

Molecular Docking Studies Involving the Inhibitory Effect of Gymnemic Acid, Trigonelline and Ferulic Acid, the Phytochemicals with Antidiabetic Properties, on Glycogen Synthase Kinase 3 (A&B)

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ABSTRACT

Type 2 diabetes mellitus is a multidimensional endocrine disorder arises due to insulin resistance coupled with insufficient insulin secretion. Chronic hyperglycemia in diabetes is known to affect most of the vital organs in the system which ultimately results in the dysfunction of major metabolic pathways. Several drugs are commercially available to maintain normoglycemia in diabetic individuals through the regulation of biological functions such as controlling the absorption of glucose in the intestine, increasing the insulin sensitivity, improvement in the secretion of insulin, prevention of excessive breakdown of glucose as well as gluconeogenesis and enhancement of glycogen synthesis. Among the various clinical approaches to maintain the blood glucose level within the physiological range, the regulation of glycogen metabolism is considered as a major target in the prognosis of diabetes mellitus. Since, most of the currently available drugs elicit undesirable side effects in addition to the development of resistance after prolonged use, the search for lead molecules preferably from plant origin still continues. Recently, we have formulated a mixture containing three phytochemicals from medicinal plants namely Gymnemic acid, Trigonelline and Ferulic acid in the ratio of 2:3:1 and systematically evaluated its antidiabetic efficacy in high fat diet fed-low dose STZ induced type 2 diabetes in rats. The present study is aimed to conduct molecular docking studies involving the inhibitory effect of individual components in the mixture, the phytochemicals with antidiabetic properties on glycogen synthase kinase 3 (A&B). The data obtained evidenced the regulatory role of GTF in the regulation of glycogen metabolism.