
QSAR modelling, molecular docking, and ADMET studies of imidazole pyridine derivatives toward anticancer drug development

Lavanya Devi G*, Liji Muthirakalayil and Venugopal Rajendiran

Department of Chemistry, School of Basic and Applied Sciences,

Central University of Tamil Nadu, Thiruvarur 610101

(Email: glavanyad@gmail.com)



Abstract

Cancer is one of the most dangerous diseases that can affect any part of our body, leading to death. In simple words, it can be defined as the proliferation of cells that prevents apoptosis. Heterocyclic derivatives play a crucial role in the discovery of cancer drugs. Imidazolepyridines are heterocyclic compounds that are biologically active and exhibit a wide range of pharmacological activities. They are formed by the fusion of an imidazole ring with a pyridine ring. Similarly, imidazolepyridine derivatives also exhibit a broad spectrum of biological activity, especially antitumor activity. In this study, the activities of different substituted imidazolepyridine derivatives such as 2-(1-phenylimidazo[1,5- α]pyridine-3-yl)-phenol (L1) and methyl (L2), methoxy (L3), fluoro (L4), nitro (L5) substituted 2-(1-phenylimidazo[1,5- α]pyridine-3-yl)-phenol were predicted through a QSAR model with different protein targets, such as tubulin and EGFR (Epidermal Growth Factor Receptor). A QSAR model for EGFR was built using the OLS (Ordinary Least Squares) method with an R² score of 0.898 and an MSE score of 0.444, whereas for tubulin, the model was built using the XGBRegressor method with an R² score of 0.611 and an MSE score of 0.213. Among the five compounds, the nitro- and methoxy-substituted heterocyclic compounds have shown the highest inhibition activity with EGFR and tubulin, respectively. Further, molecular docking and ADMET analyses also support the QSAR result. The systematic investigation will be presented.

Keywords: Anticancer drug, imidazolepyridines, QSAR, molecular docking, ADMET

Reference

Yadav, D. K., Kumar, S., Saloni, Singh, H., Kim, M. H., Sharma, P., Misra, S., & Khan, F. (2017). Molecular docking, QSAR and ADMET studies of withanolide analogs against breast cancer. *Drug Design, Development and Therapy*, 11, 1859–1870.

<https://doi.org/10.2147/DDDT.S130601>