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Research Articles

Synergistic antimicrobial activity, MD simulation studies and crystal structure of natural alcohol motif containing novel substituted cinnamates

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Abstract

A series of natural alcohols motif containing novel substituted cinnamates were developed and screened against five bacterial strains namely, *Enterococcus faecal (E. faecalis), Escherichia coli (E. coli), Bacillus subtilis (B. subtilis), Pseudomonas aeruginosa (P. aeruginosa*) and *Klebsiella pneumonieae (K. pneumonieae*). Among all cinnamates, **YS17** was identified with 100% bacterial growth inhibition across the panel, except in *E. faecalis* with MIC values of 0.25 mg/mL against *B. subtilis* and *P. aeruginosa* whereas

11/8/24, 9:24 PM Synergistic antimicrobial activity, MD simulation studies and crystal structure of natural alcohol motif containing novel substitute... Home All Journals Synergistic antimicrobial activity, MD s Volume 42, Issue 1 Synergistic antimicrobial activity, MD s Study and *in vitro* toxicity assays. Interestingly, **YS17** exhibits synergistic effect in combination with the standard drug Ampicillin (AMP). The single crystal structure analysis of **YS4** and **YS6** was also performed which reconfirmed their proposed structures. Molecular docking visualized significant non-covalent interactions between *E. coli* MetAP and **YS17** and the structural and conformational changes were further analysed using MD simulation studies. Overall, the study provided a suitable core for further synthetic alterations for their optimization as an antibacterial agent.

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Disclosure statement

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Additional information

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