

1096-VG-944

Junkoo Park* (jun-koo.park@houghton.edu), One Willard Ave., Houghton, NY 14744. *Elastic Network Model Extensions for Predicting Protein Residue-level Fluctuation*. Preliminary report.

Proteins are an important class of biomolecules, and they are fundamental research subjects of life sciences. While a protein folds to a unique structure, it makes dynamic fluctuations. These movements may correspond to certain functions and provide valuable insights for drug design. Therefore, studying the structural fluctuation is essential in protein modeling. Accurate predictions on its structural fluctuations may provide great insights into how the dynamics of the structure relate to their functions. The structural fluctuations can be analyzed theoretically for a given structure. Elastic Network Model (ENM) has been proposed recently and proved to be reasonably accurate. In this paper, we propose a refined Gaussian Network Model (GNM) which is based on atomic interaction potential, and compare the refined GNM with other elastic network models. The refined GNM has been shown to perform well for predicting residue-level structural fluctuations. The goal of this study is to extend the ENM and apply it to protein structures and analyze the results, and further improve our predictions. (Received September 11, 2013)