

Abstract Submitted  
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**From force-fields to photons: MD simulations of dye-labeled nucleic acids and Monte Carlo modeling of FRET** PEKER MILAS, BEN GAMARI, LOUIS PARROT, RICHARD BUCKMAN, LORI GOLDNER, University of Massachusetts Amherst — Fluorescence resonance energy transfer (FRET) is a powerful experimental 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 faster time scale inaccessible to experiment. 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 along with an explicit water solvent in our study of a 16mer double-stranded RNA. Cyanine dyes are attached at either the 3' or 5' ends with a three carbon linker, providing a basis for contrasting the dynamics of similar but not identical molecular structures.

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