Tentative Outline (Preliminary Proposal of Thematic Issue)

Special/Thematic Issue for the journal "Current Topics in Medicinal Chemistry"

Title of the Thematic Issue: QSAR, Molecular Docking and MD Simulation guided Lead Identification and Exploration of Binding mode of Action on Potential Targets

Guest Editor's Name: Dr. Feroz Khan

- **Scope of the Thematic Issue:**

Quantitative structure-activity relationships (QSAR) have emerged as a rational alternative in order to find new natural bioactive molecules. Many chemical descriptors can be used to describe organic molecular structure and their physico-chemical properties. Developing a predictive QSAR model for screening of bioactive natural compounds based on molecular structure is very important goal for medicinal chemist. Different chemical descriptors can be used to show correlation with bioactivity through different supervised machine learning methods such as regression. Also there are different chemical features selection methods such as correlation matrix, multicollinearity and Principal Component Analysis (PCA) can be used during QSAR modeling process. The chemical descriptors and biological activity based regression analysis and molecular docking with Molecular Dynamics (MD) simulation approaches are shown to be very successful in drug design and discovery programs. Besides, the structural similarity of compounds is so much that we may need linear models instead of non-linear ones. Once lead identified, binding mode of action or binding affinity on selected targets can be detected through molecular docking method. Further binding stability of compound on selected target can be analysed for nanosecond level through MD simulation. Therefore, QSAR, Molecular Docking and MD simulation approaches are essential tools in the pharmaceutical industry, from lead discovery, lead optimization and computer-aided drug designing & discovery programs. Moreover, QSAR studies are now suggested by regulatory bodies e.g., US FDA and European Union by the REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) regulation so that to explore the hidden factors regulating the bioactivity of compounds on selected targets. Similarly, predictive ADME (Absorption, Distribution, Metabolism, and Excretion) and predictive toxicity risk assessment can be used for detecting early bioavailability behaviour of lead compounds and high dose or long-term use toxicity risk in human respectively.

Keywords: QSAR, Docking, MD simulation, bioactivity, bioavailability, eADME, toxicity, virtual screening

Sub-topics:

Research Articles

- Antibacterial & Anticancer activity through modulation of Tubulin Microtubule Dynamics.
- Structure-Activity Relationship studies on VEGFR2 Tyrosine Kinase inhibitors for Anticancer activity.
- QSAR modeling, docking and MD simulation studies on Glycyrrhetinic acid derivatives for Anti-Tubercular activity.
- Molecular docking studies revealed the antiviral phytochemicals from medicinal plants.
- QSAR, docking and pharmacokinetics studies on Triterpene derivatives for Anticancer activity.
- Molecular modeling studies on natural Terpenoids for immunomodulatory & anticancer activity.
- Nano-formulation of extracts, in-silico studies & *in-vitro* Antibacterial evaluation.
- In-silico mechanism exploration of phytomolecules and antibiotic combinations active against drug-resistant *Staphylococcus aureus*.
- QSAR studies on selected target inhibitors for antibacterial activity.
- QSAR studies on inhibitors of Penicillin-Binding Protein 2a (PBP2a) for Anti-Methicillin Resistant *Staphylococcus aureus* (MRSA) activity.

Review Articles

- A systematic review on *in-vitro* and *in-silico* investigation of bioactive properties of Mangiferin.
- Phytomolecules targeting cell wall synthesizing protein in Methicillin Resistant Staphylococcus aureus (MRSA) for Antibacterial activity.

Schedule:

- ✧ Complete Thematic issue submission deadline: 15-Feb-23

Details of Guest Editor:

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