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From force-fields to photons: MD simulations of dye-labeled nucleic acids and Monte Carlo modeling of FRET[1]

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Fluorescence resonance energy transfer (FRET) is a powerful technique for understanding the structural fluctuations and transformations of RNA, DNA and proteins. Molecular dynamics (MD) simulations provide a window into the nature of these fluctuations on a different, faster, time scale. We use Monte Carlo methods to model and compare FRET data from dye-labeled RNA with what might be predicted from the MD simulation. With a few notable exceptions, the contribution of fluorophore and linker dynamics to these FRET measurements has not been investigated. We include the dynamics of the ground state dyes and linkers in our study of a 16mer double-stranded RNA. Water is included explicitly in the simulation. Cyanine dyes are attached at either the 3' or 5' ends with a 3 carbon linker, and differences in labeling schemes are discussed.

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