Editorial Preface

Thematic Issue on In Silico Modeling for Exploring COVID-19 Therapeutics

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At the end of 2019, a cluster of pneumonia cases occurred in Wuhan, China, which then quickly spread to other parts of the world causing a pandemic situation popularly termed as Coronavirus (CoV) Disease-2019 (COVID2019). Currently there are no curative drugs with proven efficacy against COVID-19. The devastating impact of the current COVID-19 outbreak and possibility of future CoV epidemics strongly warrant for the rapid development of new treatments and fast intervention protocols. Despite CoVs have undergone substantial genetic evolution, they still have considerable similarities, which should be a basis for the identification of promising targets for antiviral therapies against 2019-nCoV. Computational modeling and drug repurposing procedures can easily be implemented to identify suitable drugs for different identified targets (De et al., 2020; Kumar and Roy, 2020; Ojha et al., 2021; Ton et al., 2020). This approach typically relies on an integrated pipeline including a virtual screening of drug libraries to find suitable drug-target pairs using molecular similarity methods and molecular docking and binding free energy calculations used to predict drug-target interactions and binding affinity. Different tools and protocols of structure-based (molecular docking, molecular dynamics, protein-protein interaction network, etc.) and ligand based (pharmacophore mapping, quantitative structure-activity relationships or QSARs) drug design can be used for ranking and prioritization of candidate molecules in search of effective treatment strategy against coronaviruses. This thematic issue presents five articles on *in silico* modeling approaches in search of COVID-19 therapeutics.

The first article authored by Preeti Suman Saxena and colleagues provides the basics of pathophysiology, possible targets, and current treatment strategy for corona viruses along with some examples of *in silico* modeling analysis in finding anti-COVID drug candidates. The second article authored by Shahanas Naisam et al. presents virtual screening of quinoline analogues, design new ligand molecules, perform molecular interaction analysis, their molecular dynamics validation against multi targets (Spike-ACE2, TMPRSS2, and Spike Protein) of SARS-CoV-2, and suggests the most promising and effective drug molecules. The third article of Hima Vyshnavi A. M and colleagues focuses on homology modeling and evaluation of SARS-CoV-2 spike protein mutant - D614G. In the next article authored by Debanjan Sen et al., structure-based virtual screening of different compounds of *Justicia adhatoda* was performed against SARS-CoV-2 Mpro, followed by ADME filtration, molecular dynamics, and MMGBSA based binding free energy calculation. The last article of this issue authored by Anjoomaara H. Patel and colleagues has reported docking, binding free energy estimation and MD simulation of newly designed chloroquine and hydroxychloroquine analogues against the Spike- ACE2 complex of SARS-CoV-2.

I hope that the above collection of five articles will be a timely and interesting collection for the readers of IJQSPR.

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