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ABSTRACT ID - 1

Emergence of Explainable AI in Drug Discovery and Toxicity Analysis – A Review

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Conventional drug discovery is facing several challenges like time, manpower, profound knowledge, expertise when it comes to serve for more complex diseases. The field of AI and ML has transformed this field into a new dimension through employment of many models and their regular updation. Also, extensive researches open new door to discover drug, specify the respective target through the predictive ML models but the important issues in this case are the transparency and interpretability of the models. These challenges can be addressed by Explainable AI(XAI) that can analyze the drug formulation process, identify any bias and improve the interpretation of the drug design. Even after the formulation of the drug, there is a question of toxicity. So conventional ML models are not skilled to justify the toxicity as the models are without “Why?”, “How?”. In this review article, we are focusing to provide a comprehensive investigation on analytical and interpretable outlook of drug design, prediction of its components, target specification and above all “Toxicity evaluation”. This review will provide suggestions of the application of XAI in drug discovery and toxicity analysis for complex diseases. Furthermore, in this review we are trying to explore the XAI application in Neuromedicine design for Parkinson, Alzheimer’s diseases.