Tentative Outline
Special Issue for CURRENT DRUG DRUG TARGETS
Guest Editor(s): Horacio Pérez-Sánchez, Alfonso Pérez-Garrido, Sandra Gesing, Ivan Merelli and Tingjun Hou

HIGH PERFORMANCE COMPUTING IN DRUG DISCOVERY

Aims & Scope:
Drug discovery is a time-consuming, risky and expensive process, which takes generally about 15 years for successful drugs to be available on the market. Nowadays, computer-aided drug design is invaluable for investigating chemical reactions and structures and filtering the most promising substances for further experiments. The main objective of this special issue is to explore the use of emerging parallel computing architectures as well as high-performance computing systems (supercomputers, clusters, clouds, grids, GPUs, Intel Xeon Phi, multicore) in computational drug discovery. We welcome reviews and perspectives on this topic, not submitted elsewhere for review. Experts, who apply high-performance computing to drug discovery in structure-based drug design, ligand-based drug design and sequence-based approaches will be invited to contribute.

Key words: High-Performance Computing, Supercomputing, Drug Discovery, Virtual Screening, High-Throughput, QSAR

Subtopics:
- GPUs, Intel Xeon Phi, Grid Computing, Cloud Computing, Parallel/Distributed Computing in Drug Discovery
- High-Throughput Molecular Dynamics and/or Docking
- Massive Quantum Mechanical Calculations
- Quantitative Structure-Activity Relationship (QSAR)
- Pharmacophore Modeling
- Virtual Screening
- High-Throughput Screening

Schedule:

- Manuscript submission deadline: June 30th 2015
- Peer Review Due: August 30th 2015
- Revision Due: September 30th 2015
- Notification of acceptance by the Guest Editor: October 31st 2015
- Final manuscripts due: November 30th 2015