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CHEMI INTELLIGENCE: THE FUTURE PERSPECTIVE OF ARTIFICAL INTELLIGENCE

Deepti Sadana[1]* and Anima Mathur[2]

[1]Department of Research and Development, Chashaki, Faridabad, India.

[2]Department of Research and Development, Indu Raghukul Food and Chemical Pvt Ltd. Chattisgarh Raigar, India.

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***Corresponding Author**
Dr. Deepti Sadana
Department of Research and Development, Chashaki, Faridabad, India.

ABSTRACT

The synthesis of molecules continue to exist as one of the vital challenges in field of organic chemistry, often concluding in epitomized results due to repetitive and tedious tasks based on experiences. Artificial Intelligence is emerging as the modern remarkable progresses will drastically accelerate the development of novel drugs and will establish the future of chemistry. Research in Artificial Intelligence would extremely prove beneficial to humanity as well as substantial-world application realm. This review article thus focuses on importance of discovery of novel chemical compounds, planning involved in synthesis and solve the problems related to chemistry.

1. INTRODUCTION

In recent years, Artificial Intelligence techniques have depicted great potentiality in solving various problems from assembly of disciplines including designing of material and discovery of drug. A perpetual demand for the discovery of contemporary compounds in various fields of chemical industry requires the advancement of computational tools for the prophecy of molecular properties.

This new era research has generated various essential technologies such as Machine Learning, Natural Language Processing and investigation with a broad range of applications. Chemistry has a wide scope of applications in various industries viz. crop protection, food and nutrition, chemical biology, pharmaceuticals etc. These industries have significant effects on the society and human life.[1] However to improve the odds and complexities of this biological processes there is requirement of continuous research on knowledge through

investigations on literature and patents from scientific fields.[2] To enrich the projects it is necessary to integrate the statistics and data mining into molecular discovery and designing to provide computational back in molecular hypothesis formation.[3] Artificial Intelligence focuses on chemistry as translating direct benefits to the society for example drug Lipitor R (Single chemical compound, atorvastatin) generated revenue of over 12 billion dollars annually, before its patent lapsed.[4] It is important to put a lot of efforts in innovative computational tools, scrutinize and compare their real progress so to contribute to new revolution of computational tool of molecular design.[5]

2. Historical framework of artificial intelligence in chemistry

In the Past, research studies initiated for more than ten years ago to develop knowledge reasoning expert systems to solve the chemistry problems viz. Dendral and Project Halo[6,7] Synthesis and retro synthesis designing by a machine utilizing handcrafted rules was established as Reaction templates.[8] A broad chemical expertise was the utmost requirement and writing guidelines remained a time consumption work. The creative works of Free and Wilson[9] and Hansch and Fujita[10] developed the field of QSAR (Quantative structure-activity relationship) modelling. This success propelled a large emergence of research area in identification of approaches and capturing the autonomously learned representations.[11] The growing excitement and promise field of QSAR learnt disenchantment in 1990's about control experiments, model validation and other drawbacks.[12] The pioneering works of researchers led to the advancement of Artificial Intelligence technologies including Machine learning, research and planning and natural research processing etc.[13] The algorithmic principles and statistical interpretation increased the applicability domains.[14] By 2000, there was an increase in successful number of applications of Artificial intelligence techniques to design and discover drug industry, which led to the sustained development of their usage. Further, in 2015, computational advances outperformed other machine learning techniques and therefore reported as a beneficial tool for molecular designing.

3. Chemi -Intelligence technologies

Artificial technologies include various essential approaches in chemical field.

3.1 Natural language Processing and Chemical image processing

An enormous literature, patents and academic papers consists of several chemical reactions. The extraction of these consequently would lead to availability of beneficial knowledge base for machine readable format. The typical illustration of molecular structures and reactions as

textual descriptions and figures requires a combination of chemical image processing and NLP. Addition to this the approaches need to extract not only the compound structures but also the relationship between the reactants and compounds.[15] It is then used to construct the models prediction of molecular properties and designing of novel molecules.[16] However, improved text mining is still needed to extract vital information on the conditions of reactions.

3.2 Machine learning

Machine Learning is a promising approach to implement algorithms that teaches computer to learn a set of data instances. It accelerates the solution of intricate chemical problems but at the context of big Data problems. Deep Learning has emerged as the latest achievements and a strong candidate of ML techniques. There are certain challenges such as reaction data extracted with NLP and chemical image processing might contain incorrect information. Therefore, settlement is required that includes various training sets and regularization approaches.[17] Deep Learning calculates the score of developed product based on the modification of reactants.

The graph link-prediction-based recommendation algorithm accustomed a product as input to conclude the reactants.[18] In predicting reactants, a chemical compound presented as a graph is often transformed into a fingerprint that represents the structural features of the compounds.[19] Machine learning can detect the presence of active substructures viz. the part that fights a disease or completes the compound as a substantial structure.

3.3 Synthetic planning and Predictions

The approaches of Machine learning addresses the practical questions of chemistry, which includes the suitable synthesis technique for a specific compound and the optimum conditions, required viz. solvents, reactants, temperatures etc. for obtaining the maximum yield estimating the specific rate and time.[20] Prediction making in reactive chemical systems can resort to deep learning. However there are some successful examples as the recent results of chematica of assembling the relevant transformations into the extensive network.[21] The rules sometimes are incomplete or even ambiguous due to the availability of inaccurate knowledge.[22]

The Chematica platform consists of expert chemical knowledge, network theory, high performance computing and artificial intelligence to expedite the design of synthetic

pathways leading to achieve new targets.[23] There are some other prominent platforms which incorporate Machine learning algorithm viz. Chem Planner and Synthia form the data base rules for the chemical transformations to suggest possible ways to synthesize the target molecule.[24] Retro synthesis and reaction predictions are the backbone of organic chemistry. It is utilized for planning organic synthesis to convert target molecules into dynamic simpler precursors.[25] Reactivity conflicts are generally generated as the rule based procedures employed are computational for both reaction prediction and retro synthesis thus ignoring molecular context.

4. Applications of artificial intelligence in chemistry

Relevant contributions, theoretical foundations and applications of AI are stated as under:

4.1 Optimizing the predictions of chemical patterns

Patterns are pervasive in chemistry field. From the solid forms (Crystalline structures) to the multiplex combinations of functional groups, branched chains of lipid molecules, chemical patterns ascertain the properties of materials and molecules, necessary to address the vital issues of society concern.[26,27] Recent contributions in AI include different techniques for understanding and managing chemical behaviour and related systems,[28] optimizing, estimating, predicting structure-property relationships, density.[29,30] Driving generative models i.e. producing stable molecules from a set aspired properties and progressing quantum sensing.[31,32] The new data driven paradigm builds the bridge between experiments, theory, simulation and computational strategies.

4.2 Drug repurposing

Drug repositioning or repurposing is an approach in accordance with which existing drugs are used for the treatment of life threatening diseases. AI accelerates Drug repurposing as a promising approach for reduced development schedule and cost effective solutions and identification of disease targets with minimum error.[33] AI and network medicine approach are developing rapidly in a powerful way and can promote therapeutic development. The drug target network requires complete knowledge for the development of affordable and promising techniques for the treatment of complicated diseases.[34] Drug targets do not manage in separation from the proteins complex system, it becomes essential to examine the drug-target network (Bipartite graph which is composed of approved drugs and proteins linked by binary associations).[35]

5. CONCLUSIONS

Chemi-Intelligence the word itself shows the essence to master the working principles of scientific methods. This includes iterate process of scientific discovery abides observations, raising questions, proposing hypothesis, designing experiments, analysing data and withdrawing conclusions to form new theories. Researchers have made promising advancements in their respective fields.

6. Current Limitations and Future prospects

This review justifies the optimistic approach regarding the current advances and prospective for the use of Artificial intelligence in academic and industrial world. AI Techniques promises positive future focussed on chemistry concentrating on the challenges and limitations in short and long term outlook. Researchers have made promising developments and advancements in respective fields of chemistry and AI. A lot of research investigation is still required to fill the gap and produce innovations and contributions to scientific world for the benefits of humankind.

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