Special Issue

Emerging Computational Approaches in Drug Discovery and Design

Message from the Guest Editor

Computational approaches have been utilized in drug discovery and design for many decades. Given the vast amount of data generated in recent years and advancements in computational power, the field of computer-aided drug design (CADD) has evolved through efforts to integrate well-established methods with innovative techniques. In contrast, adhering to best practices in CADD remains vital, and thoroughly validating any approach is essential. In this Special Issue, we emphasize the development and application of computational approaches for drug discovery. Approaches and methods include structure- and ligand-based drug design, virtual screening, the quantitative structure–activity/property relationship (QSAR/QSPR), and machine learning. Reviews and research articles on novel method development or the use of established CADD methods are encouraged. We suggest that research manuscripts include a proper explanation of data curation before modeling. Furthermore, the reproducibility of results is highly valued (for example, exchanging codes and data, if applicable). Articles integrating computational approaches with experimental validation are also encouraged.

Guest Editor

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Message from the Editor-in-Chief

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We hope to handle your contribution to *Pharmaceuticals* soon.

Editor-in-Chief

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