# Special Issue

# Advancing Drug Discovery: Machine Learning and Virtual Screening in Phytochemical Research

## Message from the Guest Editors

"Advancing Drug Discovery: Machine Learning and Virtual Screening in Phytochemical Research" aims to explore the innovative intersection of machine learning (ML) techniques and phytochemical virtual screening in the quest for new therapeutic agents. As drug discovery evolves, the integration of computational methods to predict the bioactivity and optimize the screenings of natural compounds has become increasingly significant. This Special Issue will feature articles that discuss the application of various ML algorithms, including deep learning and random forests, in identifying promising phytochemicals from extensive databases. Contributors will also address challenges such as data curation, the incorporation of ethnopharmacological knowledge, and the enhancement of molecular docking simulations. Furthermore, discussions will extend to the prediction of pharmacokinetic properties and the drug-likeness of compounds, integrating traditional knowledge with highthroughput screening methods.

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### Deadline for manuscript submissions

closed (30 September 2025)



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You are invited to contribute either a research article or a comprehensive review for consideration and publication in *Processes* (ISSN 2227-9717). *Processes* is published in open access format – research articles, reviews, and other content are released on the internet immediately after acceptance. The scientific community and the general public have unlimited, free access to the content. As an open access journal, *Processes* is supported by the authors and their institutes through the payment of article processing charges (APCs) for accepted papers. We would be pleased to welcome you as one of our authors.

#### Editor-in-Chief

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