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In Silico Drug Testing and Optimization, Coupling Physical-Based Modeling and Machine Learning

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Message from the Guest Editors

Dear Colleagues,

In silico numerical simulations may provide additional information regarding the mechanisms guiding drug testing and optimization. The aim of this Special Issue is to use physical-based modeling methods such as continuum computational fluid dynamics (CFD), computational solid dynamics (CSD), discrete molecular dynamics (MD), dissipative particle dynamics (DPD), discrete phase modelling (DPM) and physiologically based pharmacokinetic (PBPK) coupled with machine learning to better describe drug transfer and distribution inside organs. The design of new prospective drugs, as well as carriers for their successful delivery, will be welcomed. It focuses on cardiovascular and lung biomechanics but is not limited to other organs. A comprehensive list of patient-specific features such as genetic, biological, pharmacologic and cellular aspects can be taken into account. The aim is to avoid adverse effects, drug interactions, prevent sudden patient death and shorten the time between drug treatment commencement and the achievement of desired results. In silico methods could open a new avenue for medical device and drug testing, reducing the use of real clinical trials.

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Message from the Editor-in-Chief

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