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PHYTOMOLECULES OF *Bacopa monnieri* DISPLAY POSITIVE AFFINITY FOR STEROL 14-ALPHA-DEMETHYLASE OF *Trichophyton sp*: POSSIBLE PREVENTIVE AND THERAPEUTIC USAGE IN TINEACAPITIS

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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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Short Research Article

ABSTRACT

Trichophyton sp causes Tineacapitis. Strikingly, Tineacapitis occurs primarily during specific molecular events, thus acting as a potential clinical biomarker. Further, Tineacapitis may also activate further downstream events, supporting the detrimental phase. To restrict the activity of Tineacapitis, 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 sterol14-alpha-demethylase of *Trichophyton sp* and hence bears diagnostic and therapeutic potentials against Tineacapitis.

Keywords: Phytochemical; Biovia discovery studio; *Bacopa monnieri*; metabolic pathways; Tineacapitis; *Trichophyton.*

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1. INTRODUCTION

Using phytochemicals to treat disease can be one of the best alternatives. 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 diseases like Tineacapitis, 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 recognized for being used against Tineacapitis, using a molecular docking method (BIOVIA). Brahmi (*Bacopa monnieri Linn.)* is an herb which belongs to the family Lamiaceae. Tineacapitis is a common scalp infection seen in children caused by dermatophyte infection. Tineacapitis is caused by *Trichophyton sp*. Tineacapitis affects children over the age of 6 years but before entering the puberty phase. Tineacapitis treatment requires oral administration of antifungal agent [6].

This study focuses on the identification of the phytochemical from *Bacopa monnieri* responsible to cure Tineacapitis, caused by *Trichophyton sp.*

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). The aim of this study is the identification of the phytochemical from *Bacopa monnieri*, with properties that allow their usage as treatment of Tineacapitis caused by *Trichophyton sp*.

2.2 Methodology

2.2.1 Protein structure and phytochemicals dataset collection

From the Protein Data Bank (accession: 5TZ1), the 3D structure of sterol 14-alpha-demethylase protein was accessed. For docking with the target protein, sterol 14-alpha-demethylase, several numbers of phytochemicals were considered and SDF file accession numbers were used for the purpose.

2.2.2 Molecular docking

In silico molecular docking was done by using the BIOVIA's Discovery Studio docking method (CDOCKER; Dassault Systèmes BIOVIA, 2020). The catalytic pocket of the sterol14-alpha-demethylase protein was generated and subsequently targeted for ligand interaction.

3. RESULTS AND DISCUSSION

Fig. 1 shows the active site of sterol14-alpha demethylase enzyme. Positive values of the CDOCKER Energy and CDOCKER_INTERACTION_ENERGY represent the affinity of the ligands with the receptor proteins. Ten numbers of phytochemicals (Table 1) against the sterol 14-alpha-demethylase protein revealed that apigenin and luteolin 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 did not show affinity for the active site of the sterol 14-alpha-demethylase as the docking results were failed. The chemical structure of ligand molecules showing positive affinity for the sterol14-alpha-demethylase can be studied extensively and related synthetic molecules can be developed for wide range applications.

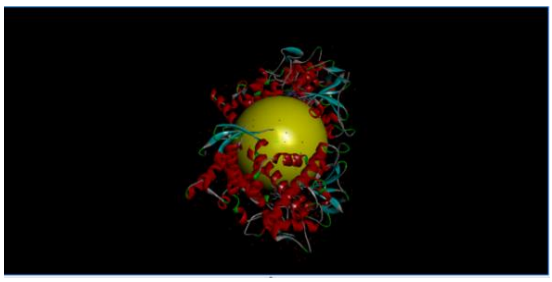

Fig. 1. Active site of sterol 14-alpha demethylase enzyme

Table 1. Results of C docking of phytochemicals with sterol 14-alpha demethylase (receptor)

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between-CDOCKER interaction energy and-CDOCKER energy
1	Apigenin	19.992	25.0511	5.0591
2	D-mannitol	-5.65502	20.5708	26.22582
3	Luteolin	24.4999	28.5708	3.5708
4	Nicotine	-5.66694	14.8624	20.52934

4. CONCLUSION

In silico molecular docking based study reveals several novel candidate molecules which can target the sterol 14-alpha-demethylase protein. It would be highly significant being confirmed in vivo. Specific phytochemical targeting sterol 14-alpha-demethylase can be employed in two ways. Firstly, these phytomolecules may act as drug by blocking the specific sites of sterol 14-alpha-demethylase, ultimately inhibiting the downstream pathways. Secondly, cost effective medical device can be developed to diagnose early stages of cancer by targeting marker proteins like sterol 14-alpha-demethylase. Phytochemicals including apigenin and luteolin may be effective. Early diagnosis being a critical issue in several cancers, appropriate ligands can be developed to be used as a diagnostic tool.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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