



Supporting Information

for

A new route for the synthesis of 1-deazaguanine and 1-deazahypoxanthine

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NMR spectra of compounds 17 to 22, 11, 31 and 30

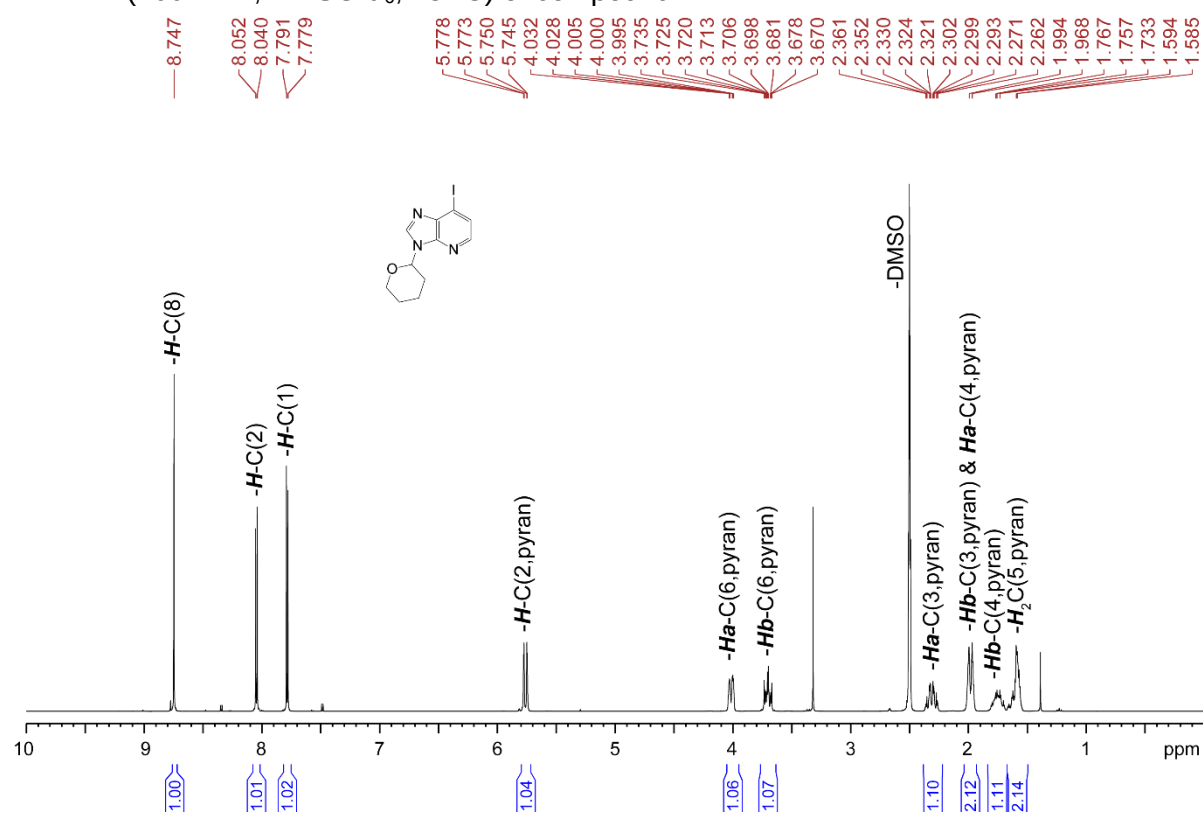
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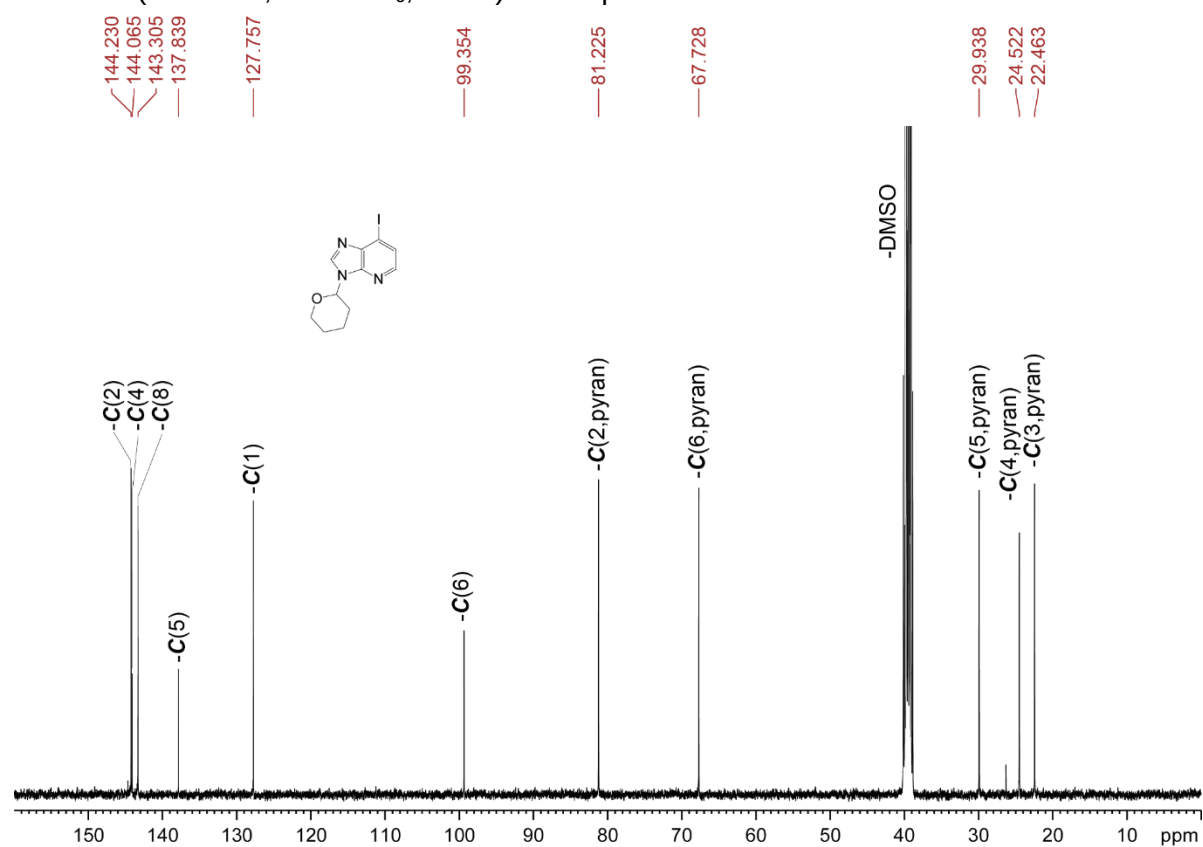
All synthetic procedures are described in the main text.

NMR spectra of compounds 17 to 22, 11, 31 and 30

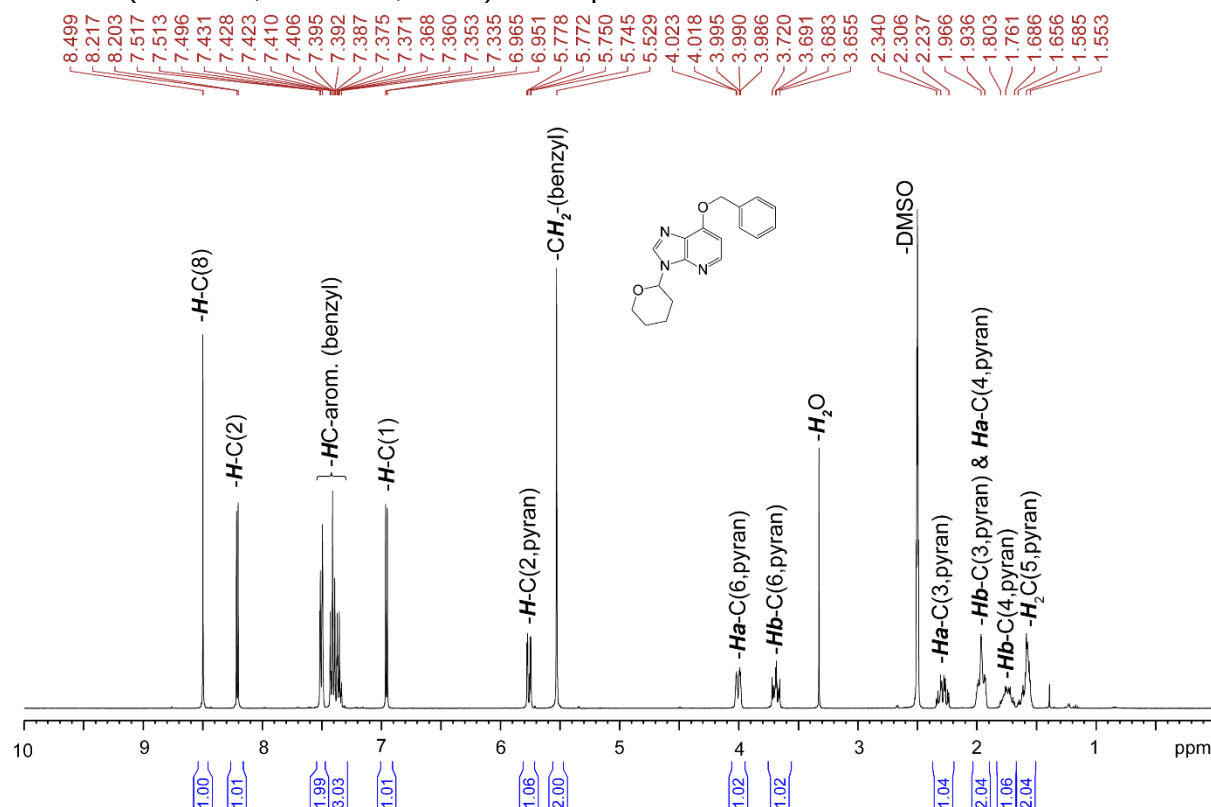
^1H NMR (400 MHz, $\text{DMSO}-d_6$, 25 °C) of compound **17**



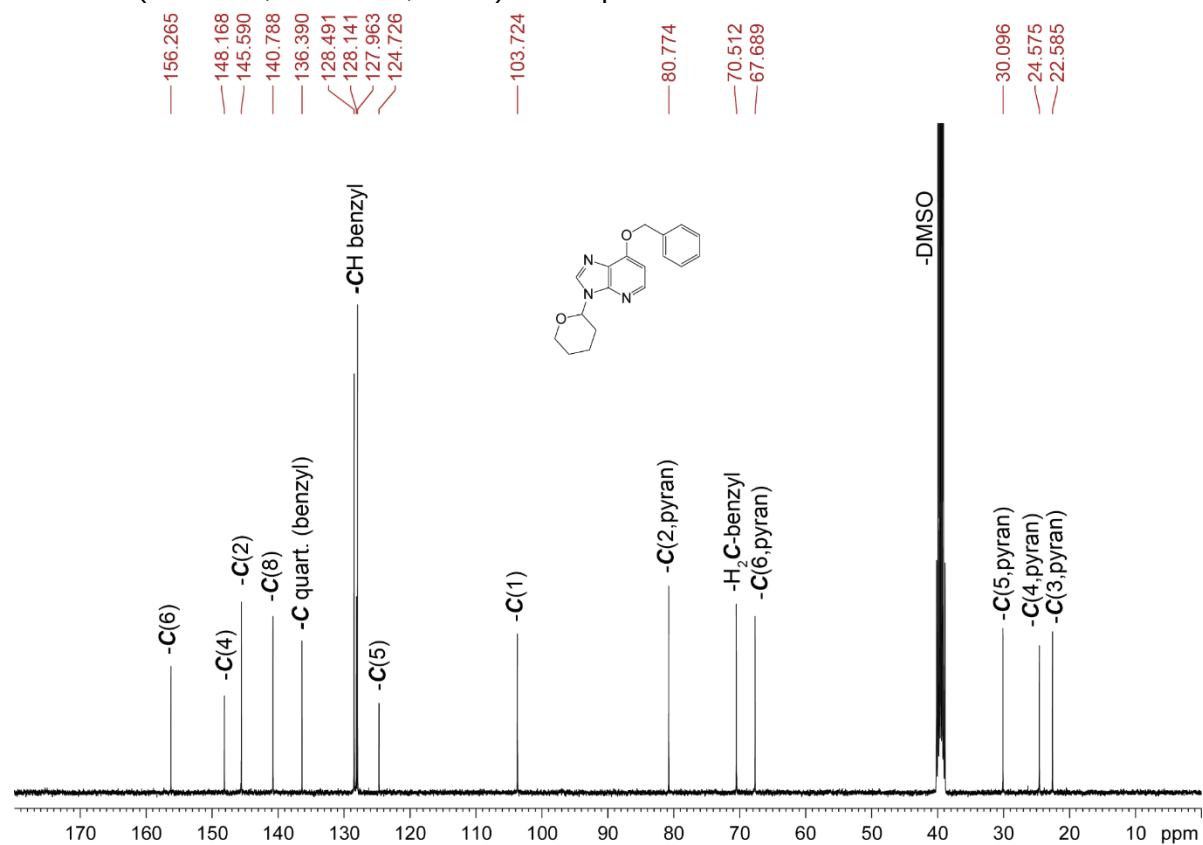
^{13}C NMR (100 MHz, $\text{DMSO}-d_6$, 25 °C) of compound **17**



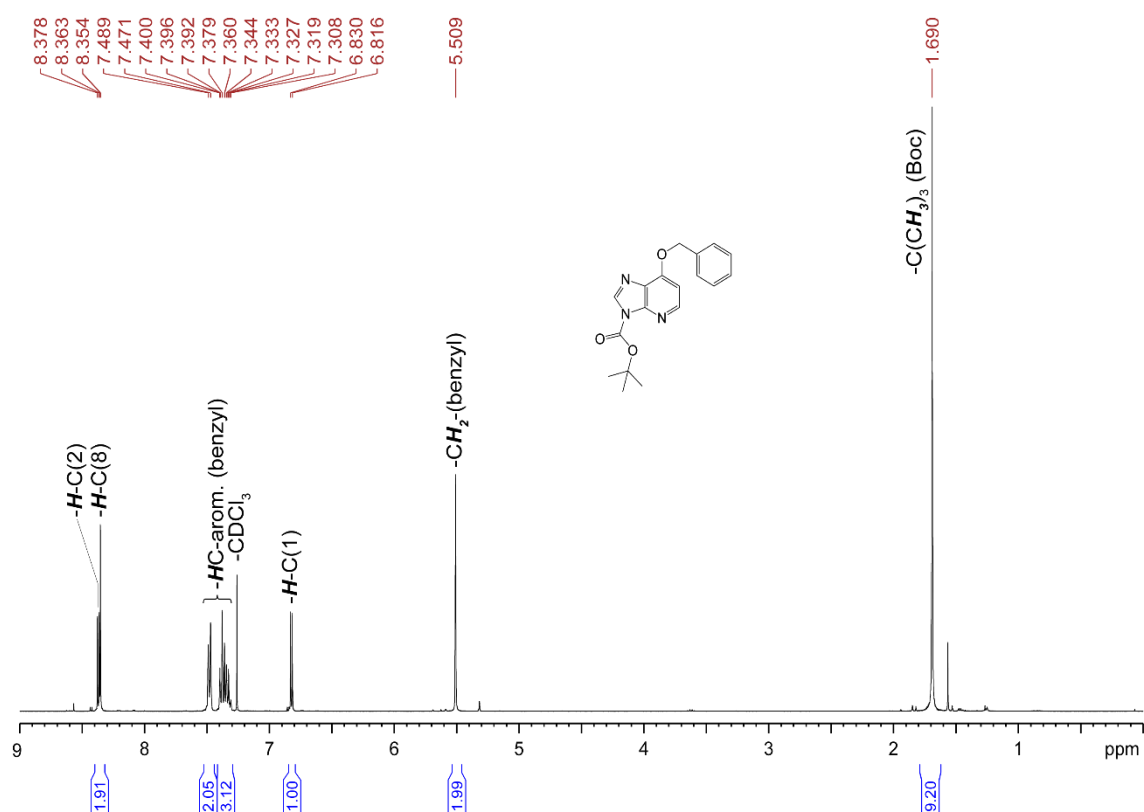
¹H NMR (400 MHz, DMSO-*d*₆, 25 °C) of compound **18**



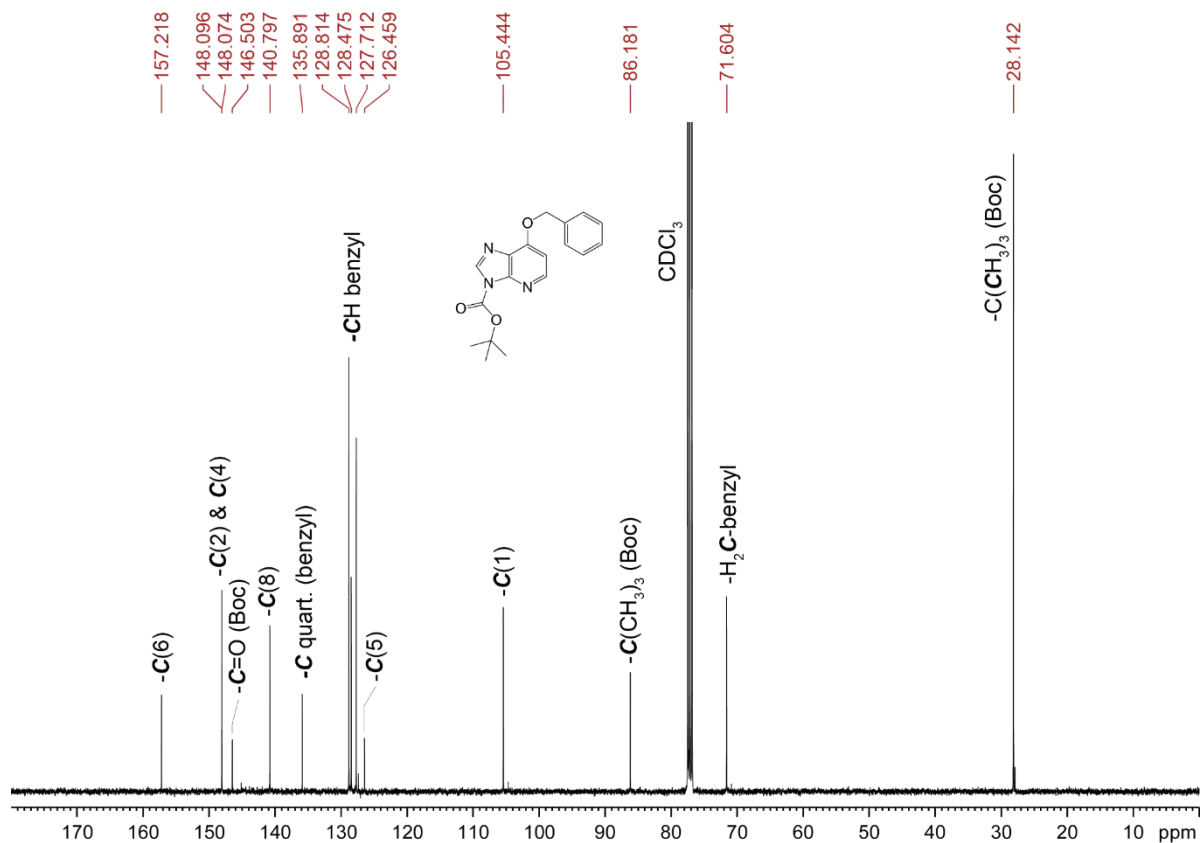
¹³C NMR (100 MHz, DMSO-*d*₆, 25 °C) of compound **18**



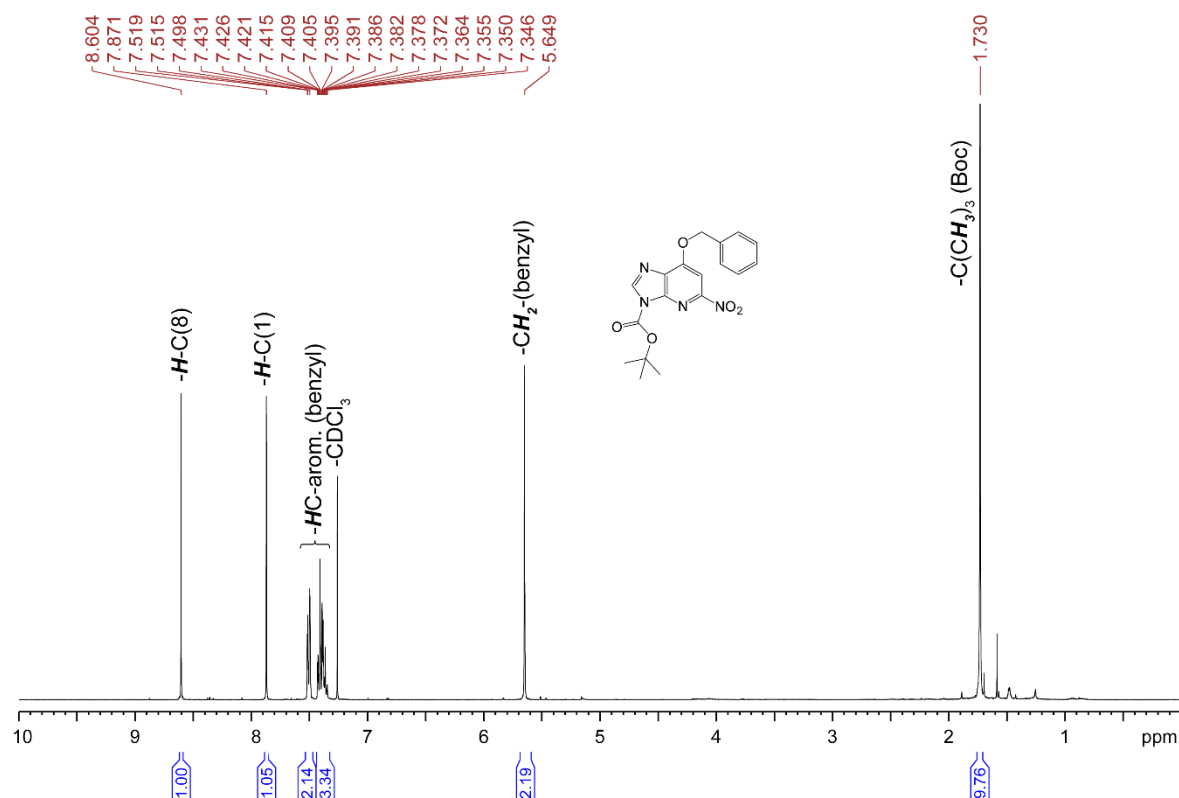
¹H NMR (400 MHz, CDCl₃, 25 °C) of compound **19**



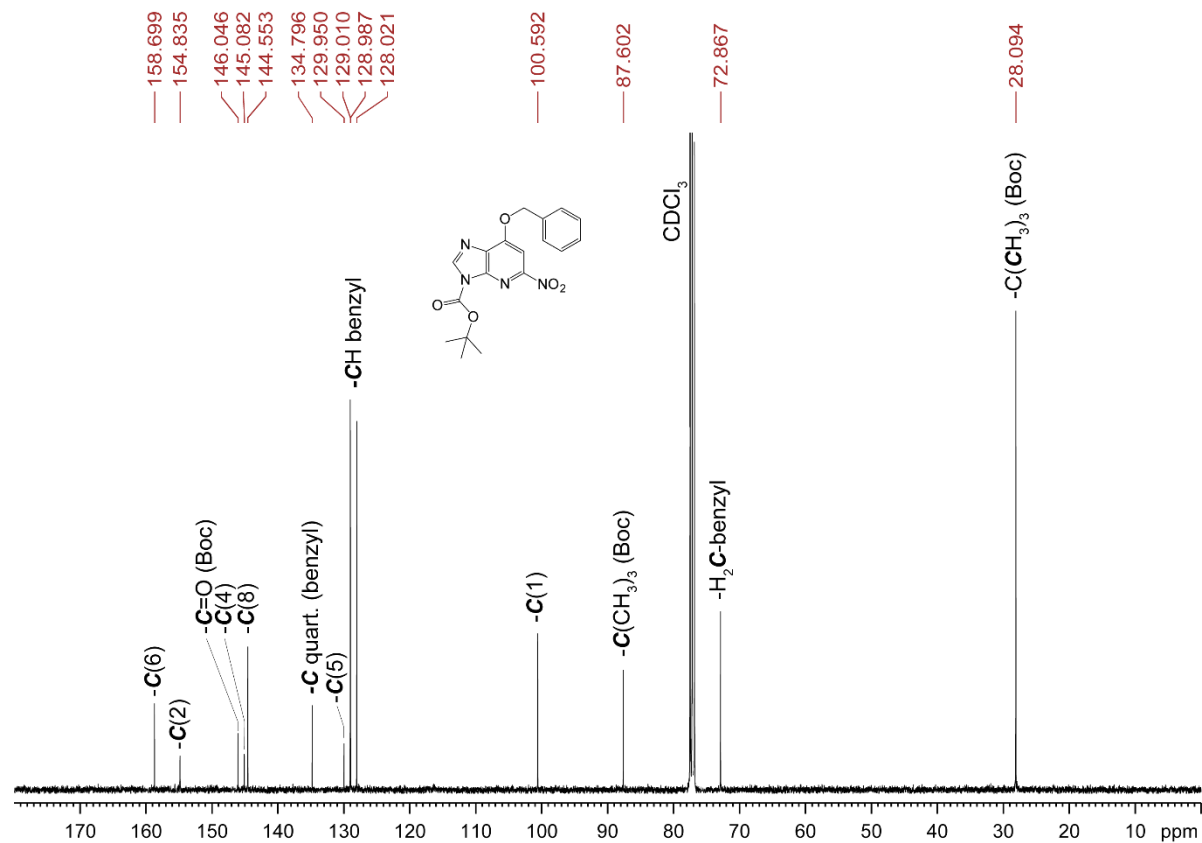
¹³C NMR (100 MHz, CDCl₃, 25 °C) of compound **19**



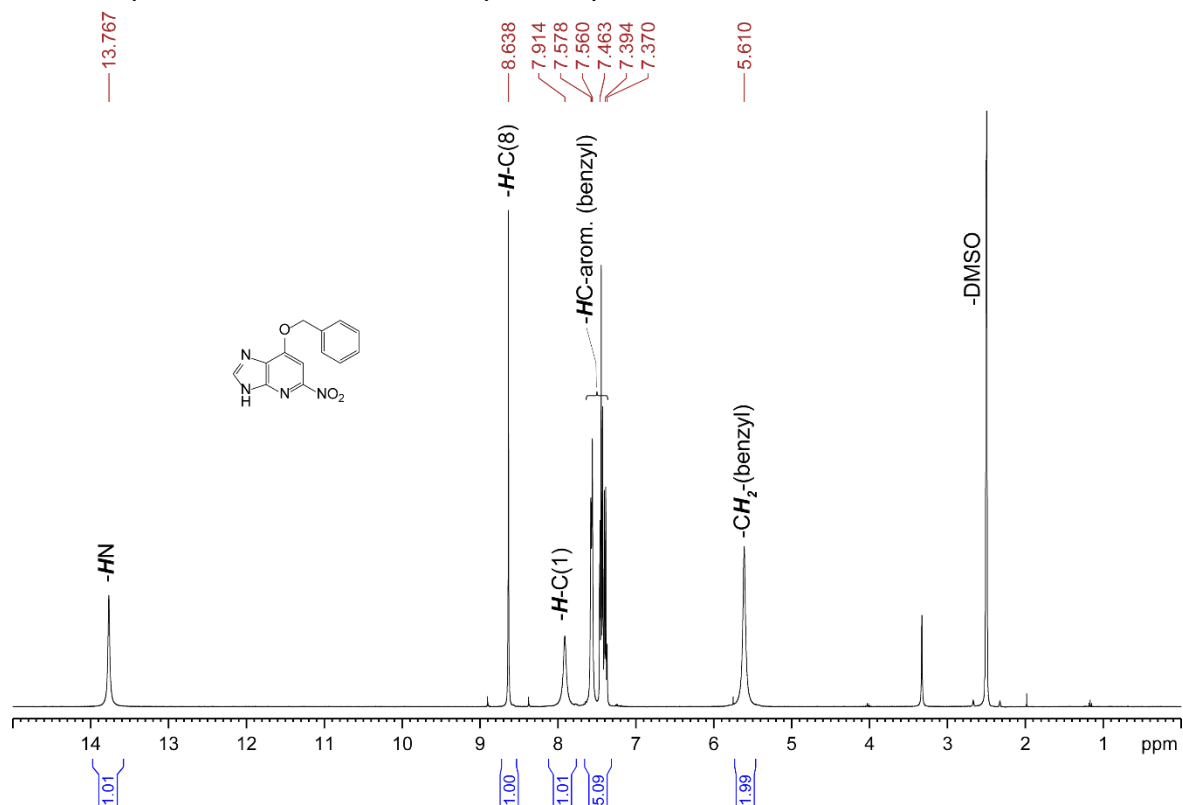
¹H NMR (400 MHz, CDCl₃, 25 °C) of compound **20**



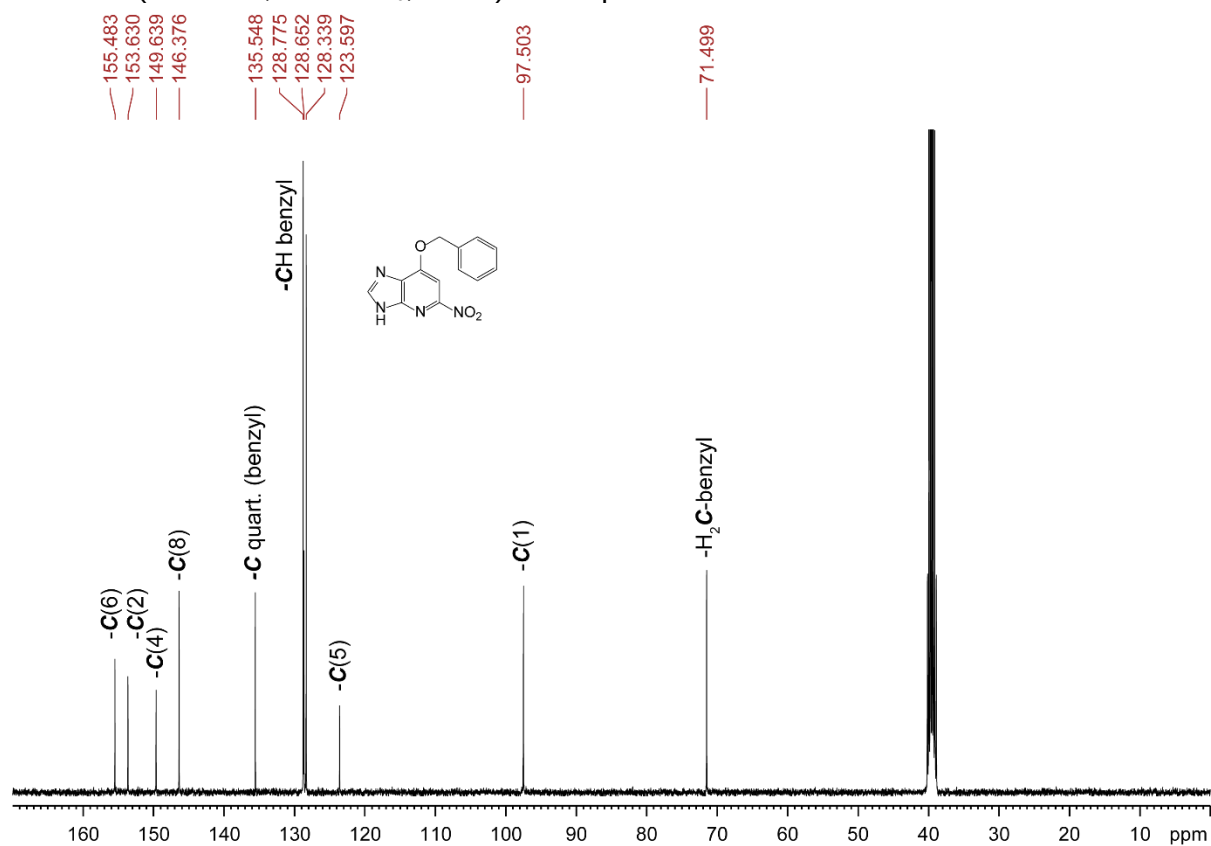
¹³C NMR (100 MHz, CDCl₃, 25 °C) of compound **20**



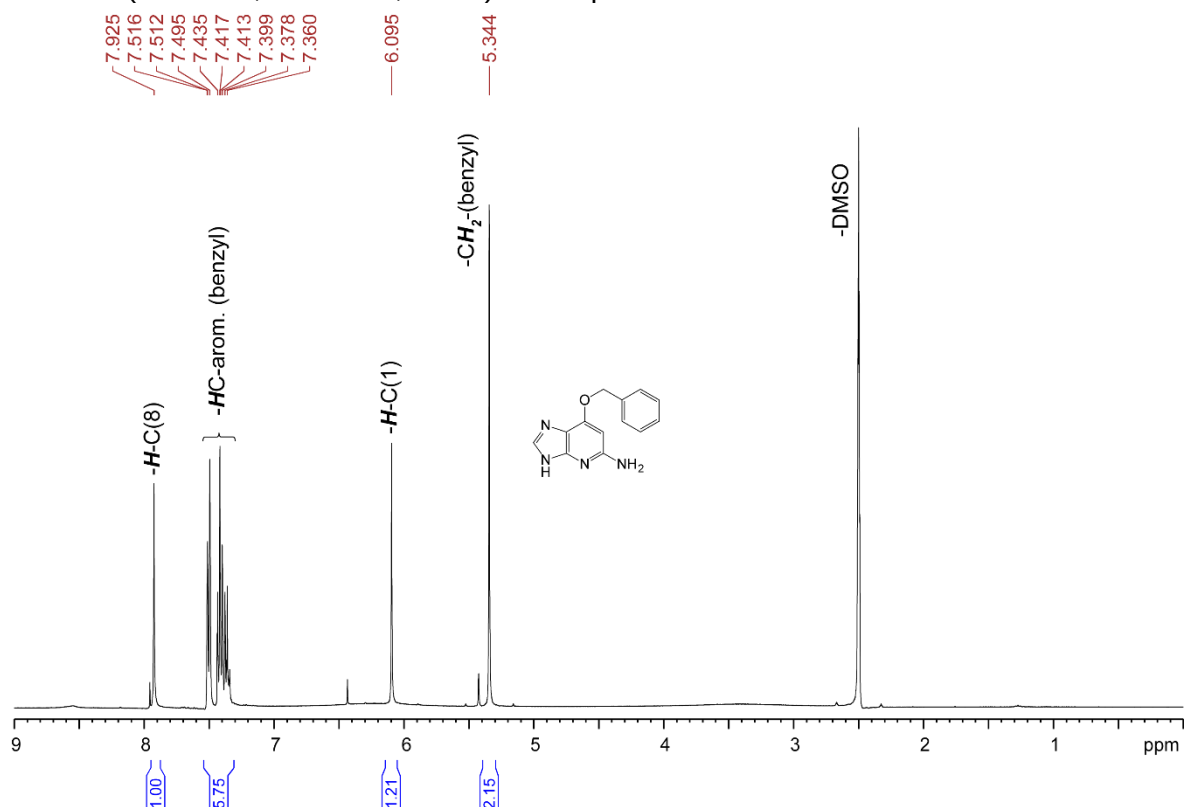
^1H NMR (400 MHz, $\text{DMSO}-d_6$, 25 °C) of compound **21**



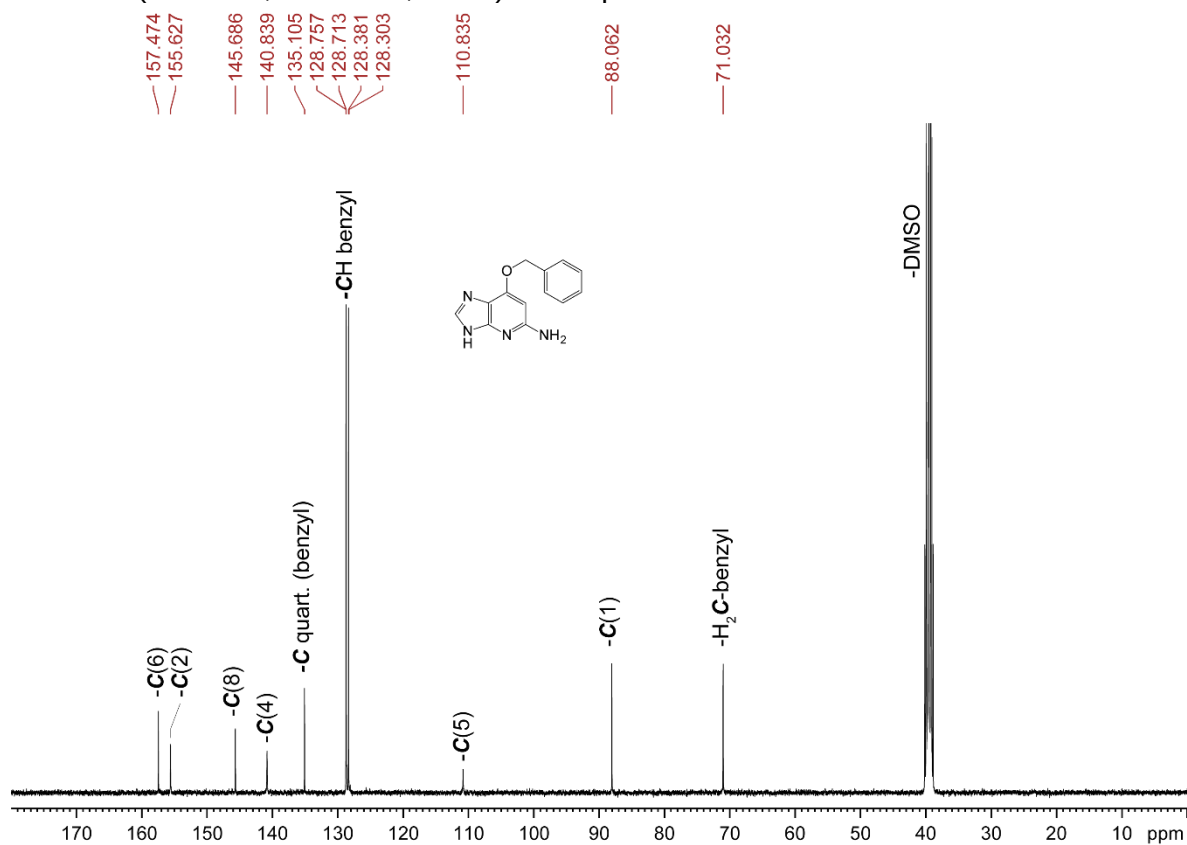
^{13}C NMR (100 MHz, $\text{DMSO}-d_6$, 25 °C) of compound **21**



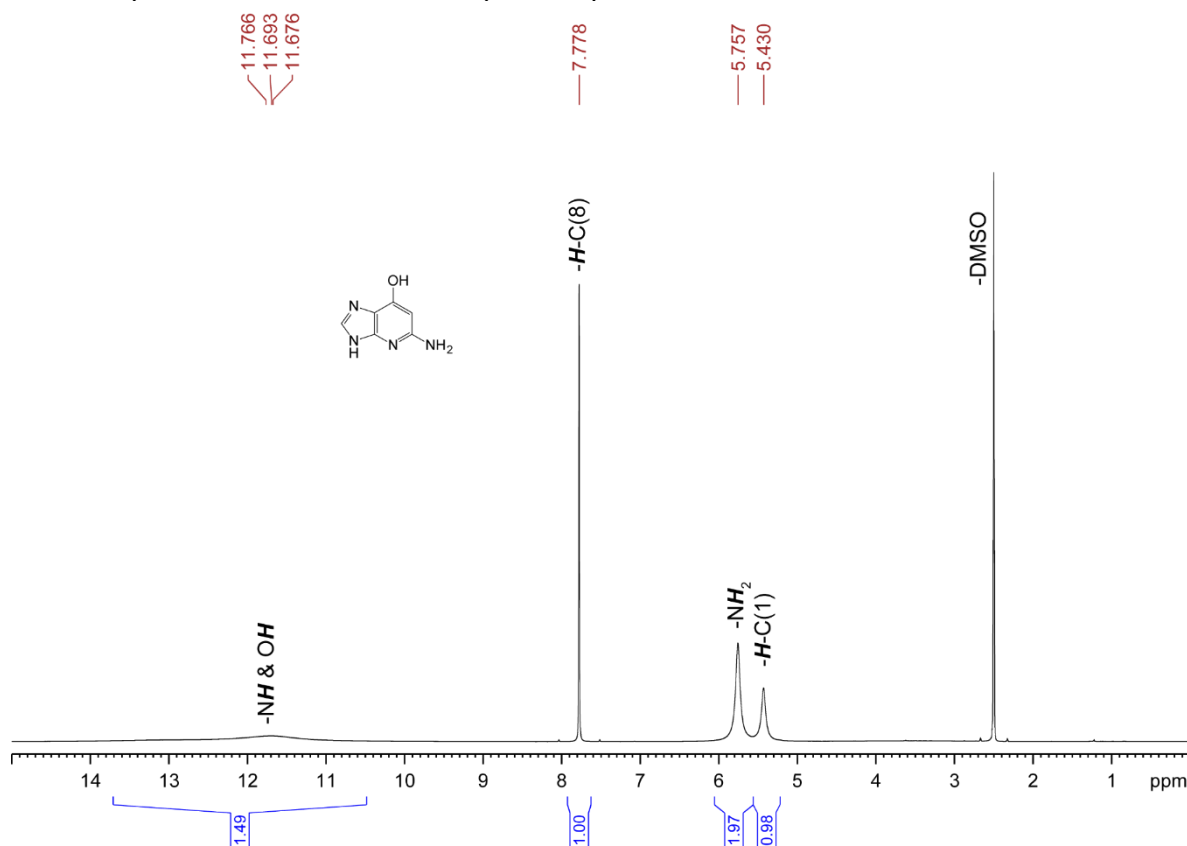
¹H NMR (400 MHz, DMSO-*d*₆, 25 °C) of compound **22**



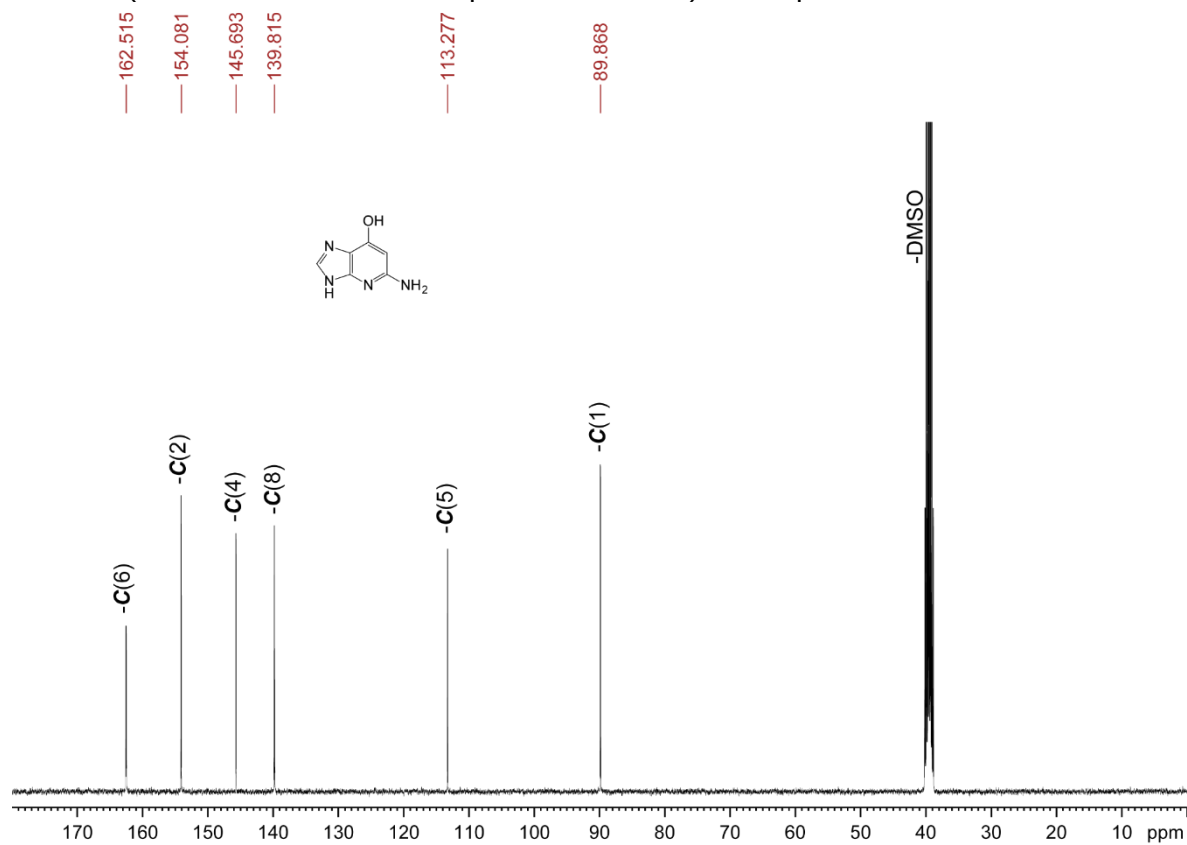
¹³C NMR (100 MHz, DMSO-*d*₆, 25 °C) of compound **22**



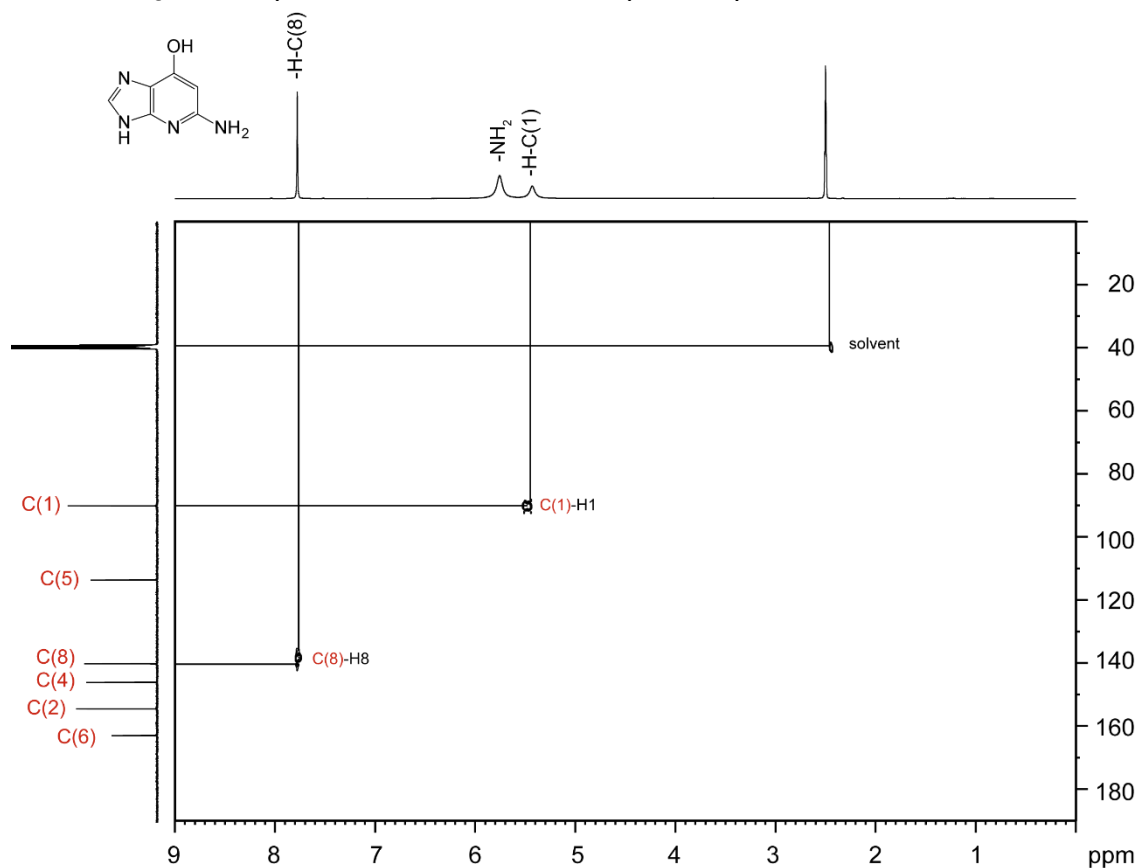
^1H NMR (400 MHz, $\text{DMSO}-d_6$, 25 °C) of compound **11**



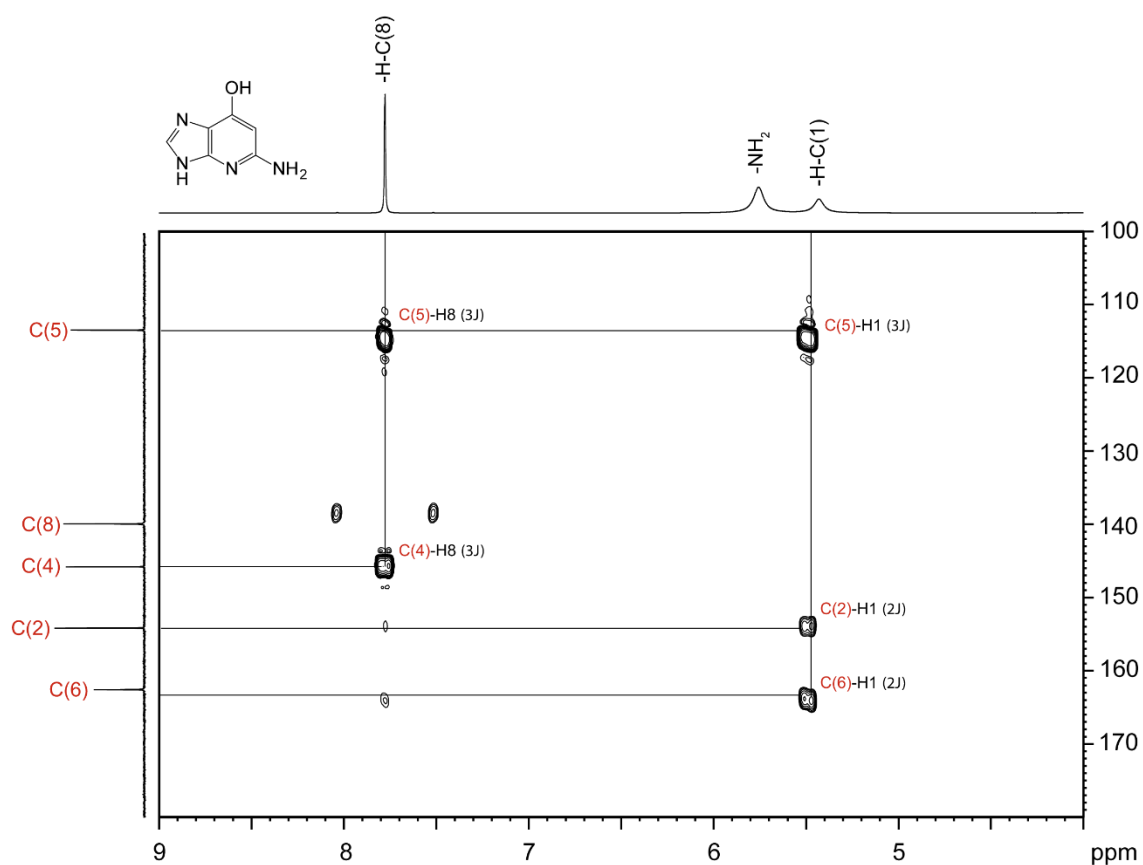
^1H NMR (100 MHz, $\text{DMSO}-d_6$ + 40 μl 5% HCl, 25 °C) of compound **11**



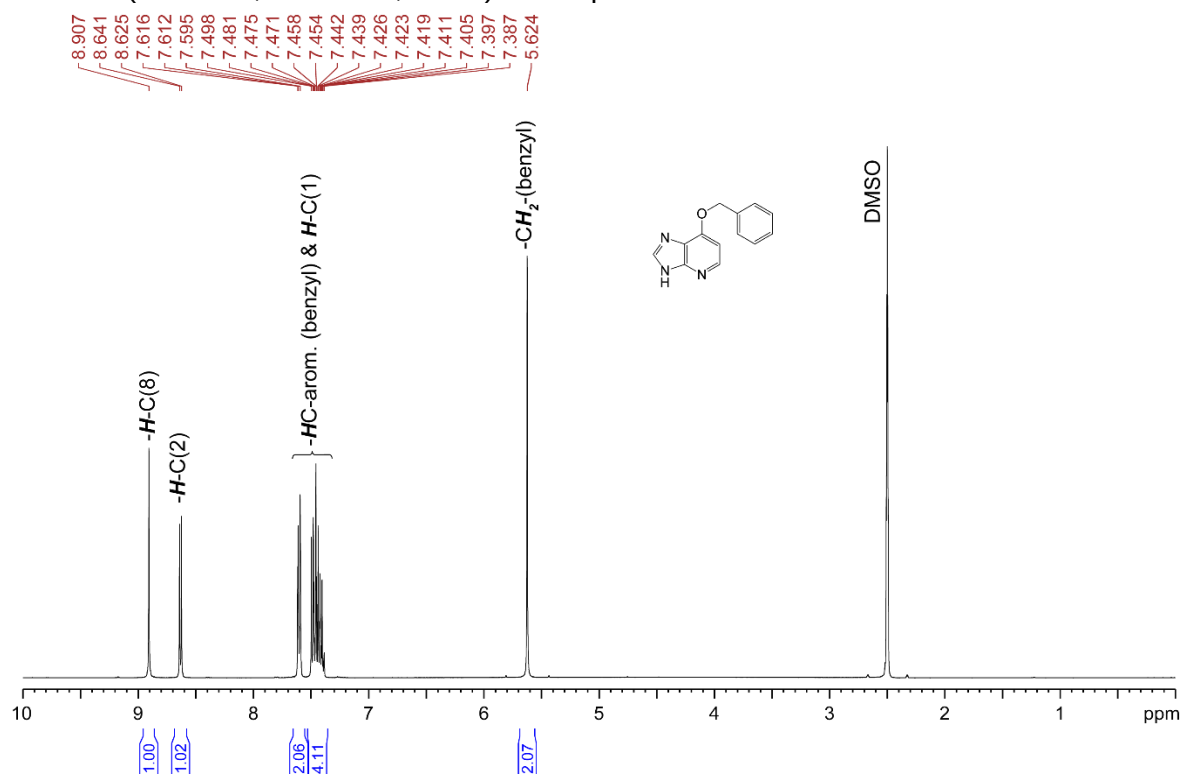
^1H , ^{13}C HSQC NMR (400 MHz, $\text{DMSO-}d_6$, 25 °C) of compound **11**



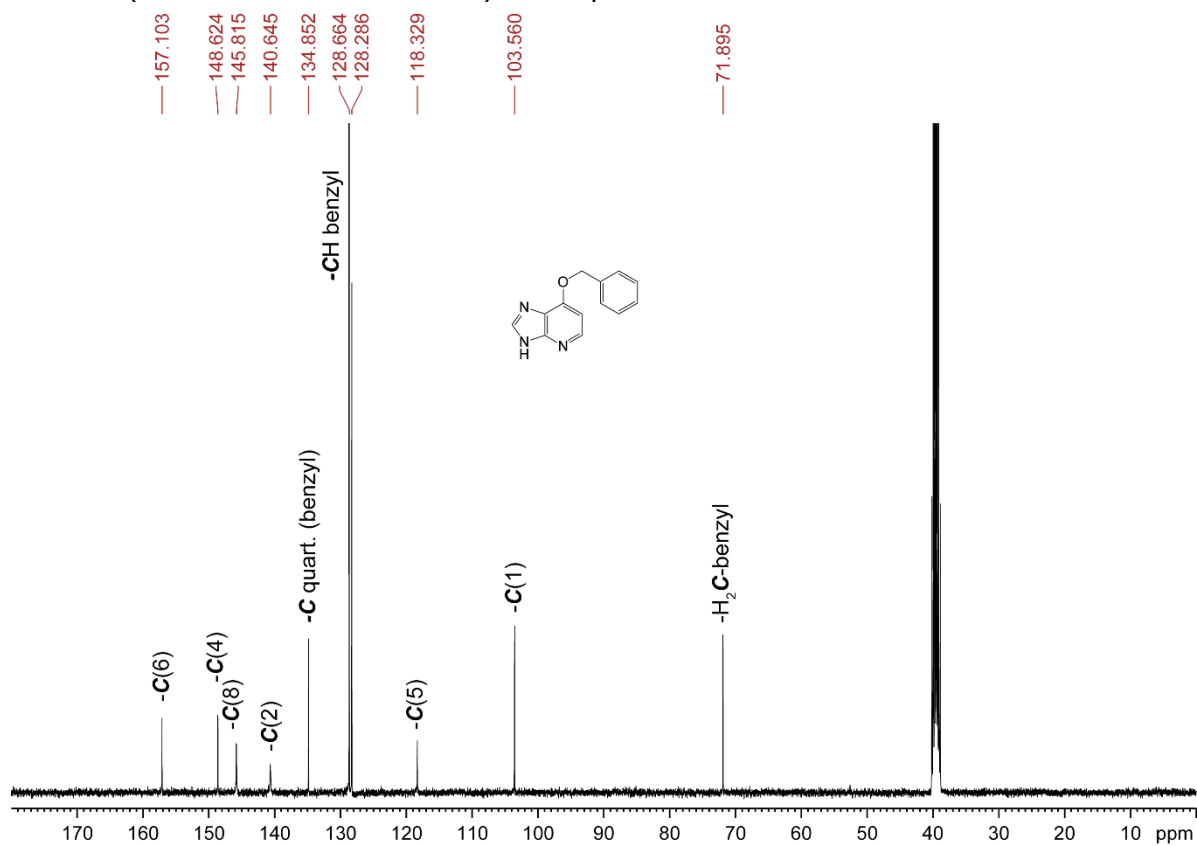
^1H , ^{13}C HMBC NMR (400 MHz, $\text{DMSO-}d_6$, 25 °C) of compound **11**



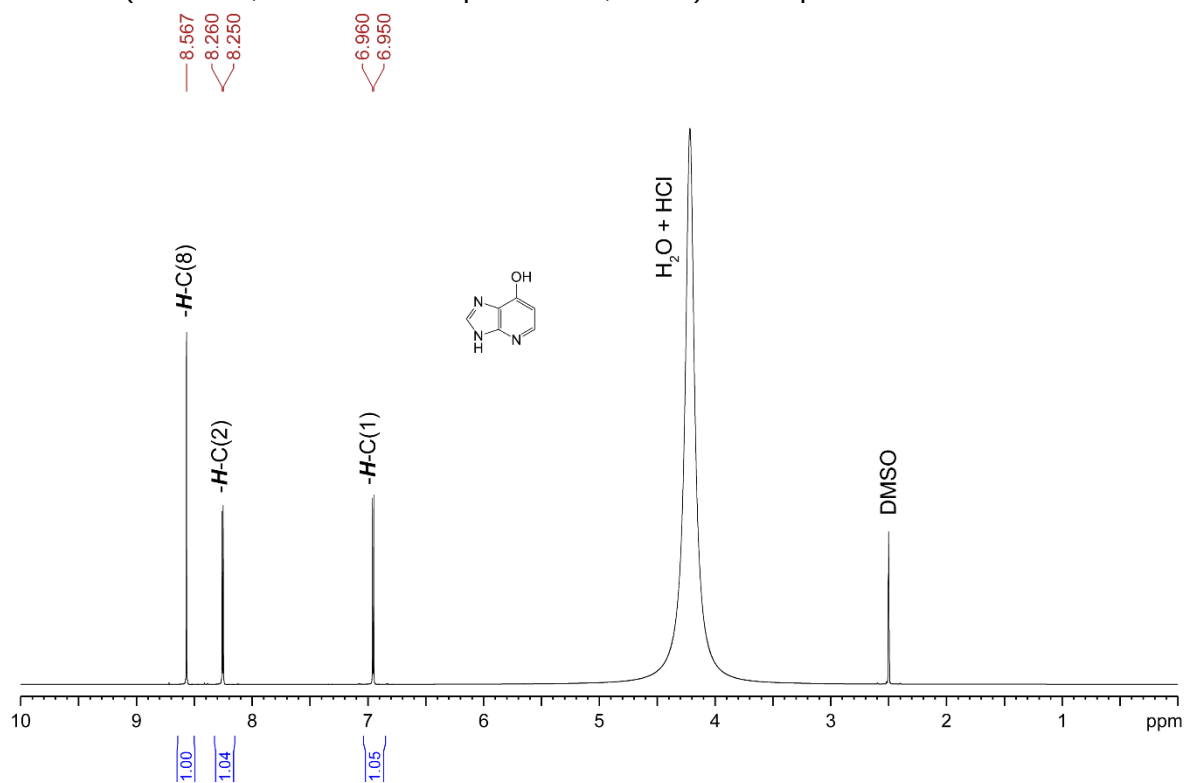
^1H NMR (400 MHz, $\text{DMSO}-d_6$, 25 °C) of compound **31**



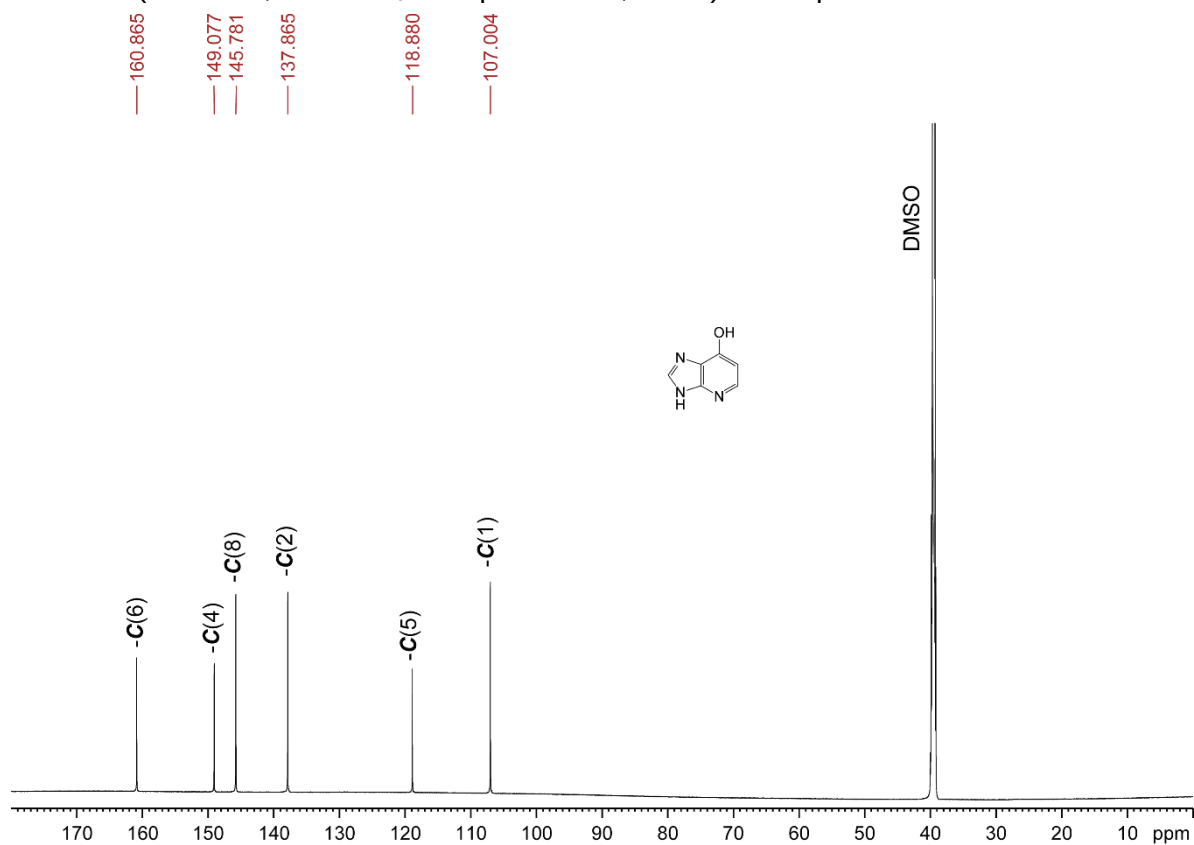
^{13}C NMR (400 MHz, $\text{DMSO}-d_6$, 25 °C) of compound **31**



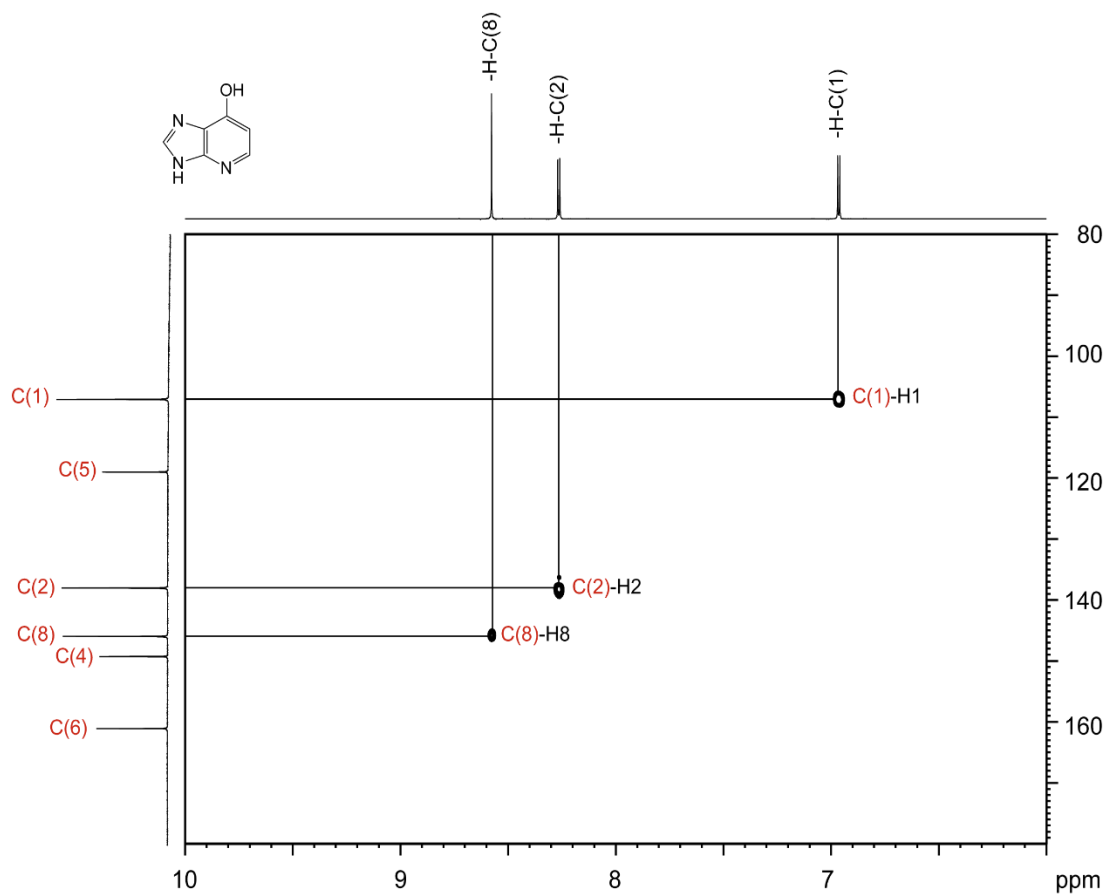
^1H NMR (700 MHz, $\text{DMSO}-d_6 + 40\ \mu\text{L}\ 5\% \text{HCl}$, 25 °C) of compound **30**



^{13}C NMR (175 MHz, $\text{DMSO}-d_6 + 40\ \mu\text{L}\ 5\% \text{HCl}$, 25 °C) of compound **30**



^1H , ^{13}C HSQC NMR (700 MHz, $\text{DMSO}-d_6$, 25 °C) of compound **30**



^1H , ^{13}C HSQC NMR (700 MHz, $\text{DMSO}-d_6$, 25 °C) of compound **30**

