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Research Article

In silico Study of Some Isolated Compound Present in *Capsicum Annum L.* against Diabetes

Nishan Chakrabarty[1], Susmita das[2], MD Jahid Hasan[3], Kutub Uddin Ahamed[1], MD Mehedi Hassan Don[2], Mohammad Manjur Rahman[4], AbidaAkter Akhi[2], MD Rakib Hasan[2], Saraban Tahora[2], and Nishat Rahman[5]*

[1]*Department of Pharmacy, Jagannath University, Bangladesh*
[2]*Department of pharmacy, Southeast University, Bangladesh*
[3]*Dept of Biochemistry and Molecular Biology, Jahangirnagar University, Bangladesh*
[4]*Department of Pharmacy, Gono University, Bangladesh*
[5]*GUSTO Research Group, Bangladesh*

***Corresponding author**
Nishat Rahman, Research Assistant, GUSTO research group Bangladesh, Email: nishatrahman.bgctub@gmail.com

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Abstract

Our pancreas makes a hormone called insulin. It's what lets our cells turn glucose from the food we eat into energy. People with type 2 diabetes make insulin, but their cells don't use it as well as they should. Since they get affected by the disease called Diabetes. Diabetes is a deep rooted illness that influences the way your body handles glucose, a sort of sugar, in your blood. From many years many experiment has taken place to discover the remarkable usage of various medicinal plants which can play an effective role against diabetes despite of chemical medications. As we know it is a very sensitive health issue many hazardous use of drugs may cause serious side effects. From this prospective we have reviewed the paper NATURAL PRODUCTS AND PLANTS AS POTENTIAL ANTIDIABETIC DRUGS. From which we have selected a medicinal plant *Capsicum annum l.* which has an active compound Phenolic acid, l Ascorbic acid, Alpha-tocopherol, Capsaicin, Carotenoids, and Capsinoids. And among them the compounds Phenolic acid, l Ascorbic acid, Alpha-tocopherol gave remarkable hypoglycemic effects on mice. Turning it to computational analysis we have the molecular docking to evaluate its role in Alpha-amylase and 1, 6-Fructose bisphosphate. These two protein enzyme plays an important role in hypoglycemic action in human body. Besides we have also analyzed the ADME properties of this compounds to find out it role in metabolism, excretion and bio-availabilities in human body.

INTRODUCTION

Capsicum annuum l. is a species native to southern North America and northern South America. Seeds were brought to Europe and *Capsicum annuum* began to be planted extensively in Portuguese colonies in Africa, India and Asia. Their popularity continues to grow across the world due to their ease of cultivation, frequently sharp taste and attractive appearance. It is now grown around the world, both commercially and domestically. This is lasting but frequently developed as a yearly in calm atmospheres, is a many-branched plant, growing up to 75 cm (30 in) in developed assortments, regularly shrubby in appearance. The leaves are basic and exchange, curved to lanceolate, with smooth edges (whole). The little blooms (around 1.5 cm, or 1 in, in measurement), are borne independently or, once in a while, in sets in the axils (where leaves join stems); they are white or incidentally purple, campanulas (chime molded), frequently with 5 projections, and contain 5 pale blue stamens. The natural products are many-seeded berries- - case like, however without any sutures-that fluctuate impressively fit as a fiddle, maturing to green, yellow, orange, red, or purple [1-10]. Cayenne is a digestive stimulant, a cardiovascular tonic, and a medical aid application for bleeding. The organic product is high in iron and vitamins A, C, E, K, and a few individuals from the B complex [11-16].

We have decided to put this experiment in further process in bioinformatics fields like molecular docking to evaluate its binding affinity with α-Amylase protein catalyst as it hydrolyses alpha obligations of extensive, alpha-connected polysaccharides, for example, starch and glycogen, yielding glucose and maltose. It is the significant type of amylase found in people and different warm blooded creatures and assumes an essential part in antidiabetic action [17-20]. We also analyzed the docking of the active compounds present in *Capsicum annum l.* with Fructose 1,6-bisphosphate exists in the glycolysis metabolic pathway and is created by phosphorylation of fructose 6-phosphate [21,22].

In the field of molecular demonstrating, docking is a technique which predicts the favored introduction of one particle to a moment when bound to each other to frame a stable complex. Knowledge of the favored introduction thusly might be utilized to predict the strength of association or binding affinity between two molecules using, for example, scoring capacities. Throughout the docking procedure, the ligand and the protein alter their compliance to accomplish a generally speaking "best-fit" and this sort of conformational change bringing about the general restricting is alluded to as "initiated fit". It involves the docking research which focusses on computationally recreating the molecular acknowledgment process. It plans to accomplish an

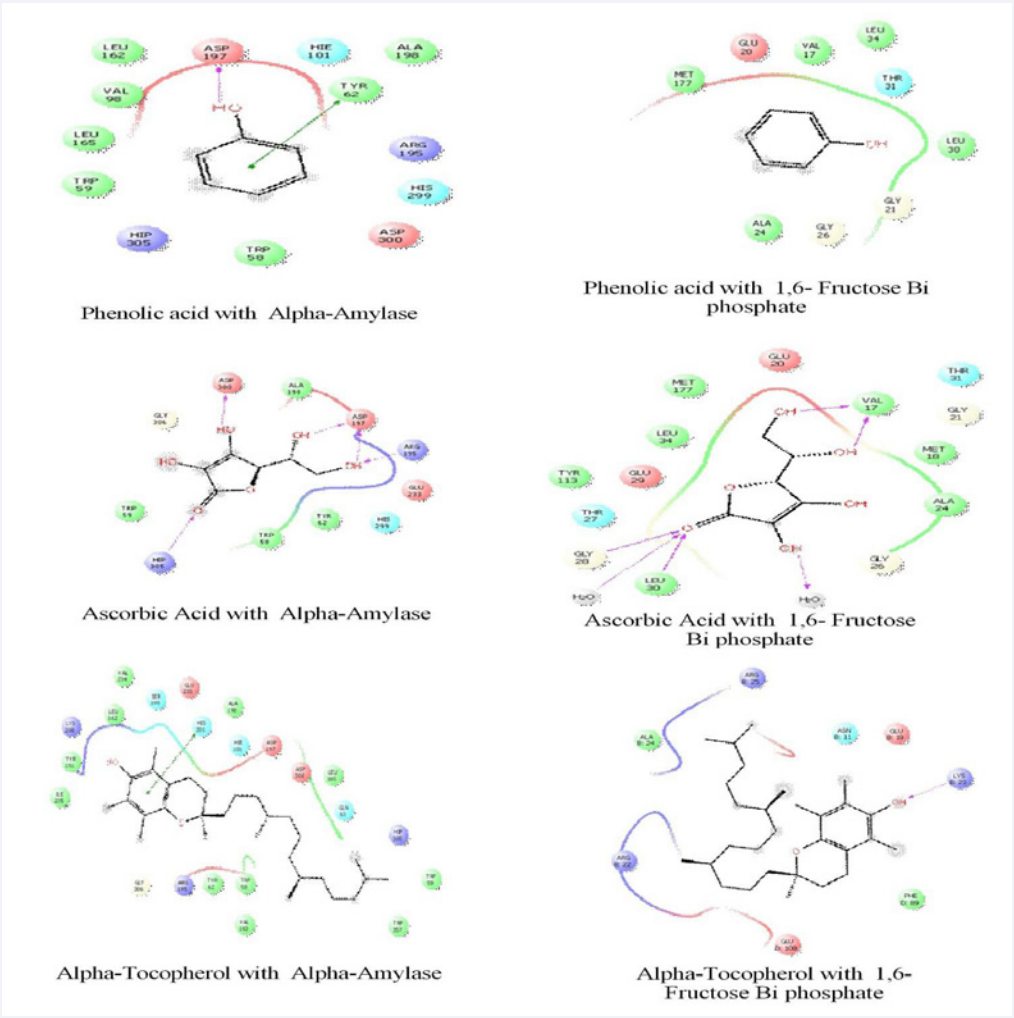

Figure 1 Docking results of Phenolic acid, Ascorbic acid and Alpha-Tocopherol with Alpha amylase and 1,6-Fructose biphosphate.

upgraded adaptation for both the protein and ligand and relative introduction amongst protein and ligand with the end goal that the free vitality of the general framework is limited [23-26].

Absorption distribution metabolism excretion (ADME) contemplates are basic in present day medicate disclosure. The reason for these investigations isn't just to comprehend the digestion, yet in addition how both parent and metabolites are killed. The data created from these investigations is helpful in deciding if the kidney or liver is a critical organ in end, and whether there is any wellbeing worry in hepatic or renally debilitated populaces [27-29].

The author of NATURAL PRODUCTS AND PLANTS AS POTENTIAL ANTIDIABETIC DRUGS have done impressive work in experimenting the effects of medicinal plant *Capsicum Annum L.* in antidiabetic properties by injecting the extract of rhizomes *Capsicum Annum L* into mice. So, we decided to experiment the ADME properties of the compounds present in *Capsicum Annum L*. This is to evaluate the absorption, distribution metabolism and excretion properties of the compound in human body.

METHODS AND MATERIAL

In silico analysis Molecular docking analysis of isolated compoundsCapsinoids, Carotenoids, Capsaicin, Phenolic acid, l Ascorbic acid, Alpha-tocopherol.

Protein preparation

Three dimensional crystal structure of Alpha-amylase (PDB id: A (1PPI) and 1,6- Fructose bisphosphate PDB id:(F 2JJK) was downloaded in pdb design from the protein data bank. From that point forward, structure was arranged and refined utilizing the Protein Preparation Wizard of Schrödinger-Maestro v10.1. Charges and bond orders were promoted, hydrogen was added to the substantial molecules, selenomethionines were changed over to methionines and all waters were erased. Utilizing power field OPLS_2005, minimization was completed setting greatest overwhelming particle RMSD (root-mean-square-deviation) to 0.30 Å.

Ligand preparation

Compounds were reprocessed from PubChem databases, i.e. Capsinoids, Carotenoids, Capsaicin, Phenolic acid, l Ascorbic acid, Alpha-tocopherol.

Glide Standard Precision (SP) ligand docking

SP adaptable ligand docking was done in Glide of Schrödinger-

Table 1: Docking results of Phenolic acid, Ascorbic acid, Alpha-Tocopherol with Alpha-amylase PDB id: A (1PPI) and 1,6-Fructose biphosphate PDB id:(F 2JJK)].

Alpha-Amylase (PDB id: A (1PPI))

Compound name	PubChem ID	Docking score	Glide emo	Glide energy
Phenolic Acid	996	-3.828	-20.765	-16.677
Ascorbic Acid	54670067	-4.12	-35.675	-28.193
Alpha-Tocopherol	14985	-2.971	-34.298	-30.323

1,6- Fructose Bi phosphate PDB id:(F 2JJK)

Compound name	PubChema ID	Docking score	Glide emo	Glide energy
Phenolic acid	996	-5.22	-25.552	-19.556
Ascorbic Acid	54670067	-0.758	-18.169	-18.034
Alpha-Tocopherol	14985	-0.758	-18.169	-18.034

Table 2: ADMET properties of Phenolic acid, Ascorbic acid, Alpha-Tocopherol by QikProp module of Schrodinger.

Compound name	Molecular weight	HB donor	HB acceptor	Log P	Molar refractivity
Phenolic Acids	94.11 g/mol	1	1	1.46	28.46
Ascorbic acid	176.12 g/mol	4	6	-1.40	35.12
Alpha-Tochopherol	430.71 g/mol	1	2	9.04	139.27

Maestro v10.1 inside which penalties were connected to non-cis/trans amide bonds. Van der Waals scaling variable and fractional charge cutoff was chosen to be 0.80 and 0.15, individually for ligand atoms. Last scoring was performed on vitality limited stances and showed as Glide score. The best docked posture with most minimal Glide score esteem was recorded for every ligand.

Ligand based ADME/Toxicity prediction: The QikProp module of Schrodinger (Maestro, version 10.1) is a speedy, precise, and simple to-utilize absorption, distribution, metabolism, and excretion (ADME) predicting configuration to deliver certain descriptors identified with ADME. It predicts both physicochemical critical descriptors and pharmacokinetically significant properties. ADME properties decide medicate like activity of ligand atoms in light of Lipinski's administer of five.

ADME/T properties of the compound (DIM) was examined utilizing QikProp 3.2 module. This investigation is finished by following server,

- http://www.scfbioiitd.res.in/software/drugdesign/lipinski. jsp # anchortag
- https://ilab.acdlabs.com/iLab2/index.php
- http://www.molinspiration.com/cgi-bin/propertiess

RESULT AND DISCUSSION

In silico analysis Molecular docking analysis

In this study, the binding mode of α-amylase enzyme and 1,6-Fructose bi-phosphate was 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 and the docking figure showed in Figure 1.

ADME and Toxicity Analysis Ligand based ADME prediction

The drug like activity of the ligand particle was arranged utilizing ADME properties by QikProp module of Schrodinger. The ADME properties of the Phenolic acid, l Ascorbic acid, Alpha-tocopherol were assessed with QikProp module of Schrodinger appeared in Table 2. The chose properties are known to impact metabolism, cell penetration, and bioavailability.

CONCLUSION

After experimenting the compound present in the plant *Capsicum Annum L.* which was suggested by the author in the research paper NATURAL PRODUCTS AND PLANTS AS POTENTIAL ANTIDIABETIC DRUGS, we got an impressive docking score. Also in ADME analysis this compounds follows the Lipinski's rule which means it may give better absorption, distribution, metabolism and excretion rate with greater bio availabilities. As it also gives hypoglycemic effects in mice which we have seen in the selected paper we can suggest this compound for further experiments.

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