



Cardamom Derived Phytochemicals against Bronchitis Caused by *Streptococcus pneumoniae*

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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 *Cardamom* plant extract can cure Bronchitis. One of the causes of Bronchitis is an infection of *Streptococcus pneumoniae*. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that 4-terpineol can effectively deactivate thymidine phosphorylase enzyme thereby interrupting the life cycle of the organism.

Keywords: *Phytochemical; Cardamom; Streptococcus pneumoniae.*

1. INTRODUCTION

In ancient years, life flourished naturally at a slow pace but in a healthy manner. Life was difficult due to several challenges of survival. Today, in

modern times, life has become more comfortable yet vulnerable, unhealthy, and stressful. 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

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different parts of plants. Different medicinal plants and their phytoextracts have shown anti-microbial action [2]. These medicinal plants play a key role in human health care. Many people rely on the use of traditional medicine [3].

Cardamom belongs to family Zingiberaceae. Cardamom extract is used to cure diseases like Bronchitis. The objective of the study is to identify the phytochemical responsible to cure the disease.

Cardamom contains phytochemicals "4-terpineol, acetic acid, cinnamaldehyde, eucalyptol, 3,7-dimethyl, Santolina alcohol" etc. These phytochemicals might act against bronchitis. However, there is no such study available.

This objective of the study is to identify the phytochemical of *Cardamom* capable of curing pneumonia-like bronchitis.

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. 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 *Cardamom* contains 4terpineol, acetic acid, cinnamaldehyde, eucalyptol, 3,7-dimethyl, Santolina alcohol, etc. It has already been established that the *Cardamom* plant belonging to the Zingiberaceae family has the potential to help controlling bronchitis. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling of bronchitis.

2.2.2 Enzyme found in *Streptococcus*

It has been reported that bronchitis can cause as a result of *Streptococcus sp.* 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 *Streptococcus sp.* bacteria. It has been found that thymidine phosphorylase enzyme (protein database code 4LHM) is involved in glycerolipid metabolism (KEGG) and very crucial for the survival of the particular microbe.

2.2.3 Molecular docking

The 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 *Cardamom* plant were downloaded from the website (www.molinstinct.com). The protein database code of the thymidine phosphorylase enzyme was identified from the website (www.rcsb.org). The active site of the enzyme was identified via the "receptor cavity" protocol found under the "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 [4]. 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 [5]. Table 1 shows that thymidine phosphorylase enzyme- acetic acid

Table 1. Results of C docking

Sl no	Ligand	- CDOCKER energy	-CDOCKER interaction energy	Difference between - CDOCKER interaction energy and - CDOCKER energy	Remarks
1	4-terpineol	-19.2812	10.2813	8.9999	Maximum inhibition of microbial enzyme
2	Acetic acid	15.8956	13.6755	2.2201	
3	Cinnamaldehyde	10.6154	14.3402	3.7248	
4	Eucalyptol	Failed	Failed	NA	
5	3,7-dimethyl	Failed	Failed	NA	
6	Santolina alcohol	Failed	Failed	NA	

interaction has the highest positive value of - CDOCKER energy (15.8956) and minimum value of the difference (2.2201) between - C DOCKER interaction energy and - C DOCKER energy followed by cinnamaldehyde. Thus the results indicated that cinnamaldehyde and acetic acid can effectively deactivate the thymidine phosphorylase enzyme thereby interrupting the biological cycle of *Streptococcus sp.* Higher positive values for acetic acid indicated that it was the most active ingredient against *streptococcus sp.* On the other hand 4-terpineol can deactivate the enzyme to a small extent (negative -CDOCKER energy but positive - CDOCKER interaction energy). Eucalyptol, 3,7-dimethyl and Santolina alcohol cannot interact with thymidine phosphorylase enzyme. Thus, the key phytochemicals preventing bronchitis caused by *Streptococcus sp.* are cinnamaldehyde and acetic acid.

4. CONCLUSIONS

It was previously known that *Cardmompl* has medicinal action against bronchitis. Bronchitis is caused by *Streptococcus 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 (4-terpineol, acetic acid, cinnamaldehyde, eucalyptol, 3,7-dimethyl, Santolina alcohol), which can have significant interaction with the vital enzyme [thymidine phosphorylase]of the microbe. It was found that cinnamaldehyde and acetic acid can form a strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. 4-terpineol were found to be

not much effective in deactivating the enzyme of the microbe. Eucalyptol, 3,7-dimethyl and Santolina alcohol cannot deactivate the enzyme. Thus, this study could explain that the presence of cinnamaldehyde and acetic acid provided the medicinal values to *Cardmom* against bronchitis caused by *Streptococcus sp.*

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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