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Synthesis of heteroannulated cyclopent[*b*]indoles: Exploration of *in vitro* cytotoxicity and molecular docking studies

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ABSTRACT

A series of novel cyclopent[*b*]indole analogues that hold isoxazolo-, pyrido-templates were designed and synthesized in good yields. The *in vitro* cytotoxicity was concerned for all the newly synthesized compounds by MTT assay against HeLa (cervix adeno carcinoma) and MCF-7 (breast cancer). These synthesized compounds were further compared with the standard drug ellipticine, 5-fluorouracil, cisplatin, and methotrexate. The synthesized heteroannulated cyclopent[*b*]indole compounds were found to show better cytotoxic activity against HeLa and MCF-7 with primary structure activity relationship studies. To identify with the nature of interactions of these molecules, we performed molecular docking studies using the protein kinase CK2 inhibitors. The docking results afforded some valuable information for the future design of more potent inhibitors.