



Santalum album L. Derived Phytochemicals against Jaundice

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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

Phytochemicals are produced by plants as secondary metabolites to protect the plants from predators. When the parts of the plant, which are rich in different phytochemical constituents, are consumed by humans, they can cure different diseases. Phytochemicals from *Santalum album* plant extract are traditionally used to cure Jaundice. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that *Isohamnetin* can effectively deactivate the enzyme, thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Santalum album; Jaundice.

1. INTRODUCTION

Nature is a major source of medicines [1]. The medicinal value of the plants is due to the phytochemicals 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

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medicine [3]. *Santalum album* extract is used to cure diseases like Jaundice. The objective of the study is to identify the phytochemical responsible to cure the disease. *Santalum album* contains "beta-pinene, alpha-pinene, p-cymene, limonene, piperazine" etc. These phytochemicals might act against Jaundice. However, there is no such study available. This objective of the study is to identify the phytochemical of *Santalum album* capable of curing Jaundice.

2. MATERIALS AND METHODS

2.1 List of Phytochemicals Used in Molecular Docking

Phytochemicals are produced by plants as secondary metabolites to protect the plants from predators. The potential threats which are caused to plants include bacteria, fungi, and virus, etc. When the parts of the plant which are rich in different phytochemical constituents are consumed by the humans they are used for curing different diseases. Published works showed that *Santalum album* L. contains flavonoids like vicenin-2, vitexin, isovitexin, orienthin, isoorienthin, chrysin-6-c-beta-Dglucopyranoside, isorhamnethin and flavan-3-ol [4].

2.2 Enzyme Found in *Leptospira interrogans* spp

It has been reported that Jaundice can be caused as a result of *Leptospira interrogans* sp. infestation. Survival of a bacteria involves various metabolic cycles, which are again regulated by different enzymes. The list of different enzymes that are present in *Leptospira interrogans* spp was identified with the help of Brenda enzyme database. It has been found that sphingomyelin phosphodiesterase *leptospira interrogans* enzyme (protein database code 5EBB) is involved in the metabolic pathway of *Leptospira interrogans* spp which is responsible for causing Jaundice and it is very crucial for the survival of the particular microbe. The phytochemical *Isohamnetin* cures the disease jaundice by affecting the biological pathway of the microbe by inhibiting the purine metabolism pathway which is required by the microbe for its survival.

2.3 Molecular Docking

The phytochemicals present in the plant extract was identified using molecular docking method. The phytochemicals which are present act as a ligand successfully inhibit the microbe by forming

a strong covalent bond with the bacterial protein. The targets are inactivated irreversibly by the covalent ligands. The target protein which is responsible for biological function can be again activated by resynthesizing the target protein. For a disease to be cured the function of the protein or the synthesis of the protein should be stopped for which it is inhibited so for such type of inhibition covalent inhibitors play a key role because it binds to the target molecule with high affinity, which leads to a long-lasting response in pharmaceutical products which requires less frequent administration [5]. 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 *Santalum album* L. plant were downloaded from the website KEGG. The protein database code of the 5EBB enzyme was identified from the website BRENDA via "receptor cavity". The active site of the enzyme was identified under "receptor-ligand interaction" menu using the -CDOCKER protocol of Biovia software. Molecular docking was done under "receptor-ligand interaction". The enzyme molecule was treated as the receptor molecule and the phytochemical was treated as the ligand. For the quality of molecular docking the "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" were used as an indicator. 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 [6,7].

3.1 Molecular Docking Using Phytochemicals of Sandalwood

Through molecular docking using biovia discovery studio we have found that *Leptospira interrogans* interaction has the highest positive

Table 1. Results of C-Docking of phytochemicals with (*Leptospira interrogans* spp) (receptor)

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and - CDOCKER energy
1	Chrysin 6-c-beta-D-glucopyranoside	9.73648	48.2791	38.54262
2	Flavan-3-ol	19.6768	29.6352	9.9584
3	Isoorientin	18.8901	46.6389	27.7488
4	Isohamnetin	36.894	44.1682	7.2742
5	Isovitexin	FAILED	FAILED	NA
6	Vicenin-2	FAILED	FAILED	NA
7	Vitexin	FAILED	FAILED	NA

value of -CDOCKER energy 36.894 and minimum value of the difference 7.2742 between -CDOCKER interaction energy and -CDOCKER energy followed by phytochemical *Isohamnetin*. Thus the results indicated that phytochemical *Isohamnetin* can effectively deactivate the *sphingomyelin phosphodiesterase Leptospira interrogans* (5EBB) enzyme thereby interrupting the biological cycle of *Leptospira interrogans* spp which is responsible for causing the disease jaundice. The higher values for *Isohamnetin* phytochemical indicated that it was the most active ingredient against *sphingomyelin phosphodiesterase Leptospira interrogans* enzyme of *Leptospira interrogans* spp. Some other phytochemicals like *Isoorientin*, *Flavan-3-ol*, *Chrysin 6-c-beta-D-glucopyranoside* also help in the deactivation of the enzyme. The other phytochemicals of sandalwood, like *Isovitexin*, *Vicenin-2*, and *Vitexin* did not show any result against the enzyme.

4. CONCLUSIONS

It was previously known that Sandalwood plant has medicinal action against Jaundice. It is caused by *Leptospira interrogans* spp. This study was carried out to identify the benefit of the phytochemicals present in the plant which help us to treat various diseases. Using Discovery studio module of Biovia software, molecular docking operation was performed to identify the phytochemical (*Isoorientin*, *Flavan-3-ol*, *Chrysin 6-c-beta-D-glucopyranoside*, *Isovitexin*, *Vicenin-2*, and *Vitexin*, *Isohamnetin*), which can have a significant interaction with the vital enzyme *sphingomyelin phosphodiesterase Leptospira interrogans* of the microbe *Leptospira interrogans* spp. It was found that phytochemical *Isohamnetin* can form a strong bond with the

enzyme *sphingomyelin phosphodiesterase Leptospira interrogans* successfully inhibiting the metabolic cycle of the microbe *Leptospira interrogans*. *Isoorientin*, *Flavan-3-ol*, and *Chrysin 6-c-beta-D-glucopyranoside* were found to be less effective in deactivating the enzyme of the microbe. *Isovitexin*, *Vicenin-2*, *Vitexin* cannot deactivate the enzyme. Thus, this study could explain that the presence of phytochemical *Isohamnetin*, *Isoorientin*, *Flavan-3-ol*, and *Chrysin 6-c-beta-D-glucopyranoside* in sandalwood provided the medicinal values for Jaundice.

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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