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Roles Of Professionals in Chemistry with Ai: A Review

Dr Bhawana Kesarwani
Assistant Professor, Department of Chemistry, Mahamaya Government Degree College, Kaushambi

***Abstract*—Artificial Intelligence (AI) is almost impossible to avoid today, even in Chemistry. Be it Synthesis Design Systems for the simulation of chemical reactions, the Structure Elucidation Systems for the interpretation of spectral data, the Molecular Modelling Systems for the visualization of chemical structures and the calculation of physicochemical parameters. AI and Chemistry applications in the healthcare industry are focused on drug discovery and development. Empowered by AI, researchers have realized more efficient optimization of process parameters and a deeper understanding of the structure-activity relationship, thus accelerating the discovery of breakthrough theoretical laws and the synthesis of innovative substances. Other areas of chemistry that will benefit from AI include compound solubility, optimizing reaction conditions and providing production methods for challenging target molecules. Significance of AI in promoting chemistry research to improve the chemical industry has evolved. The goal of the researchers is to advance drug development by creating novel medications at a minimal cost. AI assists in achieving this goal.**

***Index Terms*—Artificial intelligence (AI), analytical chemistry, biochemistry, drug design, chemoinformatic, artificial neural networks, chemometrics, properties of molecules.**

I. INTRODUCTION

AI can also alleviate chemists' manual and labour-intensive tasks and allow them to concentrate their efforts on scientifically impactful pursuits. Details include the construction of high-throughput automation platforms to realize efficient and consistent experiments, as well as the development of machine learning algorithms to automatically analyse and mine the large-volume data generated by automated experiments, thereby revealing the deep-seated laws. Liu et al. [1] reviewed the recent progress in the transformation of organic chemistry research paradigms inspired by AI. Machine learning models together with autonomous robotic systems dramatically increase the planning ability for complex molecular synthesis and accelerate the exploration pace due to the unprecedented speed and precision of automated experiments.

The methods of chemoinformatic have made accessible the huge amount of data and information and these data can be converted into knowledge to increase our understanding of chemistry and to accelerate chemical innovation. It will further be shown where new methods from AI are introduced into various fields of chemistry to further assist in understanding chemical data. [2]

Artificial intelligence (AI) refers to the ability of machines to act in seemingly intelligent ways, making decisions in response to new inputs without being explicitly programmed to do so. Whereas typical computer programs generate outputs according to explicit sets of instructions, AI systems are designed to use data-driven models to make predictions. These AI models are generally first trained on representative data sets with known output values, thereby "learning" input-output relationships. The resulting trained models can then be used to predict output values of data similar to the training set or to generate new data. Many problems involving data with complex input-output relationships are difficult or impractical to model procedurally, thus creating an opportunity for AI.

AI can feasibly be applied to various tasks in the field of chemistry, where complex relationships are often present in data sets. For example, the solubility of a new compound may be predicted either through equations based on empirical data or by using theoretical calculations. Alternatively, prediction of solubility may also be accomplished by an AI program that has developed structure-solubility relationships after being trained on numerous compounds with known solubilities. The use of AI for tasks, such as property prediction have proliferated in recent years due to explosive growth in computing power, open-source machine-learning frameworks and increasing data literacy among chemists. [3-4] AI implementations have proven to dramatically reduce design and experimental effort by enabling laboratory automation, [5] predicting bioactivities of new drugs, [6-7] optimizing reaction conditions [8] and suggesting synthetic routes to complex target molecules. [9]

II. ARTIFICIAL INTELLIGENCE (AI)

John Mc Carthy was the first who coined the term AI in 1956. AI is the ability of computers or machines to think and act as human do, represents the efforts towards computerized systems to imitate the human mind and actions. [10] The word Artificial means man-made and intelligence means the capacity to have different skills. [11] AI can be expressed as the skilful imitation of human behaviour or mind by tools or programs. [12] AI is the tool used to perform many works and the system can able to decide which work is required and that is perform. Global impact of AI more understandable for the future economy and for the future of education, which in turn, directs the economy and workforce, paving the way for the new Industrial Revolution. [13-14]

Since 2015, it has been observed that the number of scientific publications in journals and patents has increased dramatically, and the most significant has been in the fields of analytical chemistry and biochemistry, because both fields integrate AI to the maximum extent and with the highest growth rates. [15] According to reports, China and USA have provided the most journal articles and patents. The majority of commercial patent assignees for AI chemical research are medical diagnostic developers and technology corporations. Jennifer Newton questioned when an AI would be named as an author on a scientific article in January. It turns out that the response was actually quite brief. Recently, ChatGPT, the generating text algorithm that has quickly gained notoriety, was recognized as a co-author on a number of papers. [16]

III. ADOPTION OF AI IN CHEMISTRY SUBDISCIPLINES

We have identified seven major subdisciplines of Chemistry which are leveraging Artificial Intelligence: Organic Chemistry, Inorganic Chemistry, Biochemistry, Physical Chemistry, Theoretical Chemistry and Analytical Chemistry. These are discussed in this section.

A. Organic Chemistry

Synthesis of organic molecules remains one of the most important tasks in organic chemistry and the standard approach involved by Chemists is to solve a problem based on their experience, heuristics and rules of the thumb. When Chemists manually design a new drug, they not only need to design a target molecule but also need consider reaction pathways to synthesize it. They usually work backwards, starting with the molecule they want to create, followed by analysing by a process known as retrosynthesis as discussed in the previous section, in which readily available reagents and sequences of reactions could be used to produce an outcome. Researchers have tried to show that organic chemistry has a structure similar to a natural language and that the concepts of linguistic-based analysis could be used to also analyse molecules, their patterns of reactivity and their organic synthesis in the hope that Sequence-to-Sequence models for retrosynthesis and reaction prediction will be feasible in future. In this avenue, for example, IBM's neural network model trained on a dataset of 395,496 reactions has learned about prior reactions and is being used to predict what would occur under new experimental conditions.

B. Inorganic Chemistry

The variable spin, oxidation state, and coordination environments favoured by elements with well-localized electrons provide a great opportunity for tailoring properties in catalytic or functional (e.g., magnetic) materials and add layers of uncertainty to design strategy.

The High Throughput Screening uses quantum chemistry calculations to predict material properties, however, the computational complexity of these calculations often imposes a prohibitively high cost on the search for the desired material. This critical bottleneck is resolved by using deep Gaussian process-based approach to develop an emulator for quantum calculations.

C. Biochemistry

Biochemical research generates massive amounts of data which needs to be analysed, integrated, and interpreted. The need is to create a computer-enabled system that would allow biochemists without deep knowledge in carbohydrate chemistry to gain quick access to well-defined glycan assemblies and also methodology to produce large, well-defined macromolecules with programmable shape, size, and chemistry that combines reactor engineering principles and controlled polymerizations. Artificial Cells will investigate how to design artificial molecules and artificial reaction to enable the cell to solve problems. [17]

D. Physical Chemistry

Problems addressed and approaches used in Physical Chemistry are diverse. Knowledge bases can be used for storage and retrieval of databases of vapour pressures of gases or of intermolecular forces and the laws relating to physical sciences. When coupled with an Artificial Intelligence system will be able to solve quantitative problems directly by linking together code, formulas and data in the correct sequence to obtain solutions. Neural network representation of an alloy can be developed to predict composition and temperature dependent surface segregation through Monte Carlo models or use Gaussian Process approach for representing the potential energy surface which are useful for reactive scattering calculations and also can relate observed X-ray absorption near edge spectra to nanoparticle structure and composition. Researchers are using Artificial Intelligence approach to reduce the number of structures needed to be computed to arrive at a Density Functional Theory based free energy diagram in which neural networks are trained to study the performance of fourth-order gradient expansions of the Kinetic Energy Density in semi-local kinetic energy functionals depending on the density dependent variables.

E. Theoretical Chemistry

Be it Feynman diagrams in Physics or the structural elucidation in chemistry, theoretical problems can be addressed by solving graphs. A deep generative model known as SELF-referencing Embedded Strings, for example, are applied to represent chemical structures for molecules using semantically constrained graphs, SMILES, in a simple, robust, deterministic, domain-independent, model-independent way. SELFIES are based on a Chomsky type-2 grammar, augmented with two self-referencing functions for generation of valid graphs for a domain- and model-specific applications. [18]

IV. APPLICATIONS OF ARTIFICIAL INTELLIGENCE IN DIFFERENT FIELDS

AI with Pathologists

Pathologists can refer to Molecular Modelling Research for predicting the function of a compound by looking at the 2-D chemical structure for every known metabolite. Combining an advanced live-cell imaging algorithm and artificial intelligence, they can profile cancer cell extravasation within a microfluidic blood-brain niche chip to detect the minute differences between cells with brain metastatic potential and those without.

AI in Forensic

New devices are emerging for predicting Post-Mortem Interval or time of death by identifying biomarkers in different biological fluids such as blood, urine by analysing profile of different metabolites in the blood such as Lactate dehydrogenase LDH, Aspartate aminotransferase AST, triglycerides and cholesterols. In addition to this is measurement of blood pH. The use of such biochemical markers could be promising tools in forensic death investigations.

AI in Automated Lab Assistants

AI-based research tools, such as automated lab assistants, have revolutionized research laboratory in chemistry. These lab assistants enable researchers to automate the routine laboratory processes and experimental designs which accelerates and improves the research processes, ranging from preparation of sample to data analysis. Automated lab assistants enhance accuracy, reduce downtime, provide high output and free up researchers from time consuming tasks. It also offers more time to scientists to generate new ideas and conduct advanced research work in their field.

AI in Integration of Big Data

The chemical industry is all about data. It generates information from simulations, experiments, studies, research and other sources. It is essential to collect, store and analyse these data's properly, and AI will be highly useful for that. [19]

AI in Green Chemistry:

There is a trend towards more sustainable and greener chemical practices right now and AI can help achieve this faster. AI can investigate the chemical reactions and environmental impacts and used to design more efficient, environmentally friendly compounds. With the use of AI, it will be possible to minimize waste generation and promote more sustainable manufacturing practices.

AI in Automation and Robotics:
Combining AI with robotics can help to automate laboratory processes and enhance the productivity. Robotic systems that utilize AI can perform routine, repetitive tasks such as data analysis and sample preparation faster and more effectively. This helps researchers to reduce the risk of human error

AI in Reaction Prediction and Computer-Assisted Synthesis Design (CASD)
The prediction of a chemical reaction is a fundamental question for a chemist. Quantum mechanical methods can be used to calculate transition states and predict the course of a reaction. The effect of temperature or solvents on reaction are hard to calculate. With the largest reaction databases CASREACT [20] and REAXYS [21] containing 123 million reactions and 49 million reactions, respectively, there is always a fair possibility that the desired reaction or a closely related one is found. Reaction prediction is an important task in computer-assisted synthesis design (CASD) a fundamental question for an organic chemist. In a CASD system a target structure is given and a reaction that can produce this molecule has to be suggested. CASD had been taken up as a challenge from the very beginning of chemoinformatic.[22] Several research groups had embarked on the task of designing a CASD system: Ugi, [23] Gelernter, [24] Hendrickson, [25] Gasteiger, [26-27] Funatsu.[28]. Although many interesting results were obtained none of the systems came into widespread use. Organic chemists were at that time not yet prepared to accept computers for a domain they liked to do by themselves. Several decades had to pass until new attempts were made for the development of CASD systems.[29] These were largely due to the availability of large reaction databases and the development of novel search procedures. The Chematica program can successfully suggest new and interesting synthesis schemes.[30] Segler and coworkers [31] applied a combination of three different neural networks and a Monte Carlo search to extract reaction transforms from a database of 12.4 million reactions from Reaxys. The approach automatically generated successful multistep synthesis. Thus, recent work based on the combination of large reaction databases with novel data processing algorithms has provided CASD systems that are mature enough to assist organic chemists in planning laboratory work. For synthesize of a compound in drug discovery de novo design methods generate many structures. Then the medicinal chemist selects those molecules for further investigation that are more easily synthesizable. Methods for calculating values for concepts like synthetic accessibility [32] or current complexity [33] have been developed that allow the chemist to make selections which molecules should preferably be made.

AI in Drugs Discovery
Drug discovery is the most prominent field for the application of chemoinformatic methods. All drug companies have the largest employers of chemoinformatic specialists. All the drugs developed have benefitted from the use of chemoinformatic methods. The drug discovery and development process starts with the identification and validation of a protein target, then has to select a lead structure which has to be optimized and has to go through preclinical testing to make sure that properties like adsorption, solubility, distribution, excretion and metabolism
(ADME) as well as toxicity have acceptable values. Only then can a candidate be submitted to clinical development. The chemoinformatic methods used in drug discovery can be classified into ligand-based methods (when the 3D structure of the protein target is not known) and structure-based methods (when the protein structure is known). A more in-depth modelling of the biological activity of a molecule needs its 3D structure, both for ligand-based and for structure-based methods; fortunately, CORINA [34] can also generate 3D models for virtual (not yet synthesized) molecules. The methods include similarity search, pharmacophore searching, virtual screening, de novo design, docking and scoring, active site identification, xenobiotic metabolism prediction, ADME properties and toxicity prediction. Databases play an important role in the drug design process, both databases of the compounds available in the company as well as those of virtually generated structures. With the drug design and development process being so demanding both bioinformatics and chemoinformatic

methods should be used. A distinct separation between the bioinformatics and chemoinformatic methods. Often, the same mathematical procedures are used both in bioinformatics and in chemoinformatic. A gene is a chemical compound and the representation of a gene may eventually benefit from representing it by chemoinformatic methods. Various AI methods have been introduced into drug development in recent years. [35] The importance of AI in drug discovery clearly shown by the fact that more than 230 startup companies [36] have been founded that uses the AI in drug discovery, such as Merck. [37] The AI company Exscientia and Sumitomo Dainippon Pharma Co. have jointly developed a drug for obsessive- compulsive disorder that is now entering phase 1 clinical trials. The development took only one year as against an estimated 4.5 years with conventional research techniques; this amounts to massive savings. [38]

AI in Biochemical Pathways and Metabolic Engineering

Reaction databases are the gather of reaction and pathways occurring in living species. Biopath. Explore [39-41] has stored all the reactions and pathways contained on the poster distributed by Roche [42] in computer-readable form. A variety of standard chemoinformatic searches can be performed on biochemical pathways. More interesting studies of high chemical significance can be performed, particular are those where chemoinformatic and bioinformatic methods are simultaneously used.

In another approach, a chemical systems biology approach for Reverse Pathway Engineering (RPE) was established by combining chemoinformatic with bioinformatic methods. In an application for the study of Flavour-forming pathways in cheese by lactic acid bacteria, the known and novel pathways could be derived. [43] Much interest is on the redesign of pathways by redirecting the action of enzymes to produce basic organic chemicals. As an example, an optimized methanol assimilation pathway was developed by utilizing promiscuous formaldehyde-condensing aldolases in E. coli. [44] Novel AI methods such as deep learning architectures are applied to metabolic pathway prediction. [45]

AI in Regulatory Science

Due to the harmful effects of chemicals, the European Union has not only issued the Cosmetics Directive [46] but has also passed the REACH legislation on the Regulation, Evaluation, Authorization and restriction of Chemicals. [47] The REACH legislation requires companies that want to introduce large-scale production of chemicals into the market in Europe to provide a dossier that shows that these chemicals are not harmful to humans or animals. Legislation similar to REACH has been introduced in various countries such as Canada, USA, Japan, China. These laws consider toxicity testing but it is time-consuming and costly. In this situation toxicity, bioaccumulation and degradation in the environment have been developed. [48] The methods of machine learning and AI have been applied to toxicity prediction. [49-50] The predictive accuracy can be increased by augmenting the chemical structure descriptors with human transcriptome data.

AI in Material Science

The prediction of the properties of materials is the most active area of chemoinformatic. The properties that are investigated from properties of nanomaterials, materials from regenerative medicine, solar cells, homogeneous or heterogeneous catalysts, electrocatalysts, phase diagrams, ceramics or the properties of supercritical solvents and a few reviews have appeared. [51] The chemical structure of the material investigated by QSAR study. Materials can be represented by physical properties (refractive index, melting point, spectra, the components, the conditions for the production of the material etc. Use of chemoinformatic methods in material science are consider the properties of interest depend and cannot be directly calculated. A QSAR model would allow the design of new materials with the desired property. As the properties of materials are so hard to predict, AI techniques have been applied in material science. [52-53]

AI in Process Control

The problem of the detection of faults in chemical processes and process control have benefitted quite early on from the application of artificial neural networks. [54-56] An overall course on the application of artificial intelligence in process control has been developed by six European universities. [57]

The relationships between the various data produced by sensors and the amount of desired product cannot be explicitly given, making it an ideal case for the application of powerful data modelling techniques. Quite a few excellent results have been obtained for such processes as petrochemical or pharmaceutical processes, water treatment, agriculture, iron manufacture, exhaust gas denitration distillation column operation etc.

V. ARTIFICIAL INTELLIGENCE (AI) IN RETROSYNTHESIS

The plaining and synthesis of a molecule is a very important task in organic chemistry. The plaining and synthesis of an organic molecule include various steps with the help of which an organic molecule can be synthesized. For this purpose, retrosynthesis is used. Retrosynthesis is a technique in which a target molecule is transformed into a simple precursor. This process is continued until the starting molecule is obtained. [58] But if the molecule is very complex and contains many functional groups, so it is very difficult to synthesize this molecule. [59] For example, Herculean B has 32 stereo-centres and synthesis of this molecule required 47 reactions. This is very challenging and difficult retrosynthesis problem. But with the help of artificial intelligence- based algorithms, it is possible to overcome the complexity of this molecule. The goal of this algorithm is that they provide a reaction path to the target molecules so that it can convert into a simple precursor. The chemical literature has been grown increasingly, so it is very difficult to manage the decision- making process. But it is possible with the help of a network of organic chemistry, which contains all the reactions that has been published in the literature. [60]

The retrosynthesis used some reaction rules that contains a set of transformation. This rule has been encoded by some expert chemists. [61] This reaction rule represents the generic reaction that has been applied to the target molecule to generate a simple precursor. Once the rule has been finalised then the algorithm used a matrix that is used in determining the set of rules for each step of the reaction. The artificial intelligence used the Monte Carlo tree with three neural networks that helps in selecting the candidate reaction for expression. This neural network has been trained in such a way so that they can select reaction centre. But this rule-based approach is not efficient for the molecule that is beyond the scope of transformation rule. To overcome this problem a new approach that is known as deep learning has been introduced. The advantage of this approach is that it can extract the generalized patterns from a large amount of available data set. In this deep learning approach, the target molecule is encoded in the form of string that has been extracted from the SMILE string. This string has been converted into another set of character which is related to the SMILE string (simplified molecular- input- line entry system) of reactant.[61]

VI. ARTIFICIAL INTELLIGENCE (AI) IN NANOTECHNOLOGY

Artificial intelligence is mainly based on biological things, while nanotechnology combines physics, chemistry, and engineering. [62] So, the combination of artificial intelligence with nanotechnology provides new tools for information and communication technology that greatly impacts our society. The various machine learning process like decision tree, vector machine that has been applied to the association, prediction, data mining in the context of nanotechnology research. Scanning probe microscopy is the most commonly used technique in nanotechnology in which interaction between tip and sample is complicated to understand and involves many parameters. To overcome this problem, we can use the artificial intelligence technique. Combining an artificial neural network (ANN) with a principal component analysis provides simplified input data by de-correlating the data and decreasing independent variables. The ANN is trained with a numerical result that is useful to find out the dielectric constant value. The advantage of this method is that we can find the thickness of the thin-film by knowing the dielectric constant value. ANNs is used to determine the structural properties of nanomaterial like alignment and curvature. The artificial intelligence-based algorithms are used to determine the morphology of the CNT turfs. Thus, the ANN models are sufficient to relate the physical appearance of CNT turfs to Raman features. ANNs are also used in determining the properties of a complex system like a thin film. The different artificial intelligence-based training set has been used in determining the property of this nanomaterial. Artificial intelligence techniques are also used in identifying optical techniques because of the increasing growth of broad-band communication.

Artificial intelligence helps to determine the chemical kinetics parameters such as rate constant and concentration of the reactant. By using this, we get a new kinetic curve without solving the differential equation. The genetic algorithms (GA) have been used to study the clusters property of nanoparticles. The combination of genetic algorithms (GA) and DFT calculations help to obtain the equilibrium state. The ANNs is used to find out the splitting tensile strength and water absorption values which contain ZnO_2 and Cr_2O_3 nanoparticles. The main problem of nanoscale that scientists are facing is related to its simulation. It is complicated to obtain an actual optical image on a nanoscale. For this purpose, artificial intelligence has increased the quality of simulations to make them easy to interpret. [63] Artificial intelligence helps sequence the nucleotide in the translational process of Nanopore. [64] The artificial neural network-based transiting used in Nanopore sequencing provides more than 90% accuracy in sequencing. [65] Nanotechnology has many physical limitations on its working scale, and we also know that the microscopic world is entirely different from physics. So correct interpretation of the result is one of the issues. At this stage, artificial intelligence is used for correct scientific results and in Nano applications. [66]

VII. CONCLUSION

AI techniques have recently seen a rebirth in chemistry and will have to be optimized to also allow us to understand the basic foundations of chemical data. Learning from data has always been a cornerstone of chemical research. In the last sixty years computer methods have been introduced in chemistry to convert data into information and then derive knowledge from this information. This has led to the establishment of the field of chemoinformatic that has undergone impressive developments and found applications in most areas of chemistry from drug design to material science. Discovery of new drugs will be an achievement for investment of time and resources of scientific talent around the globe. Soon we are entering a world in which we can develop a new therapeutic solution in a matter of days for emerging threat or disease, rather than taking several years. And not only develop a therapeutic that is safe and effective to use, but one can also develop a stable and scalable methods of production in a matter of days. Even the roles of professionals are changing. There is a growing need for them to understand AI and its usage in their professions for productively collaborating with the technology. Focus should be given to the process of data production, curation, cleaning to further enhance the AI and these may emerge as new careers in the discipline. AI is an essential tool in modern chemistry that offers promising opportunities for the advancement of research needed to solve the most significant global challenges in the years to come. As AI continues to advance and evolve, it will play a crucial role in the future of scientific discovery.

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