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RESEARCH ARTICLE

Microwave-Promoted Multicomponent Synthesis Catalyzed by DABCO, Anti-Esophageal Cancer, Apoptotic Morphology, Kinetic Mechanism, and Computational Studies of New Pyrrole Derivatives

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ABSTRACT

In the present work, a microwave-promoted one-pot three components reaction catalyzed by 1, 4-diazabicyclo[2.2.2]octane (DABCO) was developed for the scalable synthesis of a new series of tetra-substituted pyrrole derivatives **4a-j**. The targeting pyrroles **4a-j** with a diverse functionality on the central pyrrole ring were examined for their antiproliferative activity using MTT assay on three esophageal squamous carcinoma cells (EC109, SKGT-4, and KYSE-450) in addition to two healthy cells (HET-1A and NE-1). Among the tested pyrrole derivatives, compounds **4e**, **4g**, **4h**, **4i**, and **4j** exhibited significant antiproliferative activity compared to cisplatin as a standard drug. In the cellular apoptotic test, the most potent derivatives are found to have a significant behavior for inducing apoptotic cell death in cancerous cells. After the kinetic mechanism model of enzymatic inhibition was determined, the pyrrole derivatives were conducted to molecular docking and molecular dynamics (MD) computations to investigate their potential interactions with the targeting proteins (code PDB ID: 5HZN, 6DUK, and 2LEO). The molecular docking and dynamics scores revealed that the most potent derivatives constituted good protein–ligand systems through hydrogen bonding and hydrophobic interactions. The experimental and theoretical findings revealed that the most potent pyrroles might occupy a significant position in esophageal cancer treatment.