Index of animations

This CD-ROM contains animations in two file formats (.avi for Windows and .mov for Macintosh). The animations are found in folders corresponding to the section they refer to in the thesis.

- 3.3: animation of a ligand (netropsin) sampling out the entire length of the groove through restrained molecular dynamics.

- 3.3: animation with trailing end of a ligand straying out of the groove.

- 3.5.1: CHARMm scrambled animation.

- 3.5.2: simulations for netropsin, distamycin and Hoechst 33258 both with restrained and constrained DNA.

- 3.5.3: animation with a ligand leap-frogging

- 3.6.1: animation for 2:1 ligands sliding and losing side-by-side geometry when both have a tether to the top of DNA.

- 3.6.2: animation of rigid 2:1 distamycin and thiazotropsin A.

- 3.6.3: a minimisation of two side-by-side ligands which are being expelled from the minor groove of canonical DNA.

- 3.6.3: animation showing the generation of 2:1 parameters for ISF by superimposition of generated 4-mers on an experimentally determined structure.

- 3.6.5: animation of thiazotropsin A in three binding modes (maximum overlap, one residue stagger and two residue stagger).

- 3.7: animation showing ISF of netropsin on canonical 5'GCAAATTTGCGCTATATAGC (starting from either end).

- 3.9: comparison of trajectories for ISF of netropsin using the CHARMm and cff91 force fields.