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Moringa oleifera Derived Phytochemicals against Shikimate Dehydrogenase of *Helicobacter pylori* Causing Peptic Ulcer

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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

Moringa oleifera plant extract is traditionally used to cure Peptic ulcer. It is caused by *Helicobacter pylori*. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that 9-octadecenoic acid can effectively deactivate the shikimate dehydrogenase enzyme thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Moringa oleifera; Helicobacter pylori; peptic ulcer.

1. INTRODUCTION

Nature is a major source of medicines [1]. The medicinal value of the plants is due to the phytochemicals present in it. Phytochemicals can be derived from different parts of plants.Different medicinal plants and their phytoextracts have shown anti-microbial action [2]. These medicinal

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plants play a key role in human health care. Many people rely on the use of traditional medicine [3].

Moringa oleifera belongs to family Moringaceae. *Moringa oleifera* extract is used to cure disease like peptic ulcer. The objective of the study is to identify the phytochemical responsible to cure the disease.

Moringa oleifera contains "3,7,11,15-tetramethyl-2-exadecent-1-ol, 3-ethyl-2,4-dimethylpentane, 4,8,12,16-tetramethylheptadecan-4-olide, 4-hydroxyl-4-methyl-2-pentanone, 4-hydroxyphenyltanamide-alpha-L-rhamnopyranoside, 9-octadecenoic acid" etc. These phytochemicals might act against peptic ulcer. However, there is no such study available.

This objective of the study is to identify the phytochemical of *Moringa oleifera* capable of curing peptic ulcer.

2. MATERIALS AND METHODS

2.1 Software Used

For analysis Discovery studio module of Biovia software (Dassault Systemes of France) was used. 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 of plant 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 traditional medicine and other as poison. Published works showed that *Moringa oleifera* contains 3,7,11,15-trtramethyl-2-hexadecent-1-ol, 3-ethyl-2,4-dimethylpentane, 4,8,12,16-tetramethylheptadecan-4-olide, 4-hydroxyl-4-methyl-2-pentanone, 4-hydroxyphenyltanamide-alpha-L-rhamnopyranoside, 9-octadecenoic acid etc. It has already been established that *Moringa oleifera* plant is one of the species of Moringaceae family has potential to help treating peptic ulcer. This work is focused on identification of the particular phytochemical responsible for inhibiting and controlling of peptic ulcer.

2.2.2 Enzyme found in *Helicobacter pylori*

It has been reported that Peptic ulcer can be caused as a result of *Helicobacter sp.* infestation. Various metabolic cycles have been seen in the bacterial life cycle for its survival. Different enzymes regulated these metabolic cycle. Brenda enzyme database was used to identify and list different enzymes found in *Helicobacter sp.* bacteria. It has been found that shikimate dehydrogenase enzyme (protein database code4FR5) is involved in biosynthesis of aromatic amino acid(phenylalanine, tyrosine and tryptophan) from carbohydrate 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 *Moringa oleifera* plant were downloaded from the website (https://pubchem.ncbi.nlm.nih.gov/). The protein database code of the shikimate dehydrogenase enzyme was identified from the website (www.brenda-enzymes.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 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.

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

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between - C DOCKER interaction energy and - C DOCKER energy	Remarks
1	3,7,11,15-tetramethyl-2-exadecent-1-ol	3.28977	35.9637	32.066	
2	3-ethyl-2,4-dimethylpentane	15.9778	25.4782	9.5004	
3	4,8,12,16-tetramethylheptadecan-4-olide	25.8123	43.2832	17.4709	
4	4-hydroxyl-4-methyl-2-pentanone	21.541	23.1667	1.6257	
5	4-hydroxyphenyltanamide-alpha-L-rhamnopyranoside	22.3973	25.4571	3.0598	
6	9-octadecenoic acid	27.7365	42.4509	14.7725	Maximum inhibition of microbial enzyme

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]. The results indicated 4-hydroxyl-4-methyl-2-pentanone, 4-hydroxyphenyltanamide-alpha-L-rhamnopyranoside that can effectively deactivate the shikimate dehydrogenase enzyme thereby interrupting the biological cycle of *Helicobacter sp.* Higher positive values of 4-hydroxyl-4-methyl-2-pentanone, 4-hydroxyphenyltanamide-alpha-L-rhamnopyranoside indicated that it was the most active ingredient against *Helicobacter sp.* On the other hand 9-octadecenoic acid and 3-ethyl-2,4-dimethylpentane can deactivate the enzyme to a small extent (negative -COCKER ENERGY but positive -CDOCKER INTERACTION ENERGY). Thus the key phytochemical preventing Peptic ulcer caused by *Helicobacter sp.* are 4-hydroxyl-4-methyl-2-pentanone and 4-hydroxyphenyltanamide-alpha-L-rhamnopyranoside.

4. CONCLUSIONS

It was previously known that *Moringa oleifera* plant has medicinal action against peptic ulcer. The causative agent of Peptic ulcer is *Helicobacter 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 (3,7,11,15-trtramethyl-2-hexadecent-1-ol,3-ethyl-2,4-dimethylpentane,4,8,12,16-tetramethyl heptadecan-4-olide, 4-hydroxyl-4-methyl-2-pentanone, 4-hydroxyphenyltanamide-alpha-L-rhamnopyranoside, 9-octadecenoic acid)which can have a significant interaction with the vital enzyme (shikimate dehydrogenase) of the microbe.It was found thatcan4-hydroxyl-4-methyl -2-pentanone,4-hydroxyphenyltanamide-alpha-L-rhamnopyranoside form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe.3,7,11,15-trtramethyl-2-hexadecent-1-ol and 4,8,12,16-tetramethylheptadecan-4-olide were found to be not much effective in deactivating the enzymes of the microbe. This study could explain that the presence of4-hydroxyl-4-methyl-2-pentanone,4-hydroxyphenyltanamide-alpha-L-rhamnopyranoside provided the medicinal values to *Moringa oleifera* against peptic ulcer caused by *Helicobacter 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 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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