Supplementary data for
FRET-based dual-labeled oligonucleotide probe detects target DNA by probing a minor groove environment

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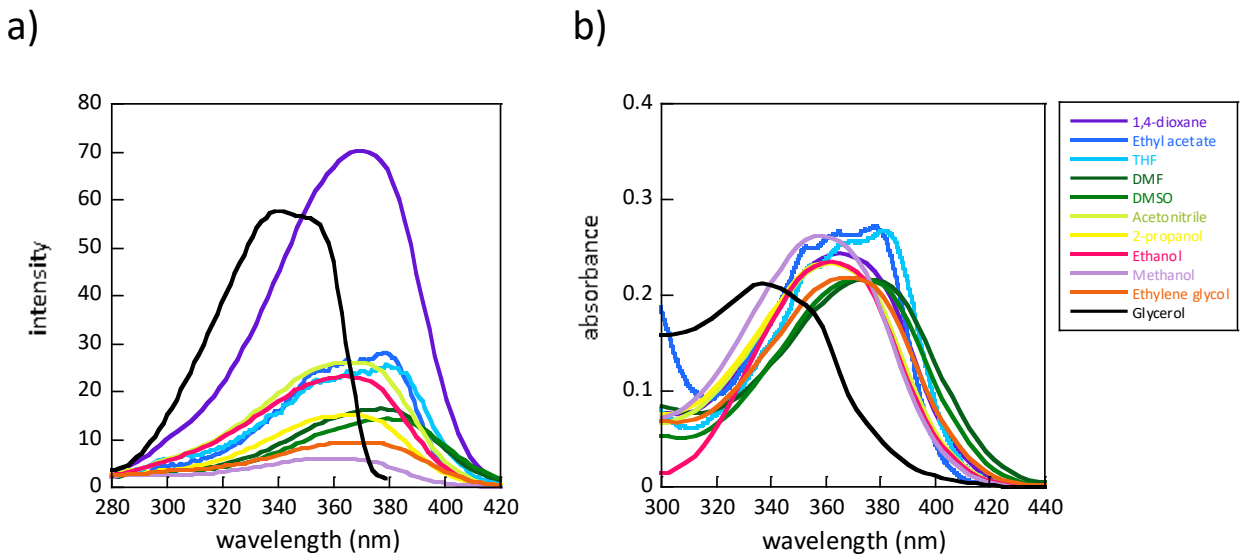


Figure S1: (a) Excitation and (b) UV absorption spectra of **^{AM37z}A** (**1**) in various solvents of different polarities. All measurements were performed at a concentration of 10 µM.

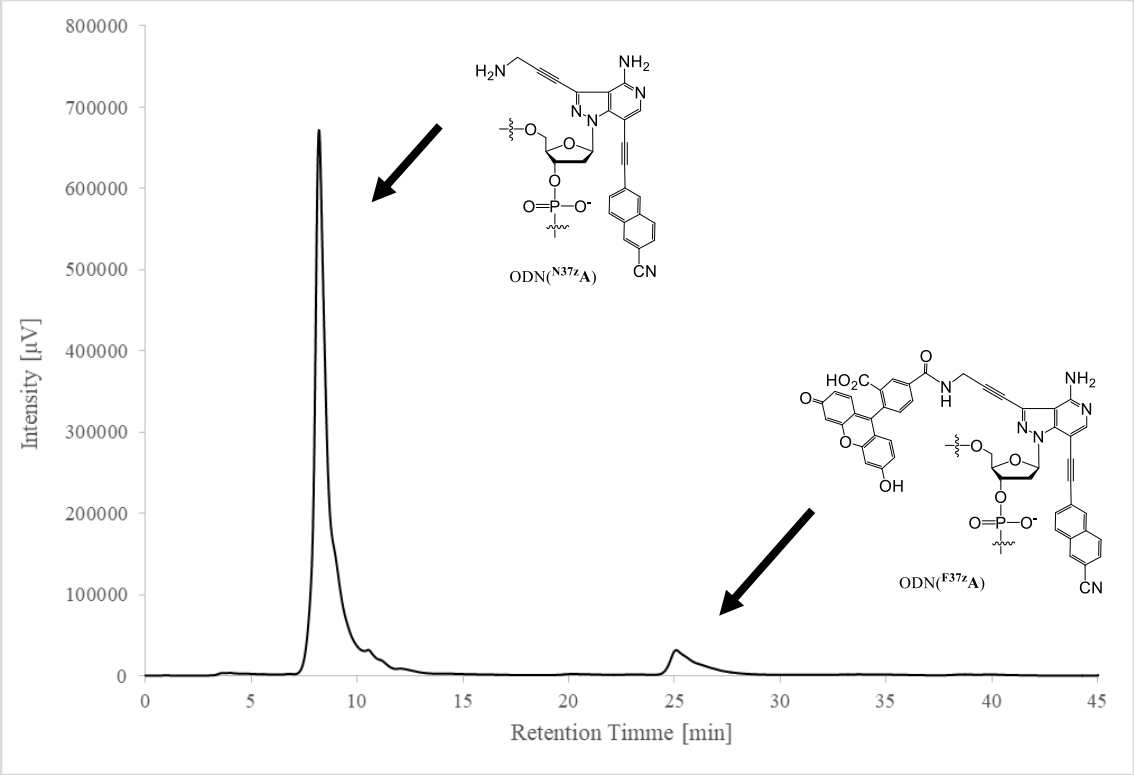


Figure S2. HPLC analysis of the reaction mixture (40°C, 15 h). The analysis was carried out on a CHEMCOBOND 5-ODS-H column (10×150 mm) eluted with 0.05 M ammonium formate buffer containing acetonitrile. Gradient from 3 to 30 % acetonitrile at a flow rate 2.0 ml/min over 45 min (UV detector at 260 nm).

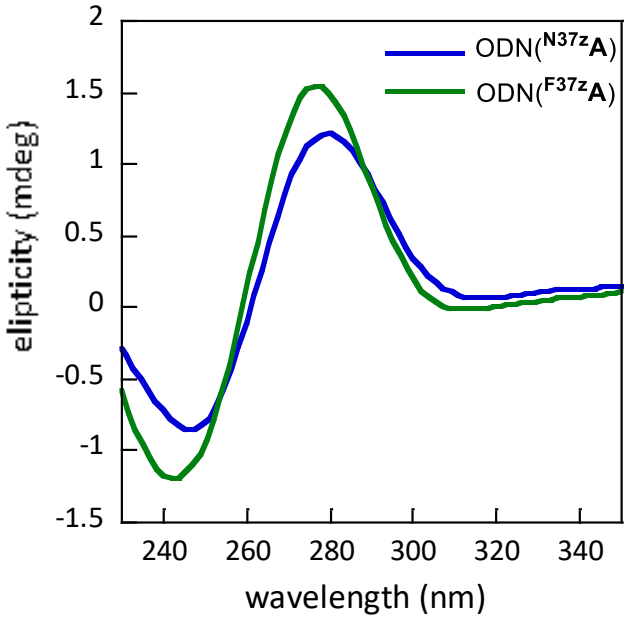


Figure S3. CD spectra of ODN(^{N37z}**A**)/cODN(T) and ODN(^{F37z}**A**) /cODN(T) (2.5 μM duplex, 0.1 M sodium chloride, 50 mM sodium phosphate buffer, pH 7.0, rt).

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

ODNs	Sequences	MALDI-TOF-MS	
		calcd. $[M + H]^+$	found $[M + H]^+$
ODN(^{N37z}**A**)	5'-d(CGCAAC ^{N37z}**A** CAACGC)-3'	4127.7	4127.5
ODN(^{F37z}**A**)	5'-d(CGCAAC ^{F37z}**A** CAACGC)-3'	4485.8	4485.1

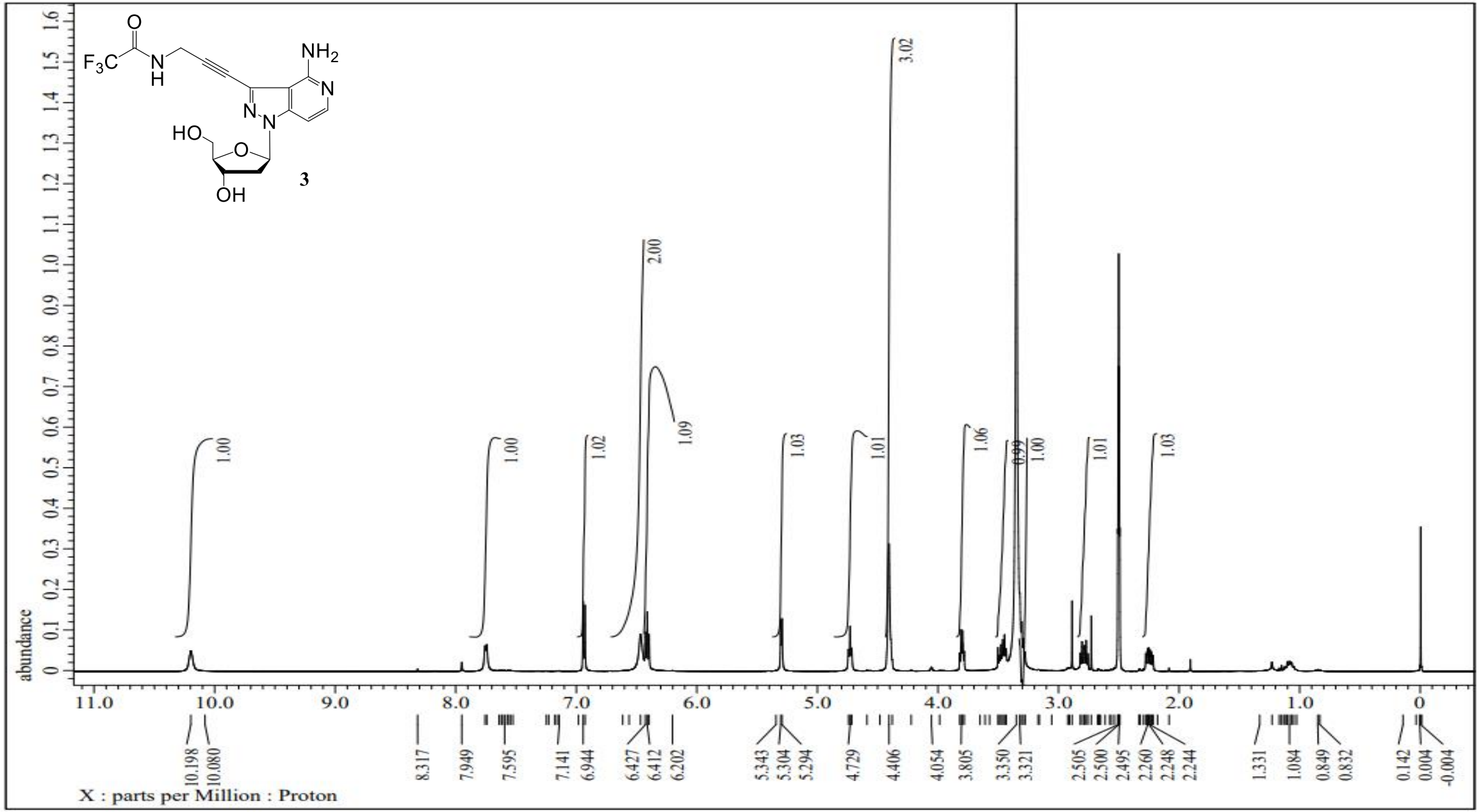


Figure S4. ^{1}H-NMR spectrum of compound **3** (DMSO-d_6)

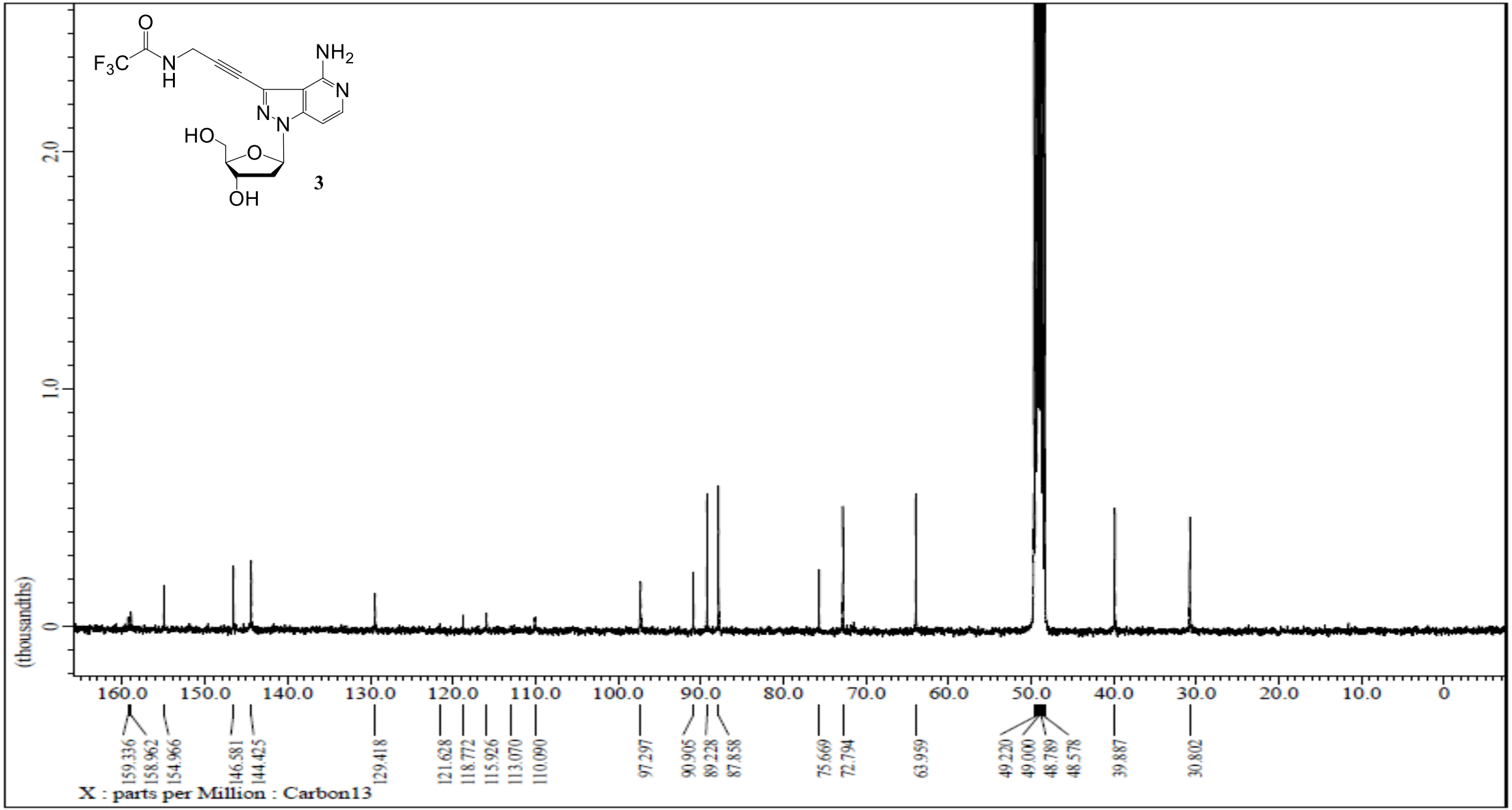


Figure S5. ^{13}C-NMR spectrum of compound **3** (CD_3OD)

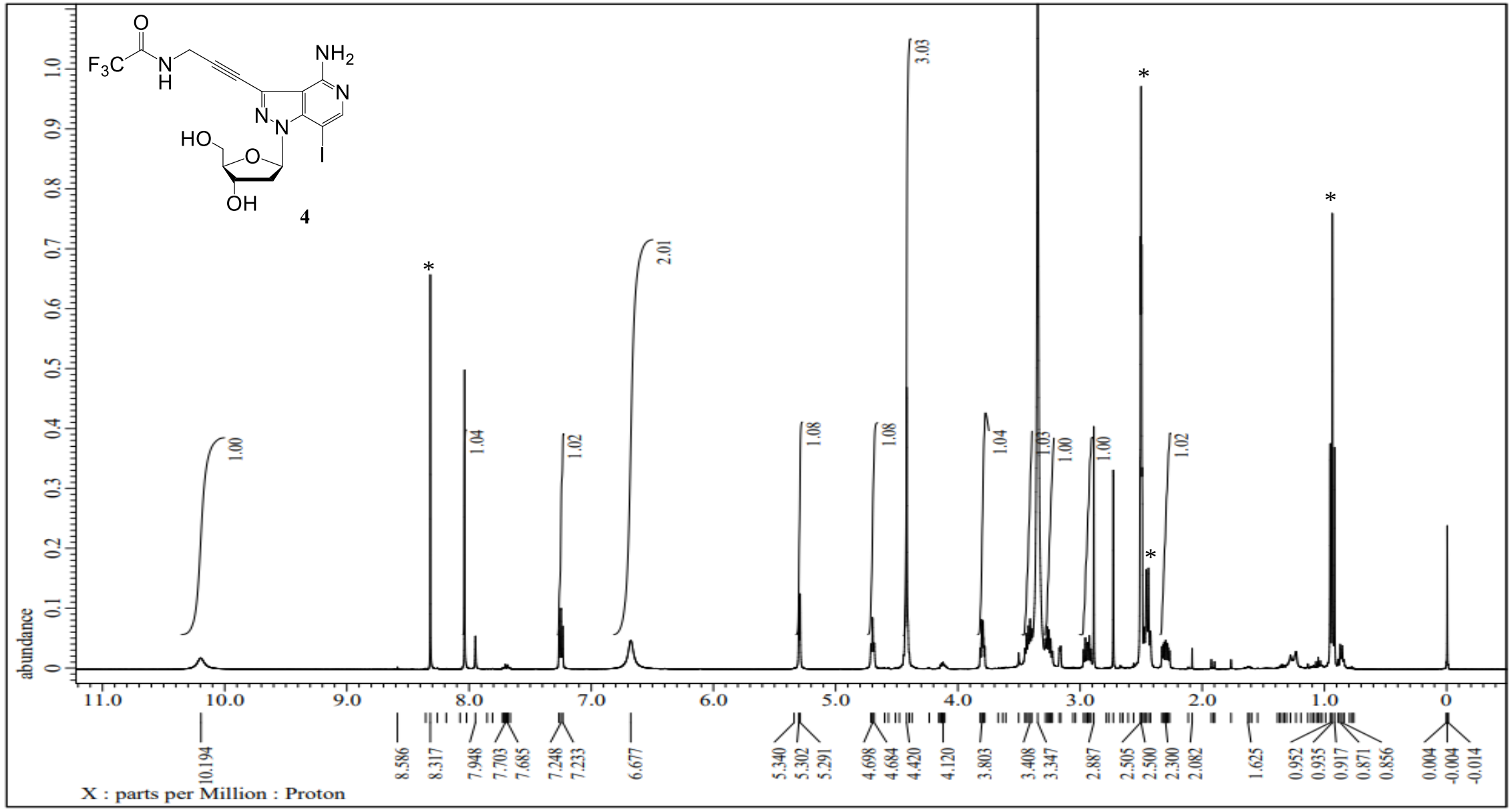
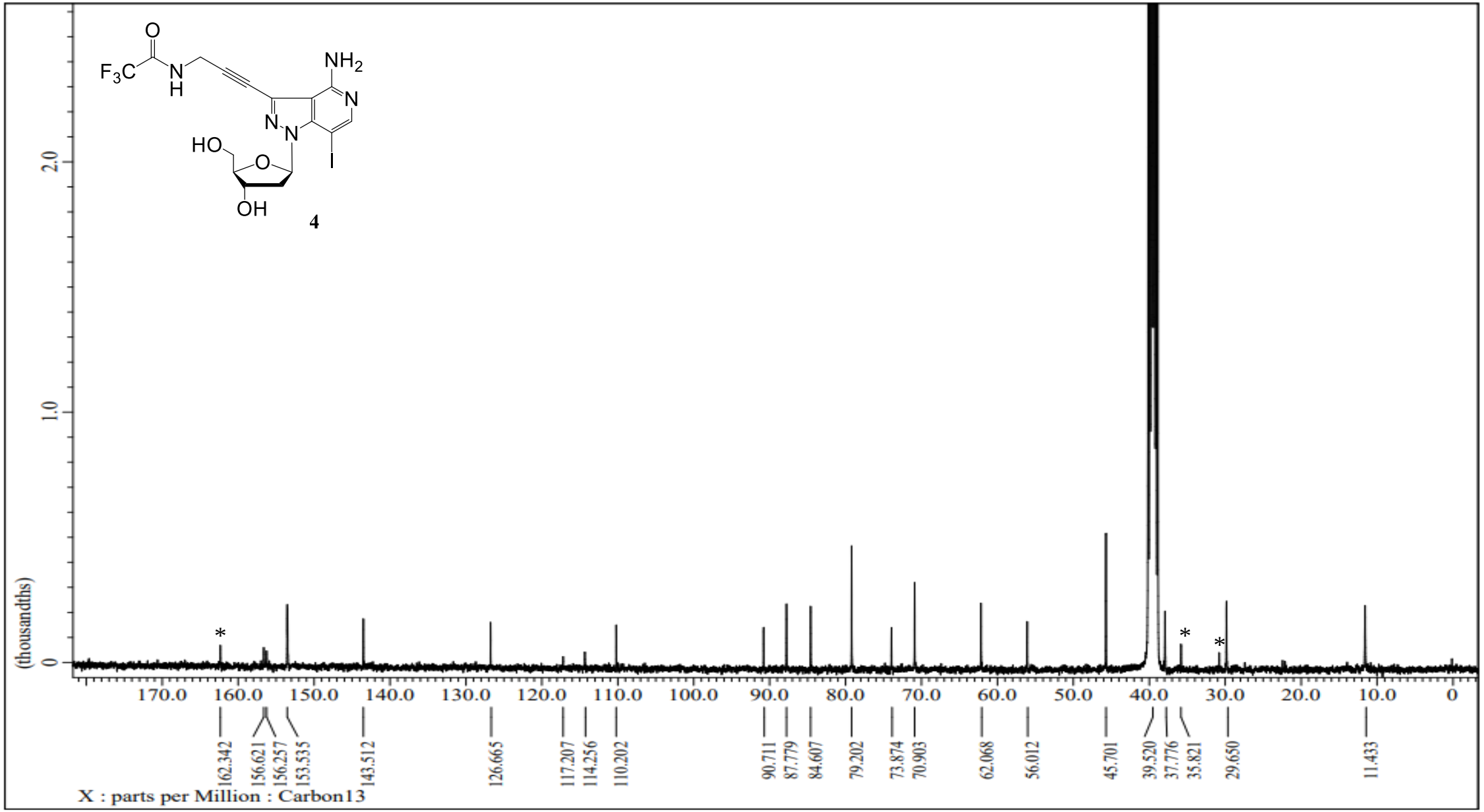


Figure S6. ^{1}H-NMR spectrum of compound **4** (DMSO-d_6)



*:solvent impurities

Figure S7. ^{13}C-NMR spectrum of compound **4** (DMSO-d_6)

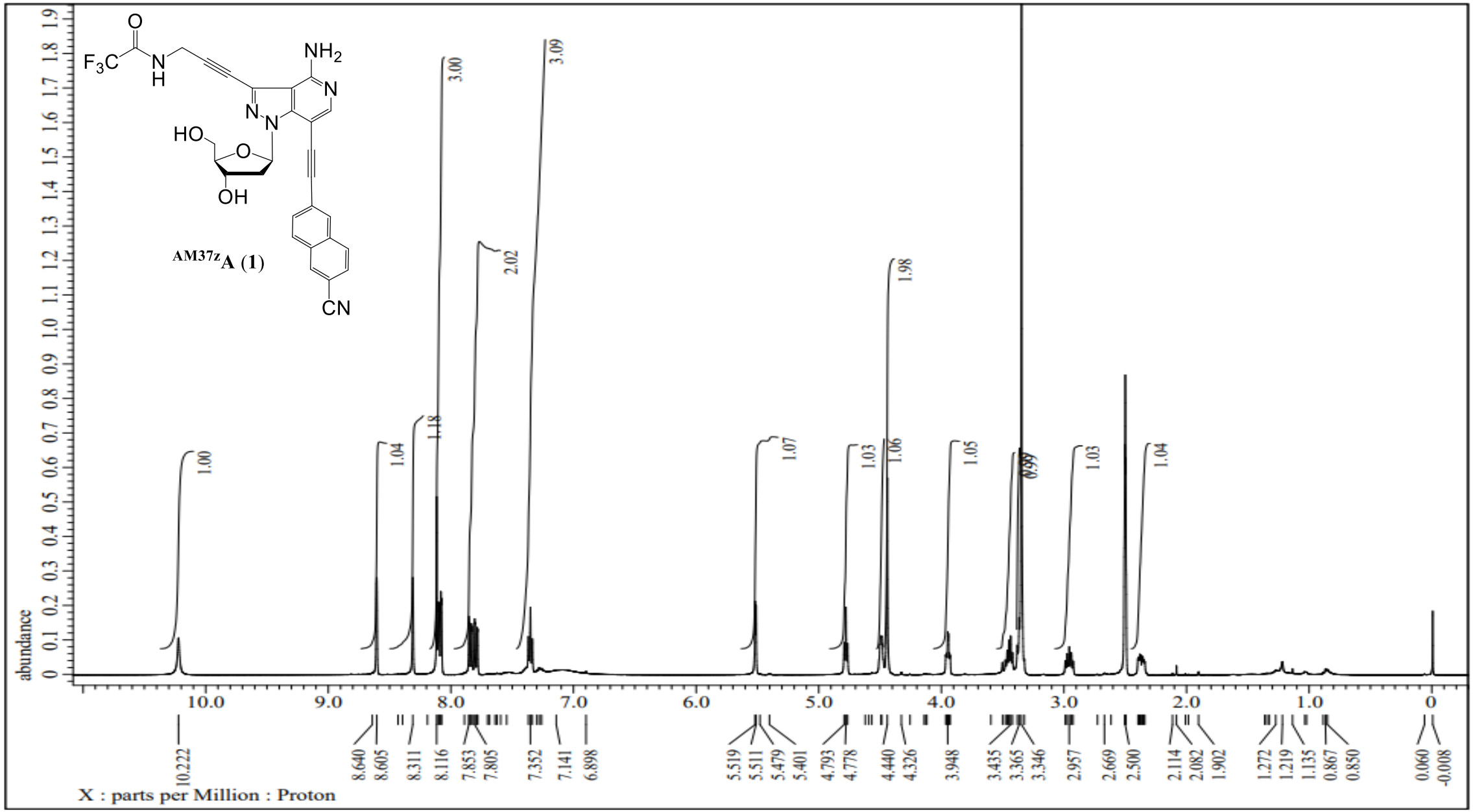


Figure S8. ^{1}H-NMR spectrum of **^{AM37z}A (1)** (DMSO-d_6)

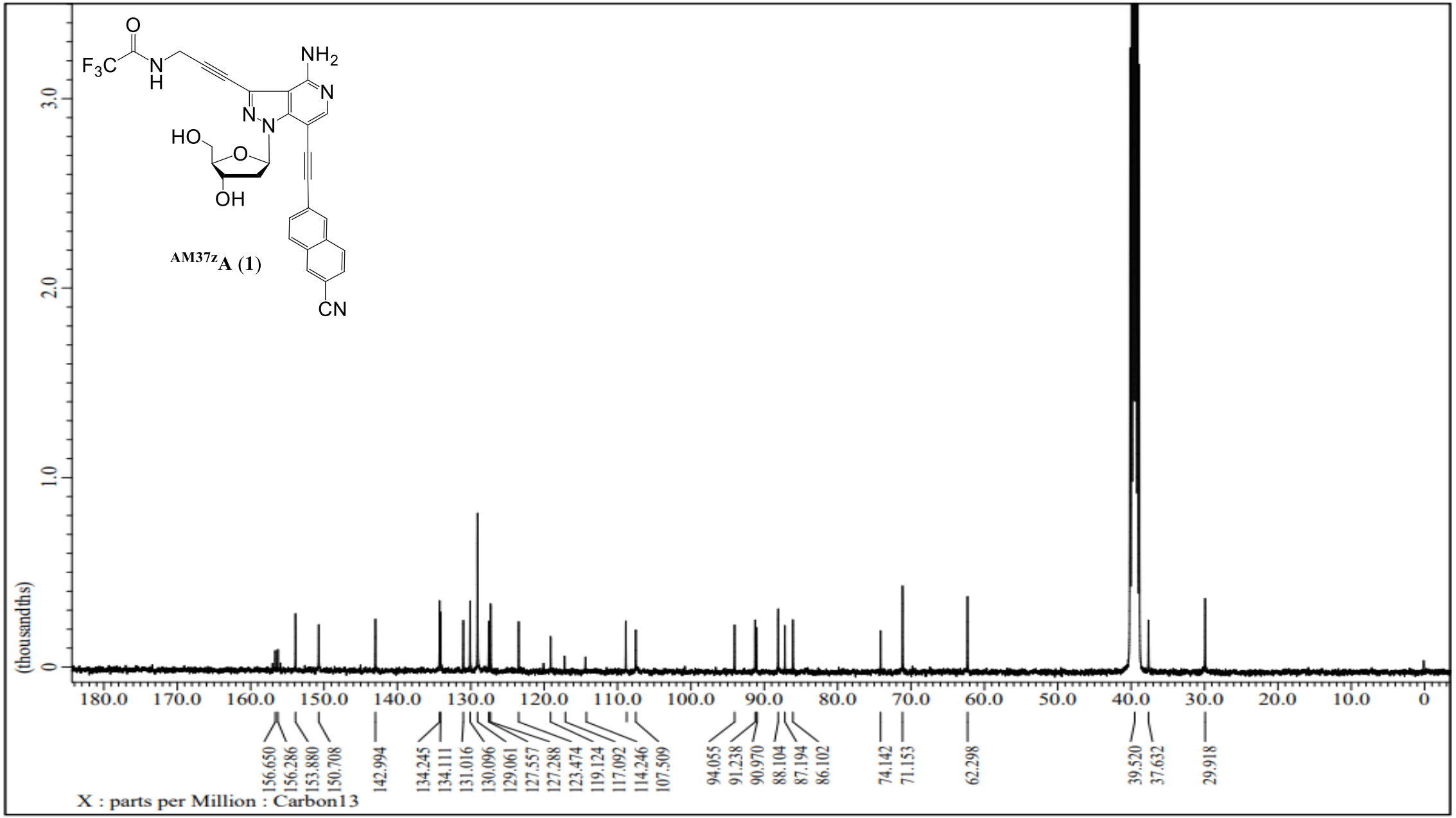


Figure S9. ^{13}C-NMR spectrum of **^{AM37z}A (1)** (DMSO-d_6)

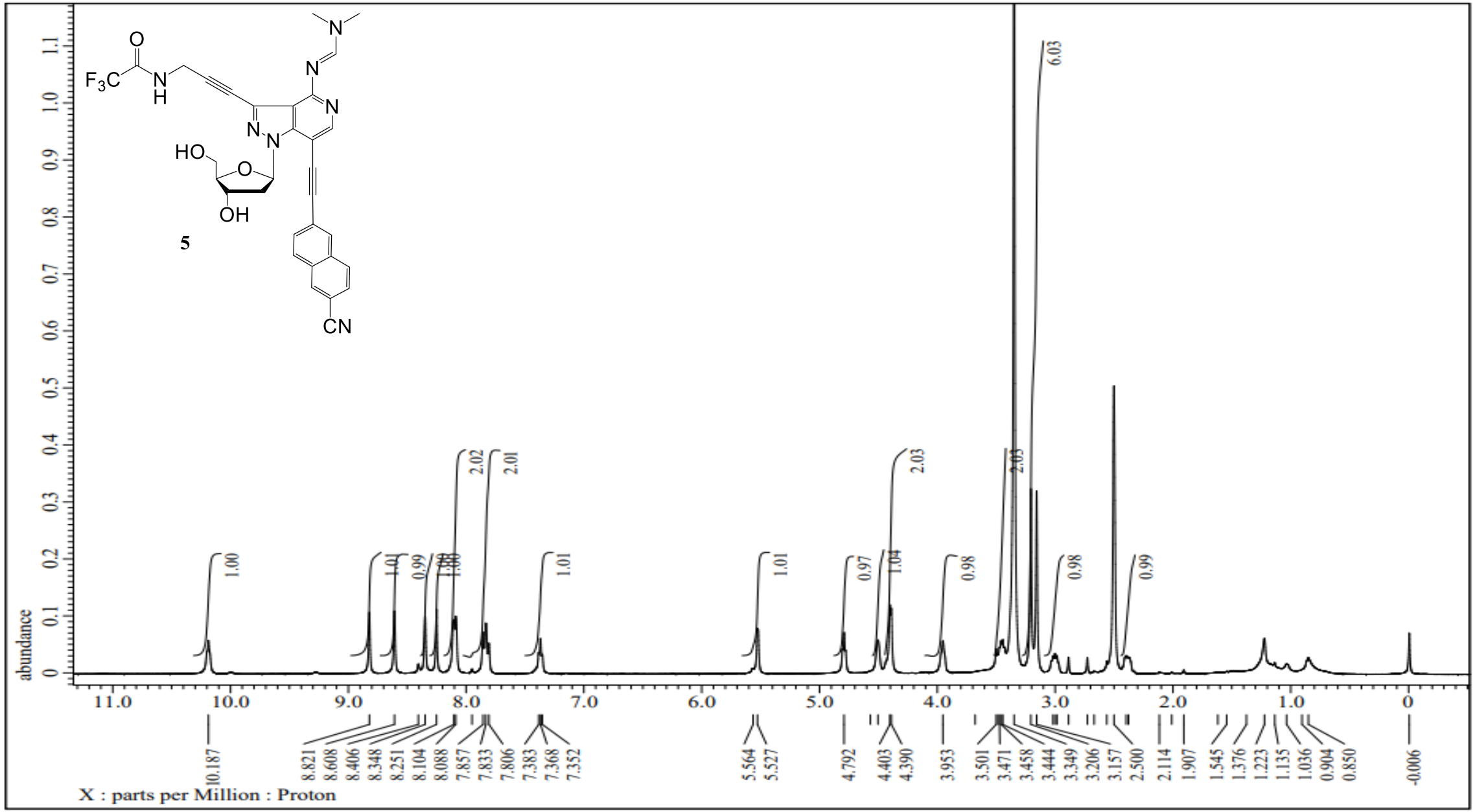


Figure S10. ^{1}H-NMR spectrum of compound **5** (DMSO-d_6)

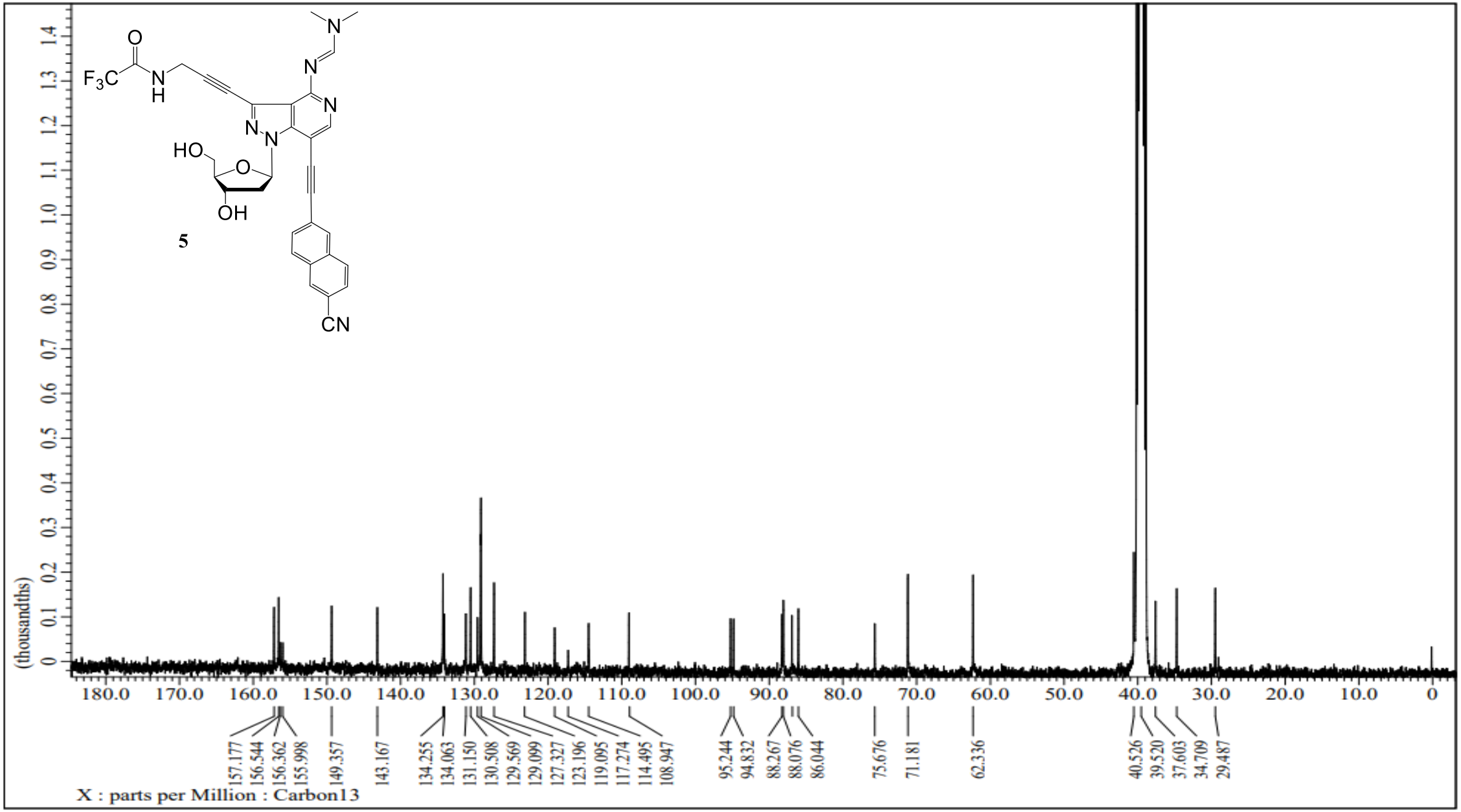


Figure S11. ^{13}C-NMR spectrum of compound **5** (DMSO-d_6)

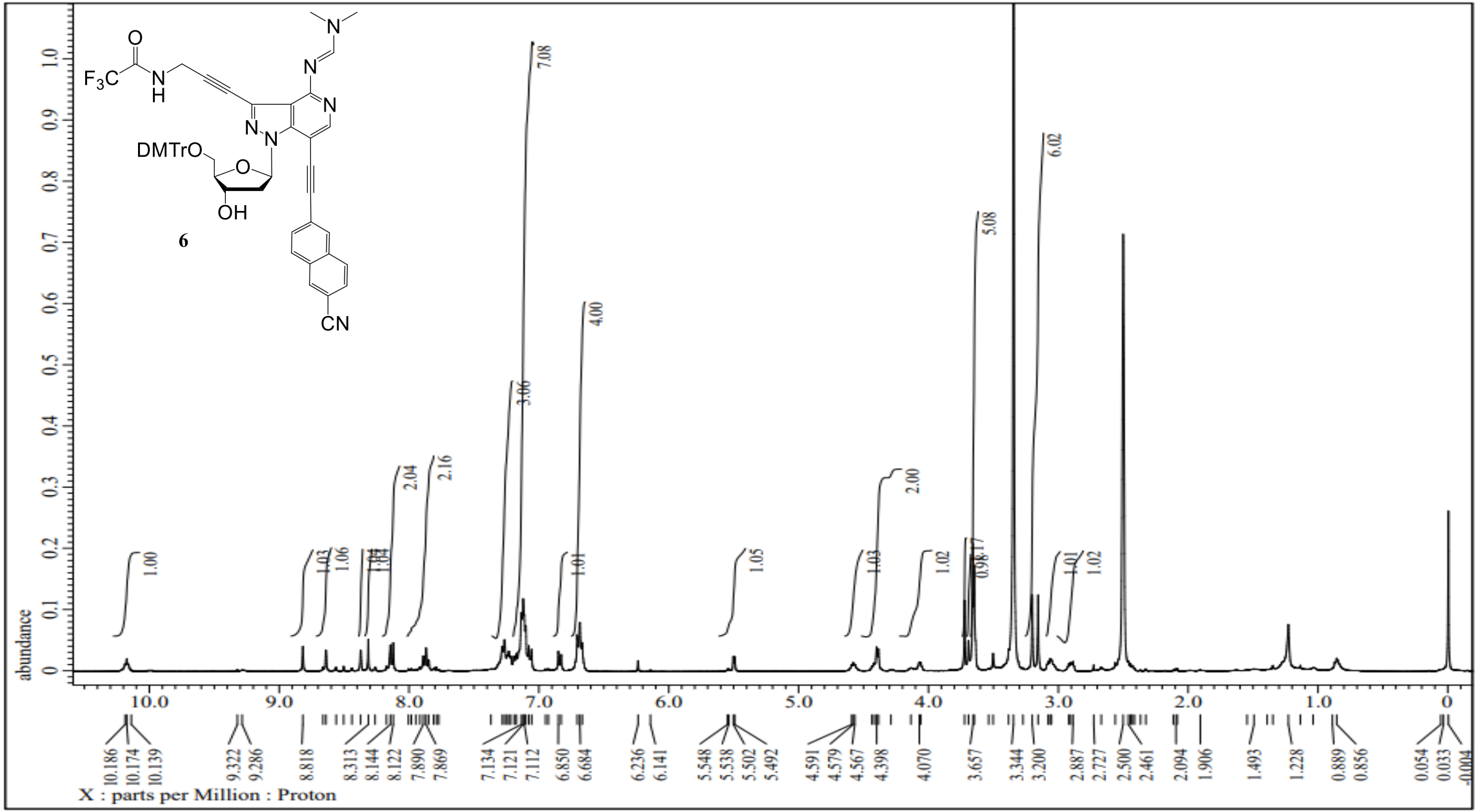


Figure S12. ^{1}H-NMR spectrum of compound **6** (DMSO-d_6)

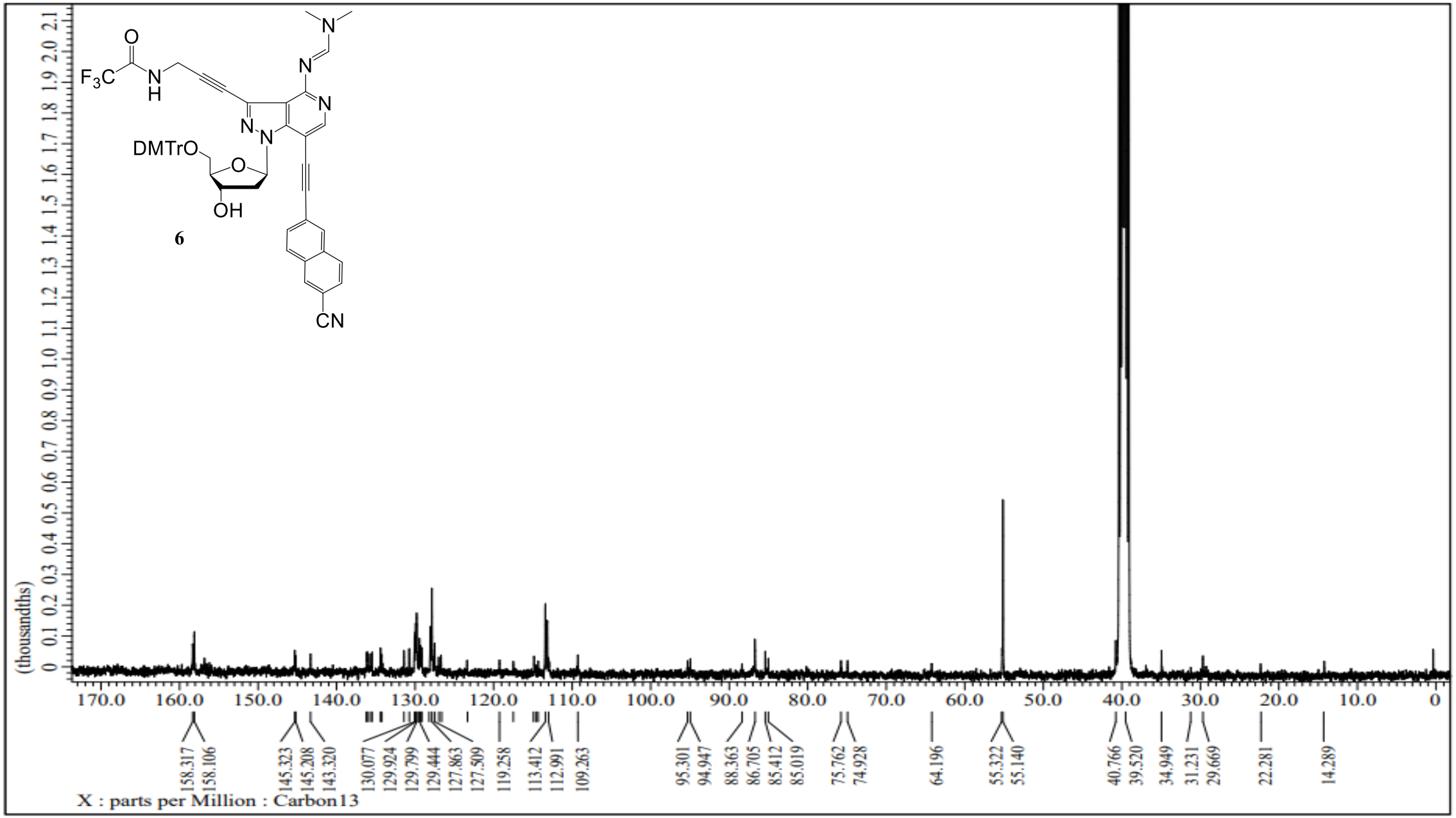


Figure S13. ^{13}C-NMR spectrum of compound **6** (DMSO-d_6)

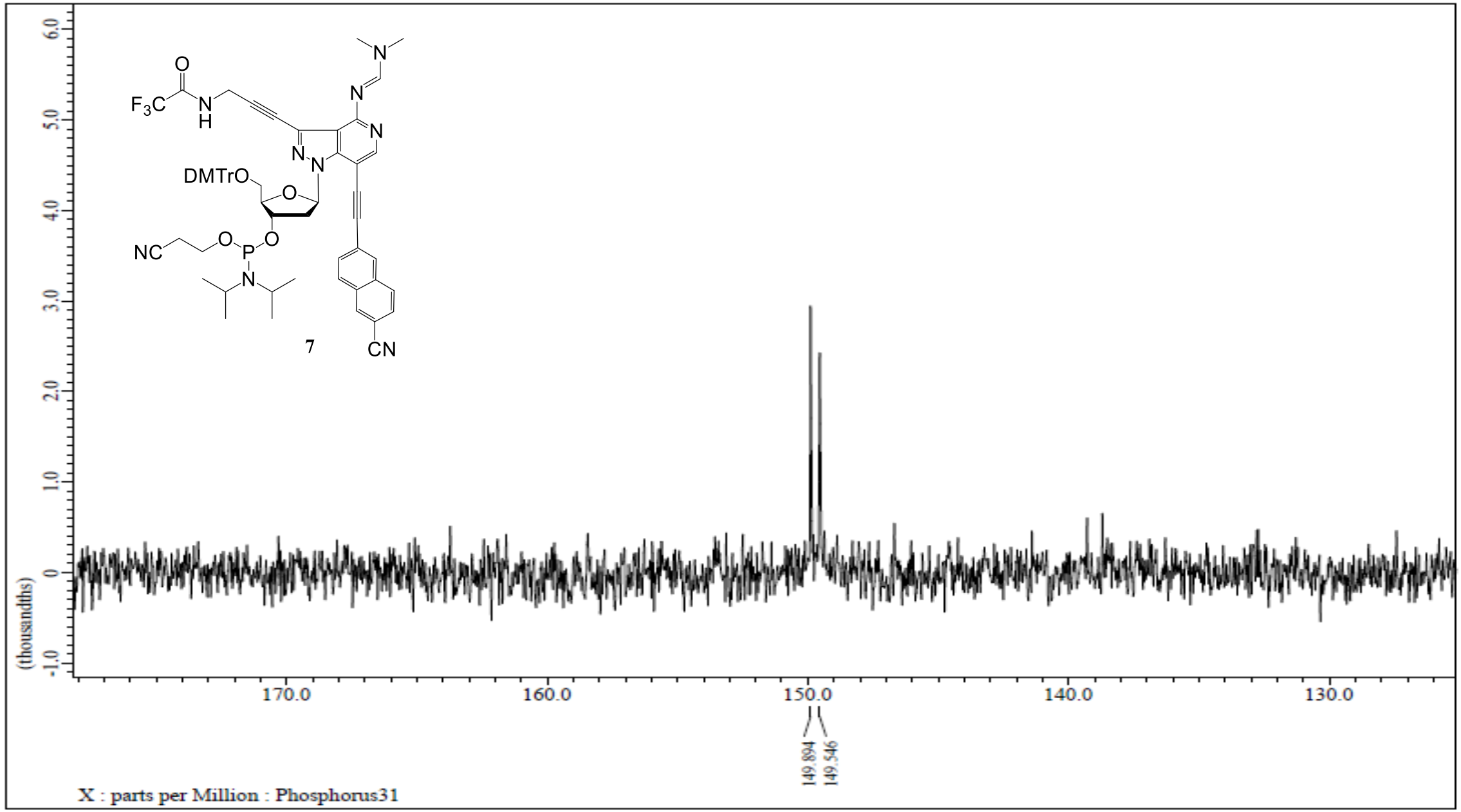


Figure S14. ^{31}P-NMR spectrum of compound **7** ($CDCl_3$)