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Bhringraj Derived Phytochemicals against *Pneumonia*

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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 *Bhringaraj* plant extract are traditionally used to cure *Pneumonia*. It is caused by *Klebsiella pneumonia.* Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that glutamic acid can effectively deactivate the dehydrogenase enzyme, thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Bhringaraj; Klebsiella pneumonia.

1. INTRODUCTION

Plants contain natural products which have medicinal value [1]. These natural products or chemical compounds present in various plant parts are enriched with anti-fungal and anti-bacterial properties. These can be used for drug formulations and used to cure deadly diseases in human [2]. More than half of the world population rely on traditional medicines which is plant based. They play a crucial role in human health [3]. The extracts of these phytochemicals can be used for medicine preparation which can be safely used to cure various infections and disaeses.

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Bhringraj extract is used to cure disease like Pneumonia. The objective of the study is to identify the phytochemical responsible to cure the disease.

Bhringraj contains"glycosides, polyacetylenes, triterpenoids, alkaloids, flavonoids" etc. These phytochemicals might act against Pneumonia. However, there is no such study available.

This objective of the study is to identify the phytochemicals of *Bhringraj* capable of curing Pneumonia.

2. MATERIALS AND METHODS

2.1 Software Used

All the operations were carried out in Discovery studio module of Biovia 2020 software (Dassault Systemes of France). Biovia 2020 discovery studio is one of the user friendly software. Its user interface is quite easy to carry out the molecular docking. The software utilizes machine learning techniques to predict the level of molecular interaction between the receptor (enzyme) and Ligand (Phytochemicals).

2.2 Methodology

2.2.1 List of phytochemicals

Phytochemicals are secondary metabolites produced by plants to fight against the predators. Phytochemicals are generally bio-active compounds which can affect animal biochemistry and metabolism. Hence they are widely examined to prove their health benefits. Published works showed that *Bhringraj* contains glycosides, polyacetylenes, triterpenoids, alkaloids, flavonoids. The polypeptides isolated from the plant yield cystine, glutamic acid, phenyl alanine, tyrosine and methionine on hydrolysis [4,5]. It has already been established that *Bhringraj* plant belonging to Asteraceae (sunflower) family has the potential to help controlling skin disease and infection. This work is focused on the identification of the particular phytochemical responsible for inhibiting and controlling of bacterial disease.

2.2.2 Enzyme found in *Aeromonas hydrophila*

Based on previously published papers it has been known that infection caused due to *Klebsiella pneumonia* infestation. For the survival of a pathogen in its host, there are specific metabolic pathways. These metabolic pathways require certain enzymes as its co-factor to function properly. Brenda enzyme database has proved useful to identify and list different enzymes found in *Klebsiella pneumonia.* It has been found that glycerol dehydrogenase (protein database code 1IWP) is involved in glutamic acid biosynthesis metabolism. This metabolism proves to be very crucial for the pathogen, thus blocking or inhibiting that pathway results in the death of the particular microbe.

2.2.3 Molecular docking

Molecular docking method has been used to identify the phytochemical from the plant extract, which act as a ligand and form a strong covalent bond with the fungal protein to successfully inhibit the microbe. The Discovery studio module of Biovia software was used for identifying molecular interaction and molecular docking was performed. First step involves collection of list of phytochemicals present in *Bhringraj* from various research papers. Second step involvesd own loading the sdf files for the phytochemicals found in the *Bhringraj* plant from various websites like PubChem, MolInstincts etc. The protein data base code of 1IWP enzyme was identified from the RCSB-PDB website. 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 phytochemicals responsible for curing the various infection 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 exissts between the protein and the ligand. The criteria for best interaction were chosen based on a) high positive value of-CDOCKER

Table 1. Results of Cdocking of phytochemicals with acetaldehyde dehydrogenase (Receptor)

Sl. no	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between - C DOCKER interaction energy and - CDOCKER energy	Remarks
1	Wedelolactone	-8.5038	16.9295	8.4256	
2	Glutamic acid	24.2267	26.4227	2.1953	Maximum inhibition of infection
3	Cystine	21.3568	23.8138	2.4578	
4	Phenylalamine	16.5296	20.9732	4.4436	
5	Luteolin	14.1622	19.6815	5.5193	
6	Apigenin	10.9574	20.2356	9.2782	
7	Triterpenic acid	FAILED	FAILED	NA	
8	Amyrin	FAILED	FAILED	NA	
9	Stigmasterol	FAILED	FAILED	NA	

energy and b) small difference between –CDOCKER energy and- CDOCKER interaction energy. Table 1 show that glycerol dehydrogenase–glutamic acid interaction has the highest positive value of-CDOCKER energy 26.4227 between-CDOCKER interaction energy and-CDOCKER energy. Thus the results indicated that glutamic acid can effectively deactivate the glycerol dehydrogenase enzyme there by interrupting the biological cycle of *Klebsiella pneumonia*. Higher positive values for indicated that it was the most active ingredient against *Klebsiella pneumonia*. On the other hand, we decollate one can deactivate the enzyme to a small extent (negative-CDocker energy but positive- CDocker interaction energy).Thus, the key phytochemicals preventing various infection by *Klebsiella pneumonia* are apigenin, luteolin, cystine, phenylalamine, apigenin.

4. CONCLUSIONS

It was previously known that *Bhringraj* plant has medicinal action against various infection. Infections are caused by *Klebsiella pneumonia*. This study was carried out to provide the theoretical basis of this observation. Molecular docking operation was executed to identify the phytochemical (coumestans, alkaloids, flavonoides, glycosides, polyacetylenes, triterpenoids) by using Discovery studio module of Biovia software, which can have a major interaction with the dynamic enzyme (glycerol dehydrogenase) of the microbe. It was found that glutamic acid can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Cystine, phenylalmine, luteolin, apigenin were found to be not much sective in deactivating the enzyme of the microbe, stigmasterol, amyrin, triterpenic acid as they fail to maintain stability. Thus, this study could explain that the presence of glutamic acid provided the medicinal values to *Bhringraj* against infections caused by *Klebsiella pneumonia*.

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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