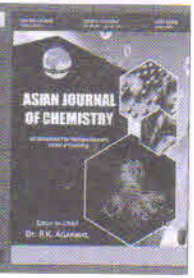
Asian Journal of Chemistry; Vol. 38, No. 1 (2026), 35-44

ASIAN JOURNAL OF CHEMISTRY

https://doi.org/10.14233/ajchem.2026.34730



Design and Synthesis of Fused 1,2,3-Triazolo-Pyrano-Quinazoline Using Copper(I) Catalysis: *In silico* Molecular Docking, *in vitro* Tyrosine Inhibition and ADMET Studies

SAIDI REDDY MODUGU[1], GOUTHAMI DASARI[2], SATHEESH KUMAR NUKALA[3,*], ASHOK KUMAR BAPURAM[4], RAJU MANNOORI[1] and BANDARI SRINIVAS[1,*]

[1]Department of Chemistry, Chaitanya Deemed to be University, Himayathnagar, Moinabad, Hyderabad-500075, India
[2]Department of Chemistry, J.B. Institute of Engineering & Technology, Yenkapally (V), Moinabad (M), Ranga Reddy (D), Hyderabad-500075, India
[3]Department of Chemistry, Government Junior College, Mustabad, Rajanna Sircilla-505404, India
[4]Department of Chemistry, Guru Nanak Institutions Technical Campus (GNITC B-Tech-I), Ibrahimpatnam, Ranga Reddy, Hyderabad-501506 India

*Corresponding author: E-mail: bandarisrinivas2005@gmail.com

Received: 20 August 2025 *Accepted*: 24 October 2025 *Published online*: 31 December 2025 AJC-22219

In this work, the synthesis of novel 1,2,3-triazolo-pyrano-quinazoline conjugates (**6a-n**) using well-known copper-catalyzed CuAAC and C-H arylation cascade reactions is carried out. The anticancer activity of these conjugates was evaluated against two human cancer cell lines, MCF-7 and HepG-2. The results showed that conjugate **6e** exhibited more potent activity compared to the standard drug erlotinib, while compounds **6b**, **6d** and **6f** displayed slightly lower activity compared to the standard drug. These four potent compounds (**6b**, **6d**, **6e** and **6f**) were assessed in a cell survival assay employing the normal breast cell line MCF-10A. None of them showed significant cytotoxicity, with IC_{50} values larger than 98.20 μM. *In vitro* tyrosine kinase EGFR inhibitory of four potent compounds were evaluated and results indicate that compound **6e** exhibited higher EGFR inhibitory activity compared to the standard drug erlotinib. On the other hand, compounds **6b** and **6f** displayed lower activity compared to both the standard drug and compound **6e**. Furthermore, the molecular docking studies were also performed on four potent conjugates and the results showed that these conjugates had more EGFR-binding interactions as compared to the standard drug erlotinib. Moreover, the *in silico* pharmacokinetic outline of the potent conjugates **6b**, **6d**, **6e** and **6f** was estimated by using SWISS/ADME and pkCSM and all the four conjugates followed Lipinski rule of five, Ghose, Veber, Egan and Muegge rules without any deviation.

Keywords: 1,2,3-Triazolo-pyrano-quinazoline conjugates, Anticancer activity, Molecular docking studies, Pharmacokinetic profile.