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INDOLIZINE DERIVATIVES AS PHOSPHODIESTERASE IV INHIBITORS: DEVELOPMENT AND VALIDATION OF PHARMACOPHORE MODELS

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The challenges of drug discovery are largely overcome by computer aided designing and among various drug designing techniques, ligand based drug designing proves to be an effective one. Looking at the usefulness, in the present investigation ligand-based pharmacophore models has been developed by analyzing common chemical features of phosphodiesterase IV (PDE4) inhibitors. A dataset of 38 indolizine derivatives was selected in order to built pharmacophore models which were developed by using pharmacophoric features *viz.* hydrogen bond acceptor (A) and aromatic ring (R). In order to build up a statistically significant model, ARRRR.30 hypothesis was selected among different developed hypothesis with a R^2 value 0.880. The selected hypothesis ARRRR.30 was further validated by performing external validation on a test set where R^2 was found to be 0.804 (between experimental and predicted activity). The developed model could be an efficient tool to develop new PDE4 inhibitors

Corresponding author: **Dr. Vipin Kumar**
Tel.: +91 9416391274

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Sharma V, Sharma PC, Kumar V*
Department of Pharmacy, School of Chemical Sciences and Pharmacy,
Central University of Rajasthan, Ajmer, Rajasthan, India
e-mail: *vipkumar@curaj.ac.in*