



Salvia rosmarinus Derived Phytochemicals against Eczema

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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

The bioactive or phytochemicals substance from the plant *Salvia rosmarinus* helps in the prevention of eczema. *Staphylococcus aureus* is the causal organism for this disease. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" indicates alcohol could deactivate the protein tyrosine phosphatase and thus interrupt enzyme *Staphylococcus aureus* life cycle.

Keywords: Bio active substance; phytochemicals; Salvia rosmarinus; Staphylococcus aureus.

1. INTRODUCTION

Mother nature has a huge reserve of medicinal plant [1]. The bioactive substance or phytochemicals present in the plants provides the therapeutic characteristics. Different bio active substances are present in various part of the plant [2]. Different plants and their bioactive substance plays an important role in therapeutic

uses. These medicinal plants play a key role in human health care. A major share of the population believes in the traditional method of healing [3].

Rosemary is a plant of Lamiaceae family. Rosemary extract is used to cure disease like eczema. The aim of the study is to evaluate the bioactive substance present in Rosemary

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responsible for inhibiting the bacteria *Staphylococcus aureus*.

Salvia rosmarinus contains “Alcohol, Linalool, Rosmarinic acid, Carnosic acid, Tannic acid and Betulinic acid” etc. These phytochemicals might act against eczema. However, there is no such study available.

This objective of the study is to identify the phytochemical of *Salvia rosmarinus* capable of curing eczema.

2. MATERIALS AND METHODS

2.1 Software Used

Discovery studio module of Biovia software (Dassault Systemes of France) was used for analysis of molecular docking of phytochemicals from plant extracts that act as a ligand and form strong covalent bond with the enzyme molecule and analyse strength of this interaction based on -CDOCKER and -CDOCKER Interaction energy. The software utilizes machine learning techniques to predict the level of molecular interaction.

2.2 Methodology

2.2.1 List of phytochemicals

Phytochemicals are bioactive non-nutrient compounds produced by plants as secondary metabolites to protect them from predators. When these plants or their parts are consumed by humans these phytochemicals provide beneficial health effects. Some phytochemicals have been used as poisons and others as traditional medicine. Published works showed that *Salvia rosmarinus* contains phytochemicals like Rosmarinic acid, carnosic acid, alcohol, tannic acid, betulinic acid, linalool etc. It has already been established that *Salvia rosmarinus* plant belonging to Lamiaceae family has potential to help control eczema. This work is focused on identification of the particular phytochemical responsible for inhibiting and controlling eczema.

2.2.2 Enzyme found in *Staphylococcus aureus*

Staphylococcus aureus is known to cause various skin diseases like eczema. Various

metabolic cycles or pathways like two component system, glycolysis, cysteine and methionine metabolism, pyruvate metabolism etc., have been seen in the bacterial life cycle for its survival (KEGG). The 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 Protein Tyrosine Phosphatase (protein database code 3ROF) is involved in Two-component system metabolism (KEGG) and very crucial for the survival of the particular microbe. Two-component signal transduction systems enable bacteria to sense and respond to stimuli by inducing changes in transcription and adapt to changes in their environment or in their intracellular state (KEGG).

2.2.3 Molecular docking

Discovery studio module of Biovia software (Dassault Systemes of France) is used for analysis of molecular docking of phytochemicals from plant extracts that act as a ligand and form strong covalent bond with the enzyme molecule and analyse strength of this interaction based on -CDOCKER and -CDOCKER Interaction energy. Molecular docking method has been used to identify the phytochemical that bind with the bacterial protein to successfully inhibit the microbe. In this process first the sdf files for the phytochemicals found in the *Salvia rosmarinus* plant were downloaded from the website (Pubchem).

The protein database code of the protein tyrosine phosphatase enzyme was identified from the website (RCSB). 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.

Table 1. Results of C docking of phytochemicals with protein tyrosine phosphatase (receptor)

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and -CDOCKER energy	Remarks
1	Alcohol	12.2901	14.2194	1.9293	Maximum inhibition of microbial enzyme
2	Linalool	-8.009	22.1796	30.1886	
3	Rosmarinic acid	-783.313	-35.881	647.432	
4	Carnosic acid	failed	failed	NA	
5	Tannic acid	failed	failed	NA	
6	Betulinic acid	failed	failed	NA	

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]. In Table 1 it is shown that protein tyrosine phosphatase-alcohol interaction has the highest positive value of -CDOCKER energy (12.2901) and minimum value of the difference (1.9293) between -CDOCKER interaction energy and -CDOCKER energy. Thus the results indicated that alcohol as a phytochemical can effectively deactivate the protein tyrosine phosphatase enzyme, thereby interrupting the biological cycle of *Staphylococcus aureus*. A higher positive value for alcohol indicated that it was the most active ingredient against *Staphylococcus aureus*. On the other hand, linalool can deactivate the enzyme to a small extent (negative -CDOCKER energy but positive -CDOCKER interaction energy). Rosmarinic acid, carnosic acid, tannic acid, betulinic acid cannot interact with protein tyrosine phosphatase enzyme. Thus, the key phytochemicals preventing eczema caused by *Staphylococcus aureus* is alcohol.

4. CONCLUSION

By studying various published journals, it is reported that *Salvia rosmarinus* plant has

therapeutic action against eczema. *Staphylococcus aureus* is known as a major causal organism of skin diseases like eczema. 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 phytochemicals (alcohol, rosmarinic acid, carnosic acid, tannic acid, betulinic acid, linalool), which can have a significant interaction with the vital enzyme (protein tyrosine phosphatase) of the microbe. From the above study it can be concluded that alcohol can form strong covalent bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Linalool is found to be less effective in deactivating the enzyme of the microbe. Rosmarinic acid, carnosic acid, tannic acid, betulinic acid are not effective in deactivating the enzyme. Thus, this study could explain that the presence of alcohol has been successful in enhancing the medicinal values to *Salvia rosmarinus* against eczema caused by *Staphylococcus aureus*. Since the alcohol-protein tyrosine phosphatase interaction has been successful in inhibiting life cycle of *Staphylococcus aureus* by blocking its metabolic pathway like two-component system hence, it is proved that phytochemical alcohol provide therapeutic values to rosemary plant against eczema diseases.

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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