



Uncovering Endophyte-Derived Antimicrobial Compounds Through Metabolomics and in Silico Approaches: A Comprehensive Review

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Abstract:

The rapid emergence of multidrug-resistant microorganisms has intensified the search for novel antimicrobial agents. Endophytes, microorganisms residing within plant tissues, have emerged as a promising source of bioactive compounds. This review highlights the potential of metabolomics and in silico studies to discover new antimicrobial agents from endophytes. Metabolomics enables comprehensive profiling of endophytic metabolites, enhancing the identification of novel bioactive compounds, while in silico tools support the prediction of bioactivity, target interactions, and pharmacokinetic properties and aid in the selection of potential drug compounds for further research. This review further discusses recent advancements, limitations, and future prospects of integrating metabolomics and computational tools for exploration of endophyte-derived antimicrobial compounds.

Keywords:

Endophytes, Antimicrobial compounds, Metabolomics, In silico drug discovery, Natural products, Antimicrobial resistance.