

Special Issue

Cheminformatics in Drug Design: Achievements and Challenges

Message from the Guest Editors

Cheminformatics is a general word implying the massive use of informatics and software engineering in the chemistry field. In particular, in this topic, the focus is on medicinal chemistry and all the methods and their assessment in developing bioactive molecules.

Experimental data should always be used to assess the cheminformatic application, whereas methodology manuscripts will be considered also in absence of experimental data, but deep comparison with state-of-the-art methods should be included.

Guest Editors

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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.

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