Special Issue

Molecular Modeling: Insights into the Enzymatic Reactions and Photochemical Processes in Biomacromolecules

Message from the Guest Editor

The molecular modeling of biochemistry-related processes is a rapidly developing field. Recent advancements in QM/MM methods and molecular dynamic simulations, as well as the development of computers and software, make it possible to obtain qualitative and quantitative models. The mechanisms of many enzymatic reactions and photochemical processes are already established. Nevertheless, there is a huge number of questions that remain unanswered. Moreover, the accumulation of novel experimental data requires its explanation from the mechanistic viewpoint. Modern molecular modeling aims to explain experimental observations and to predict novel compounds or biomacromolecular systems with the desired properties. The aim of this Special Issue is to highlight recent advancements in molecular modeling related to biomolecular processes. Contributions that cover all of these topics, as well as combined theoretical and experimental studies, are highly encouraged.

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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