Special Issue for Combinatorial Chemistry & High Throughput Screening

Guest Editor: Bijo Mathew

Computational chemistry and synthetic strategy of the design of Novel Monoamine oxidase inhibitors

Aim & Scope:
Due to the limited number of MAO-A and MAO-B inhibitors available in the clinic, several research efforts are aimed at the discovery of new inhibitors with improved properties. In particular high specificity for MAO-A and MAO-B and a reversible mode of inhibition are often cited as desirable traits, which are expected to reduce the probability of causing target disruption, less sensitivity toward pharmacokinetic parameters, and increased duration of action. Most current monoamine oxidase inhibitors lead to side effects due to lack of affinity and selectivity toward one of the isoforms. So, there is an urgent need to design novel potent, reversible and selective inhibitors of MAO-A and MAO-B. Selective inhibition of MAO-A results in the elevated level of serotonin and noradrenaline and can be used for improving the symptoms of depression . While selective MAO-B inhibitors are used with L-DOPA and/or dopamine agonists in the symptomatic treatment of Parkinson's disease. Considering the pharmacological importance of MAO inhibitors, the design of new selective MAO inhibitors is pursued by several research groups on various chemical scaffolds. The scope of the present thematic issue revealing the importance of in silico approach and design of various classes of MAO inhibitors.

Keywords:
MAO-A, MAO-B, Depression, Parkinson's disease, Dopamine agonist, Computational chemistry.

Potential topics include but are not limited to:

- Synthesis of new class of MAO inhibitors
- Reviews of various class of potent MAO inhibitors
- Molecular docking, Molecular dynamics and QSAR aspects of MAO inhibitors
- Recent development drug design strategy of MAO inhibitors

Schedule:
Manuscript submission deadline: 30 Sep 2016
Peer review due: 30 Oct 2016
Revision due: 15 Nov 2016
Notification of acceptance by the Guest Editor: 30 Nov 2016
Final manuscripts due: 8 Dec 2016