Tentative Outline

Special Issue for CURRENT COMPUTER-AIDED DRUG DESIGN

Guest Editors: Gang Yang & Zhiwei Yang

APPLICATIONS OF DOCKING AND MOLECULAR DYNAMICS IN DRUG DESIGN

Aims & Scope:

Lead compounds show activities by inhibiting or stimulating the functions of biologically relevant molecules (proteins, nucleic acids, carbohydrates and lipids). Researchers are aiming to improve certain features of the indentified lead compounds. Those to become drug candidates should bind specifically to the targets whereas not affect any other important "off-target" molecules that may even be structurally similar (i.e., no side effects). Docking and molecular dynamics have established their roles during the drug discovery and optimization processes, helping us to rank the various lead compounds, predict the binding sites and affinities as well as elucidate the binding mechanisms. With these two computational tools, obviously less time and lower cost are needed in order to “find” a potent drug candidate. This special issue is to commemorate the introduction and application of docking and molecular dynamics methods in drug design. All aspects are welcome, including the related theoretical developments.

Key words:

Docking; molecular dynamics; binding free energies; binding mechanisms; lead compounds

Subtopics:

Lead compound discovery and optimization.

Molecular recognition and docking in structure-based drug design.

Molecular dynamics for the binding mechanisms.

Protein folding and protein-protein interactions in drug design.

Free energy calculations.

Development of docking and molecular dynamics methods.

Schedule:

Manuscript submission deadline:	May 2012
Peer Review Due:	July 2012
Revision Due:	August 2012
Notification of acceptance by the Guest Editor:	September 2012
Final manuscripts due:	September 2012