

Supporting information

Two-step conversion of uridine and cytidine to variously C5-C functionalized analogs

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1. Spectral analysis of synthesized compounds

1.1. ^1H , ^{13}C and ^{19}F NMR spectra of compounds 2a and 2b

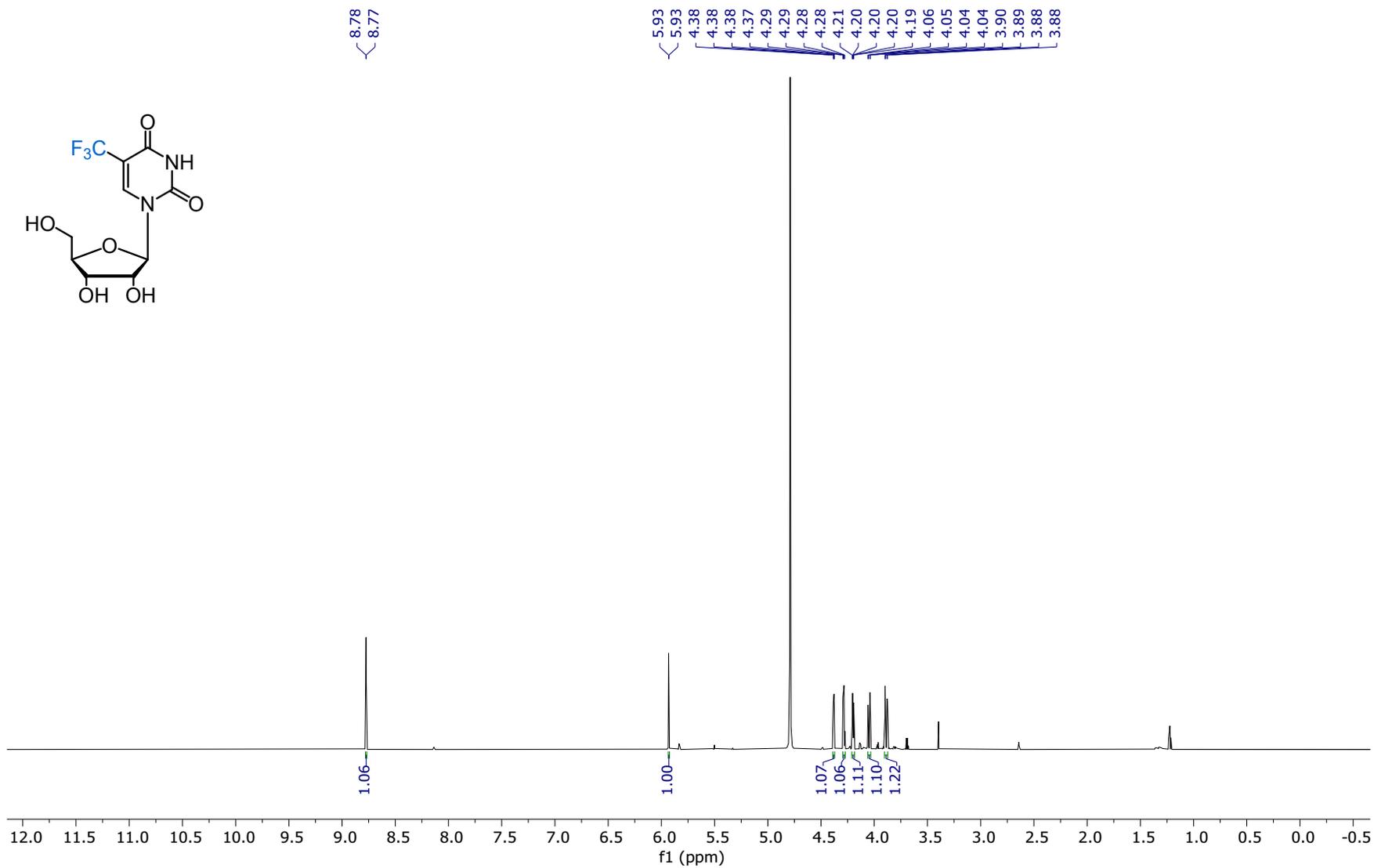


Figure S1. ^1H NMR spectrum of 2a (700 MHz, D_2O).

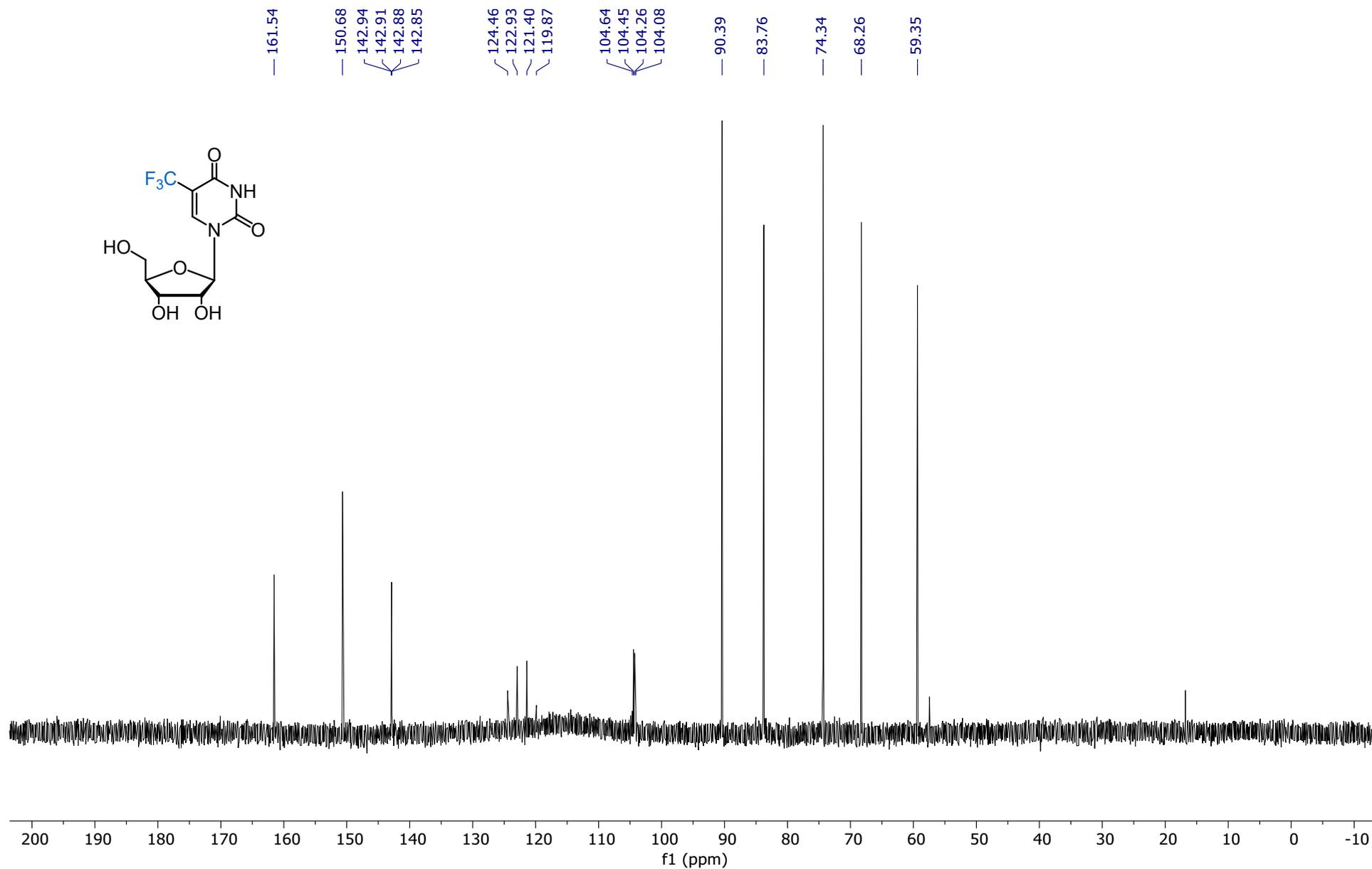


Figure S2. ^{13}C NMR spectrum of **2a** (176 MHz, D_2O).

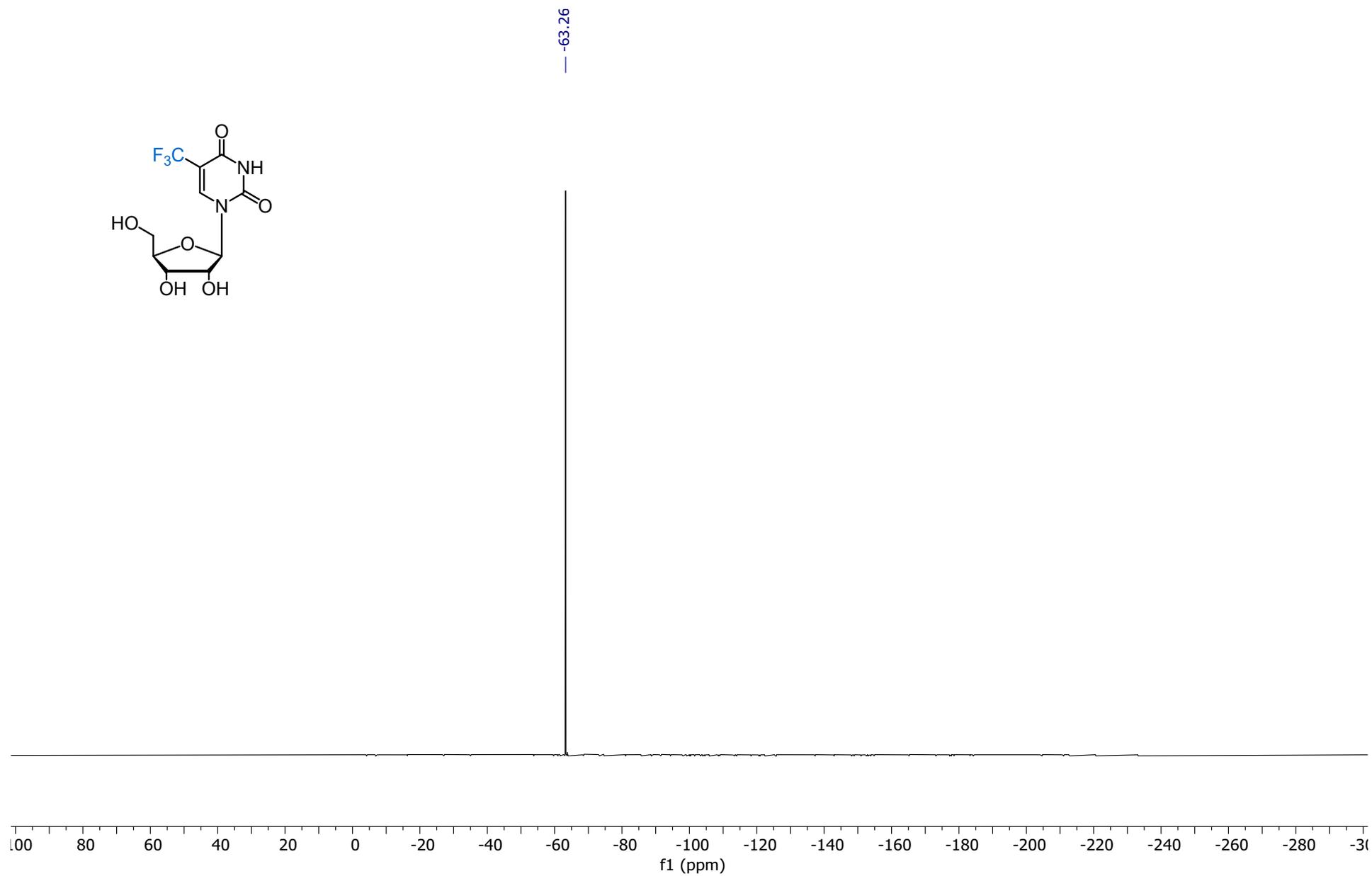


Figure S3. ^{19}F NMR spectrum of **2a** (376 MHz, D_2O).

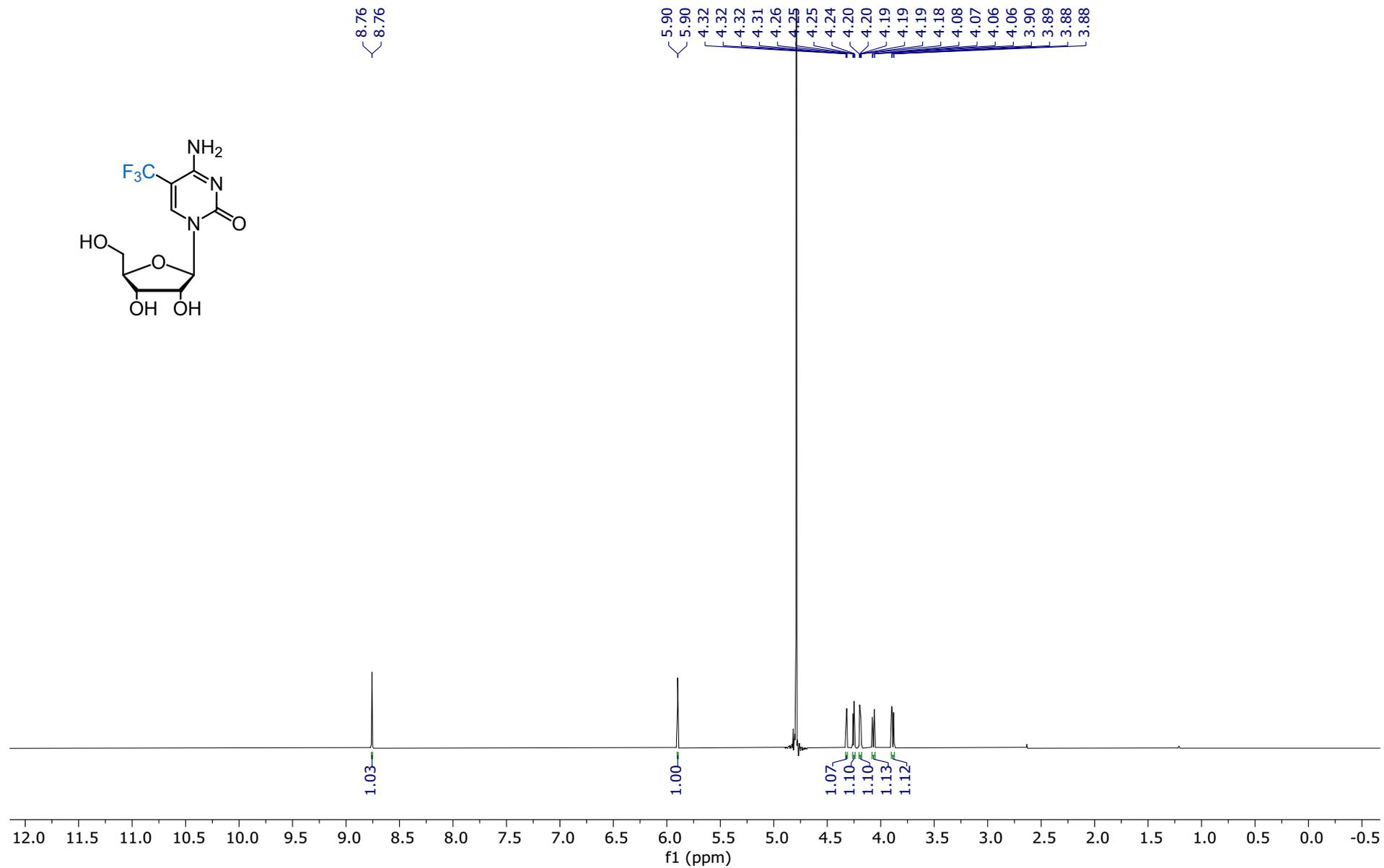


Figure S4. ¹H NMR spectrum of **2b** (700 MHz, D₂O).

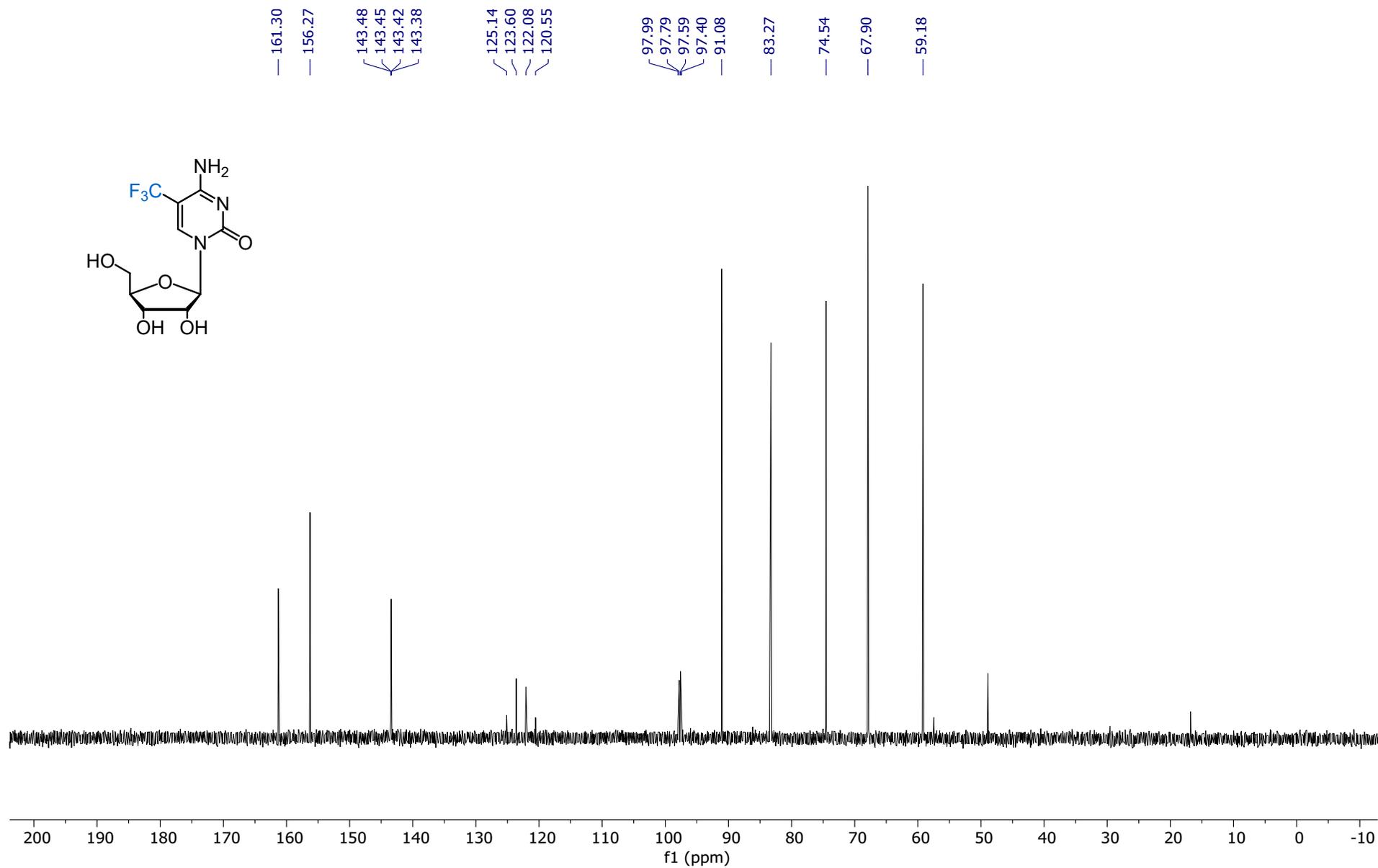


Figure S5. ^{13}C NMR spectrum of **2b** (176 MHz, D_2O).

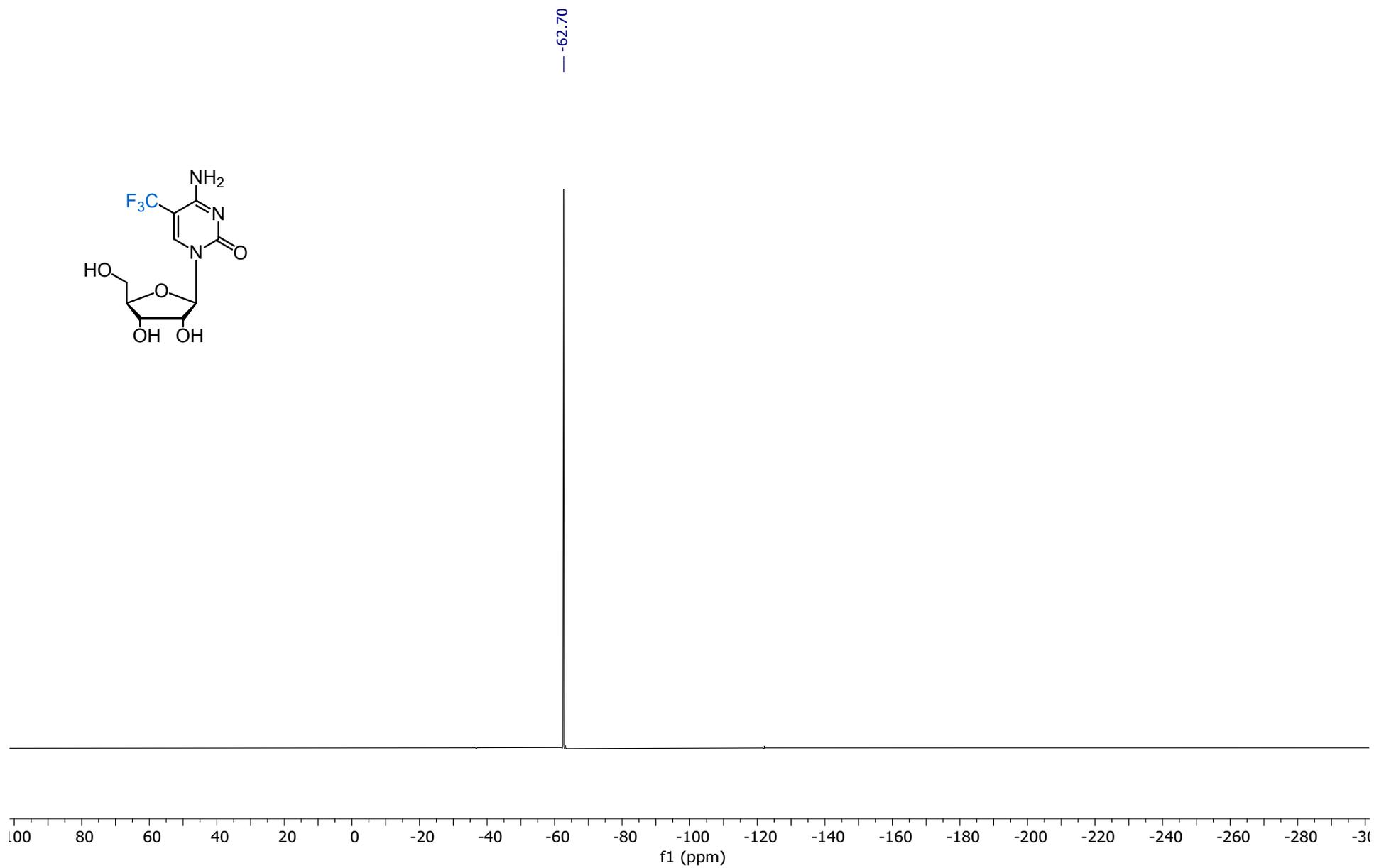


Figure S6. ^{19}F NMR spectrum of **2b** (376 MHz, D_2O).

1.2. IR and NMR spectra of uridine derivatives 3a-7a

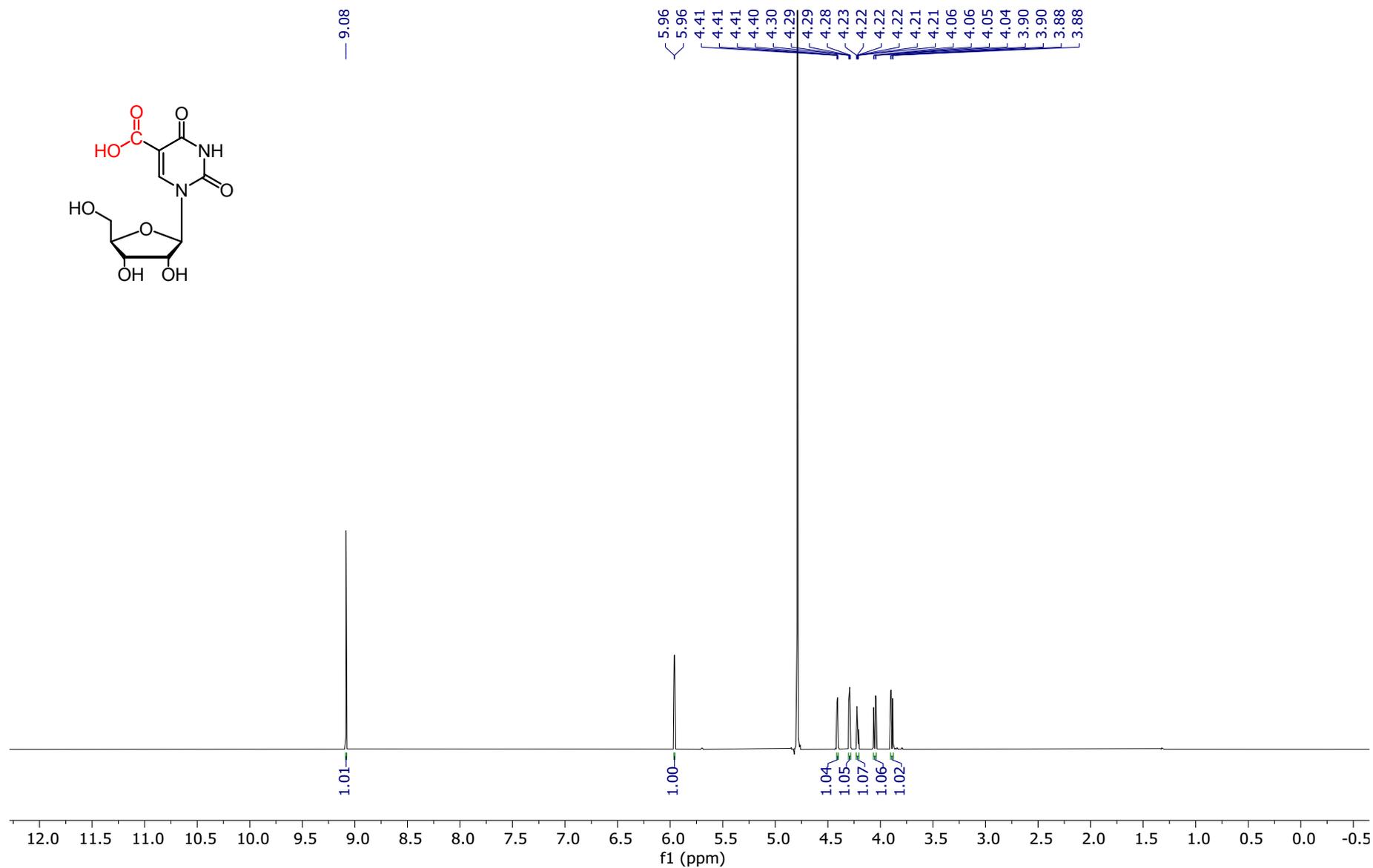
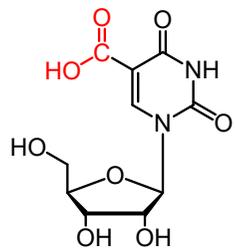


Figure S7. ¹H NMR spectrum of **3a** (700 MHz, D₂O).



166.08
164.33

150.43
149.20

103.22

90.65

83.95

74.36

68.47

59.66

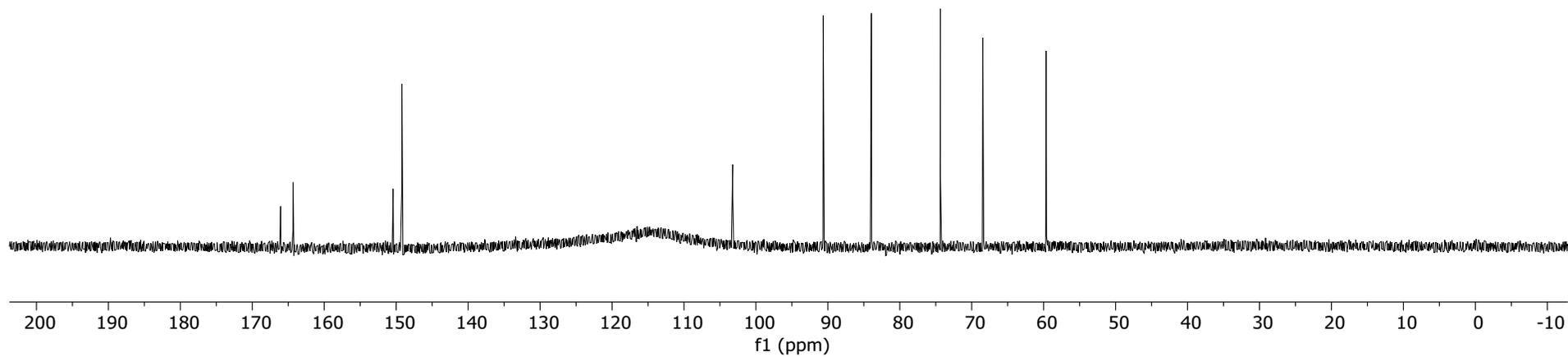


Figure S8. ^{13}C NMR spectrum of **3a** (176 MHz, D_2O)

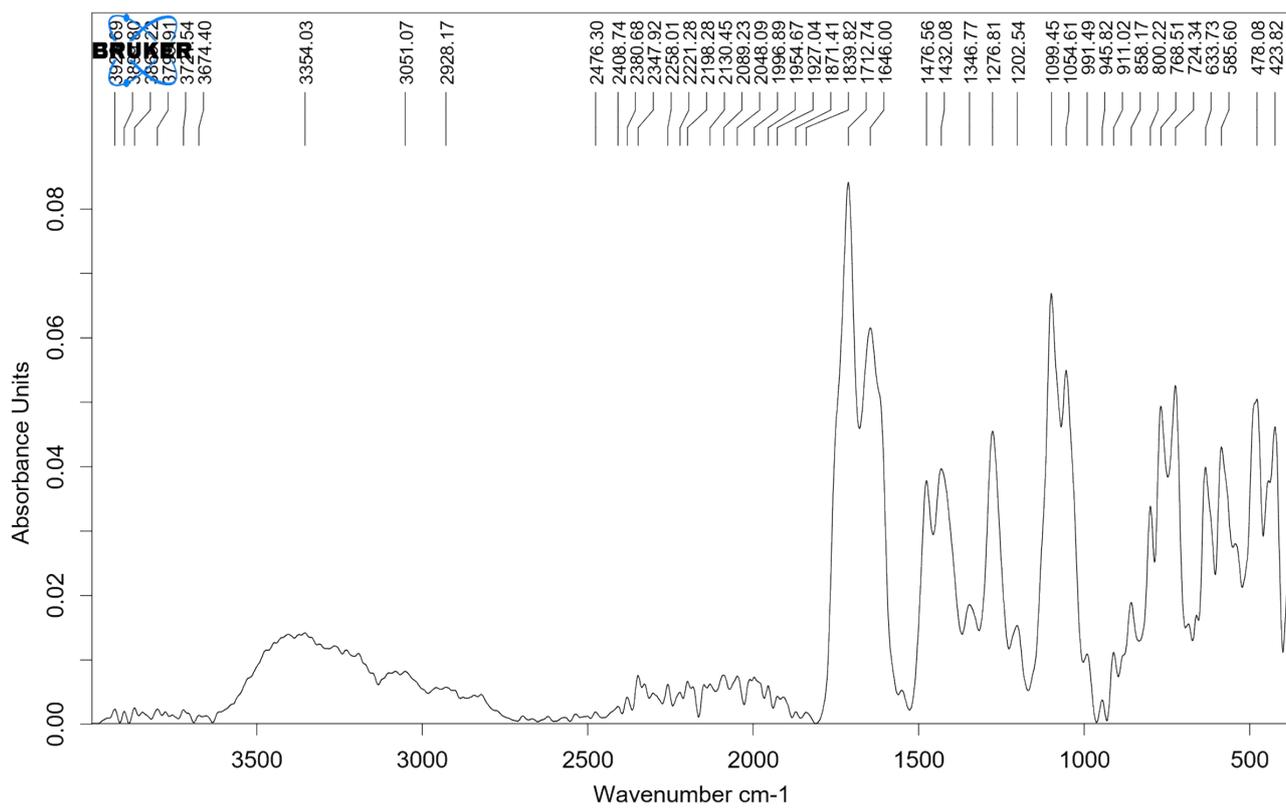


Figure S9. IR spectrum of 5-carboxyuridine (**3a**).

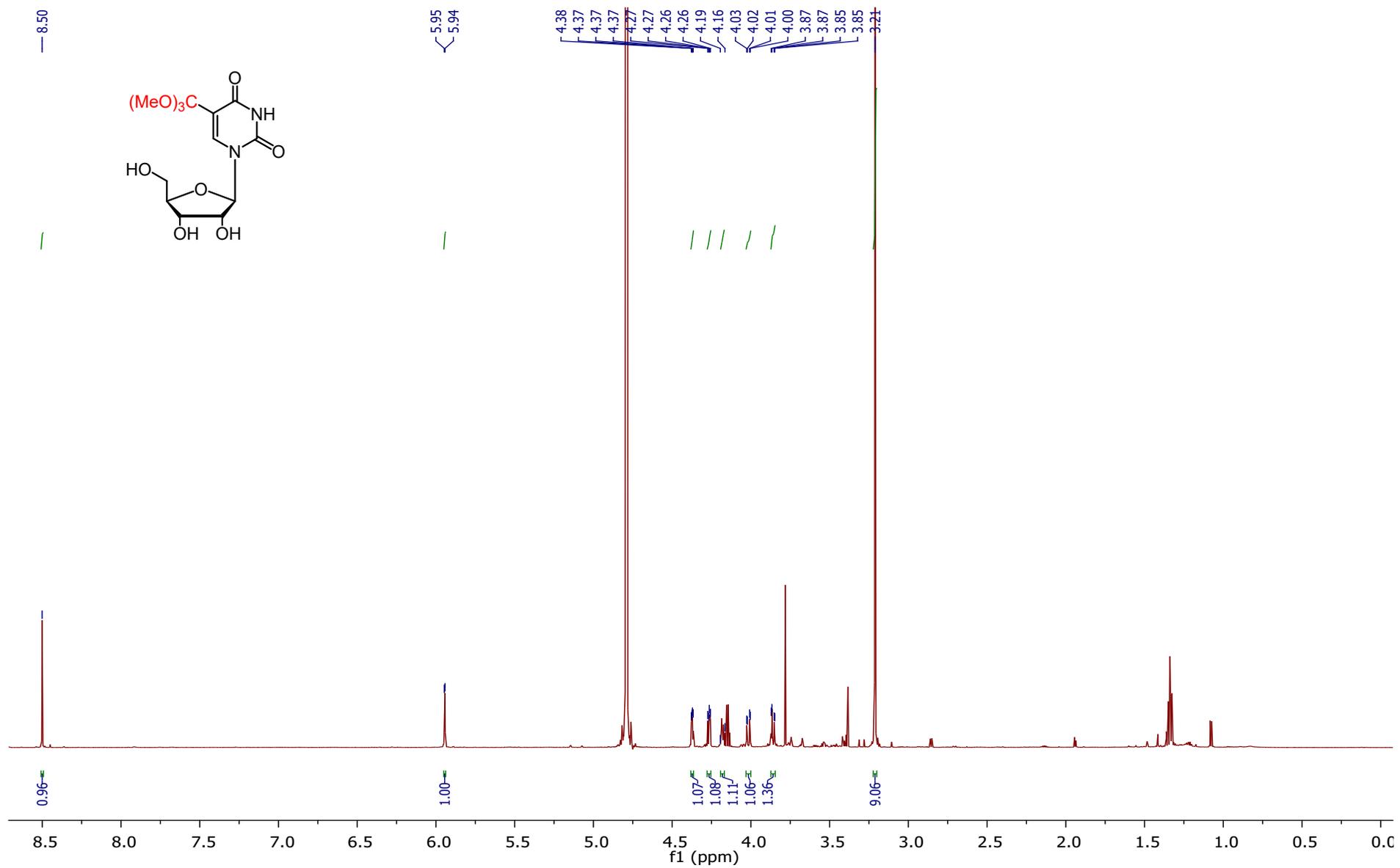


Figure S10. ¹H NMR spectrum of 5-(trimethoxymethyl)uridine (700 MHz, D₂O).

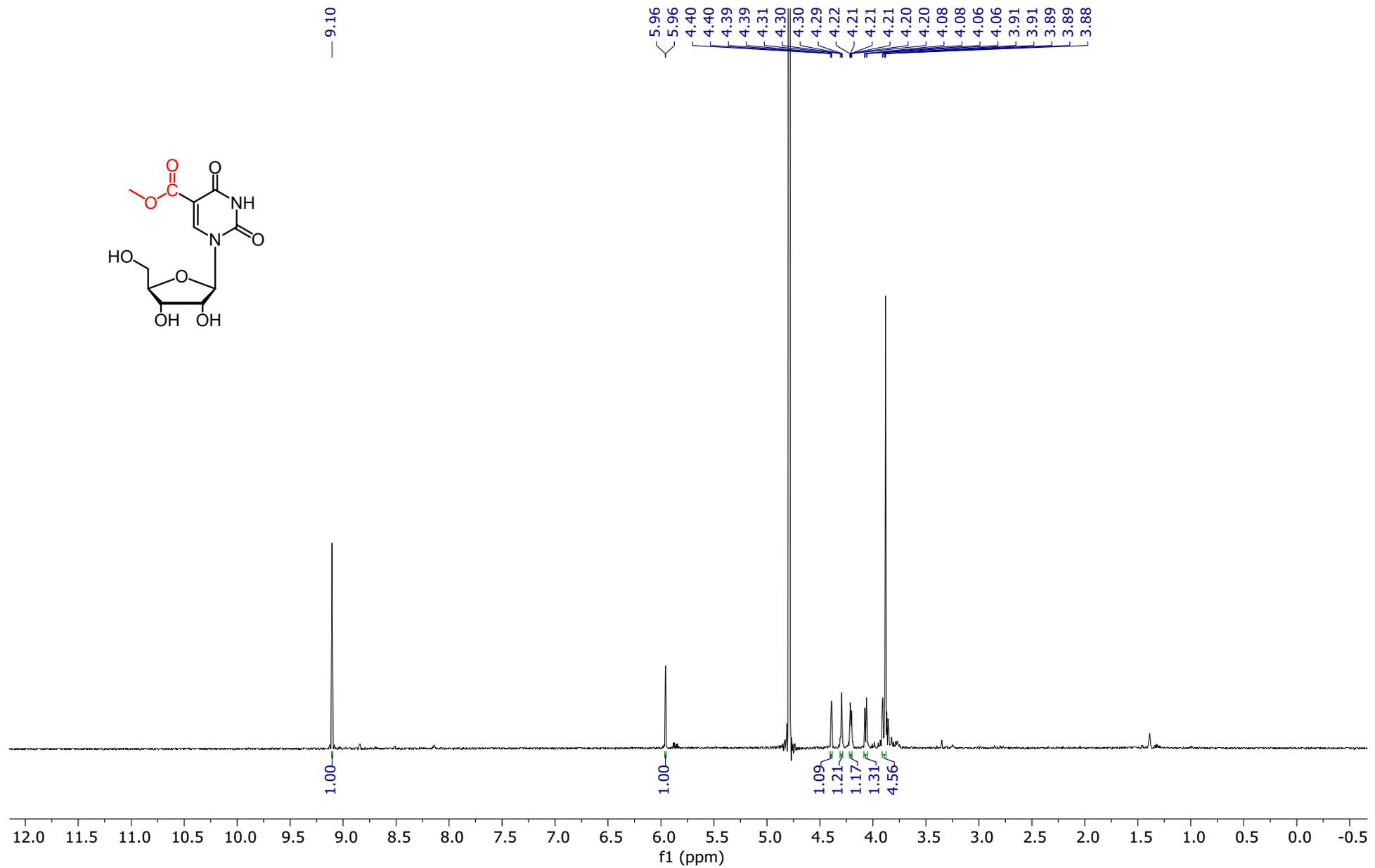
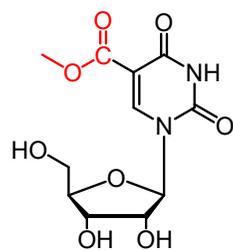


Figure S11. ¹H NMR spectrum of **4a** (700 MHz, D₂O).



— 164.73
— 162.15

— 150.61
— 149.13

— 104.17

— 90.58

— 83.78

— 74.39

— 68.35

— 59.48

— 52.43

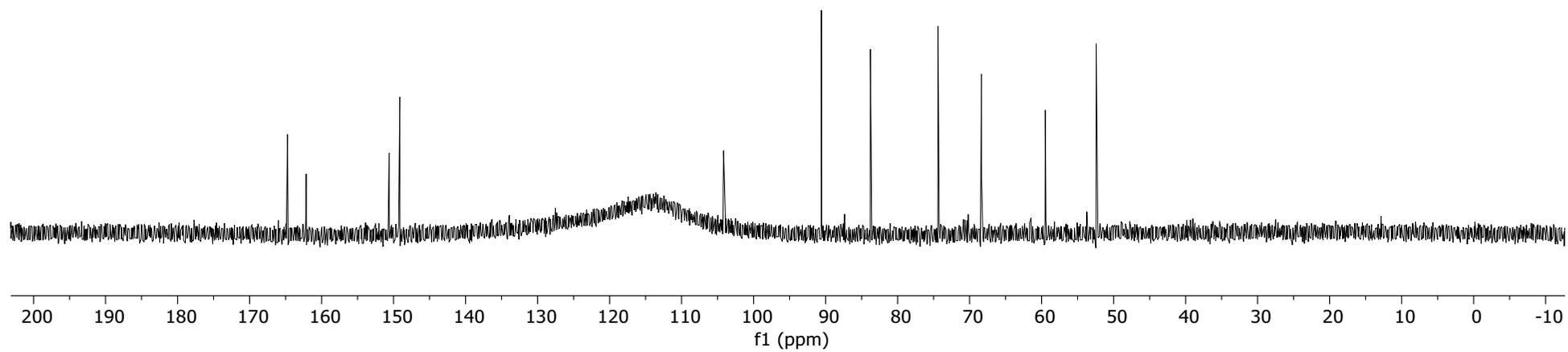


Figure S12. ¹³C NMR spectrum of 4a (176 MHz, D₂O).

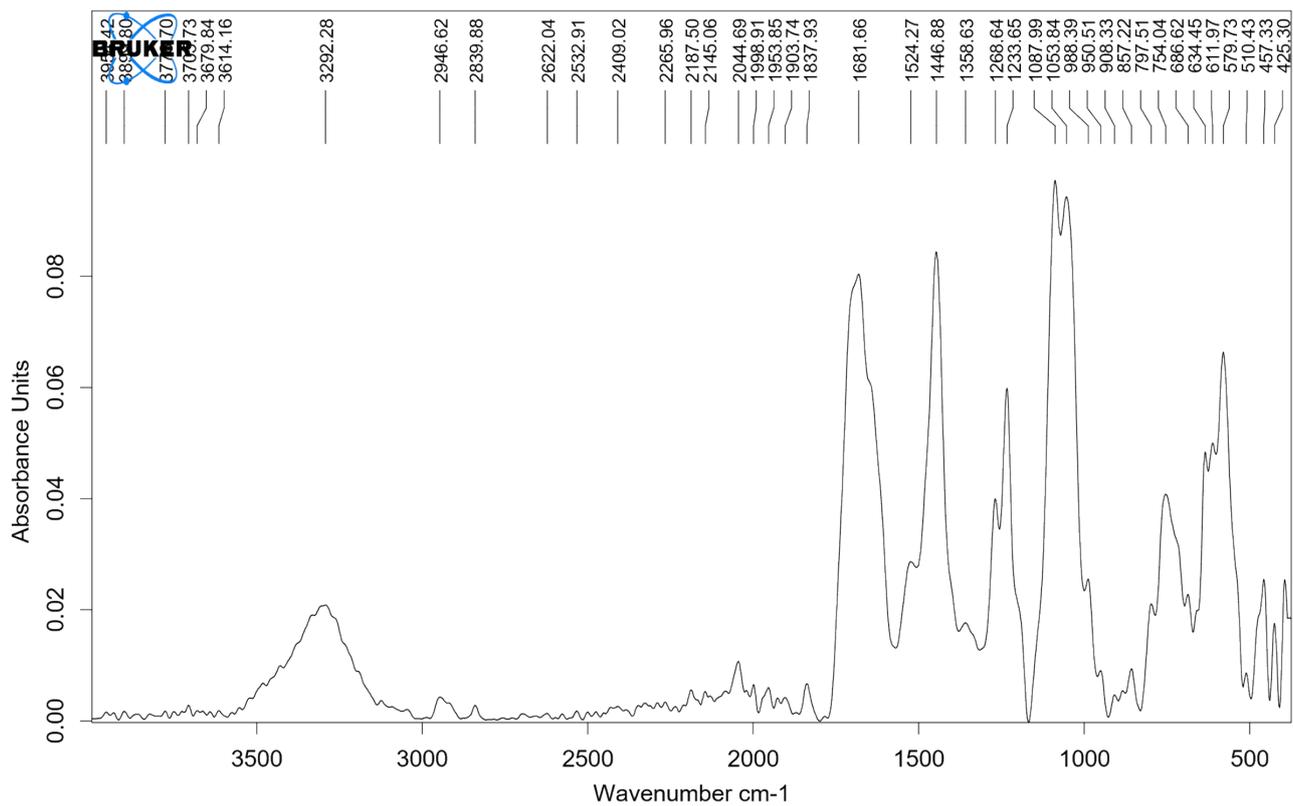


Figure S13. IR spectrum of 5-methoxycarbonyluridine (**4a**).

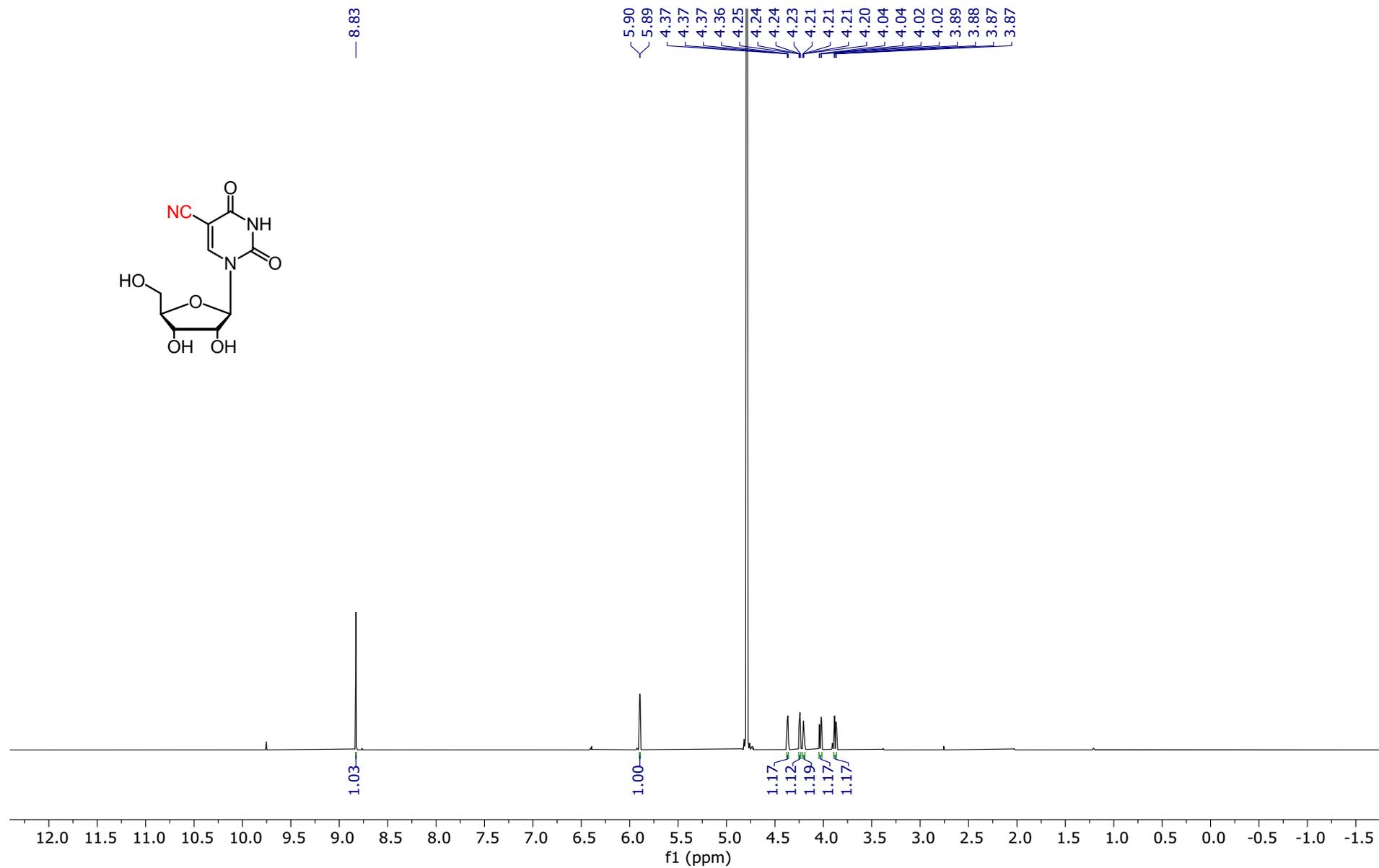


Figure S14. ¹H NMR spectrum of 5a (700 MHz, D₂O).

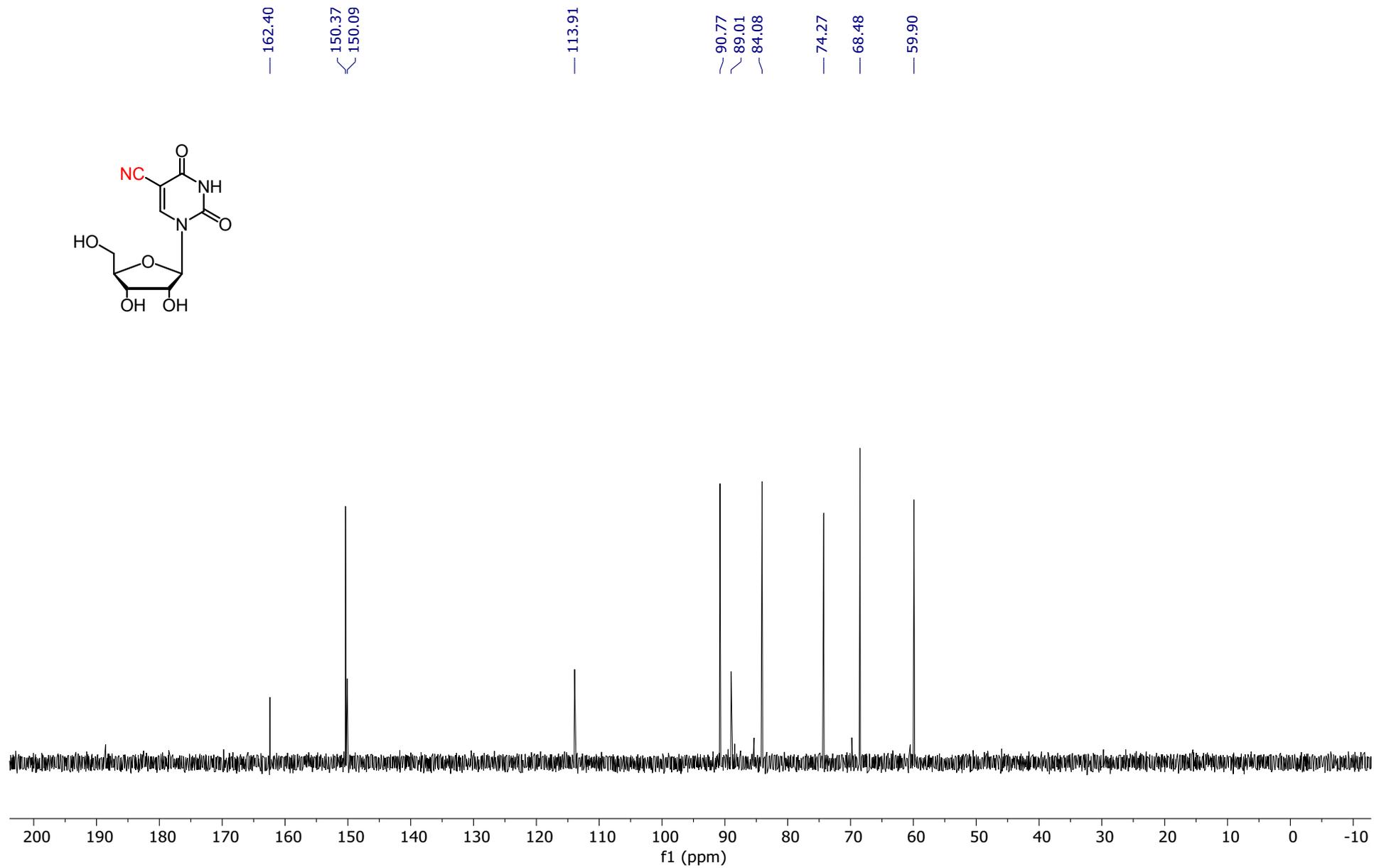


Figure S15. ^{13}C NMR spectrum of **5a** (176 MHz, D_2O).

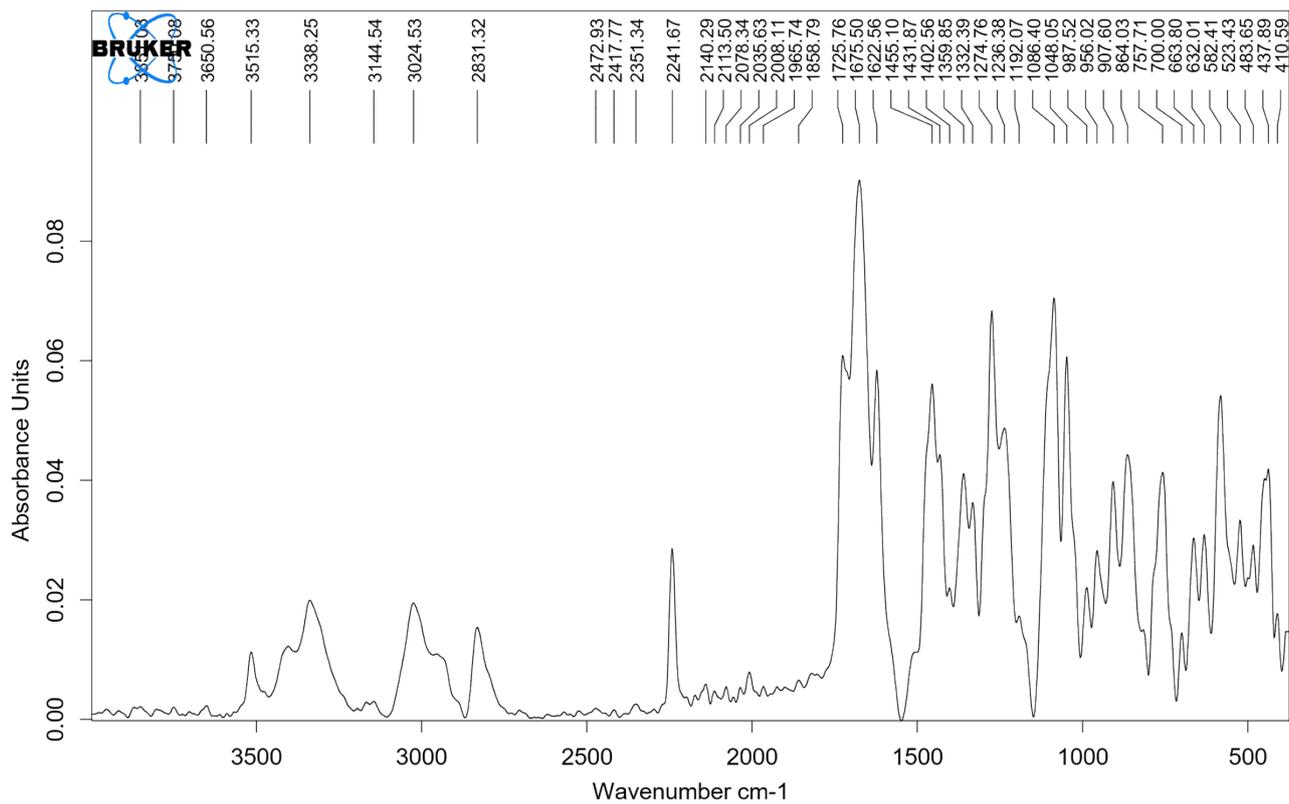


Figure S16. IR spectrum of 5-cyanouridine (**5a**).

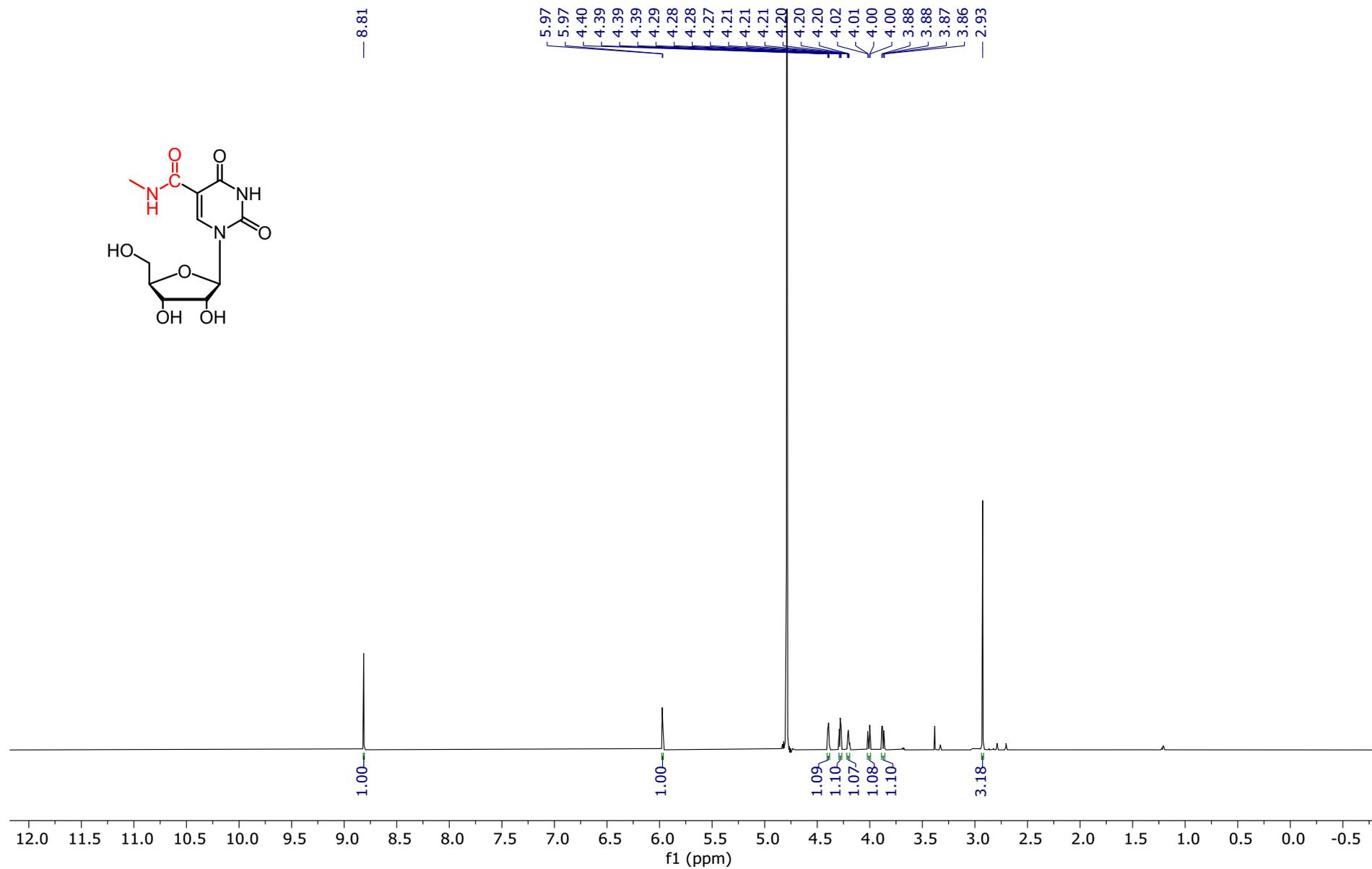


Figure S17. ¹H NMR spectrum of **6a** (700 MHz, D₂O).

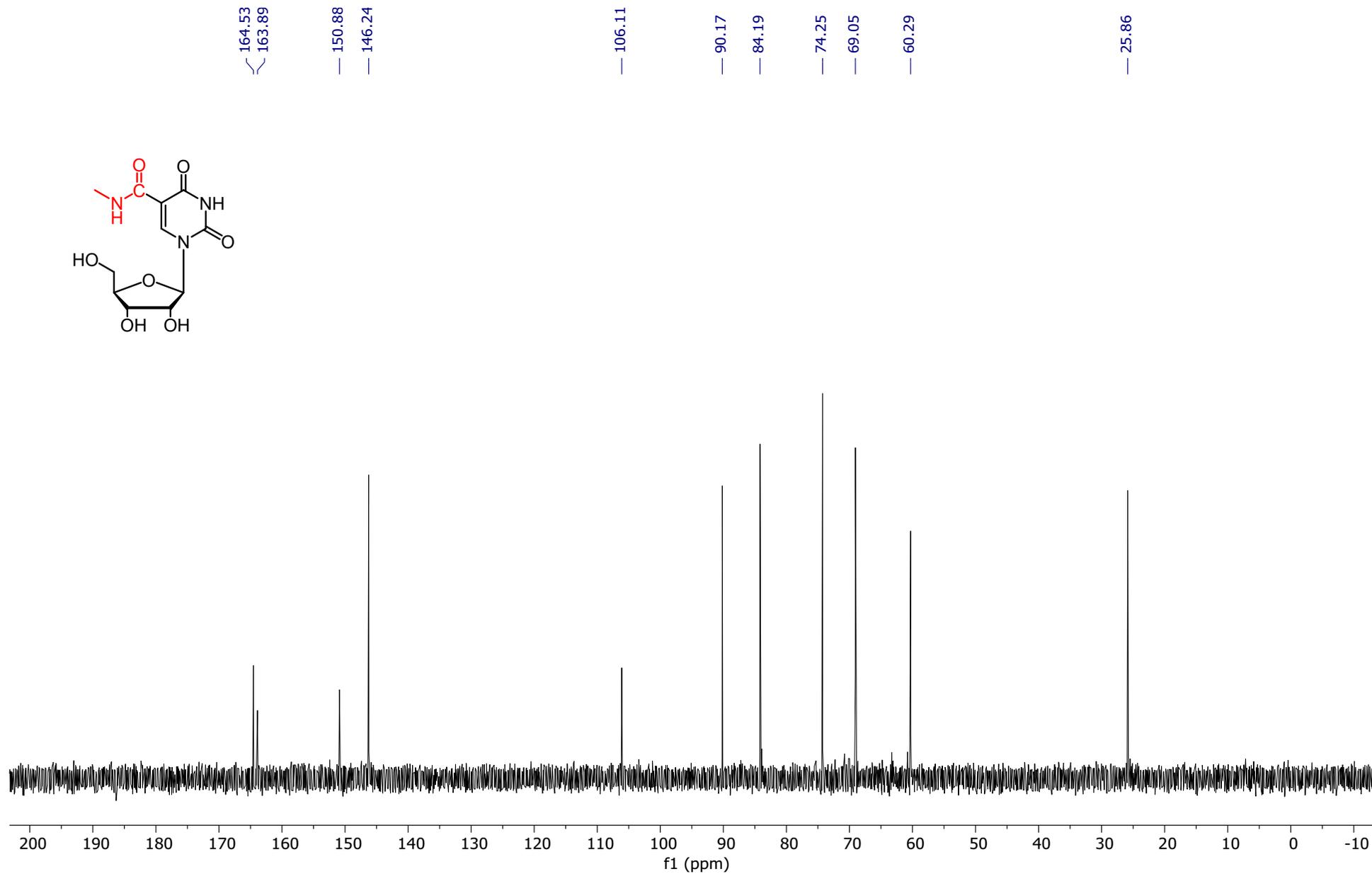


Figure S18. ¹³C NMR spectrum of **6a** (176 MHz, D₂O).

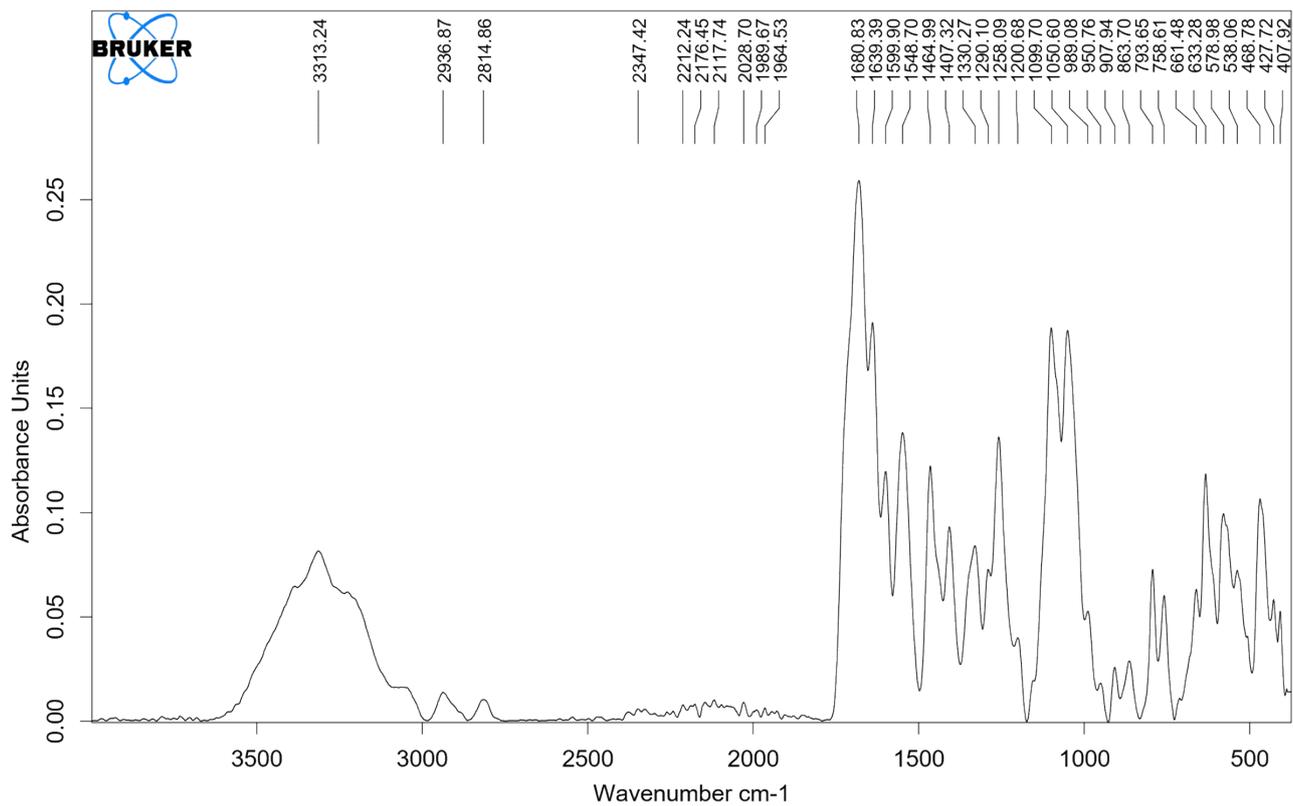


Figure S19. IR spectrum of 5-*N*-methylcarbamoyluridine (**6a**).

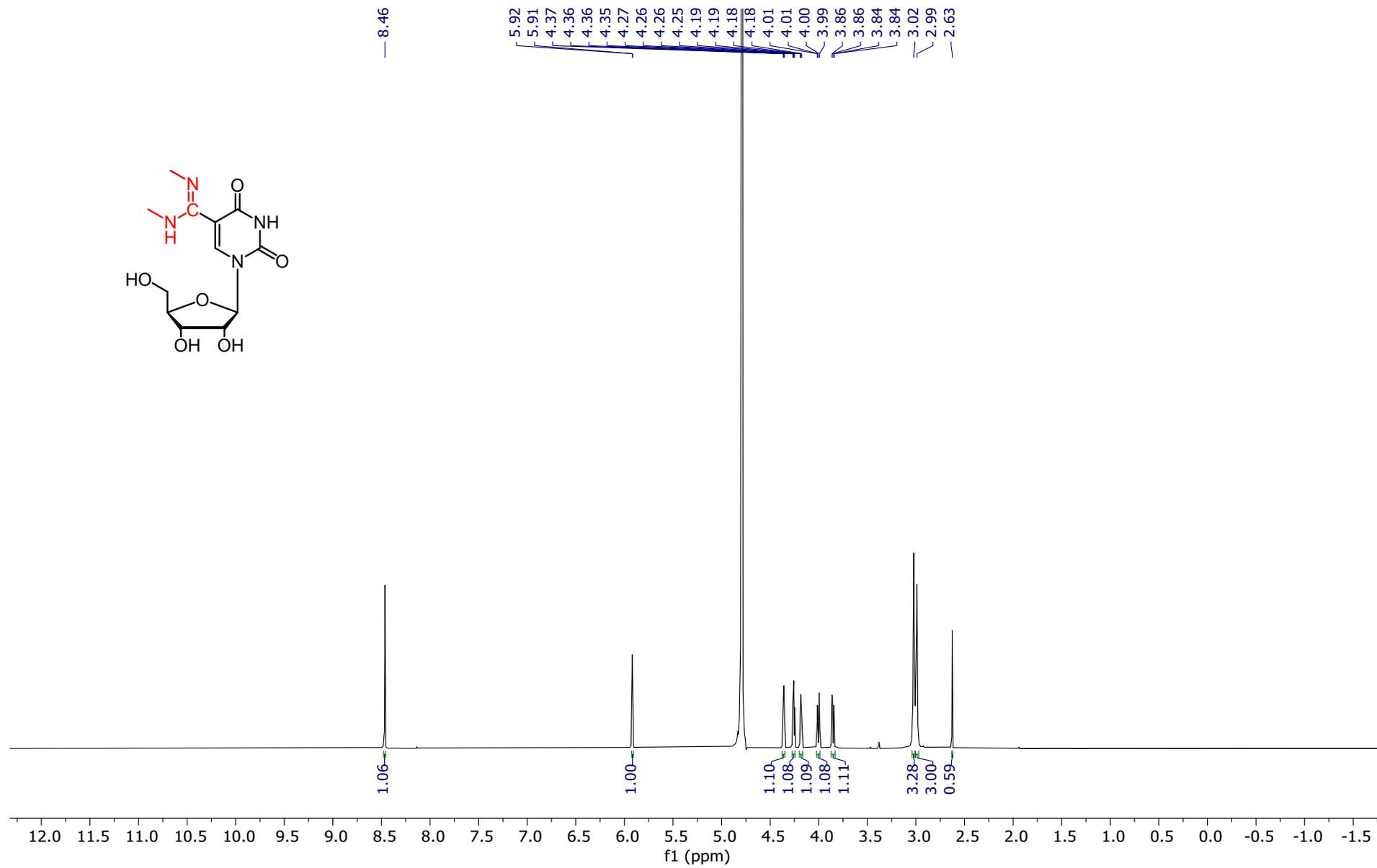


Figure S20. ¹H NMR spectrum of **7a** (700 MHz, D₂O).

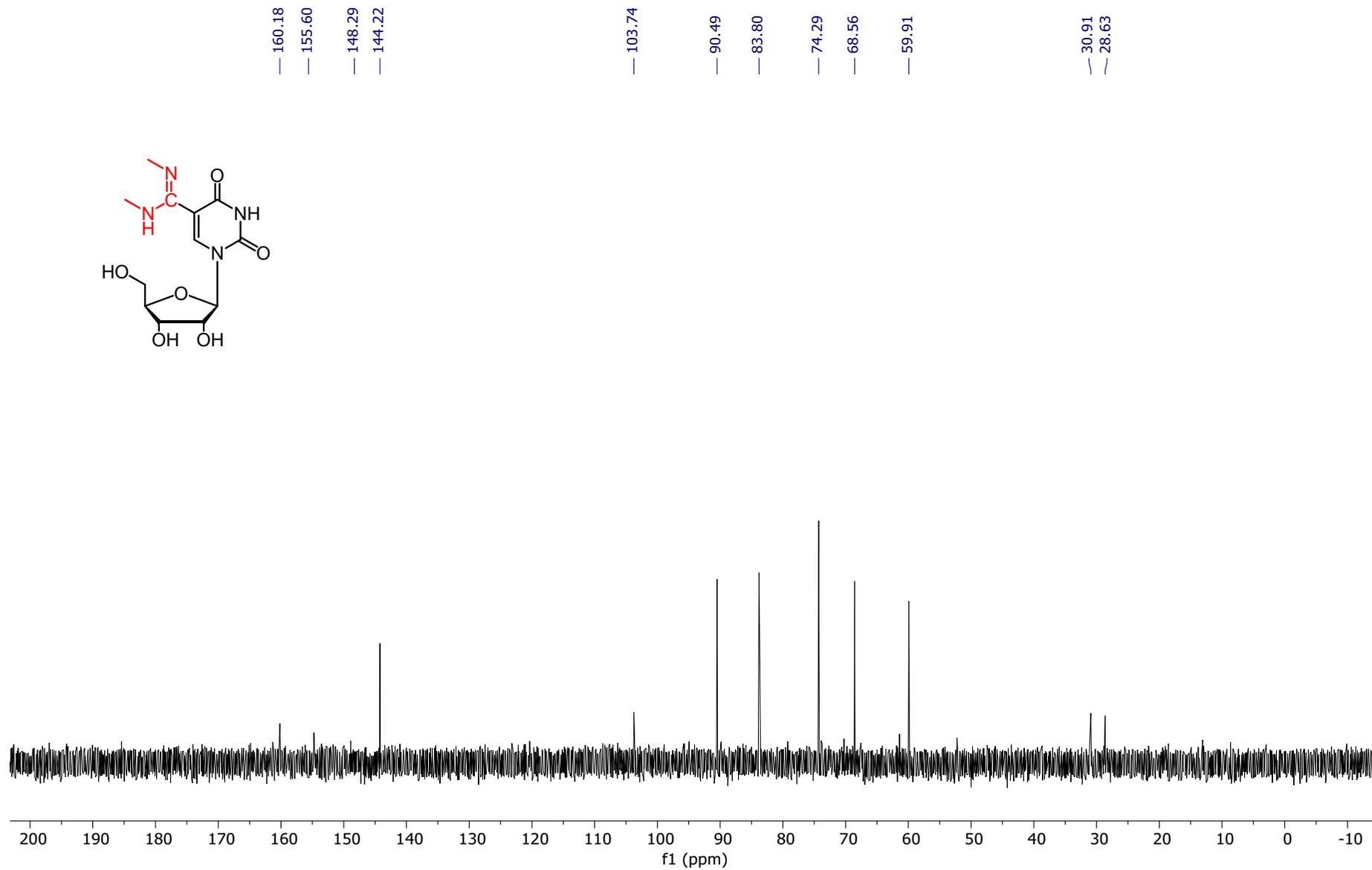


Figure S21. ¹³C NMR spectrum of **7a** (176 MHz, D₂O).

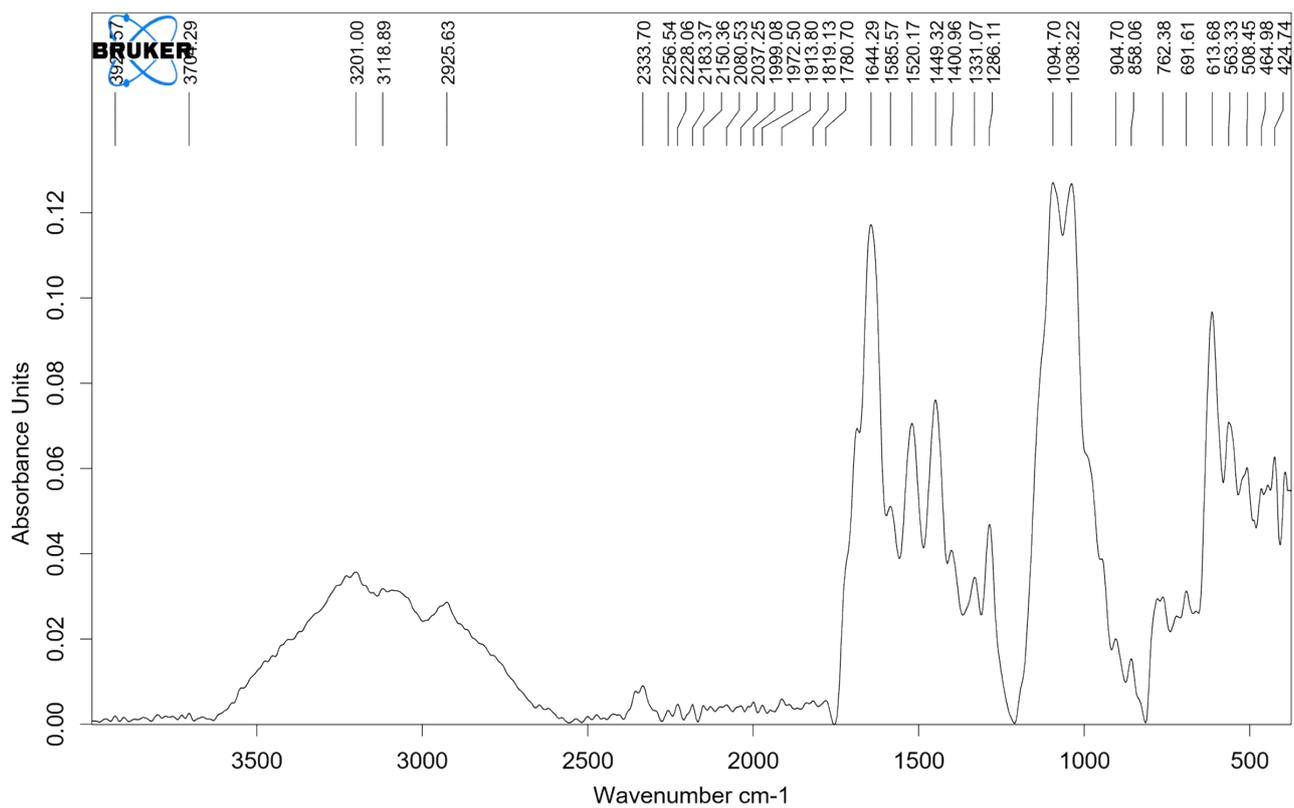


Figure S22. IR spectrum of 5-(*N,N'*-dimethylamidinyl)uridine (**7a**).

1.3. IR and NMR spectra of cytidine derivatives 3b-6b

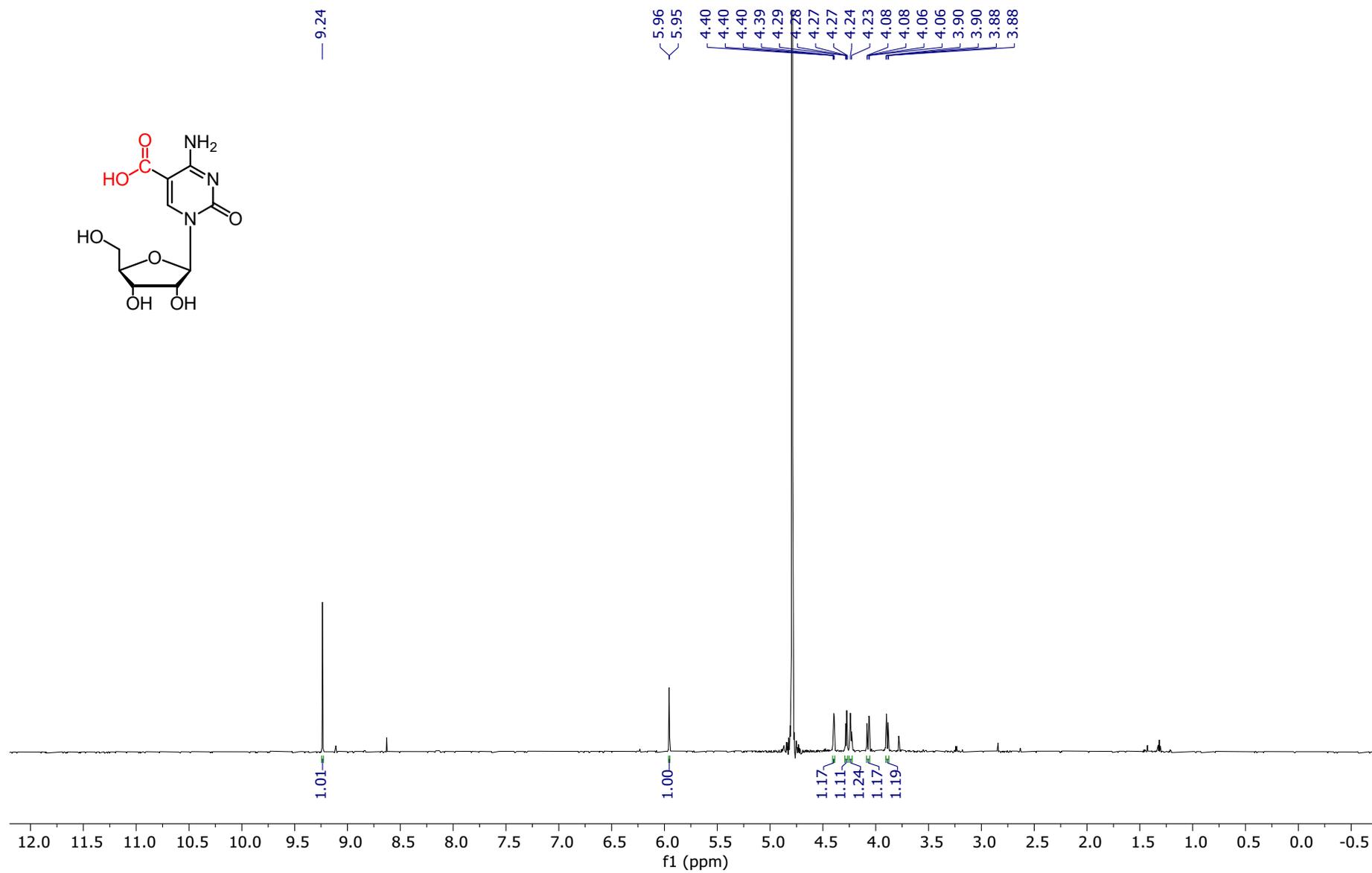


Figure S23. ¹H NMR spectrum of **3b** (700 MHz, D₂O).

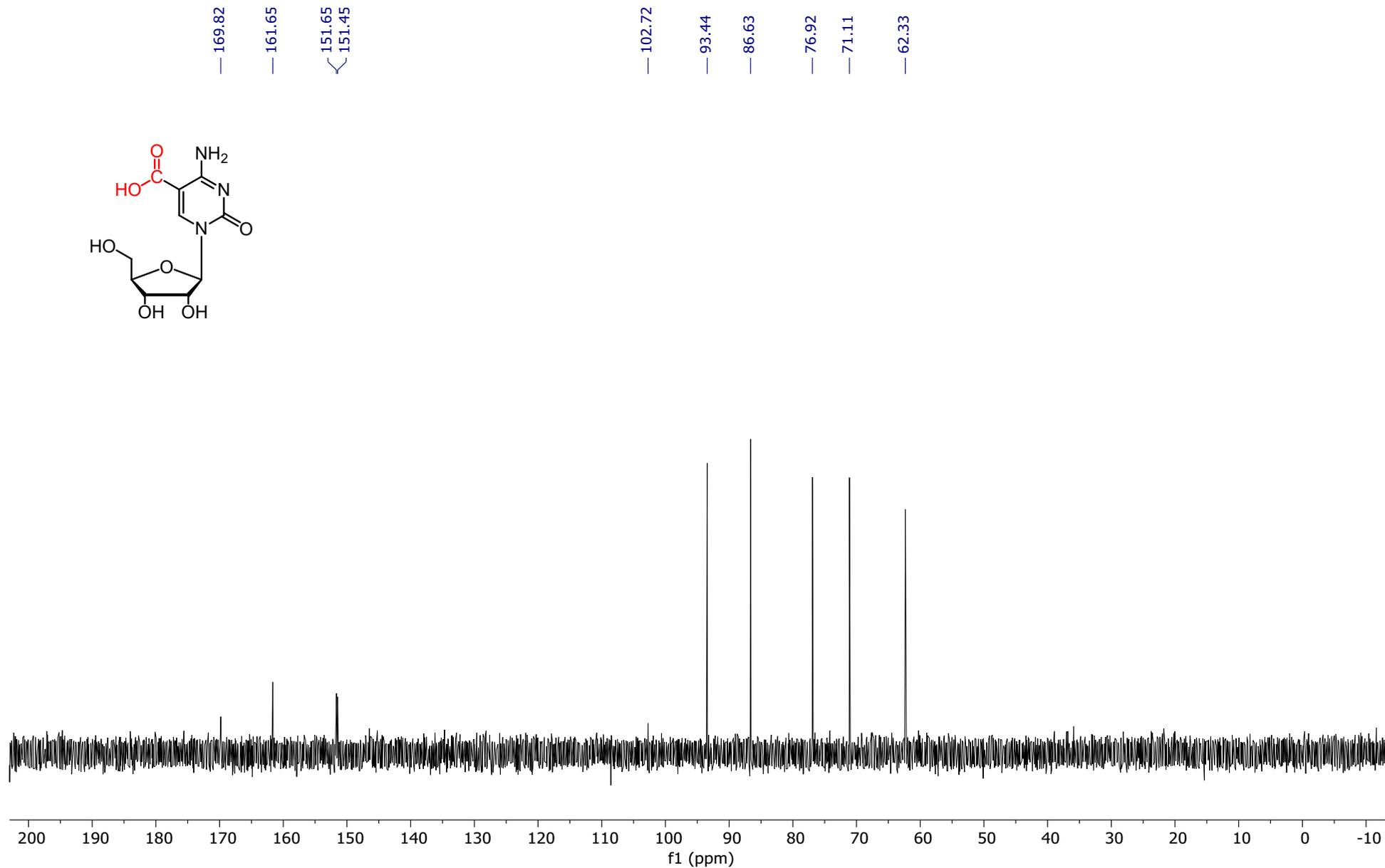


Figure S24. ^{13}C NMR spectrum of **3b** (176 MHz, D_2O).

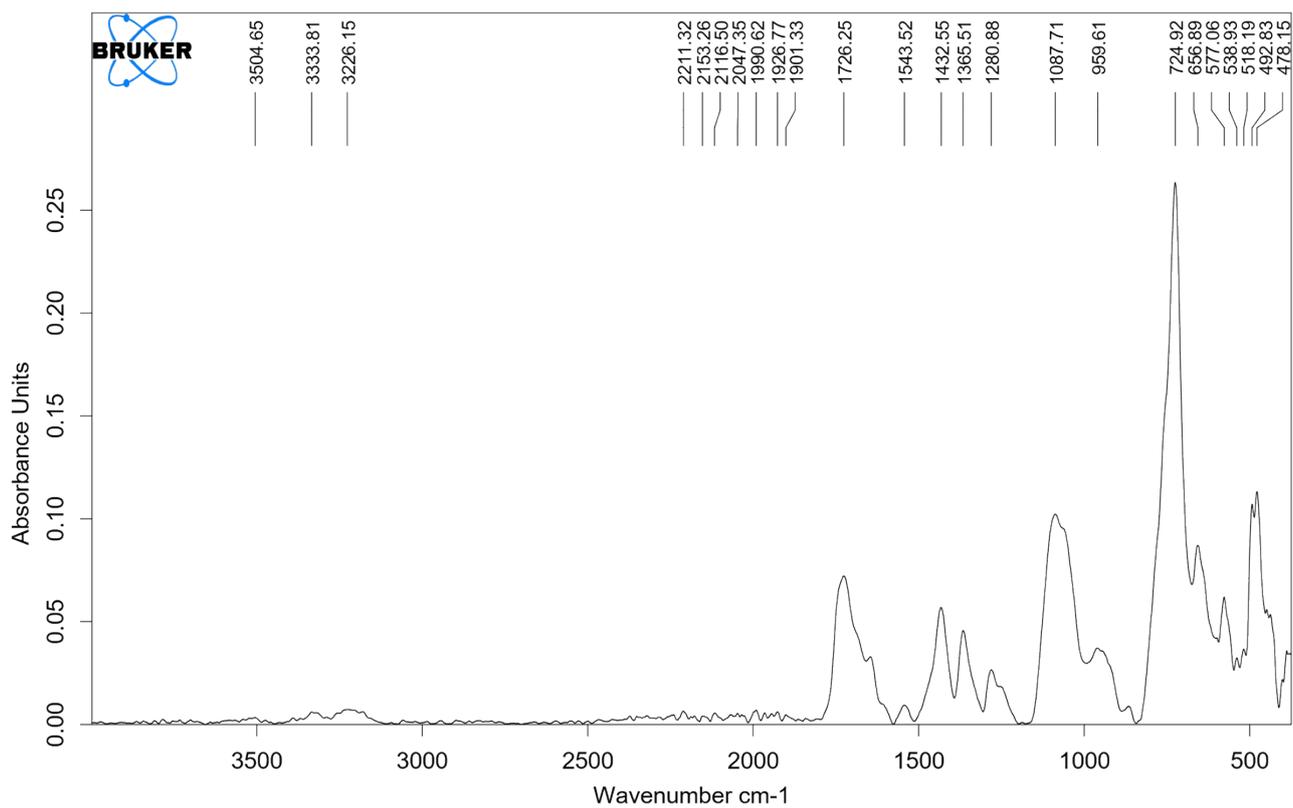


Figure S25. IR spectrum of 5-carboxycytidine (**3b**).

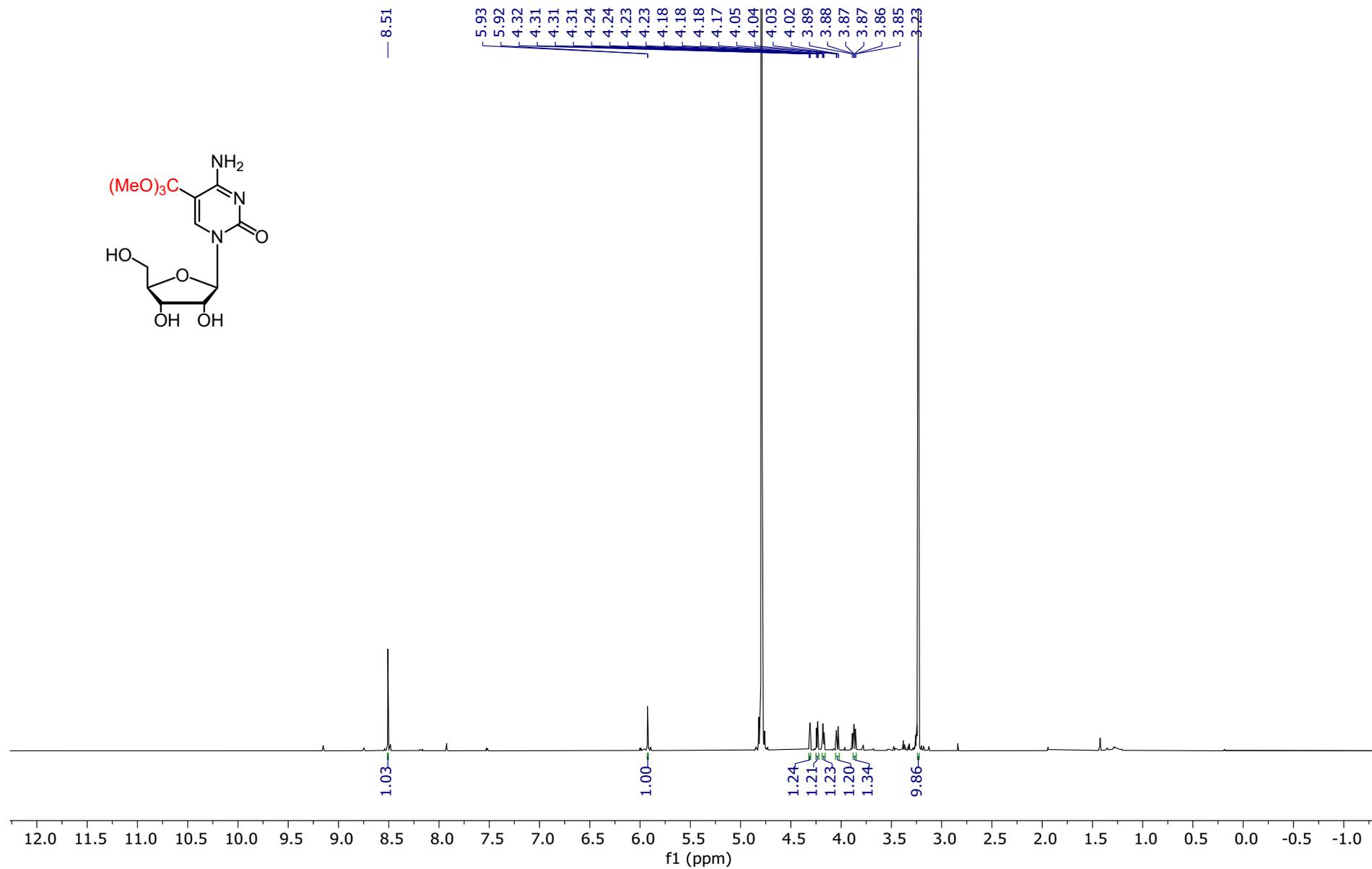


Figure S26. ^1H NMR spectrum of 5-(trimethoxymethyl)cytidine (700 MHz, D_2O).

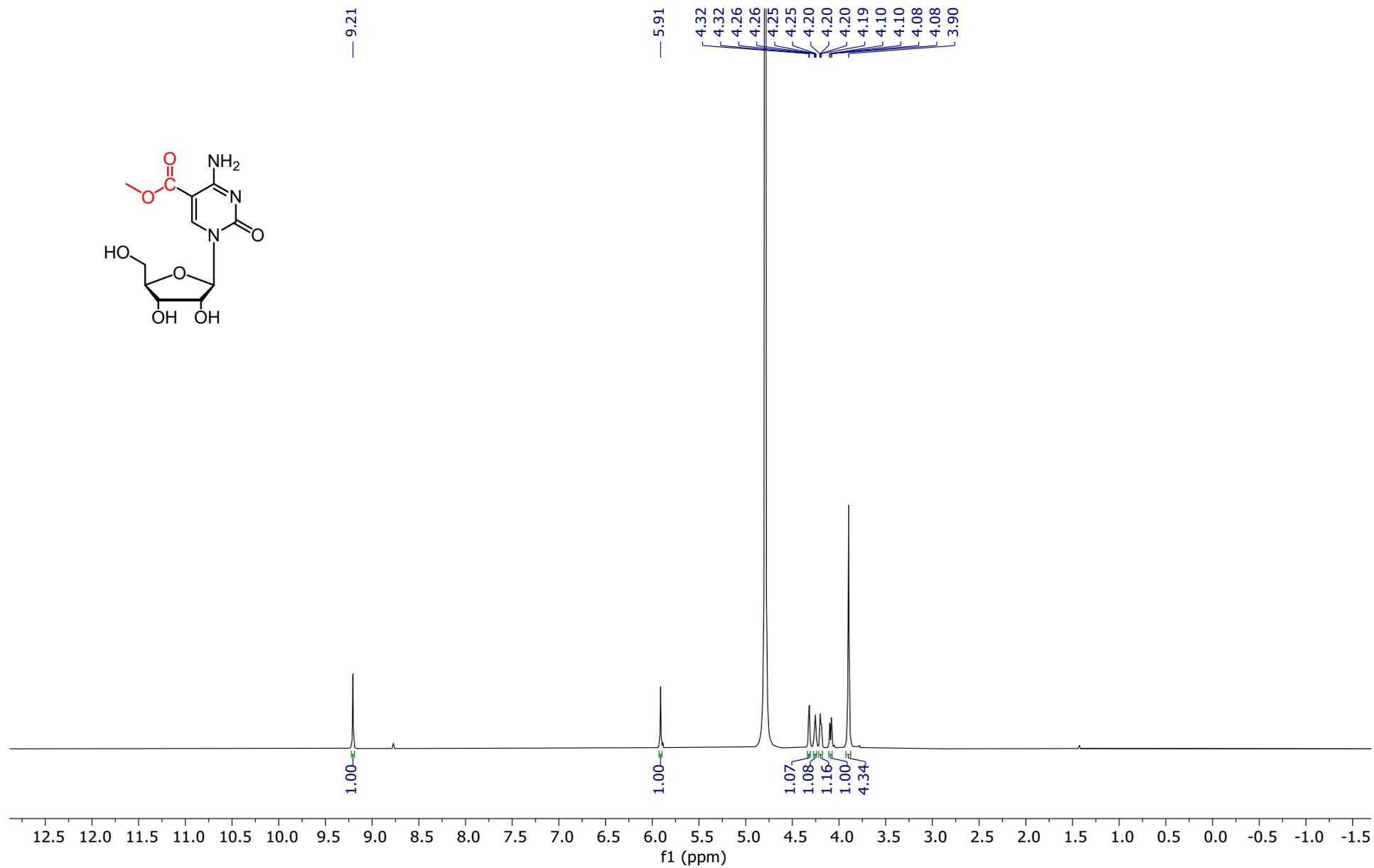


Figure S27. ¹H NMR spectrum of **4b** (700 MHz, D₂O).

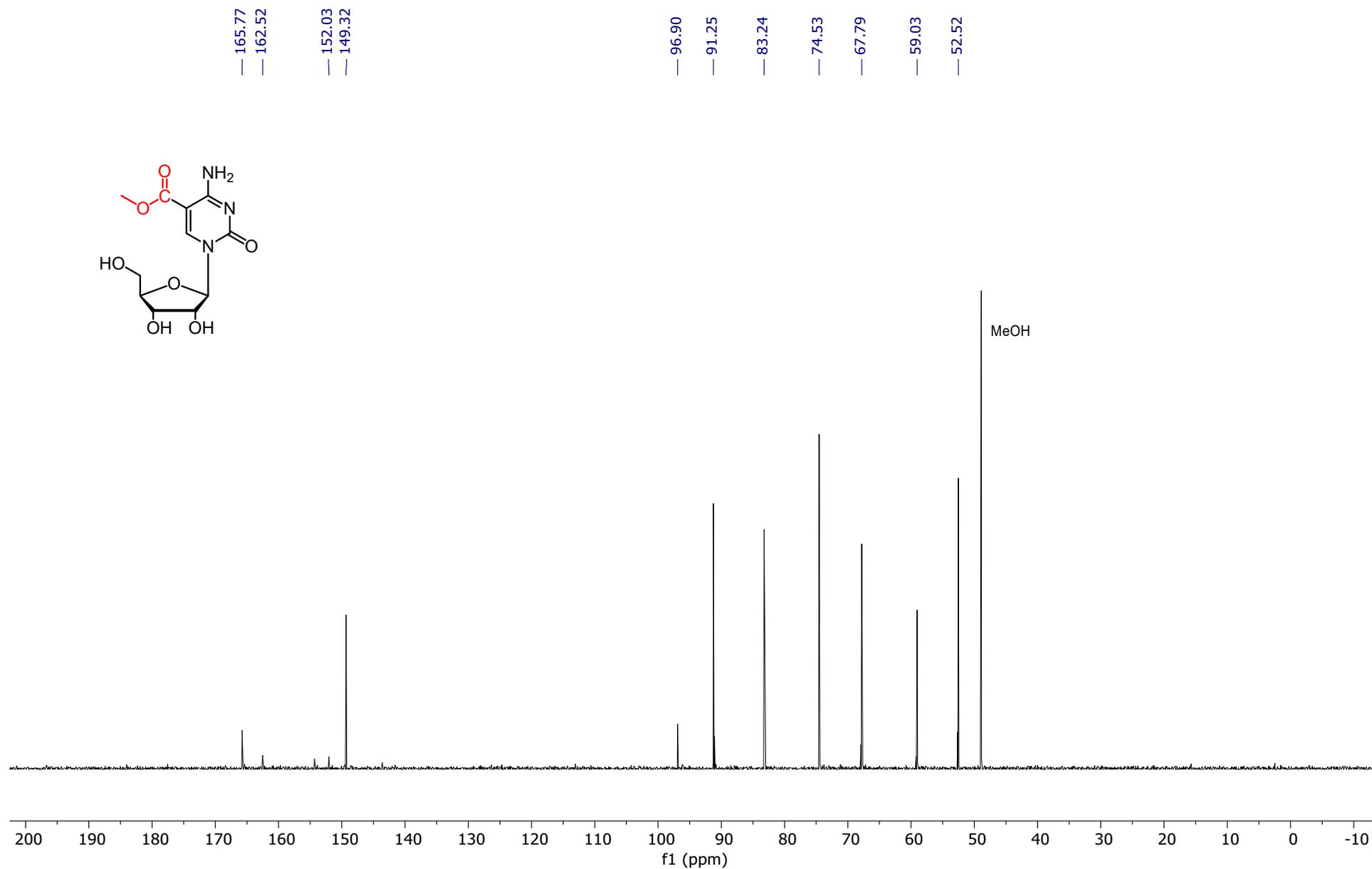


Figure S28. ¹³C NMR spectrum of **4b** (176 MHz, D₂O).

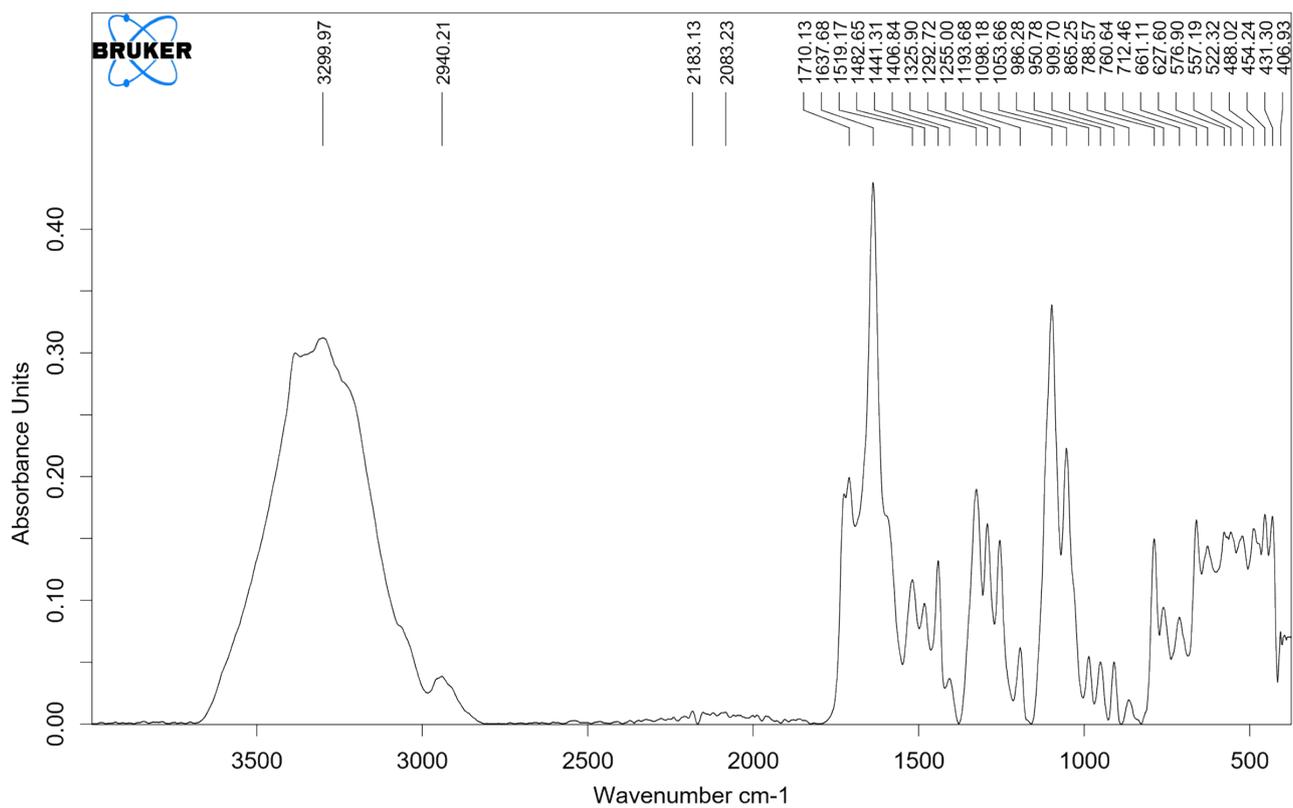


Figure S29. IR spectrum of 5-methoxycarbonylcytidine (**4b**).

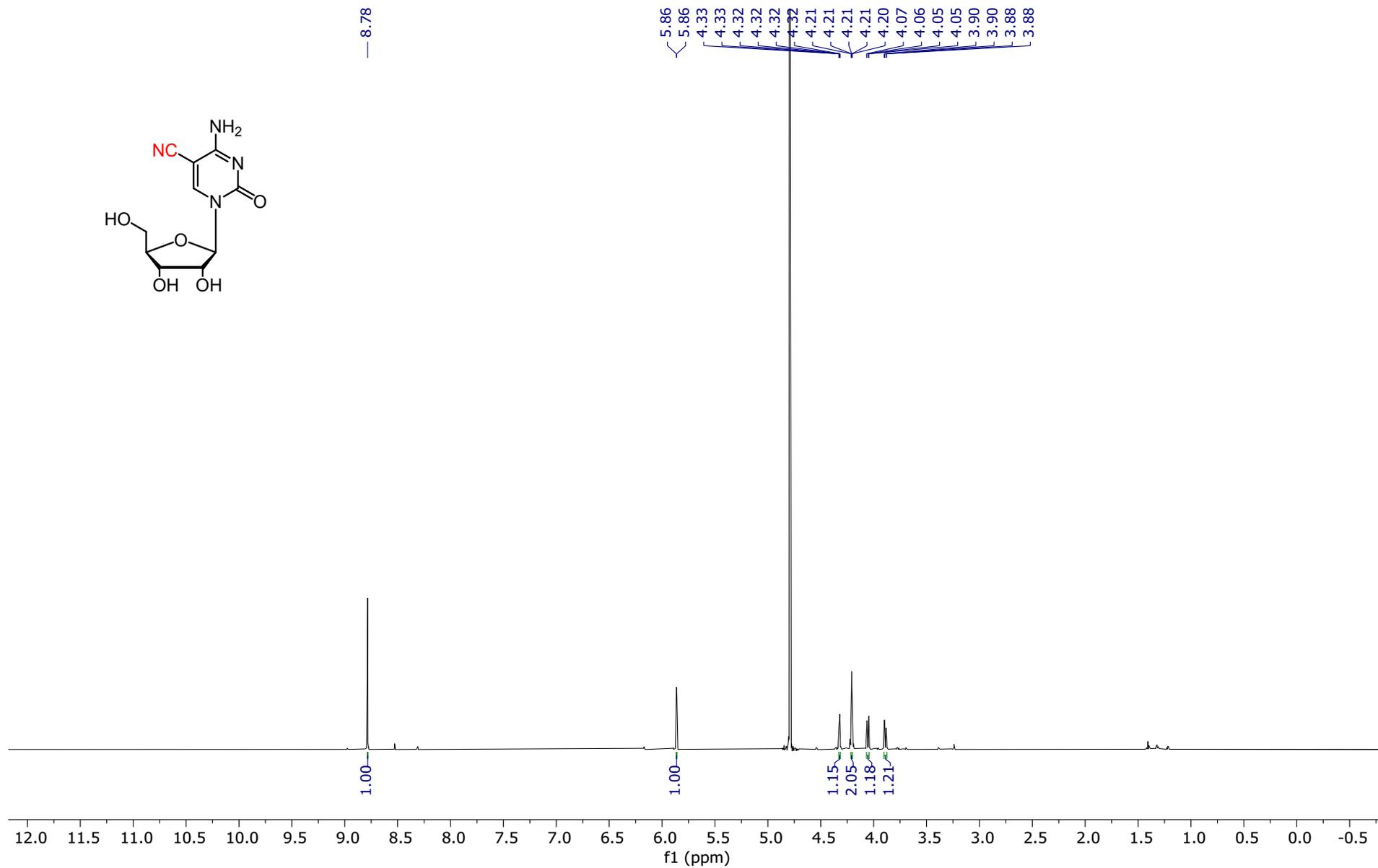


Figure S30. ¹H NMR spectrum of **5b** (700 MHz, D₂O).

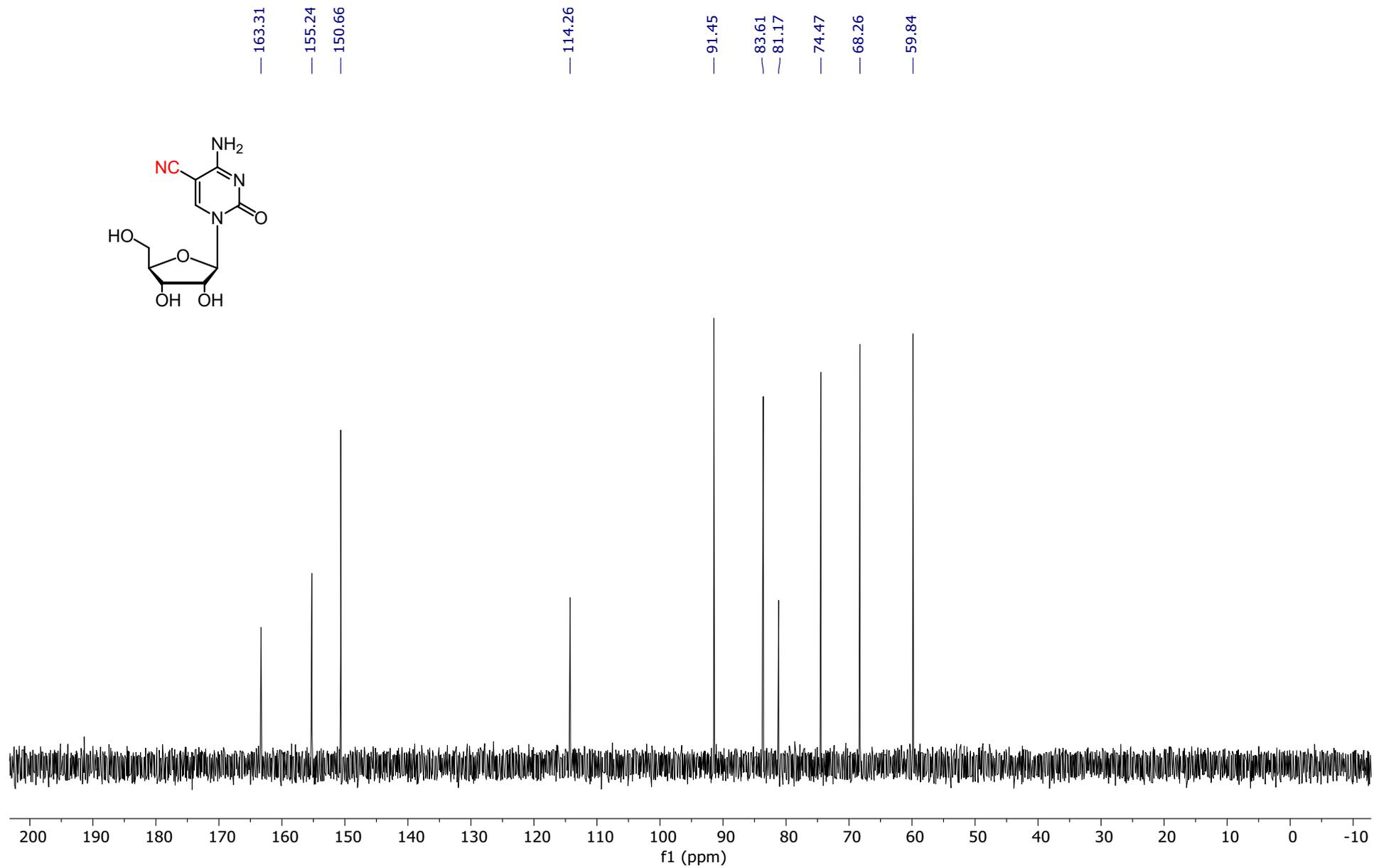


Figure S31. ¹³C NMR spectrum of **5b** (176 MHz, D₂O).

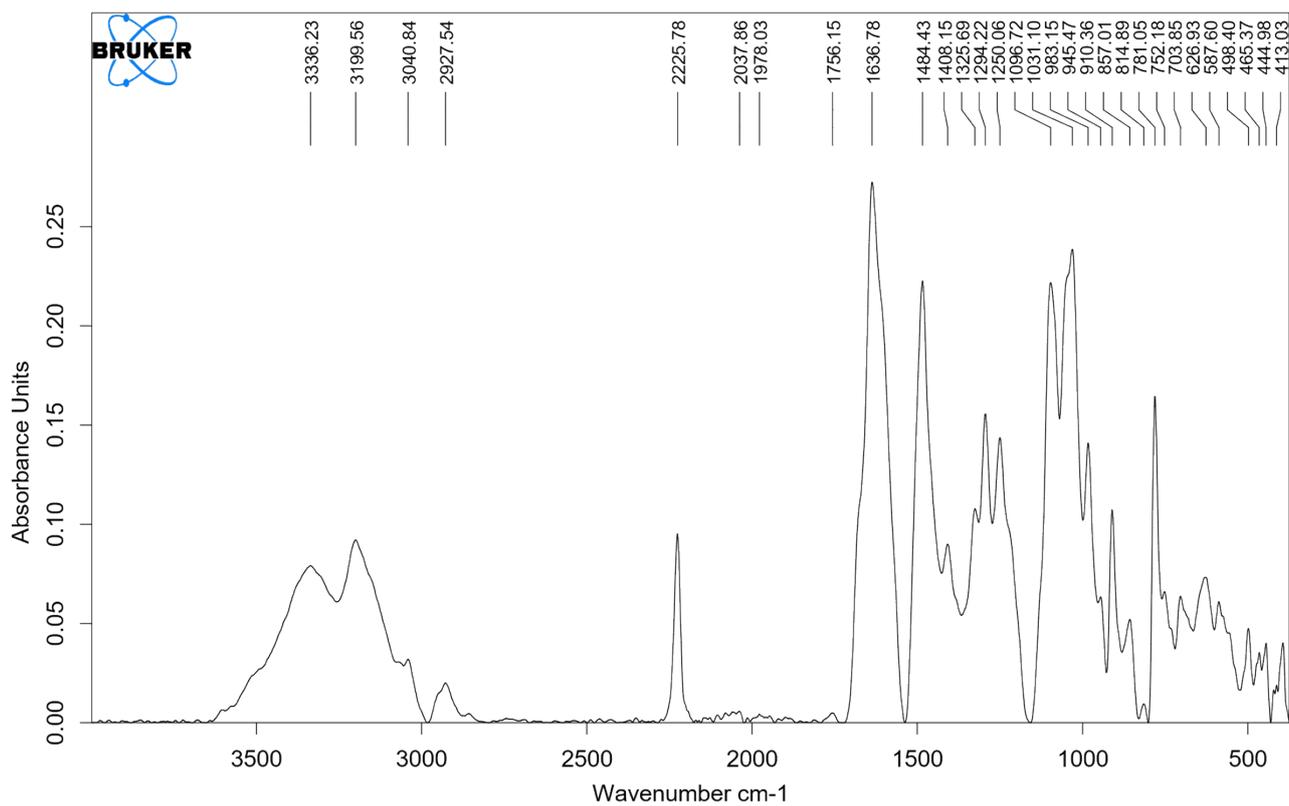


Figure S32. IR spectrum of 5-cyanocytidine (**5b**).

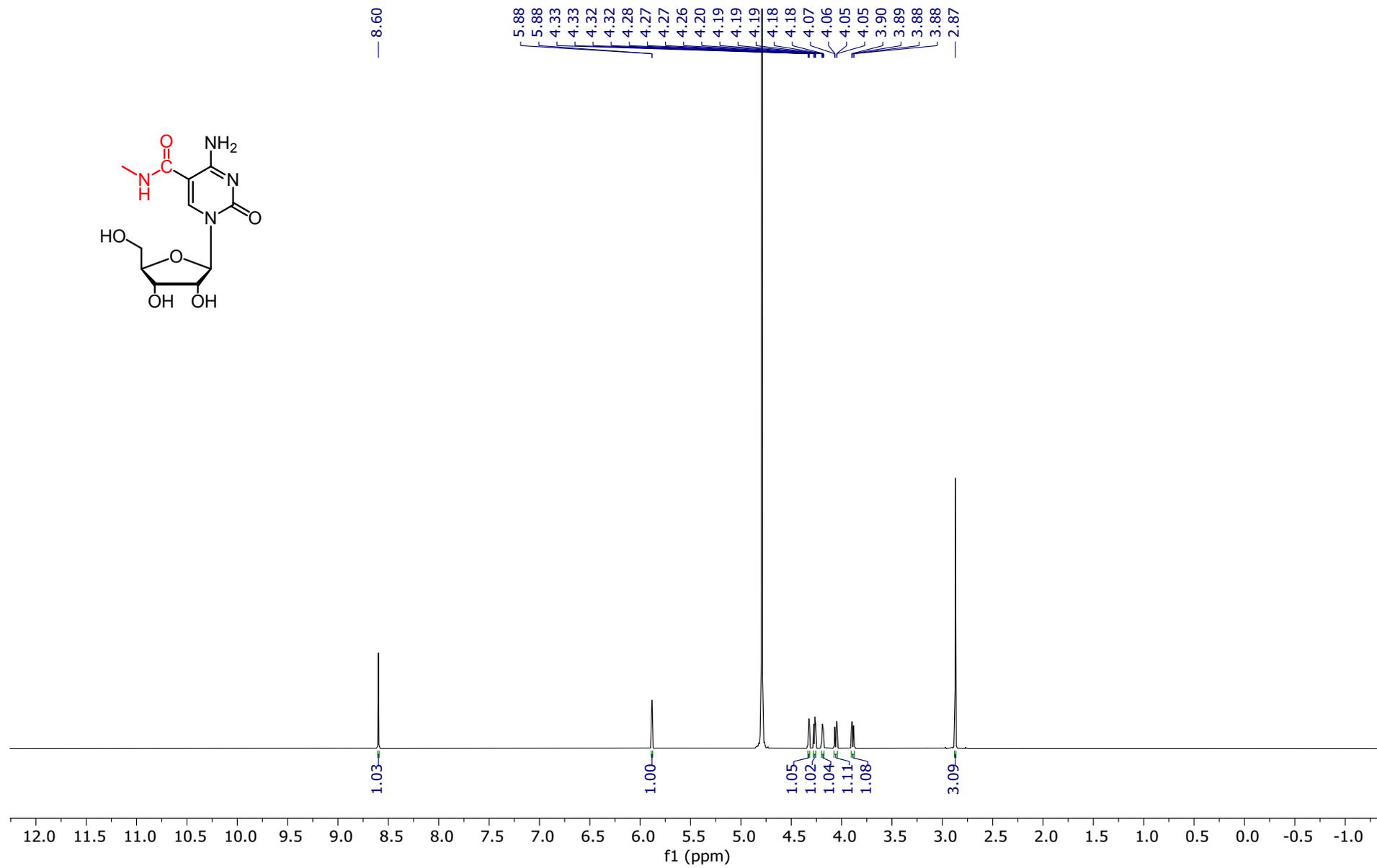


Figure S33. ¹H NMR spectrum of **6b** (700 MHz, D₂O).

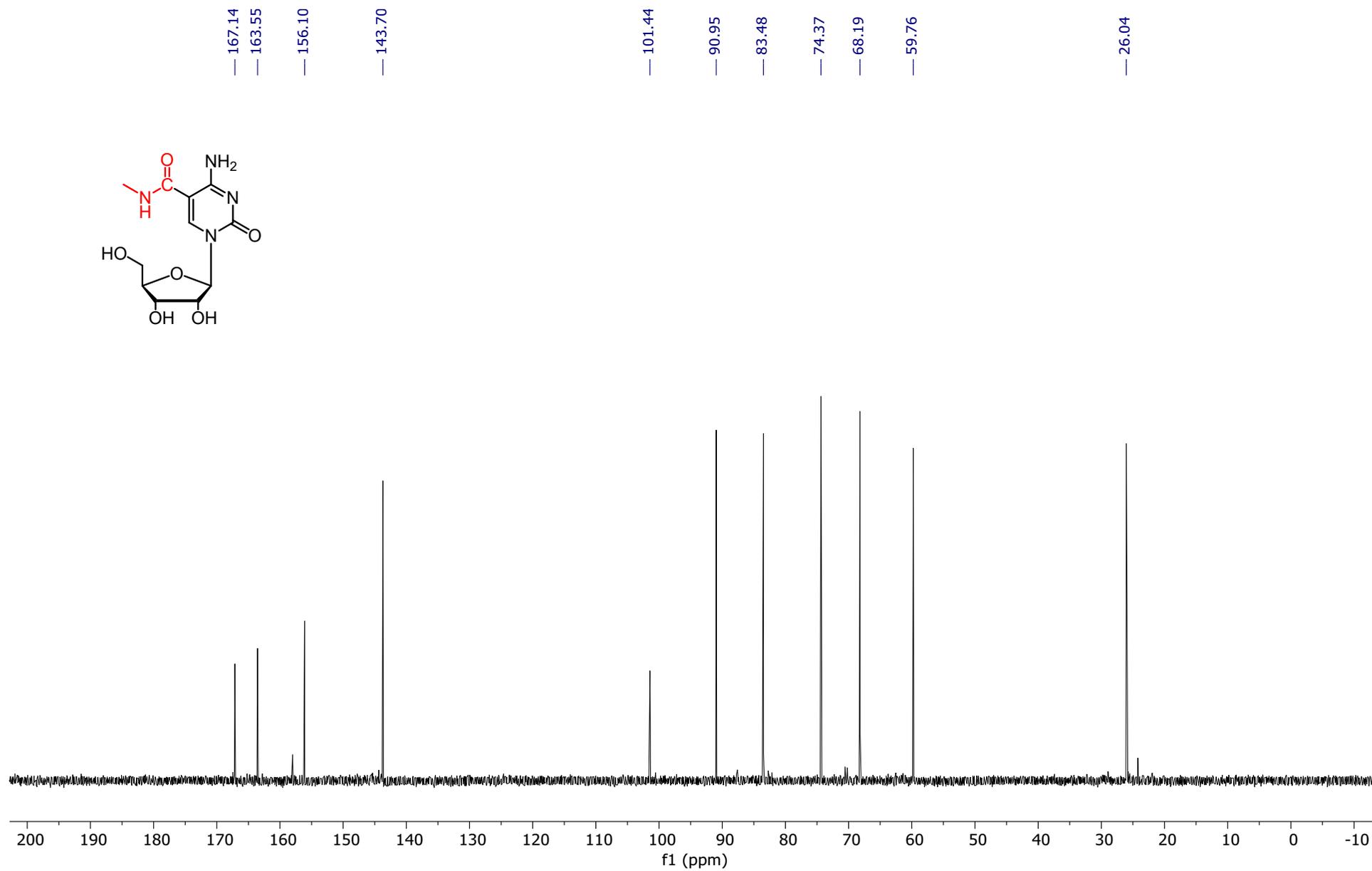


Figure S34. ^{13}C NMR spectrum of **6b** (176 MHz, D_2O).

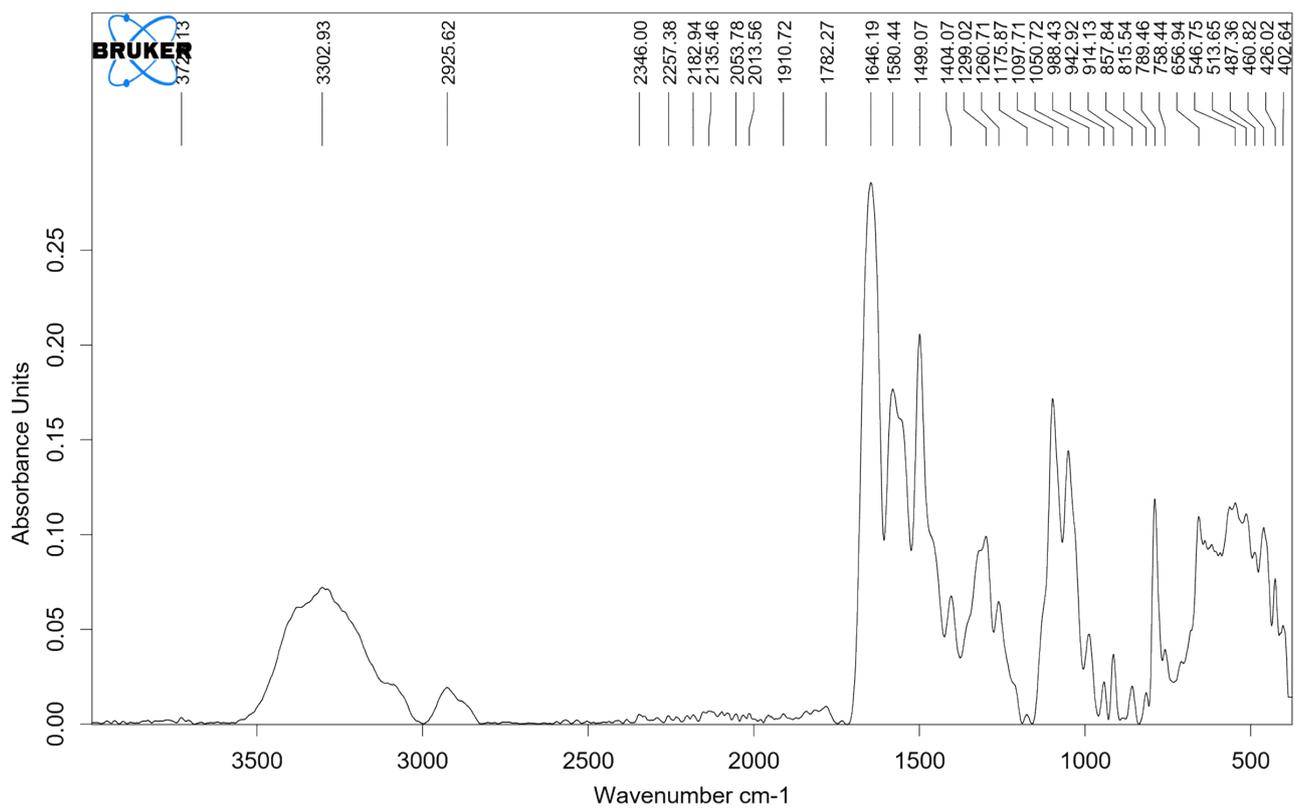


Figure S35. IR spectrum of 5-*N*-methylcarbamoylcytidine (**6b**).