

**Supplementary data for
A fluorescent 3,7-bis-(naphthalen-1-ylethynylated)-2'-deoxy-adenosine analogue reports
thymidine in complementary DNA by a large emission Stokes shift**

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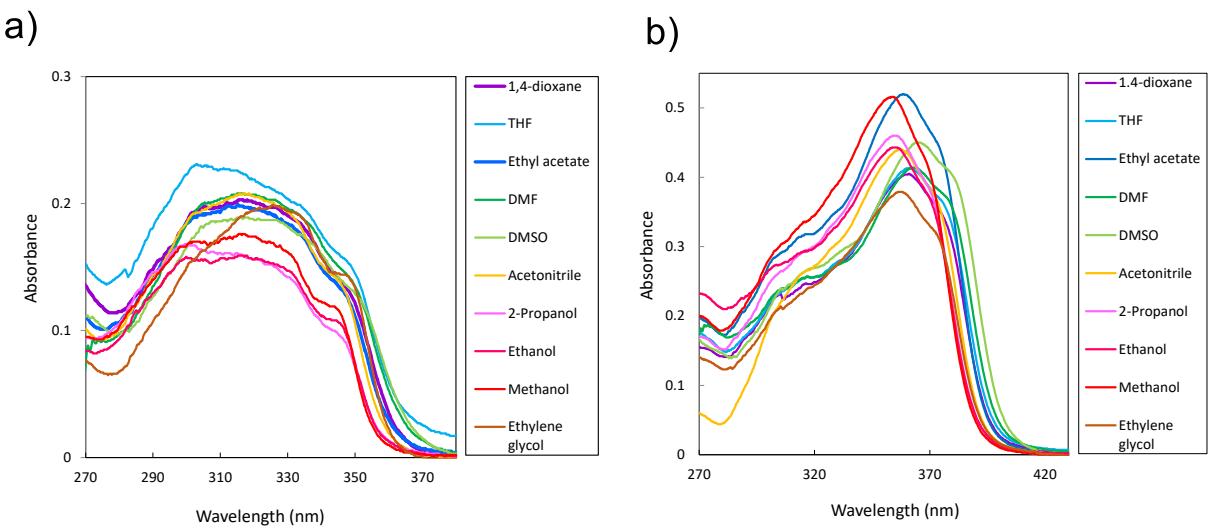


Figure S1. UV absorption spectra of (a) ^{37}nza (**2**) and (b) ^{3n7}nza (**1**) in various solvents of different polarities. All measurements were performed at a concentration of $10 \mu\text{M}$.

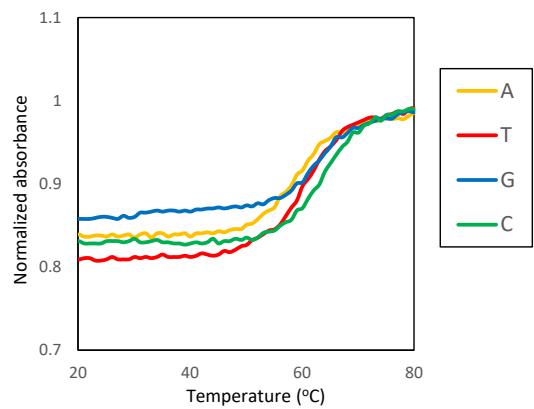


Figure S2. Thermal melting temperature (T_m) of ODN1(^{37nz}A) hybridized with cODN1(N), (N = A, T, G, or C) (2.5 μ M duplex, 0.1 M sodium chloride, 50 mM sodium phosphate buffer, pH 7.0, rt).

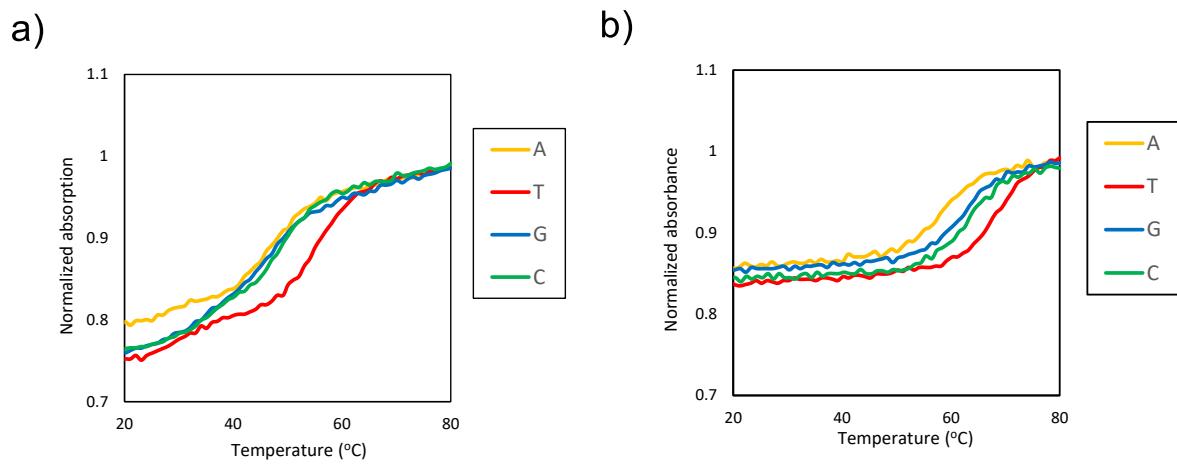


Figure S3. Thermal melting temperature (T_m) of (a) ODN1($^{3n}7^{nz}A$) hybridized with cODN1(**N**), (**N** = A, T, G, or C) and (b) ODN2($^{3n}7^{nz}A$) hybridized with cODN2(**N**), (**N** = A, T, G, or C) (2.5 μ M duplex, 0.1 M sodium chloride, 50 mM sodium phosphate buffer, pH 7.0, rt).

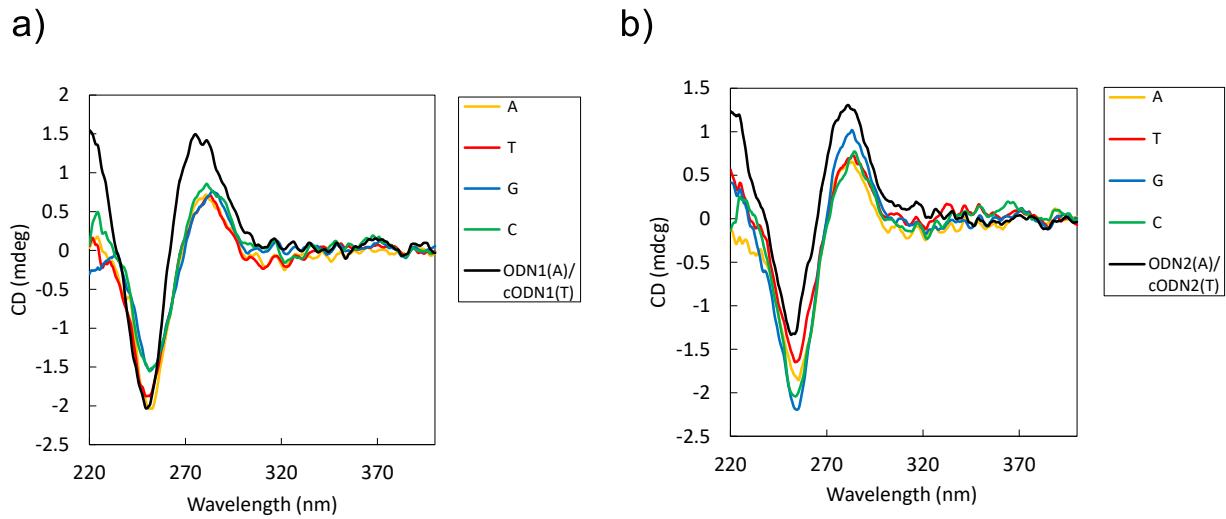


Figure S4. CD spectra of (a) ODN1(^{3n7nz}A) hybridized with cODN1(N), (N = A, T, G, or C) and (b) ODN2(^{3n7nz}A) hybridized with cODN2(N), (N = A, T, G, or C) (2.5 μ M duplex, 0.1 M sodium chloride, 50 mM sodium phosphate buffer, pH 7.0, rt).

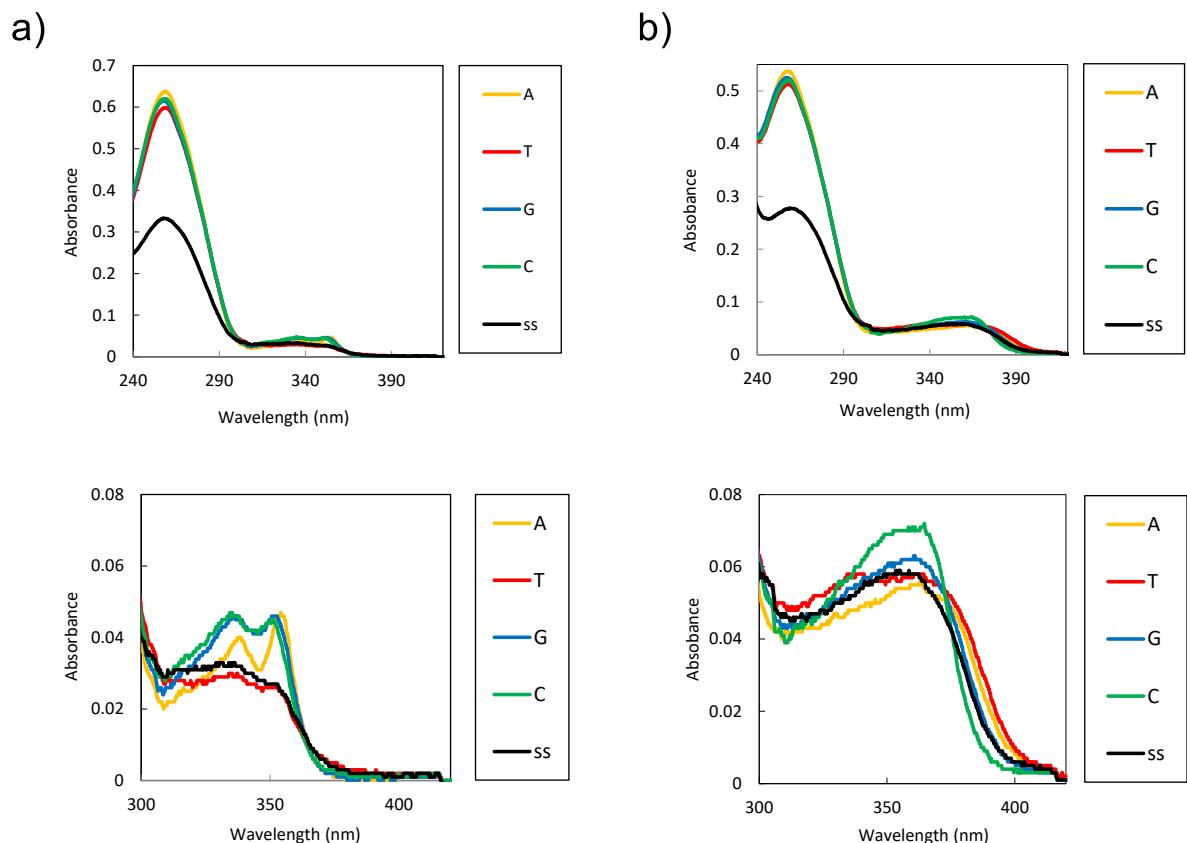


Figure S5. UV absorption spectra of (a) ODN1(^{37n}A) hybridized with cODN1(**N**), (**N** = A, T, G, or C) and (b) ODN1($^{3n}7nA$) hybridized with cODN1(**N**), (**N** = A, T, G, or C) (2.5 μ M duplex, 0.1 M sodium chloride, 50 mM sodium phosphate buffer, pH 7.0, rt).

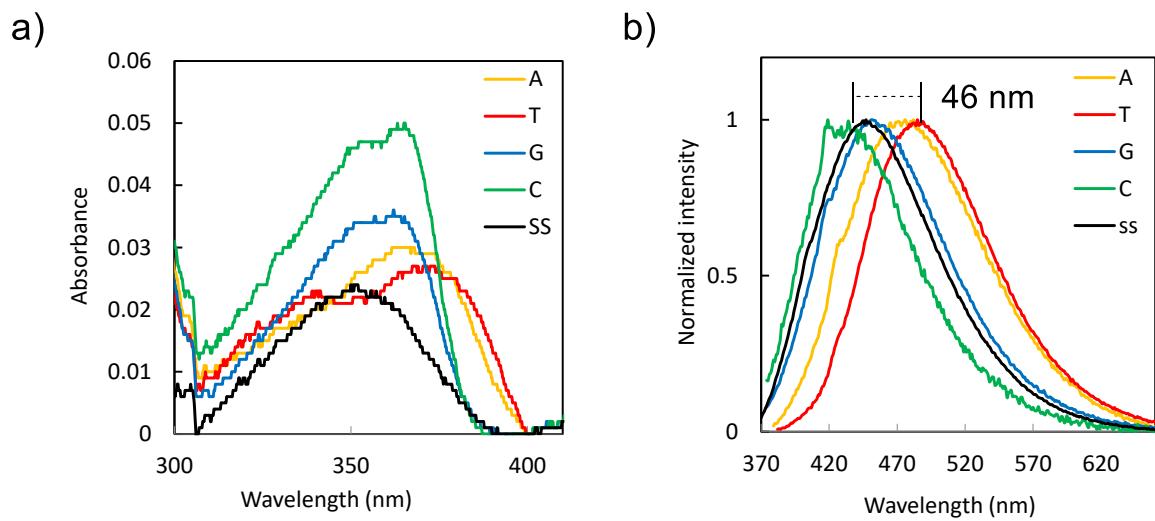


Figure S6. (a) UV absorption and (b) normalized fluorescent spectra of ODN2($^{3n}7n^zA$) hybridized with cODN2(N), (N = A, T, G, or C) (2.5 μ M duplex, 0.1 M sodium chloride, 50 mM sodium phosphate buffer, pH 7.0, rt).

Table S1. MALDI-TOF-MS spectral data for the ODNs

ODNs	Sequences	MALDI-TOF-MS	
		calcd. [M + H] ⁺	found [M + H] ⁺
ODN1(^{37nz} A)	5'-d(CGCAAT ^{37nz} A TAACGC)-3'	4077.85	4077.55
ODN1(^{3n7nz} A)	5'-d(CGCAAT ^{3n7nz} ATAACGC)-3'	4228.03	4227.83
ODN2(^{3n7nz} A)	5'-d(CGCAAC ^{3n7nz} ACAACGC)-3'	4198.01	4197.08

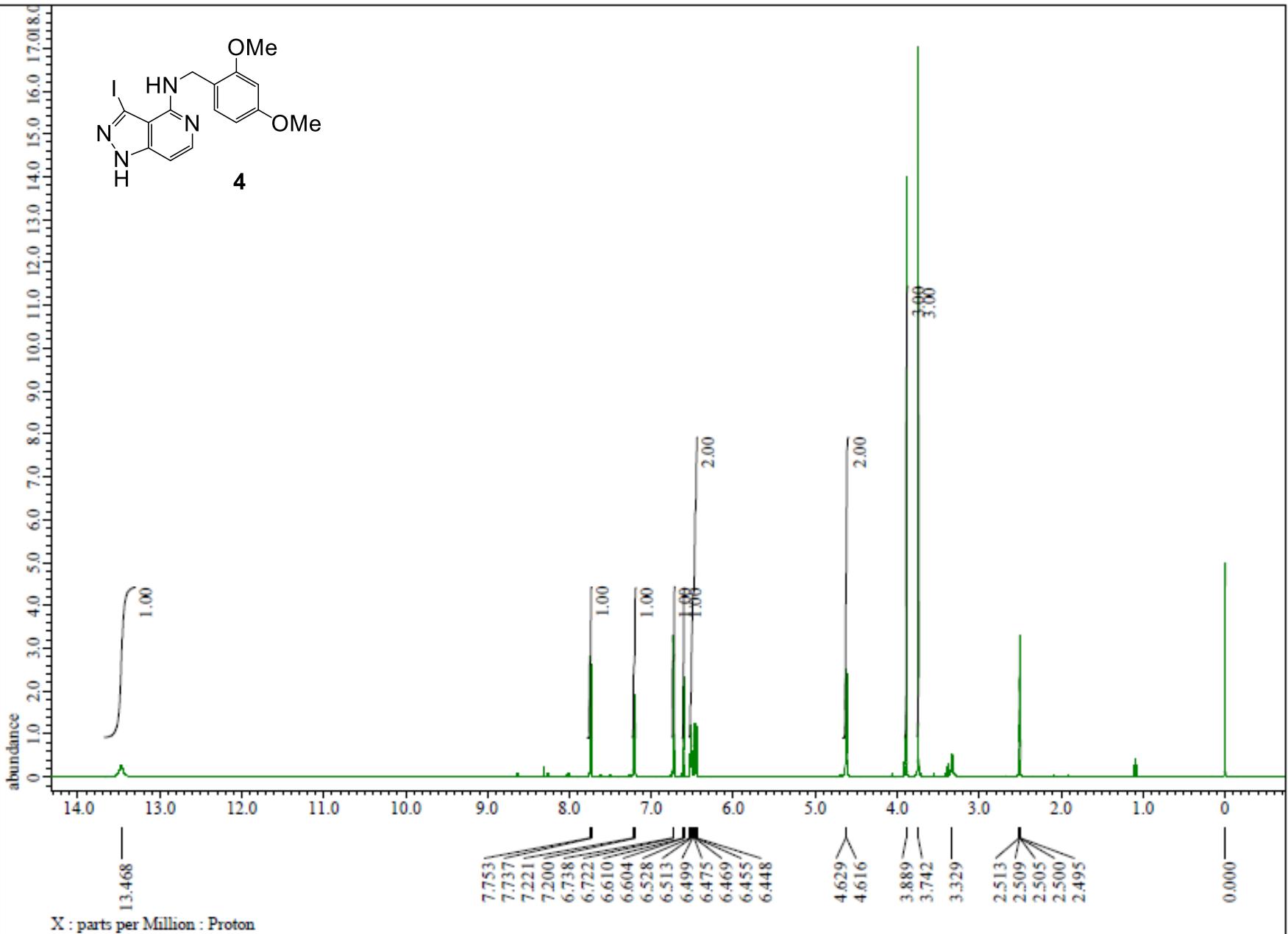


Figure S7. ^1H -NMR spectrum of compound **4** (DMSO- d_6)

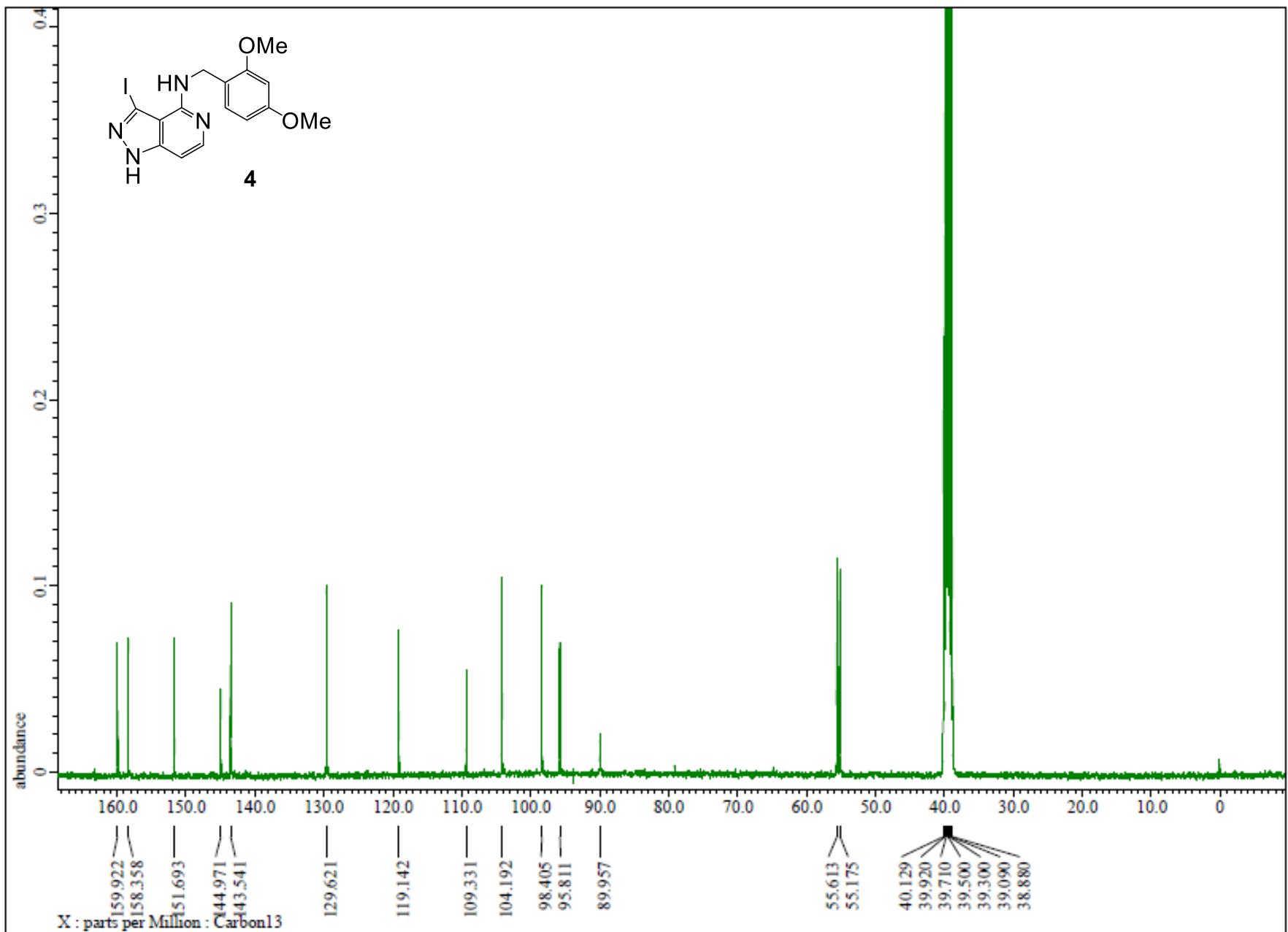


Figure S8. ^{13}C -NMR spectrum of compound **4** ($\text{DMSO}-d_6$)

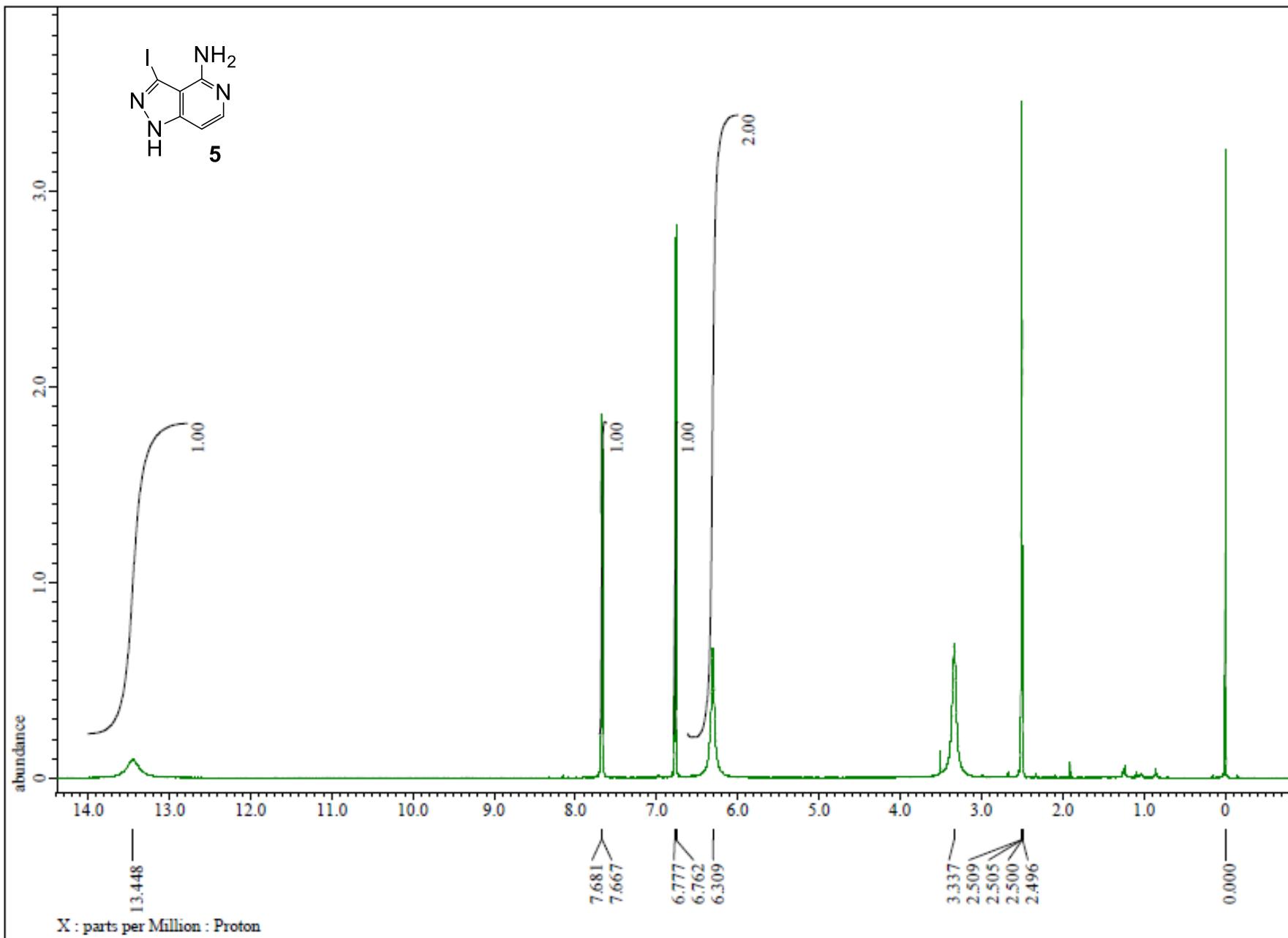


Figure S9. ^1H -NMR spectrum of compound 5 (DMSO- d_6)

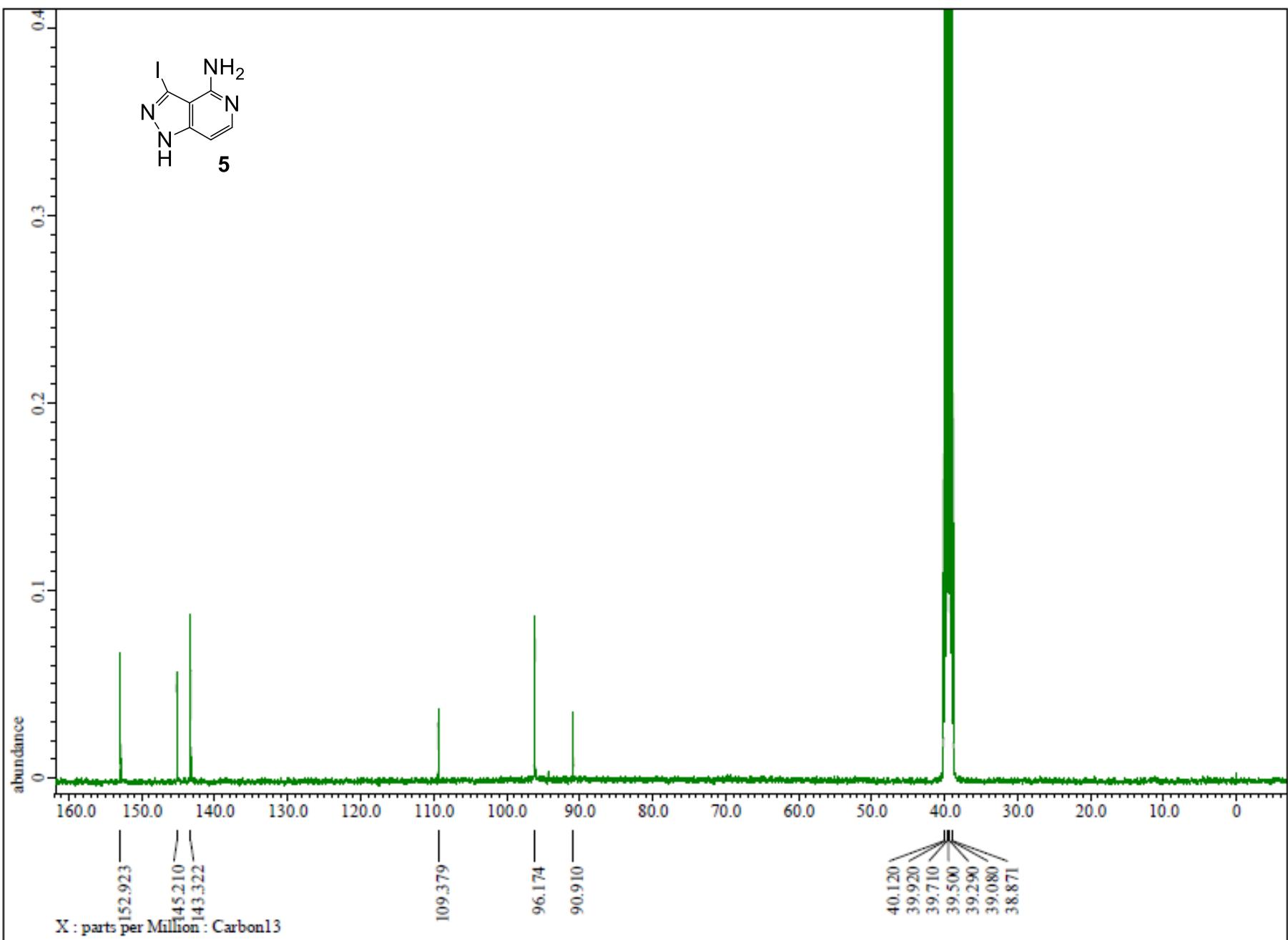


Figure S10. ^{13}C -NMR spectrum of compound **5** (DMSO- d_6)

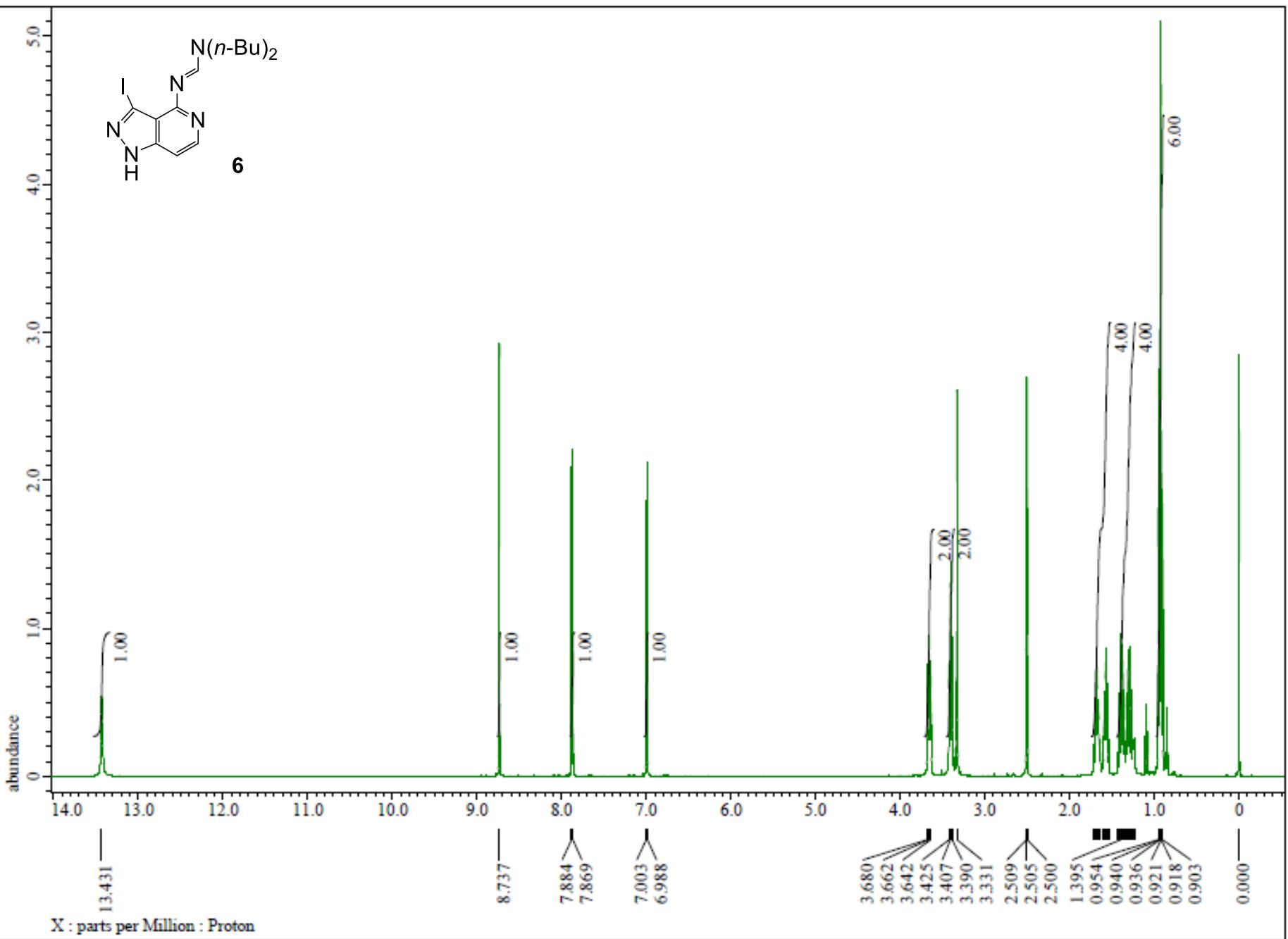


Figure S11. ¹H-NMR spectrum of compound 5 (DMSO-*d*₆)

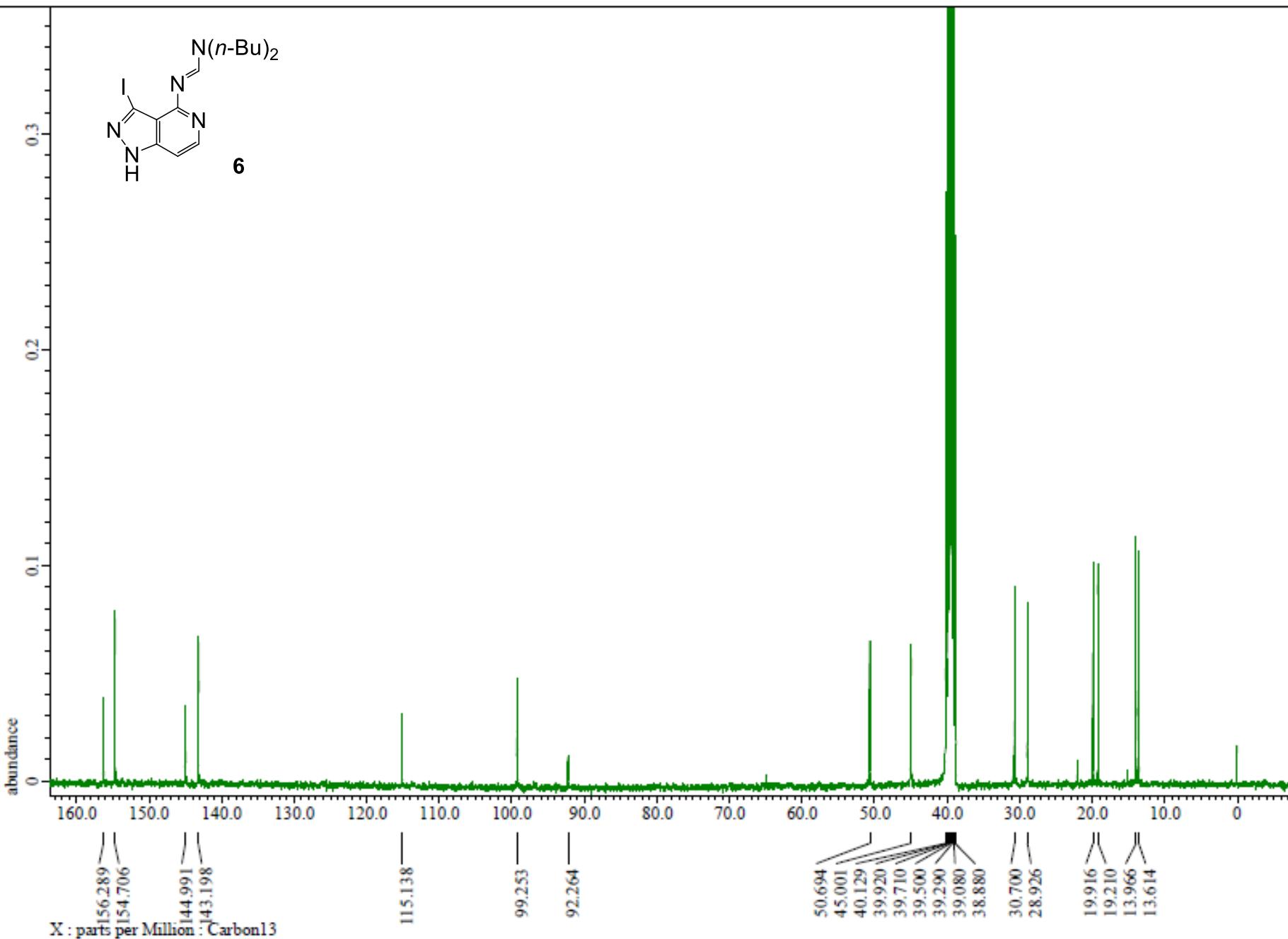


Figure S12. ^{13}C -NMR spectrum of compound 5 ($\text{DMSO}-d_6$)

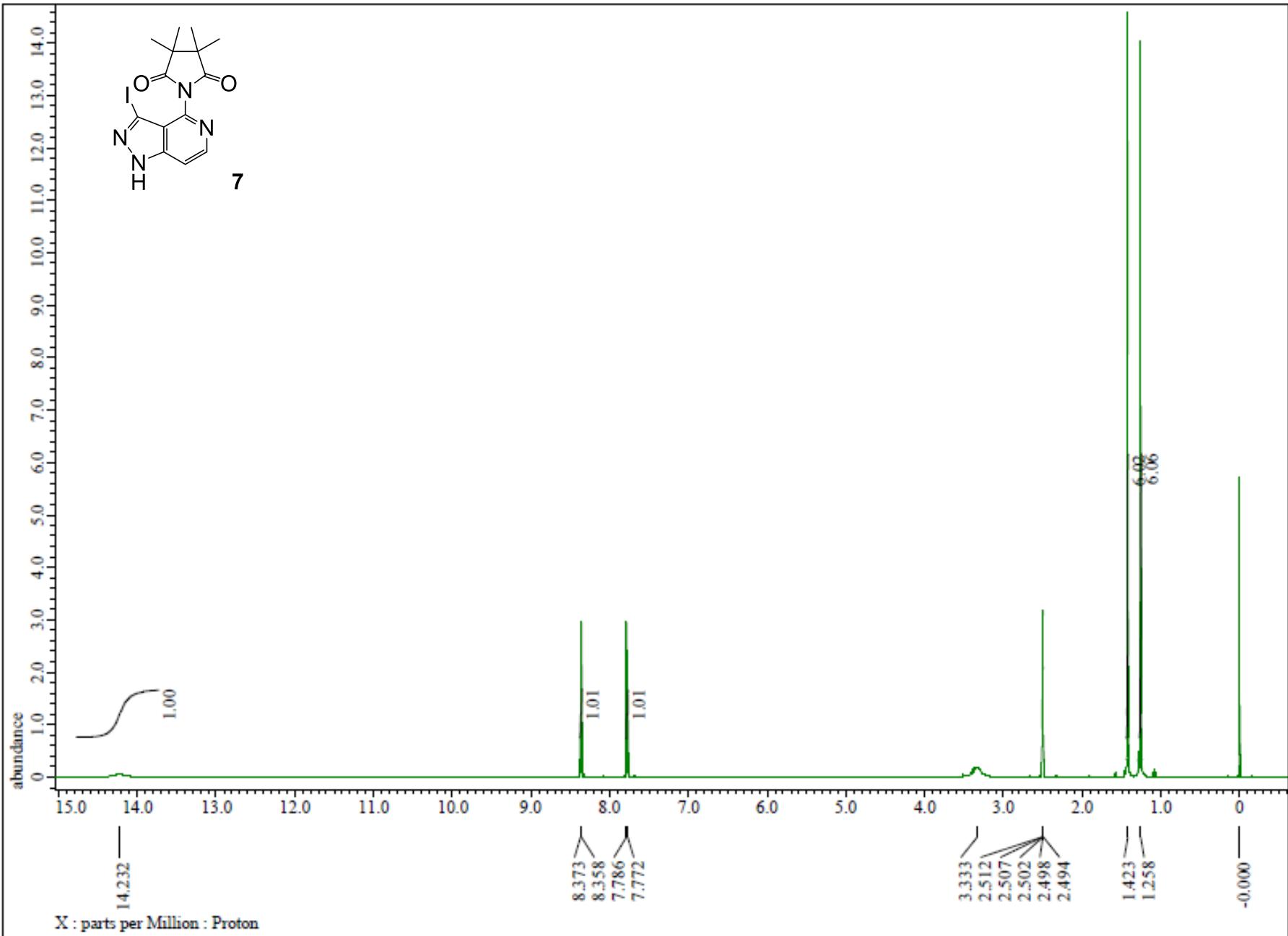


Figure S13. ^1H -NMR spectrum of compound 7 (DMSO- d_6)

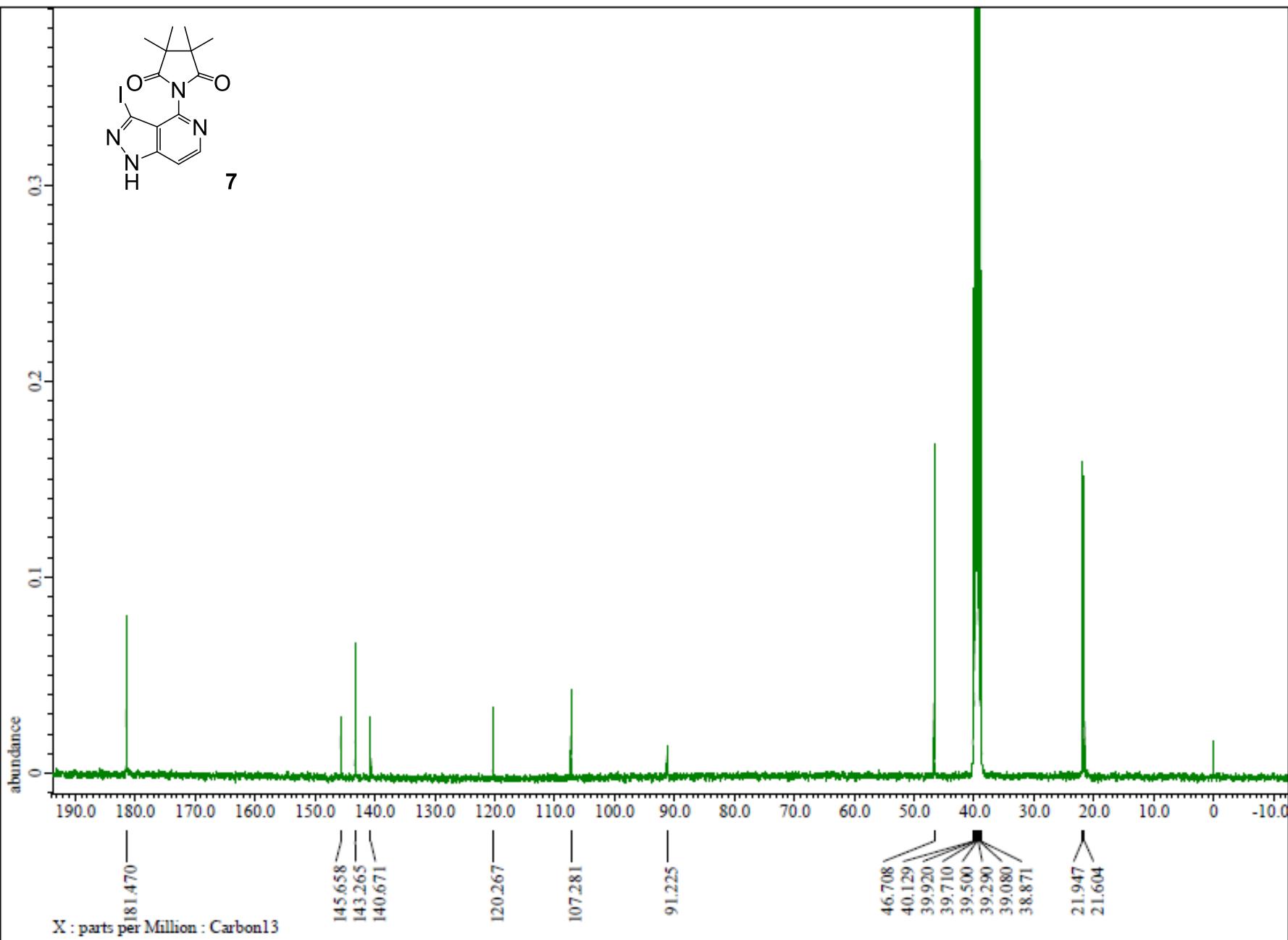


Figure S14. ^{13}C -NMR spectrum of compound 7 ($\text{DMSO}-d_6$)

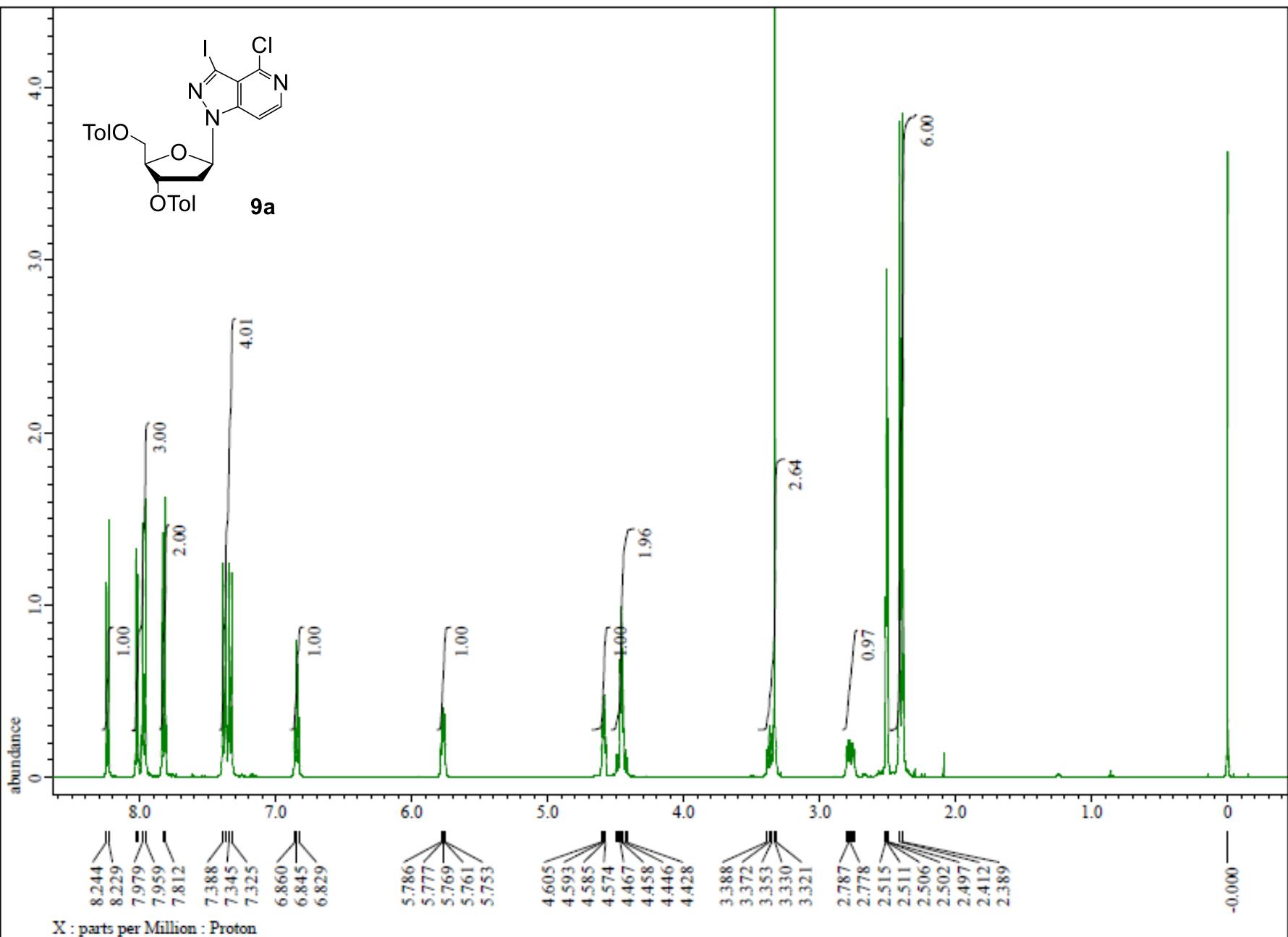


Figure S15. ^1H -NMR spectrum of compound **9a** ($\text{DMSO}-d_6$)

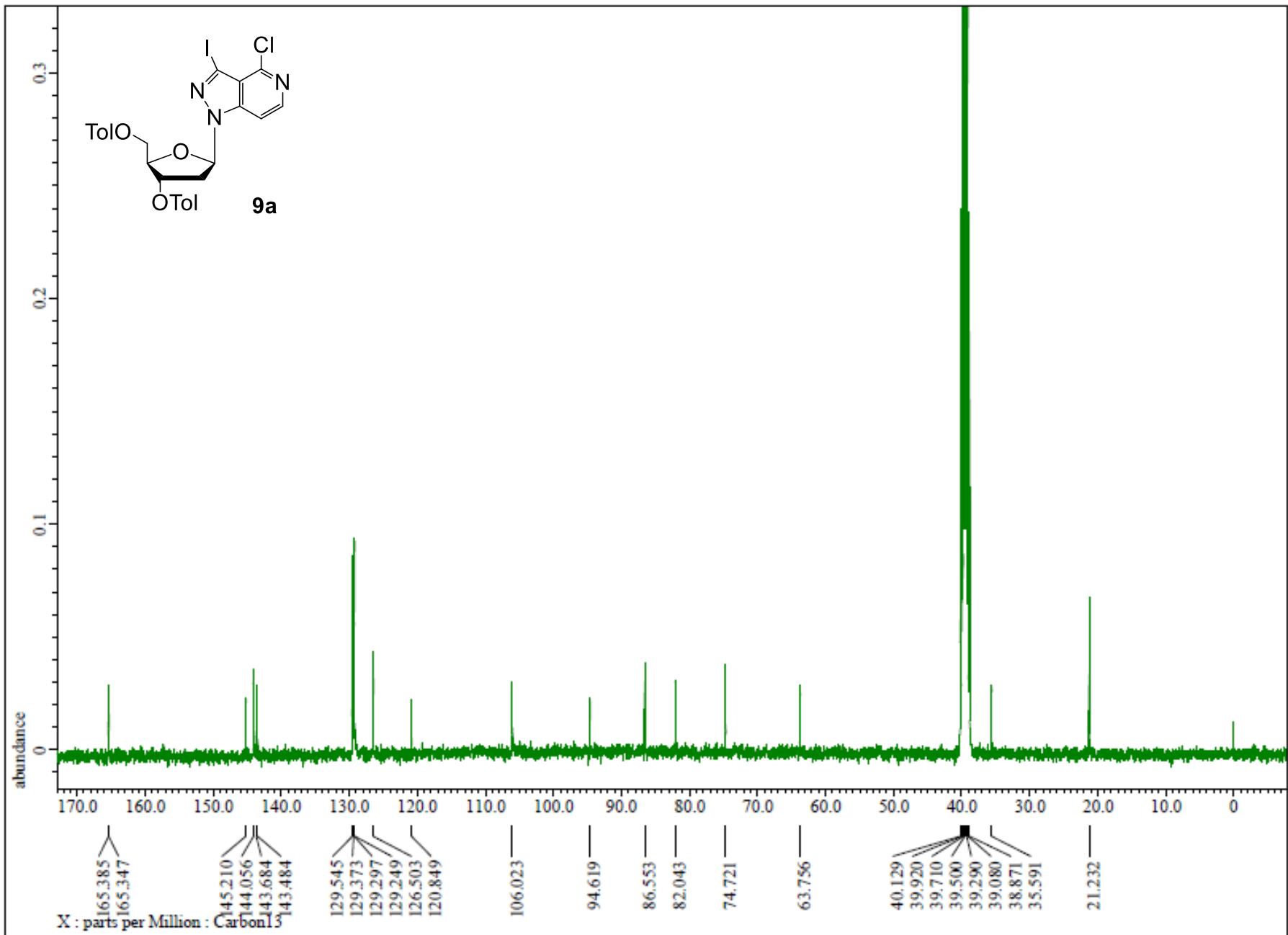


Figure S16. ^{13}C -NMR spectrum of compound **9a** ($\text{DMSO}-d_6$)

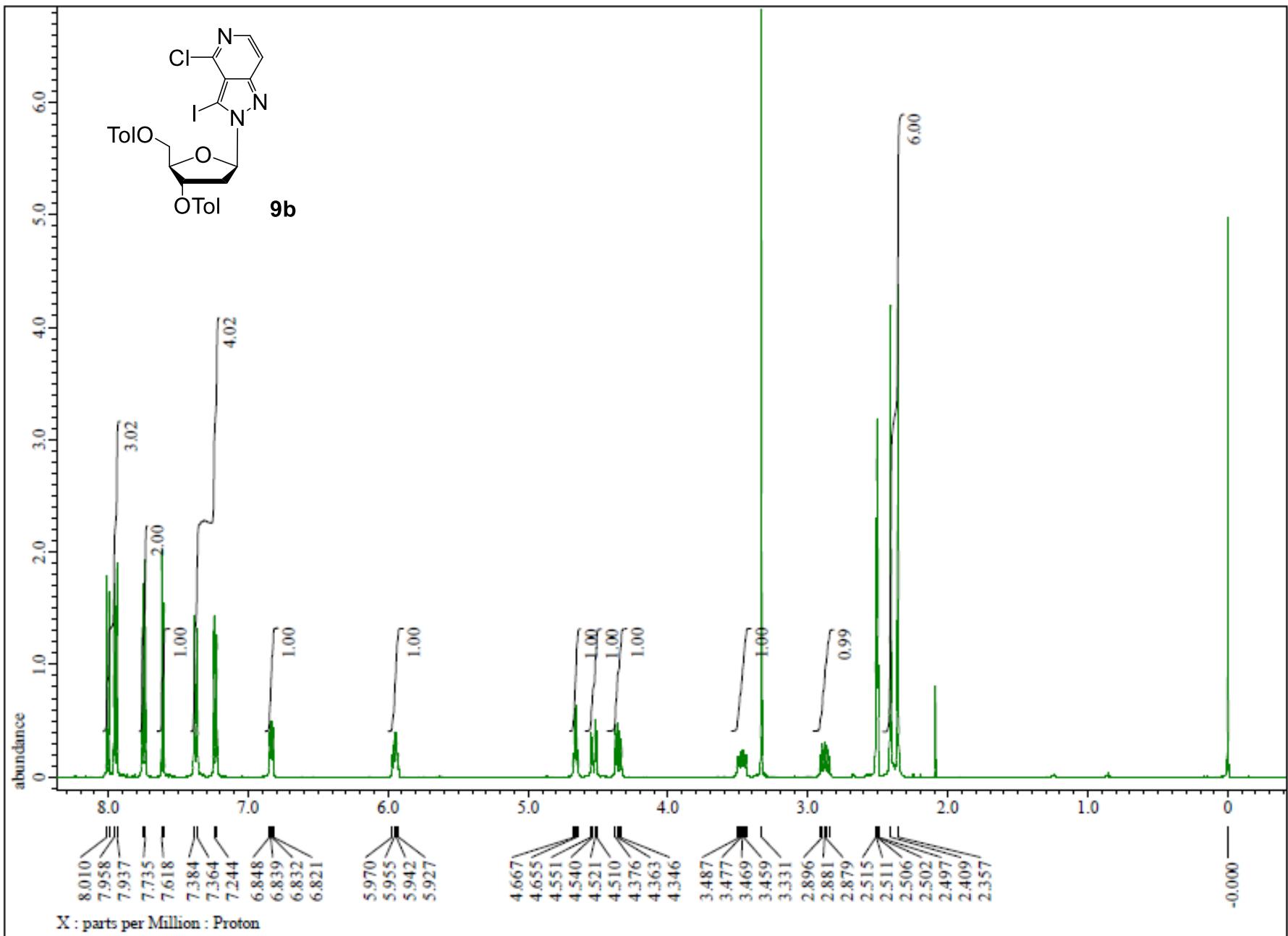


Figure S17. ^1H -NMR spectrum of compound **9b** ($\text{DMSO}-d_6$)

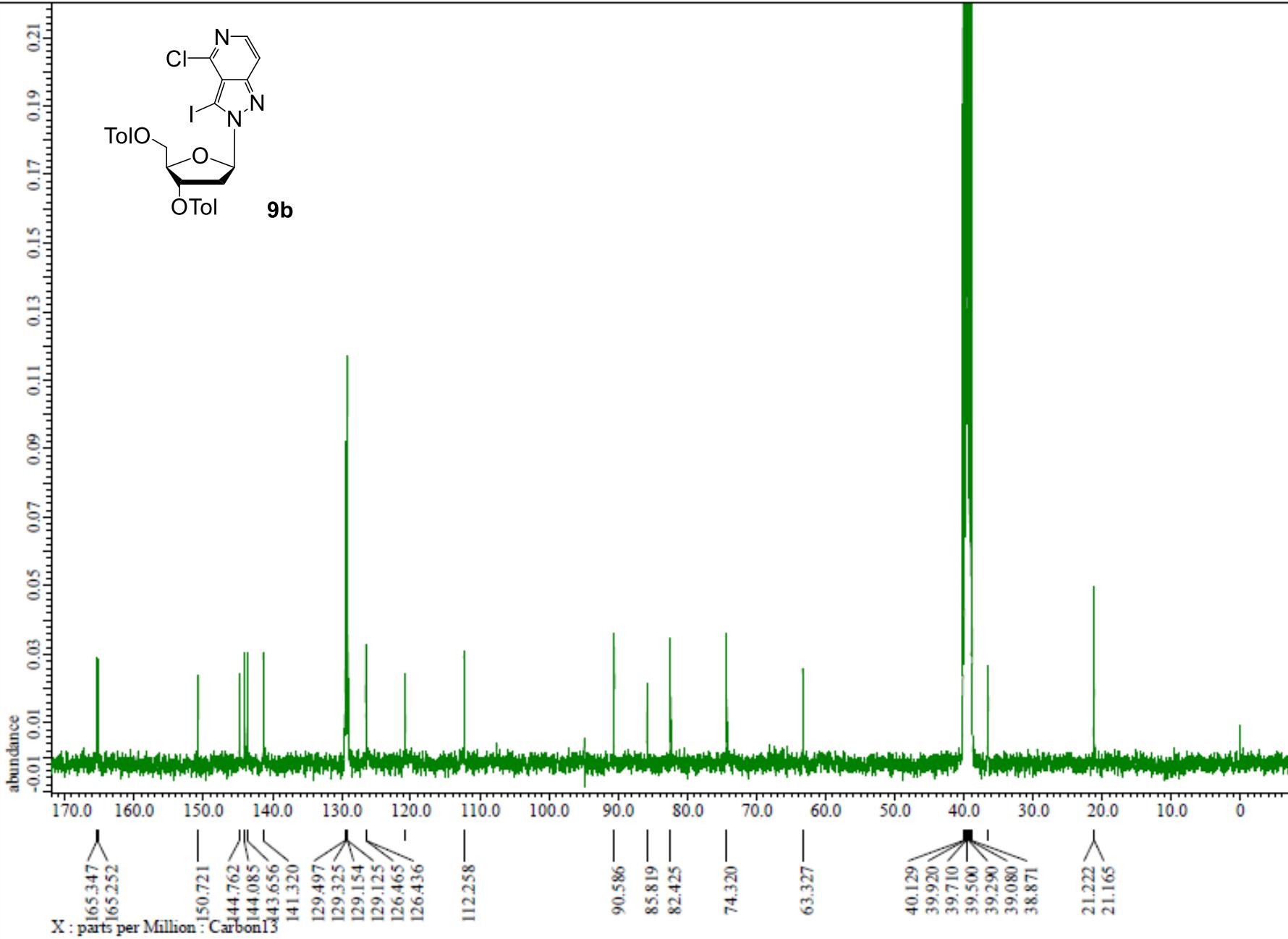


Figure S18. ^{13}C -NMR spectrum of compound **9b** ($\text{DMSO}-d_6$)

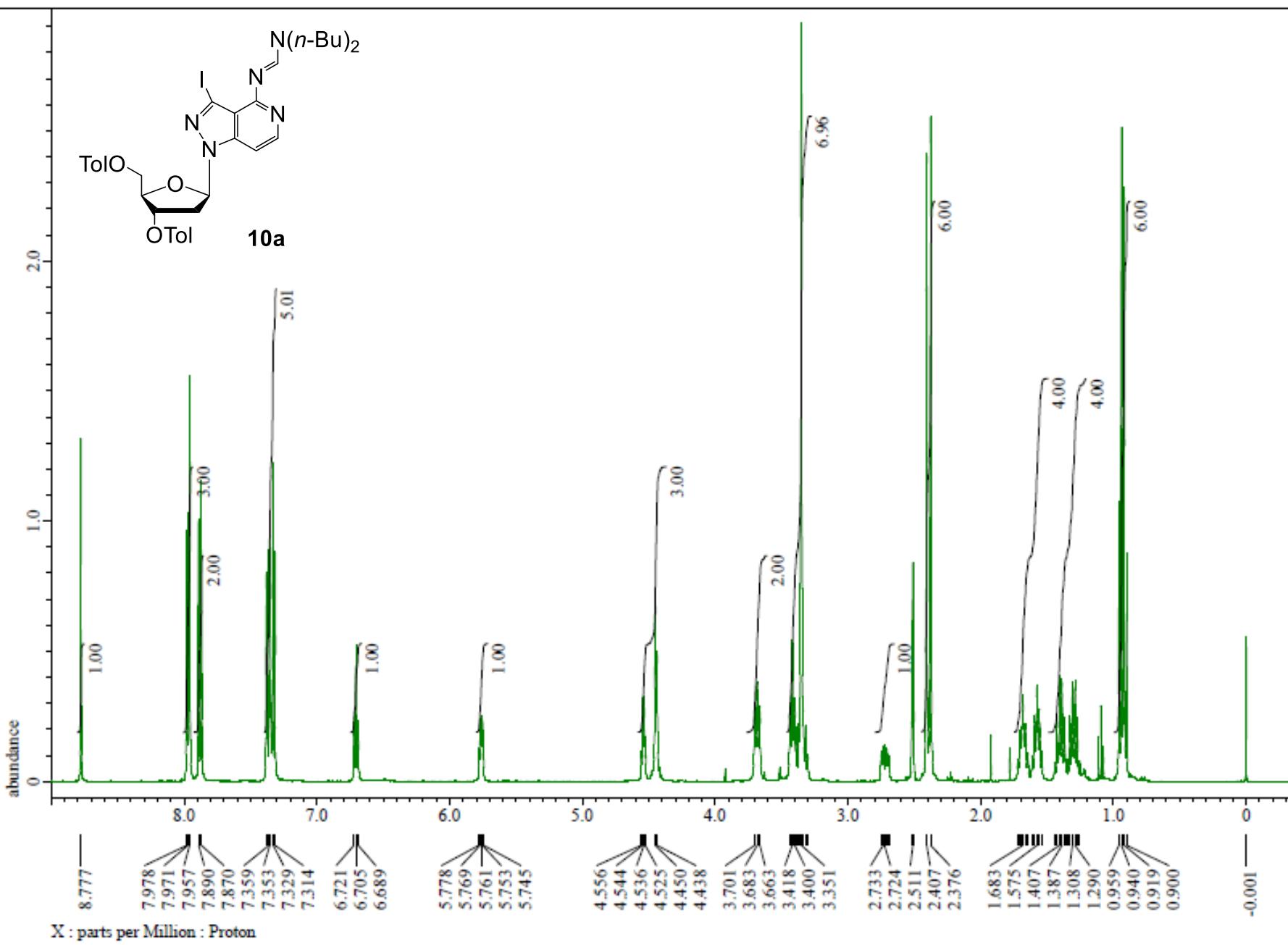


Figure S19. ^1H -NMR spectrum of compound **10a** ($\text{DMSO}-d_6$)

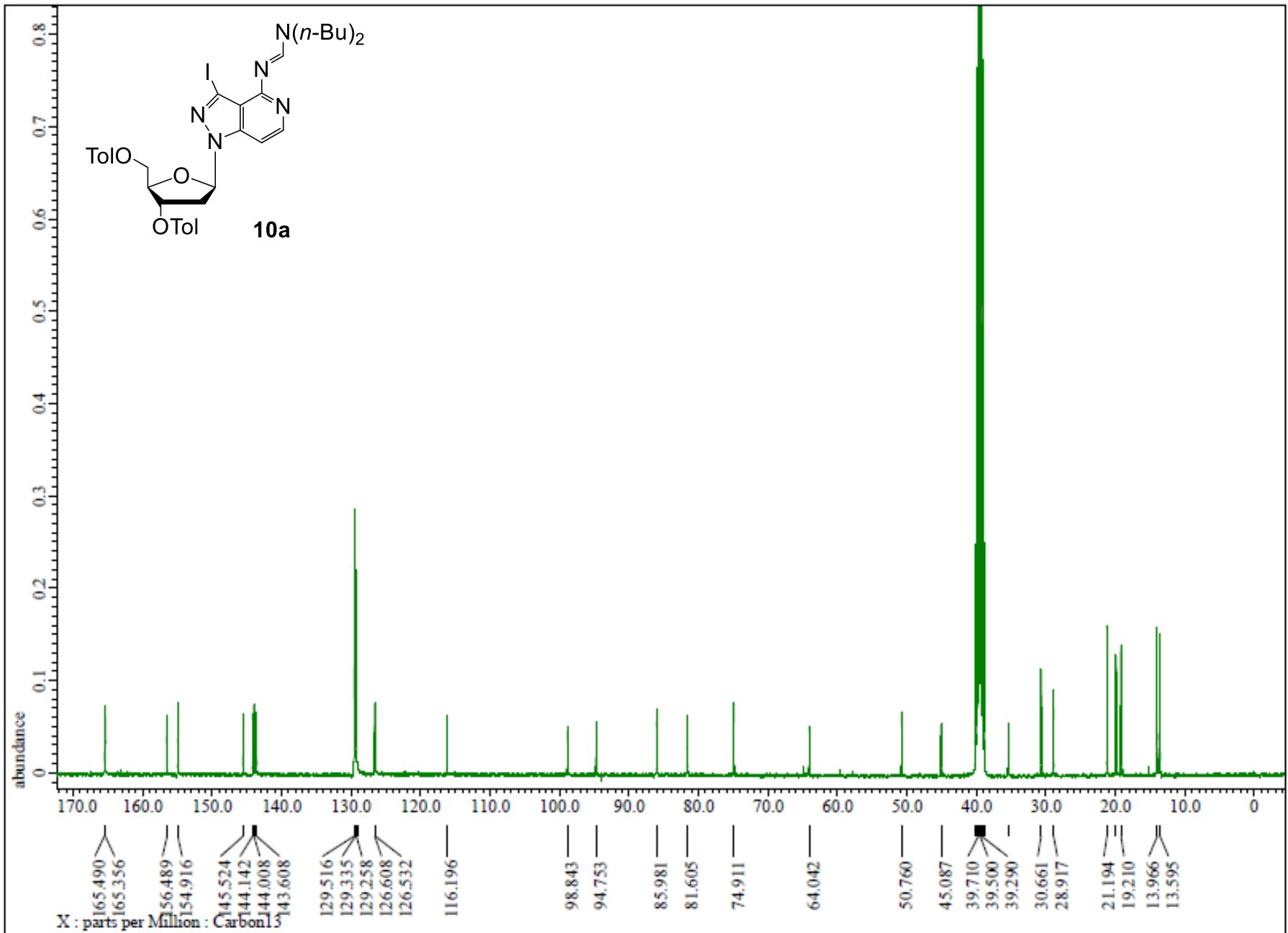


Figure S20. ^{13}C -NMR spectrum of compound **10a** ($\text{DMSO}-d_6$)

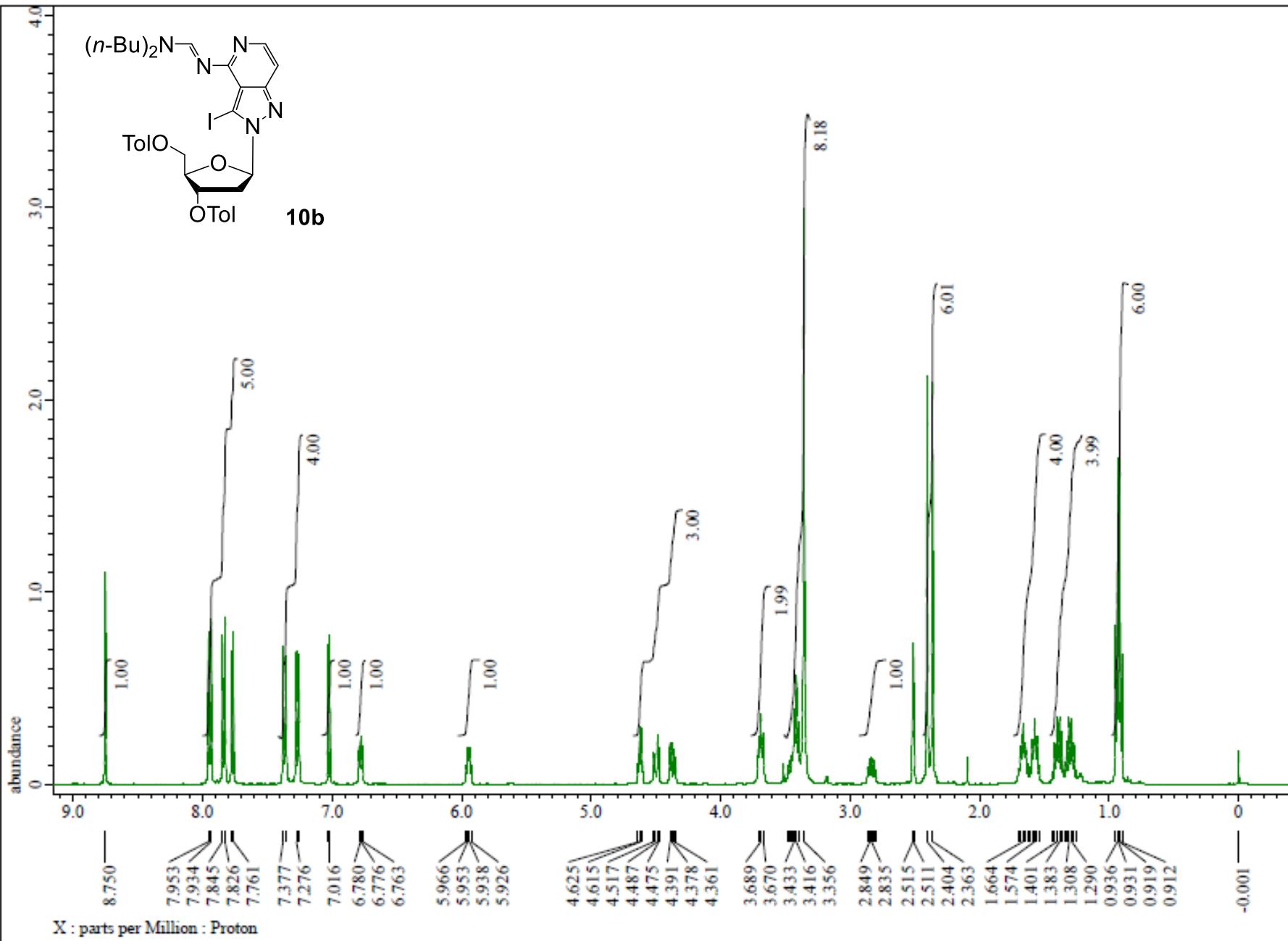


Figure S21. ^1H -NMR spectrum of compound **10b** ($\text{DMSO}-d_6$)

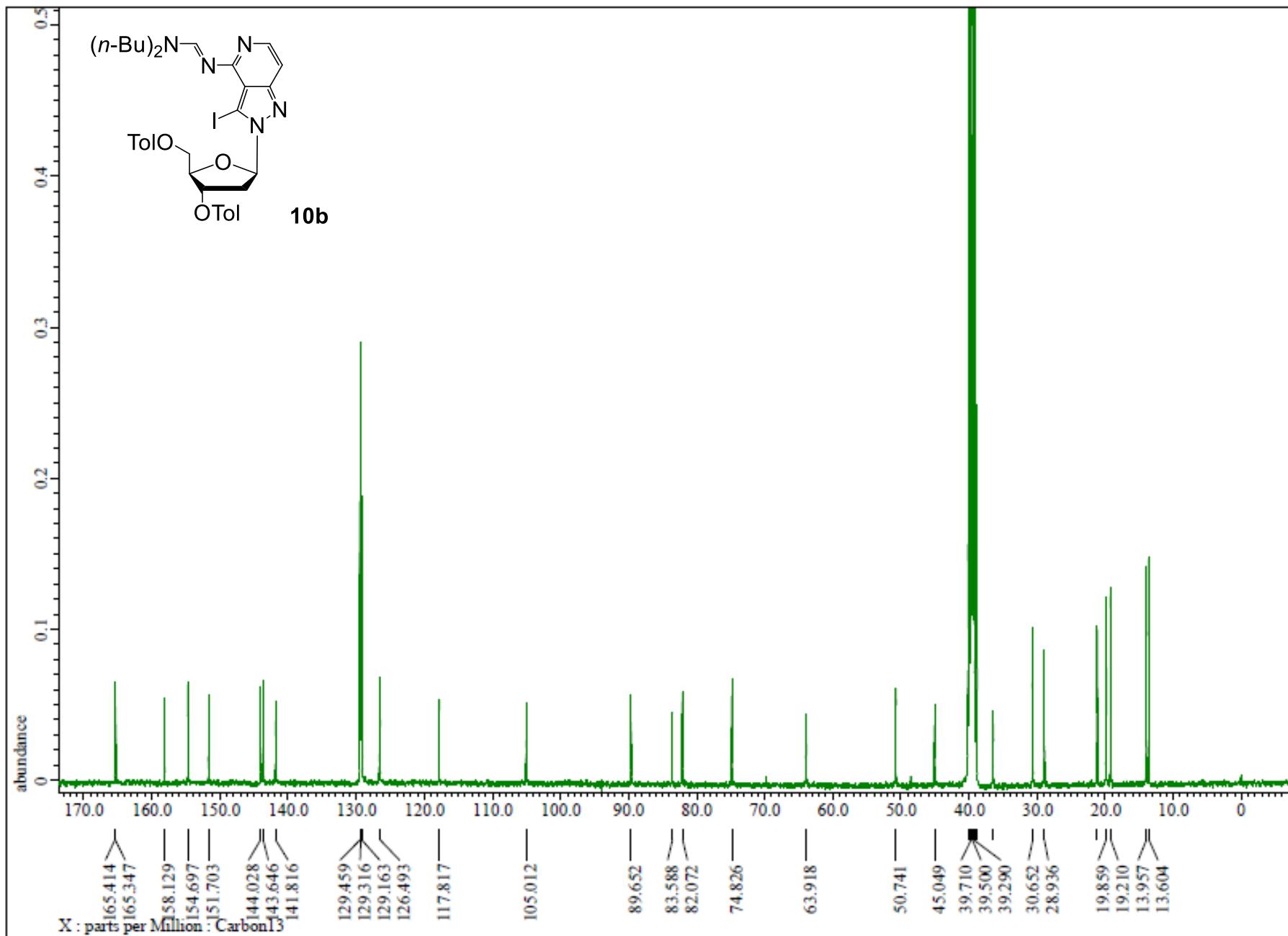


Figure S22. ¹³C-NMR spectrum of compound **10b** (DMSO-*d*₆)

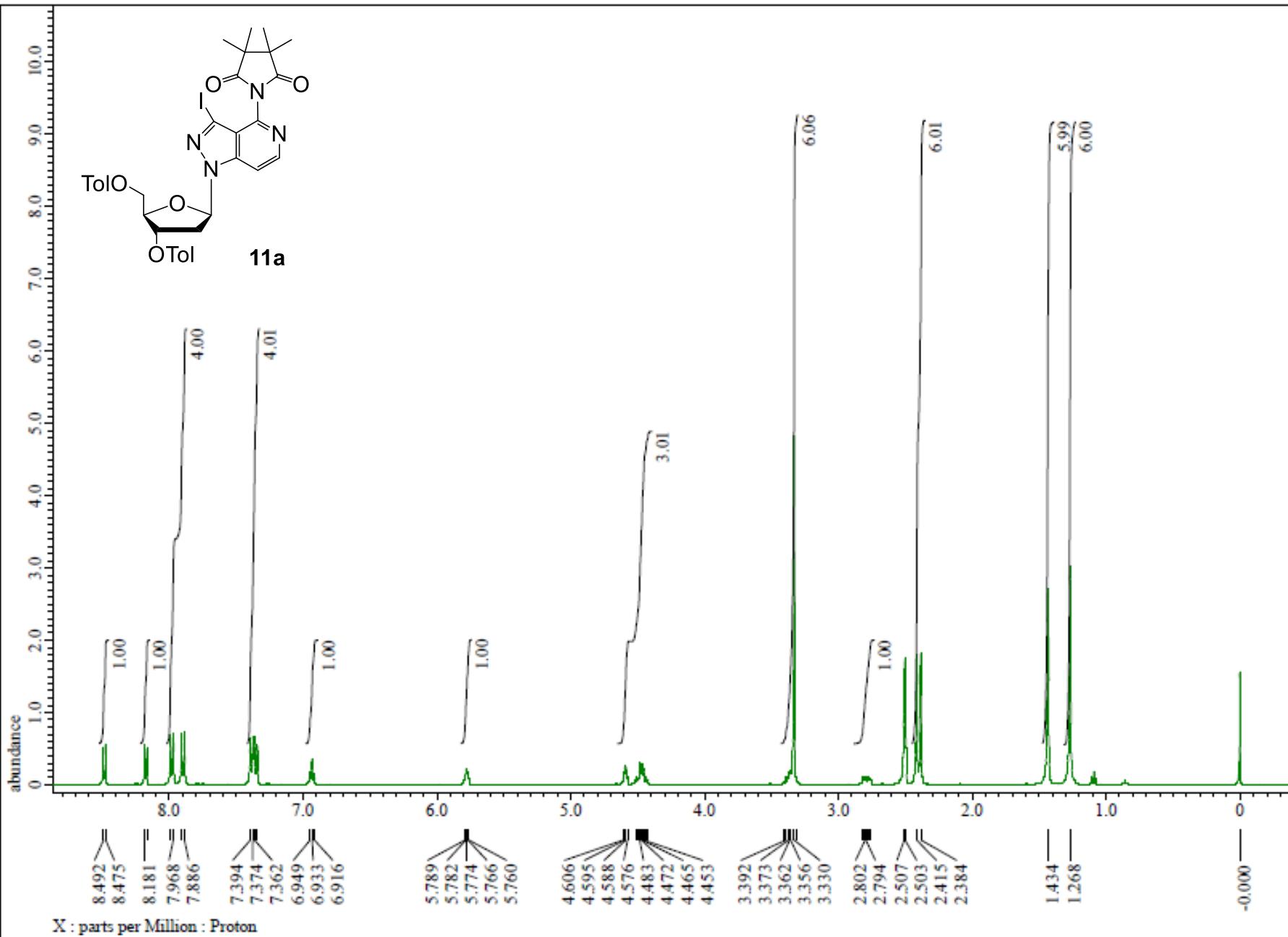


Figure S23. ¹H-NMR spectrum of compound **11a** ($\text{DMSO}-d_6$)

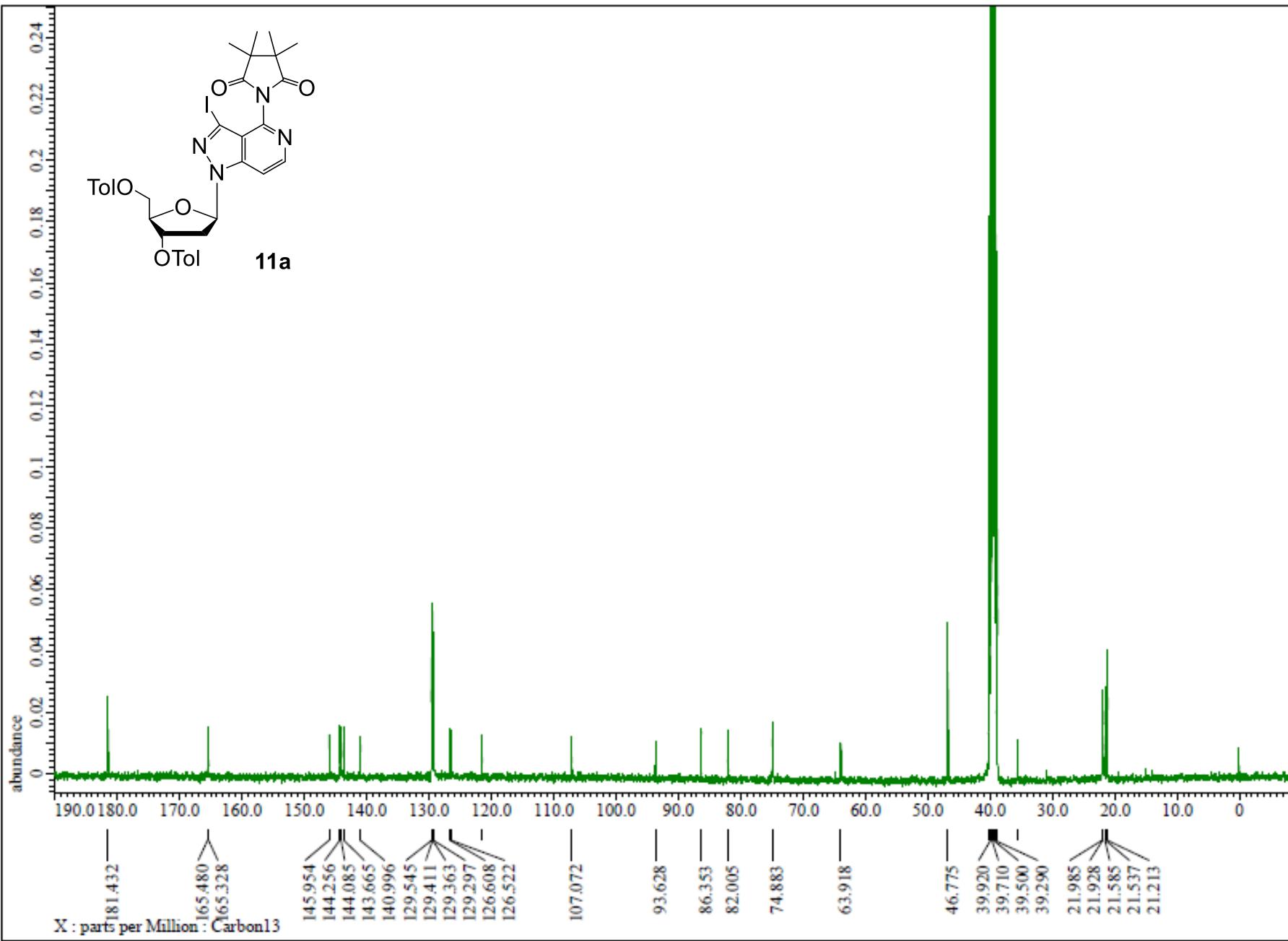


Figure S24. ^{13}C -NMR spectrum of compound **11a** (DMSO- d_6)

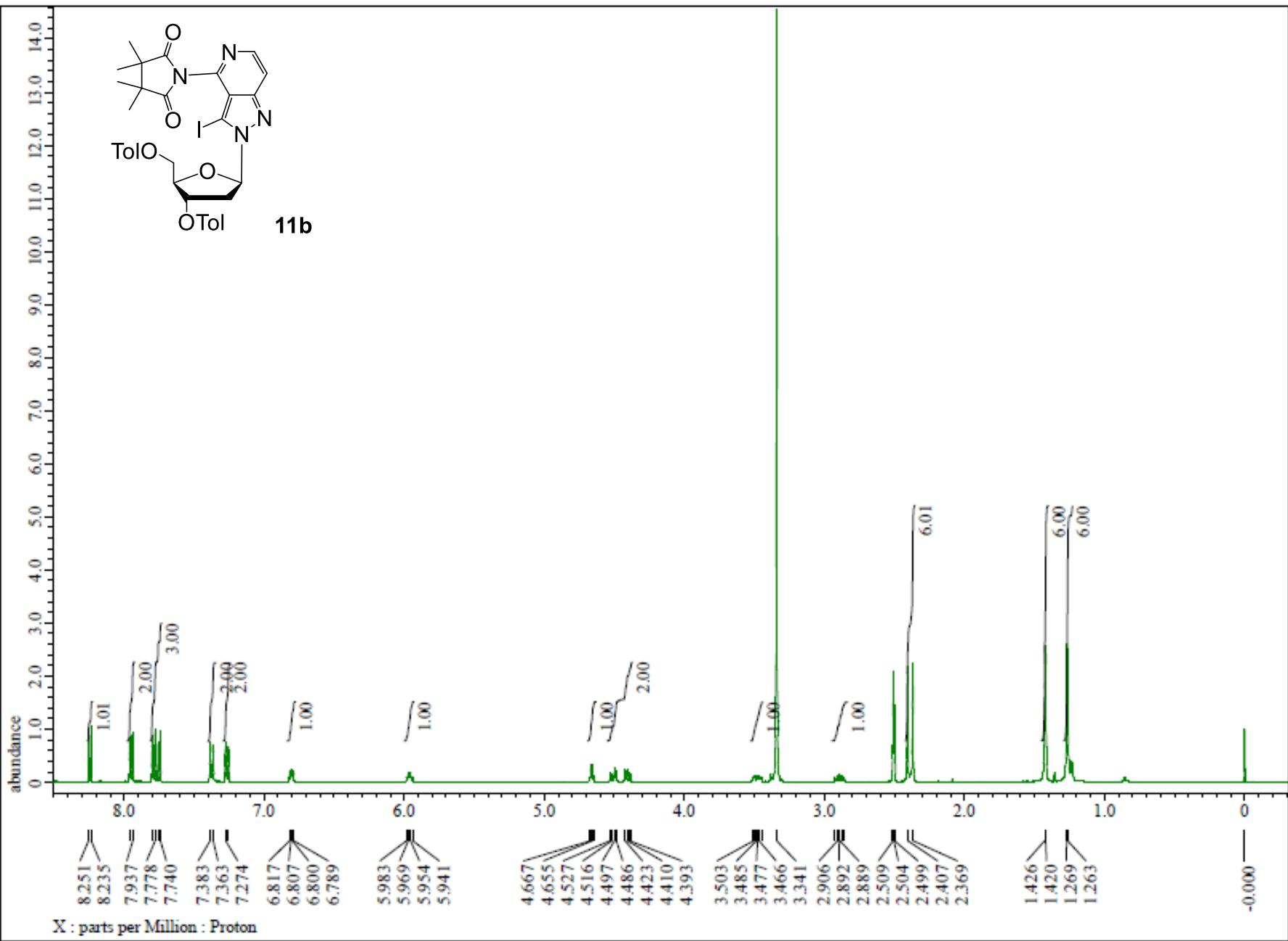


Figure S25. ¹H-NMR spectrum of compound 11b (DMSO-*d*₆)

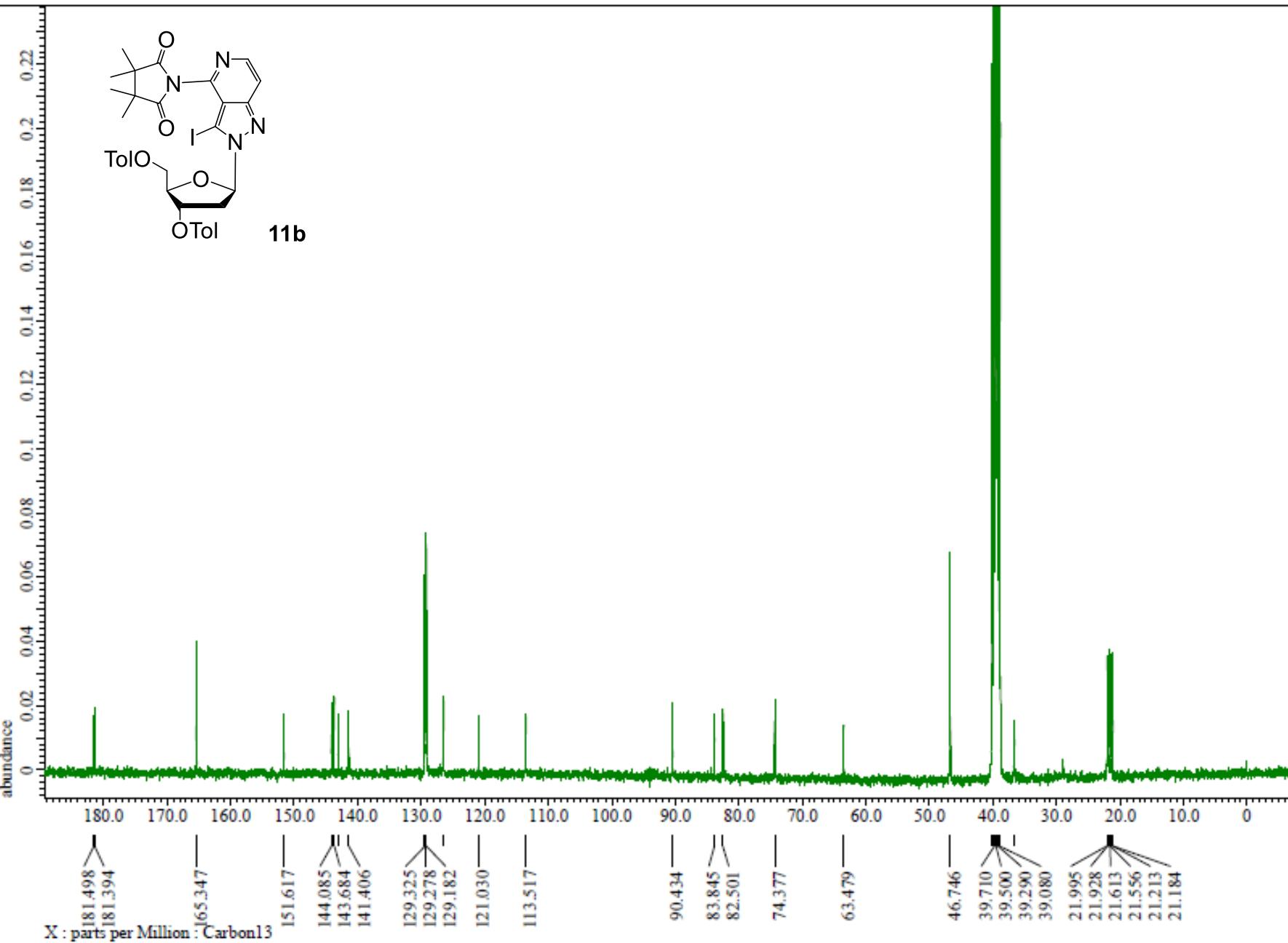


Figure S26. ^{13}C -NMR spectrum of compound **11b** ($\text{DMSO}-d_6$)

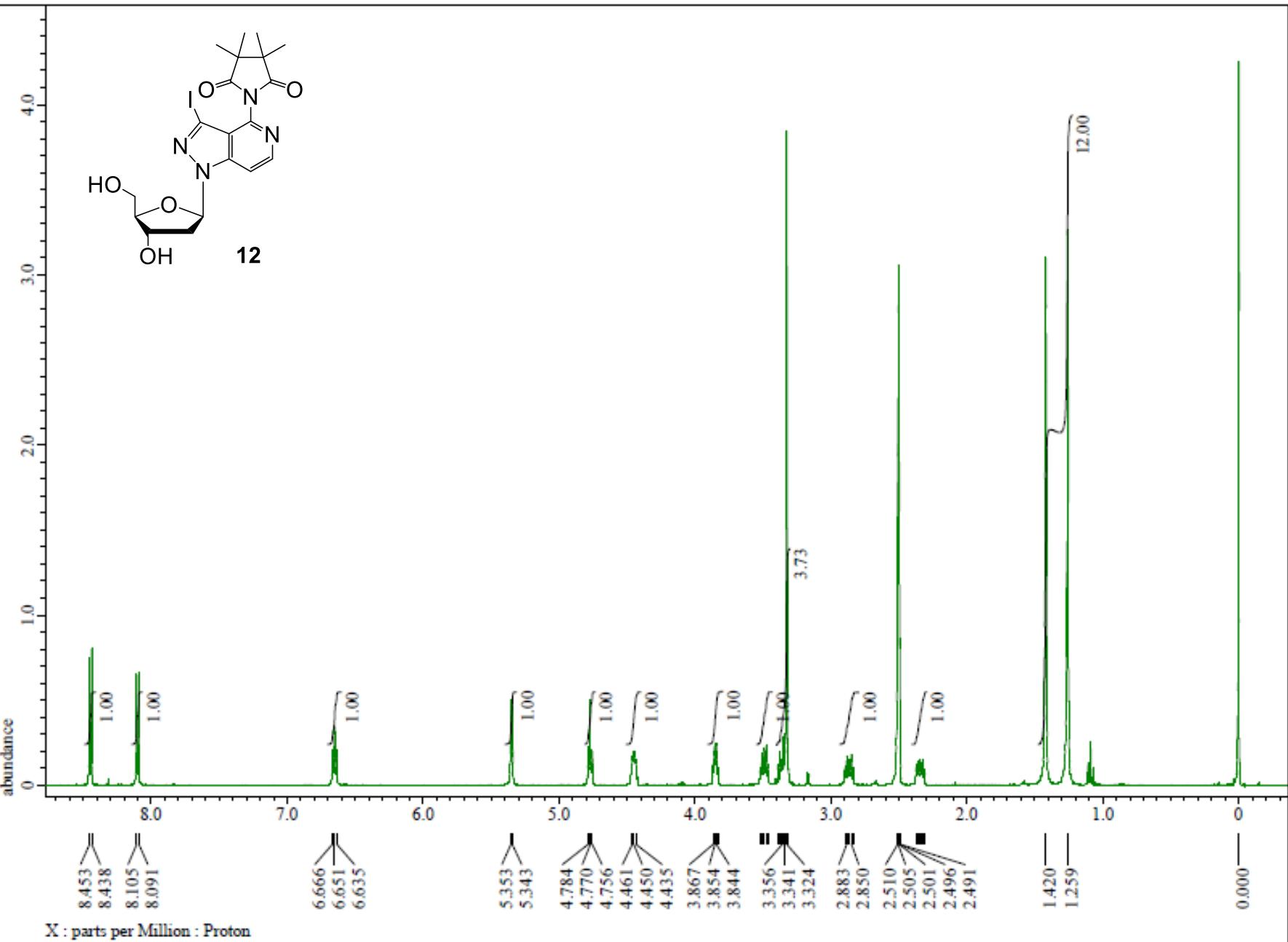


Figure S27. ^1H -NMR spectrum of compound 12 (DMSO- d_6)

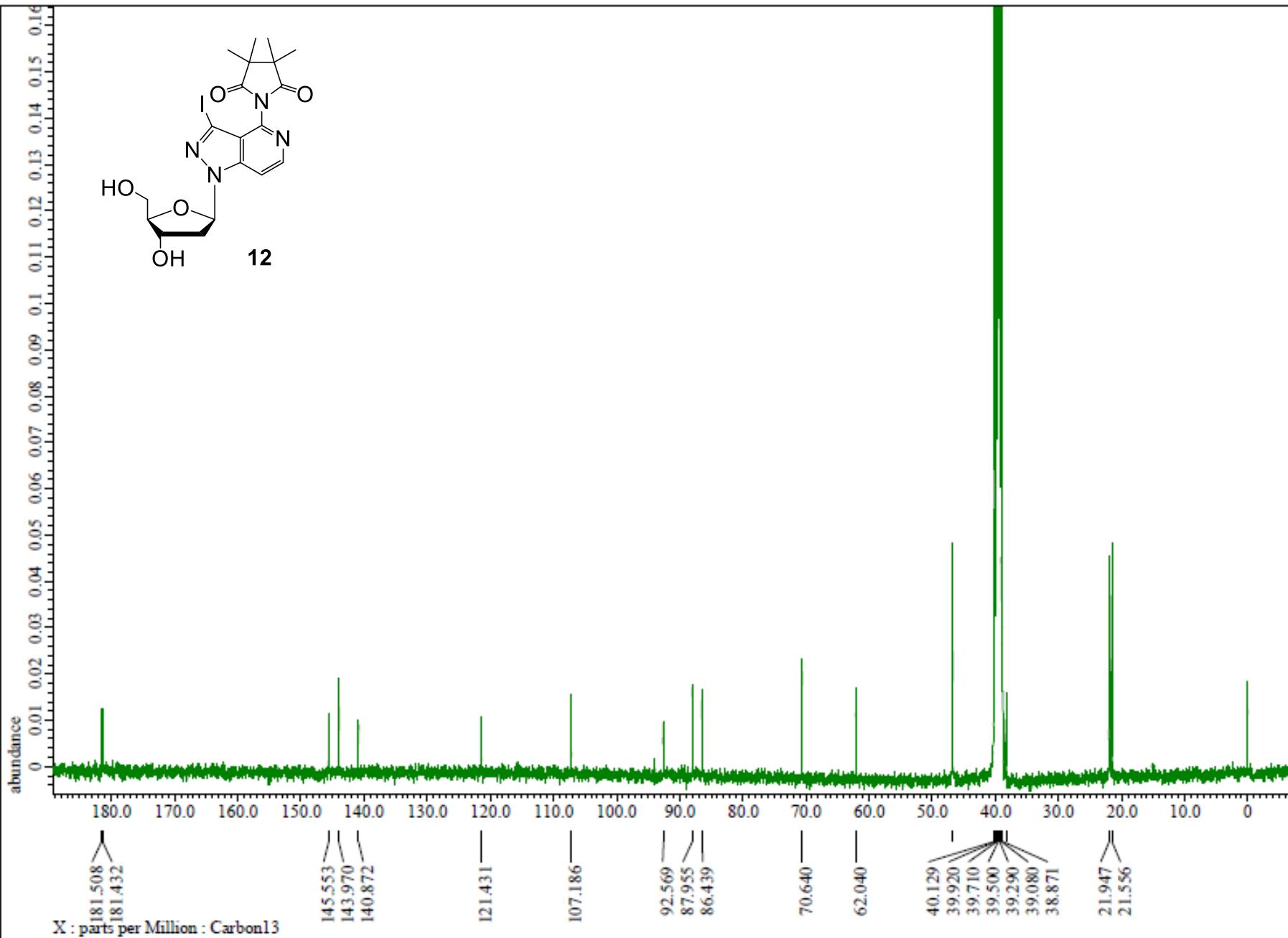


Figure S28. ^{13}C -NMR spectrum of compound 12 (DMSO- d_6)

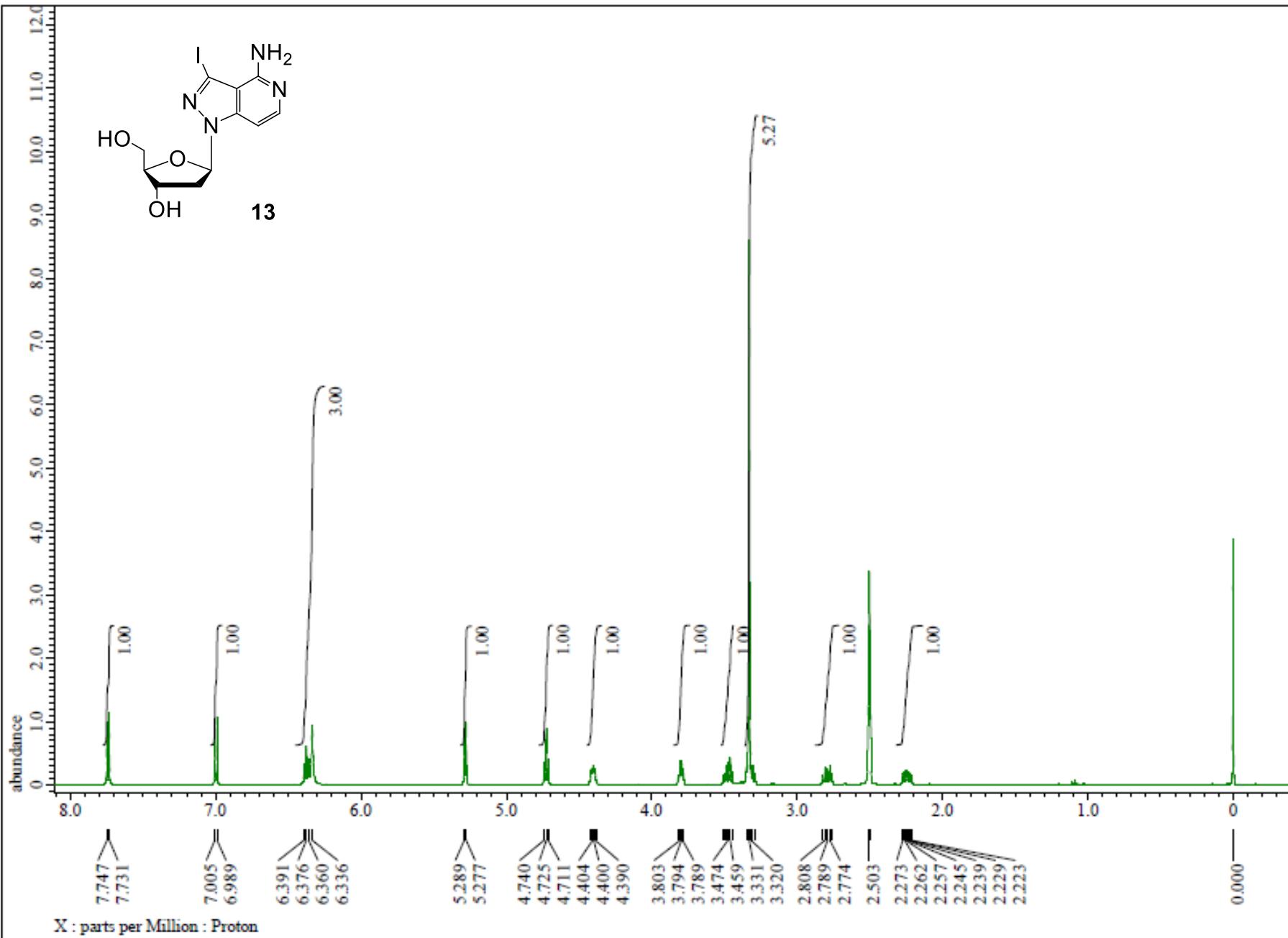


Figure S29. ¹H-NMR spectrum of compound 13 (DMSO-*d*₆)

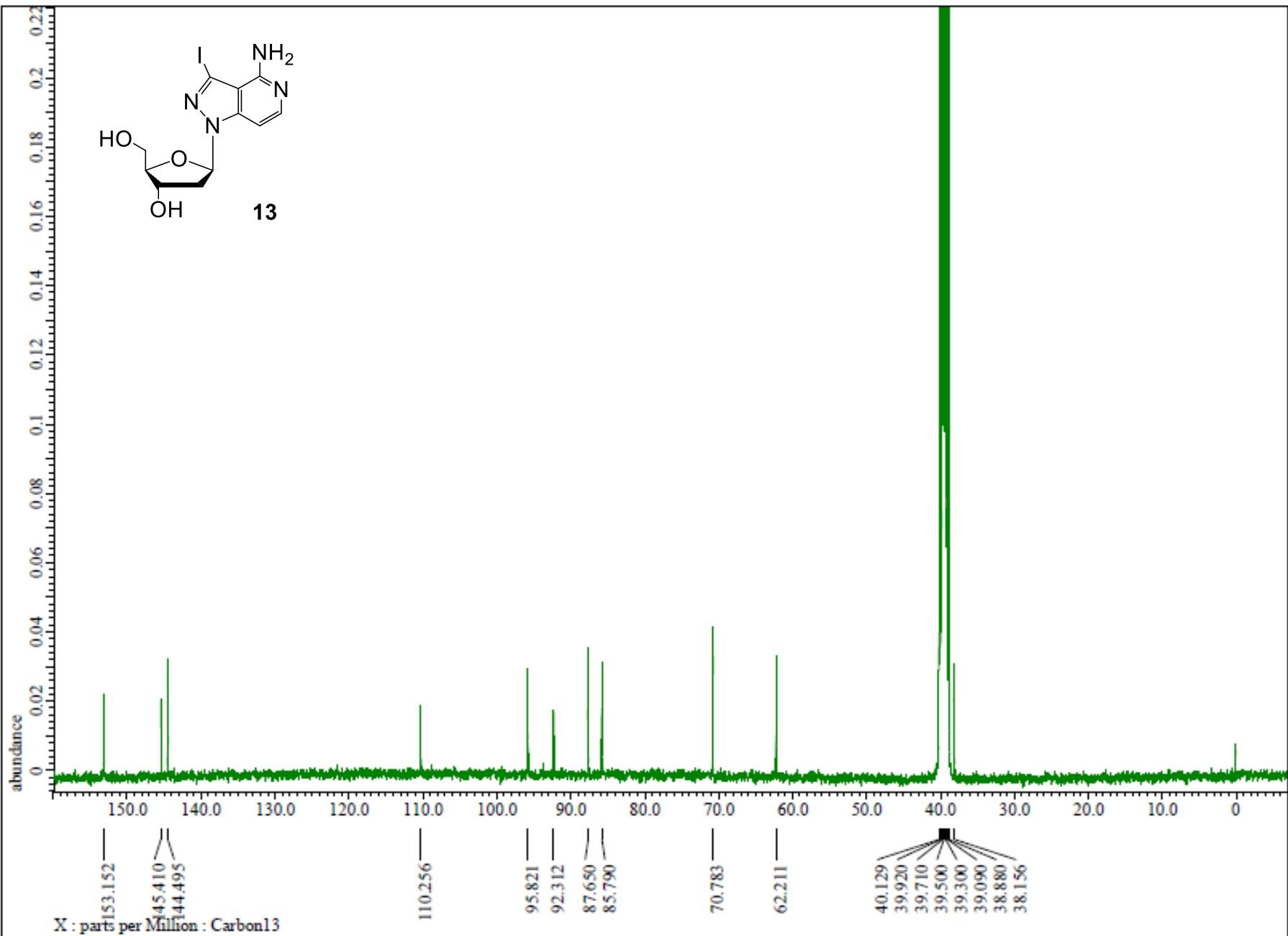


Figure S30. ^{13}C -NMR spectrum of compound 13 (DMSO- d_6)

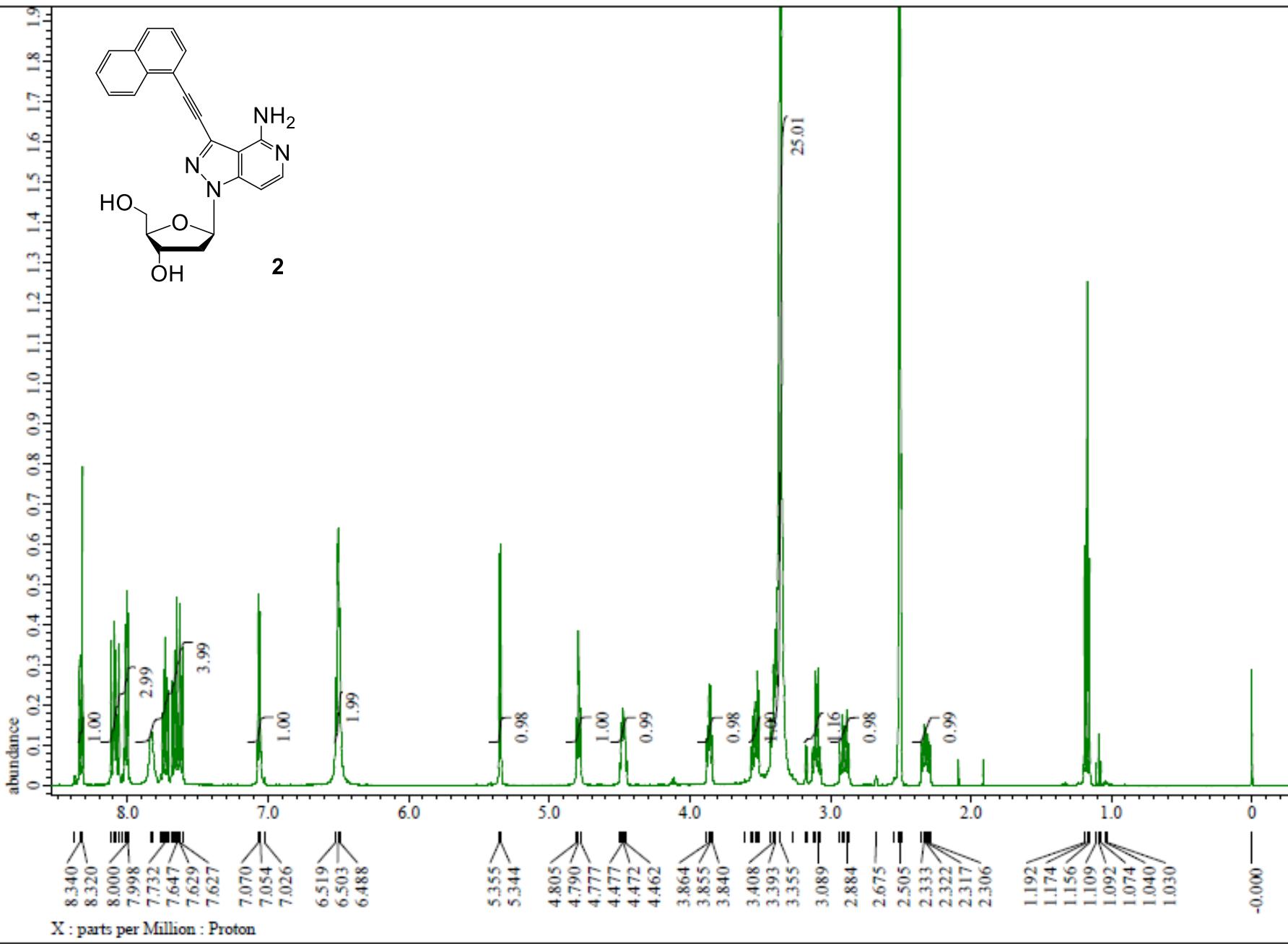


Figure S31. ¹H-NMR spectrum of compound 2 (DMSO-*d*₆)

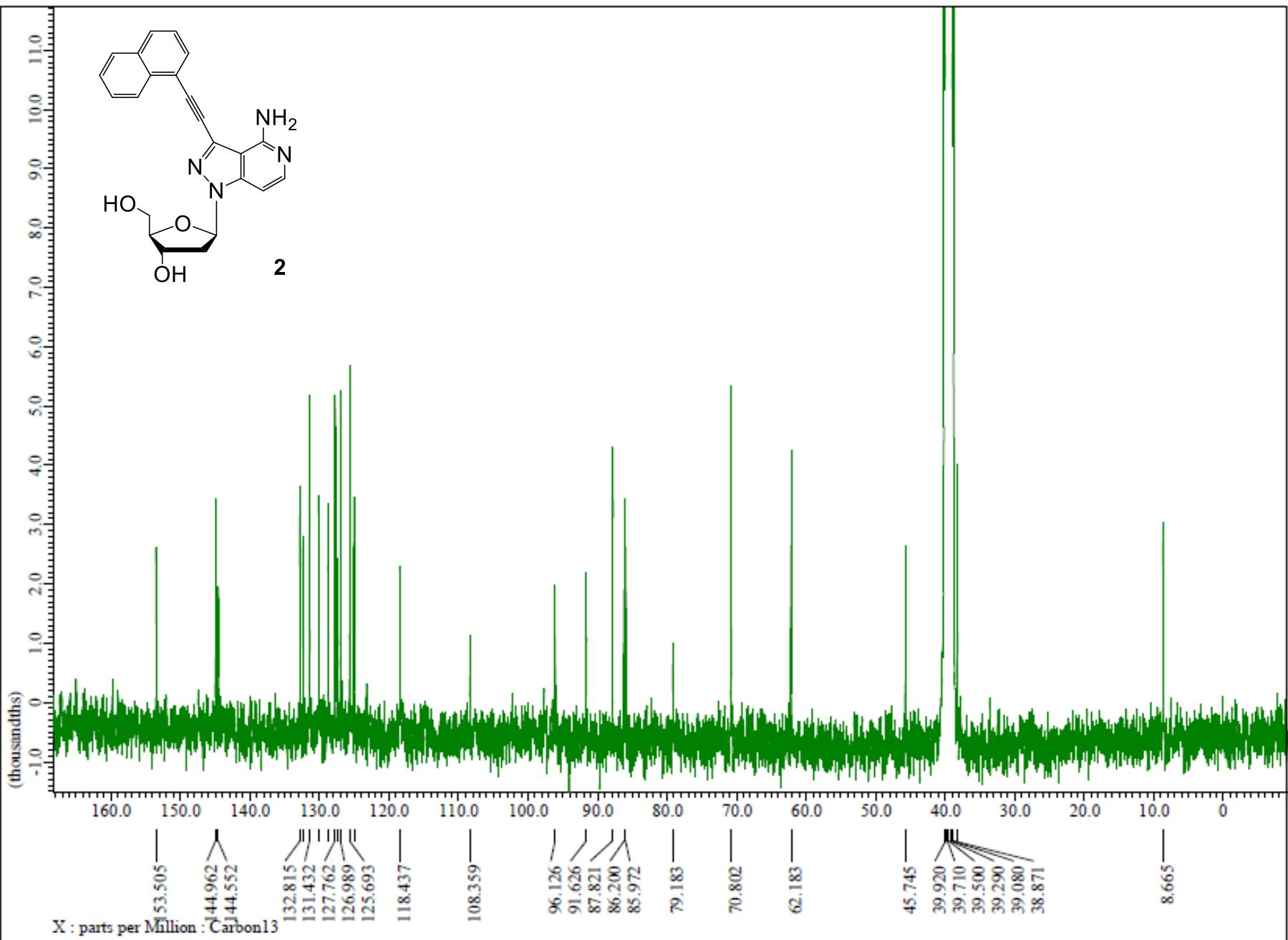


Figure S32. ^{13}C -NMR spectrum of compound **2** ($\text{DMSO}-d_6$)

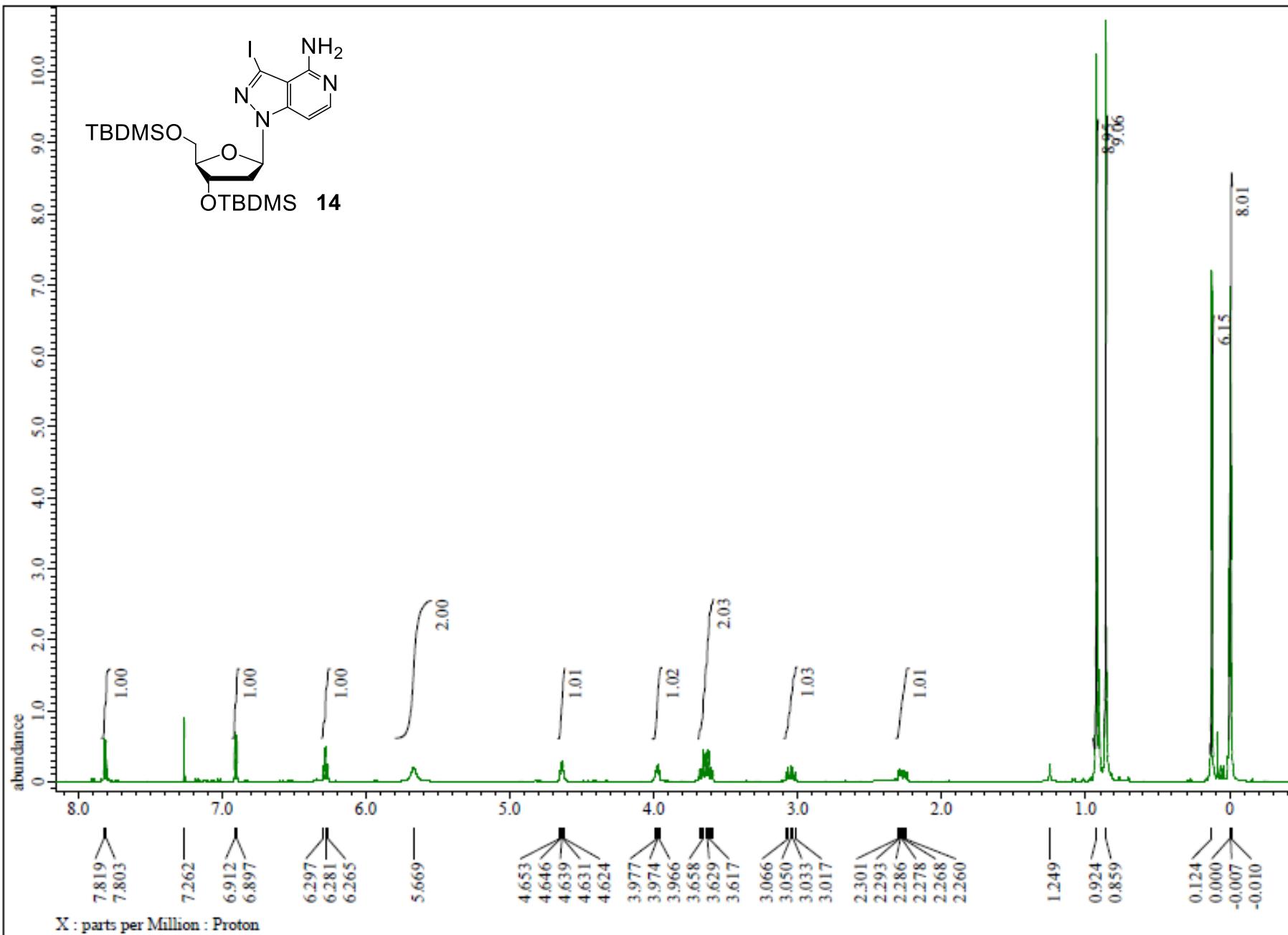


Figure S33. ^1H -NMR spectrum of compound 14 (CDCl_3)

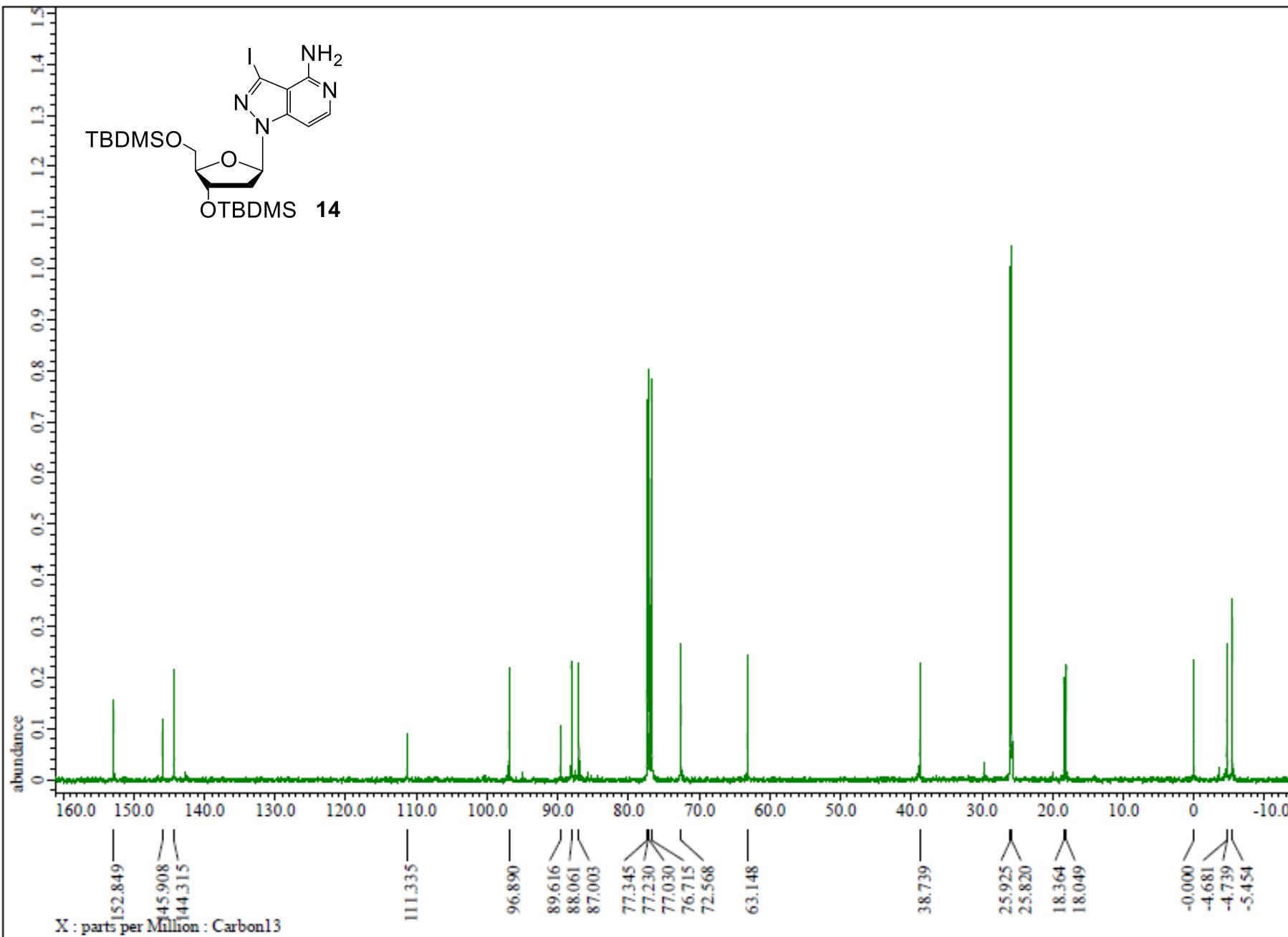


Figure S34. ^{13}C -NMR spectrum of compound **14** (CDCl_3)

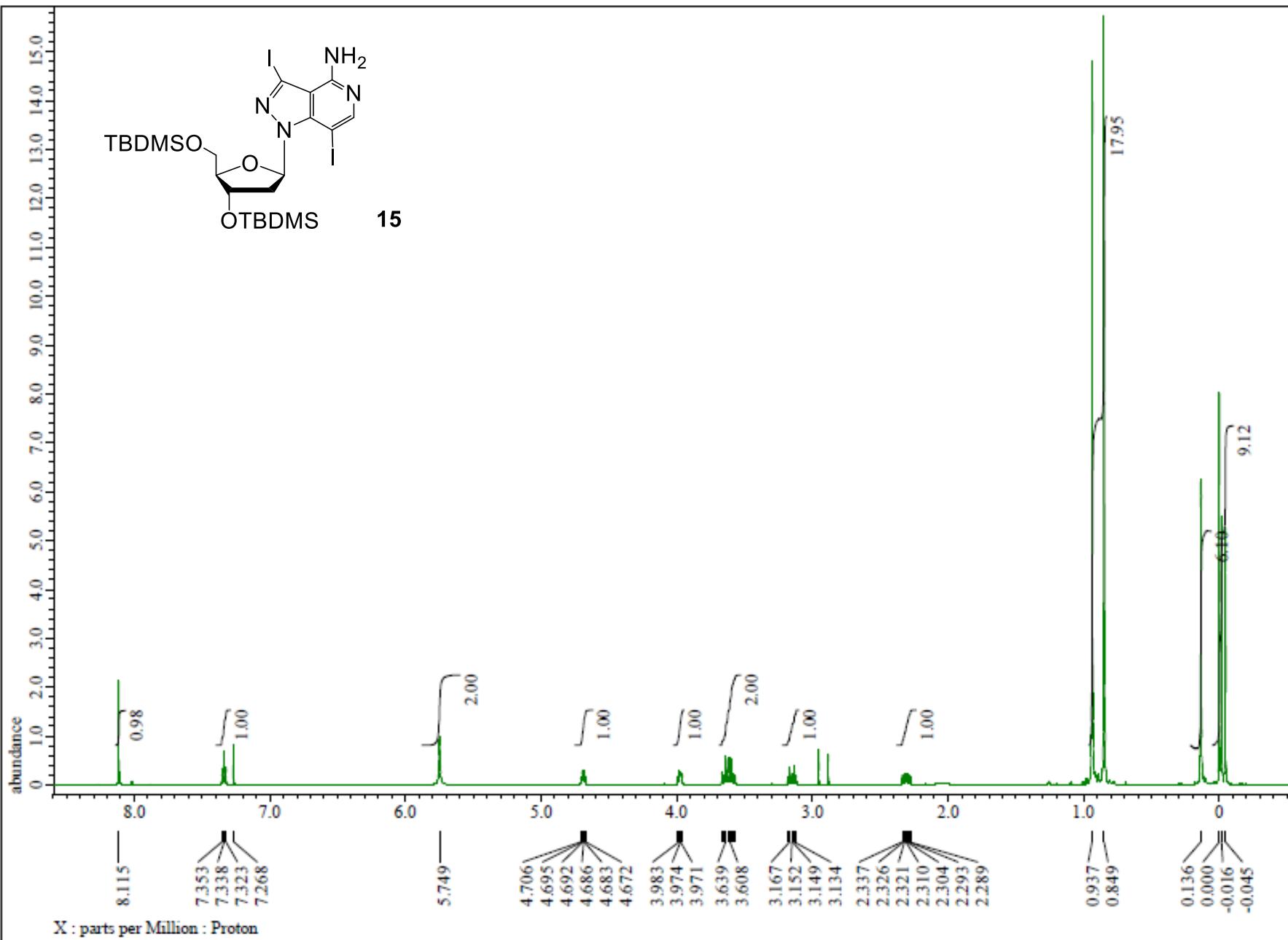


Figure S35. ^1H -NMR spectrum of compound **15** (CDCl_3)

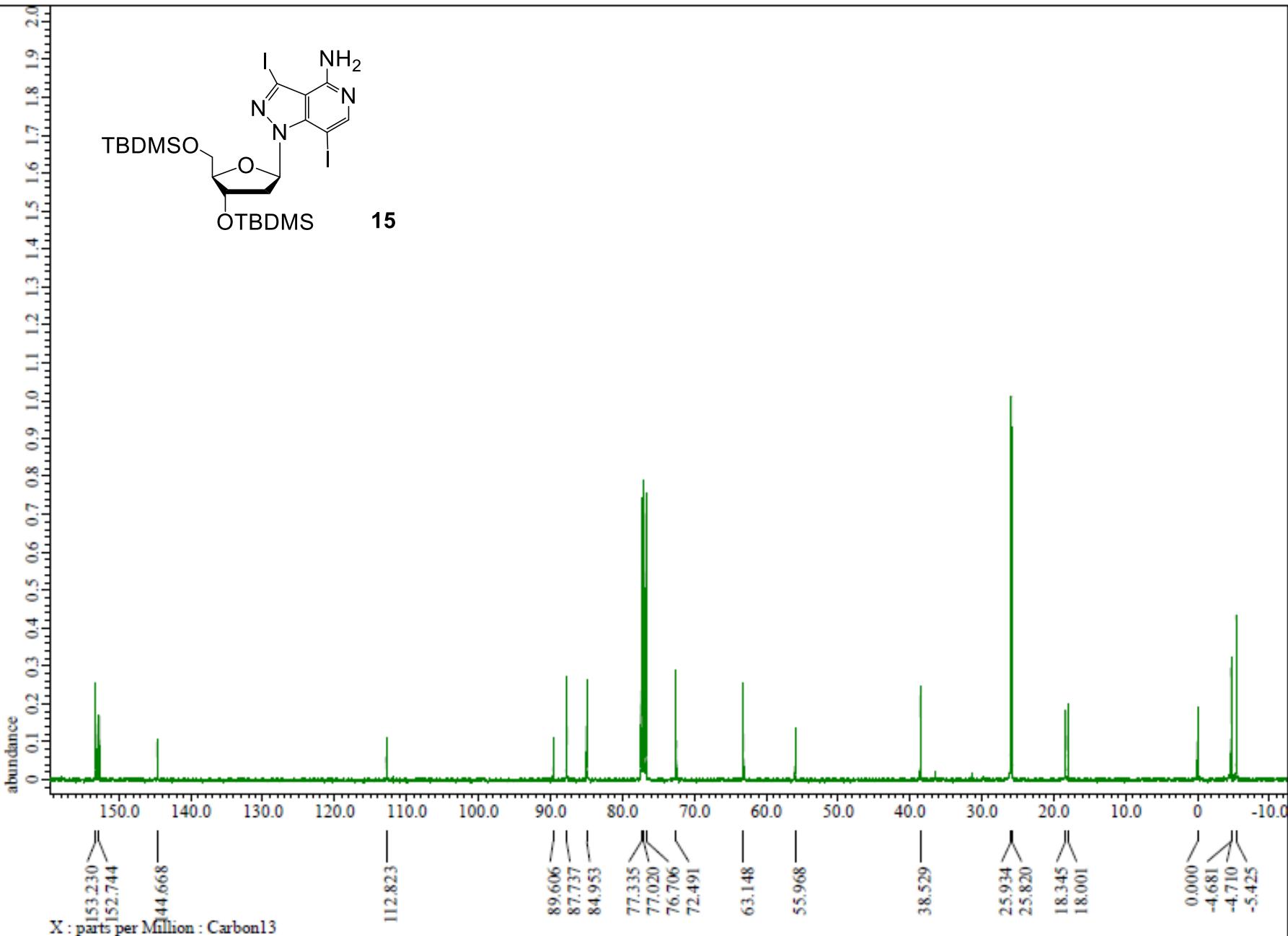


Figure S36. ^{13}C -NMR spectrum of compound **15** (CDCl_3)

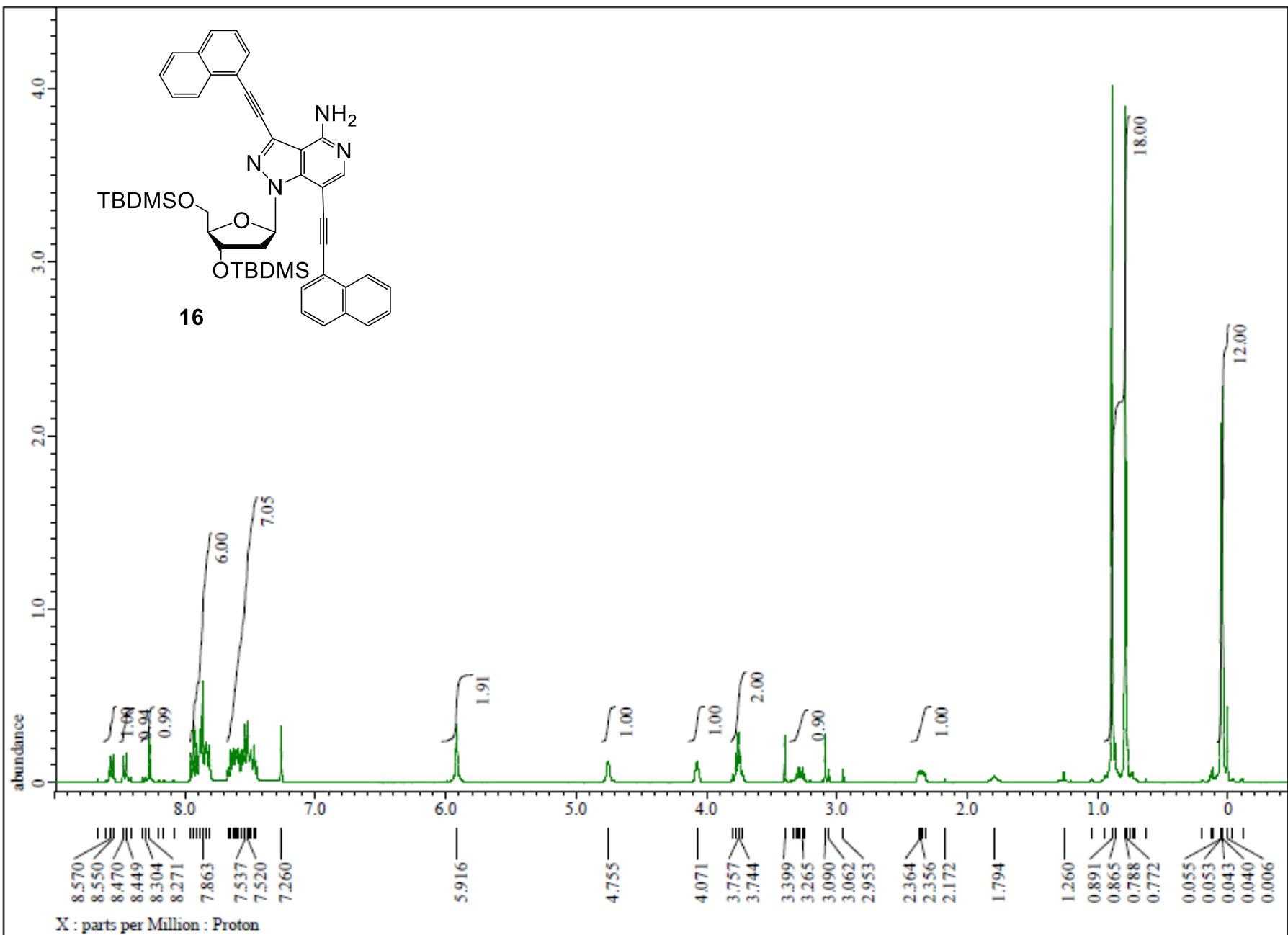


Figure S37. ^1H -NMR spectrum of compound **16** (CDCl_3)

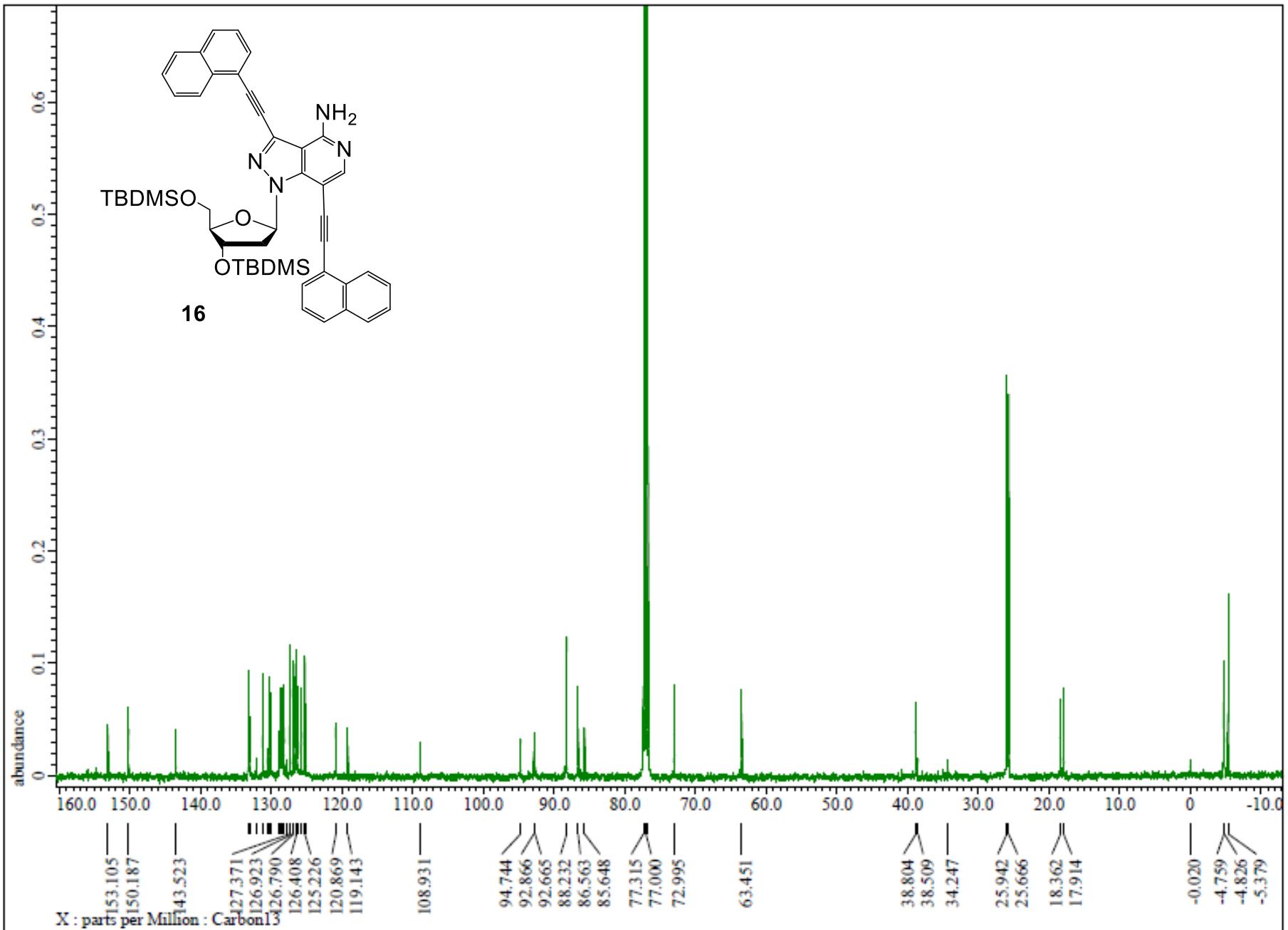


Figure S38. ^{13}C -NMR spectrum of compound 16 (CDCl_3)

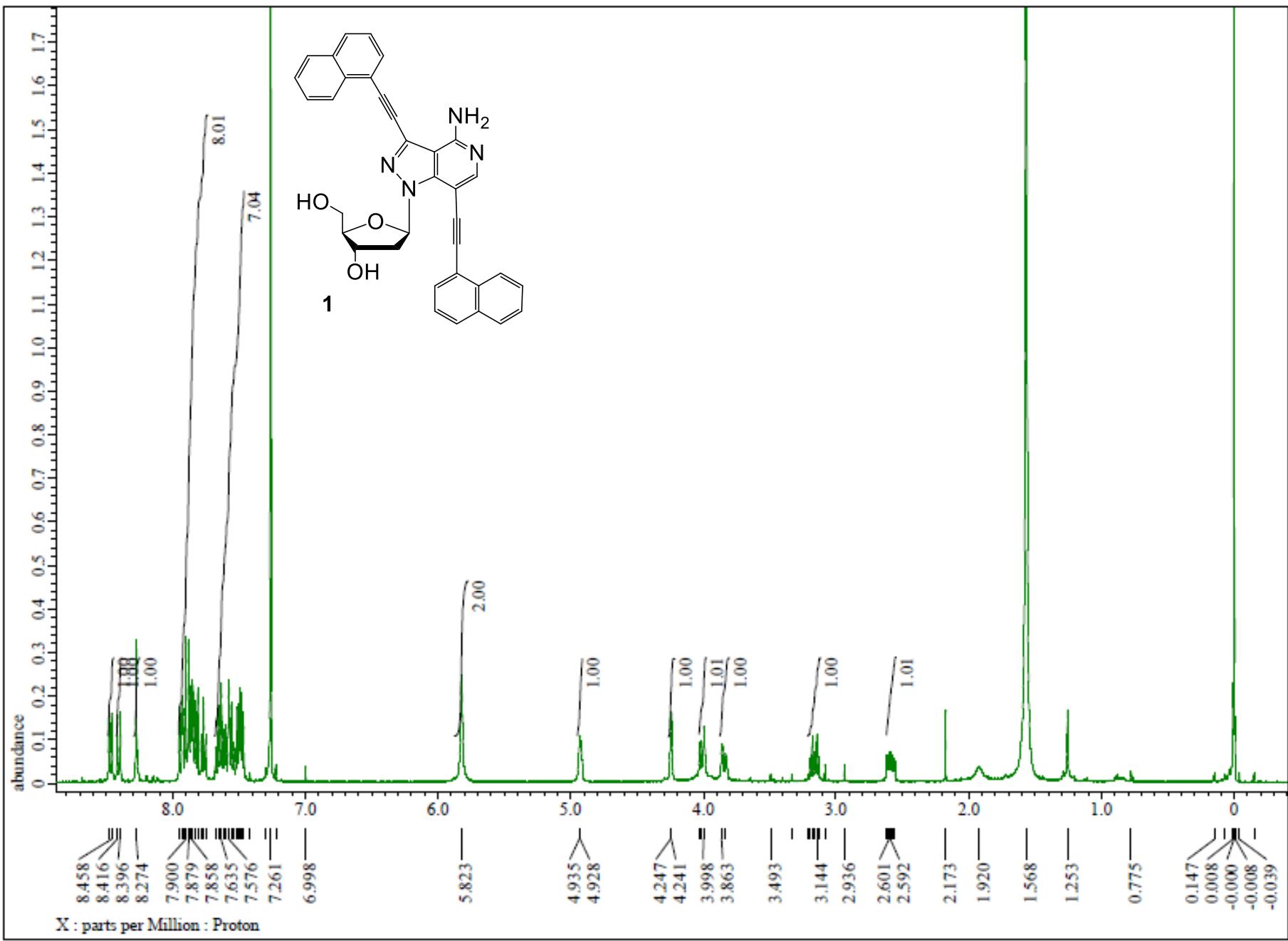


Figure S39. ¹H-NMR spectrum of compound 1 (CDCl₃)

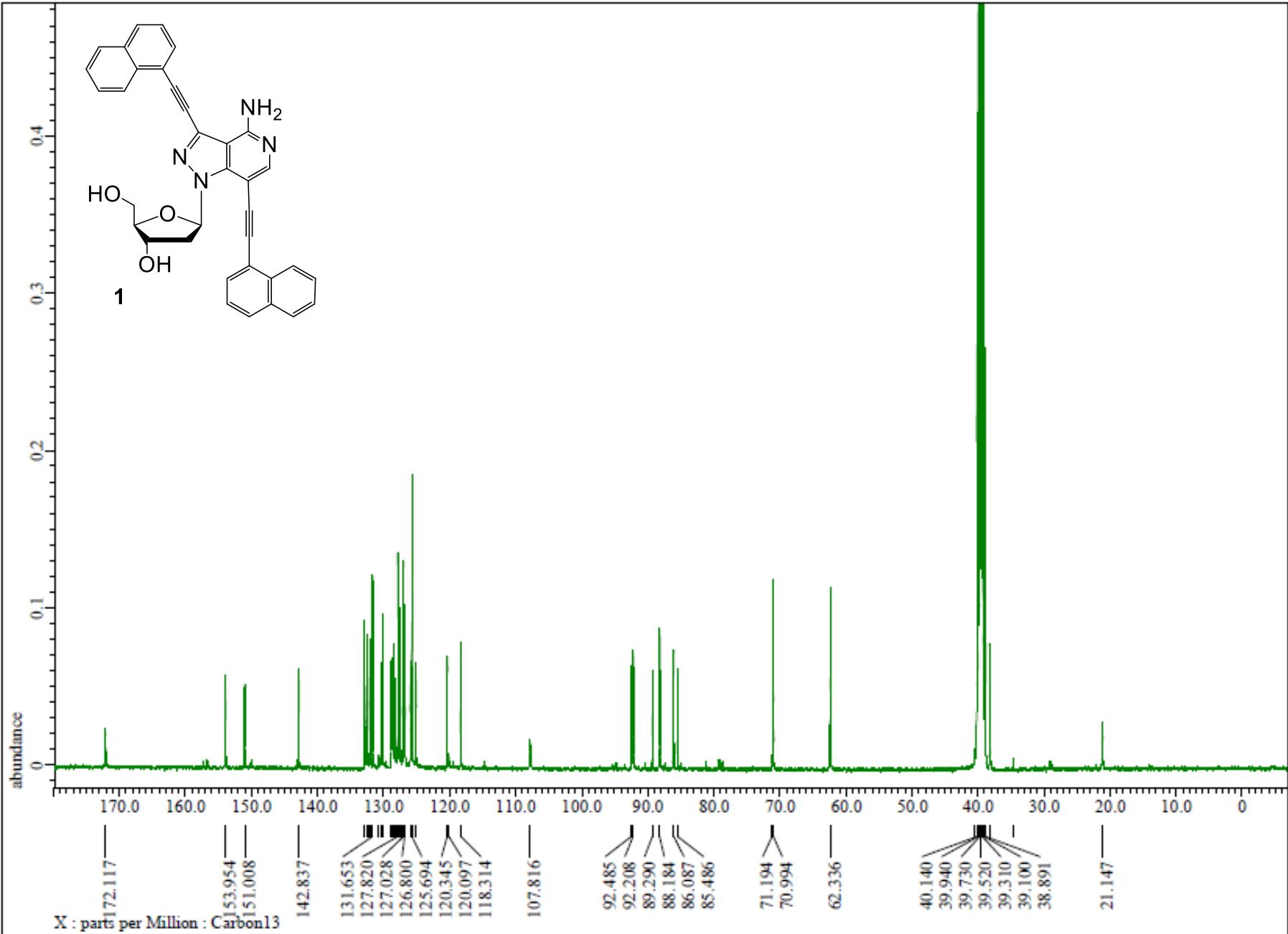


Figure S40. ¹³C-NMR spectrum of compound **1** (DMSO-*d*₆)

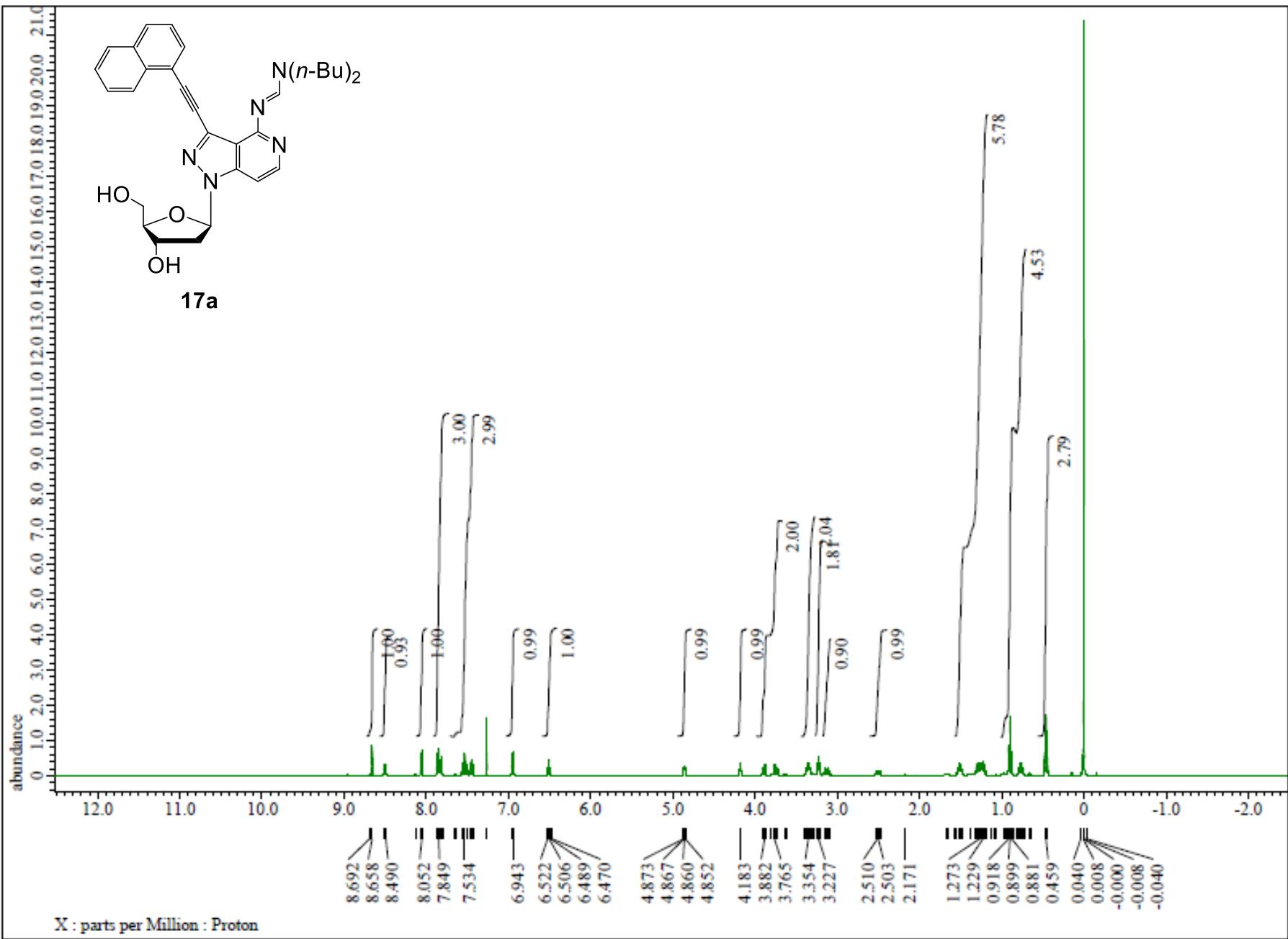


Figure S41. ¹H-NMR spectrum of compound **17a** (CDCl₃)

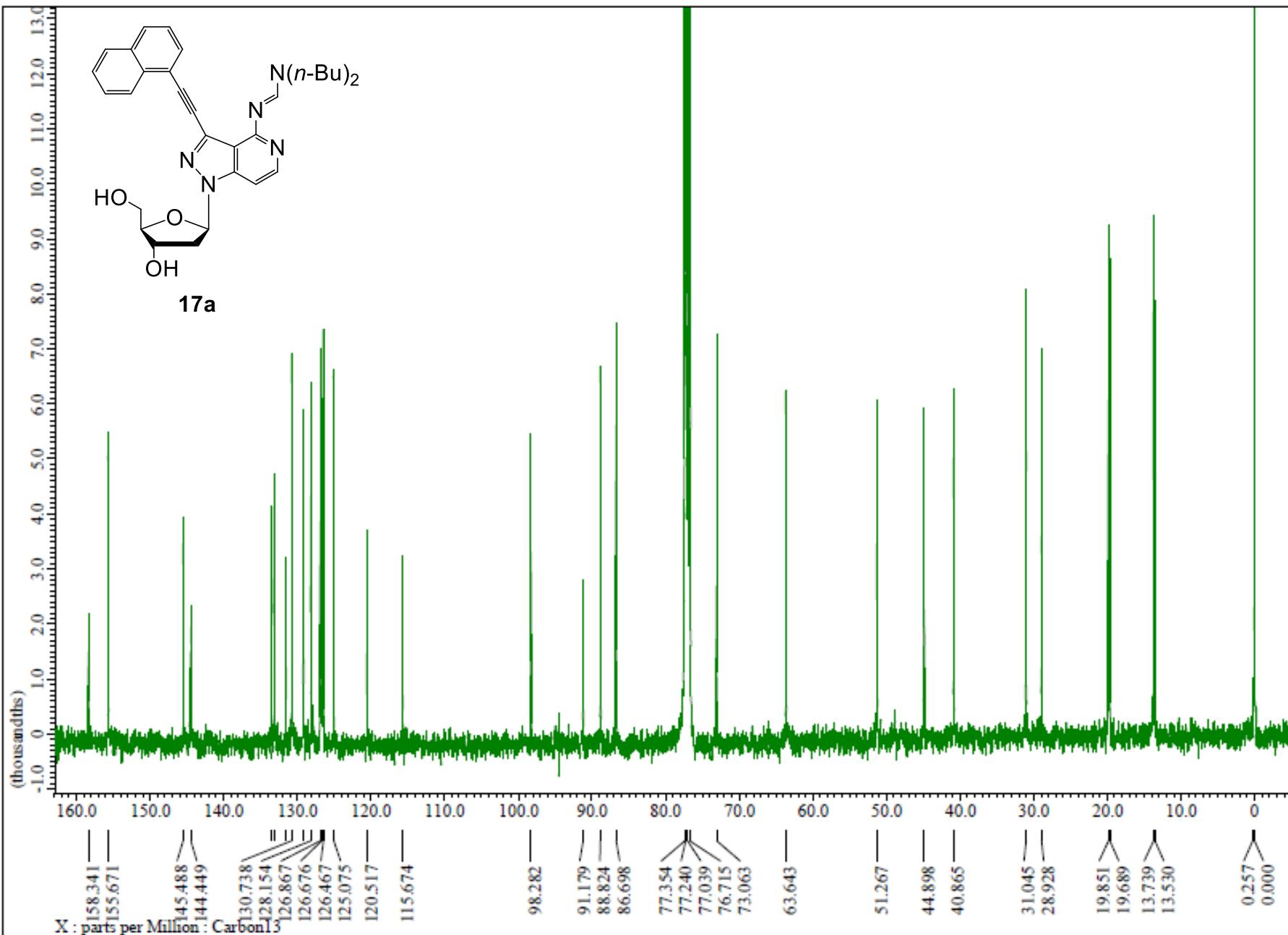


Figure S42. ^{13}C -NMR spectrum of compound **17a** (CDCl_3)

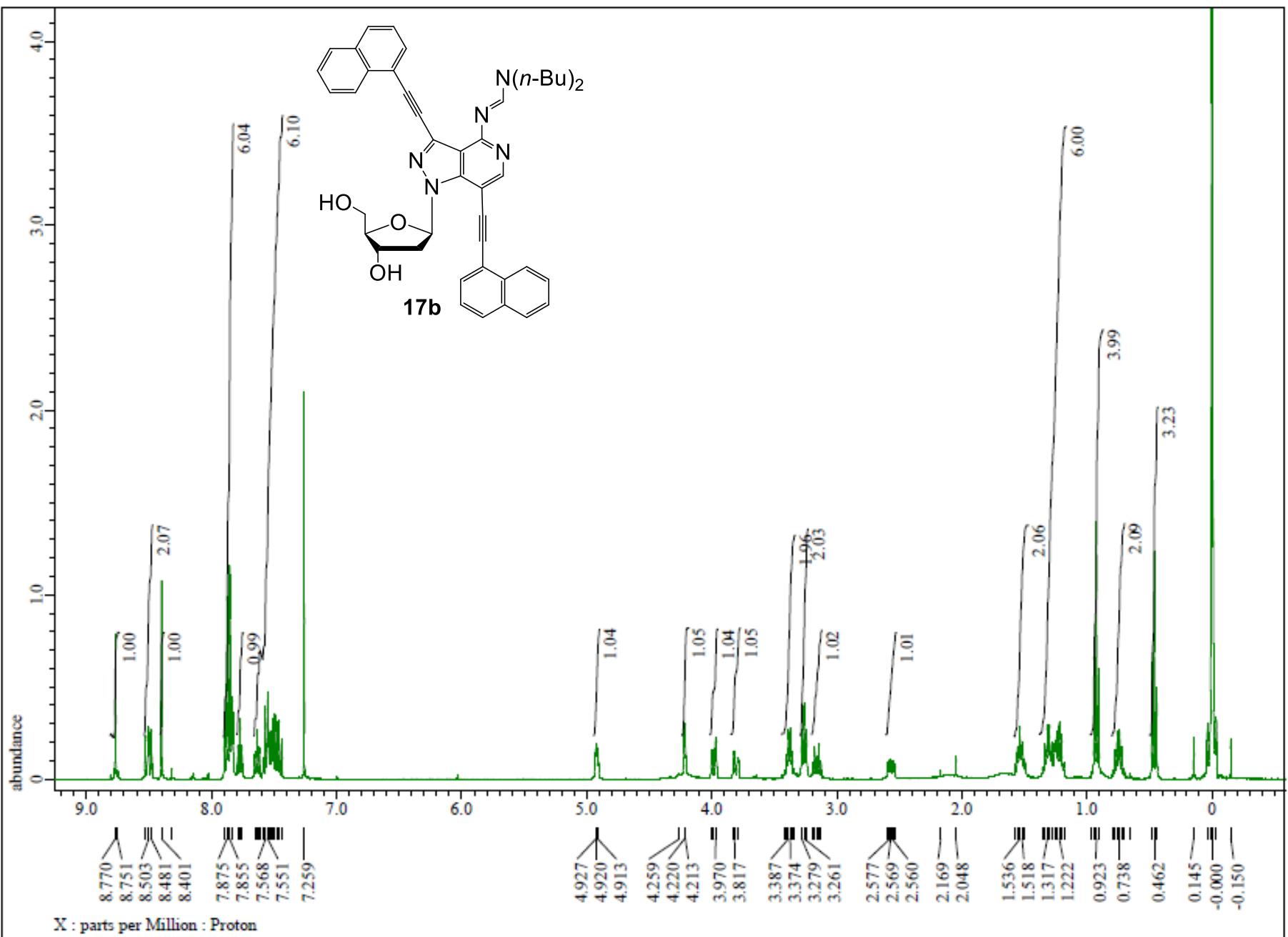


Figure S43. ^1H -NMR spectrum of compound 17b (CDCl_3)

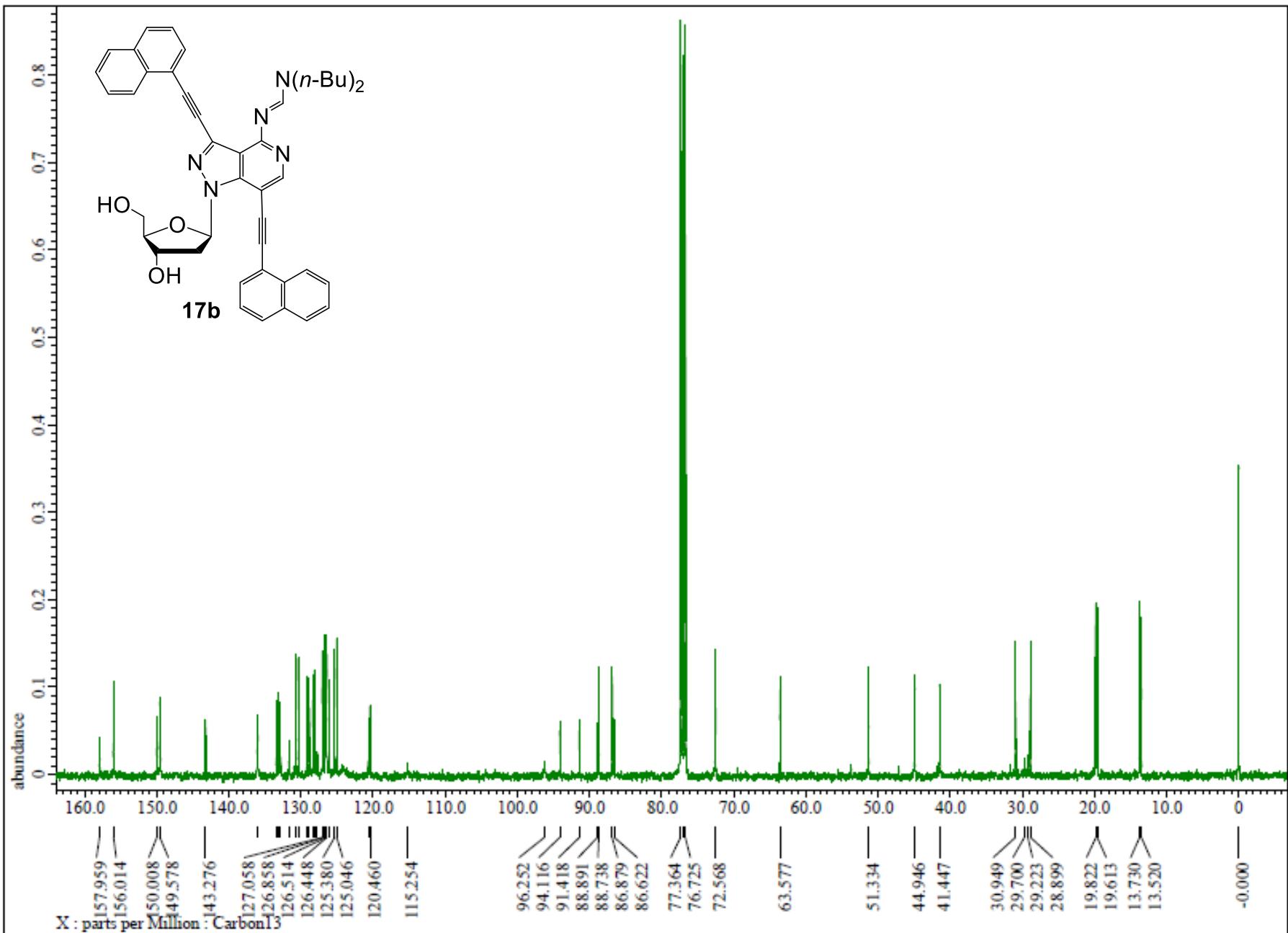


Figure S44. ^{13}C -NMR spectrum of compound **17b** (CDCl_3)

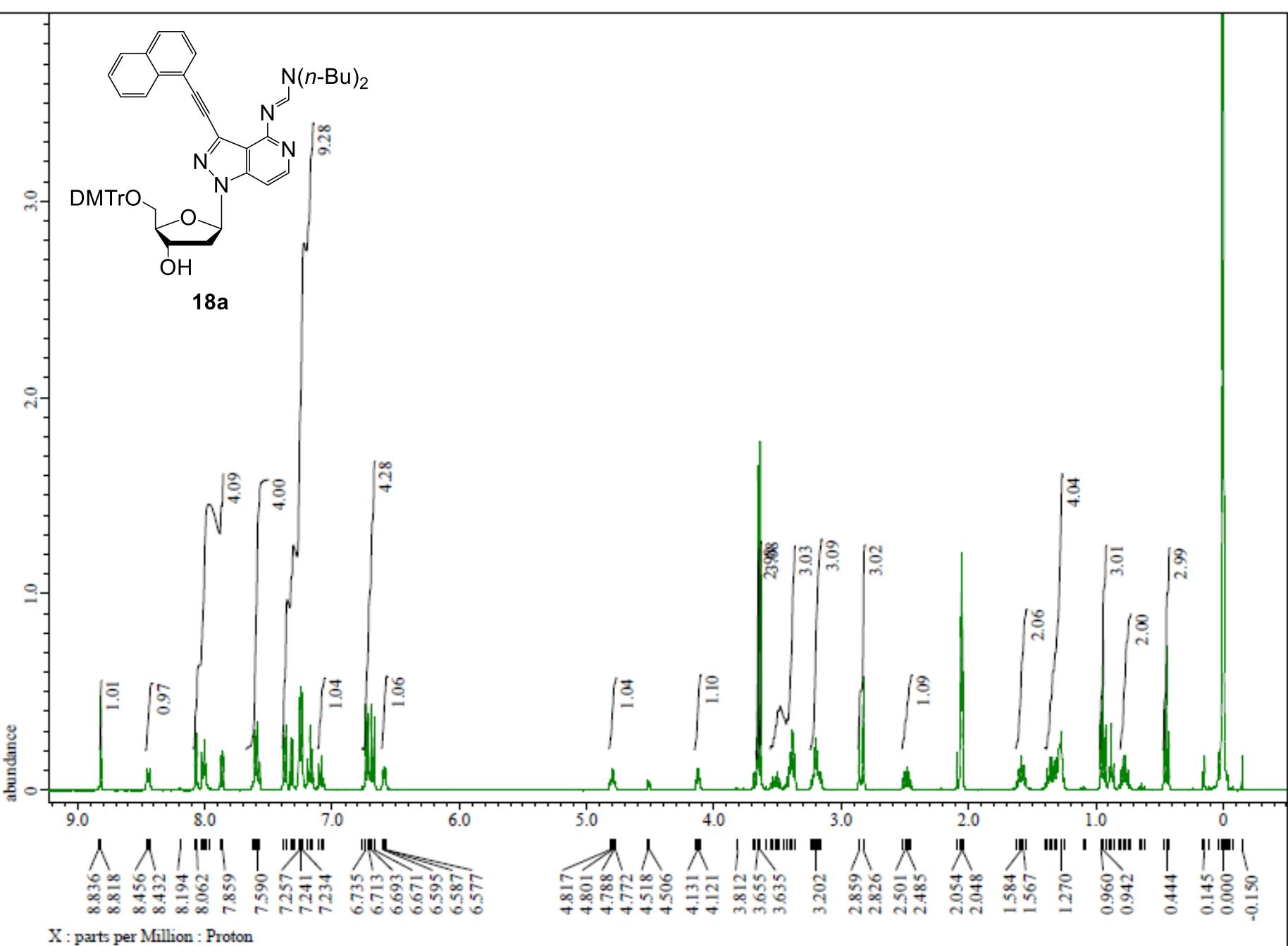


Figure S45. ¹H-NMR spectrum of compound **18a** (acetone-*d*₆)

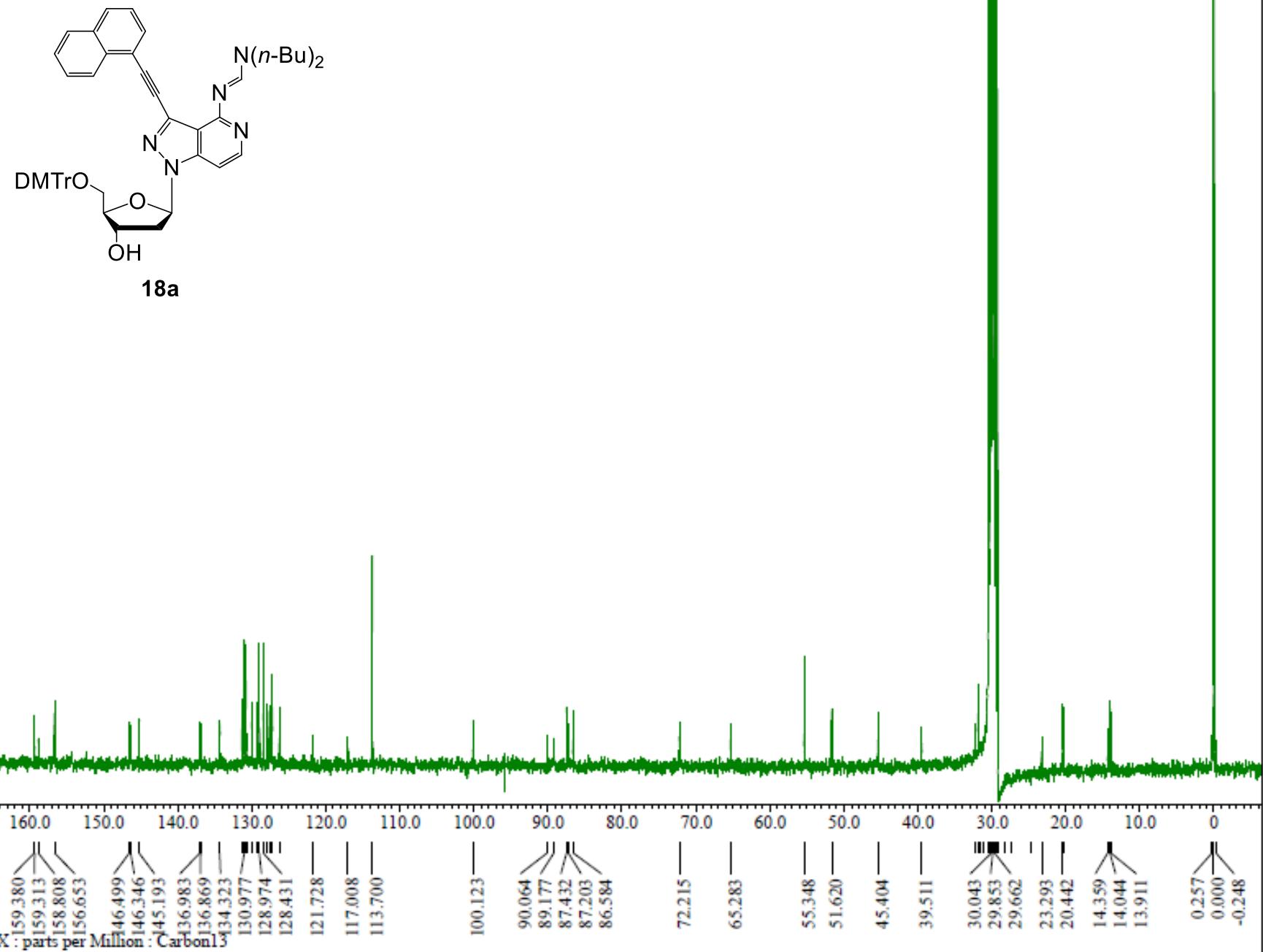


Figure S46. ¹³C-NMR spectrum of compound **18a** (acetone-*d*₆)

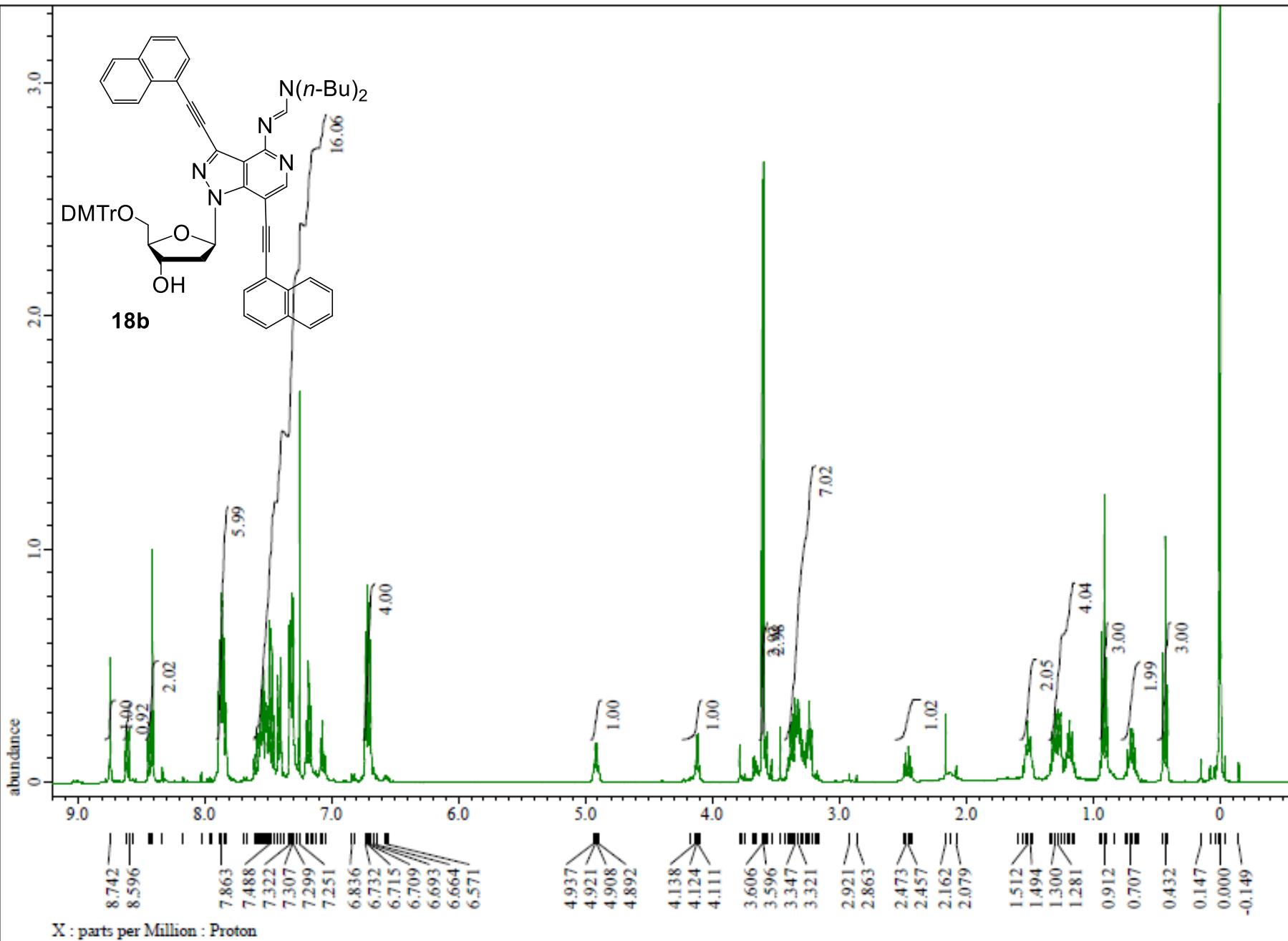


Figure S47. ^1H -NMR spectrum of compound **18b** (CDCl_3)

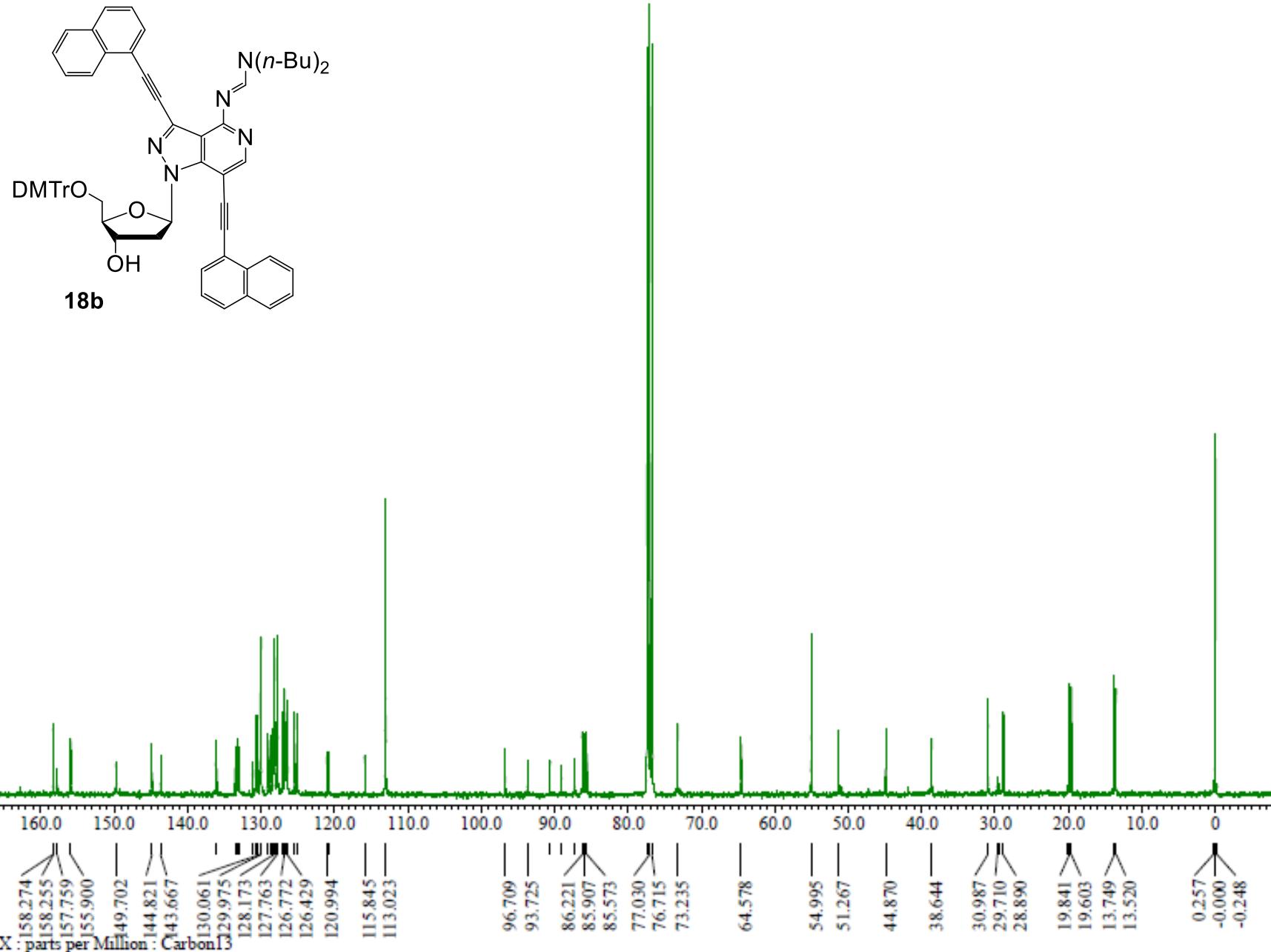


Figure S48. ^{13}C -NMR spectrum of compound **18b** (CDCl_3)