

Phytochemicals analysis of orchid buds against l-histidinol dehydrogenase of salmonella causing Dysentery: In silico

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Abstract

This present study reveals the effects of orchid buds ethanolic extract on dysentery. Dysentery is a bacterial infection and many kinds of bacteria may create dysentery. In this study one bacteria named as salmonella has taken. Salmonella is a genus of rod-shaped gram -ve bacteria of the family Enterobacteriaceae. Though salmonella poisoning is generally not a severe illness, it can be fatal in certain people and can cause dangerous dehydration phytochemicals of orchid buds were interacted with one enzyme of salmonella i.e. L-Histidinol dehydrogenase. All the phytochemicals of orchid buds were considered as ligands and the L-Histidinol dehydrogenase enzyme was taken as a receptor. All the operation was carried out in Biovia discovery studio under molecular docking menu. It gives the potential phytochemical of the taken plant which can act as a powerful drug against microbes. L (+) Aspartic acid can inhibit the enzyme involved in metabolic pathway of salmonella.

Keywords: Phytochemicals, salmonella, orchid buds, dysentery

1. Introduction

A medicinal plant is any plant which contains substances that may be similar to synthetic drugs. From phytochemical and pharmacological screening of medicinal plants it has been evaluated which parts of the plant can be used as a traditional medicine. A number of plants have been used in traditional medicine from ancient times due to its numerous applications in human life and also the plant-based drugs have no side-effect as compared to the chemical drug. The Orchid plant (*Bauhinia Variiegata*) belongs to the family Fabaceae which is commonly known as Kanchar tree has a high range of medicinal value. Most of the parts of this plant have been used for traditional medicines and it is helpful in cure of various disorder^[1]. The different sections of orchid plant like its stem, bark, seed, leaves, flowers and roots have been used for its high potentiality of medicinal importance. Diseases which can be curable by using this plant products are like Dysentery, Diabetic, Piles and Skin diseases etc.^[2] The phytochemical screening showed that Variegate contained different phytochemicals which are required for the treatment of different kinds of pathologies. This plant has a great number of pharmacological properties and studies showed that *Bauhinia Variiegata* exerted anticancer, antimicrobial, anti-inflammatory, antiulcer etc^[3, 4]. Salmonella infection is a common bacterial disease that affects the intestinal tract. These bacteria mainly live in the human and animal intestine and humans become infected through contaminated water and food. Salmonella infection develops diarrhea, dysentery, fever, abdominal cramp etc. Salmonella infection is basically called food poison and it is one type of bacteria which causes food-borne illness.^[5, 6] Dysentery is an intestinal inflammation primarily of the colon. It can lead to mild or severe stomach cramps and severe diarrhoea with mucus or blood in the faces. Dysentery is most often caused by bacteria like shigella bacteria or Salmonella bacteria. Salmonella infections are usually caused by eating raw or undercooked meat or egg products.

Most salmonella infections can be classified as stomach flu. Main aim of this present study is to identify the phytochemicals from orchid buds which are responsible for curing dysentery caused by salmonella. The phytochemicals like Aspartic acid, Glycine, Glutamic acid and Alpha-Alanine are responsible to cure dysentery by inhibiting the pathway of microbe.

2. Materials and Methods

2.1 Software used

Software used in molecular docking Biovia software (Dassault systems of France) has been used to perform molecular docking. In biovia three modules are there but a molecular docking process discovery studio is needed. This software is quite easy to understand and easy to perform molecular docking processes. This software gives the technique to predict the level of molecular interaction between the enzyme and the ligand.

2.2 Methodology

2.2.1 List of Phytochemicals

Phytochemicals are natural compounds found in the plant body. These are chemicals and play an important role in human life as they consist of antioxidant properties which are beneficial to human health. They generally have biological activities in the plant host and play a role in plant growth. Phytochemicals are mainly biocatalysts which can affect human metabolism. These are required for the benefits of human health. Orchid buds consist of phytochemicals like Aspartic acid, Glycine, Glutamic acid and Alpha-Alanine. so these phytochemicals act as ligands against Histidinol dehydrogenase enzyme of salmonella. From the published paper it has been observed that dysentery is mainly caused due to some bacteria like salmonella, Shigella and amoeba *Entamoeba histolytica* etc. The existence of pathogenic bacteria inside its biological host is totally dependent on some metabolic pathway. These

metabolic pathways are a series of chemical reactions which need some particular enzyme as its biocatalyst.

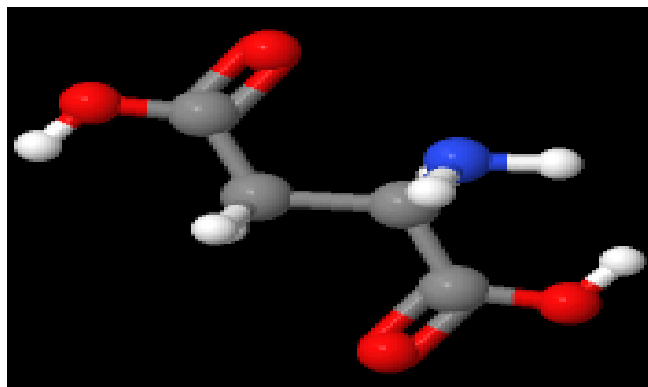


Fig 1: Aspartic acid (C_4H_7NO) Average Mass: 133.103 Da

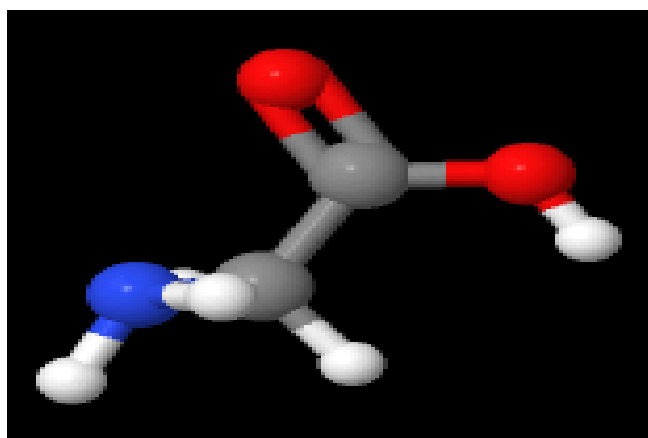


Fig 2: Glycine (C_2H_5NO) Average Mass: 75.067 Da

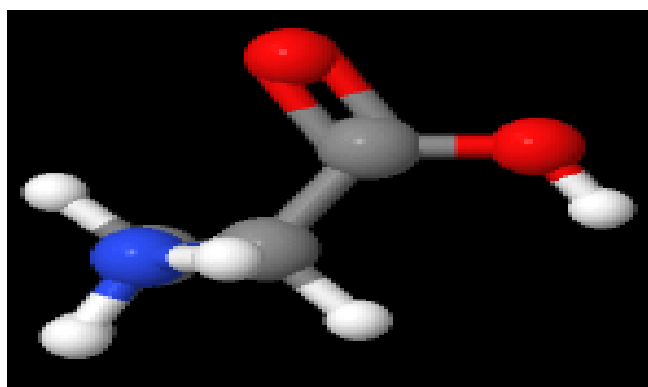


Fig 3: Alpha-Alanine (C_3H_7NO) Average Mass: 89.093 Da

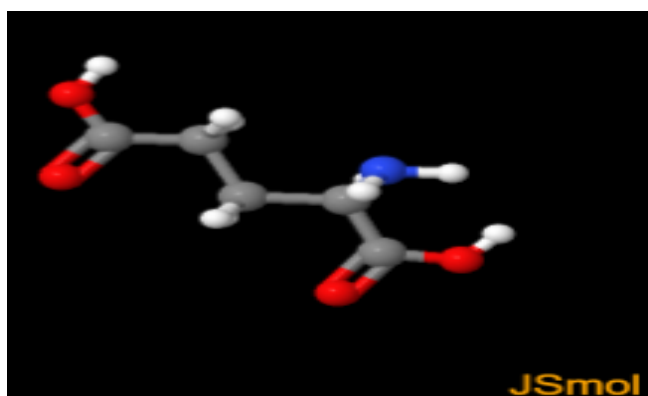


Fig 4: Glutamic acid (C_5H_9NO) Average Mass: 147.129 Da

2.2.2 Enzyme found in Salmonella bacteria

It has been shown that salmonella causes bacterial infection in the human body. It causes stomach infection, diarrhoea and dysentery like ailment. The survival of any microbe is totally dependent upon various biological pathways which is carried out inside the microbe body. For regulation of this metabolic pathway enzymes are required. So, these biochemical reactions in microbes are regulated by different enzymes which act as biocatalysts for a specific biochemical reaction. Different enzyme list can be found from Brenda enzyme database. This Brenda enzyme database was used to recognize and list down the enzymes found in salmonella. It has been found that L-Histidinol dehydrogenase of salmonella of protein database code (1KAE) is involve in dysentery.so by blocking the active sites of Histidinol dehydrogenase enzyme through specific ligands can destroy the bacteria by inhibiting the metabolic pathway of that bacteria.

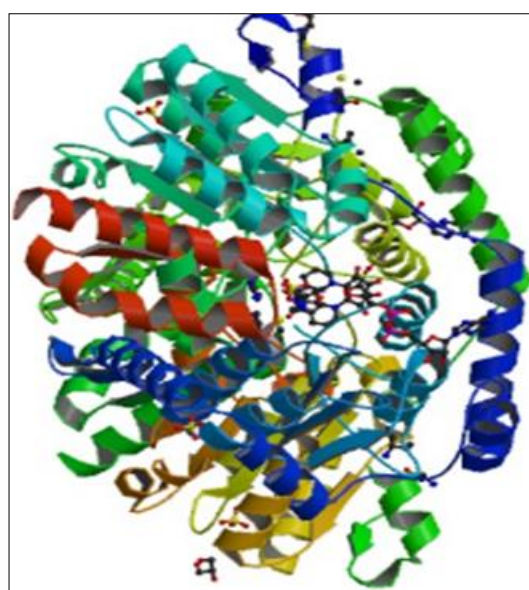


Fig 5: L-Histidinol dehydrogenase PDB Code: 1KAE

2.2.3 Molecular docking

Molecular docking is a method in biovia discovery studio which is used to block/deactivate the active site of the given enzyme by identifying the small molecule which is basically phytochemical isolated from the plant body and i.e. act as a ligand which form a strong interactive bond with the microbe protein to inhibit the bacteria successfully.

The First step is to prepare a phytochemical list present in orchid buds from google or from various published articles. Next step is downloading SDF/MOL files for the phytochemicals present in orchid buds from different websites like PubChem, Chem spider etc. Then the selected enzyme structure was downloaded from PDB RCSB website and enzyme 3D structure was copied and pasted to the remote desktop. After the opening of the structure of enzyme in the discovery studio, receptor-ligand interaction has been selected to find the active sites of the given enzyme as ligands only bind to active sites of enzyme. In receptor-ligand interaction protocol, receptor cavity is present which is then selected to identify the active site of that enzyme. Then for molecular docking two protocols are present one is C Docker which is required for ligand-protein interaction and other is Z -Docker which is required for the

protein-protein interactions. As it was a ligand-protein interaction so C-DOCKER protocol has been chosen. All the treated phytochemicals were considered as a ligand whereas the enzyme molecule was considered as a receptor as it receives the appropriate ligand into it. By selecting all

the data, it will run for 15 minutes to get the final result on the basis of two energy values i.e. -C Docker and -C Docker interaction energy. Thus, the high interaction with high positive value shows that taking phytochemical may cure dysentery.

3. Results and Discussion

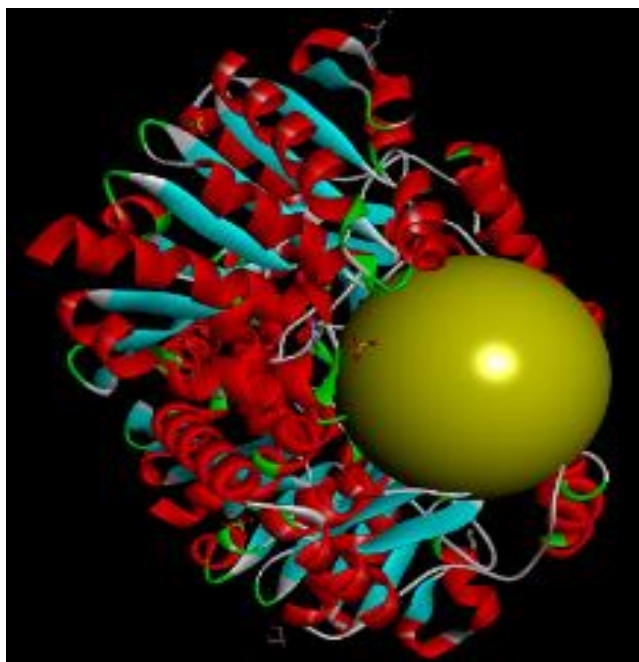


Fig 6: Active sites of Histidinol dehydrogenase enzyme

Above Fig-6 shows green colour round shape structure i.e. active sites of Histidinol dehydrogenase enzyme. It looks like green. Molecular docking is a molecular dynamic. From this dynamic's ligand is confirmed for deactivation of the active site of that enzyme. The basis for best molecular interaction was selected by taking high positive value of -C

Docker energy and small energy difference between -C Docker and -C Docker interaction energy. These two-energy values were used as a benchmark for the confirmation of molecular docking. The high positive value of -C Docking energy states that a good molecular interaction between a small molecule and the receptor molecule.

Table 1: Molecular docking energy value

Sr NO.	Small molecule (Ligand Molecule name)	-C Docker energy Value	-C Docker interaction energy Value	Difference between two energy value (between -C DOCKER interaction energy and -C DOCKER energy)
1	L(+) Aspartic acid	25.3936	24.117	1.2766
2	Glycine	16.9635	16.7285	0.235
3	Alpha-Alanine	19.6735	19.4256	0.2479
4	L(-) Glutamic acid	Failed	Failed	
5	DL Aspartic acid	Failed	Failed	

Table 1 indicates that the L (+) Aspartic acid shows highest -C Docker energy value which is highly positive among all other ligand i.e. 25.3936 with a small difference of 1.7726 between two energy values i.e. -C DOCKER interaction and -C DOCKER energy. Thus the result shows that L (+) Aspartic acid can fruitfully deactivate Salmonella Histidinol dehydrogenase enzyme and can block the metabolic pathway of the bacteria. Highest positive value of L (+) Aspartic acid confirmed that it was most effective ligand against Salmonella bacteria. so the main phytochemicals preventing dysentery by salmonella is L (+) Aspartic acid.

4. Conclusions

Orchid tree has been used as a traditional medicine from ancient times for its wide range of phytochemicals which are having numerous medicinal values towards health

disorder. Previously it was evaluated that buds of orchid trees have a healing effect against dysentery which is due to salmonella bacteria. This silico analysis gives the information of theoretical values of this observation. Orchid trees have different pharmacological properties like anticancer, antibacterial, antidiabetic and anti-inflammatory properties etc. This study was taking place in the biovia discovery studio module. From the result of molecular docking it has been observed that L (+) Aspartic acid forms stronger bonds with L-Histidinol enzyme and can inhibit the metabolic pathway of that microbe. Most significant result was found in L (+) Aspartic acid for its high +ve value of -C Docker energy followed by glycine and alpha-Alanine. But ligands like L (-) Glutamic acid and DL Aspartic acid show no result as it couldn't form any interaction with enzyme Histidinol dehydrogenase. So this study reveals that L (+)

Aspartic acid gives medicinal values to orchid buds against dysentery caused by salmonella and can be used in making drugs for dysentery.

5. References

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