



Potency of Phytochemicals from Guava (*Psidium guajava*) Seeds against *Escherichia coli* to Cure Diarrhoea: An *in silico* Analysis

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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

Machine learning to deep learning is the enduring upgrading in the pharmaceutical research field. Phytochemicals from *Psidium guajava* plant extract are traditionally used to cure Diarrhoea. The causative agent of the disease is *Escherichia coli*. To identify the secondary metabolites (ligand) which is the main responsive compound that have the capacity to inhibit the growth of microorganism was carried by molecular docking method "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that Heptadecanoic acid can effectively deactivate the *shikimate dehydrogenase enzyme* thereby interrupting the life cycle of the organism.

Keywords: *Phytoconstituents; Psidium guajava; Escherichia coli; diarrhea.*

1. INTRODUCTION

Nature always support as a golden blemish to epitomize magnificent occurrence of synergism. It has provided an outright store house of

remedies to cure affliction of mankind [1]. The phytochemicals are key supplement for the different alignments, that are found in every parts of plant [2]. People are rely on this herbal medicine for their different health issue and it

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was proved to be more beneficial than the synthetic medicine without any site effect [3].

Psidium guajava belongs to family Myrtaceae. Guava plant extract is used to cure disease like Diarrhoea. The objective of the study is to identify the phytochemical responsible to cure the disease.

Arachidic acid, Heptadecanoic acid, Lauric acid, Linoleic acid, Oleic acid, Palmitic acid, pectin, Phytic acid, Stearic acid etc. are found to be present in *Psidium guajava* plant. These phytochemicals might act against Diarrhoea. However, there is no such study available. This objective of the study is to identify the phytochemical of *Psidium guajava* capable of curing Diarrhoea.

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 biologically active, naturally occurring chemical compounds found in plants and also produced by plants as secondary metabolites 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 poisons and others as traditional medicine. Published works showed that Guava seeds contains Arachidic acid, Heptadecanoic acid, Lauric acid, Linoleic acid, Oleic acid, Palmitic acid, pectin, Phytic acid, Stearic acid. It has already been established that Guava seeds plant belonging to family Myrtaceae has potential to help controlling diarrhoea. This work is focused on identification of the particular phytochemical responsible for inhibiting and controlling of diarrhoea.

2.2.2 Enzyme found In *Escherichia coli*

It has been reported that diarrhoea can be caused as a result of *Escherichia sp.* infestation.

Various metabolic cycles like chorismite metabolism 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 *Escherichia sp.* bacteria. It has been found that shikimate dehydrogenase enzyme (protein database code 1NYT) is involved in chorismite metabolism (Brenda) 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 Guava seeds plant were downloaded from the website (www.molinstincts.com). The protein database code of the shikimate dehydrogenase enzyme 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 Bioviasoftware 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 shikimate dehydrogenase-heptadecanoic acid

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	Arachidic acid	24.9511	31.5265	6.5754	
2	Heptadecanoic acid	36.6014	39.0272	2.4258	Maximum inhibition of microbial enzyme
3	Lauric acid	29.7662	27.0767	2.6895	
4	Linoleic acid	-1.01269	31.8904	32.90309	

interaction has the highest positive value of -CDOCKER energy (36.6014) and minimum value of the difference (2.4258) between - C DOCKER interaction energy and - C DOCKER energy followed by heptadecanoic acid. Thus the results indicated that heptadecanoic acid and lauric acid can effectively deactivate the shikimate dehydrogenase enzyme thereby interrupting the biological cycle of *Escherichia* species. Higher positive values for heptadecanoic acid indicated that it was the most active ingredient against *Escherichia sp.* On the other hand, arachidic acid, linoleic acid and oleic acid can deactivate the enzyme to a small extent (negative -CDOCKER energy but positive -CDOCKER interaction energy). Thus, the key phytochemicals preventing diarrhoea caused by *Escherichia* species are heptadecanoic acid and lauric acid.

4. CONCLUSIONS

It was previously known that *Guava* plant has medicinal action against diarrhoea. Diarrhoea is caused by *Escherichia 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 (Arachidic acid, Heptadecanoic acid, Lauric acid, Linoleic acid, Oleic acid, Palmitic acid, pectin, Phytic acid, Stearic acid.), which can have a significant interaction with the vital enzyme (shikimate dehydrogenase) of the microbe. It was found that heptadecanoic acid and lauric acid can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Thus, this study could explain that the presence of heptadecanoic acid and lauric acid provided the medicinal values to *Guava* seeds against diarrhoea caused by *Escherichia 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.

REFERENCES

1. Henrich J, Heine S, Norenzayan A. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI: 10.1017/S0140525X0999152X
2. Hussain I, Ullah R, Ullah R, Khurram M, Ullah N, Basee A, Khan F, Khattak M, Zahoor M, Khan J, Khan N. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
3. Arulselvan P, Karthivashan G, Fakurazi S. Journal of Chemical and Pharmaceutical Research. 2013;5(7):233-239.

4. Das D, Das S, Pandey M, Bhattacharyay D. *In silico* analysis of phytochemicals from *Mucuna pruriens* (L.) DC against *Mycobacterium tuberculosis* causing tuberculosis. European Journal of Medicinal Plants; 2020.
5. Brinda OP, Mathew D, Shylaja MR, Davis PS, Cherian KA, Valsala PA. Isovaleric acid and avicinequinone-C are chikungunya virus resistance principles in *Glycosmis pentaphylla* (Retz.) Correa. Journal of Vector Borne Diseases. 2019;56(2):111.

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