



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

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Deadline for manuscript
submissions:
closed (15 November 2020)

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.





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Message from the Editor-in-Chief

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