## Abstract Submitted for the TSF11 Meeting of The American Physical Society

Porphyrin-Mediated Photoinduced Conformational Changes to Albumin SARAH ROZINEK, LORENZO BRANCALEON, UTSA — Many biological and nonbiological uses of protoporphyrin-IX (PPIX) depend on its ability to bind large macromolecules such as human serum albumin (HSA). HSA is both biomedically and technologically relevant to PPIX (free base and metal), and its binding site for PPIX-derivatives is well established. The irradiation of PPIX noncovalently bound to BetaLactoglobulin (BLG) is known to cause protein conformational changes that are pH-dependent due to BLG's intrinsic conformational transitions. These processes have not been extensively studied in nonphysiological pH conditions for FePPIX or PPIX bound to HSA. This study implemented a combination of optical and computational methods to compare binding characteristics of hemin and PPIX to HSA as well as structural effects of lowdose irradiation of the ligand on the protein. Spectroscopic data suggests that irradiation of the Soret band of PPIX bound to HSA is capable of modifying the globular protein structure by direct charge transfer between the porphyrin and the binding site at both physiological and acidic pH confirmations. Computational docking simulations predict lower free energy of binding for PPIX than for heme.

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