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Correlating Computational Docking Predictions with Raman Spectroscopy for Beta-Lactoglobulin-Porphyrin Complexes JAMES PARKER, LORENZO BRANCALEON, The University of Texas at San Antonio — Computational molecular docking simulations (Dock and AutoDock) may provide a wealth of structural information related to the bound configuration of protein-ligand complexes, but they require verification to ensure their predictions reflect reality. Resonance Raman spectroscopy data has been collected to correlate normal mode vibrations observed in the bound structure to computationally generated structures in order to determine the best match between the compuational model and experiment. This methodology was used to determine the bound structures at an atomistic level of β-lactoglobulin (BLG) and meso-tetrakis (p-sulfonatophenyl) porphyrin (TSPP) in aqueous solutions at pH 7 and 9. Comparisons of Raman spectra of TSPP before and after binding to BLG yield line shifts that are related to the distortions in the free molecule that are presumed to be generated by the non-covalent binding of the ligand to the protein. Our goal is to define quantitative relationships between the observed line shifts and the computed distortions in the molecular structure using normal mode analysis and DFT computational tools.

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