TITLE: SMALL MOLECULE SELECTED BY VIRTUAL SCREENING USED AGAINST ADHESION AND BIOFILM OF *CANDIDA ALBICANS*

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ABSTRACT:

Over the past decades, the increase in mortality due to fungal infections has increased worldwide. It is of crucial importance to develop new methods to control and treat these infections, since the available therapeutic arsenal is limited. Besides, antifungal resistance has been increasing and has already reached alarming marks. Currently, there are new approaches being used seeking the development of new drugs. The *in silico* method is one of them and has been used as an efficient and less expensive strategy for the new antifungals production, based on the structure of the essential genes of the fungus or virulence factors such as proteins that are essential to biofilm formation. Therefore, the aim of this study was to evaluate the anti-adhesion and anti-biofilm action of a compound selected by virtual screening of commercially available molecules in a specific database (*Life Chemicals*), which has as target the Als3 protein from the *Candida albicans* species. The methodology used was based on a standard study in the area. A *C. albicans* reference strain (ATCC 90028) was used for adhesion and biofilm assays, in the presence and absence of this compound. Carboxymethyl cellulose and DMSO (Dimethyl sulfoxide) were used in order to dilute the samples. The compound was evaluated at the concentrations 16µg/ml, 32µg/ml and 64µg/ml. The results obtained has shown that, at the concentration of 64µg/ml, the adhesion and biofilm parameters decreased 6,76% and 5,24%, respectively. In conclusion, this compound was able to reduce *in vitro* the adhesion and biofilm formation conditions showing that this molecule selected by virtual screening is promising. Although the results are not statistically significant, it is important to highlight that the target molecule can be redesigned, and consequently better results may be obtained according to the changes made.

Keywords: Virtual screening; Small molecule; *Candida albicans*; Anti-adhesion and anti-biofilm action.

Development agency: CAPES