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Synthesis, Antifungal Evaluation, Toxicity Analysis, and *in silico* Rationalization of Some 3-Aryl-1,2,4-triazolopyridines against Seed-borne Fungal Pathogens of Rice

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ABSTRACT 1,2,4-Triazolopyridines motif of great pharmacological value is almost unexplored in Agri World. The present work pertains to the synthesis of a series of 1-benzylidene-2-(pyridin-2-yl)hydrazines (**2-8**) by solid-state synthesis followed by its oxidative cyclization to obtain 3-aryl-1,2,4-triazolopyridines (**9-15**). Antifungal evaluation studies of starting reactants, intermediates, and final products against economically important seed-borne mycoflora of rice, namely, *Fusarium verticillioides, Fusarium fujikuroi*, and *Sarocladium oryzae* revealed that all the tested compounds are better fungi toxic than the standard commercial fungicides used. Interface between pymol and molecular docking suites AutoDock and Vina demonstrated them as 14-α demethylase inhibitor rationalized by docking visualization aid indicating two strong hydrogen-bonded interactions for high docking score of compound **9** than propiconazole (1H bond). Chemical reactivity indices obtained by ChemDraw ultra 3D simulation tools categorized them as "Non-doxin" like, responsible for non-persistence and less toxic behavior of the compounds. The *in silico* toxicity analysis and actual cell viability test by (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assays on mammalian stem cell revealed compound **9** (IC_{50}; 75 µg/ml) to be much lower toxic than propiconazole (IC_{50}; 41.02 µg/ml), advocating its further exploration for *in vivo* antifungal assays.

KEYWORDS 14-α Demethylase, *N*-Bromosuccinimide, Non-doxin, Oxidative cyclization, Oxone, Triazolopyridine.

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