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Design, synthesis and microbiological evaluation of *N*-substituted-2-(3-oxo-3,4-dihydro-2*H*-benzo[b][1,4]thiazin-2-yl)propionamide as antifungal agent

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ABSTRACT:

As a part of a program to develop novel antifungal agents, a series of new *N*-Substituted-2-(3-oxo-3,4-dihydro-2*H*-benzo[b][1,4]thiazin-2-yl)propionamide was design and dock into the active pocket of enzyme lanosterol 14α-demethylase (CYP51). Genetic algorithm implemented in MDS had been successfully employed to dock inhibitors into the catalytic site of the CYP51. Compounds BTMA-50, BTMA-88 were found to have good affinity for enzyme lanosterol 14α-demethylase. The design molecules were synthesized and their *in-vitro* and *in-vivo* antifungal activity were reported. All the reaction monitored by thin layer chromatography. The structures of the synthesized compounds were established by spectral techniques (IR, ^{1}HNMR, ^{13}CNMR and Mass). *In-vitro* microbiological assay indicates that the 1,4-Benzothiazine compounds show a good antifungal activity against the tested pathogenic fungi such as *Candida albicans, Trichophyton rubrum, Epidermophyton floccosum* and *Malassazia furfur.* From the result of *in-vitro* activity of benzothiazine compounds, four compounds (BTMA-24,36,50 & 88) was selected for *In-vivo* activity were tested in a murine model of systemic *Candida albicans* infection. Compound BTMA-50 was showing potent activity in *in-vivo* antifugal testing.

Keywords: Antifungal activity, 1,4-Benzothiazine, CYP51, Molecular docking.