

Tentative Outline

Special Thematic Issue for *Combinatorial Chemistry & High Throughput Screening*

Accounting Receptor Dynamic Behavior into Structure-based Design

Guest Editor: Zhiwei Yang

• **Scope of the Thematic Issue:**

Nowadays, structure-based design has been routinely applied in the drug discovery, with a better understanding about complexity of biological systems. As biological systems usually move to perform the functions, a variety of strategies have been developed for incorporating the receptor dynamic behavior into the design produces. Molecular simulation, NMR, electron microscopy and single-molecule fluorescence techniques have established their roles to present the intrinsically dynamic behavior of biomacromolecules, helping us to elucidate the physiological structures. Accordingly, this special issue is to commemorate the introduction and application of these techniques in structure-based design for the in-depth investigation on the dynamic nature of biological systems, and uncovering the receptor-ligand / protein-protein interaction modulations. All aspects are welcome, including the current efforts in theoretical developments.

Keywords: Lead compound, Molecular recognition, Protein-protein interaction, Receptor dynamics, Structural characterization, Structure-based design

Sub-topics:

The sub-topics to be covered within the issue should be provided:

- Lead compound discovery and optimization
- Molecular recognition in structure-based design
- Protein-protein interactions in structure-based design
- Receptor dynamics and conformational sampling in structure-based design
- Development of structure-based 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. Qingchuan Zheng

State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, China

Email: zhengqc@jlu.edu.cn

Title: Drug design benefits from molecular dynamics: Some examples

2. Dr. Guangyan Zhou

Department of Basic Science, Touro University at CA, USA

Email: guangyan.zhou@tu.edu

Title: Application of molecular modeling in blocking protein-protein interaction

3. Dr. Wolfgang B. Fischer

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

Email: wfischer@ym.edu.tw

Title: In silico drug targeting of viral membrane proteins

4. Dr. Lei Zhang

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

Email: zhangleio@xjtu.edu.cn

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

5. Dr. Dongfeng Dang

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

Email: dongfengdang@mail.xjtu.edu.cn

Title: Organic fluorophores with high brightness for super-resolution imaging

6. Dr. Jiajie Diao

University of Cincinnati College of Medicine

Email: diaoje@ucmail.uc.edu

Title: Detecting single molecule dynamics on lipid membranes

7. Dr. Jian Zhang

School of Medicine, Shanghai Jiaotong University

E-mail: jian.zhang@sjtu.edu.cn & jzhang.dr@gmail.com

Title: To be determined

8. Dr. Xiaojun Tian

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

Email: xiaojun.tian@asu.edu

Title: To be determined

9. Dr. Junmei Wang

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

E-mail: junmei.wang@pitt.edu.

Title: To be determined

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

Schedule:

- Thematic issue submission deadline: 30 July 2020
- Acceptance Notification from Guest Editor: 30 October 2020
- Final acceptance from the journal: 30 Nov, 2020

Contacts:

Guest Editor Name: Zhiwei Yang

Affiliation: School of Science, Xi'an Jiaotong University

Email: yzws-123@xjtu.edu.cn