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27. QSAR analysis of Second Generation Analogues of the Cancer Drug Clinical Candidate Tipifarnib for Anti-Chagas Disease

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Abstract:

In the present work, QSAR analysis was performed for second generation analogues of the cancer drug clinical candidate Tipifarnib for anti-Chagas disease. The analysis was successful in identifying the key structural features that steer the bio-action of Tipifarnib derivatives as anti-Chagas agent. Multiple modelsusing multiple splitting weredeveloped using the genetic algorithm-multilinear regression (GA-MLR) method. The developed models are biparametric with $R^2 > 0.75$, $Q^2 > 0.70$ and $R^2_{ext} > 0.80$. The models are robust with good external predictive ability. The models reveal that the anti-Chagas activity of Tipifarnib analogues has good correlation with the geometrical descriptor and topological charge descriptor.

Introduction:

Chagas disease, a disease usually spread by contact with an infected triatomine bug also called “kissing bug,” “benchuca,” “vinchuca,” “chinche,” or “barbeiro”, is one of the most neglected parasitic diseases that can cause serious heart and stomach illnesses.The disease with its major presence in the tropical regions viz. Africa and Latin America, affects more than ten million peoples each year. Trypanosoma cruzi (T. cruzi), the protozoan parasite, is the causative agent of Chagas disease. After infection, generally, the individuals become a permanent host to the parasite due to the lack of effective cure in the chronic stage of the disease. The chemotherapy heavily relies on severly toxic drugs like nitrofuran, nifurtimox, benznidazole and