UTTAR PRADESH JOURNAL OF ZOOLOGY

41(6): 59-61, 2020
ISSN: 0256-971X (P)

PREVENTION OF *Haemophilus influenza* CAUSING BRONCHITIS BY *Ocimum tenuiflorum*

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AUTHORS' CONTRIBUTIONS

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

Received: 24 April 2020
Accepted: 02 June 2020
Published: 04 June 2020

Original Research Article

ABSTRACT

Bronchitis is caused by *Haemophilus influenza.* Adenine specific DNA methyltransferase is one of its major enzymes. *Ocimum tenuiflorum* is known to cure of Bronchitis**.** 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 Rosmarinic Acid can deactivate the Adenine specific DNA methyltransferase enzyme thereby interrupting the microbe's life cycle.

Keywords: Phytochemical; *Ocimum tenuiflorum*; *Haemophilus influenza.*

1. INTRODUCTION

The use of herbal medicine increased significantly in the world including developed countries due to the pharmacological activities of plants [1,2]. The knowledge about plants have been provided by ancient people.

The stem, roots, leaves etc. were screened to get different phytochemical content [1].

Ocimum tenuiflorum belongs to family Lamiaceae and its extract can fight against disease like Bronchitis. There is 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.

Haemophilus influenza is known to cause Bronchitis.

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

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used as poisons and others as traditional medicine. Published works showed that *Ocimum tenuiflorum contains* Apigenin, Carnosic, Eugenol, Luteolin, Rosmarinic Acid etc. It has already been established that *Ocimum tenuiflorum* plant belonging to Lamiaceae family has the potential to help controlling Bronchitis. This work is focused on the identification of the specific phytochemical responsible for inhibiting and controlling of Bronchitis.

2.2.2 Enzyme found in *Haemophilus influenzae*

It has been reported that Bronchitis can cause as a result of *Haemophilus influenza* 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 *Haemophilus influenzae* bacteria. It has been found that Adenine specific DNA methyltransferase enzyme (protein database code 2NP7) is involved in adenine methylation of bacterial DNA (KEGG), (BRENDA) 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, which 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 *Ocimum tenuiflorum* plant were downloaded from the website [3]. The protein database code of the Adenine specific DNA methyltransferase enzyme was identified from the website [4]. 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 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. -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 [5,6].

Table 1 shows that (Rosmarinic Acid)-(Adenine specific DNA methyltransferase) interaction has the highest positive value of -CDOCKER energy (44.4763) and minimum value of the difference (3.3964) between -CDOCKER interaction energy and - CDOCKER energy. Thus, the results indicated that Rosmarinic Acid can effectively deactivate the Adenine specific DNA methyltransferase enzyme thereby interrupting the biological cycle of *Haemophilus influenzae*. Higher positive values for Rosmarinic Acidind icated that it was the most active ingredient against *Haemophilus influenza* followed by Luteolin, Apigenin, Eugenol. On the other hand, Carnosic Acid can deactivate the enzyme to a small extent (negative -CDocker energy but positive -CDocker interaction energy). Thus, the key phytochemicals preventing Bronchitis caused by *Haemophilus influenzae* are Rosmarinic Acid followed by Luteolin, Apigenin and then Eugenol.

Table 1. Results of C Docking of phytochemicals with Adenine specific DNA methyltransferase (receptor)

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between-CDOCKER interaction energy and - CDOCKER energy	
1	Rosmarinic Acid	41.0799	44.4763	3.3964	Highest deactivation of enzyme
2	Luteolin	28.9334	36.4063	7.4729	
3	Apigenin	21.5608	32.0484	10.4876	
4	Eugenol	12.7257	26.0864	13.3607	
5	Carnosic acid	-7.01721	32.2841	39.30131	

4. CONCLUSION

It was previously known that *Ocimum tenuiflorum* plant has medicinal action against Bronchitis. Bronchitis is caused by *Haemophilus influenzae*. 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, Carnosic, Eugenol, Luteolin, Rosmarinic Acid), which can have significant interaction with the vital enzyme Adenine specific DNA methyltransferase of the microbe. It was found that Rosmarinic Acid can form a strong bond with the enzyme followed by Luteolin, Apigenin, Eugenol, successfully inhibiting the metabolic cycle of the microbe. Carnosic Acid is found to be not much effective in deactivating the enzyme of the microbe. Thus, this study could explain that the presence of Rosmarinic Acid provided the medicinal values to *Ocimum tenuiflorum* against Bronchitis caused by *Haemophilus influenzae.*

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.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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