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One-Pot multicomponent synthesis of novel Pyrazole-Linked Thiazolyl-Pyrazolines: Molecular docking and cytotoxicity assessment on breast and lung cancer Cell-lines

Abstract:

Cancer remains a leading cause of mortality worldwide, with nearly 20 million new cases and close to 10 million deaths reported in 2022. Lung and breast cancers are among the most prevalent and deadly types, necessitating novel therapeutic approaches. Using a one-pot, multicomponent reaction strategy, this study aimed to synthesize a novel series of pyrazole-linked thiazolyl-pyrazolines. Optimal reaction conditions were identified by varying different types of bases and altering temperature, time, and solvent. The reaction gave the best yield with NaOH base at 50 oC with 2h stirring in ethanol solvent. We characterized the synthesized compounds using IR, mass spectrometry, and NMR spectroscopy. Molecular docking studies showed that these compounds strongly bind to the ErbB4 kinase, which suggests that they could be used as kinase inhibitors. Compounds 5E, 5F, and 5G exhibited potent cytotoxic effects on breast cancer cell lines, while compounds 5A, 5B, 5D, and 5G showed potent effects on lung cancer cell lines. The study highlights the importance of pyrazole-linked thiazolyl-pyrazoline scaffolds in developing effective cancer therapeutics and underscores the need for continued research in this area.

Biography

Umang Shah working as an Associate Professor at Ramanbhai Patel College of Pharmacy, CHARUSAT University, Changa. He had completed M.Pharm in Pharmaceutical Chemistry from The M.S. University of Baroda, Vadodara and Ph.D. in Pharmacy from CHARUSAT University. Dr. Shah has published more than 80 research/review articles and 02 book chapters and 10 books. Dr. Shah is one of the popular author of Pearson guide to Gpat book from Pearson Publication.