Special Issue

Applications of Computational Modeling in Disease, Infection and Drug Design

Message from the Guest Editor

Simulation techniques using computational biology, including molecular modeling, molecular dynamics, ligand docking or drug screening, allow rationalization at the molecular level of the causes of different diseases. Using these virtual modeling techniques, it is possible to understand why a variant in an amino acid causes the failure of an enzyme or a group of macromolecules in the case of diseases of genetic origin. Likewise, the interactions between viral proteins and different target proteins in the host cell can be modeled, as well as the design of new antiviral compounds. It is also possible to simulate the functioning of bacterial proteins responsible for their pathogenicity in detail. In this Special Issue, we welcome papers using virtual modeling techniques in computational biology, alone or in combination with in vitro or in vivo strategies, for the characterization and therapy of diseases, whether of genetic origin, or viral or bacterial infections, including the design of new drugs and therapies.

Guest Editor

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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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