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Temperature Dependent Solvation Dynamics of the Chromophore Environment in the Far-Red Fluorescent Protein mPlum[1]
CHOLA REGMI, PREM CHAPAGAIN, BERNARD GERSTMAN, Florida International University — We used molecular dynamics (MD) simulations to investigate the solvation dynamics of the chromophore environment in the far red fluorescent protein mPlum. Low temperature experiments on mPlum show a reduced Stokes shift compared to the room temperature. This suggests that the flexibility of the chromophore environment is related to the large Stokes shift in the red fluorescent protein mPlum. We performed MD simulations at various temperatures and systematically explored the protein-chromophore hydrogen bond pattern as well as the dynamics of the internal water molecules near the chromophore. We also investigated the dynamics of the hydrogen bond formed between residues E16 and I65, which is considered to play an important role in the observed large red shift in the emission spectrum. We quantify the hydrogen bonding pattern as a function of temperature to show how the Stokes shift in mPlum is correlated to the E16-I65 hydrogen bond dynamics.

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