

Supplementary data for
The fluorescently responsive 3-(naphthalene-1-ylethynyl)-3-deaza-2'-deoxyguanosine
discriminates cytidine via the DNA minor groove

Azusa Suzuki,^a Masaki Yanagi,^a Takuya Takeda,^a Robert H. E. Hudson,^b and Yoshio Saito^{a*}

*a) Department of Chemical Biology and Applied Chemistry, College of Engineering,
Nihon University, Koriyama, Fukushima 963-8642, Japan*

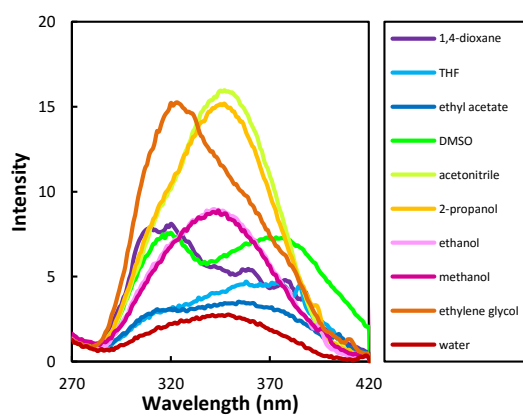
Email Address: saitoy@chem.ce.nihon-u.ac.jp

*b) Department of Chemistry, The University of Western Ontario,
London, Ontario, Canada N6A 5B7.*

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a)



b)

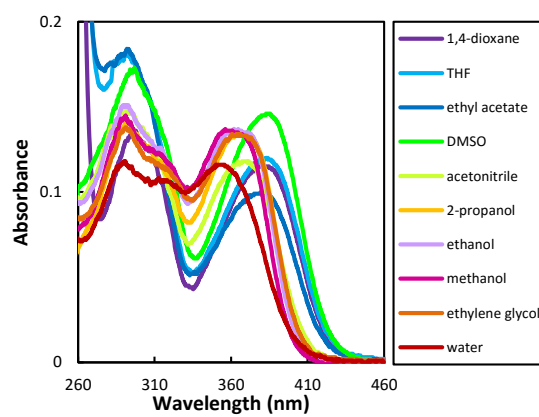


Figure S1: (a) Excitation and (b) UV absorption spectra of ^{3nz}G (1) in various solvents of different polarities. All measurements were performed at a concentration of 10 μM .

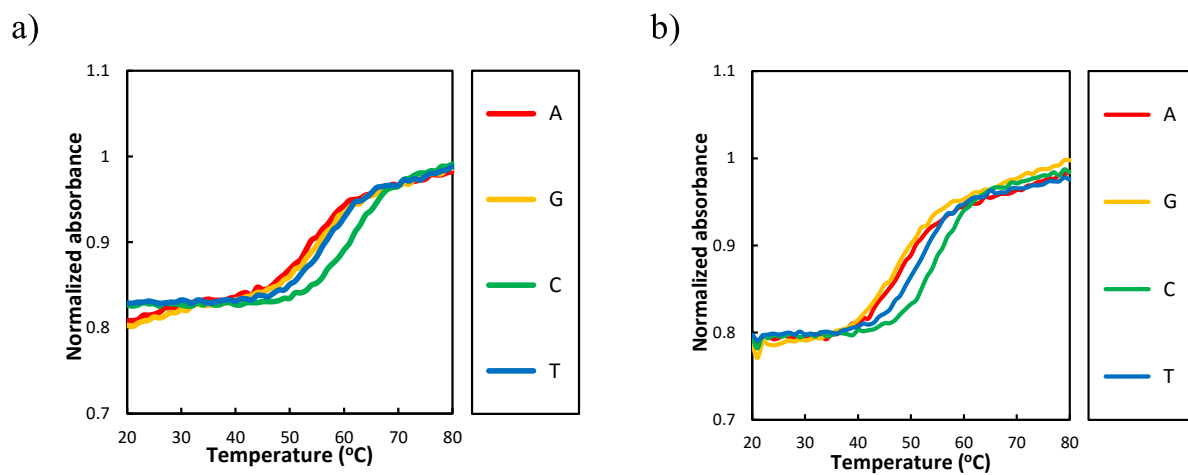


Figure S2: Thermal melting temperature (T_m) of (a) ODN1($^{3nz}\mathbf{G}$) hybridized with cODN1(N), (N = A, G, C, or T) and (b) ODN2($^{3nz}\mathbf{G}$) hybridized with cODN2(N), (N = A, G, C, or T) (2.5 μM duplex, 0.1 M sodium chloride, 50 mM sodium phosphate buffer, pH 7.0, rt).

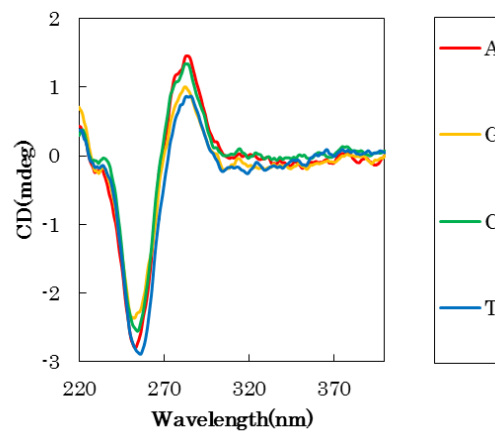


Figure S3: CD spectra of ODN1(^{3nz}G) hybridized with cODN1(N), (N = A, G, C, or T) (2.5 μ M duplex, 0.1 M sodium chloride, 50 mM sodium phosphate buffer, pH 7.0, rt).

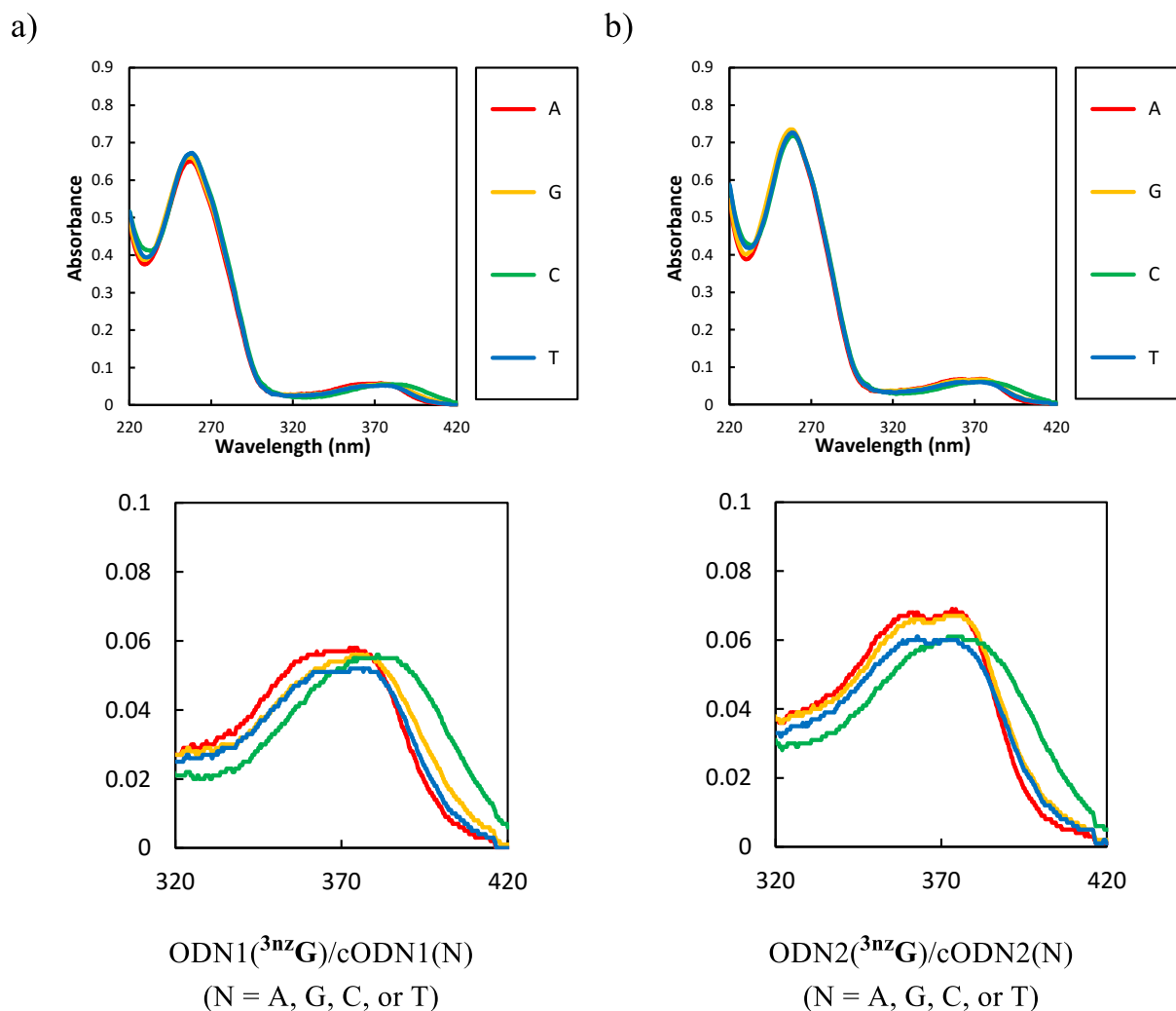


Figure S4: UV absorption spectra of (a) ODN1(^{3nz}G) hybridized with cODN1(N), (N = A, G, C, or T) and (b) ODN2(^{3nz}G) hybridized with cODN2(N), (N = A, G, C, or T) (2.5 μ M duplex, 0.1 M sodium chloride, 50 mM sodium phosphate buffer, pH 7.0, rt).

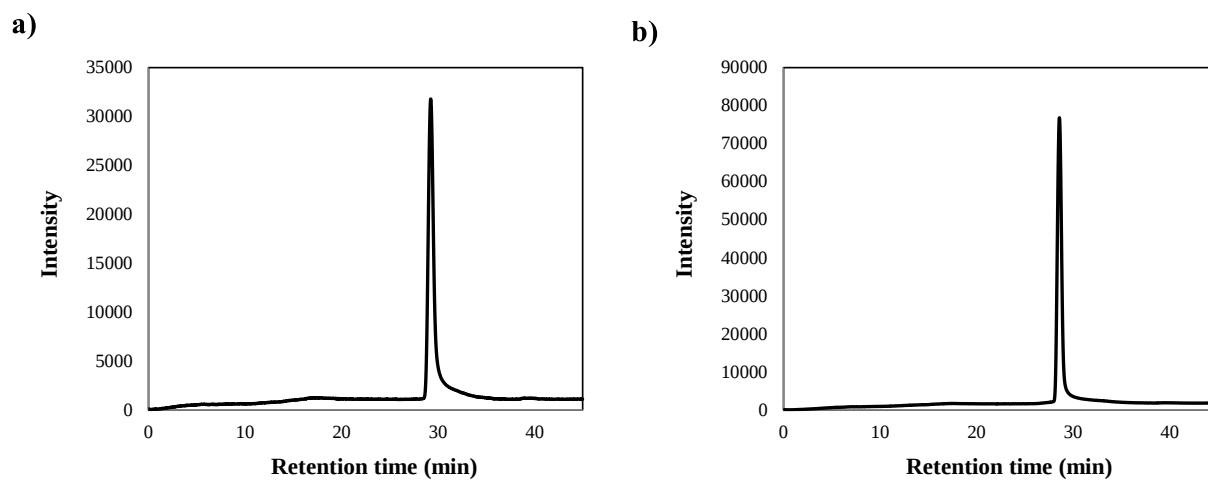


Figure S5. HPLC profiles determined at 260 nm of single-stranded oligonucleotides. a) ODN1(^{3nz}G), and b) ODN2(^{3nz}G). HPLC analysis was performed on a CHEMCOBOND 5-ODS-H column (10 × 150 mm) eluted with 50 mM ammonium formate buffer containing acetonitrile. Gradient: from 3 to 20 % acetonitrile at a flow rate 2.0 ml/min over 45 min.

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

ODNs	Sequences	MALDI-TOF-MS	
		calcd. $[M + H]^+$	found $[M + H]^+$
ODN1(^{3nz} G)	5'-d(CGCAAC ^{3nz} GCAACGC)-3'	4063.83	4063.34
ODN2(^{3nz} G)	5'-d(CGCAAT ^{3nz} GTAACGC)-3'	4093.85	4093.99

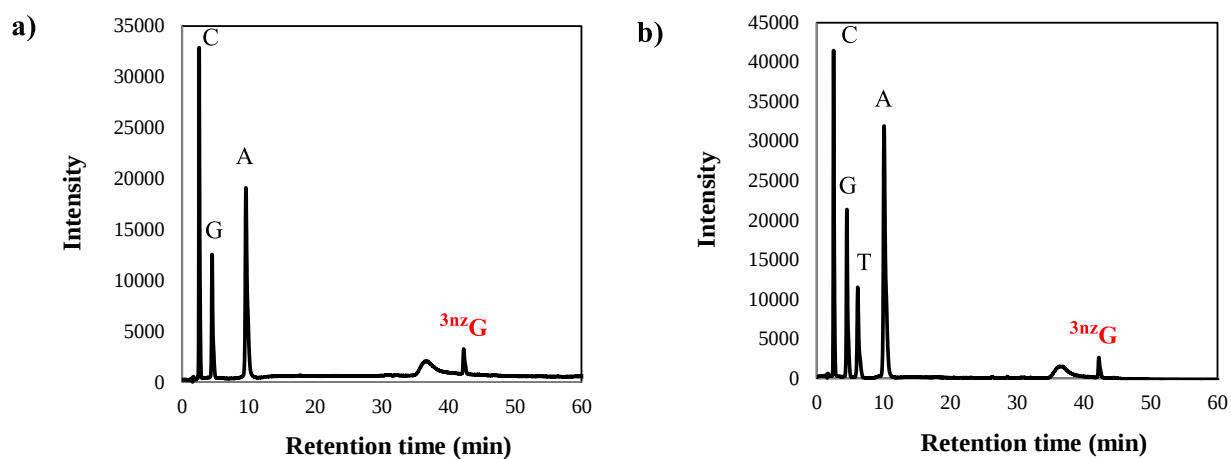


Figure S6. HPLC data for the products of the enzymatic digestion of a) ODN1(^{3nz}G), and b) ODN2(^{3nz}G). HPLC analysis was performed on a COSMOSIL 5-ODS-H column (4.6 × 150 mm) eluted with 50 mM ammonium formate buffer containing acetonitrile. Gradient: from 3 to 50 % acetonitrile at a flow rate 1.0 ml/min over 60 min. Broad signal at around 36 min. is a system peak.

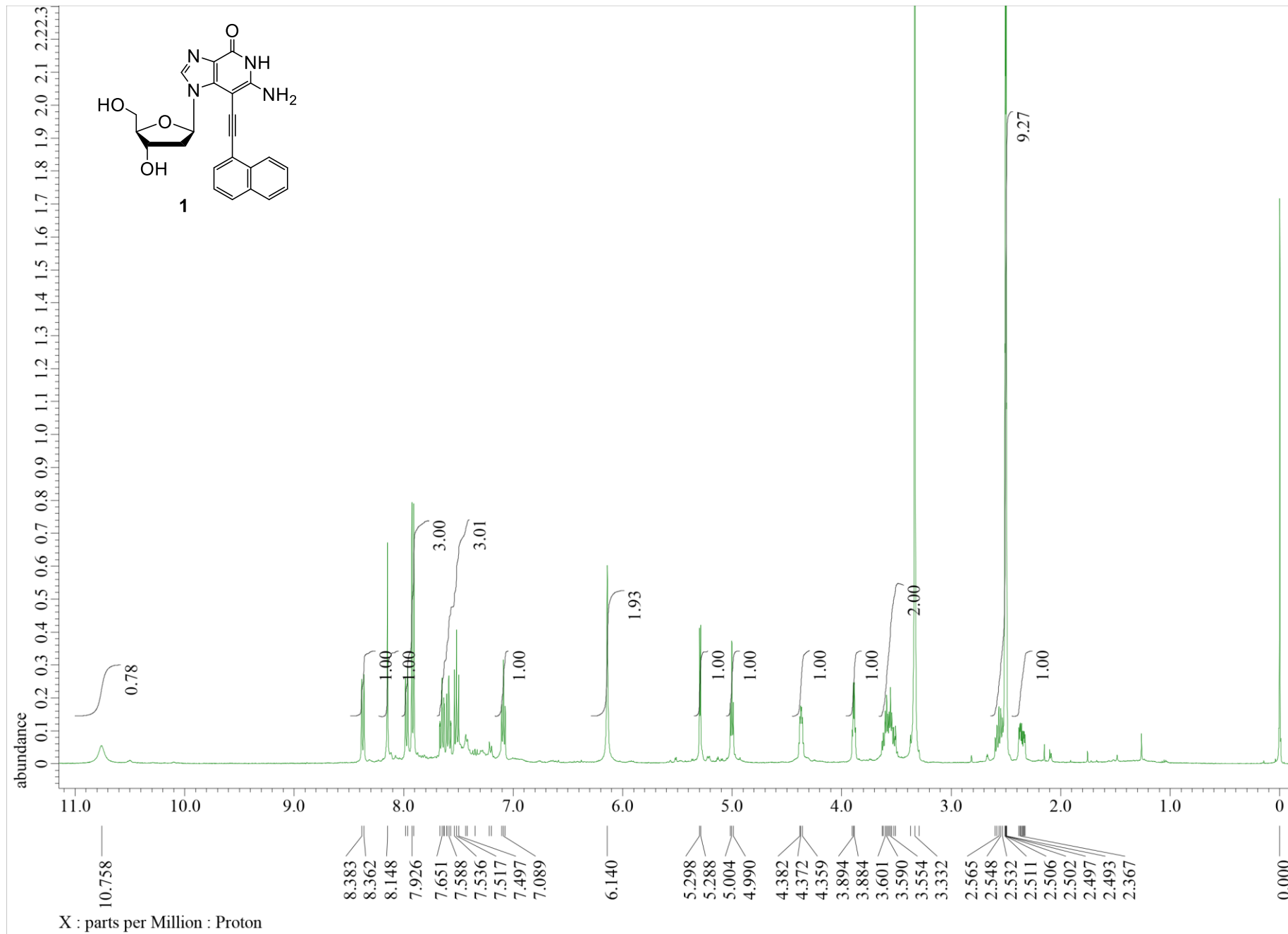


Figure S7. ^1H -NMR spectrum of compound **1** ($\text{DMSO}-d_6$)

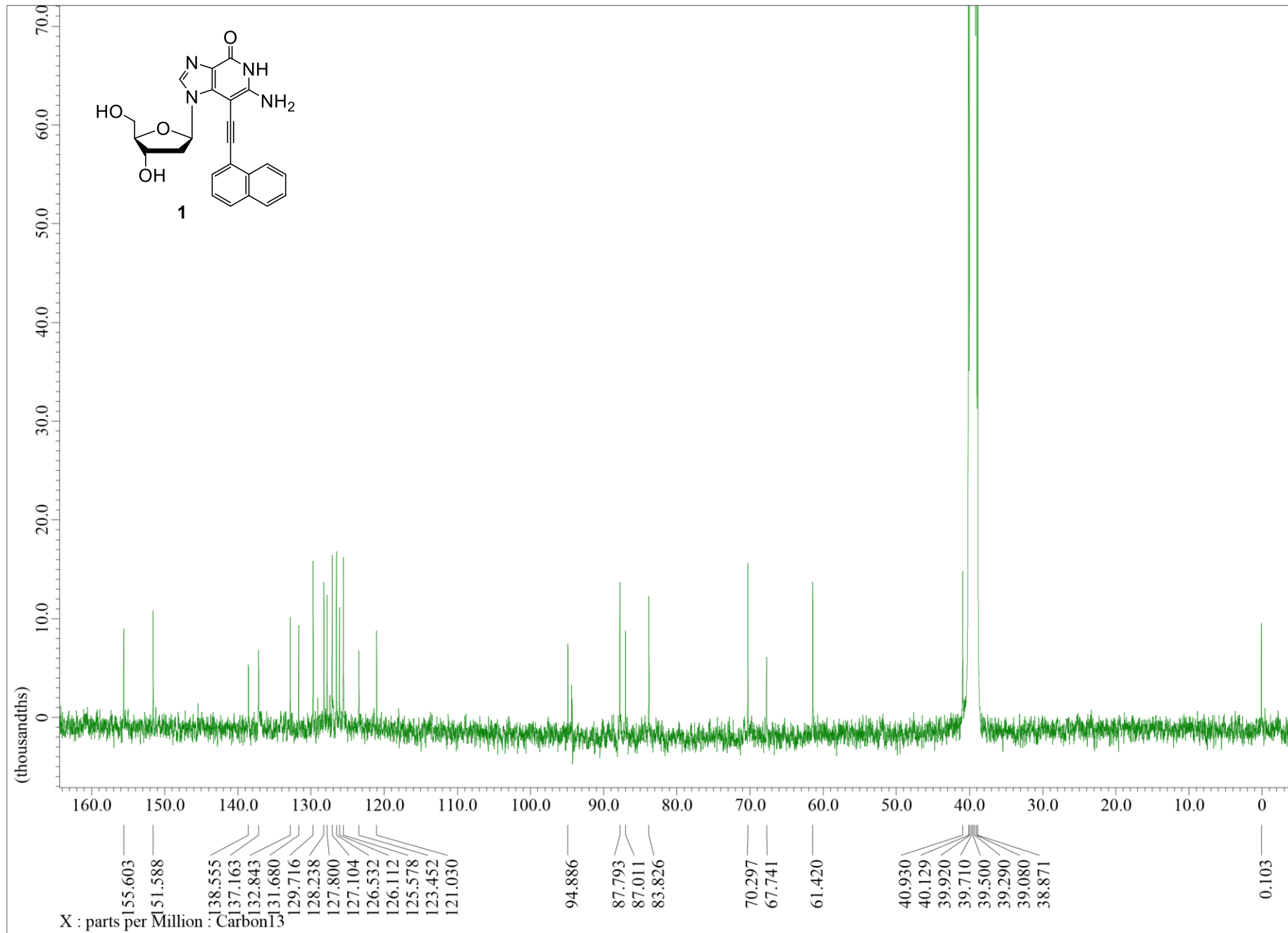


Figure S8. ^{13}C -NMR spectrum of compound **1** ($\text{DMSO}-d_6$)

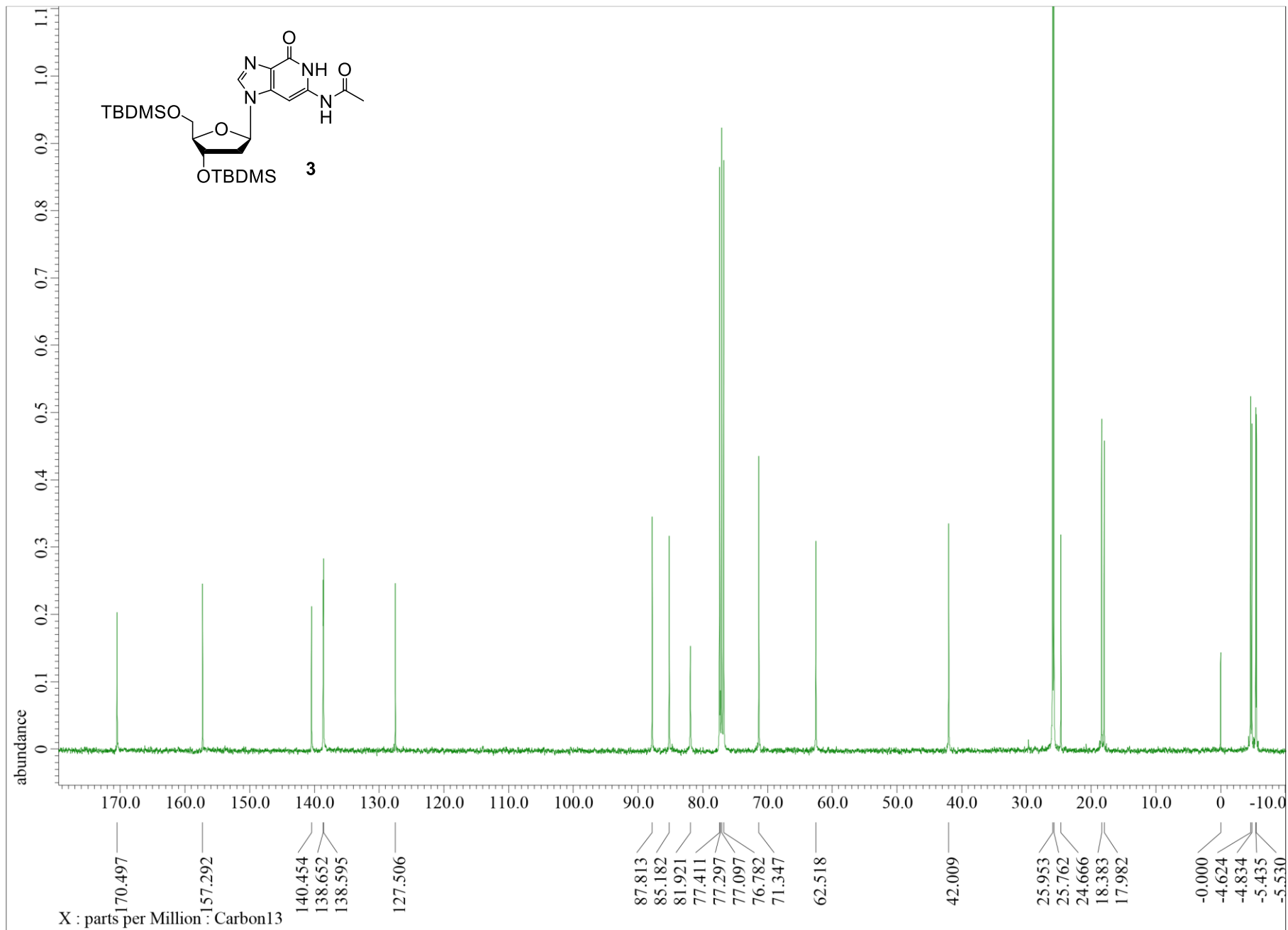


Figure S10. ¹³C-NMR spectrum of compound **3** (CDCl₃)

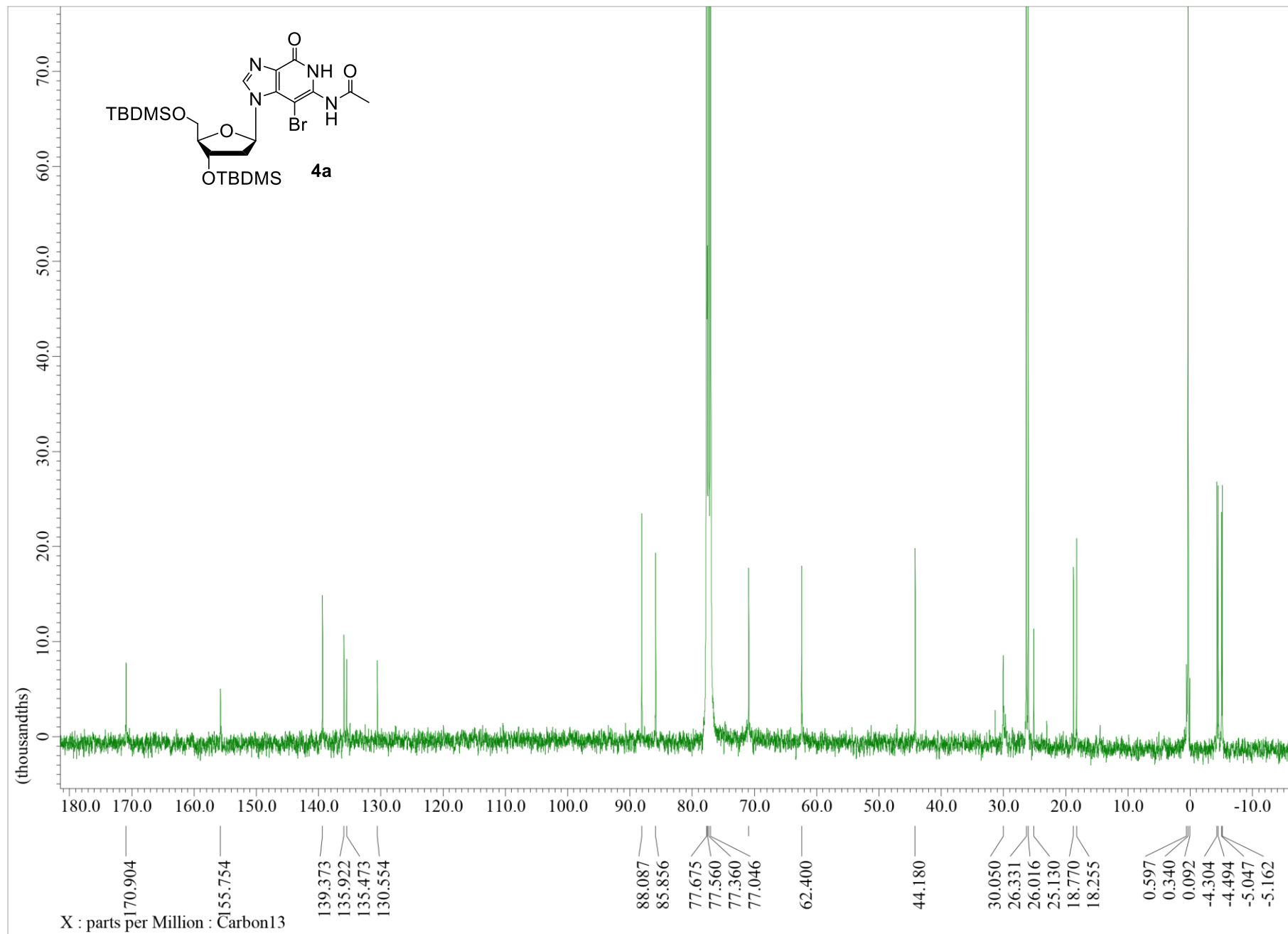


Figure S12. ¹³C-NMR spectrum of compound **4a** (CDCl₃)

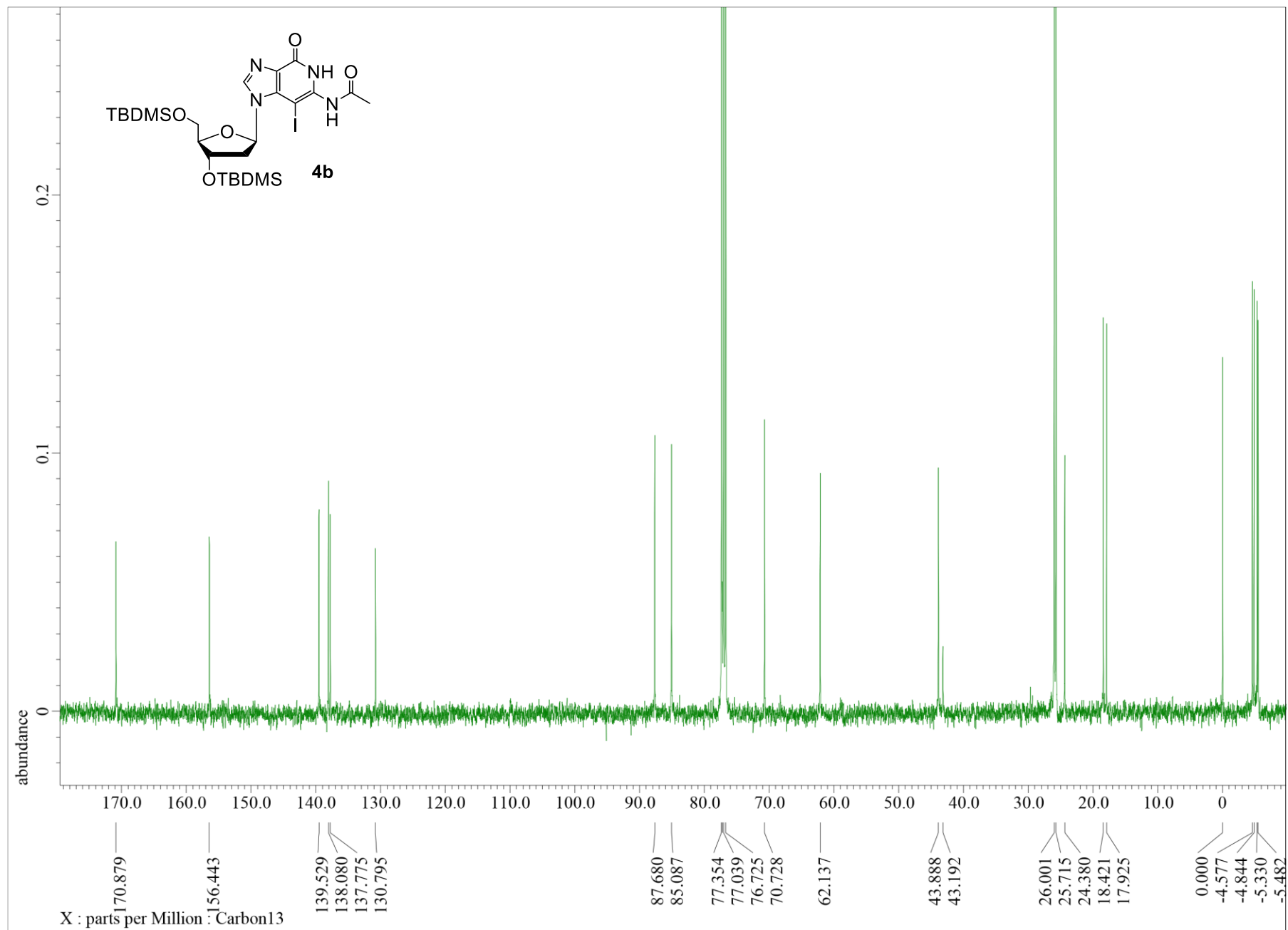


Figure S14. ¹³C-NMR spectrum of compound **4b** (CDCl₃)

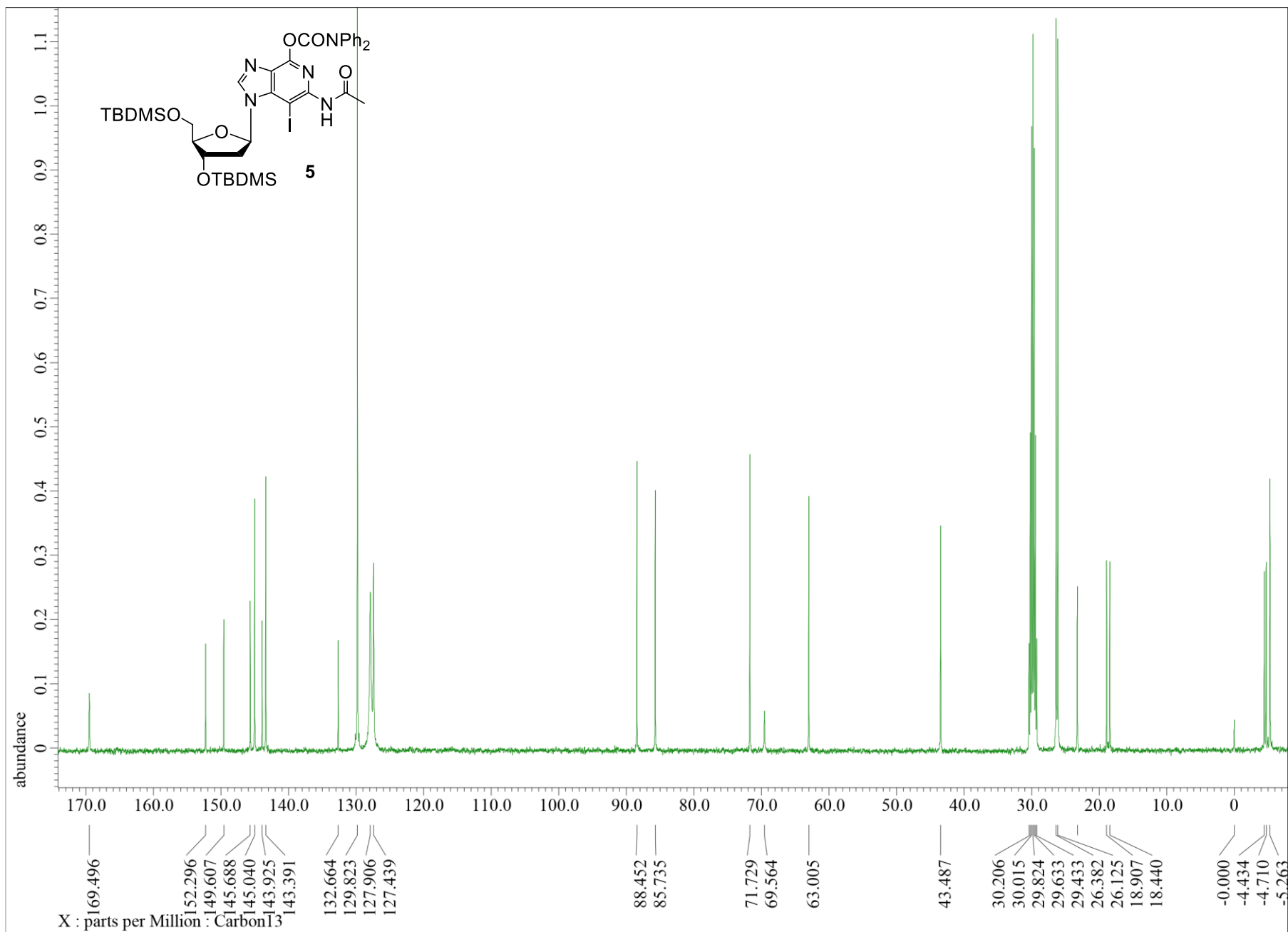


Figure S16. ¹³C-NMR spectrum of compound 5 (Acetone-*d*₆)

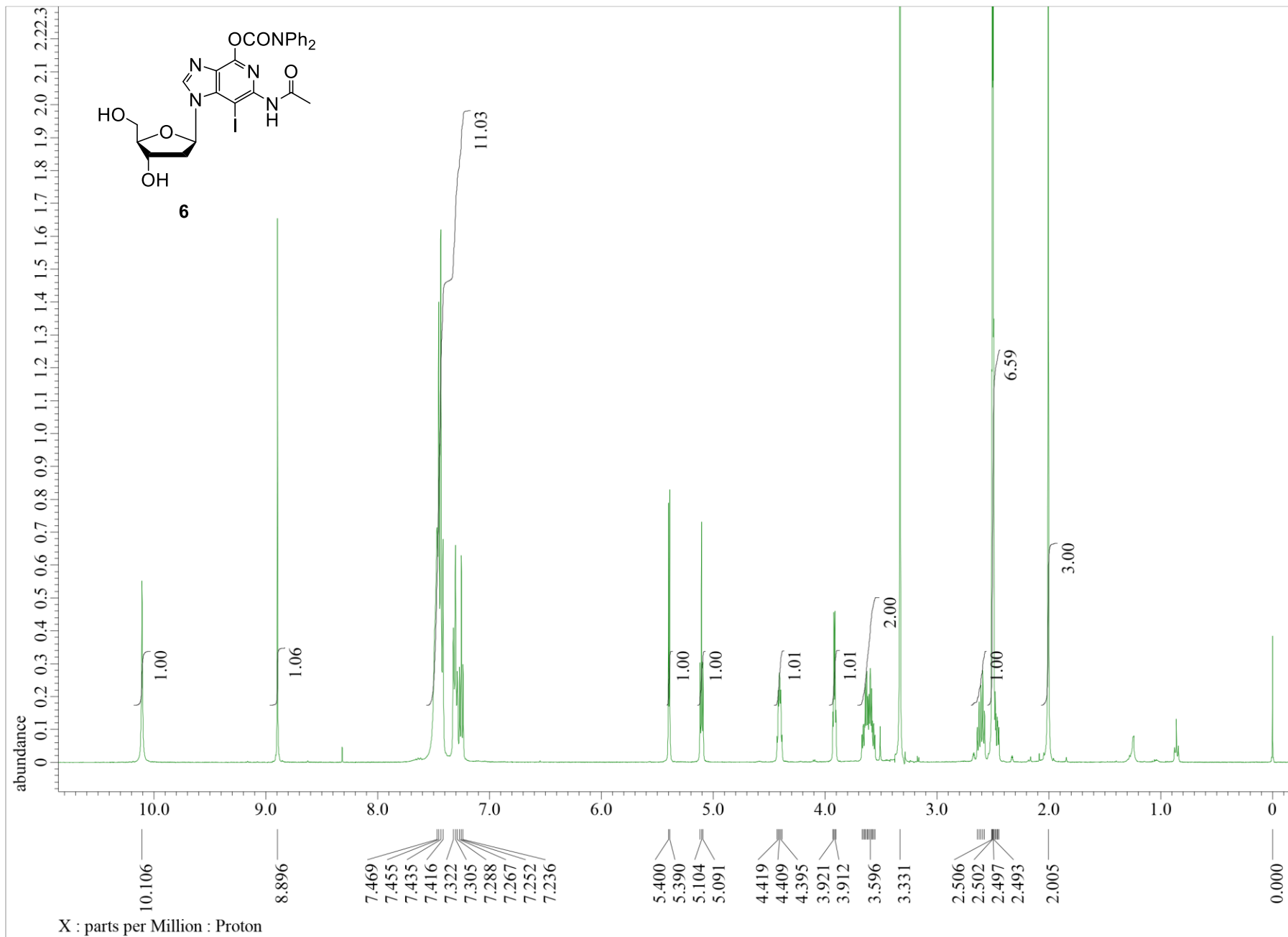


Figure S17. $^1\text{H-NMR}$ spectrum of compound **6** (DMSO- d_6)

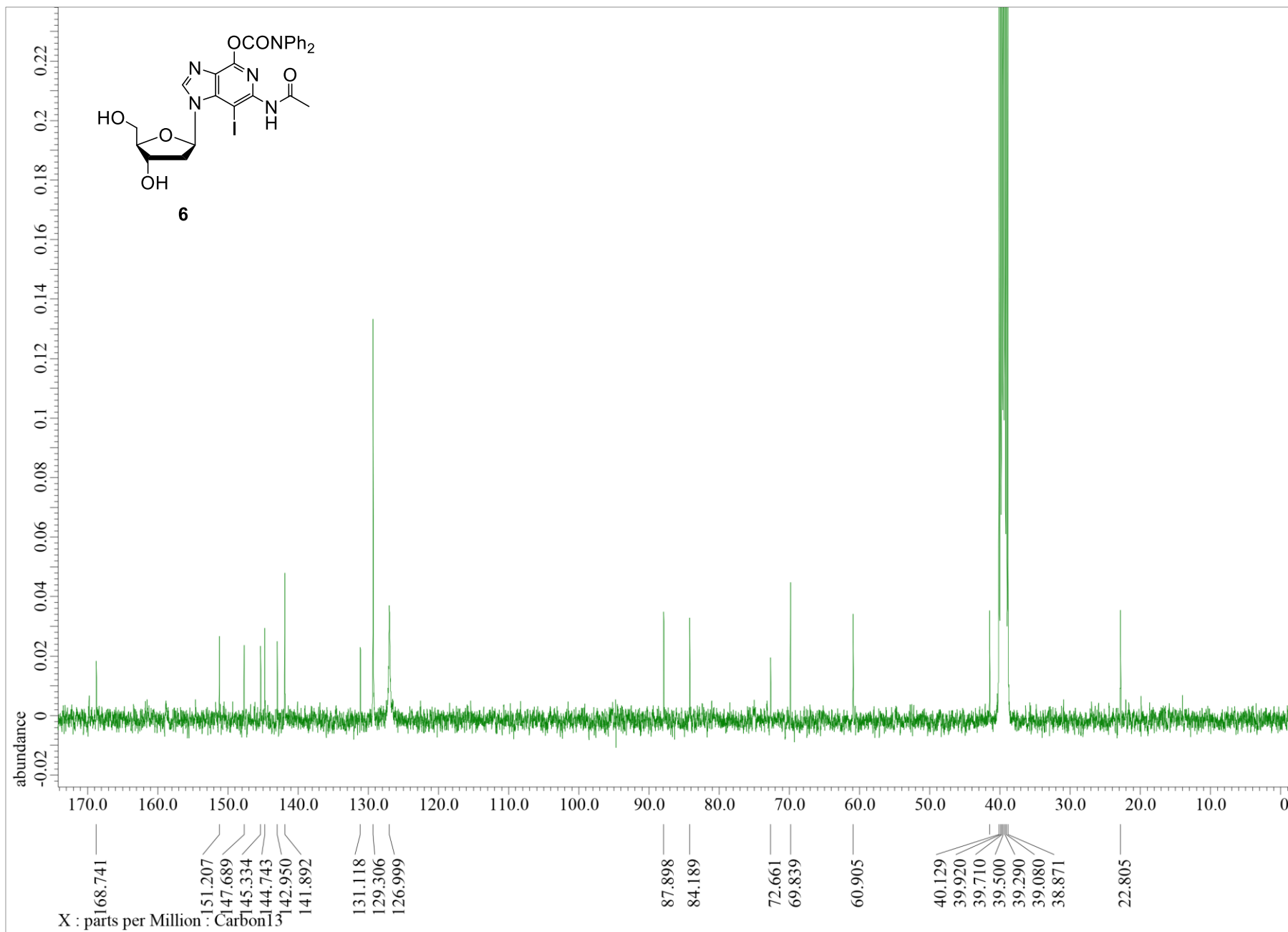


Figure S18. ^{13}C -NMR spectrum of compound **6** (DMSO- d_6)

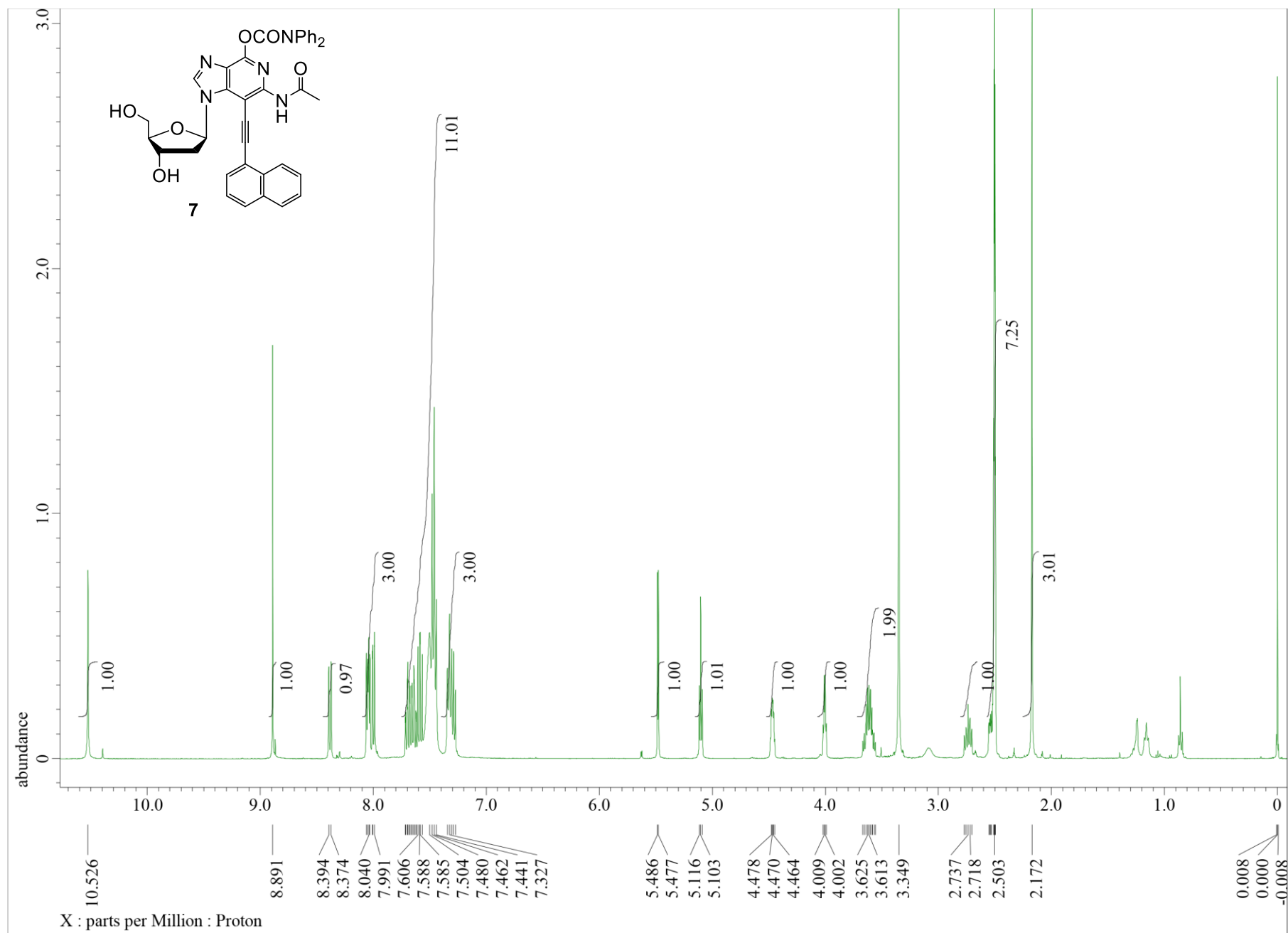


Figure S19. ¹H-NMR spectrum of compound 7 (DMSO-*d*₆)

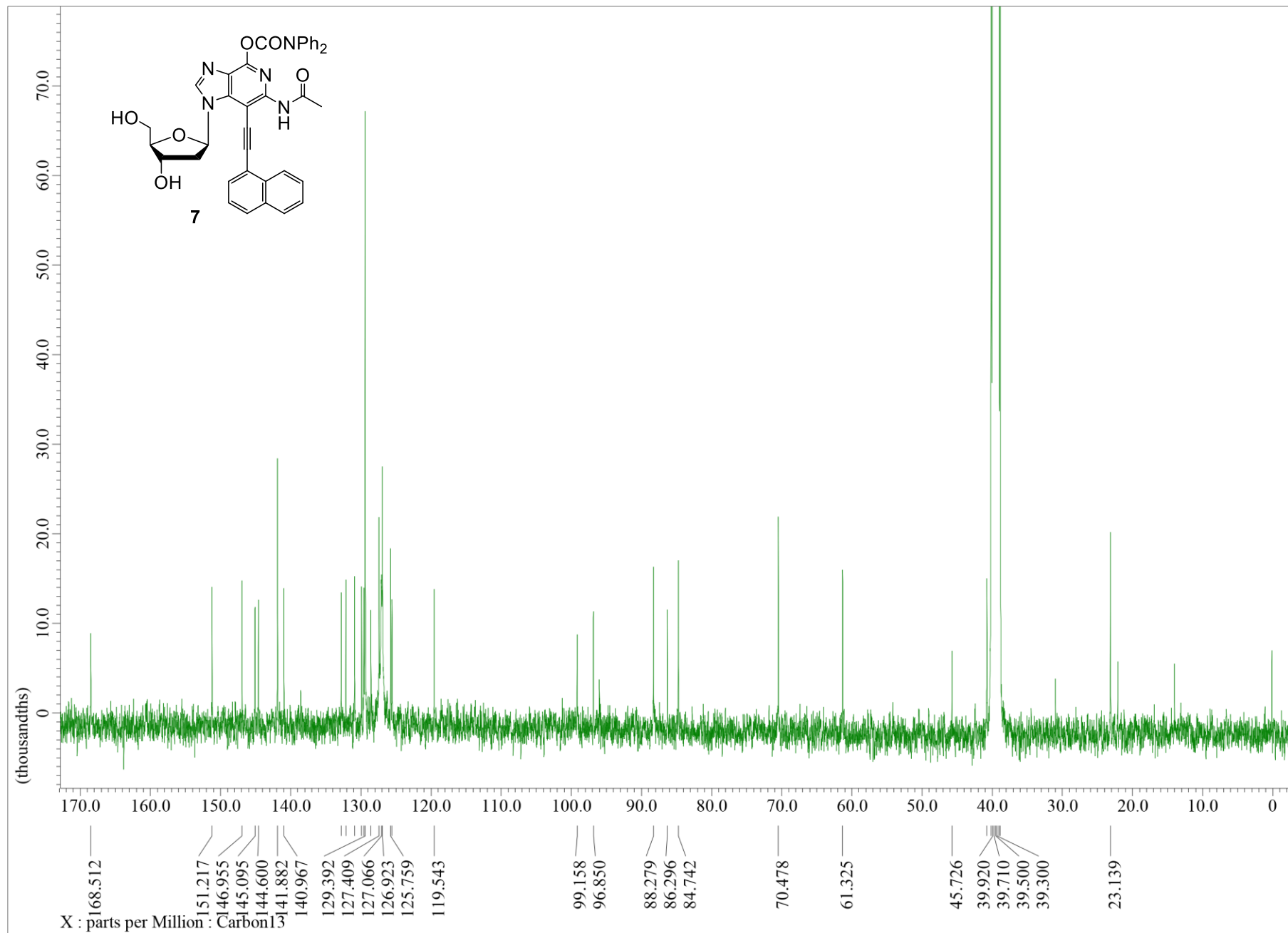


Figure S20. ^{13}C -NMR spectrum of compound 7 (DMSO- d_6)

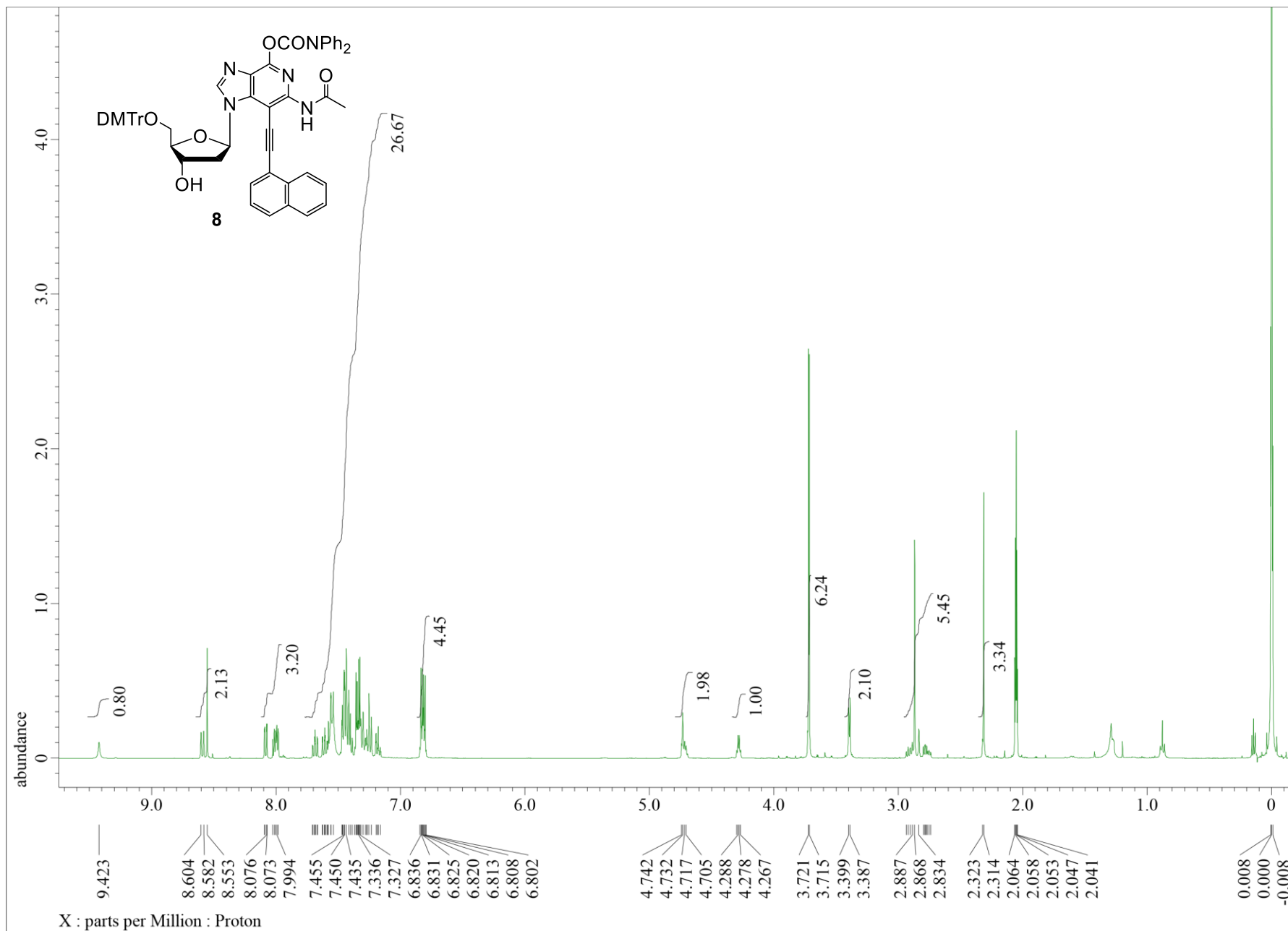


Figure S21. ¹H-NMR spectrum of compound **8** (Acetone-*d*₆)

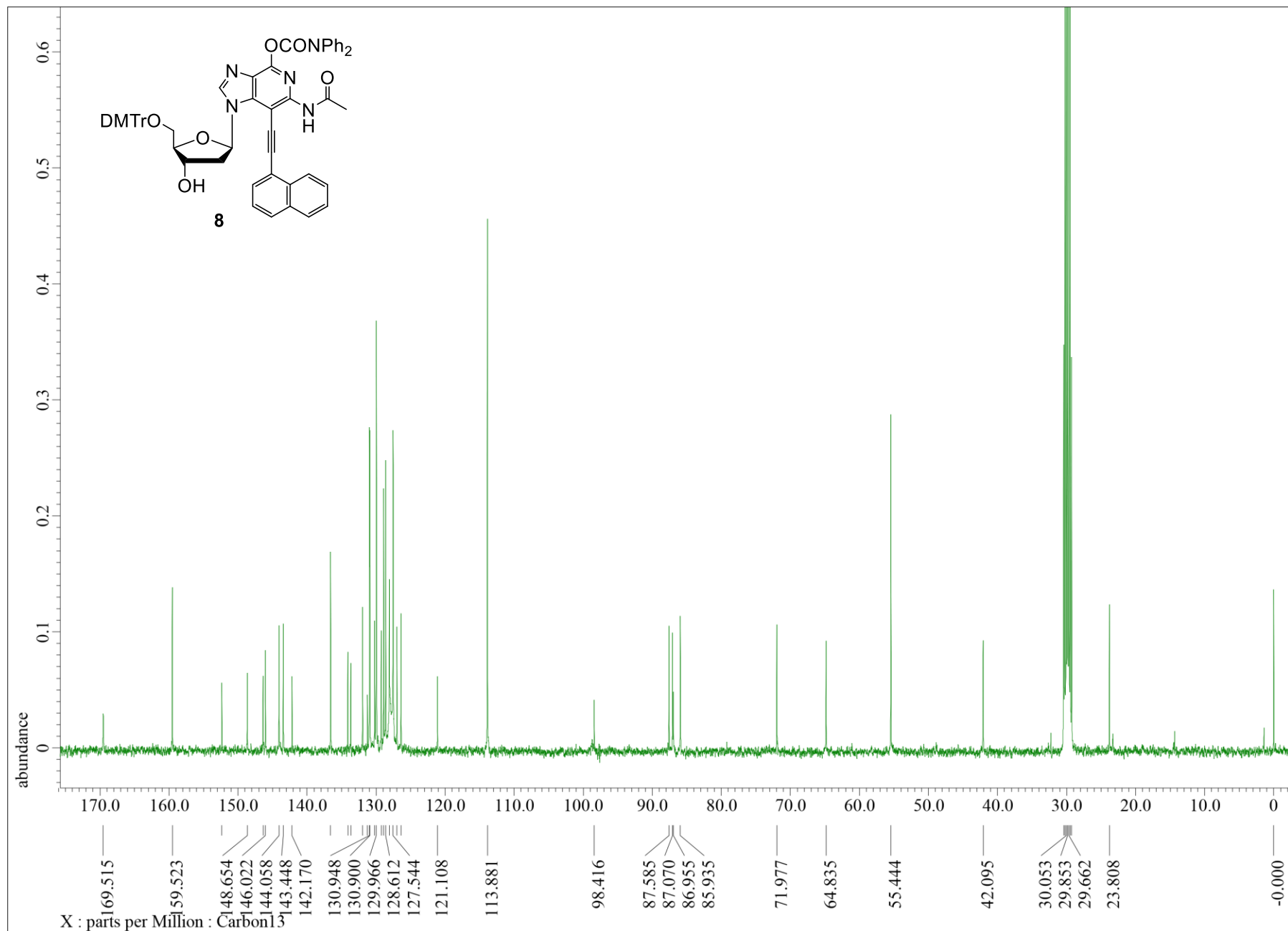


Figure S22. ¹³C-NMR spectrum of compound **8** (Acetone-*d*₆)