Non-edible part of *Capsicum annuum*- novel source of Acetylcholinesterase inhibition: Molecular docking and in vitro enzymatic studies

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Abstract

Alzheimer's disease (AD) is the most common form of dementia effecting the aging population of the world. It is more fatal than other diseases like cancer, stroke, and heart disease. Enhancement of acetylcholine levels in the brain is one means of treating the disease. However, the drugs presently used in the management of the disease have various drawbacks. New treatments are required to get the potential inhibitors. In this study, extract of *Capsicum annuum* were evaluated to determine their antioxidant and Acetylcholinesterase inhibitory (AChEI) activity. The DPPH and β-carotene assays were used to determine antioxidant activity and Ellman's colorimetric method to quantify AChEI activity. Although both ethanolic and aqueous extracts showed activity in both assays, the ethanolic extract of *C. annuum* was found to contain the highest AChEI activity (IC_{50} = 0.03 ± 0.08 mg/ml) and the antioxidant activity (β-carotene; IC_{50} = 0.14 ± 0.08 mg/ml and DPPH; IC_{50} = 0.23 ± 0.01 mg/ml). The results suggest that the tested plant may provide a substantial source of secondary metabolites, which act as natural antioxidants and acetylcholinesterase inhibitors, and may be beneficial in the treatment of AD.

AChE structure shows that the enzyme possesses a deep narrow gorge which penetrates halfway into the enzyme, where the catalytic site resides (Kryge et al., 2000). The binding site of AChE consists of five subsites: a peripheral anionic site (PAS), an acyl binding pocket (ABP), the esteratic site (ES), an oxyanion hole (OH) and an anionic subsite (AS).

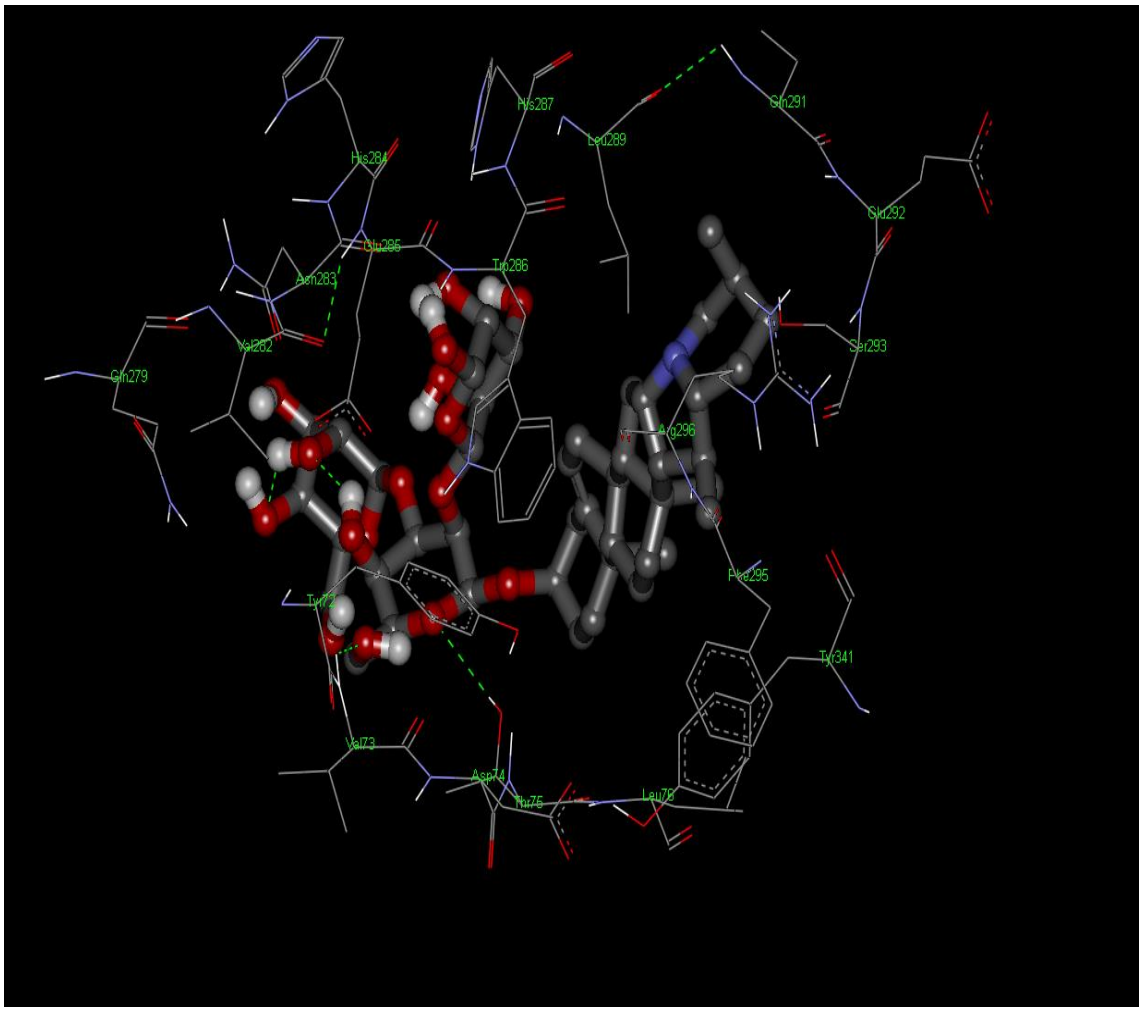

Figure 1: Representations of the molecular model of the complex formed between α-solanine and AChE. 3D representation of the ligand-enzyme binding interactions. α-chaconine is represented as a dark grey sticks and hydrogen bonds as green dashed lines.

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