

Tentative Outline

**Special Thematic Issue for the journal Special "Thematic Issue for the journal Current Topics in Medicinal Chemistry"
(Science Citation Index Expanded (SCI-E), Quartile:Q3, Impact Factor:3.570)**

Title of the Thematic Issue: Structure-Activity Relationship of New compounds

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• **Scope of the Thematic Issue:**

The development of novel anti-cancer drugs is one of the most important themes in cancer research. One is worried about developing breast cancer risk, has just been diagnosed, is going through breast cancer treatment, or is trying to stay well after treatment, this detailed information can help you find the answers you need. Great effort has been done to find the target of anti-cancer drugs. A further target-specific compound is being developed to cure cancer. Correlation between structure and function is one of the important aspects of the success of anti-cancer compounds. Researchers around the world are working to find better ways to prevent, detect, and treat breast cancer and their valuable contribution to the expansion in the field of medicinal chemistry.

Keywords: Cell culture, apoptosis, cytotoxicity, anticancer drug/agents, synthesis characterization and biological activity such as anticancer, apoptosis, antioxidant, enzyme, etc, QSAR, Inhibitor, bioinformatic, molecular docking, breast cancer

Sub-topics:

- What Is Breast Cancer?
- Cells of Breast cancer
- Triple-negative Breast Cancer
- Apoptosis
- Apoptosis on Breast cancer
- Cell Culture treatment in Breast cancer
- Anticancer agent/ drug
- Anticancer activity
- Cytotoxicity in Breast cancer
- Estrogen/Progesterone
- Her2/neu marker
- Breast cancer metabolism
- Breast cancer drug therapy
- Enzymatic studies in Breast cancer
- Molecular and genetic studies
- BRCA1 and BRCA2 gene mutations
- P53, CA 15-3 etc
- Signal Pathway
- Inhibitor
- DNA binding
- QSAR
- Bioinformatic
- Molecular docking
- In silico analysis
- Structure and Function
- Medicinal chemistry
- Developing better synthetic compounds /ligands: Targeting the receptor, oncogene, signaling pathway, DNA-Protein interaction
- Drug delivery system
- Pharmacology
- Target-Based Anticancer Drug Discovery
- Method Studies

Tentative titles of the articles:

- Structure-Activity Relationships and Quantitative Structure-Activity Relationships for Breast Cancer Resistance Protein (ABCG2).
- Inhibition of Cancer-Associated Mutant Isocitrate Dehydrogenases: Synthesis, Structure-Activity Relationship, and Selective Antitumor Activity.
- Platinum(II) compounds with chelating ligands based on pyridine and pyrimidine: Synthesis, characterizations, DFT calculations, cytotoxic assays and binding to a DNA model base.
- Investigation of the Structure-Activity Relationships of Psilocybin Analogues.
- Anticancer Diiron Vinyliminium Complexes: A Structure-Activity Relationship Study.
- Structure-activity relationship of novel acridone derivatives as antiproliferative agents.
- Review of anticancer potentials and structure-activity relationships (SAR) of rhodanine derivatives.
- Structure-Activity Relationships of Thiophene Carboxamide Annonaceous Acetogenin Analogs: Shortening the Alkyl Chain in the Tail Part Significantly Affects Their Growth Inhibitory Activity against Human Cancer Cell Lines.
- Anticancer agents based on Plastoquinone analogs with N-phenylpiperazine: Structure-activity relationship and mechanism of action in breast cancer cells.
- Synthesis, characterization, DNA binding and anticancer activities of the imidazolidine-functionalized (NHC)Ru(II) complexes.
- Folic Acid and Poly(ethylene glycol) Decorated Paclitaxel Nanocrystals Exhibit Enhanced Stability and Breast Cancer-Targeting Capability.
- Identification and Preliminary Structure-Activity Relationship Studies of 1,5- Dihydrobenzo[e][1,4]oxazepin-2(3H)-ones That Induce Differentiation of Acute Myeloid Leukemia Cells In Vitro.
- Selected heterocyclic compounds as antioxidants. Synthesis and biological evaluation.
- Design, Synthesis, and Anticancer Activity Studies of Novel Quinoline-Chalcone Derivatives.
- Novel Benzenesulfonate Scaffolds with a High Anticancer Activity and G2/M Cell Cycle Arrest.
- Synthesis, Characterization, DNA/HSA Interactions, and Anticancer Activity of Two Novel Copper(II) Complexes with 4-Chloro-3-Nitrobenzoic Acid Ligand.
- Quinazoline analogues as cytotoxic agents; QSAR, docking, and in silico studies
- Cytotoxicity and pro-apoptosis activity of synthetic 1,3-thiazole incorporated phthalimide derivatives on cancer cells.
- Hexokinase 2 Inhibition and Biological Effects of BNBZ and Its Derivatives: The Influence of the Number and Arrangement of Hydroxyl Groups.
- Transition metal complexes of phenanthrenequinone thiosemicarbazone as potential anticancer agents: synthesis, structure, spectroscopy, electrochemistry and in vitro anticancer activity against human breast cancer cell-line, T47D.
- Novel tubulin-targeting agents: anticancer activity and pharmacologic profile of epothilones and related analogues.
- Cyclin-Dependent Kinase 4 and 6 Inhibitors in Cell Cycle Dysregulation for Breast Cancer Treatment.
- Targeting the ROS/PI3K/AKT/HIF-1 α /HK2 axis of breast cancer cells: Combined administration of Polydatin and 2-Deoxy-d-glucose.

- Molecular docking, synthesis and anticancer activity of thiosemicarbazone derivatives against MCF-7 human breast cancer cell line.
- Chemical inhibitor anticancer drugs regulate mechanical properties and cytoskeletal structure of non-invasive and invasive breast cancer cell lines: Study of effects of Letrozole, Exemestane, and Everolimus.
- Antitumor activity of Z-endoxifen in aromatase inhibitor-sensitive and aromatase inhibitor-resistant estrogen receptor-positive breast cancer.
- Antiproliferative and Pro-Apoptotic Effects of Thiazolo[3,2-b][1,2,4]triazoles in Breast and Cervical Cancer Cells.
- Synthesis, crystal structure, and anti-breast cancer activity of a novel metal-porphyrinic complex [YK(TCPP)(OH)₂•(solvents)_x].
- N-substituted hydroxynaphthalene imino-oxindole derivatives as new class of PI3-kinase inhibitor and breast cancer drug: Molecular validation and structure-activity relationship studies.
- Mechanisms of disease: understanding resistance to HER2-targeted therapy in human breast cancer
- HER-2/neu induces p53 ubiquitination via Akt-mediated MDM2 phosphorylation
- Combination of dasatinib and okadaic acid induces apoptosis and cell cycle arrest by targeting protein phosphatase PP2A in chronic myeloid leukemia cells

Schedule:

- ✧ Thematic issue submission deadline: 21-March-23

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