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Alpinia galanga Derived Phytochemicals against Shikimate Dehydrogenase 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

Phytochemicals can be derived from different parts of plants. Different medicinal plants and their phytoextracts have shown anti-microbial action. These medicinal plants play a key role in human health care. Phytochemicals from *Alpinia galanga* plant extract are traditionally used to cure Peptic Ulcer. The objective of the study is to identify the phytochemical of *Alpinia galanga* capable of curing Peptic Ulcer. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that *Alpinia galanga* derived Phytochemicals cannot act effectively against Peptic Ulcer caused by *Helicobacter pylori*.

Keywords: Phytochemical; Alpinia galangal; peptic ulcer; Helicobacter pylori.

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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 plants play a key role in human health care. Many people rely on the use of traditional medicine [3]. *Alpinia galanga* extract is used to cure diseases like Peptic Ulcer. The objective of the study is to identify the phytochemical responsible to cure the disease. *Alpinia galanga* contains "beta-pinene, alpha-pinene, p-cymene, limonene, piperazine" etc. These phytochemicals might act against Peptic Ulcer. However, there is no such study available. The objective of the study is to identify the phytochemical of *Alpinia galanga* capable of curing Peptic Ulcer.

2. MATERIALS AND METHODS

2.1 Software Used

The 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, and fungi. 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 *Alpinia galanga* contains β-farnesene, α-fenchyl acetate, β-bisabolene, β-bergamotene, β-pinene. It has already been conventional that *Alpinia galanga* plant belonging to Zingiberaceae family has the potential to help controlling Peptic Ulcer. This work is focused on the 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 cause as a result of *Helicobacter pylori* infestation. In the bacterial life cycle, various metabolic cycles have been seen for its existence. These metabolic cycles are controlled by different enzymes. A list of different enzymes found in *Helicobacter pylori* bacteria is detected by using Brenda enzyme database. It has been found that Shikimate Dehydrogenase enzyme (protein database code 4FR5) is involved in chorismate metabolism (BRENDA) and very essential for the existence of the specific microbe.

2.2.3 Molecular docking

The 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 *Alpinia galanga* plant were downloaded from the website (pubchem.ncbi.nlm.nih.gov). The protein database code of the Shikimate Dehydrogenase enzyme was identified 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 the "receptor cavity" protocol. Molecular docking was done under the "receptor-ligand interaction" and "Dock ligand" menu by using the CDOCKER protocol of Biovia software. The enzyme act as the receptor molecule and the phytochemical act as the ligand. The quality of molecular docking was 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 value of

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

Sl. no	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and -CDOCKER energy
1	β-pinene	-5.01216	19.5254	24.53756
2	α-fenchyl acetate	-22.075	28.5576	50.6326
3	β-farnesene	-20.0517	35.2585	55.3102
4	β-bergamotene	-21.9437	33.8794	55.8231
5	β-bisabolene	-36.2115	29.2627	65.4742

-CDOCKER energy, -CDOCKER interaction energy and minimum value of the difference between - C DOCKER interaction energy and - C DOCKER. Thus the results in the table indicate that β-farnesene, α-fenchyl acetate, β-bisabolene, β-bergamotene and β-pinene can deactivate the enzyme to a small extent due to negative -CDOCKER energy but positive -CDOCKER interaction energy. Thus, these phytochemicals cannot act effectively against Peptic Ulcer caused by *Helicobacter pylori*.

4. CONCLUSION

It was previously known that *Alpinia galanga* plant has medicinal action against Peptic Ulcer. Peptic Ulcer is caused by Helicobacter pylori. 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 (β-farnesene, α-fenchyl acetate, β-bisabolene, β-bergamotene, β-pinene), which can have significant interaction with the dynamic enzyme (shikimate dehydrogenase) of the microbe. It was found that these phytochemicals cannot form a strong bond with the enzyme successfully to inhibit the metabolic cycle of the microbe. β-farnesene, α-fenchyl acetate, β-bisabolene, β-bergamotene, β-pinene were found to be not much effective in deactivating the enzyme of the microbe. Thus, this study could explain that the presence of β-farnesene, α-fenchyl acetate, β-bisabolene, β-bergamotene, β-pinene could not provide any medicinal values to *Alpinia galanga* against Peptic Ulcer caused by Helicobacter pylori.

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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