Supplementary Material (ESI) for *Organic and Biomolecular Chemistry*

Electronic Supplementary Information

Synthesis and modelling of DNA junction and minor groove zipper motifs incorporating the double-headed nucleoside 5′(*S*)-*C*-(thymine-1-ylmethyl)-thymidine

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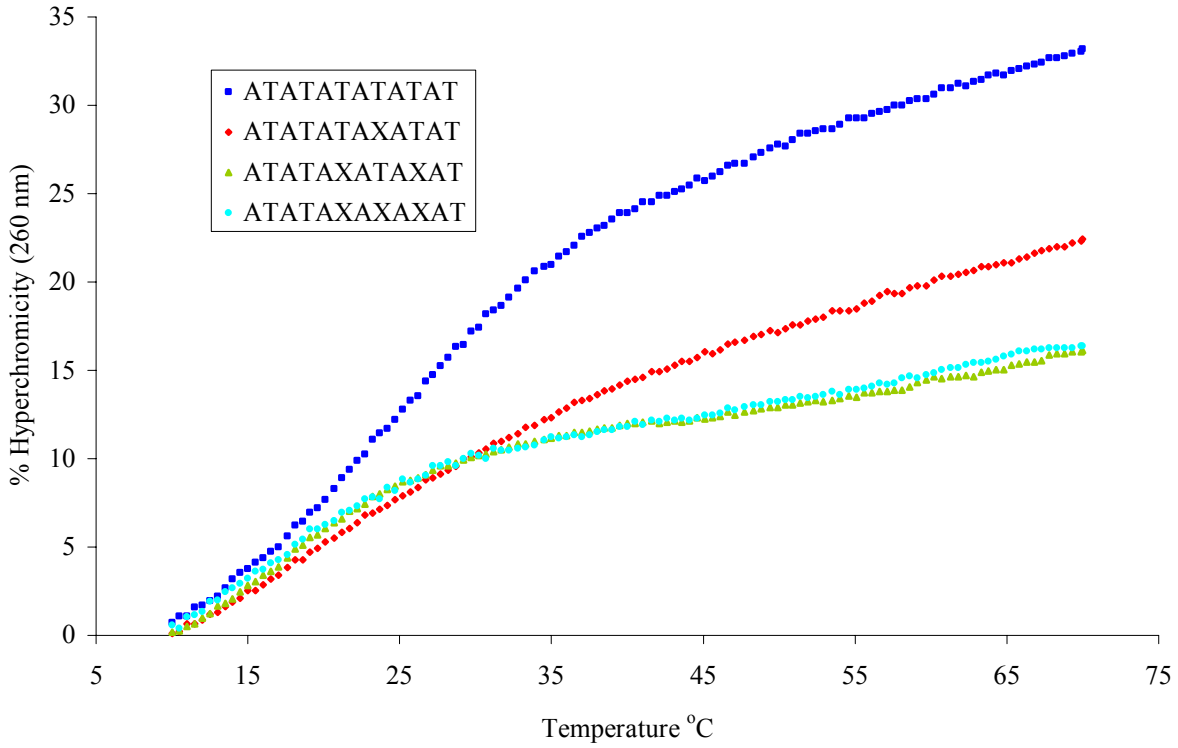
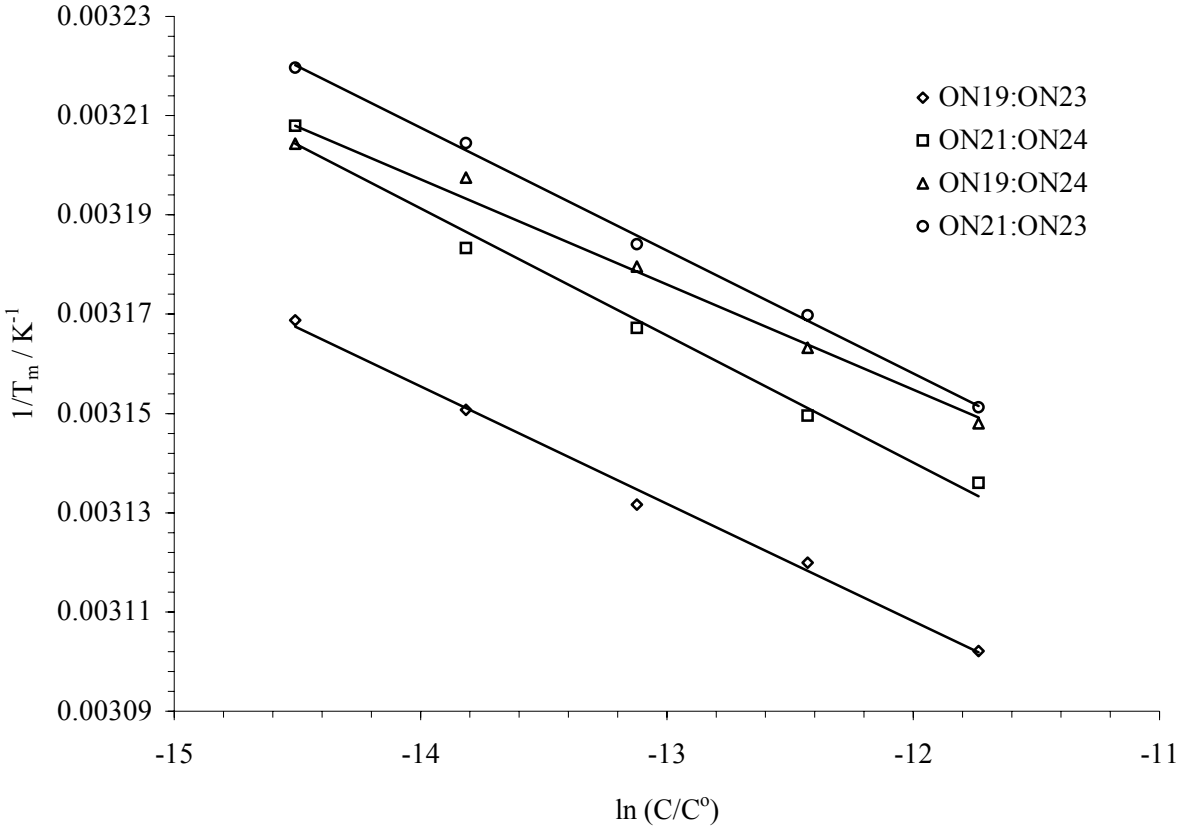
- UV-melting profiles for self-complementary sequences **27-30** (ESI-Figure 1).
- Van´t Hoff plots for obtaining the data in Table 6 (ESI-Figure 2).
- Modelling data; Root mean squared deviation (ESI-Figure 3) and alignment of dipole vectors (ESI-Figure 4).

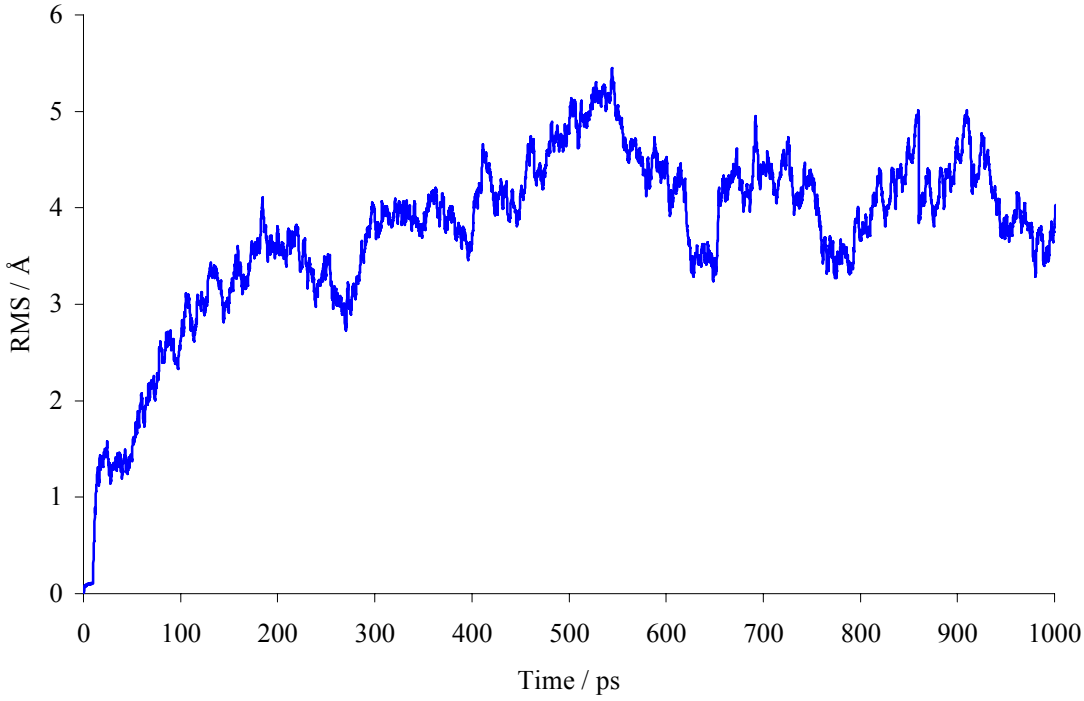
ESI-Figure 1. UV-melting profiles for the 5´-ATATATATATAT-3´ zipper motifs. % Hyp. = (Abs(T)/Abs(10°C)-1)·100%.



ESI-Figure 2. $1/T_m$ vs. ln(C) plots of the four combinations (110 mM Na^+, pH 7.0, C° = 1 mol/l).



ESI-Figure 3. Root mean squared deviation (Å) for the conformational fit of the backbone to the initial A-type conformation during the 1000 ps simulation.



ESI-Figure 4. Alignment of the two extra thymidine nucleobases electric dipoles during the 1000 ps simulation.