SCIENCE CHINA
Chemistry

• EDITORIAL •
• SPECIAL TOPIC • Chemistry for Life Sciences

October 2013 Vol.56 No.10: 1331–1332
doi: 10.1007/s11426-013-4982-x

Preface

In life sciences, molecules are categorized into biological macromolecules (protein, DNA, RNA etc.) and small molecules (neurotransmitters, vitamins, drugs, natural products, water etc.). The main methodology of chemistry for life sciences is using chemical techniques and tools to explore and manipulate the functions of biological macromolecules. This methodology can be traced back to Wöhler's synthesis of urea from "inorganic" compounds in 1828. Today, we realize that chemistry can advance a molecular understanding of biology, and the harnessing of biology can advance chemical knowledge as well [1–4]. Chemicals are widely used as probes to investigate biological functions [5–7].

The completion of the human genome project has boosted the developments of chemical biology, chemical genomics, proteomics, metabolomics, medicinal chemistry, synthetic biology, and other interdisciplinary studies. The key is to understand structure based bio-molecular interactions and transformations. The chemistry of life sciences involves the construction of networks to map the diversity of biological macromolecules and small molecular diversity as well.

In this special topic, a number of active researchers in this field have been invited to outline their recent progresses. Many drug targets are G protein coupled receptors (GPCRs). One of important GPCR groups is Muscarinic acetylcholine receptor (mAChR) family, which plays crucial roles in various physiological functions and pathophysiological processes. Dr. Chen and his group [8] are known for the discovery of mAChR modulators. In their review paper, the mAChR modulators derived from natural toxins and diverse interaction modes are outlined. Dr. Wang at University of California in Davis discussed the structural complexity of GPCRs and their interaction modes with the ligands [9].

G-quadruplexes (also known as G-tetrads or G4-DNA) are potential drug targets, which are being taken note of by scientists in the fields of drug discovery. Dr. Huang and her group [10] have made significant achievement in discovering new ligands for these targets, and their mechanisms of actions. Here they summarize recent progress on discovering G-quadruplex ligands from natural products.

Three articles report on molecular simulations and chemoinformatics applied in predicting or classifying bioactive compounds. Dr. Yan and her colleagues [11] report their work on classification of hERG potassium ion channel blockers with support vector machine approach; Zhang and colleagues [12] report their work on predicting hiCE inhibitors based upon pharmacophore models derived from the receptor and its ligands; and Dr. Liao [13] describes the diverse evolution and Polo-like kinase 1 inhibitors.

One of the bottlenecks in drug innovation is to acquire new and diverse small molecule scaffolds.

Three articles outline the progresses on seeking new biological small molecule agents by biological or chemical syntheses, and extraction from traditional medicine. Dr Sun's group [14] gives a perspective on the biosynthesis of tetronate antibiotics; Dr. Zhou [15] at Shanghai Jiao Tong University outlined a privileged small molecule scaffold for antifungal, antibacterial, antiviral, anti-parasite, and anti-inflammatory activities; Dr. Zhou and colleagues at [16] Soochow University review natural products derived from lycorine (traditional Chinese medicine) and their biological functions. PubChem is a well-known chemical compound database providing information on the biological activities of small molecules, and is organized as three linked databases (PubChem Substance, PubChem Compound, and PubChem BioAssay) within the NCBI's Entrez information retrieval system. Since it was released in 2004, PubChem has become one of the most important resources for research in life sciences. Drs. Bryant, Wang and colleagues [17] have described the PubChem information system to help researchers to discover agents with novel biological functions.

Chemistry for Life Sciences has a broad spectrum of areas. It is impossible to cover all of them in this special topic with ten articles. By reviewing these articles, we hope the readers can get a picture of this booming discipline.

We highly appreciate Editors Dr. Xiaowen Zhu and Dr. Xuemei Zhang for their continuing supports to us in organ-

izing and editing this issue. Dr. Qiong Gu has dedicated a lot of time on processing the submissions for this issue. We are grateful to all the authors for their supports. We appreciate any comments and suggestions from the readers.

Jun Xu (Sun Yat-sen University)
Arnold T. Hagler (University of Massachusetts, Amherst)
August 10, 2013

1 Breslow R. Artificial enzymes, cancer chemotherapy, conjugation and nanoelectronics, and prebiotic chemistry. *Sci China Chem*, 2011, 54: 1803–1814
2 Gan JH, Sheng J , Huang Z. Chemical and structural biology of nucleic acids and protein-nucleic acid complexes for novel drug discovery. *Sci China Chem*, 2011, 54: 3–23
3 Wang F, Chen Y, Huang Y, Jin HW, Zhang LR, Yang ZJ, Zhang LH. Synthesis, physicochemical and biological properties of oligonucleotides incorporated with amino-isonucleosides. *Sci China Chem*, 2012, 55: 70–79
4 Chen X, Hao ZY, Chen PR. Protein photocrosslinking reveals dimer of dimers formation on MarR protein in *Escherichia coli*. *Sci China Chem*, 2012, 55: 106–111
5 Chen MJ, Qu DZ, Chi WL, Wang W, Ren XS, Cong SJ, Liang PZ, Feng SP, Zhang BL. 5-Ethynyl-2′-deoxyuridine as a molecular probe of cell proliferation for high-content siRNA screening assay by "click" chemistry. *Sci China Chem*, 2011, 54: 1702–1710
6 Zhao DS, Chen YX, Liu Q, Zhao YF, Li YM. Exploring the binding mechanism of thioflavin-T to the β-amyloid peptide by blind docking method. *Sci China Chem*, 2012, 55: 112–117
7 Sun W, Li J, Li WH, Su LJ, Du LP, Li MY. Design of OFF/ON fluorescent thiol probes based on coumarin fluorophore. *Sci China Chem*, 2012, 55: 1776–1780
8 Xu JR, Wang H, Chen HZ. Muscarinic acetylcholine receptor modulators derived from natural toxins and diverse interaction modes. *Sci China Chem*, 2013, 56: 1333–1343
9 Wang Ting. The complexity of G-protein coupled receptor-ligand interactions. *Sci China Chem*, 2013, 56: 1344–1350
10 Shan C, Tan JH, Ou TM, Huang ZS. Natural products and their derivatives as G-quadruplex binding ligands. *Sci China Chem*, 2013, 56: 1351–1363
11 Xuan SY, Liang H, Wang Z, Yan AX. Classification of blocker and non-blocker of hERG potassium ion channel using a support vector machine. *Sci China Chem*, 2013, 56: 1413–1423
12 Zhang GD, Ge H, Gu Q, Xu J. Predicting hiCE inhibitors based upon pharmacophore models derived from the receptorand its ligands. *Sci China Chem*, 2013, 56: 1402–1412
13 Liao C, Yao RS. Diversity evolution and jump of Polo-like kinase 1 inhibitors. *Sci China Chem*, 2013, 56: 1392–1401
14 Tao WX, Zhu MH, Deng ZX, Sun YH. Biosynthesis of tetronate antibiotics: A growing family of natural products with broad biological activities. *Sci China Chem*, 2013, 56: 1364–1371
15 Zhang J, Zhu MY, Lin YN, Zhou HC. The synthesis of benzoxaboroles and their applications in medicinal chemistry. *Sci China Chem*, 2013, 56: 1372–1381
16 Cao ZF, Yang P, Zhou QS. Multiple biological functions and pharmacological effects of lycorine. *Sci China Chem*, 2013, 56: 1382–1391
17 Hao M, Cheng T, Wang Y, Bryant HS. Web search and data mining of natural products and their bioactivities in PubChem. *Sci China Chem*, 2013, 56: 1424–1435

XU Jun received his Ph.D. degree from University of Science & Technology of China in 1989 and conducted his postdoctoral research work at Australian National University (ANU) and McGill University in 1990–1993. He worked in the US pharmaceutical industry for over 20 years, held the senior positions, such as, R&D Director, Research Fellow, etc. for Bio-Rad Sadtler Labs, DPI/Biofocus, Boehringer Ingelheim Pharmaceuticals, Inc. (BIPI), OMG (now Accelrys) and Tripos. He became a Professor in Medicinal Chemistry & CADD and founding Director of Research Center for Drug Discovery (RCDD) at Sun Yat-sen University since 2009. His recent research interests include anti-virus or metabolic syndrome drug discovery, and high performance computing algorithm applied in biomedical innovations.

HAGLER T. Arnold was a theoretical/computational chemist in the labs of Harold Scheraga at Cornell and then Shneior Lifson at the Weitzman Institute. Following his postdoc with Shneior he joined the faculty of the Weitzman. In 1984, Dr. Hagler founded Biosym, and served as CEO. His company introduced a variety of software tools for structure based drug design. From 2000 to 2003, he served as President of Structural Proteomics and VP of Discovery Partners, a CRO of which it was a subsidiary. Dr. Hagler is currently VP of computational structural biology at Shifa and adjunct professor in the departments of Chemistry and Biochemistry and Molecular Biology at University of Massachusetts, Amherst (UMass Amherst) and adjunct professor of Pharmaceutical Chemistry at University of California, San Francisco (UCSF). He is focusing on the design of ligands to target the androgen receptor, a prostate cancer target.