

Molecular Docking Approaches in Evaluating Antidiabetic, Neuroprotective, and Wound Healing Potential of Plant-based Nanosuspensions

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Abstract

Diabetes mellitus is a chronic metabolic disorder associated with debilitating complications such as cognitive dysfunction and impaired wound healing. Conventional therapies largely focus on glycemic control and remain insufficient to address the complex molecular mechanisms underlying these complications. Plant-derived bioactive compounds exhibit antidiabetic, neuroprotective, and wound-healing properties; however, their clinical application is limited by poor solubility and low bioavailability. Plant-based nanosuspensions have emerged as an effective delivery strategy to enhance the pharmacological performance of phytochemicals. Molecular docking plays a crucial role in elucidating ligand-protein interactions and identifying key molecular targets involved in glucose metabolism, neuroinflammation, neurodegeneration, angiogenesis, and extracellular matrix remodeling. This review highlights docking-guided insights into the multitarget activity of phytochemicals incorporated into nanosuspensions and correlates *in silico* predictions with experimental evidence. Advances in docking methodologies, nanotechnology, and systems pharmacology support the rational development of multifunctional herbal nanosystems for the management of diabetes and its associated complications.

Key words: Diabetes mellitus, molecular docking, herbal nanosuspensions, phytochemicals, neuroprotection, wound healing, multitarget therapy