

## Tentative Outline

### Special Thematic Issue for Letters in Drug Design & Discovery

**Title of thematic issue: Antimalarial drug discovery - Exploration of novel structural scaffolds towards development of potent antimalarial agents**

**Guest Editors: Mithun Rudrapal, Dipak Chetia**

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

Malaria is a growing infectious disease burden across the globe. In spite of all efforts to eradicate and control of malaria by World Health Organization (WHO), it continues to be a major problem to public-health worldwide. Over the past few decades, the emergence and spread of multi-drug resistant strains of malaria parasites, particularly *Plasmodium falciparum* has become an increasingly serious concern in malaria chemotherapy. The emergence of drug resistance has limited the clinical usefulness of existing antimalarial drugs. To address this challenging issue, the discovery and development of potent antimalarial drugs is urgently required. The development of novel antimalarial drugs may be an effective alternative approach in malaria chemotherapy to counter the spread and emergence of malaria parasites that are resistant to existing antimalarial agents. To develop new and potent antimalarial molecules, multiple modern approaches of rational drug design (RDD) such as modification of natural lead molecule, analogue design based on bio-active scaffold, virtual screening and QSAR, design of hybrid molecules, inhibitors designing based on receptor molecule, drug repositioning are currently under practice. The novelty of disease target and the bio-potential of structural scaffolds play a vital role in RDD besides the application computational and virtual screening tools. For example, triazolopyrimidine-based inhibitor (DSM265) is being developed as *P. falciparum* dihydroorotate dehydrogenase enzyme (*Pf* DHOD) inhibitors for treating resistant malaria. With this perspective, this thematic issue of Letters in Drug Design and Discovery has been focused to bring together the on-going research activities on recent developments in the discovery and development of potent antimalarial leads or drug molecules.

**Keywords:** Malaria, *P. falciparum*, Drug Resistance, Antimalarial, Structural Scaffold, Drug Discovery

#### **Subtopics:**

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

- Structure-based drug design and virtual screening
- Computational inhibitor design and docking
- Design, chemical synthesis and QSAR
- Natural bioactive scaffolds and lead design
- Disease target and drug repositioning
- Hybrid scaffolds and multi-target approach

#### **Schedule:**

- ✧ Manuscript submission deadline: June 30, 2019
- ✧ Peer Review Due: July 20, 2019
- ✧ Revision Due: August 10, 2019
- ✧ Announcement of acceptance by the Guest Editors: August 20, 2019
- ✧ Final manuscripts due: September 10, 2019

**Contacts:****Lead Guest Editor: Mithun Rudrapal**

**Affiliation:** Department of Pharmaceutical Sciences, Dibrugarh University, Dibrugarh-786 004, Assam, India

**Email:** rudrapal.m03@gmail.com

**Guest Editor: Dipak Chetia**

**Affiliation:** Department of Pharmaceutical Sciences, Dibrugarh University, Dibrugarh-786 004, Assam, India

**Email:** dchetia@dibru.ac.in

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