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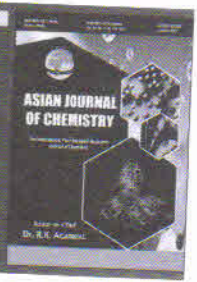

Synthesis, Antimicrobial and DFT Studies of 1,3,4-Oxadiazole Linked Quinoline Carbaldehyde Derivatives

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A novel series of oxadiazole-linked quinoline derivatives was synthesized and evaluated for antimicrobial activity and electronic properties. The synthetic pathway involved the preparation of 4-substituted benzohydrazides, subsequent cyclization to yield 5-(4-substituted phenyl)-1,3,4-oxadiazole-2-thiols, and their coupling with 6/8-subst:tuted-2-chloroquinoline-3-carbaldehydes to obtain the target compounds *viz*. 2-((5-(4-substituted phenyl)-1,3,4-oxadiazol-2-yl)thio)-6/8-substituted quinoline-3-carbaldehydes (**7a-l**) in moderate to good yields. Antibacterial activity was assessed against *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli* and *Pseudomonas aeruginosa*, while antifungal activity was evaluated against *Candida albicans* using minimum inhibitory concentration (MIC) methods. Most compounds exhibited promising antimicrobial activity. Notably, compounds **7g** and **7k**, bearing *p*-nitro phenyl substitution on the oxadiazole ring and chloro substitution on the quinoline nucleus, showed superior antibacterial and antifungal activities comparable to standard drugs.

Keywords: Oxadiazole–quinoline hybrids, Antimicrobial activity, Density functional theory, HOMO-LUMO analysis.