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Model development for P-glycoprotein inhibitors using Random forest method

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Drug discovery is very expensive as it involves expenditure of large amount of money, manpower and time. It involves biological evalution of large set of diverse molecules. However, now a days drug discovery has been facilitated by numerous computational methodologies to shorten the lengthy process. QSAR (Quantitative structure-activity relationship) tools are well know for the prediction of activity of closely related analogs. However these methods significantly depends on the nature of training sets and have high predictive power when applied to compounds structurally related to the compounds included in the training set. And have poor predictive power when applied to structually diverse molecules. In the current study of P-glycoprotein inhibitors. Model development carried out on more than 150 compounds. The compounds along with activities has been devided into training sets (for model development) and test compounds (for validation). Descriptors generaed using DRAGONH. Random forest (Number of tress used is 1000) used for model development with Q2 more than 0.75.

Biography

Veerendhar has completed his PhD in Organic Chemistry from University of Hyderabad and Postdoctoral studies from The Hebrew University of Jerusalem, Israel. He has two US patents to his credit. He is working as a Principal Scientist in a premier Pharmaceutical industry and also persuing Business Analytics and Master Black Belt at Indian Statistical Institute. He has published his research work in eight reputed journals.

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