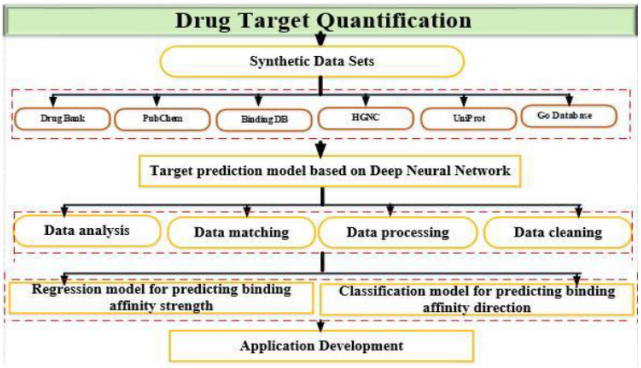
# Molecular diagnosis: Drug target evaluation based on deep neural network prediction techniques

**AR JUNEJO, Li Xiang**
Harbin Institute of Technology, China

With the continuous improvement of computer performance and related technology, the combination of Artificial Intelligence (AI) and Bioinformatics can find new drugs more efficiently. However, most of the current researches focus on the prediction of drug target binding affinity and the determination of drug targets. In this work, the quantitative prediction model of drug target is established by combining of Network Bioinformatics and Deep Neural Network (DNN). It includes a regression model for predicting the strength of drug target binding affinity and a classification model for predicting the direction of drug target. After collecting, processing, and matching the data in the major bioinformatics databases, a classification and a regression model are built based on KERAS online library. Moreover, the performance of the model is verified by cross-validation techniques. Finally, the prediction of the strength and direction of binding affinity between drugs and targets is achieved. In addition, to expand the application of the model, by combining Genetic Ontology Database, by combining medicine, a multi-layer network model is recognized. Our works aims to establish a drug target quantification model, in the future reveal the theoretical basis of medicine, and serve for drug screening, drug reorientation, drug development and other fields. After improving of model, the characteristics of data are analyzed, which is composed of similarity vector of 7306 - dimension and drug selection. The model is single output regression model, the partition ratio of data set is 98:1:1, the loss function is MSE, and the evaluation criteria are consistent with each other. The model in the performance of the test set is categorical-cross entropy = 0.2201□categorical-accuracy = 0.9816, F1 score, precision and recall are 0.9648, 0.9646 and 0.9640respectively.



## Biography

AR JUNEJO has expertise in evaluation and analysis in improving the Drug Target and Deep Neural Network, Artificial Intelligence (AI), Molecular Diagnosis. His open and contextual evaluation model based on responsive constructivists creates new pathways for improving healthcare. He has built this model after years of experience in research, Deep Innovation 2B Lab, and Technology Innovation building Lab science park, Harbin Institute of Technology. The methodology that utilizes the previous generations of evaluation: measurement, description and judgment. It allows for value-pluralism. This approach is responsive to all stakeholders and has a different way of focusing.