**Mentor:** Patricia Soto  
**Department:** Physics  

**Research area:** Protein conformational dynamics and pathological folding

The overarching goal of the Computational Molecular Biophysics group is to elucidate the mechanisms by which proteins hallmark of neurodegenerative diseases, such as prion disease and Alzheimer’s disease, interact with the cell membrane to induce cytotoxicity. The nature of the protein- membrane lipid interactions makes multi-scale computer modeling a unique technique to probe the complexity of the interactions at an atomic level currently unreachable by experimental techniques. The INBRE funded project focuses on prion diseases, also known as transmissible spongiform encephalopathies, a family of inevitably fatal diseases in mammals, including humans. Prions, molecular aggregates responsible for prion diseases, propagate biological information by conversion of the non pathological version of the prion protein, PrP\textsuperscript{c}, to the infectious isoform, PrP\textsuperscript{Sc}. Our project examines the mechanism by which the cellular form of the prion protein, PrP\textsuperscript{c}, interacts with plasma membrane microdomains rich in cholesterol. The outcome of our project will shed light into our fundamental understanding of prion diseases, will aid in the interpretation of wet lab experiment results and, importantly, will identify targets for therapeutics.

**Keywords (research topics):** pathological protein folding, amyloid, prion, Alzheimer’s, protein-lipid interactions

**Keywords (skills/techniques):** biomolecular modeling, continuum electrostatics, molecular docking, normal mode analysis, molecular dynamics simulations.