*Journal of Pharmaceutical Research International*

***32(7): 88-92, 2020; Article no.JPRI.56464***
***ISSN: 2456-9119***
*(Past name: British Journal of Pharmaceutical Research, Past ISSN: 2231-2919, NLM ID: 101631759)*

# *Murraya koenigii* Derived Phytochemicals against Dysentery

**Ashima Mishra[1], Diksha Mohanta[1], Sarthak Siddhant Mishra[1], Sunil Jha[1] and Dipankar Bhattacharyay[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/v32i730513
Editor(s):
(1) Syed A. A. Rizvi, Nova Southeastern University, USA.
Reviewers:
(1) Maria Bintang, IPB University (Bogor Agricultural University), Indonesia.
(2) Sandeep Onkar Waghulde, University of Mumbai, India.
(3) K. Ashokkumar, Kerala Agricultural University, India.
Complete Peer review History: http://www.sdiarticle4.com/review-history/56464

***Original Research Article***

***Received 05 April 2020***
***Accepted 23 May 2020***
***Published 24 May 2020***

## ABSTRACT

Phytochemicals are any of various biologically active compounds found in plants. These are produced by plants and have biological activity. It has been reported that *Murraya koenigii* leaf extract is traditionally used to cure dysentery. Dysentery is an intestinal inflammation, primarily of the colon. It can lead to mild or severe stomach cramps and severe diarrhoea with mucus or blood in the faeces. It is the infection in the intestinal tract. One enzyme, which is involved in its biochemical pathway, is known as alcohol dehydrogenase (which have pdb id.1Y9A). The molecular docking was studied by biovia discovery studio. In which the interaction is done between the phytochemical of the plant with the enzyme. The stability of the interaction was evaluated based on –CDocker energy and –CDocker interaction energy.

*Keywords: Phytochemical; biovia; discovery studio; Murraya koenigii; Entamoeba histolytica.*

---

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

## 1. INTRODUCTION

Diseases are any harmful deviation from the normal structural or functional state of an organism, generally associated with certain signs and symptoms and differing in nature from physical injury. Nowadays, diseases are more fatal and dangerous due to many reasons like life is fast-faced, comfortable, readymade, stressful and unhealthy. It can cause blood pressure, diabetes, obesity, etc. [1].

Thousands of years from now, we are using traditional methods to cure a disease by preparing medicines from different medicinal plants. The plants part like bark, leaves, flowers, roots, fruits, and seeds are used to prepare medicines which have chemicals substance that produce a definite physiological action on the human body. These are used by 80% of the world's population as a traditional medicine because of its safety and their cost-effectiveness. The chemical substances present in the plant part are called the phytochemicals, and its extract is known as phytoextract have effective properties like anti-oxidant, anti-inflammatory, anti-microbial and also the anti-cancer properties. About 25% of the modern pharmaceutical drug have botanical origins [2].

Curry leaves (Murraya koenigii) belongs to family Rutaceae. Its leaves extract are used to cure many diseases like dysentery, dierrhea, and eczema etc. Curry leaves are rich in carbohydrates, fibres, calcium, phosphorous, irons and vitamin A, vitamin B, vitamin E, iron, folic acid, carotenoids (Lutein and β-carotene) and Flavonoids (catechin and quercetin) [3,4,5]. It can improve digestion, lowers cholesterol and prevent greying of hair. Curry leaves contain phytochemicals like alpha-pinene, beta-caryophyllene, cinnamic acid, ferulic acid, girinimbine, myrcene, nerolidol, sabinene, and terpinen-4-ol [6]. Curry leaves extract are used to cure dysentery.

Dysentery is blood diarrhoea caused by infection with certain bacteria or parasites. It lasts for about 14 or more days in which subjects are passing grossly blood stools [7,8,9]. Dysentery may be bacillary or may be amoebic. The amoebic dysentery is caused by the amoebas. It is much more chronic and insidious than the bacillary disease and is more challenging to treat.

Entamoeba Histolytica is an anaerobic parasitic amoebozoan. It lives in the human intestine. It transmits commonly through contaminated water or food [10].

This study focuses on the identification of the phytochemical of Murraya koenigii responsible for curing dysentery caused by Entamoeba histolytica.

## 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 between the enzymes with the phytochemicals of the plant [11].

### 2.2 Methodology

#### 2.2.1 List of phytochemicals

Phytochemicals are non- nutritive compounds present in the plants. It is a threat to 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. It has already been established that plant Murraya koenigii belonging to Rutaceae family has potential to help controlling dysentery [12]. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling of dysentery. List of phytochemicals is prepared produced by the Murraya koenigii like alpha pinene, beta caryophyllene, cinnamic acid, ferulic acid, girinimbine, myrcene, nerolidol, sabinene, and terpinen-4-ol [13].

#### 2.2.2 Enzyme found in entamoeba histolytica

It has been reported that dysentery can cause as a result of Entamoeba Histolytica infestation [14]. 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 Entamoeba Histolytica bacteria. It has been found that alcohol dehydrogenase enzyme (protein database code. 1Y9A) is involved in tryptophan metabolism and methionine metabolism (www.brenda-enzymes.org) and very crucial for the survival of the particular microbe.

### 2.2.3 Molecular docking

Molecular docking method has been used to identify the phytochemicals 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 Murraya koenigii plant were downloaded from the website (pubchem.ncbi.nlm.nih.gov). The protein database code of the alcohol dehydrogenase was identified from the website (www.rcsb.org). 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 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 curing the disease.

## 3. RESULTS AND DISCUSSION

Results showed that the active site of the alcohol dehydrogenase enzymes Fig. 1 and Table 1. It appears as a light green colour. CDOCK is a molecular dynamics (MD) simulated-annealing- based algorithm. It is a grid-based molecular docking method and optimized for accuracy. The ligand conformations were obtained by Molecular Dynamic methods.

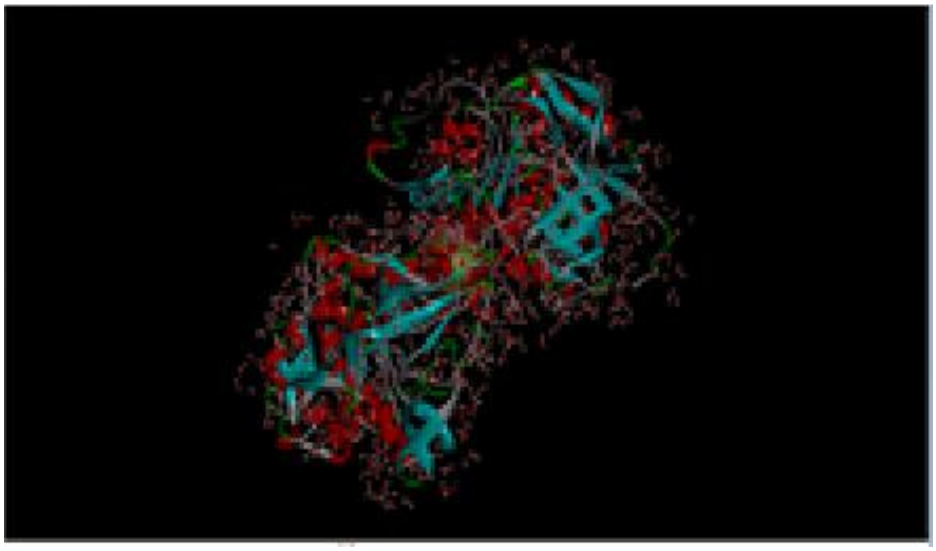

**Fig. 1. The active site of alcohol dehydrogenase enzyme**

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

| Sl. no. | Ligand | - CDOCKER energy | - CDOCKER interaction energy | Difference between - CDOCKER interaction energy and - CDOCKER energy |
|---|---|---|---|---|
| 1 | Cinnamic acid | 13.7791 | 15.3708 | 1.5917 |
| 2 | Ferulic acid | 17.7324 | 20.2813 | 2.5489 |
| 3 | Girinimbine | -2.31892 | 20.757 | 23.07592 |
| 4 | Alpha pinene | -12.0502 | 13.0062 | 25.0564 |
| 5 | Myrcene | -15.2807 | 14.6179 | 29.8986 |
| 6 | Beta caryophyllene | -25.5772 | 16.8965 | 42.4737 |

-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.
b) Small difference between -CDOCKER energy and -CDOCKER interaction energy [15].

## 4. CONCLUSION

As we have known that Murraya koenigii plant has medicinal action against dysentery which is caused by *Entamoeba histolytica*. This study here was carried out to provide the theoretical basis of observation. Here the use of Discovery studio module of Biovia software enables us to perform molecular docking operation was performed to identify the phytochemical (Alpha pinene, beta caryophyllene, cinnamic acid, ferulic acid, girinimbine, myrcene, nerolidol, sabinene, terpinen-4-ol) with which the vital enzyme (alcohol dehydrogenase) of microbe interact significantly.

It was found that cinnamic acid and ferulic acid confirm strong bond with enzyme successfully which inhibit the metabolic pathway (tryptophan metabolism and methionine metabolism) of microbe. Whereas girinimbine, alpha pinene, myrcene, beta caryophyllene were not found much effective in the activating the enzyme of microbe. Thus this study explains the presence of cinnamic acid and ferulicacid provide efficient medicinal value to Murraya koenigii 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 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. Pfeiffer LM, Dupont LH. Journal of Infection - Elsevier. 2012;64:374-386.
2. Ashokkumar K, Kumarakurubaran S, Saradha Devi KM. Reverse phase- high performance liquid chromatography- diode array detector (RP-HPLC-DAD) analysis of flavonoids profile from curry leaf (*Murraya koenigii* L). Journal of Medicinal Plants Research. 2013;7(47):3393-3399.
3. Ashokkumar K, Pandian A, Murugan M, Dhanya MK, Sathyan T, Sivakumar P, Surya R, Warkentin TD. Profiling bioactive flavonoids and carotenoids in select south Indian spices and nuts. Natural Products Research; 2019.
DOI: 10.1080/14786419.2018.1557179
4. Ashokkumar K, Arun Shivkumar Shunmugam. Chapter 18: Curry leaf (*Murraya koenji* L. Spreng): Its phytochemistry and pharmacological properties - A review. Medicinal Plants: Phytochemistry, Pharmacology and Therapeutics. Edited by V. Gupta, and Published by M/S Daya Publishing House, New Delhi. 2016;4:375-390.
5. Jain M, Gilhotra R, Singh RP, Mittal J. Curry leaf (Murrayakoenigii): A spice with medicinal property. MOJ Biol Med. 2017;2(3):00050.
6. Dutt R, Dalal J, Singh G, Gahalot SC, Chandolia RK. Medicinal Uses of *Murraya koenigii* and *Aegle marmelos* for fertility augmentation in animals: A review. Int. J. Curr. Microbiol. App. Sci. 2018;7(9):645-657.
7. Bhandari PR. Curry leaf (*Murraya koenigii*) or cure leaf: Review of its curative properties. Journal of Medical Nutrition and Nutraceuticals. 2012;1(2):92.
8. Handral HK, Pandith A, Shruthi SD. A review on *Murraya koenigii*: Multipotential

medicinal plant. Asian Journal of Pharmaceutical and Clinical Research. 2012;5(4):5-14.
9. Nowak P, Mastalska K, Loster J. Entamoeba histolytica-pathogenic protozoan of the large intestine in humans. J Clin Microbiol Biochem Technol. 2015; 1(1):010-017.
10. Singh S, More PK, Mohan SM. Curry leaves (*Murraya koenigii* Linn. Sprengal)-a mircale plant. Indian Journal of Scientific Research. 2014;4(1):46-52.
11. Saini SC, Reddy GBS. A review on curry leaves (*Murraya koenigii*): Versatile multi-potential medicinal plant. Am J Phytomed Clin Ther. 2015;3:363-8.
12. Gahlawat DK, Jakhar S, Dahiya P. *Murraya koenigii* (L.) Spreng: An ethnobotanical, phytochemical and pharmacological review. Journal of Pharmacognosy and Phytochemistry. 2014;3(3):109-119.
13. Brinda OP, Deepu Mathew, Shylaja MR, Sangeetha Davis P, Anita Cherian K, Valsala PA. Isovaleric acid and avicequinone-C are chikungunya virus resistance principles in *Glycosmis pentaphylla* (Retz.) Correa. 2019;56(2): 111-121.
14. Nishan M, Subramanian P. *Murraya koenigii* (curry leave)-A review on its potential. Int. J. Pharm Tech Res. 2015; 7(4):566-572.
15. Kumar SR, Loveleena D, Godwin S. Medicinal property of *Murraya koenigii*-A review. International Research Journal of Biological Sciences. 2013;2(9): 80-83.



*Peer-review history:*
*The peer review history for this paper can be accessed here:*
*http://www.sdiarticle4.com/review-history/56464*