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Synthesis, Characterization, and Biological Evaluation of 1,3,4-Mercaptooxadiazole Ether Derivatives Analogs as Antioxidant, Cytotoxic, and Molecular Docking Studies

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Abstract : Oxadiazoles and their derivatives with thioether functionalities represent a new and exciting class of physiologically active heterocyclic compounds. Several molecules with these moieties play a vital role in pharmaceuticals because of their diverse biological activities. This paper describes a new class of 1,3,4- oxadiazole-2-thioethers with acetophenone, coumarin, and N-phenyl acetamide residues (S-alkylation), with the hope that the addition of various biologically active molecules will have a synergistic effect on anticancer activity. The structure of the synthesized title compounds was determined by the combined methods of IR, proton-NMR, carbon-13-NMR, and mass spectrometry. Further, all the newly prepared molecules were assessed against their antioxidant activity. Furthermore, four compounds were assessed for their molecular docking interactions and cytotoxicity activity. The synthesized derivatives have shown moderate antioxidant activity compared to the standard BHA. The IC50 of the tilted molecules (11b, 11c, 13b, and 14b) observed for in vitro anti-cancer activities were 11.20, 15.73, 59.61, and 27.66 g/ml at 72-hour treatment time against the A549 cell lines, respectively. The tested compounds' biological evaluation showed that 11b is the most effective molecule in the series.

Keywords : antioxidant activity, cytotoxicity activity, molecular docking, 1, 3, 4-Oxadiazole-2 thioether derivatives
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