Water Exchange at the Beta-Barrel “Holes” of Several Far-Red Fluorescent Proteins

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There is a desire to improve several physical characteristics of far-red fluorescent proteins. One hypothesis is that the access of water to the fluorophore has some effect on these characteristics. Simulations of several temperatures as well as two water models have been performed on the Neptune, mCardinal, and mCrimsonT fluorescent proteins. Water exchange appears to be minimal below 320K. There also does not appear to be significant differences between the two water models used.