Special Issue

In Silico Approaches in Drug Design

Message from the Guest Editor

In the last few decades, computational methods have been successfully applied by the pharmaceutical community. This is mainly due to the development of both new theoretical approaches and new hardware and software technologies. In this context, in silico approaches such as molecular simulations, QM/MM simulations, chemoinformatics, artificial intelligence, etc., became fundamental in the drug design process. To celebrate the success story and advances in the important synergistic combination of drug design and in silico investigation, the journal Pharmaceuticals invites fellow scientists to submit original papers or reviews, which will be published in a Special Issue on "In silico Approaches in Drug Design". Such an issue will contemplate the following topics: computer-aided drug design, molecular dynamics simulations, Monte Carlo simulations, QM/MM simulations, molecular docking, chemoinformatics, in silico databases, data mining, machine learning, pharmacophore-based virtual screening, combinatorial chemistry, QSAR, and in silico ADMET. Looking forward to your contribution.

Guest Editor

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Message from the Editor-in-Chief

Because of your expertise in the field of drug sciences, I kindly invite you to consider publishing your current work, in the form of a research article or a review, in the open access electronic journal *Pharmaceuticals*. *Pharmaceuticals* is characterized by an active editorial board and a dynamic editorial staff. Manuscripts are peer-reviewed and a final decision is provided to authors within 4–6 weeks after submission. Papers are published on the web immediately after acceptance. For details on the submission process or any other matter, please do not hesitate to contact us.
We hope to handle your contribution to *Pharmaceuticals* soon.

Editor-in-Chief

Prof. Dr. Amélia Pilar Rauter
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