Journal of Basic and Applied Engineering Research
p-ISSN: 2350-0077; e-ISSN: 2350-0255; Volume 6, Issue 4; April-June, 2019, pp. 246-246

http://www.krishisanskriti.org/Publication.html

Synthesis of 3-aryl-1,2,4-triazolopyridines for Mycocidal Evaluation as Potent 14-alpha Demethylase Inhibitors

Heena[1]*, Anjali Sidhu[1] and Anju Bala[2]

[1]Department of Chemistry, Punjab Agricultural University, Ludhiana
[2]Department of Plant Breeding and Genetics, Punjab Agricultural University, Ludhiana
*E-mail: *heenabajaj1996@gmail.com*

Abstract —*A series of 3-aryl-1,2,4-triazolopyridines were synthesized in a multistep reaction mechanism. Some initial steps were carried out in solid state by microwave oriented reaction enhancement methodology till the formation of hydrazones, with quite reduction in reaction time and solvents used. The synthesized hydrazones were further cyclized using N-bromosuccinimide and oxone in 1:1 to give 3-aryl-1,2,4-triazolopyridines in excellent yield. Screening of the synthesized compounds for antifungal evaluation revealed one of the compound inflicting maximum mycocidal potential against all the test fungi, better than the standard commercial fungicide propiconazole (Tilt 25 EC). The in silico evaluation, docking score and pesticide likeliness factors corresponded well with the actual results. The HOMO-LUMO energy differences and Toxtree analysis indicated the non doxin like non persistant category of chemicals belonging to class III of pesticides, advocating their exploration for further trials.*

Keywords*: 14-α Demethylase. N-bromosuccinimide. 1,2,4-Triazolopyridine. Oxidative cyclization. Oxone.*