SUPPLEMENTARY INFORMATION

Sequence-dependent response of DNA to torsional stress: a potential biological regulation mechanism

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Figure S1. Time evolution of twist for the steps most affected by the imposed twist in each oligomer: TpA in ACGT and AGCT, CpG in ACGA and CCGA. The central panels show the behaviour of these steps in the relaxed oligomer, while the left and right hand panels show the impact of undertwisting (-5°) or overtwisting (+5°) with respect to the average base pair step twist of the restrained segments (34.9°). The time series are coloured as a function of the BI/BII state of the 3'-flanking phosphate junctions for the Watson (w) and Crick (c) strands.
Figure S2. Time evolution of shift for TpA and CpG dinucleotide steps during the simulations of the ACGT and CCGA oligomers. For overtwisted DNA (+5.0° with respect to the average twist per base pair step for the restrained segments, 34.9°), these YpR steps show a bimodality in shift (see Figure S2). Changes in shift are coupled to BI/BII transitions in the YpR junctions: BI Watson (i.e. 5' → 3' strand) and BII Crick (i.e. 3' → 5' strand) leading to positive shift (coloured yellow above), while the reverse leads to negative shift (coloured green above).