TITLE: Multi-Scale Approaches in Medicinal Chemistry of Anticancer Agents

Aims & Scope:

Cancers comprise a group of life-threatening diseases characterized by an uncontrolled cell growth, and they have the potential to spread to other parts of the body. Nowadays, cancers have a highly negative impact on modern societies in terms of prevalence and mortality, with millions of new cases and deaths each year worldwide.

Science has experienced great progresses, and through the process known as drug discovery, the pharmaceutical industry has provided a plethora of therapeutic alternatives for the treatment of diverse types of cancer. Nevertheless, cancers have become resistant to most antineoplastic drugs, which in addition are associated with serious side effects. Consequently, nowadays, the scientific community working in cancer research currently faces great challenges toward the discovery of new, versatile, and efficient anti-cancer drugs.

Drug discovery is an expensive and time-consuming process. Advances in both experimental and theoretical/computational methods envisage that the greatest challenges in anticancer drug discovery can be addressed from a multi-scale optic, i.e., through the use of different approaches, dissimilar research areas, and multiple biological data involving chemical species at different levels of diversity and complexity, which can remarkably impact and speed up the design and development of more potent and safer chemotherapeutic agents.

This special issue will be devoted to reporting reviews and original research contributions written by experts in the field of multi-scale approaches in anticancer drug discovery. In this context, topics will include (but will not be limited to) cutting edge works on medicinal chemistry (organic compounds of natural and/or synthetic origin), chemical biology, computational biology and chemogenomics approaches, complex network analysis (drug-target interactions), fragment-based computational design of promising anti-cancer leads, and polypharmacology. All types of cancer can in principle be included, but special emphasis will be given to cancers of the following organs: lung, breast, prostate, colon, stomach, liver, and brain.

Key words: Anti-cancer; chemical biology; chemogenomics; complex networks; computational; drug discovery; polypharmacology; fragments; medicinal chemistry; multi-scale.

Subtopics:

1- Computational Biology and Chemogenomics of Anti-Cancer Agents.

2- Polypharmacology.

3- Chemical Biology and Medicinal Chemistry of Anti-Cancer Agents.

4- Complex Network Analysis in Anti-Cancer Drug Discovery.
5- Advanced Computational Approaches in Anti-Cancer Drug Discovery.
6- Medicinal Chemistry of Natural Products in Cancer Research.
7- Virtual Screening of Anti-Cancer Compounds.
8- Fragment-Based Computational Design of Potential Anti-Cancer Leads.

Schedule:
Manuscript submission deadline: May 31st, 2017
Peer Review Due: From June 1st to July 1st, 2017
Revision Due: July 2 to July 21, 2017
Notification of acceptance by the Guest Editor: July 22 to July 24, 2017
Final manuscripts due: July 24 to July 31st, 2017