Supporting Information

Urea Induced Unfolding Dynamics of Flavin Adenine Dinucleotide (FAD): Spectroscopic and Molecular Dynamics Simulation Studies from Femto-second to Nano-second Regime

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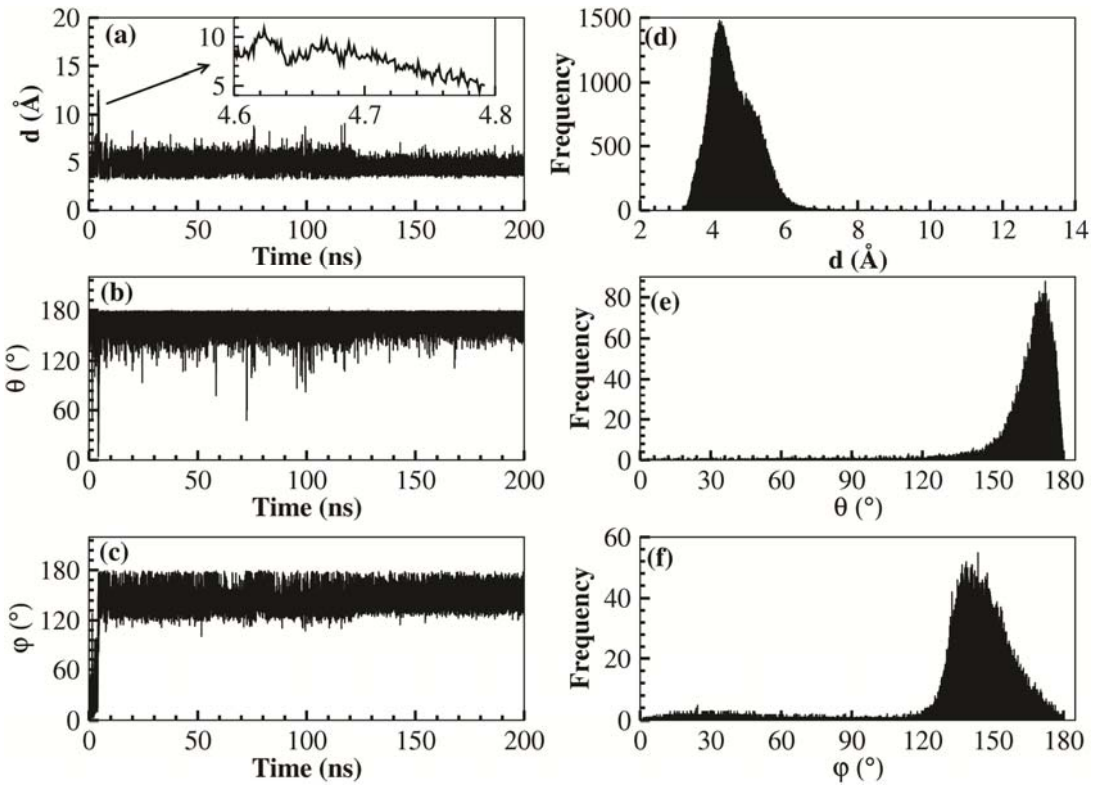

Figure S1: (a), (b) and (c) show the variation of d, θ, φ, respectively with time in water. (d), (e) and (f) are the distribution of the three parameters (d, θ and φ) in water solvent. When $d \leq 6Å^1$, and the angles is $40^\circ \geq \{\theta, \varphi\} \geq 140^\circ$, we defined these conformations as stack conformations.

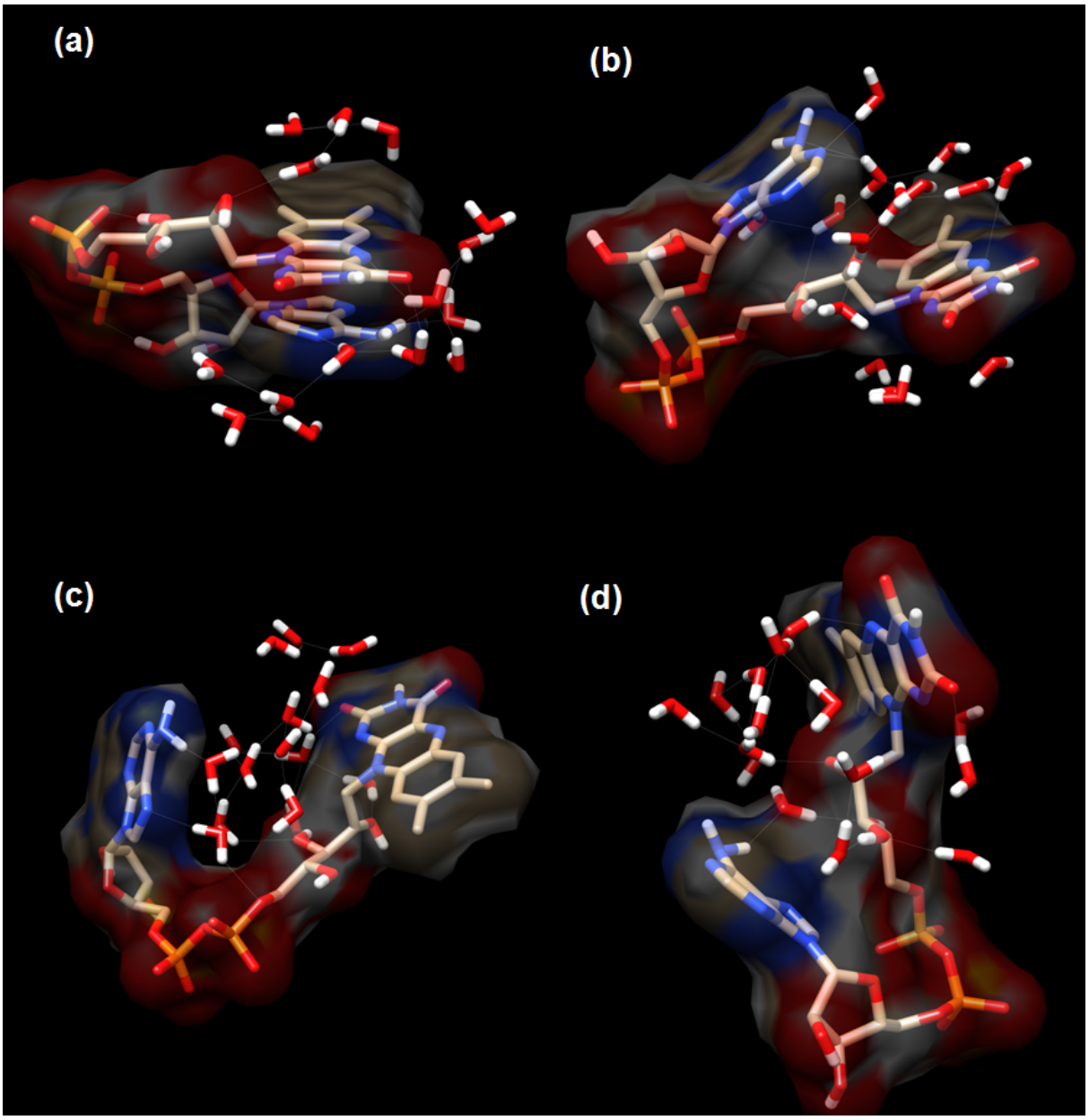

Figure S2: Orientations of water molecules around adenine and isoalloxazine rings of FAD at different time points in the trajectory.

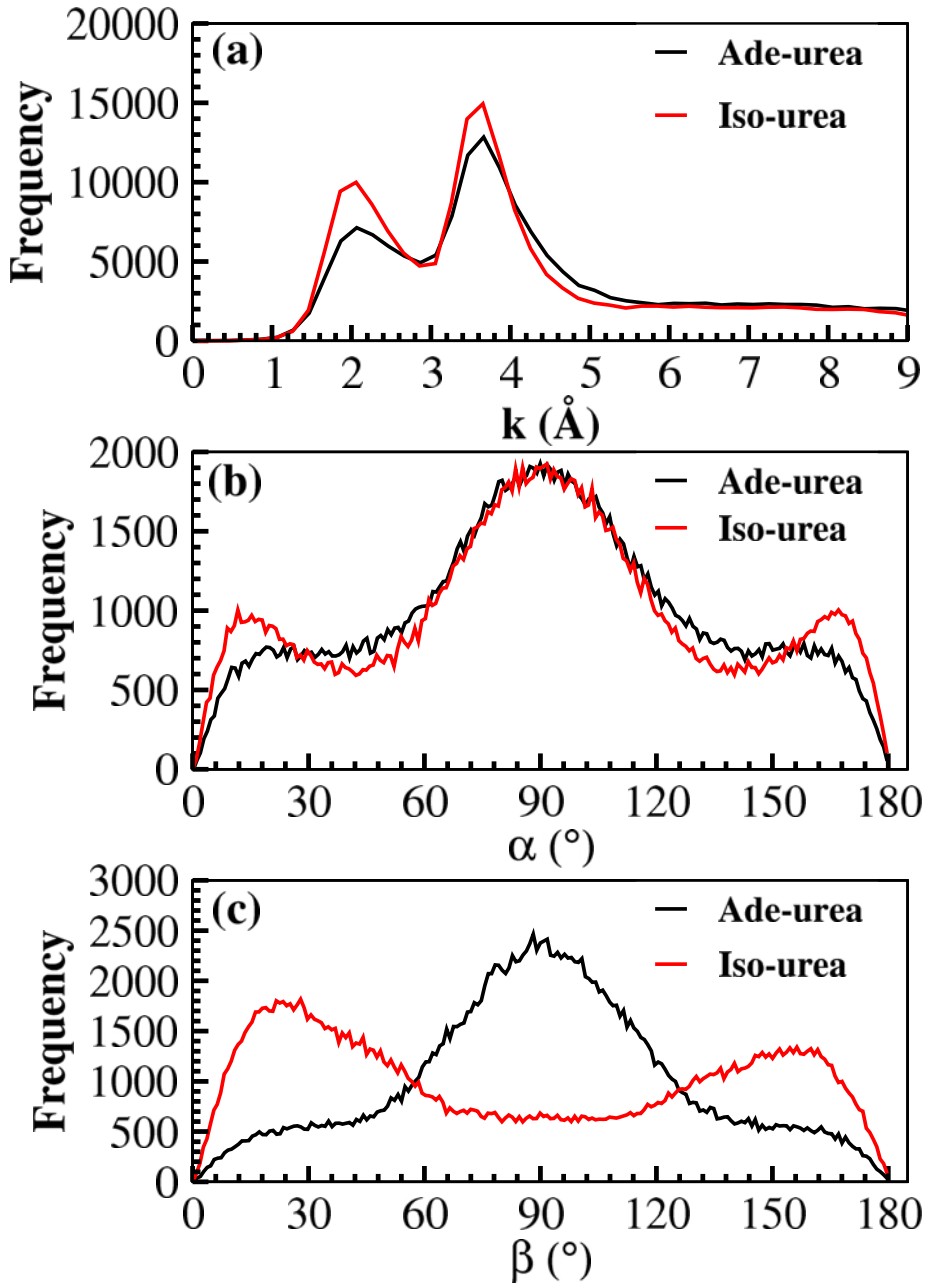

Figure S3: Distribution of k, α and β for Ade/Iso with urea. (a) distribution of distance (k) between the COMs of Ade and urea, Iso and urea. (b) Distribution of angle (α) between the Ade and urea, Iso and urea. (c) Distribution of angle (β) between Ade and urea, Iso and urea.