



Applications of Computational Chemistry Methods in Viral Diseases Research

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Message from the Guest Editors

Computational chemistry has achieved maturity and, nowadays, is one of the central scientific fields in the pharmaceutical industry. It is crucial for planning the early stages of drug design projects, such as designing more efficient and economic synthetic routes for chemical administration, the screening of huge databases, as well as proposing hypotheses for the probable mechanisms of action of drugs in biological systems. Such endeavors are extremely complex and require the usage of modern and sophisticated approaches, such as artificial intelligence, data science, computational molecular simulations through classical mechanics and quantum mechanics, cheminformatics, applied mathematics, and biostatistics. This Special Issue of *Molecules* is dedicated to the application of these methods in medicinal computational chemistry, and we invite our fellow scientists to submit original papers or reviews that will enrich the state of the art in this field.





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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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