

Thursday June 11, 15:10-15:50:

SPEAKER: Edoardo SARTI (SISSA, Trieste)

TITLE: "Statistical scoring functions for protein folding and docking pose recognition"

ABSTRACT:

Although it is widely accepted that the tridimensional structure - and thus, function - of a protein depends only on its amino acid sequence, the issue of finding a correspondence between a particular sequence and its stable conformation is still far from being solved.

A key role in investigating this problem is played by statistical potentials. In particular, scoring functions constitute a wide class of algorithms whose aim is to assess the quality of some collection of objects. In this context, they are employed to evaluate the stability of a number of different putative conformations (poses) of a protein whose stable (native) state is unknown. First, the theoretical foundations of the subject will be delineated, then an example will be given by introducing BACH, a knowledge-based, statistical scoring function to assess the quality of both folding and docking poses.