

Special Issue

Natural Product and Enzyme Inhibition for Disease Management

Message from the Guest Editors

Bioactive compounds from natural sources have gained significant attention for their potential therapeutic applications, particularly in the inhibition of enzymes associated with human diseases. The inhibition of disease-relevant enzymes is an essential strategy in the treatment of various conditions. Research involves both in vitro and in silico approaches to understand the mechanisms and efficacy of these bioactive compounds: the former allow for the direct assessment of enzyme inhibition and the compounds' effect on cellular processes, while the latter, including molecular docking and molecular dynamics simulations, provide insights into the binding interactions and predict the compounds' biological activity. Combining these approaches enables a comprehensive evaluation of bioactive compounds, facilitating the identification of promising natural candidates for drug development. The combination of natural product research with modern technological advances holds the promise of discovering new and effective treatments for enzymatic dysregulation-driven diseases.

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