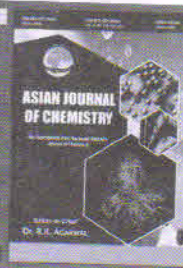


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## Novel Functional Acrylic Copolymers: Synthesis, Characterization, Molecular Docking and Biological Efficacy

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In this study, the functional methacrylate monomers 2,4-dichlorophenyl methacrylate (2,4-DMA) and vanillin methacrylate (VMA) were synthesized and subjected to free-radical (co)polymerization at controlled feed ratios to generate a compositionally tunable copolymer series. Monomer-to-polymer conversion and chain microstructure were verified using FT-IR, <sup>1</sup>H NMR and HPLC. The disappearance of vinyl proton resonances and the loss of C=C stretching bands, combined with high chromatographic purity (>99%), confirmed efficient propagation and minimal side reactions. Compositional variations in the copolymers were further reflected in systematic shifts in carbonyl and aromatic vibrational domains, consistent with differing contributions of the 2,4-dichlorophenyl and vanillin units to the polymer backbone. Biological evaluation demonstrated a clear composition-dependent antimicrobial response, with 2,4-DMA-rich copolymers exhibiting the highest inhibition against both bacterial and fungal strains. To complement the experimental findings, a molecular docking analysis was also performed against *E. coli* DNA gyrase (PDB: 1KZN). The selected copolymer fragment displayed a binding affinity of -5.20 kcal/mol, supported by hydrogen bonding with ASN46 and stabilizing  $\pi$ -alkyl,  $\pi$ -sigma, and alkyl interactions with residues such as ALA47, THR165, VAL43 and VAL167, consistent with the observed antibacterial potency. Based on the results, this study establishes 2,4-DMA/VMA copolymers as a structurally adaptable platform with tunable antimicrobial performance enhanced by favorable protein-binding interactions. These materials show promising aspects for antimicrobial coatings, protective films and biologically responsive polymer systems.

**Keywords:** Acrylic copolymers, 2,4-Dichlorophenyl methacrylate, Vanillin methacrylate, Docking studies, Antimicrobial activity.