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3D QSAR studies of Salicylanilide benzoates derivatives & generation of new leads as Mycobacterium tuberculosis inhibitors

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Abstract : Tuberculosis is one of the tenth primary cause of death throughout the world. The increasing number of drug resistance TB cases day by day and the patient poor compliance for the prolong treatment crating a alarming situation. The best tool to create the lead compounds for any disease is can only be achieved through the Combination of ligand and structure-based approaches. We have carried out comparative molecular field analysis(CoMFA) and comparative molecular similarity indices analysis (CoMSIA) on the reported series of Salicylanilide 4-(trifluoromethyl)benzoates&2-hydroxy-N-phenylbenzamides derivatives as Mycobacterium tuberculosis inhibitors. In CoMFA model, the cross validated q^2 and the non-cross validated r^2 value for training set were found as0.643and 0.945, respectively; while in CoMSIA model, q^2 value was 0.819and r^2 value was 0.954. The generated contour maps (CoMFA & CoMSIA) fields were used for the design of 35 novel2 & 3-(4-aminobenzamido) benzoic acid derivatives and the prediction the pMIC of the design series were carried out. The series is also checked for the toxicity using osiris property explorer which could be explored in future to identify novel Mycobacterium tuberculosis inhibitors.

Keywords : 3D QSAR, CoMFA, CoMSIA, Salicylanilide Benzoates, Mycobacterium Tuberculosis.

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