

# Tentative Outline

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

### *In silico methodologies applied to anti-infections drug discovery*

**Guest Editors: Luciana Scotti and Marcus T. Scotti**

#### **Aims & Scope:**

The WHO defines that infectious diseases are caused by pathogenic microorganisms, such as bacteria, viruses, parasites or fungi; the diseases can be spread, directly or indirectly, from one person to another. Zoonotic diseases are infectious diseases of animals that can cause disease when transmitted to humans. Pharmacological design applied to the discovery of pharmacophores has expanded the use of CADD tools; from drug lead identification to receptor-based screening; and to identify aspects in active compounds (when located at a similar distances) that are both common and essential. A pharmacophore's importance is based on its molecular recognition in biological systems, for examples: in molecular ligand-receptor and in DNA-protein couplings. The *in silico* methods are based on an examination of the chemical structure of compounds, identifying features responsible for specific biological activity, thus enabling the estimation of theoretical data and the validation of any statistical model of a large set of compounds before they are synthesized, contributing significantly to accelerating the design/discovery process and reducing the need for expensive lab work and clinical trials. Theoretical studies using *in silico* methods have aided in the process of drug discovery. Technological advances in the areas of structural characterization, computational science, and molecular biology have contributed to faster planning of new feasible molecules. Chemoinformatic studies show that a large fraction of compounds are "drug-like" or at least, "lead-like" having structural and physicochemical properties that render them as potential drugs or leads. This thematic issue will bring together theoretical studies of different methodologies, such as QSAR, docking, chemometric tools, artificial intelligence and other applied in order to optimize the search for new drugs for the cure and treatment of infectious diseases.

**Keywords: infectious diseases, in silico, drug discovery**

#### **Subtopics:**

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

- QSAR
- Docking
- Neural networks
- Any CADD (Computer-aided drug discovery) in the research against infectious diseases.

#### **Schedule:**

- ✧ Manuscript submission deadline: 30 December, 2019
- ✧ Peer Review Due: 30 January, 2020
- ✧ Revision Due: 28 February, 2020
- ✧ Announcement of acceptance by the Guest Editors: 30 March, 2020
- ✧ Final manuscripts due: 15 April, 2020

#### **Contacts:**

Guest Editor: Luciana Scotti

Federal University of Paraíba, Campus I; 58051-970, João Pessoa, PB, Brazil.

E-mail: [luciana.scotti@gmail.com](mailto:luciana.scotti@gmail.com)

Co-Editor: Marcus Tullius Scotti

Federal University of Paraíba, Campus I; 58051-970, João Pessoa, PB, Brazil.

E-mail: [mtscotti@gmail.com](mailto:mtscotti@gmail.com); [mtscotti@ccae.ufpb.br](mailto:mtscotti@ccae.ufpb.br)

Any queries should be addressed to [cchts@benthamscience.org](mailto:cchts@benthamscience.org)