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ABSTRACT

A breach in epithelial lining from trauma or disease leads to wound formation. Wounds can vary in depth and can be incised, chopped, lacerated or a complex type depending upon the inducing agent and the direction of force applied. An untreated wound follows the natural course of healing that comprises of four phases. Prior to remodeling, the final phase in wound healing, proliferation phase initiates when the fibroblasts start depositing new extracellular matrix. Sometimes, the remodeling is compromised and there is excessive matrix deposition. This phenomenon is termed fibrosis. A number of signal transduction pathways orchestrate the wound healing and a disparity in the interaction leads to fibrosis. Transforming Growth Factor Beta (TGF-β) pathway acts as a hub in the whole interaction of wound healing and an abnormal response in its receptor has been confirmed to be the root cause of fibrosis. In the current project, TGF-β receptor was investigated as the target protein to alleviate fibrosis using bioinformatics tool. Briefly, the structures of TGF-β receptors were retrieved from PDB. A series of natural and synthetic drugs were searched and the corresponding structures were retrieved from PUBCHEM database. Ligand-receptor docking was done using Swiss-dock software. The structure of best docked ligand i.e. α-tocopherol was modified in ChemSketch followed by docking. Both virgin and the modified α-tocopherol can act as novel drug against excessive fibrosis; however it needs final validation *in vitro* and *in vivo*.

Key Words – Wound; Fibrosis; TGF-β; Bioinformatics tools; Docking