



Trigonella foenum-graecum Derived Phytochemicals against Cellulitis

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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

Cellulitis is a common and sometimes painful bacterial skin infection. *Trigonella foenum-graecum* extract is traditionally used to cure diseases like cellulitis. Phytochemicals from *Trigonella foenum-graecum* plant extract can cure Cellulitis. The objective of the study is to identify the phytochemical of *Trigonella foenum-graecum* capable of curing Cellulitis. Molecular docking method applied using "Biovia Discovery Studio". "The experiment shows that the phytochemical sarginine, carpaine, choline, gentianine and diosgenin failed to deactivate the UDP-glucose 6-dehydrogenase enzyme of *Streptococcus pyogenes* for treating Cellulitis.

Keywords: Phytochemical; cellulitis; *Trigonella foenum graecum*.

1. INTRODUCTION

Cellulitis is a common and sometimes painful bacterial skin infection. It is a common and potentially serious bacterial skin infection. With cellulitis, the bacteria enter the skin and the skin

appears swollen and red. Nature is a major source of medicines [1] to treat many diseases like Cellulitis. 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

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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].

Trigonella foenum-graecum extract is traditionally used to cure diseases like cellulitis. These phytochemicals might act against cellulitis. However, there is no such study available.

The objective of the study is to identify the phytochemical of *Trigonella foenum-graecum* capable of curing Cellulitis.

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 have been used as poisons and others as traditional medicine. Published works showed that *Trigonella foenum-graecum* contains Arginine, Carpaine, Choline, Diosgenin, Gentianine, Gitogenin, Histidine, L-tryptophan, Sarsapogenin, Trigonelline, Vitamin-E-acetate etc. It has already been established that *Trigonella foenum-graecum* plant belonging to family Fabaceae has the potential to help controlling cellulitis. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling of cellulitis.

2.2.2 Enzyme found in *Streptococcus pyogenes*

It has been reported that cellulitis can be caused as a result of *Streptococcus pyogenes* infection. Various metabolic cycles are critical 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 *Streptococcus pyogenes* bacteria. It has been found that UDP-glucose 6-dehydrogenase enzyme (protein database code 1DLJ) is involved in catalyzing the formation of UDP-glucuronic acid which is required for capsular hyaluronic acid synthesis [4].

2.2.3 Molecular docking

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 to successfully inhibit the microbe. The Discovery studio module of Biovia software was used for identifying molecular interaction and to perform molecular docking. In this process first, the sdf files for the phytochemicals found in the *Trigonella foenum-graecum* plant were downloaded from the website (<https://tinyurl.com/yckwbhr9>). The protein database code of the enzymes was identified from the website (RCBS 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 Bioviasoftware 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 [5, 4]. 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. Table 1 shows that the phytochemical sarginine, carpaine, choline, gentianine and diosgenin failed to deactivate the UDP-glucose 6-dehydrogenase enzyme of *Streptococcus pyogenes* for treating Cellulitis.

Table 1. Results of C Docking of phytochemicals with UDP-glucose 6-dehydrogenase (receptor)

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and –CDOCKER energy
1	Arginine	31.3562	31.694	0.3378
2	Carpaine	Failed	Failed	NA
3	Choline	Failed	Failed	NA
4	Diosgenin	Failed	Failed	NA
5	Gentianine	Failed	Failed	NA

4. CONCLUSIONS

It was previously known that *Trigonella foenum-graecum* plant has medicinal action against cellulitis. Cellulitis is caused by *Streptococcus pyogenes*. 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 (Arginine, Carpaine, Choline, Diosgenin, Gentianine), which can have significant interaction with the vital enzyme (UDP-glucose 6-dehydrogenase) of the microbe. It was observed that the phytochemical sarginine, carpaine, choline, gentianine, and diosgenin of *Trigonella foenum-graecum* cannot deactivate the UDP-glucose 6-dehydrogenase of *Streptococcus pyogenes* for the treatment of Cellulitis. However, docking of the sephyto chemicals with other enzymes of *Streptococcus pyogenes* may give some better results.

DISCLAIMER

The products used for this research are commonly and predominantly use products in our area of research and country. There is 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 the 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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