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Bixa orellana Derived Phytochemicals against *Entamoeba histolytica* Causing Dysentery

Sonali Parida[1], Jogesh Kumar Nayak[1], Anindita Jena[1], Arsia Tabish[1], Archita Sahoo[1], Ananya Pani[1] and Rukmini Mishra[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.

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ABSTRACT

Phytochemicals from *Bixa orellana* plant extract are traditionally used to cure Dysentery. It is caused by *Entamoeba histolytica.* Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that benzoin acid can effectively deactivate the alcohol dehydrogenase enzyme thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Bixa orellana; Entamoeba histolytica.

1. INTRODUCTION

Plants are rich in bioactive compounds which act as a natural defense system and protect them from invading pathogens [1]. These compounds are rich in medicinal properties and can be used for to cure different diseases. The plant extracts from these medicinal plants can be used to formulate drugs which are more safe and cost effective [2]. They plant an important role in human health care. Traditional medicines are always preferred [3].

**Corresponding author: E-mail: rukmini.mishra@cutm.ac.in;*

Bixaorellana belongs to family bixaceae. *Bixaorellana* extract is used to cure disease like Dysentery. The objective of the study is to identify the phytochemical responsible to cure the disease.

Bixaorellana contains “norbixin, phytol, phenol, acetic acid, anthraquinone, benzoic acid and farnesyl acetone” etc. These phytochemicals might act against Dysentery. However, there is no such study available.

This objective of the study is to identify the phytochemical of *Bixa orellana* capable of curing Dysentery.

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 secondary metabolites produced by plants to protect them from predators. The potential threats to plants include bacteria, viruses and fungi. When these plants or their parts are consumed by humans these phytochemicals resist threats to health. Some phytochemicals have been used as poisons and others as traditional medicine. Published works showed that *Bixa orellana* contains norbixin, phytol, phenol, acetic acid, anthraquinone, benzoic acid and farnesyl acetone. It has already been established that *Bixa orellana* plant belonging to Bixaceae family has potential to help controlling Dysentery. This work is focused on the identification of specific phytochemical liable for inhibiting and controlling of Dysentery.

2.2.2 Enzyme found in *Entamoeba histolytica*

It has been stated that dysentery can causeas a result of *Entamoeba histolytica* invasion. In the bacterial life cycle various metabolic cycles have been seen for its existence. These metabolic cycles are controlled by different enzymes. List of different enzymes found in *Entamoeba histolytica* bacteria are detected by using Brenda enzyme database. It has been found that alcohol dehydrogenase enzyme (protein database code 1Y9A) is involved in ethanol fermentation, methionine, Tryptophan, valine, phenylalanine, leucin metabolism and tyrosine metabolism (BRENDA) and very essential for the existence of the specific 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 *Bixa orellana* plant were downloaded from the website (www.molinstincts.com). The protein database code of the alcohol dehydrogenase enzyme was recognized from the website (www.rcsb.org). The active site of the enzyme was found under "receptor-ligand interaction" and “define and edit binding site” menu via “receptor cavity” protocol. Molecular docking was doneunder “receptor-ligand interaction” and “Dock ligand” menu by using the CDOCKER protocol of Biovia software. The enzyme acts as the receptor molecule and the phytochemical act as the ligand. The quality of molecular docking were indicated by the “-CDOCKER_ENERGY” and “-CDOCKER_INTERACTION_ENERGY”. The high positive value of “-CDOCKER_ENERGY” and “-CDOCKER_INTERACTION_ENERGY” between the ligand and the receptor indicates a good interaction. Thus, the interactions with high values might specify the major phytochemical liable 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 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 between -CDOCKER energy and -CDOCKER interaction energy [4,5]. Table 1 shows that alcohol dehydrogenase-benzoic acid interaction has the highest positive value of -CDOCKER

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

Sl. no	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between - C DOCKER interaction energy and - C DOCKER energy	Remarks
1	Benzoic acid	12.6197	13.6892	1.0695	Maximum inhibition of infection
2	Acetic acid	12.1717	10.3064	1.8653	
3	Phenol	8.30143	19.4032	2.10177	
4	Anthraquinone	12.5373	17.9321	5.3948	
5	Phytol	3.62936	25.8629	22.23354	
6	Norbixin	-6.92316	31.9345	38.85766	

energy (12.6197) and minimum value of the difference (1.0695) between - C DOCKER interaction energy and - C DOCKER energy followed by acetic acid, phenol and anthraquinone. Thus the results indicated that benzoic acid, acetic acid, phenol and anthraquinone can efficiently deactivate the alcohol dehydrogenase enzyme thereby interfering the biological cycle of *Entamoeba histolytica*. Higher positive values for benzoic acid, acetic acid, phenol and anthraquinone showed that these are the most dynamic constituent against *Entamoeba histolytica*. On the other hand norbixin and farnesyl acetone can deactivate the enzyme to a small extent due to negative -CDOCKER energy but positive -CDOCKER interaction energy. Thus, the important phytochemicals preventing Dysentery caused by Entamoeba histolyticaare benzoic acid, acetic acid, phenol and anthraquinone.

4. CONCLUSIONS

It was previously known that *Bixa orellana* plant has medicinal action against Dysentery. Dysentery is caused by *Entamoeba histolytica*. This study was carried out to provide the theoretical basis of this observation. Molecular docking operation was executed to identify the phytochemical (benzoic acid, acetic acid, phenol, anthraquinone, phytol, nor-bixin, farnesyl acetone) by using Discovery studio module of Biovia software, which can have a majorinteraction with the dynamic enzyme (alcohol dehydrogenase) of the microbe. It was found that benzoic acid, acetic acid, phenol and anthraquinone can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Phytol, nor-bixin and farnesyl acetone were found to be not much effective in deactivating the enzyme of the microbe as they fail to maintain stability. Thus, this study could explain that the presence of benzoic acid, acetic acid, phenol and anthraquinone delivered the medicinal values to *Bixa orellana* against Dysentery caused by *Entamoeba histolytica*.

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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