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Computer-Aided Drug Design Strategies

Guest Editor:

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Message from the Guest Editor

Dear Colleagues,

Computer-aided drug design is nowadays a widespread research field that is continuously taking ground, raising more and more interest in the scientific community. This is undoubtedly due to the increasing use of machine learning (ML) and other artificial intelligence (AI) approaches in drug design and discovery. AI models demonstrated their reliability in a plethora of applications, including the prediction of physical-chemical properties and biological activities of small molecules, in silico evaluation of ADME and toxicological profiles of chemicals, as well as protein structures and ligand–protein complex prediction. Nevertheless, thanks to the constant improvement of computation power and efficiency, classic ligand-based and receptor-based in silico strategies still provide invaluable help in drug discovery, design and optimization. Long molecular dynamics (MD) simulations, allowing us to evaluate complex protein motions are now becoming more affordable, and MD studies for evaluating stability and potential binding affinity of predicted ligand–protein complexes are now commonly performed in hit finding, hit-to-lead and lead optimization campaigns.

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Message from the Editor-in-Chief

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