

Development of selective human matrix metalloproteinases-9 (hMMP-9) inhibitors as potent diabetic wound healing agents

Authors : Geetakshi Arora, Danish Malhotra

Abstract : Diabetic wounds are serious health issues and often fail to heal, leading to limb amputation that makes the life of the patient miserable. Delayed wound healing has been characterized by an increase in matrix metalloproteinase-9 (MMP-9). Thus research throughout the world has been going on to develop selective MMP-9 inhibitors for aiding diabetic wound healing. Bioactive constituents from natural sources always served as potential leads in drug development with high rates of success. Considering the need for novel selective MMP-9 inhibitors and the importance of natural bioactive compounds in drug development, we have screened a library of bioactive constituents from plant sources that were effective in diabetic wound healing on human MMP-9 (hMMP-9) using molecular docking studies. Screened constituents are ranked according to their dock score, ΔG value (binding affinity), and Ligand efficiency evaluated from FlexX docking and Hyde scoring modules available with drug designing platform LeadIT. Rhamnocitrin showed the highest correlation between dock score, ΔG value (binding affinity), and Ligand efficiency was further explored for binding interactions with hMMP-9. The overall study suggest that Rhamnocitrin is sufficiently decorated with both hydrophilic and hydrophobic substitutions that perfectly block hMMP-9 and act as a potential lead in the design and development of selective hMMP-9 inhibitors.

Keywords : MMP-9, diabetic wound, molecular docking, phytoconstituents

Conference Title : ICCPAPC 2022 : International Conference on Clinical Pharmacology and Advanced Pharmaceutical Chemistry

Conference Location : Auckland, New Zealand

Conference Dates : December 02-03, 2022