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In silico ANALYSIS OF EFFECT OF PHYTOCHEMICALS FROM *Pavonia odorata* AGAINST *Epidermophyton floccosum* CAUSING ATHLETES FOOT DISEASE

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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

Epidermophyton floccosum causes athletes foot disease. Strikingly, athlete's foot disease rises primarily during specific molecular events, thus acting as a potential clinical biomarker. Further, athlete's foot disease may also activate further downstream events, supporting the detrimental phase. To restrict the activity of athletes foot disease, several bio molecules can be deployed, of which the phytochemicals can be the best alternative. Molecular docking-based screening of a few phytochemicals revealed that the phytochemicals effectively associate with the active site of the protein and hence bears diagnostic and therapeutic potentials against athletes' foot disease.

Keywords: Phytochemical; biovia; discovery studio; atheletes foot disease; epidermophyton.

1. INTRODUCTION

Nature has been a complete storehouse provider of remedies to cure all the aliments of mankind. Several categories of phytochemicals are found in the plant parts like fruit, leaf, stem, root, flower and bark which contain immense pharmaceutical functionalities [1]. For treating several diseases, phytochemical compounds like tocopherols, carotenoids, anthocyanins, phenolics etc. are effective [2,3]. Several phytochemicals act as natural antioxidants, which supplements the need of the human body [4]. Across the globe, it is recommended for consumption of fruits and vegetables, primarily to improve the state of health [5]. We primarily screened a few phytochemicals, which are not yet globally

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recognized for being used against athlete's foot disease, using a molecular docking method (BIOVIA). *Pavonia odorata* wild belongs to the family Malvaceae. It is known as sugandhabala in native Indian sub-tropical areas.

A group of fungus belonging to genus Epidermophyton generally cause Athletes foot disease. They are smooth, thin-walled, club-shaped microconidia. Epidermophyton infection (tineapedis) is a common fungus disease that affects the keratinized tissue, skin, nails, foot. The aim of this study is the identification of the phytochemical from *Pavonia odorata*, with properties that allow their usage as treatment of Athletes Foot Disease caused by *Epidermophyton floccosum*.

2. MATERIALS AND METHODS

2.1 Protein Structure and Phytochemicals Dataset Collection

From the Protein Data Bank (accession: 3H3N), the 3D structure of protein was accessed. For docking with the target protein, subsequently phytochemicals were considered and SDF file accession numbers were used for the purpose.

2.2 Molecular Docking

In silico molecular docking was done by using the BIOVIA's Discovery Studio docking method (CDOCKER; Dassault Systèmes BIOVIA). The catalytic pocket of the Glycerol Kinase protein was generated and subsequently targeted for ligand interaction. 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 fungal protein to successfully inhibit the microbe.

3. RESULTS AND DISCUSSION

Fig. 1 shows the active site of the Glycerol Kinase enzyme. The positive values of the CDOCKER Energy and CDOCKER_INTERACTION_ENERGY represent the affinity of the ligands with the receptor proteins. Several number of phytochemicals (Table 1) against the protein, revealed that caproic acid, palmitic acid, acetone are potential binding ligands as evident from their higher CDOCKER ENERGY and CDOCKER_INTERACTION_ENERGY (Table 1). These are very common and easily available. Phytochemicals including Hesperidin, Epicatechin, Tangeretin, Allicin, Sulforaphane, Cyanidin and Malvidin didnot show affinity for the active site of the protein as the docking results were failed. The chemical structure of ligand molecules showing positive affinity for the protein can be studied extensively and related synthetic molecules can be developed for wide range applications in the field of therapeutics.

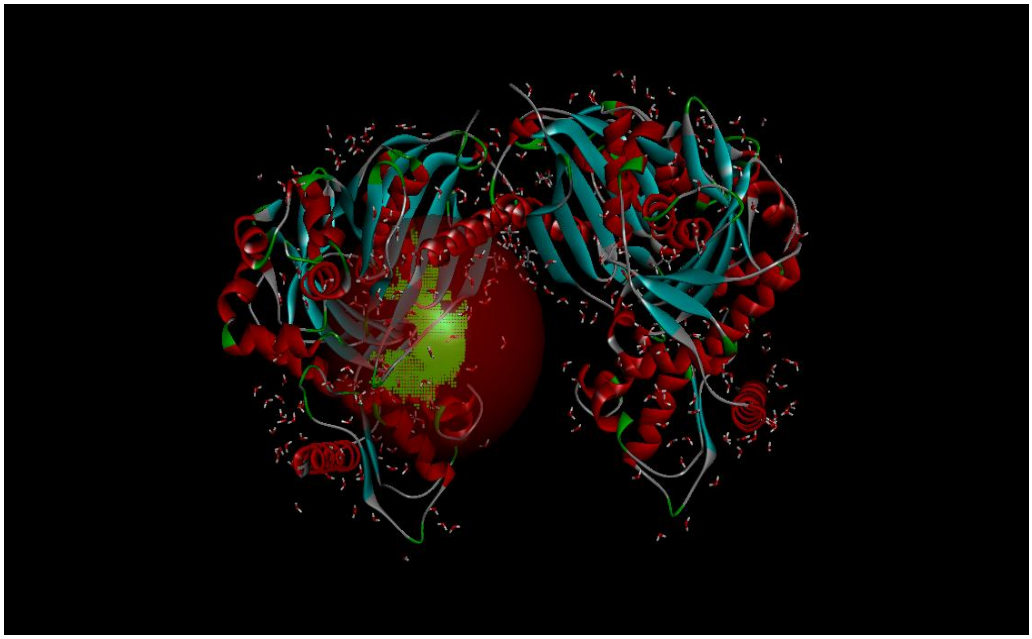

Fig. 1. Active site of Glycerol kinase *Epidermophyton floccosum* enzyme

Table 1. Results of C Docking of phytochemicals with Glycerol kinase of *Epidermophyton floccosum* (receptor)

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and -CDOCKER energy
1	Acetone	14.8336	14.4788	0.3548
2	Palmitic acid	45.6905	44.1445	1.546
3	Caproic acid	26.7473	24.4257	2.3216
4	Pinocarveol	2.64117	23.7693	21.12813
5	Alpha-pinene	-5.17094	19.8271	24.99804
6	Alpha-eudesmol	1.49052	31.9229	30.43238
7	Alpha-terpine	-16.3262	20.7197	37.0459

4. CONCLUSIONS

In silico molecular docking based study reveals several novel candidate molecules which can target the Glycerol Kinase protein. It would be highly significant being confirmed *in vivo*. Specific phytochemical targeting Glycerol Kinase protein can be employed in two ways. Firstly, these phytomolecules may act as drug by blocking the specific sites of Glycerol Kinase protein, ultimately inhibiting the downstream pathways. Secondly, cost effective medical device can be developed to diagnose early stages of disease by targeting marker proteins like Glycerol Kinase enzyme. Phytochemicals including caproic acid, palmitic acid, and acetone may be effective. Since, Glycerol Kinase is highly significant in modulating the growth factor signaling and promotes cancerous activity; they should be restricted being over activated by blocking their active site. Early diagnosis being a critical issue in several diseases, appropriate ligands can be developed to be used as a diagnostic tool.

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.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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