



## **Guava Seeds Derived Phytochemicals against Dysentery**

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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 are the secondary metabolites that are known as nonnutritive but extremely beneficial for the defensive system for the organism. These phytochemicals can be obtained from all the plants and they play a major role in curing different diseases. The extract of the guava seed contains various phytochemicals that can cure the disease like dysentery, caused by the protozoa parasite, namely *Entamoeba histolytica*. "Biovia Discovery Studio" was used for the molecular docking process. "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that Heptadecanoic acid can effectively deactivate the alcohol dehydrogenase enzyme further inhibiting the biological process of the causative organism.

**Keywords:** Heptadecanoic acid; Guava; *Entamoeba histolytica*.

### **1. INTRODUCTION**

Nature has been an abundant source of medicinal agents for thousands of years and an

impressive number of modern drugs have been derived from natural plant resources or their derivatives [1]. The medicinal value of the plants lies in some chemical substances that produce

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definite physiological actions on the human body. These substances are called phytochemicals [2]. These phytochemicals can be extracted from any part of the plant and they have shown to have key role in human health science [3].

*Psidium guajava* is common tropical fruit belongs to the family Myrtaceae. The objective of the study is to identify the phytochemical responsible for curing the disease. Guava seeds are known to contain “phytochemicals like Arachidic acid, Heptadecanoic acid, Lauric acid, Linoleic acid, Oleic acid, Palmitic acid, pectin, Phytic acid, Stearic acid” [4]. These phytochemicals might act against dysentery. This study focuses on the identification of the phytochemical of Guava seeds responsible for curing dysentery caused by a protozoan *Entamoeba histolytica*.

## 2. MATERIALS AND METHODS

### 2.1 Software Used

Discovery studio module of Biovia software (Dassault Systemes of France) was used for analysis. It uses 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, 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. Guava seeds contain lipids. It has already been established that Guava seeds plant belonging to family Myrtaceae has the potential to help controlling dysentery.

#### 2.2.2 Enzyme found in *Entamoeba histolytica*

Various metabolic cycles have been seen in the protozoan life cycle for its survival. These metabolic cycles are regulated by different enzymes that have been listed to be found in *Entamoeba histolytica*. It has been stated that

alcohol dehydrogenase is involved in Methionine, Tryptophan and Tyrosine metabolism and essential for the existence of the specific microbe.

### 2.2.3 Molecular docking

Molecular docking method has been used to identify the phytochemical from the plant extract, which acts as a ligand and forms 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](http://www.molinstincts.com)). The protein database code of the alcohol dehydrogenase enzyme was recognized from the website([www.rcsb.org](http://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 quality of molecular docking was indicated “-CDOCKER\_ENERGY” and “-CDOCKER\_INTERACTION\_ENERGY”. 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 that is accountable 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 [5,6]. On the other hand, lauric acid, linoleic acid and oleic acid can deactivate the enzyme to a small extent. (negative -CDOCKER energy but positive -CDOCKER interaction energy).

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

Sl. no.	Ligand	-C DOCKER Energy	-C DOCKER Interaction Energy	Difference Between -C DOCKER interaction energy and -C DOCKER energy	Remarks
1	Arachidic Acid	37.7428	32.888	4.854	
2	Heptadecanoic Acid	34.643	34.0749	0.568	Maximum inhibition in microbial enzyme
3	Lauric Acid	27.2742	23.3699	3.9043	
4	Linoleic Acid	5.01096	27.108	22.097	
5	Oleic Acid	19.7223	32.7585	13.0362	
6	Palmitic Acid	30.5667	28.1648	2.4019	

#### 4. CONCLUSIONS

It was previously known that *Guava* plant has medicinal action against dysentery. Dysentery is caused by a protozoan *Entamoeba histolytica*. 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 significant interaction with the vital enzyme of the microbe. It was found that heptadecanoic acid and palmitic acid can form a 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 palmitic acid provided the medicinal values to *Guava* seeds against dysentery.

#### 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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