# Special Issue

## Structure-Based Design of Drugs and Biologically Active Molecules Based on Computer-Aided Drug Discovery

**Message from the Guest Editor**

Computer-Aided Drug Discovery (CADD) has advanced significantly, particularly with Structure-Based Drug Design (SBDD). SBDD uses three-dimensional models of biological targets, obtained by techniques such as X-ray crystallography and nuclear magnetic resonance (NMR), to guide the creation and optimization of bioactive molecules. SBDD allows the precise identification of ligands with high affinity and specificity, essential for therapeutic efficacy.

Computational tools, such as molecular docking and molecular dynamics, are employed to predict the conformation of ligands and their binding energies to the biological target. Molecular docking remains a vital tool in SBDD, allowing the prediction of the preferred orientation of a molecule in a protein target.

CADD and SBDD not only significantly reduce the time and cost associated with developing new drugs but also increase the accuracy in identifying promising compounds. The integration of computational and experimental methods is crucial for successful drug discovery, facilitating the identification and optimization of new drug candidates.

**Guest Editor**

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