

Special Issue

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

Message from the Guest Editors

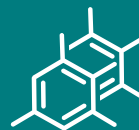
Cheminformatics techniques form have been interesting tools in the effort to explore large chemical spaces, reducing at the same time animal testing as well as costs in terms of materials and human resources on drug discovery processes in medicinal chemistry. In addition, with the emergence of nanotechnologies, 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

Prof. Dr. Humbert González-Díaz
Dr. Aliuska Duardo-Sanchez
Prof. Dr. Alejandro Pazos Sierra

Deadline for manuscript submissions

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Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th 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.

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

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