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The Role of Artificial Intelligence (AI) in Organic Chemistry

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Abstract

Aim: AI systems in organic chemistry can facilitate chemical reactions by enforcing catalysts and recognizing chemical properties with the help of space structure and cause possible reactions to provide, therefor AI in organic chemistry plays an important role and can be a helpful tool for design with de novo strategies drugs and prediction molecular domain of chemical compound.

Methods: To evaluate this goal in this narrative paper we searched PubMed, CINAHl, and psyc INFO, and a total of 3567 papers were recognized, and 26 articles were selected in this review.

Conclusion: there are very types of machine learning for the use of AI in organic chemistry for predicting and designing new chemical molecules that can be proper treatment approaches in curing disease, also this study evaluates some machine learning methods that are the best for designing drugs for patients, but the researcher's in all of the world belong the little of their time to research about applied AI in organic chemistry and for more evaluate accuracy, specificity, and sensitivity of reagents chemical in the recent century, with notice scarce accessible to drug discovery chemist scientists in the world should more research about this aim in future years that can be drug consumption is very feasible for individual with different disorders.

Keywords: Biochemistry; Biological Variation; Clinical Molecular Diagnostics; Pharmacokinetics

Introduction

We aim to achieve this review paper by explaining AI's role in chemistry specifically in drug design and molecular modeling. If we want to describe AI using computer intelligence in the prediction structure of molecules and atoms in the chemical organic structure it can help the human mind potentially design and create chemical structures for predicting and analyzing drugs for the treatment of human diseases that are not cured with possible drugs [1]. In the pharmaceutical industry, AI can reach vast success in drug design research, this is because using AI technology can help scientists with the use of novel methods can design new drugs for treatment persons in the world and can reduce human manual error in designing drugs from structures of chemical complicate compound and it can help to hopeful landscape in future in pharmacology science in the world [2]. One another important key that we can apply to it is the selection of proper compounds in drug design strategies. The compound that is selected for more study should well physiochemical properties and ADMET standard items, all this process is done by using AI and machine learning in the pharmacy industry because AI can represent vast chemical information for choosing profit compounds in the drug design approach for chemists [3]. If we want to introduce AI can say it is a machine that constitutes human and can do every work such as humans and it may be applied in vast works education, study, research, lifestyle, and … AI is computer-based human intelligence and can be the error that human with higher mind potent can restrict activity it in some cases [4]. Another term that I intend to explain is organic chemistry means compounds that have non-aquatic reactions they can solve in compounds that have similar specificity to them. Furthermore, organic chemistry consists of all compounds that have in their structure carbon atom and non-organic chemistry includes all atoms without carbon [5]. At this time there are very need to use AI in creating drugs for patients. In the past delivery of drugs to the individual was a very time-consuming and complicated process that AI scientists could use with faster activity these drugs create for individuals that require them, also patients should be trained in consumer from this novel technology that may be long for 3 or 4 years [6]. Studies that down in recent years show that producing new drugs can be time-long, expensive, and very scarce in availability to patients with the help of data from AI and machine learning can be this issue solved but it needs more try and study in the future [7]. AI technique can integrate the help of machine learning from structures in organic chemistry to predict and propel new drugs that can be very useful in the therapy of rare disorders but are applicable from AI with limitations such as information, availability, and error, in this subject requires more clear options [8]. This review paper intends to research using collection information from other manuscripts in AI technology applied in the process design novel drugs from evaluating chemical structures for the treatment of different disorders. The main goal of this paper is to help variant AI approaches and machine learning strategies compare the differences and similarities of these methods can explain these results and reach a proper conclusion in designing novel drugs for individuals with different conditions. One research question on this topic is to evaluate the proper and non-proper effects of AI applied in drug design and molecular modeling in this process and that reply to this question is very hard and requires more clearing issues and research in this discipline. translating information from AI language to design novel drugs can play an important role in retaining the health of patients all over the world. As told later in the above text the creation of one drug for a specific disease is a very complex, long-time, and high cost in the world this use of innovative technology can be more helpful to scientists and patients in getting their health. Therefore, we can compare the main ideas of other authors to understand which method is the best choice for scientists to save time, is cheaper, and is more effective in creating drugs for diseases. One of the most important and routine programs used for the application of AI in organic chemistry is the SYNCHEM program. This approach system helps chemists resolve complicated chemical structures that with user handling, work is very hard for scientists specifically in stereochemistry content [11]. Scientists in organic chemistry in the use of AI in organic chemistry can achieve this success with the use of an axiomatizing program that can resolve optimum synthetic chemical organic reactions that chemists with only cannot find the best resolve method to proceed them [12]. One of the novel approaches that scientists use of AI in organic chemistry is using of novel logic languages for resolving and optimizing re-

actions chemical that easy methods cannot find, this novel method is done by a Prolog planner in the organic chemistry discipline [13]. One of the challenges in organic chemistry is designing and creating novel drugs for different conditions. Many chemists cannot chemical structures in organic chemistry to predict and design new drugs because it is time-consuming and high-cost to perform experimental work that uses artificial intelligence approaches to help chemist researchers synthesize new and novel drugs for rare fatal diseases all over the world [14]. In the new center, Scientists can use AI tools and organic chemistry software for the fast production of drugs that are very limited in different regions of the world and they successfully could teach this algorithm to students in academic universities and teaching places that this successful goal in near future is provided soon [15]. One of the methods in drug design is AI technology can help researchers with different machine learning to easily analyze chemical data and apply them to create novel drugs that can help patients in the world reduce their disease furthermore, AI technology can reach scientists with more accuracy and efficiency predict behavior of different drugs for various disease [16]. Table (1) summaries results from the use of AI in optimization chemical reactions:

Table 1

A study that was done by Nayak et all in 2017 year(24)	A study that was done by Shen et all in 2023 year(23)	A study that was done by Samuel et all in 2024 year(22)	A study that was done by Puri et all in 2024 year(21)	A study that was done by Cao et all in 2019 year(20)	A study that was done by Chen et all in the 2024 year(19)	A study that was done by Kim et all in the 2021 year(18)	A study that was done by Xu et all in the 2024 year (17)
Result	Result	Result	Result	Result	Result	Result	Result
This study shows that the use of AI in chemical reaction neural networks can increase the accuracy and sensitivity of chemical reactions and optimize chemical processes implying an important role	The result of this study represents that applying AI and dependent techniques to it can enhancement speed of chemical reactions and produce efficient materials via optimized flow chemistry	This research explains that the use of machine learning in the AI approach can help to enhance optimization in chemical reactions via promoting catalysis activity and increase reproduce new chemical materials	Results of this study show that the use of AI and machine learning can help to optimize chemical reactions or enhance precision and reduce time-consume for chemical reactions and this key can help one progress in designing drugs and pharmaceutical technology	They can minimize entropy generation with transfer mass causes optimization of chemical reactions and enhance reproduce yield in one chemical reaction	These results show that with use of machine learning, chemistry engineering, and data science can enhance optimization in chemical reactions with AI, in therefore global model can reproduce new reactions and local models cause an increased yield and selectivity of reaction	These scientists use AI with approach machine learning in converse methane gas to c2 formation and coke they can apply AI to reduce the production of coke and enhance the creation of c2 and amount error reach <5%	Using AI in the optimization of chemical reactions both causes improved economic conditions and environmental performance and also reduces greenhouse gases on earth

Research Material

We can use in this review manuscript different approaches of machine learning in the direction of better use of AI in drug design with the help of organic or inorganic chemistry structures. Machine learning is the very best technique that can analyze information from AI faster in creating different drugs with vast organic chemistry structures that in condition usually this work is backbreaking and time-consuming. For example, the eToxPred model of machine learning can easily evaluate the amount of toxicity of small organic chemistry molecules with high efficiency. One of the methods evaluated in this paper is using of the QSAR model helps scientists interpret the quantitative specificity of organic molecules in chemistry science, also the method can help in predicting biological activity from the chemical structure which can be very useful in this project.

Table 2

Random forest	Support vector machines	QSAR	EToxPred	The types of machine learning platforms in AI in organic chemistry
High accuracy, handling non-linearity, feature importance, robustness, versatility, balanced performance	Interpret high dimensional data, is very effective in resolving optimal decision limitations, effective in	Enhance predictive performance, the inclusion of diverse data sources, ability to handle high dimensional data,	Determine toxicity drug discovery candidate efficiency	Benefit
Lack of interpretability, computational complexity, overfitting, imbalanced datasets	Modulating small dataset SVM is very poor in evaluating big chemical data, it can cause noise in classification chemical structures, and unrecognized accurate kernel parameters can approach to cause error	The efficiency of model update Sensitivity to quality of input data, potential for overfitting is prevalent, applicability of domains accessibility, problem in interpretation complexity of data, lack of understanding about molecular interpret data input	Reliability of the training data, interpretability of the model predictions, generalizability, regulatory acceptance	limitations
Quantitative-structure-activity prediction, chemical risk assessment, applicable in anticipating chemical domains	Predictive toxicology, structure-activity relationships, computational chemistry, environmental chemistry	Molecular modeling in organic chemistry integrates quantum chemistry with machine learning, enhancement of chemical research	Toxicity prediction, synthetic accessibility, enhancing research efficiency	Applicability in organic chemistry

Main Body

In a study done by pu and et all in 2019, they used from eToxPred model of machine learning to assess the amount of toxicity of their chemical agents the result shows that this method can be useful in virtual screening and can be a good matter for evaluating the toxicity of chemical compounds [9], while another study by Ai and et all in 2019 ex-

press that this model has accuracy, sensitivity, and specificity for evaluate toxicity chemical agents in an aquatic system that as implicate in above text first case was good in virtual screening and the second model is the best for aquatic system [10]. From the interview of these two models, we can conclude that the eToxPred model only explores toxicity in the virtual system, and in another method this specificity ass in aquatic systems, and also both two matters are proper but notice which condition is ready scientists in chemistry science can apply these approaches for evaluate and fasting their results in their research. Furthermore, in these two models, there are other machine-learning strategies in vast studies of organic chemistry explained by authors that we implicate in this section shortly. One other method is supervised learning which evaluates the properties of the compound chemical from possible information, scientists say that this matter is the best and most useful when we have elementary data from one chemical structure and we don't have the properties of this agent. This matter has 3 algorithms: 1. support vector machines: that from structure chemical information predict chemical properties of compounds that scare chemists. 2. Random forests: this method anticipates the properties of chemical compounds with the help of tree design in their matter which also causes high accuracy and both useful for complicated chemical structures. 3: Deep neural networks that is useful for predicting molecular properties of chemical compounds. Another approach is unsupervised learning this method is best when chemical information is scarce and with the help of sub-methods can predict chemical information. 1. Clustering algorithm: by visualization of chemical structures in space can reach this data and 2. Principal component analysis: useful for solving complicated chemical structures. Later model machine learning is transfer learning that is used when data chemical is limited and can be evaluated chemical properties from this scarce information, and the end approach is reinforcement learning that is useful for predicting efficiency conditions in chemical reactions. Scientists in chemistry can help these types of machine learning easily evaluate and predict chemical structures that can be important key points in innovation strategy in chemistry science.

Conclusion

This qualitative review has evaluated the effect of using AI technology in organic chemistry with the help of applying different types of machine learning approaches. In this review paper, we can reach these outcomes that each matter in its situation can be helpful and belong to a specific chemical structure and reaction with unique properties. But until now there have been limited studies that explain this concept in their paper and a few studies carried out on this topic. To clarify this issue in chemistry science young researchers should try to provide vast information about the use of each method in machine learning and applied AI technology in organic chemistry until now there are very gaps that should be filled to solve chemical issues in structure and performance for molecular modeling and design novel drugs in de novo approach for enhance accuracy, efficiency and short- time produce drugs technology. In Table 2 applicability of these AI approaches in organic chemistry is shown.

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