INSTITUTE COLLOQUIUM

Friday, 27 February 2015 4:00 p.m. Fermion

Speaker:

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Title:

Exploring the universe of protein folds

Abstract:

It is currently believed that the atlas of existing protein structures is faithfully represented in the Protein Data Bank. On the contrary, in this talk I will show that it is more plausible that the known folds form a rather small subset of the full ensemble of possible conformations. This statement is based on a sophisticated numerical approach that allows for an exhaustive exploration of the conformational space of a 60 amino acid polypeptide chain described with an accurate all-atom interaction potential.

Our analysis suggests that natural folds are characterized by a smaller value of the contact orders (average distance between amino acids in contact) with respect to the complete structural space. This suggests the presence of an evolutionary bias, possibly related to kinetic accessibility, towards structures with shorter loops between contacting residues. Moreover this result implies the existence of new folds that have not (or not yet) used by Nature. Beside their conceptual relevance, these new structures open a range of practical applications such as the development of accurate structure prediction strategies, the optimization of force fields, and the identification and design of novel folds. In the last part of the talk I will briefly illustrate recent advanced in derivation of statistical potentials that can be used to design these completely new structures.
