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Research article

3D-descriptors in modeling the dipeptidyl peptidase IV (DPP-4) inhibition activity: Derivatives of β-Aminoamide bearing subsituted triazolopiperazines

Raghuraj Parihar, Afsar Jahan, Brij Kishore Sharma*

Department of Chemistry, Government College, Bundi-323 001 (Rajasthan), India.

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***Corresponding Author: Brij Kishore Sharma,** Department of Chemistry, Government College, Bundi-323 001 (Rajasthan), India.
Email id: bksharma_sikar@rediffmail.com

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Abstract

The DPP-4 and DPP-8 inhibitory activity of triazolopiperazines have been quantitatively analyzed in terms of 3D-Dragon descriptors. The derived QSAR models have shown that atomic properties played pivotal role in terms of weighted radial distribution functions, 3D-MoRSE signals, component symmetry directional WHIM index and moment expansions. The CP-MLR indentified RDF, 3D-MoRSE, WHIM and GETAWAY descriptors, unweighted or weighted with atomic properties endow relevant molecular 3D informations about molecular size, shape, symmetry, atom distribution, effective position of substituents and fragments in the molecular space, hold promise for rationalizing the DPP-4 and DPP-8 inhibitory actions of triazolopiperazines. The values of statistical parameters, Q^2_{LOO} and r^2_{Test} ensure that the models have validated internally and externally, both and the predictions are reliable and acceptable. PLS analysis has further confirmed the dominance of the CP-MLR identified descriptors. Applicability domain analysis revealed that the suggested models have acceptable predictability. All the compounds are within the applicability domain of the proposed models and were evaluated correctly.