ORIGINAL RESEARCH ARTICLES

MOLECULAR DOCKING AND ADMET BASED MINING OF NATURAL COMPOUNDS FROM *PTEROCARPUS MARSUPIUM* AGAINST PRIME TARGETS OF DIABETES MELLITUS

Siddhi S. Tambe[a]*, Rohini R. Pujari[a], Vishnu P. Chaudhari[a] and Sandesh Lodha[b]

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ABSTRACT

In the Ayurvedic system of medicine, *Pterocarpus marsupium* Linn bark extract is used for the treatment of diabetes. It has a rich profile of chemical constituents. However, phytochemicals with antidiabetic activity are not reported yet. To comprehend more about this plant's antidiabetic mechanism of action, 26 reported phytochemicals, namely, pterostilbene, marsupsin/ carpusin, 7-O-α-L-rhamnopyranosyloxy-4′-methoxy-5-hydroxy isoflavone, (-)-epicatechin, pterosupin, liquiritigenin, vijayoside, pteroside, propterol-b, beta-eudesmol, pseudobaptigenin, isoliquiritigenin, garbanzol, 5-de-oxykaempferol, catechol, gallic acid, 3,4-dihydroxybenzoic acid, naringetol, 4-hydroxybenzaldehyde, trans-stilbene, 3,7,4′-trihydroxyflavone, 7,4′-dihydroxyflavone, (2*S*)-7-hydroxyflavanone, oleanolic acid, lupeol and marsupol/ebanol, were subjected to molecular docking studies using six targets of diabetes, namely, *C* and *N*-terminal subunits of human maltase-glucoamylase, glucagon like peptide-1, *N*-terminal sucrase-isomaltase, human peroxisome proliferator-activated receptor –α and ϒ. The docking studies were carried out using PyRx and AutoDock Vina 1.1.2 software. Compounds with optimum binding affinity were subjected to evaluate drug likeliness and toxicity using SwissADME and admetSAR web tools. Vijayoside was found to have maximum affinity (-8.5 Kcal mol^{-1}) with *N*-terminal subunit of human maltase-glucoamylase. The binding energies of O-α-L-rhamnopyranosyloxy-4'-methoxy-5-hydroxy isoflavone was found to be maximum with *C*-terminal (-10.0 Kcal mol^{-1}). Danugliprion, a standard, was found to have maximum binding affinity (-11.4 Kcal mol^{-1}) with glucagon-like peptide-1. Pteroside was found to bind favorably (-7.5 Kcal mol^{-1}) with *N*-terminal sucrase-isomaltase.7-O-α-L-rhamnopyrancsyloxy-4′-methoxy-5-hydroxy isoflavone has exhibited stable interactions with other receptors (-10.2 and -8.2 Kcal mol^{-1} for human peroxisome proliferator-activated receptor–α and ϒ). These three phytochemicals also exhibited druggability properties. Further *in vitro* and *in vivo* studies may fully validate the results.