



Capsicum anum L. Derived Phytochemicals against *Haemophilus influenzae* 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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ABSTRACT

Phytochemicals from *Capsicum anum* L. plant extract are traditionally used to cure bronchitis. Bronchitis is caused by *Haemophilus influenzae*. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that myrcetin and quercetin can effectively deactivate the Palmitoyl-CoA hydrolase enzyme thereby interrupting the life cycle of *Haemophilus influenzae*.

Keywords: *Phytochemical; Capsicum anum L.; Haemophilus influenzae.*

1. INTRODUCTION

Plants are used as medicine throughout the world and are the major resources of medicine [1]. Phytochemicals present in these plants are

used for treating various diseases. These plant-based chemical substances are derived from different parts of plants. The plant extracts show antimicrobial action against different microorganisms [2]. These medicinal plants play

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a key role in human health care. Many people rely on the use of traditional medicine [3]. *Capsicum anum* L. belongs to family Solanaceae. *Capsicum anum* L. extract is used to cure diseases like bronchitis. The objective of the study is to identify the phytochemical responsible to cure the disease.

Capsicum anum contains “phytochemicals like 1, 8-cineole, apigenin, camphene, capsaicin, linalool, luteolin, myrcene, myricetin, quercetin” 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 *Capsicum anum* capable of curing bronchitis.

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 *Capsicum* contains 1,8-cineole, Apigenin, camphene, capsaicin, linalool, luteolin, myrcene, rutin, β -carotene. It has already been established that *Capsicum* plant belonging to Solanaceae 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 *Haemophilus influenzae*

It has been reported that bronchitis can be caused as a result of *Haemophilus influenzae* 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 *Haemophilus influenzae* bacteria. It has been found that palmitoyl-CoA-hydrolase enzyme (protein database code 1YLI) is involved in lipid metabolism (KEGG) and very crucial for the survival of the particular microbe. The enzyme is involved in the esterification of fatty acids to form triglycerides [4].

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 *Capsicum* plant were downloaded from the website [5]. The protein database code of the palmitoyl-CoA-hydrolase enzyme was identified from the website [6]. 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 [7,8]. Table 1 shows that palmitoyl-CoA hydrolase-Myricetin interaction has the highest positive value of -CDOCKER energy

Table 1. Results of C docking of phytochemicals with palmitoyl-CoAhydrolase (receptor)

Sl. no	Ligand	-C DOCKER Energy	-C DOCKER Interaction Energy	Difference Between - C DOCKER Interaction Energy And - C DOCKER Energy
1	Myricetin	27.0749	29.2435	2.1686
2	Quercetin	25.7857	30.0193	4.2336
3	Luteolin	22.9727	27.648	4.6753
4	Apigenin	21.4293	26.8581	5.4288
5	Capsaicin	17.7672	36.111	18.3438
6	Linalool	-10.2877	22.9628	33.2505
7	1,8-cineole	-13.8487	13.337	27.1857
8	Myrcene	-14.3327	17.1876	31.5203
9	β -carotene	Failed	Failed	Failed

(27.0749) and minimum value of the difference (2.1686) between - C DOCKER interaction energy and - C DOCKER energy followed by Quercetin. Thus, the results indicated that myricetin and quercetin can effectively deactivate the palmitoyl-CoAhydrolase enzyme thereby interrupting the biological cycle of *Haemophilus influenzae*. Higher positive values for luteolin indicated that it was the most active ingredient against *Haemophilus influenzae*. On the other hand, 1,8-cineole, linalool, myrcene and camphene can deactivate the enzyme to a small extent (negative -CDOCKER energy but positive -CDOCKER interaction energy). β -carotene cannot interact with palmitoyl-CoAhydrolase enzyme. Thus, the key phytochemicals preventing bronchitis caused by *Haemophilus influenzae* are myricetin and quercetin.

4. CONCLUSIONS

It was previously known that the Capsicum plant has medicinal action against bronchitis. Bronchitis is caused by *Haemophilus influenzae*. 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 (1,8-cineole, Apigenin, capsaicin, linalool, luteolin, myrcene, myricetin and quercetin), which can have significant interaction with the vital enzyme (palmitoyl-CoAhydrolase) of the microbe. It was found that luteolin and apigenin can form a strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. 1,8-cineole, capsaicin, linalool, myrcene, camphene, rutin were found to be not much effective in deactivating the enzyme of the microbe. β -carotene cannot deactivate the enzyme. Thus, this study could explain that the presence of luteolin and apigenin provided the

medicinal values to Capsicum against bronchitis caused by *Haemophilus influenzae*.

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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