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In Association with: Association of Pharmaceutical Teachers of India (APTI) – Tamil Nadu Branch
ISBN: 978-81-971041-0-7 **08th January, 2026**

ECP-EP-012

DESIGN, SYNTHESIS, AND BIOLOGICAL ASSESSMENT OF 1,3,4-THIADIAZOLYL-BENZAMIDE DERIVATIVES AS PROMISING BRAF KINASE INHIBITORS: A COMBINED COMPUTATIONAL AND EXPERIMENTAL STUDY

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Objective: The primary objective of this study was to design, synthesize, and evaluate a novel series of 1,3,4-thiadiazolyl-benzamide derivatives as potential BRAF^V600E inhibitors for treating melanoma. This involved assessing their binding affinity via molecular docking, predicting pharmacokinetic properties through computational ADMET analysis, and determining in vitro cytotoxicity against melanoma cell lines to identify promising leads that overcome resistance to existing BRAF inhibitors like dabrafenib.

Methodology: Molecular docking using the BRAF crystal structure (PDB ID: 4LMN) revealed several candidates with strong predicted binding affinities and key interactions comparable to dabrafenib, with compound IA25 exhibiting the best docking score (−9.7 kcal/mol) and forming hydrogen bonds with Asn221 and Phe209. Computational ADMET evaluation suggested desirable pharmacokinetic behavior, chemical stability, and low toxicity.

Results: In vitro cytotoxicity screening against M-14 and B16-F1 melanoma cell lines demonstrated that IA25, IA11, and IA8 showed potent antiproliferative efficacy with IC_{50} values in the range of 33.93–40.62 nM. Overall, these results indicate that the synthesized thiadiazole–benzamide hybrids hold significant promise as potential BRAF-targeted anticancer leads for further optimization and preclinical studies.

Conclusion: Molecular docking using the BRAF crystal structure (PDB ID: 4LMN) revealed several candidates with strong predicted binding affinities. In vitro cytotoxicity screening against M-14 and B16-F1 melanoma cell lines demonstrated that IA25, IA11, and IA8 showed potent antiproliferative efficacy with IC_{50} values in the range of 33.93–40.62 nM.

Keywords: BRAF kinase, melanoma, 1,3,4-thiadiazole, benzamide derivatives, molecular docking, kinase inhibition, drug design.