Dipartimento di Scienze della Vita e dell'Ambiente

Seminari A.A. 2016/2017

10 Novembre 2016, ore 12:00, Aula Azzurra

"*De novo* protein folding and design"

Dr. Ivan Coluzza

Department of Physics

University of Vienna

Protein folding and design are major biophysical problems, the solution of which would lead to important applications especially in medicine. Here we provide evidence of how a novel parametrization of the Caterpillar model may be used for both quantitative protein design and folding. With computer simulations it is shown that, for a large set of real protein structures, the model produces designed sequences with similar physical properties to the corresponding natural occurring sequences. The designed sequences require further experimental testing. For an independent set of proteins, previously used as benchmark, the correct folded structure of both the designed and the natural sequences is also demonstrated. The equilibrium folding properties are characterized by free energy calculations. The resulting free energy profiles not only are consistent among natural and designed proteins, but also show a remarkable precision when the folded structures are compared to the experimentally determined ones. Ultimately, the updated Caterpillar model is unique in the combination of its fundamental three features: its simplicity, its ability to produce natural foldable designed sequences, and its structure prediction precision. It is also remarkable that low frustration sequences can be obtained with such a simple and universal design procedure, and that the folding of natural proteins shows funnelled free energy landscapes without the need of any potentials based on the native structure.

Può essere utilizzato per il riconoscimento di crediti da parte degli studenti della laurea magistrale e di dottorato.