Special Issue

Advances in Elucidating Disease Mechanisms and Designing Therapeutics Using Computer-Aided Simulations and Modeling

Message from the Guest Editor

Drug design for discovering new therapies for a large range of illnesses has been one of the most prominent and quickly developing areas of chemistry. Recent advances in computer-aided modeling can help circumvent these costs by predicting which drugs will be effective and avoiding those that will be ineffective in experiments. In addition, the elucidation of the disease mechanism through the protein structure and dynamics can also aid in designing new therapeutics. The development of machine learning algorithms can predict and design new drugs for specific types of illnesses, thus making computer-aided drug design even more efficient. The main aim of this Special Issue is to develop collaboration between computer-aided drug design methods and experimental studies to design news therapeutics more efficiently. Topics of this Special Issue may include, but are not limited to: Fragment-based drug design, G-protein signaling, enzyme kinetics, G-protein receptors, cellular signaling, biostructures, ligand docking, machine learning for drug design, and lead optimization.

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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