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Protein barrel fluctuations and the barrel permeability: A comparison between Green and Red Fluorescent proteins CHOLA REGMI, PREM CHAPAGAIN, BERNARD GERSTMAN, Department of Physics, Florida International University, THEORETICAL BIOPHYSICS TEAM — As compared to the Green Fluorescent Proteins (GFP), the monomeric variants of the Red Fluorescent Proteins (RFP), also known as mFruits, are substantially less photostable, possibly due to the barrel permeability for molecular oxygen into the protein barrel. We performed molecular dynamics simulations to compare the protein barrel fluctuations of the GFP as well as a monomeric variant of the RFP. We also performed implicit ligand sampling for uncovering the pathways for molecular oxygen entry into the barrels. We found that, as compared to the GFP barrel, the RFP barrel has significantly larger structural fluctuations and these large barrel fluctuations lead to clear pathways through which molecular oxygen or other ions can enter the barrel more easily.

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