



## **Trigonella foenum-graecum Derived Phytochemicals against Cough**

**Bidyashree Tripathy<sup>1</sup>, Elina Sahoo<sup>1</sup>, Sunil Jha<sup>1</sup> and Dipankar Bhattacharyay<sup>1,2\*</sup>**

<sup>1</sup>Centurion University of Technology and Management, Odisha, India.

<sup>2</sup>Go to Market Laboratory, Gram Tarang, Odisha, India.

### **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 Cough. There are many reasons for cough. It has been reported that cough can be caused as a result of *Bordetella sp.* infection. The objective of the study is to identify the phytochemical of *Trigonella foenum-graecum* capable of curing Cough. Molecular docking method applied using "Biovia Discovery Studio". The research clearly indicates that choline, arginine, and gentianine cannot effectively deactivate the enzyme histidinekinase of the microbe. On the other hand, carpaine and diosgenin failed to deactivate the enzyme. Thus, none of these phytochemicals can effectively deactivate the histidinekinase enzyme of *Bordetella sp.* and thus cannot be used to treat cough caused by this particular microbe.

**Keywords:** *Phytochemical; Trigonella foenum-graecum; cough.*

\*Corresponding author: E-mail: [dipankar.bhattacharyay@cutm.ac.in](mailto:dipankar.bhattacharyay@cutm.ac.in);

## 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 phyto-extracts 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* belongs to family-graecum. *Trigonella foenum-graecum* extract is traditionally used to cure diseases like cough. *Trigonella foenum-graecum* contains "beta-pinene, alpha-pinene, p-cymene, limonene, piperazine" etc. These phytochemicals might act against *Trigonella foenum-graecum*. However, there is no such study available.

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

## 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 [4]. 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 cough. This work is focused on the identification of the particular phytochemical

responsible for inhibiting and controlling of cough [5].

#### 2.2.2 Enzyme found in *Bordetella sp.*

There are many reasons of cough. It has been reported that cough can be caused as a result of *Bordetella sp.* infection [6]. 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 *Bordetella sp.* bacteria. It has been found that histidinekinase enzyme (protein database code 3A0S) is involved in signal transduction pathways upstream of virulence pathways and 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 acts as a ligand and forms 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 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 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

**Table 1. Results of C docking of phytochemicals with histidine kinase (receptor)**

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and –CDOCKER energy
1	Choline	Failed	Failed	NA
2	Arginine	29.619	28.5921	1.0269
3	Gentianine	Failed	Failed	NA
4	Carpaine	Failed	Failed	NA
5	Diosgenin	Failed	Failed	NA

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 [7,8]. Table 1 shows that choline, arginine and gentianine have higher negative –CDOCKER energy as well as –CDOCKER interaction energy and maximum value of the difference between –CDOCKER interaction energy and –CDOCKER energy. This indicates that choline, arginine and gentianine cannot effectively deactivate the enzyme histidinekinase of the microbe. On the other hand, carpaine and diosgenin failed to deactivate the enzyme. Thus, none of these phytochemicals can effectively deactivate the histidinekinase enzyme of *Bordetella sp.* and thus cannot be used to treat cough caused by this particular microbe.

#### 4. CONCLUSIONS

It was previously known that *Trigonella foenum-graecum* plant has medicinal action against cough. Cough is caused by *Bordetella sp.* 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 (histidinekinase) of the microbe. It was found that choline, arginine and gentianine cannot effectively inhibit the histidinekinase enzyme activity of *Bordetella sp.* Carpaine and Diosgenin were unable to react with the enzyme and therefore failed to show any results indicating that they can never be used to inhibit the histidinekinase enzyme of *Bordetella sp.* for treating cough. However, these phytochemicals

may show good enzyme deactivating capabilities against some other enzymes of the microbe.

#### 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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