STRUCTURAL BIOINFORMATICS OF MEMBRANE PROTEINS

Summary

Our genome is composed of 20–30 % of membrane proteins but number of structures of these proteins known and deposited in public databases is still small. However, new achievements in experimental techniques, especially microfocusing of X-ray beam enabling diffracting of microcrystals, as well as mutagenesis leading to obtaining of thermostable mutants are real hope for quick emerging of new structures. Theoretical methods for determination of structure of membrane proteins are still in infant phases. Usage of homology modeling is limited by small number of membrane proteins which are necessary to serve as templates whereas ab-initio methods are confined to predicting of small membrane proteins or parts of larger ones only. The area which the bioinformatics is foremost in is prediction of dynamical behavior of proteins in lipid bilayer which is still mostly inaccessible to experimental methods. Full-atom as well as coarse-grain molecular dynamics methods are used to describe investigated systems in different time scales and with different accuracy.