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

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A novel series of pyrazole conjugates were synthesized using molecular hybridization approach through Vilsmeier-Haack reaction. The structure elucidation of the synthesized compounds was established using 1HNMR, 13CNMR, IR and elemental analyses. All compounds were tested 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)*. 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) emerged as 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. Molecular docking studies of the compounds into the crystal structure of topoisomerase II and topoisomerase IV suggested that compounds 3a and 4b preferably interact with the target through hydrogen bonding.

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