Supporting Information

Thermodynamic Profiles and NMR Studies of Oligonucleotide Duplexes Containing Single Diastereomeric Spiroiminodihydantoin Lesions

Irine Khutsishvili, Na Zhang, Luis A. Marky, Conor Crean, Dinshaw J. Patel, Nicholas E. Geacintov, and Vladimir Shafirovich

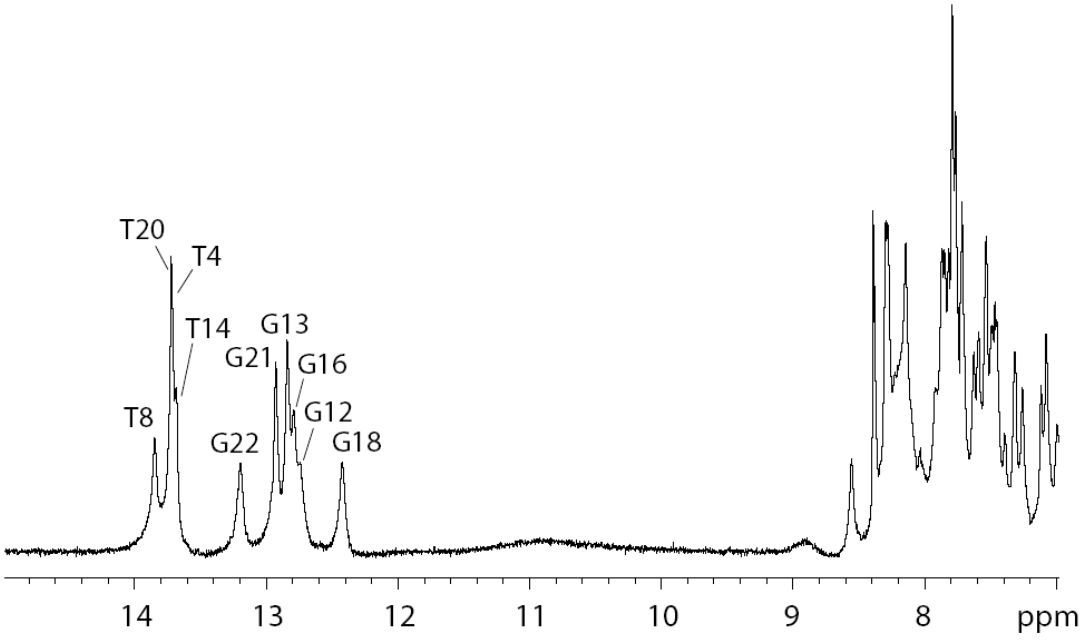

Figure S1. NMR spectrum (7.0–15.0 ppm) of the Sp-*S* 11-mer duplex in 100 mM NaCl, 10 mM sodium phosphate H_2O buffer, pH 6.8 at 0 °C. The imino proton assignments are labeled.

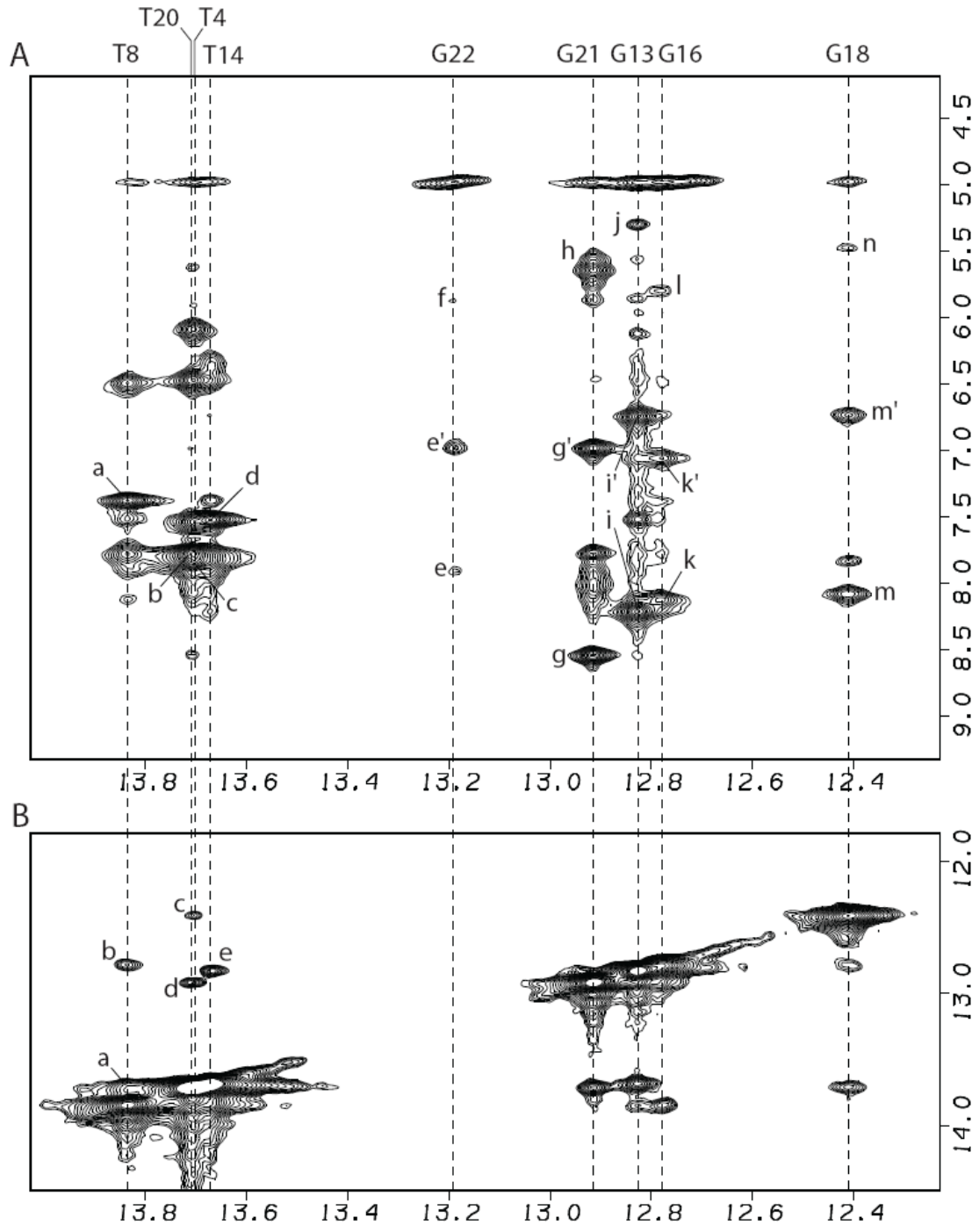

Figure S2. Expanded NOESY (200 ms mixing time) contour plots for the Sp-*S* 11-mer duplex in 100 mM NaCl, 10 mM phosphate, H_2O buffer solution, pH 6.8 at 0 ^{o}C. Panel A identifies NOEs between imino protons (12.2 to 14.0 ppm), amino and non-exchangeable protons (4.5 to 9.0 ppm), with NOE cross peaks a to n characteristic of Watson-Crick base pairs. Cross-peaks a to n

are assigned as follows: a, T8(NH3)-A15(H2); b, T20(NH3)-A3(H2); c, T4(NH3)-A19(H2); d, T14(NH3)-A9(H2); e,e′, G22(NH1)-C1(NH_2); f, G22(NH1)-C1(H5); g,g′, G21(NH1)-C2(NH_2); h, G21(NH1)-C2(H5); i,i′, G13(NH1)-C10(NH_2); j, G13(NH1)-C10(H5); k,k′, G16(NH1)-C7(NH_2); l, G16(NH1)-C7(H5); m,m’, G18(NH1)-C5(NH_2); n, G18(NH1)-C5(H5). Panel B identifies NOEs between imino protons, with the cross peaks labeled a to e, which are assigned as follows: a, T8(NH3)-T14(NH3); b, T8(NH3)-G16(NH1); c, T4(NH3)-G18(NH1); d, T20(NH3)-G21(NH1); e, T14(NH3)-G13(NH1).

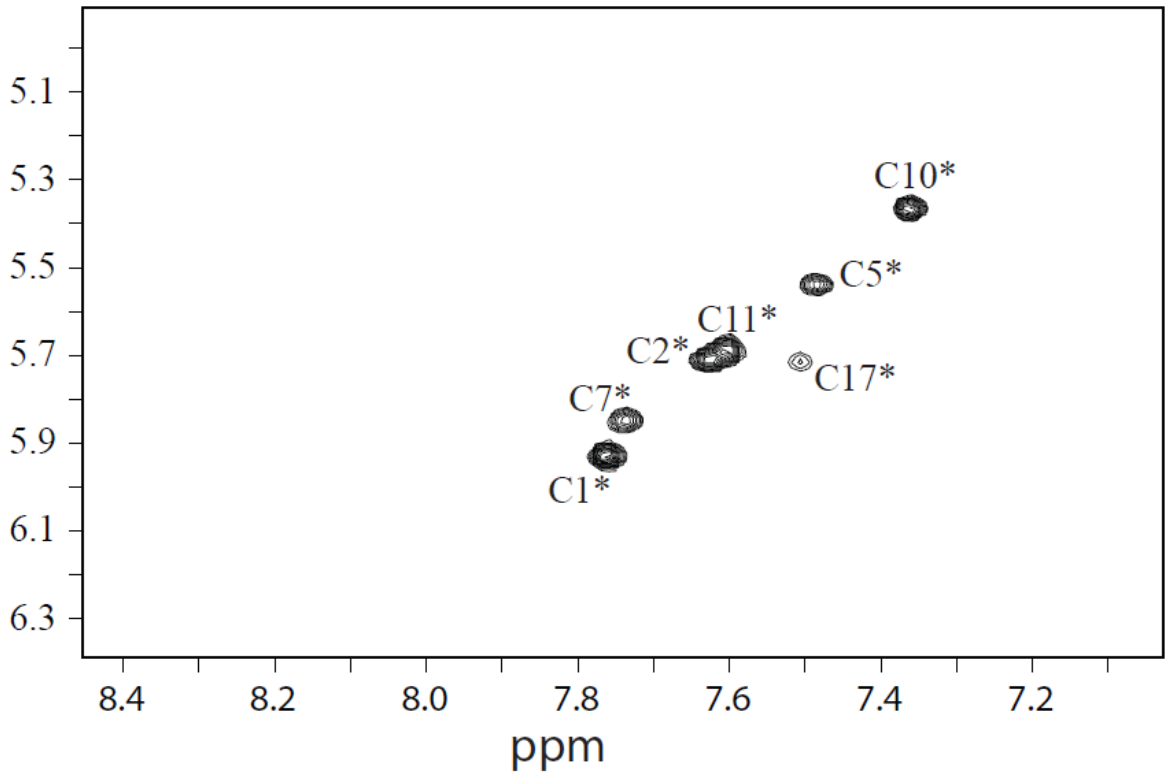

Figure S3. COSY NMR contour plots of the Sp-*S* 11-mer duplex. This NOE spectrum was determined with the 11-mer duplex dissolved in 100 mM NaCl, 10 mM sodium phosphate 10% D_2O aqueous buffer solution, pH 6.8 at 0 °C. The through-bond connectivities between base protons H6 and H5 of all cytosines are labeled as asterisks.