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Trigonella foenum-graecum Derived Phytochemicals against Tuberculosis

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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 from *Trigonella foenum-graecum* plant extract are traditionally used to cure Tuberculosis. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that this plant extract can effectively deactivate the dihydrofolate reductase enzyme thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Trigonella foenum-graecum; Tuberculosis.

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

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plants play a key role in human health care. Many people rely on the use of traditional medicine [3].

Trigonella foenum-graecum belongs to family Piperaceae. Fenugreek extract is used to cure diseases like Tuberculosis. The objective of the study is to identify the phytochemical responsible for curing the disease.

These phytochemicals might act against Tuberculosis. However, there is no such study available.

This objective of the study is to identify the phytochemical of *Trigonella foenum-graecum,* capable of curing Tuberculosis.

2. MATERIALS AND METHODS

2.1 Software Used

Discovery studio module of Biovia software (DassaultSystemesof 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.It has already been established that *Trigonella foenum-graecum* plant belonging to family Fabaceae has the potential to help controlling Tuberculosis [4]. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling Tuberculosis.

2.2.2 Enzyme found in *Mycobacterium tuberculosis*

It has been reported that Tuberculosis can be caused as a result of *Mycobacterium tuberculosis* infection. 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 *Mycobacterium tuberculosis* bacteria. It has been found that shikimate dehydrogenase enzyme (protein database code 4P4G) is involved in biosynthesis of aromatic amino acids (phenylalanine, tyrosine and tryptophan) from the metabolism of carbohydrates and is very crucial for the survival of the particular microbe.

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 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://www.sciencedirect.com/science/article/pii/S1658077X15301065*). 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 Bioviasoftwere under “receptor-ligand interaction”. The enzyme molecule was treated as the receptor molecule and the phytochemical was treated as the ligand [5]. 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 [6,7]. Table 1 shows that shikimate

Table 1. Results of CDocking of phytochemicals with shikimate dehydrogenase (receptor)

Sl no	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and -CDOCKER energy	Remarks
1	Arginine	35.321	35.1289	0.1921	Maximum inhibition of microbial enzyme
2	Choline	17.6663	27.9548	10.2885	
3	Gentianine	13.3482	25.1868	11.8386	
4	Diosgenin	-93.4624	20.5678	114.0302	
5	Carpaine	Failed	Failed	NA	

dehyrogenase-arginine interaction has the highest positive value of –CDOCKER energy (35.321) and minimum value of the difference (-0.1921) between –CDOCKER interaction energy and –CDOCKER energy followed by Choline and Gentianine. So, the results indicated that arginine, choline and gentianine can effectively deactivate the shikimate dehydrogenase enzyme, thereby interrupting the biological cycle of *Mycobacterium tuberculosis*. Higher positive values for Arginine indicated that it was the most active ingredient against *Mycobacterium tuberculosis.* On the other hand, Diosgenin can deactivate the enzyme to a small extent because of the more negative –CDOCKER energy but positive –CDOCKER interaction energy. The phytochemical Carpaine failed to interact with the enzyme shikimate dehydrogenase. Thus, the key phytochemicals preventing Tuberculosis caused by *Mycobacterium tuberculosis* are Arginine, Choline and Gentianine.

4. CONCLUSIONS

It was previously known that *Trigonella foenum-graecum* plant has medicinal action against Tuberculosis. Tuberculosis is caused by *Mycobacterium tuberculosis*. 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 (shikimate dehydrogenase) of the microbe. It was found that arginine, choline, and gentianine can form strong bonds with the enzyme successfully inhibiting the biosynthesis of aromatic amino acids in the life cycle of *Mycobacterium tuberculosis.* Diosgenin is not effective in deactivating the enzyme of the microbe. Further, carpaine cannot deactivate the enzyme of the microbe. Thus, this study could explain that the presence of arginine, choline, gentianine provided the medicinal values to *Trigonella foenum-graecum* against Tuberculosis caused by *Mycobacterium tuberculosis.*

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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