

In vitro and in silico evaluations of diarylpentanoid series as α -glucosidase inhibitor

ABSTRACT

A series of thirty-four diarylpentanoids derivatives were synthesized and evaluated for their α -glucosidase inhibitory activity. Eleven compounds (19, 20, 21, 24, 27, 28, 29, 31, 32, 33 and 34) were found to significantly inhibit α -glucosidase in which compounds 28, 31 and 32 demonstrated the highest activity with IC₅₀ values ranging from 14.1 to 15.1 μ M. Structure-activity comparison shows that multiple hydroxy groups are essential for α -glucosidase inhibitory activity. Meanwhile, 3,4-dihydroxyphenyl and furanyl moieties were found to be crucial in improving α -glucosidase inhibition. Molecular docking analyses further confirmed the critical role of both 3,4-dihydroxyphenyl and furanyl moieties as they bound to α -glucosidase active site in different mode. Overall result suggests that diarylpentanoids with both five membered heterocyclic ring and polyhydroxyphenyl moiety could be a new lead design in the search of novel α -glucosidase inhibitor.

Keyword : Diarylpentanoids; α -Glucosidase inhibitory activity; Docking; Polyhydroxyphenyl; Furanyl