GC-MS and molecular docking studies of *Hunteria umbellata* methanolic extract as a potent antidiabetic agent

The purpose of this study was to investigate the diabetic effect of phytocompounds synthesized from *Hunteria umbellata* using GC-MS analysis and molecular docking studies. Peroxisome proliferator-activated receptor gamma (PPAR-γ) agonists are beneficial in the treatment of diabetes by stimulating insulin sensitivity and antagonizing hepatic gluconeogenesis. The aim of the present study was to investigate PPAR-γ agonist property of phytocompounds from *Hunteria umbellata* using in silico approach. Molecular docking of *Hunteria umbellata* on human PPAR-γ protein was determined by Auto/Vina in Pymol 4.2 and compared with Glibenclamide, a known agonist of PPAR-γ. Our present study reports the phytochemical analysis of the extracts of the seeds and leaves of *Hunteria umbellata*. Twenty one compounds were revealed through GC-MS analysis and screened using AutoDock/Vina against PPAR-γ. Docking studies recommended that 2,2-Benzylidenebis (3-methylbenzofuran) an existing phytochemical from the seed of *Hunteria umbellata* had the highest fitness score of -11.3 Kcal/mol and hence could be a potent antidiabetic drug. *Hunteria umbellata* seed extract and its compound 2,2-Benzylidenebis (3-methylbenzofuran) have a significant antidiabetic activity against PPAR-γ. Molecular binding interaction of an in silico data demonstrated that 2,2-Benzylidenebis (3-methylbenzofuran) has more specificity towards the PPAR-γ binding site and could be a potent antidiabetic compound.

Biography

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