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Beet Root Derived Phytochemicals against *Escherichia coli* Causing Diarrhea

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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 from *Beet Root (Beta vulgaris)* plant extract are traditionally used to cure Diarrhea. It is caused by *Escherichia coli.* Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that caffeic acid can effectively deactivate the *Shikimate dehydrogenase* enzyme thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Beta vulgaris; Shikimate dehydrogenase.

1. INTRODUCTION

Plants produce several phytochemicals that have medicinal properties [1]. These compounds have several health benefits and can be effectively used to prepare medicines against various diseases. They show antimicrobial activities and thus help us fight against different infections [2]. The medicinal plants are a great source of bioactive compounds that are vital to human health. Traditional medicines are reliable and safe [3].

Beet root belongs to family *Amaranthaceae*. Beet root extract is used to cure disease like Diarrhea. The objective of the study is to identify

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the phytochemical responsible to cure the disease.

Beet root contains “caffeic acid, chlorogenic acid, ellagic acid, ferulic acid, kaempferol acid, myricetin, quercetin, rutin, syngric acid vanallic acid” etc. These phytochemicals might act against Diarrhea. However, there is no such study available.

This objective of the study is to identify the phytochemical of *Beet root* capable of curing Diarrhea.

2. MATERIALS AND METHODS

2.1 Software Used

Discovery studio module of Biovia software (Dassault Systems 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, 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 *beet root* contains caffeic acid, chlorogenic acid, ellagic acid, ferulic acid,kaempferol acid, myricetin, quercetin, rutin, syngric acid, vanallic acid, etc. It has already been established that *beet root* plant belonging to Amaranthaceae family has the potential to help controlling diarrhea [4]. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling of Diarrhea.

2.2.2 Enzyme found in *Escherichia coli*

It has been reported that Diarrhea can be caused as a result of *E. coli* infestation. Various metabolic cycles 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 *E. coli* bacteria. It has been found that shikimate dehydrogenase enzyme (protein database code1NYT) is involved in the biosynthesis of aromatic amino acids (phenylalanine, tyrosine, and tryptophan) from the metabolism of carbohydrates.

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 Beat root plant were downloaded from the website (PUBCHEM). The protein database code of the isocitrate dehydrogenase enzyme was identified from the website (BRENDA). 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 [5,6]. The CDOCKER_ENERGY” and “-CDOCKER_INTERACTION_ENERGY” were used as an 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 [7,8]. Table 1 shows that shikimate dehydrogenase-caffeic acid interaction has the highest positive value of -CDOCKER energy (27.8151) and minimum value of the difference (1.4196) between -CDOCKER interaction energy and - C DOCKER energy of ferulic acid. Thus the results indicated that caffeic acid and ferulic acid can effectively deactivate the isocitrate dehydrogenase enzyme thereby

Table 1. Results of C Docking

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between C DOCKER interaction energy- and C DOCKER energy	Remarks
1	Caffeic acid	27.8951	29.3097	1.4196	Maximum inhibition of microbial infection
2	Ferulic acid	23.9788	31.7808	7.801	
3	Kaempferol	19.2729	27.5693	8.2967	
4	Vannilic acid	20.6596	30.0964	9.4368	
5	Myricetin	23.1677	33.2406	10.0729	
6	Quercetin	23.9742	34.5755	10.6013	
7	syringic acid	20.638	31.1896	10.5516	
8	Chlorogenic acid	8.8433	30.7256	21.8823	
9	Ellahic acid	-1.94538	25.7596	27.70498	
10	rutin	failed	failed	NA	

interrupting the biological cycle of *Escherichia sp*. Higher positive values for caffeic acid indicated that it was the most active ingredient against *Escherichia sp*. On the other hand, ferulic acid, vanillic acid, syringic acid, quercetin, myricetin, kaempferol, ellagic acid, chlorogenic acid also can deactivate the enzyme but lesser extent as compared to the caffeic acid. Therefore the key phytochemicals preventing Diarrhea caused by *Escherichia* species are caffeic acid and ferulic acid.

4. CONCLUSIONS

It was previously known that *Beta vulgaris* plant has medicinal action against Diarrhea. Diarrhea is caused by *E. coli 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 which can have a significant interaction with the vital enzyme (shikimate dehydrogenase) of the microbe. It was found that caffeic acid and ferulic acid can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe while quercetin, ellagic acid, myricetin, kaempferol, syringic acid, chlorogenic acid were found to have good positive value more than expected and rutin failed to make any interaction with the protein. Thus this study could explain that the presence of caffeic acid and ferulic and also the remaining phytochemicals provide the best medical values to beet root against Diarrhea caused by *Escherichia* species.

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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