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Synthesis, *in vivo*, and molecular docking studies of 1,3,4-oxadiazole-quinoline conjugates as anticonvulsant agents

Neeru Rani[1]*, Pushpendra Kumar Shukla[2] and Rajnish Kumar[3]

[1]Research Scholar, Department of Pharmaceutical Chemistry, Teerthanker Mahaveer College of Pharmacy, Teerthanker Mahaveer University, Moradabad-244001, India

[2]Associate Professor, Department of Pharmaceutical Chemistry, Teerthanker Mahaveer College of Pharmacy, Teerthanker Mahaveer University, Moradabad-244001, India

[3]Associate Professor, Department of Pharmaceutical Chemistry, Noida Institute of Engineering and Technology (Pharmacy Institute), Greater Noida-201306, India

ABSTRACT A series of new benzylidene-{5-[2-(substituted phenyl)-1,2-dihydro-quinolin-4-yl]-[1,3,4]oxadiazol-2-yl} amines **(7a-o)** was synthesized by the reaction of (5-amino-[1,3,4]oxadiazol-2-yl)-[2-(substituted-phenyl)-1,2-dihydro-quinolin-4-yl]methanones **(6a-o)** with benzaldehyde and evaluated for antiepileptic potential. *In vivo* assessments were carried out using the maximal electroshock seizure (MES) and subcutaneous pentylenetetrazole (scPTZ) models, while molecular docking analyses were performed with AutoDock version 4.2. Among the tested compounds, **7c**, **7d**, **7h**, and **7l** exhibited notable anticonvulsant activity as compared to the standard phenytoin, without inducing neurotoxicity. The compounds, protected both MES and scPTZ models, also demonstrated antidepressant-like effects, as confirmed through motor activity testing with an actophotometer. These antidepressant effects suggested a dual mechanism of action, supporting the compounds' role as antiepileptic agents. Molecular docking studies further validated this by revealing interactions with key neurological targets, including the $GABA_A$ receptor. Compounds **7c**, **7d**, **7h**, and **7l** exhibited the highest binding affinities (−7.74–−9.39 kcal/mol) and showed strong interactions with amino acid residues VAL A:50, ARG A:192, GLU A:72, PHE A:98, ARG A:114, TYR A:126, and ASN A:149.

KEY WORDS 1,3,4-Oxadiazole, Quinoline, Antiepileptic activity, *In silico* studies, Maximal electroshock seizure, Subcutaneous pentylenetetrazole.

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