Deciphering the Composition and Bioactivity of Malaysian Syzygium Essential Oils: Insights from Multivariate Chemometrics and Molecular Docking Studies

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Abstract

The genus Syzygium, an important member of the Myrtaceae family, comprises over 1200 species, primarily found in the tropical regions of Asia. Syzygium species are valued throughout their range for their medicinal and economic importance. Characterized by aromatic shrubs and trees, these species are prolific producers of essential oils that are widely used for their natural therapeutic effects in food, medicine, and cosmetics. In recent years, studies have focused on the essential oils of Malaysian Syzygium species, many of which have reported interesting pharmacological activities. This review attempts to summarize the information on the essential oils of Malaysian Syzygium species in terms of their medicinal uses, chemical composition, and bioactivity. The information on Syzygium species was collected through electronic searches (PubMed, SciFinder, Scopus, Google

Scholar, and Web of Science) and a library search for articles published in peer-reviewed journals. Our results cover eight Syzygium species in Malaysia and highlight eugenol, caryophyllene, α-pinene, α-humulene, and viridiflorol as the predominant components. Multivariate chemometric analyses, including hierarchical cluster analysis (HCA) and principal component analysis (PCA), were used to discriminate the essential oils based on their chemical profiles. Antibacterial and cytotoxic activities were the most frequently reported bioactive properties. In addition, molecular docking simulations provided insights into the binding interactions of the major components with the active sites of enzymes related to these bioactivities. This review aims to provide comprehensive information on the chemical components and biological properties of the essential oils of Malaysian Syzygium species and provide guidance for the selection of accessions or species with optimal chemical profiles.

Author keywords

binding affinity; essential oil; molecular dynamics; multivariate; Myrtaceae; Syzygium

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