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Boswellia serrata Roxb. ex Colebr. Derived Phytochemicals against Skin Disease

Diptiprajnya Sahoo[1], Chinmayee Naik[1], Ashwini Kumar Mahanti[1], Mukundjee Pandey[1] and Gyanranjan Mahalik[1*]

[1]Centurion University of Technology and Management, Odisha, India.

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 *Boswellia serrata* Roxb. ex Colebr plant extract are traditionally used to cure skin disease. It is caused by *Staphylococcus aureus.* 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 shikimate dehydrogenase enzyme thereby interrupting the life cycle of the organism.

Keywords: Boswellia serrata; phytochemical; Staphylococcus aureus; skin disease.

1. INTRODUCTION

Many people rely on the use of traditional medicine [1].

The environment is a significant wellspring of medications [2]. The traditional medicinal estimation of the plants is because of the phytochemicals present in it. Phytochemicals can be gotten from various pieces of plants. Diverse therapeutic plants and their phytoextracts have shown inhibiting microbial action [3]. These traditional plants assume a key job in human social healthcare. Numerous individuals depend on the utilization of ethnomedicinal medication [1].

**Corresponding author: E-mail: gyanranjan.mahalik@cutm.ac.in;*

Boswellia serrata belongs to family Burseraceae. *B. serrata* extract is traditionally used to cure skin disease. The objective of the study is to identify the phytochemical responsible to cure the skin disease.

B. serrata contains “P-cymene, boswellic acid” etc. These phytochemicals might act against skin diseases. However, there is no such study available.

This objective of the study is to identify the phytochemical of *B. serrata* capable of curing skin diseases.

2. MATERIALS AND METHODS

2.1 Software Used

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. 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. It has already been established that *Boswellia serrata* plant belonging to Burseraceae family has potential to help controlling skin disease. This work is focused on identification of the particular phytochemical responsible for inhibiting and controlling of skin disease.

2.2.2 Enzyme found in *Staphylococcus aureus*

It has been reported that skin disease can be caused as a result of *Staphylococcus aureus* 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 *Staphylococcus aureus* bacteria. It has been found that shikimate dehydrogenase (protein database code 1NYT) is involved in chorismate metabolism (KEGG) and very crucial for survival of the particular microbe.

2.2.3 Molecular docking

Molecular docking method has been used to identify the phytochemical from the plant extract, that act 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 (www.molinstinct.com). The protein database code of the shikimate dehydrogenase enzyme was identified from the website (www.rcsb.org). 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 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.Thecriteria 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 shikimate dehydrogenase-P-cymene interaction has the highest minimum value of the difference (0.33347) between - C DOCKER interaction energy and - C DOCKERenergy followed by boswellic acid(has the highest positive value i.e. 12.5266). Thus, the

Table 1. Results of C Docking of phytochemicals with shikimate dehydrogenase (receptor)

Ligand	- CDOCKER energy	- CDOCKER interaction energy	Difference between - C DOCKER interaction energy and - C DOCKER energy	Remarks
P-cymene	4.41674	4.75021	0.33347	Maximum inhibition of microbial enzyme
Boswellic acid	12.5266	25.7663	13..2397	
Sabinene	-16.1732	12.4186	28.5918	
Terpinen-4-ol	-17.4794	15.4128	32.8922	Minimum inhibition of microbial enzyme
D-limonene	-24.1232	16.9494	41.0726	
Incensole acetate	FAILED	FAILED	NA	-

results indicated that P-cymene can effectively deactivate the shikimate dehydrogenase enzyme thereby interrupting the biological cycle of *Staphylococcus aureus*. Higher positive values for boswellic acid also indicated that it was the most active ingredient against *Staphylococcus aureus*. On the other hand, sabinene, terpinen-4-ol and D-limonene can deactivate the enzyme to a small extent (negative -CDOCKER energy but positive -CDOCKER interaction energy). Incensole acetate cannot interact with shikimate dehydrogenase enzyme. Thus, the key phytochemicals preventing skin disease caused by *Staphylococcus aureus* is P-cymene.

4. CONCLUSIONS

It was previously known that *Boswellia serrata* plant has medicinal action against skin disease. Skin disease is caused by *Staphylococcus aureus*. 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 (Boswellic acid, D-limonene, Incensole acetate, P-cymene, Sabinene, Terpinen-4-ol), which can have a significant interaction with the vital enzyme (shikimate dehydrogenase) of the microbe. It was found that P-cymene can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. D-limonene, sabinene and terpinen-4-olwere found to be not much effective in deactivating the enzyme of the microbe. Incensole acetate cannot deactivate the enzyme. Thus, this study could explain that the presence of P-cymene provided more medicinal values to *Boswellia serrata* against skin disease caused by *Staphylococcus aureus*.

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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