Homology modeling and molecular docking studies on Type II diabetes complications reduced PPAR γ receptor with various ligand molecules

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ABSTRACT

Peroxisome proliferator-activated receptor gamma (PPAR γ), a type II nuclear receptor present in adipose tissue, colon and macrophages. It reduces the hyperglycemia associated metabolic syndromes. Particularly, type II diabetes-related cardiovascular system risk in human beings. The fatty acid storage and glucose metabolism are regulated by PPAR γ activation in human body. According to recent reports commercially available PPAR γ activating drugs have been causing severe side effects. At the same time, natural products have been proved to be a promising area of drug discovery. Recently, many studies have been attempted to screen and identify a potential drug candidate to activate PPAR γ . Hence, in this study we have selected some of the bio-active molecules from traditional medicinal plants. Molecular docking studies have been carried out against the target, PPAR γ . We Results suggested that Punigluconin has a efficient docking score and it is found to have good binding affinities than other ligands. Hence, we concluded that Punigluconin is a better drug candidate for activation of PPAR γ gene expression. Further studies are necessary to confirm their efficacy and possibly it can develop as a potential drug in future. © 2017 Elsevier Masson SAS. All rights reserved.