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2-Thioimidazole Analogues: Synthesis, in silico Studies and in vitro Anticancer and Antiprotozoal Evaluation

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Abstract : Substituted 2-Thioimidazole analogues have been synthesized and confirmed by advanced spectroscopic techniques. Among them, ten compounds have been selected and evaluated for their in vitro anti-cancer activity at the National Cancer Institute (NCI) for testing against a panel of 60 different human tumor cell lines derived from nine neoplastic cancer types. Furthermore, synthesized compounds were tested for their in vitro antiprotozoal activity, and none of them exhibited significant potency against antiprotozoans. It was observed that the tested all compounds seem effective on the UACC-62 melanoma cancer cell line as compared to other cancer cell lines and also exhibited the least potent in the Non-Small Cell Lung Cancer cell line in one-dose screening. In silico studies of these derivatives were carried out by molecular docking techniques and Absorption, Distribution, Metabolism, and Excretion (ADME) using Schrödinger software to find potent B-Raf kinase inhibitor (PDB ID: 3OG7). All the compounds have been performed for docking study; Compound D4 has a good docking score for melanoma cancer as compared with other.

Keywords : anticancer activity, cancer cell line, 2-thio imidazole, one-dose assay, molecular docking
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