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Advanced In Silico Methods and Digital Platforms for Rational Drug Design and Predictive Toxicology

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Message from the Guest Editors

Dear Colleagues,

In recent years, the unprecedented advancements in computer-assisted drug discovery and predictive toxicology have allowed powerful and reliable models to be built from large amounts of data. In this respect, pharmaceutical companies and academia have made remarkable investments to generate customizable tools, services, and technologies that are capable of reaching impressive standards.

For this Special Issue, we call on medicinal chemists and toxicologists to share their experiences on the design of novel methods and the implementation of digital platforms, in order to provide practical answers to challenging issues related, but not limited to, drug repurposing, target fishing, bioactivity prediction, de novo design, molecular docking, molecular dynamics, homology modeling, virtual screening, QSAR, and alternative methods for the prediction of toxicological endpoints.

In light of this, we are delighted to invite international scientists to contribute to this Special Issue with research articles, mini-perspectives, and brief articles describing recent methods and platforms for drug discovery and predictive toxicology.

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Message from the Editor-in-Chief

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