Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Probing the role of dispersion energy on structural transformation of double-stranded xylo- and ribo- nucleic acids

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Table S1. H-rise, rise, h-twist and twist parameters obtained following 3DNA analysis for the double-stranded RNA and XNA at various time points.

Scaling Factor for ε →	**0.01**		**1.00**		**5.00**	
	h-rise (rise)	h-twist (twist)	h-rise (rise)	h-twist (twist)	h-rise (rise)	h-twist (twist)
RNA (Initial)	3.4 (3.4)	36.3 (36.2)	3.4 (3.4)	36.3 (36.2)	3.4 (3.4)	36.3 (36.2)
RNA (0 ns)	3.4 (3.4)	37.5 (37.0)	3.3 (3.4)	37.4 (35.9)	3.3 (3.4)	37.4 (35.9)
RNA (20 ns)	4.6 (6.7)	6.4 (12.5)	3.2 (3.5)	32.9 (30.6)	3.1 (3.3)	39.9 (38.8)
RNA (80 ns)			2.6 (3.3)	31.9 (28.4)	2.8 (3.2)	49.8 (46.7)
XNA (Initial)	3.5 (3.2)	15.5 (11.2)	3.5 (3.2)	15.5 (11.2)	3.5 (3.2)	15.5 (11.2)
XNA (0 ns)	2.5 (3.6)	18.7 (12.0)	3.1 (3.7)	17.2 (12.1)	2.5 (3.6)	18.7 (12.0)
XNA (20 ns)	3.2 (5.2)	-5.9 (1.0)	2.8 (3.3)	-1.1 (0.1)	1.9 (3.1)	-0.9 (1.4)
XNA (80 ns)	--	--	1.5 (3.5)	7.2 (4.9)	3.1 (3.5)	-1.6 (-3.1)

In Table S1 “Initial” indicates the starting structure for the simulation while “0 ns” indicates the equilibrated structure prior to production run.

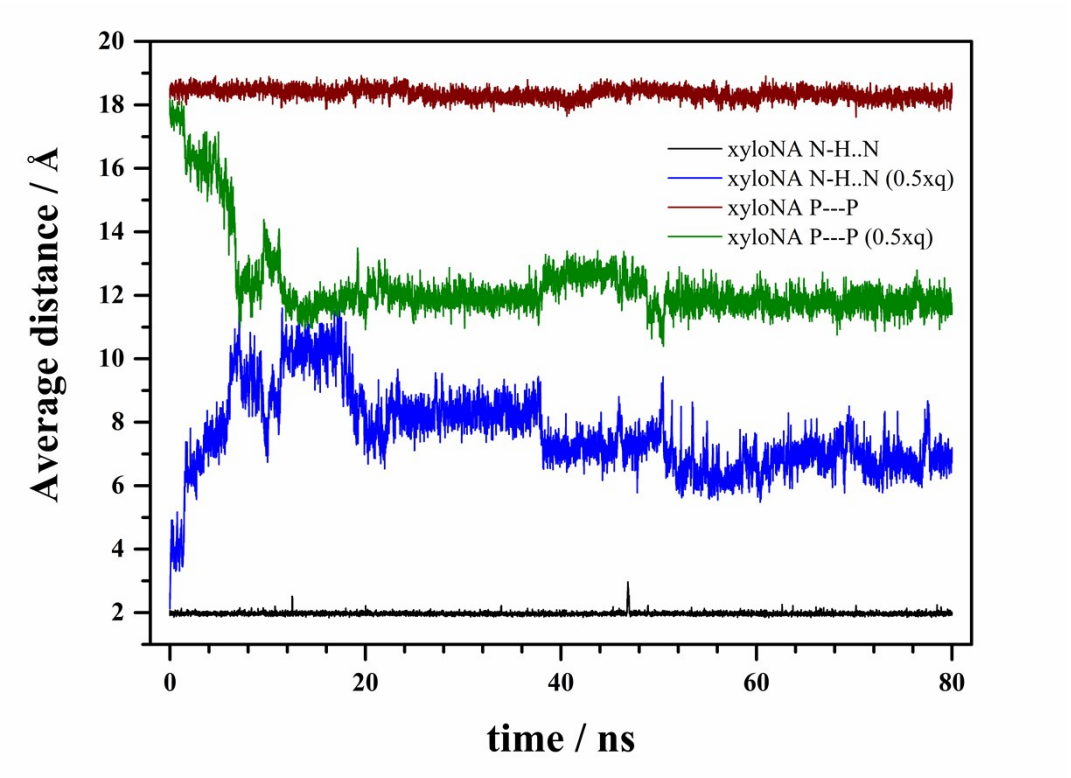

Fig. S1. Plots of average inter-strand N–H···N hydrogen bonded distance (black – unscaled; blue – scaling factor for the charges 0.5) and average inter-strand distance between phosphorus atoms (brown – unscaled; green – scaling factor of the charges 0.5) for the double-stranded XNA as a function of simulation time. Various curves correspond to simulations carried out by scaling electrostatic energy (charges). The decrease in the electrostatic energy leads to almost instantaneous change in the double-helix structure due breaking of the N–H···N hydrogen bonds followed by base flipping, which is captured by increase in the N–H···N hydrogen bonded distance and decrease in the inter-strand P---P distance.

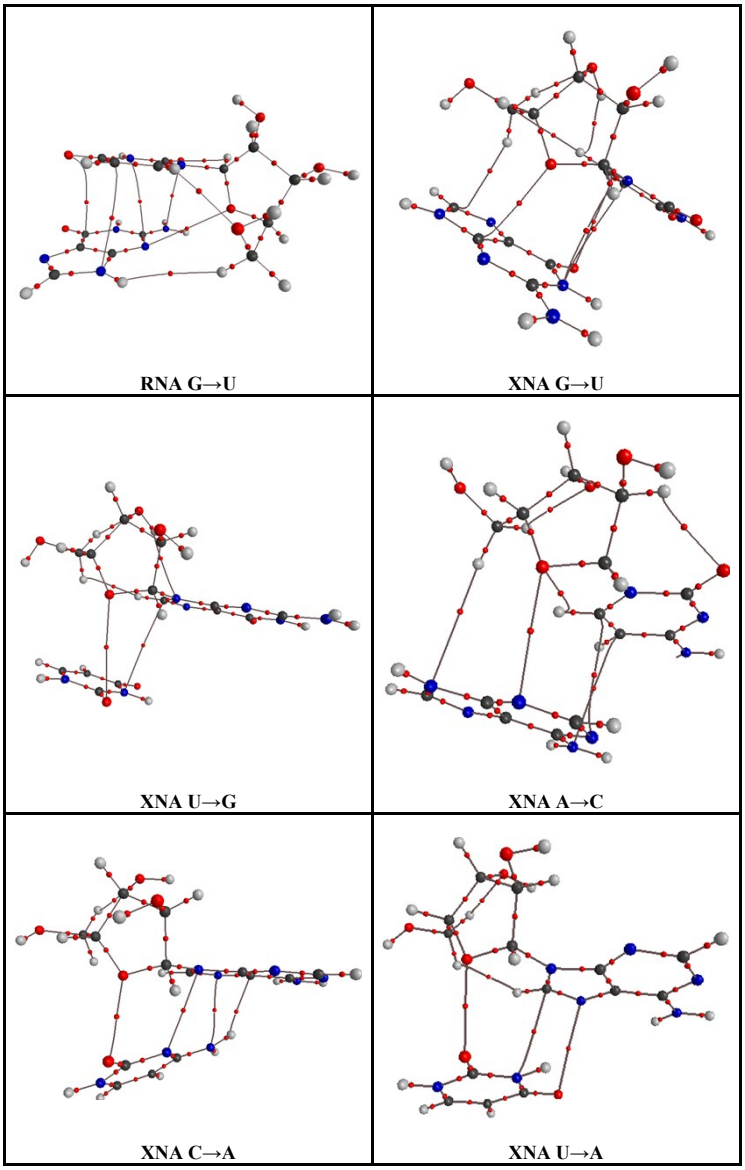

Fig. S2. Molecular graphs for the XNA, depicting the presence of bond critical point for the Lp···π interaction between the oxygen atom of the xylose and the adjacent nucleobase in XNA. Also shown is for RNA for sake of comparison, which does not show a bond critical point corresponding to Lp···π interaction.