عنوان مقاله:

Synthesis, Molecular Docking, and Anticancer Evaluation of New Azo-Based Sulfonamides against MCF ۷ Human Breast Cancer Cell Line

محل انتشار:

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خلاصه مقاله:

We synthesized a series of new azo-based sulfonamides ۸a-l via multistep chemical processes including chlorosulfonation, nucleophilic substitution, diazotization, and coupling reactions. The synthesized compounds were characterized using various physical and spectral techniques such as melting point, IR, ۱H- and ۱۳C-NMR, Mass, and elemental analysis. We evaluated the antibacterial and anticancer activities of compounds ۸a-l. The cytotoxicity of these compounds was assessed on the MCF-۷ breast cancer cell line and the MCF-۱۰ human normal cell line after ۴۸ h exposure. Notably, compound ۸h demonstrated significantly higher cytotoxicity against MCF-۷ ($IC_{۵۰}$ = ۰.۲۱ μM) while showing minimal toxicity towards the MCF-۱۰ human normal cell line. To gain insights into the molecular interactions, we utilized molecular docking to predict the binding affinity of these compounds to the FGFR۲ kinase receptor structure (PDB ID : ۴J۹۸). Compound ۸h exhibited the highest docking score, consistent with our experimental results and demonstrating favorable protein-substrate interactions. In addition, we performed ADME prediction of the compounds, indicating their potential as lead drug candidates. Furthermore, we evaluated the antibacterial activity of compounds ۸a-l against Gram-positive and Gram-negative bacteria. Compound ۸i showed the strongest antibacterial activity against Staphylococcus aureus, a Gram-positive pathogen. This study provides valuable insights into the biological activities .of azo-based sulfonamide derivatives, establishing their potential as both anticancer agents and antibacterial compounds

کلمات کلیدی:

Azo-based sulfonamide, Sulfonamide, breast cancer, Molecular docking, Cytotoxicity, antibacterial