Chalcones: As Potent α-Amylase Enzyme Inhibitors; Synthesis; *In Vitro*, and *In Silico* Studies

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ABSTRACT

Introduction: Chalcone possesses a wide range of biological activities. Trans-chalcone (1,3-diphenyl-2-propen-1-one), is found abundantly in edible plants and acts as a precursor for the biosynthesis of flavonoids and isoflavonoids. Theα, β-unsaturated character in chalcones is responsible for their pharmacological properties i.e. anticancer, antioxidant, antifungal, anti-inflammatory, antiprotozoal, antimalarial, antibacterial [19], and tyrosinase, β-lactamase and α-amylaseenzymes inhibition. The inhibition of α-amylase enzyme is one of the best therapeutic approaches for the management of type II diabetes mellitus.

Objective: In the current study chalcone derivatives (**1-17**) were synthesized and evaluated their inhibitory potential against α-amylase enzyme

Method: For that purpose, a library of substituted (*E*)-1-(naphthalene-2-yl)-3-phenylprop-2-en-**1**-ones was synthesized by Claisen-Schmidt condensation reaction of 2-acetonaphthanone and substituted aryl benzaldehyde in the presence of base and characterized via different spectroscopic techniques such as EI-MS, HREI-MS, ^{1}H-, and ^{13}C-NMR.

Result: seventeen synthetic chalcones were evaluated for *in vitro* porcine pancreatic α-amylase inhibition. All the chalcones demonstrated good inhibitory activities in the range of IC50 = 1.25 ± 1.05to 2.40 ± 0.09 μM as compared to the standard commercial drug acarbose (IC50 = 1.34 ± 0.3 μM).

Conclusion: Chalcone derivatives (**1-17**) were synthesized, characterized, and evaluated for their α-amylase inhibition. SAR revealed that electron donating groups in the phenyl ring have more influence on enzyme inhibition. However, to insight the participation of different substituents in the chalcones on the binding interactions with the *α*-amylase enzyme, *in silico* (computer simulation) molecular modeling analyses were carried out.

Keywords: Chalcones, synthesis, diabetes mellitus, α-amylase enzyme inhibition, in vitro, molecular docking.

REFERENCES

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