Journal of Research in Biology
An International Scientific Research Journal

ISSN No: Print: 2231 –6280; Online: 2231- 6299

Systematic Review

Deciphering the Antioxidant and Therapeutic Potential of Lamiaceae Phytochemicals: Insights from Density Functional Theory and *In Silico* Approaches

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ABSTRACT:

The Lamiaceae family represents one of the most pharmacologically significant groups of medicinal plants, comprising over 7,000 species distributed across diverse ecological regions. These plants are rich in structurally diverse phytochemicals, including phenolic acids, flavonoids, and terpenoids, many of which exhibit potent antioxidant, anti-inflammatory, antimicrobial, antiviral, and anticancer activities. In recent years, computational chemistry particularly Density Functional Theory (DFT) combined with in silico methodologies such as molecular docking, molecular dynamics simulations, Quantitative StructureActivity Relationship (QSAR) modeling, and ADMET profiling, has significantly advanced the mechanistic understanding of these bioactive compounds.

This review systematically examines the application of DFT and complementary computational techniques in elucidating the antioxidant mechanisms and therapeutic potential of key Lamiaceae phytochemicals, including rosmarinic acid, lauteolin, carnosic acid, thymol, carvacrol, and ursolic acid. Particular emphasis is placed on quantum chemical descriptors such as Bond Dissociation Enthalpy (BDE), Ionization Potential (IP), Proton Affinity (PA), and Frontier Molecular Orbital (FMO) energies, which govern radical scavenging activity. Additionally, the integration of DFT-derived descriptors with molecular docking and ADMET predictions is discussed to highlight multi-target drug discovery potential.

Despite substantial progress, challenges remain in accurately modeling solvent effects, conformational flexibility, and biological environments. Future directions include the integration of machine learning with quantum chemical descriptors and the development of multi-target therapeutic frameworks. This review provides a consolidated and critically evaluated foundation for advancing computational phytochemistry in Lamiaceae-based drug discovery.

Keywords:
Lamiaceae; Density Functional Theory; Antioxidants; Molecular Docking; Phytochemicals; QSAR; ADMET; In Silico Drug Discovery

Article Citation:
Kores. J. J. (2025). Deciphering the Antioxidant and Therapeutic Potential of Lamiaceae Phytochemicals: Insights from Density Functional Theory and In Silico Approaches. **Journal of Research in Biology 15(4): 1-15**

Web Address:
http://jresearchbiology.com/documents/RA0902.pdf

Dates:
Received: 25 Aug. 2025 **Accepted:** 25 Nov. 2025 **Published:** 15 Dec. 2025