International Journal of Computer
Science and Engineering (IJCSE)
ISSN (P): 2278–9960; ISSN (E): 2278–9979
Vol. 12, Issue 2, Jul–Dec 2023; 11–20

International Academy of Science,
Engineering and Technology
Connecting Researchers; Nurturing Innovations

AN INSIGHT REVIEW ON BIG DATA ANALYTICAL MODELS OF COMPUTATIONAL PHARMACOLOGY IN ATTENTION-DEFICIT/HYPERACTIVITY DISORDER (ADHD)

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ABSTRACT

Attention-deficit/hyperactivity disorder (ADHD) is the foremost neurodevelopmental disorder in childhood. Trouble in paying attention and controlling impulsive behaviour. Predominant hyperactive and Impulsive behaviour are the various symptoms of ADHD. Drug Analysis is the most cogent process in the pharmaceutical industry. The main aspect of this Review is to scrutinize vvarious computational methods and models that curtail the cost and time of drug analysis. Multiscale computational methods used in identifying the drug efficacy of an individual drug with combinations& dosage levels of drugs, half-life period, and level of drug ligand interactions to identify the immunological reactivity of drugs in the human body were conferred in this Review. Various algorithms, namely Rank Correlations and scoring Functions, Association Rules,Artificial Neural Networks (ANN), Quantitative Association Rule,Decision trees (DT), convolutional neural networks (CNN), K-nearest neighbours (KNN), random forests (RF), Support vector machines (SVM), Advances in Deep Learning, principal component analysis (PCA) and independent component analysis (ICA), the Apriori algorithm, hierarchical clustering, and Anomaly detection was launched for drug analysis. These were compared with the conventional techniques of online screening systems (e.g., Pharmacophore Modelling, QSAR and molecular docking) forligand-based, novo drug design. This proves that the machine learning algorithms accord more accuracy and desired results in time with rapid drug analysis. Future trends in drug design and screening will involve combining various methodologies to handle complex problems of many sizes and dimensions.

KEYWORDS: *Virtual Screening, Multiscale Model, Machine Learning, De Novo Design, ADHD, ANN, K-Mean, KNN, PCA, QSAR, Molecular Docking, Pharmacophore Modelling*

Article History

Received: *02 Dec 2023* | ***Revised:*** *20 Dec 2023* | ***Accepted:*** *31 Dec 2023*