Alignment Independent 3D-QSAR Study of AT1 Inhibitors as Anti- hypertensive Drugs

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Abstract: The renin-angiotensin system (RAS) plays an important role in the regulation of blood pressure through the actions of angiotensin II (AT1) (vasoconstriction, aldosterone secretion, renal sodium reabsorption). Excessive activity of the AT1 causes increased blood pressure thus is an appropriate target for developing novel anti-hypertensive drugs. In order to understand the structural characteristics correlated with the potency of AT1 inhibitors, a Molecular Interaction Fields (MIF) based alignment independent three-dimensional quantitative structure-activity relationship (3D-QSAR) study was conducted. The resulted model PLS analysis indicated that the computed activities were in excellent agreement with experimentally observed values (R^2 = 0.89, Q^2_{LOO} = 0.83 and R^2_{Pred} = 0.873) [1-3].

Keywords: 3D-QSAR; anti-hypertension ; AT1

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