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Supporting Information

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Chemoenzymatic Synthesis of *arabino*-configured Bicyclic Nucleosides

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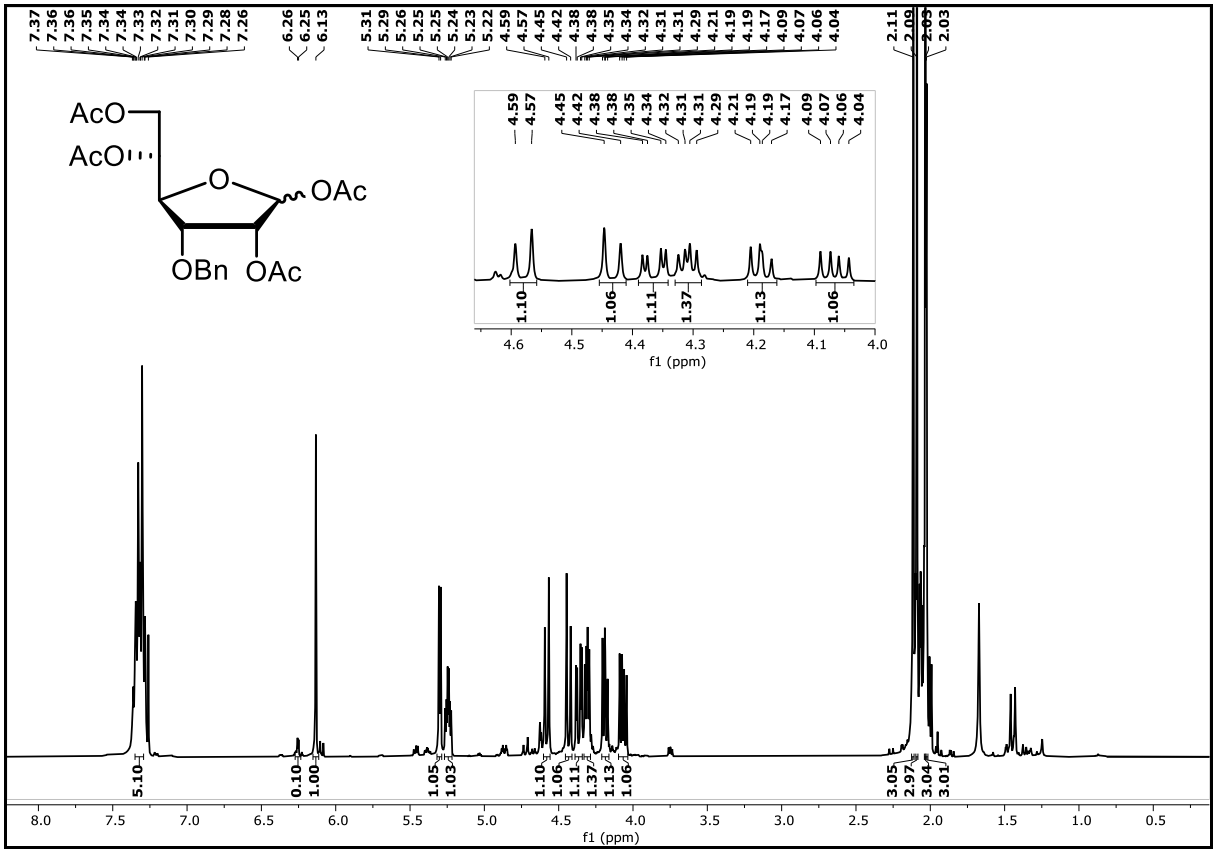

Figure 1: ^{1}H NMR spectrum of compound **2** (400 MHz, $CDCl_3$)

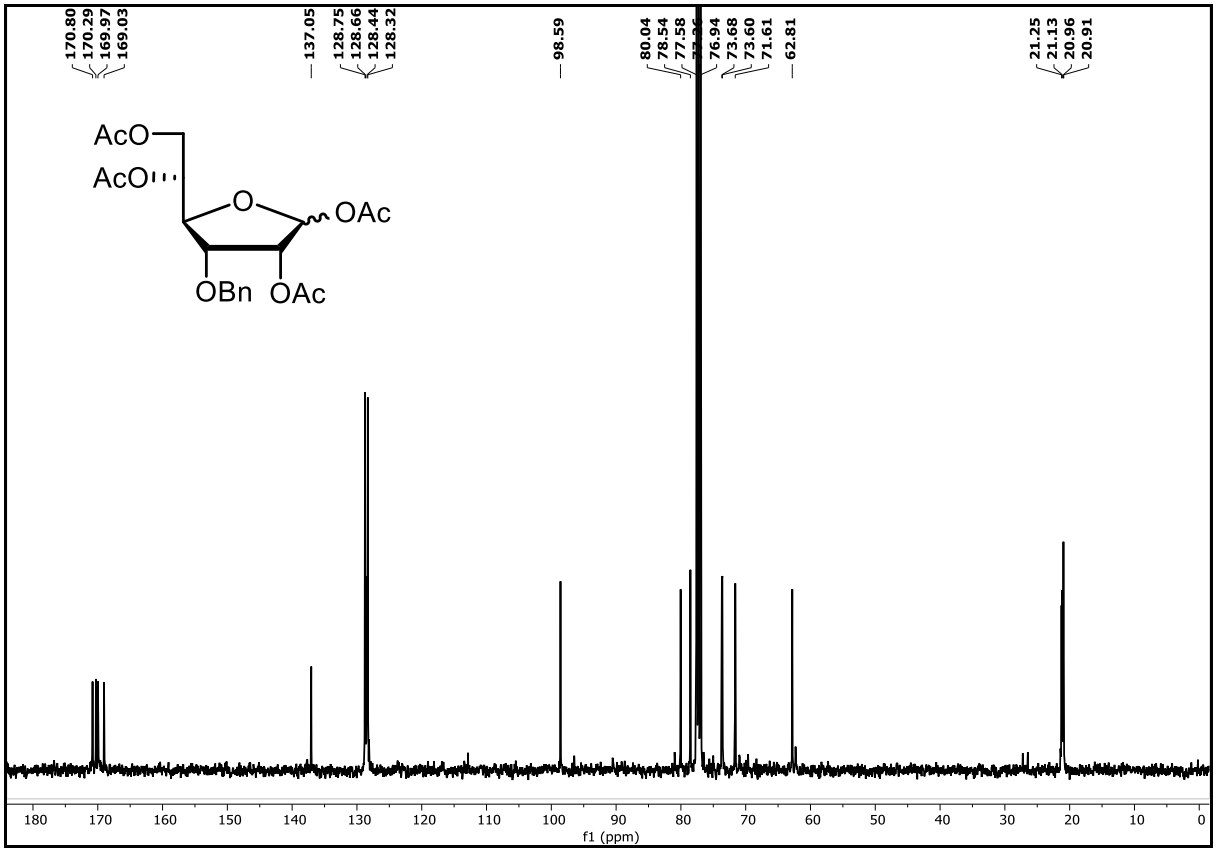

Figure 2: ^{13}C NMR spectrum of compound **2** (100.6 MHz, $CDCl_3$)

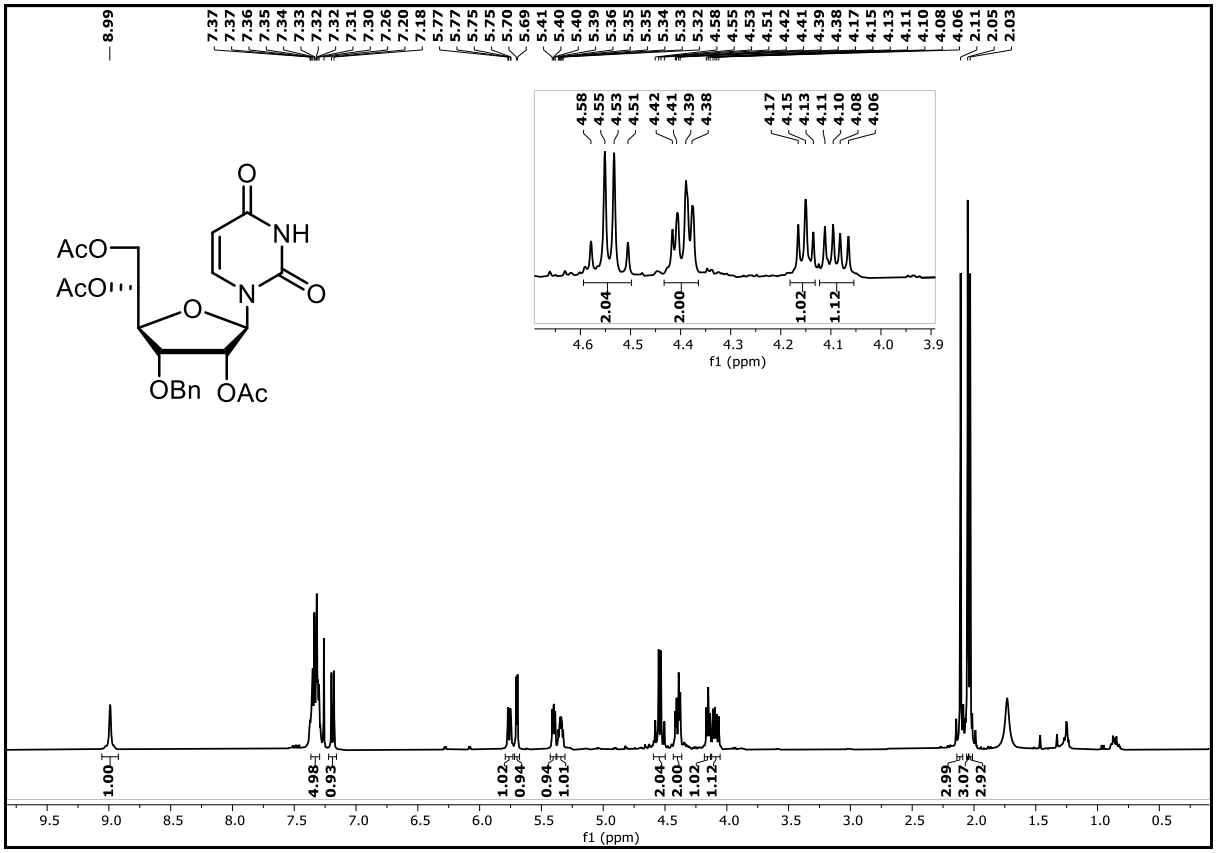

Figure 3: ^{1}H NMR spectrum of compound **3a** (400 MHz, $CDCl_3$)

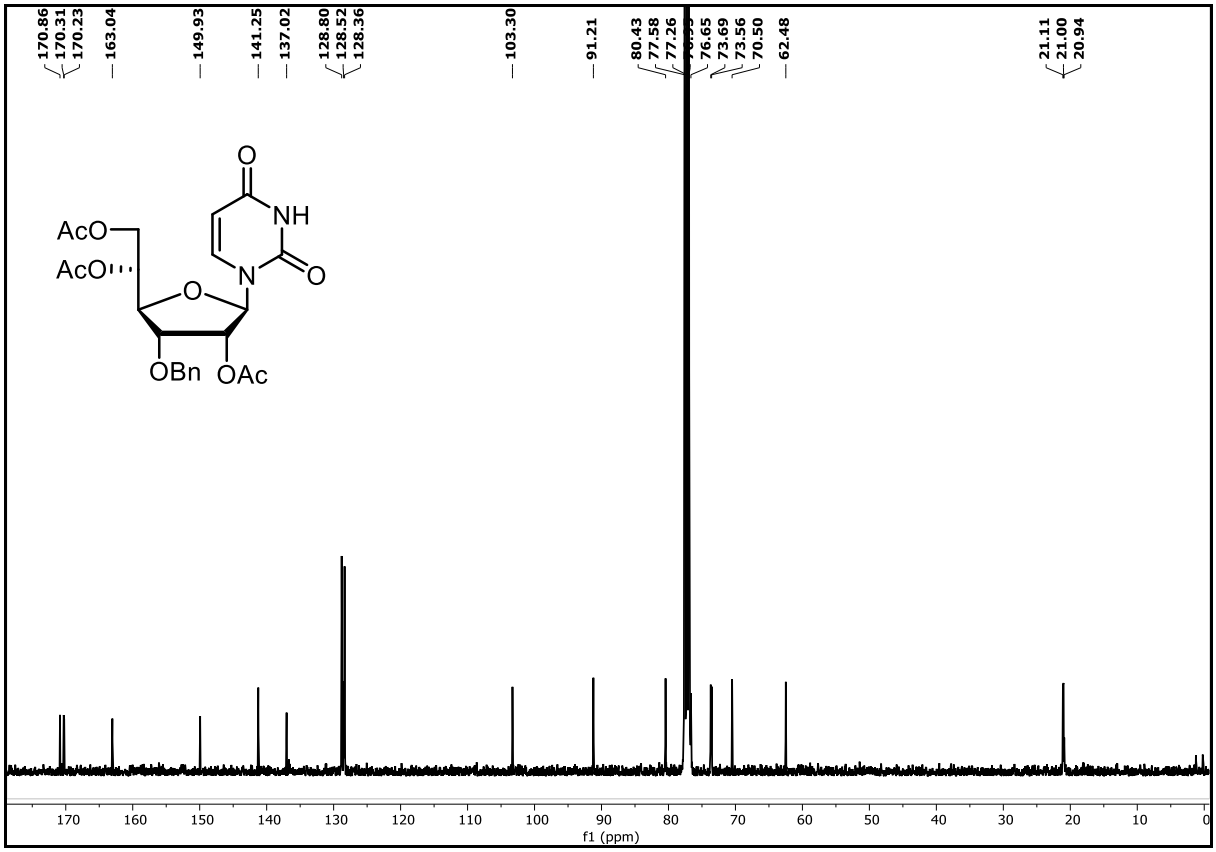

Figure 4: ^{13}C NMR spectrum of compound **3a** (100.6 MHz, $CDCl_3$)

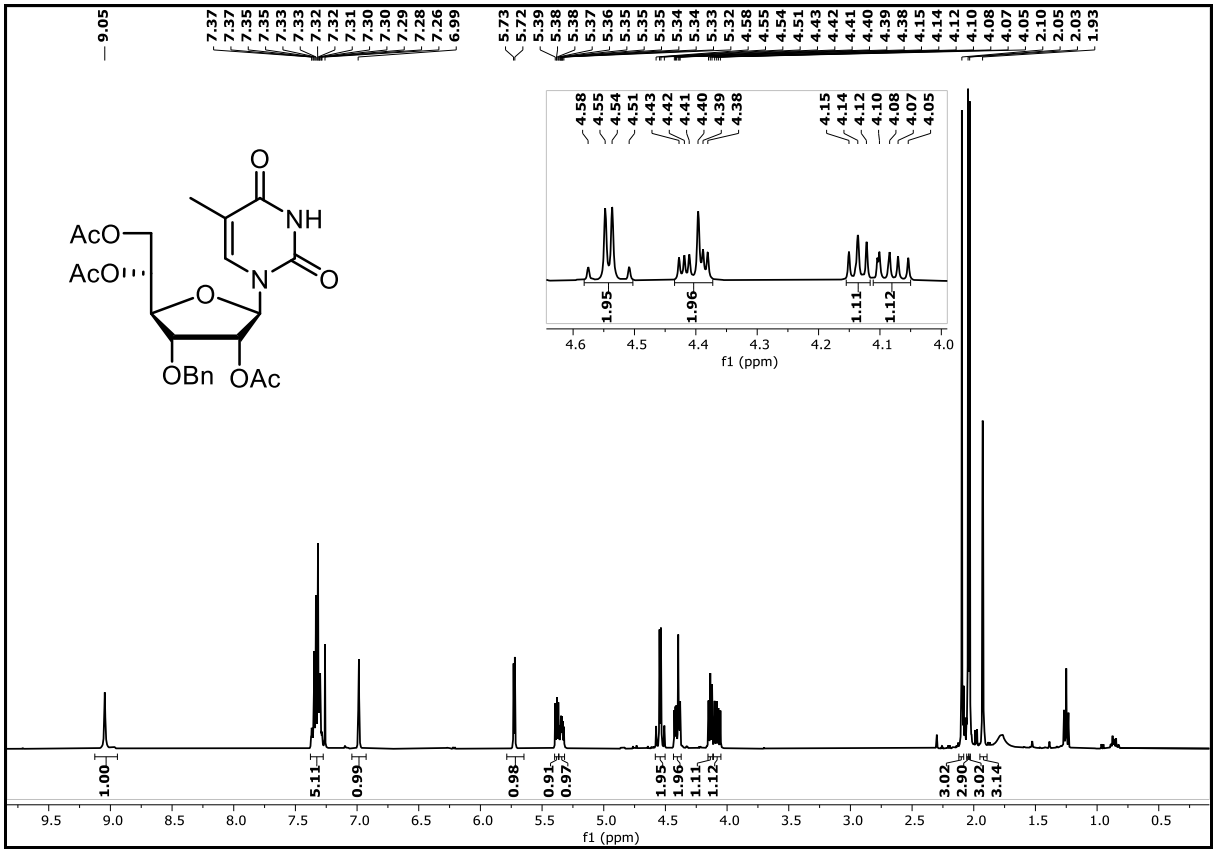

Figure 5: ^{1}H NMR spectrum of compound **3b** (400 MHz, $CDCl_3$)

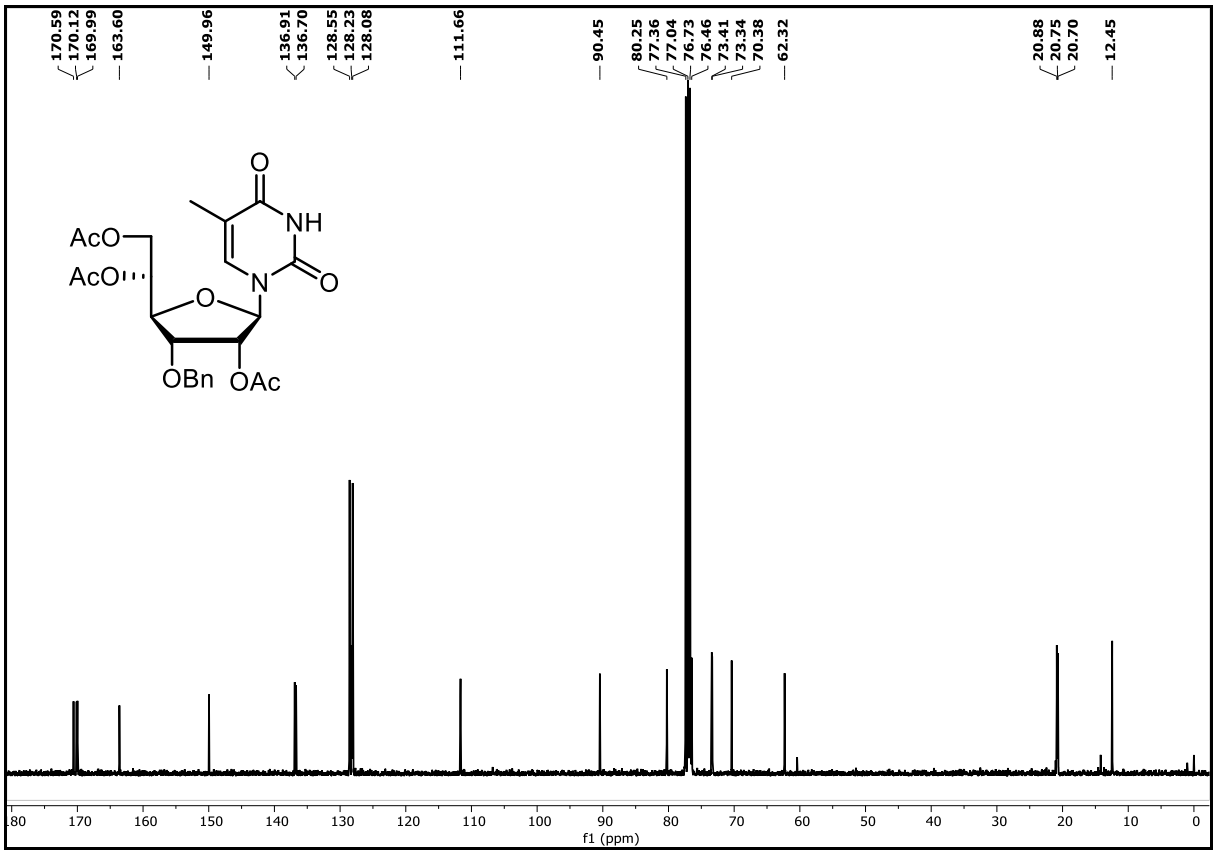

Figure 6: ^{13}C NMR spectrum of compound **3b** (100.6 MHz, $CDCl_3$)

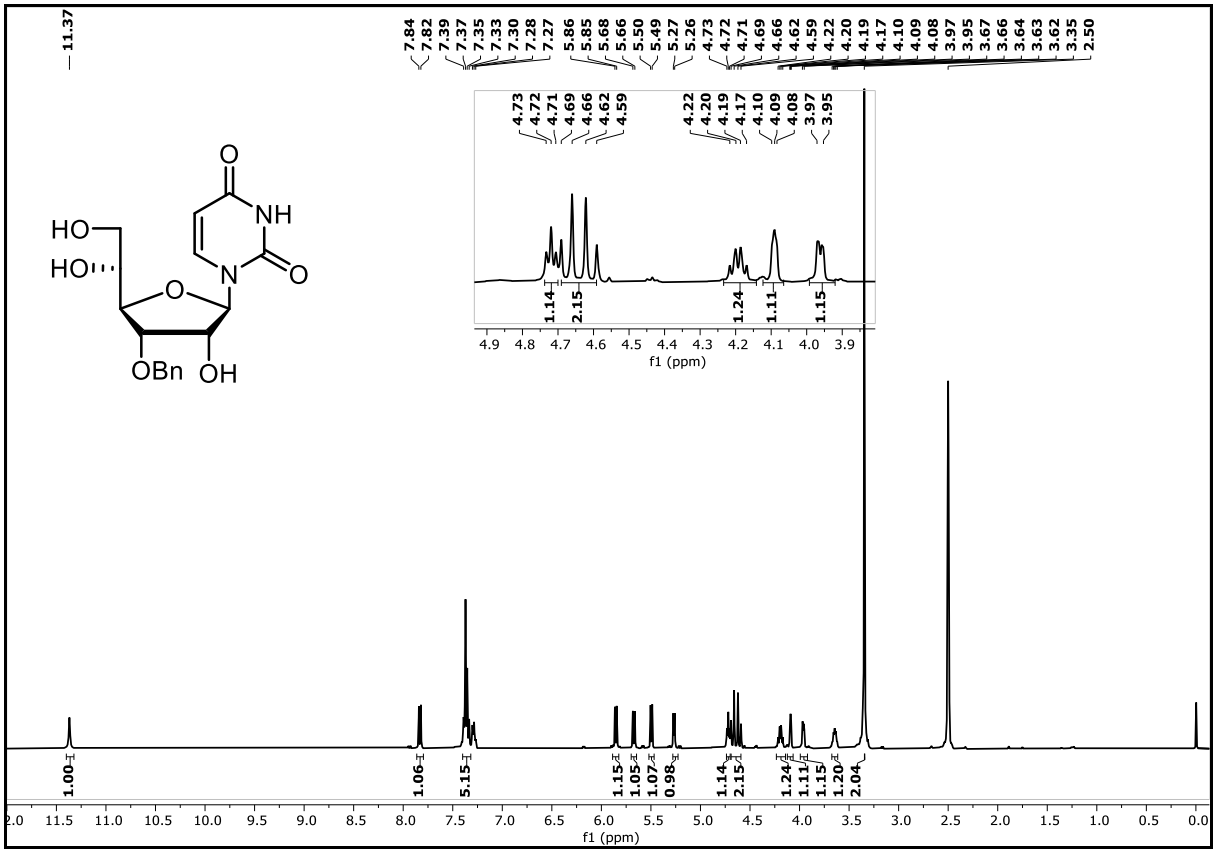

Figure 7: ^{1}H NMR spectrum of compound **4a** (400 MHz, DMSO-d_6)

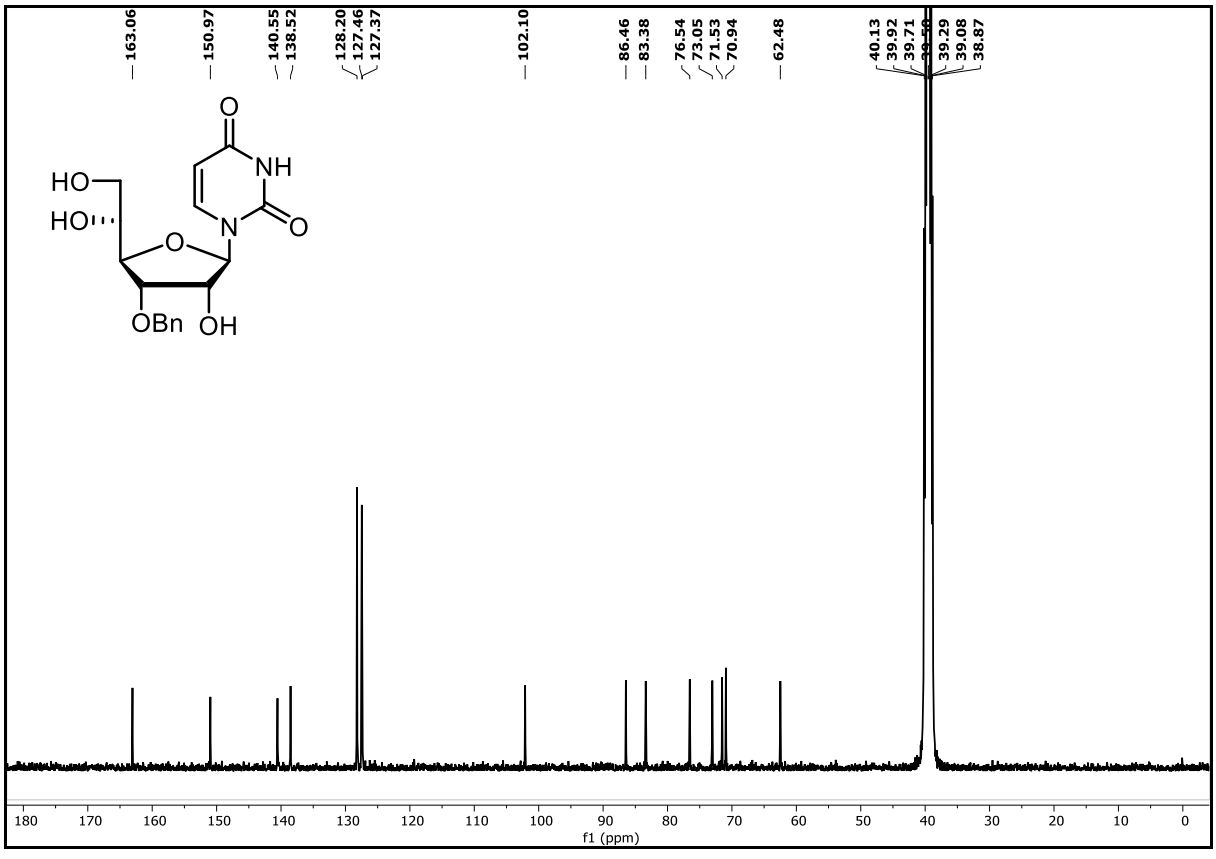

Figure 8: ^{13}C NMR spectrum of compound **4a** (100.6 MHz, DMSO-d_6)

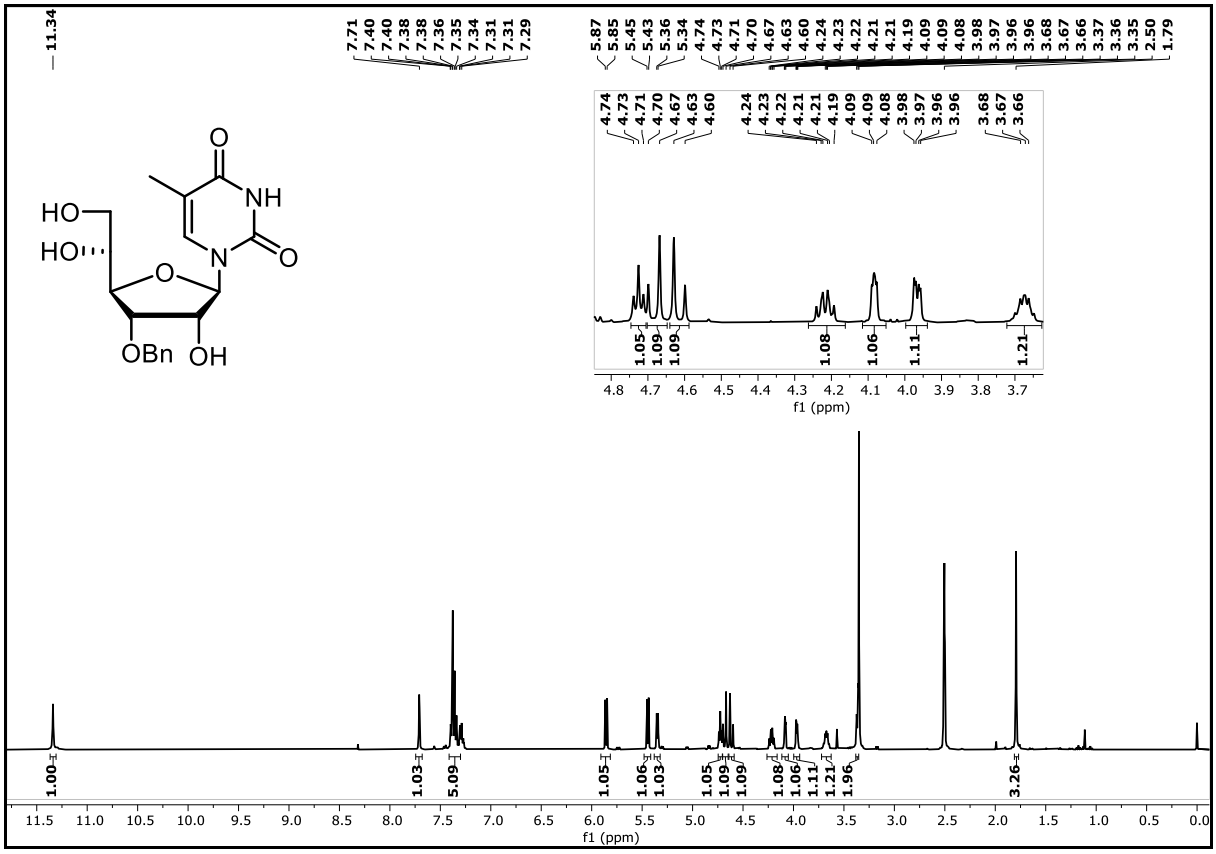

Figure 9: ^{1}H NMR spectrum of compound **4b** (400 MHz, DMSO-d_6)

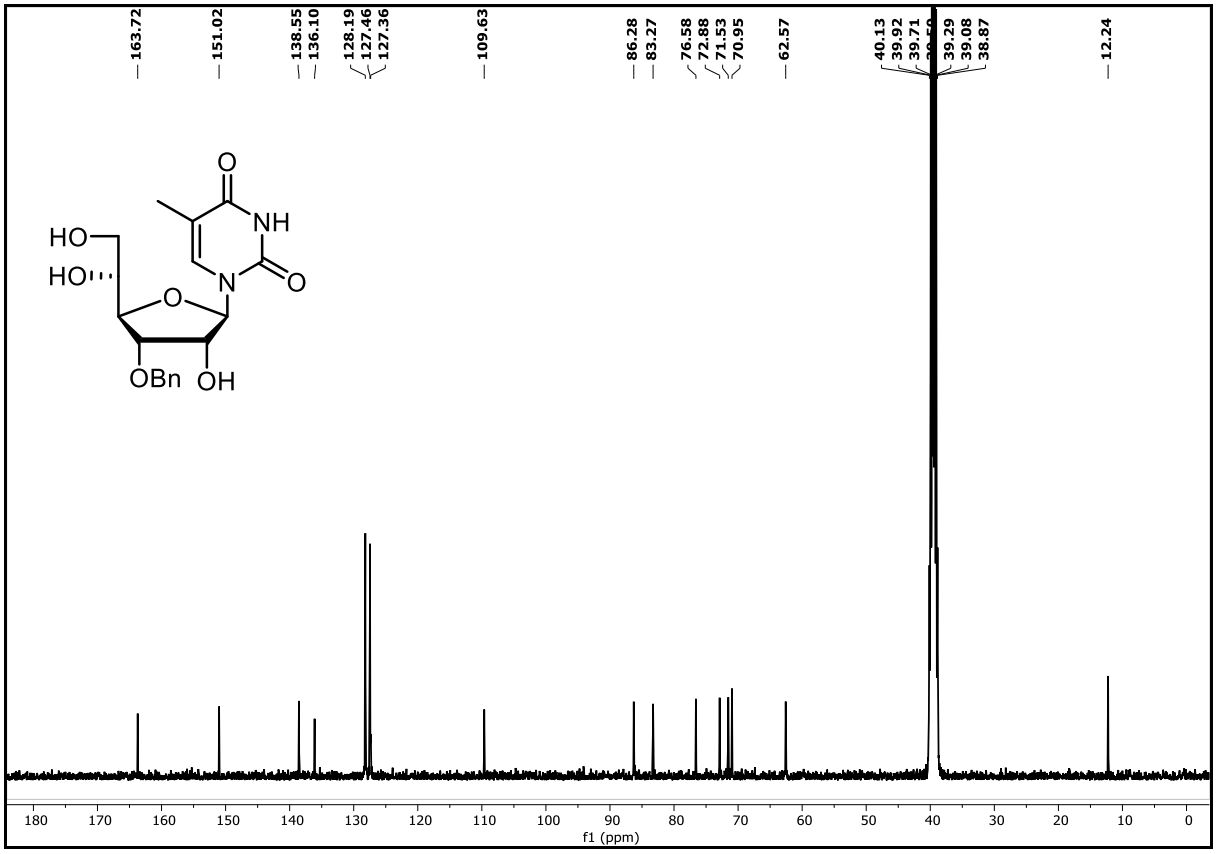

Figure 10: ^{13}C NMR spectrum of compound **4b** (100.6 MHz, DMSO-d_6)

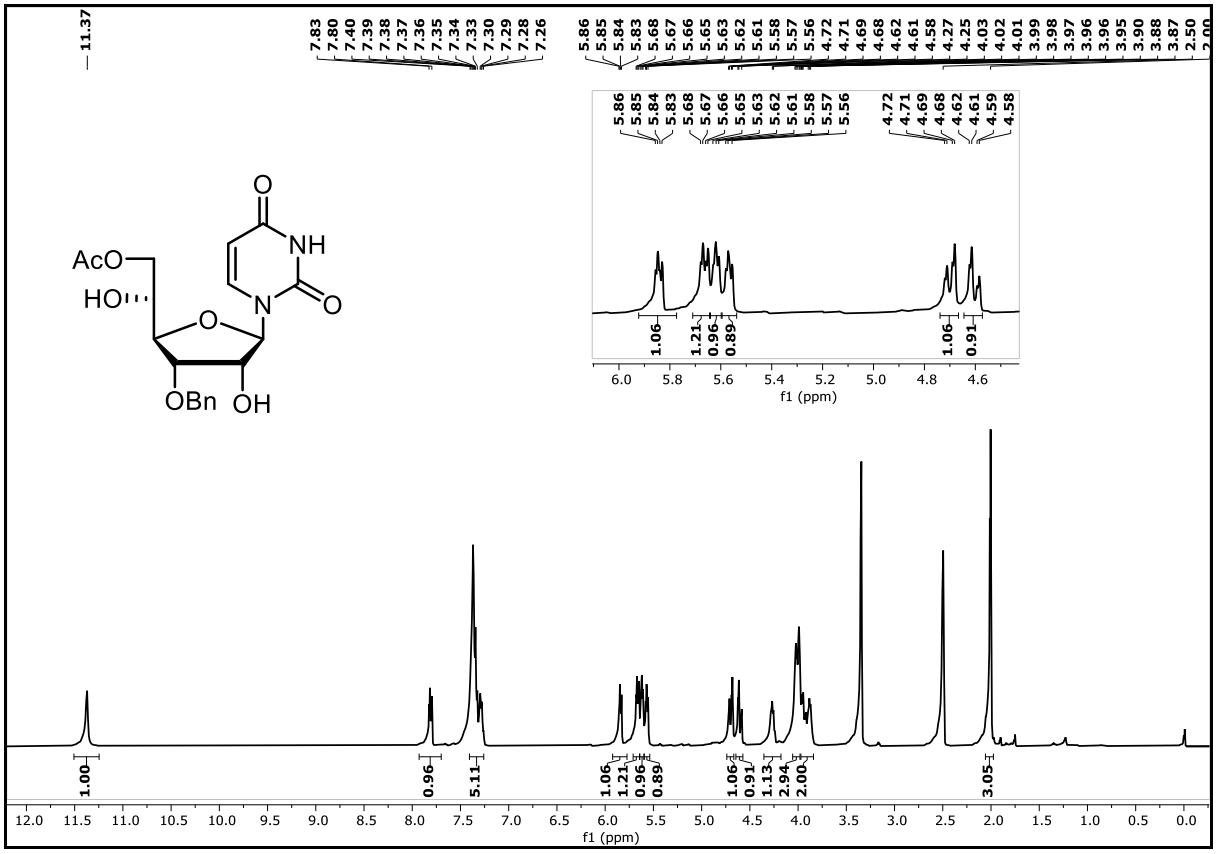

Figure 11: ^{1}H NMR spectrum of compound **5a** (400 MHz, DMSO-d_6)

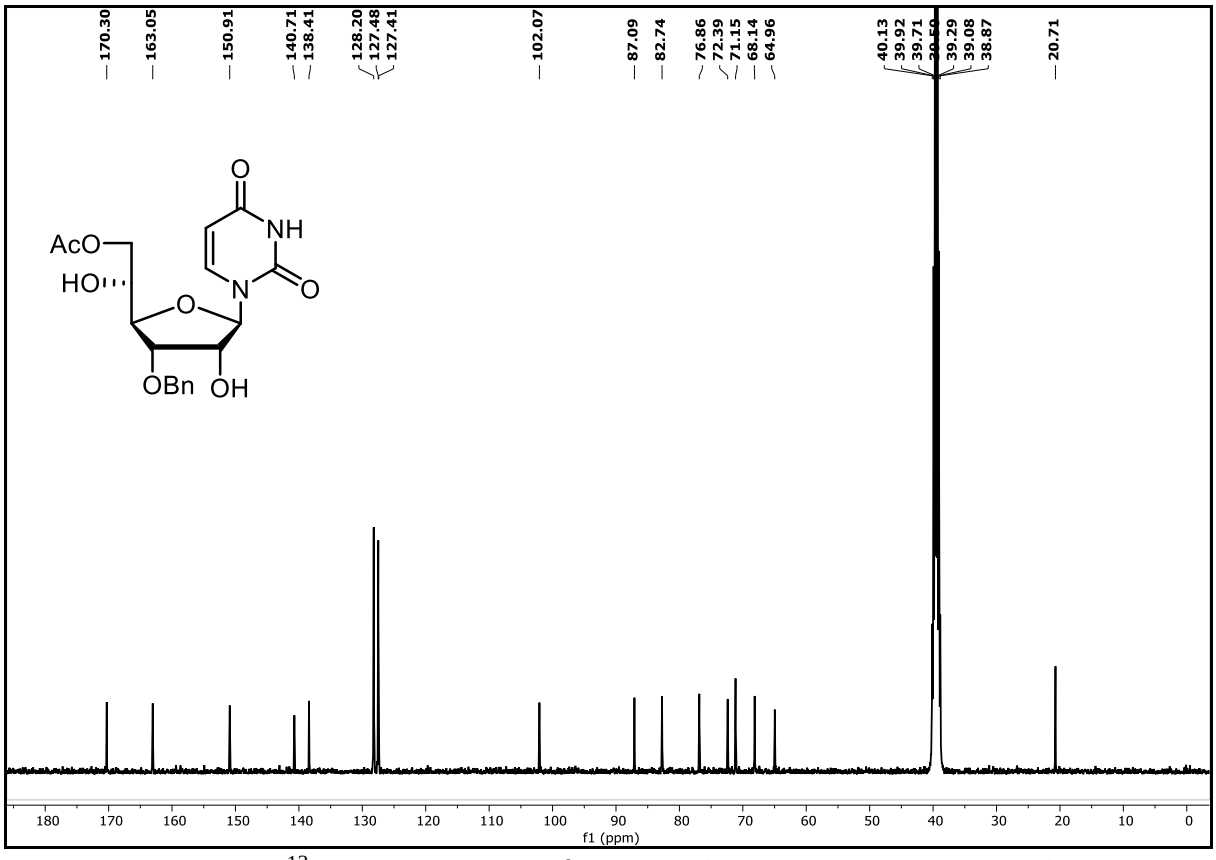

Figure 12: ^{13}C NMR spectrum of compound **5a** (100.6 MHz, DMSO-d_6)

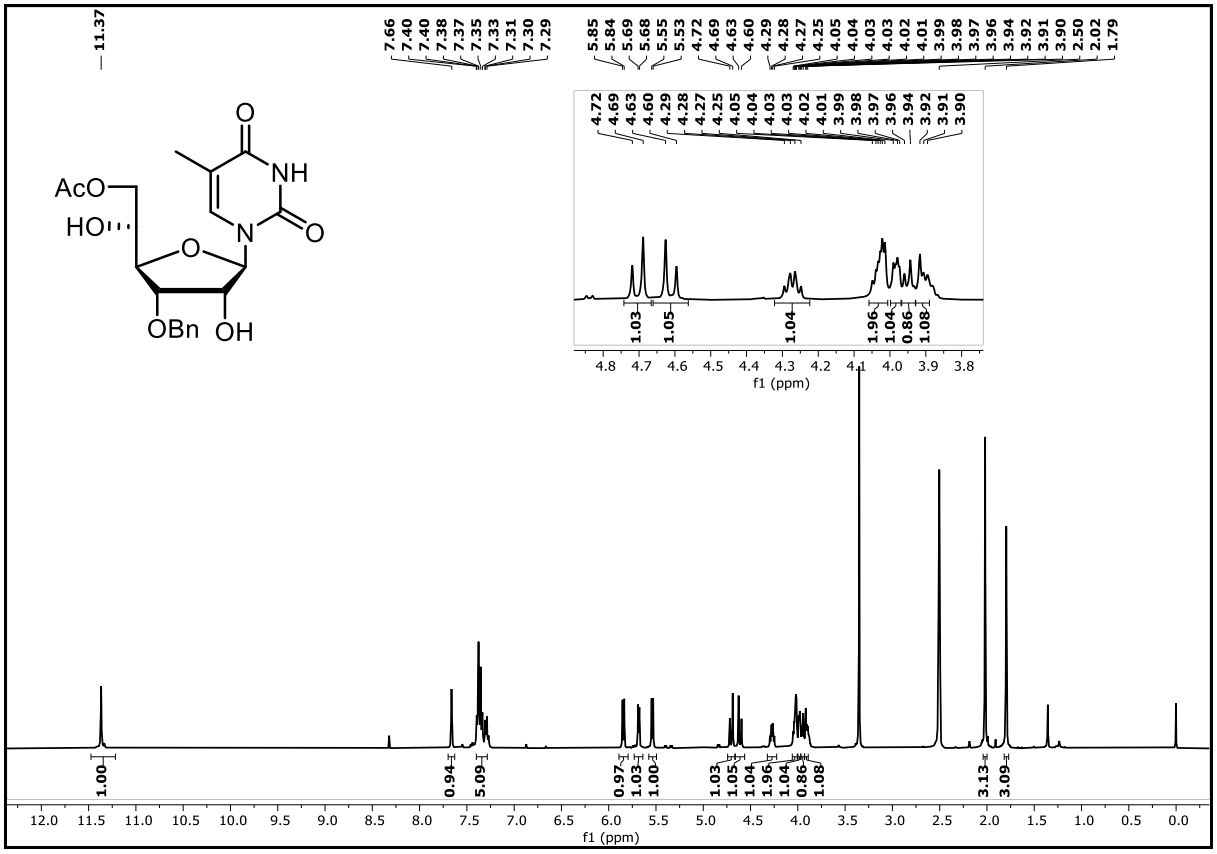

Figure 13: ^{1}H NMR spectrum of compound **5b** (400 MHz, DMSO-d_6)

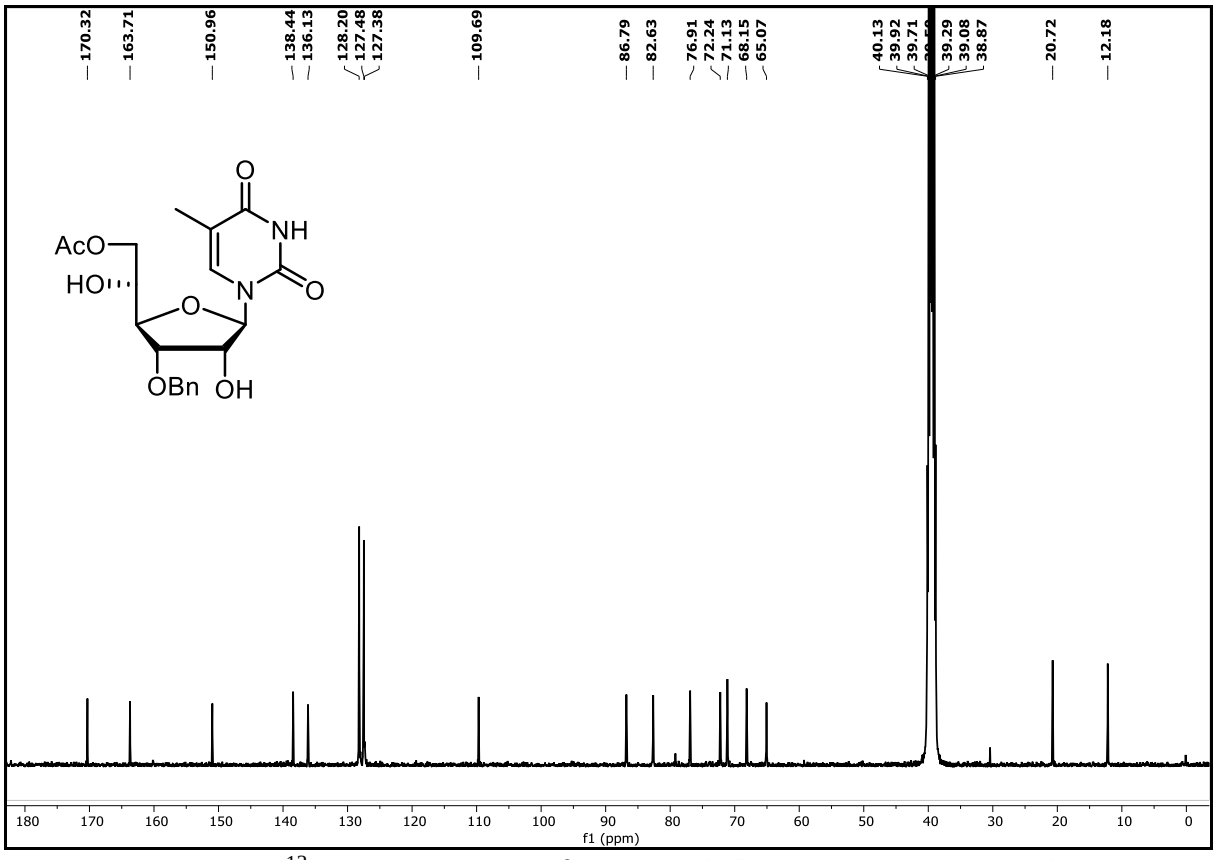

Figure 14: ^{13}C NMR spectrum of compound **5b** (100.6 MHz, DMSO-d_6)

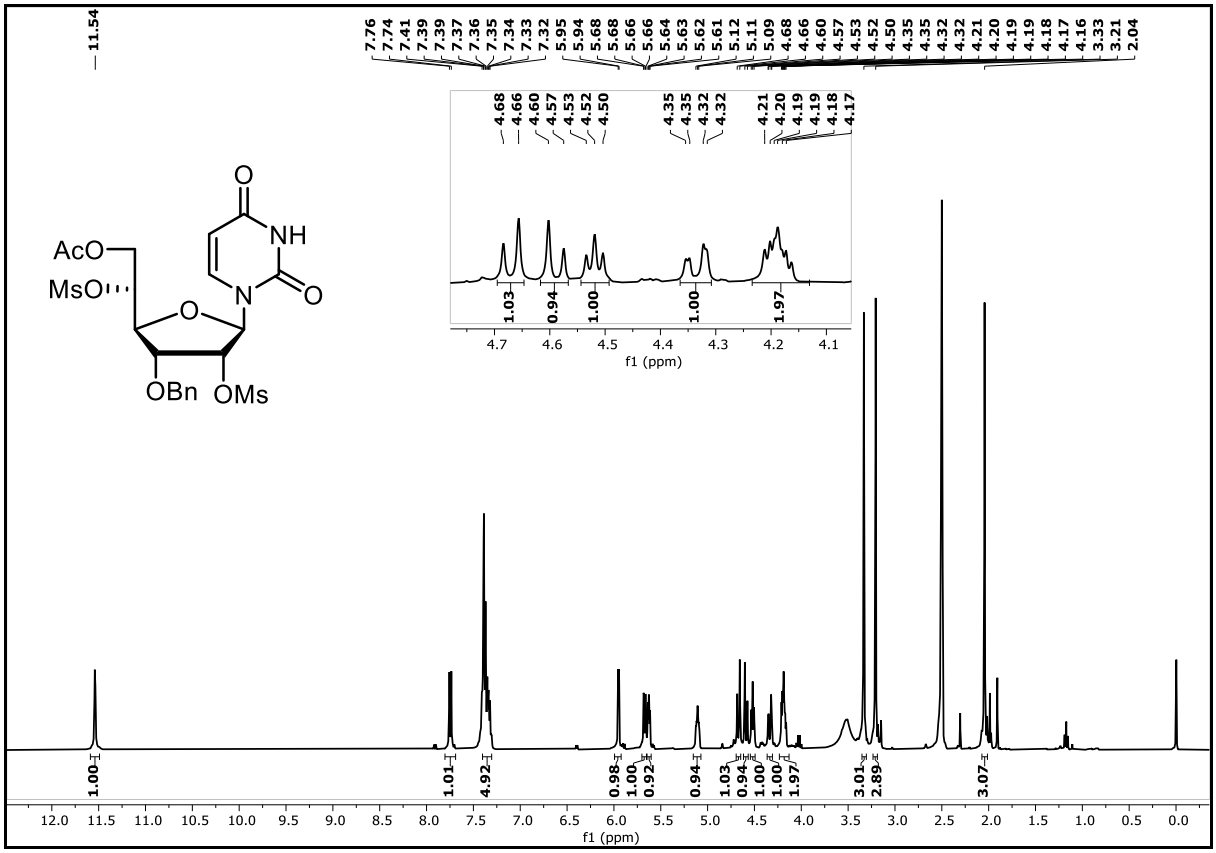

Figure 15: ^{1}H NMR spectrum of compound **6a** (400 MHz, DMSO-d_6)

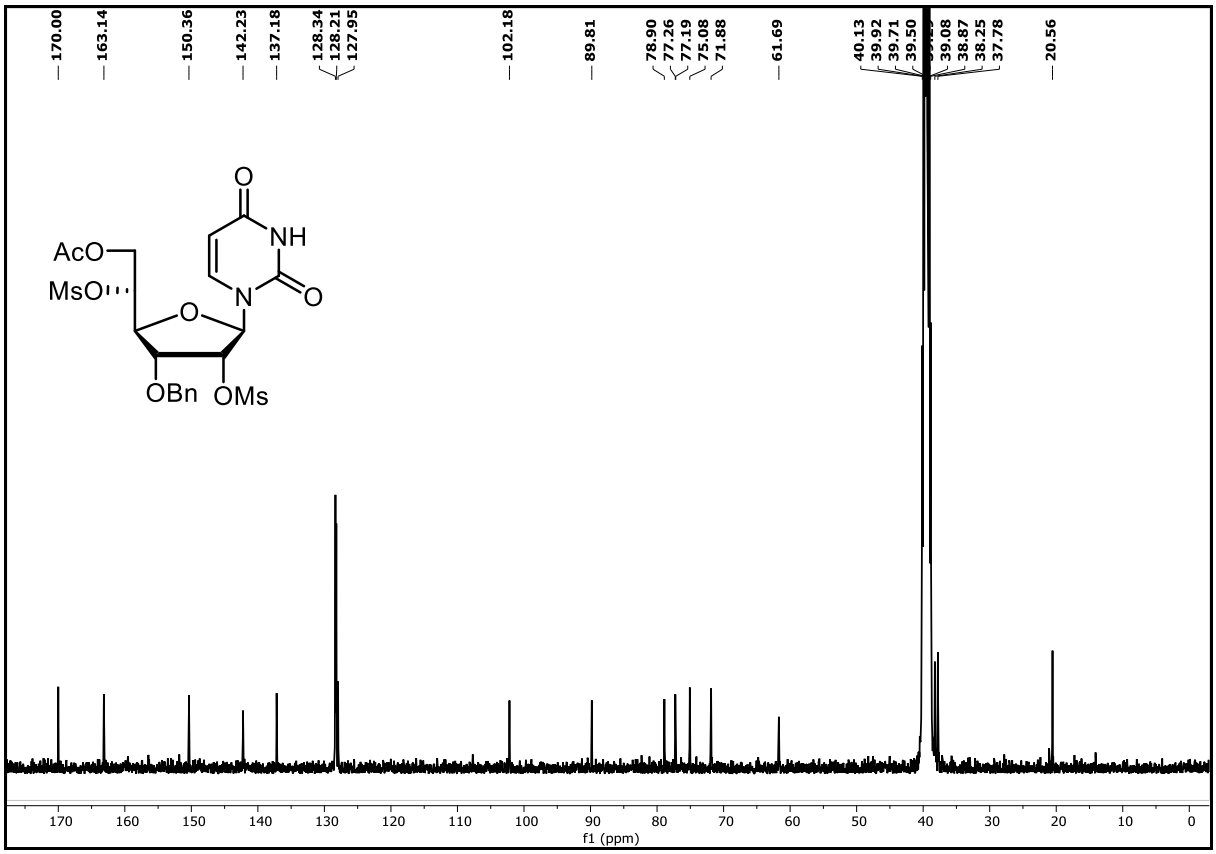

Figure 16: ^{13}C NMR spectrum of compound **6a** (100.6 MHz, DMSO-d_6)

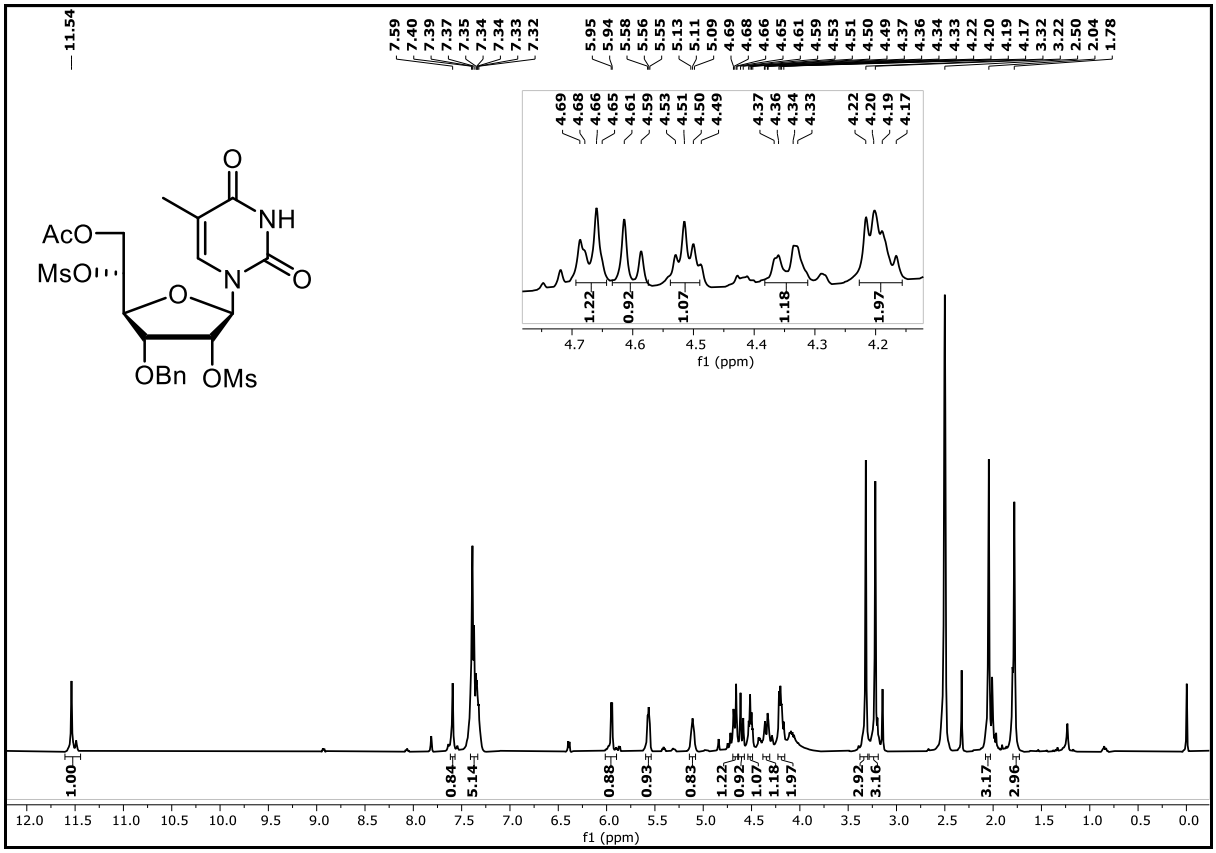

Figure 17: ^{1}H NMR spectrum of compound **6b** (400 MHz, DMSO-d_6)

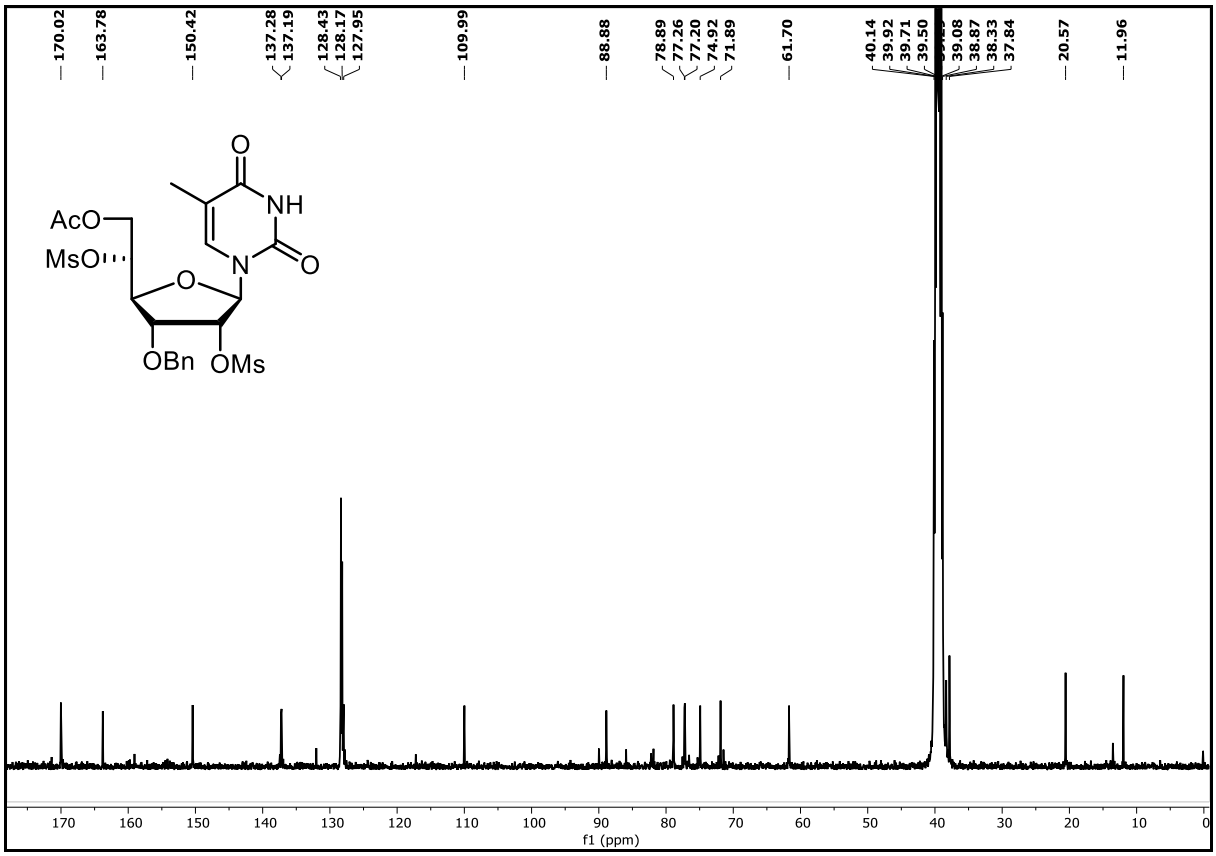

Figure 18: ^{13}C NMR spectrum of compound **6b** (100.6 MHz, DMSO-d_6)

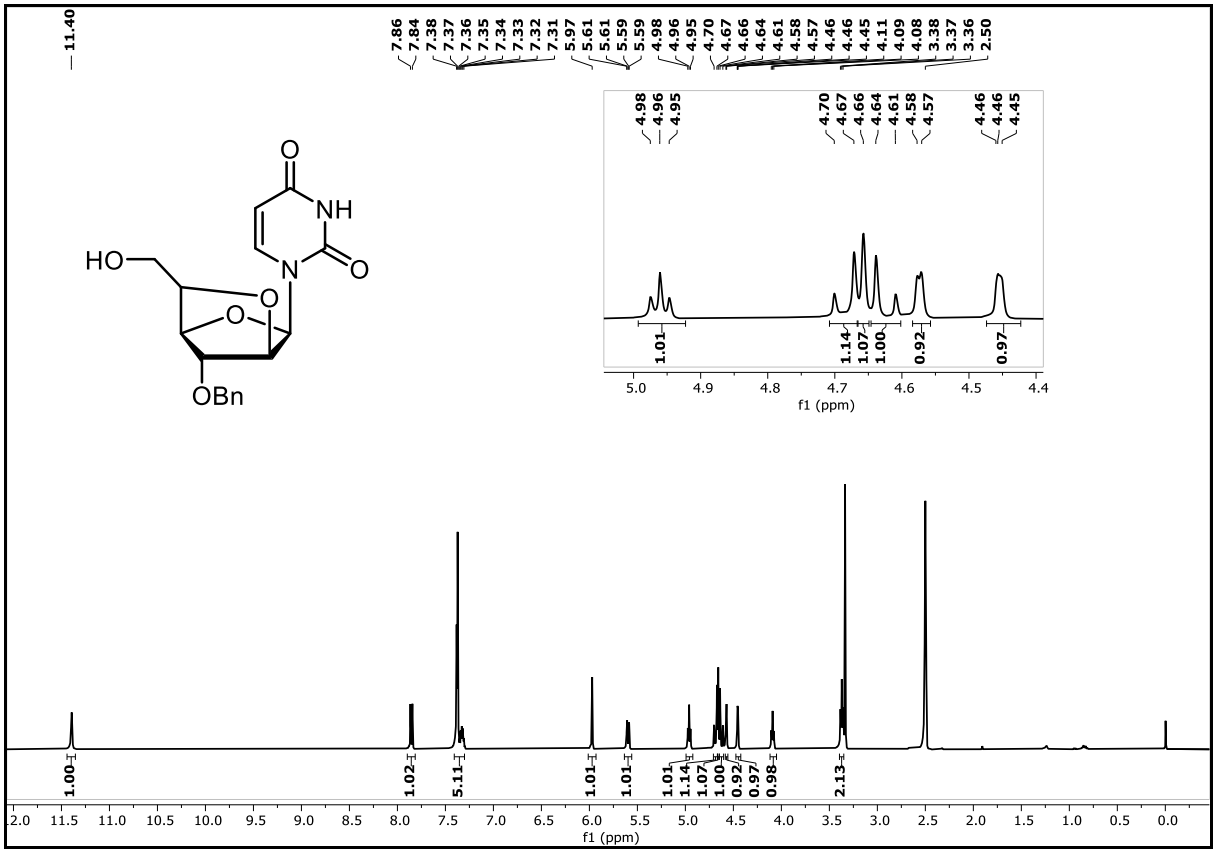

Figure 19: ^{1}H NMR spectrum of compound **7a** (400 MHz, DMSO-d_6)

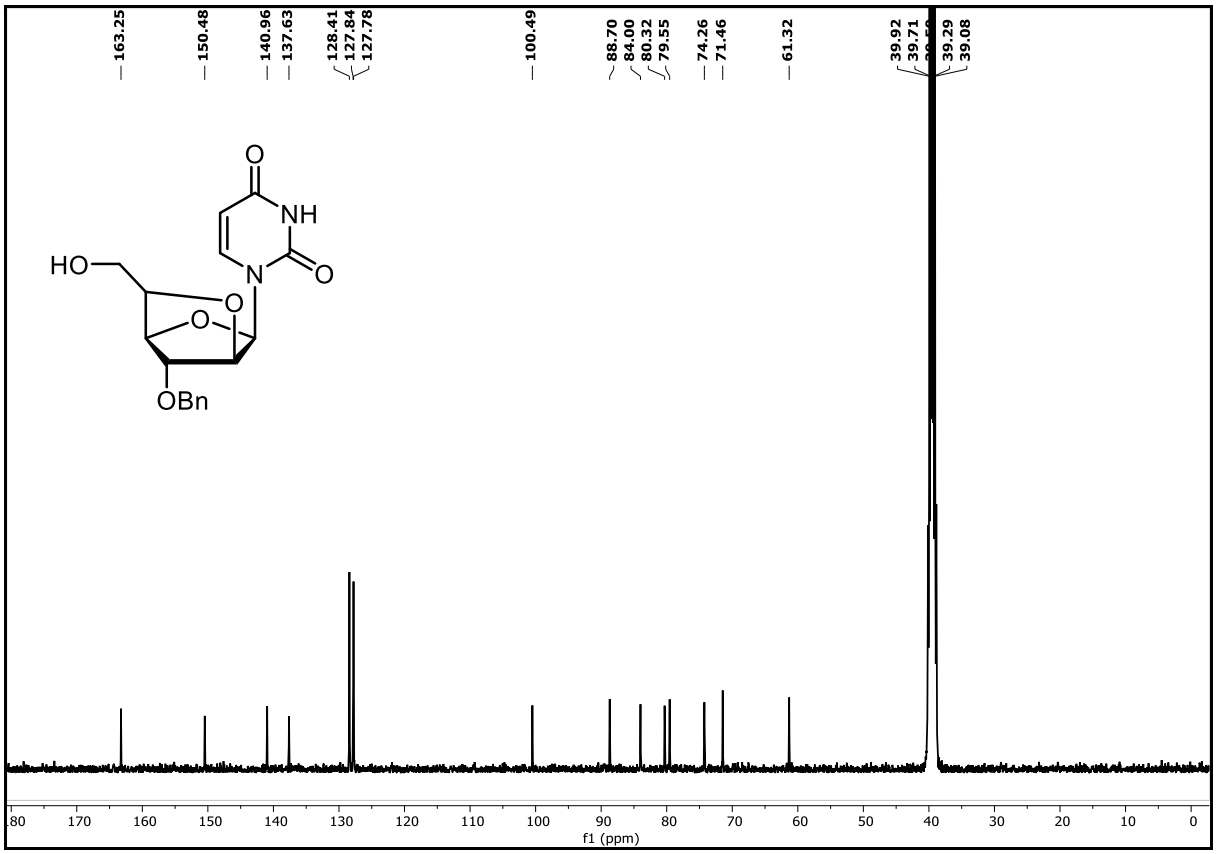

Figure 20: ^{13}C NMR spectrum of compound **7a** (100.6 MHz, DMSO-d_6)

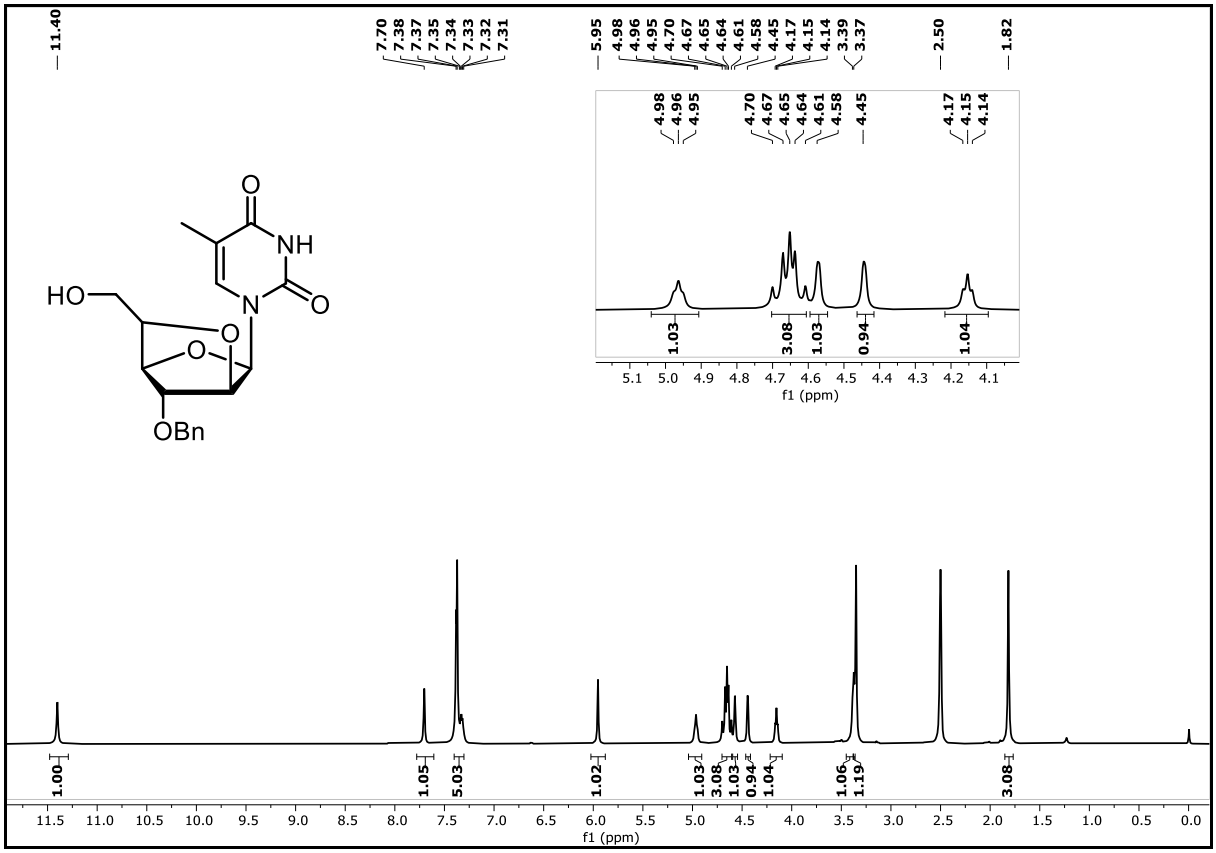

Figure 21: ^{1}H NMR spectrum of compound **7b** (400 MHz, DMSO-d_6)

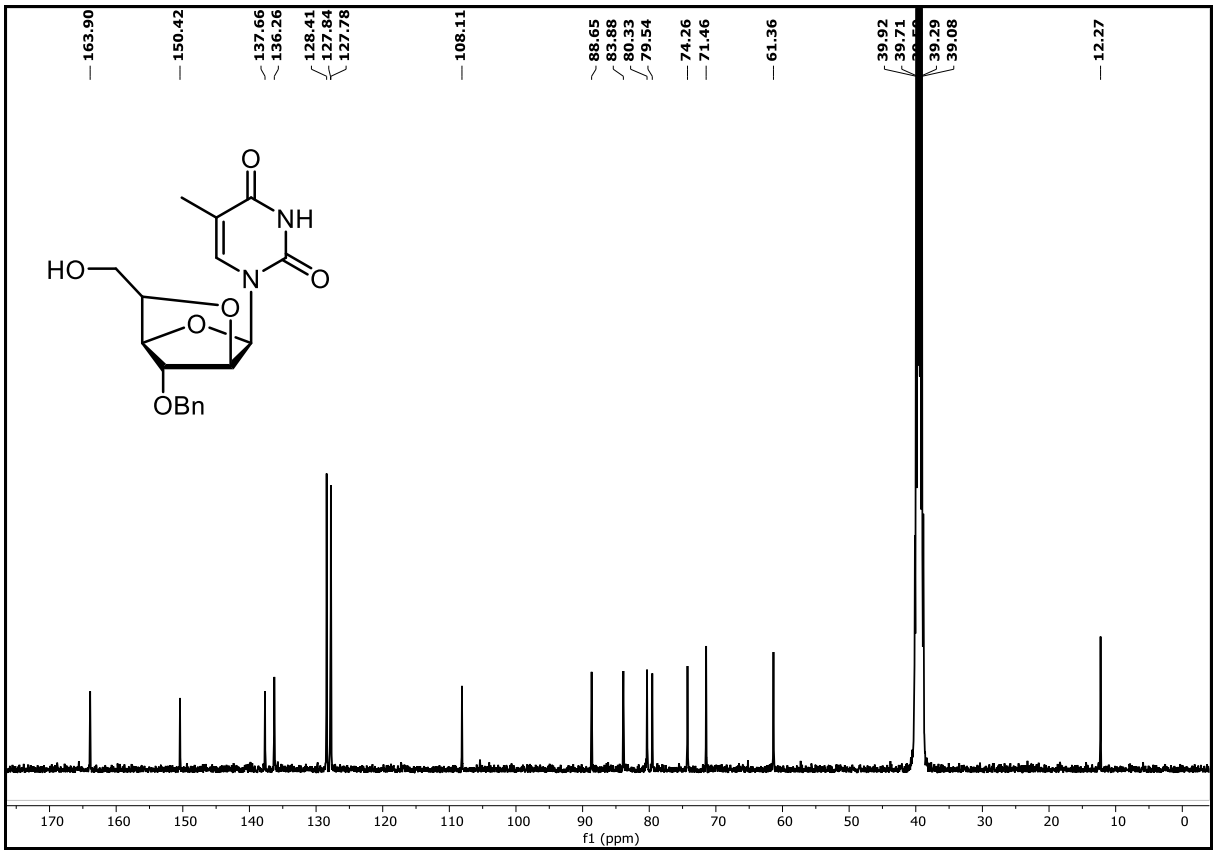

Figure 22: ^{13}C NMR spectrum of compound **7b** (100.6 MHz, DMSO-d_6)

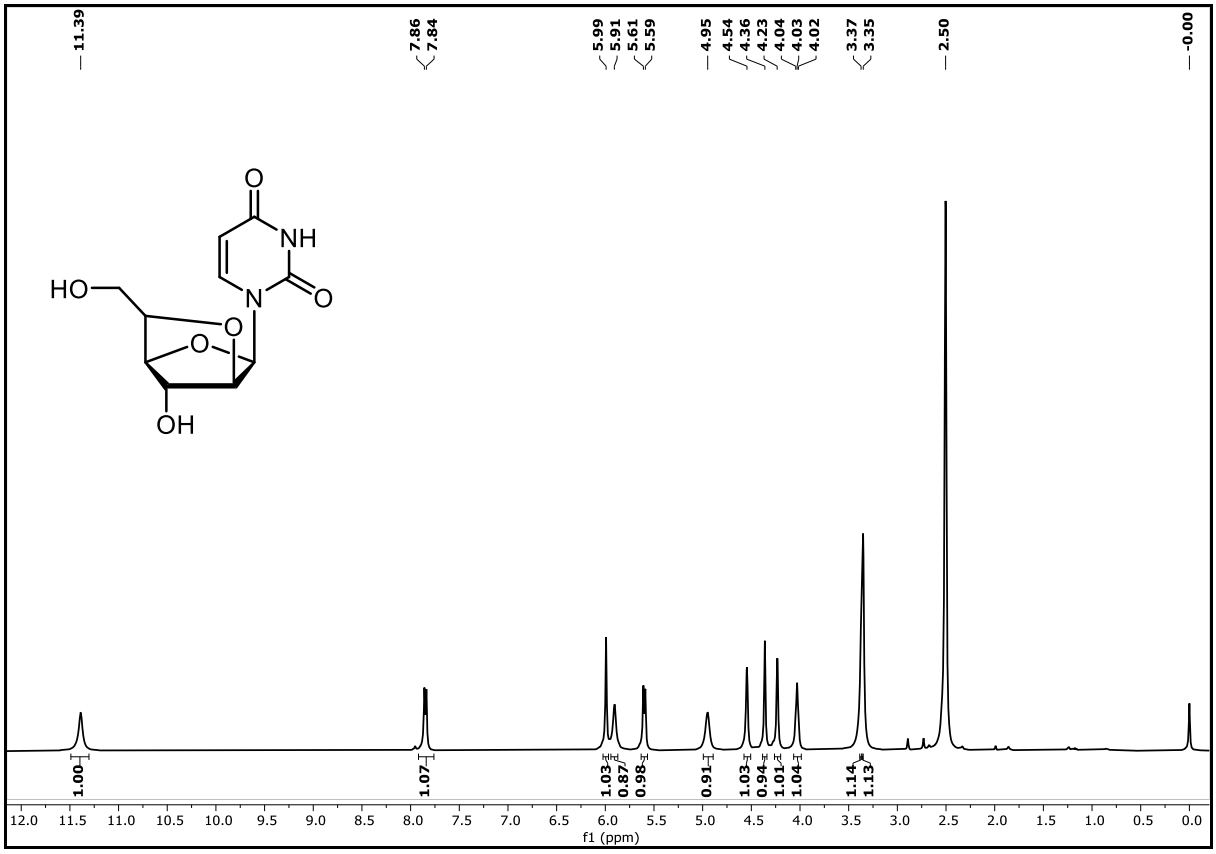

Figure 23: ^{1}H NMR spectrum of compound **8a** (400 MHz, DMSO-d_6)

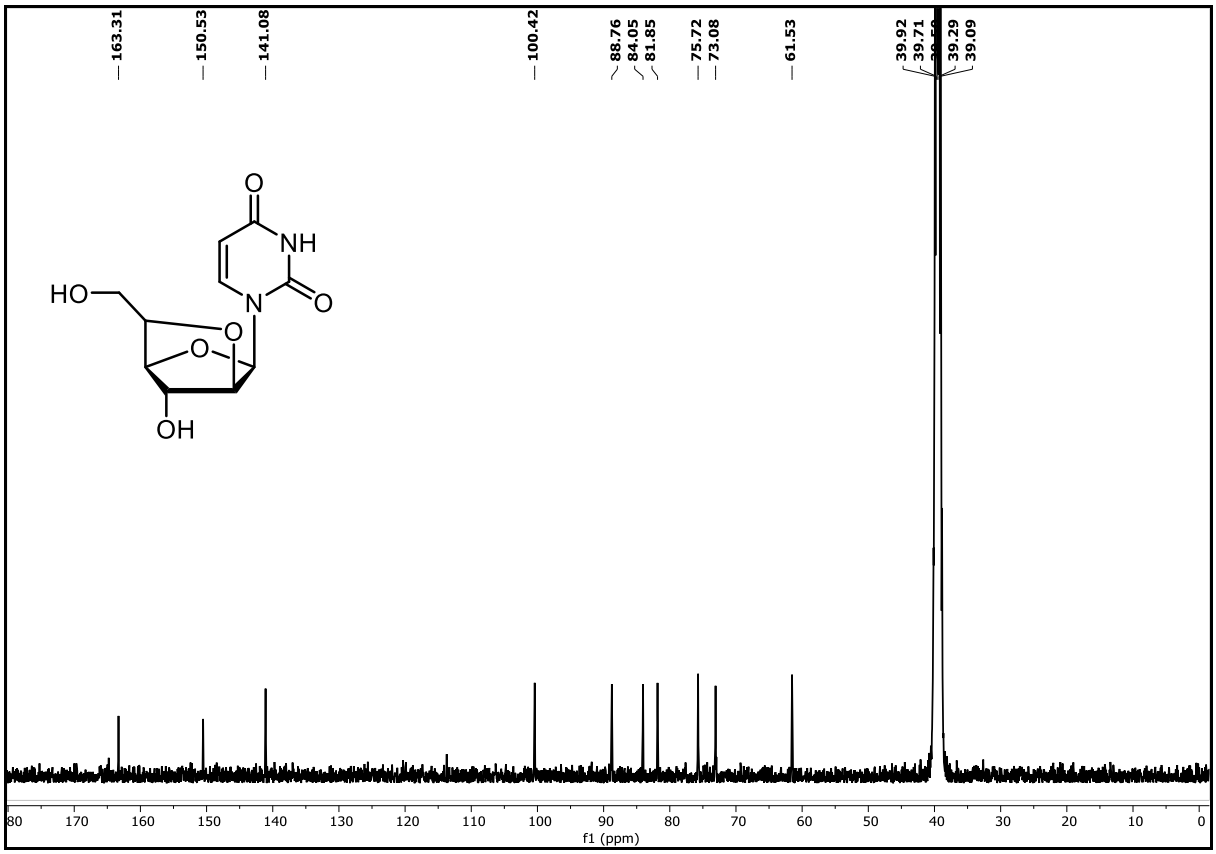

Figure 24: ^{13}C NMR spectrum of compound **8a** (100.6 MHz, DMSO-d_6)

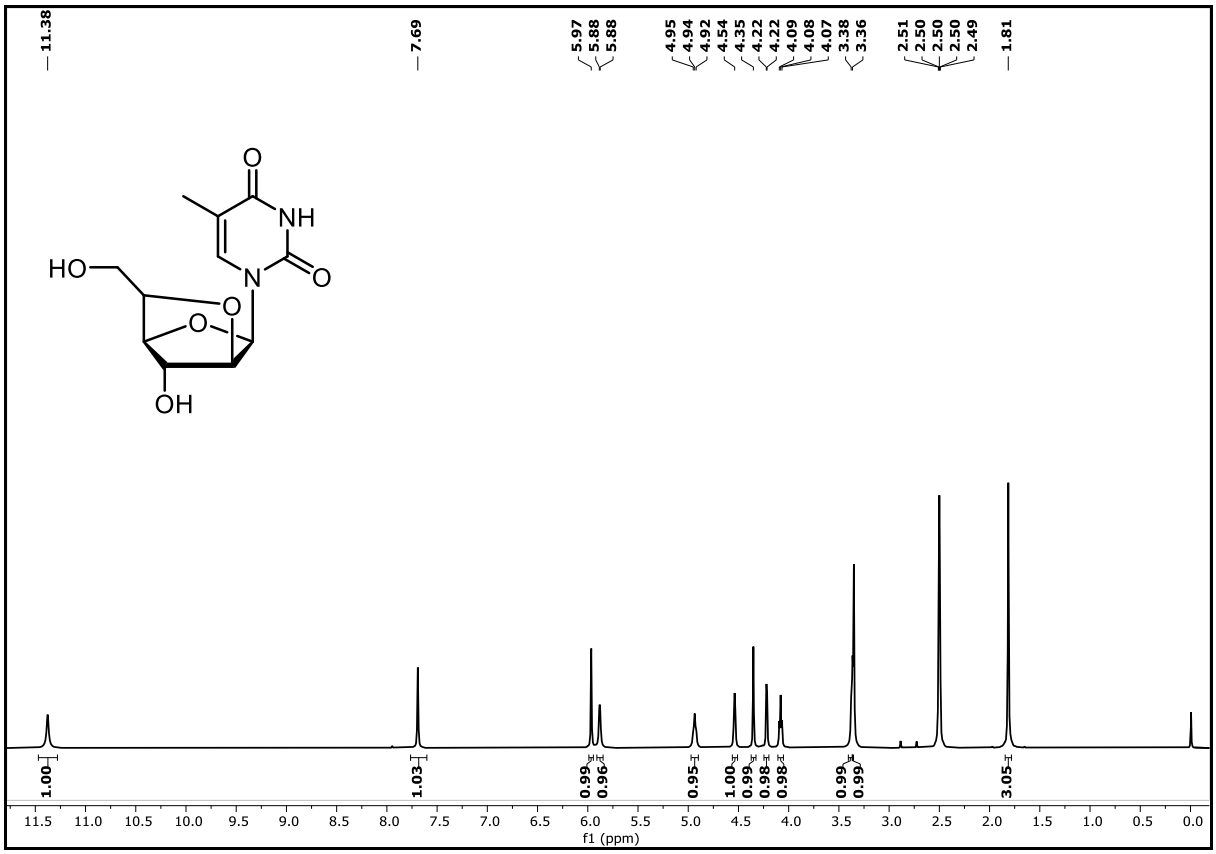

Figure 25: ^{1}H NMR spectrum of compound **8b** (400 MHz, DMSO-d_6)

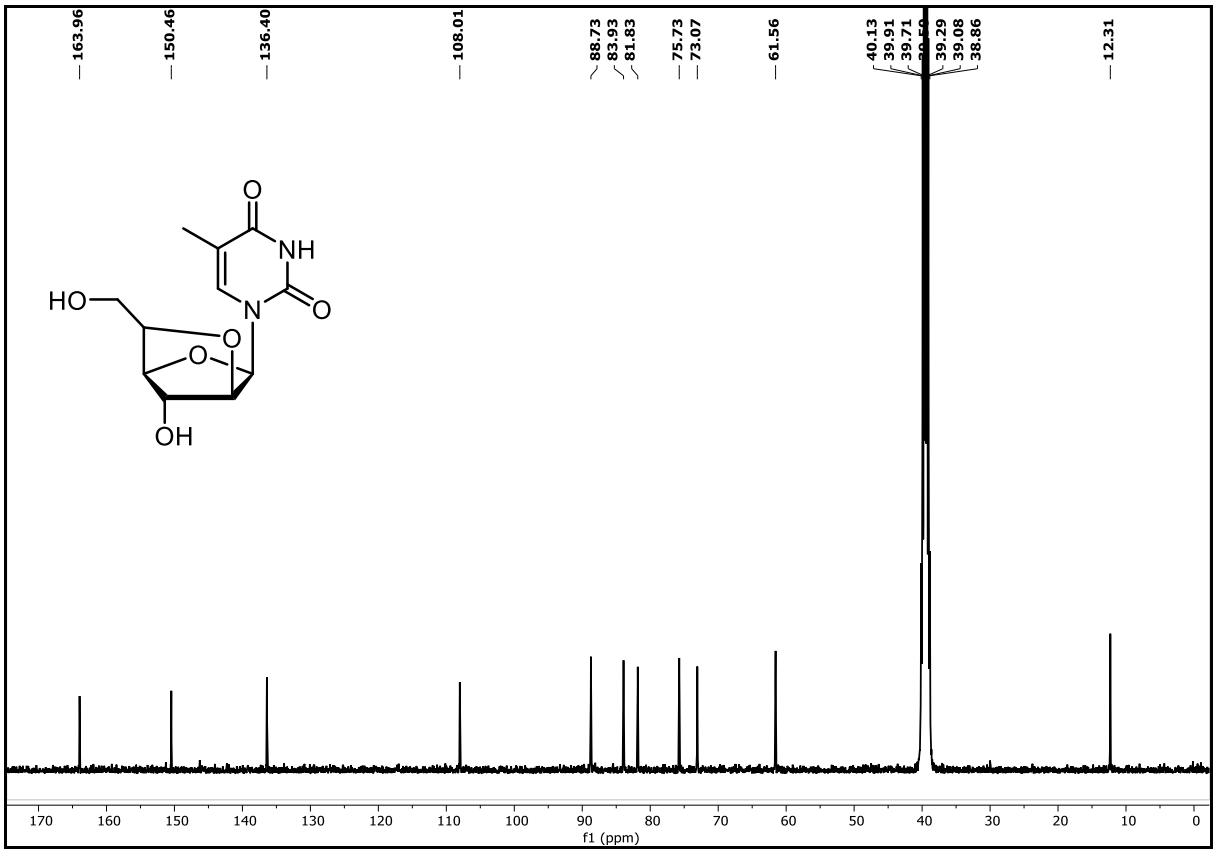

Figure 26: ^{13}C NMR spectrum of compound **8b** (100.6 MHz, DMSO-d_6)

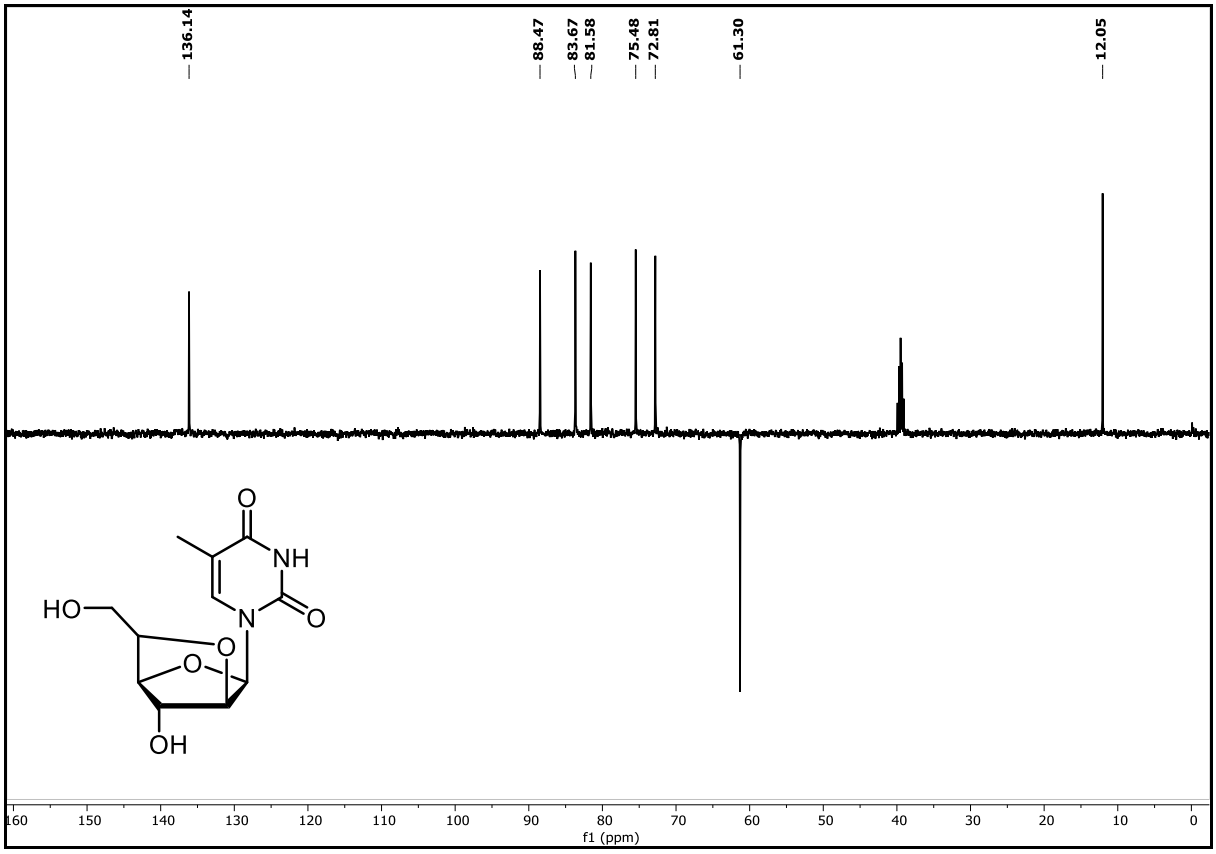

Figure 27: DEPT-135 ^{13}C NMR spectrum of compound **8b** (100.6 MHz, DMSO-d_6)

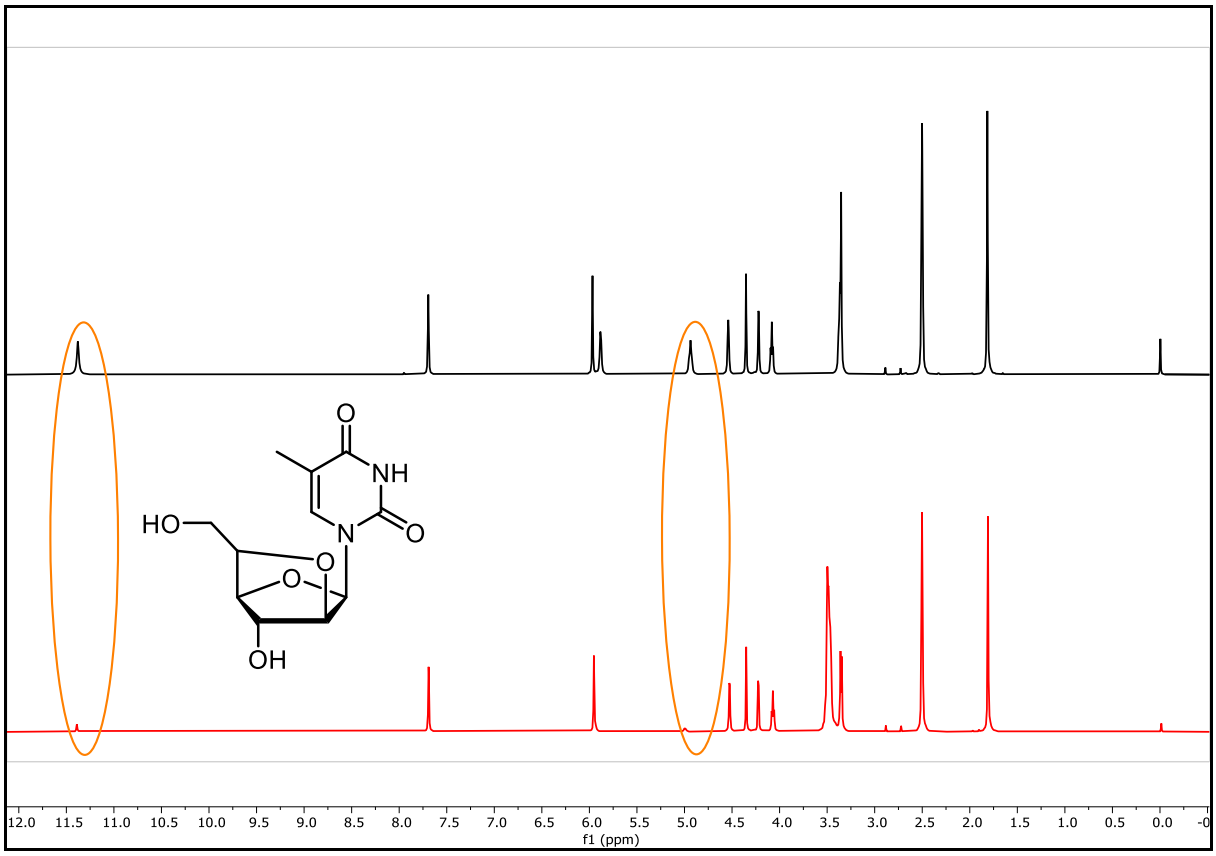

Figure 28: D_2O Exchange ^{1}H NMR spectrum of compound **8b** (400 MHz, DMSO-d_6)

Single crystal X-ray diffraction analysis of 1-((1*S*,3*R*,4*S*,7*R*)-7-hydroxy-6-(hydroxymethyl)-2,5-dioxabicyclo[2.2.1]heptan-3-yl)-5-methylpyrimidine-2,4(1*H*,3*H*)-dione (8b)

Compound **8b** was dissolved in a mixture of methanol and chloroform (1:1) to grow single crystals appropriate for X-ray diffraction studies by allowing slow evaporation of the solvent at room temperature. The X-ray diffraction data was collected on X'calibur CCD diffractometer with graphite monochromatized Mo/Kα radiation (λ = 0.71073 Å) at temperature 298 K. The structure was solved by direct methods using SHELXS-97 and refined by the full-matrix least-squares method on F^2 (SHELXL-97). All calculations were done with the help of WINGX package of crystallographic programs. For the molecular graphics, the program Mercury was used. The selected bond lengths, bond angles, etc. are given in Table 1.

Table 1. Crystal data and structure refinement for compound **8b**.

Identification code	**8b**
Empirical Formula	$C_{11}H_{14}N_2O_6$
Formula Weight	270.24
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P21
Unit cell dimensions	a = 5.9070(2) Å, α = 90°
	b = 11.2782(4) Å, β = 90.116(3)°
	c = 8.7658(3) Å, γ = 90°
Volume	583.98 (3) $Å^3$
Z	2
Density (calculated)	1.537 g/cm^3
Absorption coefficient	0.127 mm^{-1}
F (000)	284.0
Crystal size	0.1 × 0.1 × 0.1
Theta range for data collection	3.449 to 31.142

Index ranges	$-8 \leq h \leq 7$, $-14 \leq k \leq 14$, $-11 \leq l \leq 12$
Reflections collected	13929
Independent reflections	3788 [R(int) = 0.0346, R_{sigma} = 0.0263]
Refinement method	Full-matrix least-squares on F^2
Data/restrains/parameters	3788/1/179
Goodness-of-fit on F^2	0.854
Final R indices [1≥ 2sigma(I)]	R_1 = 0.0347, wR_2 = 0.1053
R indices (all data)	R_1 = 0.0400, wR_2 = 0.1118
CCDC No.	2240085