

Special Issue

Cheminformatics, Past, Present, and Future: From Chemistry to Nanotechnology and Complex Systems

Message from the Guest Editors

Cheminformatics techniques form have been interesting tools in the effort to explore large chemical spaces, reducing at the same time animal testing as well as costs in terms of materials and human resources on drug discovery processes in medicinal chemistry. In addition, with the emergence of nanotechnologies, cheminformatics needs to deal with drug–nanoparticle systems used as drug delivery systems, drug co-therapy systems, etc. This brings to mind the application of cheminformatics in areas beyond drug discovery such as the fuel industry, polymer sciences, materials science, and biomedical engineering. In this context, we propose to open this new issue to discuss with all colleagues worldwide all the past, present, and future challenges of cheminformatics. The present Special Issue is also associated with MOL2NET-05, the International Conference on Multidisciplinary Sciences, ISSN: 2624-5078, MDPI SciForum, Basel, Switzerland, 2019. The link of the conference: <https://mol2net-05.sciforum.net/>. We especially encourage submissions of papers from colleagues worldwide to the conference (short communications) and complete versions (full papers) to the present Special Issue.

Guest Editors

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Deadline for manuscript submissions

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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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