Special Issue

Recent Advances in Computational Drug Discovery: From In Silico Screening to Multiscale De Novo Drug Design

Message from the Guest Editor

Diseases continue to plague modern societies, and over time, through the process known as drug discovery, a plethora of therapeutic options has been introduced to cure illnesses. Unfortunately, the scientific community still faces several challenges in drug development. On one hand, it is well-established that the chemical space to be covered in the search for new drugs is vast, being formed by approximately 1060 small molecules. On the other hand, diseases are difficult to treat because of their multifactorial nature, such as drug resistance. Consequently, designing a new drug is increasingly expensive, complex, and time-consuming.

To accelerate and improve drug discovery, in silico approaches have become an integral part of all the drug discovery projects, helping to rationalize the design of potent and versatile therapeutic agents.

We are inviting the scientific community to submit original research contributions, short communications, or review articles that highlight the most recent advances in the applications of in silico approaches to all the areas involved in drug discovery.

Guest Editor

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Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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