Tentative Outline

In silico studies in the drug research against the neurodegenerative diseases

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Aims & Scope:

Neurodegenerative diseases include Alzheimer's disease (AD), amyotrophic lateral sclerosis (ALS), Parkinson's disease (PD), and Huntington's disease. These diseases involve different aspects of reward processing (primary rewards, secondary rewards, reward-based learning, and reward-based decision-making). About 70% of the population with 65 years or more are affected by these progressive neurodegenerative disorders of the central nervous system and characterized by gradual loss of cognitive function, progressive memory loss, disorientation, language impairment, abnormal behavior, personality changes, etc.  

Theoretical studies using in silico methods have aided in the process of drug discovery. Technological advances in the areas of structural characterization, computational science, and molecular biology have contributed to faster planning of new feasible molecules. Chemoinformatic studies show that a large fraction of compounds are “drug-like” or at least, “lead-like” having structural and physicochemical properties that render them as potential drugs or leads. This thematic issue will bring together theoretical studies of different methodologies, such as QSAR, docking, chemometric tools, artificial intelligence and other applied in order to optimize the search for new drugs for the cure and treatment of neurodegenerative diseases.

Key words: neurodegenerative diseases, in silico, drug discovery

Subtopics of interest include, but are NOT limited to:
- Chemometric tools applied to drug discovery against neurodegenerative diseases
- Molecular modeling tools, including docking, applied to drug discovery against neurodegenerative diseases
- QSAR, CoMFA, CoMSIA applied to drug discovery against neurodegenerative diseases

Schedule:

Manuscript submission deadline: 15 January, 2017
Peer Review Due: 10 March, 2017
Revision Due: 5 April, 2017
Notification of acceptance by the Guest Editor: 10 April, 2017
Final manuscripts due: 15 APRIL, 2017