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Molecular Dynamics-Based Structural Sampling: Case Studies of Stilbene, Urea, and Carotenoid Complexes

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Hydrogen bonding plays an important role in nature, from carotenoids and stilbenes to urea [1-6]. Carotenoids are responsible for the coloration of leaves, fruits, flowers, and other organisms, and they play a critical role in photosynthesis through light-harvesting and photoprotective functions. In these processes, hydrogen bonding can be significant, which motivates the need to understand the effects of polar solvents [2−4]. Stilbenes are diarylethenes that exhibit fluorescence and reversible photoisomerization upon UV excitation. The influence of the environment, such as polystyrene, on stilbene geometry remains an open question [5]. Urea is an efficient hydrogen-bond donor and acceptor, making it a suitable model compound for studying polar interactions [6].

A polar environment can induce new molecular arrangements, and molecular dynamics (MD) is a suitable tool for exploring such structural diversity. In this work, we show how stilbene-based complexes are formed, discuss the challenges of obtaining stable complexes in a realistic urea solvent, and finally present possible new complexes involving carotenoids - with particular emphasis on fucoxanthin - in protic and aprotic polar solvents.

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