Recent Progress on the Structural Basis of Activation and Post-translational Modification of Proteins

Aims & Scope:

Medicinal chemistry is a discipline at the intersection of chemistry and various biological and pharmacological research areas, where the chemical synthesis and the design of bio-active molecules are highly involved. At the biological interface, medicinal chemistry combines to form a set of highly interdisciplinary sciences, such as biochemistry, molecular biology, structural biology and computational biology. The principal aim of this special issue is to report recent progress of medicinal chemistry incorporating experimental and computational biology. The review articles of this hot issue will focus on researches of structure-based computational drug design, protein-based therapeutics, biopharmaceuticals, protein-drug interaction predictions, prediction and determination of protein-ligand complex, as well as druggability assessment of protein-drug interfaces. All these researches will provide new insights into the molecular mechanisms in understanding organization and functioning of biological systems, as well as the structural basis for drug design.

Keywords: Structural biology, bioinformatics, NMR spectroscopy, X-ray crystallography, 3D protein structure, drug discovery and design, protein-protein interaction, protein-drug interaction, pseudo amino acids.

Subtopics:

1. Activation and deactivation of drug-target proteins
2. Determination of phosphorylation sites
3. Post-translational modification of proteins
4. Submolecular mechanism of diseases
5. Druggability assessment of protein-protein interfaces;
6. Prediction and determination of protein complex structure based on structural bioinformatics, X-ray cryptography and NMR spectroscopy;
7. Approaches for detection and analysis of protein-biomolecule interactions.

Schedule: July, 2016