Special Thematic Issue proposal for the journal 'MEDICINAL CHEMISTRY'

Title of the issue: Natural products inspired drug discovery for infectious diseases

Guest Editor(s): Dr. Harish C. Upadhyay & Dr. Santosh K. Srivastava

Scope of the Thematic Issue:

Infectious diseases are caused by pathogenic microorganisms such as bacteria, viruses, and fungi, and are considered contagious or communicable. Following the development of the antibiotics penicillin and streptomycin, chemotherapy saw a resurgence. These medicines were a miracle that cured millions of people of severe diseases like tuberculosis and pneumonia up to the 1980s. After the 1980s, a period of contempt for the existing systems of therapy began, giving credence to the current era of drug resistance. The emergence of new strains of multidrug-resistant (MDR) organisms with novel penicillin-binding proteins (PBPs), enzymatic mechanisms of drug modification, mutated drug targets, increased efflux pump expression, and altered membrane permeability over time is the consequence of ongoing selective pressure from various antibacterial drugs. According to the WHO, antibacterial resistance is a worldwide and endangering problem because the existing antimicrobials are insufficient to meet the challenges. The WHO identified 12 human pathogenic bacteria (the "dirty dozen"), including *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and *Enterobacteriaceae,* that urgently require new drugs due to drug resistance and a lack of available medicines. Similar to these, other pathogenic bacteria and viruses have spread like a pandemic around the world with few treatment options, posing major risks to global health.

Natural products, including medicinal plants, have always provided new and important leads against various pharmacological targets. The bioactive plant secondary metabolites themselves have provided many exciting drugs of clinical use. Many times, the semi-synthetic approaches by modifying the existing functional groups of natural products have produced many druggable leads with improved efficacy over the parent compounds. Not only druggable molecules, but also synthetic modifications for structure activity relationship studies (SAR) have provided enough information for synthetic chemists to offer a strategy for designing new leads or drugs. The mastery of natural products in drug discovery is ever more evident as more than half of all the drugs of today contain compounds originally identified from plants or their derivatives. Exploring nature's treasure for drug discovery is successful and continues to be an effort. The entry of the computer-aided drug design (CADD) approach applying diverse computerised methods enabled a speedy boost-up in the drug discovery process, minimising the time and cost. The innovative drug discovery programme for the advent of efficient and cost-effective drugs with a broad range of functionality may be focused on exploring natural products for novel pharmacophores and virtual design of molecules taking a scaffold of natural origin for the source of potential therapeutic agents.

This thematic issue is aimed at summing up the recent advances in the field of natural product-inspired drug discovery for infectious diseases. The scope of this thematic issue will cover all areas of medicinal chemistry, including current developments in rational drug design, synthetic chemistry, bioorganic chemistry, high-throughput screening, combinatorial chemistry, compound diversity measurements, drug absorption, drug distribution, metabolism, new and emerging drug targets, pharmacogenomics, and structure-activity relationship approaches applied for the discovery and development of novel antimicrobial (viz. antibacterial, antifungal, antitubercular, antimalarial, antifilarial, antihelmintic, and antiviral) leads.

Keywords: Medicinal plants, Natural product, Hybrid molecules, Structure activity relationship, Antibacterial, Antifungal, Antiviral, Antimicrobial drug resistance, Computer-aided drug design

Sub-topics:

- Phytochemical investigations medicinal plants/natural products and bio-evaluations for the search of novel antimicrobial and antiviral leads.
- Antimicrobial nano-herbal formulations using medicinal plants.
- Structure activity relationship (SAR) studies of new antimicrobial and antiviral agents.
- Synthesis of natural product-based hybrid molecules as potential antimicrobial agents.
- Computational approaches for rational antimicrobial drug design.
- Current developments in target-based drug discovery of new antimicrobials.

Schedule:

- ✧ Thematic issue submission deadline: January 05, 2023
- ✧ Peer Review Due: January 20, 2023
- ✧ Revision Due: January 30, 2023
- ✧ Announcement of acceptance by the Guest Editor(s): February 10, 2023
- ✧ Final manuscripts due: February 20, 2023

Contacts:

1. Dr. Harish C. Upadhyay, PhD (CSIR-CIMAP, India)
   Assistant Professor Chemistry, Department of Applied Sciences, Rajkiya Engineering College (Affiliated with Dr. A.P.J. Abdul Kalam Technical University, Lucknow), Churk, Sonbhadra-231206, India. Email: harishcu@gmail.com, harishcu@recsonbhadra.ac.in; Mo.: +91-9415164409
2. Dr. S.K. Srivastava, PhD
   Emeritus medical Scientist, Ex-chief Scientist & head, medicinal Chemistry Department, CSIR-Central Institute of medicinal and Aromatic Plants, Lucknow, India
   Email: skscimap@gmail.com