

Tentative Outline

Special Thematic Issue for Current Topics in Medicinal Chemistry

Accounting Conformational Dynamics into Structural Modeling and Drug Discovery

Guest Editors: Zhiwei Yang

Aims & Scope:

Nowadays, protein structure prediction / modeling has been routinely applied in drug discovery to increase the effectiveness. It provides essential contributions in successful predictions (e.g. antivirals for COVID-19) at the leading edge of a battle against a pandemic, and understanding of the functional complexity of living systems. However, there are two main issues to be solved to implement reliable predictions, i) accurate modeling of the protein structure and "binding pocket", ii) correct incorporating the intrinsically dynamic behavior of proteins. A variety of algorithms and strategies have been and are currently developed for the ever-improving estimation of structural modeling and drug discovery with accounting for conformational dynamics, including molecular simulation, deep learning, NMR, cryo-electron microscopy and single-molecule fluorescence techniques. Accordingly, this special issue is to collect a series of state-of-the-art examples of the recent progress in this rapidly changing field, and uncovering the ligand-protein / peptide-protein / protein-protein interaction modulations. All aspects are welcome, including the current efforts in theoretical developments.

Keywords: Structural modeling, Docking, Molecular recognition, Conformational dynamics, and Rational drug design

Subtopics:

The subtopics to be covered within this issue are listed below:

- Advances in protein structure prediction and design
- Frontiers in cryo-EM and NMR of dynamic structure modeling
- Advances in ligand / peptide / protein-protein docking
- Integrating conformational dynamics in drug discovery
- Development of rational drug design

Tentative titles of the articles and list of contributors:

Tentative titles of the articles and list of contributors with their names, designations, addresses and email addresses should be provided.

1. Dr. Junmei Wang

Department of Pharmaceutical Sciences, University of Pittsburgh, 3501 Terrace Street, Pittsburgh, Pennsylvania

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Title: Extended Linear Interaction Energy Method Perform in Accurate Binding Free Energy Calculations

2. Dr. Jian Zhang

School of Medicine, Shanghai Jiaotong University

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Title: Discovery of Allosteric Modulators Using Reversed Allosteric Communication

3. Dr. Wolfgang B. Fischer

Institute of Biophotonics, School of Biomedical Science and Engineering, National Yang-Ming University, Taiwan

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Title: Drugs against Viral Channel Forming Proteins

4. Dr. Shuichi Miyamoto

Exploratory Chemistry Research Laboratories, Sankyo Co., Ltd., 1-2-58, Hiromachi, Shinagawa-ku, Tokyo
140-8710, Japan

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Title: Conformational Analysis and Docking Study of Potent Inhibitors

5. Dr. Fabio Lannutti

Dipartimento di Scienze del Farmaco, Università "G d'Annunzio" di Chieti-Pescara, Via dei Vestini 31, I-66100
Chieti, Italy

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Title: A Cross-docking Approach for Rational Drug Design

6. Dr. Tingjun Hou

College of Pharmaceutical Sciences, Zhejiang University, Hangzhou, China

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Title: Machine Learning-Based Scoring Functions in Structure-Based Virtual Screening

7. Dr. Thomas Balle

Department of Medicinal Chemistry, Faculty of Pharmaceutical Sciences, University of Copenhagen,
Universitetsparken 2, Denmark

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Title: Prediction of the Receptor Conformation for Agonist Binding

8. Dr. Qingchuan Zheng

Institute of Theoretical Chemistry, Jilin University, China

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Title: Protein-Ligand Interactions Uncovered by Multiscale Simulations

9. Dr. Lei Zhang

School of Physics, Xi'an Jiaotong University, Xi'an, China

Email: zhangleio@xjtu.edu.cn

Title: Bio-macromolecular dynamic structures reflected by Cryo-EM

10. Dr. Guanghong Wei

Department of Physics, Fudan University, Shanghai, China

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Title: Conformational Ensembles of Intrinsically Disordered Proteins

11. Dr. Jiajie Diao

University of Cincinnati College of Medicine

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Title: Detecting Single Molecule Dynamics in Synaptic Membrane Fusion

12. Dr. Xiaojun Tian

School of Biological and Health Systems Engineering, Arizona State University, Tempe, AZ.

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Title: How do cells communicate with each other through paracrine and autocrine?

- More submission will be invited from the Xi'an Jiaotong University, Arizona State University, University of Cincinnati, University of Pittsburgh, and the universities and colleges in North America

Schedule:

- ✧ Manuscript submission deadline: 30 July 2021
- ✧ Peer Review Due: 30 August 2021
- ✧ Revision Due: 30 September 2021
- ✧ Announcement of acceptance by the Guest Editors: 30 October 2021
- ✧ Final manuscripts due: 30 November 2021

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