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

Supporting Information for :

Probing interaction of a trilysine peptide with DNA behind formation of guanine-lysine cross-links: insights from molecular dynamics. †

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1) Protocol for the molecular dynamics simulations

All molecular dynamic simulations and post-processing were performed with the Amber 16 Molecular Dynamics software package. The force-field parameters were taken from parm99. Each system (KKK, TGT and the double-stranded 15-bp) was previously built using the tleap and nucleic acid builder (nab) programs within the Antechamber suite of programs. KKK was left uncapped with $–NH_3^+$ and $–COO^-$ termini to match the experimental setup by one of us. We stress out that the trilysine was not arbitrarily added close to guanine, but was placed at a distance of ~6 Å in order to avoid biaising the self-association process.

For the KKK-15bp system, four independent trajectories were run for 200 or 500ns (see Table 1, thus 1.4 µs in total). It is to be noted that Trajectories 1 and 2 were run using a time step of 2fs, where as trajectories 3 and 4 were run using a time step of 4fs taking advantage of the Hydrogen Mass Repartitioning scheme (HMR).

After all dynamic molecular simulations, a cluster analysis was performed using the cpptraj module of AMBER, and thermodynamic parameters were extracted using the MM-GBSA method with internal and external dielectric constants set to 1 and 80, respectively. The salt concentration was set to 0.15 M.

2) Cartoon representations for the TGT oligonucleotides and KKK@15-bp system before interactions

a) KKK-TGT system

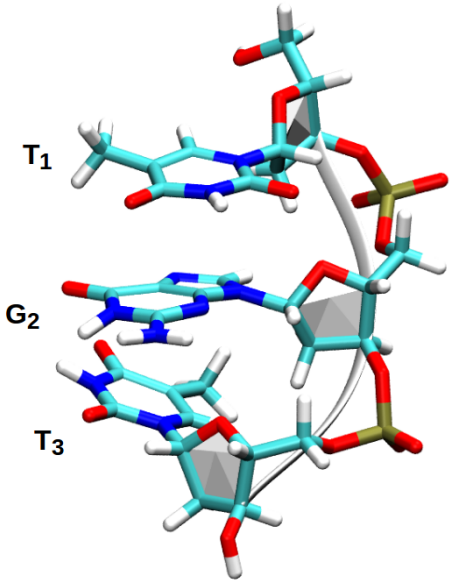

Figure S1. *Representative structure of isolated TGT trinucleotide after 200ns of simulation. Obtained by cluster analysis. One observes a π-stacking interaction.*

b) KKK-15-bp system

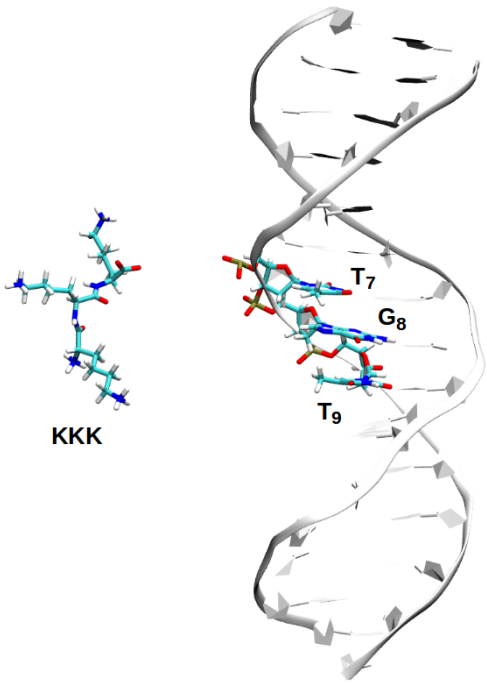

Figure S2. *Initial configuration of the 15-bp oligonucleotide with the KKK peptide placed near the center of the duplex.*