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3D QSAR Pharmacophore based Virtual Screening and Molecular Docking for Identification of Potential IGF1R Inhibitors for Cancer Treatment

Yesuraju Konda[1], Bajibaba Shaik[2], Kalyani Paidikondala[2], Rambabu Gundla[2]* and Aparna Pasula[1]*

1. Department of Chemistry, Jawaharlal Nehru Technology University, Hyderabad, Telangana, **INDIA**
2. Department of Chemistry, GITAM deemed to be University, Hyderabad, **INDIA**

Email: rgundla@gmail.com, aparnapasula@jntuh.ac.in

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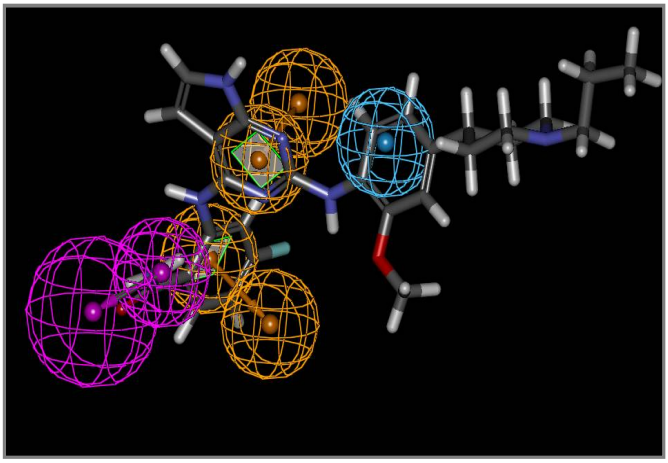
ABSTRACT

3D pharmacophore models were developed using chemical features for IGF1R based on the known inhibitors using Discovery Studio 2.0 and validated using external test set. The best pharmacophore model, Hypo1, includes hydrogen bond donor, hydrophobic and ring aromatic features, which has the highest correlation coefficient (0.90), cost difference (77.80), low RMS (1.55), as well as it shows a high goodness of fit and enrichment factor. Hypo1 was used as a 3D query for virtual screening to retrieve potential inhibitors from GOSTAR and ZINC databases. The hit compounds were subsequently subjected to molecular docking studies and finally, 44 compounds were obtained based on consensus scoring function for biological evaluation.

Graphical Abstract



Best pharmacophore model Hypo1 aligned to training set active Compound 1-1.

Keywords: IGF1R, Pharmacophore, HYPOGEN, Molecular docking, Ligand Fit, Cancer.