Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Fluorescence spectroscopy investigation and molecular docking simulation of the interaction of β-lactoglobulin A (BLGA) with meso-tetrakis(4-sulfonatophenyl) porphyrin (TSPP) IVAN SILVA, LORENZO BRANCALEON, SAM SANSONE, University of Texas at San Antonio — The interaction of TSPP and β-lactoglobulin A (BLGA) was studied as a function of pH (6.0-9.0). TSPP is a dye that is currently in clinical trials for its application in photodynamic therapy of cancer, and BLGA is a well known globular protein. Binding to the protein affects the photophysics of the dye, hence its potential in clinical applications. Data from TSPP fluorescence experiments were analyzed and modeled by computational methods. Protein-dye interaction was studied using fluorescence spectroscopy to record the spectral shift (from 643nm to 649nm) to quantify bound and free dye with use of Gaussian curve fitting. TSPP-induced quenching of protein fluorescence determined the binding constant and the number of binding sites through S-V and double-log plots. Fluorescence lifetime characterized the effects of the binding and the location of the binding site through FRET. Unlike the binding of protoporphyrin IX, pH dependence of the TSPP binding to BLG is not modulated by the pH conformational change of the protein. Molecular simulation of the docking of TSPP monomers to BLGA dimers were done using the Arguslab software. Simulations reveal that the interaction is driven by the four negative charges on TSPP which keep it on the surface of the protein.

Ivan Silva
University of Texas at San Antonio

Date submitted: 13 Dec 2007 Electronic form version 1.4