

JBP

Journal of Biochemicals and Phytomedicine

eISSN: 2958-8561



Biochemical and Antimicrobial Studies of Metallic Nanoparticles Synthesized from *Justicia carnea* Extract: Molecular Docking of Its Phytochemicals for Anti-Anaemic Potential

Adebayo Seun Gbadamosi ^{1*}, Oloketuyi Kikelomo Boluwatife ², Margaret Oladunni Oseni ³, Olatunde Abass Oseni ⁴

¹ National Biotechnology Research and Development Agency, Abuja, Nigeria

² Department of Science Laboratory Technology, Ekiti State University, Ado-Ekiti, Nigeria

³ Department of Chemistry, Federal University, Oye-Ekiti, Nigeria

⁴ Department of Medical Biochemistry, College of Medicine, Ekiti State University, Ado-Ekiti, Nigeria

Journal Pre-proof

ARTICLE INFO

Article Type:

Review

Article History:

Received: 29 May 2025

Revised: 18 Aug 2025

Accepted: 10 Sept 2025

Available online: 18 Oct 2025

Keywords:

Natural products,
Molecular docking,
Anaemia,
Nanoparticles,
Antimicrobial activities,
Justicia carnea

* Corresponding author:

E-mail:

adebayoseungbadamosi@gmail.com

ABSTRACT

Introduction: Anaemia affects over 1.6 billion people worldwide. This study explored *Justicia carnea* and its green-synthesized metallic nanoparticles as potential anti-anaemic agents, combining biochemical evaluation and molecular docking of key phytochemicals

Methods: Phytochemical composition, antioxidant capacity, antimicrobial activity, and green synthesis of three metallic NPs were analyzed using standard techniques. Eight phytochemicals were docked against anaemia-related targets (EPOR, MIF, ER α , transferrin, DHFR) using SwissDock. Binding interactions were profiled with PLIP, and drug-likeness predicted with SwissADME.

Results: Screening revealed bioactive constituents including steroids, alkaloids, flavonoids, phenols, and terpenoids, indicating broad medicinal potential. The extract showed strong antioxidant activity and free-radical scavenging, potentially mitigating oxidative stress associated with anaemia. Significant antifungal activity was observed in the extract, whereas the NPs exhibited notable antibacterial effects. FTIR confirmed phenolics, carboxylic acids, and amines. Docking revealed ursolic acid binding EPOR ($\Delta G = -7.82$ kcal/mol), rosmarinic acid interacting with ER α , β -amylin and ursolic acid targeting MIF, and rutin binding transferrin ($\Delta G = -8.69$ kcal/mol), supporting iron transport. Kaempferol and rosmarinic acid displayed favorable ADME profiles, suggesting drug-like potential.

Conclusion: *Justicia carnea* and its biosynthesized nanoparticles demonstrate significant antioxidant, antimicrobial, and anti-anaemic activities, highlighting their potential as safe, cost-effective, and multifunctional therapeutic agents against anaemia.

Please cite this paper as:

Gbadamosi AS, Oloketuyi KB, Oseni MO, Oseni OA. Biochemical and antimicrobial studies of metallic nanoparticles synthesized from *Justicia carnea* extract: molecular docking of its phytochemicals for anti-anaemic potential. Journal of Biochemicals and Phytomedicine. In press. doi: 10.34172/jbp.2025.x11