

Special Issue

Computer Simulation for Drug Design and Medical Bioengineering

Message from the Guest Editors

The discovery of natural and synthetic chemical compounds as candidates for pharmaceutical drugs is essential scientifically, socially, and economically in medical and bioengineering fields. Improvements in bioinformatics and computational biology have increased the efficiency of many stages of the drug discovery pipeline. Computer-aided tools which are used in drug discovery are critical for many human pathologies. Special attention has been paid to drug design for cancers and brain pathologies and, in the last two years, for SARS-CoV2 infection. Bioinformatics methods such as molecular dynamics, molecular docking, fragment-based screening (FBS), and QSAR, are strategically used when new chemicals being considered for potential drugs. Pharmacological features, represented by pharmacokinetic (ADME), pharmacodynamic (targets discovery), and toxicity profiles are critical for assessing proposed chemical structures for new candidate drugs. Additionally, bioengineering tools being employed to develop in silico tools. We welcome your submission for our Special Issue in *Pharmaceutics*, "Computer Simulation for Drug Design and Medical Bioengineering".

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