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Realização

Sociedade
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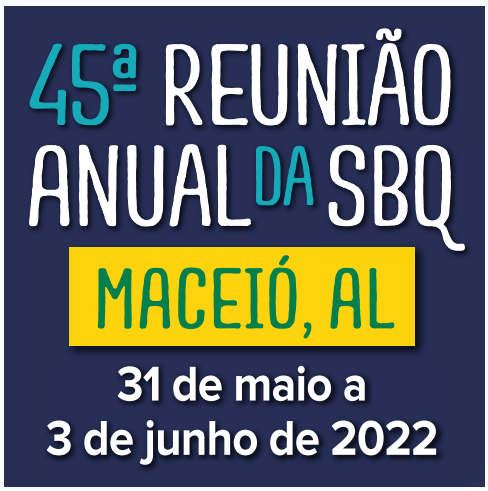
FERNANDO DE CARVALHO DA SILVA

Anais da 45ª Reunião Anual da SBQ



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Molecular Docking and Quantum Studies of Lawsone Dimers Derivatives: New Investigation of Antioxidant Behavior and Antifungal Activity

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Key words: Antifungals, Antioxidant, *C. albicans,* Lawsone, Molecular Docking.

Highlights

Verification of the antioxidant potential using different techniques: *in vitro* tests, DFT and cyclic voltammetry. Rationalization of data obtained in antifungal tests through molecular docking.

Abstract

In general, fungal species are characterized by their opportunistic character and can trigger various infections in immunocompromised hosts. The emergence of infections associated with high mortality rates is due to the resistance mechanisms that these species develop. This phenomenon of resistance denotes the need for the development of new and effective therapeutic approaches. In this work, we report the investigation of the antioxidant and antifungal behavior of dimeric naphthoquinones derived from lawsone whose antimicrobial and antioxidant potential has been reported in the literature. Seven fungal strains were tested, and the antioxidant potential was tested using the combination of the methodologies: reducing power, total antioxidant capacity and cyclic voltammetry. Molecular docking studies (**PDB ID 5V5Z** and **1EA1**) were conducted which allowed the derivation of structure-activity relationships (SAR) (Figure 1). Compound **1-i**, derived from 3-methylfuran-2-carbaldehyde showed the highest antifungal potential with an emphasis on the inhibition of *Candida albicans* species (**MIC = 0.5 µg/mL**) and the highest antioxidant potential.

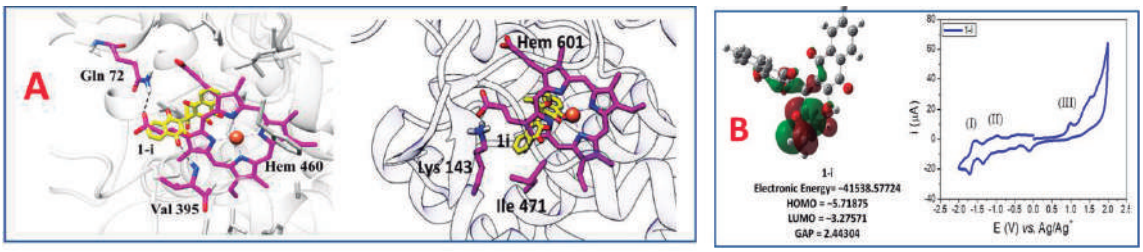

Figure 1: A) Best score docking poses for **1-i** (PDB 1EA1) (left) and best scoring docking poses for **1-i** (PDB 5V5Z) (right). B) Molecular orbital energy level and HOMO shapes. Cyclic voltamomgrams from **1-f** and 1-i obtained at glassy carbon electrode in 0.1 M $TBAPF_6$ in acetonitrile at a scan rate of 100 mV s^{-1}.

A combination of molecular modeling data and *in vitro* assays can help to find new solutions to this major public health problem.

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