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Molecular modeling of the conformational dynamics of the cellular prion protein[1] CHARLES NGUYEN, Department of Physics, Creighton University, IAN COLLING, Department of Biology, Creighton University, JASON BARTZ, Department of Medical Microbiology and Immunology, Creighton University, PATRICIA SOTO, Department of Physics, Creighton University — Prions are infectious agents responsible for transmissible spongiform encephalopathies (TSEs), a type of fatal neurodegenerative disease in mammals. Prions propagate biological information by conversion of the non-pathological version of the prion protein to the infectious conformation, PrP^{Sc}. A wealth of knowledge has shed light on the nature and mechanism of prion protein conversion. In spite of the significance of this problem, we are far from fully understanding the conformational dynamics of the cellular isoform. To remedy this situation we employ multiple biomolecular modeling techniques such as docking and molecular dynamics simulations to map the free energy landscape and determine what specific regions of the prion protein are most conductive to binding. The overall goal is to characterize the conformational dynamics of the cell form of the prion protein, PrP^{c}, to gain insight into inhibition pathways against misfolding.

[1]NE EPSCoR FIRST Award to Patricia Soto

Charles Nguyen
Creighton University

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