Supplementary Information

Understanding Mixed Sequence DNA Recognition by Novel Designed Compounds: The Kinetic and Thermodynamic Behavior of Azabenzimidazole Diamidines

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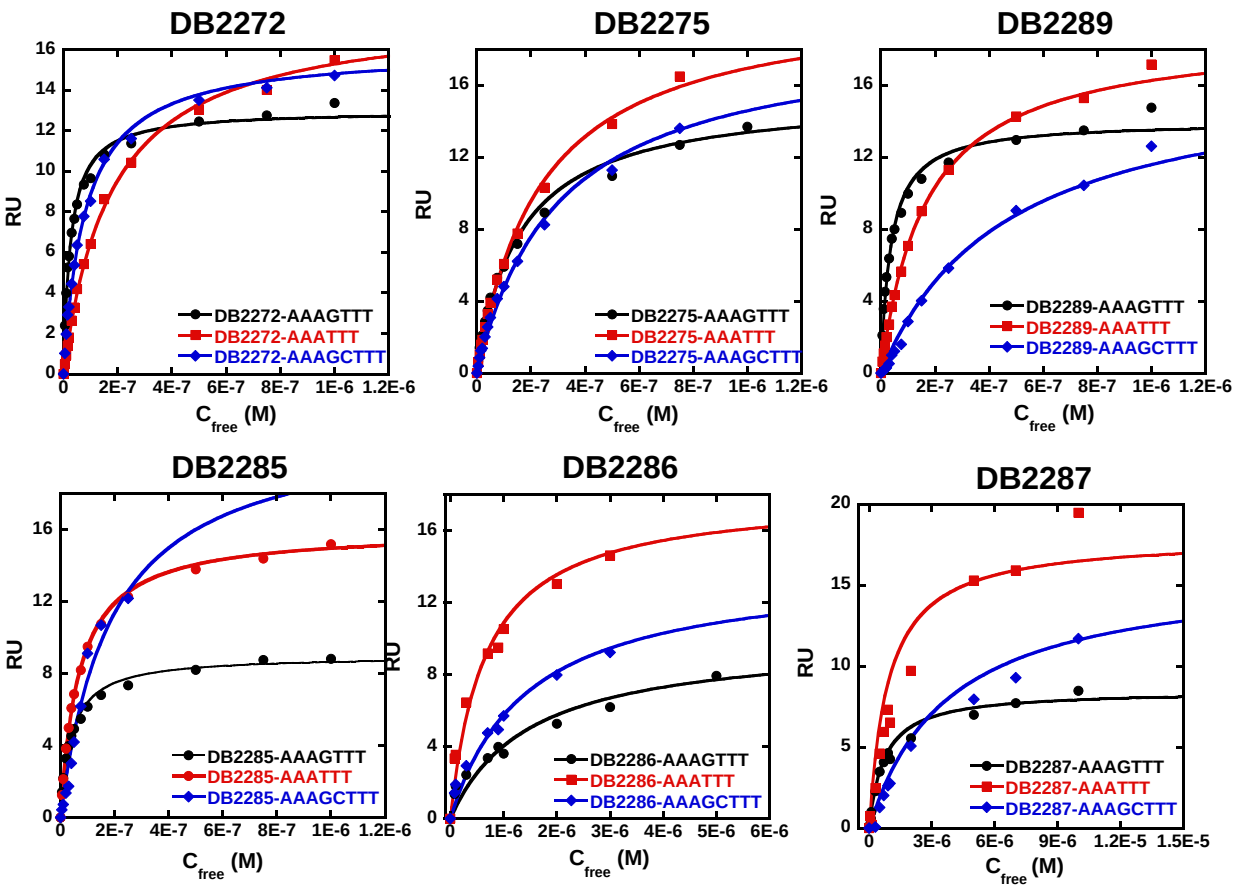

Figure S1: SPR equilibrium binding plots of selected diamidines with AAA**G**TTT, AAATTT and AAA**GC**TTT sequence at 100 mM NaCl concentrations and 25 °C. The steady state response values were fitted as a function of free ligand concentration to a single-site interaction model. The binding affinities are listed in Table 1.

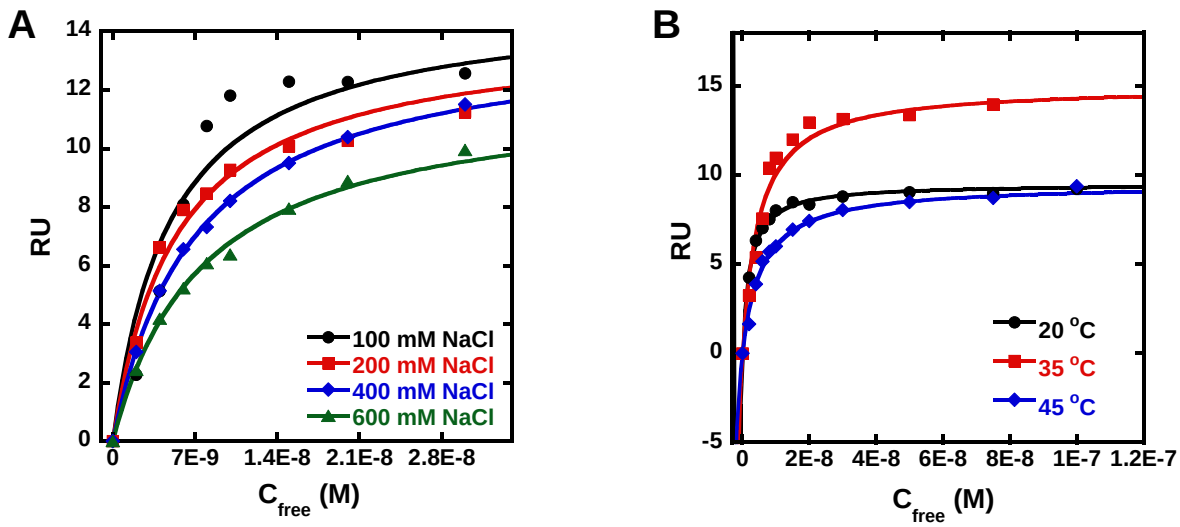

Figure S2: SPR equilibrium binding plots of DB2277 with AAA**G**TTT hairpin DNA sequence, (A) different salt concentrations at 25 ^{o}C and (B) different temperatures at 200 mM NaCl concentration. The steady state response values were fitted as a function of free ligand concentration to a single-site interaction model. The binding affinities are listed in the inset and in Table 2 and 3.

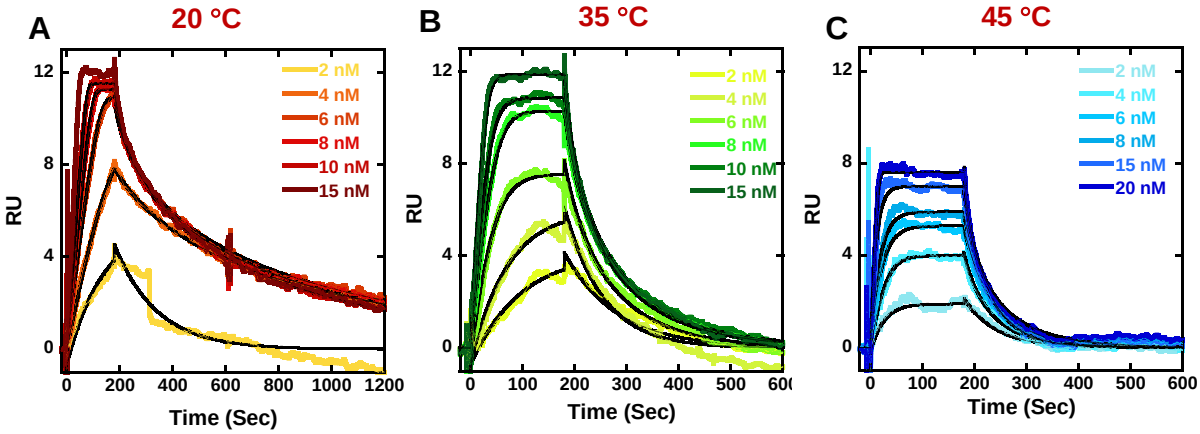

Figure S3: (A-C) SPR sensorgrams (color) and global kinetic fits (black overlays) for DB2277 with the AAA**G**TTT DNA sequence at different temperatures as mentioned above.

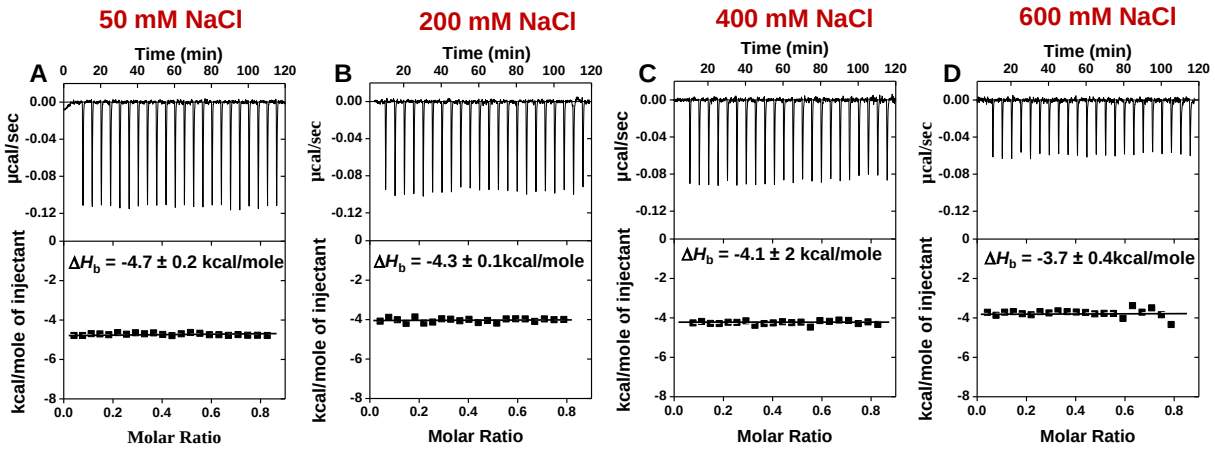

Figure S4: (A-E) ITC data for the titration of DB2277 and AAA**G**TTT hairpin duplex DNA at different salt concentrations.

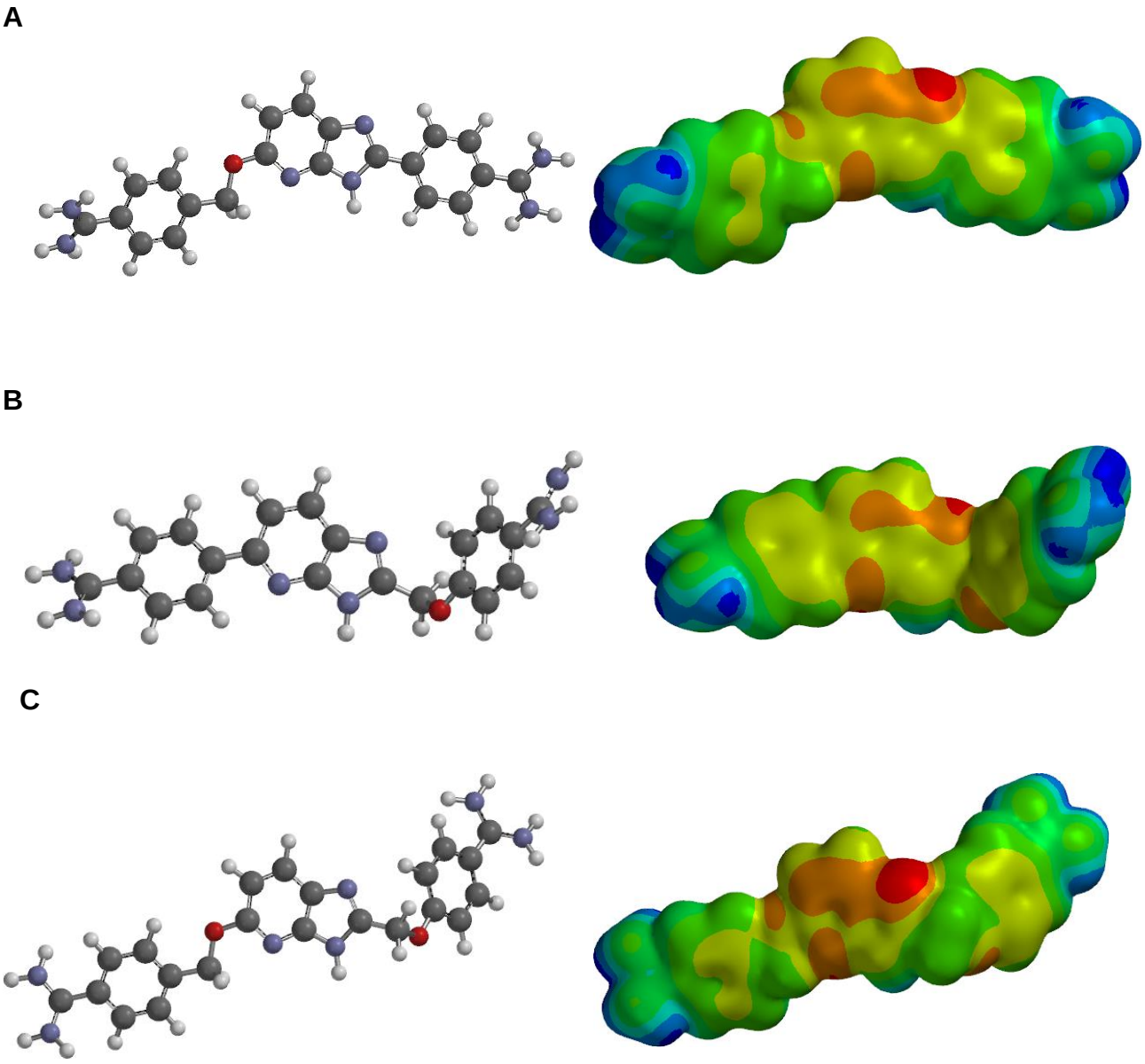

Figure S5: DFT ab initio calculations at the 6-31G* (p,d) level of theory for DB2277 (A), DB2275 (B) and DB2272 (C) with their respective electrostatic potential maps