

## QSAR Study of Derivatives for Antimicrobial Evaluation of Novel Benzimidazole Type of Fluconazole Analogues Invoking Quantum Mechanical Based Descriptors

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Recently, Zhang *et al.* [1], have reported the novel series of benzimidazole type of fluconazole analogues and their synergistic effects with chloromycin, norfloxacin and fluconazole. The authors screened new compounds for their antimicrobial activities *in vitro* conditions using two-fold serial dilution technique. In their study, they evaluated that the 3,5-*bis*(trifluoromethyl)phenyl benzimidazoles gave comparable or even stronger antibacterial and antifungal efficiency while comparing with reference drugs chloromycin, norfloxacin and fluconazole. In present research work, local reactivity as well as global reactivity parameters are evaluated invoking quantum mechanical based descriptors to validate the above mentioned experimental facts. Experimental and theoretical correlation supports the research findings.

### Reference

1. H.-Z. Zhang, G. L. V. Damu, G.-X. Cai and C.-H. Zhou, European Journal of Medicinal Chemistry, 64, 2013, 329-344.