

Special Issue

Advancing Cheminformatics—A Theme Issue in Honor of Professor Jürgen Bajorath

Message from the Guest Editor

In the last 15–20 years, Prof. Dr. Jürgen Bajorath has been one of the leading figures in cheminformatics and in chemical information sciences. We would like to dedicate a Special Issue in honor of Prof. Jürgen Bajorath with a collection of reviews and original articles from his research areas.

- molecular similarity analysis and computer-based hit and lead identification;
- analysis, characterization, and visualization of systematical structure–activity relationships;
- analysis of lead optimization efforts;
- analysis of big data in medicinal chemistry.

You are welcome to visit the [webiste](#) and submit your paper [here](#). If you have any questions, please feel free to contact the managing editor Larry Li (larry.li@mdpi.com). We look forward to hearing from you.

Guest Editor

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Deadline for manuscript submissions

closed (30 September 2021)



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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 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.

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