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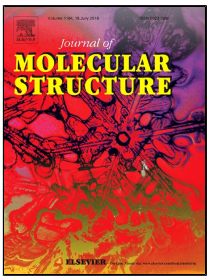

QSAR Studies of TIBO derivatives as HIV-1 reverse transcriptase inhibitors Using HQSAR, CoMFA and CoMSIA

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QSAR Studies of TIBO derivatives as HIV-1 reverse transcriptase inhibitors Using HQSAR, CoMFA and CoMSIA

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Abstract: The study deals with CoMFA, CoMSIA and HQSAR to explore the important features of tetrahydroimidazo[4,5,1-jk][1,4]benzodiazepinone (TIBO) derivatives for exerting potent HIV-1 reverse transcriptase (HIV-1 RT) inhibitors activity. The cross-validated q^2 value of CoMFA model is 0.641 and the non-cross-validated r^2 value is 0.847. The best cross-validated q^2 value of CoMSIA Model is 0.706 and the non-cross-vaildated r^2 value is 0.939. The most effective HQSAR model was obtained that the cross-validation q^2 value of 0.839, the non-cross-validated r^2 value of 0.942, the standard error of prediction SD_{CV} value of 0.604, and the best hologram length value of 307 using atoms and bonds as fragment distinctions. The statistical parameters from models indicate that the data are well fitted and have high predictive ability. Furthermore, Molecular docking was employed to explore the binding requirements between the ligands and the receptor protein which included several hydrogen bonds between the TIBO inhibitors and active site residues. Observations derived from these QSAR modeling study may be utilized further in designing promising HIV-1 reverse transcriptase inhibitors.

Key Words: HIV-1 reverse transcriptase inhibitors; CoMFA ; CoMSIA; HQSAR; Molecular docking

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