UTTAR PRADESH JOURNAL OF ZOOLOGY

41(7): 44-46, 2020
ISSN: 0256-971X (P)

In-silico ANALYSIS OF PHYTOCHEMICALS FROM *Linum usitatissimum* AGAINST *Staphylococcus aureus* CAUSING ECZEMA

ATASI ROUTRAY[1], PRAJNA PRIYADARSINI SETHI[1], RUNKI PRIYADARSINI SAMAL[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: 25 April 2020
Accepted: 10 June 2020
Published: 12 June 2020

Original Research Article

ABSTRACT

Eczema is caused by "*Staphylococcus aureus"*. Aspatate semialdehyde "dehydrogenase" is one of its major enzyme. *Linum usitatissimum* is known to cure eczema**.** The plant extract contains different phytochemical compounds. By using "Biovia Discovery Studio", "molecular docking" of the phytochemicals with the enzymes was studied. The results showed that *Linum usitatissimum* can deactivate the aspatate semialdehyde dehydrogenase enzyme in that way interrupting the microbe's life cycle.

Keywords: Phytochemicals; *Linum usitatissimum*; *Staphylococcus aureus.*

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 has been provided by ancient people.

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

Flax or linseed is a member of the genus Linum belonging to family Linaceae. Flax seed extract can cure diseases like eczema.

They are high opportunity of above "phytochemicals" plays an important role in curative eczema. However, there was no details to identify exact "phytochemical" responsible for treat eczema. However, there is no report distinguishing the particular phytochemical capable to fix eczema. The study aims "identification of the phytochemical of *Linum usitatissimum* responsible for treatment eczema caused by *Staphylococcus aureus"*.

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.

**Corresponding author: Email: dipankar.bhattacharyay@cutm.ac.in;*

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 *Linum usitatissimum* contains ferulic acid, linamarin, p-coumaric acid, salicylic acid, sinapic acid, syringic acid, anillc acid etc.It has already been established that plant *Linum usitatissimum* belonging to Linaceae family has potential to help in controlling of eczema. This work is focused on identification of the particular phytochemical responsible for inhibiting and controlling eczema.

2.2.2 Enzyme found in *Staphylococcous*

It has been reported that eczema can be caused as a result of *Staphylococcous aureus* 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 *Staphylococcous sp.* bacteria. It has been found that aspartate-semialdehyde dehydrogenase enzyme (protein database code 3VOS) is involved in glycine, serine, and threonine metabolism (KEGG) and is very crucial for survival of the particular microbe.

2.2.3 Molecular docking

The 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 *Linum usitatissimum* plant were downloaded from the website [3]. The protein database code of the aspartate semialdehyde dehydrogenase (3VOS) 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 aspartate- semialdehyde dehydrogenase –feruic acid interaction has the highest positive value of -CDOCKER energy (17.3055) and minimum value of the difference (5.6773) between - C DOCKER interaction energy and - C DOCKER energy. Thus the results indicated that feruic acid can

Table 1. Results of CDocking of phytochemicals with aspartate semialdehyde dehydrogenase (receptor) dehydrogenase (Receptor)

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Feruic acid	17.3055	22.9828	5.6773
2	Linamarin	-21.2656	19.1867	2.0789
3	p-coumaric acid	15.5349	18.o469	2.512
4	Salicylic acid	5.64209	9.79796	4.15587
5	Sinapic acid	-10.7992	8.74336	2.05584
6	Syringic acid	6.85673	13.4213	6.56457
7	Vanillic acid	9.82962	18.2659	8.43628

effectively deactivate the aspartate- semialdehyde dehydrogenase enzyme thereby interrupting the biological cycle of *Staphylococcous sp.* Higher positive values for aspartate semihaldehyde dehydrogenase indicated that it was the most active ingredient against *Staphylococcous sp.* On the other hand syringic acid, linamarin acid, sinapic acid, salicylic acid, can deactivate the enzyme to a small extent (negative -CDocker energy but positive -CDocker interaction energy). Thus, the key phytochemicals preventing eczema caused by *Staphylococcous sp.* are asprtate semialdehyde dehydrogenase.

4. CONCLUSION

It was previously known that *Linum usitatissimum* plant has medicinal action against eczema. Eczema is caused by *Staphylcoccous aureus*. 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 phytochemicals ferulic acid, linamarin, p-coumaric acid, salicylic acid, sinapic acid, syringic acid, vanillc acid, which can have significant interaction with the vital enzyme aspartate – semialdehyde dehydrogenase of the microbe. It was found that feruic acid and p-coumaric acid can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe.

Syringic acid, linamarin acid, sinapic acid, salicylic acid were found to be not effective in deactivating the enzyme of the microbe. Thus, this study could explain that the presence of feruic acid and p-coumaric acid provided the medicinal values to *Linum usitatissimum* against eczema caused by *Staphylococcou aureus.*

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. Mol-Instincts | Chemical Property Database | Available:www.molinstincts.com
4. Enzyme Database – BRENDA | Available:www.brenda-enzymes.org
5. 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.
6. 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.