Special Issue

Recent Advances in Computer Aided Drug Design

Message from the Guest Editors

Computer-aided drug design (CADD) is an effective strategy for accelerating and economizing the drug discovery and development process. Because of the dramatic increase in the availability of information on biological macromolecules and small molecules, the applicability of computational drug discovery has been extended and broadly applied to nearly every stage in this process workflow. The present scenario could greatly benefit from accepted methods such as molecular docking, pharmacophore modeling and mapping, de novo design, molecular similarity calculation, and sequence-based virtual screening, which have been greatly improved with AI technology and applications.

This Special Issue aims to collect new approaches developed to overcome the main issues faced by medicinal chemists in drug discovery and the biological evaluation of these promising drug targets. A further aim is to address challenging biological validations by testing in cell-culture and animal models. This drug target identification is an intermediate step prior to successful clinical trials, making it truly essential for modern researchers in the fields of drug discovery and structural bioinformatics.

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