

1139-92-173

Erica Flapan* (eflapan@pomona.edu), **Adam He** and **Helen Wong**. *A new model of protein knot folding*. Preliminary report.

How knotted proteins fold has remained controversial since the identification of deeply knotted proteins nearly two decades ago. Both computational and experimental approaches have been used to investigate protein knot formation. In this talk, we describe a new model of knot folding that could explain the formation of all currently known protein knot types and predict knot types that might be identified in the future. Our model is motivated by computer simulations of Virnau and coworkers for the $+6_1$ -knotted DehI protein which implicate a loop flipping mechanism that results in the simultaneous threading of two loops. We analyze fingerprint data from crystal structures of protein knots as evidence that particular protein knots fold according to specific configurations from our model. (Received February 08, 2018)