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# Design of Novel Target-Oriented Chemotherapeutic Anti-cancer Agents with ADME Pharmacokinetics

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Deadline for manuscript submissions:
**closed (31 July 2023)**

## Message from the Guest Editors

Dear Colleagues,

Cancer is the second-leading cause of death worldwide. Anti-cancer activity presents a promising area of research for finding effective and selective anti-cancer agents. In the context of updated and continuous drug discovery, "computer-aided drug design" (CADD) refers to a wide variety of theoretical and computational methodologies that have been employed in predicting the three-dimensional molecular structures of receptors, enzymes, and nucleic acids as molecular models of drug–receptor complexes for designing novel inhibitors with altered recognition and receptor-affinity properties. CADD helps in finding rationalized synthetic compounds or semisynthetic natural compounds against apoptosis, angiogenesis, and metastasis downstream signaling pathway. Additionally, rationalized design helps in studying drug metabolism, drug–target interactions, and ADME pharmacokinetics.

Therefore, this Special Issue deals with designing novel chemotherapeutic agents (synthetic- or natural-based compounds) against both cellular and molecular pathways as selective anti-cancer agents.

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## Editor-in-Chief


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## Message from the Editor-in-Chief

The metabolome is the result of the combined effects of genetic and environmental influences on metabolic processes. Metabolomic studies can provide a global view of metabolism and thereby improve our understanding of the underlying biology. Advances in metabolomic technologies have shown utility for elucidating mechanisms which underlie fundamental biological processes including disease pathology. *Metabolites* is proud to be part of the development of metabolomics and we look forward to working with many of you to publish high quality metabolomic studies.

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