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1,2,3-Triazole tethered acetophenones: Synthesis, bioevaluation and molecular docking study

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ABSTRACT

A small focused library of eighteen new 1,2,3-triazole tethered acetophenones has been efficiently prepared *via* click chemistry approach and evaluated for their antifungal and antioxidant activity. The antifungal activity was evaluated against five human pathogenic fungal strains: *Candida albicans*, *Fusarium oxysporum*, *Aspergillus flavus*, *Aspergillus niger*, and *Cryptococcus neoformans*. Among the synthesized compounds, **9c**, **9i**, and **9p** found to be more potent antifungal agents that the reference standard. These 1,2,3-triazole based derivatives were also evaluated for antioxidant activity, and compound **9h** was found to be the most potent antioxidant as compared to the standard drug. Furthermore, molecular docking study of the newly synthesized compounds was performed and results showed good binding mode in the active site of fungal *C. albicans* enzyme P450 cytochrome lanosterol 14α-demethylase. Moreover, the synthesized compounds were also analyzed for ADME properties and showed potential as good oral drug candidates.