Tentative Outline

Special Thematic Issue for Medicinal Chemistry

Insights on SARS-COVID-19 and its linkage with cancer using rational drug design: Bioactive compounds using computational approaches

Guest Editors: Potla Durthi Chandrasai and Prof. Mohammad Amjad Kamal

Aims & Scope:
Recently, many studies have focused on SARS-COVID-19 based models to describe biological systems and on Bioactive compounds to treat Cancer. Biological molecules, including DNA, miRNAs, proteins, and other small molecules, are complicated at the cellular system level, which is the basis of all biological processes. Bioinformatics and computer-aided drug design can help in finding possible drug-like candidates and can achieve a new stage of drug discovery. Many studies have tried to combine the computer-aided drug design with the model of the biological system to explore the mechanism of life.

Subtopics:
The subtopics to be covered within this issue are listed below:
- In silico screening of drug candidates as a potential candidate against SARS/COVID-19.
- Computational approaches against Cancer using bioactive compounds.
- Rational drug designing towards SARS COVID19 and cancer.
- High throughput virtual screening for the understanding of binding affinities towards the existing anti-retroviral drug candidates.
- Drug-Target associations/interactions and Drug repurposing/combination prediction with the computational approach
- Network-based pharmaceutical studies and Network-based disease markers.
- Critical reviews on bioactive compounds for the management of COVID-19.
- Computational approaches for enhanced production of bioactive compounds towards Cancer using Artificial Neural Networks.
- Computational approaches for enhanced production of bioactive compounds towards Cancer using Genetic Algorithm.
- Computational approaches for enhanced production of bioactive compounds towards Cancer using Genetic Programming.

Schedule:
- Manuscript submission deadline: 15th November, 2020
- Peer Review Due: 15th December, 2020
- Revision Due: 30th March, 2021
- Announcement of acceptance by the Guest Editors: 10th May, 2021

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