Computational study of the interaction of sulfoindocyanine dye Cy3 with single- and double-stranded DNA

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Many fluorescent studies of biologically relevant systems employ sulfoindocyanine dye Cy3 as a label. Energy transfer and distance correlations are usually studied using Forster theory. To interpret such studies correctly one has to be able to separate the effects of the environment from the effects of the dynamics of the system on the fluorescence of the dye. In this work, we report results of the simulation of Cy3 dye attached to single- , double- and mixed-DNA. Our results indicate that Cy3-DNA interaction consists predominantly of two modes: interaction of Cy3 indole rings with nearby bases and hydrogen bonding of Cy3 CH_2OH side-group to accessible H bond acceptors of the backbone and bases. We will use our data to help interpret recent experiment form the Levitus' lab at Arizona State University.