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MOLECULAR DOCKING & IN SILICO ADME STUDIES OF PHYTOCHEMICAL CONSTITUENTS ADHATHODA VASICA AGAINST SUPERFAMILY SUBGROUP OF TREHALOSE -6- PHOSPHATE PHOSPHATASE.

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ABSTRACT

Trehalose-6-phosphate phosphatase (TPP) enzymes are used by many pathogenic microorganisms in their process of infection and proliferation to biosynthesise the sugar trehalose from trehalose-6-phosphate (T6P). As a result, the current work uses in silico techniques to build novel candidate medications that block TPP. *Adhathoda Vasica* commonly known as Vasaka or Malabar nut. It belongs to the Acanthaceae family and has been used in traditional Ayurvedic and Unani medicine for centuries are a promising source of phytochemicals, particularly vasicine and vasicinone, quinazoline alkaloids, including vasicinolone, vasicol, and adhatodine. These compounds are known for their bronchodilatory and expectorant properties. Swiss ADME software was accessed in a web server that displays the Submission page of Swiss ADME in Google was used to estimate individual ADME behaviors of the compounds from the plant. Advanced ADME studies were performed for confirmation of vasicine, adhatodine and Epitaraxenol compounds to be orally bioavailable or not. The present work is an approach to design new generation candidate drugs to inhibit TPP through *in silico* methods on pulmonary activity using 1YMQ. Docking studies of 3D model of TPP with many phytochemicals revealed most of them have good binding affinity to an enzyme with adothodine exhibiting highest affinity with Docking score -7.4 having more responsible for inhibiting infection on pulmonary activity compared to the compound Vasicine with the docking score: -6.5, and epitaraxerol with the docking score: -7.0. Hence the current research proves that the phytochemical compound of *Adhatoda vasica* act as promising lead as Trehalose-6-phosphate phosphatase

Keywords: *Trehalose-6-phosphate phosphatase, Adhatoda vasica, Swiss ADME, Molecular Docking.*

INTRODUCTION

Adhatoda vasica, commonly known as Vasaka or Malabar nut, is a medicinal plant native to the Indian subcontinent and other parts of Southeast Asia. It belongs to the Acanthaceae family and has been used in traditional Ayurvedic and Unani medicine for centuries. The plant is a small, evergreen shrub that typically grows to a height of 1-2 meters. It has thick, lance-shaped leaves with serrated edges and clusters of white or purple flowers [1]. The plant's leaves, roots, and flowers are the parts commonly used for medicinal purposes. Adhatoda vasica has a long history of use in treating respiratory ailments. It is known for its expectorant, bronchodilator, and antitussive properties. The plant contains several bioactive compounds, including alkaloids like vasicine and vasicinone, which are believed to be responsible for its therapeutic effects [2].

Figure 01: Adhatoda vasica

In traditional medicine, Adhatoda vasica has been used to alleviate symptoms of respiratory conditions such as asthma, bronchitis, cough, and common cold. It is believed to help loosen and expel mucus from the respiratory tract, reduce inflammation, and soothe coughs. The plant has also been used for its antimicrobial and anti-inflammatory properties [3,4].

Modern scientific research has also investigated the medicinal properties of Adhatoda vasica. Several studies have demonstrated its potential benefits in respiratory conditions, including bronchial asthma and chronic obstructive pulmonary disease (COPD). It has been shown to have bronchodilatory effects and help improve lung function [5].

It is important to note that while Adhatoda vasica has a long history of traditional use and shows promising results in some studies, further research is still needed to fully understand its mechanisms of action and establish its efficacy and safety.

As with any herbal remedy, it is recommended to consult with a healthcare professional or a qualified herbalist before using Adhatoda vasica or any other herbal treatment, especially if you have an existing medical condition or are taking other medications [6-9].

TAXONOMICAL CLASSIFICATION

Kingdom: Plantae (Plants)

Phylum: Magnoliophyta (Flowering Plants) Class: Magnoliopsida (Dicotyledons) Order: Lamiales

Family: Acanthaceae (Acanthus family) Genus: Adhatoda

Species: vasica

Phytochemical Compounds of Adhatoda Vasica

Adhatoda vasica (Vasaka) contains various phytochemical compounds that contribute to its medicinal properties. Here are some of the major phytochemical compounds found in Adhatoda vasica:

Vasicine, Vasicinone, Quinazoline alkaloids like vasicinolone, vasicol, and adhatodine for many of its therapeutic effects, including bronchodilatory, expectorant, and anti-inflammatory properties. Flavonoids, such as quercetin and kaempferol. phenolic compounds, including caffeic acid, ferulic acid, and chlorogenic acid. These compounds exhibit antioxidant and anti-

Phenolic compounds: Adhatoda vasica contains various phenolic compounds, including caffeic acid, ferulic acid, and chlorogenic acid. These compounds exhibit antioxidant and anti-inflammatory activities [10].

Health Benefits

Adhatoda vasica, known for its medicinal properties. It has been used in traditional Ayurvedic and Unani medicine for various respiratory conditions. While scientific research is ongoing, here are some potential health benefits associated with Adhatoda vasica. Adhatoda vasica has been traditionally used for respiratory ailments like asthma, bronchitis, and cough. It is believed to have bronchodilatory and expectorant properties, helping to relieve congestion, promote mucus expulsion, and ease breathing. Adhatoda vasica has shown antimicrobial properties against certain bacteria and fungi. It may have potential in fighting respiratory infections caused by these pathogens. Some studies suggest that Adhatoda vasica exhibits anti-inflammatory properties, which may help in reducing inflammation in the respiratory tract and other body systems.Antioxidant Activityand anti-asthmatic effects also seen [11].

MATERIALS AND METHOD

Materials

Collection of plant material

J. adhatoda (Adhatoda): Disease-free fresh leaves were gathered from the J. adhatoda plant and were rinsed in tap water 2–3 times and once with sterile distilled water. Subsequently, the leaves were air-dried on a sterile blotter under shade and then oven dried at 50°C for 4–5 days until the weight became constant. The withered plant materials were powdered by a mechanical grinder.

Preparation of plant extract

Powdered plant extracts weighing 50 g were soaked in 200 ml of methanol with stirring for 5 days. After soaking, it was strained through double layers of muslin, Whatman filter paper No. 1, and then evaporated and dried at 40°C to obtain filtrated extracts. The resultant extracts were weighted and refrigerated in a small bottle at 5°C.

The HPLC- grade solvents including menthanol, Ethyl acetate, Sodium bicarbonate, Sodium bicarbonate were from Spectrum reagents and chemicals Pvt.Ltd (Edayar, Cochin.) 90-99.5% Ethanol were from Coating & Coating (India) Pvt.Ltd (Hill view industrial estate, Amrut Nagar). Using distilled water and a RO water purification system, deionized water was created.

Instruments

The high-speed centrifuge (R-24) was from Remi Instruments, Mumbai. The Sonicator PCi Instruments, Mumbai. The pH meter INFRA DIGI. Magnetic Stirrer (1MLH) was from Remi Instruments, Mumbai.

Methods

Qualitative phytochemical analysis

Steroids: An aliquot of the skin extract (1 mL) was dissolved in 10 mL chloroform, and an equivalent volume of strong sulphuric acid was added to the test tube by the sides. The upper layer glows red, while the sulphuric acid layer turns yellow and fluoresces green. This suggested that steroids were present [12].

Terpenoids To 2ml of acetic anhydride and concentrated H_2SO_4, an aliquot of the skin extract (2ml) was added. The presence of terpenoids is shown by the creation of blue green rings [13].

Tannins: The presence of tannins was determined by mixing a portion of the skin extract (2ml) with a few drops of 1 percent lead acetate. The reddish precipitate showed the presence of tannins [14].

Saponins: An aliquot of the skin extract (5ml) was combined with 20ml distilled water and agitated for 15 minutes in a graduated cylinder. The presence of Saponins is shown by the formation of foam [15].

Anthocyanins: To 2ml of 2 N HCl and ammonia, an aliquot of the skin extract (2ml) was added. The presence of anthocyanins is indicated by the appearance of pink-red that fades to blue-violet [16].

Glycosides: In a 5ml extract, 2ml glacial acetic acid, one drop of 5% $FeCl_3$, and conc. H_2SO_4 were added; the formation of a brown ring indicated the presence of glycosides [17].

Alkaloids: Mayer's test: Mayer's regent (Potassium mercuric iodide solution) was added to the acidic solution. The presence of alkaloids is indicated by a cream-colored precipitate [18].

Phenol: When half a ml of $FeCl_3$ solution was added to two ml of test solution, a strong colour was produced, indicating the presence of phenols [19].

Flavonoids: A test tube was filled with a small amount of skin extract (2-3ml) and a few drops of sodium hydroxide solution. The presence of flavonoids is shown by the formation of a bright yellow colour that faded to white after a few drops of weak HCl were added [20].

Druglikeness ADME Studies

Druglikeness is a qualitative concept used in drug design for how "druglike" a substance is with respect to factors like bioavailability. It is estimated from the molecular structure before the substance is even synthesized and tested.

Which can be done by using Lipinski's rule states that, in general, an orally active drug has no more than one violation of the following criteria: No more than 5 hydrogen bond donors (the total number of nitrogen–hydrogen and oxygen–hydrogen bonds) No more than 10 hydrogen bond acceptors (all nitrogen or oxygen atoms).

The adhatoda vasica medicinal plant was selected for the identification of phytochemicals based on their inhibitory property against TPP. More than 9 phytochemicals from the plant, it were retrieved from extensive literature survey for ligand (inhibitor) preparation to act against TPPs of pathogens. Their respective two-dimensional chemical structures in structured data format (SDF) were retrieved from PubChem-NCBI database and SDF format was converted into Protein data bank (PDB) format using Pymol for further analysis [21].

Molecular Docking Studies

Analysis of Molecular Docking Protein Structure Preparation the Protein Data Bank (PDB) website contains 3D structures of big biological substances such as proteins and nucleic acids.

The structure of the T proteins, PDB ID 4BGH and 5ZWJ, was downloaded from the protein data bank with resolutions of 1.95A° and 2.9A°, respectively. http://www.rcsb.org/pdb/.

Hydrogen atoms are introduced to replace all heavy atoms, water molecules, and metal ions in the system. which are then stabilised with the least amount of energy using "Add Energy" → Kollman Charge, Gasteiger Charge were added in the Autodock MGL Tool.

Ligand Preparation Drug compound resveratrol Was drawn using the ACD/Chemsketch software as MOL format and then converted to pdb format using "OpenBabel" of MGL Tool.

In Autodock MGL Input the PDB format of Ligand from the OpenBabel software, and save the output as. PDBQT format. Now Add the Grid by input the macromolecule and select the ligand. In Grid Box set the x, y, z dimension as 60X60X60 and pick the atom from Atom toolbar, Save the atom grid as .TXT config file and Output was saved as. GPF (Grid Parameter File). Run the AutoGrid, and do the docking manual select macromolecule and ligand, In Search Parameter set the genetic algorithm RA run as 25. Save the Output as Lamarckian GA (4.2) DPF. Run AutoDock, In docking save the output as Vina Config (config.txt). Run AutoDock Vina and save as out pdbqt file [22, 23].

RESULTS

Non-nutrient chemical substances known as phytochemicals have been shown to help prevent non-communicable diseases. These chemical molecules are produced by plants to protect themselves, and they are also thought to protect humans from certain diseases. Phytochemicals that have biological activity, such as saponins, terpenoids, flavonoids, tannins, steroids, and alkaloids, have anti-inflammatory properties [24,25]. Hypoglycemic properties are found in glycosides, flavonoids, tannins, and alkaloids. Analgesic effects were found in steroids and triterpenoids.

Table 01: Phytochemical Screening result

PHYTOCHEMICAL CONSTITUENT	ETHANOL EXTRACT OF GRAPE SEED
Alkaloids	++
Glycosides	++
Saponins	++
Phenols	++
Flavonoid	+++
Tannis	+++
Anthocyanins	++
Terpenoids	+
Steroids	++
Terpenoids	+

Steroids, terpenoids, anthocyanins, glycosides, flavonoids, and phenols were found in the phytochemical contents of grape skin extract table-1.

Alkaloids, flavonoids, glycosides, polyphenol and flavonoids, tannins, and sterols were found in the ethanolic extract of *Adathoda Vasica*. Alkaloids, flavonoids, saponins, and tannins are phytochemicals that have been implicated as key bioactive substances in the medicinal use. In traditional medicine, the plant's source should be obvious and specific.

SWISS ADME Results

Table 02: ADME parameter results of phytochemical of *Adhatoda vasica*.

Compound	MW g/mol	#Heavy atoms	#Aromatic heavy atoms	#Rotatable bonds	#H-bond acceptors	#H-bond donors	MR	TPSA	Consensus Log P
1	188.23	14	0	6	2	1	62.11	35.83 Å²	1.23
2	335.40	25	12	4	3	1	106.02	53.93 Å²	3.07
3	426.72	31	0	0	1	1	134.88	20.23 Å²	7.22

Table 03:

Compound	GI absorption	BBB permeant	Pgp substrate	Lipinski #violations	Bioavailability Score	Synthetic Accessibility
1	High	No	No	0	0.55	3.36
2	High	Yes	Yes	0	0.55	3.92
3	low	No	No	Yes; 1 violation: MLOGP= 7.22	0.55	6.04

Insilico Docking Studies

Pulmonary Activity:

Vasicine: The binding affinity score given by atomic contact energy (ACE) value for Vasicine at superfamily subgroup of trehalose 6 Phosphate Phosphatase enzyme is -6.5 and the hydrogen bond interaction formed by Vasicine at superfamily subgroup of trehalose 6 Phosphate Phosphatase enzyme is shown in figure a) & b) along with their visualization

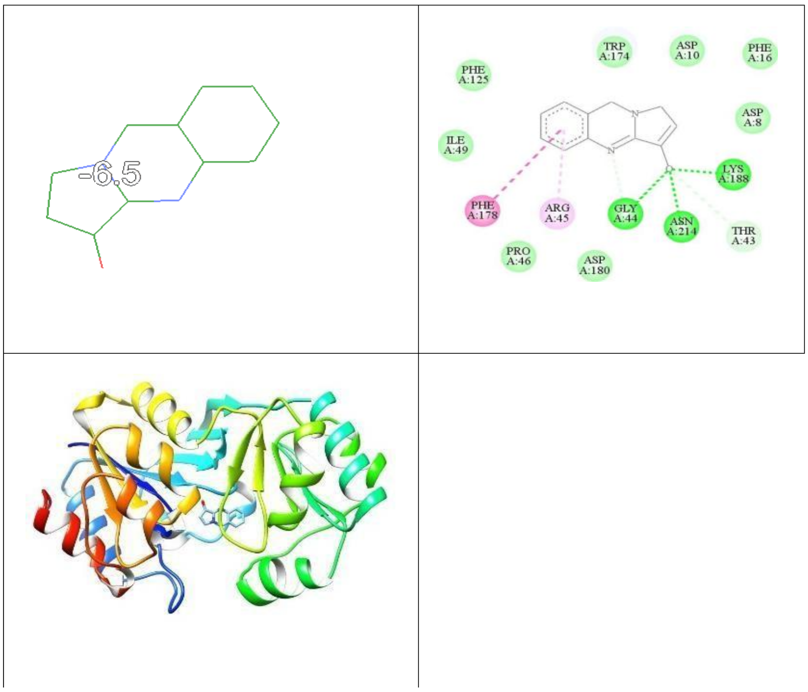


Figure 02: Docking image of Vasicine at superfamily subgroup of trehalose 6 Phosphate Phosphatase e enzyme.

Adhatodine: The binding affinity score given by atomic contact energy (ACE) value for Adhatodine at superfamily subgroup of trehalose 6 Phosphate Phosphatase enzyme is -7.0 and the hydrogen bond interaction formed by Adhatodine at superfamily subgroup of trehalose 6 Phosphate Phosphatase enzyme is shown in figure a) & b) along with their visualization c).

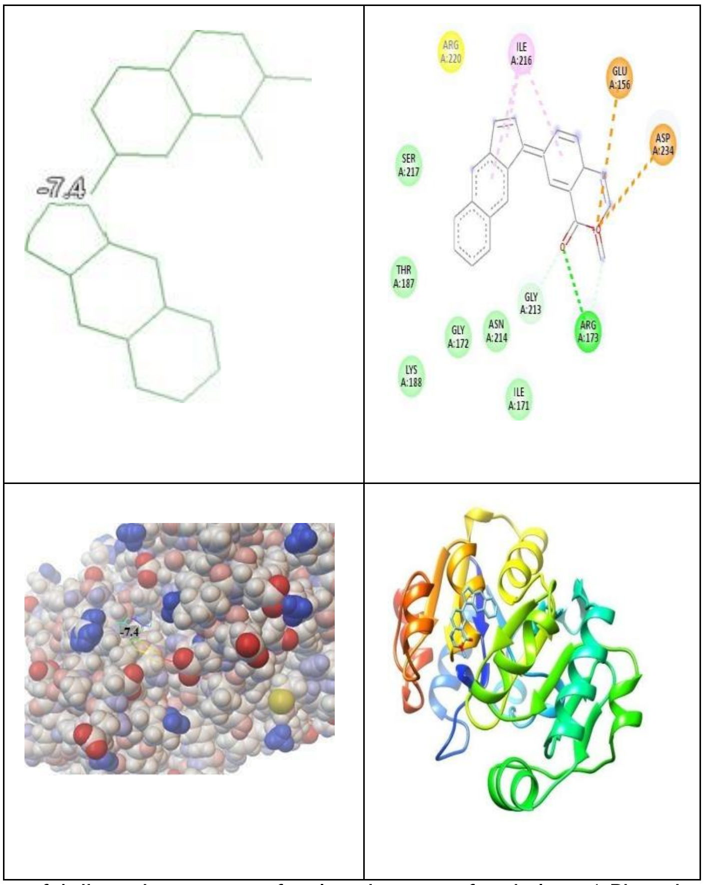


Figure 03: Docking image of Adhatodine at superfamily subgroup of trehalose 6 Phosphate Phosphatase enzyme.

Epitaraxenol: The binding affinity score given by atomic contact energy (ACE) value for Epitaraxenol at superfamily subgroup of trehalose 6 Phosphate Phosphatase enzyme is -7.0 and the hydrogen bond interaction formed by Epitaraxenol at superfamily subgroup of trehalose 6 Phosphate Phosphatase enzyme is shown in figure a) & b) along with their visualization c).

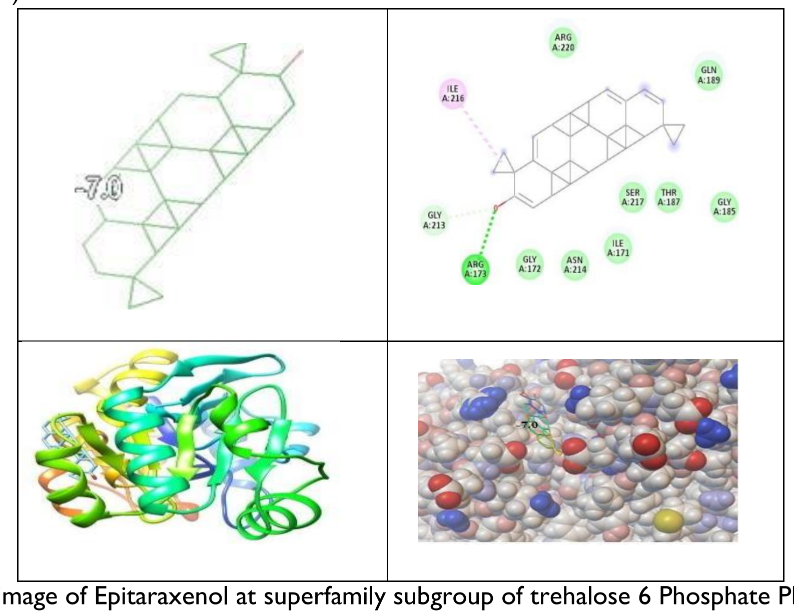


Figure 04: Docking image of Epitaraxenol at superfamily subgroup of trehalose 6 Phosphate Phosphatase enzymeā

Table 04: Structure of Ligands

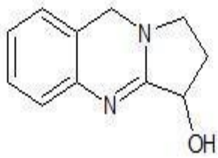
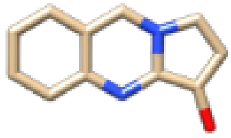
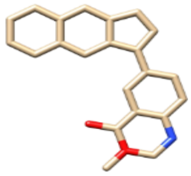
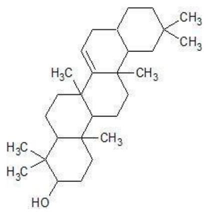
STRUCTURE	COMPOUND	PDB STRUCTURE
	1	
	2	
	3	

Table 05: Binding Energy of the Molecular Docking study of compound ligands with the Protein 1YMQ

S.NO	Compound	Conformation	Binding Energy	No of Hydrogen Bonds	Hydrogen Contacts
1	Vasicine	2	-6.5	5	ARG 45, GLY44, PHE 178, LYS 188, ASN 214.
2	Adhatodine	1	-7.4	5	GLU 156, ARG 173, GLY 213, ILE 216, ASP 234
3	Epitaraxenol	2	-7.0	3	ARG 173, GLY 213, ILE 216

DISCUSSION

Natural source of medicine is the main aim of our research which was developing in recent days. As conventional medicine is showing various side effects in treatment. Natural sources as therapeutics is important resource of novel medicine developing in recent era. Hence, our study where research on pulmonary activity of various phytochemical compound from adhatoda vasica, procedure where quite promising So as the Readers & Researchers will find interest in natural products as a source of therapeutics Compound which have played important role in the development of modern–day-medicines. The present study showed that the active compounds of Adhotoda vasica is rich in basic nutrients. Qualitative phytochemical screening showed that it is abundant in phytochemicals such as Vasicine, adhatodine, epitaraxerol, etc.

Inslico Docking studies done in the present research of pulmonary activity where 1YMQ PDB id were selected and binds with the phytochemicals of Adhatoda vasica compounds and it is performed and obtain the good hydrogen bonding and binding energy with Docking Score: Vasicine: -6.5, Adhatodine: -7.4, Epitaraxerol:

CONCLUSION

Molecular docking presents a powerful approach for investigating the potential of Adhatoda vasica phytochemical compounds on pulmonary activity. Through the identification of target proteins, prediction of binding modes, and validation through experimental studies, the therapeutic potential of these compounds for respiratory diseases can be explored. The successful application of molecular docking in this context may lead to the development of novel treatments and contribute to improved respiratory health outcomes for individuals worldwide.

In this study we have done SWISS ADME studies and among 3 phytochemical constituents 2 satisfied all factors of Lipinski rule., ie., Vasicine, Adhathodine, and Epitaraxerol satisfies Lipinski rule with one violation. So both phytochemical constituents are orally bioavailable according to Lipinski rule. The current study establishes that Adhatoda vasica compound epitaraxeerol is more effective than Vasicine and epitaraxerol shows significant response on pulmonary activity on 1YMQ respectively. By Molecular docking studies reveals that Compound adhatodine with Docking score -7.4 having more responsible for pulmonary activity compared to the compound Vasicine with the docking score: -6.5, and epitaraxerol with the docking score: -7.0. Hence the current research proves that the phytochemical compound of Adhatoda vasica act as promising lead as pulmonary agent. Further research which includes Invitro activity, Stability and Toxicity profile studies needs to be assessed for establishing better result prior to clinical use.

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NIL

CONFLICT OF INTEREST

Not declared

AUTHOR CONTRIBUTION

All authors are contributed equally.

INFORM CONSENT AND ETHICAL CONSIDERATIONS

Not applicable

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