Indian Journal of Heterocyclic Chemistry
Vol. 35 - Number 04 (Oct-Dec 2025) 845-852
https://connectjournals.com/01951.2025.35.845
https://doi.org/10.59467/IJHC.2025.35.845

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Ethyl 5-methyl-7-(1,3-diaryl-1*H*-pyrazolyl)-4,7-dihydrotetrazolo[1,5-a] pyrimidine-6-carboxylate hybrids: Synthesis, biological, molecular docking, and ADME studies

Ayyanar Suguna Devi, Rajendran Aarthi and Chennan Ramalingan*
Department of Chemistry, School of Advanced Sciences, Kalasalingan Academy of Research and Education (Deemed to be University), Krishnankoil, Tamil Nadu, India

ABSTRACT Five ethyl 5-methyl-7-(1,3-diaryl-1*H*-pyrazolyl)-4,7-dihydrotetrazolo[1,5-a]pyrimidine-6-carboxylates **(7a-7e)** were designed and synthesized from aralkyl ketone and phenyl hydrazine through condensation, cyclization, and multi-component reactions. The outcome of radical scavenging evaluation reflects that all the synthesized molecular hybrids exhibited good activity, with the highest one being the hybrid **7d** (~83%), which is comparable to the standard ascorbic acid (~85%). Cytotoxicity examination indicates that molecular hybrids **7a** and **7d** showed appreciable activity and, among them, **7d** was identified as the most active one against SW1990 (IC_{50} ~19 μM) as well as MDA-MB-231 (IC_{50} ~28 μM). On comparing with the standard gemcitabine, **7d** exhibited superior activity. Further, **7d** displayed a significant binding affinity (−8.8 kcal/mol) while employing molecular docking with the protein BCL-2 (B-cell lymphoma 2). The outcome of the pharmacokinetics and physicochemical properties prediction analysis implies that **7d** has the potential to be developed into a successful medication.

KEY WORDS