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Design, synthesis and *in vitro* antiproliferation activity of some 2-aryl and -heteroaryl benzoxazole derivatives

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Abstract

Background: Phortress produces reactive electrophilic metabolites that form DNA adducts only in sensitive tumor cells. The authors converted the 2-phenylbenzothiazole nucleus in phortress to 2-aryl and -heteroaryl benzoxazole derivatives (11 new and 14 resynthesized). All synthesized compounds were studied for antitumor activity in various cancer cells. **Materials & methods:** Cytotoxicity, cell morphology, flow cytometry and cell-cycle analyses of compounds were performed and more active derivatives were tested in the MCF-7 cell line. **Conclusion:** Methyl 2-(thiophen-2-yl)benzo[d]oxazole-6-carboxylate (**BK89**) has a higher effect than fluorouracil to induce apoptotic cell death (apoptosis value of 49.44%). Cell-cycle analysis shows that the compounds **BK89** and methyl 2-(furan-2-yl)benzo[d]oxazole-6-carboxylate (**BK82**) can be used as potential cell-cycle blockers by arresting MCF-7 cells in G0/G1 phase at rates of 63% and 85%, respectively.

Plain language summary

There is an urgent need to develop potent and selective anticancer agents. In this study, the design and applications of compounds sensitive to specific cancer cells and targeting cancer cells were investigated. The results show that the synthesized compounds can be antiproliferative drug

candidates for breast cancer. These compounds may shed light on cancer treatment and cancer research.

Keywords: apoptosis • benzoxazole • cell-cycle • cytotoxicity • flow cytometry • molecular docking • phortress

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