

Tentative Outline

Special Thematic Issue for the journal : Anti-Cancer Agents in Medicinal Chemistry

Title of the Thematic Issue: Discovery of promising anticancer agents via computational and experimental approach

Sectional Editor: Kaushik Chanda

• **Scope of the Thematic Issue:**

Cancer refers to a group of disorders in which cellular proliferation is unregulated, resulting in increased cell growth and decreased cell death. The fundamental basic underlying mechanism for disease development and progression is genetic changes, which can be inherited or caused by environmental factors. Accelerated growth, evasion of scheduled cell death, evasion of immunological checkpoints, and the ability to penetrate distant organs are all characteristics of malignant cells. Mutations in genes involved in the regulation of cell proliferation and growth, such as proto-oncogenes and tumour suppressor genes, cause these aberrant cellular features. Furthermore, mutations in genes involved in DNA repair compromise the integrity of DNA sequences, allowing numerous DNA lesions to accumulate in cancer cells. A large number of heterocyclic molecules including natural products have shown potent anticancer activity. This thematic issue intends to highlight the anti-cancer activities of various scaffolds through computational as well as experimental approach. Therefore, all the submitted Review Articles/Mini-reviews should focus on anti-cancer activities of promising scaffolds via computational and experimental approach.

Keywords: Natural Product, Synthetic compounds, Cancer Biology, Computational Chemistry, In vitro and in vivo study, Molecular dynamics simulation, MM-GBSA, Machine learning

Sub-topics:

- Heterocyclic moieties as potential anticancer agents
- Natural products as anticancer agents
- Computational study of heterocyclic moieties as possible anticancer agents
- In vitro and in vivo study of heterocyclic molecules as potent anticancer agents
- Machine Learning
- Drug Repurposing
- Breast cancer

Tentative titles of the articles:

- A comprehensive review on the anticancer potential of N heterocycles
- Per-residue footprints approach for discovery of potential inhibitors against myeloid leukaemia.
- In silico screening and anti-proliferative study of natural product analogues coumapherine and piperidongumine against CD46 and CD559
- Cytotoxic activity of Psilocybe mushroom: Combined in silico and in vitro strategy

Schedule:

- ✧ Manuscript Submission deadline: Aug 30, 2022
- ✧ Notification of acceptance by the Guest Editor: October 30, 2022
- ✧ Final manuscripts due: November 15, 2022

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