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Investigating Docking Predictions for Beta-Lactoglobulin-Porphyrin IX Complexes in Monomer and Diamer Forms JAMES PARKER, The University of Texas at San Antonio — Molecular docking of protein-ligand complexes are largely focused upon filtering a large database of ligands. Our goal is to determine the exact binding site(s) of a known binding ligand, porphyrin IX (PPIX), to beta-lactoglobulin (BLG) to enable better descriptions of conformational changes that occur during the binding of the ligand-protein complex as well as physical/chemical changes that occur in the presence of other stimuli such as laser-tissue heating. The first step involved examining four conformations of BLG (1 diamer, 1BEB and 3 monomers, 1BEB chain A, 1BEB chain B, and 1DV9) for use in docking with PPIX. The computed bound state for the diamer configuration placed the ligand over the gap between the two monomers. For the monomer, the ligand bound along the exposed face of the polypeptide. The relative binding strengths of the two configurations differ by 2 parts in 100. This result was verified by experiment in which the ligand bound to a diamer configuration of BLG did not precipitate out of solution when a denaturing agent was added to divide the diamer.

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