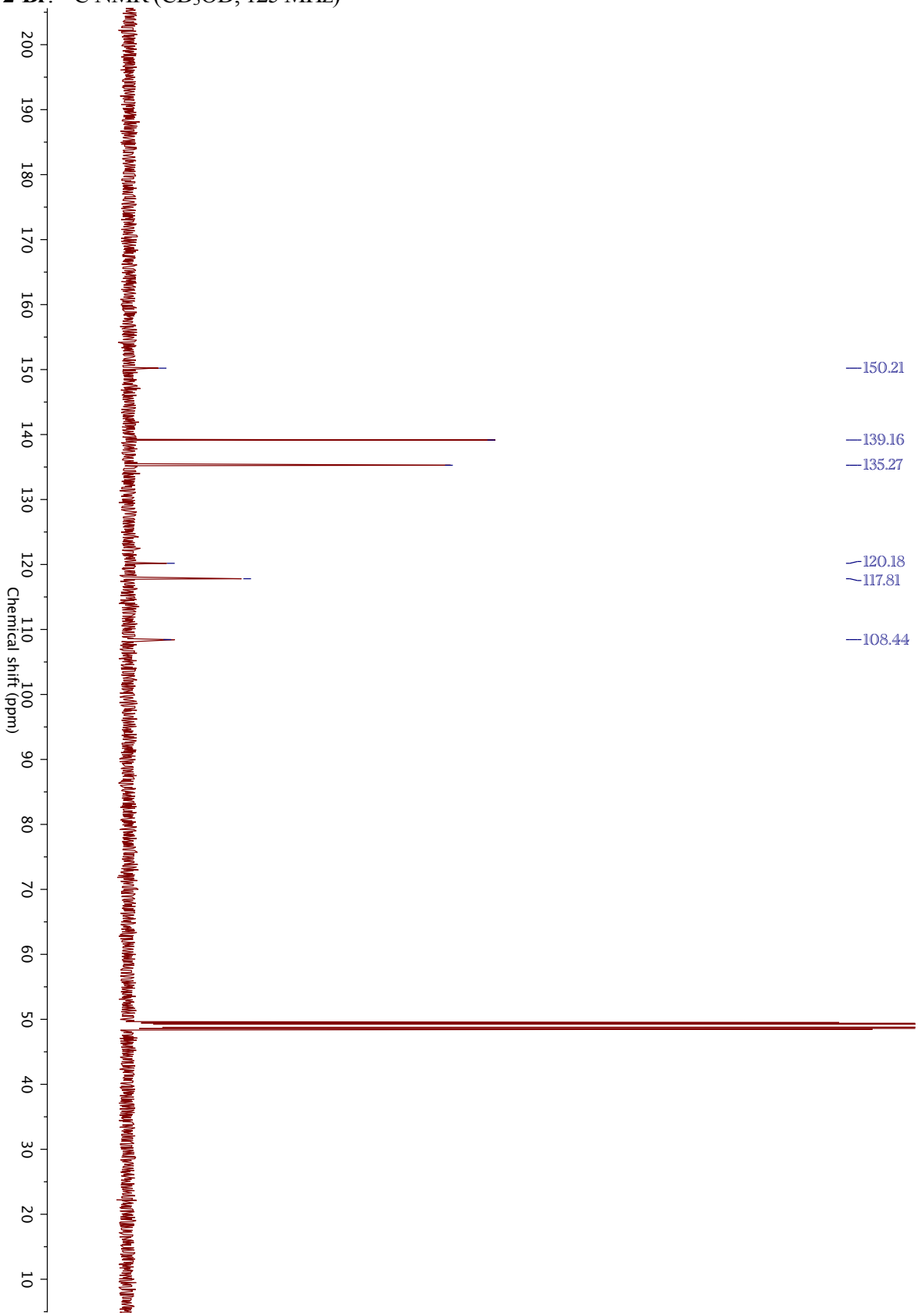
**1-I$_2$**: $^1$H NMR ($CDCl_3$, 125 MHz)



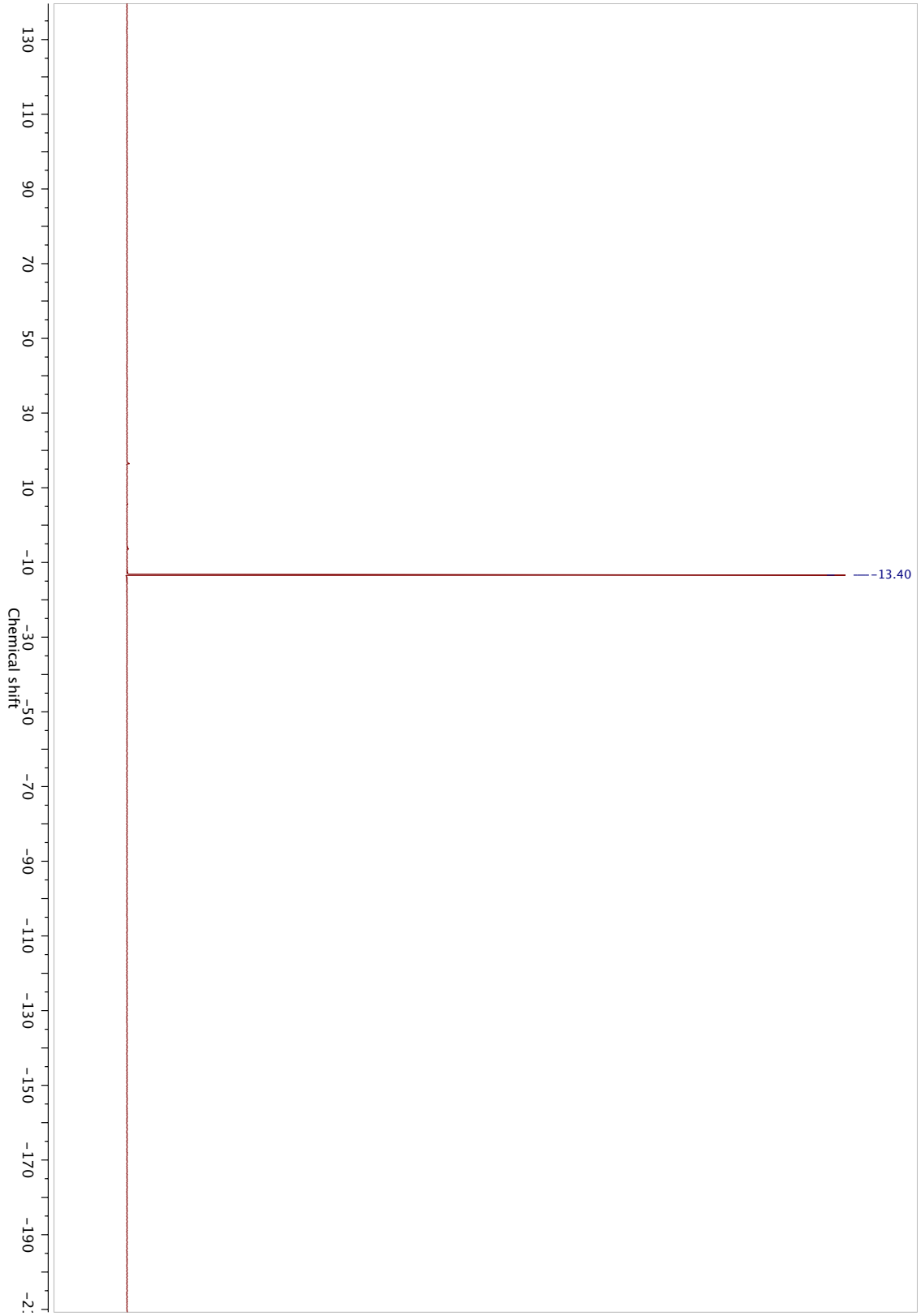
**2-Br**: $^{1}$H NMR ($CD_3OD$, 500 MHz)



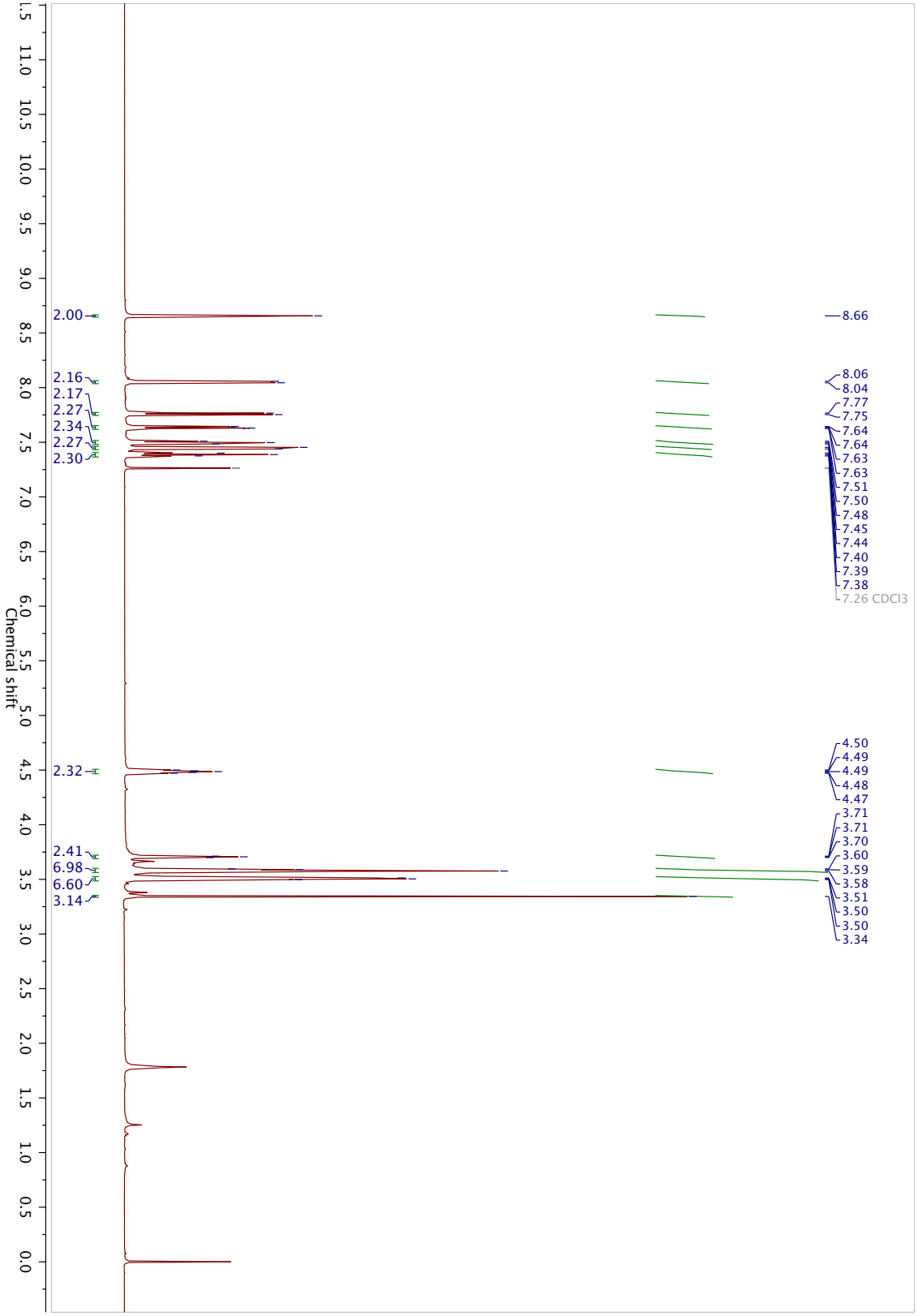
**2-Br**: $^{13}C$ NMR ($CD_3OD$, 125 MHz)



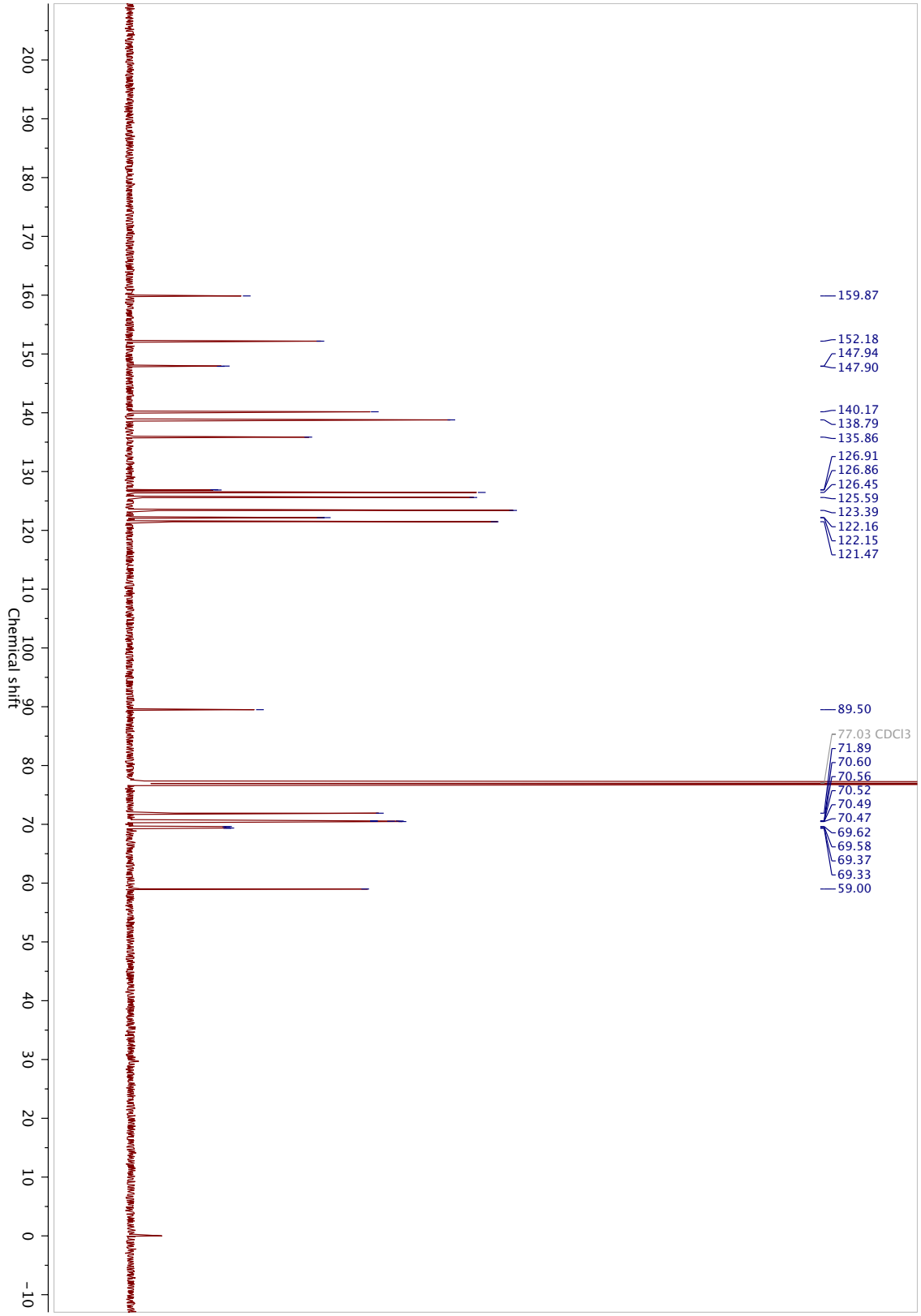
**6-I**: $^{31}P$ NMR ($CDCl_3$, 240 MHz)



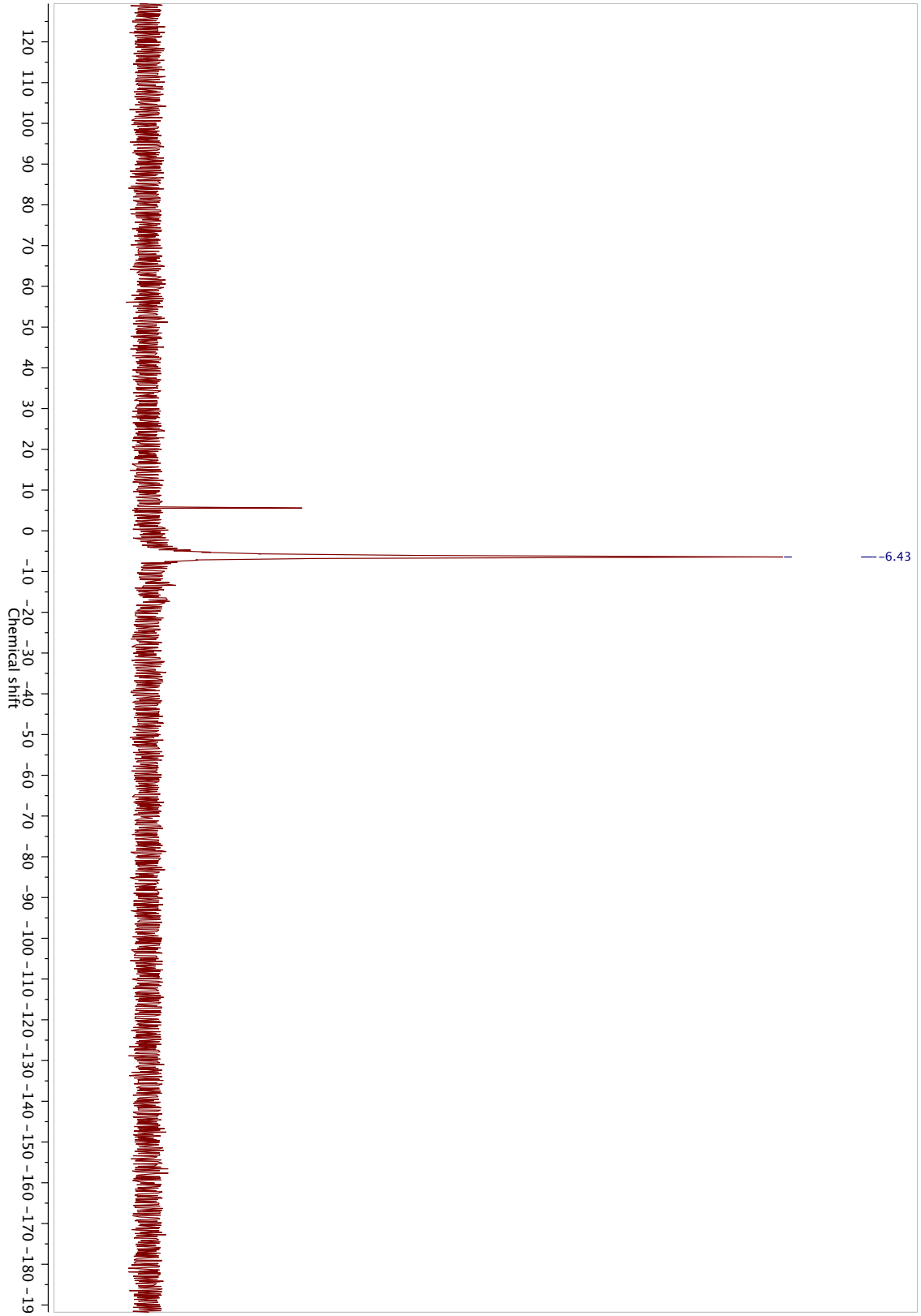
**6-I**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



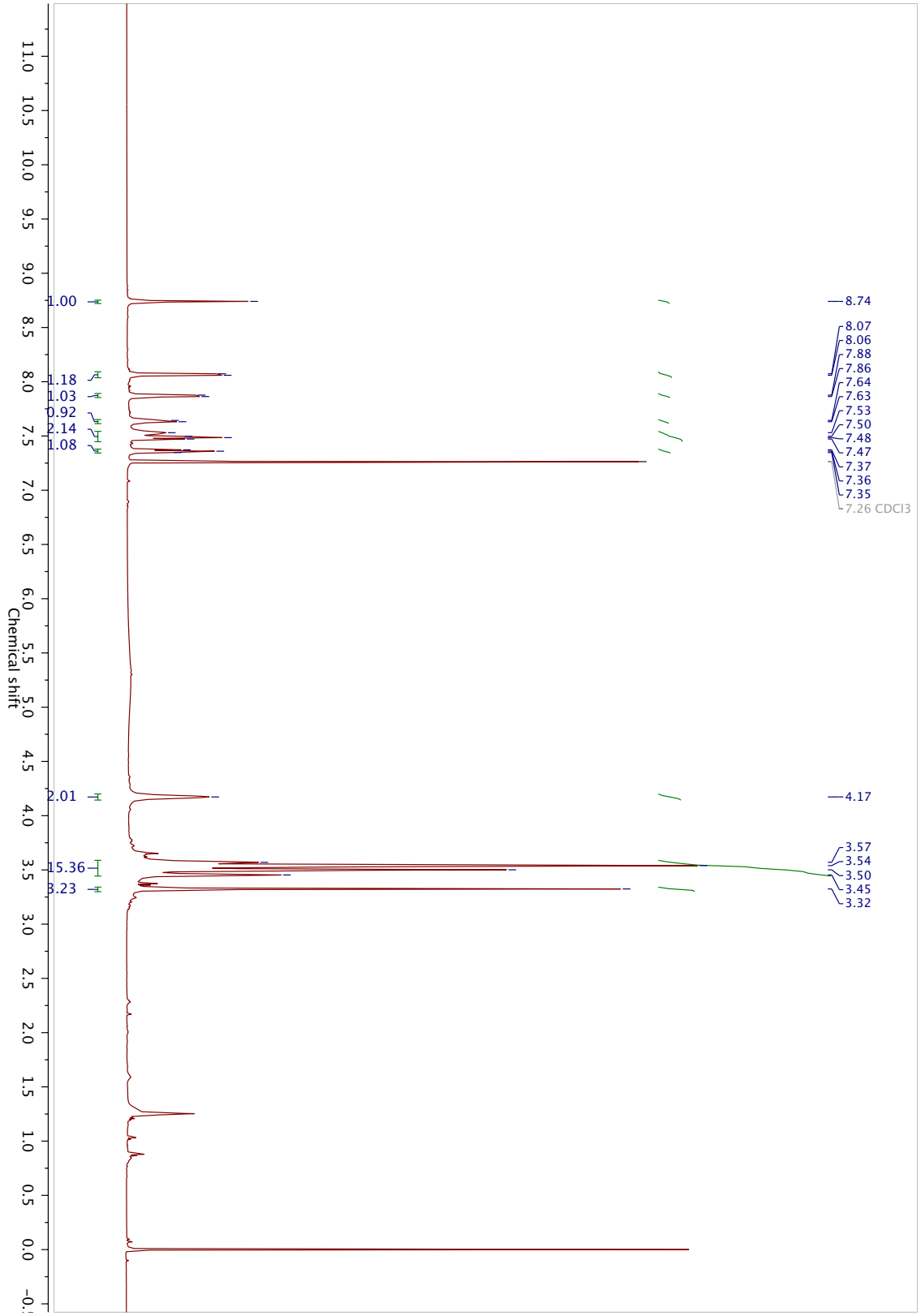
**6-I**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



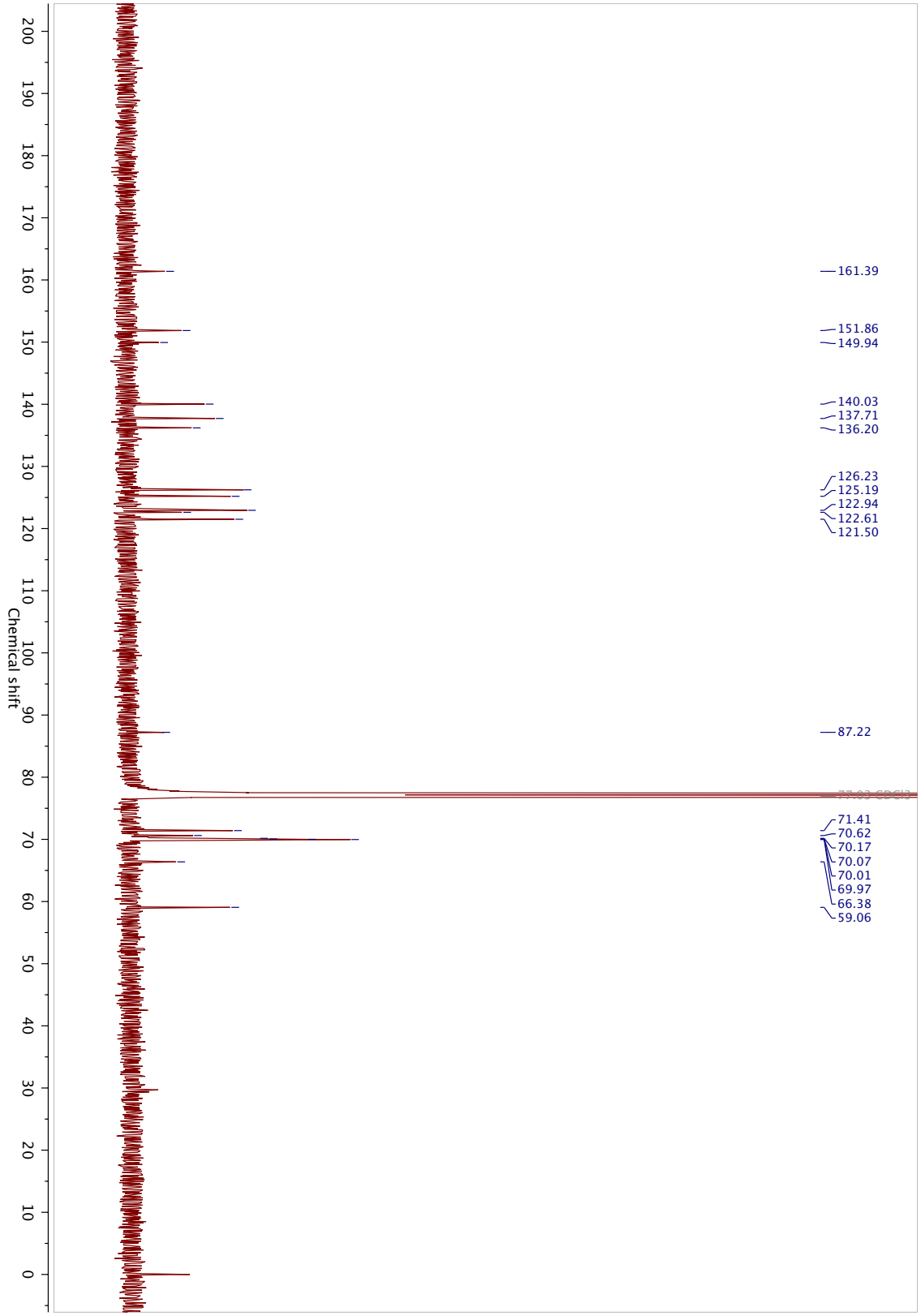
**7-I**: $^{31}P$ NMR ($CDCl_3$, 240 MHz)



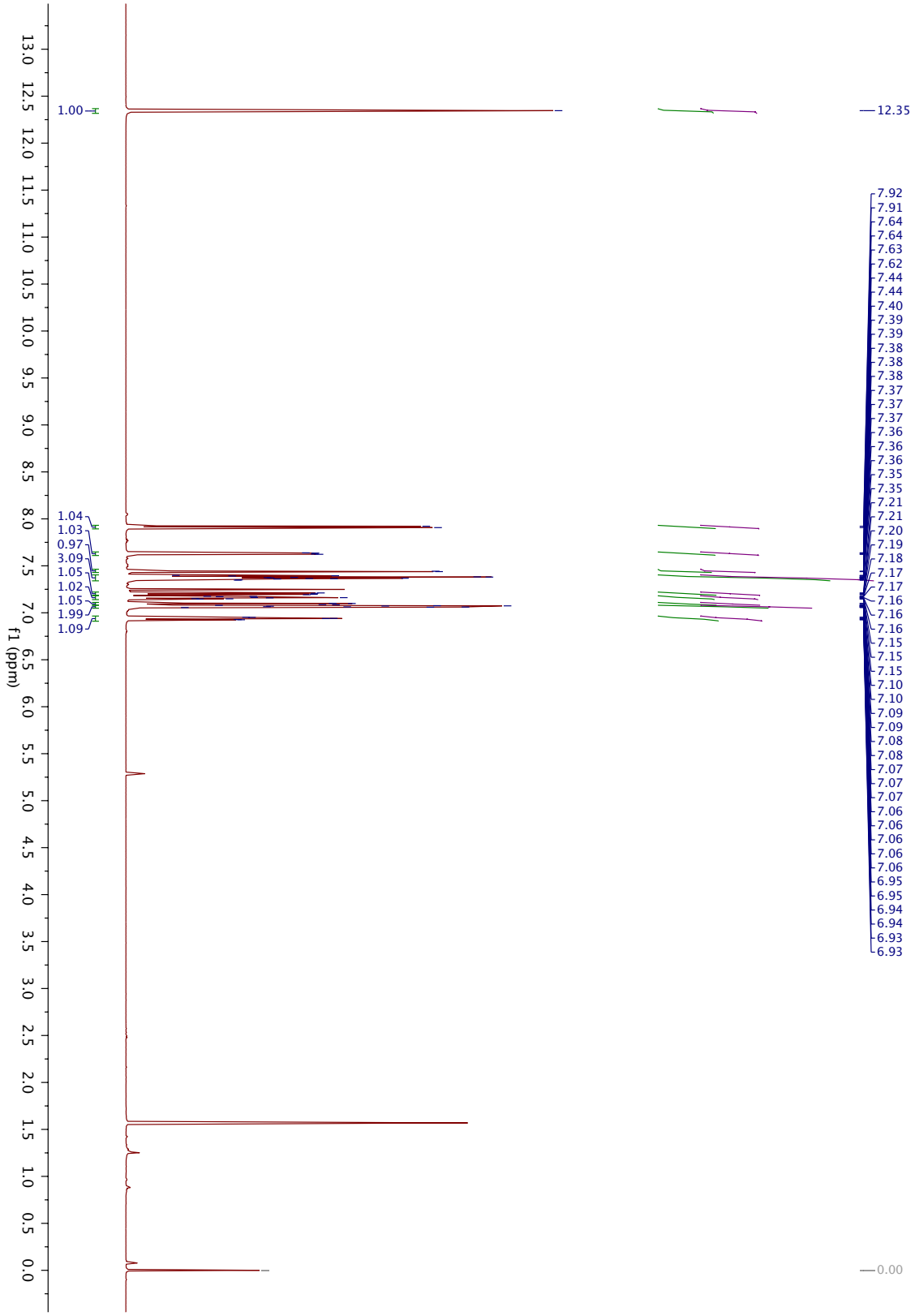
**7-I**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



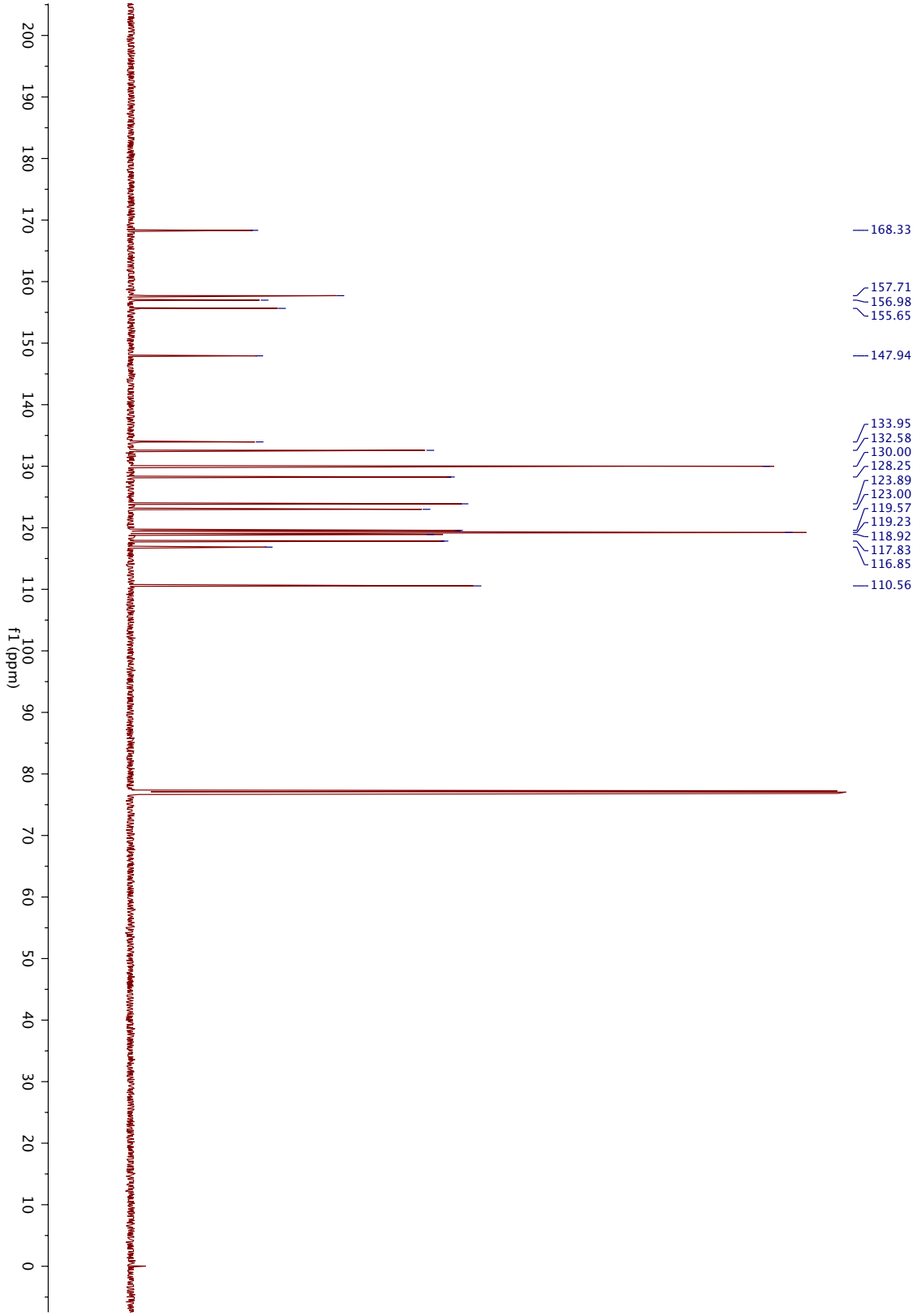
**7-I**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



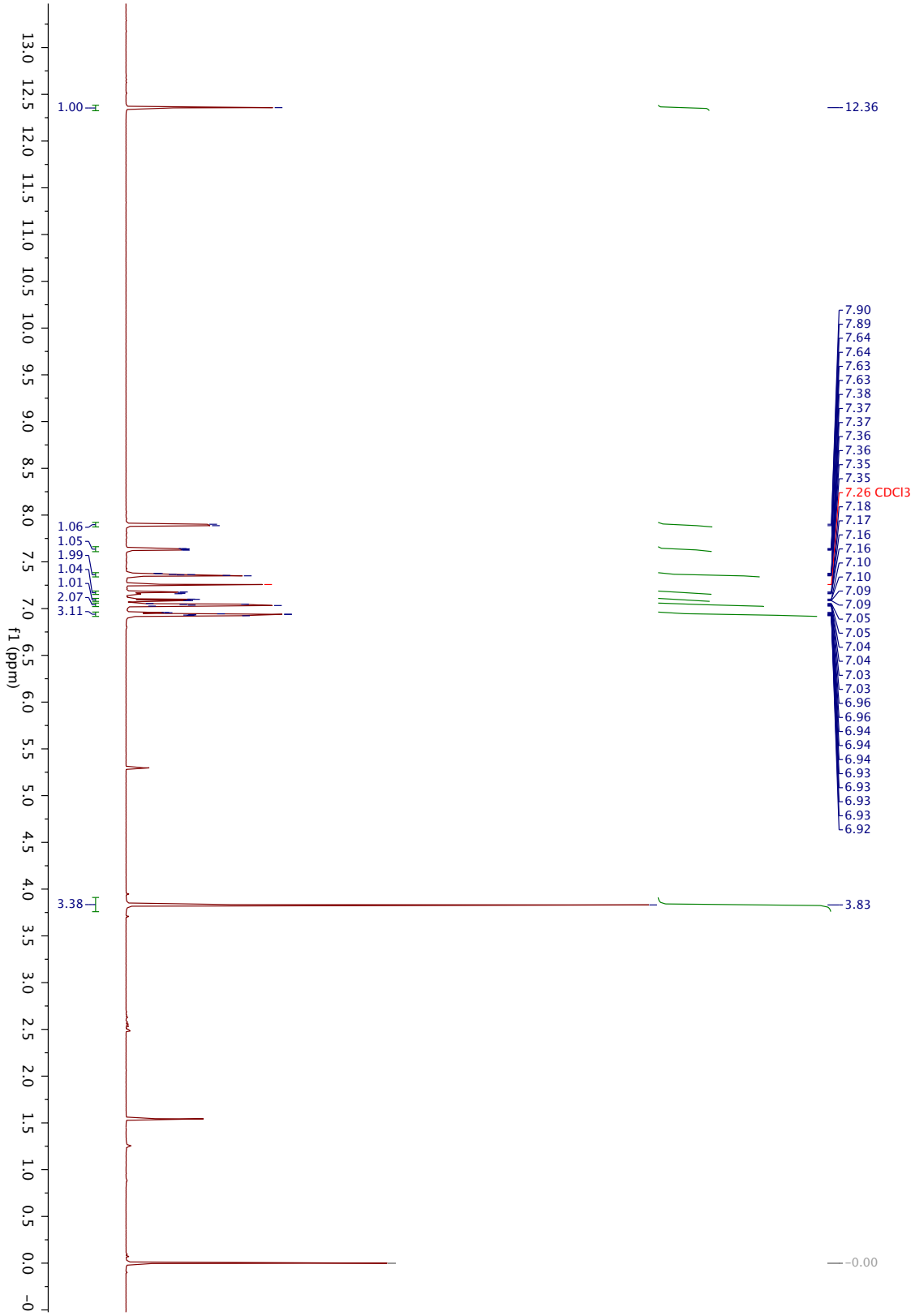
**9a**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



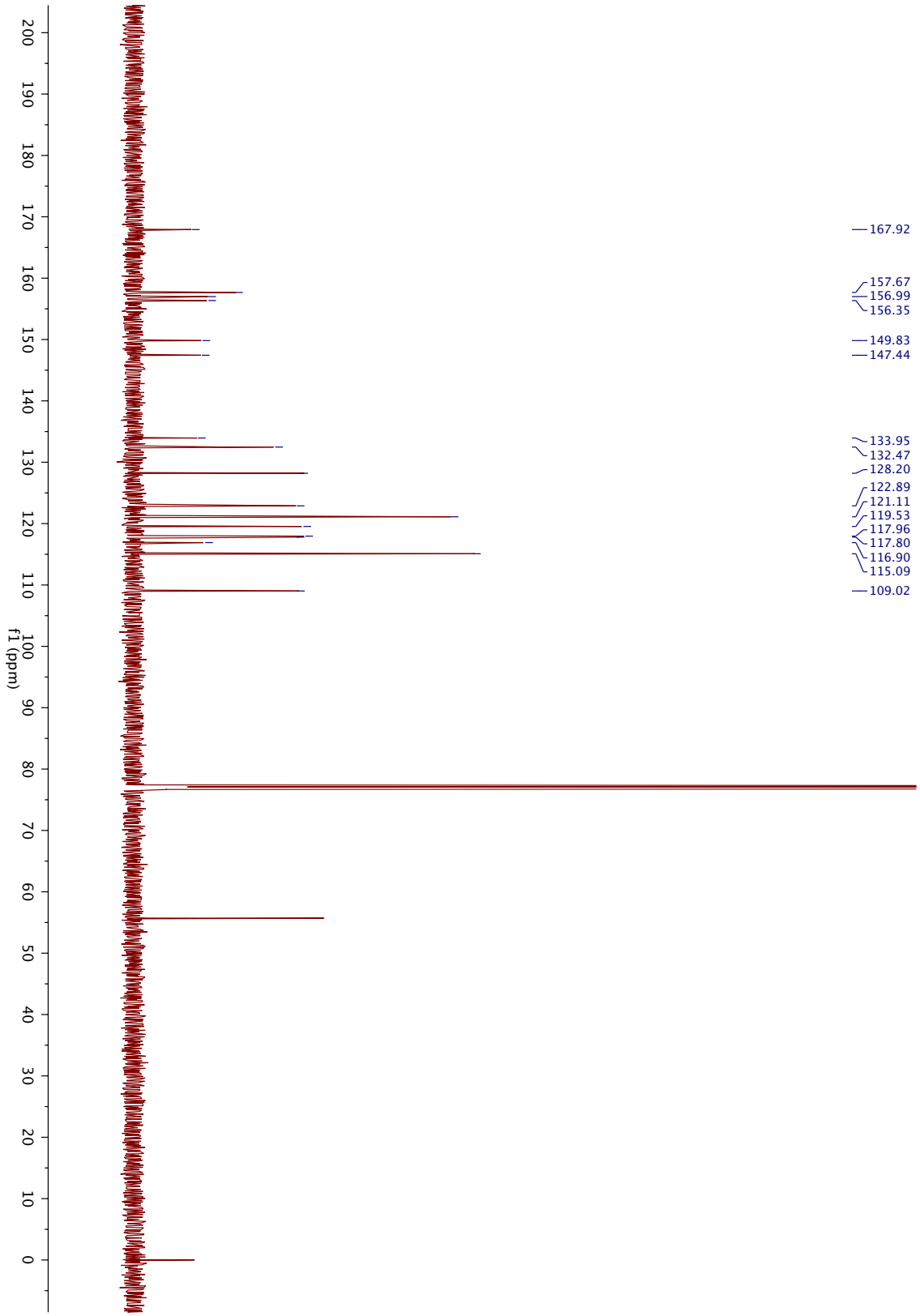
**9a**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



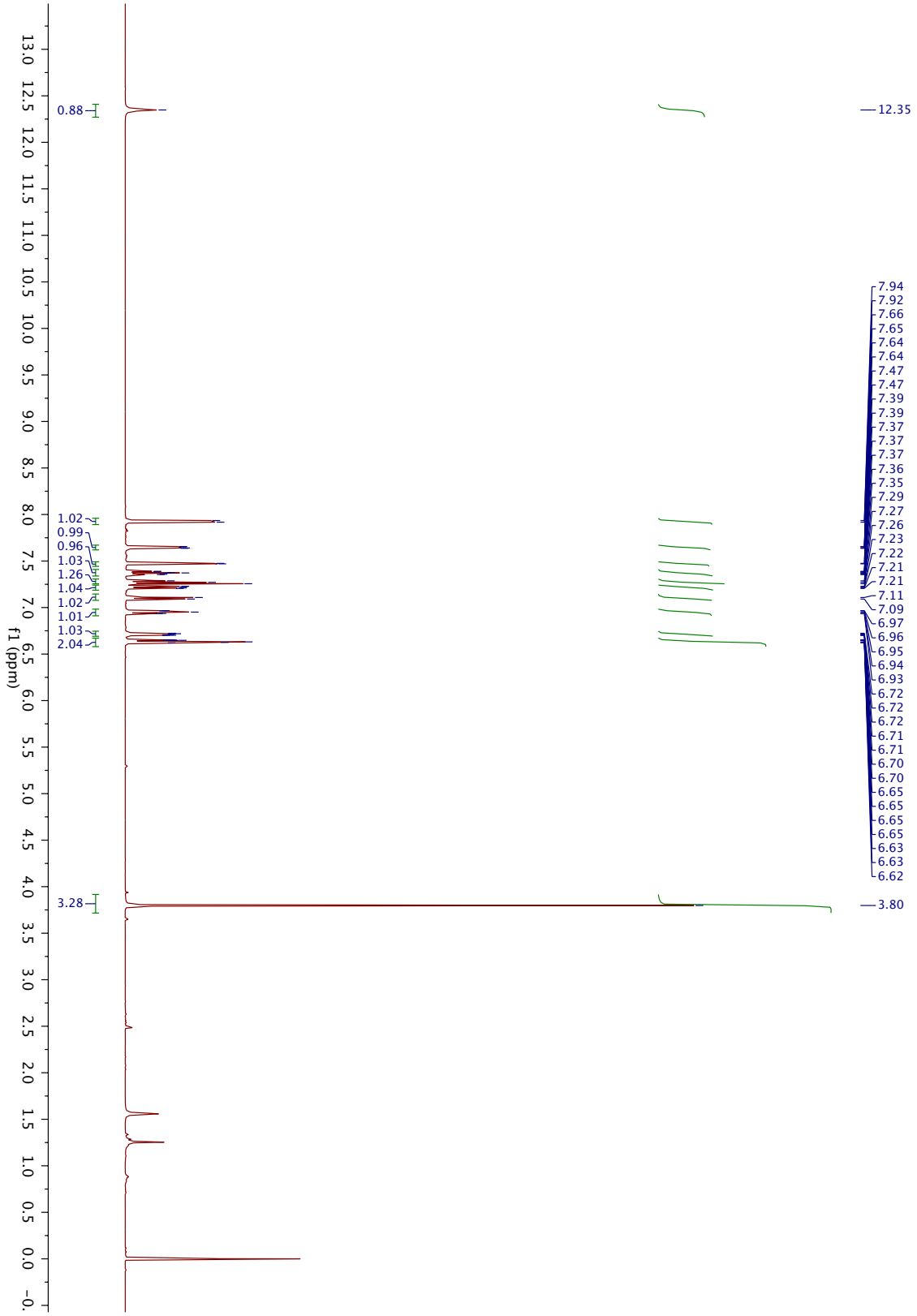
**9b**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



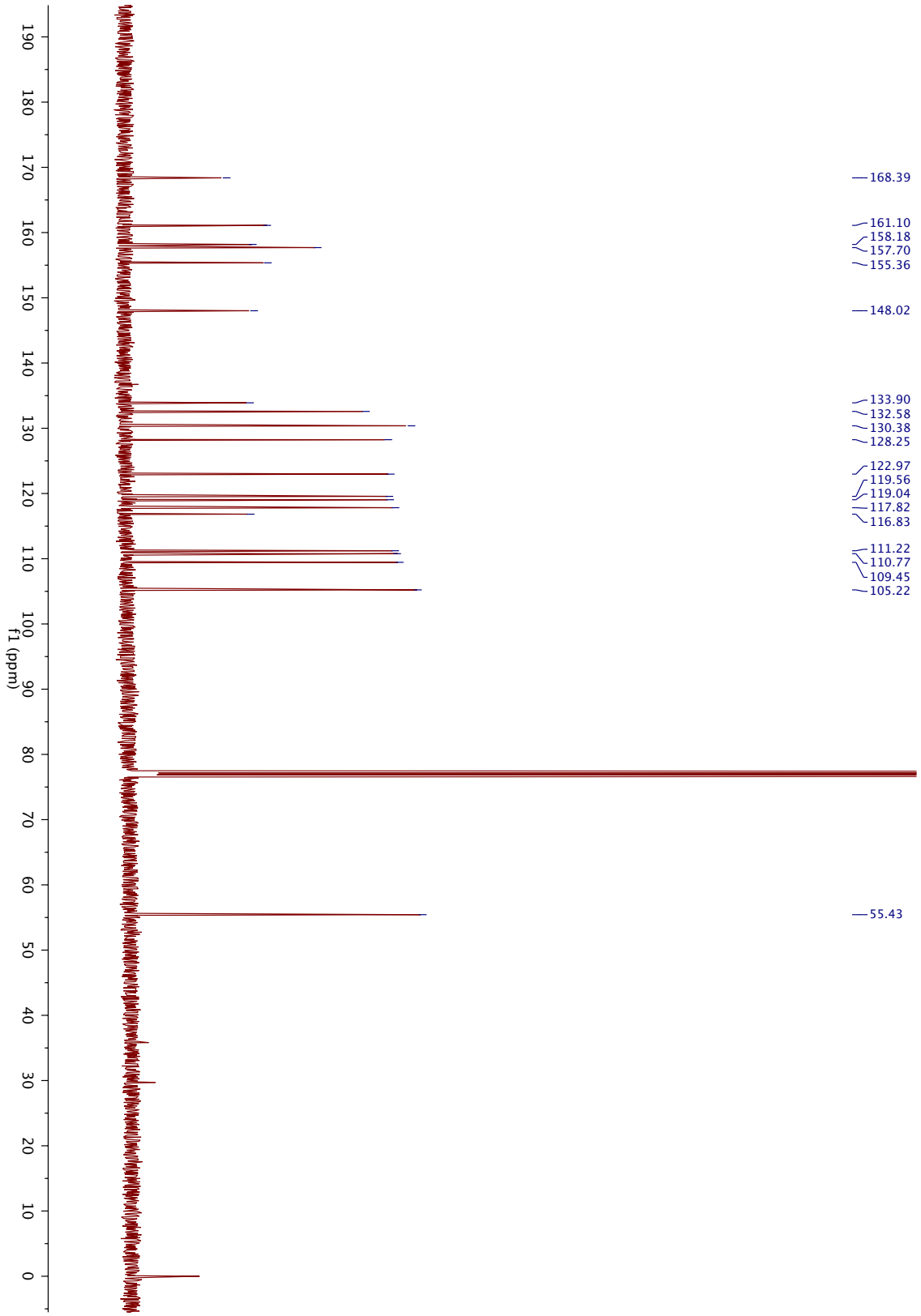
**9b**: $^{13}C$ NMR ($CDCl_3$, 75 MHz)



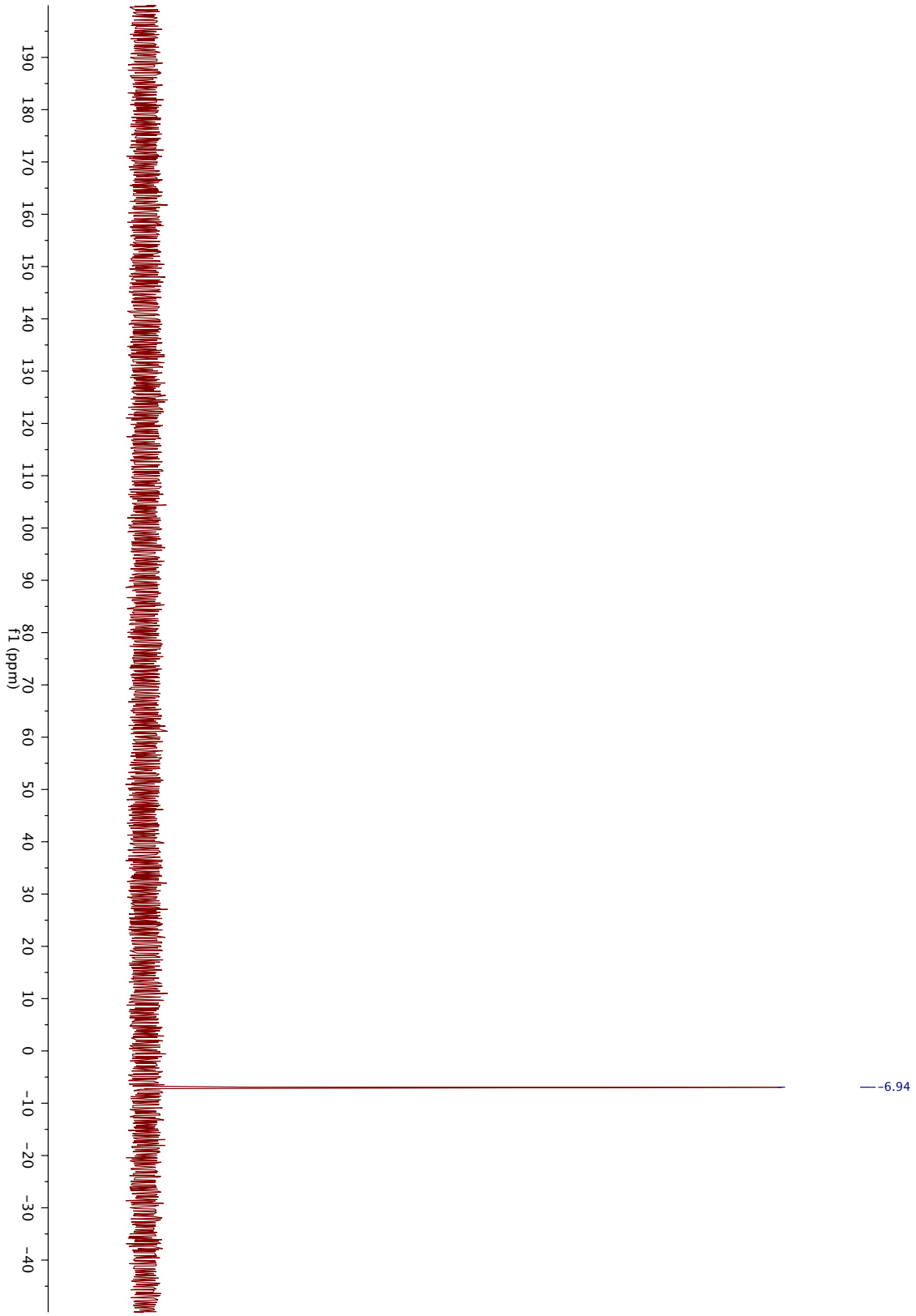
**9c**: $^{1}$H NMR ($CDCl_3$, 500 MHz)



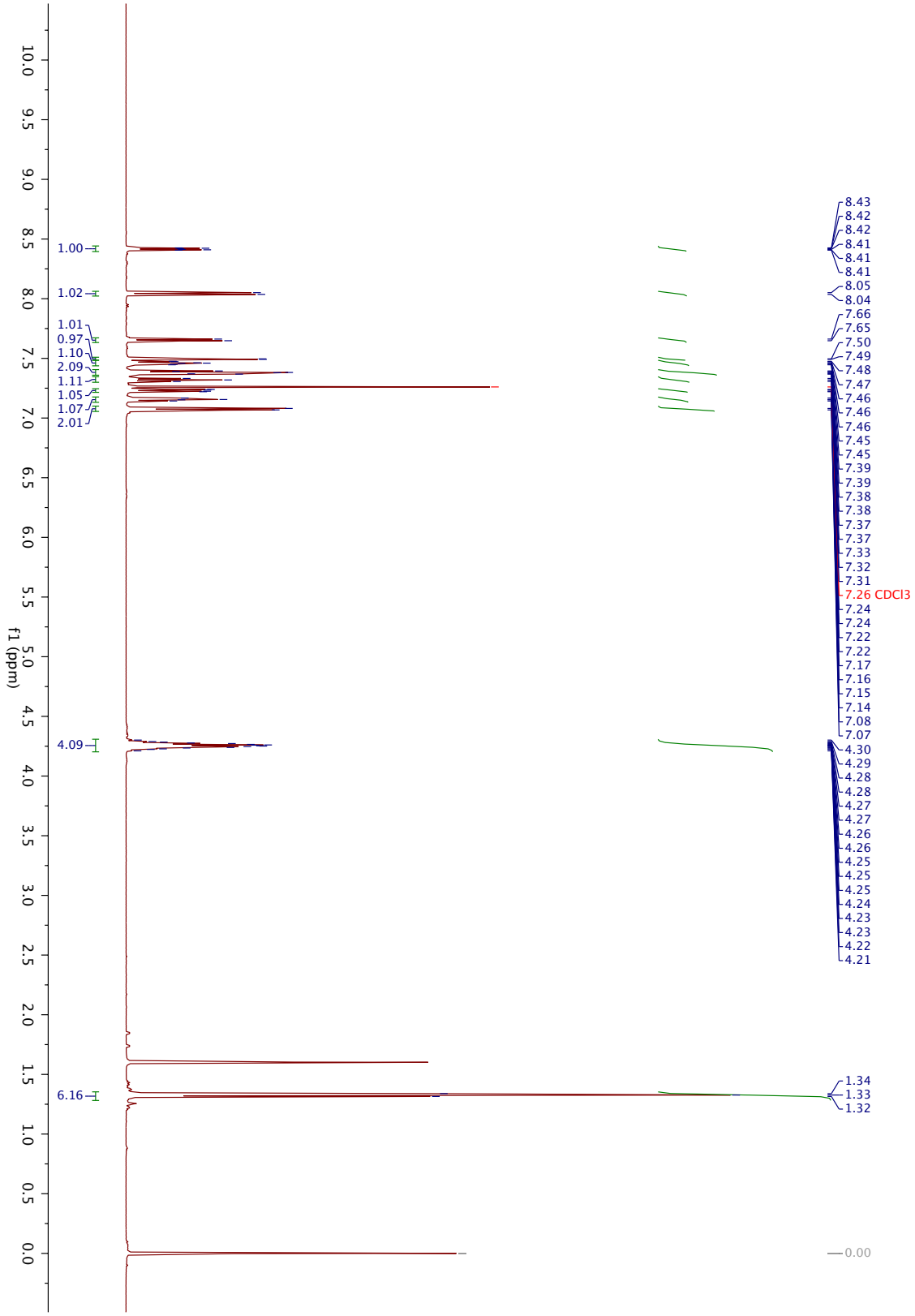
**9c**: $^{13}C$ NMR ($CDCl_3$, 125 MHz)



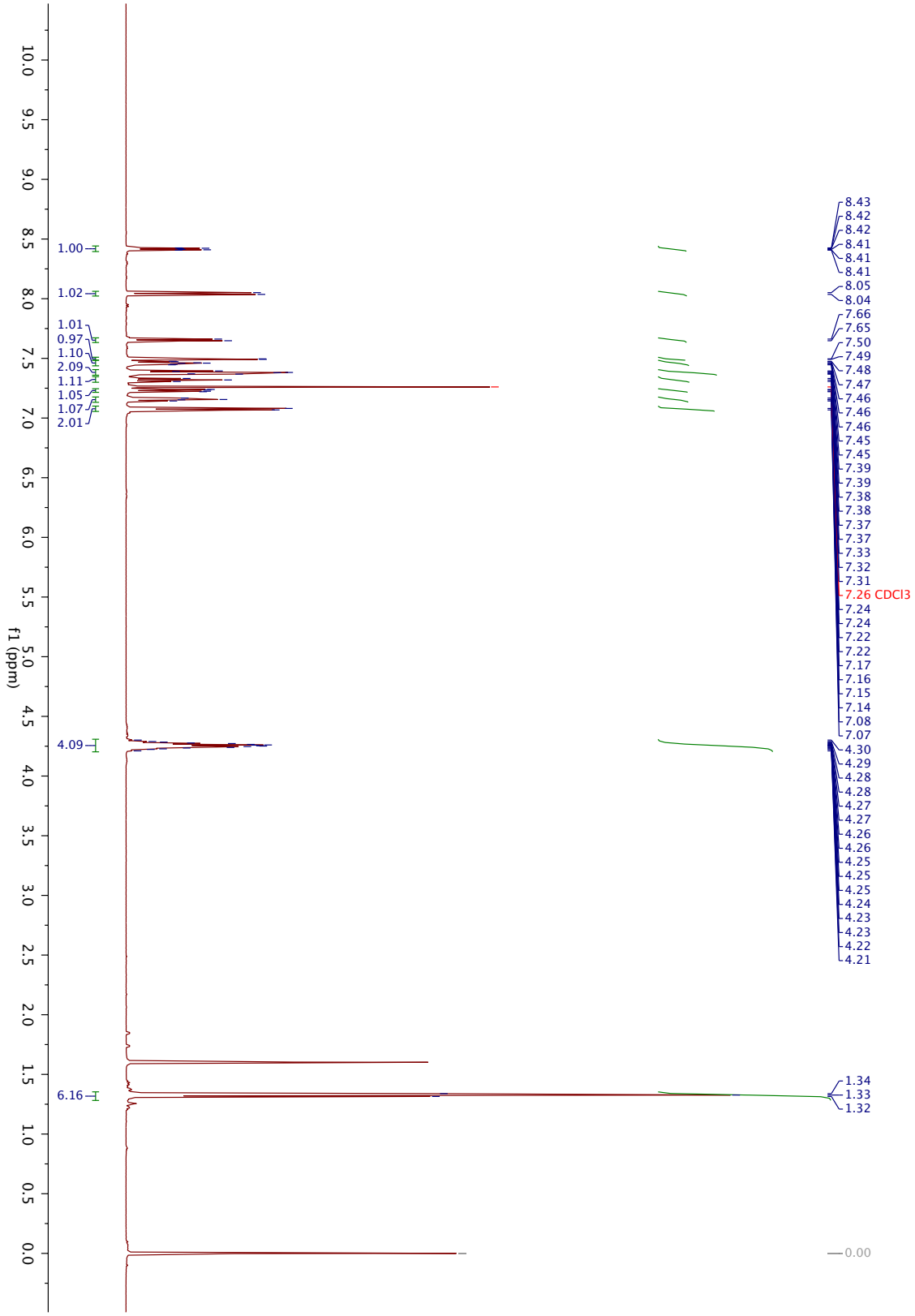
**10a**: $^{31}P$ NMR ($CDCl_3$, 160MHz)



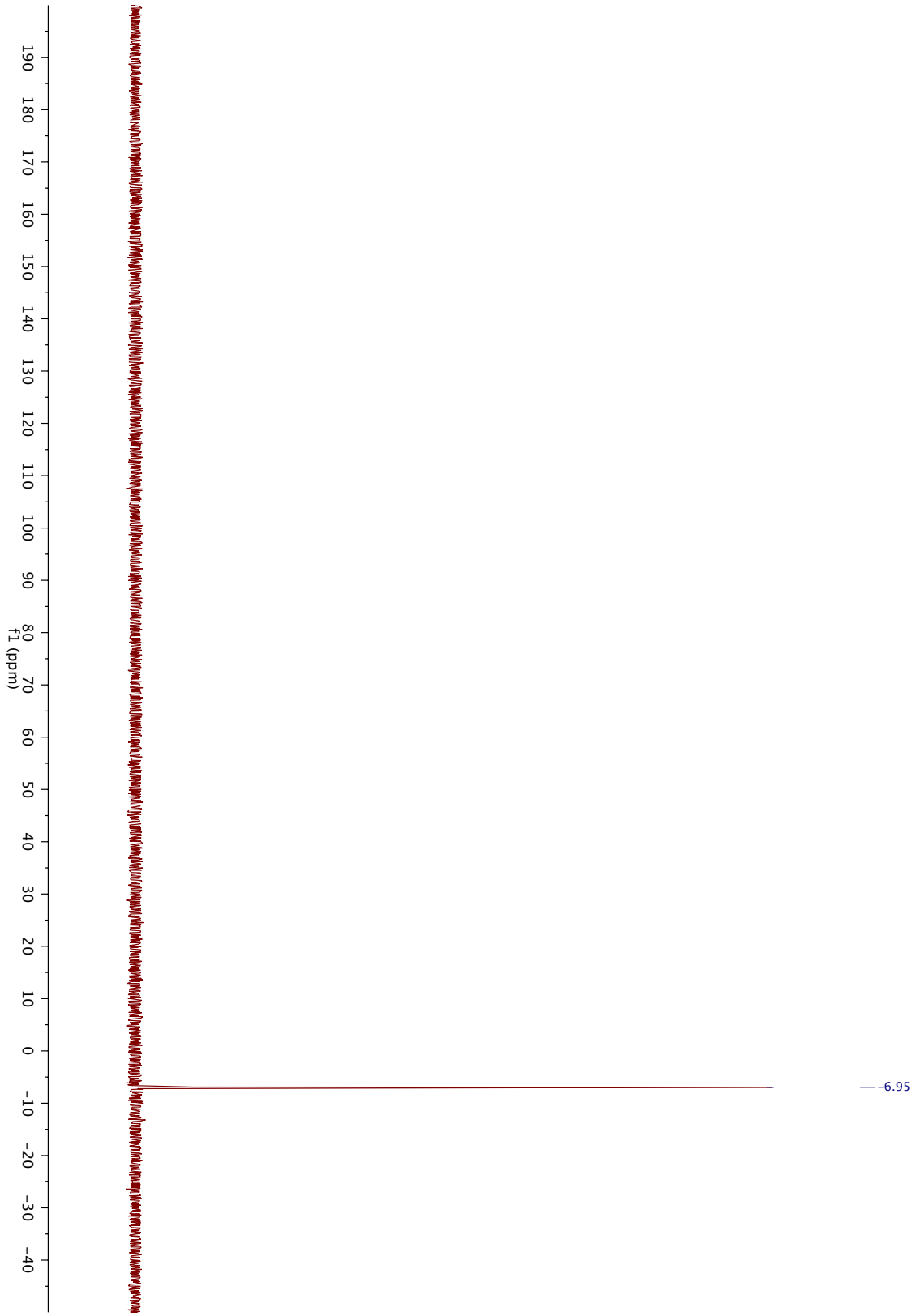
**10a**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



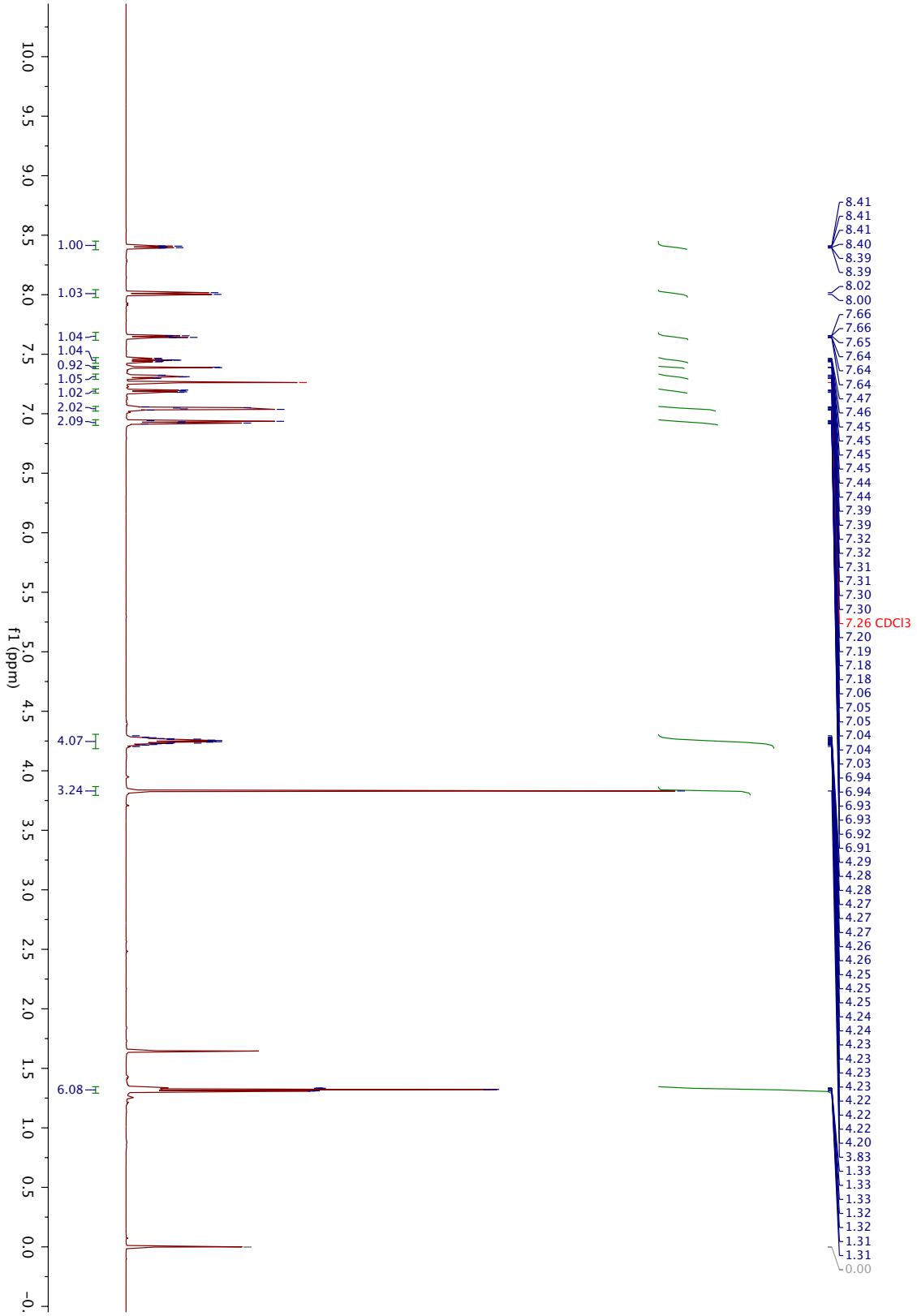
**10a**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



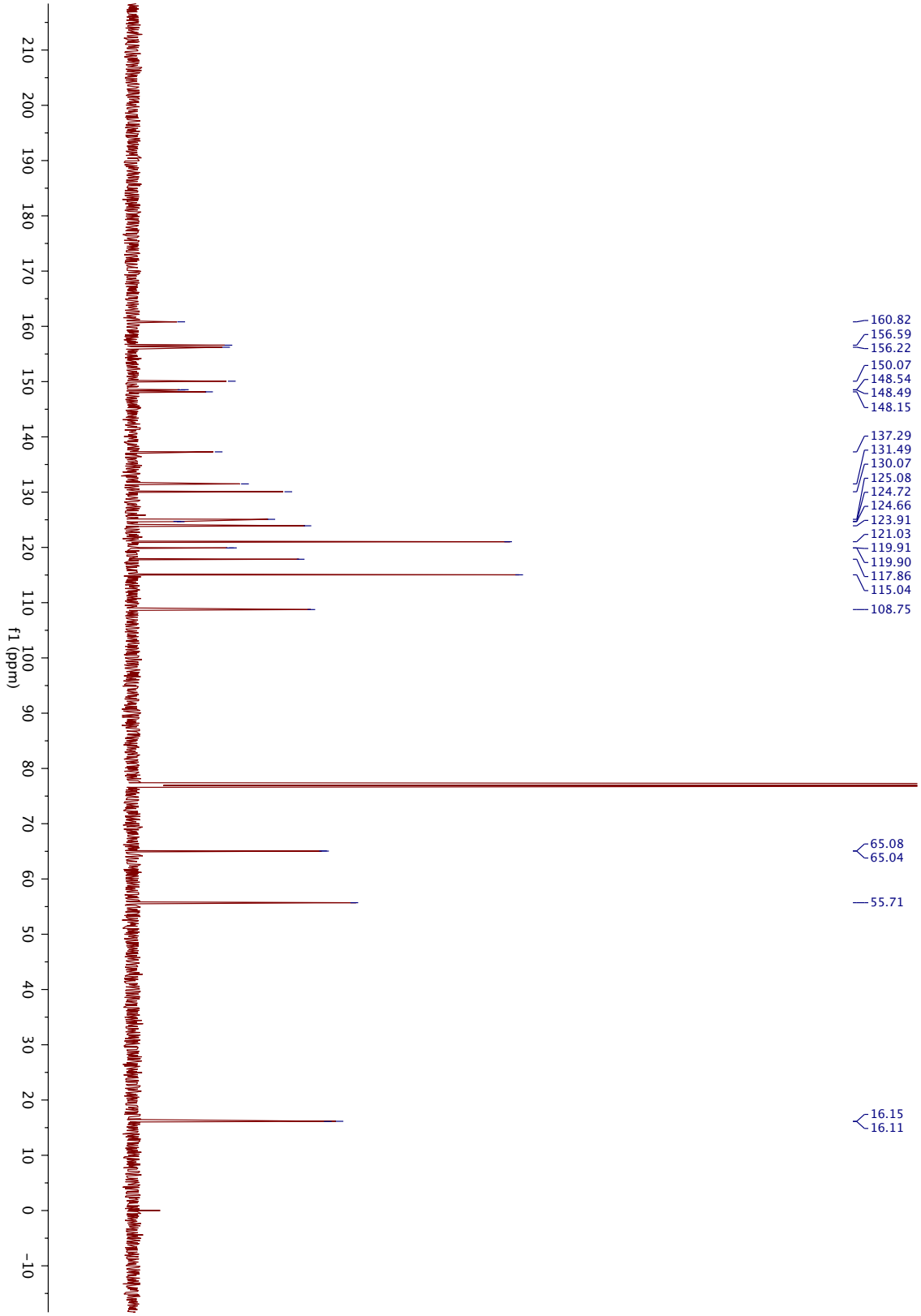
**10b**: $^{31}P$ NMR ($CDCl_3$, 160MHz)



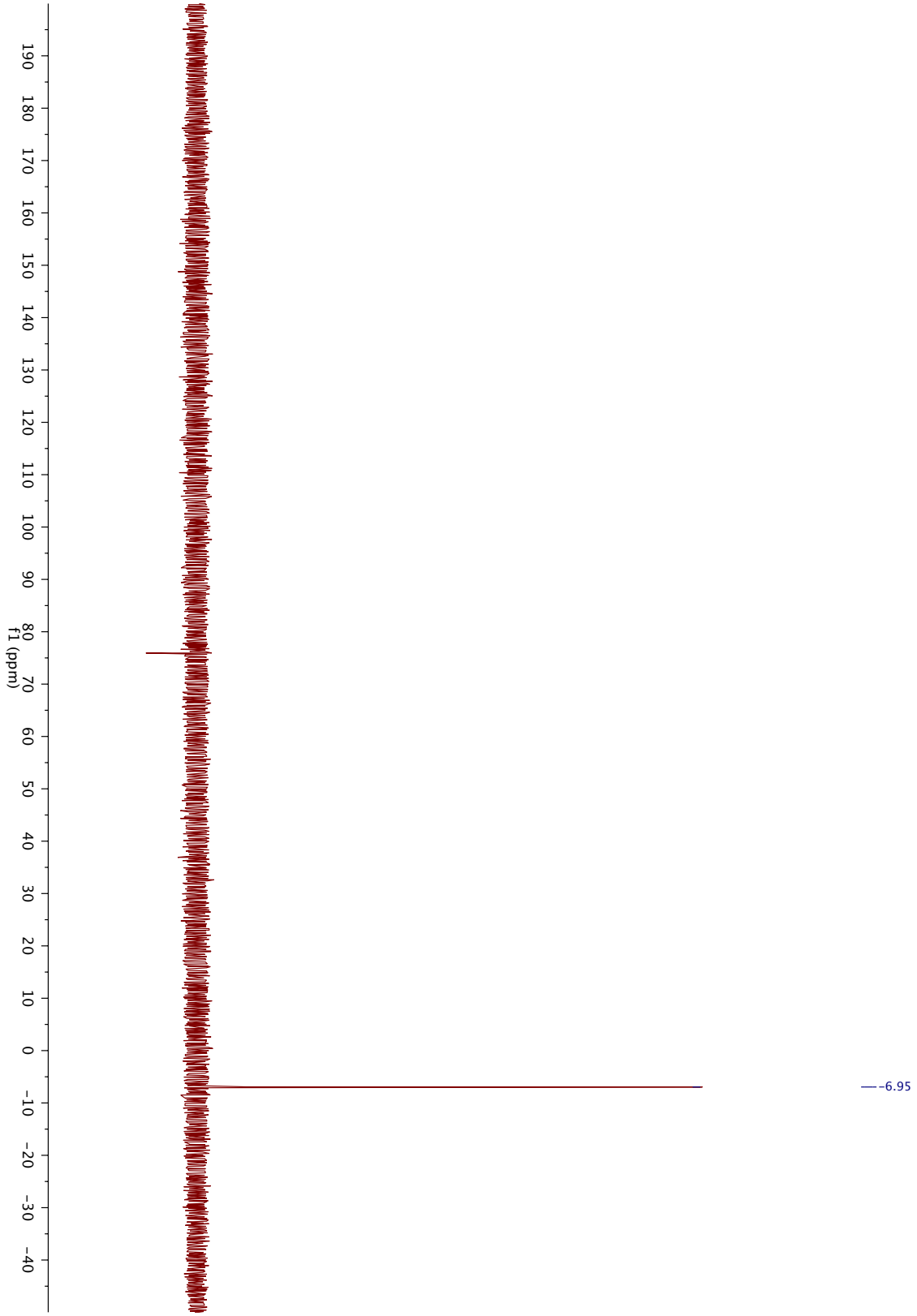
**10b**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



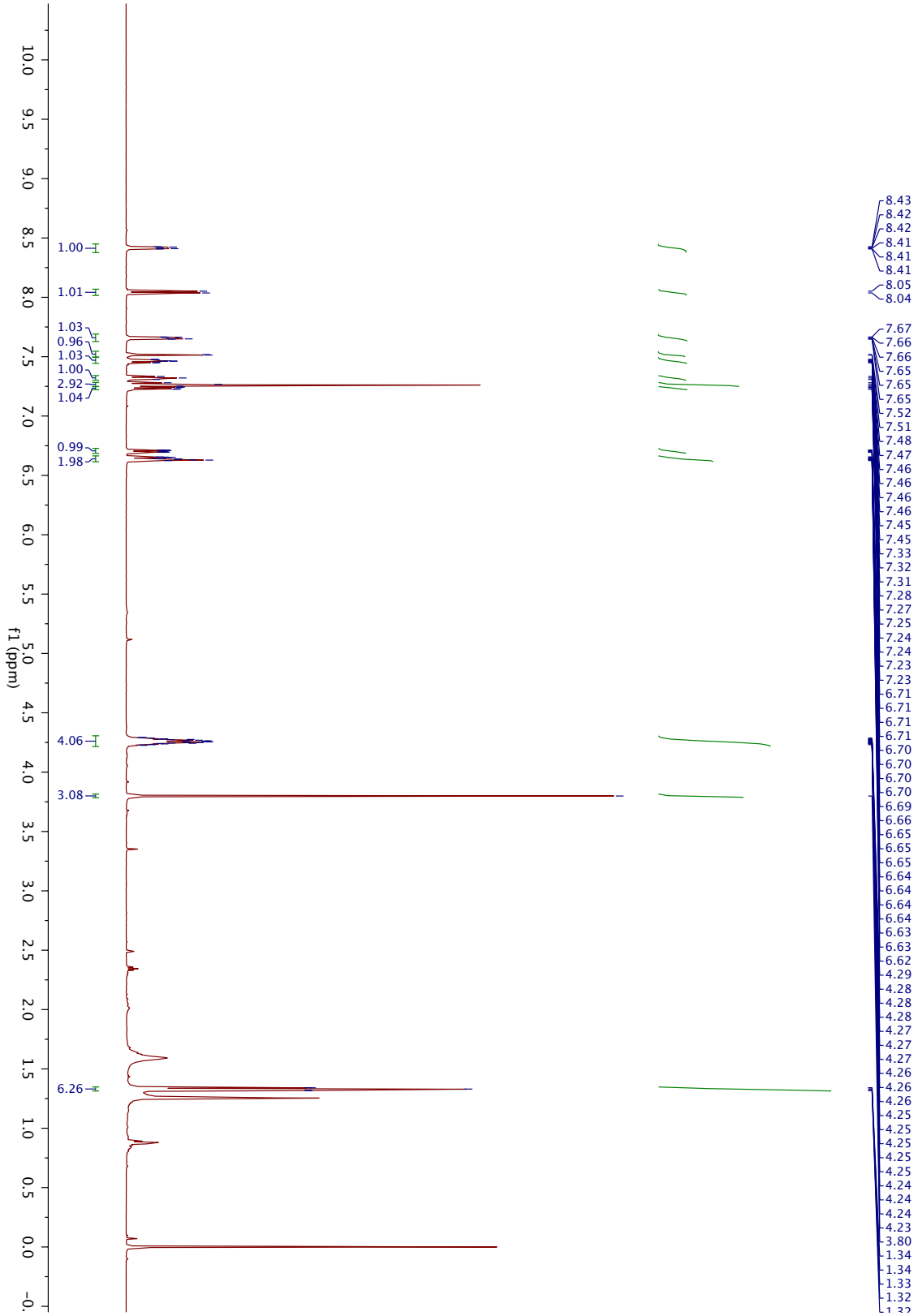
**10b**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



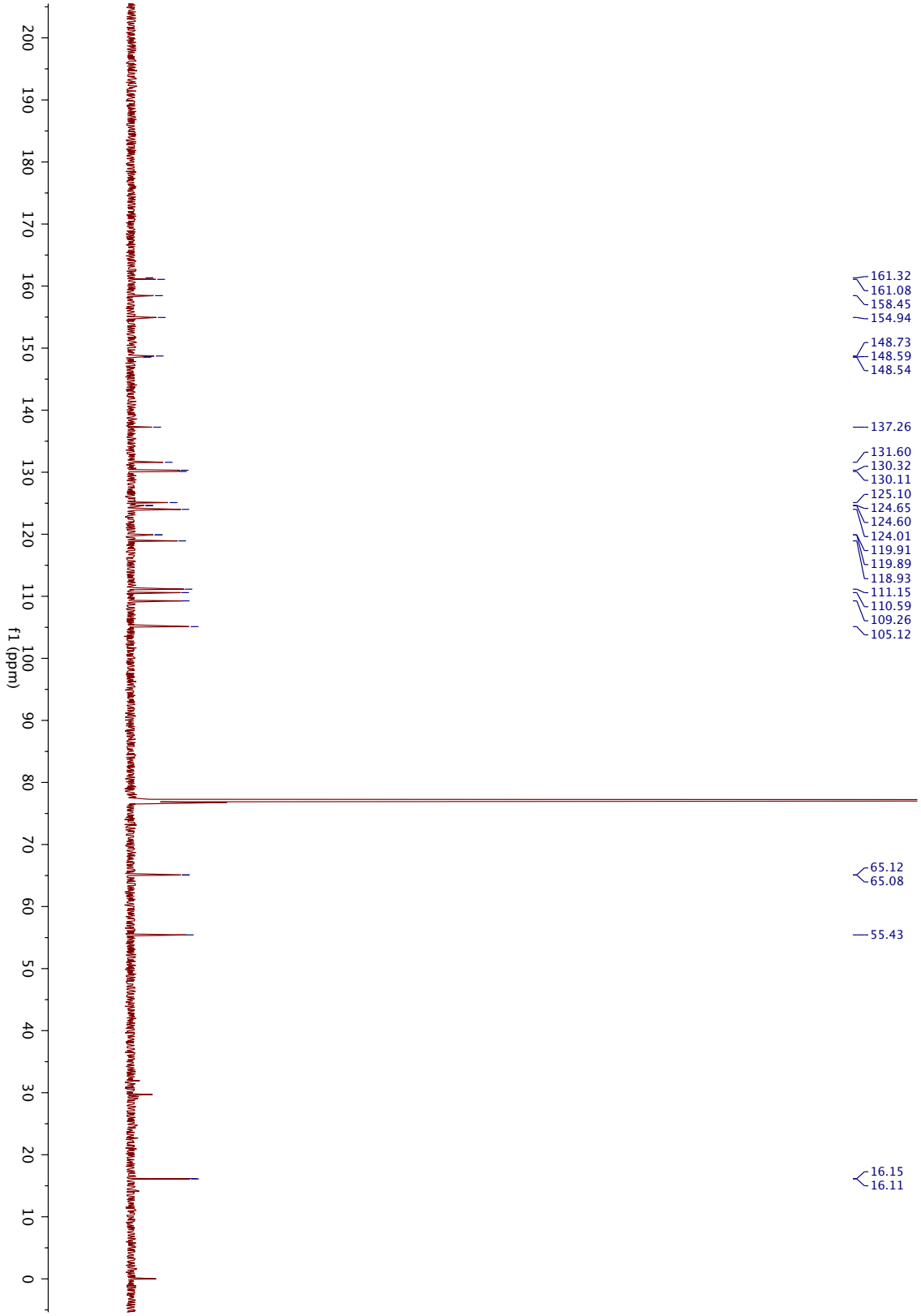
**10c**: $^{31}P$ NMR ($CDCl_3$, 160MHz)



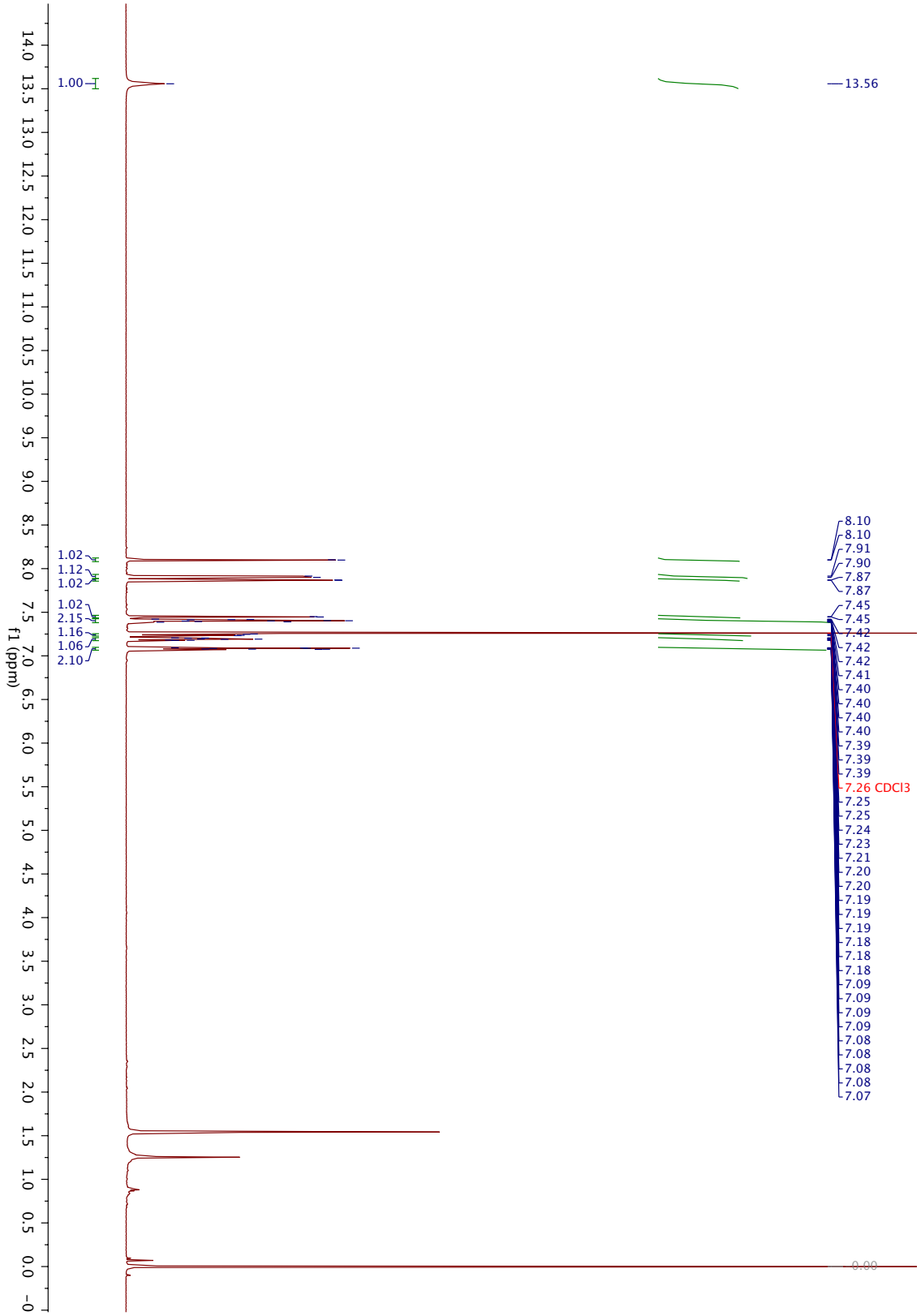
**10c**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



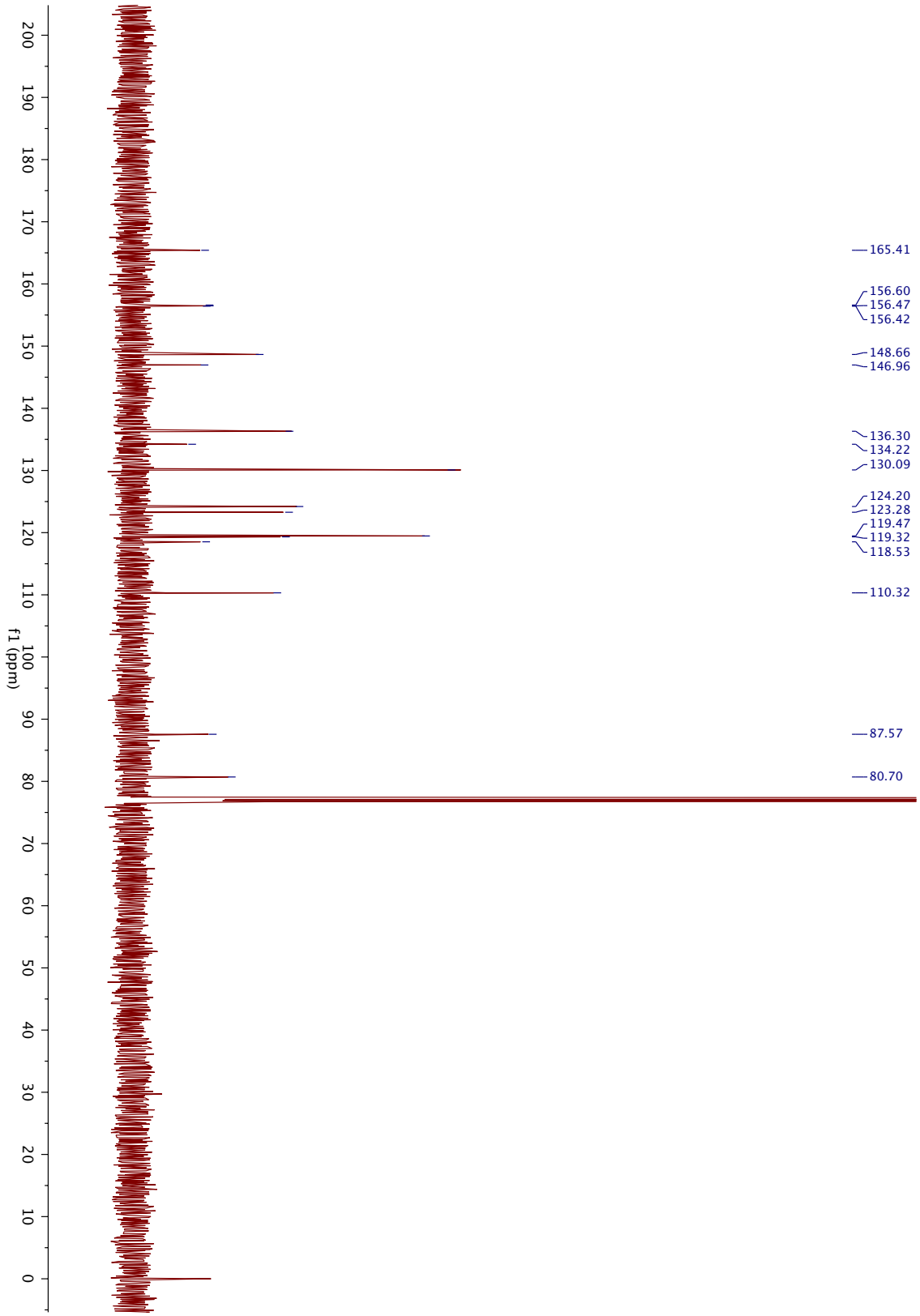
**10c**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



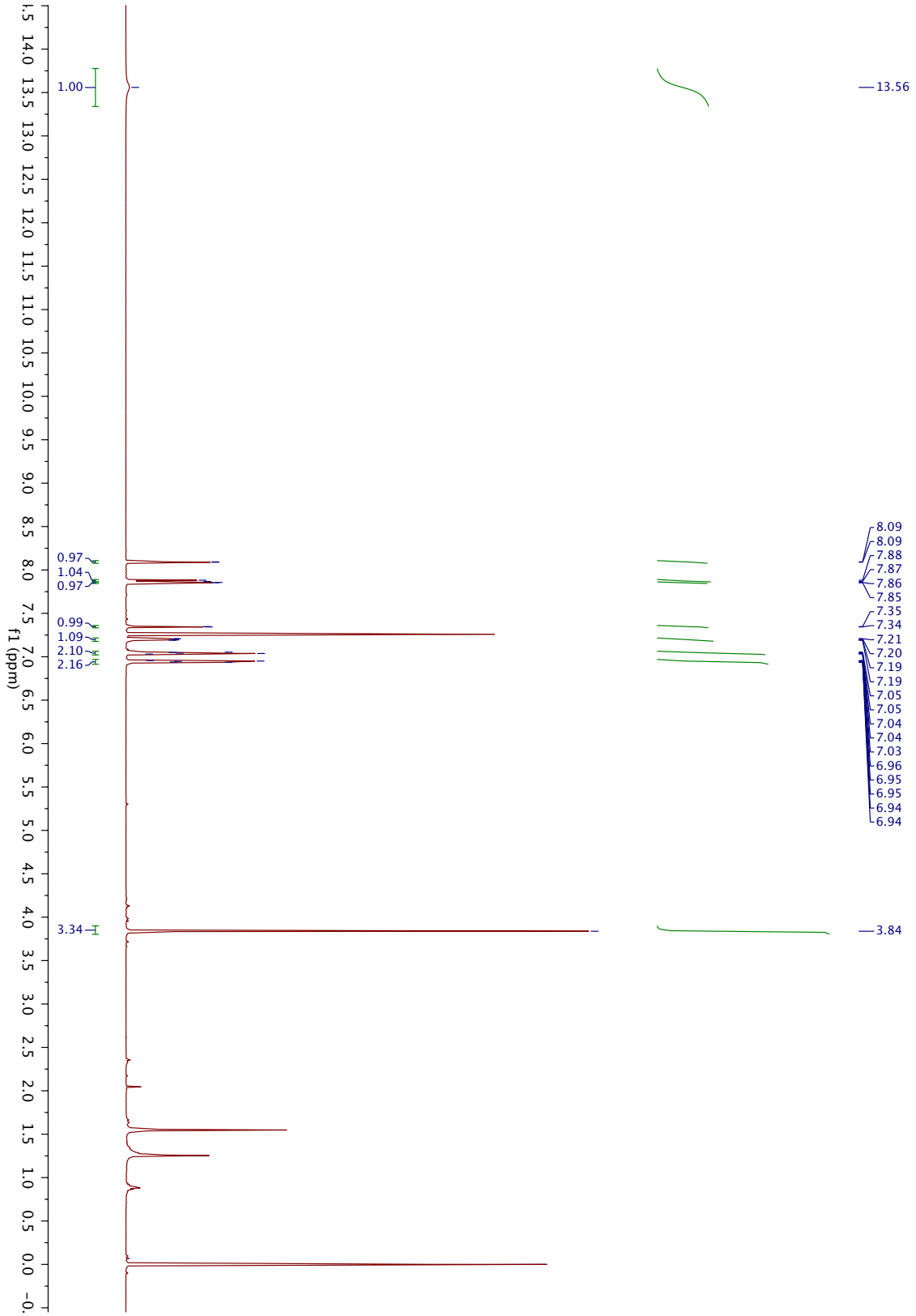
**12a**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



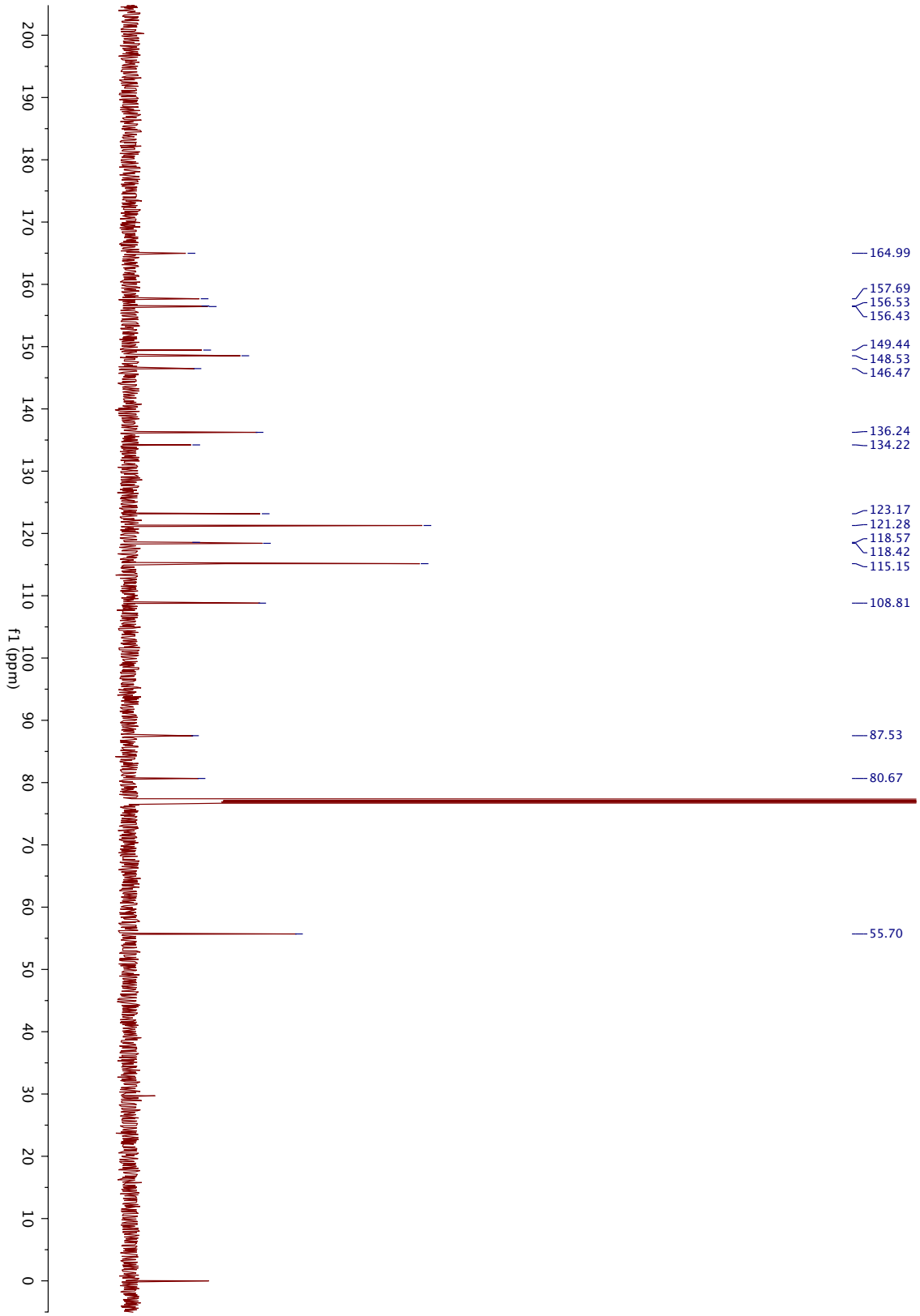
**12a**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



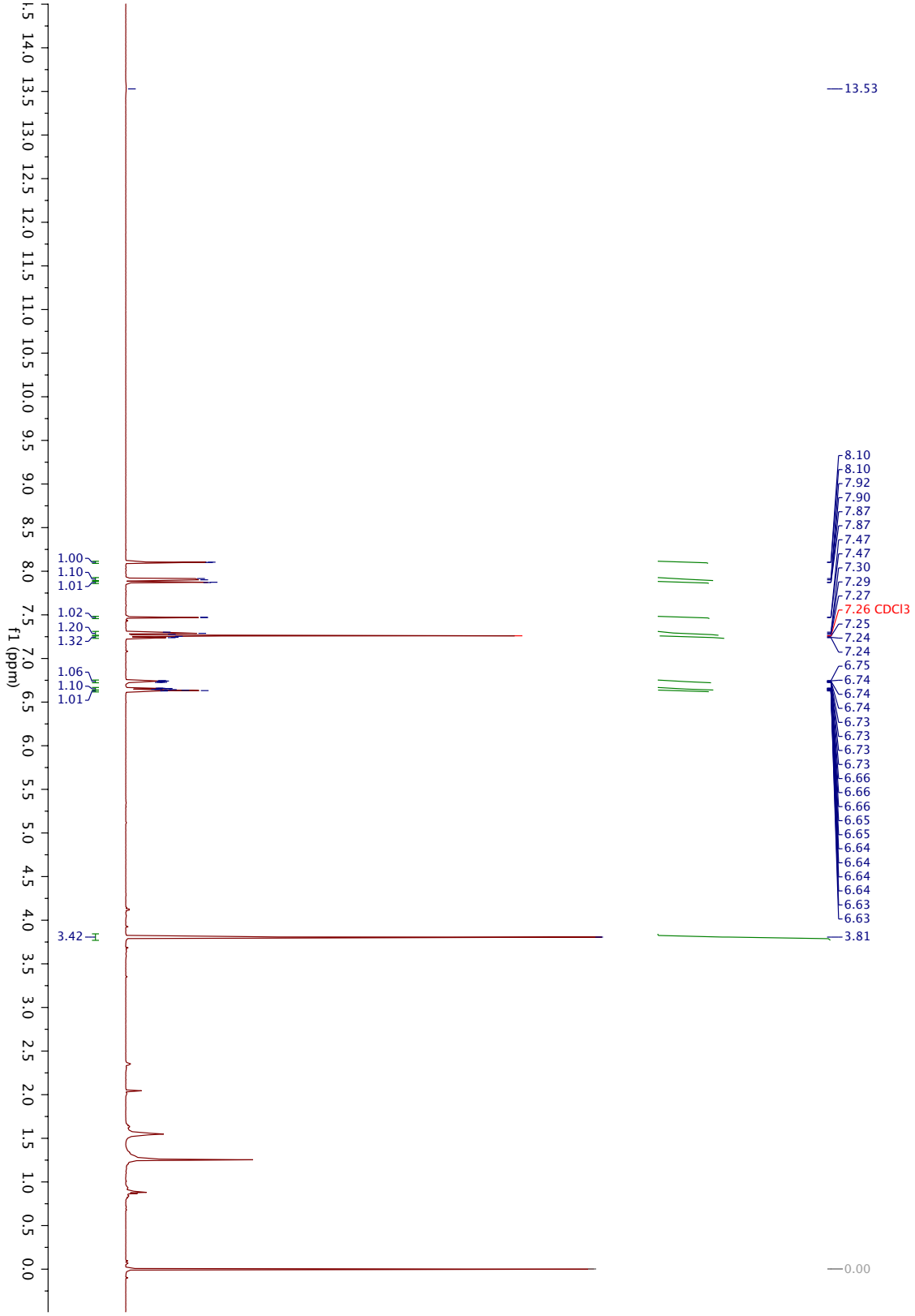
**12b**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



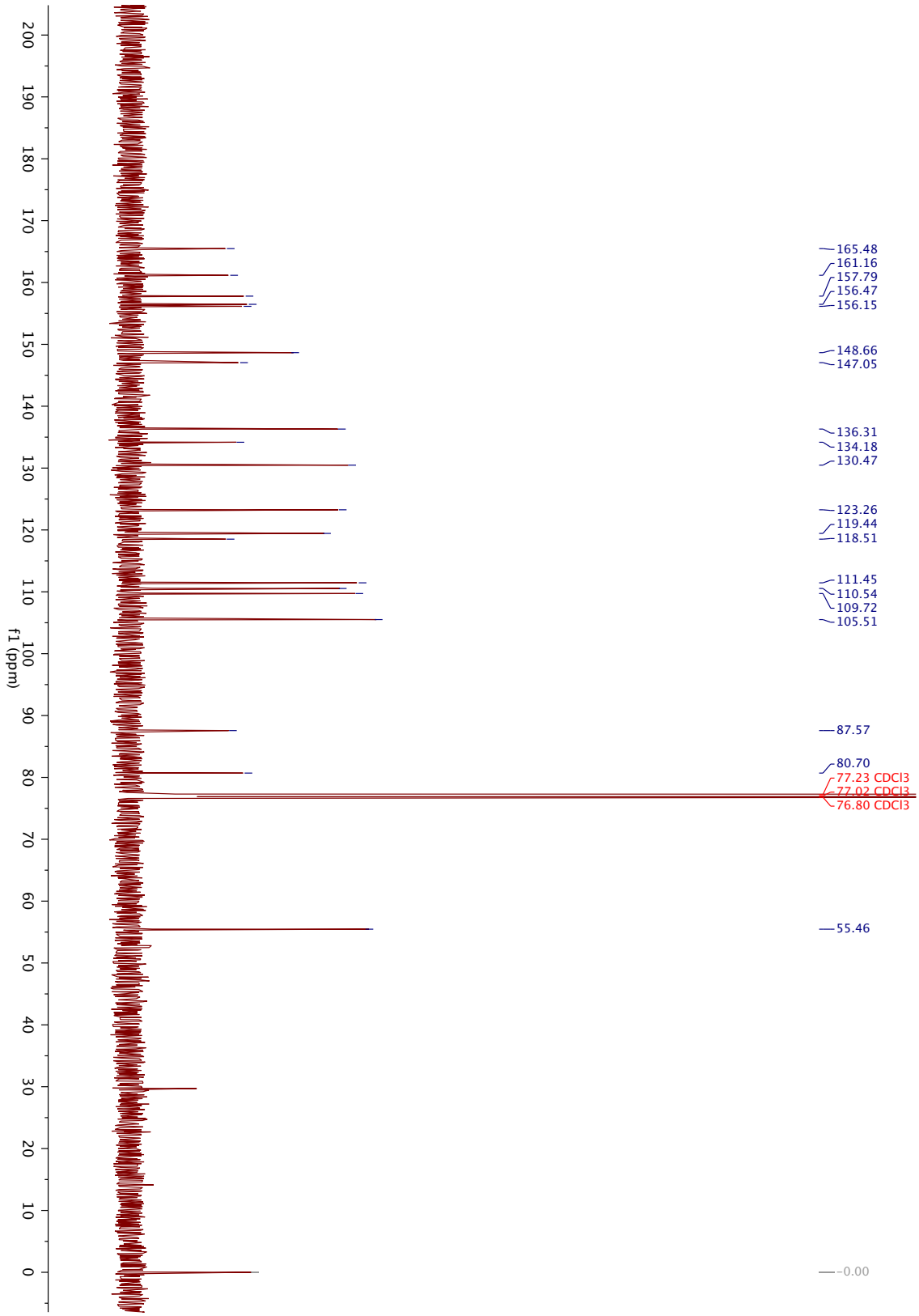
**12b**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



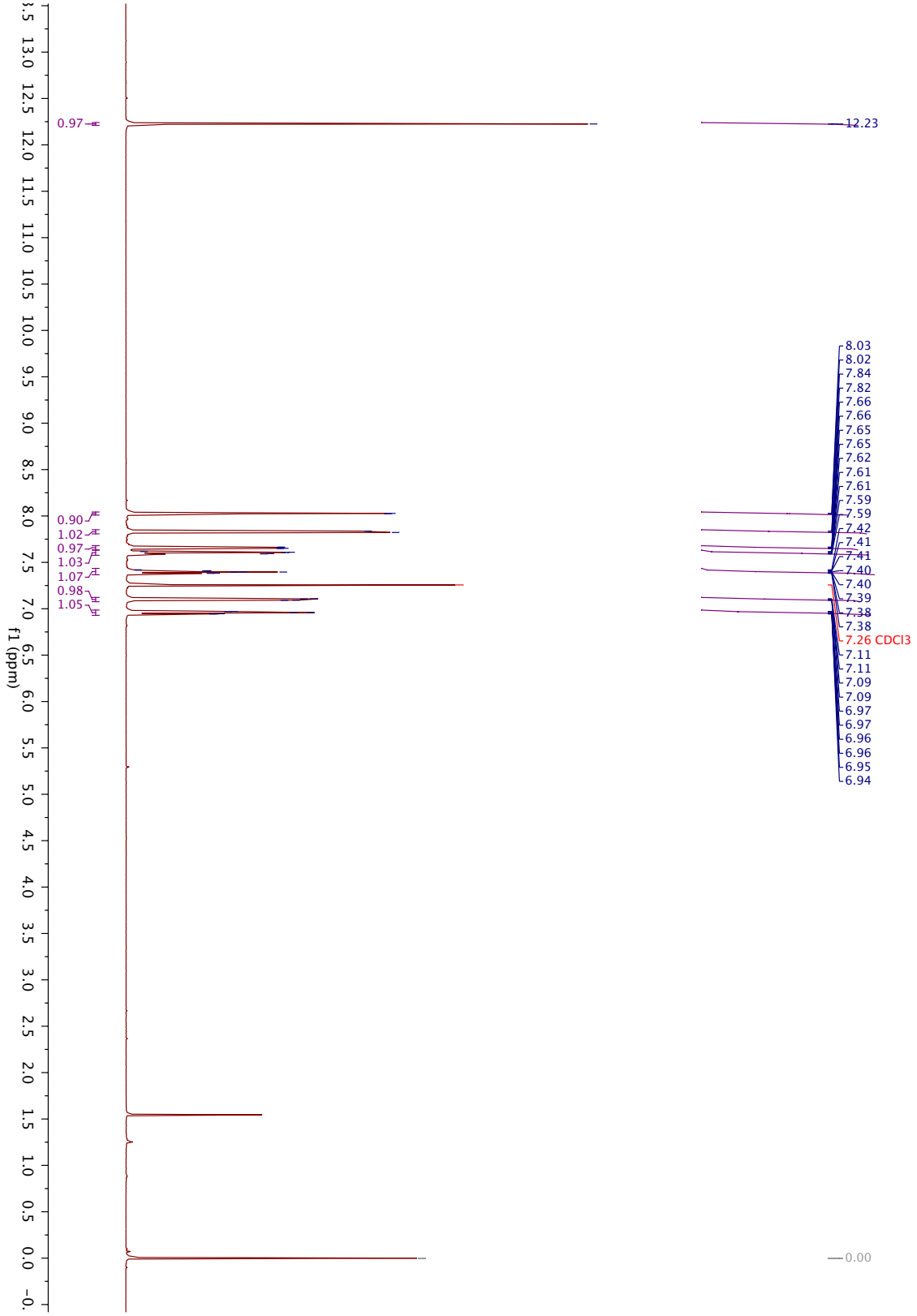
**12c**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



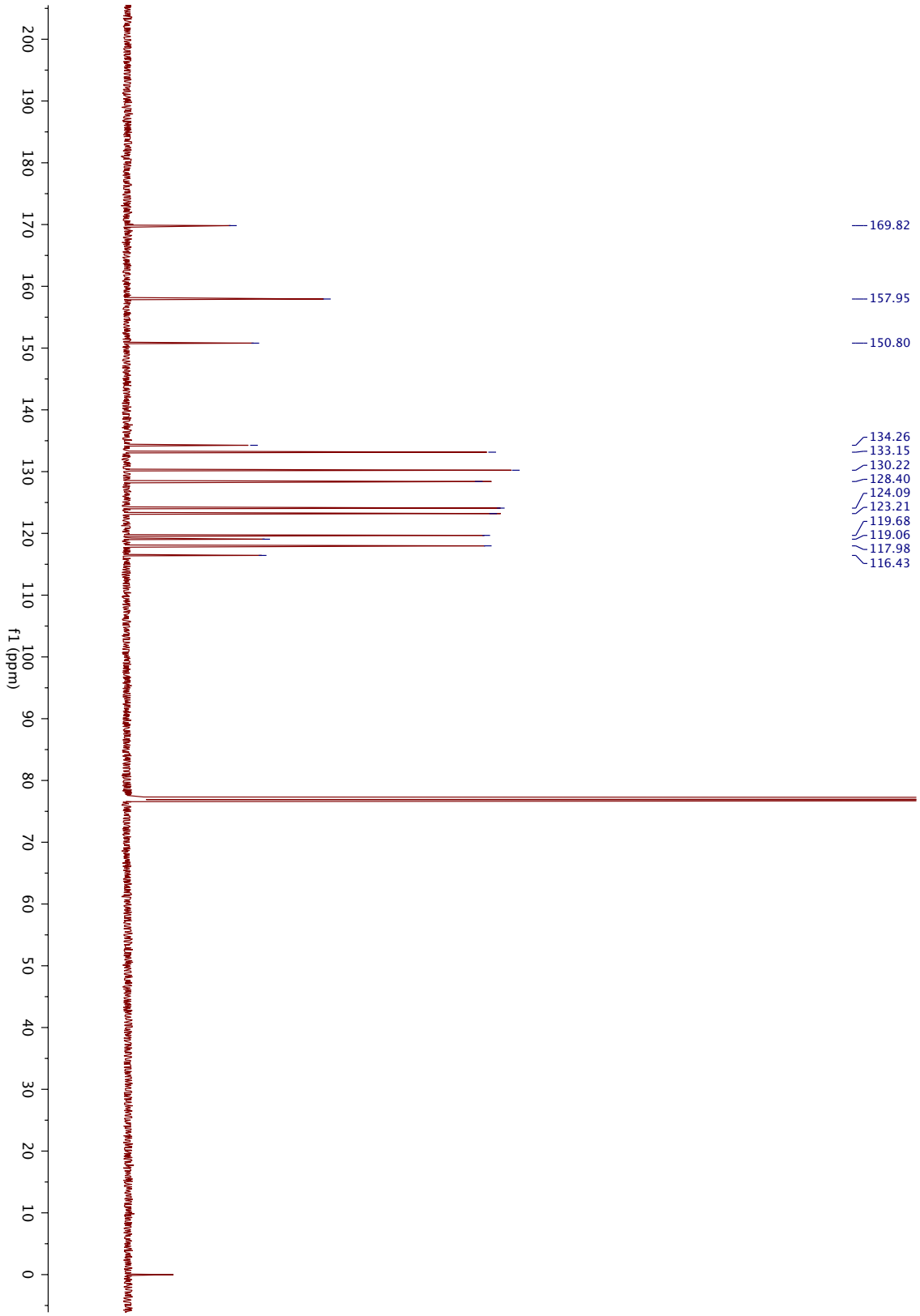
**12c**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



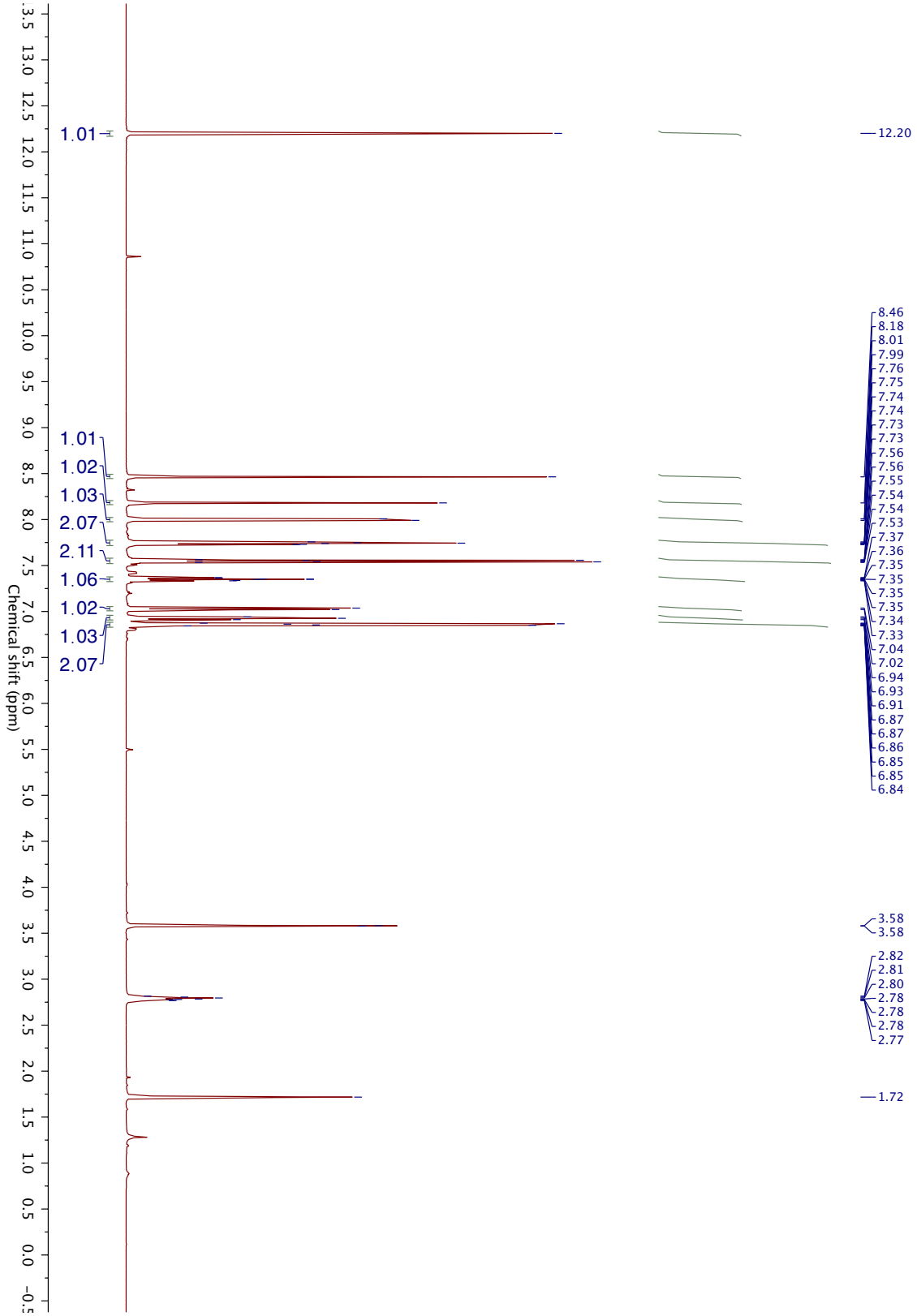
**14**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



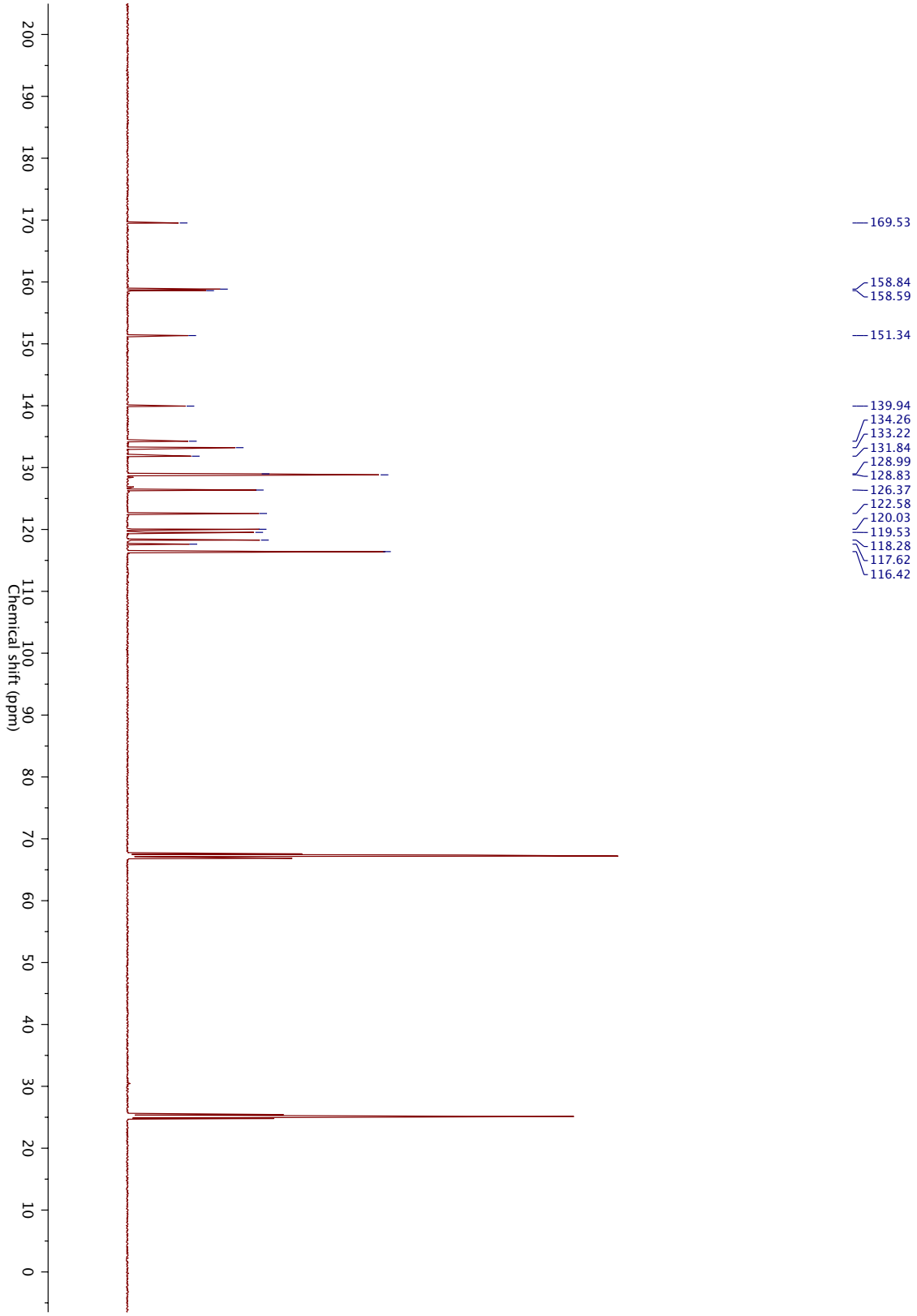
**14**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



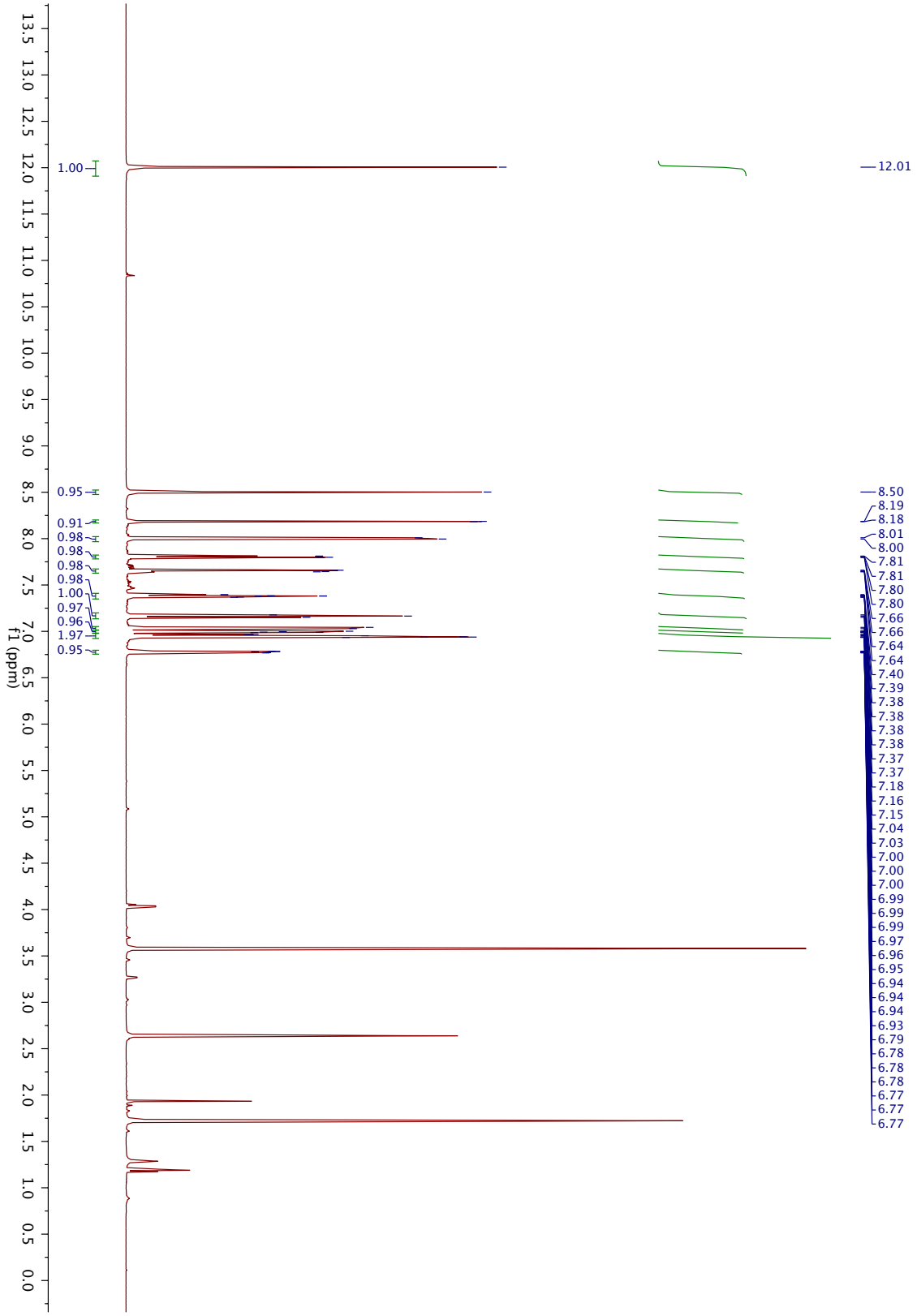
**15**: $^{1}$H NMR (THF-$d_8$, 500 MHz)



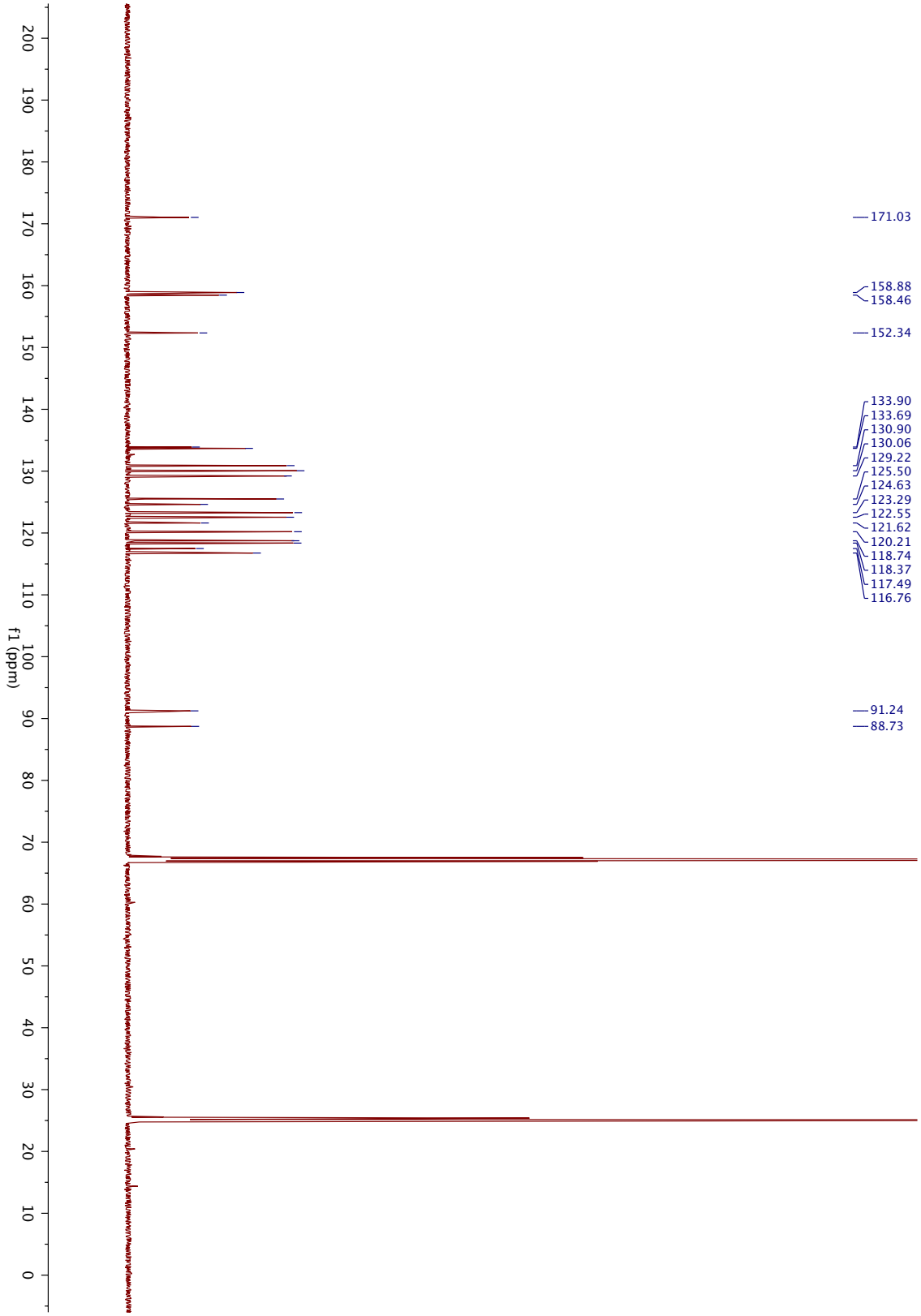
**15**: $^{13}$C NMR (THF-$d_8$, 125 MHz)



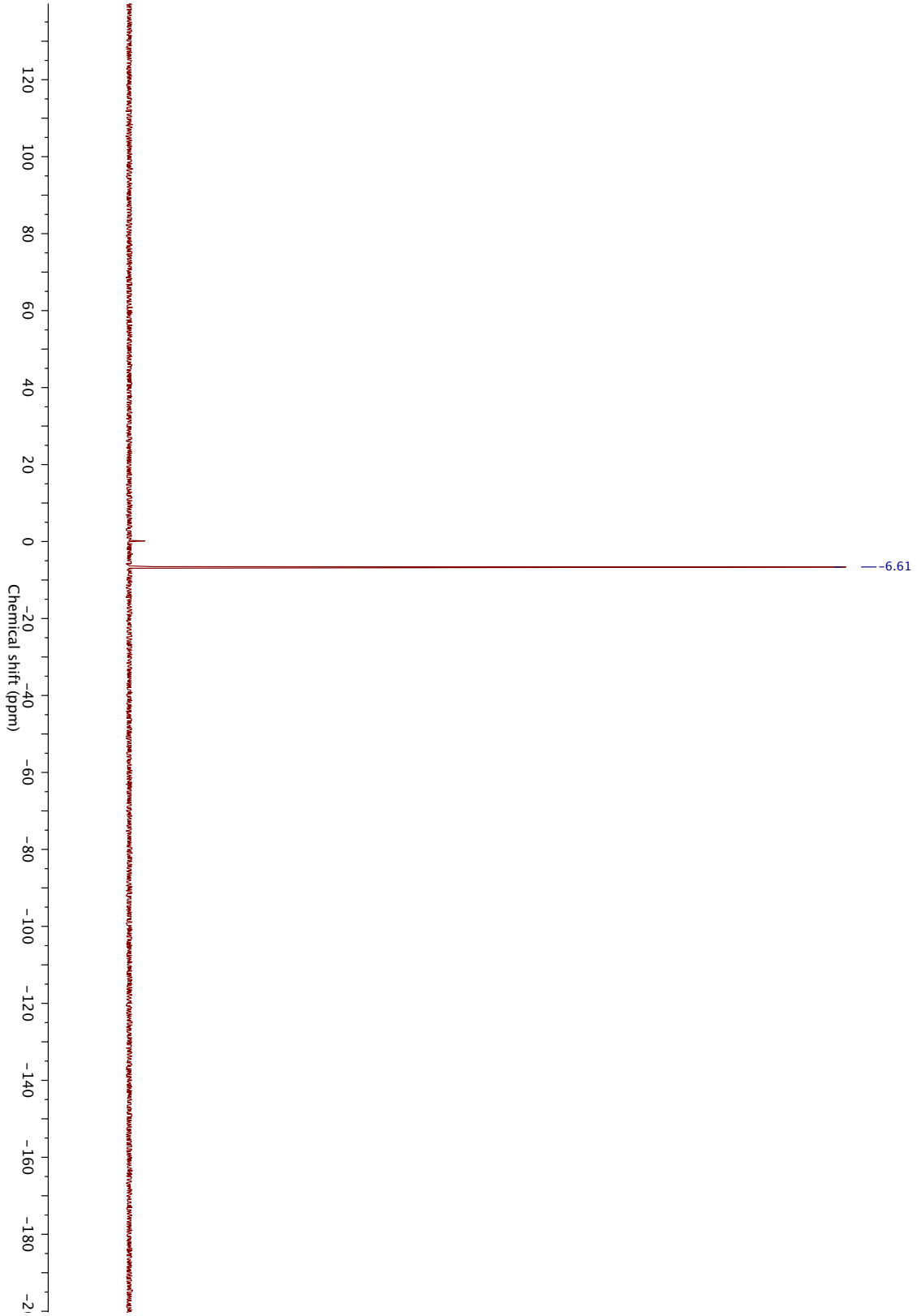
**16**: $^{1}$H NMR (THF-$d_8$, 600 MHz)



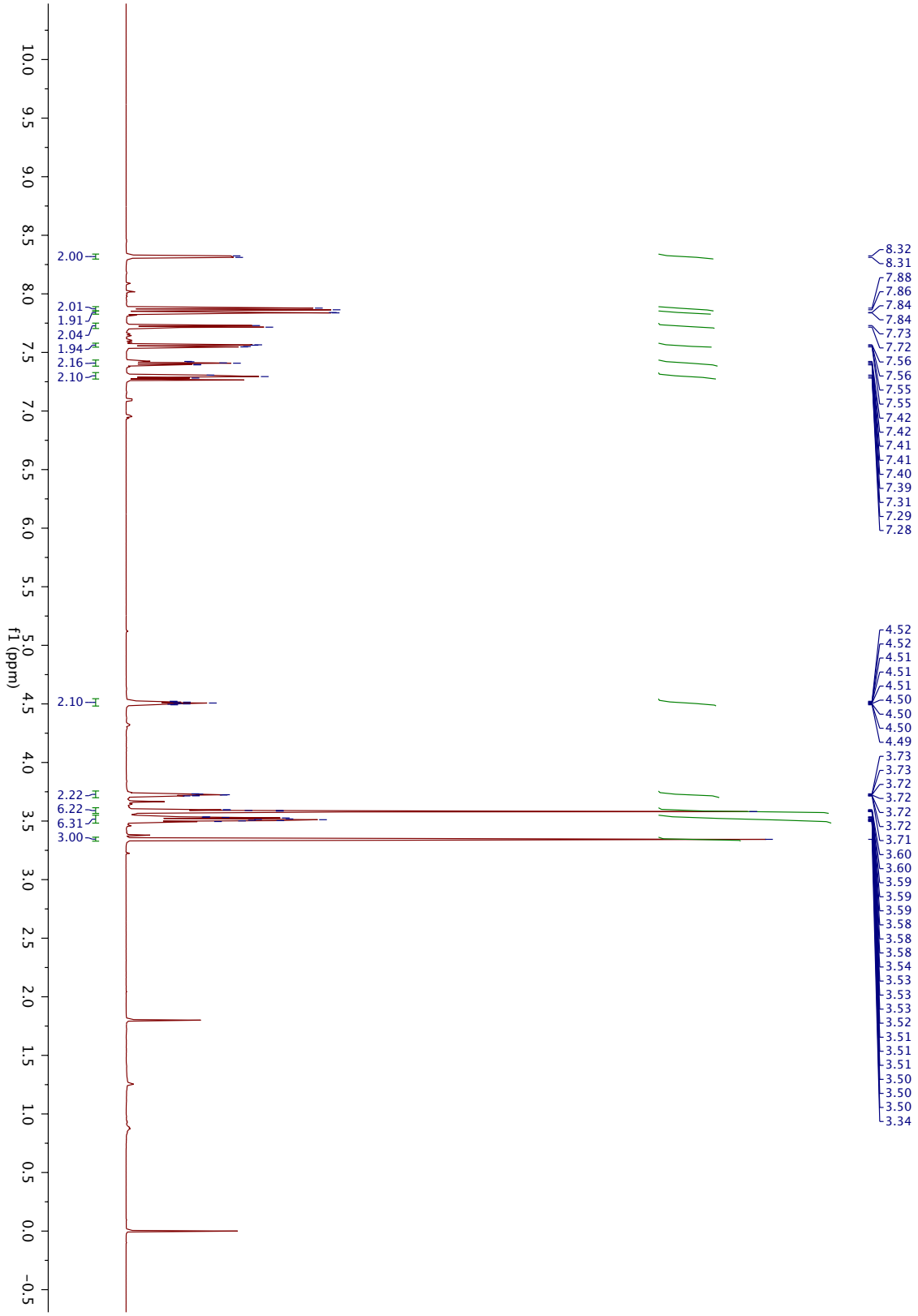
**16**: $^{13}$C NMR (THF-$d_8$, 150 MHz)



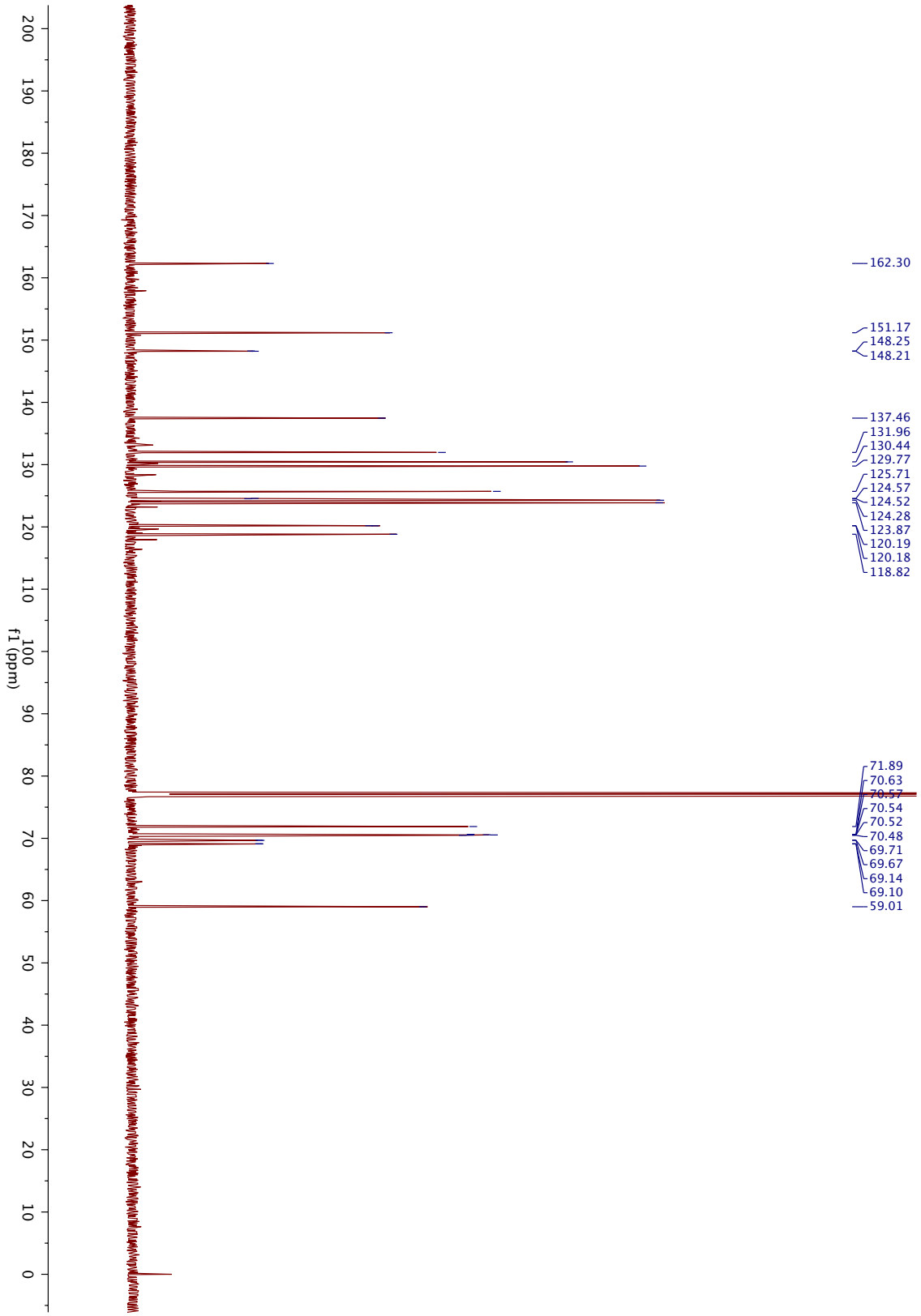
**17**: $^{31}P$ NMR (CDCl3, 240 MHz)



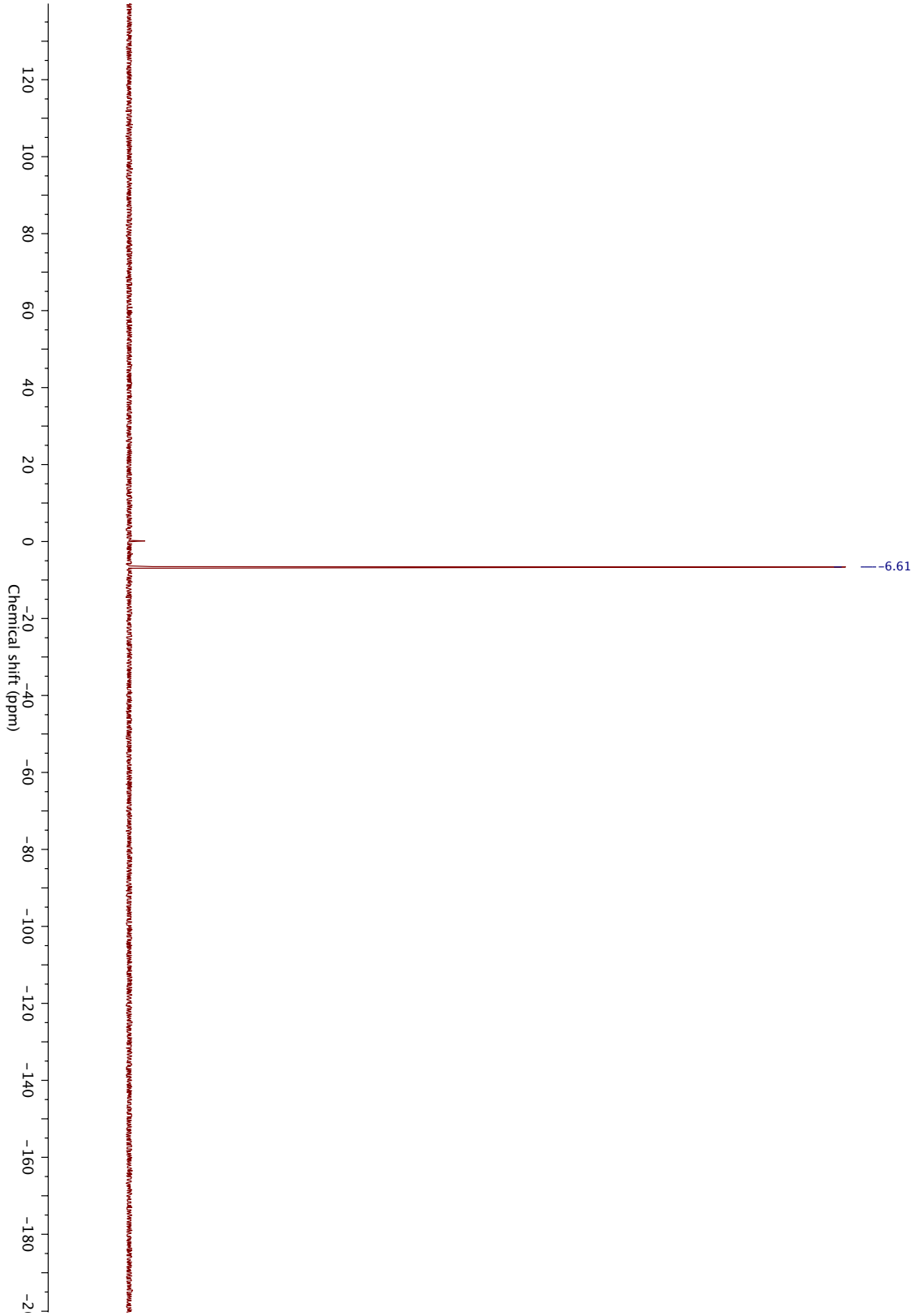
**17**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



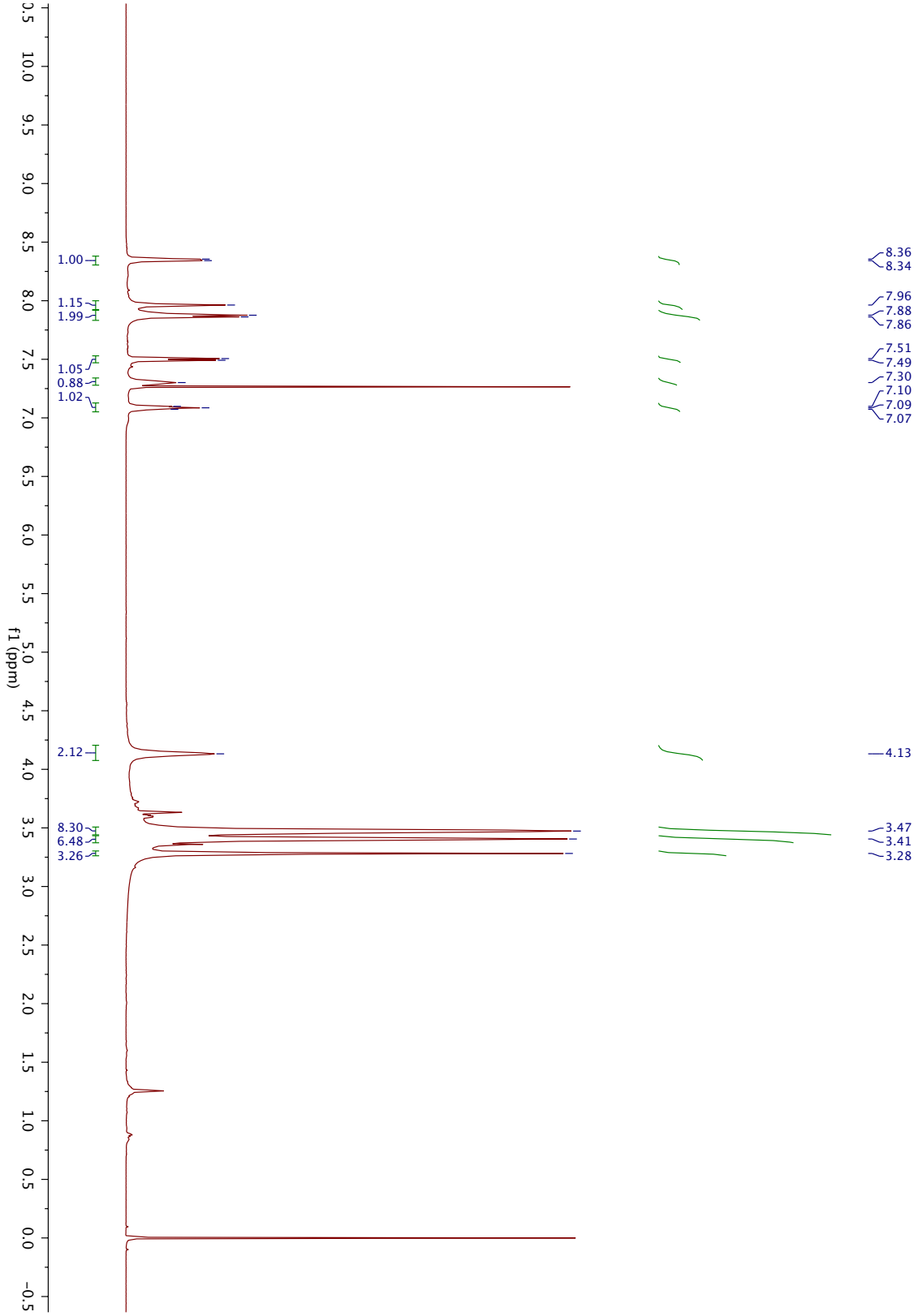
**17**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



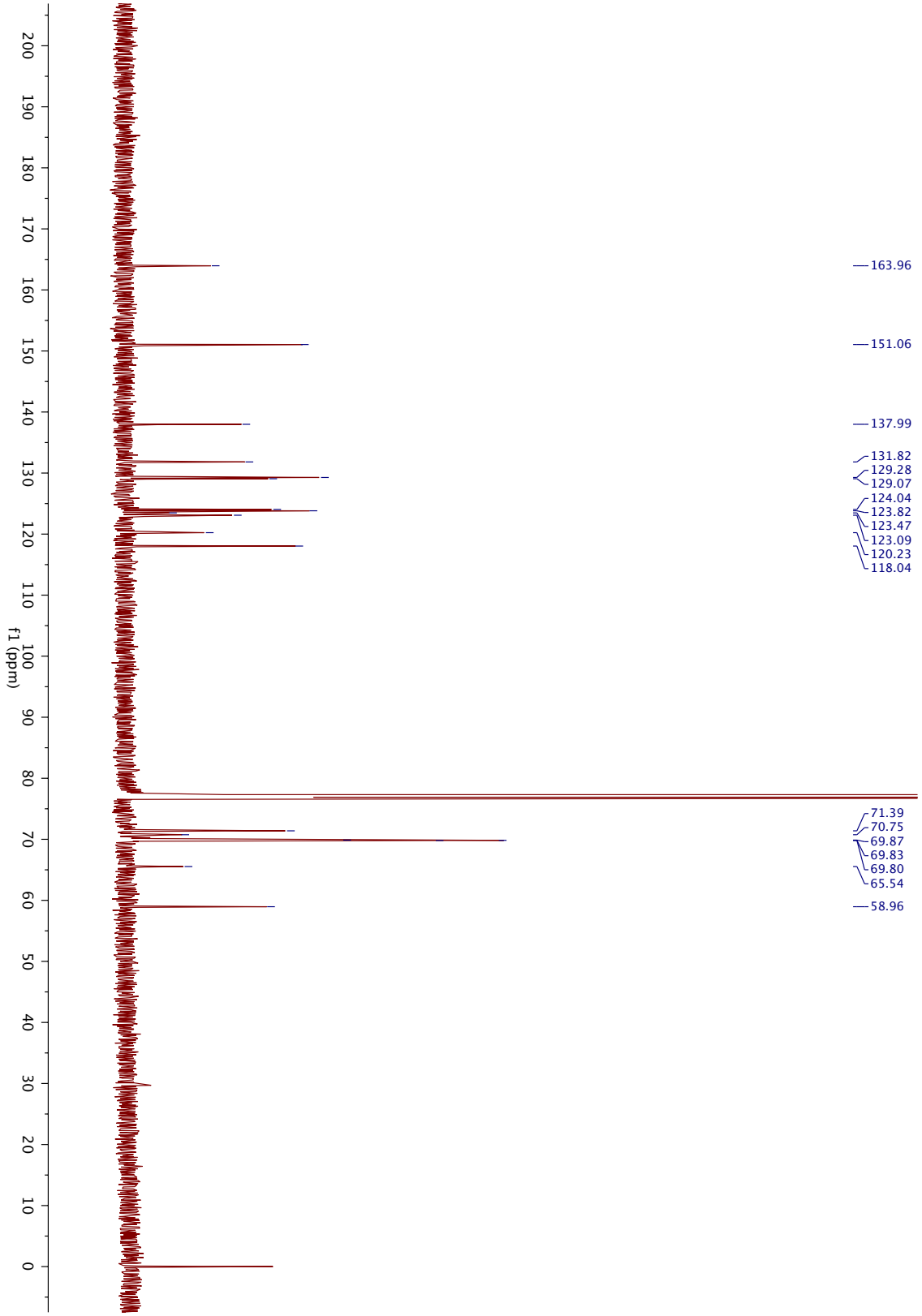
**18**: $^{31}$P NMR (CDCl3, 200 MHz)



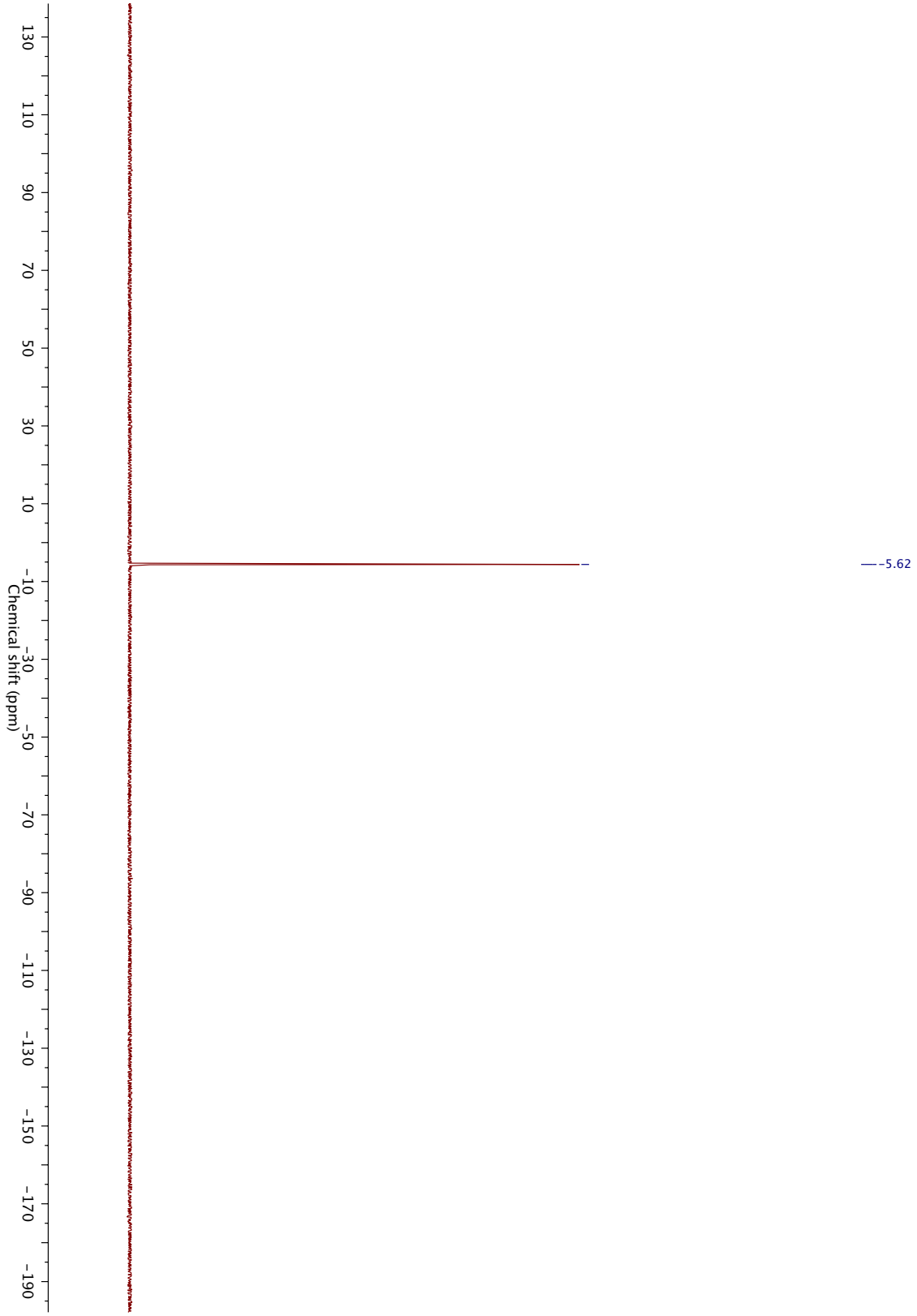
**18**: $^{1}$H NMR ($CDCl_3$, 600 MHz)



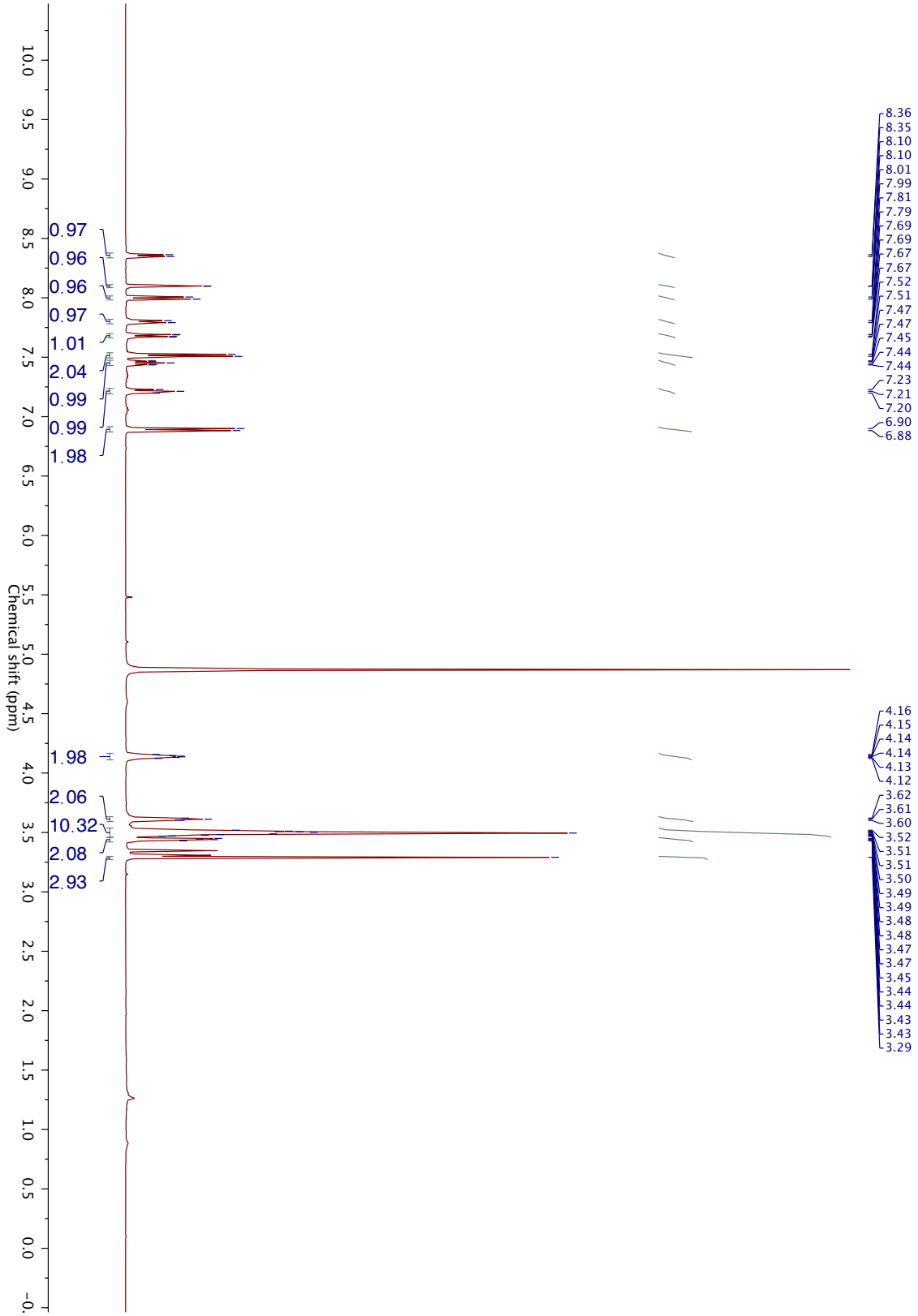
**18**: $^{13}C$ NMR ($CDCl_3$, 150 MHz)



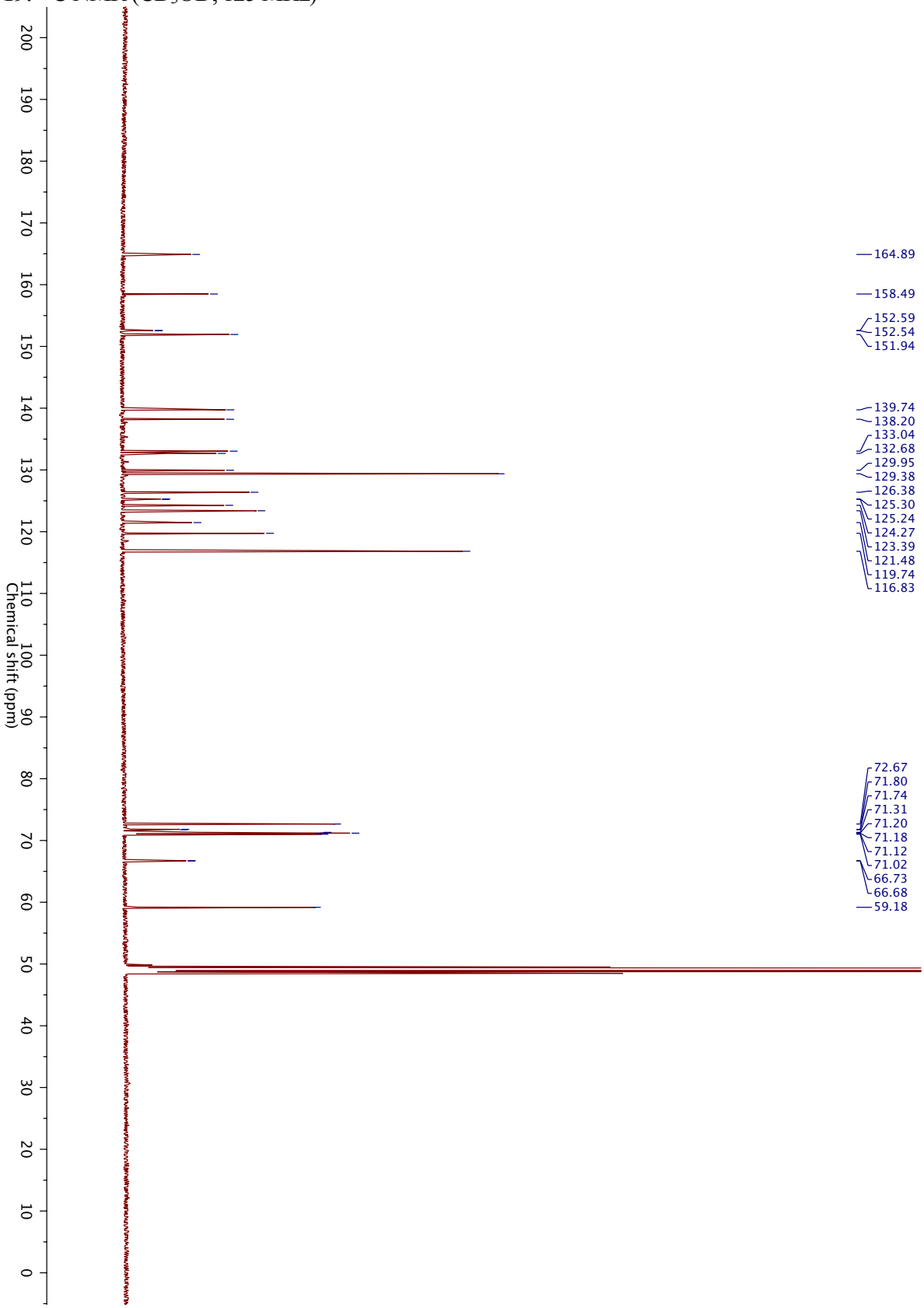
**19**: $^{31}P$ NMR ($CD_3OD$, 200 MHz)



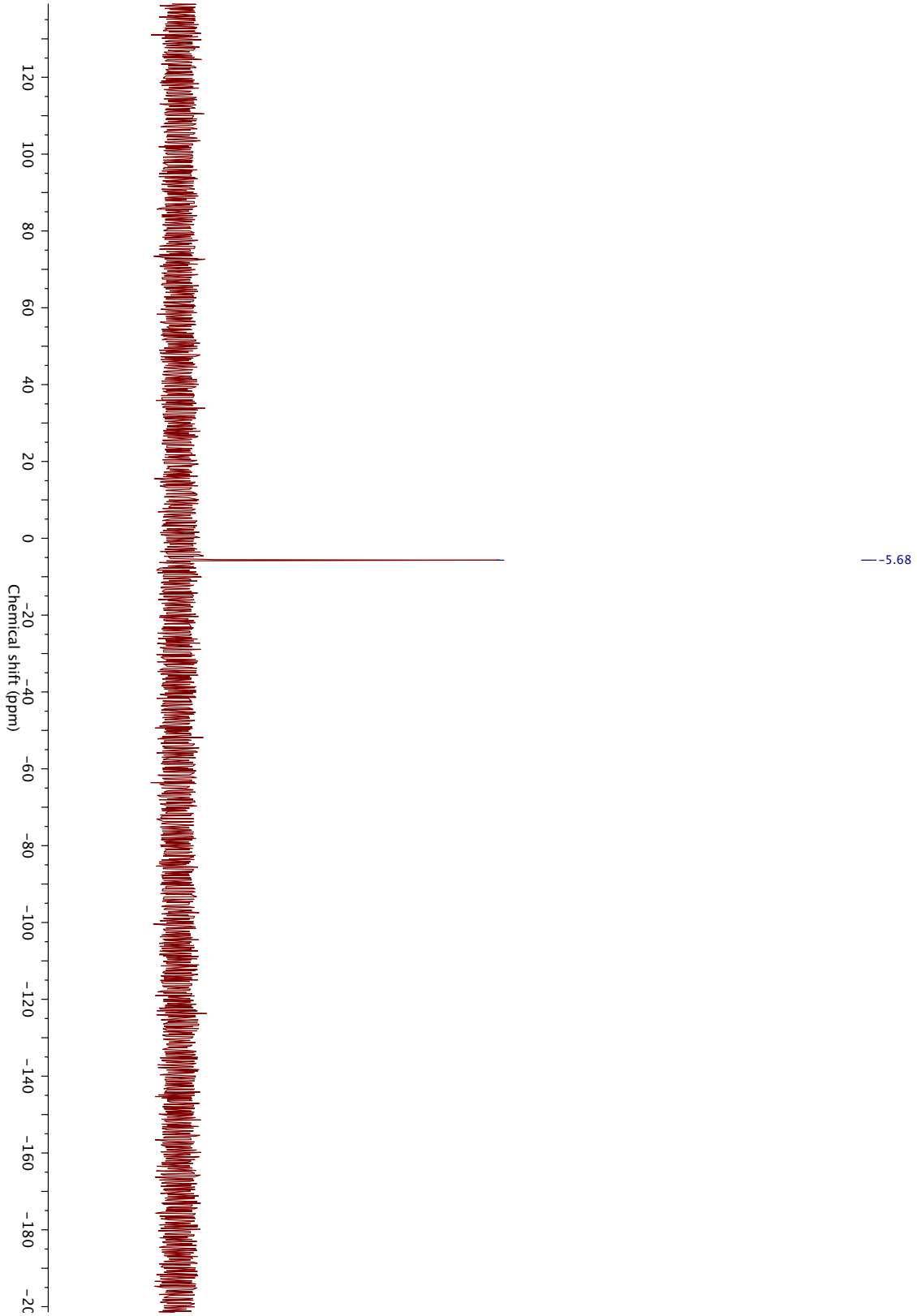
**19**: $^{1}$H NMR ($CD_3OD$, 500 MHz)



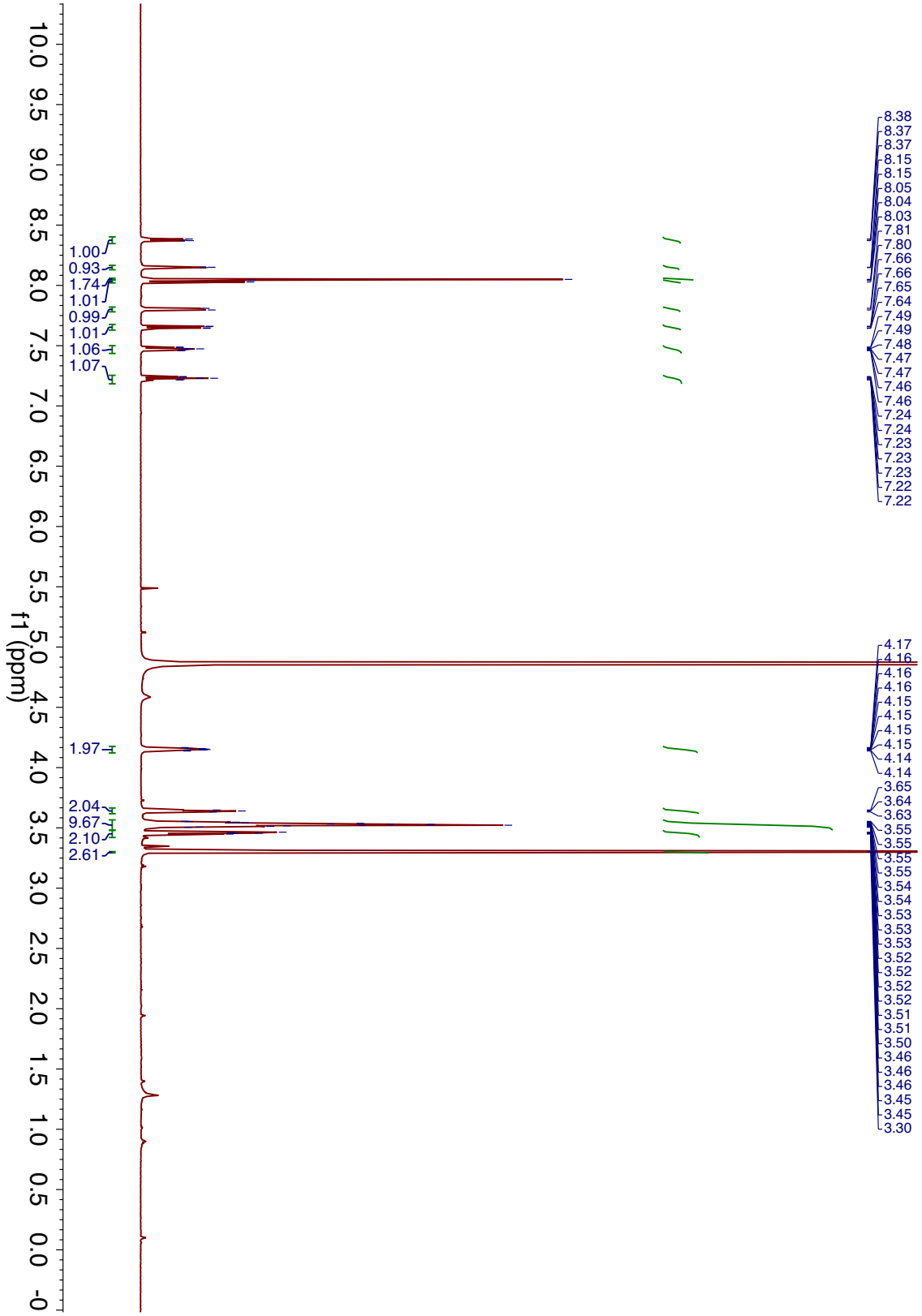
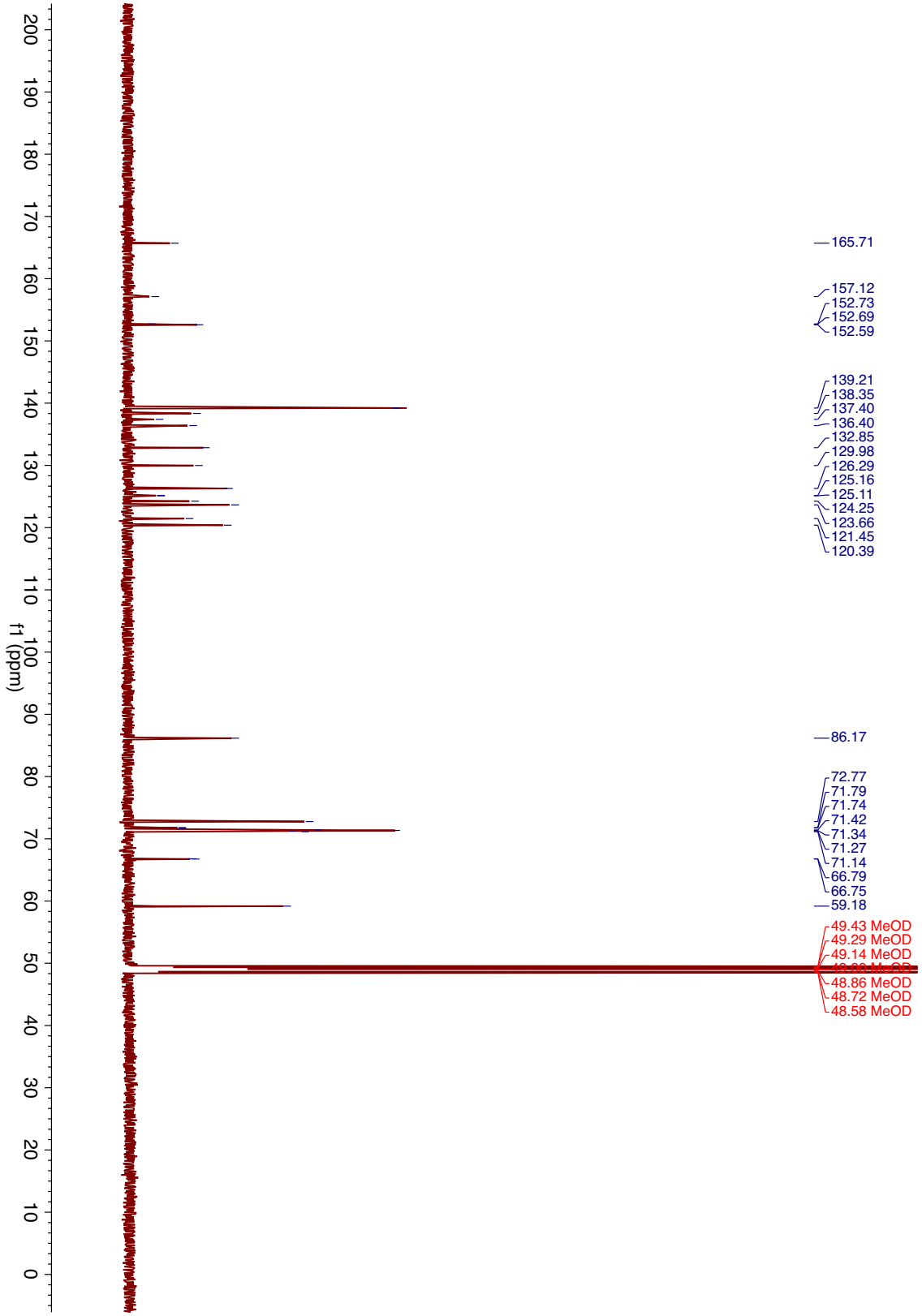
**19**: $^{13}C$ NMR ($CD_3OD$, 125 MHz)



**19-I$_2$**: $^{31}$P NMR ($CD_3OD$, 200 MHz)



**19-I$_2$**: $^1$H NMR ($CD_3OD$, 600 MHz)



**19-I$_2$**: $^{13}$C NMR ($CD_3OD$, 150 MHz)