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## Synthesis, anti-bacterial activity and molecular docking of novel pyrazole-thiazolidinone conjugates

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A novel series of pyrazole conjugates were synthesized through Vilsmeier Haack and nucleophilic substitution reaction. The chemical structures of these compounds were established using 1HNMR, 13CNMR, IR and elemental analyses. The synthesized compounds were assayed for antimicrobial activity against two Gram positive bacteria (methicillin-resistant *Staphylococcus aureus, Staphylococcus aureus*) and four Gram negative bacteria (Escherichia coli, *Salmonella typhimurium*, *Klebsiella pneumonia* and *Pseudomonas aeruginosa*). Interestingly, among the compounds tested, 3-(2,4-dichlorophenyl)-1-(2,4-dinitrophenyl)-1pyrazoyl)methylene)hydrazinecarbothioamide (3a) and 2-((3-(2-chlorophenyl)-1-(2,4-dinitrophenyl)-1H-pyrazol-4-yl)methyleneamino)thiazolidin-4-one (4b) were the most cogent antimicrobial compounds with minimum bacterial concentration (MBC) of 0.08, 0.08, 0.16 and 0.16 μg/mL against MRSA and S. aureus respectively. To explore the antimicrobial result on a structural basis, molecular docking studies of the synthesized compounds into the crystal structure of topoisomerase II and topoisomerase IV using AutoDock Vina suggested that compounds 3a and 4b would form hydrogen bonds with the active site of the target.

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