Special Issue

Artificial Intelligence for Drug Design and Discovery

Message from the Guest Editor

Given the growing implication of Artificial Intelligence methods in drug design (note the sharp increase in the number of publications devoted to this technique in PubMed), it seems necessary to review the status, opportunities, developments, challenges, and prospects in these methods and in their role to establish more efficient research strategies. Thus, the goal of this Special Issue would be to allow the drug designers involved in competitive research to measure the real interest in new algorithms for discovering innovative and more effective drugs. It is also important to point out the present limitations of the new methods in order to allow the readers to have an honest idea about the real contribution of AI for them.

Guest Editor

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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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