

## THEMATIC ISSUE

### Development of new enzyme inhibitors and their use in medicinal chemistry: synthetic, biological and computational aspects

#### Aims & Scope:

Current Medicinal Chemistry covers all the latest and outstanding developments in medicinal chemistry and rational drug design. Each issue contains a series of timely in-depth reviews and guest edited thematic issues written by leaders in the field covering a range of the current topics in medicinal chemistry. Current Medicinal Chemistry is an essential journal for every medicinal chemist who wishes to be kept informed and up-to-date with the latest and most important developments.

#### Abstract:

Evaluation of enzyme inhibitors in drug discovery is a valuable reference work that clearly addresses the need for medicinal chemists and pharmacologists to communicate effectively in the difficult and demanding world of drug discovery. Enzymes are considered by many in the pharmaceutical community to be the most attractive targets for small molecule drug intervention in human diseases. The attractiveness of enzymes as targets stems from their essential catalytic roles in many physiological processes that may be altered in disease states.

The structural determinants of enzymes with the aim of identifying inhibitory molecules that may serve as the starting points for drug discovery and development efforts. Drugs that function as enzyme inhibitor constitute a significant portion of theoretically bioavailable therapeutic agents that are in clinical use today. Likewise, much of the drug discovery and development efforts at present are focused on identifying and optimizing drug candidates that act through inhibition of specific enzyme targets. The attractiveness of enzymes as targets for drug discovery stems from the high levels of disease association (target validation) and druggability (target tractability) that typically characterize this class of proteins. Recent and continuous advances in new synthetic methodologies, biological tools and computational chemistry allow a better understanding not only in the drug-enzyme interaction, but also in the validation and identification of targets involved in a specific disease. Our special issue will be focused on the synthesis, isolation, mechanism of action and possible ways of computational /prediction-modelling of compounds whose influence on enzymatic receptors could exercise an inhibition to improve the therapeutic action on related diseases in both mental disorders or neuromotor dysfunctions.

#### Guest Editor:

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#### Important Dates

**Submission deadline:**

February, 2017

**Tentative publication date:**

June, 2017

