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Synthesis and molecular docking studies of 3-methyl-1,4-diarylazetidin-2-ones

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The *trans* isomers of 3-methyl-1,4-diarylazetidin-2-ones have been isolated from the reactions of *N*-1-diarylmethanimine with the ketene generated from propionyl chloride *via* [2+2] cycloaddition protocol. The reaction has been optimised by varying different parameters such as temperature, solvent and bases. The *trans* β-lactams are obtained as the major diastereomers and the structure has been confirmed from the coupling constants of the respective hydrogens from the ^{1}H NMR spectra. The structures of the β-lactams have been elucidated by ^{1}H and ^{13}C NMR spectral techniques and ESI-MS spectroscopy. The synthesized compounds have been evaluated for their binding affinities. To gain insights into the mechanism of action, the interactions between the synthesized compounds and the selected microbial target *S. aureus* DNA Gyrase B protein have been examined. These investigations have shed light on the potential binding modes of (±) *trans* 3-methyl-1,4-diarylazetidin-2-ones, enhancing our understanding of the mechanism of action.

Keywords: 1,4-Diarylazetidin-2-ones, Molecular docking, β-Lactams, Antibacterial agents