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ABSTRACT BOOK

International Graduate Student Conference on Pharmaceutical Sciences (IGSCPS) 2023

Theme

"Pharmacy and Pharmaceutical Science Contributions to Sustainable Development Goals: Good Health and Well-being"

Faculty of Pharmacy Universitas Airlangga

OP012

SYNTHESIS AND EVALUATION OF ACRYLAMIDE DERIVATIVE AS PROSPECTIVE IMAGING AGENT FOR LUNG CANCER

Muammar FAWWAZ (1,2,*), Kenji MISHIRO (3), Muzakkir BAITS (1), Mamat PRATAMA (1), Ryuichi NISHII (4), Kazuma OGAWA (2),

1 Laboratory of Pharmaceutical Chemistry, Faculty of Pharmacy, Universitas Muslim Indonesia, Indonesia
2 Graduate School of Medical Sciences, Kanazawa University, Japan
3 Institute for Frontier Science Initiative, Kanazawa University, Japan
4 Biomedical Imaging Sciences, Department of Integrated Health Sciences, Graduate School of Medicine, Nagoya University, Japan.
muammar.fawwaz@umi.ac.id

ABSTRACT

The use of radiotracer in cancer diagnostics has attracted attention because it is accurate and non-invasif. Radioimaging agents based on third generation tyrosine kinase inhibitors (TKIs) have been developed to assess the sensitivity of non small cell lung cancer (NSCLC) patients to therapy. However, these radiotracers have not been able to stratify sensitive patients to the TKIs therapy. Thus, this study aims to provide an iodine-induced olmutinib derivative (I-OTB) with prospects for development as a radioactive imaging agent for NSCLC patients. Molecular docking was used to estimate the interaction of the I-OTB receptor complex by the AutoDock Vina program package. The synthesis method used to prepare the novel compound refers to previous studies by incorporating an iodine atom into the phenyl group in the 3-arylocyanilide structure. Furthermore, I-OTB activity was evaluated through a cytotoxicity test against NSCLC cell lines. The half inhibitory concentration (IC50) was determined using a 2-(2-methoxy-4-nitrophenyl)-3-(4-nitrophenyl)-5-(2,4-disulfophenyl)-2H tetrazolium monosodium salt (WST-8) assay. Docking studies show that I-OTB can carry out similar interactions with the parent compound. The binding energies of OTB and I-OTB in complex with EGFR T790M are -8.7 and -7.9 kcal/mol, respectively. We successfully synthesized I-OTB by multisteps reaction. The WST-8 assay exhibited that the cytotoxic effect of I-OTB was comparable to that of OTB. I-OTB had an affinity for the EGFR L858R/T790M mutation with an IC50 of 10.49 ± 5.64 μM compared to EGFR wild type with an IC50 of more than 10 μM. These results indicate that the iodine substituent in OTB could retain the selectivity of the parent compound against the EGFR L858R/T790M. Therefore, I-OTB stands out for radioiodination, and [123/124I]I-OTB may be a promising candidate for imaging the EGFR L858R/T790M mutation

Keyword: Acrylamide, molecular docking, NSCLC, olmutinib, tyrosine kinase inhibitor

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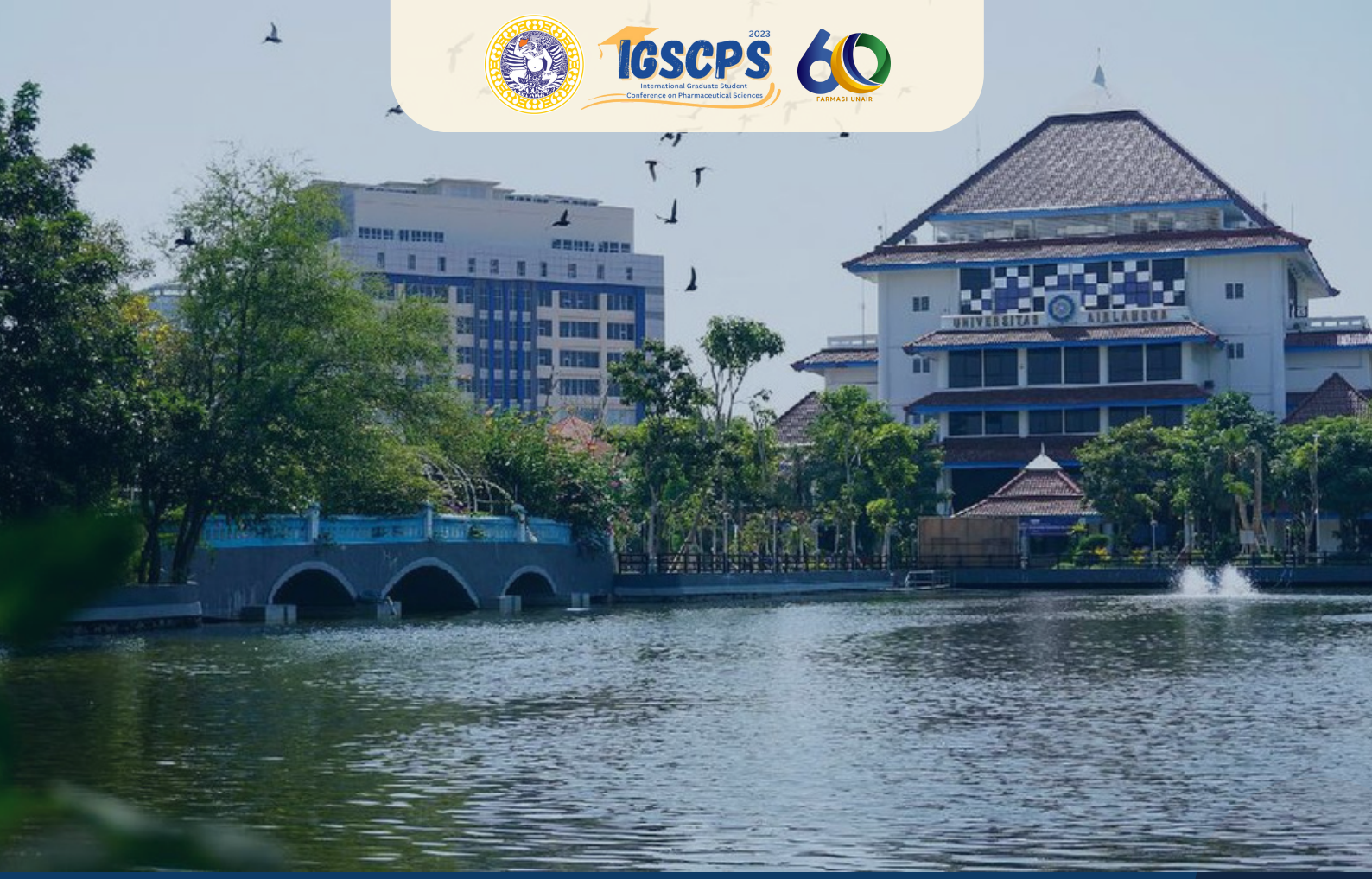

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