



Vaccinium corymbosum L. Derived Phytochemicals against 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 *Vaccinium corymbosum* L. 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 thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; *Vaccinium corymbosum*; Shikimate dehydrogenase.

1. INTRODUCTION

Nature is a noteworthy wellspring of meds [1]. The restorative estimation of the plants is a direct result of the phytochemicals present in it. Phytochemicals can be gotten from different bits of plants. Assorted restorative plants and their Phytoextracts have shown the foe of microbial

action [2]. These therapeutic plants accept a key activity in human social protection. Various people rely upon the usage of standard medicine [3].

Vaccinium corymbosum L. belongs to family Ericaceae. *V. corymbosum* extract is used to cure diseases like diarrhoea. The objective of the

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study is to identify the phytochemical responsible to cure the disease.

V. corymbosum contains “caffeic acid, Aloe-emodin” etc. These phytochemicals might act against diarrhoea. However, there is no such study available.

This objective of the study is to identify the phytochemical of *V. corymbosum* 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 *Vaccinium corymbosum* contains etc. It has already been established that *Vaccinium corymbosum* plant belonging to the Ericaceae family has the potential to help controlling diarrhea. 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 cause as a result of *Escherichia 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 *Escherichia coli* bacteria. It has been found that shikimate dehydrogenase (protein database code 1NYT) is involved in chorismate metabolism (Brenda enzyme database) 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 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 *Vaccinium corymbosum* plant were downloaded from the website (www.molinstinct.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 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 shikimate dehydrogenase-caffeic acid interaction has the highest positive value of -CDOCKER energy (30.2204) and minimum value of the difference (1.02) between -CDOCKER interaction energy and -CDOCKER energy followed by aloe-emodin. Thus the results indicated that caffeic acid and aloe-emodin can more effectively deactivate the shikimate dehydrogenase enzyme thereby interrupting the biological cycle of *Escherichia coli*. Higher positive values for caffeic acid indicated that it

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

Ligand	-CDOCKER Energy	-CDOCKER Interaction Energy	Difference between -CDOCKER interaction energy and - CDOCKER energy	Remarks
Caffeic acid	30.2204	31.2404	1.02	Maximum inhibition
Aloe-emodin	23.5801	28.2584	4.6783	
Anthraquinone	8.1267	16.098	7.9713	
Apigenin	16.7773	24.9363	8.159	
Resveratrol	19.3412	29.4724	10.1312	
Cinnamyl-alcohol	5.74496	19.4129	13.66794	Minimum inhibition

was the most active ingredient against *Escherichia coli*. On the other hand, anthraquinone, apigenin, resveratrol and cinnamyl-alcohol can also deactivate the enzyme and are also much effective. (positive -CDOCKER energy and -CDOCKER interaction energy). Thus, all the phytochemicals are effective to cure the disease Diarrhoea but the key phytochemicals preventing diarrhoea caused by *Escherichia coli* are caffeic acid and aloe-emodin.

4. CONCLUSIONS

It was previously known that *Vaccinium corymbosum* plant has medicinal action against diarrhea. Diarrhea is caused by *Escherichia coli*. 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 (caffeic acid, aloe-emodin, anthraquinone, apigenin, resveratrol, cinnamyl-alcohol), which can have significant interaction with the vital enzyme (shikimate dehydrogenase) of the microbe. It was found that caffeic-acid and aloe-emodin can form strong bonds with the enzyme successfully inhibiting the metabolic cycle of the microbe. Anthraquinone, apigenin, resveratrol, and cinnamyl-alcohol were also found to be effective in deactivating the enzyme of the microbe. Thus, this study could explain that the presence of all the phytochemicals provided the medicinal values to *Vaccinium corymbosum* against caused diarrhea by *Escherichia coli* but caffeic acid and aloe-emodin are more effective against diarrhea.

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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