



***Eclipta alba* Derived Phytochemicals against Jaundice**

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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 otherwise known as secondary metabolites means the small organic molecules that are not essential for growth, development and reproduction but can protect from various diseases. Infact these phytochemicals are the key source of medicine. Secondary metabolites from *Eclipta alba* plant extract are traditionally used to cure Jaundice which is caused by *Leptospira interrogans*. The curative property of *Eclipta alba* against *Leptospira interrogans* was proved by molecular docking method in "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" recommended that pentadecan, heptadecane, 6,10,14-trimethyl-2-petadecanone can successfully deactivate the thioredoxin-disulfide reductase enzyme thereby disrupting the cellular function as well as the lifecycle of causative organism.

Keywords: *Phytochemical; Eclipta alba; Leptospira interrogans; jaundice.*

1. INTRODUCTION

For herbal medicine, people rely on the nature so we can say medicine is the nature's best gift we ever know [1]. And the medicinal properties of the plant are due to the phytochemicals present in it. These phytochemicals can be found in every part of the plant like in roots, stem, leaves, seed and flower etc. One plant can contain a large number of phytoconstituents and because of the defensive mechanism of these phytoconstituent it can be used against various diseases which are mainly caused by microorganisms [2]. From the prehistoric period people have been depending on herbal medicines for their different ailments. And now a day these medicinal plants are again playing the key role in pharmaceutical sectors [3].

Eclipta alba commonly known as bhringraj or false daisy belongs to the family Asteraceae. It is believed that Bhringraj is one of the most effective herbs for being a liver tonic and also it is beneficial for hair growth, diabetes and eye care. The leaf extract of the *Eclipta alba* is used for curing Jaundice. And the objective of the recent study is to find out the effective phytoconstituents which going to inhibit the causative organism of the Jaundice. Bhringraj contains phytochemicals like "6,4,10-trimethyl-2-pentadecanone, 7,11-Dimethyl-3-methyl-1,6,10-dodecatriene, Echinocystic acid, Heptadecane, Octa-9-enoic-acid, pentadecane, phytol" [4]. Jaundice can be curable by these phytochemicals but there is no such study available yet. In the present study aim is to identify the most effective bioactive compound that will bound the enzyme of the thioredoxin-disulfide reductase and there by inhibiting the activity of the enzyme resulting in the disrupting the cellular NADPH reduction process for active site disulfide formation in cell which will control the life cycle of the causative organism.

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 used as poisons and others as traditional medicine. Published works showed that *Eclipta alba* contains 6,10,14-trimethyl-2-pentadecanone, 7,11-Dimethyl-3-methylene-1,6Z,10-dodecatriene, Echinocystic acid, Heptadecane, Octa-9-enoic-acid Pentadecane etc. It has already been established that *Eclipta alba* belonging to *Asteraceae* family has potential to help controlling jaundice. This work is focused on identification of the particular phytochemical responsible for inhibiting and controlling of jaundice.

2.2.2 Enzyme found in *Leptospira*

It has been reported that jaundice can be caused as a result of *leptospira* 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 *Leptospira interrogans* bacteria. It has been found that Thioredoxin-disulfide reductase (protein database code 3R9U) is involved in selenocompound metabolism (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. In this process first the sdf files for the phytochemicals found in the *Eclipta alba* plant were downloaded from the website [4]. The protein database code of the thioredoxin-disulfide reductase 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 Bioviasoftware 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 energy [5,6]. Table 1 shows that thioredoxin-

disulfide reductase-pentadecane interaction has the highest positive value of -CDOCKER energy (37.6504) and minimum value of the difference (-0.2203) between- C DOCKER interaction energy and - C DOCKER energy followed by heptadecane and 6,10,14-trimethyl-2-pentadecanone. Thus the results indicated that pentadecane, heptadecane, 6,10,14-trimethyl-2-pentadecanone can effectively deactivate the thioredoxin-disulfide reductase enzyme thereby interrupting the biological cycle of *Leptosira*. Higher positive values for pentadecane indicated that it was the most active ingredient against *Leptosira interrogans*. The octa-9-enoic acid is also effectively deactivate the thioredoxin-disulfide reductase. On the other hand 7,11-Dimethyl-3methylene-1,6Z,10-dodecatriene deactivate the enzyme to a small extent (negative -Cdocker energy but positive-CDocker interaction energy) Echinocystic acid cannot interact with thioredoxin-disulfide reductase enzyme. Thus, the key phytochemicals preventing jaundice caused by *Leptosira interrogans* are pentadecanone, heptadecanone, 6,10,14-trimethyl-2-pentadecanone.

Table 1. Results of C Docking of phytochemicals with thioredoxin-disulfide reductase (receptor)

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between- CDOCKER interaction energy and - CDOCKER energy	Remark
1	Pentadecane	37.6504	37.4301	-0.2203	Maximum inhibition microbial enzyme
2	Heptadecane	34.5131	41.6951	7.182	
3	6,10,14-trimethyl-2-pentadecanone	35.397	45.4577	10.0607	
4	Octa-9-enoic acid	33.9538	50.0175	16.0637	
5	7,11-Dimethyl-3-methylene-1,6Z,10-dodecatriene	-25.7864	36.1636	61.95	
6	Echinocystic acid	Failed	Failed	NA	

4. CONCLUSIONS

It was previously known *Ecliptaalba* plant has medicinal action against jaundice. Diarrhea is caused by *Leptosira interrogans*. 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 (pentadecane,heptadecane,6,10,14-trimethyl-2-pentadecanone,octa-9-enoic acid,7,11-Dimethyl-3-methylene-1,6Z,10dodecatriene,echinocystic acid), which can have a significant interaction with the vital enzyme (thioredoxin-disulfide reductase) of the microbe. It was found thatpentadecane, heptadecane,6,10,14-trimethyl-2-pentadecanone can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Octa-9-enoic acid were and 7,11-Dimethyl-3methylene-1,6Z,10-dodecatriene found to be not much effective in deactivating the enzyme of the microbe. Echinocystic acid cannot deactivate the enzyme.Thus, heptadecane, 6,10,14-trimethyl-2-pentadecanoneprovided the medicinal values to *Eclipta alb* against jaundice caused by *Leptosira interrogans*.

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.

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