

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.

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Message from the Editor-in-Chief

Because of your expertise in the field of drug sciences, I kindly invite you to consider publishing your current work, in the form of a research article or a review, in the open access electronic journal *Pharmaceuticals*.

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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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