# 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 high-throughput screening methods.

## Guest Editors

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## Deadline for manuscript submissions

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## Editor-in-Chief

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