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Buddleja asiatica Derived Phytochemicals against Diarrhea

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Author's contribution

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

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ABSTRACT

Plants produce nonnutritive compounds that are often extracted to make herbal medicines. It has been reported that extracts of *Buddleja asiatica* are effective to treat diarrhea. One of the causes of Diarrhea is an infection by *Campylobacter jejuni.* The objective of the study is to identify the phytochemical of *Buddleja asiatica* capable of curing Diarrhea. ATP-phosphoribosyl transferase enzyme plays an important role in Purine Metabolism. 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 transferase enzyme thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Buddleja asiatica; diarrhea.

1. INTRODUCTION

Diarrhea is characterized by loose, watery stools or a frequent need to have a bowel movement. It usually lasts a few days. Nature is a major source of medicines [1] for diseases like Diarrhoea. 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

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in human health care. Many people rely on the use of traditional medicine [3].

Buddleja asiatica belongs to family Scrophulariaceae. Extract of *Buddleja asiatica* is used to cure diseases like Diarrhea. The objective of the study is to identify the phytochemical responsible to cure the disease.

Buddleja asiatica contains "Lignoceric acid, Apigenin, caryophyllene oxide, Alpha amyrin and Stigmasterol" etc. These phytochemicals might act against Diarrhoea. However, there is no such study available.

The objective of the study is to identify the phytochemical of *Buddleja asiatica* capable of curing Diarrhea.

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 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 are harmful to humans and others used as traditional medicine. Published works showed that *Budlejaasiatica* contains *Apigenin, Lignoceric acid, B caryophyllene oxide, Alpha amyrin, Stigmasterol J,* etc. [3]. It has already been established that *Budleja asiatica* plant belonging to *Scrophulariaceae* family has the potential to help controlling diarrhea. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling diarrhea [4].

2.2.2 Enzyme found in *Campylobacter jejuni*

It has been reported that diarrhea can cause as a result of *Campylobacter jejuni* 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 *Campylobacter jejuni* bacteria. It has been found that ATP-phosphoribosyl transferase enzyme (protein database code 5UBH) is involved in Purine Metabolism (KEGG) and 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 that acts as a ligand and form a strong covalent bond with the bacterial protein 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 (www.pubchem.ncbi.nlm.nih.gov). The protein database code of the ATP-phosphoribosyl transferase enzyme was identified from the website (https://www.rcsb.org/pdb). 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 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 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. Nonbonded interaction that exists between the protein and the ligand is given by CDOCKER interaction. The criteria for best interaction was chosen based on:

a) The high positive value of -CDOCKER energy and
b) The small difference between -CDOCKER energy and -CDOCKER interaction energy [5].

Table 1. Results of C docking

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and -CDOCKER energy	Remarks
1	Lignoceric acid	43.2715	57.5326	14.2611	Maximum inhibition of the microbial enzyme
2	Apigenin	34.3806	42.1425	7.7619	
3	βcaryophyllene oxide	5.64752	29.7792	24.13168	
4	Alpha amyrin	-144.598	9.79372	154.39172	
5	Stigmasterol	-148.84	14.721	163.531	

Table 1 shows that ATP-phosphoribosyltransferase-Lignoceric acid interaction has the highest positive value of -CDOCKER energy (43.2715) Apigenin has a minimum value of the difference (7.7619) between - C DOCKER interaction energy and - C DOCKER energy [6,7]. Thus the results indicated that can effectively deactivate the ATP-phosphoribosyl transferase enzyme thereby interrupting the biological cycle of *Campylobacter jejuni.* Higher positive values for Lignoceric acid indicated that it was the most active ingredient against *Campylobacter jejuni*. Apigenne having a lower difference between -CDOCKER energy and -CDOCKER interaction energy is the most active ingredient.

β-caryophyllene oxide having both positive interactions can also slightly affect the enzyme. Whereas Alpha amyrin and Stigmasterol with (negative -CDOCKER energy but positive -CDOCKER interaction energy) can deactivate the enzyme but up to a small extent Table 1 shows ATP-phosphoribosyl transferase and phytochemicals interaction was found to have the highest interaction.

4. CONCLUSIONS

It was previously known that *Buddleja asiatica* plant has medicinal action against diarrhea. Diarrhea is caused by *Campylobacter jejuni.* 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 (Apigenin, Lignoceric acid, B caryophyllene oxide, Alpha amyrin, Stigmasterol), which can have significant interaction with the vital enzyme (ATP-phosphoribosyl transferase) of the microbe. It was found that apigenin and lignoceric acid can form a strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. β-caryophyllene oxide was found to be less effective in deactivating the enzyme of the microbe. Alpha amyrin and stigmasterol cannot deactivate the enzyme effectively. Thus, this study could explain that the presence of Apigenin and Lignoceric acid provided the medicinal values to *Buddleja asiatica* against diarrhea caused by *Campylobacter jejuni.*

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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