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In-Silico Analysis And Antidiabetic Effect Of A-Glucosidase Inhibitory Of Active Compounds Of Pterocarpus Marsupium

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History

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Abstract: -

The identification of anti-diabetic natural compounds is a thriving field of opportunity in the drug discovery sector. P. marsupium has traditionally been used to treat diabetes and contains important phytochemicals. We investigated the TPC, TFC, antioxidant and antidiabetic activities of methanolic extract of P.marsupium. Total amount of phenols, flavonoids in methanolic extract of leave, stem, bark of P.marsupium were found to be 6.25, 12.613, 10.863 µg/ml respectively. The flavonoid content was found in P.marsupium leave (5.043), stem (19.246) and bark (13.782) µg/ml. In DPPH scavenging activity of plants parts found of P.marsupium, IC_{50} values were found to be leaves (96.146 µg/ml.), stem (21.705.µg/ml) and bark (27.177 µg/ml). Alpha-glucosidase of P.marsupium plants IC_{50} values were found to be leave (107.77µg/ml), stem (23.64µg/ml) and bark (60.123µg/ml). In-silico studies were investigated to determine the binding affinity of phytoconstituents of P. marsupium in additional with the crystal structure of alpha-glucosidase (PDB ID: 5ZCD). Thirty one active constituents derived from P.marsupium, and standard (maltotriose) docked with target proteins. Result of molecular docking showed that the pterosupin, (-11.0 kcal/mol) had best docked against alpha-glucosidase as related to native ligand maltoriose (-10.04kcal/mol). This study provides valuable insights into the therapeutic potential of P.marsupium plant compounds for managing diabetes and warrants further research and clinical investigation for practical applications in diabetes treatment and prevention.

Keywords: TPC, TFC, Antioxidant, Diabetes mellitus, Alpha-glucosidase, P.marsupium, Molecular docking.

1. Introduction:

Diabetes mellitus (DM) is a high metabolic disorder leading to a high rate of blood sugar morbidity and mortality that affects people all over the world[1,2] and characterized by a loss of glucose homeostasis with disturbances[3] of carbohydrate, fat and protein metabolism attributed to low production of insulin[4].The Latin term "Mellitus" means "sweetened with honey," while the Greek word "Diab" is the source of the word

"diabetes." Ancient Hindu physicians believed that "Madhumeha" was a condition in which a patient passed delicious urine and displayed sweetness throughout their body, including in their perspiration, mucous, breath, and blood[3]. It occurs because the pancreas does not make enough insulin or because the body cannot use the insulin adequately, and it is a chronic condition[6,7]. Healthy eating, frequent exercise, the use of synthetic or natural medications, and upholding a healthy lifestyle are all effective ways to treat diabetes mellitus[8,9].

Type 1 Diabetes Mellitus (T1DM) and type 2 Diabetes Mellitus (T2DM) are the two most prevalent forms of the disease. Insulin-dependent diabetes is the term used to describe type 1 diabetes. It is a catabolic condition brought on by an immune system response. Only 10% of type 1 diabetes patients have the condition, which requires them to need insulin injections for the remainder of their lives because their bodies no longer produce insulin[10]. Additionally, they must monitor normal blood glucose levels by performing routine blood tests[8]. Non-insulin-dependent diabetes is another name for type 2 diabetes. It is a diverse set of diseases, with T2DM affecting the majority of diabetics and accounting for 90% of cases. The body's cells do not react to insulin because of a malfunction in how it is secreted and used [10, 7, 11]. It manifests as hyperglycemia as a result of pancreatic beta-cell malfunction and insulin resistance[12,2]. Some people may be able to manage their T2DM symptoms by exercising frequently, watching their blood sugar levels, decreasing weight and maintaining a balanced diet. Reducing glucose absorption by preventing carbohydrate digestion is one of the most effective approaches to managing T2DM. In the digestive tract, two enzymes of intestinal alpha-glucosidase and pancreatic alpha-amylase help break down of carbohydrates to produce absorbable glucose[13]. When carbohydrates are broken down by the enzyme alpha-amylase (glucose), disaccharides are broken down or converted to monosaccharides[14,15]. These inhibitions might postpone the intestinal breakdown of carbohydrates, which would assist to reduce T2DM[16,17]. One of the therapeutic approaches being researched for the treatment of diabetes is the inhibition of glucosidase and amylase activity, and herbal plants are providing a therapeutic approach to treat diabetic Mellitus (DM) because they are a rich source of various bioactive compounds that have either directly or indirectly been used in the treatment of various diseases and ailments.

*P. marsupium*is an important medicinal plant belonging to family Fabaceae and commonly known as Red Kino Tree (English), Vijaysar (Hindi), is one of the most valuable multipurpose forest trees that yields excellent timber for the international trade market. Vijaysar helps to manage blood sugar levels by preventing the damage to pancreatic cells and promoting insulin secretion due to its antioxidant and anti-inflammatory activity. Role of *P. marsupium* is found in Ayurveda, Homeopathic and Unani systems of medicine[18,19]. *P. marsupium* is well known in India and its neighboring countries for more than 2000 years, as one of the most versatile medicinal plants having a wide spectrum of biological activity. Every part of the tree has been used as traditional medicine for household remedy against various human ailments[20]**.** Its flowers are used in fever, hemostati, and rejuvenating. The gum (kino) obtained from the tree is used for the treatment of diarrhea, pyrosis and toothache. Leaves are used for various skin diseases. Stem are used for the treatment of neurological problems. The wood of this plant is used for chest pain, body pain and also be used for the treatment of diabete[21]. The bark is used for the treatment of stomachache, cholera, dysentery, urinary complaints, tongue diseases and toothache[22]**.**

In the current study, it intends to extract *P. marsupium* plant and carried out their anti-oxidative and anti-diabetic properties (in-vitro & in-silico research). This research work is also aimed to find out the interaction of reported active compound with the target protein, this findings could be useful for the discovery of new, potent and active α-glucosidase inhibitors.

2 Materials and Methods

2.1 Biological assay

2.1.1 Plant materials and extraction

P. marsupium plant parts of leaves and stem were collected from the Arogyadham campus, Chitrakoot, Satna (M.P. India) is washed with water and then washed with ethanol and allowed to dry in shade at room temperature. Dried parts of plant grind and store in an airtight container for further use. Take 20gm of powder of *P. marsupium* leave, stem and bark then added 100ml (80%) methanol and use the cold maturation method for extraction. The extract was filtered through the Whatman No.1 filter paper. The filtrate was concentrated at room temperature for dryness.

2.1.2Extraction of plants procedure

The powdered samples were subjected to extraction with 80% methanol by maceration method using a rotatory shaker. Maceration method was adapted from Tiwari etal[23]. In this process, the 20 gram powdered sample is kept in a stoppered container then dissolved in 100 ml of methanol (80%) and allowed to stand in water bath shaker for 72 hours (at room temperature). After 72 hours, sample was taken out and filtered through filter paper (Whatman No. 1) Pour the filtrate in a petriplate or bowl and kept it for drying in hot air oven at 35 ^{0}C. After sufficient drying, the material is collected in eppendrop tubes for further uses.

2.1.3 Estimation of total Polyphenolic content

The total Polyphenolic content of extracts was measured by using Folin-Ciocalteu reagent. The 50 µl of plant extract diluted with 50 µl water followed by addition of 150 µl of Folin-Ciocalteu reagent (1N) & 25 µl of Na_2CO_3(20%w/v) and incubated at 45ºC for 60 min then absorbance was measured spectrophotometrically at 765nm (BioTek$^{Synergy\ H4}$multimode micro plate reader, BioTek instrument, IncWinoosci, VT, USA). Quantification was performed with respect to the standard curve of Catechol (Y=0.0044x+0.1586, r^2 =0.9941). Results were expressed as milligram of Catechol equivalent per ml of extract[24].

2.1.4 Determination of Flavonoids contents

Total flavonoids in the plant extract in brief 50 µl of sample, followed by 50µl of $AlCl_3.6H_2O$ in ethanol and 25µl Sodium acetate, solution added. The absorbance at 430nm was taken (BioTek^{synergyH4} multi-mode microplate reader, BioTek Instruments, Inc Winooski, VT, USA), after 2.5 h of incubation at 20^0 C. Total flavonoids contents were calculated with respect to the standard curve of the flavonoids quericetin dehydrate (Y=0.0069x+0.0613, r^2 =0.9646). Results were expressed as micrograms of quericetin dehydrate equivalents (QE) per ml of the extract[25].

2.1.5 DPPH free radical scavenging assay

The assay for free radical DPPH was done by using 2, 2-diphenyl-1-picrylhydrazyl (DPPH) method. In brief, a 96-well microplate, 30 µl of various dilutions (10-100 µg /ml) of methanolic extract 100 µl of tris–HCl buffer (0.1M, pH 7.4) and 150 µl of DPPH solution (0.004% w/v in methanol) were added. The reaction mixture was shaken well. The DPPH decolonization was recorded at 517 nm on a BioTek Synergy H4 hybrid multimode micro plate reader (BioTek instruments, Inc Win-oosci, VT, USA.), after 30 min incubation in dark. The percentage of DPPH scavenging by plant extracts obtained in terms of ascorbic acid equivalent concentration[26]. Quantification was performed with respect to the standard curve of Ascorbic acid equation. Result was expressed as milligram of Ascorbic acid equivalent per ml of extract. Experiment was done in triplicates. DPPH radical's concentration was calculated using the following equation:

DPPH scavenging effect (%) = Ao – A1 / Ao X 100

Where Ao was the absorbance of the control and A1 was the absorbance in the presence of the sample.

2.1.6 α-Glucosidase Inhibition Activity

α-glucosidase inhibitory activity was performed following the method of Tripathi etal.[24] In brief Rat-intestinal acetone powder was dissolved in 4 ml of 50 mM ice cold phosphate buffer and sonicated for 6 minutes at 4°C. After vortexing for 20 minutes, the suspension was centrifuged (10,000 rpm, 4°C, 30 minutes) and the resulting supernatant was used for the assay. A reaction mixture containing 50 µl of phosphate buffer (50 mM; pH 6.8), 20 µl of rat α -glucosidase (1 U/ml) and 25 µl of sample of varying concentrations was pre-incubated for 5 min at 37°C, and then 25 µl of 3 mM PNPG was added to the mixture as a substrate. After incubation at 37°C for 30 min, enzymatic activity was quantified by measuring the absorbance at 405 nm in a micro titer plate reader (Bio-TEK, USA). Acarbose was used as a positive control and water as negative control. The percentage of enzyme inhibition by the sample was calculated by the following formula:

% Inhibition = $\frac{(A_0 - A_1)}{A_0} \times 100$

Where A_0= Absorbance of control

A_1 = Absorbance of sample

The concentration of an inhibitor required to inhibit 50% of enzyme activity under the mentioned assay conditions is defined as the IC_{50} value.

2.2 In-silico analysis (Molecular docking)

2.2.1 Collection of protein and ligand for insilico study

The three-dimensional 3D structure of intestinal alpha-glucosidase protein (PDB ID: 5ZCD) in complex with maltoriose. Protein (PDB ID: 5ZCD) was retrieved as a receptor downloaded from the RCSB Protein Data Bank[27](https://www.rcsb.org/,). The compounds used in this study for molecular docking against the proteins catalytic site were active compounds derived from the plant *P. marsupium*. A total of 31 active compounds were retrieved from a *P. marsupium* plant (show in Table-1) in database of IMPPAT (Indian Medicinal Plants, Phytochemistry and Therapeutics)[28] https://doi.org/10.1038/s41598-018-22631-zPubChem and pubchem database (https://pubchem.ncbi.nlm.nih.gov/) in SDF formate[29].

Table 1 Name, IMPPAT and PubChem CID of P. marsupium compounds

S.N	Name of compound	IMPPAT	CID Code
1	Pterosupin	IMPHY009654	CID:133775
2	propterol b	IMPHY011467	ND
3	Naringetol	IMPHY010550	CID:439246
4	(-)-Epicatechin	IMPHY014908	CID:72276
5	7,4'-Dihydroxyflavone	IMPHY010592	CID:5282073
6	Liquiritigenin	IMPHY001869	CID:114829
7	Garbanzol	IMPHY000908	CID:442410,
8	3,7,4'-Trihydroxyflavone	IMPHY005430	CID:5281611
9	7-Hydroxy-5,4'-dimethoxy-8-methylisoflavone 7-O-rhamnoside	IMPHY013393	CID:44257328
10	3,4-Dihydroxybenzoic acid	IMPHY011883	CID:72,
11	Marsupsin	IMPHY009579	CID:134369
12	Propterol	IMPHY005318	CID:185124,
13	4-Hydroxybenzaldehyde	IMPHY009356	CID:126
14	(+) abscisic acid,	IMPHY011652	CID:5280896,
15	Isoliquiritigenin	IMPHY006489	CID:638278,
16	Gallic acid	IMPHY012021	CID:370
17	Pseudobaptigenin	IMPHY004580	CID:5281805
18	Pterostilbene	IMPHY004573	CID:5281727
19	(2S)-7-hydroxyflavanone	IMPHY011492	CID:688857
20	Catechol	IMPHY004079	CID:289
21	Ebanol	IMPHY006496	CID:6437266,
22	beta-Eudesmol	IMPHY011542	CID:91457,
23	Oleanolic acid	IMPHY011826	CID:10494,
24	Lupeol	IMPHY012473	CID:259846
25	Linoleic acid	IMPHY014990	CID:5280450
26	trans-Stilbene	IMPHY006487	CID:638088,
27	Arachidic acid	IMPHY011394	CID: 10467
28	Oleic acid	IMPHY011797	CID: 445639
29	Palmitic acid	IMPHY007327	CID: 985
30	Stearic acid	IMPHY004631	CID: 5281
31	Myristic acid	IMPHY000060	CID: 11005

2.2.2 Molecular docking analysis

Before molecular docking analysis, the selected compounds against the alpha-glucosidase active site, for which the target protein and the ligands were prepared using the Protein Preparation Wizard (PrepWizard) and LigPrep Module of Schr€odinger suite[30], respectively. The protein was prepared by adding the missing residues and assigning the formal and partial charges to the structure. The native ligands and the co-crystallized water molecules were deleted from the protein structure to allow the docking of new ligands into the active catalytic pocket.and the ligand was pre-proceed using the default parameters of the LigPrep module in the Schro¨dingersuite[31], the ligands were prepared by generating their tautomeric confirmations with OPLS3e force field and EPIK state penalty at pH 7.0±2.0. A variety of software tools are available for molecular docking purpose. In this study Glide XP programs of schrodinger suit package was used for molecular docking experiment[32].

3 Result and discussion:-

3.1 Biological analysis

3.1.1 Total Polyphenolic content

The total polyphenolic contents quantify in the plant extracts is convey in designate of cathecol equivalent the standard curve equation: (Y=0.0044x+0.1586, r^2 =0.9941).

The complete quantification of Polyphenolic material is represented in terms of Cathecol. Cathecol 's standard graph was presented in fig-1-A and the all analyzed plants sample data is given in table- 2

In the present study, it was found that total polyphenolic content was found to be the highest in *P. marsupium stem.* The polyphenolic content was found in *P.marsupium* leave (6.25), stem (12.613) and bark (10.863) µg/ml.

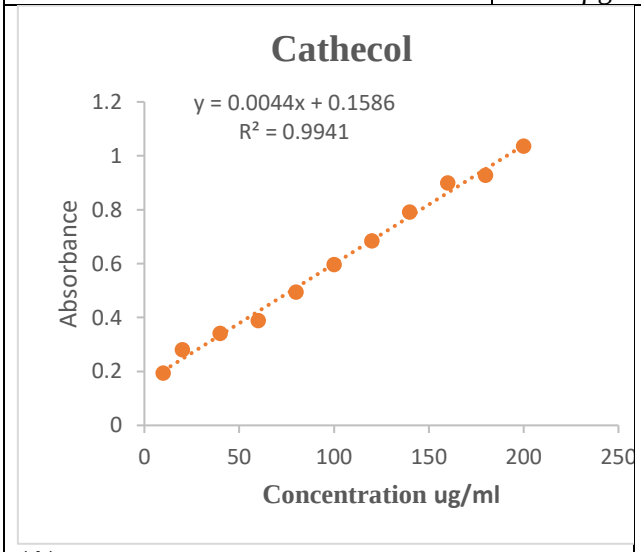
3.1.2 Total flavonoids content

The total flavonoid contents quantify in the plant extracts is convey in designate of quericetin equivalent the standard curve equation: (Y=0.0069x+0.0613, r^2 =0.9646). In the plant extract the overall quantify of flavonoid content is expressed in term of the standard curve quericetin. Quericetin's standard graph was presented in fig-1-B and the all analyzed plants sample data is given in table-2

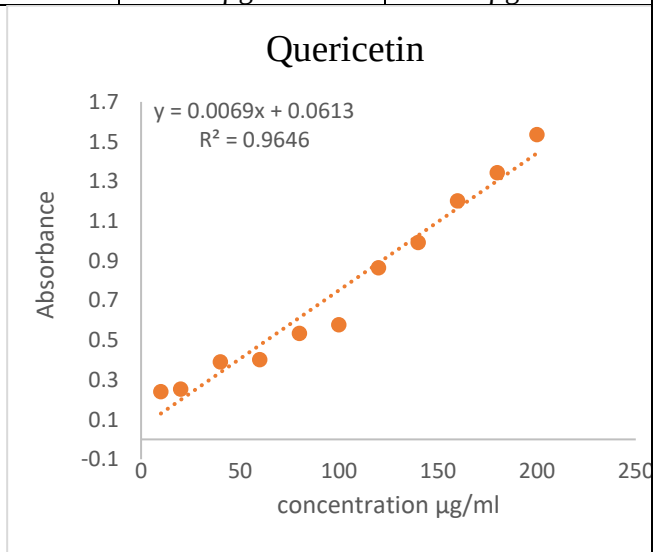
In the present study, it was found that total flavonoid content was found to be the highest in *P.marsupium* stem. The flavonoid content was found in *P.marsupium* leave (5.043), stem (19.246) and bark (13.782) µg/ml.

Table-2Quantitative phytochemical analysis of *P.marsupium* plant

Quantitative test	***Pterocarpus marsupium***		
	Leave	**Stem**	**Bark**
Total Phenolic content	6.25 µg/ml	12.613 µg/ml	10.863 µg/ml
Total flavonoid content	5.043 µg/ml	19.246 µg/ml	13.782 µg/ml



(A)



(B)

Figure -1 Represent the standard graph of cathecol (A) and quericetin (B)

3.1.3 Antioxidant activities(1,1-diphenyl 2- picrylhydrazyl(DPPH) assay)

In present investigation antioxidant activities of all the plant extracts were determined in terms of IC_{50} values. For antioxidant assays, (DPPH) activity compare to ascorbic acid. Ascorbic acid was used as reference standard.

Result of DPPH scavenging activity are shown in table -3 and statistical result of the data shown in graph-2-A shows the standard curve of ascorbic acid and graph-2-B show the curve of *P.marsupium* . The test is based on the ability of the stable DPPH free radical to decolourize in the presence of antioxidants.

In the present investigation, IC_{50} value of standard ascorbic acid is calculated to be 20.45ug/ml. Outcome of our work designate that *P.marsupium* plant exhibited excellent antioxidant activity.

Maximum antioxidant activity was shown in *P.marsupium* stem with less IC_{50} value (21.705 µg/ml.) which was very near the standard ascorbic acid, while the lowest antioxidant activity was found in *P.marsupium*

leaves with highest IC_{50} value of 96.146 µg/ml. DPPH activity of selected medicinal plants parts found of *P.marsupium* leaves (96.146 µg/ml.), stem (21.705.µg/ml) and bark (27.177 µg/ml).

Table-3 IC_{50} values of Antioxidant activity of *P.marsupium* plants (DPPH activity)

Concentration µg/ml	***PterocarpusMarsupium***		
	Leaf	***Stem***	Bark
10	24.47917	40.81439	30.39773
25	27.55682	52.88826	49.50284
50	31.10795	78.19602	69.46023
100	51.70455	89.60701	75.78125
200	71.35417	93.37121	83.19129
400	95.50189	95.9517	95.50189
IC_{50} values	**96.146 µg/ml**	**21.705 µg/ml**	**27.177 µg/ml**

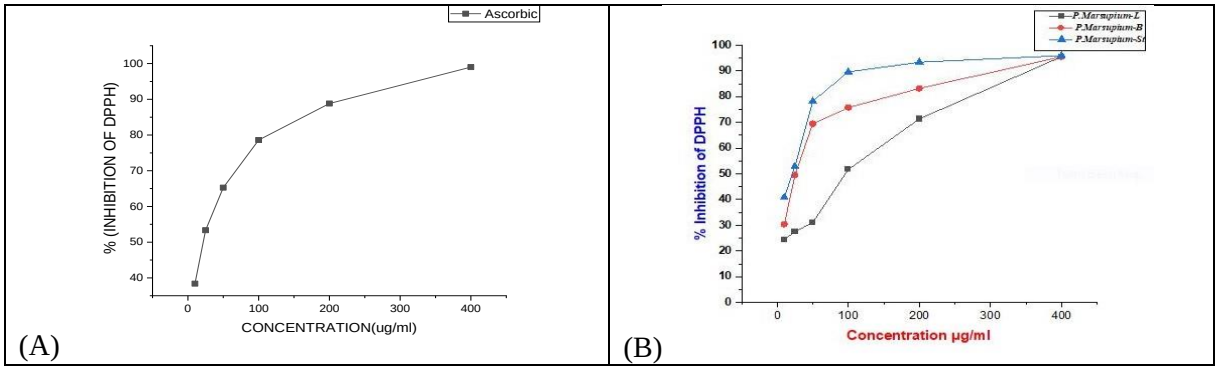


Fig 2- Represent the standard curve of Ascorbic acid (A) and the *P.marsupium* plant parts (B)

3.1.4 Alpha-glucosidase-

We evaluated the in-vitro alpha-glucosidase inhibition of selected plants as compared with acarbose and expressed IC_{50} value and percentage inhibition. The result of alpha-glucosidase activity was presented in table-4 and the acarbose curve is shown in fig-3(A) and statistical analysis of data present in fig-3(B).

In the present investigation, IC_{50} value of standard acarbose is calculated to be 92.6128 ug/ml. The *P.marsupium plant* exhibited excellent antidiabetic activity. Maximum antidiabetic activity was found in *P.marsupium* stem with less IC_{50} value (23.64µg/ml) which was also better than standard ascorbic acid. Alpha-glucosidase of selected medicinal plants parts found that IC_{50} values of P.marsupium leave (107.77µg/ml), stem (23.64µg/ml) and bark (60.123µg/ml).

Table-4 IC_{50} values of Anti-diabetic activity of *P.marsupium* plant (Alpha Glucosidase activity)

Concentration µg/ml	***Pterocarpus Marsupium***		
	Leaf	***Stem***	***Bark***
10	9.278351	30.24055	23.71134
25	24.74227	52.92096	32.64605
50	44.3299	62.54296	49.07216
100	49.82818	84.08935	56.70103
200	56.35739	93.95189	63.23024
400	72.16495	95.05155	79.0378
IC_{50} values	**107.77** µg/ml	**23.64** µg/ml	**60.123** µg/ml

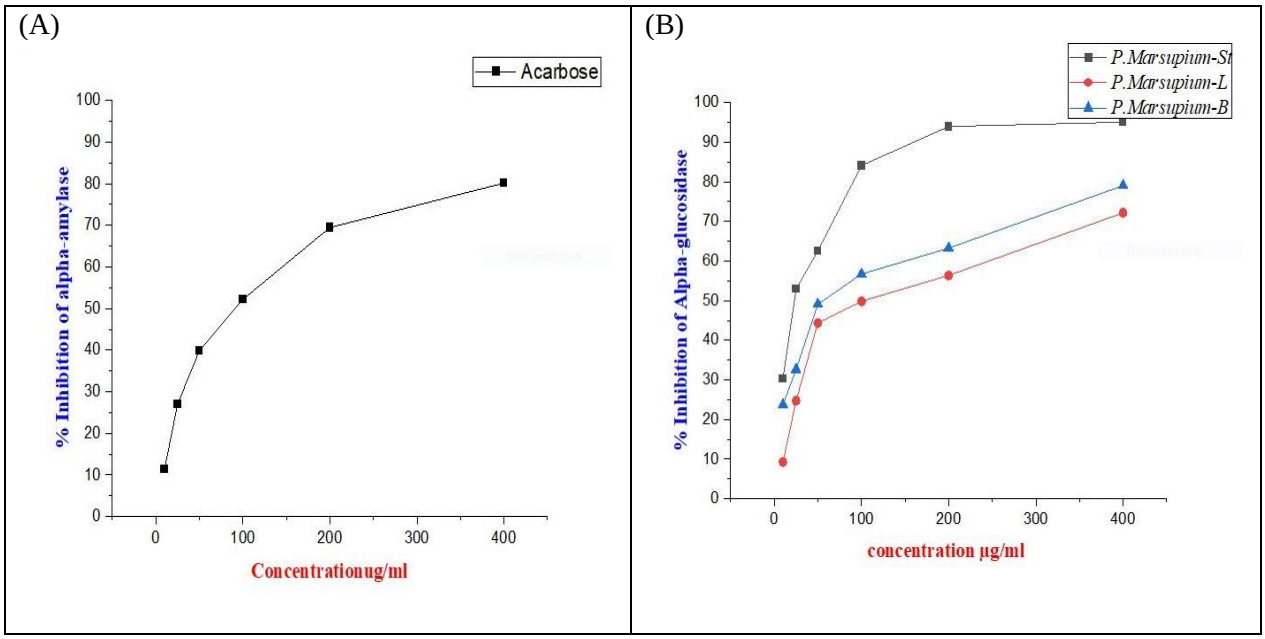


Fig-3 Represent the standard curve of Acarbose (A) and the *P. marsupium* plant parts (B)

3.2 In-silico Assay

3.2.1Molecular Interaction analysis

The target protein's binding site creates a number of ligand binding poses when a ligand is docked into it, and those with the best docking scores and lowest binding energies are taken into consideration for further analysis. In this study, the docking analysis was performed to predict the binding potential of all compounds from selected medicinal plants against alpha-glucosidase proteins (PDB ID-5ZCD). The total 31 compounds of *P.marsupium* medicinal plants were found.

The top 5 best docking compounds were selected from *P. marsupium* with alpha-glucosidase proteins under -11 kcal/molto -7.4 kcal/mol. Additionally, control compound maltotriose with alpha-glucosidase docking energy (-10.04 kcal/mol) as a control. The top docking compounds were chosen for identification of intermolecular interaction with 2D and 3D diagram showed with the protein fig 4.

Alpha- glucosidase (5ZCD) and *pterocarpus marsupium* complexes:

Molecular interaction analysis of *pterocarpus marsupium* compounds of top five docking energy compounds name, Pterosupin, Naringetol, (-)-Epicatechin, Isoliquiritigenin and 7-Hydroxy-5,4'-dimethoxy-8-methylisoflavone7-O-rhamnoside, compounds showed a strong binding complex of -11.0 kcal/mol, -9.1kcal/mol, -8.2 kcal/mol, -7.5 kcal/mol and -7.4 kcal/mol respectively.

Alpha- glucosidase and Pterosupin docked complex :

The interaction analysis (figure-4(a,b)) of top most Pterosupin docked complex generated five hydrogen bonds with the target proteins residues His^{203}, Asn^{258}, Gln^{256}, Asp^{382}. In which, His^{203}, Asn^{258}, Asp^{382} formed only one-one hydrogen bond except Gln^{256} formed two hydrogen bonds with the ligand. While, the hydrophobic interaction showed nine residues Ala^{200}, Phe^{144}, Phe^{163}, Phe^{282}, Met^{385}, Phe^{225}, Ile^{143}, Tyr^{388} and Met^{229}.

Alpha- glucosidase and Naringetoldocked complex:

The interaction (figure-4(c,d)) of top two docked complex Naringetol showed three hydrogen bonds with the target proteins residues His^{203}, Asn^{258}, Gln^{256}. While, total eight residues Ala^{200}, Phe^{144}, Phe^{163}, Phe^{282}, Met^{385}, Phe^{225}, Ile^{143} and Met^{229} showed the hydrophobic interaction. Along with, Phe^{144} residue formed pi-pi stacking.

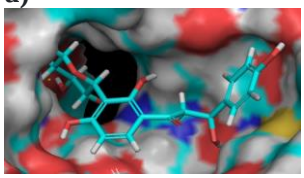
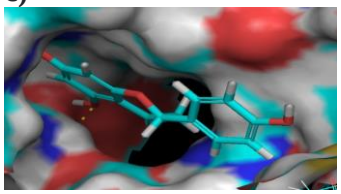
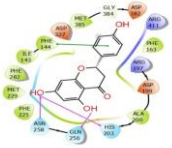
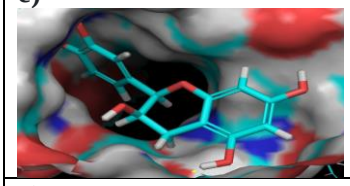
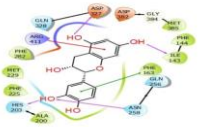
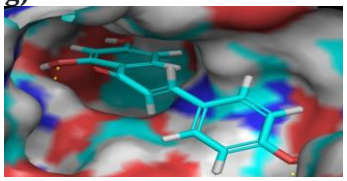
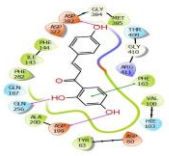
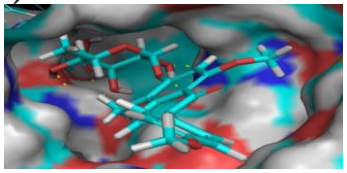
Alpha- glucosidase and (-)-Epicatechindockedcomplex :

The interaction analysis (figure-4(e,f)) of top three docked complex(-)-Epicatechindisplayed four hydrogen bonds with the target proteins residues His^{203}, Asn^{258}, Ile^{143}, Asp^{327}. Additionally, total eight residues Ala^{200}, Phe^{144}, Phe^{163}, Phe^{282}, Met^{385}, Phe^{225}, Ile^{143} and Met^{229} discovered the hydrophobic interaction. while, Phe^{163} residue formed pi-pi stacking and Arg^{411} residue formed pi-pi cation.

Alpha- glucosidase and Isoliquiritigenin docked complex:
The interaction analysis (figure-4(g,h)). of top four docked complex Isoliquiritigenin generated three hydrogen bonds with the target proteins residues Asn^{199}, Gln^{256}, Asp^{382}. While, total eight residues Ala^{200}, Phe^{144}, Phe^{163}, Phe^{282}, Met^{385}, Ile^{143}, Tyr^{63} and Met^{385} discovered the hydrophobic interaction. Along with, Phe^{163} residue formed pi-pi stacking.

Alpha-glucosidase and 7-Hydroxy-5,4'-dimethoxy-8-methylisoflavone7-O-rhamnoside docked complex:
The interaction analysis (figure-4(I,j)) of top five strong docked complex 7-Hydroxy-5,4'-dimethoxy-8-methylisoflavone7-O-rhamnoside showed three hydrogen bonds with the target proteins residues Gln^{256}, Asp^{327}. In which, Asp^{327} formed one hydrogen bond and Gln^{256} formed two hydrogen bonds with the ligand. Whereas, the hydrophobic interaction generated eight residues Ala^{200}, Phe^{144}, Phe^{163}, Phe^{282}, Met^{385}, Phe^{225}, Ile^{143}, and Trp^{288}.

Alpha- glucosidase and maltotriose docked complex:
The molecular interaction analysis (figure-4.(c,d)) of control docked complex maltotriose formed nine hydrogen bonds with target protein Asn^{258}, Gln^{256}, Hie^{103}, Asp^{199}, Asp^{60}, Arg^{411}, Arg^{197}, Asp^{307}. In which, Asn^{258}, Gln^{256}, Hie^{103}, Asp^{199}, Asp^{60}, Arg^{411}, and Arg^{197}formed only one-one hydrogen bonds except for Asp^{307} which formed two hydrogen bonds with the ligand. Additionally, the hydrophobic interaction showed eight residues Phe^{144}, Ile^{143}, Phe^{282}, Phe^{163}, Phe^{225}, Val^{100}, Tyr^{63}, and Ala^{200}.
The molecular interactions of the top five docked complex are presented in descending order: Pterosupin, (-)-Epicatechin, Naringetol,Isoliquiritigenin, 7-Hydroxy-5,4'-dimethoxy-8-methylisoflavone7-O-rhamnoside. Pterosupin complex was the best interaction compared to (control) maltotriose.

3D Structure	2D Structure
a) 	b) 
c) 	d) 
e) 	f) 
g) 	h) 
i) 	j) 

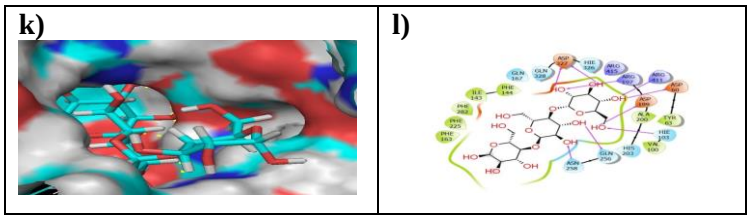


Fig: 4 3D and 2D poses of the selected natural compounds of *PterocarpusMarsupium* i.e, (a,b) Pterosupin, (c,d) Naringetol, (e,f) (-)-Epicatechin, (g,h) Isoliquiritigenin (i,j) 7-Hydroxy-5,4'-dimethoxy-8-methylisoflavone7-O-rhamnoside. In 2D interaction maps, pink arrow (H-bond), green line (π-π stacking, red-violet (salt bridge), red (negative), violet (positive), green (hydrophobic), and blue (polar) colour residues exhibits the interactions in the respective docked complexes.

Conclusion:

The *P. marsupium* is important medicinal plant to cure various disease because it contain variety of phytochemicals in different parts. The overall result obtain by present study we observed that the stem part of *P.marsupium* shows strong antioxidant and antidiabetic activity. According to their binding energy, the active constituents Pterosupin, Naringetol, (-)-Epicatechin, Isoliquiritigenin and 7-Hydroxy-5,4'-dimethoxy-8-methylisoflavone7-O-rhamnoside of *P.marsupium* might be responsible for antidiabetic activity in diabetic patients .

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