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Exploring and scoring Proteomes: A computational approach

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It is currently believed that the atlas of *existing* protein structures is faithfully represented in the Protein Data Bank. However, whether this atlas covers the full universe of all possible protein structures is a debated issue. If all protein structures that are compatible with basic physico-chemical principles have not been already explored by evolution, novel 'artificial' protein structures could be created and used as building stones for novel proteomes. By using a sophisticated numerical approach, we generated 'in silico' a database of around 30,000 protein-like compact folds of a 60 residue polypeptide chain. This ensemble plausibly represents the universe of possible protein folds of similar length and indeed, all the known folds are represented in the set with good accuracy. However, they form a rather small subset, biased towards structures with shorter loops between contacting residues (lower contact order). This raises the question of why this bias exists in natural folds and of whether novel artificial protein structures can be designed. In assessing the role of protein structures within the proteome it is important to evaluate their ability to interact with other proteins and to avoid possibly aberrant pathogenic interactions. I will discuss how simple scoring functions can be developed, based on a statistical analysis of existing protein structures, that allow to predict 'in silico' i) the propensity of a protein sequence to aggregate into cross-β amyloid structures, ii) the quality of a model protein or protein complex, iii) the binding affinity of a protein complex formation.

Biography

Antonio Trovato received in 2000 his Ph.D. in Condensed Matter Physics from SISSA (International School for Advanced Studies) in Trieste, working in the statistical mechanics of bio-polymers with Prof. Amos Maritan. He has held post-doctoral positions at the Niels Bohr Institute in Copenhagen and later at the National Insitute of Matter Physics (INFM) and at the University of Padova, developing coarse-grained modeling techniques for protein and DNA molecules. In 2008 he obtained a permanent staff position in the Physics Department of the University of Padua. Dr. Trovato is teaching quantum physics in the Material Science course.

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