Special Issue

Small Molecule Drug Discovery: Driven by In-Silico Techniques

Message from the Guest Editor

Small molecules are one type of drugs that are commonly used in medicine. They are typically synthesized chemically and are generally less complex than biologics. Generally, small molecules are designed to interact with specific targets involved in disease processes, such as enzymes or receptors.Moreover, the field of small-molecule drug design is a constantly developing area that benefits from advances in computational tools and methodologies. With the help of these tools, scientists can better design and optimize small-molecule drug candidates. In particular, ligand-based methods are critical tools for virtual screening, with pharmacophore modeling, 3D-QSARs, CoMSIA, and CoMFA being the most significant. Structure-based drug design is a highly specific, efficient, and rapid process that focuses on the 3D structure of a target protein and the disease knowledge at the molecular level. This Special Issue aims to present the latest advances in the discovery, design, synthesis, and pharmacological evaluation of small molecules driven by computational approaches.

Guest Editor

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

Editor-in-Chief

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