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RESEARCH ARTICLE

In Silico Study of Some Isolated Compound Present in Ageratum *Conyzoides against* Diabetes

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Abstract

The present study aims to investigate the α-amylase inhibition by *in silico* molecular docking used for some selected compounds 6-methoxyquinoline-1-oxide, Alpha-cubebene, Beta-caryophyllene, Beta-sitosterol, Hydrogen Cyanide, Kaempferol and Quercetin-3, 7-diglucoside from *Ageratum conyzoides* to identify whether these compounds interact with the responsible protein (α-amylase enzyme). A wide range of docking score found during molecular docking by Schrodinger. 6-methoxyquinoline-1-oxide, Alpha-cubebene, Beta-caryophyllene, Beta-sitosterol, Hydrogen Cyanide, Kaempferol and Quercetin-3,7-diglucoside showed the docking scores -4.508 kj/mol, -4.892 kj/mol, -5.495 kj/mol, -3.783 kj/mol, -2.952 kj/mol, -7.706 kj/mol and -5.73 kj/mol respectively. Among all the compounds, Kaempferol showed highest docking score. So, Kaempferol is the best compounds for α-amylase inhibition, as it possessed higher value in Molecular docking. Further *in vivo* investigation need to identify whether isolated compounds from *Ageratum conyzoides* have α-amylase inhibitory activity or not.

Keywords: Ageratum conyzoides; Diabetes mellitus; Molecular docking; Kaempferol

Introduction

Diabetes has turned into a typical ailment these days. Individuals of various ages can be influenced by various kind diabetes because of failure of pancreas to deliver enough insulin or the safe cells to insulin. This is called Diabetes mellitus. As indicated by WHO Diabetes mellitus is an unending infection caused by acquired and additionally obtained inadequacy underway of insulin by the pancreas, or by the incapability of the insulin created. Such a lack brings about expanded convergences of glucose in the blood, which thus harm a significant number of the body's frameworks, specifically the veins and nerves. There are two principle forms of diabetes - Type 2 diabetes (formerly known as insulin-dependent) in which the pancreas fails to produce the insulin which is essential for survival.

This form develops most frequently in children and adolescents, but is being increasingly noted later in life. Type 2 diabetes (formerly named non-insulin-dependent) which results from the body's inability to respond properly to the action of insulin produced by the pancreas. Type 2 diabetes is substantially more typical and records for around 90% of all diabetes cases around the world. It happens most regularly in grown-ups, however is being noted progressively in young people too. As of late incorporated review information of WHO demonstrates that roughly 150 million individuals have diabetes mellitus around the world, and that this number may well twofold continuously 2025. Quite a bit of this expansion will happen in creating nations and will be because of populace development, maturing, undesirable eating regimens, stoutness and inactive ways of life [1-7].

Molecular docking is an imperative instrument in the improvement of new medications. Docking strategy permits describing the conduct of a test little particle in the coupling site of the receptor target of interest. A fruitful docking technique must have the capacity to effectively anticipate the local ligand represent the receptor restricting site (i.e.to locate the trial ligand geometry inside a specific resistance confine) and the related physical-compound molecular associations [8-11].

Ageratum conyzoides is a species of flowering plant of the genus *Ageratum* in the Asteraceae family. Tropical America, especially Brazil, and considered an invasive weed in many other regions. It is an herb that is 0.5–1 m. high, with ovate leaves 2–6 cm long, and flowers are white to mauve. It is a herb that is 0.5– 1 m. high, with praise leaves

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2– 6 cm long, and blooms are white to mauve [12,13]. We have selected the plant *Ageratum conyzoides* which gave remarkable anti-diabetic effects on rats. The hypoglycaemic and antihyperglycaemic properties of the aqueous extracts of the leaves of *Ageratum conyzoides L.* were evaluated in normoglycemic and in streptozotocin-induced diabetic rats, in order to validate its use in folk medicine. So, we selected this plant for *in silico* computational analysis to examine its effects on Alpha- amylase protein enzyme. This two protein enzyme plays important role in controlling the blood glucose level. Also to analyses the effects of bio availabilities of these plant in human body [14-18].

As a therapeutic plant, *Ageratum conyzoides* is generally utilized by numerous customary societies, against loose bowels and diarrhea.It is additionally a bug spray and nematicide. *A. conyzoides* is inclined to turning into an uncontrolled ecological weed when become outside of its normal range. It is an obtrusive weed in Africa, Australia, Southeast Asia and the USA.It is viewed as a direct weed of rice development in Asia.

Methods and Materials

Protein preparation

Three dimensional protein structure of Alpha-amylase (PDB ID: 1PPI) was downloaded in pdb sort out from the protein data bank. Starting there forward, structure was arranged and refined using the Protein Preparation Wizard of Schrödinger-Maestro v10.1. Charges and bond orders were assigned, hydrogens were added to the staggering particles, selenomethionines were changed over to methionines and all waters were eradicated. Using power field OPLS_2005, minimization was finished setting most extraordinary considerable particle RMSD (root-mean-square-deviation) to 0.30 Å.

Ligand preparation

Compounds were reprocessed from PubChem databases i.e 6-methoxyquinoline-1-oxide (Pubchem ID: 253821), Alpha-cubebene (Pubchem ID: 86609), Beta-caryophyllene (Pubchem ID: 5281515), Beta-sitosterol (Pubchem ID: 222284), Hydrogen Cyanide (Pubchem ID: 768), Kaempferol (Pubchem ID: 5280863) and Quercetin-3,7-diglucoside (Pubchem ID: 10121947).

Receptor grid generation

Receptor grids were calculated for prepared proteins such that various ligand poses bind within the predicted active site during docking. In Glide, grids were generated keeping the default parameters of van der Waals scaling factor 1.00 and charge cutoff 0.25 subjected to OPLS 2001 force field. A cubic box of specific dimensions centred on the centroid of the active site residues (Reference ligand active site) was generated for receptor. The bounding box was set to 14 Å × 14 Å × 14 Å for docking experiments.

Glide standard precision (SP) ligand docking

SP adaptable ligand docking was done in Glide of Schrödinger-Maestro v10.1 inside which disciplines were related with non-cis/trans amide bonds [19,20]. Van der Waals scaling variable and fragmentary charge cutoff was being 0.80 and 0.15, only for ligand particles. Keep going scoring was performed on imperatively limited positions and showed up as Glide score. The best docked posture

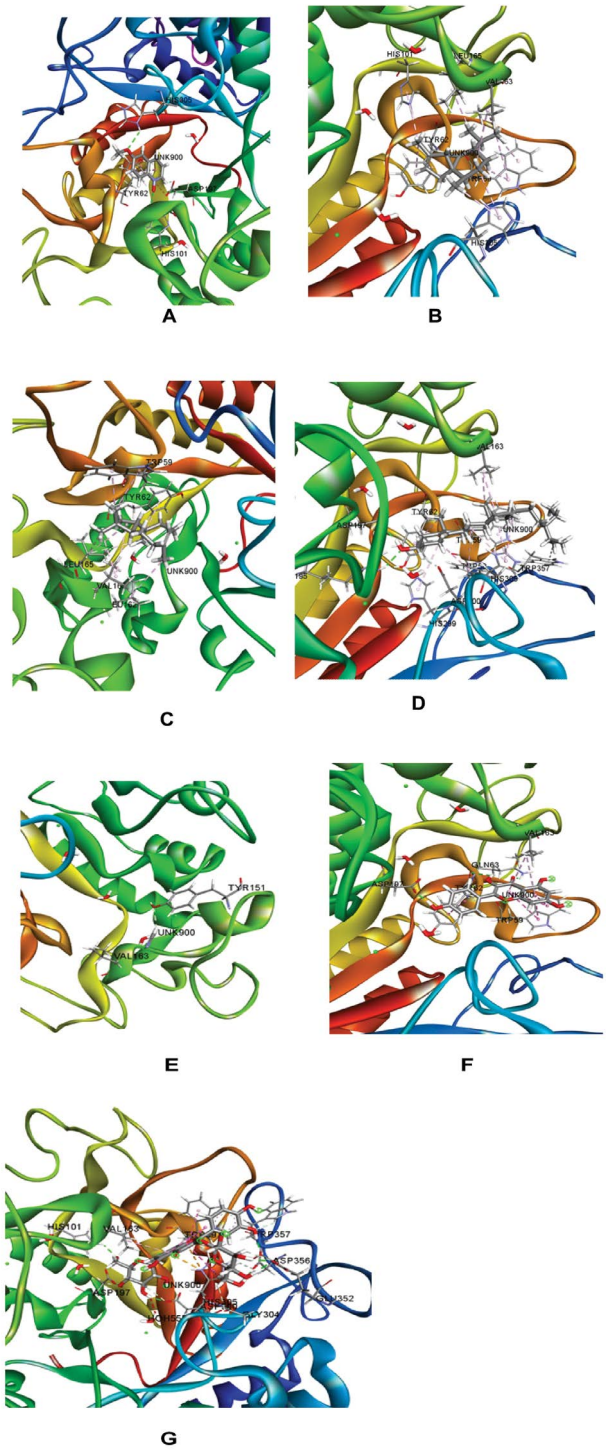

Figure 1: Docking analysis pose of A (6-methoxyquinoline-1-oxide), B (Alpha-cubebene), C (Beta-caryophyllene), D (Beta-sitosterol), E (Hydrogen Cyanide), F (Kaempferol) and G (Quercetin-3, 7-diglucoside) with Alpha amylase.

Compound Name	Compound ID	Docking Score	Glide Energy
6-methoxyquinoline-1-oxide	253821	-4.508	-20.364
Alpha-cubebene	86609	-4.892	-21.166
Beta-caryophyllene	5281515	-5.495	-20.109
Beta-sitosterol	222284	-3.783	-32.412
Hydrogen Cyanide	768	-2.952	-5.225
Kaempferol	5280863	-7.706	-43.246
Quercetin-3,7-diglucoside	10121947	-5.73	-63.943

Table1: Docking results of 6-methoxyquinoline-1-oxide, Alpha-cubebene, Beta-caryophyllene, Beta-sitosterol, Hydrogen Cyanide, Kaempferol and Quercetin-3, 7-diglucoside with Alpha-amylase PDB id: 1PPI.

with most unimportant Glide score respect was recorded for every ligand.

Result

In silico analysis Molecular docking analysis

In this examination, the coupling technique for α-amylase protein was investigated by doing computational examination, skim docking. Both Glid standard (SP) and extra exactness (XP) mode had been introduced, where extra precision mode used for cross approval reason. The consequences of docking examination were depicted in table 1 and the docking figure appeared in figure 1.

Discussion

Docking studies by Maestro v 10.1 (Schrodinger) showed that Kaempferol of *Ageratum conyzoides* had the lowest docking score respectively against both α-amylase enzymes which is -7.706 kj/mol. Kaempferol of *Ageratum conyzoides* 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

From above discussion we can assume that this plant can play a prominent role for anti-diabetic activity. As it has been accepted in following three experiments, we can suggest *Ageratum conyzoides* for further research to amend the activity of anti-diabetic for better effect.

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