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Computational Docking Study of Mangiferin with Human Umbilical Cord and Umbilical Cord Derived Exosomal Protein Targets

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ABSTRACT

Introduction

Colorectal cancer is one of the leading causes of cancer-related mortality worldwide, highlighting the need for improved therapeutic strategies. Natural bioactive compounds have gained attention due to their diverse pharmacological activities and lower toxicity. Mangiferin, a xanthone glycoside from Mangifera indica, is known for its antioxidant, anti inflammatory, and anticancer properties. In regenerative medicine, human umbilical cord–derived mesenchymal stem cells and their extracellular vesicles (exosomes) play an important role in cell communication and therapeutic applications. These vesicles contain proteins and signaling molecules that can influence cellular processes. Therefore, the present study aims to evaluate the molecular interaction between mangiferin and selected human umbilical cord and umbilical cord-derived exosomal protein targets using in-silico molecular docking analysis.

Methods The three-dimensional structure of mangiferin was obtained from chemical databases and prepared as the ligand for docking analysis. Protein structures related to human umbilical cord tissues and umbilical cord-derived exosomes were retrieved from protein databases. Molecular docking studies were carried out using AutoDock-based computational tools to determine binding affinity and interaction patterns between mangiferin and the selected protein targets. The docked complexes were further analyzed using molecular visualization software to identify binding energy values, hydrogen bond interactions, and amino acid residues involved in ligand–protein binding.

Results Docking results indicated that mangiferin exhibited stable binding interactions with several human umbilical cord and exosome-associated protein targets. The ligand demonstrated favorable binding energies and formed multiple hydrogen bonds and hydrophobic interactions within the active sites of the proteins, suggesting strong molecular affinity and stable ligand–protein complexes.

Conclusion This in-silico docking study indicates that mangiferin interacts with human umbilical cord and exosomal protein targets, suggesting potential relevance in regenerative, exosome-based therapeutic approaches and supporting further studies on its possible role in cancer research