World Academy of Science, Engineering and Technology
International Journal of Pharmacological and Pharmaceutical Sciences
Vol:17, No:11, 2023

Construction of QSAR Models to Predict Potency on a Series of substituted Imidazole Derivatives as Anti-fungal Agents

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Abstract : Quantitative structure–activity relationship (QSAR) modelling is one of the main computer tools used in medicinal chemistry. Over the past two decades, the incidence of fungal infections has increased due to the development of resistance. In this study, the QSAR was performed on a series of esters of 2-carboxamido-3-(1H-imidazole-1-yl) propanoic acid derivatives. These compounds have showed moderate and very good antifungal activity. The multiple linear regression (MLR) was used to generate the linear 2d-QSAR models. The dataset consists of 115 compounds with their antifungal activity (log MIC) against «Candida albicans» (ATCC SC5314). Descriptors were calculated, and different models were generated using Chemoffice, Avogadro, GaussView software. The selected model was validated. The study suggests that the increase in lipophilicity and the reduction in the electronic character of the substituent in R1, as well as the reduction in the steric hindrance of the substituent in R2 and its aromatic character, supporting the potentiation of the antifungal effect. The results of QSAR could help scientists to propose new compounds with higher antifungal activities intended for immunocompromised patients susceptible to multi-resistant nosocomial infections.

Keywords : quantitative structure–activity relationship, imidazole, antifungal, candida albicans (ATCC SC5314)
Conference Title : ICPP 2023 : International Conference on Pharmacy and Pharmacology
Conference Location : Paris, France
Conference Dates : November 27-28, 2023