International Journal of Medicinal Chemistry

Hindawi

Special Issue on
Computational Design of Therapeutics

CALL FOR PAPERS

Computational tools and resources are increasingly becoming part of the drug discovery process in medicine. Some of the recent drug discovery processes have included the usage of machine learning techniques in classifying putative small molecule drugs, employing structure-based optimization techniques to improve drug affinity, and web based mining tools to filter putative drug molecules. As the field progresses and computers become more and more powerful, newer methods are required in understanding the underlying drug discovery processes.

This special issue of International Journal of Medicinal Chemistry focuses on "computational design of therapeutics." The computational aspect will focus on the development of novel approaches/methods or application of techniques, such as machine learning, algorithm design, data mining, databases, optimization, and visualization methods that have a potential in aiding drug discovery techniques, whereas the therapeutics aspect will focus on the structure/ligand -based drug designing processes.

Potential topics include but are not limited to the following:

- Computational methods and algorithms for developing small molecule drugs
- Computational models for predicting biological activity
- Development of databases and visualization tools to enhance drug discovery

Authors can submit their manuscripts through the Manuscript Tracking System at https://mts.hindawi.com/submit/journals/ijmc/cdt/.

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