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Cardamom Derived Phytochemicals against Mycoplasma pneumonia Causing Bronchitis

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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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Original Research Article

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ABSTRACT

Bronchitis is inflammation of the bronchi in the lungs. Bronchitis is mainly caused by a viral infection and a small number of cases are caused by a bacterial infection like *Mycoplasma pneumonia*. Cardamom extract is a traditional medicine that is used to treat Bronchitis. The objective of the study is to identify the phytochemical of *Cardamom* capable of curing pneumonia-like bronchitis Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that acetic acid can effectively deactivate glycerophosphodiester phospho diesterase enzyme thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Cardamom; Mycoplasma pneumoniae.

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1. INTRODUCTION

Bronchitis is inflammation of the bronchi in the lungs. Bronchitis is mainly caused by a viral infection and a small number of cases are caused by a bacterial infection like *Mycoplasma pneumonia*. The symptoms of Bronchitis is aggravated by tobacco smoke, dust, and other air pollution.

Nature is a major source of medicines [1] for many diseases like Bronchitis. The medicinal value of the plants is due to the phytochemicals present in it. Phytochemicals can be derived from different parts of plants. Different medicinal plants and their phytoextracts have shown antimicrobial action [2]. These medicinal plants play a key role in human health care. Many people rely on the use of traditional medicine [3]. Cardamom extract is such a traditional medicine that is used to treat Bronchitis.

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

The 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 *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 *Mycoplasma*

It has been reported that bronchitis can be caused as a result of *Mycoplasma sp.* infestation. Various metabolic cycles are important 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 *Mycoplasma sp.*bacteria. It has been found that glycerophosphodiester phosphodiesterase enzyme (protein database code1YDY) 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, 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 cardamom plant were downloaded from the website (www.molinstinct.com). The protein database code of the glycerophosphodiester phosphodiesterase 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" [4]. 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 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

SI. no.	Ligand	- CDOCKER energy	-CDOCKER interaction energy	Difference between - CDOCKER interaction energy and - CDOCKER energy	Remarks
1	4-terpineol	-88.7821	-27.6802	61.1019	
2	Acetic acid	17.7754	16.1053	1.6701	Maximum inhibition of microbial enzyme
3	Cinnamaldehyde	6.24877	13.4099	7.16113	
4	Eucalyptol	Failed	Failed	NA	
5	3,7-dimethyl	Failed	Failed	NA	
6	Santolina alcohol	Failed	Failed	NA	

Table 1. Results of C docking of phytochemicals with glycerophosphodiester phosphodiesterase (receptor)

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 shows 1 that glycerophosphodiester phosphodiesterase enzyme- acetic acid interaction has the highest positive value of -CDOCKER energy (17.7754) and minimum value of the difference (1.6701) between - C DOCKER interaction energy and - C DOCKER energy followed by cinnamaldehyde. Thus the results indicated that acetic acid and cinnamaldehyde can effectively deactivate the glycerophosphodiester phosphodiesterase enzyme thereby interrupting the biological cycle of Mycoplasma sp. Higher positive values for acetic acid indicated that it was the most active ingredient against mycoplasma sp. On the other hand, 4-terpineol and cinnamaldehyde 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 with glycerophosphodiester phosphodiesterase enzyme.

Thus, the key phytochemicals preventing bronchitis caused by *mycoplasma sp.* are acetic acid and cinnamaldehyde. Table 1 shows glycerophosphodiester phosphodiesterase – acetic acid interaction was found to have the highest interaction.

4. CONCLUSIONS

It was previously known that *Cardmom*plant has medicinal action against bronchitis. Bronchitis is

caused by Mycoplasma 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 (4terpineol. acid, cinnamaldehvde. acetic 3,7-dimethyl, Santolina alcohol), eucalyptol, which can have significant interaction with the vital enzyme [glycerophosphodiester phosphodiesterase] of the microbe. It was found that acetic acid and cinnamaldehyde can form a strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe 4terpineol 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 Cardamom against bronchitis caused by Mycoplasma 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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