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PHYTOMOLECULES OF *Commiphora wightii* DISPLAY POSITIVE AFFINITY FOR DEHYDROGENASE OF *Commiphora wightii*: POSSIBLE PREVENTIVE AND THERAPEUTIC USAGE IN SKIN DISEASE

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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

Skin disease is caused by *Staphylococcus sp.* One of the key enzymes involved in its biochemical pathway is dehydrogenase Plant extract of *Commiphora wightii* can be effectively used against skin disease. The molecular docking of the phytochemicals with the enzyme was studied using Biovia Discovery Studio. Molecular docking-based screening of a few phytochemicals revealed that the phytochemicals effectively associate with the active site of the protein and hence bears diagnostic and therapeutic potentials skin disease. Phytochemicals including α-pinene and eugenol may effectively deactivate the dehydrogenase enzyme thereby interrupting the life cycle of *Staphylococcus*.

Keywords: Phytochemical; biovia; discovery studio; *Commiphora wightii*; *Staphylococcus aureus*.

1. INTRODUCTION

In olden days, life was natural, slow, difficult at times but healthy. Today, in modern times, life is fast paced, comfortable, readymade, stressful and unhealthy. For treating several diseases, phytochemical compounds like tocopherols, carotenoids, anthocyanins, phenolics etc. are effective [1,2]. Several phytochemicals act as natural antioxidants, which supplements the need of the human body [3]. Across the globe, it is recommended for consumption of fruits and vegetables, primarily to improve the state of health [4]. We primarily screened a few phytochemicals, which are not yet globally recognized, using a molecular docking method (BIOVIA). Commiphora wightii belongs to family burseraceae. Commiphora

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wightii extract is used to cure disease like skin disease [5]. *Commiphora wightii* is known to contain phytochemicals like, eugenol, α-terpineolz-guggulsterone, α-pinene and linalool etc [6]. A group of bacteria belonging to genus Staphylococcus generally cause skin disease. They are round shaped Gram positive bacteria. Staphylococcus infection is a common bacterial disease that affects the upper respiratory tract and on the skin. Staphylococcus bacteria typically live in animal and human respiratory and are shed through faeces. Humans become infected most frequently through contaminated water or food [3]. This study focuses on the identification of the phytochemical of *Commiphora wightii* responsible to cure skin disease caused by *Staphylococcus sp.*

2. MATERIALS AND METHODS

2.1 Bacterial Protein's Structure and Phytochemicals Dataset Collection

From the Protein Data Bank (accession: 3P7X), the 3D structure of protein was accessed. For docking with the target protein, subsequently phytochemicals were considered and SDF file accession numbers were used for the purpose.

2.2 Molecular Docking

In silico molecular docking was done by using the BIOVIA's Discovery Studio docking method (CDOCKER; Dassault Systèmes BIOVIA). The catalytic pocket of the protein was generated and subsequently targeted for ligand interaction. Molecular docking method has been used to identify the phytochemical from the plant extract, which 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 performs molecular docking. In this process first the sdf files for the phytochemicals found in the *Commiphora wightii* plant were downloaded from the website. 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

Fig. 1 shows the active site of the dehydrogenase enzyme. The positive values of the CDOCKER Energy and CDOCKER_INTERACTION_ENERGY represent the affinity of the ligands with the receptor proteins. Molecular docking of several numbers of phytochemicals present in the *Commiphora wightii* (Table 1) against the protein revealed that α-pinene and eugenol are potential binding ligands as evident from their higher CDOCKER ENERGY and CDOCKER_INTERACTION_ENERGY (Table 1). These are very common and easily available. Phytochemicals including Hesperidin, Epicatechin, Tangeretin, Allicin, Sulforaphane, Cyanidin and Malvidin didnot show affinity for the active site of the protein as the docking results were failed. The chemical structure of ligand molecules showing positive affinity for the protein can be studied extensively and related synthetic molecules can be developed for wide range applications in the cancer therapeutics.

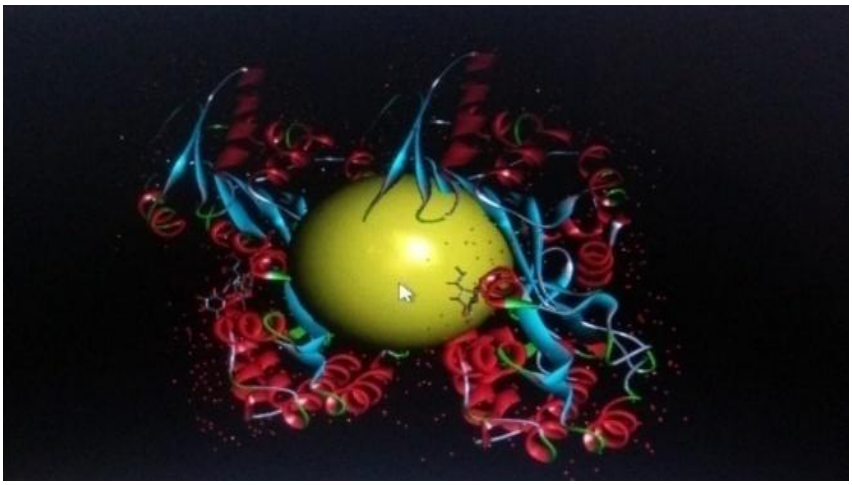

Fig. 1. Active site of dehydrogenase enzyme

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

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -C DOCKER interaction energy and - C DOCKER energy
1	α-terpineol	-4.1872	23.9957	28.1829
2	z-guggulsterone	-34.9821	32.0597	67.0424
3	Eugenol	13.8639	28.1447	14.2808
4	α-pinene	12.7957	27.3069	14.5112
5	linalool	-3.9798	25.9235	29.9033

4. CONCLUSION

In silico molecular docking based study reveals several novel candidate molecules which can target the dehydrogenase protein. It would be highly significant being confirmed *in vivo*. Specific phytochemical targeting dehydrogenase protein can be employed in two ways. Firstly, these phytomolecules may act as drug by blocking the specific sites of dehydrogenase protein, ultimately inhibiting the downstream pathways. Secondly, cost effective medical device can be developed to diagnose early stages of disease by targeting marker proteins like dehydrogenase enzyme. Phytochemicals including α-pinene and eugenol may be effective. Since, dehydrogenases are highly significant in modulating the growth factor signaling and promote cancerous activity; they should be restricted being over activated by blocking their active site. Early diagnosis being a critical issue in several diseases, appropriate ligands can be developed to be used as a diagnostic tool.

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.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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