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In Silico Drug Design for GPCRs: Big Data for Small Molecule Discovery

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Message from the Collection Editor

The current drug discovery process increasingly relies on data-driven computational approaches. Among many aspects of computational revolution, one can name (1) the explosion of high-resolution structural information and molecular modeling capabilities for the target receptors, (2) improvement of virtual screening and rational design algorithms, (3) rapid growth of virtual combinatorial libraries, supported by fast parallel synthesis of compounds, (4) application of machine learning approaches to the analysis of chemogenomics information and predictions of multitarget ligand activity profiles, and (5) advanced computational approaches for predicting affinities and potencies of derivatives. The exponentially growing data sources and improved tools, supported by access to highly parallel GPU and cloud computing, are poised to revolutionize the field both in academia and industry, making data-driven computational analysis and design the backbone of drug discovery.

This Special Issue of *Biomolecules* will showcase recent examples of computationally intensive data-driven approaches that contribute to the different aspects of small molecule drug discovery for GPCR targets.

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