Frontiers in Pharmaceutical, Material, and Environmental Sciences: Innovative Approaches and Applications

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Chapter – 5

Synthesis of oxindole Schiff's base derivatives: Drug likeness and ADMET studies

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Abstract

Our research goes to the synthesis of oxindole derivatives as newly drug-like small molecules. However, we synthesized oxindole-Schiff's bases (3a–b) and demonstrated computational chemistry and comparative studies with the standard multi-purpose FDA-approved Bevacizumab anticancer drug. All the synthesized compounds (3a and 3b) were characterized using UV and FT-IR spectral analysis. Further the drug-likeness properties of the synthesized compounds were demonstrated through *in–silico* studies as a preliminary investigation. We found that synthesized compounds showed drug-like properties due to the molecular weight (M.W. < 500 Da), the number of H-bond donors (HBDs: < 5), H-bond acceptors (HBAs: < 10), rotatable bonds (<10), topological polar surface area (TPSA) not higher than the thresholds of 140 $Å^2$, and the octanol-water partition coefficient (Log P) not exceeding the value of 5 constitute a number of these descriptors. In the future, the newly synthesized oxindole derivatives could be analyzed as anticancer properties against various cancer cell lines through *in-vitro* as well as *in-vivo* studies.

Keywords: Oxindole, Schiff base, ADMET, drug-likeness

[14] Van Beijnum, J. R., Huijbers, E. J. M., van Loon, K., Blanas, A., Akbari, P., Roos, A., Wong, T. J., Denisov, S. S., Hackeng, T. M., Jimenez, C. R., Nowak-Sliwinska, P., & Griffioen, A. W., (2022). Extracellular vimentin mimics VEGF and is a target for anti-angiogenic immunotherapy. *Nature Communications 2022 13:1*, *13*(1), 1–20

[15] Wang, X., Liu, J., Xu, L., Hao, Z., Wang, L., & Xiao, J., (2015). Friedel–Crafts alkylation of heteroarenes and arenes with indolyl alcohols for construction of 3,3-disubstituted oxindoles. *RSC Advances*, *5*(123), 101713–101717

[16] Waring, M. J., Ben-Hadda, T., Kotchevar, A. T., Ramdani, A., Touzani, R., Elkadiri, S., Hakkou, A., Bouakka, M., & Ellis, T., (2002). 2,3-Bifunctionalized quinoxalines: synthesis, DNA interactions and evaluation of anticancer, anti-tuberculosis and antifungal activity. *Molecules*, *7*(8), 641–656

[17] Yu, Q., Guo, P., Jian, J., Chen, Y., & Xu, J., (2018). Nine-step total synthesis of (-)-strychnofoline. *Chemical Communications*, *54*(9), 1125–1128

[18] Zhang, J. L., Ye, W. L., Zhang, J., Hu, X. Q., & Xu, P. F., (2021). Enantioselective Construction of Polycyclic Indazole Skeletons Bearing Five Consecutive Chiral Centers through an Asymmetric Triple-Reaction Squence. *Organic Letters*, *23*(13), 5033–5038

[19] Zhao, Y. H., Le, J., Abraham, M. H., Hersey, A., Eddershaw, P. J., Luscombe, C. N., Boutina, D., Beck, G., Sherborne, B., Cooper, I., & Platts, J. A., (2001). Evaluation of human intestinal absorption data and subsequent derivation of a quantitative structure - Activity relationship (QSAR) with the Abraham descriptors. *Journal of Pharmaceutical Sciences*, *90*(6), 749–784.