UTTAR PRADESH JOURNAL OF ZOOLOGY

41(6): 53-55, 2020
ISSN: 0256-971X (P)

PREVENTION OF *Escherichia coli* CAUSING DIARRHOEA BY *Foeniculum vulgare*

ABINASH MOHAPATRA[1], RAKESH KUMAR GOCHHAYAT[1], MUKUNDJEE PANDEY[1,2*] AND DIPANKAR BHATTACHARYAY[1,2]

[1]Centurion University of Technology and Management, Odisha, India.
[2]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.

Received: 20 April 2020
Accepted: 31 May 2020
Published: 02 June 2020

Original Research Article

ABSTRACT

Diarrhea is caused by *Escherichia coli.* Shikimate dehydrogenase is one of its major enzymes. *Foeniculum vulgare* is known to cure Diarrhea. The plant extract contains different phytochemical compounds. By using "Biovia Discovery Studio", the molecular docking of the phytochemicals with the enzymes was studied. The results showed that caprylic can deactivate the shikimate dehydrogenase enzyme thereby interrupting the microbe's life cycle.

Keywords: Phytochemical; *Escherichia coli*; *Foeniculum vulgare*.

1. INTRODUCTION

Traditional medicines have gained importance as they are safe and reliable. The medicinal properties of the phytochemicals make them suitable to be used as medicines to fight against various diseases [1,2]. This knowledge can be effectively used for human health care.

Various plant parts were extracted and screened to get different phytochemical content [1].

Foeniculum vulgare belongs to family Apiaceae. Its extract can fight against diseases like Diarrhea. There is a high likelihood that these phytochemicals assume a significant job in relieving a disease. Anyway, there is no report distinguishing the particular phytochemical capable to fix eczema.

Escherechia coli is known to cause 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 have been

**Corresponding author: Email: mukundjee.pandey@cutm.ac.in;*

used as poisons and others as traditional medicine. Published works showed that *Foeniculum vulgare* contains eriodictyol-7 rutinoside, kaempferol-3-arabinoside, queccetin-3-rutinoside, rosmarinic acid, behenic acid, caproic acid, caprylic acid, lauric acid, myristic acid, oleic acid, stearic acid, undecanoic acid, 1,3-o-dicaffeoylquinic acid, 3-o- caffeoylquinic acid, 4-o-caffeoylquinic acid, 5-o-caffeoylquinic acid etc. It has already been established that *Foeniculum vulgare* plant belonging to Apiaceae family has the potential to help to control of diarrhea. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling of diarrhea.

2.2.2 Enzyme found in *Escherichia coli*

It has been reported that diarrhea can cause as a result of *Escherichia coli* 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 *Escherichia coli*. It has been found that shikimate dehydrogenase (1NYT) is involved in Phenylalanine, tyrosine and tryptophan biosynthesis (KEGG) 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 perform molecular docking. In this process first, the sdf files for the phytochemicals found in the *Foeniculum vulgare* plant were downloaded from the website (PubChem). The protein database code of shikimate dehydrogenase enzyme was identified from the website RCSB PDB. 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 softwere 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. 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 [3,4].

Table 1 shows that Shikimate dehydrogenase and caprylic acid interaction has the highest positive value of -CDOCKER energy (25.9286) and minimum value

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

Sl. no.	Ligand	- CDOCKER energy	- CDOCKER interaction energy	Difference between –C DOCKER and –C DOCKER interaction energy	Remarks
1	Caprylic acid	25.928	25.906	0.0219	Highest deactivation of the enzyme
2	Caprolic acid	24.116	25.4351	1.318	
3	5-o-caffeoylquinic acid	19.113	36.731	17.113	
4	4-o-caffeoylquinic acid	12.954	31.912	18.957	
5	3-o-caffeoylquinic acid	10.771	36.712	25.941	
6	Behenic acid	FAILED	FAILED	NA	

of the difference (0.0219) between - C DOCKER interaction energy and - C DOCKER energy. Thus the results indicated that caprylic acid can effectively deactivate the enzyme thereby interrupting the biological cycle of *Escherichia coli*. Higher positive values for shikimate dehydrogenase indicated that it was the most active ingredient against diarrhea. On the other hand, 3-o-caffeoylquinic acid can deactivate the enzyme to a small extent (negative -CDOCKER energy but positive -CDOCKER interaction energy). 1,3-O-dicaffeoylquinic acid, behenic acid cannot interact with shikimate dehydrogenase. Thus, the key phytochemicals preventing diarrhea caused by *Escherichia coli* are caprylic acid and caproic acid.

4. CONCLUSION

It was previously known that plant has *Foeniculum vulgare* medicinal action against diarrhea. Diarrhea is caused by *Escherichia coli*. 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 (behenic acid, caproic acid, caprylic acid, 1,3-o-dicaffeoylquinic acid, 3-o-caffeoylquinic acid, 4-o-caffeoylquinic acid, 5-o-caffeoylquinic acid), which can have significant interaction with the vital enzyme shikimate dehydrogenase of the microbe. It was found that caprylic acid and caproic acid can form a strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. 3-o-caffeoylquinic acid is found to be not much effective in deactivating the enzyme of the microbe. 1,3-O-dicaffeoylquinic acid, behenic acid cannot deactivate the enzyme. Thus, this study could explain that the presence of caprylic acid and caproic acid provided the medicinal values to *Foeniculum vulgare* against diarrhea caused by *Escherichia coli*.

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 personal efforts of the authors.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Mario Gajdacs, Edit Urban. The relevance of anaerobic bacteria in brain abscesses: A ten-year retrospective analysis (2008–2017), from infectious disease. 2019;15:789-781.
2. Farckkarahan, Kamhuravsar, et al. Antimicrobial and antioxidant activities of medicinal plant *Glycyrrhiza glabra* var; glandulifera from deffination habitats. 2016; 30(4):797-804.
3. Marissa L. Puzan, Belete Legesse, Ryan A. Koppes, Hicham Fenniri, Abigail N. Koppes. Bioactive organic rosette nanotubes support sensory neurite outgrowth. ACS Biomater. Sci. Eng. 2018;4(5):1630-1640.
4. Brinda OP, Deepu Mathew, Shylaja MR, Sangeetha Davis P, Anita Cherian K, Valsala PA. Isovaleric acid and avicequinone-C are Chikungunya virus resistance principles in *Glycosmis pentaphylla* (Retz.) Correa. 2019; 56(2):111-121.