DNA-Dye-Conjugates: Conformations and Spectra of Fluorescence Probes

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Extensive molecular-dynamics (MD) simulations were used to investigate DNA-dye and DNA-photosensitizer conjugates, which act as reactants in templated reactions leading to the generation of fluorescent products in the presence of specific desoxyribonucleic acid sequences (targets). Such reactions are potentially suitable for detecting target nucleic acids in live cells by fluorescence microscopy or flow cytometry. The simulations show how the attached dyes/photosensitizers influence DNA structure and melting behavior, and reveal the relative orientations of the chromophores with respect to each other. Our results will help to optimize the reactants for the templated reactions, especially length and structure of the spacers used to link reporter dyes or photosensitizers to the oligonucleotides responsible for target recognition. Furthermore, we demonstrate that the structural ensembles obtained from the simulations can be used to calculate steady-state UV-vis absorption and emission spectra. These data will be used in a subsequent study to develop a detailed model of fluorescence kinetics, including quenching of the reporter dye via fluorescence resonance energy transfer (FRET).