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 how these interactions change with mutations and how these mutations affect protein variants 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

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