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Design, molecular modeling, synthesis and biological evaluations of alkyl (aryl) amido 2,2-dichloroacetate derivatives based on Passerini multicomponent reaction

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Abstract

Dichloroacetate (DCA) as an orally available small molecule, that stimulates the activity of pyruvate dehydrogenase (PDH) enzyme by inhibiting the pyruvate dehydrogenase kinase (PDK), increases the flux of pyruvate into the mitochondria, navigating the cellular metabolism from glycolysis to glucose oxidation. This reverses the suppressed mitochondrial apoptosis and making cancer cells vulnerable towards apoptosis. In this study, a series of novel alkyl (aryl) amido 2,2-dichloroacetate derivatives were synthesized and their cytotoxic activities against various human cancer cell lines including MCF-7, HT-29, and Hela were evaluated. These compounds showed satisfactory potencies against the studied cancer cell lines. Docking studies were also done to find their binding site to PDK isoenzymes. Compounds A1 and A2 as the best cytotoxic compounds were also used to induce HT-29 cells apoptosis. Results show that these compounds might have a potential value for further study in drug development.

Biography

Davoud Afshar Faroji is an Associate professor in the Department of Microbiology and Virology, School of Medicine, Zanjan University of Medical Sciences, Zanjan, Iran. He has completed his Ph.D. in Tehran University of Medical Sciences, Iran. He have done about 70 publications.

Publications

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