Journal Name

ARTICLE

Electronic supplementary information

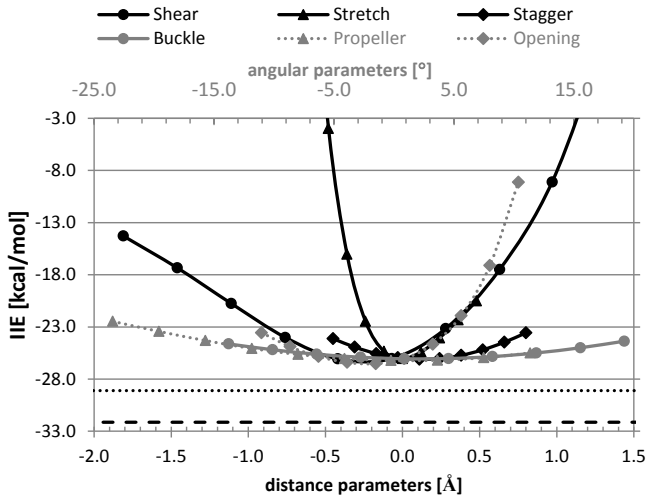

Fig.S7. The diversity of intermolecular interaction energy of canonical G-C pair in conformations characteristics to B-DNA double helix. Black lines represent variations of IIE as a function of displacement parameter, while grey curves stand for angular parameters. The corresponding energy of the ground state level (after full optimization) is denoted by dashed line. The dotted line represent the IIE without correction for monomer geometry relaxation.

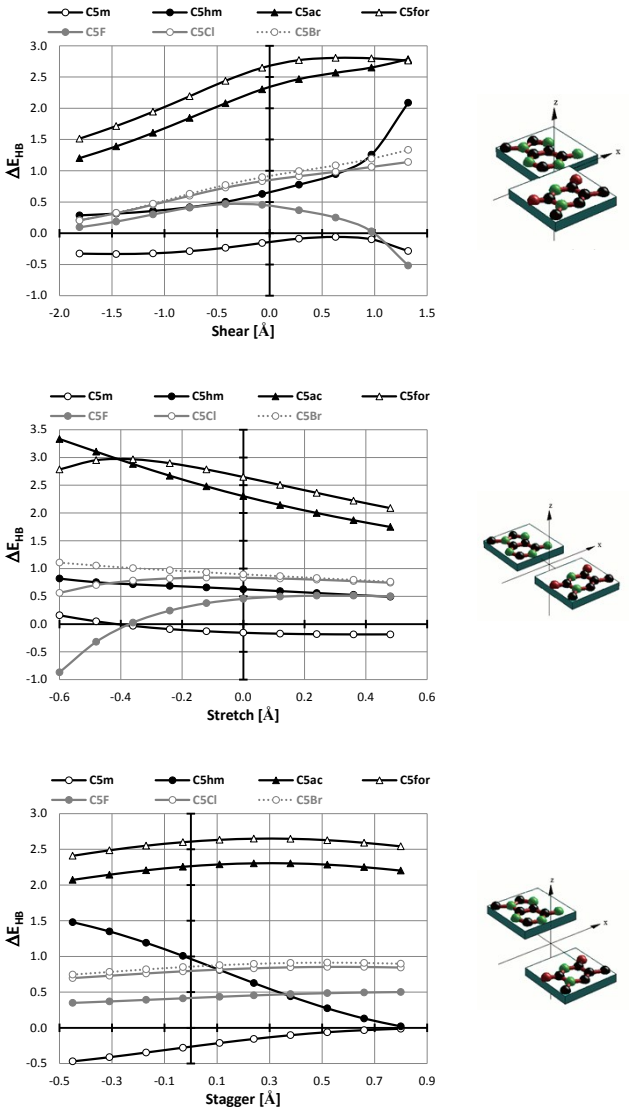

Fig.S8. Scan of the relative intermolecular interaction energies of canonical guanine with 5-modified cytosine derivatives as a function of hydrogen bonding separation parameters defining. The reference points corresponds to values characterizing G-C pair documented in Fig.7. The positive values indicate lower pairs stability compared to analogical conformations of canonical G-C pair.

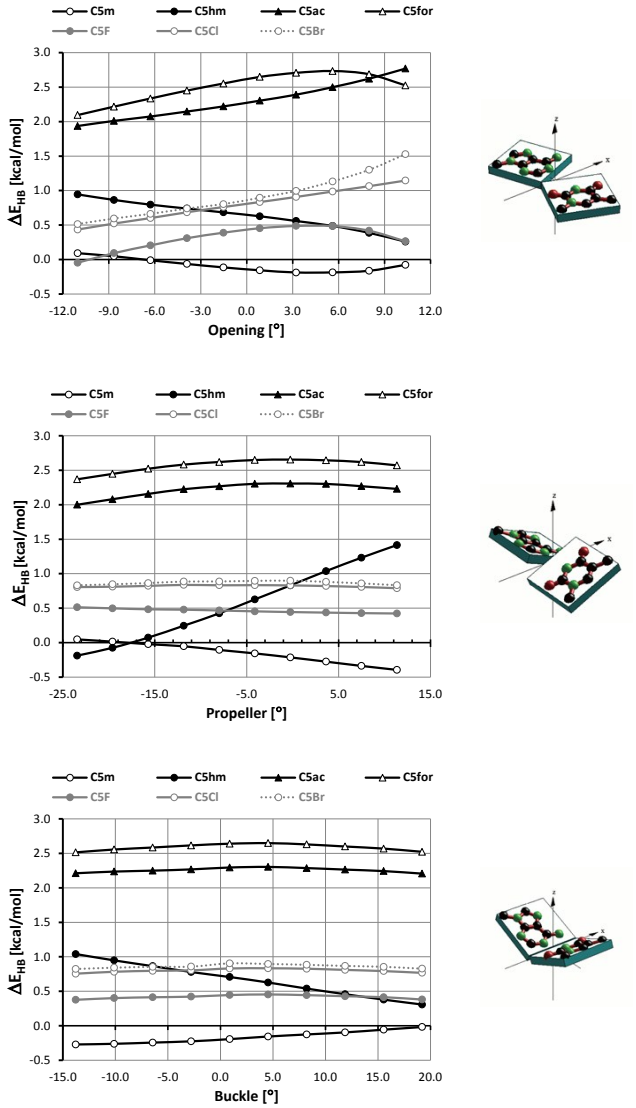

Fig.S9. Scan of the relative intermolecular interaction energies of canonical guanine with 5-modified cytosine derivatives as a function of hydrogen bonding angle parameters defining. The reference points corresponds to values characterizing G-C pair documented in Fig.7. The positive values indicate lower pairs stability compared to analogical conformations of canonical G-C pair.