Tentative Outline
Special Thematic Issue for Current Pharmaceutical Design

"Recent Updates in the Computer Aided Drug Design Strategies for the Discovery of Agonists and Antagonists of Adenosine Receptors"

Aims & Scope:

Adenosine receptors (ARs) belong to the G protein coupled receptors (GPCRs) and are classified into four subtypes viz. A_1, A_{2A}, A_{2B} and A_3 ARs. These receptors show different tissue distribution and signalling pathways, and are considered as pivotal drug targets for developing potential therapeutic agents for modulating several physiological and pathological processes involving cardiovascular, respiratory, renal, immune and central nervous system. Thus, it is essential to gain proper insight into the active site topology of these receptors as well as the physicochemical properties of ligands required for effective binding and modulating the ARs. In this regard, the discovery of the 3D X-ray crystal structure of the A_1 and A_{2A} ARs has greatly augmented the researchers' comprehension about these receptors in the pursuit of rational design of new subtype-selective drugs with novel chemotypes targeting ARs. Moreover, the crystal structures of the A_1 and A_{2A} ARs have also greatly facilitated the construction of improved homology models of A_{2B} and A_3 ARs.

It has been postulated from the failure of plenty of potential lead molecules at different stages of the development process of clinical trials that the major emphasis should be given at the early stages of rational drug design and discovery process for identifying new drug-like molecules in order to save time as well as to enhance the success rate of novel drug development. In this regard, *in silico* computer aided drug design (CADD) strategies are continuously emerging as a potential tool for the discovery of new drugs. This special thematic issue will be focused on various aspects of recent advances/developments in CADD strategies to facilitate the discovery of novel adenosine receptors agonists and antagonists while overcoming the numerous challenges. Special emphasis will be given on the structure-based drug design (SBDD) strategies including homology modelling, molecular docking and dynamics studies of ARs. This issue will also be contextualized with ligand-based drug design (LBDD) approaches like 3D-QSAR and pharmacophore modelling that are currently being explored in search of novel and selective ligands for ARs.

For this thematic issue of *Current Pharmaceutical Design*, review papers are invited from the potential contributors in various aspects of the CADD strategies employed for the discovery of novel ligands targeting ARs in search of potential therapeutic agents.

Keywords: Adenosine Receptors, Agonists and Antagonists, structure-based drug design, homology modelling, molecular docking, molecular dynamics, ligand-based drug design, 3D-QSAR, pharmacophore modelling

Subtopics:

1. Recent advances in the *in silico* ligand-based (QSAR and pharmacophore modelling) and structure-based (homology modelling, molecular docking and molecular dynamics) approaches for the design and discovery of agonists and antagonists of A_1, A_{2A}, A_{2B} and A_3 adenosine receptors (ARs).
2. Molecular dynamics simulations of adenosine receptors: advances, applications and trends
3. 3D-QSAR and pharmacophore modelling of adenosine receptors: advances, applications and trends

Schedule:

- Manuscript submission deadline: **November 2018**
- Peer Review Due: **November 2018**
- Revision Due: **December 2018-January 2019**
- Announcement of acceptance by the Guest Editors: **February 2019**
- Final manuscripts due: **February 2019**

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