Journal of Pharmaceutical Research International

32(7): 112-115, 2020; Article no.JPRI.57274
ISSN: 2456-9119
(Past name: British Journal of Pharmaceutical Research, Past ISSN: 2231-2919, NLM ID: 101631759)

Eclipta alba L. Derived Phytochemicals against *Escherichia coli* Causing Diarrhea

Krishna Rani[1], Aischarya Mohanty[1], Sagarika Parida[1], Manisha Mohanty[1*], Subhashree Sahu[1], Sanchayita Nayak[1] and Sutapa Mohanty[1]

[1]Centurion University of Technology and Management, 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/v32i730519
Editor(s):
(1) Dr. R. Deveswaran, University of Applied Sciences, India.
Reviewers:
(1) N. K. Udaya Prakash, Vels Institute of Science, Technology and Advanced Studies (VISTAS), India.
(2) Ochieng O. Anthony, Sumait University, Tanzania.
(3) Lassina Ouattara, Université Nazi Boni, Burkina Fao.
Complete Peer review History: http://www.sdiarticle4.com/review-history/57274

Original Research Article

Received 04 April 2020
Accepted 22 May 2020
Published 25 May 2020

ABSTRACT

Phytochemicals from *Eclipta alba* L. plant extract are traditionally used to cure Diarrhea. It is caused by *Escherichia coli*. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that Pentadecanone can effectively deactivate the alcohol dehydrogenase enzyme (protein database code 4GKV) thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Eclipta alba L.; Escherichia coli; diarrhea.

1. INTRODUCTION

Herbal therapy is the use of medicinal plants for the prevention and treatment of diseases [1]. Phytochemicals present in plants are responsible for attributing the medicinal properties. Different plant parts compose different phytochemicals. Literature data revealed that extracts from different plant sources have shown antimicrobial activity against different micro-organisms [2]. Plant based drugs play a major role in human health care. Because of safety and efficacy of medicinal plants, many people rely on traditional medicine [3]. *Eclipta alba* L. belongs to family

**Corresponding author: E-mail: mohantymanisha14@gmail.com;*

Asteraceae. *Eclipta alba* L. extract is used to cure disease like Diarrhea. The objective of the study is to identify the phytochemical responsible to cure the disease. *Eclipta alba* L. contains "pentadecanone, Echinocystic acid, heptadecane, octadea-9-enoic acid 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

Biovia software (Dassault Systemes of France) is a software company that provide software for advanced biological, chemical and material research for pharmaceutical, aerospace, energy and chemical industries.

Discovery studio module of Biovia software (Dassault system, is a software company) is used for analysis of molecular docking of phytochemicals from plant extracts that act as a ligand and form strong covalent bond with the enzyme molecule and analysis strentgh of this interaction based on -CDOCKER and -CDOCKER interaction energy. The software utilizes machine learning techniques to predict the level of molecular interaction.

2.2 Methodology

2.2.1 List of phytochemicals

Phytochemicals are biologically active compounds found in 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 c*ontains phytochemicals like 10,14-trimethyl-2-pentadecanone,7,11-Dimethyl3methylene1 ,6Z1,Echinocystic acid, heptadecne,octadea-9-enoic acid etc. It has already been established that *Eclipta alba*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 *E. coli*

It has been reported that Diarrhea can cause as a result of *E. coli sp.* 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 *E. coli sp.* bacteria. It has been found that alcohol dehydrogenase enzyme (protein database code 4GKV) is involved in glycerolipid metabolism (KEGG) and very crucial for survival of the particular microbe.

2.2.3 Molecular docking

Discovery studio module of Biovia software 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. In this process first the sdf files for the phytochemicals found in the *Eclipta alba* plant were downloaded from the website (PubChem). The protein database code of the alcohol dehydrogenase enzyme was identified from the website (RCSB). 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 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

Table 1. Results of C Docking of phytochemicals with alcohol dehydrogenase (receptor)

Sl. no.	Ligand	- CDOCKER energy	- CDOCKER interaction energy	Difference between - C DOCKER interactions energy and C DOCKER energy
1	Heptadecane	25.3549	25.2566	0.0983
2	Pentadecanone	26.5968	28.8642	2.2674
3	Octadea-9-enoic acid	21.3031	30.3726	9.0695
4	Echinocystic	-65.0034	33.3124	98.3158
	Dodecatriene	-40.3559	16.44	56.7959

energy [4,5]. Table 1 shows that glycerol dehydrogenase- heptadecaneinteraction has the highest positive value of -CDOCKER energy (25.3549) and minimum value of the difference (0.0983) between -CDOCKER interaction energy and -CDOCKER energy followed by pentadecanone. Thus the results indicated that Pentadecanone and heptadecane can effectively deactivate the alcohol dehydrogenase enzyme, thereby interrupting the biological cycle of *E. coli sp.*. Higher positive values for heptadecane indicated that it was the most active ingredient against *E. coli sp.*. On the other hand 7,11-dimethyl 3 methylene 1,6,10 dodecatriene and echinocystic acid can deactivate the enzyme to a small extent (negative -CDOCKER energy but positive -CDOCKER interaction energy).

4. CONCLUSIONS

After analysing different published journals it is concluded that *Eclipta alba* plant has medicinal action against Diarrhea (NCBI). Diarrhea is caused by *E. coli sp.*. 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 (10,14-trimethyl-2-pentadecanone ,7,11-Dimethyl-3methylene1,6Z1,Echinocystic acid, heptadecane,octadea-9-enoic acid), which can have a significant interaction with the vital enzyme (alcohol dehydrogenase) of the microbe. It was found that heptadecane and pentadecanone can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Thus, this study could explain that the presence of pentadecanone, enoic and heptadecane provided the medicinal values to *Eclipta alba* against Diarrhea caused by *E. coli Sp.*

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 the 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.

Peer-review history:
The peer review history for this paper can be accessed here:
http://www.sdiarticle4.com/review-history/57274