



Syzygium aromaticum Derived Phytochemicals against Infections in Feet Crack Caused by Trichophyton rubrum

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

Article Information

DOI: 10.9734/JPRI/2020/v32i630503

Editor(s):

(1) Dr. R. Deveswaran, M. S. Ramaiah University of Applied Sciences, India.

Reviewers:

(1) S. Danish Kadir, University of Rajshahi, Bangladesh.

(2) Phillip Minnaar, Agricultural Research Council, South Africa.

(3) Fuad Al-Rimawi, Al-Quds University, Palestine.

Complete Peer review History: <http://www.sdiarticle4.com/review-history/56446>

Received 06 April 2020

Accepted 14 May 2020

Published 15 May 2020

Original Research Article

ABSTRACT

Phytochemicals from *Syzygium aromaticum* plant extract traditionally used to cure Feet Crack. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that Myricetin can effectively deactivate the dihydrofolate reductase enzyme thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Syzygium aromaticum; Trichophyton rubrum.

1. INTRODUCTION

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 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

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medicine [3]. *Syzygium aromaticum* extract is used to cure disease like Gonorrhoea. The objective of the study is to identify the phytochemical responsible to cure the disease. *Syzygium aromaticum* contains “beta-pinene, alpha-pinene, p-cymene, limonene, piperazine” etc. These phytochemicals might act against Feet Crack. However, there is no such study available. This objective of the study is to identify the phytochemical of *Syzygium aromaticum* capable of curing Feet Crack.

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 *Syzygium aromaticum* contains Beta-caryophyllene, Campesterol 3-beta-d-glucoside, Eugenol, Gallic acid, Kaempferol, Myricetin, Oleanoid acid, Rhamnetin, Stigmasterol, vanillin etc. It has already been established that *Syzygium aromaticum* plant belonging to Myrtaceae family has potential to help controlling the infection. This work is focused on identification of the particular phytochemical responsible for inhibiting and controlling of the infection in feet cracks.

2.2.2 Enzyme found in *Trichophyton rubrum*

It has been reported that infection in feet crack can cause as a result of *Trichophyton rubrum* 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 *Trichophyton rubrum*. It has been found that

Laccase enzyme (protein database code 1KYA) is involved in oxidation of phenolic and non-phenolic compound for the fungus 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 act as a ligand and form 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 *Syzygium aromaticum* plant were downloaded from the website [4]. The protein database code of the Laccase enzyme was identified from the website [5]. 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 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.

Table 1 shows that (Myricetin)- (Laccase) interaction has the highest positive value of -CDOCKER energy (30.7642) and minimum value of the difference (5.6837) between -CDOCKER interaction energy [6,7] and -CDOCKER energy. Thus, the results indicated that Myricetin can effectively deactivate the Laccase enzyme

Table 1. Results of CDocking of phytochemicals with Laccase enzyme (receptor)

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and -CDOCKER energy
1	Myricetin	30.7642	36.4479	5.6837
2	Rhamnetin	25.8526	31.7149	5.8623
3	Gallic acid	24.6676	22.3528	-2.3148
4	Kaempferol	23.2967	28.4838	5.1871
5	Vanillin	14.7127	17.7633	3.0506
6	Eugenol	9.43861	20.3223	10.88369
7	Beta-caryophyllene	-19.5183	22.9212	42.4395
8	Stigmasterol	-41.0718	39.2297	80.3015
9	Compesterol 3-beta-d-glucoside	-45.9939	53.1614	99.1559
10	Oleanoid acid	-79.5527	31.1846	110.7373

thereby interrupting the biological cycle of *Trichophyton rubrum*. Higher positive values for Myricetin indicated that it was the most active ingredient against Laccase followed by Rhamnetin, Gallic acid, Kaempferol, Vanillin and Eugenol. On the other hand, Beta-caryophyllene, Stigmasterol, Compesterol 3-beta-d-glucoside, Oleanoid acid can deactivate the enzyme to a small extent (negative -CDOCKER energy but positive -CDOCKER interaction energy). Thus, the key phytochemical preventing Oral infections caused by *Trichophyton rubrum* is Myricetin.

4. CONCLUSIONS

It was previously known that *Syzygium aromaticum* plant has medicinal action against Infections in Oral cavity. This infection is caused by *Trichophyton rubrum*. 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 (Beta-caryophyllene, Compesterol 3-beta-d-glucoside, Eugenol, Gallic acid, Kaempferol, Myricetin, Oleanoid acid, Rhamnetin, Stigmasterol, vanillin), which can have a significant interaction with the vital enzyme Laccase of the microbe. It was found that Myricetin can form strong bond with the enzyme followed by Rhamnetin, Kaempferol, Gallic acid, Vanillin and Eugenol successfully inhibiting the metabolic cycle of the microbe. While Beta-caryophyllene, Stigmasterol, Compesterol 3-beta-d-glucoside, Oleanoid acid were found to be not much effective in deactivating the enzyme of the microbe. Thus, this study could explain that the presence of Myricetin provided the medicinal

values to *Syzygium aromaticum* against Oral infections caused by *Trichophyton rubrum*.

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.

REFERENCES

1. Henrich J, Heine S, Norenzayan A. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI: 10.1017/S0140525X0999152X
2. Hussain I, Ullah R, Ullah R, Khurram M, Ullah N, Basee A, Khan F, Khattak M, Zahoor M, Khan J, Khan N. Phytochemical

- analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10:7487-7492.
3. Arulselvan P, Karthivashan G, Fakurazi S. Journal of Chemical and Pharmaceutical Research. 2013;5(7):233-239.
 4. Mol-Instincts, Chemical Property Database. Available:www.molinstincts.com
 5. Enzyme Database – BRENDA. Available:www.brenda-enzymes.org
 6. Das D, Das S, Pandey M, Bhattacharyay D. *In silico* analysis of phytochemicals from *Mucuna pruriens* (L.) DC against *Mycobacterium tuberculosis* causing tuberculosis. European Journal of Medicinal Plants; 2020.
 7. Brinda OP, Deepu Mathew, Shylaja MR, Sangeetha Davis P, Anita Cherian K, Valsala PA, Isovaleric acid and avicequinone-C are chikungunya virus resistance principles in *Glycosmis pentaphylla* (Retz.) Correa. 2019;56(2): 111-121.

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Peer-review history:
The peer review history for this paper can be accessed here:
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