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Abstract

In Silico Approaches to Evaluate the Binding Affinity of Verbascoside on Sirtuin1 (SIRT1) Receptor for the Treatment of Diabetic Wound Healing †

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Abstract: Diabetes mellitus is one of the leading metabolic disorders which leads to chronic wounds of the lower limbs. Complications such as abnormal vasculopathy and functioning of endothelial cells, decreased glucose-6-phosphate dehydrogenase, inadequate remodeling of extracellular matrix, decreased nitric oxide synthase, neuropathy, and secondary infections delay the process of wound healing, which finally leads to amputation of the lower extremities. In vitro and in vivo studies exploring the role of the SIRT1 receptor in diabetic wounds have shown decreased expression of the receptor along with an increase in the levels of reactive oxygen species (ROS). Treatment with specific SIRT1 agonists in animal models has demonstrated an increase in angiogenesis and a faster rate of wound healing. Verbascoside has a potential role in wound healing by proliferation and keratinocyte migration, synthesis of extracellular matrix, increasing neutrophil and macrophage function, and increasing angiogenesis. Thus, a molecular docking study was conducted to evaluate the interaction between Verbascoside and the SIRT1 receptor (PDB ID: 4ZZJ). The least binding energy was found to be −9.6 kcal/mol, which suggested a high binding interaction between the receptor and the ligand. The interacting amino acids include ARG274, GLU467, PRO468, LEU469, PRO470, PHE474, GLU477, ARG649, and VAL657, which is the common binding pocket for polyphenols. However, in vitro and in vivo studies are required to further evaluate the activity of verbascoside in diabetic wound healing.

Keywords: binding interaction; chronic wounds; extracellular matrix; metabolic disorders; reactive oxygen species

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