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Title of the Thesis : Synthesis, Characterization and Therapeutic Potential of Novel Azole Derivatives

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Abstract

Cancer is a group of diseases involving cell or collection of cells exhibiting unrestrained growth, invasion and occasionally metastasis. These three characteristics of malignant cancers separate them from benign tumors, as they are self- controlled, and thus do not spread to other parts. Majority of cancers results in tumor formation.

In the quest of developing an effective heterocyclic compounds exhibiting anticancer activities more than 30 compounds were synthesized and characterized. The structure elucidation and assessment of purity of the compounds were confirmed through various spectroscopic techniques such as FT-IR, ^{1}HNMR, ^{13}CNMR, ESI-MS and CHN analysis.

1,3,4-oxadiazole with mercapto substituents were synthesized and evaluated for their anticancer activity against HepG2, (liver cancer cell line) and MCF-7 (breast cancer cell line) and their cytotoxicity were screened against human embryonic kidney epithelial (HEK-293) , 4 compounds showed better anticancer activity with more specificity and less toxicity in comparison to the standard anticancer drug Doxorubicin. Also, compound *2-(butylthio)-5-(p-aminophenyl)- 1,3,4-oxadiazole* act as potent apoptotic inducer and STAT3 inhibitor for MCF-7

breast cancer cell line. Compounds which include N-benzhydrylpiperazine-1, 3, 4-oxadiazoles conjugates, piperazine -2-azetidinones hybrids and imidazole clubbed with 2- azetidinone derivatives were screened for anticancer activity against Hela c(cervical cancer cell line) and their toxicity was evaluated on HEK-293 , among them 6 compounds bearing nitrogen and oxygen within ring framework showed much higher anticancer activity than the standard anticancer drug 5-Fluorouracil. Also, compounds *N-benzhydryl-4-((5-(4-aminophenyl)-1, 3, 4-oxadiazol-2-yl) methyl) piperazine, (N-(3-chloro-2-(3-nitrophenyl)-4-oxoazetidin-1-yl)-2-(4-phenylpiperazin-1-yl) acetamide)* and *(N-(2-amino-3-chloro-2-(4-oxoazetidin-1-yl)-2-(4-ethylpyridin-2-yl)-1H-imidazole-1-carboamideacetamide)* showed potential to induce apoptosis in HeLa cancer cells.

Incorporation of one or more pharmacophores into a single molecule lead to improvement in activity due to the synergistic effect of the two scaffolds.