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Effects of pressure on the protein barrel and the chromophore interactions in mCherry YUBA BHANDARI, PREM CHAPAGAIN, CHOLA REGMI, BERNARD GERSTMAN, Florida International University — Fluorescent proteins (FP) can be attached to proteins of interest, which makes it possible to study the movement, localization and many other physiological processes of the tagged proteins. A number of fluorescent proteins have been genetically engineered to enhance their intensity, photo-stability, pH-stability etc. The structural fluctuations of FPs determine the ease of access of small molecules like oxygen and may be an important consideration for their fluorescence spectrum and stability. A protein's response to pressure perturbations provides useful insights for understanding their folding and dynamics. Experiments have shown that application of pressure affects both the fluorescence peak as well as the quantum yield of the protein. We report on molecular dynamics computational investigations of the effect of pressure on the fluctuations of the beta barrel and the structure of the chromophore of a well characterized Red Fluorescent Protein, mCherry. We discuss our results on how pressure affects the ability of water and other ions to penetrate the barrel to reach the chromophore, as well as the effect on the time dependent hydrogen bonding network in the chromophore's cavity region.

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