Integrated Anti-Inflammatory Compounds Database for Wound Management Using Phyto-Fabricated Zinc Oxide Nanoparticles; In Vitro, In Vivo and Computational Approach

Arusa Aftab*
Department of Botany, Lahore College for Women University, Lahore, Pakistan.
*E-mail: arusakashif@gmail.com

ABSTRACT

Introduction: Green nanoparticles being sustainable, having small size, large surface area, and controlled release capabilities can easily penetrate to deeper layers. These are ideal carriers for targeted drug delivery to the affected skin areas slowly and steadily and have least side effects. Inflammation, is characterized by swelling, redness and pain. The excessive use of anti-inflammatory drugs i.e., diclofenac, ibuprofen, naproxen and aspirin cause drastic effects on the vital organs like kidney, liver and digestive tract.

Objectives: The present study was planned to evaluate the in vitro anti-inflammatory (protein denaturation inhibition and hemolysis assay) and in vivo (wound healing in rabbits) associated with antioxidant and antibacterial (against inflammation causing microbes) from Solanum nigrum L. and Solanum americanum M.

Methodology: The aqueous leaf extract and phytofabricated ZnO nanoparticles were assessed during the procedure. The nano-coated bandage was formulated and checked its efficacy in wound healing among rabbits (Odongo *et al*., 2023). The macerated aqueous extract was prepared using leaf samples from both plants at 50 µL, 100 µL and 150 µL concentrations (Chen *et al.*, 2022; Lyimo *et al*., 2022). The wound healing of tissues was analyzed through histopathological analysis (Chandran *et al.*, 2017).

Key Findings: The results indicated that T7 (Aqueous extract of S. nigrum) and T14 (S. americanum mediated ZnO NPs) bandages showed best wound healing. The ZnO nanocoated bandage exhibited paramount anti-inflammatory property hence could be a better source to manage inflammation in replacement of allopathic drugs. Phytochemical constituents of the aqueous leaf extract were analyzed through GCMS analysis and their inflammatory disease-associated targets were assessed through network pharmacology (in silico approach). The phytocheicals identified through GC-MS and network pharmacology were (12-Methyl-E, E-2, 13-octadecadien-1-ol, kaempferol, 9,9-Dimethoxybicyclo[3.3.1]nona-2,4-dione, oleic acid, 13-tetradecenal, quercetin and cis-5-Methl-2-isopropyl-2-hexen-1-ol), pterosterone, cannabisin F, 6-Hydroxyluteolin 7-sophoroside, kaempferol, ursolic acid, rutin, N-trans-pcoumaroyloctopamine, N-methylsolasodine, N-trans-p-feruloyloctopamine and N-trans-p-feruloytyramine).

Conclusion: The compounds; kaempferol and quercetin were identified from both GCMS and network pharmacological analysis. Protein-protein interaction (PPI) network identified 112 inflammation associated gene targets. The top 3 hub genes were TNF, IL6 and AKT1 were found to replace synthetic medications targeting TNF, AKT1, and EGFR through drug repurposing like. Revitalization analysis also highlighted three genes (TNF, AKT1 and EGFR) strongly correlated with FDA-approved drugs. Summary of outcomes, implications, and recommendations.

Keywords: Drug Revitalization, Inflammation, *In-silico*, Pharmaceutical, Repurposing.

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