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Barrel fluctuation and oxygen diffusion pathways in the monomeric fluorescent proteins CHOLA REGMI, PREM CHAPAGAIN, YUBA BHANDARI, ILAN CHEMMAMA, BERNARD GERSTMAN, Florida International University — Fluorescent proteins are valuable tools as biochemical markers for studying cellular processes. Improving the photostability of the FPs is highly desirable in biochemical, biomedical and cell biology. Oxygen is necessary for the proper maturation of the chromophore in fluorescent proteins (FPs), but photobleaching of FPs is also oxygen sensitive. The photobleaching of the monomeric variant of RFPs has been attributed to the lack of proper shielding against oxygen or other small molecules, ions or halides. We use molecular dynamics simulation to investigate the protein barrel fluctuations in mCherry, one of the most useful monomeric mFruit variant of RFPs. We also employ oxygen diffusion simulations to search for possible pathways of oxygen to the chromophore. The ultimate goal is to use the results of these calculations to propose amino acid substitutions that will block the oxygen pathways and prevent photobleaching in the engineered proteins.

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