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Photoinduced Localized Unfolding of Tubulin Dimers Bound to a Water Soluble Porphyrin and the Search for Binding Location Using Docking Simulations Guided by a Combination of Resonance Raman Spectroscopy and Density Functional Theory[1] BRADY MCMICKEN, LORENZO BRANCALEON, The University of Texas at San Antonio, Department of Physics and Astronomy, ROBERT THOMAS, Optical Radiation Bioeffects Branch, Bioeffects Division, JBSA Fort Sam Houston — The ability to modify the conformation of a protein by controlling its partial unfolding may have practical applications such as inhibiting its function. One method of locally unfolding a protein involves the use of a photosensitizer non-covalently bound to a protein which triggers photochemical reactions upon irradiation leading to protein conformational changes. We investigate the photoinduced conformational changes of tubulin mediated by a bound water soluble porphyrin which acts as a photosensitizer. Also of interest is how conformational changes of tubulin affect its function such as forming microtubules and the mechanism responsible for the structural change. To better understand the conformational change we must find the binding location between the porphyrin and protein. Density functional theory calculations will be combined with Resonance Raman spectroscopy to correlate the changes in vibrational modes of the porphyrin with changes in its physical structure upon binding to tubulin. This will allow us to determine the distorted conformation 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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Brady McMicken
Univ of Texas, San Antonio

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