# **Special Issue**

# Secondary Metabolites as Drug Leads: Bridging Experimental Discovery and Computational Innovation

## Message from the Guest Editors

Secondary metabolites, derived from plants. microorganisms, and marine organisms, have long been a cornerstone in efforts toward the discovery of novel therapeutic agents, owing to their structural diversity and wide spectrum of biological activities. Recent advances in computational chemistry and bioinformatics, synergistically combined with experimental methodologies, have significantly enhanced the identification, characterisation, and optimisation of these bioactive compounds. This Special Issue will provide an interdisciplinary platform for research in this area, emphasising the critical importance of integrating computational strategies with experimental validation to elucidate mechanisms of action, predict pharmacokinetic profiles, and optimise therapeutic efficacy. This approach aligns directly with the scope of Pharmaceuticals, promoting a multidisciplinary perspective that bridges medicinal chemistry, pharmacology, biotechnology, and computational sciences. By showcasing integrative studies, this Special Issue will foster innovation in secondary metabolite research, ultimately advancing the development of safer and more effective therapeutic agents.

### **Guest Editors**

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#### Deadline for manuscript submissions

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## Message from the Editor-in-Chief

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We hope to handle your contribution to *Pharmaceuticals* soon.

#### Editor-in-Chief

#### Prof. Dr. Amélia Pilar Rauter

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