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Insilico molecular docking analysis of isolated compounds of *Ocimum sanctum* against two related targets to diabetes

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Abstract
Background: To investigation antidiabetic activity of the isolated compounds of *Ocimum sanctum* against two responsible proteins α-amylase enzyme and Glucokinase.
Methodology: For this purpose we subjected the active compounds of *Ocimum sanctum* of to reveal its potentiality by molecular docking analysis to find out its potent compound against Diabetics which was done by Maestro v 10.1 (Schrodinger) docking analysis.
Results: A wide range of docking score found during molecular docking by Maestro v 10.1 (Schrodinger). Among of the compounds Carvacrol had the lowest docking score against α-amylase enzyme and Glucokinase which is -5.581 kj/mol and -7.322 kj/mol respectively.
Conclusion: Carvacrol from *Ocimum sanctum* detected with significant docking score which may be a potent antidiabetics compound because the less the docking score will be, the compound will be more potent.

Keywords: *Ocimum sanctum*, α-amylase enzyme, glucokinase, molecular docking

Introduction
Diabetes mellitus is a major cause of morbidity and mortality and its global prevalence is growing rapidly [1-3]. It causes serious endocrine syndrome with poor metabolic control and responsible for increased risk of diseases such as atherosclerosis, renal failure, blindness [4-6]. The most common endocrine disorders are characterized by hyperglycemia, hypercholesterolemia and hypertriglyceridemia, resulting from defects in insulin secretion or reduced sensitivity of the tissue to insulin (insulin resistance) and/or combination of both [7-9]. A large number of studies are ongoing to spot natural substances that are effective in reducing the severity of diabetes. Ayurveda is a science that uses herbal medicines. From earlier period, a number of these herbal preparations are used in the treatment of diabetes. Even The World Health Organization (WHO) approves the use of plant drugs for various diseases, together with diabetes mellitus [10, 11]
Molecular docking is an importance methodologies in the making plans and layout of new drugs. These strategies goal to expect the experimental binding mode and affinity of a small molecule within the binding site of the receptor target of interest. A successful docking methodology must be able to correctly predict the native ligand pose the receptor binding site (i.e.to find the experimental ligand geometry within a certain tolerance limit) and the associated physical-chemical molecular interactions [12, 13]
Ocimum sanctum L. (also known as Ocimum tenuiflorum, Tulsi) has been used for thousands of years in Ayurveda for its diverse healing properties. Tulsi, the Queen of herbs, the legendary 'Incomparable one' of India, is one of the holiest and most cherished of the many healing and healthy giving herbs of the orient. The sacred basil, Tulsi, is renowned [14, 15] for its religious and spiritual sanctity, as well as for its important role in the traditional Ayurvedic and Unani system of holistic health and herbal medicine of the East [13]. The leaves are demulcent, expectorant and antipyretic; juice is used for the treatment of coughs, colds, catarrh and bronchitis; useful in gastric disorder, earache, ringworm, leprosy and itches. An infusion of the leaves is used as a stomachic in gastric disorders of childrens, and in hepatic affections. The dried leaves are powdered and employed as a snuff in ozoena. The plant drives away mosquitoes. [16] Essential oil of the leaves and inflorescences possess good antifungal and

antibacterial properties [17]. Water extract showed significant biological activity against Mycobacterium tuberculosis [18]

Materials and Methods

In silico analysis

Molecular docking analysis of isolated compounds

Protein Preparation

Three-dimensional crystal Structure of Alpha amylase (PDB ID: 1PPI) and Glucokynase (PDB ID: IVAS) was downloaded in pdb format from the protein data bank. After that, the structure was prepared and refined using the Protein Preparation Wizard of Schrödinger-Maestro v10.1. Charges and bond orders were assigned, hydrogens were added to the heavy atoms, selenomethionines were converted to methionines, and all waters were deleted. Using force field OPLS_2005, minimization was carried out setting maximum heavy atom RMSD (root-mean-square-deviation) to 0.30 Å.

Ligand Preparation

Compounds were retrieved from PubChem databases, i.e. Carvacrol, Palmitic Acid, Stearic Acid and Vicenin. Then Ligands are prepared by Schrödinger-Maestro v10.1.

Glide Standard Precision (SP) ligand docking

SP flexible ligand docking was carried out in Glide of Schrödinger-Maestro v 10.1 [19, 20] within which penalties were applied to non-cis/trans amide bonds. Van der Waals scaling factor and partial charge cutoff were selected to be 0.80 and 0.15, respectively for ligand atoms. Final scoring was performed on energy-minimized poses and displayed as Glide score. The best-docked pose with lowest Glide score value was recorded for each ligand.

Results

In silico analysis

Molecular docking analysis

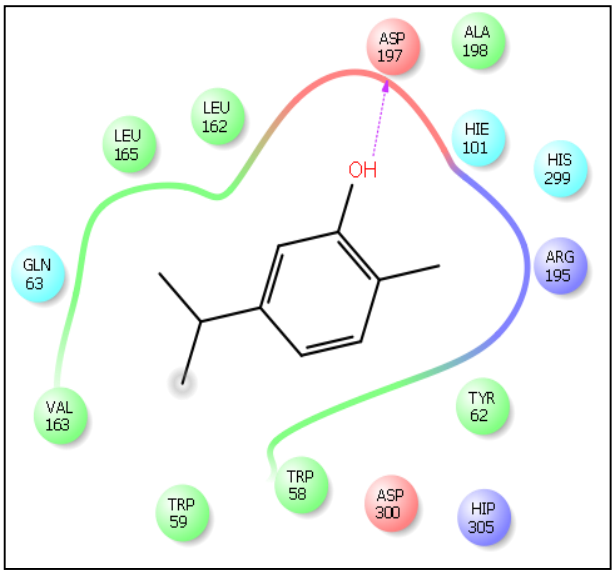
In this study, the binding mode of α-amylase enzyme and Glucokynase were investigated by doing computational analysis, glide docking. Both glide standard (SP) and extra precision (XP) mode had been introduced, where extra precision mode used for cross validation purpose. The results of docking analysis were described in Table 1 & 2 and the docking figure showed in Figure 1 & 2. Among all the compounds, Carvacrol showed well docking score againt both α-amylase enzyme and Glucokynase repectively.

Table 1: Docking results with Carvacrol, Palmitic Acid, Stearic Acid, Vicenin in the α-amylase enzyme (PDB: 1PPI).

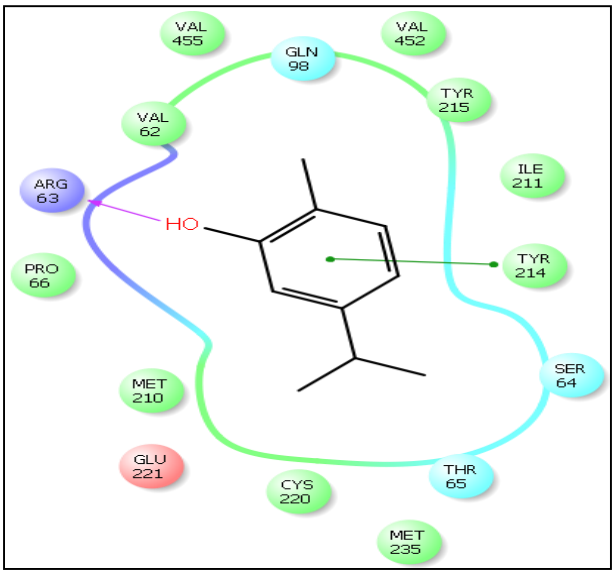
Compound name	Compound ID	Docking energy
Carvacrol	10364	-5.581
Palmitic Acid	985	1.377
Stearic Acid	5281	2.27
Vicenin	13644663	-5.495

Table 2: Docking results with Carvacrol, Palmitic Acid, Stearic Acid, Vicenin in the Glucokynase enzyme (PDB: IVAS)

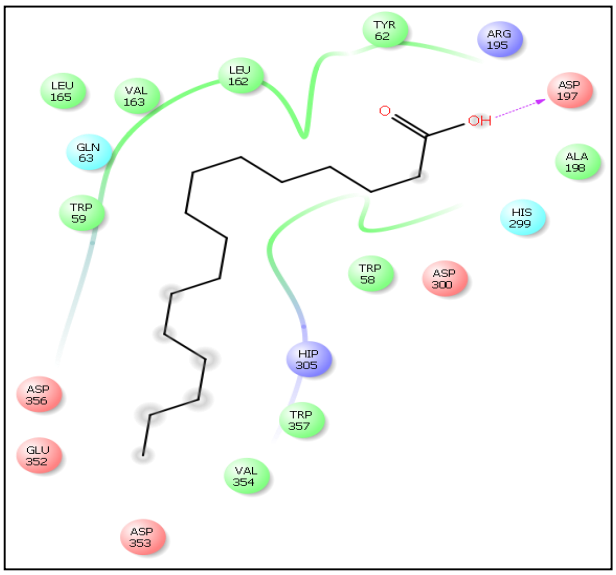
Compound name	Compound ID	Docking energy
Carvacrol	10364	-7.322
Palmitic Acid	985	-1.528
Stearic Acid	5281	1.034
Vicenin	13644663	-3.486



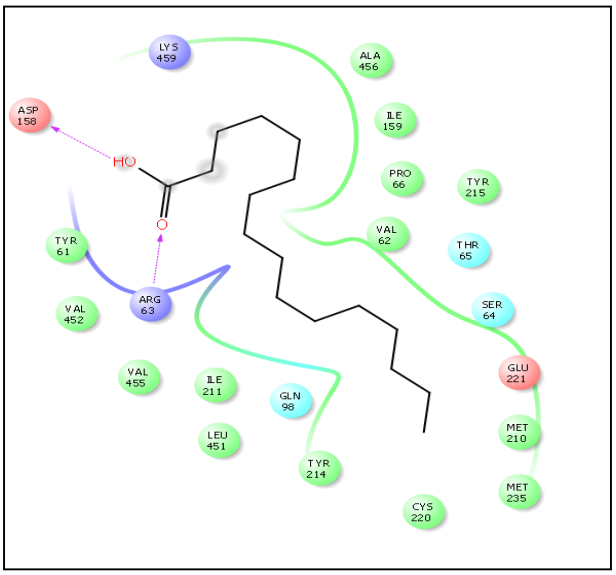
Carvacrol with Alpha amylase



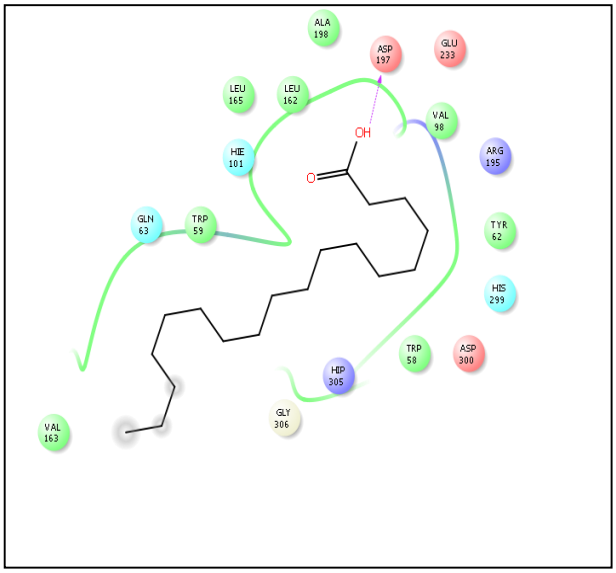
Carvacrol with Glucokynase



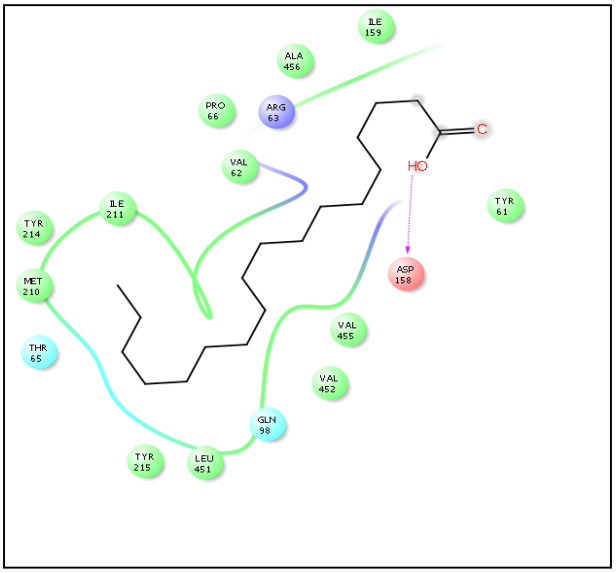
Palmitic Acid with Alpha amylase



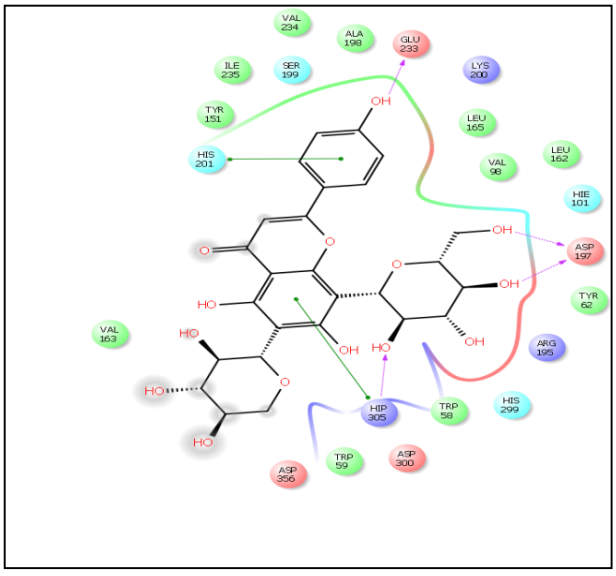
Palmitic Acid with Glucokynase



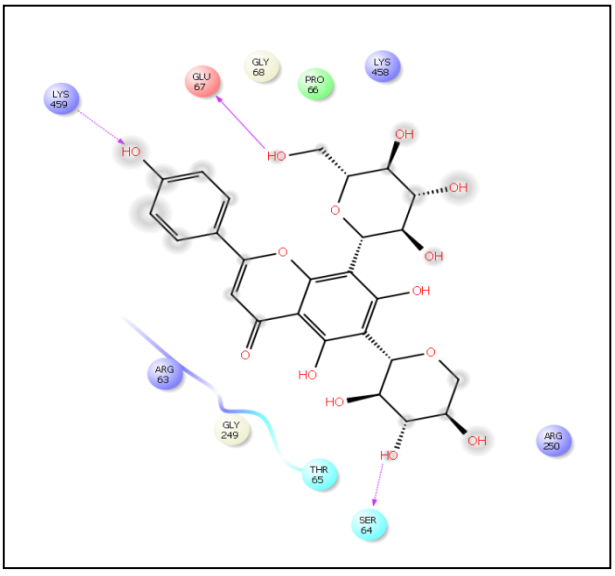
Stearic Acid with Alpha amylase



Stearic Acid with Glucokynase



Vicenin with Alpha amylase



Vicenin with Glucokynase

Fig 1: Docking figure of Carvacrol, Palmitic Acid, Stearic Acid, Vicenin with Alpha amylase (PDB ID: 1PPI) and Glucokynase (PDB ID: IVAS)

Discussions

Docking studies by Maestro v 10.1 (Schrodinger) showed that Carvacrol of *O. Snectum* had the lowest docking score respectively against both α-amylase enzyme and Glucokynase which are --5.581 kj/mol and -7.322 kj/mol. Carvacrol from *O. Snectum* detected with significant docking score which may be a potent anti-diabetic compound because the less docking score, the compound will be more potent.

Conclusion

Among all the compounds Carvacrol showed best docking score towards α-amylase enzyme and Glucokynase. So, Carvacrol is the best compounds for inhibiting of both, as it possessed best value in Molecular docking. Further *in vitro* and *in vivo* investigation need to identify α-amylase enzyme and Glucokynase inhibitory activity of isolated compounds from Ocimum sanctum.

Competing Interests

The authors declare that they have no competing interests.

Acknowledgment

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