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Eclipta alba L. Derived Phytochemicals against *Campylobacter* Causing Diarrhea

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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 *Eclipta alba* L. plant extract are traditionally used to cure Diarrhea. It is caused by *Campylobacter.* Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDocker energy and -CDocker interaction energy" suggested that 6, 10, 14-trimethyl-2-pentadecanone can effectively deactivate the Argininedecarboxylase enzyme (protein database code 3N29) thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Eclipta alba L.; campylobacter; Diarrhea.

1. INTRODUCTION

Medicinal plants are the valuable resources of new drugs [1]. Herbal derived remedies need a powerful and deep assessment of their pharmacological efficacy. Different types of phytochemicals are responsible for the medicinal properties. Plant extracts derived from different parts show anti microbial activity against different micro-organisms [2]. Herbs are natural products and play a major role in human health care. Therefore, traditional medicines are given importance to treat different diseases [3]. *Eclipta alba* L. belongs to family Asteraceae. *Eclipta alba* L. extract is used to cure disease like Gonorrhoea. The objective of the study is to identify the phytochemical responsible to cure the disease. *Eclipta alba* L. contains

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phytochemicals like "6,10,14-trimethyl-2-pentadecanone,7,11-Dimethyl-3-methylene-1,6,10-dodecatriene, Heptadecane, Echinocysticacid, Octadea-9-enoic acid, Pentadecane, Phytol" etc. These phytochemicals might act against Diarrhea. However, there is no such study available. This objective of the study is to identify the phytochemical of *Eclipta alba* L. capable of curing Diarrhea.

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. Some phytochemicals have been used as poisons and others as traditional medicine. Published works showed that *eclipta alba*contains6,10,14-trimethyl-2-pentadecanone,7,11-dimethyl-3-methylene,1-6-10-Dodecatriene, Heptadecane, Pentadecane, Phytol, Octadea-9-enoic acid, Echinocystic acid etc.It has already been established that *Ecliptaalba* plant belonging to Asteraceae family has potential to help controlling Diarrhea. This work is focused on identification of the particular phytochemical responsible for inhibiting and controlling of Diarrhea.

2.2.2 Enzyme found in *Campylobacter*

It has been reported that diarrhea can causeas a result of *Campylobacter* 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 *Campylobacter* bacteria. It has been found that Arginine decarboxylase enzyme (protein database code 3N29) is involved in Urea cycle (KEGG) and very crucial for 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 act as a ligand and form 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. Molecular docking is a kind of bioinformatic modelling which involves the interaction of two or more molecules to give the stable adduct. Depending upon binding properties of ligand and target, it predicts the three-dimensional structure of any complex. In this process first the sdf files for the phytochemicals found in the *Ecliptaalba* plant were downloaded from the website [4]. The protein database code of the Arginine decarboxylase enzyme was identified from the website [5]. 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 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 forbest interaction was chosen based on (a) high positive value of -CDOCKER energy and (b)small difference between -CDOCKER energy and -CDOCKER interaction energy [4,5]. Table 1 shows that Arginine decarboxylase-Pentadecane interaction has the highest positive value of –CDOCKER energy [28.7582] and minimum value of the difference [1.0881] between –CDOCKER energy followed by 6,10,14-trimethyl-2-pentadecanone. Thus the results indicated that pentadecane,6,10,14-trimethyl-2-pentadecanone and Heptadecane

Table 1. Results of C Docking of phytochemicals with Arginine decarboxylase (receptor)

Sl. no.	Ligand	- C DOCKER energy	- C DOCKER interaction energy	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Pentadecane	28.7582	29.8463	1.0881
2	6,10,14-trimethyl-2-pentadecanone	34.5337	37.2345	2.7008
3	Heptadecane	31.6099	34.739	3.1291
4	Octadea-9-enoic acid	24.7439	38.4364	13.6925
5	Phytol	10.6643	37.2641	26.5998
6	7,11-dimethyl-3-methylene-1,6,10-dodecatriene	-31.396	24.7486	56.1446
7	Echinocystic acid	Failed	Failed	NA

can effectively deactivate the Arginine decarboxylase enzyme, thereby interrupting the biological cycle of *campylobacter*. Higher positive values for pentadecane indicated that it was the most active ingredient against *campylobacter*. On the other hand Phytol and 7,11-dimethyl-3-methylene-1,6,10-dodecatriene [negative CDOCKER energy and positive -CDOCKER INTERACTION energy] can deactivate the enzymes to a small extent. On the other hand, Echinocystic acid can not interact with Arginine decarboxylase enzyme.

4. CONCLUSIONS

It was previously known that *Eclipta alba* has medicinal action against Diarrhea. Diarrhoea is caused by *campylobacter*. This study was carried out to provide the theoretical basis of the observation. Using Discovery studio Molecule of Biovia software, Molecular docking operation was performed to identify the phytochemical [6,10,14-trimethyl-2-pentadecanone,7,11-Dimethyl-3-methylene,1,6,10-dodecatriene, pentadecane, echinocystic acid, octadea-9-enoic acid, Heptadecane, Phytol, which have significant interaction with the vital enzyme [Arginine decarboxylase] of the microbe. It was found that Pentadecane,6,10,14-trimethyl-2-pentadecanone, And Heptadecane can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Thus, this study could explain that the presence of pentadecane,6,10,14-trimethyl-2-pentadecanone and Heptadecane provided the medicinal values to *Eclipta alba* against Diarrhea caused by *Campylobacter*.

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.

CONSENT

It is not applicable.

ETHICAL APPROVAL

It is not applicable.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Henrich J, Heine S, Norenzayan A. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI: 10.1017/S0140525X0999152X
2. Hussain I, Ullah R, Ullah R, Khurram M, Ullah N, Basee A, Khan F, Khattak M, Zahoor M, Khan J, Khan N. Phytochemical analysis of selected medicinal plant.

African Journal of Biotechnology. 2011;10: 7487-7492.

3. Arulselvan P, Karthivashan G, Fakurazi S. Journal of Chemical and Pharmaceutical Research. 2013;5(7):233-239.
4. Das D, Das S, Pandey M, Bhattacharyay D. *In silico* analysis of phytochemicals from *Mucuna pruriens* (L.) DC against *Mycobacterium tuberculosis* causing tuberculosis. European Journal of Medicinal Plants; 2020.
5. Brinda OP, Mathew D, Shylaja MR, Davis PS, Cherian KA, Valsala PA. Isovaleric acid and avicequinone-C are chikungunya virus resistance principles in *Glycosmis pentaphylla* (Retz.) Correa. Journal of Vector Borne Diseases. 2019;56(2):111.

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