New approaches to the prediction of protein structure and interactions
The combined exploration of the sequence and structure spaces with large scale simulations leads to a new generation of highly accurate prediction methods useful in applications such as the design of new drugs.

Summary

The study and characterization of structural and dynamical features of protein-protein interactions is of paramount importance. Understanding these interactions will expand our knowledge on the mechanisms by which mutations contribute to diseases, including cancer.

Objectives

- Detection of species-specific coevolution
- Prediction of functional consequences of mutations