# Pyrimidine Nucleosides with Reactive (β-Chlorovinyl)sulfone or (β-Keto)sulfone Group at C5 Position, Their Reactions with Nucleophiles and Electrophiles, and Polymerase-catalyzed Incorporation into DNA

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# SUPPORTING INFORMATION

$^{1}H$, $^{13}C$, and $^{31}P$ NMR spectra for all new compounds: Figures S1-S59; Pages S2-S60.

**Figure S1.** $^{1}H$ NMR, (400 MHz), $CDCl_3$

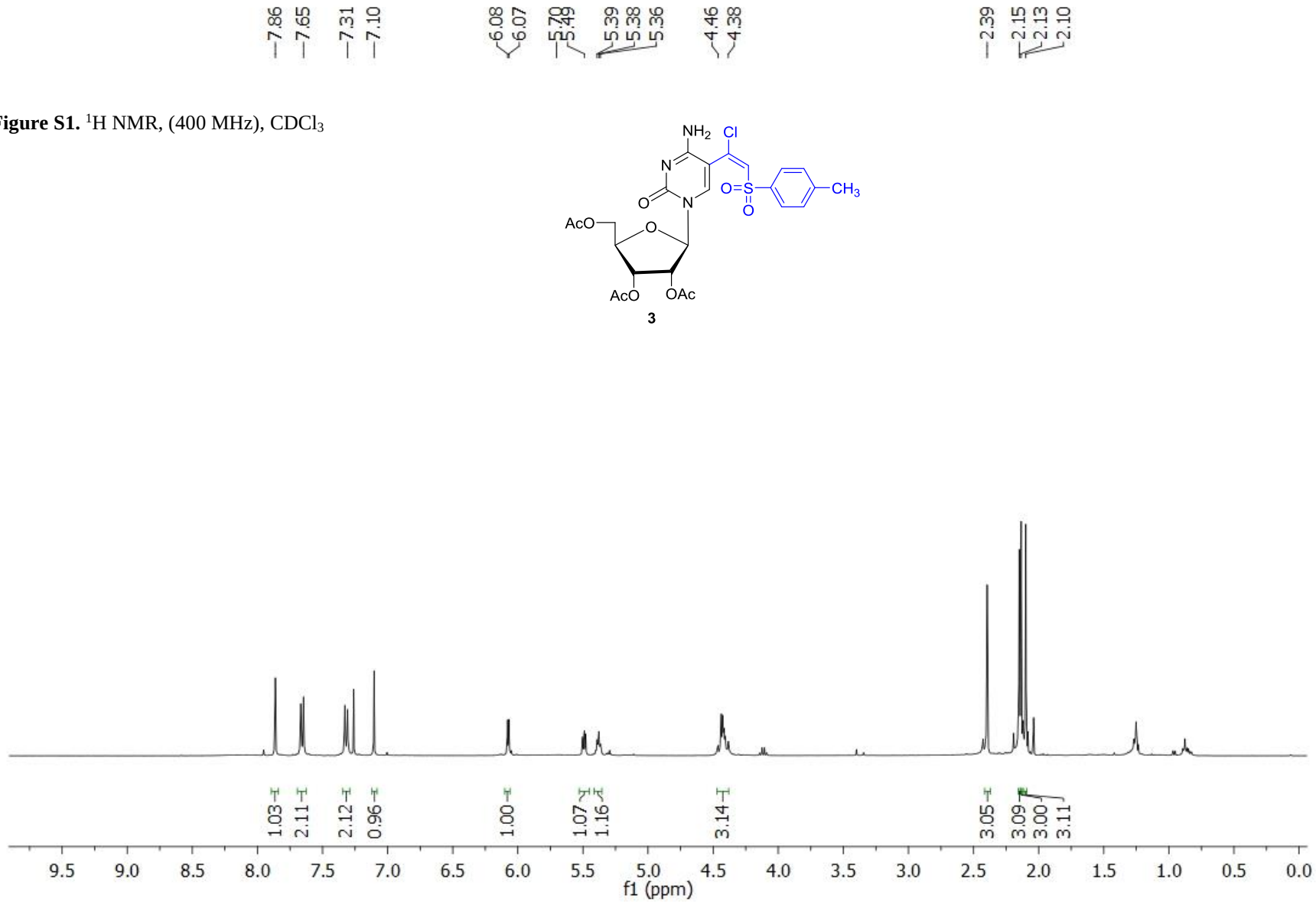


**Figure S2.** $^{13}C$ NMR, (100 MHz), $CDCl_3$

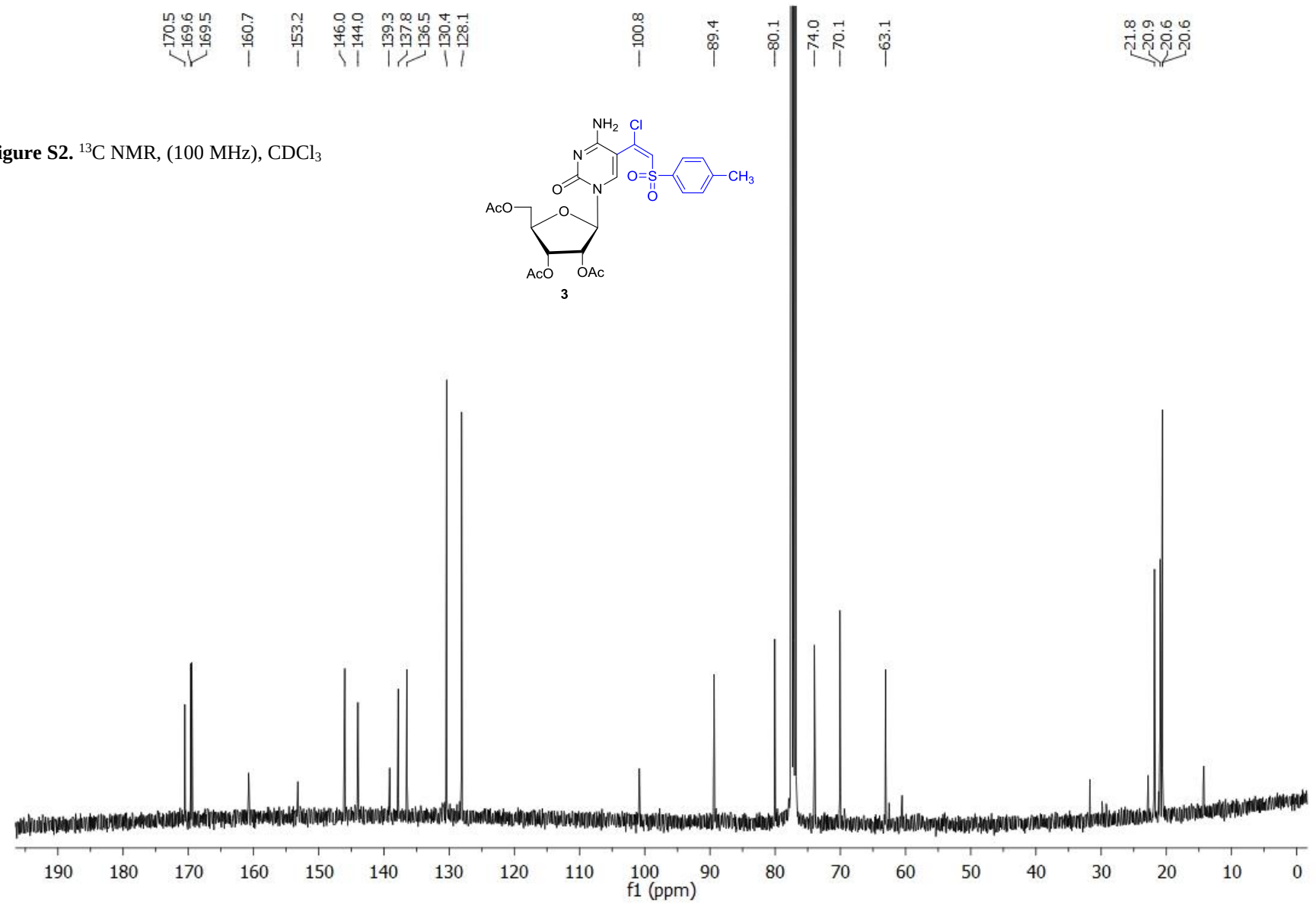


**Figure S3.** $^{1}H$ NMR, (400 MHz), $CDCl_3$

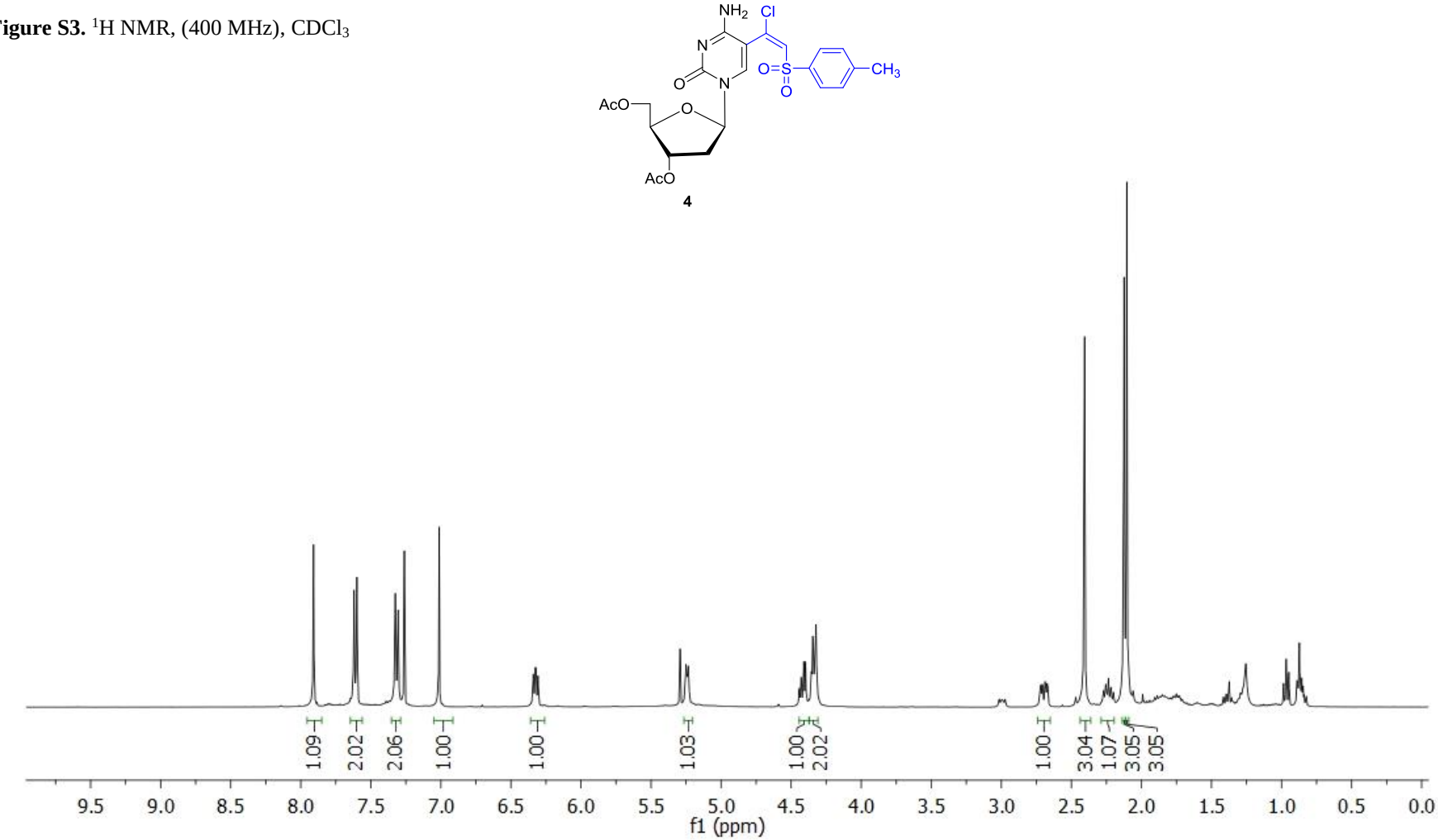


**Figure S4.** $^{13}C$ NMR, (100 MHz), $CDCl_3$

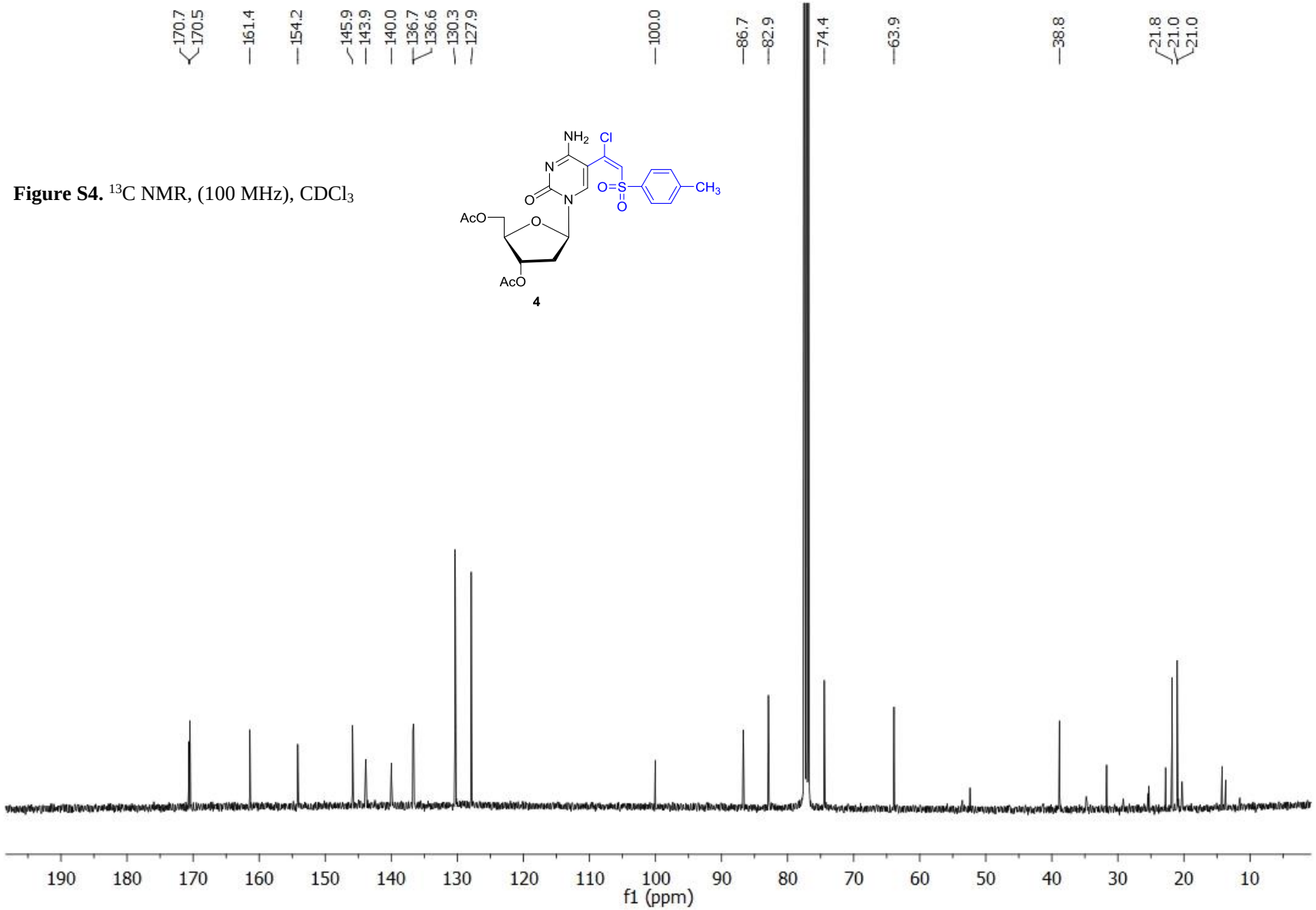
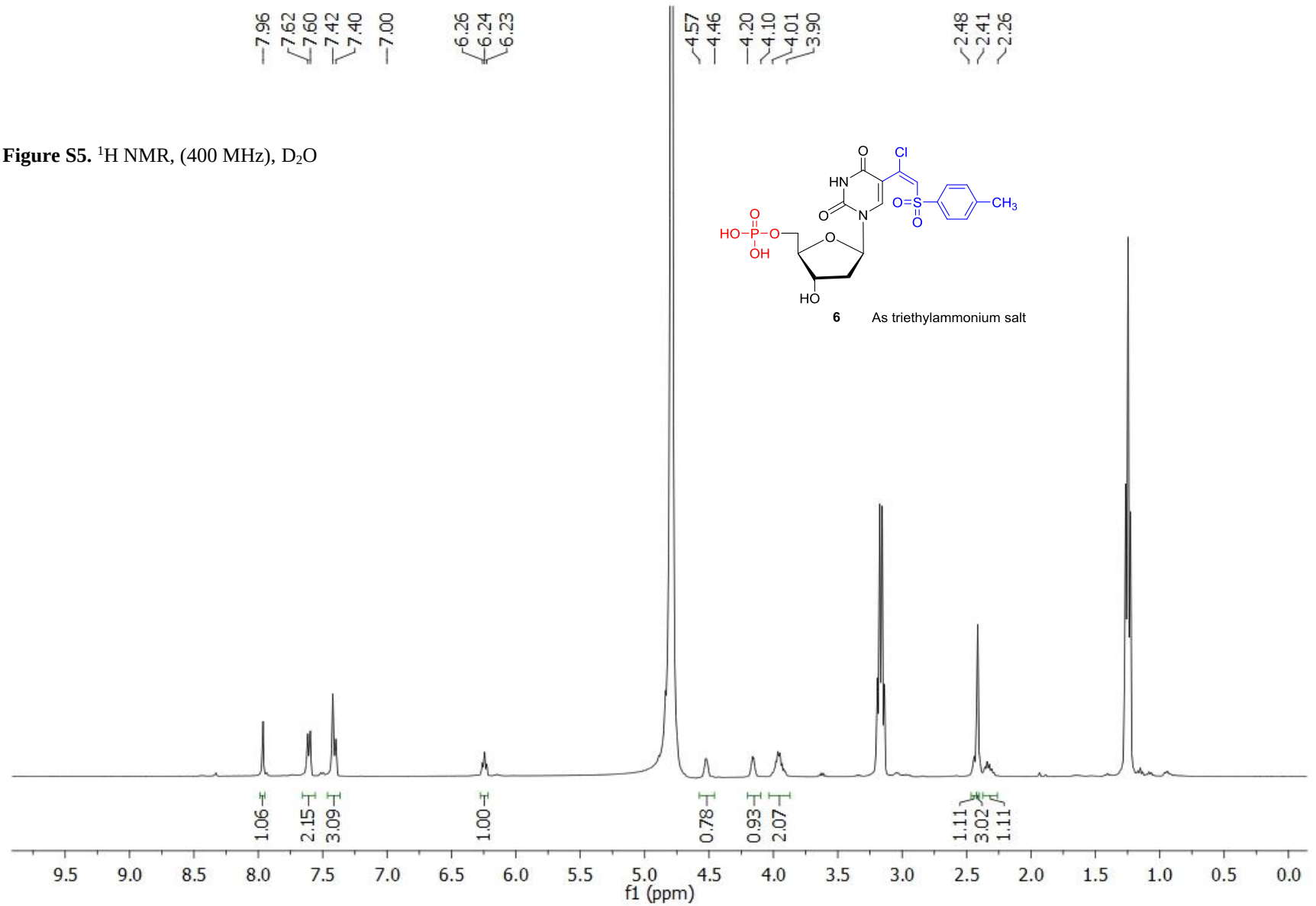


**Figure S5.** $^{1}H$ NMR, (400 MHz), $D_2O$







**6** As triethylammonium salt

**Figure S6.** $^{13}C$ NMR, (100 MHz), $D_2O$

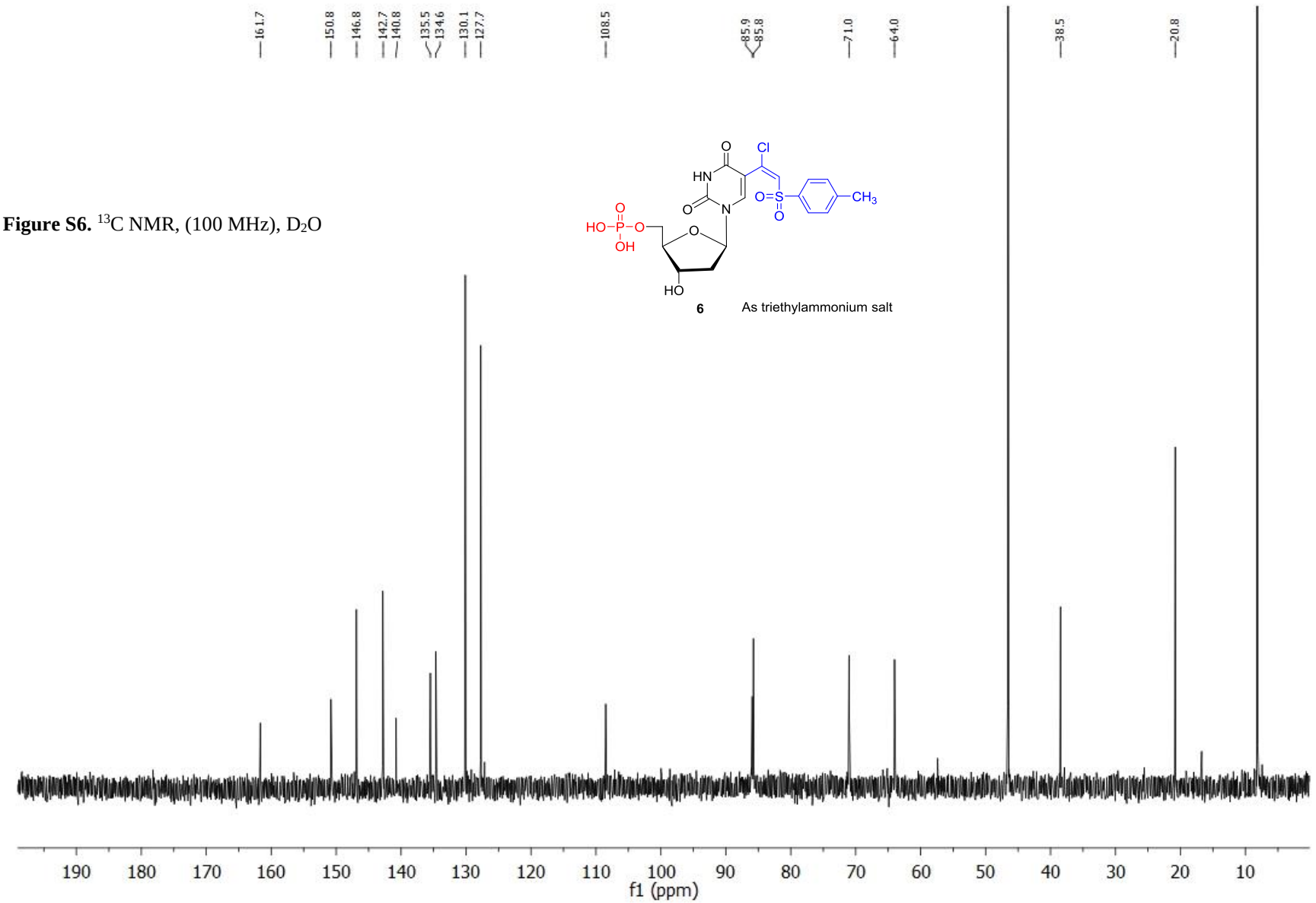
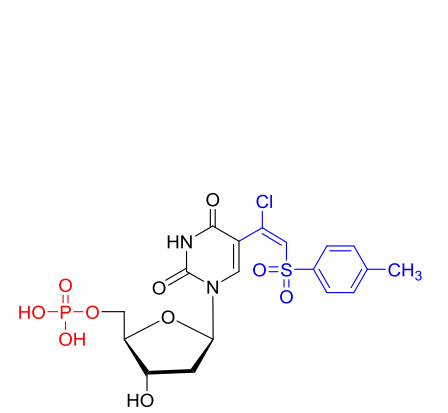


**Figure S7.** $^{31}P$ NMR, (162 MHz), $D_2O$



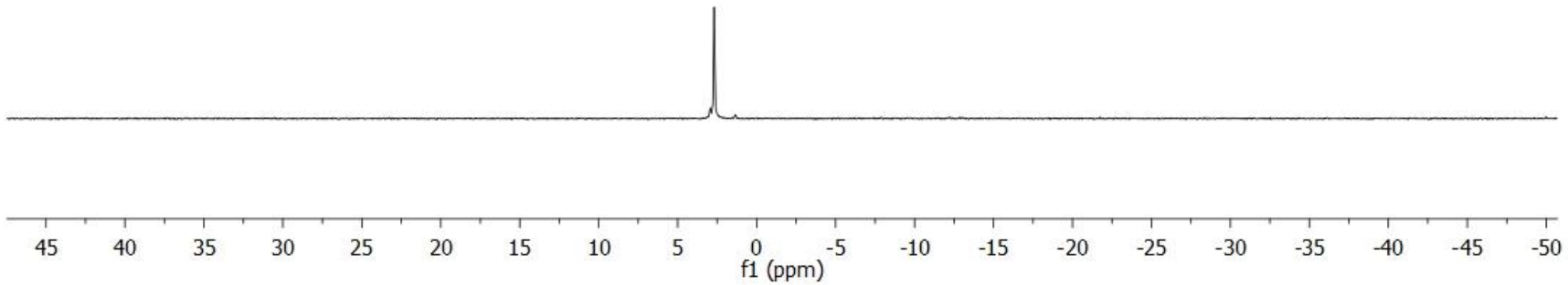



**Figure S8.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

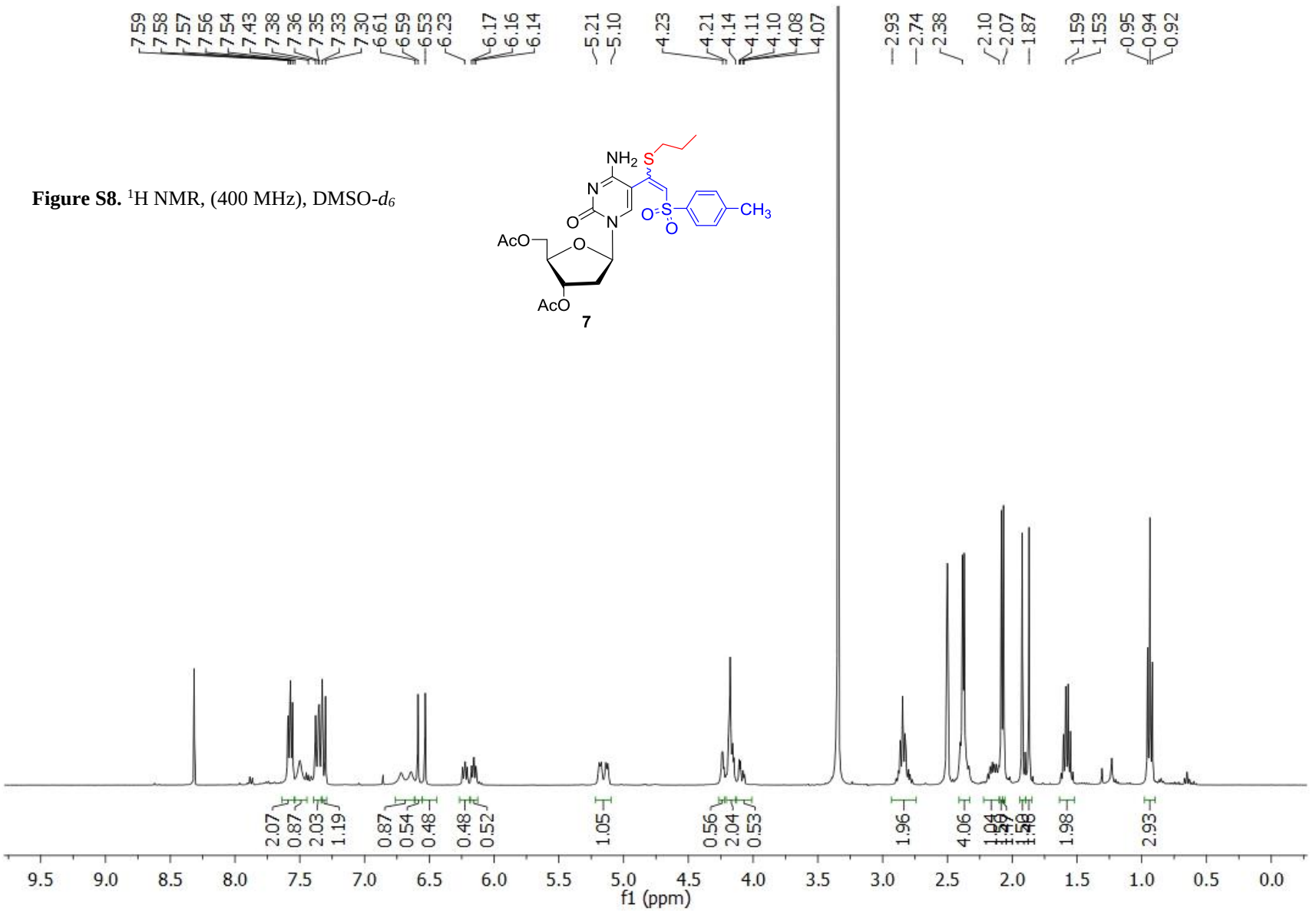
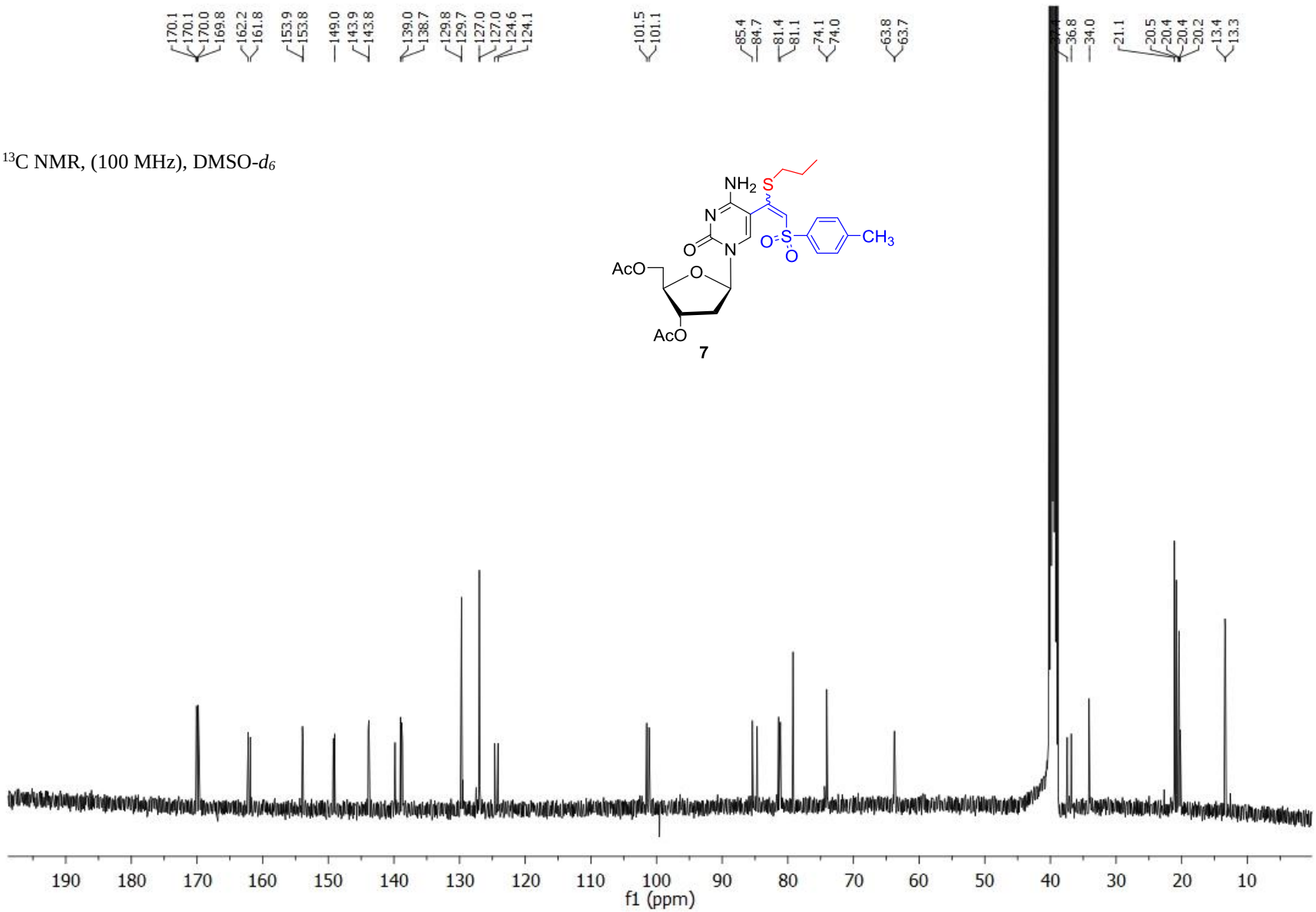
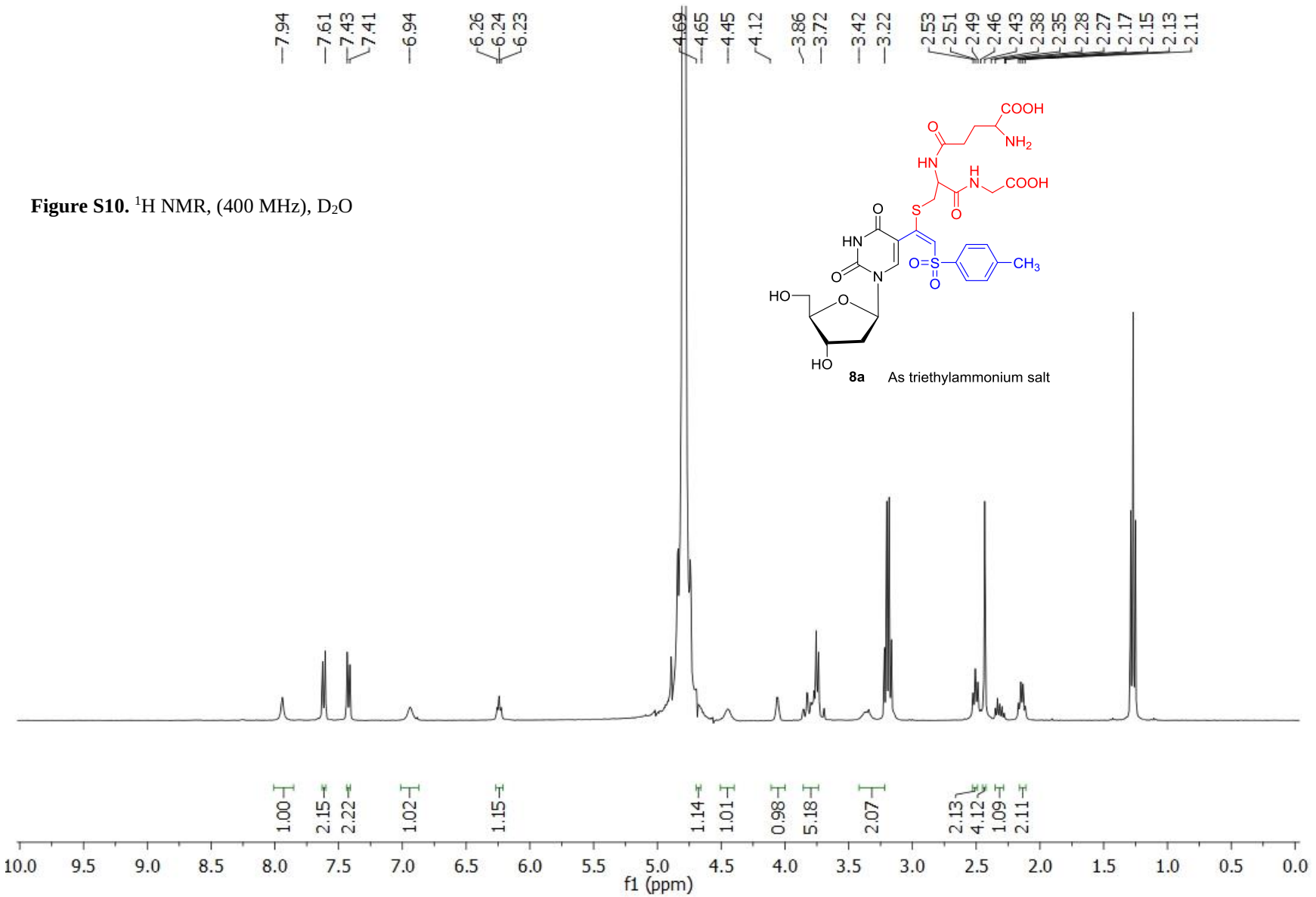


**Figure S9.** $^{13}C$ NMR, (100 MHz), DMSO-$d_6$






**8a** As triethylammonium salt

**Figure S10.** $^{1}H$ NMR, (400 MHz), $D_2O$

**Figure S11.** $^{13}C$ NMR, (100 MHz), $D_2O$

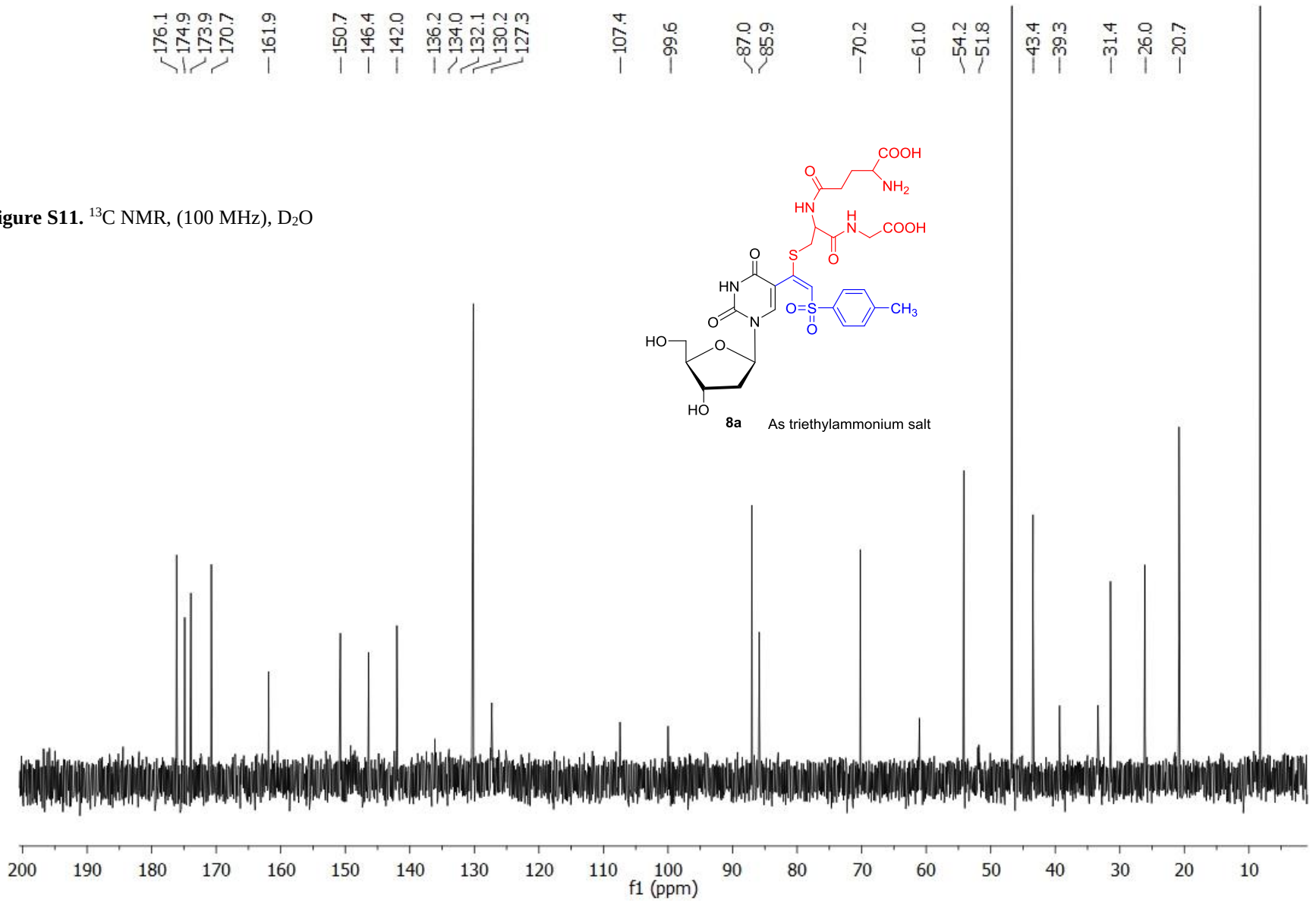


**Figure S12.** $^{1}H$ NMR, (400 MHz), $D_2O$

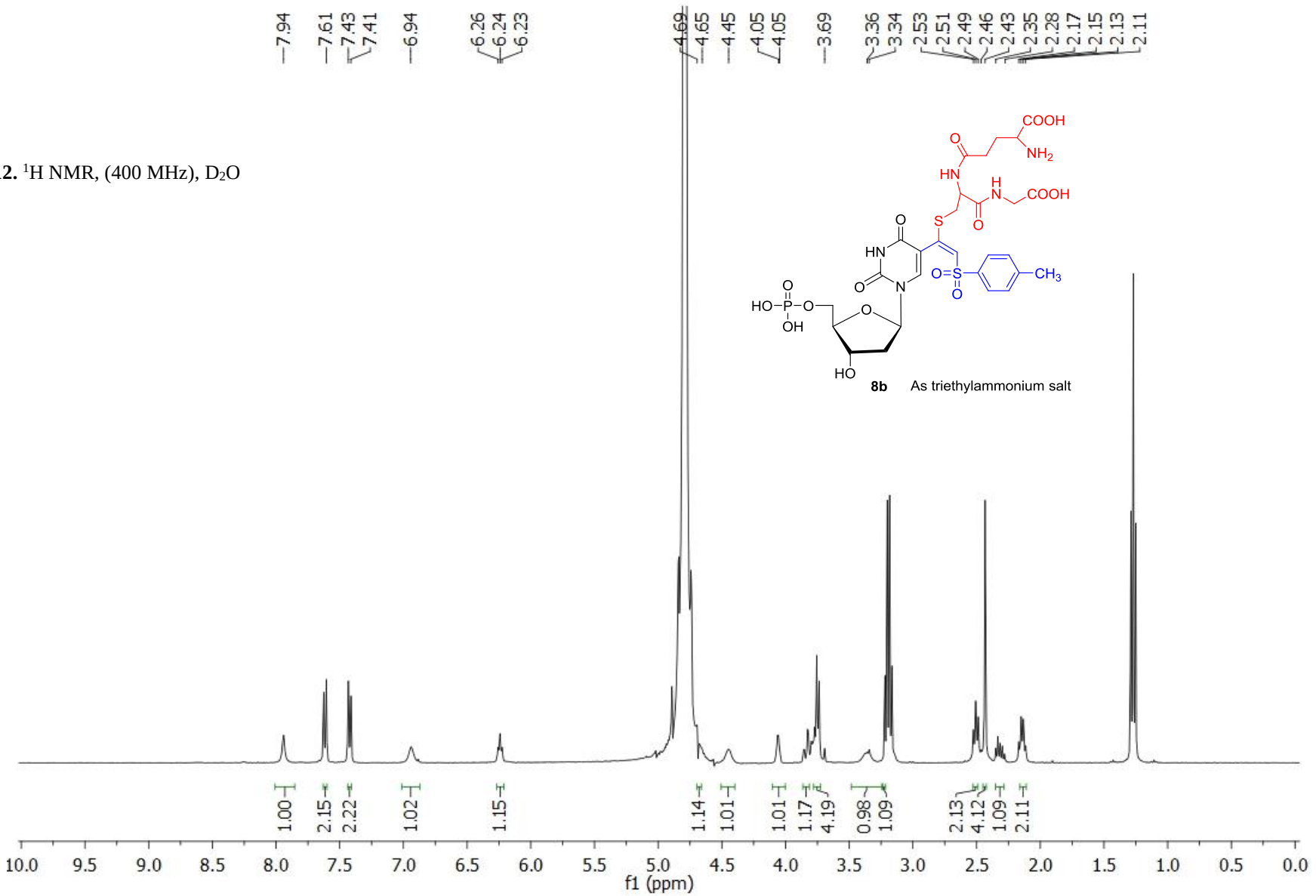


**Figure S13.** $^{13}C$ NMR, (100 MHz), $D_2O$

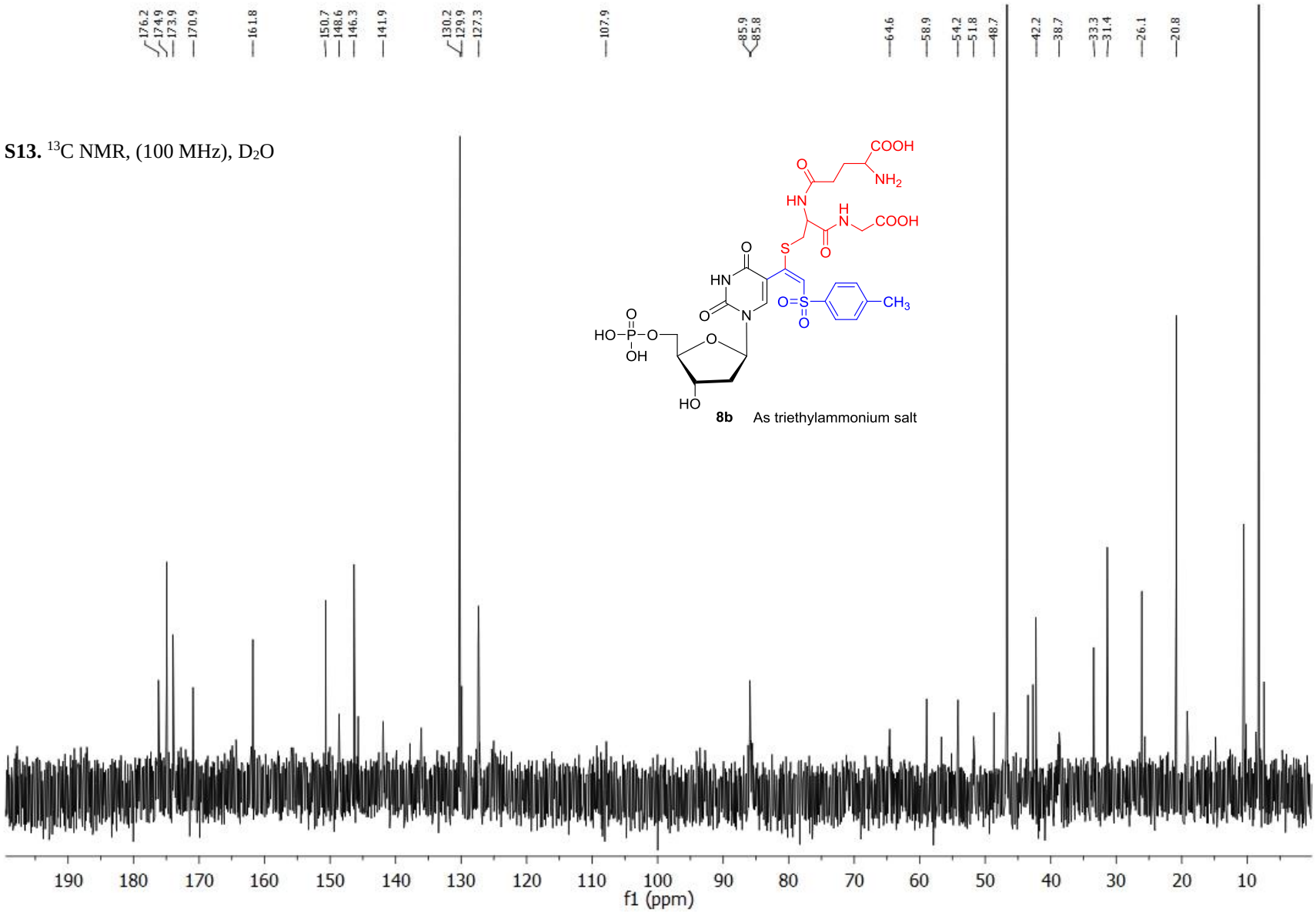
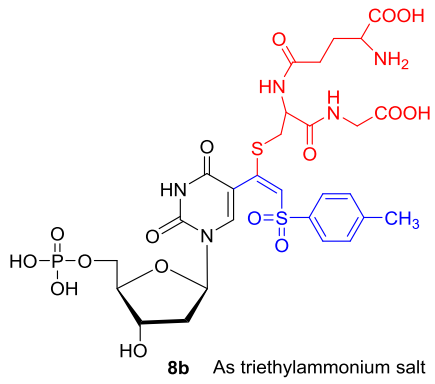


**Figure S14.** $^{31}P$ NMR, (162 MHz), $D_2O$




**8b** As triethylammonium salt

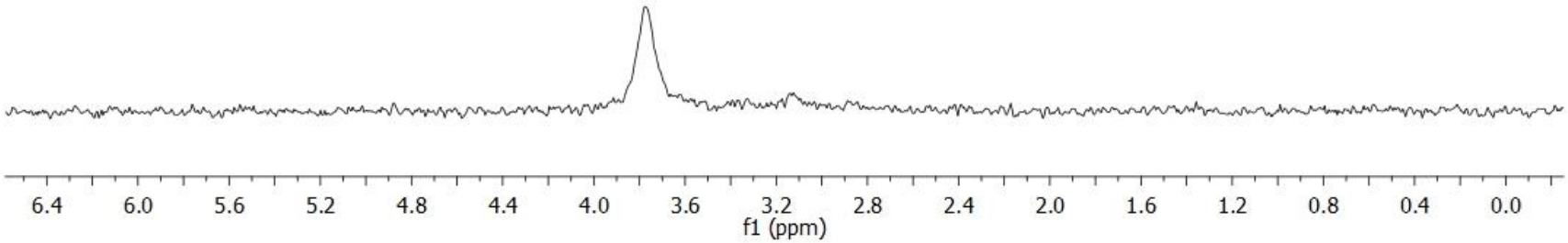


**Figure S15.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

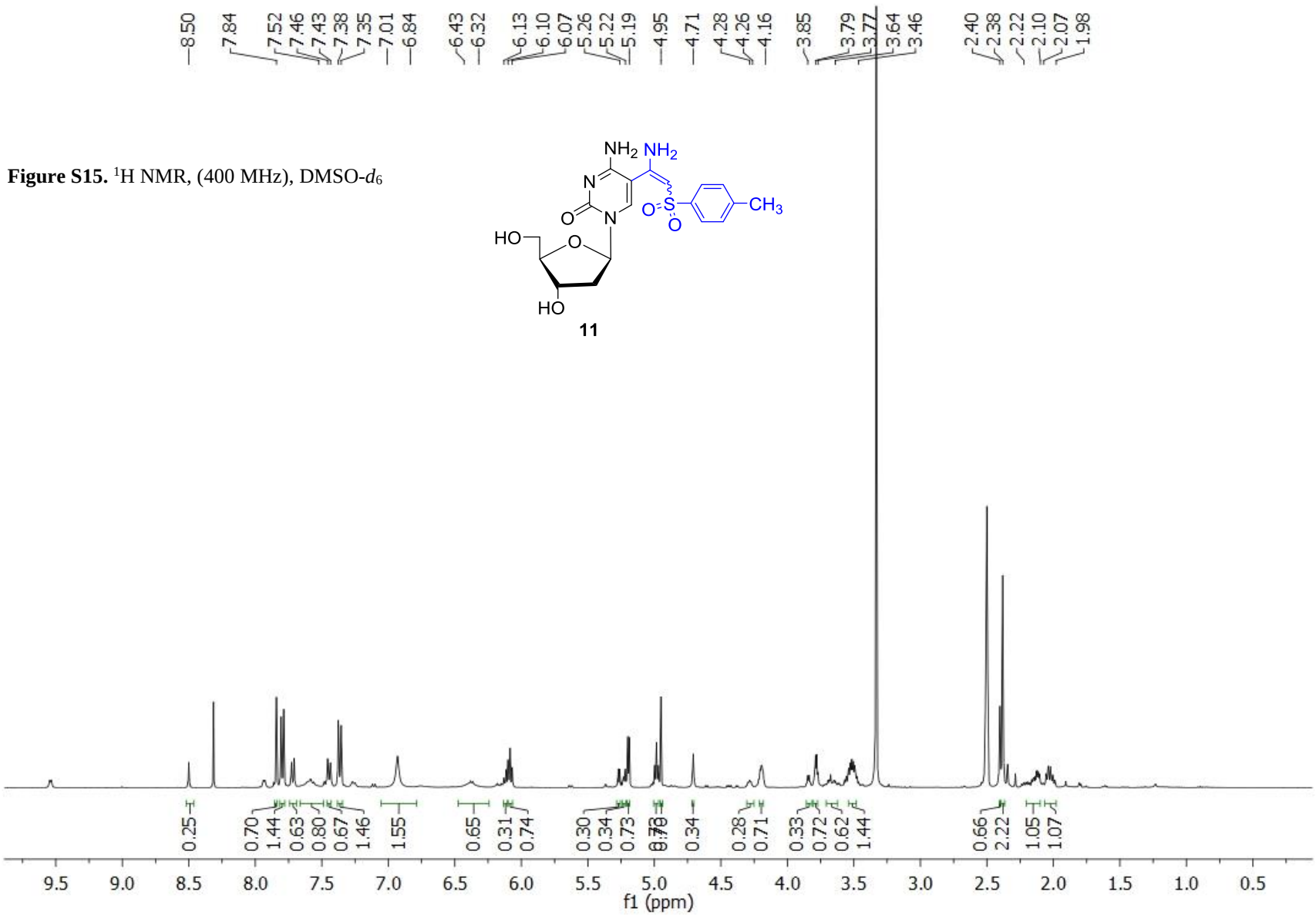


**Figure S16.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

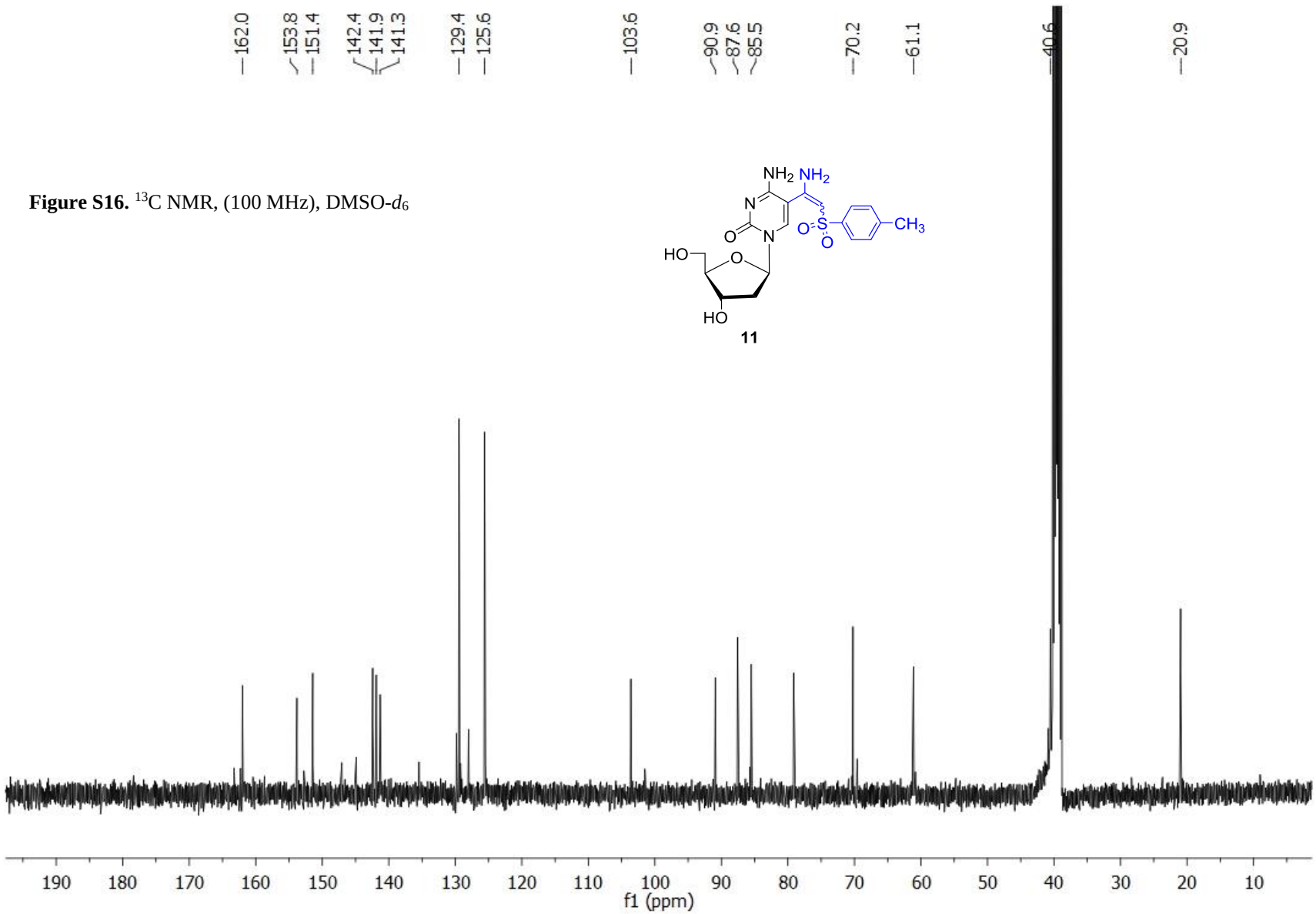


**Figure S17.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

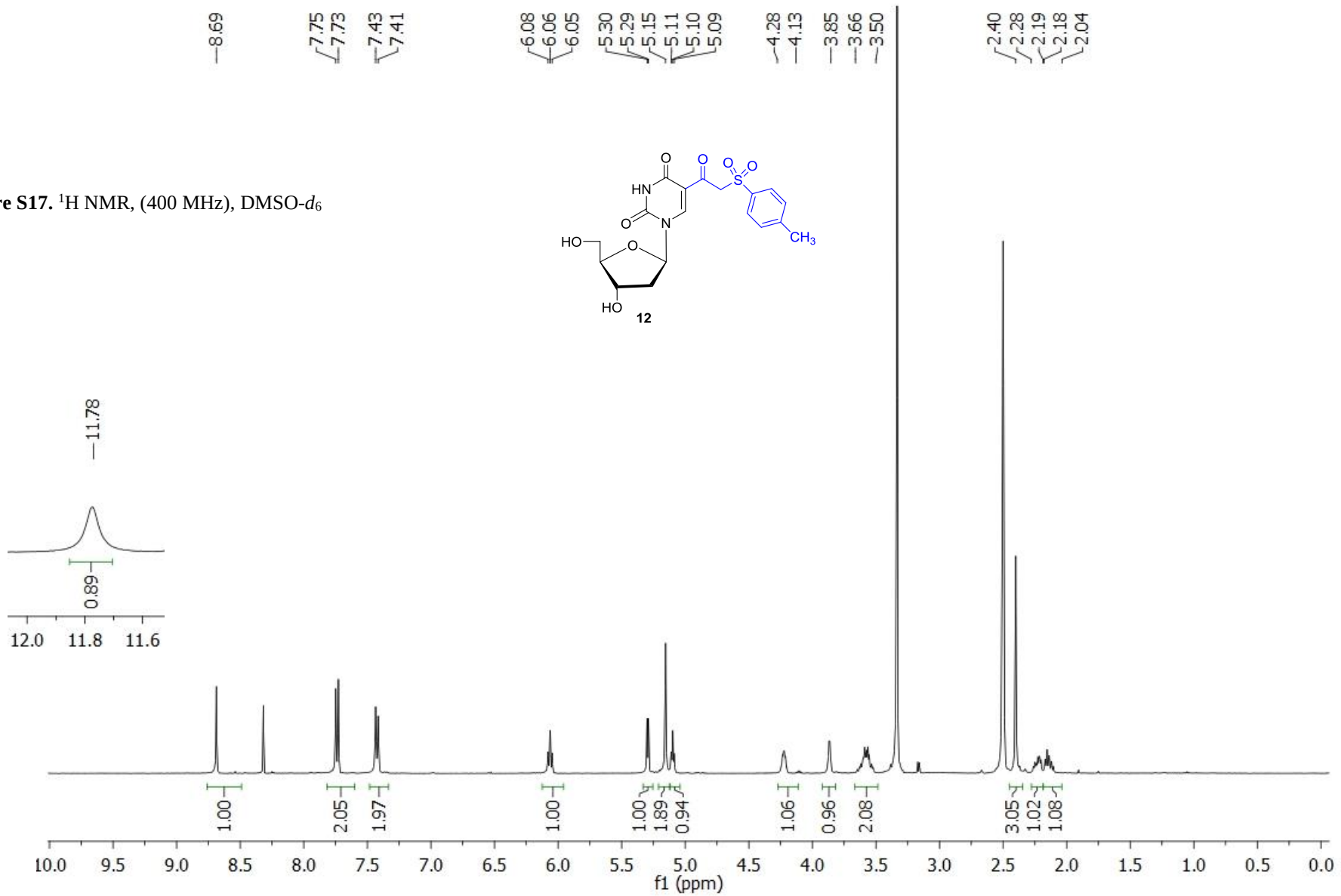
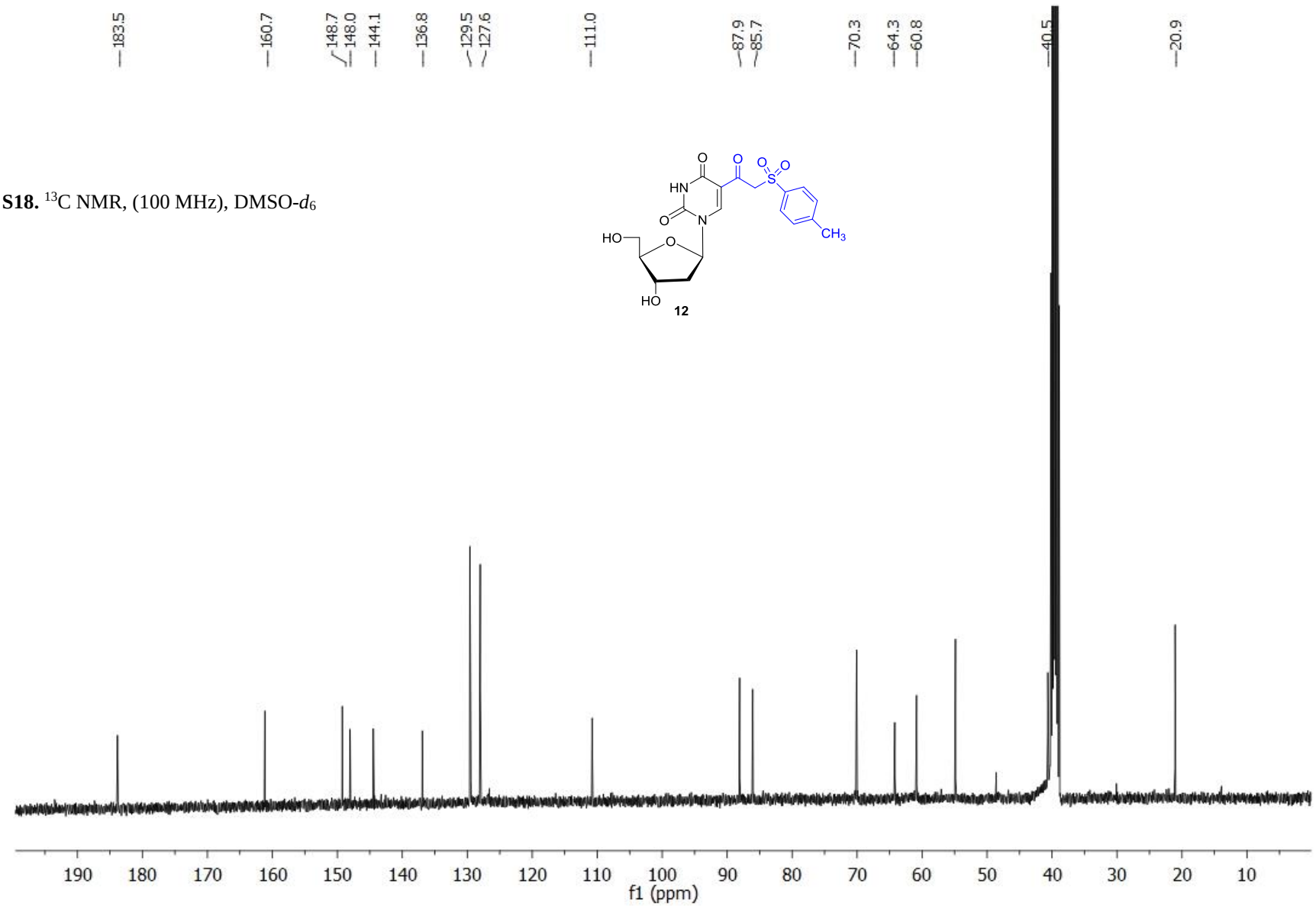


**Figure S18.** $^{13}C$ NMR, (100 MHz), DMSO-$d_6$



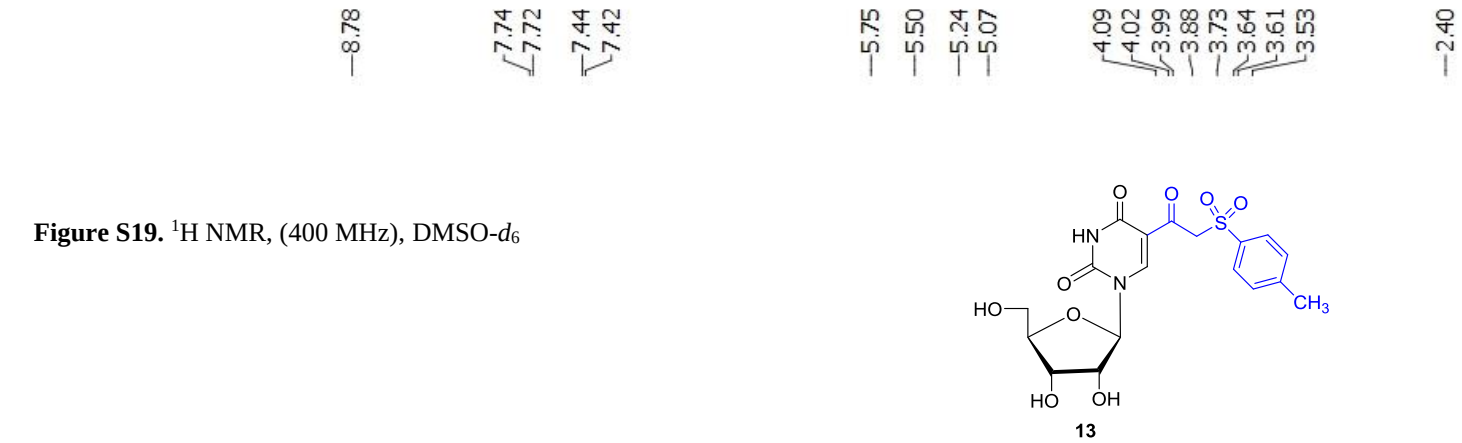



**Figure S19.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

**Figure S20.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

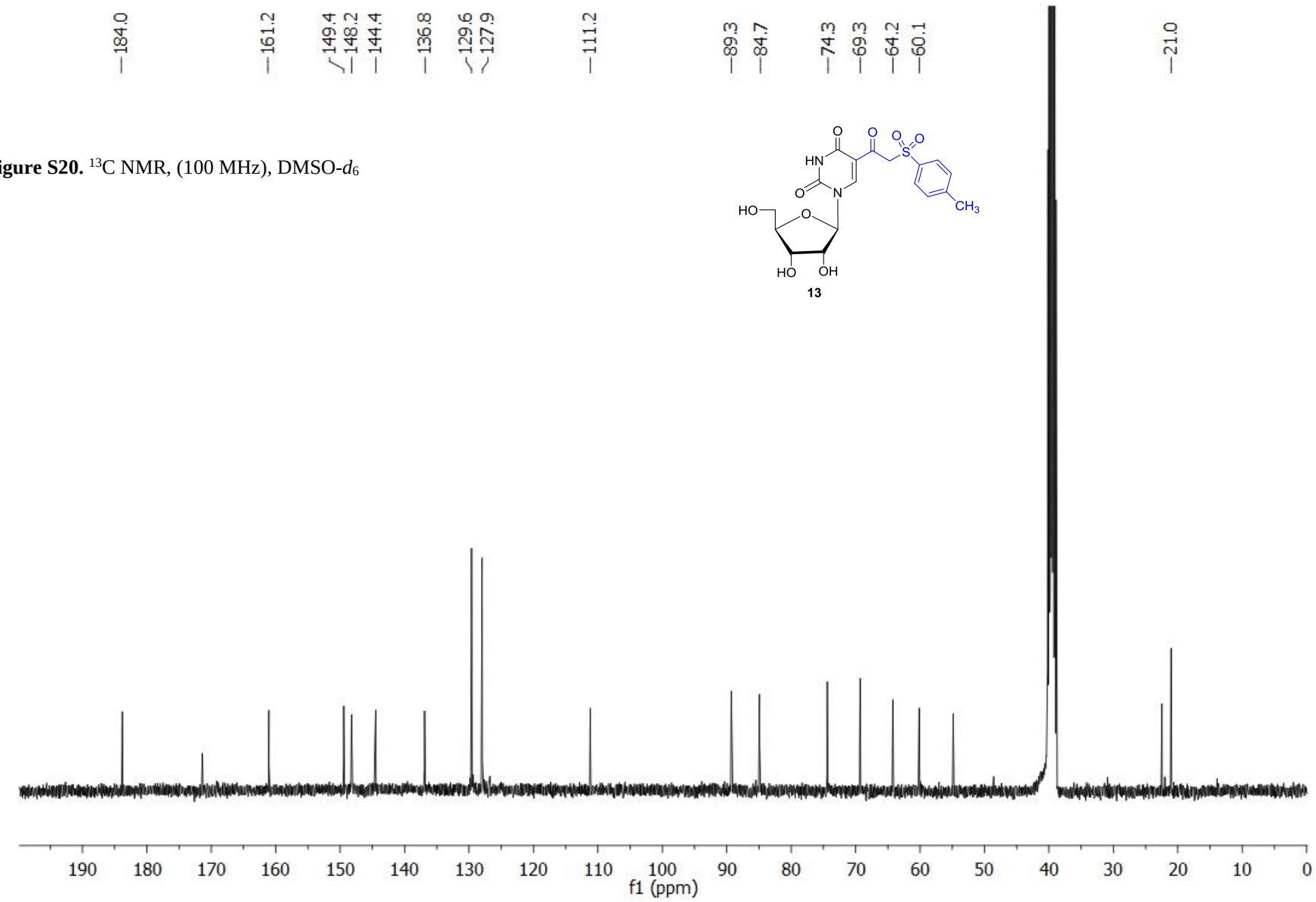


**Figure S21.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

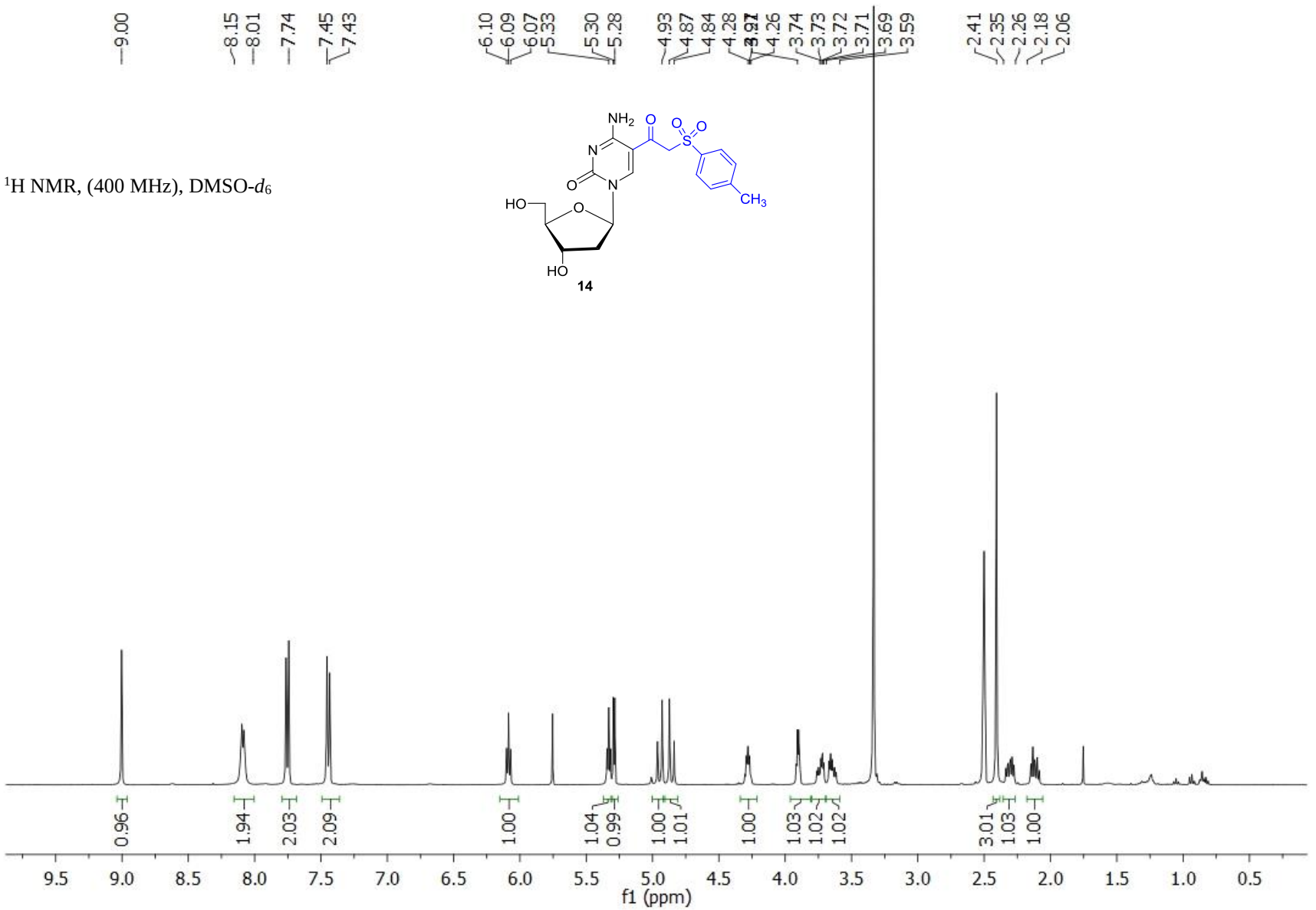


**Figure S22.** $^{13}C$ NMR, (100 MHz), DMSO-$d_6$

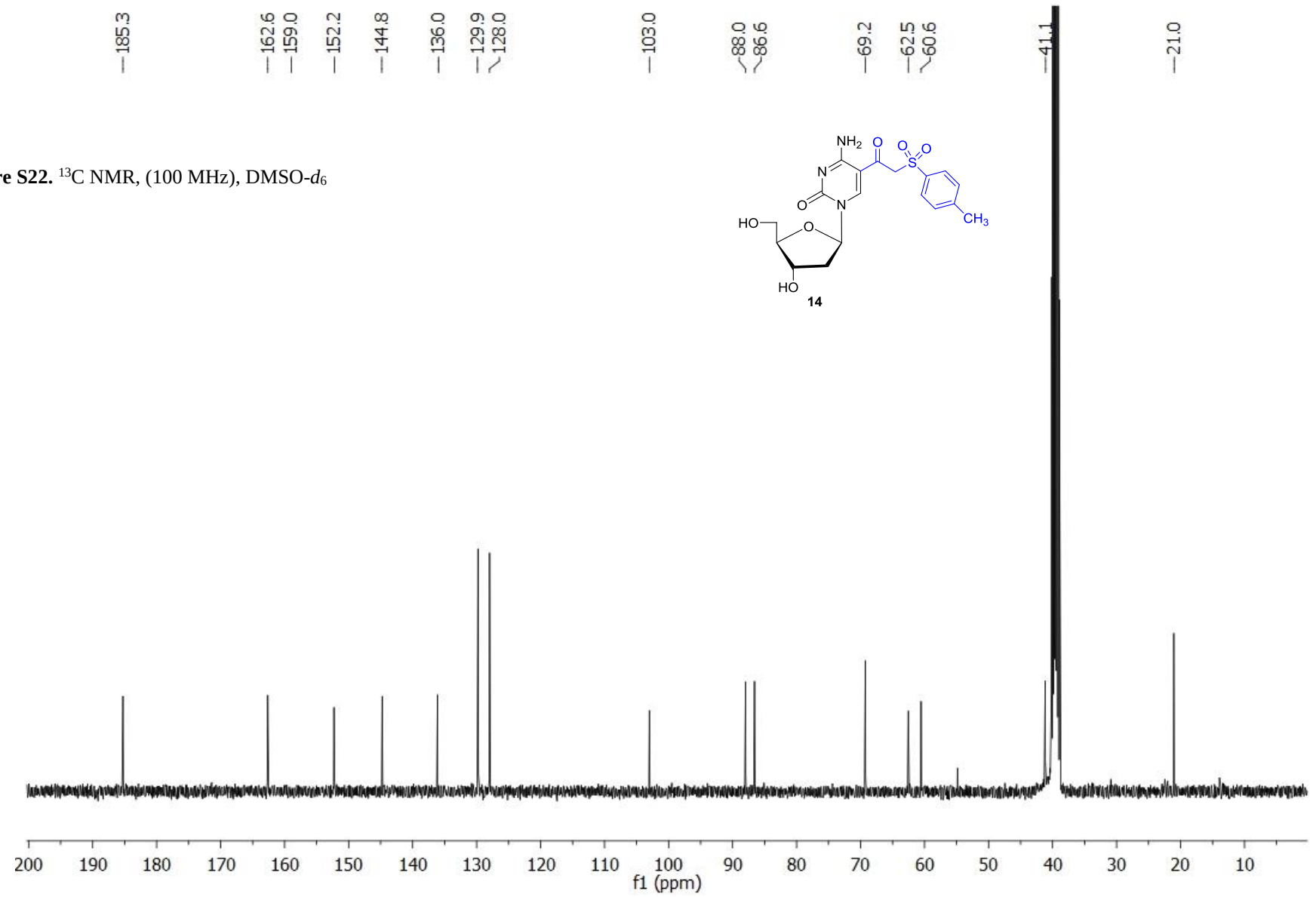


**Figure S23.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

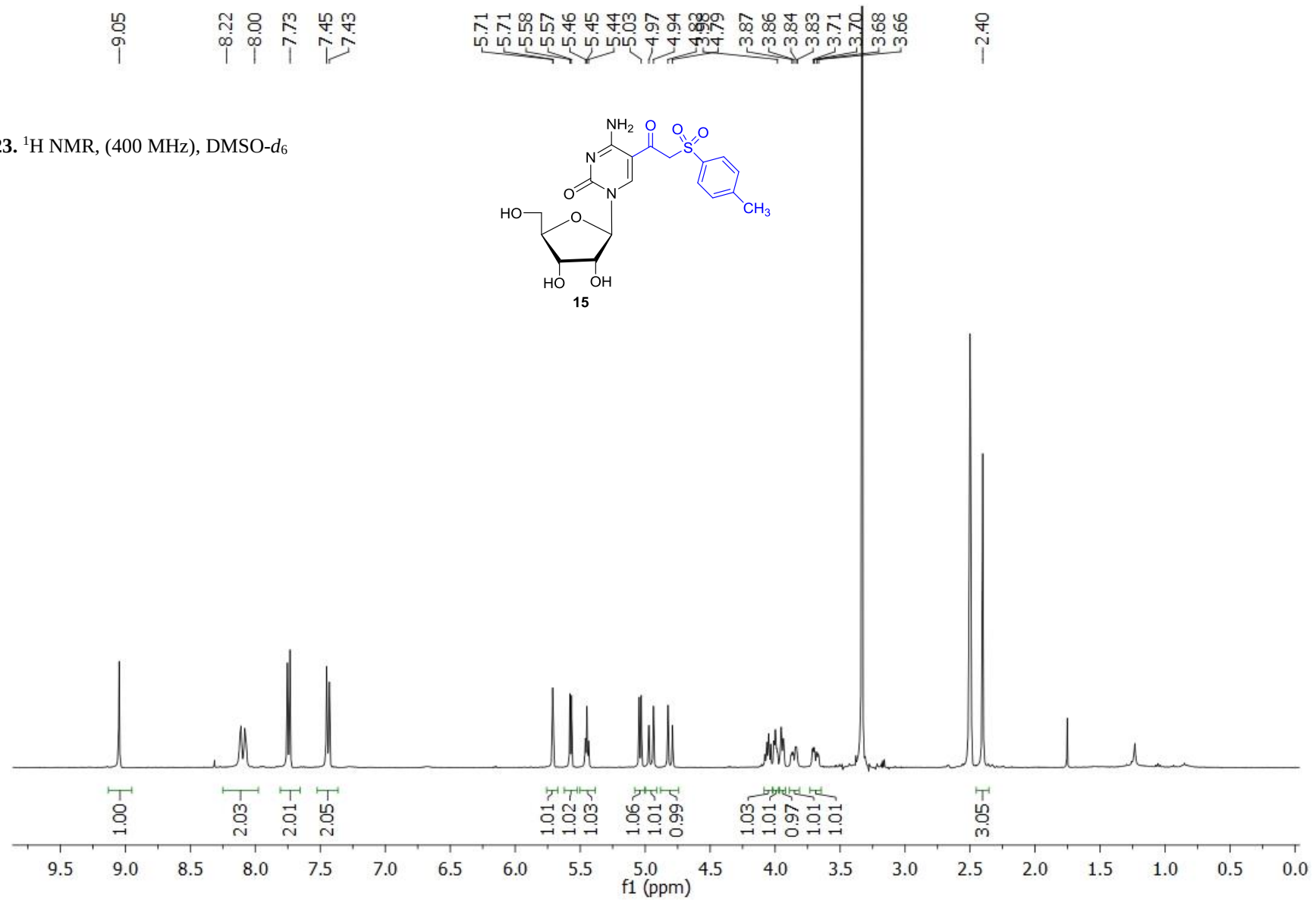


**Figure S24.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

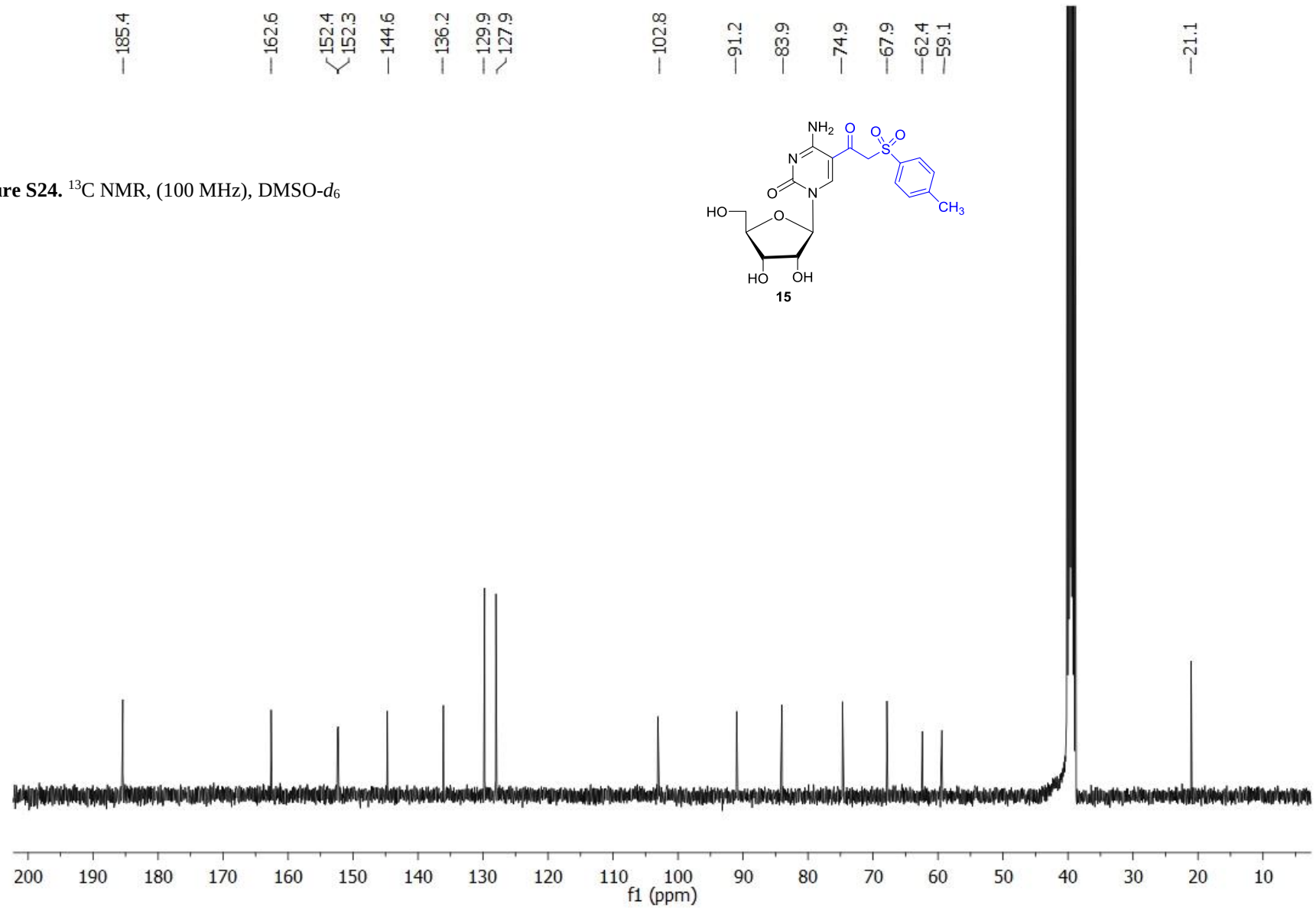


**Figure S25.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

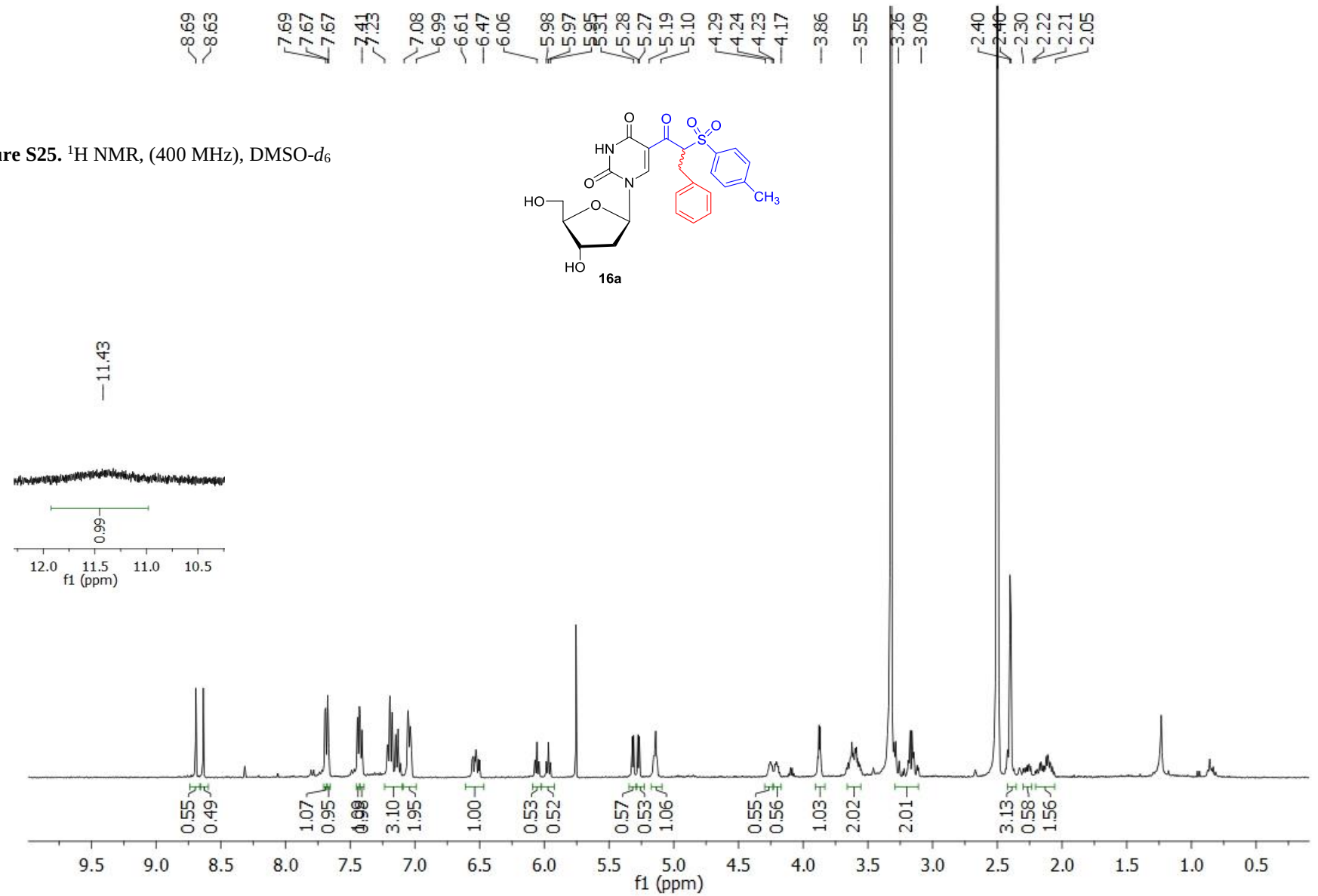


**Figure S26.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

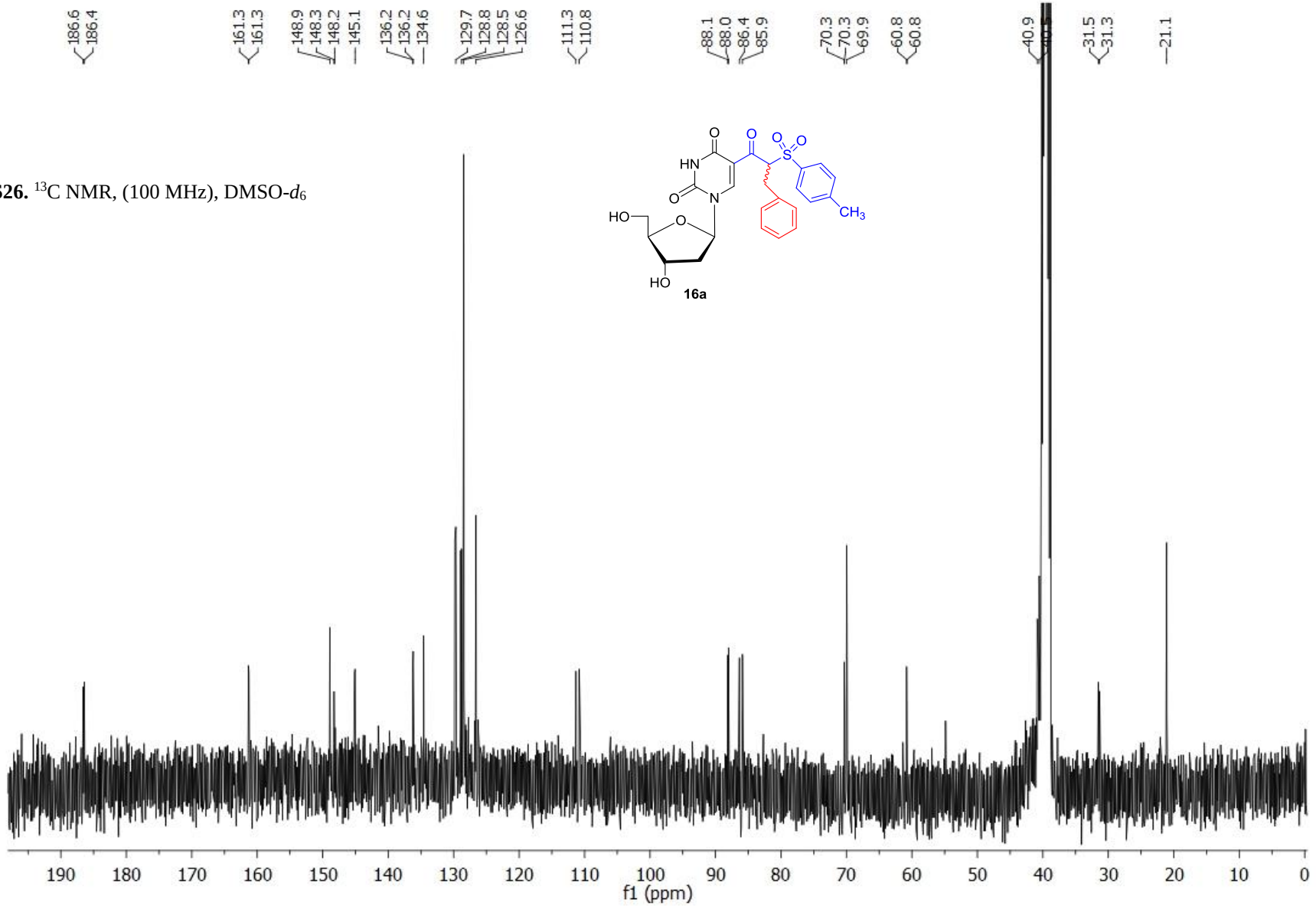


**Figure S27.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

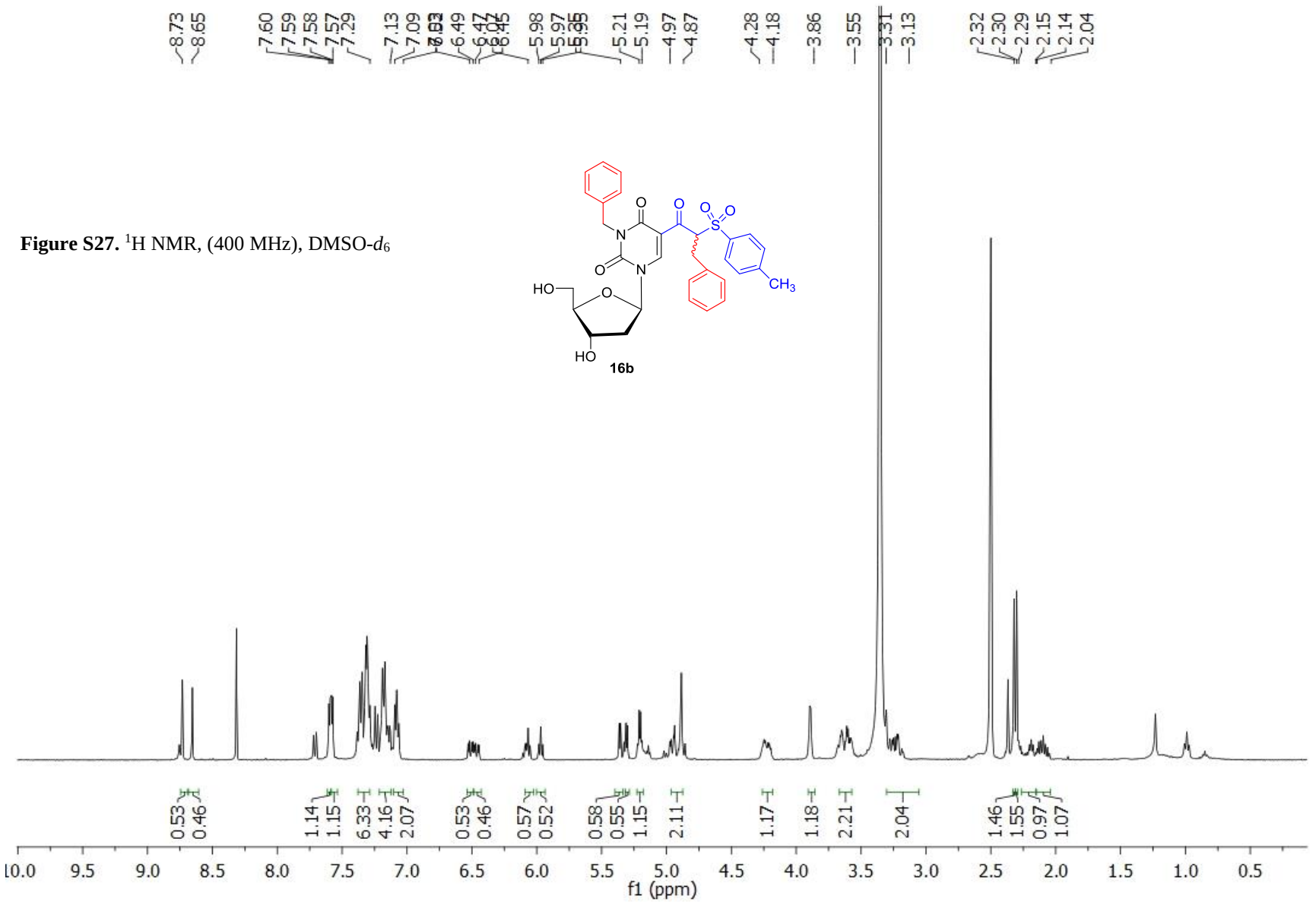


**Figure S28.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

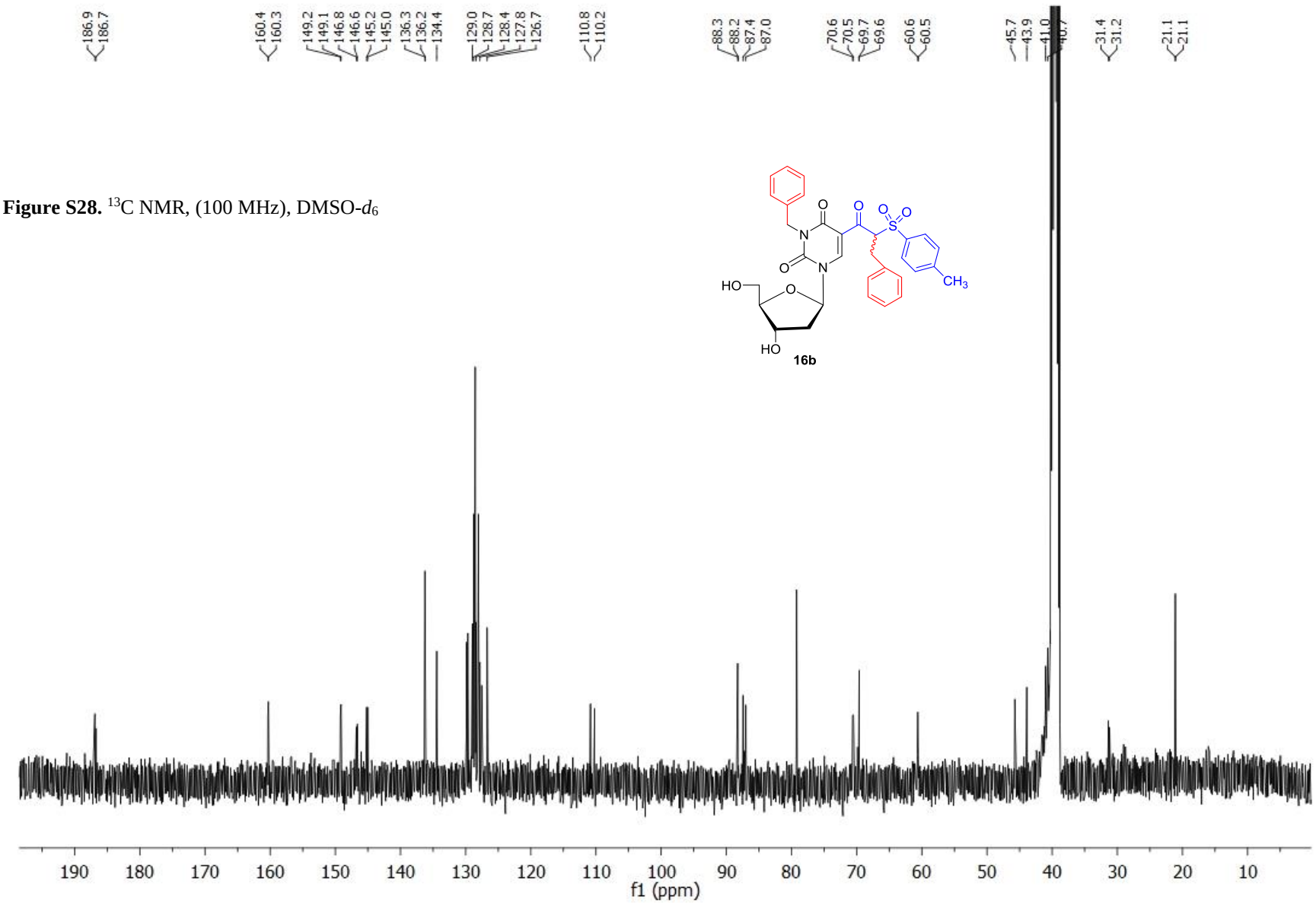


**Figure S29.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

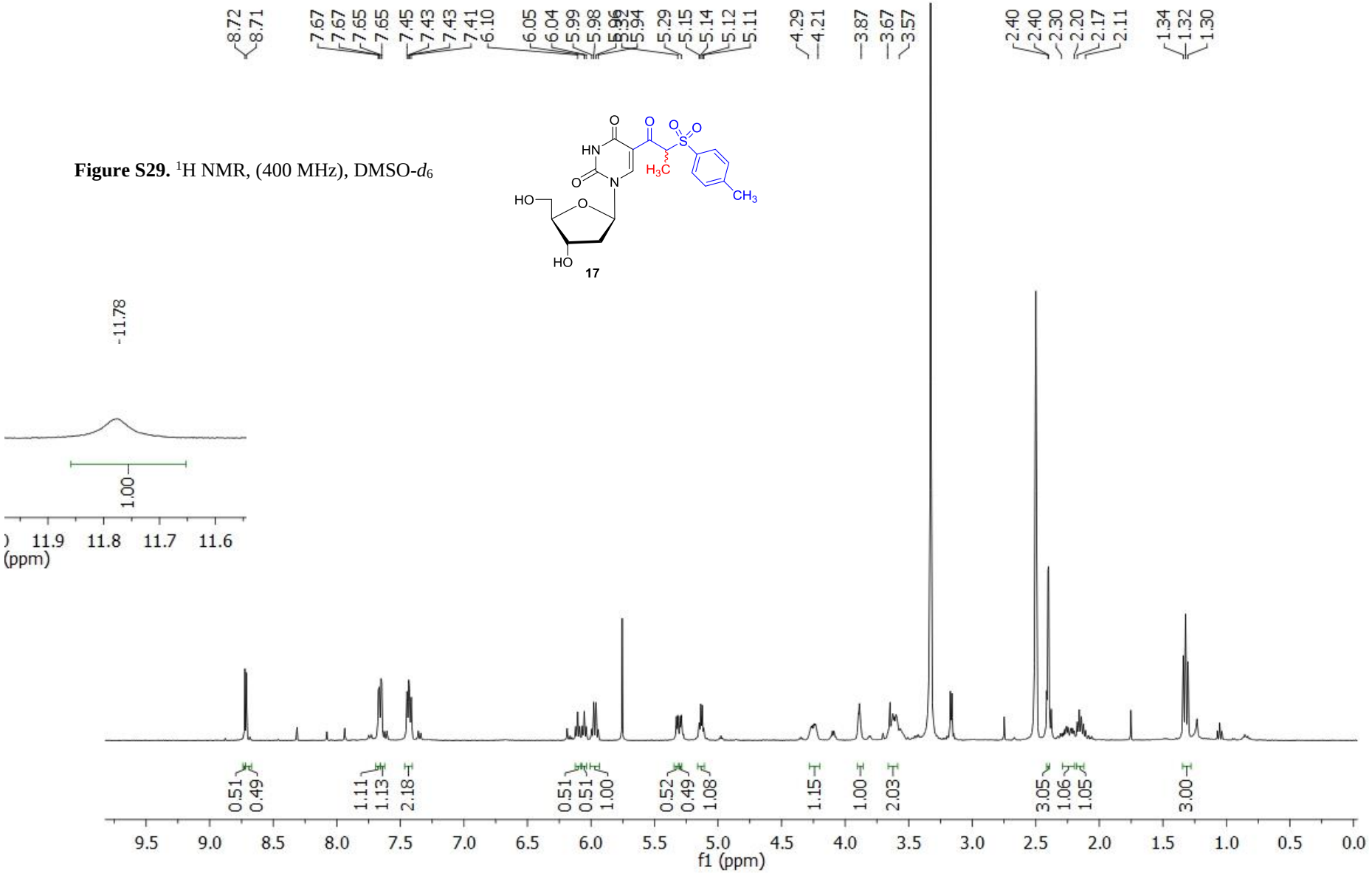


**Figure S30.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

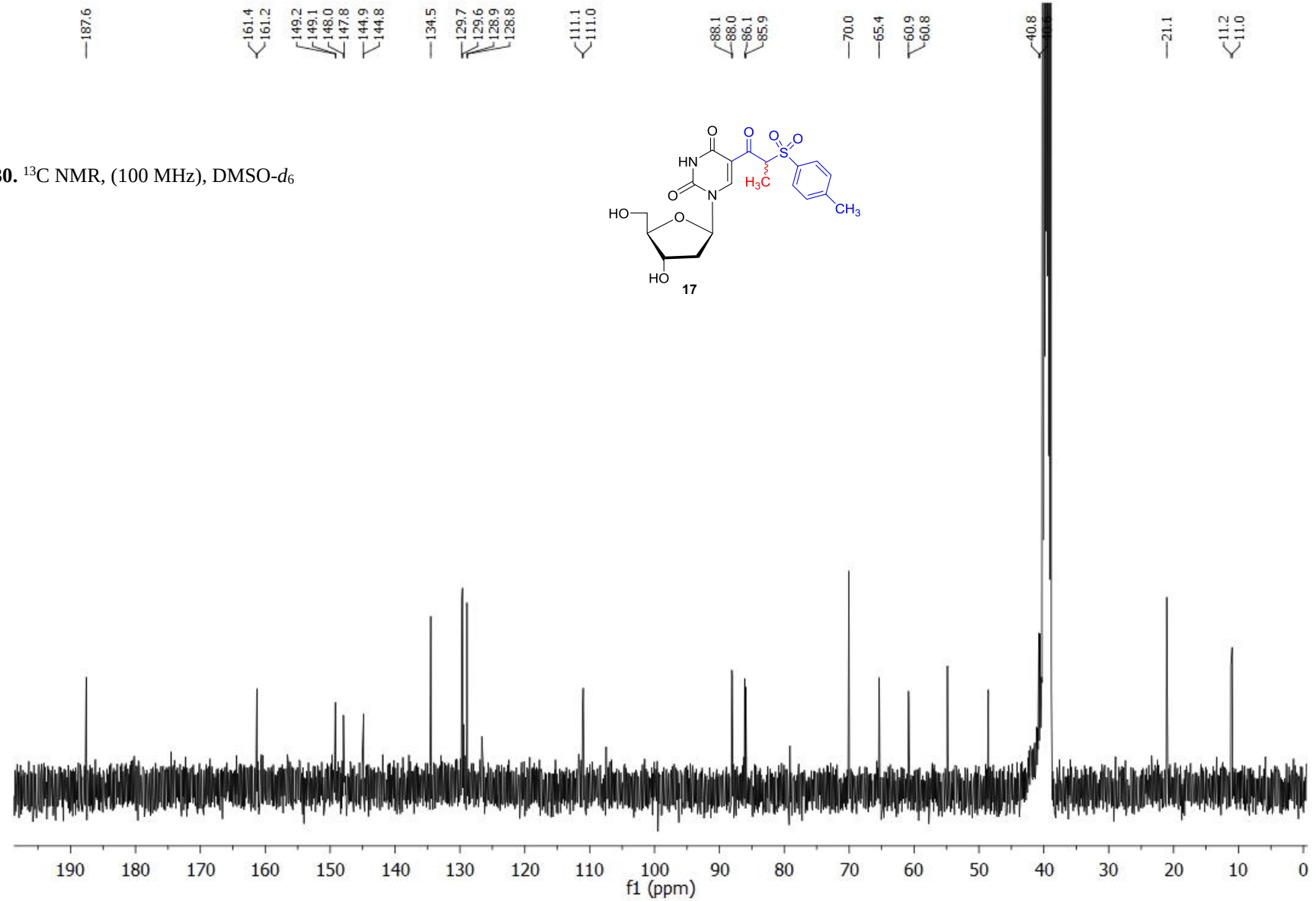


**Figure S31.** [1]H NMR, (400 MHz), DMSO-$d_6$

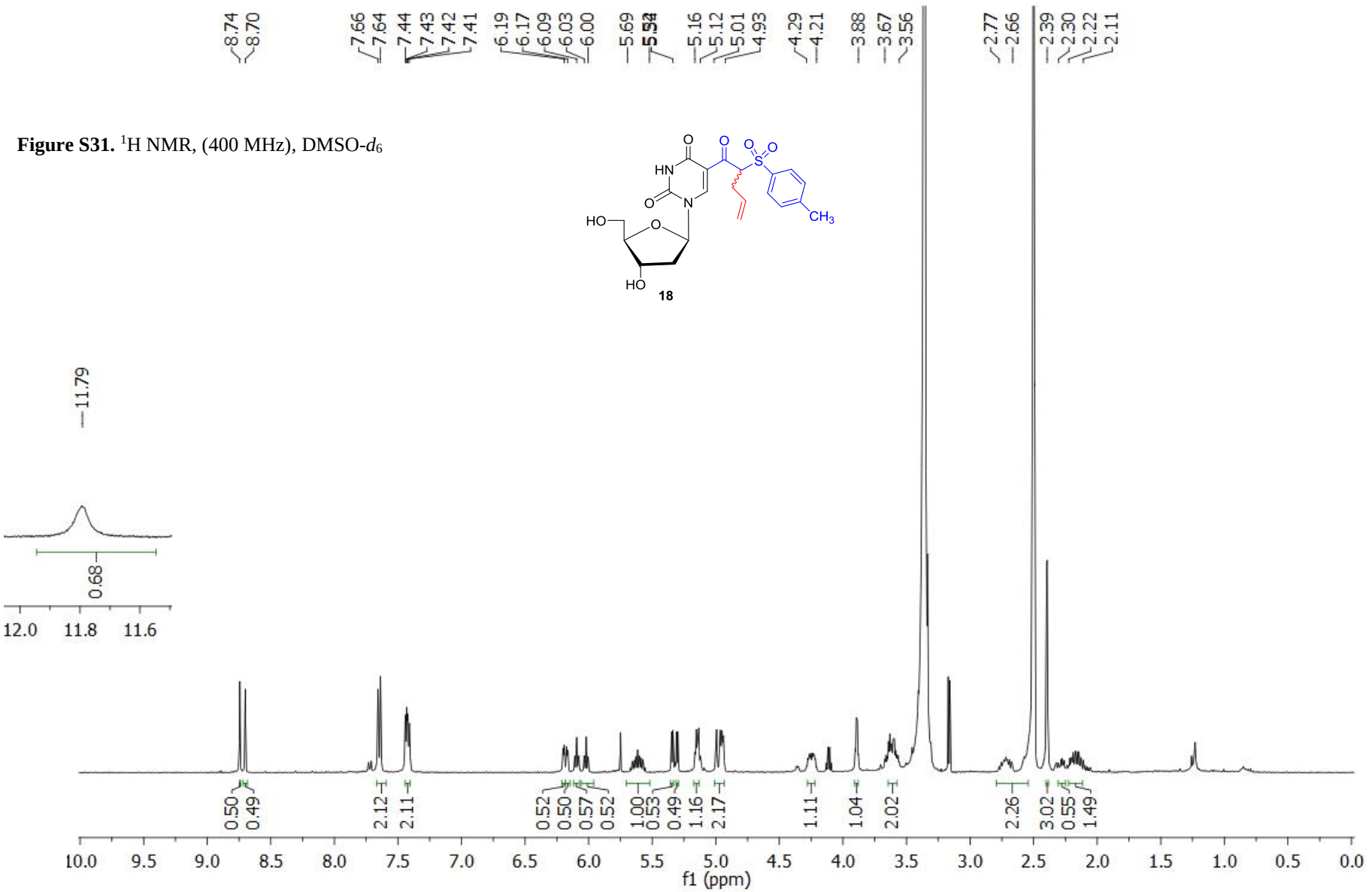


**Figure S32.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

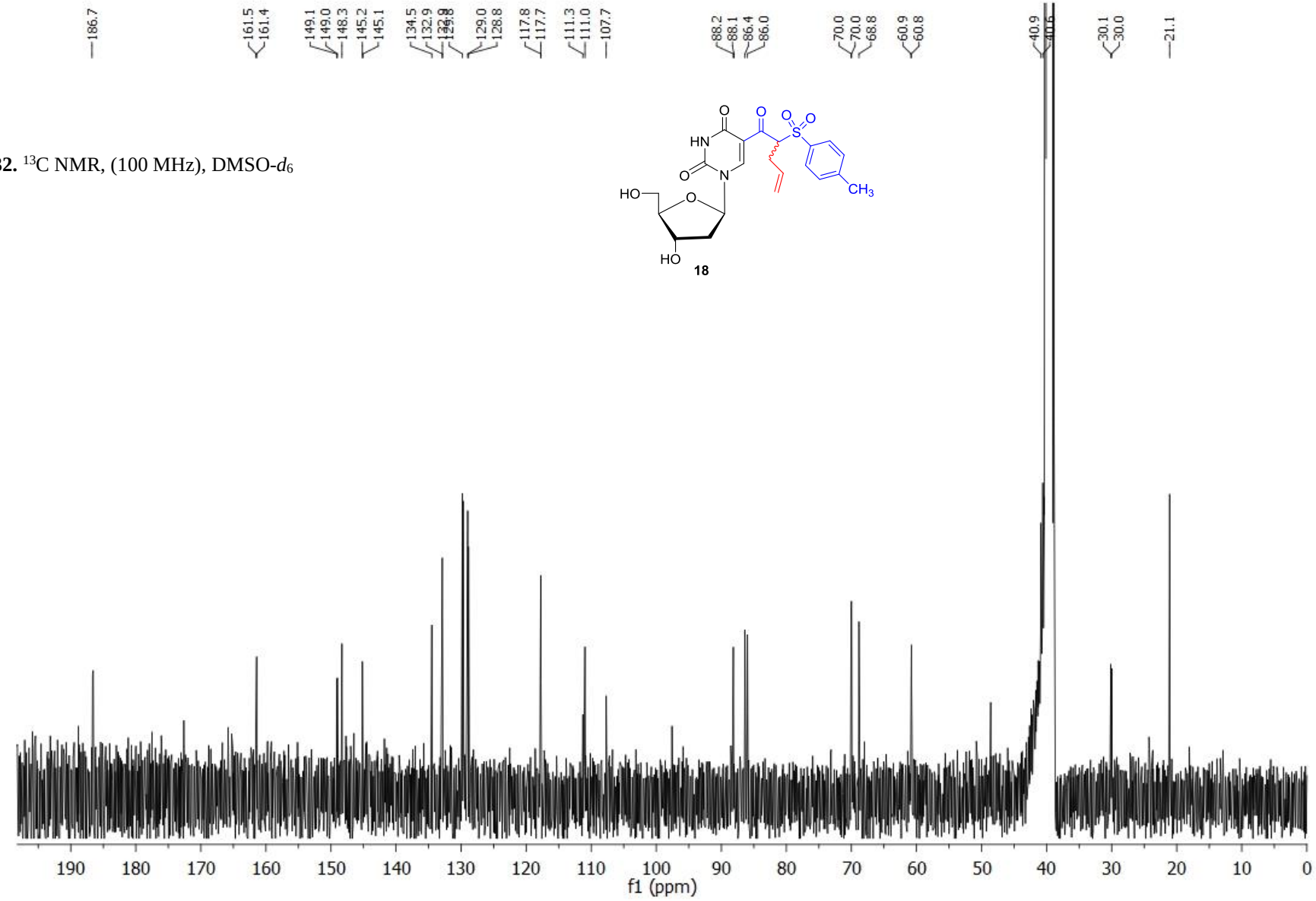


**Figure S33.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

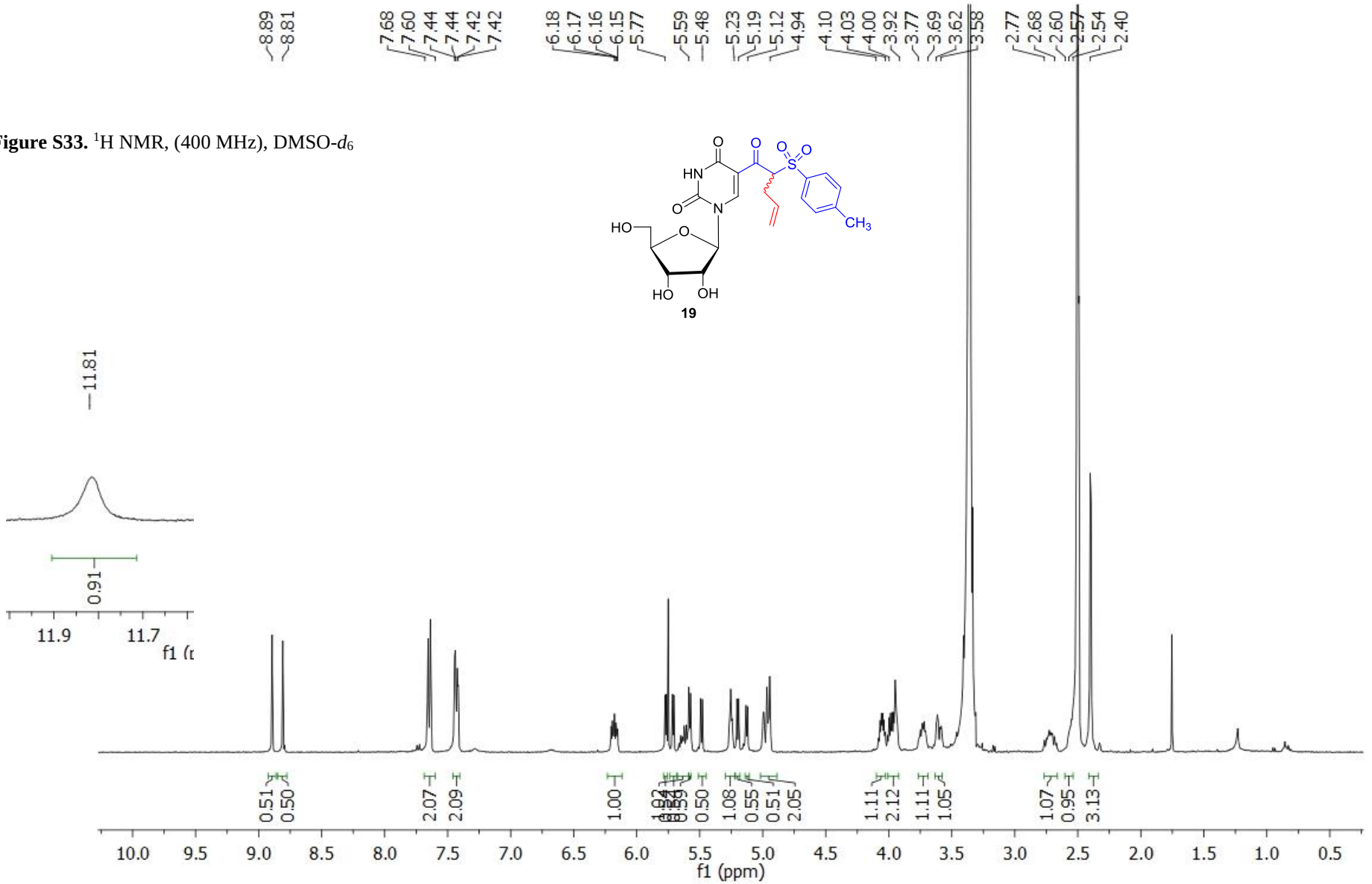


**Figure S34.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

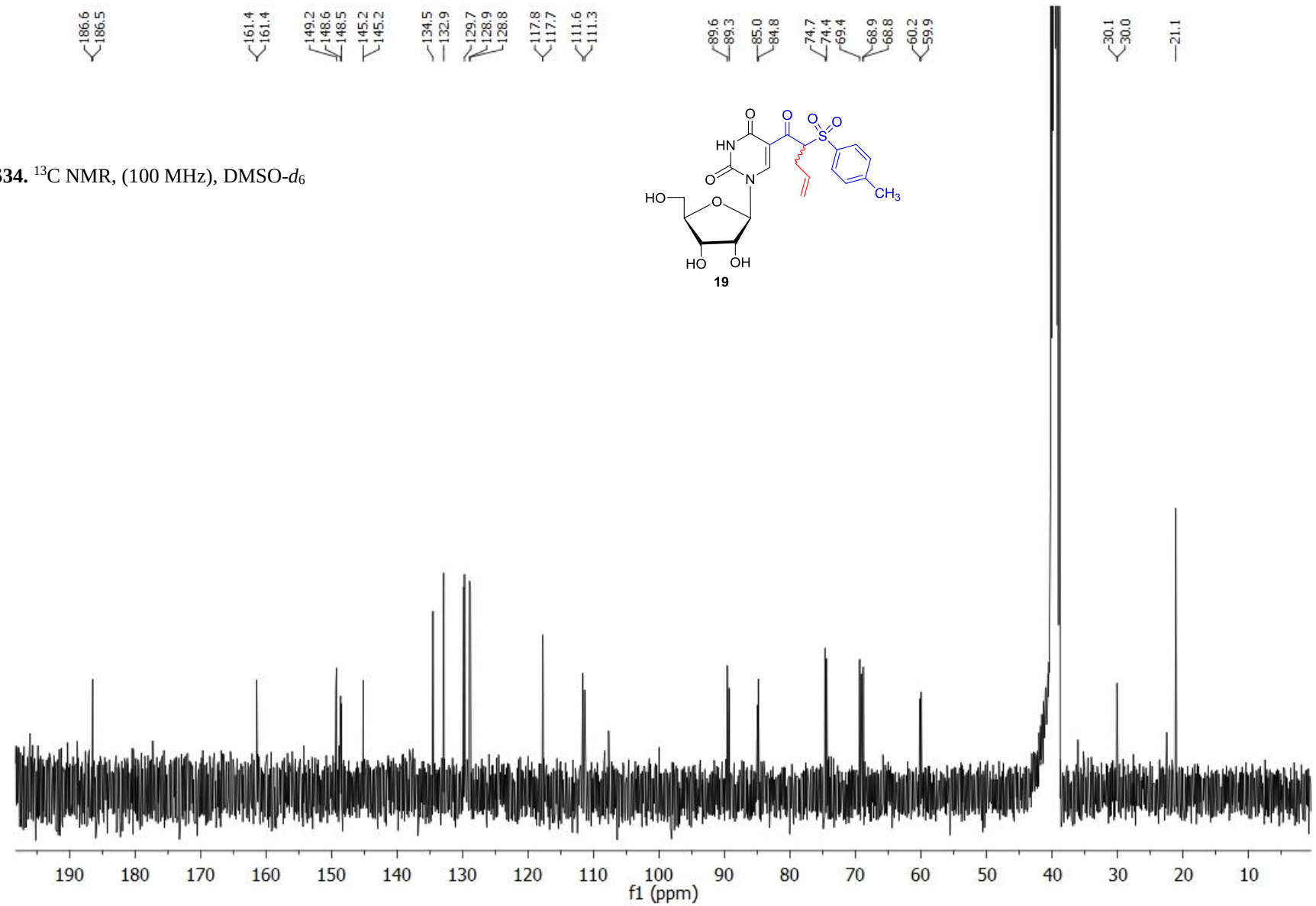


**Figure S35.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

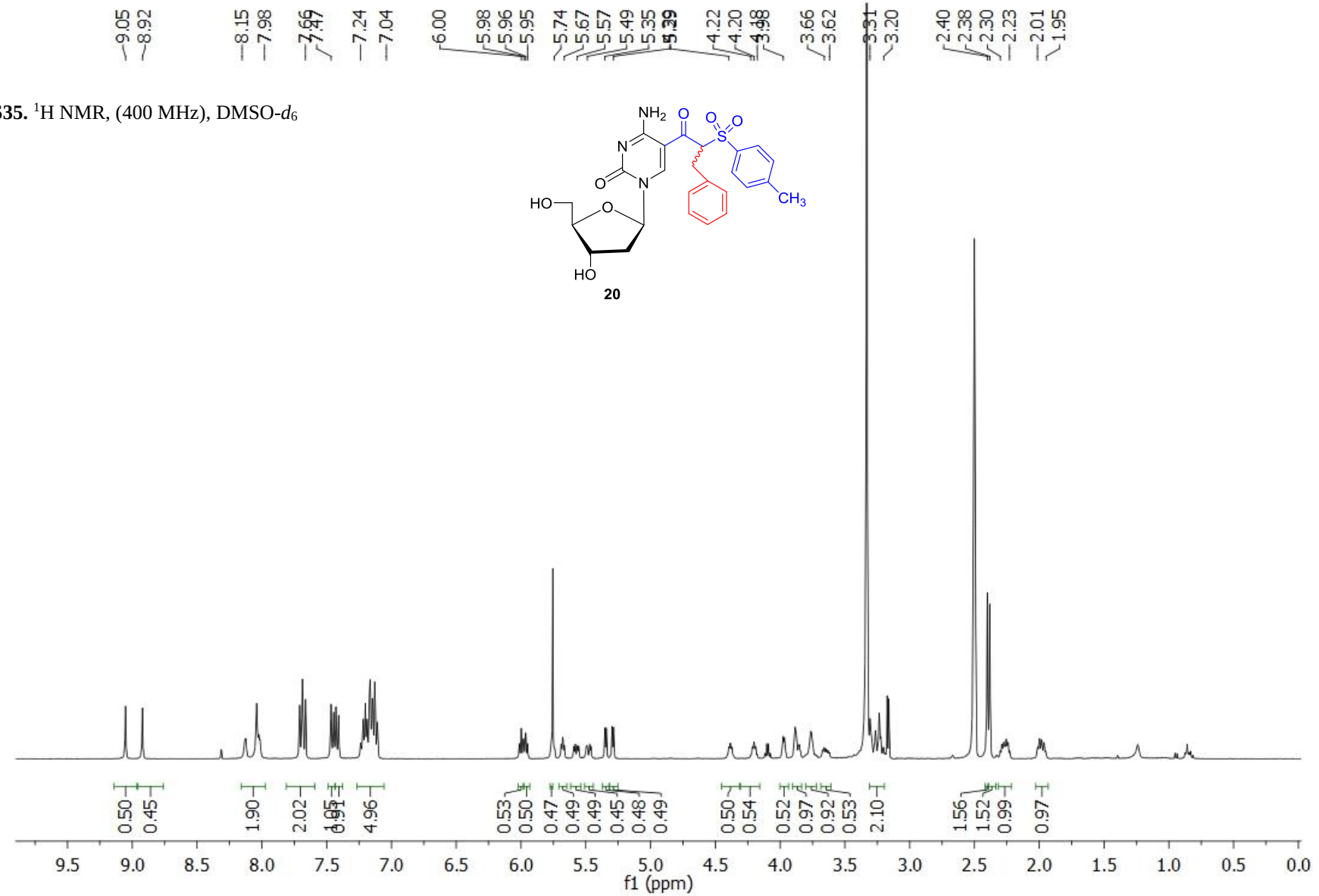


**Figure S36.** $^{13}C$ NMR, (100 MHz), DMSO-$d_6$

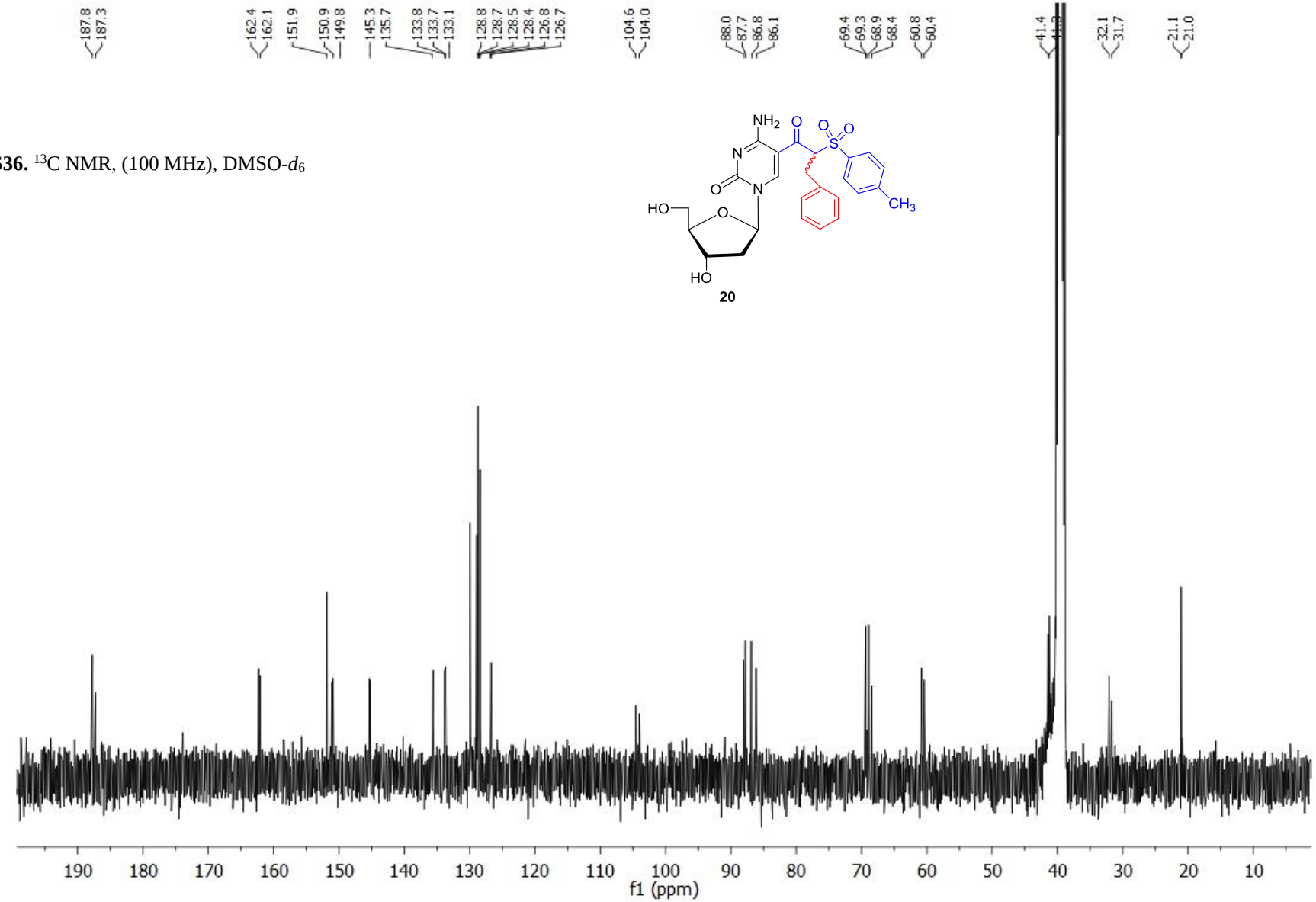


**Figure S37.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

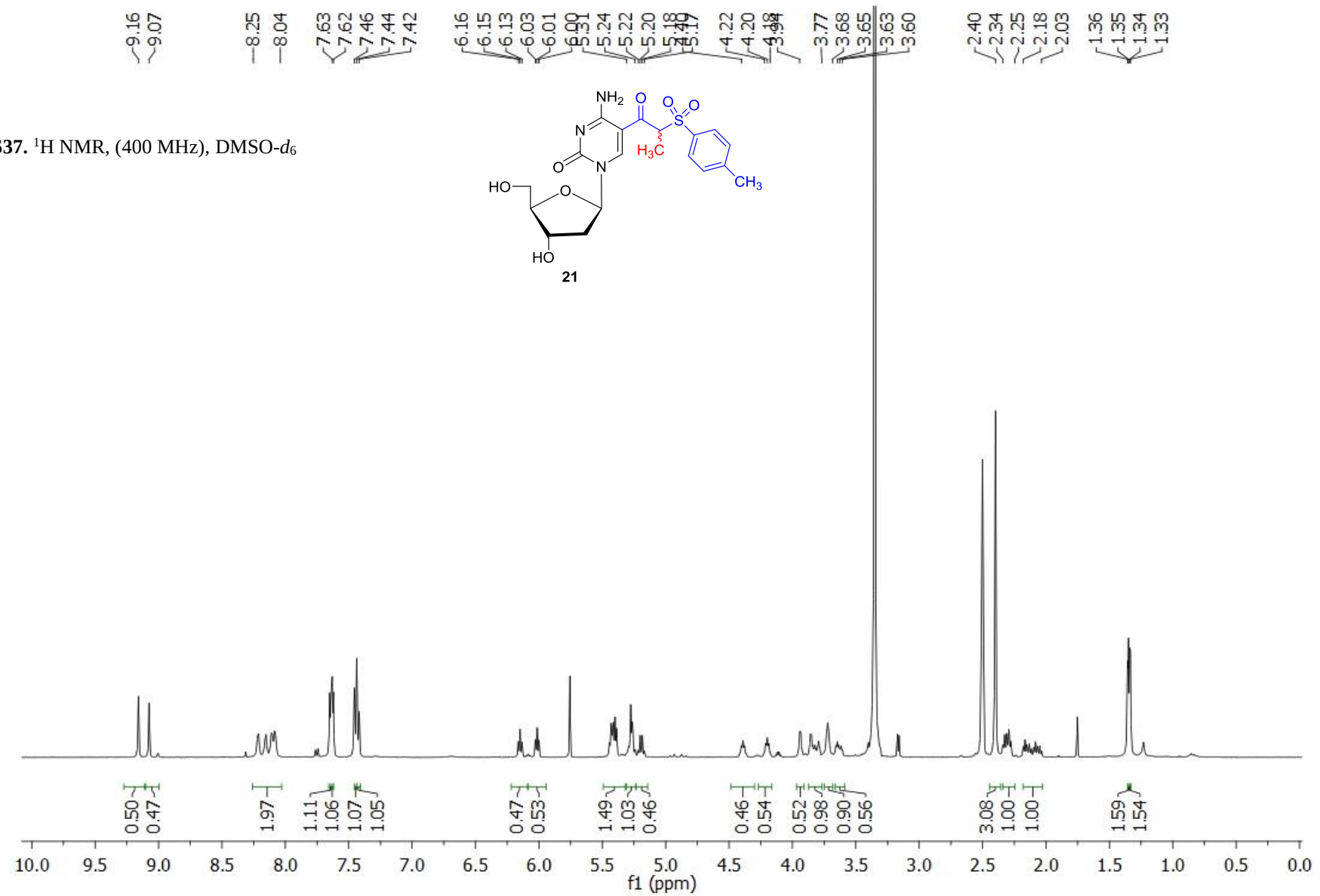


**Figure S38.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

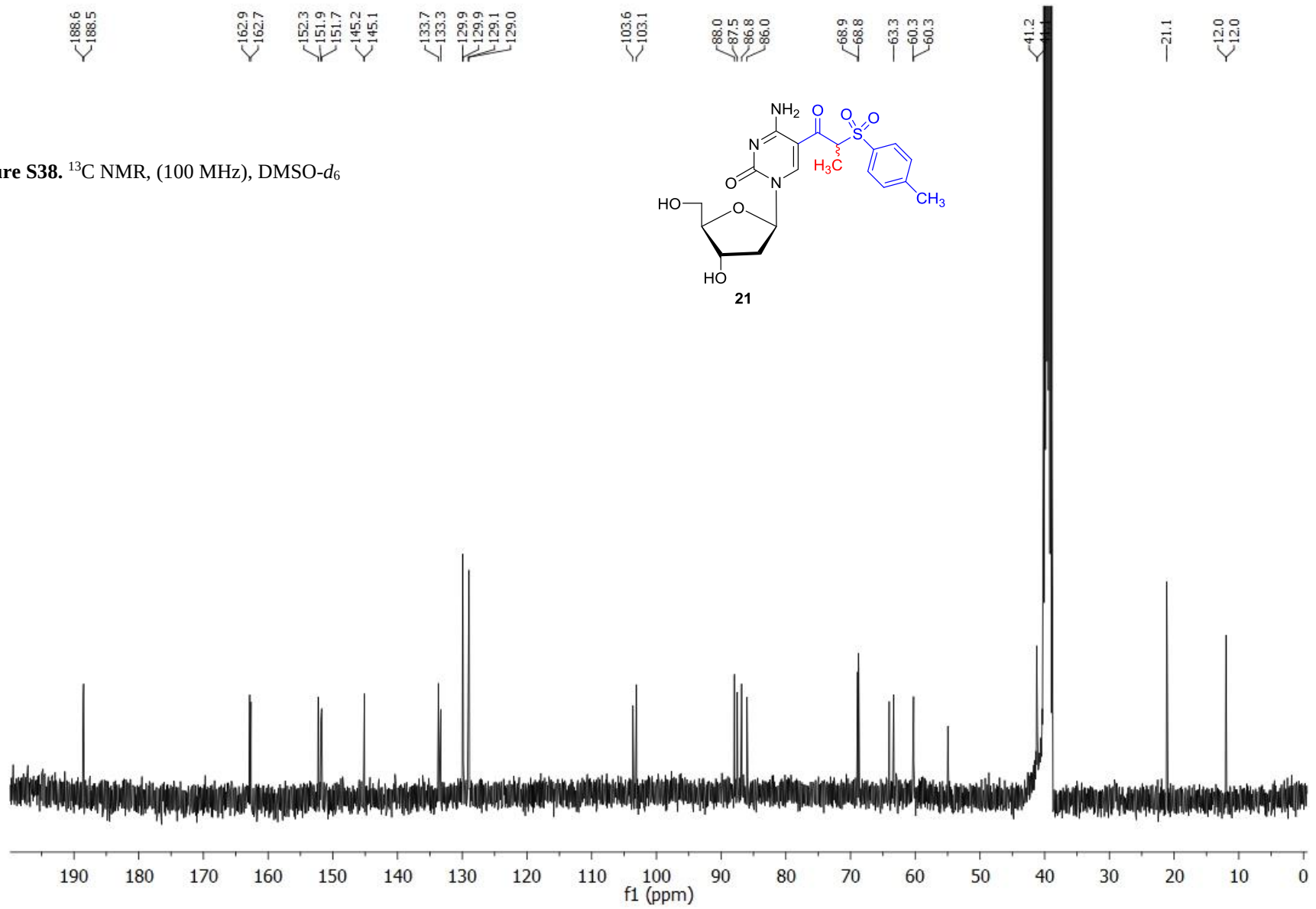


**Figure S39.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

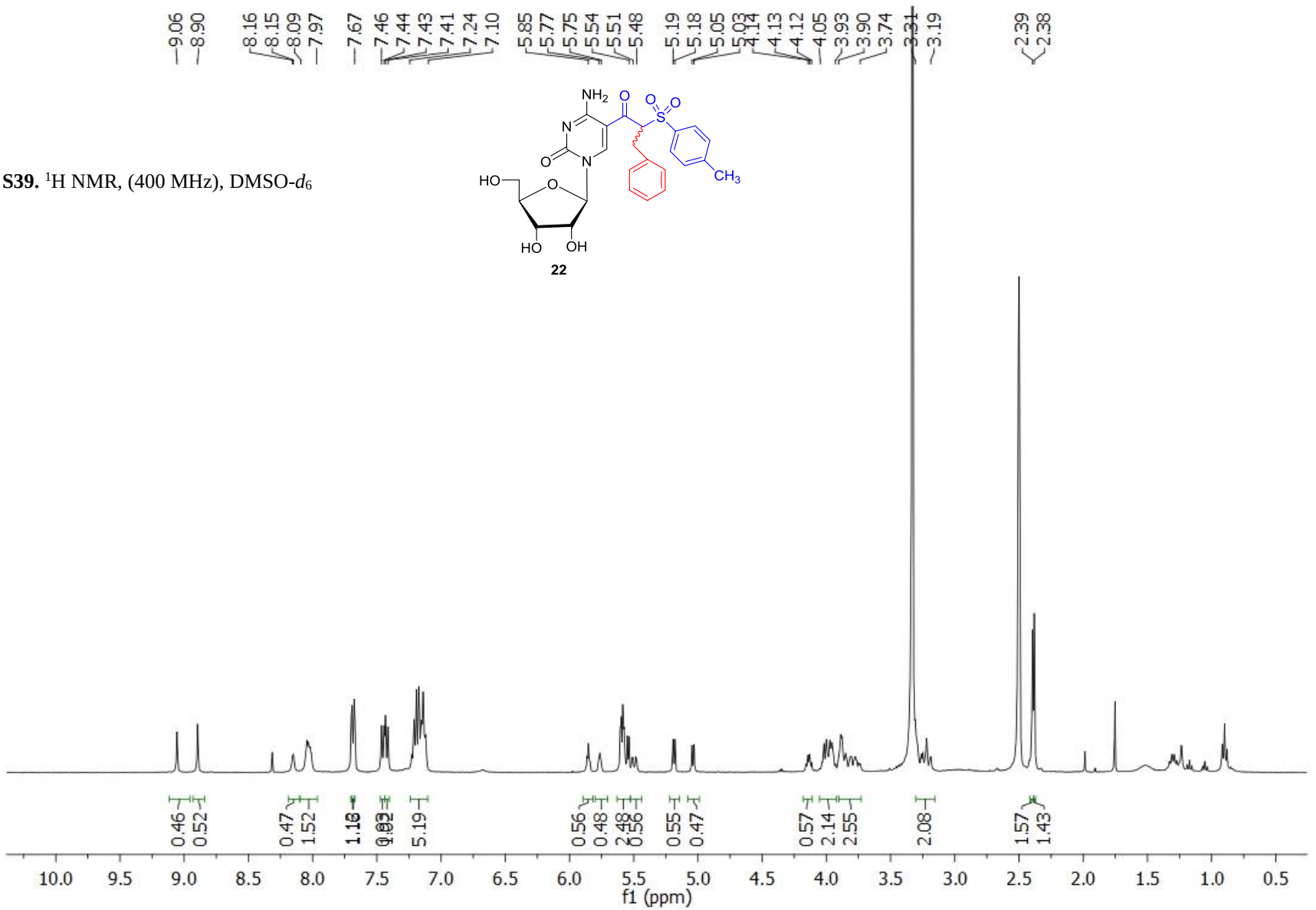


**Figure S40.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

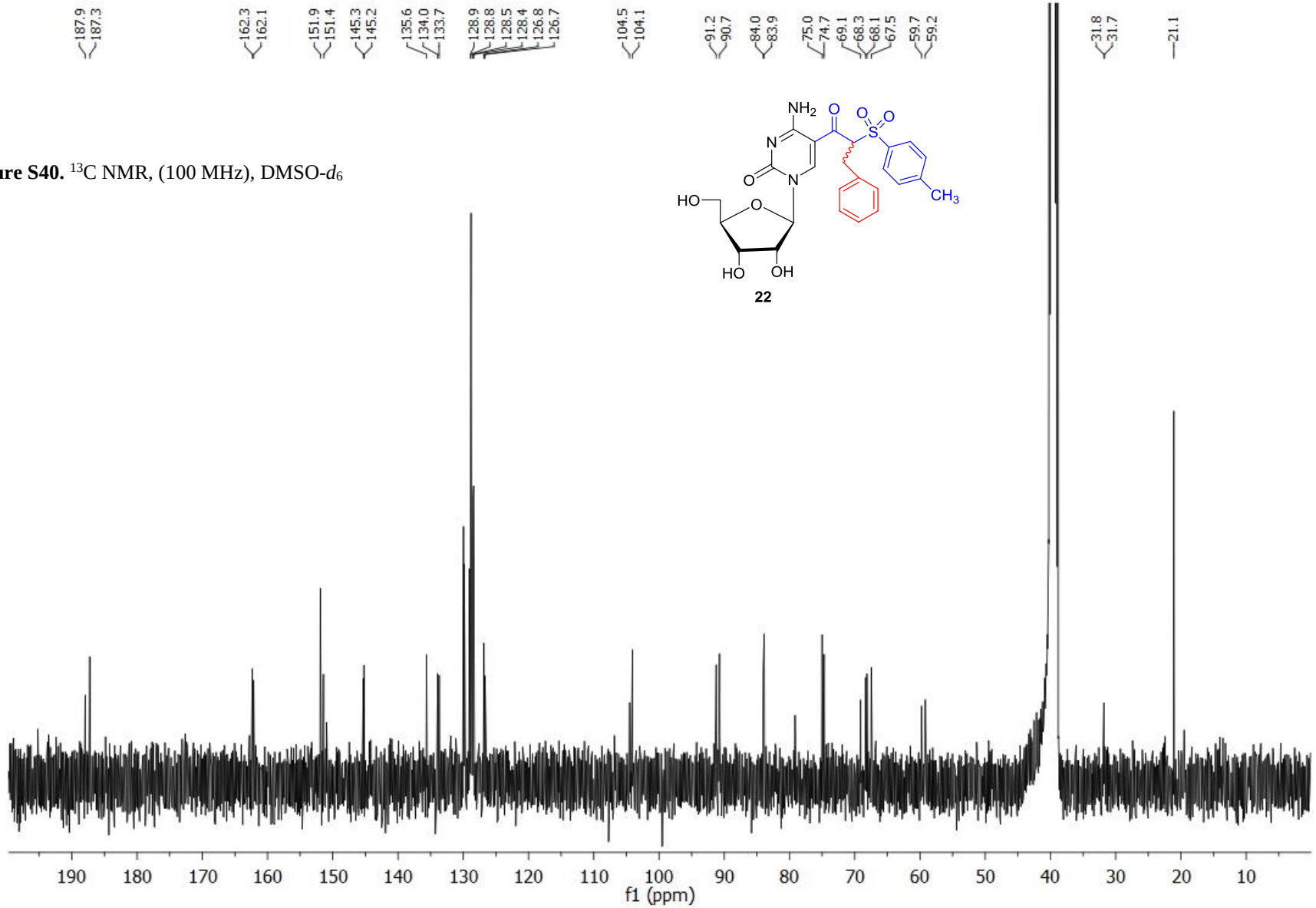


**Figure S41.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

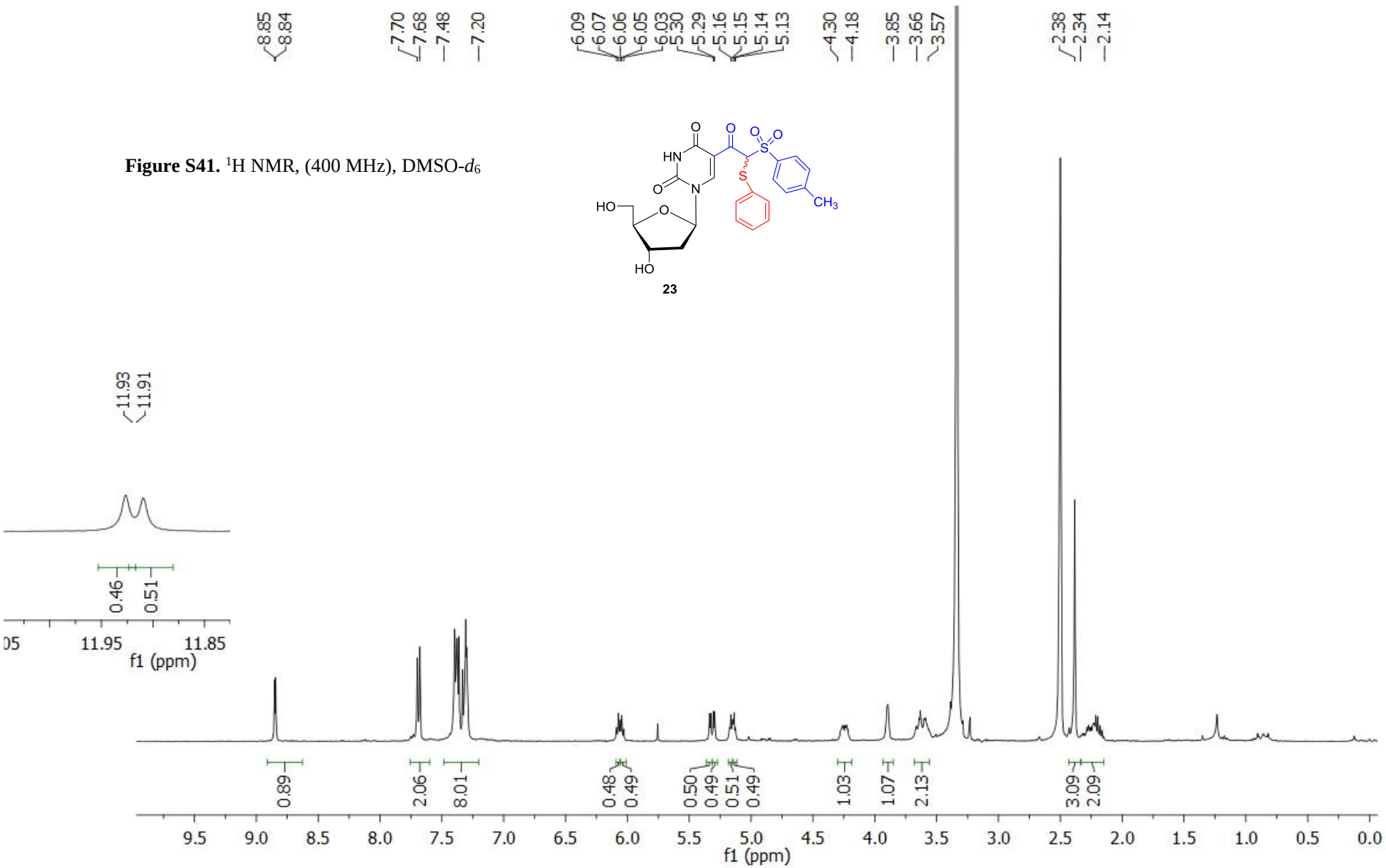


**Figure S42.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

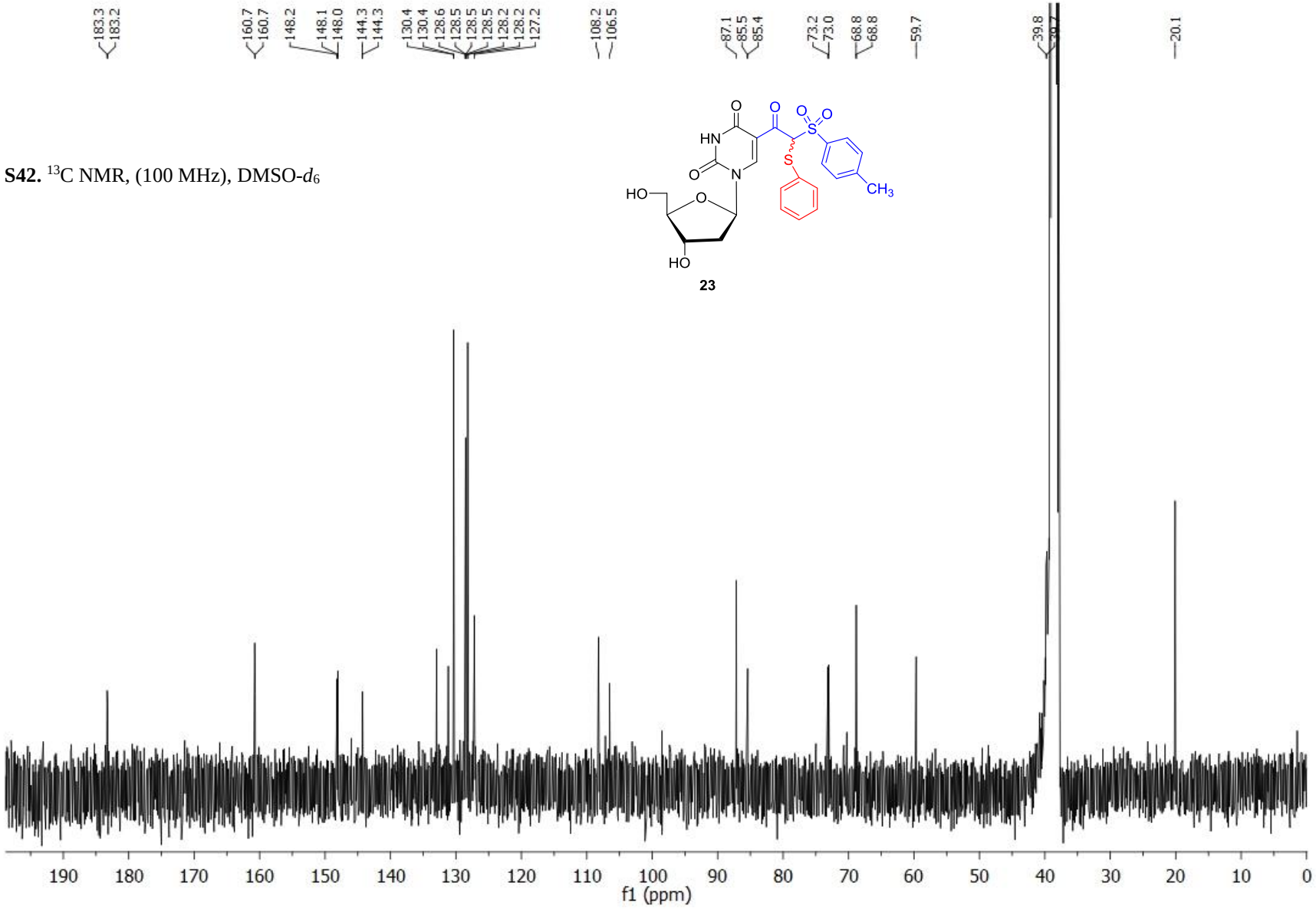


**Figure S43.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

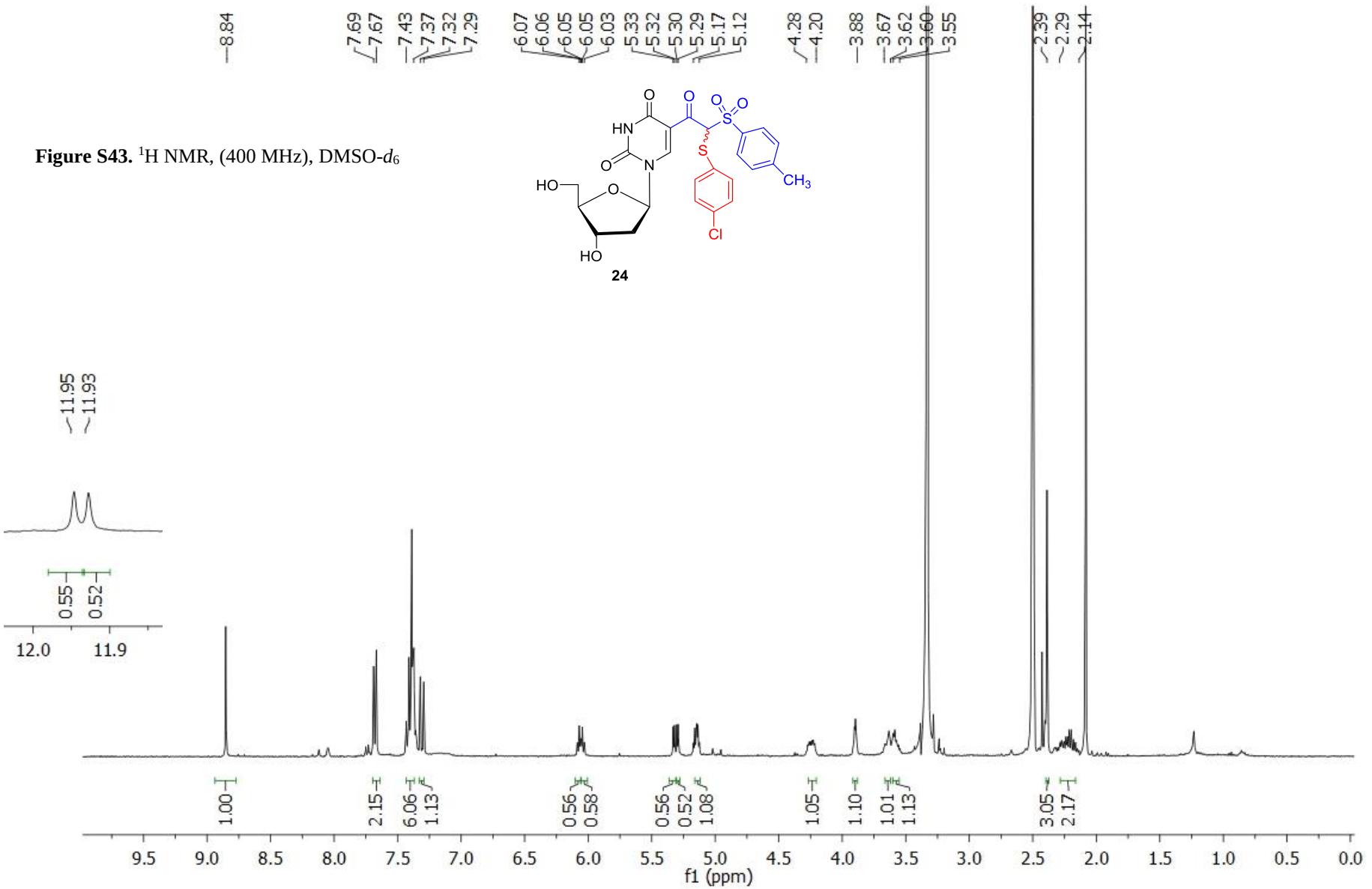


**Figure S44.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

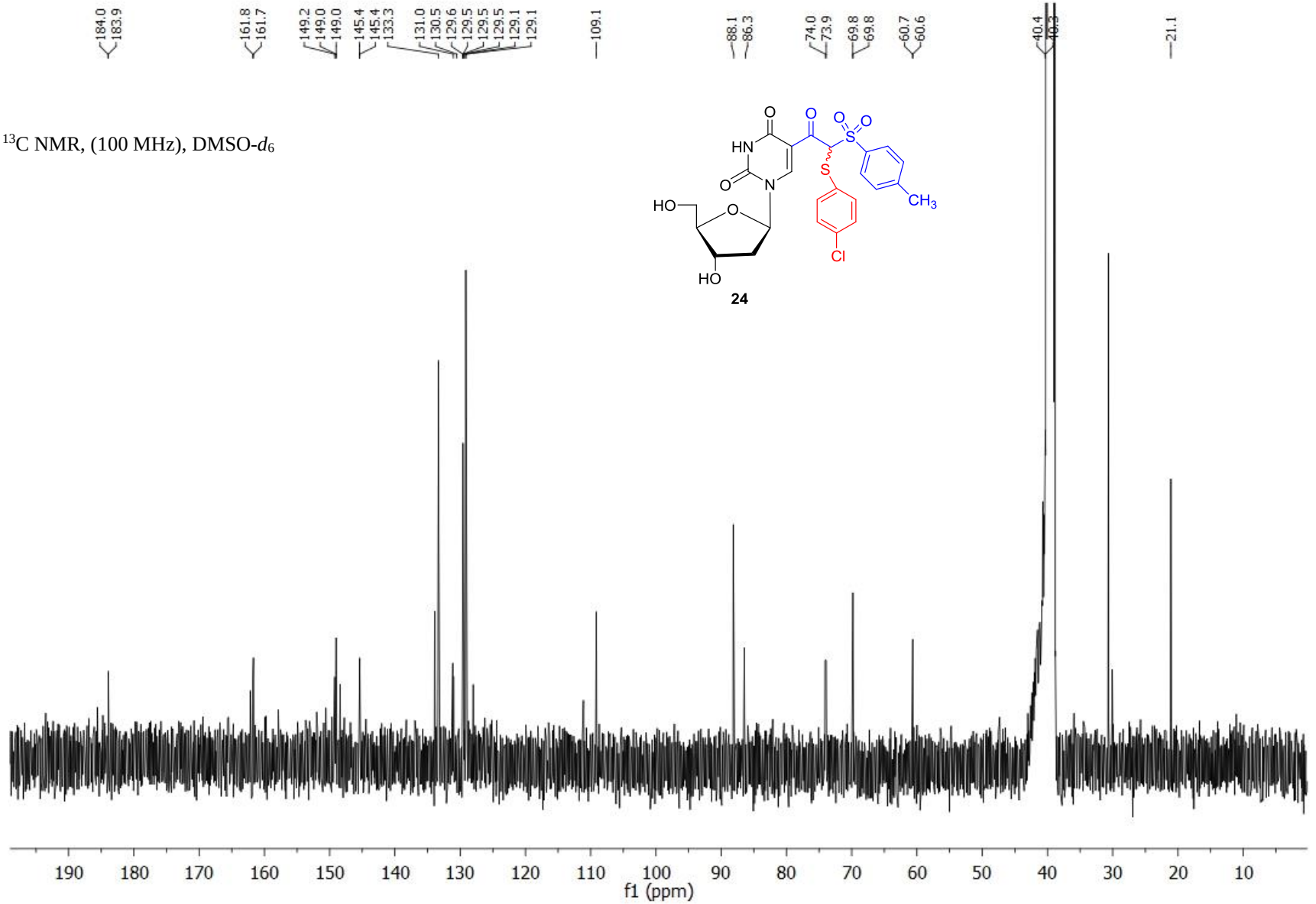
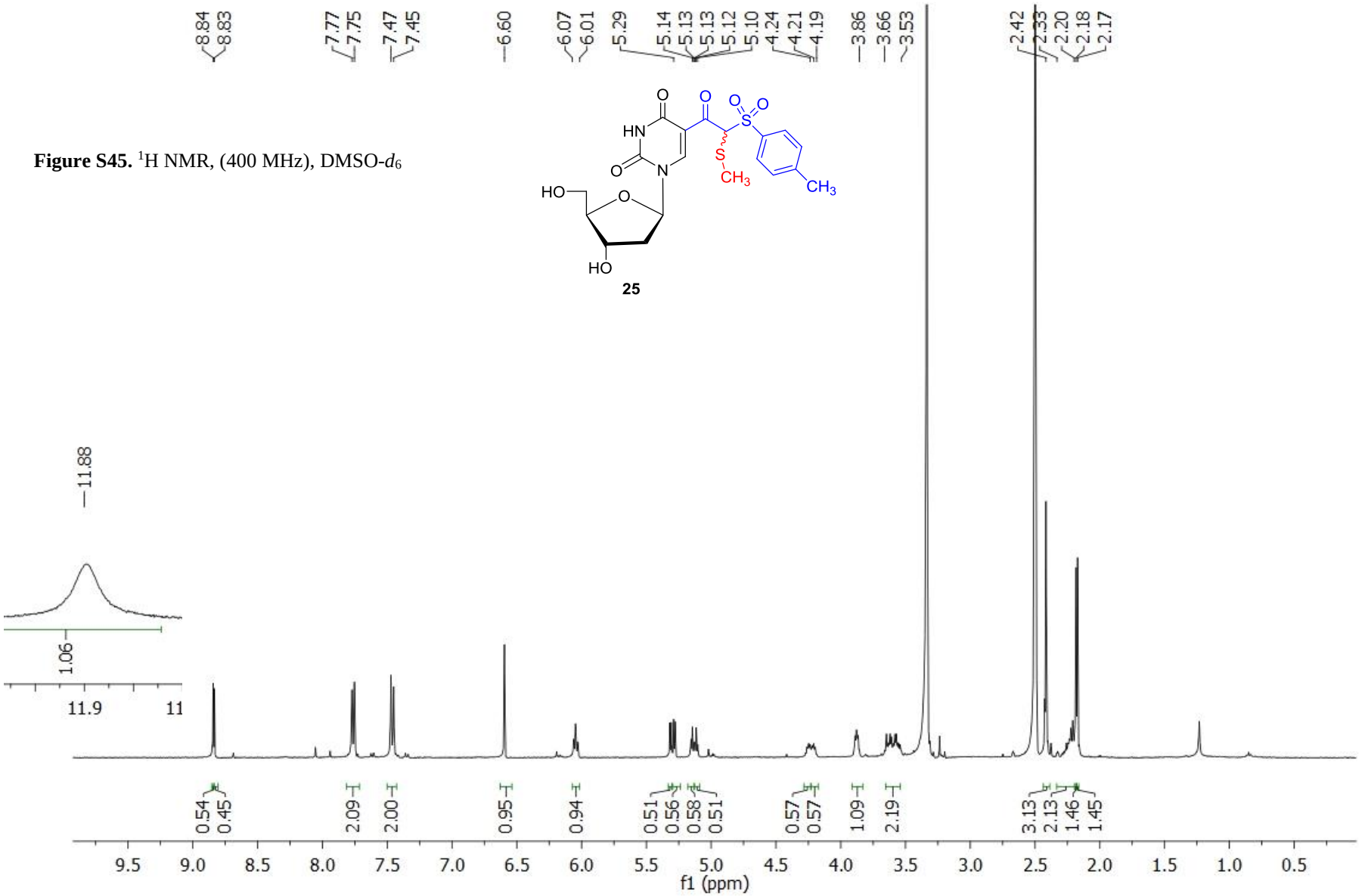


**Figure S45.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$




**25**

**Figure S46.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

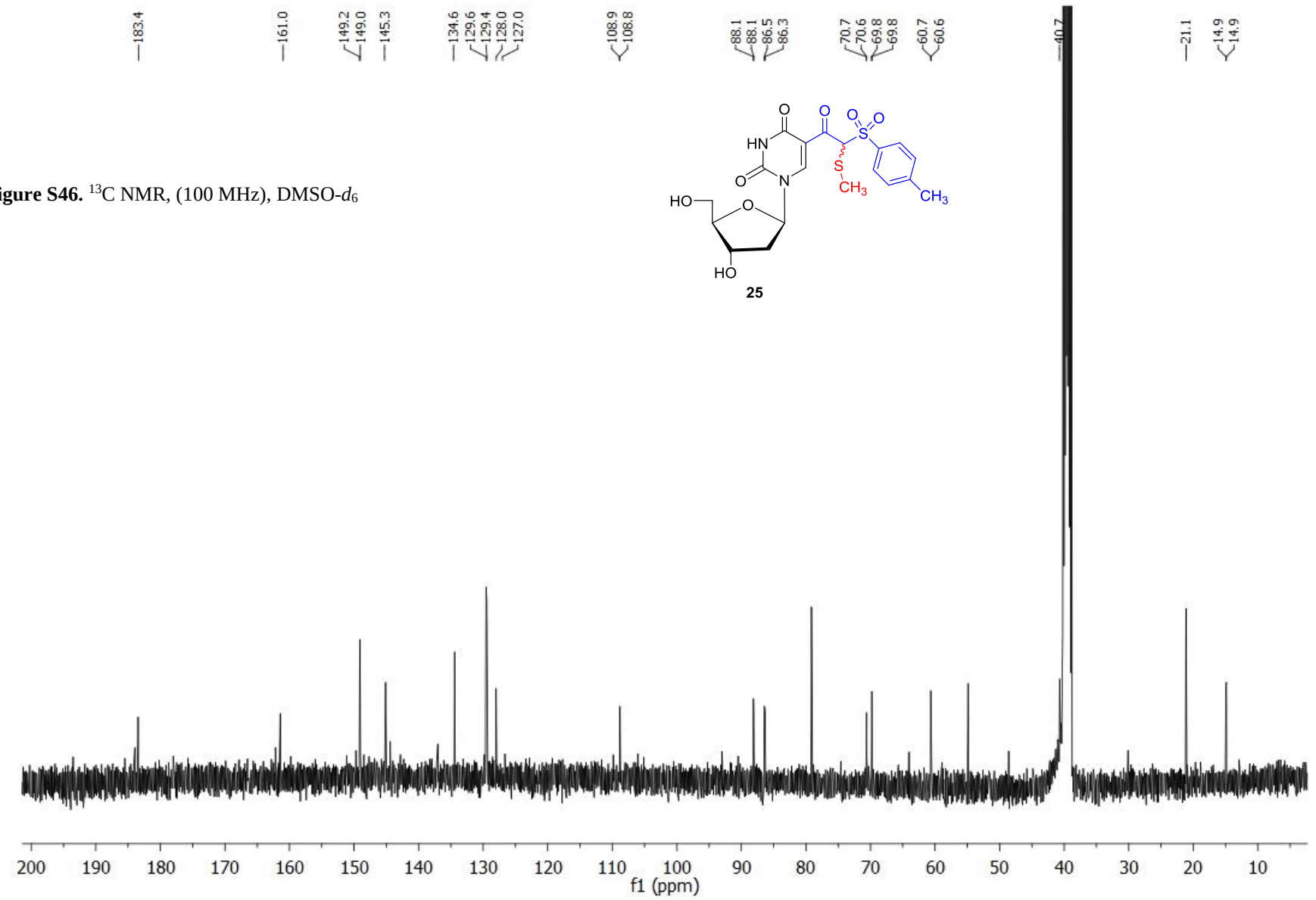


**Figure S47.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

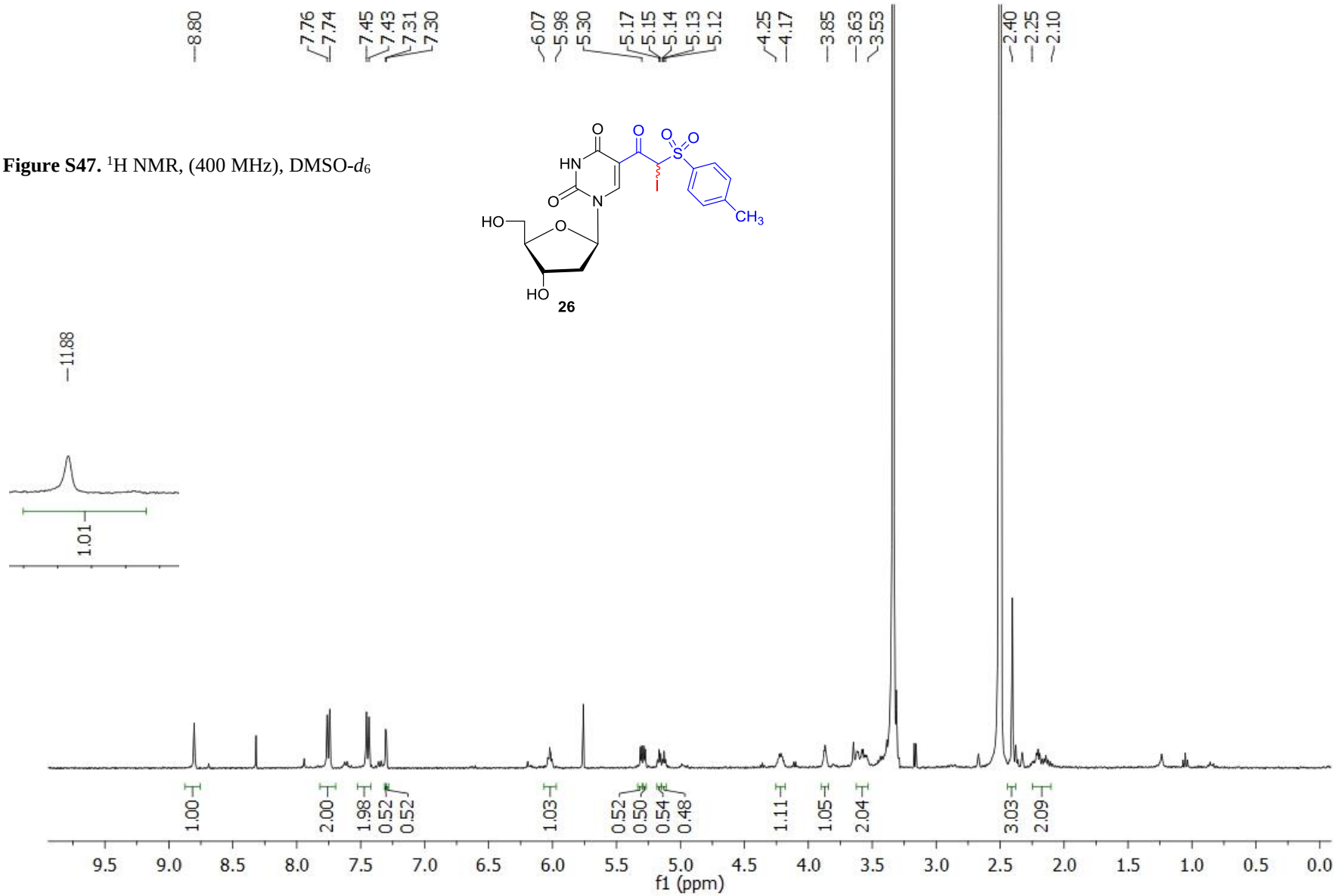


**Figure S48.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$

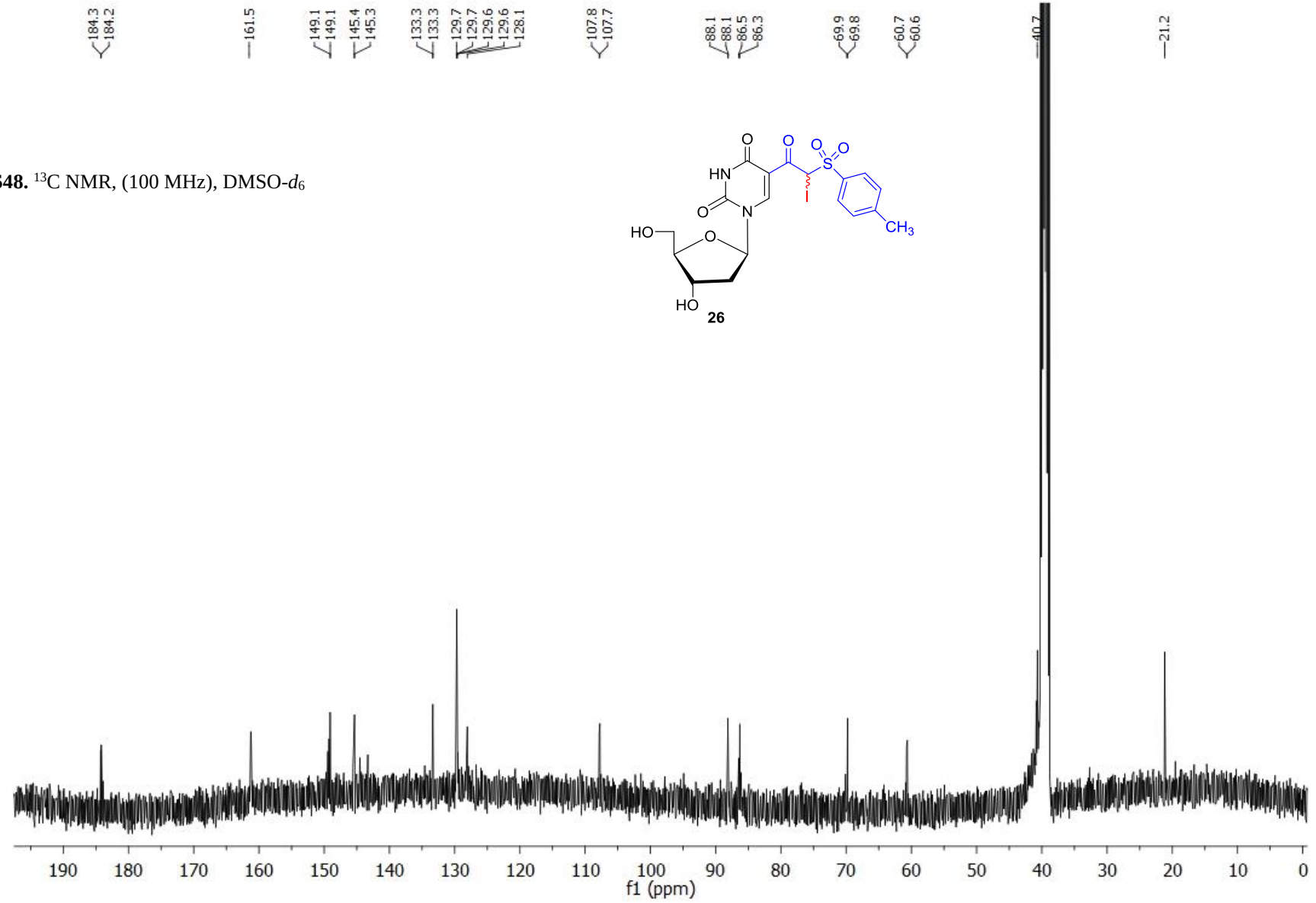


**Figure S49.** $^{1}$H NMR, (400 MHz), DMSO-$d_6$

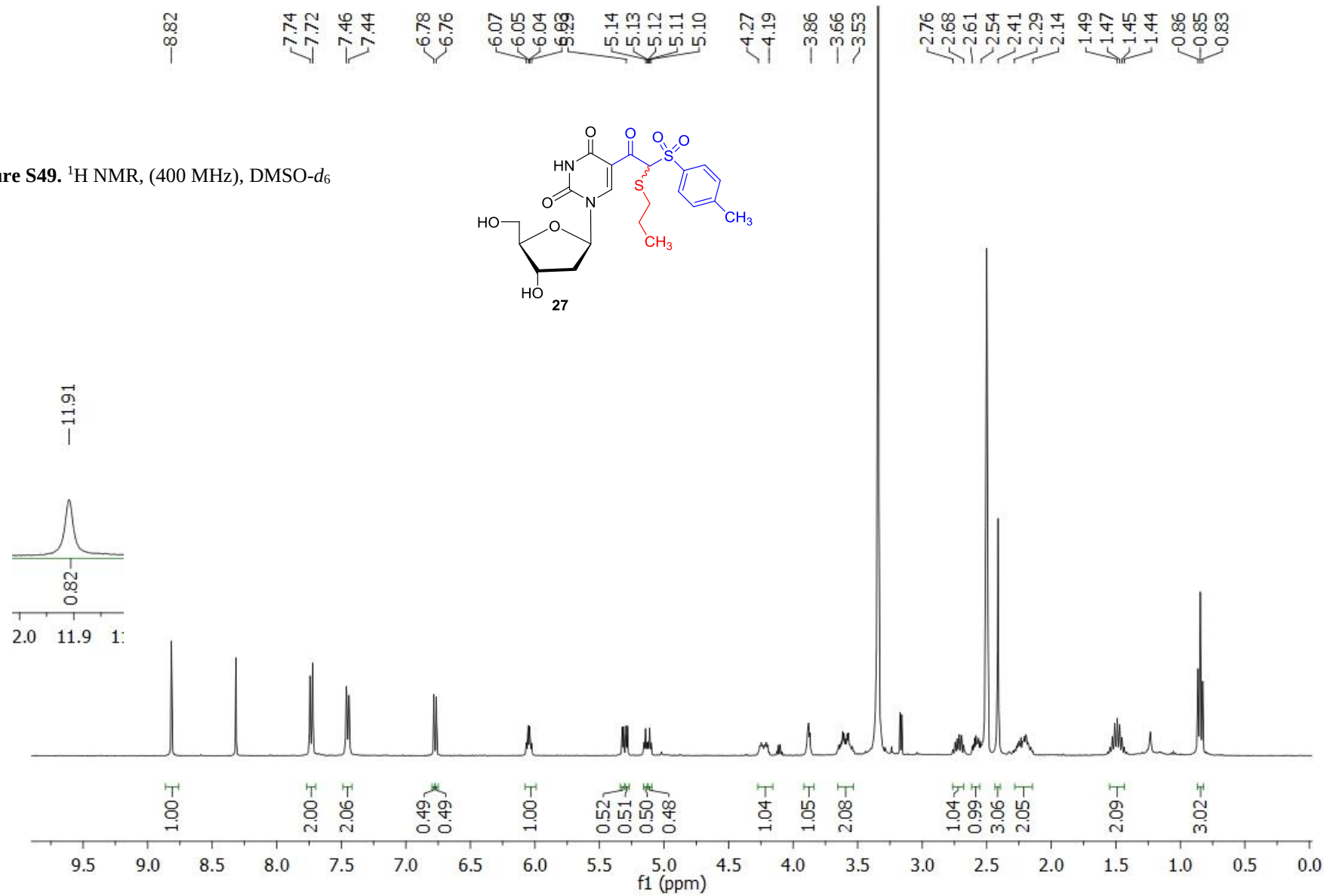


**Figure S50.** $^{13}$C NMR, (100 MHz), DMSO-$d_6$




27

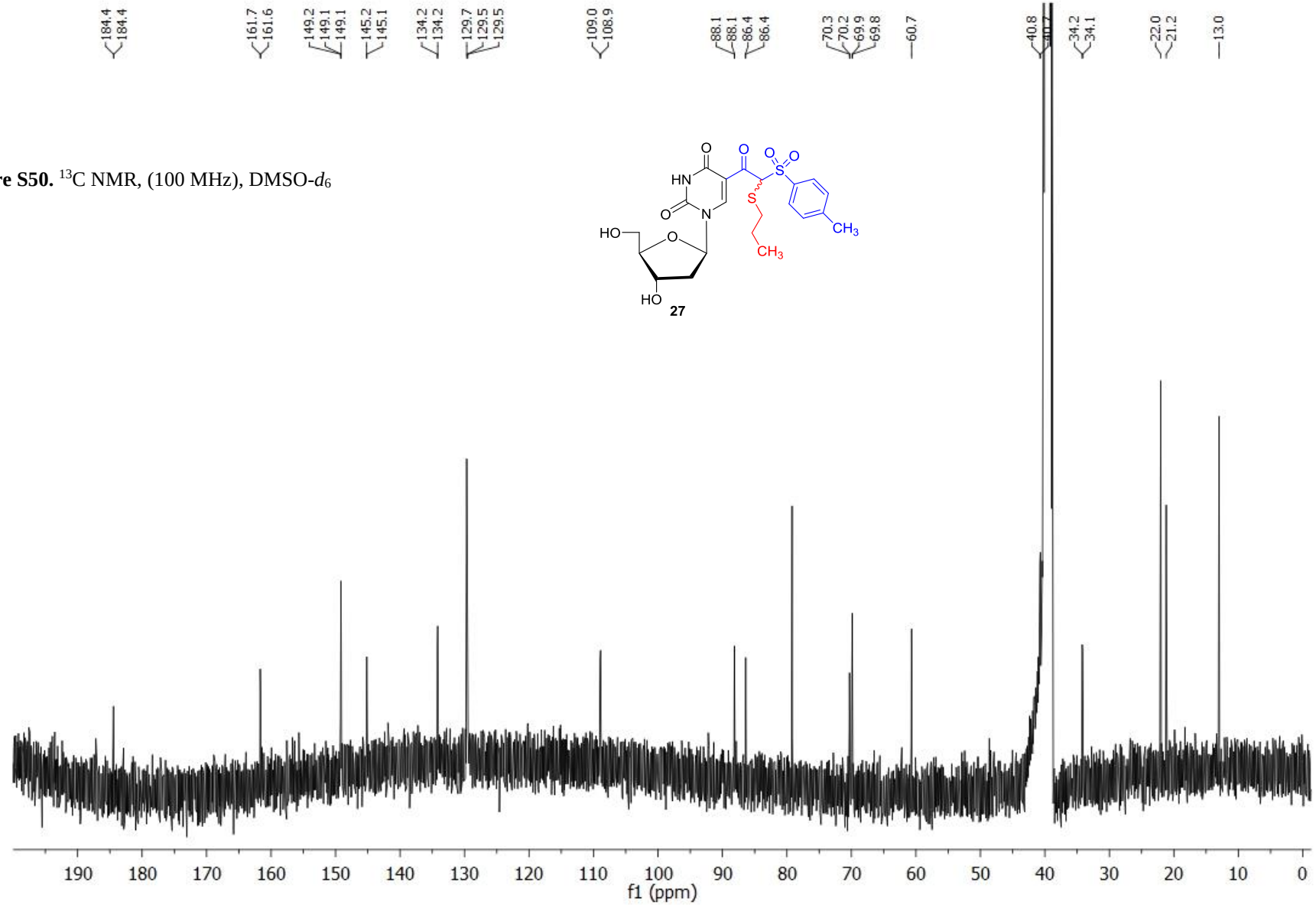
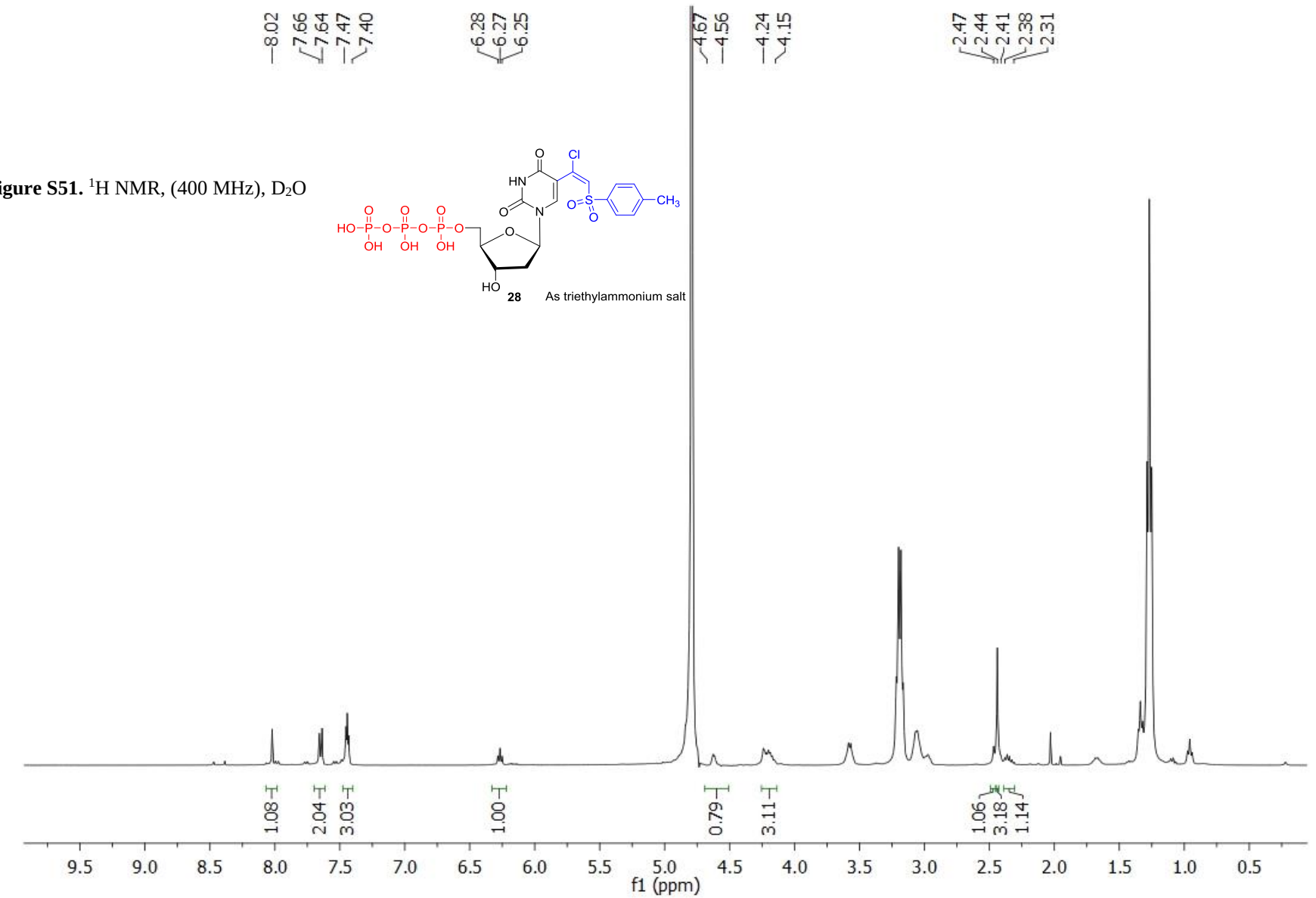


**Figure S51.** $^{1}H$ NMR, (400 MHz), $D_2O$




**28** As triethylammonium salt

**Figure S52.** $^{13}C$ NMR, (100 MHz), $D_2O$

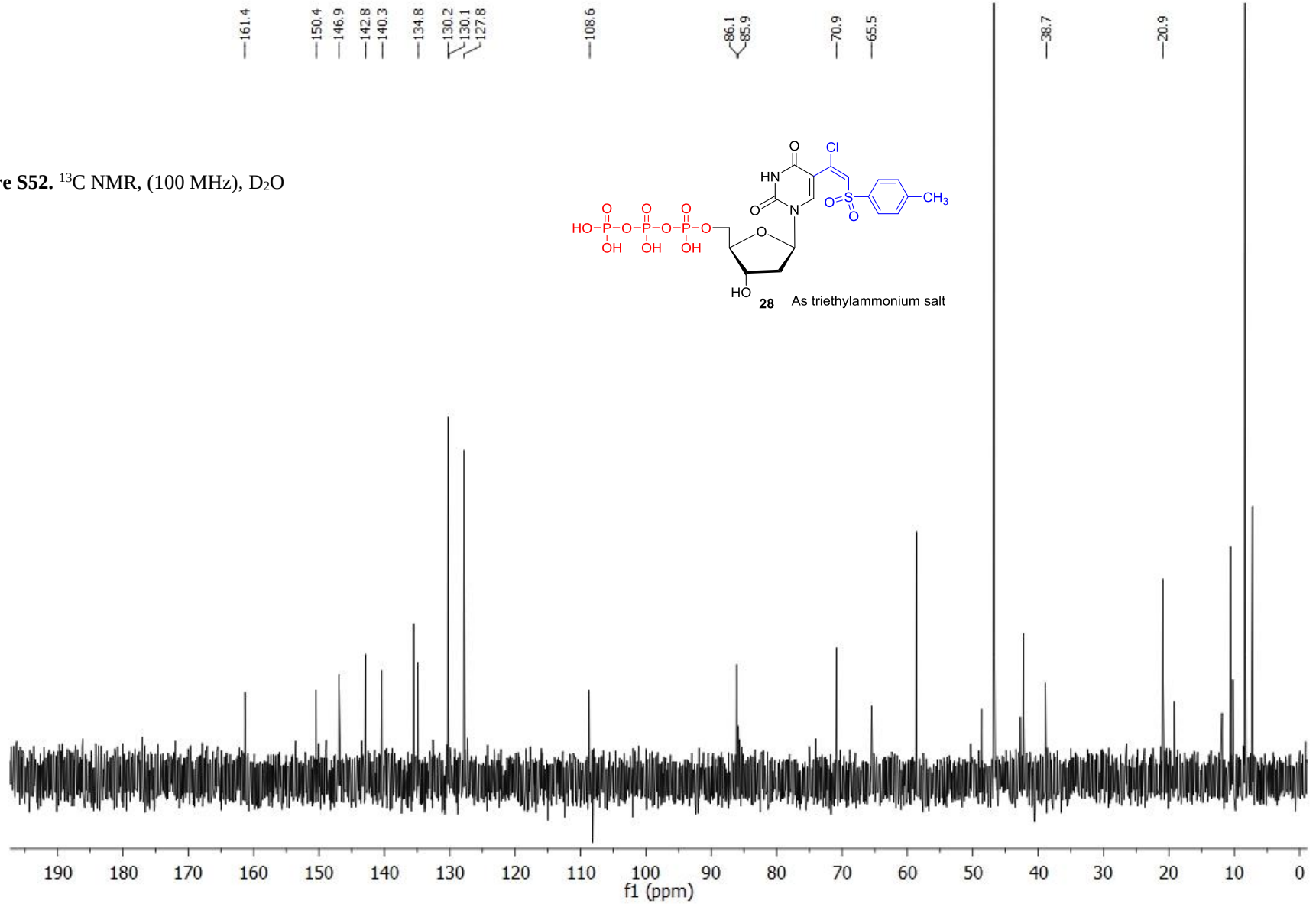


**Figure S53.** $^{31}P$ NMR, (162 MHz), $D_2O$

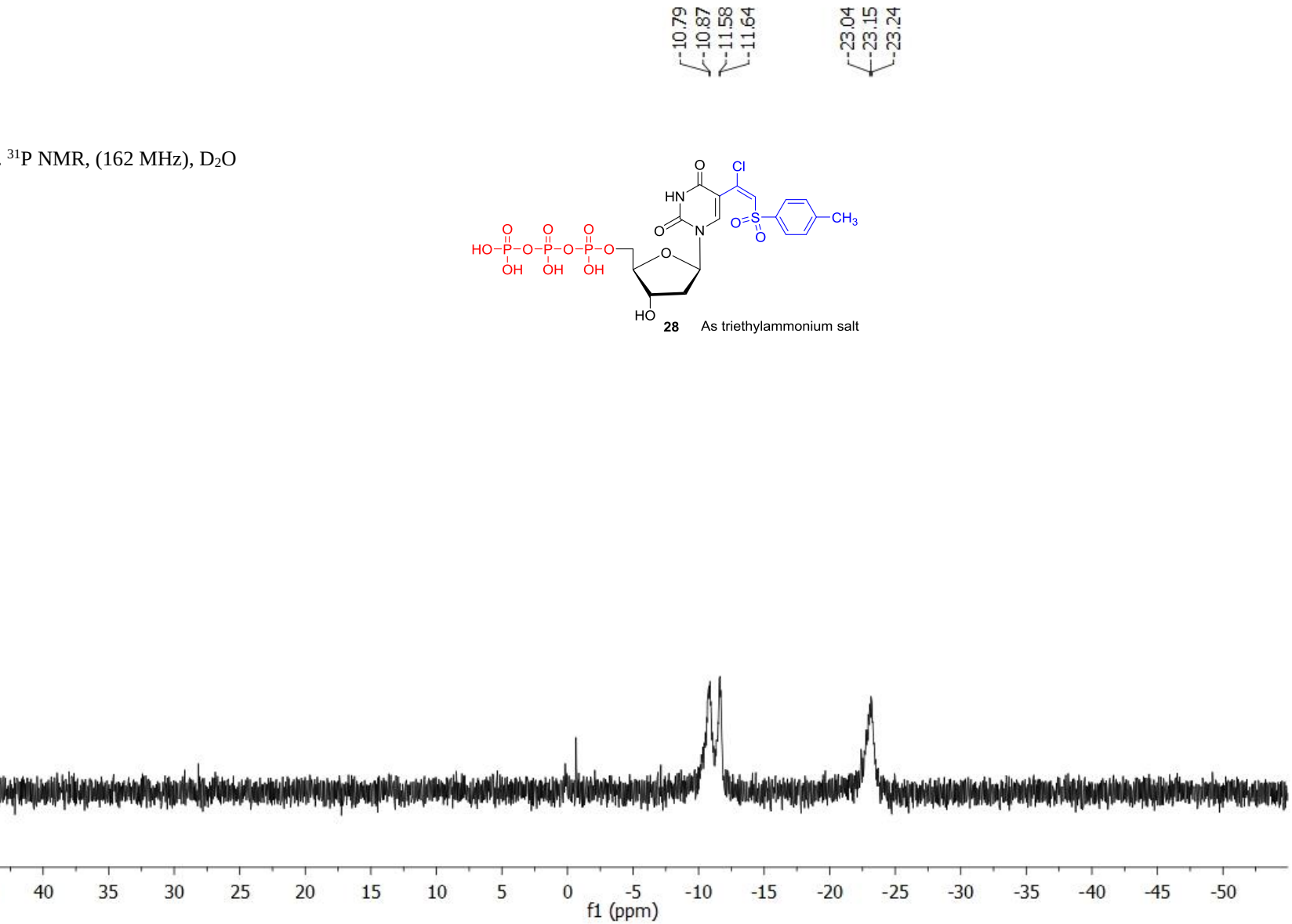


**Figure S54.** $^{1}H$ NMR, (400 MHz), $D_2O$




**29** As triethylammonium salt

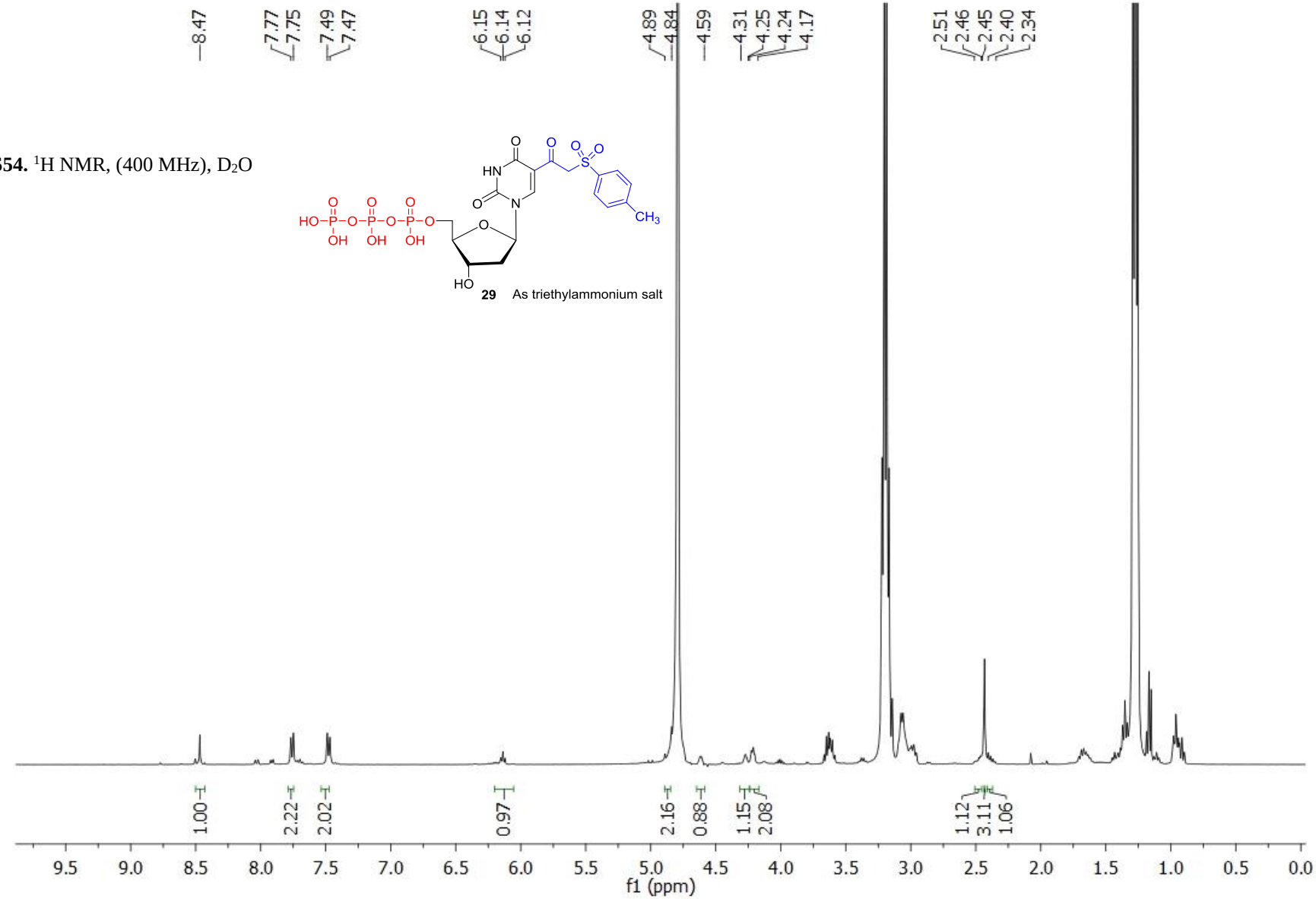


**Figure S55.** $^{13}C$ NMR, (100 MHz), $D_2O$

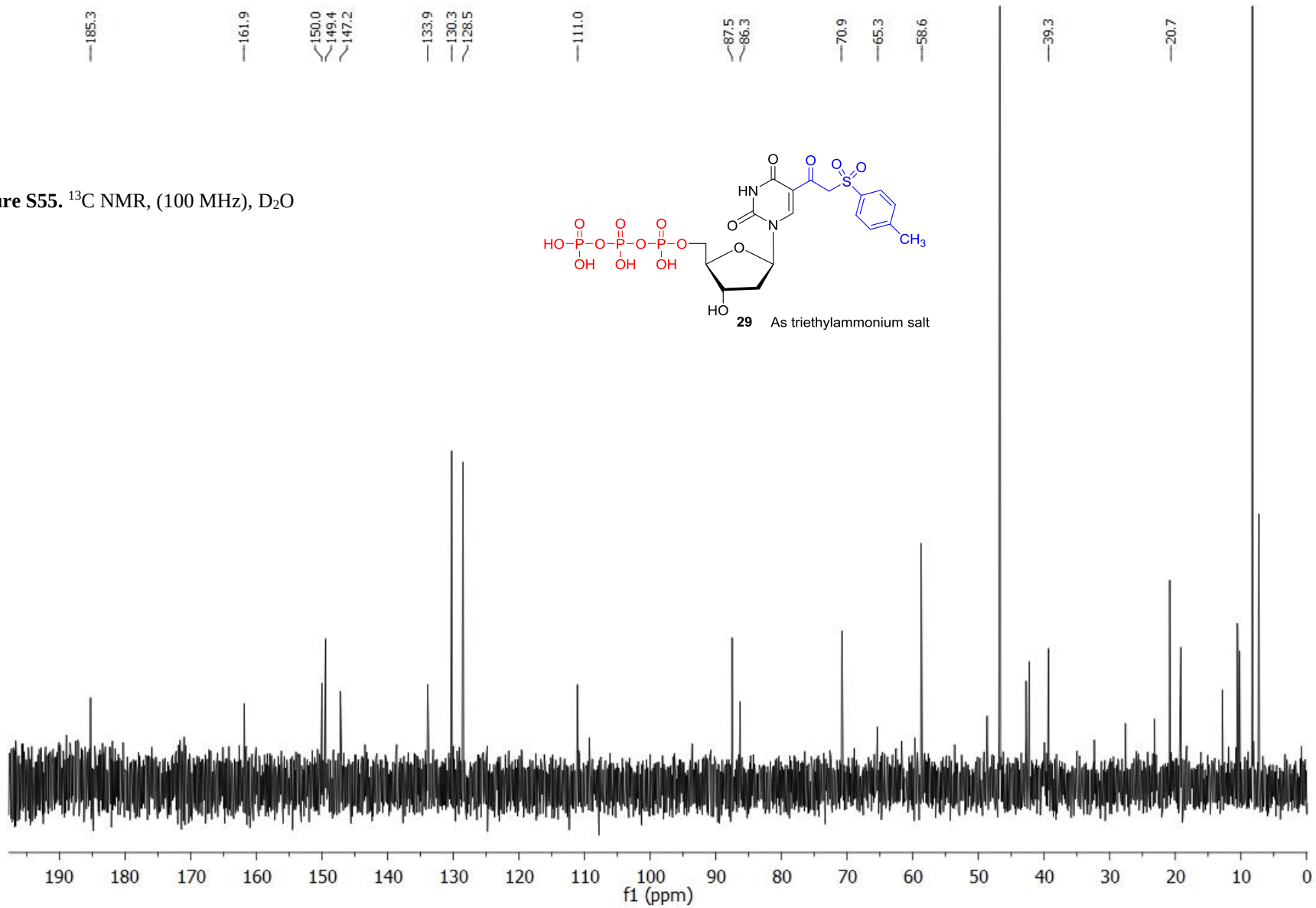


**Figure S56.** $^{31}P$ NMR, (162 MHz), $D_2O$

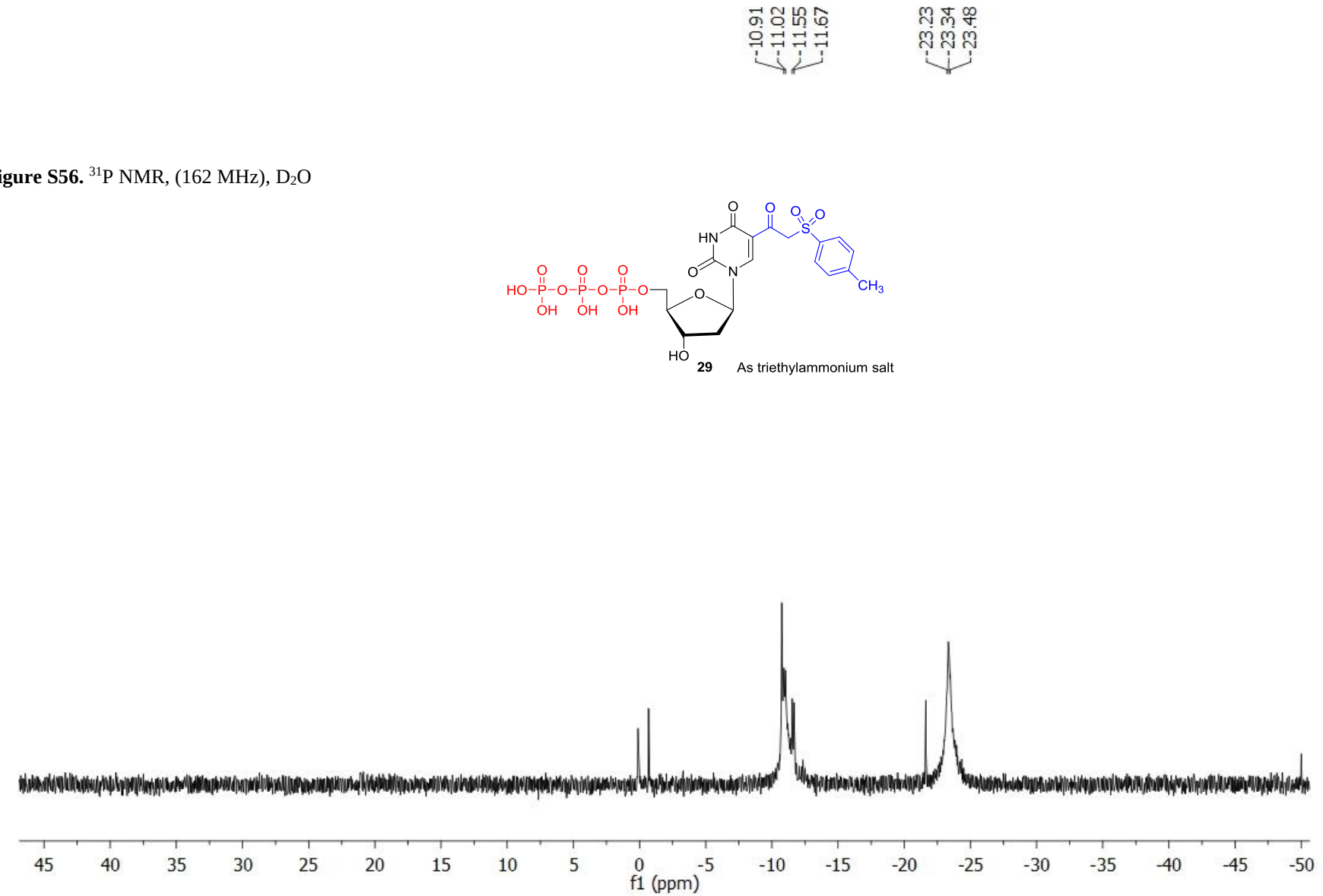


**Figure S57.** $^{1}H$ NMR, (400 MHz), $D_2O$

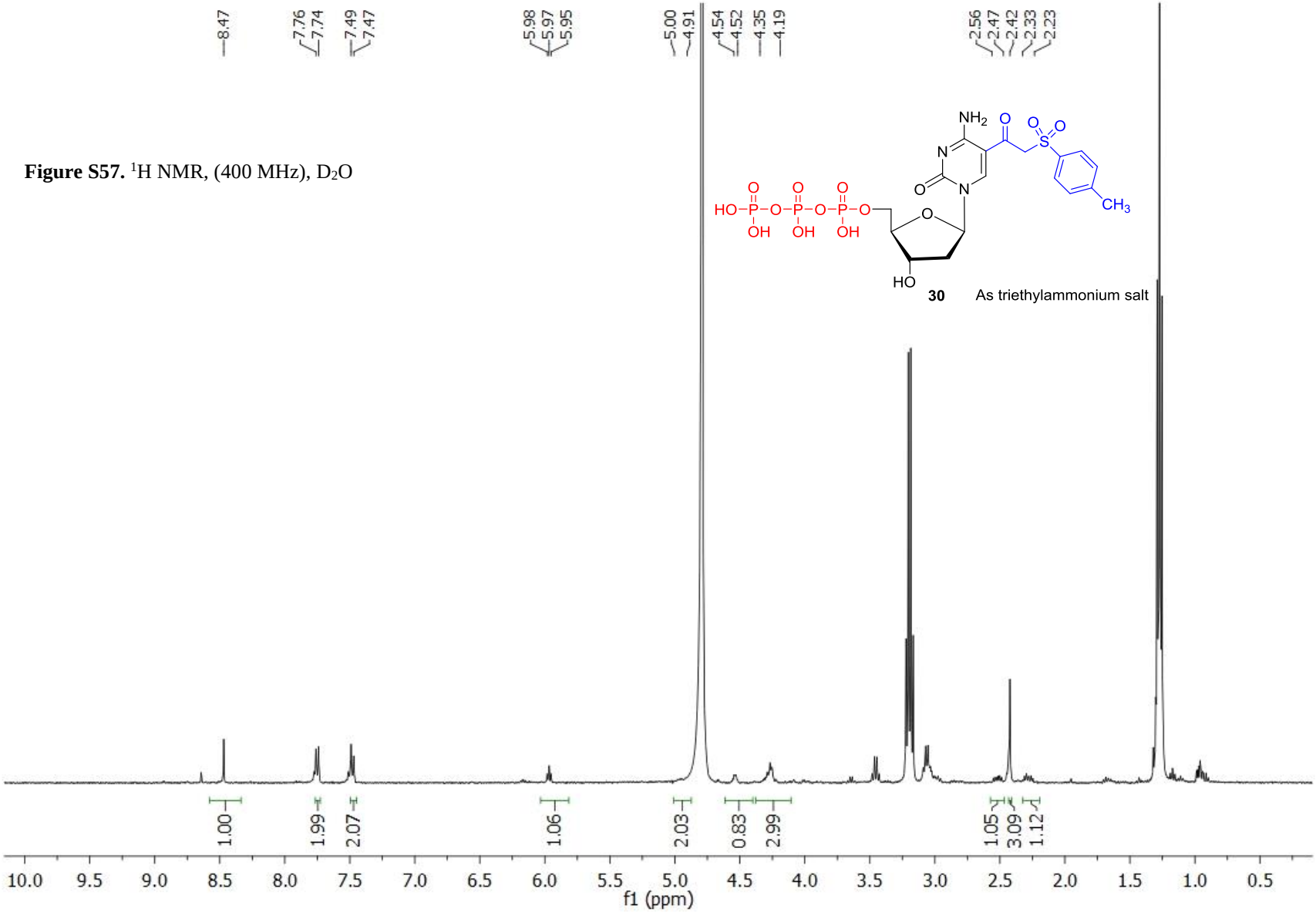
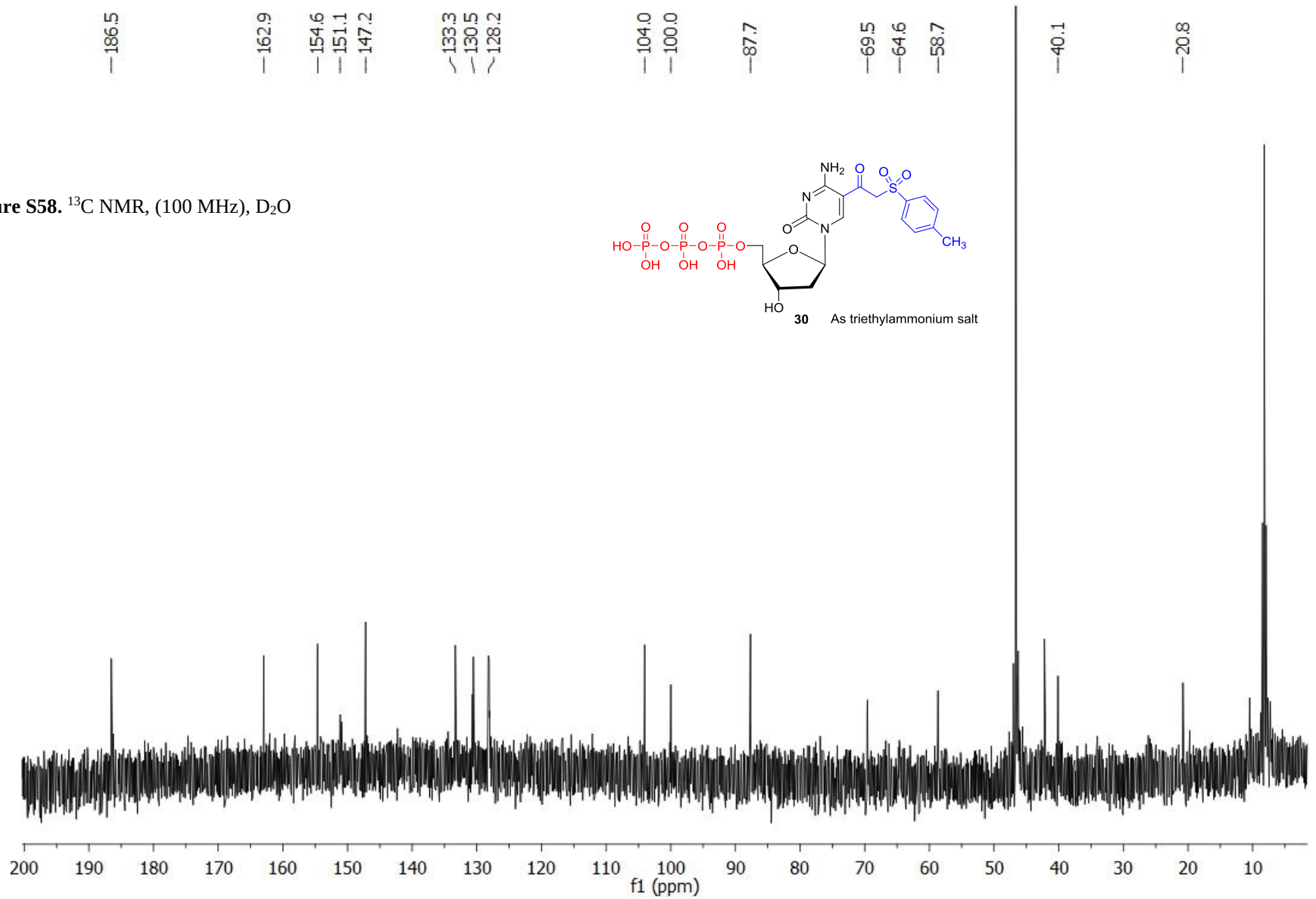
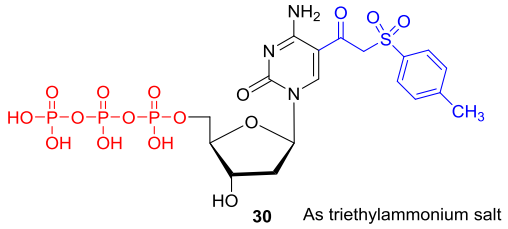


**Figure S58.** $^{13}C$ NMR, (100 MHz), $D_2O$




**30** As triethylammonium salt


**Figure S59.** $^{31}P$ NMR, (162 MHz), $D_2O$




**30** As triethylammonium salt