Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

8-Aza-7-deazaguanine Nucleosides and Oligonucleotides with Octadiynyl Side Chains: Synthesis, Functionalization by the Azide-Alkyne 'Click' Reaction and Nucleobase Specific Fluorescence Quenching of Coumarin Dye Conjugates

Frank Seela [a, b *], Hai Xiong [a, b], Peter Leonard [a] and Simone Budow [a]

[a] *Laboratory of Bioorganic Chemistry and Chemical Biology, Center for Nanotechnology, Heisenbergstraße 11, 48149 Münster, Germany and*

[b] *Laboratorium für Organische und Bioorganische Chemie, Institut für Chemie, Universität Osnabrück, Barbarastraße 7, 49069 Osnabrück, Germany.*

Table of contents

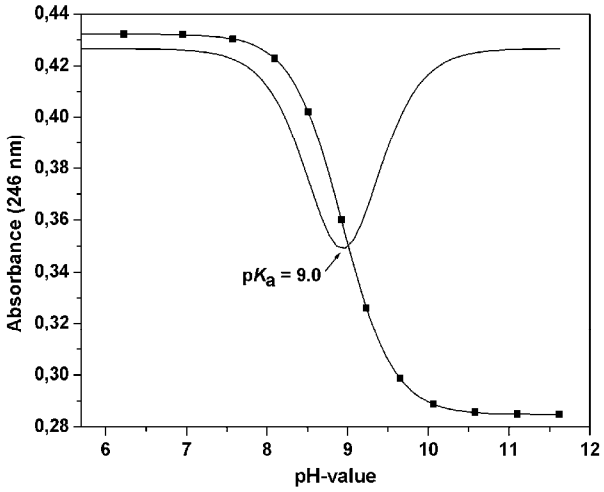
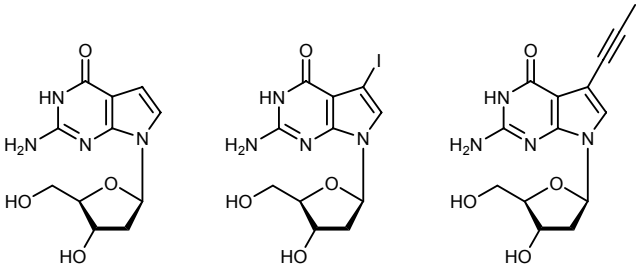


Figure S1 UV spectrum of nucleoside **2d** as a function of pH values measured in phosphate buffer (7.8 g of $NaH_2PO_4 \cdot H_2O$ in 500 ml H_2O) from pH = 2.0-12.5 at 246 nm.

Table S1 pK_a-values of nucleosides. [a]

Compd.	Wavelength[b] [nm]	pK_a[c]	Ref
c^7G_d (**1a**)	295	10.2	25
$I^7c^7G_d$ (**1b**)	-	10.3	25
Prop c^7G_d (**1c**)	300	10.2	25
Octa c^7G_d (**1**)	302	10.4	14
$c^7z^8G_d$ (**2a**)	248	9.3	26
$I^7c^7z^8G_d$ (**2b**)	240	8.9	
Prop $c^7z^8G_d$ (**2c**)	245	8.9	
Octa $c^7z^8G_d$ (**2d**)	246	9.0	



[a] Measured in phosphate buffer (0.1 M NaH_2PO_4) from pH 2 to pH 12.5.

[b] Wavelength of measurements as indicated. [c] Deprotonation.

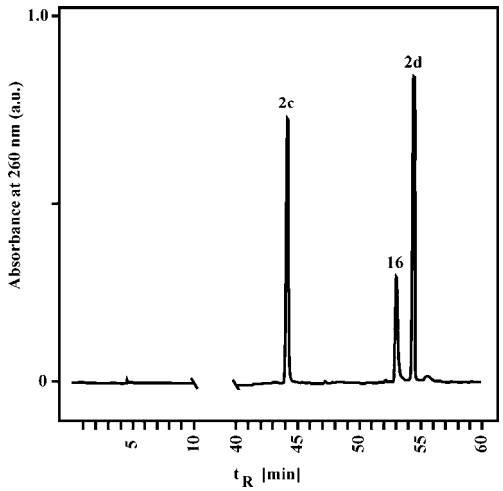


Figure S2 HPLC profile of an artificial mixture of the nucleosides **2c**, **2d** and **16** on a RP-18 (250 x 4 mm) column. Gradient: 0-25 min 100% B, 25-60 min 0-50% A in B with a flow rate of 0.7 ml/min. The following solvent systems were used: MeCN (A) and 0.1 M (Et_3NH)OAc (pH 7.0)) – MeCN, 95 : 5 (B).

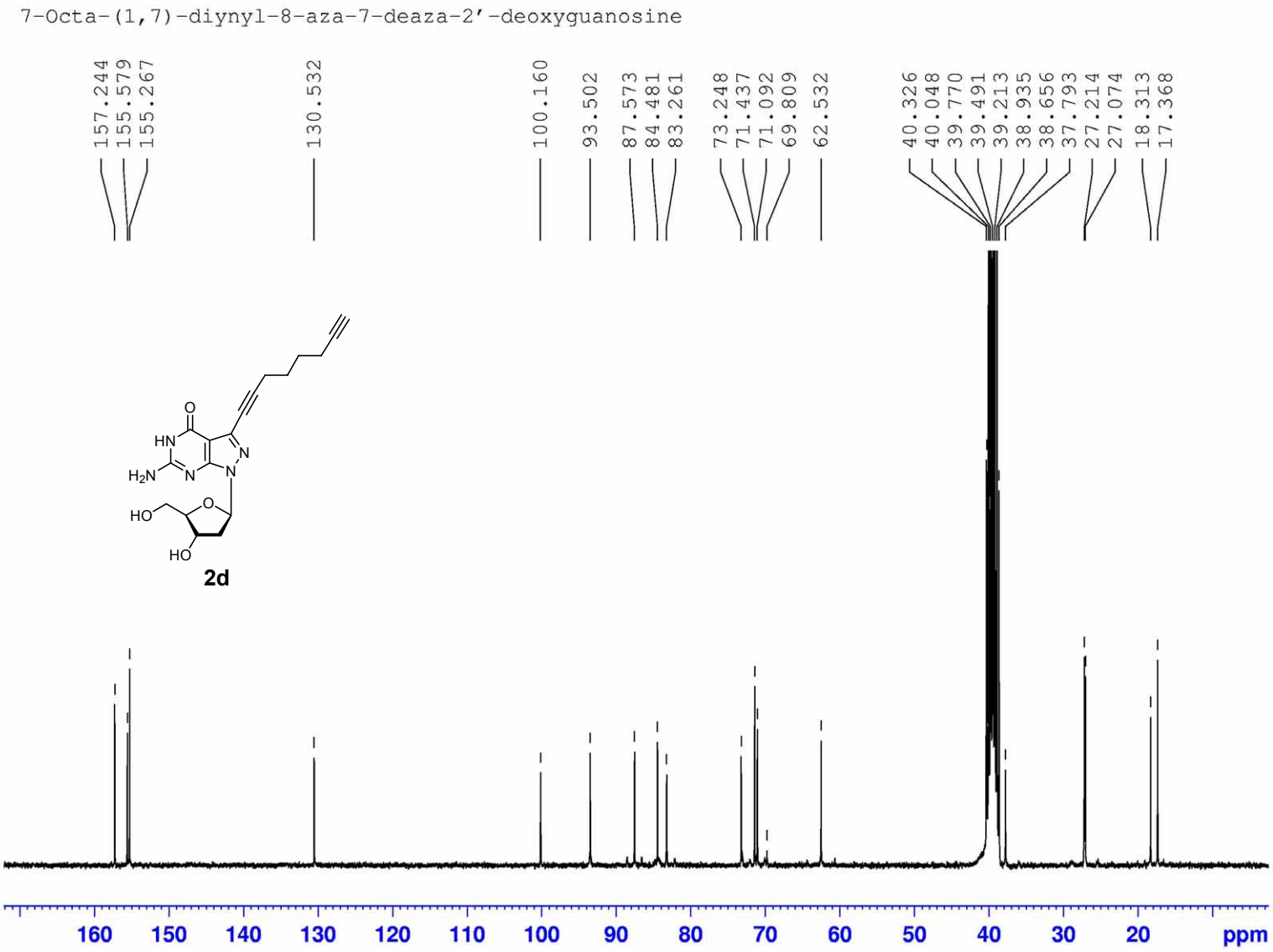


Figure S3. ^{13}C-NMR spectrum of compound 2d.

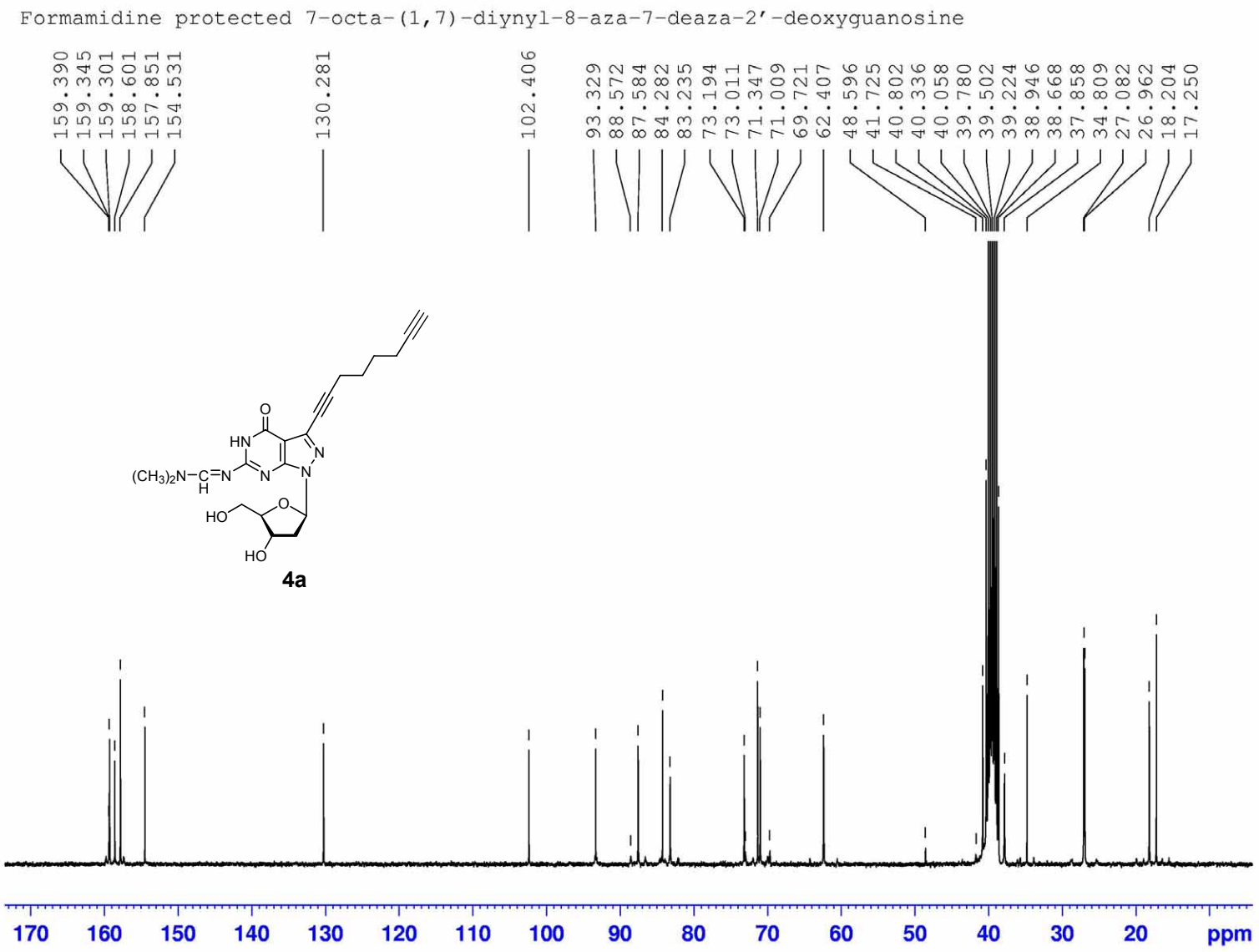


Figure S4. ^{13}C-NMR spectrum of compound 4a.

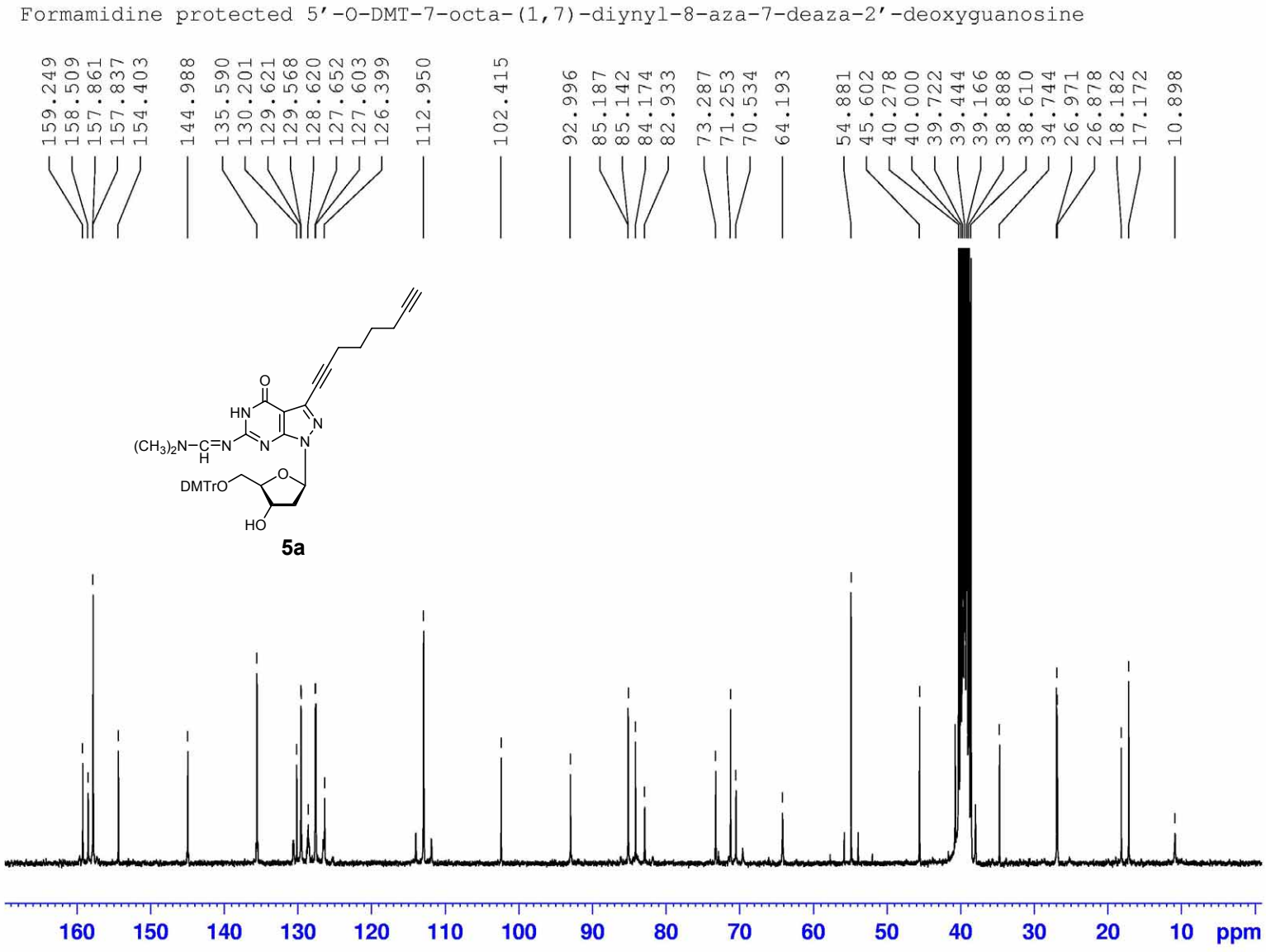


Figure S5. ^{13}C-NMR spectrum of compound 5a.

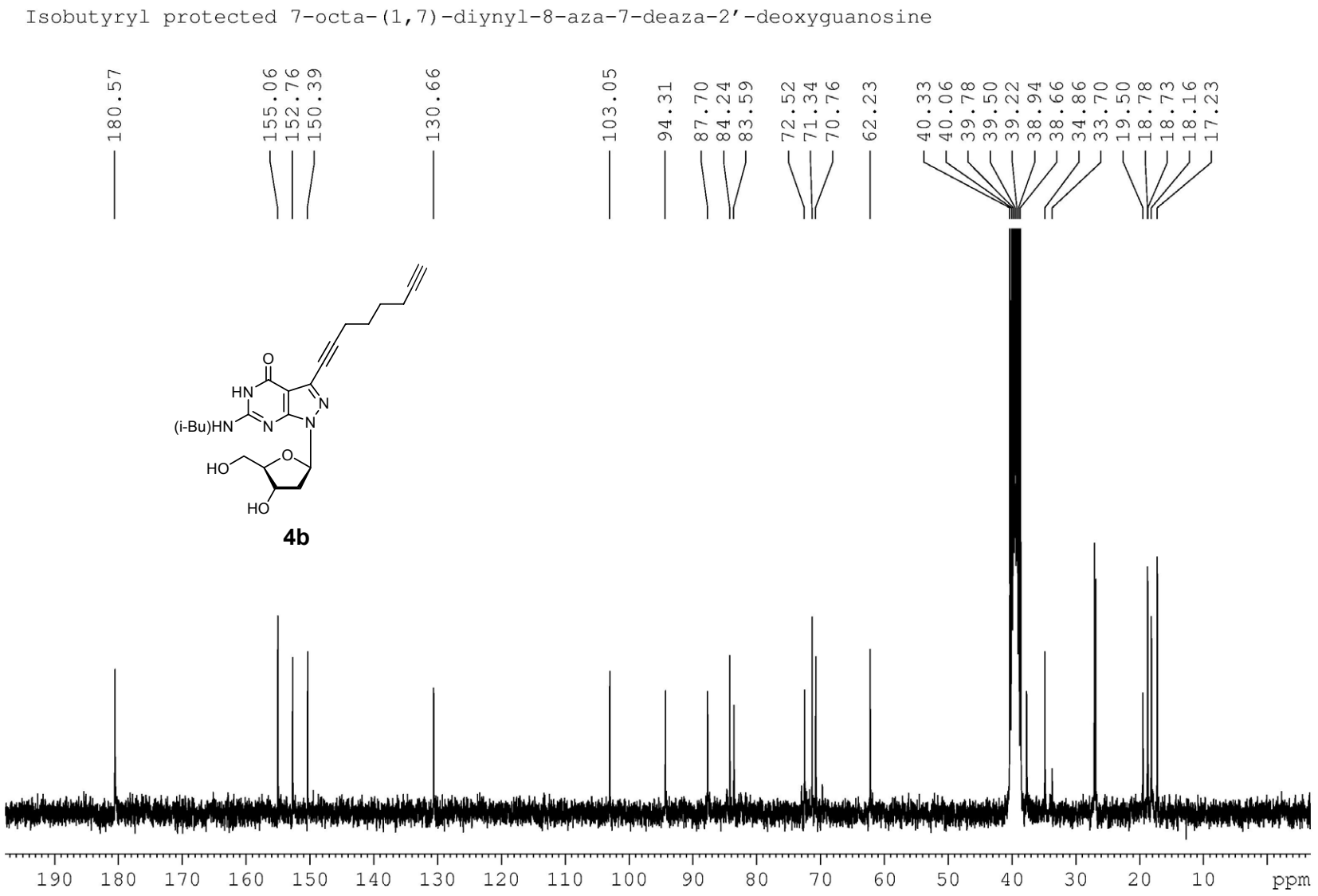


Figure S6. ^{13}C-NMR spectrum of compound 4b.

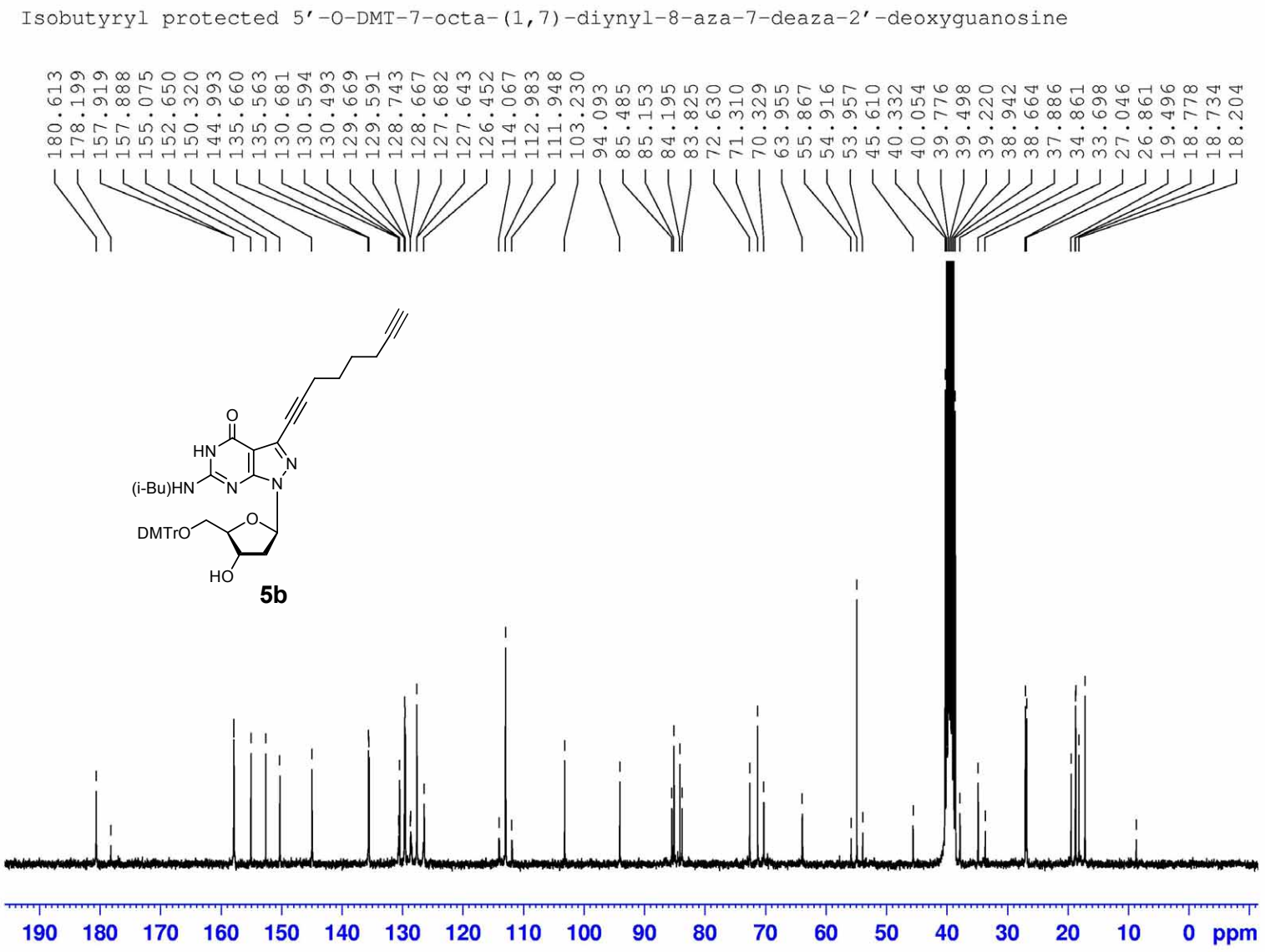


Figure S7. ^{13}C-NMR spectrum of compound 5b.

Supp
This

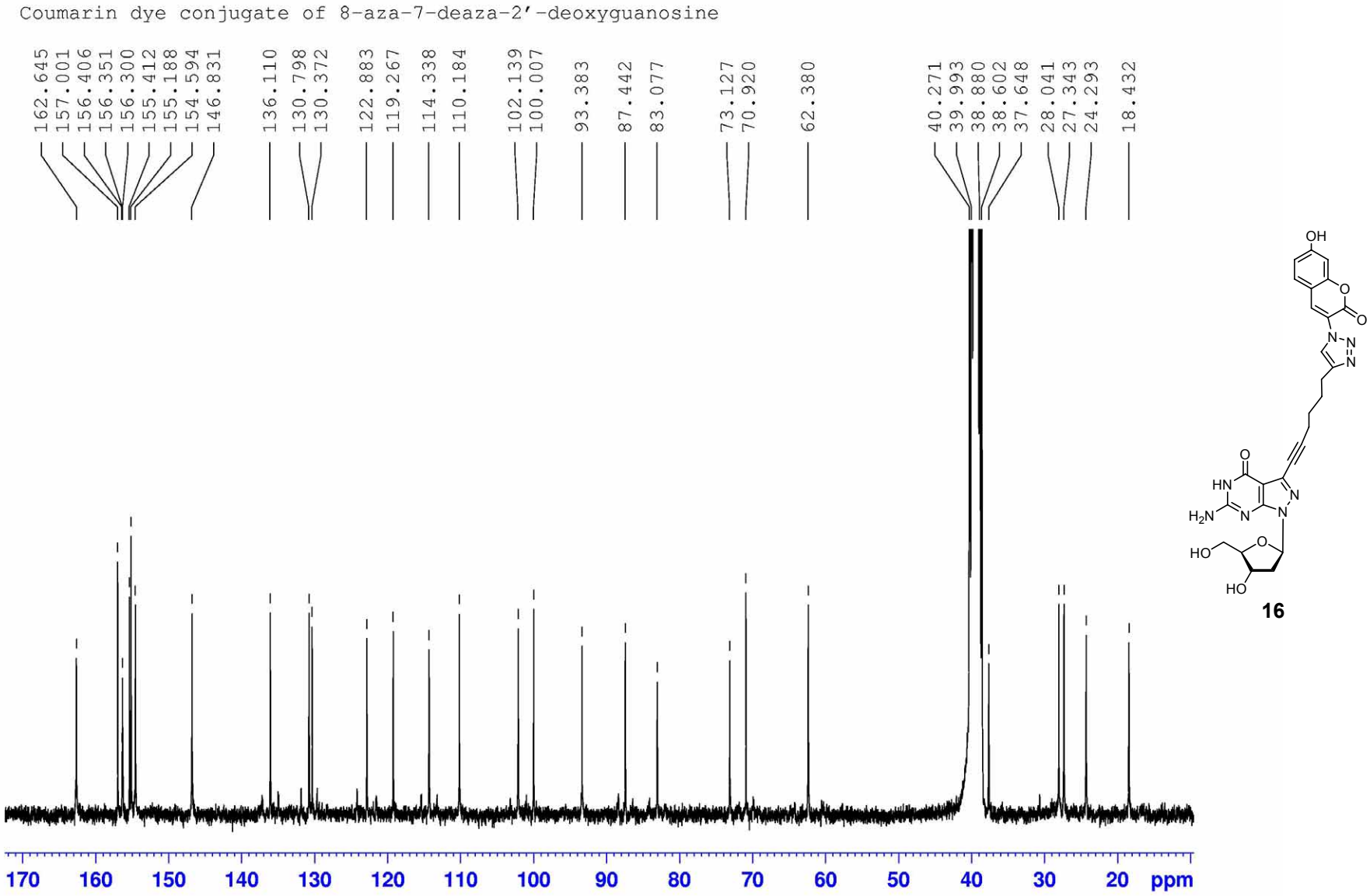


Figure S8. ^{13}C-NMR spectrum of compound 16.

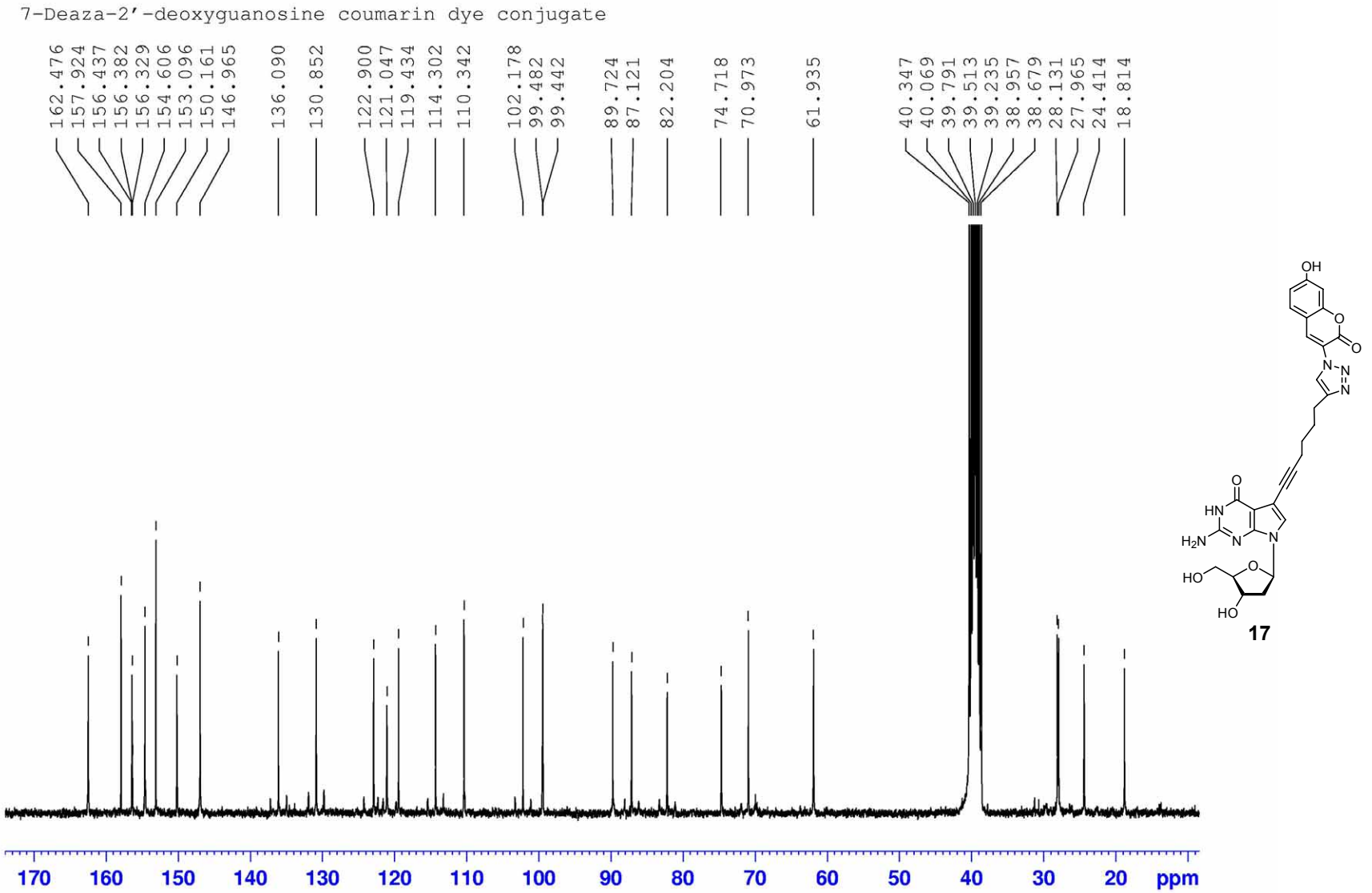


Figure S9. ^{13}C-NMR spectrum of compound 17.