

Special Issue

Natural Bioactive Compounds for Biomedical Applications: Experimental and Theoretical Studies

Message from the Guest Editors

Interactions between biological targets and organic molecules, particularly xenobiotics and macromolecules, are essential for many biological processes. Investigations of these interactions are carried out by a variety of spectral methods. New lead compounds are introduced to the market every year. In the field of computational drug design, the identification and characterization of biological targets of interest represent a significant step. Despite the growing number of resolved protein structures, structural determination remains challenging for many heterocyclic ligands and drug targets. In these cases, computational spectral analyses and/or ligand-based drug design methods may be used successfully. Advances in structural chemistry methods have provided information on many molecules, making structure-based drug design a powerful tool for drug discovery in both academia and pharmaceutical industry. We kindly invite researchers worldwide to submit their original papers or reviews featuring recent developments in the synthesis of natural bioactive compounds and in the analysis of their interactions in the respective chemical environments.

Guest Editors

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Deadline for manuscript submissions

closed (15 November 2021)



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Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal *Applied Sciences* has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

Editor-in-Chief

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