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RESEARCH

Synthesis, Characterization, and Biological Evaluation of Quercetin-Boronate@Cu-hNFs and Quercetin-Boronate@Zn-hNFs: AChE Inhibition, Antioxidant, Anticancer, Antibacterial, Antibiofilm Activity Against Multidrug-Resistant Bacteria and Molecular Docking Studies

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Abstract

In this study, hybrid nanoflowers (hNFs) were synthesized using quercetin-boronate as the organic component and zinc (Zn^{2+}) and copper (Cu^{2+}) ions as the inorganic components. The obtained nanostructures were characterized using field emission scanning electron microscopy (FE-SEM), energy-dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), and elemental mapping techniques. To evaluate their bioactivities, antioxidant properties, acetylcholinesterase (AChE) enzyme inhibition, anticancer effects against the human lung adenocarcinoma (A549) cell line, and antibacterial activities were investigated against non-resistant strains of *Staphylococcus aureus* (*S. aureus*), *Enterococcus faecalis* (*E. faecalis*), *Escherichia coli* (*E. coli*), and *Pseudomonas aeruginosa* (*P. aeruginosa*), as well as drug-resistant methicillin-resistant *S. aureus* (MRSA) and multidrug-resistant *E. coli* (MDR *E. coli*). Additionally, antibiofilm activities were examined against MRSA and MDR *E. coli* strains. Molecular docking studies were performed to investigate the interactions of the quercetin-boronate ligand with target proteins including 1EVE, 4EY7, 2W9S, 1JIJ, 3U2D, 6P9Z, and 6QXS, in correlation with the observed bioactivities. Notably, Quercetin-Boronate@Zn-hNFs exhibited greater activity compared to Quercetin-Boronate@Cu-hNFs in 2,2-diphenyl-1-picrylhydrazyl (DPPH), 2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS), and AChE inhibition assays, with IC_{50} values of 15.6, 2.7, and 43 µg/mL, respectively. The strongest antibacterial activity was exhibited by Quercetin-Boronate@Zn-hNFs against *S. aureus and E. faecalis*, with MIC values of 16 and 32 µg/mL, respectively. In contrast, Quercetin-Boronate@Cu-hNFs demonstrated activity against MRSA and MDR *E. coli* strains with a MIC value of 256 µg/mL. Furthermore, these hybrid nanoflowers exhibited dose-dependent antibiofilm activity. Docking scores for the quercetin-boronate ligand ranged from −5.598 to −9.152 kcal/mol, with the highest binding affinity observed against the 2W9S protein.

Keywords Nanoflower · Antimicrobial · Anticancer · Molecular docking · Quercetin boranate

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1 Introduction

Nanoflowers, also referred to as flower-shaped nanostructures, have garnered significant interest in recent years due to their unique properties, such as high surface area, non-toxicity, facile and cost-effective synthesis [1, 2]. In addition to their therapeutic properties, these structures have demonstrated a broad range of applications, including enzyme immobilization [3, 4], energy storage [5], and biosensor technologies [6]. The morphology and dimensions of synthesized nanoflowers vary depending on the type of metal used during synthesis [7]. Moreover, both the metal ions and the chemical agents employed in their fabrication have

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