Dihedral freedom of the ligand Bilirubin in the UnaG protein.

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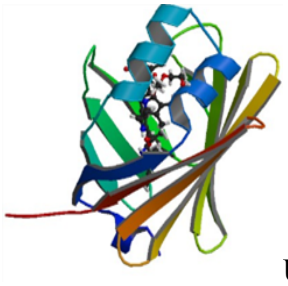

UnaG, a fatty-acid-binding protein (FABP), is the first fluorescent protein identified in a vertebrate. UnaG is found in the muscle fibers of the Japanese Freshwater Eel and is suspected to help relieve muscle stress during long migration. Its fluorescence is triggered by the presence of the ligand bilirubin, the yellow breakdown product of heme catabolism. This finding enabled researchers to develop a sensitive assay to determine the bilirubin levels in human serum. In addition UnaG presents other promising applications as its fluorescence is oxygen-independent. This study focuses on better understanding the conformational changes available to the ligand bilirubin in the excited state. This is accomplished through performing a series of 50ns molecular dynamic simulations; two molecular dynamic simulations with freely rotating dihedrals that approximate the first excited state as well as a typical "ground state" simulation. Simulation results suggest that τ_{AB} and φ_{AB} dihedral angles have great rotational freedom, while τ_{CD} and φ_{CD} dihedral angles with lesser rotational freedom rotate in a negatively correlated hula twist (figure 1).

Figure 1: