2021 IEEE 2nd International Congress of Biomedical Engineering and Bioengineering, CI-IB and BI 2021 • 2021 •
2nd IEEE International Congress of Biomedical Engineering and Bioengineering, CI-IB and BI 2021 • Bogota • 13 October 2021through 15 October 2021 • Code 175151

Virtual screening of new targets and inhibitors for Candida albicans infection control

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Document type
Conference Paper
Source type
Conference Proceedings
ISBN
978-166540855-4
DOI
10.1109/CI-IBBI54220.2021.9626093
Publisher
Institute of Electrical and Electronics Engineers Inc.
Sponsors
Colombia Section of IEEE
Original language
English
View less

Abstract

Infection by Candida albicans fungus is considered of biomedical interest, producing significant mortality and comorbidity. The development of pathogen resistance during pharmacological treatments is increasing, thus, the pursuit for new inhibitors is necessary. Virtual screening is one of the bioinformatics tools used for the search of new drugs, and potential targets for disease management. The aim of the present study was to analyze a library of potential targets, and to identify suppressors for C. albicans using virtual screening. 50 protein targets with restraining potential were examined, choosing GPI-Anchored hemophore PGA10 protein (RBT5) as the target, since it is involved in C. albicans survival and nutrients acquisition. Meanwhile, through the implementation of AutoDock Vina and PyRx software, the molecular affinity of 25 molecules available in ZINC15 database was analyzed, obtaining favorable results for the following compounds: ZINC000000065058, ZINC000000065374 and ZINC000000072389, displaying affinity with the same region of the target protein. These results provide a potential target for the development of novel suppressors, as well as guidelines for three new drugs that could aid in C. albicans suppression. © 2021 IEEE.

Author keywords

Bioinformatics; Candidiasis; Drug treatment; Molecular docking

Indexed keywords