**Buddleja asiatica** Lour. Derived Phytochemicals against *Staphylococcus aureus* Causing Skin Diseases

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**Authors’ contributions**

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

**Article Information**

DOI: 10.9734/JPRI/2020/v32i830529

(1) Dr. Syed A. A. Rizvi, Nova Southeastern University, USA.

Reviewers:

(1) Uzuazokaro M. Agatemor, Novena University, Nigeria.
(2) Maria Bintang, IPB University, Indonesia.

Complete Peer review History: [http://www.sdiarticle4.com/review-history/57269](http://www.sdiarticle4.com/review-history/57269)

**ABSTRACT**

Phytochemicals from *Buddleja asiatica* plant extract are traditionally used to cure skin diseases. It is caused by *Staphylococcus aureus*. Molecular docking method applied using “Biovia Discovery Studio”. “High positive values of -CDOCKER energy and -CDOCKER interaction energy” suggested that lignoceric acid can effectively deactivate the L-lactate dehydrogenase enzyme thereby interrupting the life cycle of the organism.

**Keywords:** Buddleja asiatica; phytochemical; Staphylococcus aureus; skin diseases.

**1. INTRODUCTION**

Plants have a major source of herbal medicine [1]. The medicinal properties of the plants is due to the secondary metabolites present in it. Secondary metabolites can be derived from various parts of plants. Different traditional plants and their bioactive compound have shown antimicrobial activity [2]. These traditional plants play a key role in human health care. Now a days

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many people depend on the use of traditional medicine because of less side effect [3].

*Buddleja asiatica* belongs to family Scrophulatiaceae. *B. asiatica* extract is used to cure disease like skin diseases.

*Buddleja asiatica* contains “lignoceric acid, apigenin” etc. These phytochemicals might act against skin diseases. However, there is no such study available.

This objective of the study is to identify the phytochemical of *Buddleja asiatica* capable of curing skin diseases.

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 secondary metabolites produced by plants to protect them from predators and infection. They act as biologically active compounds. When humans consumed these plants and their parts these phytochemicals fight off threats to health. From all these phytochemicals some have been used as traditional medicines and others as poisons. By analyzing the Published works it was found that *Buddleja asiatica* contains α-amyrin, apigenin, lignoceric acid, B caryophyllene, stigmasterol etc. The established work shows that plant *Buddleja asiatica* comes under the family Loganiaceae which has the potential to help in controlling skin disease. The main aim of this work is to identify the particular responsible phytochemical which helps in inhibiting and controlling of skin diseases.

2.2.2 Enzyme found in *Staphylococcus*

It has been reported that *Staphylococcus aureus* causes the skin diseases. It is one of the major bacteria responsible for skin infection. The metabolic pathways of *Staphylococcus aureus* are glycolysis / gluconeogenesis, cysteine and methionine metabolism, pyruvate metabolism, propanoate metabolism, biosynthesis of secondary metabolites, microbial metabolism in diverse environments and biosynthesis of antibiotics (KEGG) that are involved in its life cycle and are responsible for its survival. Enzymes of the bacteria regulate these metabolic pathways. The list of different enzymes of *Staphylococcus aureus* bacteria were found by using Brenda enzyme database. It has been found that L-lactate dehydrogenase enzyme (protein database code 3DOO) is involved in glycolysis pathway (KEGG). Glycolysis is a central pathway of *Staphylococcus aureus* that produces important precursor metabolites. In this pathway L-lactate dehydrogenase enzyme helps in the propanoate metabolism (KEGG).

2.2.3 Molecular docking

Molecular docking method has been used to identify the phytochemical from the plant extract, that 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 perform molecular docking. In this process first the sdf files for the phytochemicals found in the *Buddleja asiatica* plant were downloaded from the website (PubChem). The protein database code of the L-lactate dehydrogenase 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.

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
Table 1. Results of C Docking of phytochemicals with L-lactate dehydrogenase
*Staphylococcus aureus* (receptor)

| Sl. no. | Ligand            | -CDOCKER energy | -CDOCKER interaction energy | Difference between -CDOCKER interaction energy and -CDOCKER energy | Remarks                                      |
|---------|-------------------|-----------------|----------------------------|-----------------------------------------------------------------|----------------------------------------------|
| 1       | Lignoceric acid   | 40.2074         | 44.8178                    | 4.6104                                                          | Highest inhibition of microbial enzyme       |
| 2       | Apigenin          | 22.2116         | 37.4669                    | 15.2553                                                         |                                               |
| 3       | α –amyrin         | -573.848        | -77.1648                   | 496.6832                                                        | Lowest inhibition of microbial enzyme        |
| 4       | B caryophyllene oxide | -3.41393 | 21.5523                    | 24.96623                                                        |                                               |
| 5       | Stigmasterol      | -76.2703        | 26.0164                    | 102.2867                                                        |                                               |

based on a) high positive value of -CDOCKER energy and b) small difference between -CDOCKER energy and -CDOCKER interaction energy [4,5]. Table 1 shows that L-lactate dehydrogenase – lignoceric acid interaction has the highest positive value of -CDOCKER energy (40.2074) and minimum value of the difference (4.6104) between - C DOCKER interaction energy and - C DOCKER energy followed by apigenin. Thus the results indicated that lignoceric acid and apigenin can effectively deactivate the L-lactate dehydrogenase enzyme thereby interrupting the biological cycle of *Staphylococcus aureus*. Higher positive values for lignoceric acid indicated that it was the most active ingredient against *Staphylococcus aureus*. On the other hand B caryophyllene oxide and Stigmasterol can be less effective (negative -CDOCKER energy but positive -CDOCKER interaction energy). α-amyrin can not deactivate the enzyme (both negative -CDOCKER energy and -CDOCKER interaction energy). Thus, the key phytochemicals preventing skin disease caused by *Staphylococcus aureus* are lignoceric acid and apigenin.

4. CONCLUSIONS

*Staphylococcus aureus* is the major causing organism for skin disease. By analysing the published work it has been known that *Buddleja asiatica* plant has medicinal value against skin disease. To provide the theoretical basis of this observation this study was carried out. The molecular docking interaction was performed to identify the phytochemicals (α-amyrin, apigenin, lignoceric acid, B-caryophyllene oxide, Stigmasterol) which can have a significant interaction with the vital enzyme (L-lactate dehydrogenase) of the *Staphylococcus aureus*. The molecular docking is done by using the Discovery studio module of Biovia software. From the observation of molecular docking it was found that lignoceric acid and apigenin can form strong bond with the enzyme successfully inhibiting the metabolic cycle (glycolysis) of the *Staphylococcus aureus*. B caryophyllene oxide and Stigmasterol was found to be not much effective in deactivating the enzyme of the *Staphylococcus aureus*. α-amyрин cannot deactivate the enzyme (L-lactate dehydrogenase). Thus, this study could explain that the presence of lignoceric acid and apigenin provided the medicinal values to *Buddleja asiatica* against skin disease 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 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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