

P022 Molecular dynamics study of chemically engineered GFP mutants: comparison of intramolecular FRET efficiency
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Due to its unusual spectroscopic properties, green fluorescent protein (GFP) has become a useful tool in molecular genetics, biochemistry and cell biology. Here, we computationally explore the behaviour of two GFP constructs, designed as bioprobes for enzymatic triggering using intramolecular fluorescence resonance energy transfer (FRET). These constructs differ in the location of the intra-molecular FRET partner, an attached chemical chromophore (either at a N-terminal or C-terminal site). We apply the temperature replica exchange molecular dynamics (REMD) method to the two flexible constructs, permitting efficient sampling of protein/chromophore phase space. The calculated efficiency of FRET was derived from the inter chromophore distance and orientational factor, κ^2 . In agreement with experiment, the construct with the C-terminally attached dye was found to have higher energy transfer efficiency than observed for the N-terminal construct. The molecular basis for this observation is discussed.