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3D-QSAR studies of Benzoxazinones: Analogs of Efavirenz

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Surendra Kumar · Reena Rachel Jacob · Meena Tiwari

Abstract

In the present study, a set of 14 analogs of Efavirenz with human immunodeficiency virus-1 (HIV-1) reverse transcriptase (RT) inhibitory activity, were subjected to 3D-QSAR studies. Various combinations of thermodynanic, electronic and steric descriptors were used in order to understand the physicochemical properties desirable for interaction with the receptor. Multiple linear regression analysis was performed, using VALSTAT, to select the descriptors and to generate various models that relate the structural features to the biological activity. Among them, an informative and statistically significant model both in fitting and predictive ability (r = 0.9354 and r cv2 = 0.8059) was selected. Cross-validation was performed using leave-one-out (LOO) and bootstrapping method. The significant model indicated that the thermodynamic descriptors, viz., Henry's law constant and stretch bend energy play an important role in RT inhibitory activity. Consequently, the best QSAR model will be of major importance to aid the design of new HIV-1 reverse transcriptase inhibitor.