Indian Journal of Heterocyclic Chemistry
Vol. 36 - Number 01 (Jan-Mar 2026) 23-28
https://connectjournals.com/01951.2026.36.23
https://doi.org/10.59467/IJHC.2026.36.23

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

Docking studies of 1,2,4-oxadiazole incorporated (2-(oxazol)-1*H*-imidazole) derivatives as anticancer agents

Suresh Bairi[1], Ramgopal Appani[2] and Laxminarayana Eppakayala[3]*

[1]Department of Pharmaceutical Chemistry, University College of Pharmaceutical Sciences, Palamuru University, Mahabubnagar, Telangana, India
[2]Department of Pharmaceutical Chemistry, School of Pharmacy, Anurag University, Hyderabad, Telangana, India
[3]Deapartment of Chemistry, Anurag University, Venkatapur, Ghatkesar, Hyderabad, Telangana 500088, India

ABSTRACT A new series of 1,2,4-oxadiazole-incorporated (2-(oxazol)-1H-imidazole) derivatives was designed and assessed through molecular docking to explore their potential as anticancer agents. The strategic fusion of oxadiazole and imidazole scaffolds was proposed to enhance pharmacological activity by strengthening binding affinity and molecular stability. In silico studies, including molecular docking against the tyrosine kinase targets epidermal growth factor receptor and human epidermal growth factor receptor 2, along with toxicity evaluations, were conducted to identify promising drug candidates. Several of the designed compounds demonstrated strong binding affinities and favorable interactions with key active-site amino acid residues. Among them, compound 1d showed the best overall balance of Absorption, Distribution, Metabolism, and Excretion properties and toxicity parameters, positioning it as the most promising anticancer lead.

KEY WORDS Oxadiazole–imidazole hybrids, Molecular docking, Epidermal growth factor receptor/human epidermal growth factor receptor 2 inhibitors, *In silico* absorption, distribution, metabolism, and excretion profiling, Anticancer drug design.

How to cite this article: Bairi, S., Appani, R. and Eppakayala, L. Docking studies of 1,2,4-oxadiazole incorporated (2-(oxazol)-1*H*-imidazole) derivatives as anticancer agents, *Indian J. Heterocycl. Chem.*, **2026**, *36*, 23–28. *https://doi.org/10.59467/IJHC.2026.36.23*