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Molecular Advances in Computational Chemistry for Drug Design

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Message from the Guest Editor

Dear Colleagues,

The impressive recent progress made advancing the richness of scientific data and enhancing commonly available computational power is supporting the development of innovative computational approaches for drug design. Overall, the field has benefited from the power of the artificial intelligence (AI) algorithms implemented in countless applications, including ligand- and structure-based methods. Innovative AI-based methods have been reported for rational de novo design of promising compounds, property prediction, ADME/Tox profiling, docking simulations, and MM/MD calculations and analysis. In parallel, enhanced computational power has allowed the development of targeted MD/MM approaches capable of extensively simulating the molecular recognition processes, thus gaining information concerning the complex stability and free energy from the corresponding interaction.

Overall, this Special Issue aims to publish manuscripts dealing with novel computational approaches in drug design by considering both methodological and applicative studies, with a view to offering a picture of the fields in which computational chemistry can impact the drug discovery process.

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Message from the Editor-in-Chief

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