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3D QSAR of 4, 5-diaryl imidazoline as P2X7 receptor antagonists, using pharmacophore based alignment

Nisha M[1], Sukhvir C[1], Malkeet Singh B[2] and **Om S[1]**
[1]Punjabi University, India
[2]Bar Ilan University, Israel

Introduction: Purinergic receptors, also known as purinoceptors, are ligand-gated membrane ion channels involved in many cellular functions. Among all identified purinergic receptors, P2X7 subform is unique since it induces the caspase activity, cytokine secretion, and apoptosis. The distribution of P2X7 receptors and the need of high concentration of ATP required to activate this receptor exhibited its ability to function as a 'danger' sensor associated with tissue inflammation and damage. Present work describes the atom based 3D QSAR analysis using pharmacophore-based alignment to explore the essential three-dimensional structural feature requirements of study molecules for better antagonism of P2X7 receptor.

Method: The best pharmacophore model (HPRRR.13) was developed and used to align study molecules for 3D QSAR analysis. The best QSAR model (HPRRR.134) generated with PLS factor 4 showed good values of statistical parameters i.e. R2 training, SD, F-value, q2 test, and Pearson-rtest.

Results: The contours of different properties generated using the best model was able to explain the variation in the activity of dataset with respect to these properties. The best pharmacophore model was subjected to screen in-house database where it picks some molecules that are reported as COX-2 inhibitors in the literature. Thus, generated pharmacophore based 3D QSAR model may successfully be used to design new potent congener representatives.

Conclusion: In this article, we tried to explore various aspects of $P2X_7$ receptors including therapeutic potential, and recent discoveries and developments of $P2X_7$ receptor antagonists. The newly developed potent antagonists of $P2X_7$ receptor would serve as a novel therapeutic agent to combat various inflammatory conditions.

nishamehta0009@gmail.com