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Docking Prediction of a Water Soluble Porphyrin and Tubulin Assisted with Resonance Raman and Vibrational Mode Analysis BRADY MCMICKEN, Univ of Texas, San Antonio; 711th Human Performance Wing, Optical Radiation Bioeffects Branch, LORENZO BRANCALEON, Univ of Texas, San Antonio, ROBERT THOMAS, 711th Human Performance Wing, Optical Radiation Bioeffects Branch, JAMES PARKER, Univ of Texas, San Antonio; 711th Human Performance Wing, Optical Radiation Bioeffects Branch — The ability to modify protein conformation by controlling its partial unfolding may have practical applications such as diminishing its function or blocking its activity. One method used to induce partial unfolding of a protein involves the use of a photosensitizer noncovalently bound to a protein that triggers photochemical reactions upon irradiation leading to protein conformational changes. We are investigating the photoinduced conformational changes of tubulin mediated by a bound water-soluble porphyrin that acts as a photosensitizer. Analysis of how tubulin conformational changes affect its function including polymeric assembly forming microtubules is of interest to uncover the mechanism responsible for the structural change. Our approach to better understand the conformational change, we first plan to discover the binding location between the porphyrin and protein. Use of vibrational mode analysis using density functional theory and resonance Raman experiments targeting the porphyrin molecule will be used to correlate Raman peaks with vibrational modes. The relative intensities of the porphyrin bound to tubulin can be used to calculate the equilibrium geometry observed from Raman spectra. These data will provide the relative distortion of the porphyrin when bound to tubulin, which will subsequently be used in docking simulations to find the most likely binding configuration.

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