



# **Michelia champaca Derived Phytochemicals against Skin Disease**

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## **Author's contribution**

The sole author designed, analysed, interpreted and prepared the manuscript.

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## **ABSTRACT**

Phytochemicals from *Michelia champaca* plant extract can cure skin disease. Skin disease can be caused by many reasons. Infections due to *Staphylococcus aureus* is one of the main reasons for skin disease. This objective of the study is to identify the phytochemical of *Michelia champaca* capable of curing skin diseases. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that Magnoflorine can effectively deactivate thymidylate synthase thereby interrupting the life cycle of the organism.

**Keywords:** Phytochemical; *Michelia champaca*; *Staphylococcus aureus*.

## **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 medicine [3].

*Michelia champaca* belongs to family Magnoliaceae. *Michelia champaca* extract is

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used to cure diseases like skin disease. The objective of the study is to identify the phytochemical responsible to cure the disease.

*Michelia champaca* contains "parthenolide,  $\beta$ -sitosterol, liriodenine, micheliolde, magnoflorine and ushinsunine" etc. These phytochemicals might act against skin disease. However, there is no such study available.

This objective of the study is to identify the phytochemical of *Michelia champaca* capable of curing skin diseases.

## 2. MATERIALS AND METHODS

### 2.1 Software Used

Discovery studio module of Bivia 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 threats to health. Some phytochemicals have been used as poisons and others as traditional medicine. Published works showed that *Michelia champaca* contains parthenolide [4],  $\beta$ -sitosterol [5], liriodenine [6], micheliolde [7], magnoflorine and ushinsunine [8]. It has already been established that *Michelia champaca* plant belonging to the Magnoliaceae family has the potential to help controlling skin disease. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling 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 thymidylate synthase enzyme (protein database code 4DQ1) is involved in pyrimidine metabolism (BRENDA), which is very crucial for the survival of the particular microbe.

### 2.2.3 Molecular docking

The 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 Bivia software was used for identifying molecular interaction and perform molecular docking. In this process first, the sdf files for the phytochemicals found in the *Michelia champaca* plant were downloaded from the website (PUBCHEM). The protein database code of the thymidylate synthase enzyme was identified from the website (RCSB). The active site of the enzyme was identified via the "receptor cavity" protocol found under the "receptor-ligand interaction" menu. Molecular docking was done using the CDocker protocol of Bivia 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 [9,10]. Table 1 shows that thymidylate synthase-magnoflorine interaction has the highest value out of all other interactions -CDOCKER energy (6.21843) and minimum value of the difference (33.87937) between -CDOCKER interaction energy and -CDOCKER energy. Thus the result indicated that

**Table 1. Results of C docking of phytochemicals with thymidylate synthase (receptor)**

Sl no	Ligand	- CDOCKER energy	- CDOCKER interaction energy	Difference between - CDOCKER interaction energy and - CDOCKER energy	Remarks
1	Magnoflorine	6.21843	40.0978	33.87937	Maximum inhibition of the microbial enzyme
2	Ushinsunine	-4.55439	29.6732	34.22759	
3	Liriodenine	-13.8035	28.1892	41.9927	
4	Parthenolide	-33.9671	26.0171	59.9842	
5	Micheliolide	-52.2247	25.2948	77.5195	
6	$\beta$ -sitosterol	FAILED	FAILED	NA	

magnoflorine can effectively deactivate the thymidylate synthase enzyme thereby interrupting the biological cycle of *Staphylococcus aureus*. Negative values for all of the reactions indicated that these were not the most active ingredients against *Staphylococcus aureus*. That is, ushinsunine, liriodenine, parthenolide, micheliolide can deactivate the enzyme to a small extent (negative -CDOCKER energy but positive -CDOCKER interaction energy).  $\beta$ -sitosterol cannot interact with the thymidylate synthase enzyme. Thus, these phytochemicals may not be able to prevent skin diseases of different conditions caused by *Staphylococcus aureus* when considering about thymidylate synthase enzyme of the bacteria. But the key phytochemical in deactivating the thymidylate synthase enzyme was found to be magnoflorine which may be also responsible for curing the disease.

#### 4. CONCLUSIONS

It was previously known that *Michelia champaca* 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 (magnoflorine, ushinsunine, liriodenine, micheliolide, parthenolide,  $\beta$ -sitosterol), which can have significant interaction with the vital enzyme (thymidylate synthase) of the microbe. It was found that magnoflorine can form a better bond in comparison to the other phytochemicals. Ushinsunine, liriodenine, parthenolide, micheliolide were found to be less effective in deactivating the thymidylate synthase enzyme of

the microbe.  $\beta$ -sitosterol cannot interact with the enzyme at all. Thus, this study could conclude that the presence of the phytochemical magnoflorine provides medicinal value to the plant *Michelia champaca* in curing *Staphylococcus aureus* associated skin disease.

#### CONSENT

It is not applicable.

#### ETHICAL APPROVAL

It is not applicable.

#### COMPETING INTERESTS

Author has declared that no competing interests exist.

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