

## Special Issue

# Computational Investigation on Molecular Design, Structure, and Solvation

### Message from the Guest Editor

Theoretical and computational chemistry as a research field has grown to complement experiments and assumed the mantle of guiding force in predictions and explorations in the fields of chemistry, biology, drug design, and all the interdisciplinary areas encompassed by these three. A rapid development and accessibility of computational hardware, robust code developments, and parallel deployments of codes in these new hardware have helped theoretical and computational chemistry to grow in leaps and bounds. This Special Issue titled “Computational Investigation on Molecular Design, Structure, Reactivity, and Solvation” aims to bring the latest developments in the research areas covering molecular structure and/or activity prediction, chemical reactivity problems, chemical processes in liquid media, machine learning, and artificial intelligence in (bio)chemical (re)activity predictions.

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### Guest Editor

Dr. Dipankar Roy

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### Deadline for manuscript submissions

closed (31 July 2023)



## Molecules

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## About the Journal

### Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 30th 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 all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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### Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

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