Journal of Pharmaceutical Research International

32(7): 84-87, 2020; Article no.JPRI.56455
ISSN: 2456-9119
(Past name: British Journal of Pharmaceutical Research, Past ISSN: 2231-2919, NLM ID: 101631759)

Cinnamomum zeylanicum (*Cinnamon*) Derived Phytochemicals against Aspartate Semialdehyde Dehydrogenase of *Aspergillus fumigatus* Causing Aspergillosis

Biswajit Jena[1], Minati Rani Muni[1], P. K. Prusty[1], Sunil Jha[1] and Deepankar Bhatttacharyay[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.

Article Information

DOI: 10.9734/JPRI/2020/v32i730512
Editor(s):
(1) Prof. Mostafa A. Shalaby, Cairo University, Egypt.
Reviewers:
(1) Sandeep Onkar Waghulde, University of Mumbai, India.
(2) Mosad Ahmed Ghareeb, Theodor Bilharz Research Institute, Egypt.
Complete Peer review History: http://www.sdiarticle4.com/review-history/56455

Original Research Article

Received 05 April 2020
Accepted 22 May 2020
Published 24 May 2020

ABSTRACT

Aspergillosis is an infection caused by a type of fungus. The illnesses is caused by aspergillosis infection and usually attack the respiratory system, but their signs and severity vary greatly. It has already been established that plant *Cinnamomum zeylanicum* belonging to the Lauraceae family has the potential to help controlling aspergillosis. This work is focused on the identification of the particular phytochemical responsible for inhibiting and decreasing the effect of aspergillosis. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that cinnamic acid can effectively deactivate aspergillosis.

Keywords: Phytochemical; Cinnamomum zeylanicum; Aspergillus fumigates.

**Corresponding author: E-mail: dipankar.bhattacharyay@cutm.ac.in;*

1. INTRODUCTION

Aspergillosis is an infection caused by a type of fungus. The illnesses caused by aspergillosis infection usually attack the respiratory system, but their signs and severity vary greatly. Aspergillosis is the name given to a wide variety of diseases caused by fungal infections from species of *Aspergillus*. Nature is a major source of medicines [1] of many diseases like Aspergillosis. 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 plants play a key role in human health care. Many people rely on the use of traditional medicine [3].

This objective of the study is to identify the phytochemical of *Cinnamomum zeylanicum* capable of curing Aspergillosis.

2. MATERIALS AND METHODS

2.1 Software Used

Discovery studio module of BIOVIA software (Dassault Systems 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. Published works showed that *Cinnamomum zeylanicum* contains Procyanidin, A2, eugenol 3D, catechin, cinnamic acid curcumin, nicotine, quercetin, vanillin. It has already been established that plant *Cinnamomum zeylanicum* belonging to the Lauraceae family has the potential to help controlling aspergillosis. This work is focused on the identification of the particular phytochemical responsible for inhibiting and decreasing the effect of aspergillosis.

2.2.2 Enzyme found in *Cinnamomum zeylanicum*

It has been reported that aspergillosis can be caused as a result of *Aspergillus fumigatus* infestation. Various metabolic cycles have been seen in the fungi life cycle for its survival. These metabolic cycles are regulated by different enzymes. Brenda enzyme database was used to find the list of different enzymes found in *Aspergillus fumigatus* fungi. It has been found that aspartate semialdehyde dehydrogenase enzyme (protein base code 5JW6) is involved in amino acid metabolism (mainly synthesis the amino acids like glycine, serine, threonine, cysteine, methionine, lysine) [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, 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 *Cinnamomum zeylancium* plant were downloaded from the website (PUBCHEM). The protein database code of the aspartate semialdehyde dehydrogenase enzyme was found 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 with the help CDOCKER protocol of BIOVIA software under “receptor-ligand interaction” [4]. 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 controlling 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 non-bonded 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

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

Sl. no.	Ligand	- CDOCKER energy	- CDOCKER interaction energy	Difference between - CDOCKER interaction energy and - CDOCKER energy	Remarks
1	P-CYMENE	14.2999	14.9983	0.6984	
2	PIPERAZINE	1.99172	11.6549	9.66318	
3	ALPHA-PINENE	-13.7461	11.3739	25.4992	
4	BETA-PINENE	-10.941	13.485	24.426	
5	LIMONENE	-26.5154	12.0783	38.5937	
6	QURECITINE	FAILED	FAILED	FAILED	
7	PIPERINE	FAILED	FAILED	FAILED	

between -CDOCKER energy and CDOCKER interaction energy [5]. Table 1 shows that aspartate semialdehyde dehydrogenase cinnamic acid interaction has the highest positive value of -CDOCKER energy (21.7962) and minimum value of the difference (2.7916) between - C DOCKER interaction energy and - C DOCKER energy followed by vallinin Thus the results indicated that cinnamic acid and vallinin can effectively deactivate the aspartate semialdehyde dehydrogenase enzyme thereby interrupting the biological cycle of *Aspergillus fumigatus.* Table 1 shows interaction was found to have the highest interaction.

Higher positive values for cinnamic acid indicated that it was the most active component against *Aspergillus fumigatus.* On the other hand, quercetin, catechin, eugenol 3D, curcumin, nicotine can deactivate the enzyme to a small extent. Procyanidin A2 cannot interact with aspartate semialdehyde hydrogenase enzyme. Thus, the key phytochemicals preventing aspergillosis caused by *Aspergillus fumigatus* are cinnamic acid and vallinin.

4. CONCLUSIONS

It was previously known that that *Cinnamon zeylancium* plant has medicinal action against aspergillosis. Aspergillosis is caused by *Aspergillus fumigatus*. This study was carried out to provide the theoretical knowledge of this observation. Using Discovery studio module of BIOVIA software, molecular docking operation was performed to identify the phytochemical (cinnamic acid, vallinin, quercetin, catechin, eugenol 3D, curcumin, nicotin, procyanidin A2), which can have significant interaction with the vital enzyme (aspartate semialdehyde dehydrogenase) of the microbe. It was found can form a strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Curcumin and nicotin were found to be not much effective in deactivating the enzyme of the microbe. Procyanidin A2 cannot deactivate the enzyme. Thus, this study could explain that the presence of cinnamic acid and vallinin provided the medicinal values to Cinnamomum *zeylanicum* against aspergillosis caused by *Aspergillus fumigates*.

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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Peer-review history:
The peer review history for this paper can be accessed here:
http://www.sdiarticle4.com/review-history/56455