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Molecular Simulation of the docking of meso-tetrakis(4-sulfonatophenyl) porphyrin (TSPP) to b-lactoglobulin dimer. IVAN SILVA, SAMUAL SANSONE, LORENZO BRANCALEON, University of Texas at San Antonio — Data from fluorescence-quenching experiments and fluorescence-lifetime reveal that TSPP interacts with the Trp residues of BLGA. Fluorescence-lifetime measurements were compiled and identified possible Trp residues responsible for binding. We have run molecular simulation of the docking of TSPP monomers to BLGA dimmers using the Arguslab software. Simulations reveal that the interaction is driven by the four negative charges on TSPP which keep the porphyrin on the surface of the protein.

Samual Sansone
University of Texas at San Antonio

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