ABSTRACT

Diabetes mellitus (DM) is a complex mulitifactorial metabolic disorder resulting from either insulin insufficiency or insulin dysfunction. In the present study, the phytocompounds were selected from traditionally used medicinal plants and nutraceuticals and the selected targets for Diabetes Mellitus were Peroxisome Proliferator Activate Receptor gamma, Fructose 1-6 bisphosphate and Dipeptidyl peptidase IV. Using Glide (Schrodinger module), in silico docking of the phytocompounds with these targets was carried out and their efficacy was evaluated against DM. The docking results of the phytocompouds were compared with the corresponding synthetic drugs in order to explore the multi -targeting efficiency of the phytocompounds for treating diabetes. Of the 27 selected compounds from 12 plants, Glucobrassicin present in Capparis spinosa and Brassica oleracea (Broccoli) and Epigallocatechin gallate (EGCG) present in Camellia sinensis showed better interactions and glide score with all the 3 receptors than the corresponding drugs / inhibitor. From the present study it is concluded that the phytocompounds can be used as an appropriate lead molecules against diabetes. Further the nutraceuticals, Aegle marmelos, Brassica oleracea, Glycine max, Zingiber officinale, Capparis spinosa and Trigonella foenum graecum can be added as food supplement to reduce the risk of diabetes.