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Atom based 3D-QSAR of Quinoline derivatives and pharmacophore based virtual screening for identification of selective Phosphodiesterase 4B inhibitors

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Phosphodiesterase 4B (PDE4B) hydrolyses cyclic adenosine monophosphate (cAMP) and thus regulates its intracellular levels. The enzyme has been proposed as a potential drug target against diseases like inflammation and chronic obstructive pulmonary disease. But use of current PDE4B inhibitors is limited due to dose-dependent nausea and vomiting. Adverse effects associated with current PDE4B inhibitors are possibly results of PDE4D inhibition, a highly similar homolog of PDE4B. Here we considered quinoline analogs and applied ligand-based pharmacophore and atom based 3D-QSAR modeling with structure-based docking and ADME approach. A 5-point pharmacophore model was developed and used to derive a predictive 3D-QSAR model for studied dataset. The obtained r2 and q2 values were 0.96 and 0.91 respectively. The result suggested that the generated 3D-QSAR model is reliable and can be considered for PDE4B activity prediction. Further, pharmacophore model was employed for virtual screening to identify potent PDE4B inhibitors. The selective ligands for PDE4B identified through docking and prime binding energy analysis of ligands in both PDE4B and PDE4D. ADME analysis was performed to confirm the drugeability of selective ligand.

Biography

Vidushi Sharma is a Ph.D student in the deptt of pharmaceutical chemistry in Delhi Institute of Pharmaceutical Sciences and Research (DIPSAR) (affiliated to university of Delhi). After finishing her masters in pharmaceutical chemistry (from DIPSAR) she worked as an assistant professor (~ 2 years). She is currently doing her PhD on a "Departent of Science and Technology (DST)" funded project which is entitled as "Design, synthesis and biological evaluation of phosphodiesterase-4b inhibitors". She has one national and two international publications (recently accepted).

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