Indian Journal of Chemistry
Vol. 63, March 2024, pp. 286-292
DOI: 10.56042/ijc.v63i3.6682

Synthesis, spectral analysis and *in vitro* anticancer activity of 1,2,3-triazole derivatives and their molecular docking studies

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Received 9 November 2023; accepted (revised) 23 February 2024

Triazole derivatives are an absolutely essential class of compounds as they are involved in such a diverse range of pharmacological effects. In the field of medical chemistry, these nitrogen-containing heterocycles are used in the role of therapeutic medicines. The molecule with the given name has been synthesized by using click chemistry [Copper-Catalyzed Azide-Alkyne Cycloaddition (CuAAC)] with 1-propargyl-6-methoxy benzimidazolone as the dipolarophile and benzylazide as the dipole. A majority of the compounds show moderate to excellent efficacy when tested for anticancer properties against several cancer cell lines. The MCF-7 cell line is the most resistant to compounds **1a** and **1e**, with an IC_{50} value of 1.82 and 1.90 μM respectively. In contrast, the MDA - MB-231 and HeLa cell lines respond favorably to compounds **IVb**, **IVc** and **IVd**. Compound **IVa** is docked in the active site with EGFR as the target molecule. ^{1}H and ^{13}C NMR, IR and ESI-HRMS have been used to determine the structures of the newly synthesized compounds.

Keywords: Triazole, 1,3-Dipolar cycloaddition, Click reaction, Anticancer activity