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Pavonia odorata Derived Phytochemicals against *Entamoeba histolytica* Causing Dysentery

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

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ABSTRACT

Phytochemicals from *Pavonia odorata* plant extract are traditionally used to cure Dysentery. It is caused by *Entamoeba histolytica*. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that palmitic acid can effectively deactivate the *Alcohol dehydrogenase* enzyme thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Pavonia odorata; Entamoeba histolytica.

1. INTRODUCTION

Plants contain secondary metabolites that can be used formulated to drugs [1]. The bioactive compounds derived from various plant parts contain medicinal properties. The extracts of these phytochemicals exhibit antibacterial and antifungal properties [2]. They play a vital role in enhancing the immune power and health of people [3].

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Pavonia odorata extract is used to cure diseases like Dysentery. The objective of the study is to identify the phytochemical responsible to cure the disease.

Pavonia odorata contains “palmitic acid, caporic acid, Hexahydrofarnesyl acetone, Alpha-terpinene, Alpha-pinene, Alpha-eeudesmol” etc. These phytochemicals might act against Dysentery. However, there is no such study available.

This objective of the study is to identify the phytochemical of *Pavonia odorata* capable of curing Dysentery.

2. MATERIALS AND METHODS

2.1 Software Used

Discovery studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques to predict the level of molecular interaction.

2.2 Methodology

2.2.1 List of phytochemicals

Phytochemicals are produced by plants as secondary metabolites to protect them from predators. The potential threats to plants include bacteria, viruses, fungi, etc.. When these plants or their parts are consumed by humans these phytochemicals fight off threats to health. Some phytochemicals have been used as poisons and others as traditional medicine. Published works showed that *Pavonia odorata* contains palmitic acid, caporic acid, Hexahydrofarnesyl acetone, Alpha-terpinene, Alpha-pinene, Alpha-eeudesmol etc. It has already been established that *Pavonia odorata* plant belonging to Malvaceae family has potential to help controlling Dysentery. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling of Dysentery.

2.2.2 Enzyme found in salmonella

It has been reported that Dysentery can cause as a result of *Entamoeba histolytica* infestation. Various metabolic cycles have been seen in the bacterial life cycle for its survival. These metabolic cycles are regulated by different enzymes. Brenda enzyme database was used to identify and list different enzymes found in *Entamoeba histolytica*. It has been found that Alcohol dehydrogenase *Entamoeba histolytica* enzyme (protein database code 1Y9A) is involved in different metabolisms like Tryptophan metabolism, Tyrosine metabolism, Phynylalanine metabolism, Leucine metabolism, Valine metabolism, Methyonine metabolism, Ethanol formatation, Propanol degradation (BRENDA) and very crucial for the survival of the particular microbe.

2.2.3 Molecular docking

The molecular docking method has been used to identify the phytochemical from the plant extract, which acts as a ligand and form a strong covalent bond with the bacterial protein to successfully inhibit the microbe. The Discovery studio module of Biovia software was used for identifying molecular interaction and perform molecular docking. In this process first, the SDF files for the phytochemicals found in the *Pavonia odorata* plant were downloaded from the website (Pub-Chem). The protein database code of the Alcohol dehydrogenase *Entamoeba histolytica* enzyme was identified from the website (Brenda-enzyme database). The active site of the enzyme was identified via “receptor cavity” protocol found under "receptor-ligand interaction" menu. Molecular docking was done using the CDOCKER protocol of Biovia software under “receptor-ligand interaction”. The enzyme molecule was treated as the receptor molecule and the phytochemical was treated as the ligand. The “-CDOCKER_ENERGY” and “-CDOCKER_INTERACTION_ENERGY” were used as an indicator for the quality of molecular docking. The high positive value of those indicators presented a good interaction between the ligand and the receptor. Thus, the interactions with high values might indicate the major phytochemical responsible for curing the disease.

3. RESULTS AND DISCUSSION

-CDOCKER energy was calculated based on the internal ligand strain energy and receptor-ligand interaction energy. -CDOCKER interaction signifies the energy of the nonbonded interaction that exists between the protein and the ligand. The criteria for best interaction was chosen based on a high positive value of -CDOCKER energy and b) small difference between -CDOCKER energy and -CDOCKER interaction energy [4,5]. Table 1 shows that Alcohol dehydrogenase *Entamoeba histolytica* palmitic

Table 1. Results of C Docking of phytochemicals with Alcohol dehydrogenase *Entamoeba histolytica* (receptor)

Sl. no.	Ligand	-CDOCKER Energy	-CDOCKER Interaction Energy	Difference between -CDOCKER interaction energy and -CDOCKER energy	Remarks
1	Palmitic acid	35.7412	33.204	2.5372	Maximum inhibition of microbial infection
2	Caproic acid	17.994	14.9688	3.0252	
3	Hexahydrofarnesyl acetone	14.4432	10.7125	3.7307	
4	Pinocarveol	-6.49664	13.8402	20.33684	
5	Alpha-eudesmol	-11.8495	18.295	30.1445	
6	Alpha-pinene	-12.0895	12.9466	25.0361	
7	Alpha-terpine	-20.765	14.0157	34.7807	

acid interaction has the highest positive value of -CDOCKER energy (35.7412) and minimum value of the difference (2.5372) between - C DOCKER interaction energy and - C DOCKER energy followed by caporic acid. Thus the results indicated that palmitic acid and caporic acid can effectively deactivate the Alcohol dehydrogenase enzyme of *Entamoeba histolytica*, thereby interrupting the biological cycle of *Entamoeba histolytica*. Higher positive values for palmitic acid indicated that it was the most active ingredient against *Entamoeba histolytica*. On the other hand, Alpha-terpinene, Alpha-pinene and Alpha-eudesmolcan deactivate the enzyme to a small extent (negative -CDOCKER energy but positive –CDOCKER interaction energy). Alpha-terpine and Alpha-pinene cannot interact with Alcohol dehydrogenase *Entamoeba histolytica* enzyme. Thus, the key phytochemicals preventing Dysentery caused by *Entamoeba histolytica* are palmitic acid, caporic acid and Hexahydrofarnesyl acetone.

4. CONCLUSIONS

It was previously known that *Pavonia odorata* plant has medicinal action against Dysentery. Dysentery is caused by *Entamoeba histolytica*. This study was carried out to provide the theoretical basis of this observation. Using Discovery studio module of Biovia software, molecular docking operation was performed to identify the phytochemical (palmitic acid, caporic acid, Hexahydrofarnesyl acetone, Alpha-terpinene, Alpha-pinene, Alpha-eudesmol), which can have significant interaction with the vital enzyme (Alcohol dehydrogenase *Entamoeba histolytica*) of the microbe. It was found that palmitic acid, caporic acid, and Hexahydrofarnesyl acetone can form a strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Alpha-terpinene, Alpha-pinene, and Alpha-eudesmol were found to be not much effective in deactivating the enzyme of the microbe. Thus, this study could explain that the presence of palmitic acid, caporic acid and Hexahydrofarnesyl acetone provided the medicinal values to *Pavonia odorata* against Dysentery caused by *Entamoeba histolytica.*

DISCLAIMER

The products used for this research are commonly and predominantly use products in our area of research and country. There is absolutely no conflict of interest between the authors and producers of the products because we do not intend to use these products as an avenue for any litigation but for the advancement of knowledge. Also, the research was not funded by the producing company rather it was funded by personal efforts of the authors.

CONSENT

It is not applicable.

ETHICAL APPROVAL

It is not applicable.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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