



Kewda (*Pandanus odorifer*) Flower Derived Phytochemicals against Salutaridine Reductase of Hepatitis Virus Causing Hepatitis A

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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

Pandanus odorifer plant extract is traditionally used to cure Hepatitis A. It is caused by Hepatitis virus. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that 1, 2, 3-benzene triol can effectively deactivate the salutaridine reductase enzyme thereby interrupting the life cycle of the organism.

Keywords: *Phytochemical; Pandanus odorifer; hepatitis virus; hepatitis A.*

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].

Pandanus odorifer belongs to family pandanaceae. Kewda flower extract is used to cure disease like Hepatitis A. The objective of the study is to identify the phytochemical responsible to cure the disease.

Pandanus odorifer contains "1,2,3-benzene triol, 1,2-benzene dicarboxylic acid, heptanes, naphthalene, octadecanedioic acid, quinic acid" etc. These phytochemicals might act against Hepatitis A. However, there is no such study available.

This objective of the study is to identify the phytochemical of *Pandanus odorifer* capable of curing Hepatitis A.

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 [2]. 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 Kewda flower contain 1,2,3-benzene triol, 1,2-benzene dicarboxylic acid, heptane, naphthalene, octadecanedioic acid and quinic acid. This work is focused on identification of the particular phytochemical responsible for inhibiting and controlling of hepatitis.

2.2.2 Enzyme found in Hepatitis A

It has been reported that hepatitis can cause as a result of Hepatitis A infestation. Various metabolic cycles have been seen in the Viral 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 Hepatitis A virus. It has found that salutaridine reductase (NADPH) enzyme having protein database code 3O26 (www.rcsb.org) is involved in Arginine and proline metabolism (KEGG).

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 Viral 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 Kewda flower were downloaded from the website.

The protein database code of the enzyme salutaridine reductase (NADPH) 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 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 [4,5].

Table 1 shows that salutaridine reductase (NADPH)-heptane interaction has the highest positive value of -CDOCKER energy (15.9219)

Table 1. Results of C Docking of phytochemicals with salutaridine reductase (receptor)

SI no	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between - C DOCKER interaction energy and -CDOCKER energy	Remarks
1	Heptane	15.9219	15.0922	0.8297	
2	1,2,3-benzene triol	18.176	17.0502	1.1258	Maximum inhibition of microbial enzyme
3	1,2-benzene dicarboxylic acid	14.6107	16.5203	1.9096	
4	Napthalene	0.0582512	12.3889	12.3306488	
5	Quinic acid	3.48199	25.4051	21.92311	
6	Octadecanedioic acid	Failed	Failed	Failed	

and minimum value of the difference (0.8297) between -CDOCKER interaction energy and - C DOCKER energy followed by 1,2,3-benzene triol. Thus the results indicated that heptanes, 1,2,3-benzene triol, 1,2-benzene dicarboxylic, naphthalene and quinic acid can effectively deactivate the salutaridine reductase enzyme thereby interrupting the biological cycle of hepatitis. But the Octadecanedioic acid failed to interact with this enzyme. Higher positive values for heptane indicated that it was the most active ingredient against hepatitis A. Thus, the key phytochemicals preventing hepatitis caused by hepatitis A are heptanes and 1,2,3-benzene triol.

4. CONCLUSIONS

It was already known that *Kewda flower* has curative action against hepatitis. Hepatitis are caused by hepatitis A. 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 (heptanes, 1,2-benzene dicarboxylic acid, octadecanedioic acid, naphthalene, quinic acid and 1,2,3-benzene triol), which can have a significant interaction with the salutaridine reductase (NADPH) enzyme of the microbe. It was found that heptanes, 1,2-benzene triol can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Naphthalene, 1,2-benzene dicarboxylic acid and Quinic acid were found to be less effective than heptanes and 1,2,3-benzene triol in deactivating the enzyme of the microbe and the octadecanedioic acid failed to interact with this

enzyme. Thus, this study could explain that the presence of heptanes and 1,2,3-benzene triol provided the medicinal values to *Kewda flower (Pandanus odorifer)* against hepatitis caused by hepatitis A.

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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