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Synthesis of thiazolo[3,2-*a*]pyrimidine molecules, in vitro cytotoxic evaluation and molecular docking studies

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Abstract

Novel hybrid molecules of thiazolopyrimidine 4a–j have been prepared starting from various thiazoles 3a–j. The reaction of thiazoles 3a–j with thiourea yielded hybrid molecules 4a–j in an excellent yield. These molecules were screened for their anticancer activities against human breast carcinoma cell line (MCF-7), human lung adenocarcinoma cell line (A549) and human cervical cancer cell line (HeLa) using MTT assay. Among all molecules, compounds 4g and 4f exhibited potent cytotoxic activity. Compound 4g with IC_{50} value of 3.1 ± 0.4 µM and IC_{50} value of 9.8 ± 0.4 µM against A549 and HeLa cell line, respectively. Compound 4f with IC_{50} value of 6.8 ± 0.7 µM against MCF-7 molecular docking study of all synthesized molecules 4a–j was performed on

topoisomerase II using the AutoDock technique. All the synthesized thiazolopyrimidine hybrid molecules have been characterized and confirmed using spectroscopic techniques.

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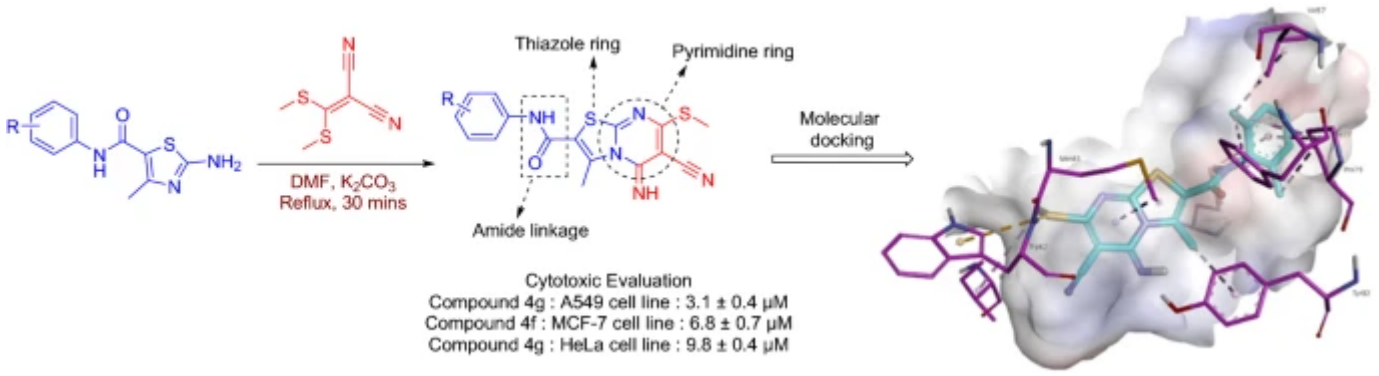

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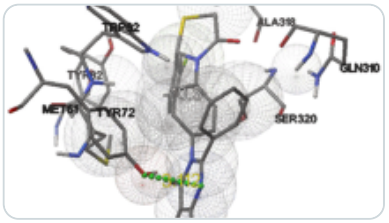

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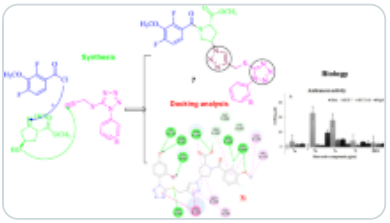

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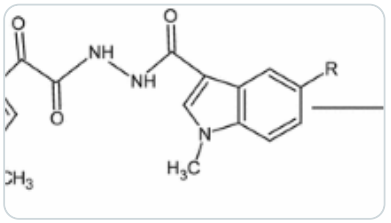

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Ethics declarations

Conflict of interest

The authors declare that they have no conflict of interest.

Ethical approval

This article does not contain any studies with animals performed by any of the authors.

Informed consent

Informed consent was obtained from all individual participants included in the study.

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