

Supporting Information

8-Aza-2'-deoxyguanosine: Base Pairing, Mismatch Discrimination and Nucleobase Anion Fluorescence Sensing in Single-Stranded and Duplex DNA

Frank Seela*, Dawei Jiang, Kuiying Xu

Laboratory of Bioorganic Chemistry and Chemical Biology, Center for Nanotechnology, Heisenbergstraße 11, 48149 Münster, Germany and Laboratorium für Organische und Bioorganische Chemie, Institut für Chemie, Universität Osnabrück, Barbarastraße 7, 49069 Osnabrück, Germany

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Table S1 Fluorescence excitation and emission wavelengths at different pH values utilized for the determination of the pK_a value.

pH value	Excitation wavelength [nm]	Emission wavelength [nm]
4.4	254	346
5.2	255	346
5.8	256	347
6.3	272	351
7.1	277	358
8.0	277	359
8.4	277	359
8.7	278	359
9.3	278	358
9.8	278	358
10.2	278	359
10.8	278	359

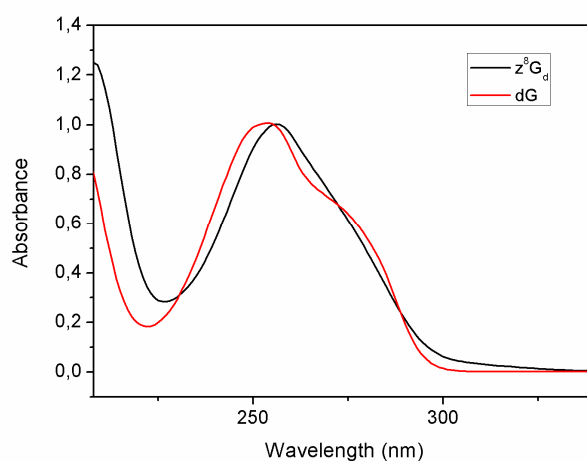


Figure S2 UV spectra of dG and nucleoside **9**, measured in MeOH (at identical concentrations).

Extinction coefficients: dG $\epsilon_{254} = 13450$, $\epsilon_{260} = 11900$; z^8G_d (**9**) $\epsilon_{257} = 13400$, $\epsilon_{260} = 12660$.

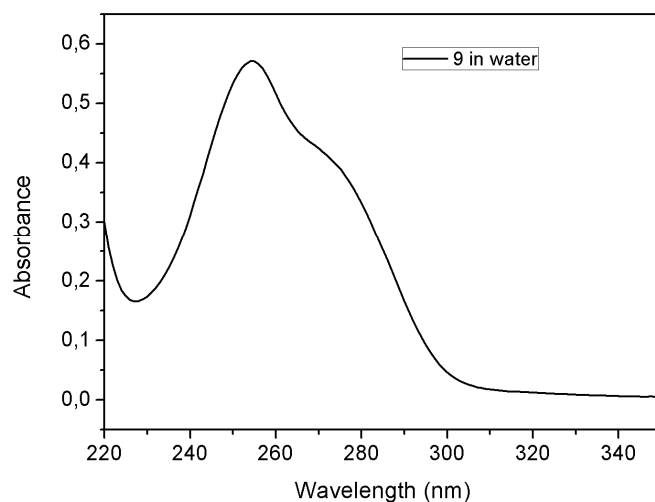


Figure S3 UV spectra of nucleoside **9**, measured in H₂O.

Extinction coefficients: z^8G_d (**9**) $\epsilon_{254} = 11400$, $\epsilon_{260} = 10300$.

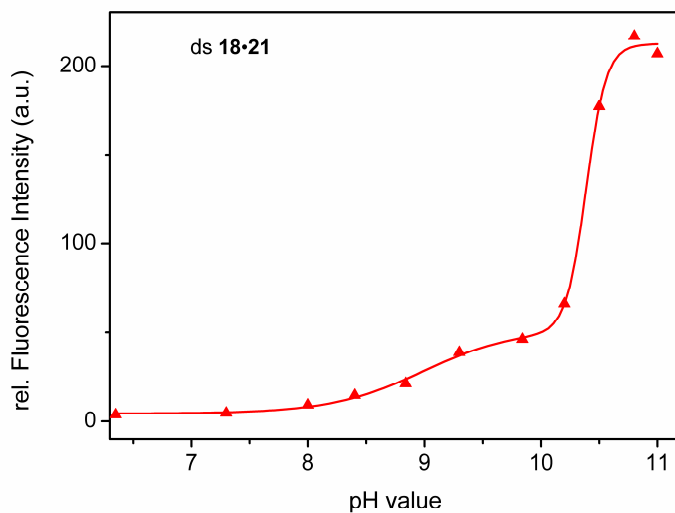


Figure S4 Expanded spectrum of the pH-dependent fluorescence emission curve of duplex **18•21** (see manuscript Figure 5). Measurements were performed in 1.0 M NaCl, 60mM Na-cacodylate buffer (5 μ M concentration for each ss oligonucleotide). Excitation wavelength = 277 nm; emission at 360 nm. The pK_a values are 9.1 and 10.4.

8-Aza-2'-deoxy-3',5'-di-O-(4-toluoyl)-guanosine

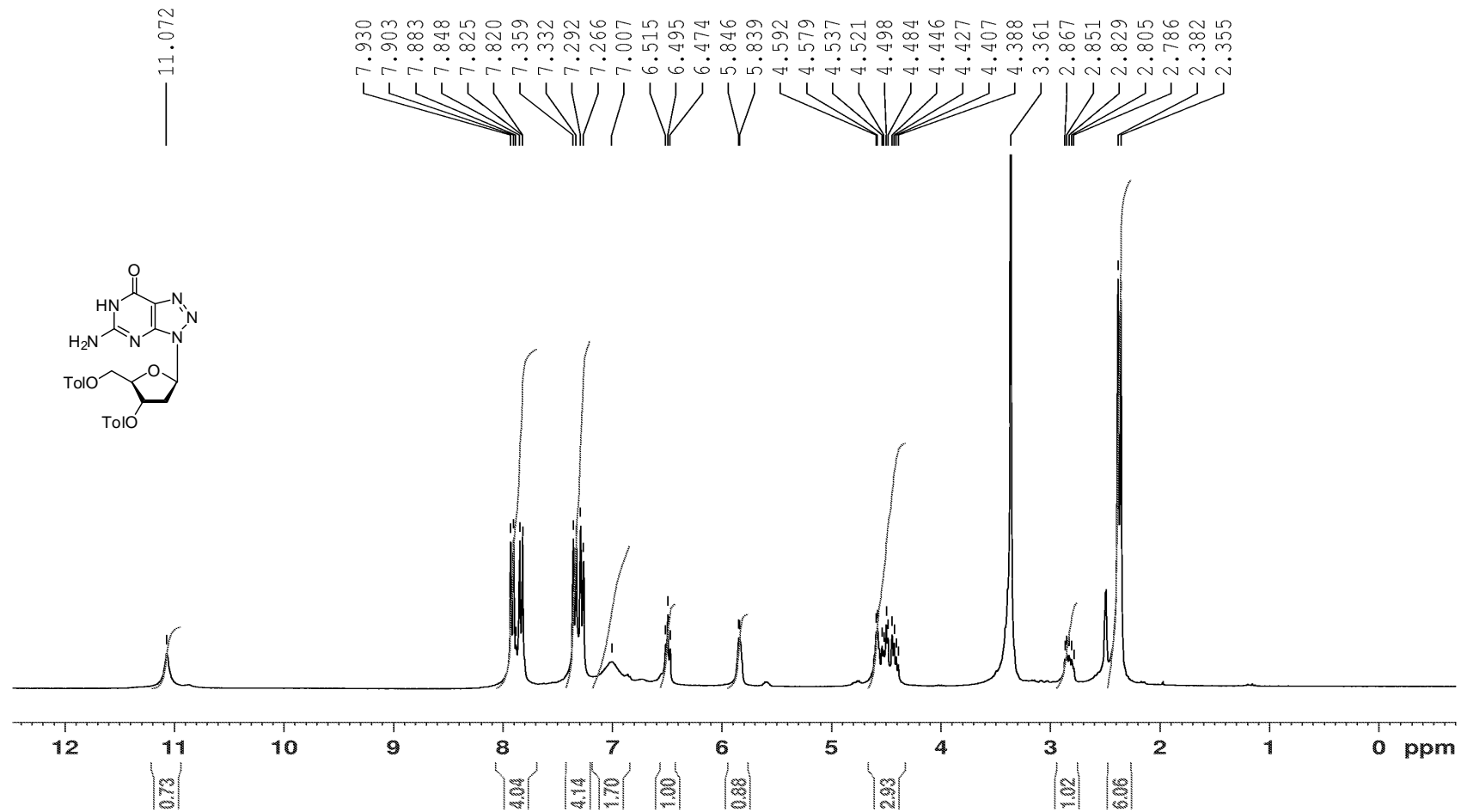


Figure S5. ¹H-NMR spectrum of compound 15.

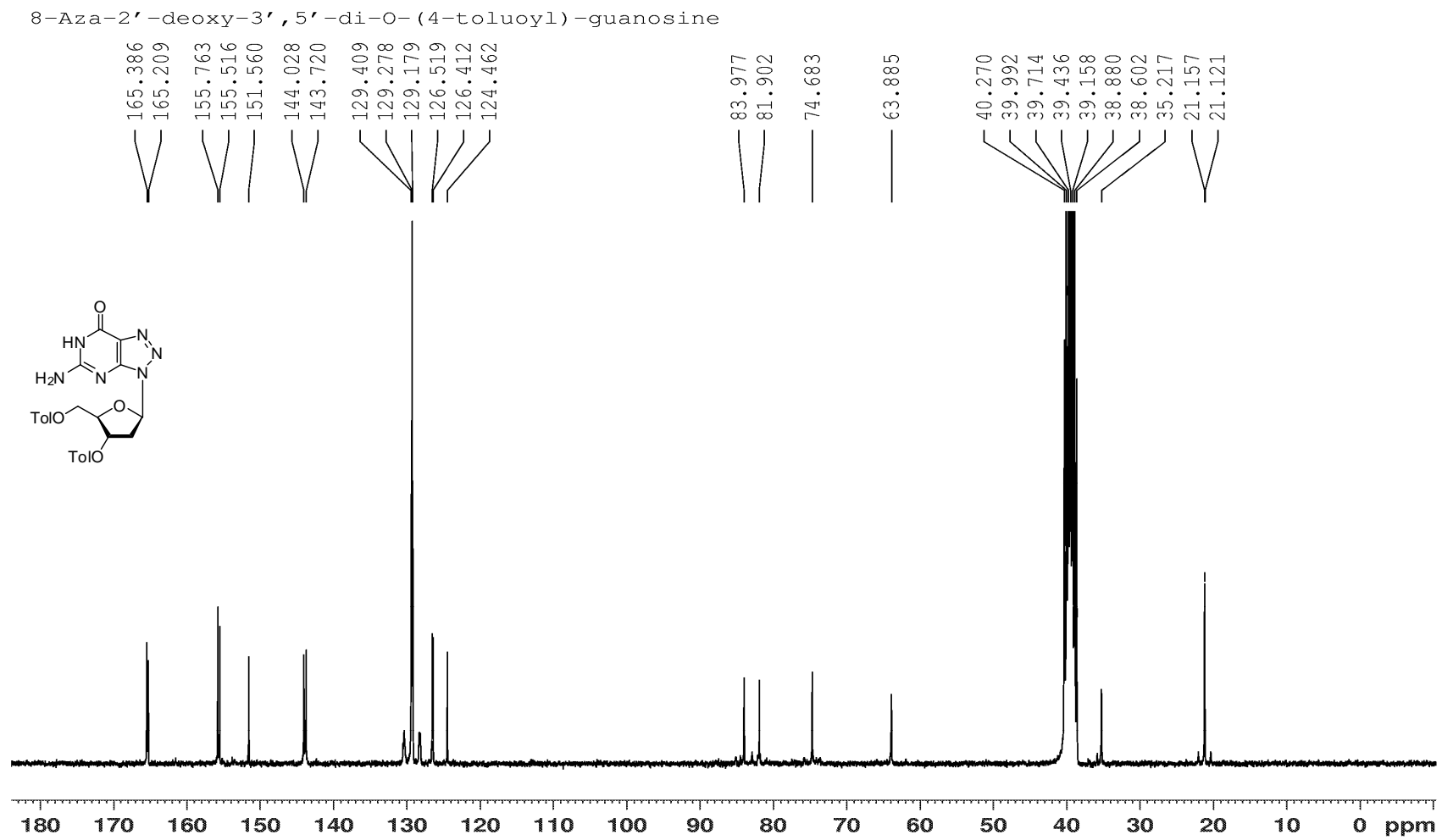


Figure S6. ^{13}C -NMR spectrum of compound 15.

8-Aza-2'-deoxyguanosine

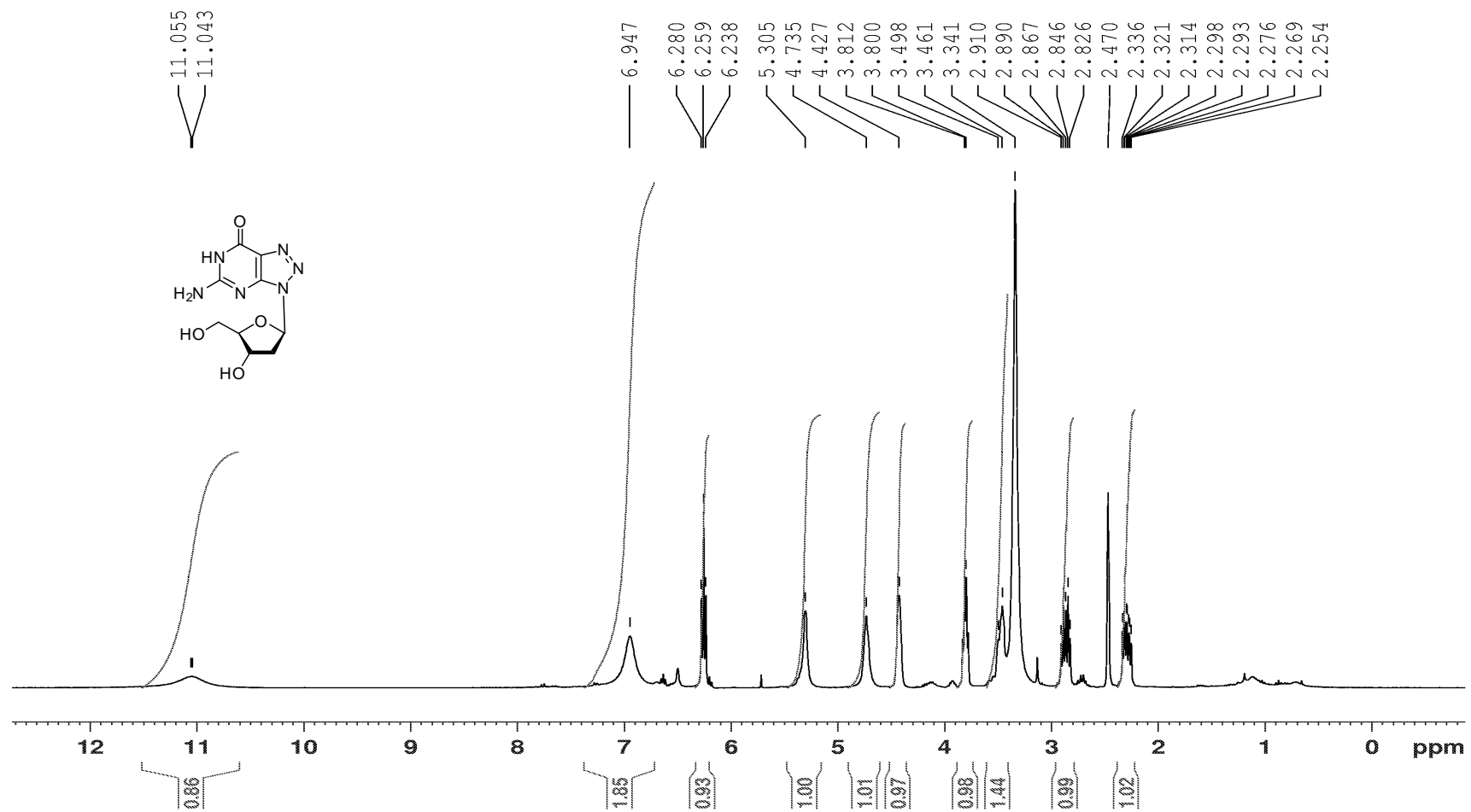


Figure S7. ¹H-NMR spectrum of compound 9.

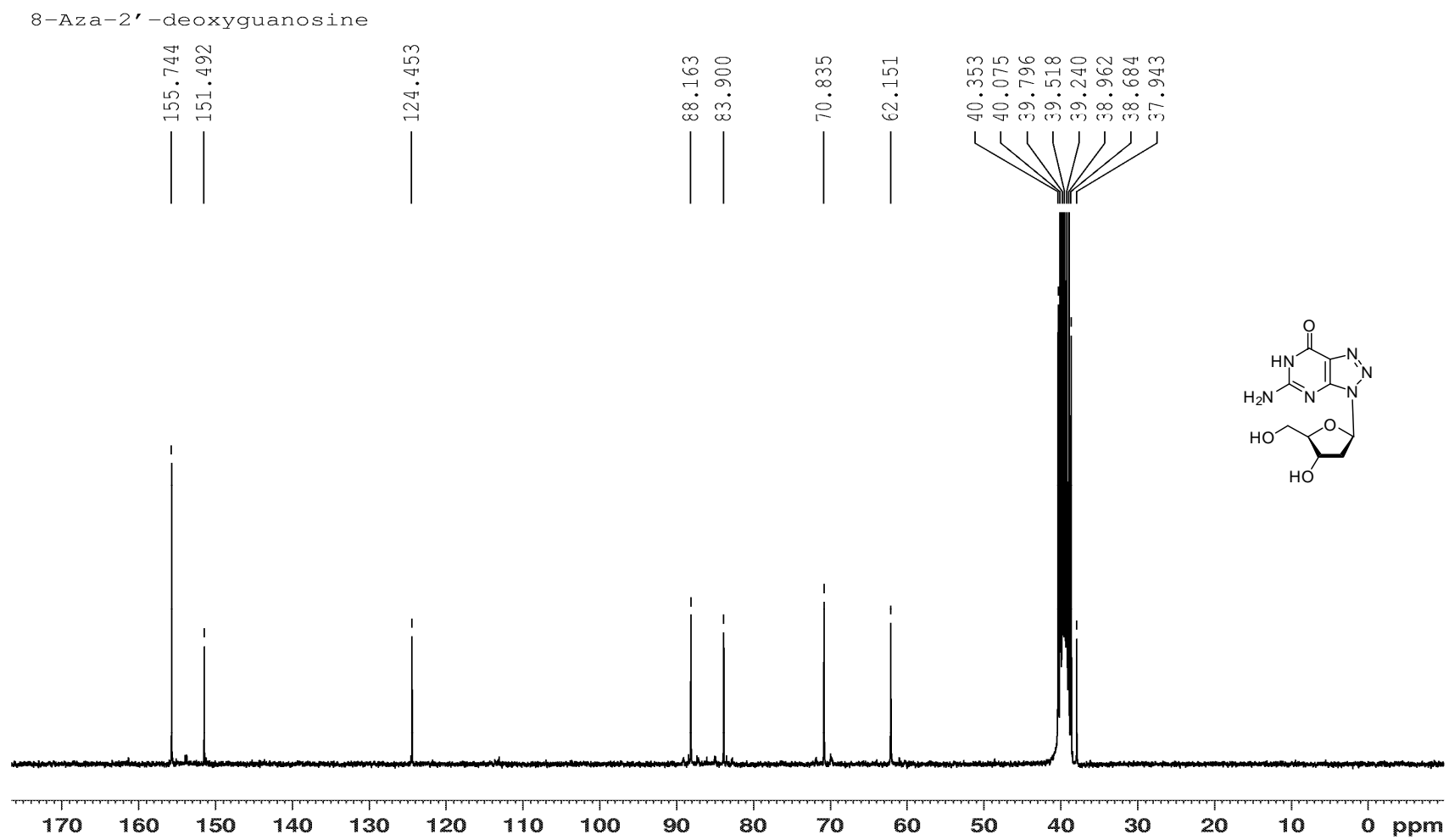


Figure S8. ^{13}C -NMR spectrum of compound 9.

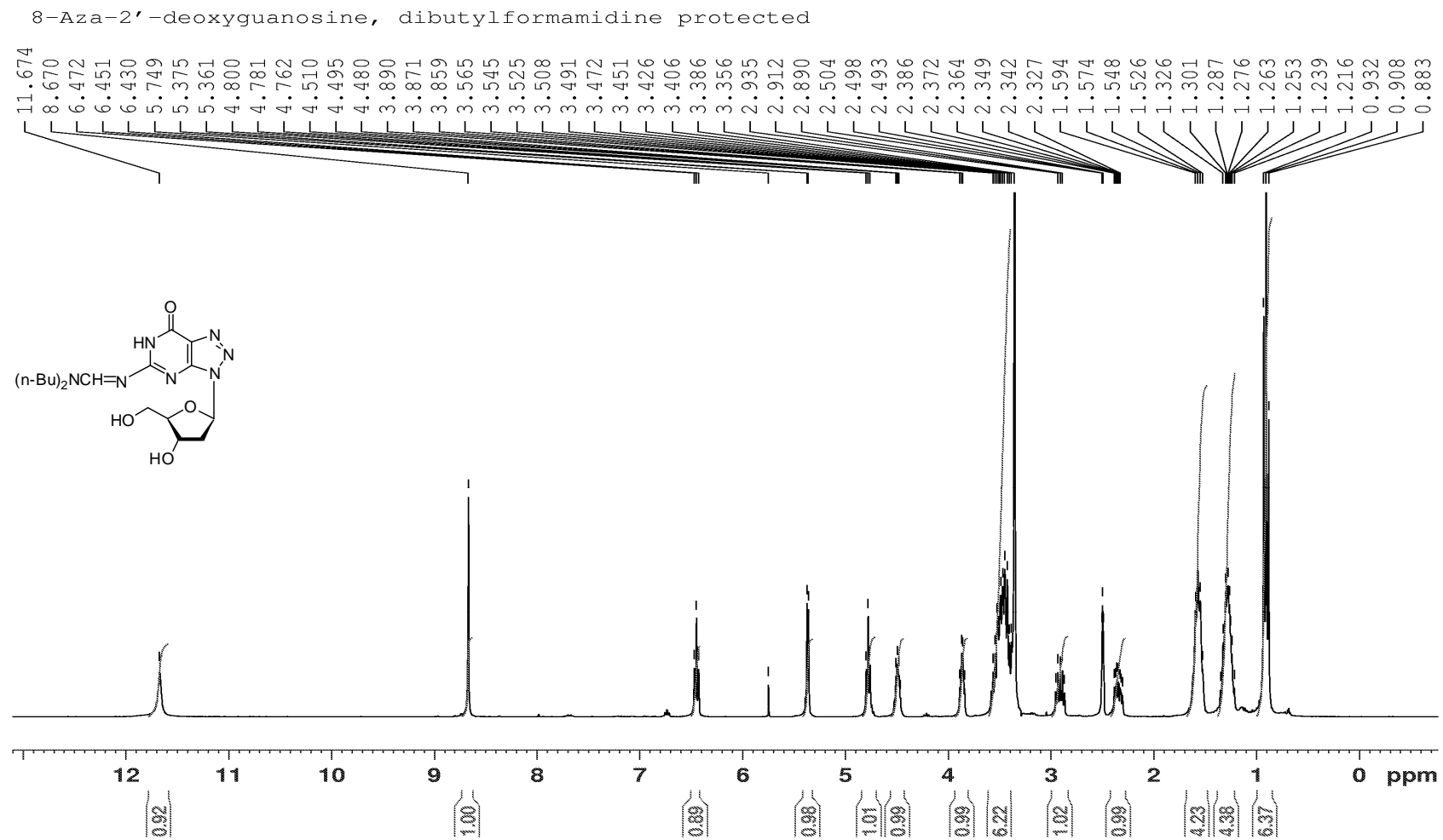


Figure S9. ^1H -NMR spectrum of compound 16.

8-Aza-2'-deoxyguanosine, dibutylformamidinium protected

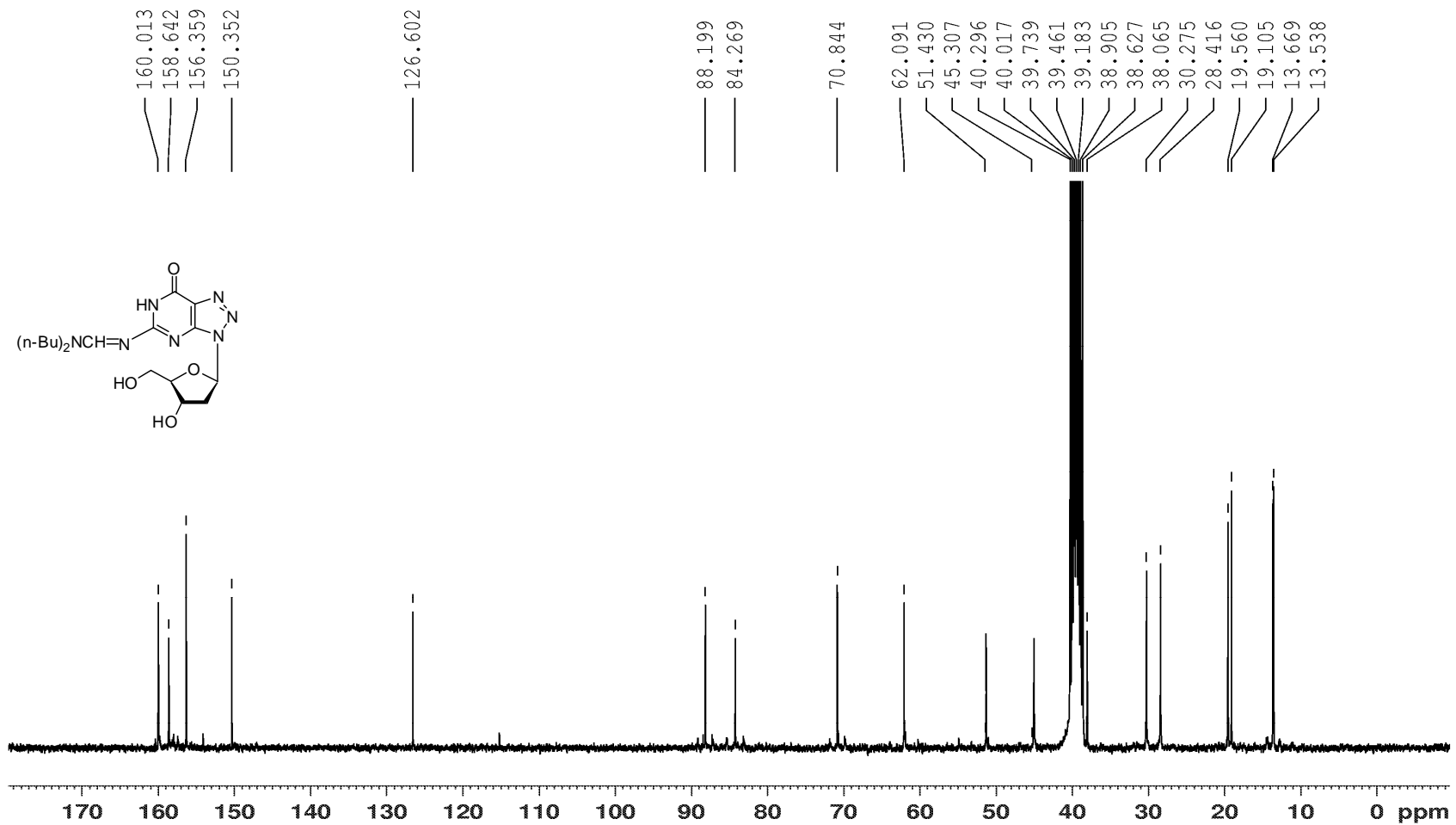


Figure S10. ¹³C-NMR spectrum of compound 16.

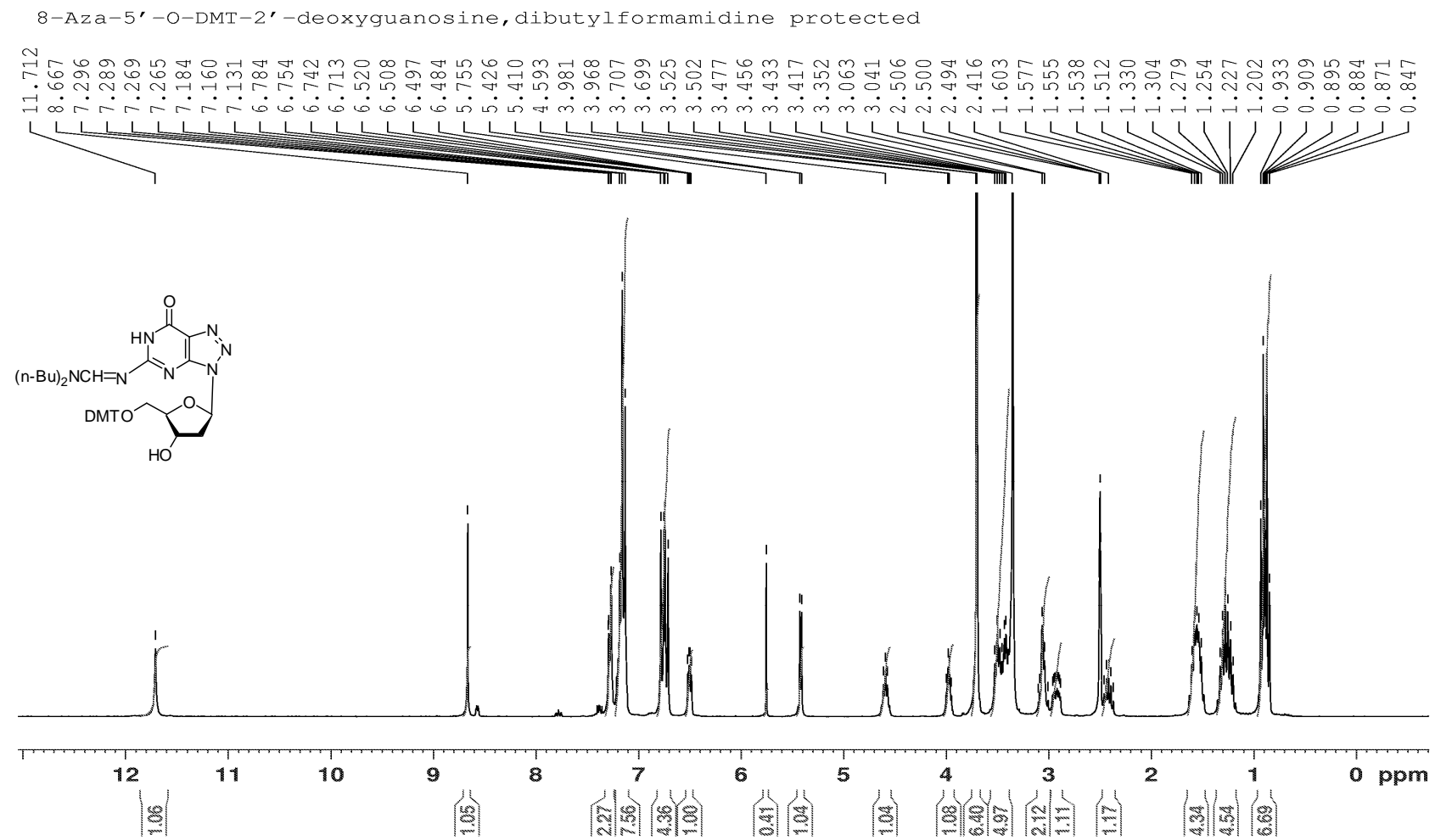


Figure S11. $^1\text{H-NMR}$ spectrum of compound 17.

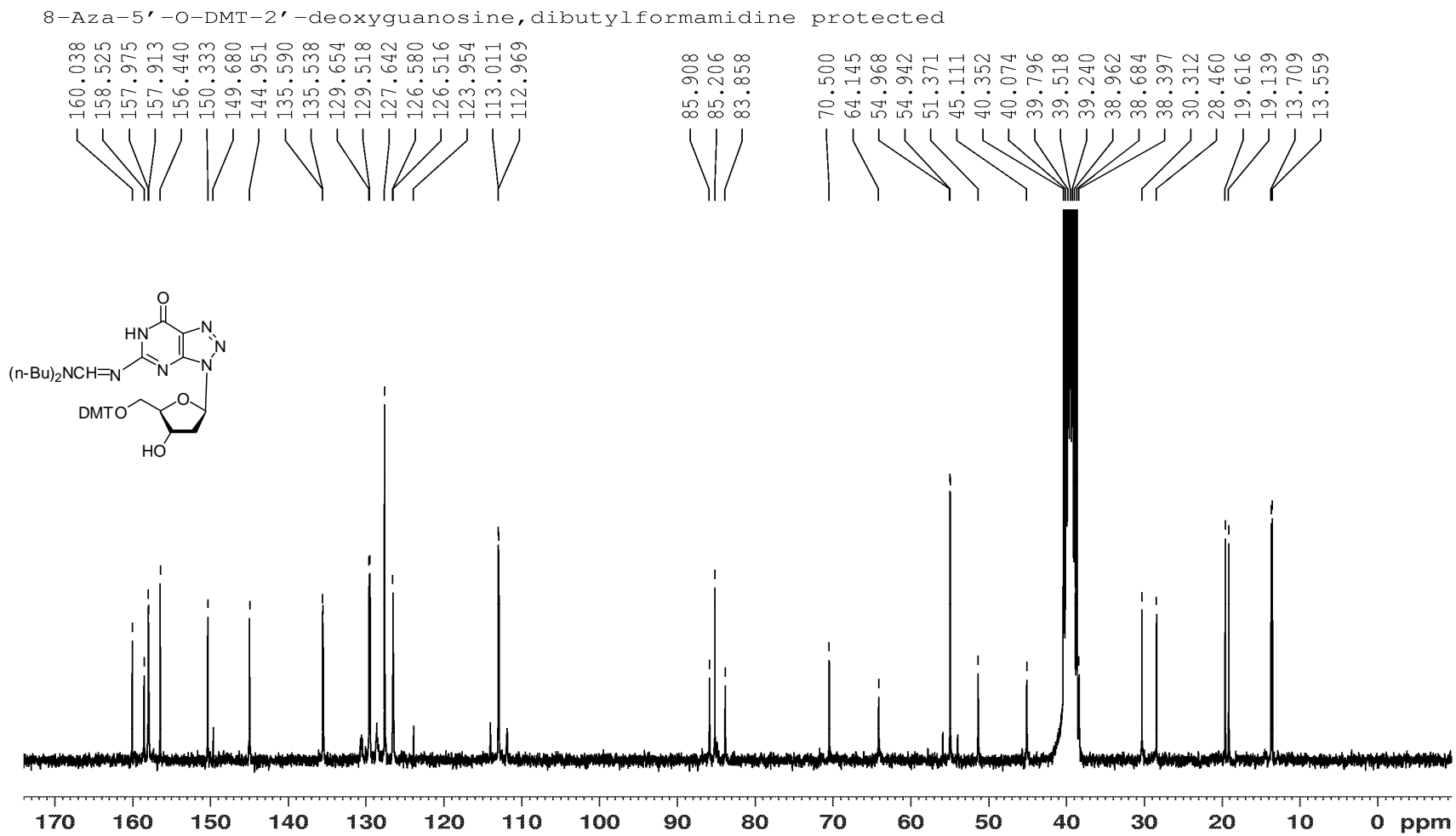


Figure S12. ¹³C-NMR spectrum of compound 17.

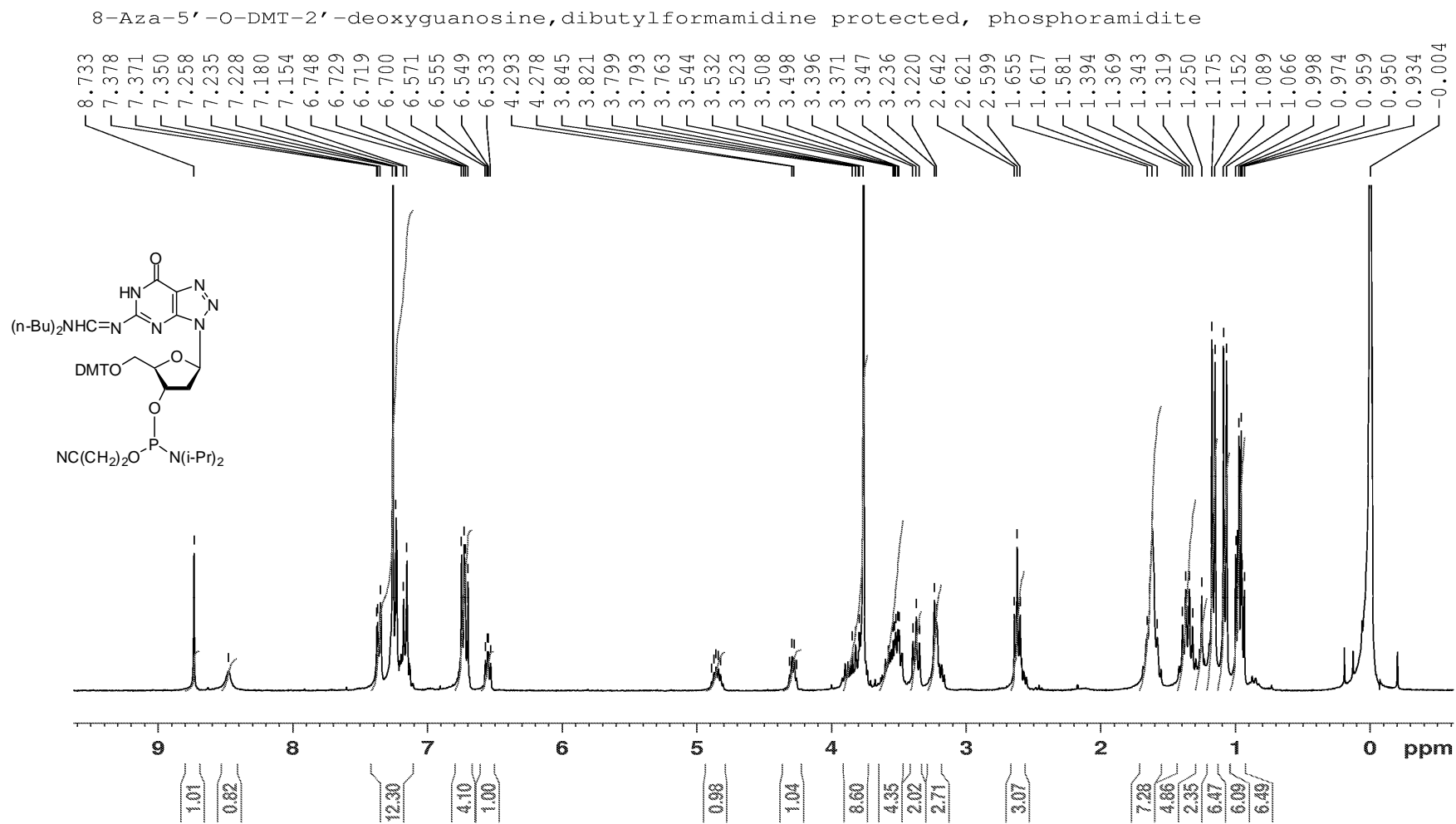


Figure S13. $^1\text{H-NMR}$ spectrum of compound 11.

8-Aza-5'-O-DMT-2'-deoxyguanosine, dibutylformamidinium protected, phosphoramidite

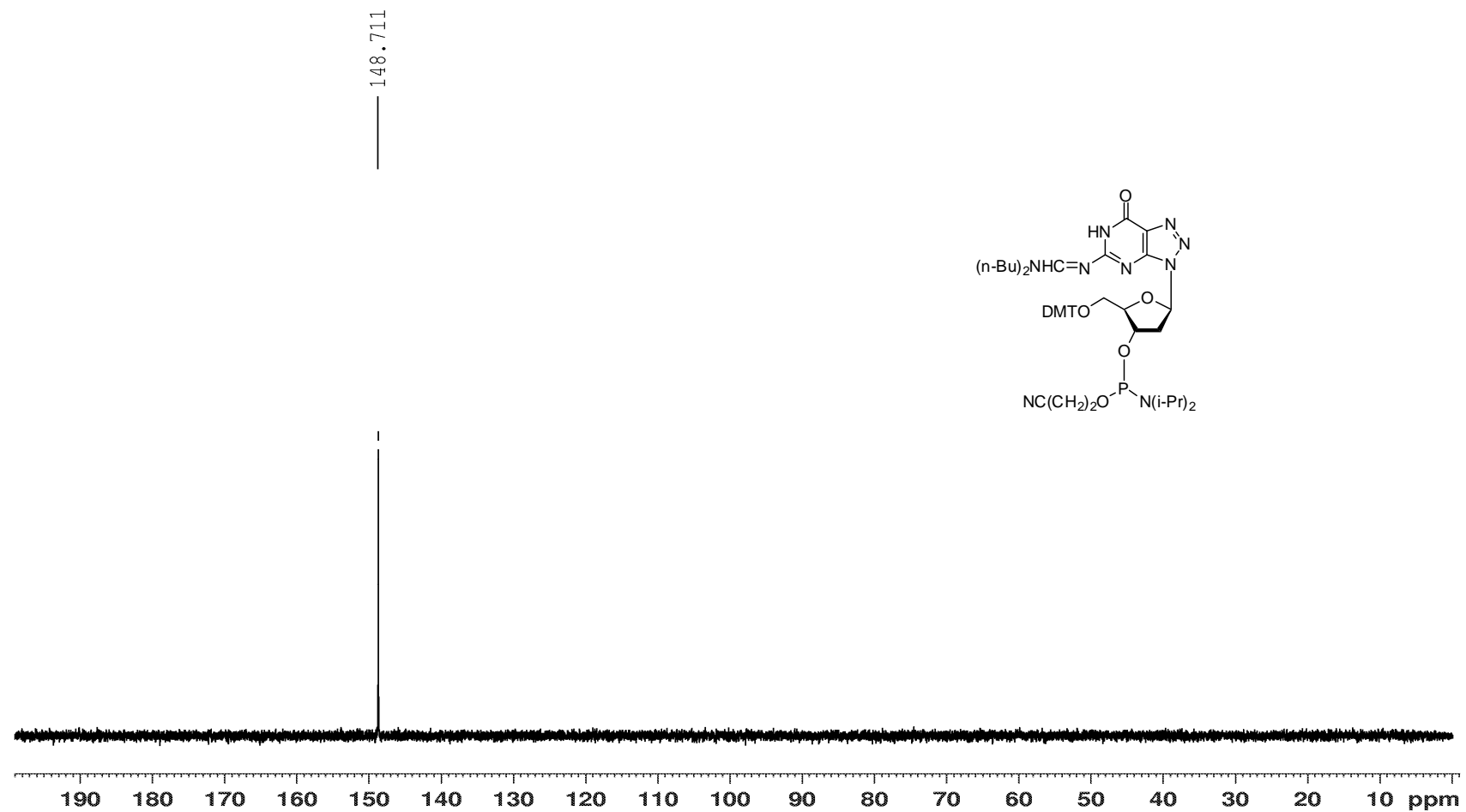


Figure S14. ^{31}P -NMR spectrum of compound 11.