Tentative Outline

Special Issue for Current Medicinal Chemistry

Guest Editor: Zunnan Huang
Co-Guest Editor: Ruo-Xu Gu

Development and Application of Computational Methods in Biology and Medicine

Aims & Scope:

During the past decades, computational biology has become a well-established research area and it finds many applications in a substantial number of scientific fields, ranging from genetics to nano and biomaterials. The boosting of computational biology is attribute to the accumulation of massive biological data, as well as the development of high performance computing.

Several major computational methods, such as density functional theory, molecular dynamics (MD) simulation, Monte Carlo (MC) simulation, virtual screening and some bioinformatics approaches, play a pivotal role in the field of computational biology. The developments and widely applications of these methods not only improve our standing of the mechanisms of biological processes, but also facilitate the diagnosis and therapy of diseases. For instance, high throughput virtual screening is a rational drug design method that benefits the discoveries and developments of drug candidates targeting specific proteins.

We invite authors to contribute review articles that will create a multidisciplinary forum of discussion on recent advances in these computational methods and their applications to study the structure, dynamics, and functions of biomolecules that involved in targeted drug design, diagnosis and therapy of diseases, as well as the understanding of the mechanisms of critical biological processes.

Keywords: Virtual screening, hybrid QM/MM techniques, molecular dynamics, allosteric ligand binding, arylamine N-acetyltransferase, receptor tyrosine kinases type III inhibitors.

Sub topics:

1. Recent developments and applications of high throughput virtual screening methods in rational drug design.
2. Applications of MD or MC simulations in the characterization of the structure and function relationship of biomolecules and the ligand-protein interactions.
3. Recent developments and applications of the molecular simulations and density functional theory methods in the design of nano and biomaterials.
4. Recent progresses of the hybrid QM/MM techniques in the study of the enzymatic catalysis.
5. Recent advances of bioinformatics approaches in the diagnosis and therapy of diseases.
6. Recent progresses of method developments in computational biology.

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