Supporting Information

NMR Imino Proton Exchange Experiments on Duplex DNA Primarily Monitor the Opening of Purine Bases

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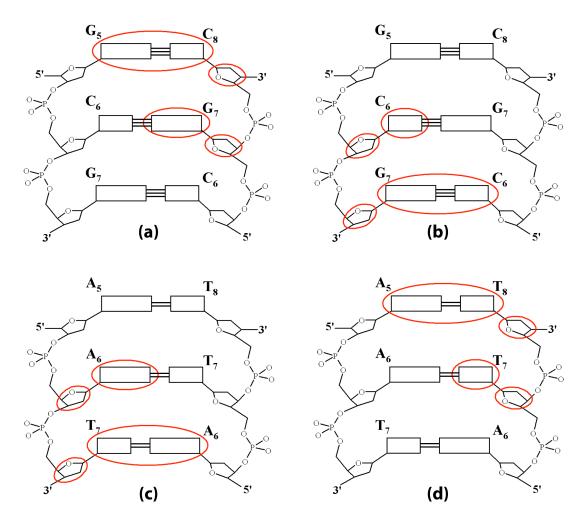


Figure S1: The pseudodihedral angle is defined as the dihedral angle formed by the center of masses (COM) of four sets of atoms: the non-hydrogen atoms in the (a) flipping base, (b) its sugar moiety, (c) the sugar moiety of the adjacent nucleotide on the 3' side, and (d) the adjacent base pair on the 3' side. For the base opening of G, C, A and T, the four sets of atoms chosen to define the COM pseudodihedral angle are given in (a), (b), (c) and (d) respectively.