

عنوان مقاله:

Synthesis, characterization, molecular docking studies and biological evaluation of some novel hybrids based on quinazolinone, benzofuran and imidazolium moieties as potential cytotoxic and antimicrobial agents

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خلاصه مقاله:

Objective(s): Hybridization of bioactive natural and synthetic compounds is one of the most promising novel approaches for the design of hit and lead compounds with new molecular structures. In this investigation, a series of novel hybrid structures bearing quinazolinone, benzofuran and imidazolium moieties were designed and synthesized. Materials and Methods: Novel hybrid compounds were prepared and their structures were characterized by spectral and analytical data. In order to evaluate the biological activities, the synthesized hybrid compounds were studied for in vitro antibacterial activity against three Gram positive bacteria (*Staphylococcus aureu*, *Bacillus subtilis*, *Listeria monocitogenes*) and three Gram-negative bacteria (*Escherichia coli*, *Pseudomonas aeruginosa*, *Salmonella entritidis*) and also, *Candida albicans* as one yeast-like fungi strain. Cytotoxic activities of the synthesized compounds were also evaluated by the MTT assay in the human breast cancer cell line (MCF- γ) and finally docking studies of cytotoxic derivatives were performed on aromatase enzyme. Results: The results of antimicrobial activity showed that compound 14e, with two halogen atoms on quinazolinone and benzofuran was the most active against all the tested strains of microorganisms with the MIC value 16-128 $\mu\text{g/ml}$. Some of the tested compounds showed good cytotoxicity on MCF- γ , and compound 14c with $\text{IC}_{50} = 0.59$ micromolar (μM) was found to be the most cytotoxic compound among the studied hybrid derivatives. The docking analysis showed acceptable binding interactions for these compounds. Conclusion: Based on the obtained results, the hybrid derivatives of quinazolinone, benzofuran and imidazolium could be regarded as efficient candidates for further molecular developments of anticancer and antimicrobial agents.

کلمات کلیدی:

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