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Boswellia serrata Derived Phytochemicals against 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

Dysentery is an intestinal inflammation, primarily of the colon. Nature is a major source of medicines for different diseases like Dysentery. Phytochemicals from *Boswellia serrata* plant extract can cure Dysentery. This objective of the study is to identify the phytochemical of *Boswellia serrata* capable of curing Dysentery. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that p-cymene can effectively deactivate the enzyme, thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Boswellia serrata; Dysentery; molecular docking; traditional medicine.

1. INTRODUCTION

Dysentery is an intestinal inflammation, primarily of the colon. Dysentery is often spread through contaminated food or water. It can lead to mild or severe stomach cramps and severe diarrhoea with mucus or blood in the feces. It is reported that Dysentery is caused by *Entamoeba histolytica,* an anaerobic parasitic amoebozoan. Nature is a major source of medicines [1] for different diseases like Dysentery. The medicinal value of the plants is due to the phytochemicals

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present in it. Phytochemicals can be derived from different parts of plants. Different medicinal plants and their phytoextracts have shown anti-microbial action [2]. These medicinal plants play a key role in human health care. Many people rely on the use of traditional medicine [3]. *Boswellia serrata* extract is used to cure diseases like Dysentery. The objective of the study is to identify the phytochemical responsible to cure the disease. *Boswellia serrata* contains "beta-pinene, alpha-pinene, p-cymene, limonene, piperazine" 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 *Boswellia serrata* capable of curing Dysentery.

2. MATERIALS AND METHODS

2.1 Software Used

The Discovery studio module of Biovia software (Dassault Systems 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 *Boswellia serrata* contains boswellic acid, D-limonene, Incensole acetate, P-cymene, sabinene, Terpinen-4-ol, etc. It has already been established that *Boswellia serrata* plant has the potential to help controlling Dysentery. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling Dysentery.

2.2.2 Enzyme found in *Entamoeba histolytica*

It has been reported that Dysentery can cause as a result of Entamoeba sp. Infection. 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 *E. histolytica*. It has been found that alcohol dehydrogenase enzyme (protein database code 1Y9A) is involved in different metabolism like Tryptophan metabolism, Phenylalanine metabolism, Valine metabolism, Methionine metabolism, Ethanol formation, Propanol degradation (BRENDA) and is 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 *Boswellia serrata* plant were downloaded from the website (Pub-Chem). The protein database code of the alcohol dehydrogenase enzyme was identified from the website (www.rcsb.org). The active site of the enzyme was identified via the "receptor cavity" protocol found under the "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 P-cymene interaction has the highest value of -CDOCKER energy (12.4406) and minimum value

Table 1. Results of CDocking of phytochemicals with Alcohol dehydrogenase (receptor)

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and -CDOCKER energy
1	p-cymene	12.4406	12.9227	0.4821
2	Boswellic acid	6.07175	15.5173	9.44555
3	Terpinen-4-ol	-13.4773	15.3683	28.8456
4	Sabinene	-17.4056	13.9505	31.3561
5	D-limonene	-24.0287	14.2101	38.2388
6	Incensole acetate	-38.1204	24.839	62.9594

of the difference (0.4821) between -CDOCKER interaction energy and -CDOCKER energy followed by boswellic acid. Thus the results indicated that P-cymene and Boswellic acid can deactivate the alcohol dehydrogenase enzyme thereby interrupting the biological life cycle of *E. histolytica*.

A higher positive value of P-cymene indicates that it is the most active ingredient against the microbe. On the Other hand, D-limonene, Incensole acetate, Sabinene, and terpinen-4-ol can deactivate the enzyme to a small extent (negative -CDOCKER energy and positive -CDOCKER interaction energy) by bind to its active side. Thus the key phytochemicals preventing Dysentery caused by *E. histolytica* are P-cymene and Boswellic acid.

4. CONCLUSIONS

It was previously known that *Boswellia serrata* plant has medicinal action against Dysentery. Dysentery is caused by *E. histolytica*. This study was carried out to provide the theoretical basis of this observation. Using the Discovery studio module of Biovia software, molecular docking operation was performed to identify the phytochemical (Boswellic acid, D-limonene, P-cymene, Incensole acetate, sabinene, Terpinene-4-ol), which can have significant interaction with the vital enzyme alcohol dehydrogenase of the microbe. It was found that P-cymene and Boswellic acid can form a strong bond with the enzyme thereby inhibiting the metabolic cycle of the microbe. Other phytochemicals are not much effective in deactivating the enzyme of the microbe. Thus, this study could explain that the presence of P-cymene and Boswellic acid phytochemicals provide medicinal value to *Boswellia serrata* against *E. histolytica*.

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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