International Journal of Medicinal Chemistry

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Special Issue on

In Silico Approaches Enabling Discovery towards Emerging Drug Targets

CALL FOR PAPERS

In silico molecular modeling methodologies are nowadays considered as an indispensable part of most drug discovery campaigns. Indeed, theoretical simulations and cheminformatics tools are extensively utilized in the early stages of the discovery workflow, either for facilitating the identification of hit compounds with promising drug-likeness and high originality or for rationalizing medicinal chemistry efforts towards hit-to-lead and drug optimization processes. Such computational tools continuously gain accuracy and efficiency, while their collective successful application is apparent in the fact that they currently constitute a *sine qua non* stage fully integrated in the pipelines of most academic laboratories involved in drug or chemical probe discovery as well as in the pharmaceutical industries.

At the same time, the successful application of structural genomics projects and the advances in molecular biology have unveiled a continuously increasing number of protein structures that constitute potential drug targets of high importance. To efficaciously validate those targets and to enable dissection of their possible roles in a medical or therapeutic perspective, small-molecule cell-active and highly selective modulators of their biological activity are needed. In this aspect, incorporation of the various molecular modeling tools and algorithms in such bioactive compound discovery projects can highly advance efficient exploration of the available chemodiversity so that the whole procedure may rationally be guided towards the most favored and suitable chemical space, thus maximizing the success rate for developing high quality chemical probes or drug candidates.

We invite authors to contribute original research articles of high quality as well as review articles that will highlight the impact of *in silico* methodologies in medicinal chemistry endeavors towards well-established and emerging drug targets. Emphasis will be given to the application of novel techniques and algorithms such as those involving modelling of solvation effects in binding, free energy simulations, consensus scoring methods, or molecular similarity approaches, while special focus will be on the computational exploration of bioactivity of natural products.

Potential topics include but are not limited to the following:

- *In silico* assisted bioactive compound discovery towards emerging targets such as protein kinases, transmembrane receptors, metabolic enzymes, and epigenetic modules
- Virtual screening of large compound collections and evaluation of method performance and combined and comparative application of theoretical and experimental screening techniques
- Implementation of structure-based and ligand-based algorithms for lead discovery
- High-accuracy simulation methodologies including FEP and sophisticated MD algorithms in lead optimization
- Mapping and characterization of solvation effects in rational drug design
- *In silico* fragment-based drug discovery approaches
- Pharmacophore modeling and exploration of the biological activity profile of natural products
- Characterization of bioactive compounds in terms of optimal physicochemical and PK/Tox properties

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

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