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PHYTOMEDICINAL EFFECT OF *Nardostachys jatamansi* AGAINST DERMATITIS CAUSING *Staphylococcus aureus*: AN *In silico* ANALYSIS

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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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Short Research Article

ABSTRACT

Dermatitis is caused by *Staphylococcus aureus.* Alcohol dehydrogenase is one of its major enzymes. *Nardostachys jatamansi* is known to cure of dermatitis**.** The plant extract contains different phytochemical compounds. By using "Biovia Discovery Studio", the molecular docking of the phytochemicals with the enzymes was studied. The results showed that phytochemicals1-octacosanol and beta-sitosterol can deactivate the alcohol dehydrogenase enzyme thereby interrupting the microbe's life cycle.

Keywords: Phytochemical; *Nardostachys jatamansi; Staphylococcus epidermidis.*

1. INTRODUCTION

The use of herbal medicine increased significantly in the world including developed countries due to the pharmacological activities of plants [1,2]. The knowledge about plants has been provided by ancient people.

The stem, roots, leaves etc. were screened to get different phytochemical content [1]. Jatamansi belongs to family Caprifoliaceae. Its extract can fight against diseases like dermatitis. There is high likelihood that these phytochemicals assume a significant job in relieving a disease. Anyway, there is no report distinguishing the particular phytochemical capable to fix eczema.

Staphylococcus epidermidis is known to cause dermatitis.

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

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threats to health. Some phytochemicals have been used as poisons and others as traditional medicine. Published works showed that *Nardostachys jatamansi* contains 1-Octacosanol, Beta-sitosterol, Oleanolic Acid, Ursolic Acid etc. It has already been established that *Nardostachys jatamansi* plant belonging to Caprifoliaceae family has the potential to help to control Epidermitis. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling of Epidermitis.

2.2.2 Enzyme found in *Staphylococcus*

It has been reported that Dermititis 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 alcohol dehydrogenase enzyme (protein database code 4RQT) is involved in valine metabolism (KEGG) and very crucial for the survival of the particular microbe.

2.2.3 Molecular docking

Molecular docking method has been used to identify the phytochemical from the plant extract, which acts as a ligand and forms 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 *Nardostachys jatamansi* plant were downloaded from the website (PUBCHEM). The protein database code of the alcohol dehydrogenase enzyme was identified from the website (brenda-enzymes.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 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 [3,4].

Table 1 shows that alcohol dehydrogenase-1-octacosanol interaction has the highest positive value of -CDOCKER energy (52.7539) and minimum value of the difference (5.9638) between - CDOCKER interaction energy and - C DOCKER energy. Thus the results indicated that 1-octacosanol can effectively deactivate the alcohol dehydrogenase enzyme thereby interrupting the biological cycle of *Staphylococcus aureus*. Higher positive values for 1-octacosanol indicated that it was the most active ingredient against *Staphylococcus aureus*. On the other hand, Beta-sitosterol can deactivate the enzyme to a small extent (negative -CDOCKER energy but positive -CDOCKER interaction energy). Oleanolic acid and Ursolic acid cannot interact with the alcohol dehydrogenase enzyme. Thus, the key phytochemicals preventing dermititis caused by *Staphylococcus aureus* are is 1-octacosanol.

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

Sl. no.	Ligand	- CDOCKER energy	- CDOCKER interaction energy	Difference between- C DOCKER interaction energy and - CDOCKER energy
1	1-Octacosanol	52.7539	58.7177	5.9638
2	Beta-sitosterol	-68.126	34.2181	102.3441
3	Oleanolic Acid	Failed	Failed	NA
4	Ursolic Acid	Failed	Failed	NA

4. CONCLUSION

It was previously known that *Nardostachys jatamansi* plant has medicinal action against Dermititis. Dermititis 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 (1-Octacosanol, Beta-sitosterol, Oleanolic Acid, Ursolic Acid), which can have significant interaction with the vital enzyme alcohol dehydrogenase of the microbe. It was found that 1-octacosanol can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Beta-sitosterol was found to be not much effective in deactivating the enzyme of the microbe. Oleanolic acid and Ursolic acid cannot deactivate the enzyme. Thus, this study could explain that the presence of 1-octacosanol provided the medicinal values to *Nardostachys jatamansi* against dermititis 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 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.

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COMPETING INTERESTS

Authors have declared that no competing interests exist.

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