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In Silico Approaches in Drug Design

Guest Editor:

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Deadline for manuscript submissions:
closed (30 April 2022)

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.

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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*.

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We hope to handle your contribution to *Pharmaceuticals* soon.

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