Applications of Artificial Intelligence Based Techniques on the Analysis of Chemical Data: A Review

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***Abstract*—Artificial Intelligence based techniques such as Deep Learning, Machine Learning, Chemometrics have recently begun to replace chemical heuristics. They are promising tools that can be used to gain insight on the characteristics, processes and interactions of a chemical sample and to a clearer and better understanding of chemical data. The focus of this review paper is on the recent developments on the applications of Artificial Intelligence based techniques for different chemical scenarios of computational chemistry, quantum chemistry, synthetic route design, drug delivery, analysis of spectral data and analytical chemistry.**

Keywords— Spectroscopic Measurements, Deep Learning, Chemometrics, Machine Learning, Artificial Intelligence,

I. INTRODUCTION

Artificial Intelligence, Chemometrics, Machine Learning, Deep Learning are currently present in every branch of science and technology, including chemistry. They are promising techniques that lead to a greater understanding and clarity of data. There are patterns in Chemistry, such as the periodic system of elements, crystalline structures of solids, branched chains organic compounds, atomic radii, functional groups, ionization energy, ionic radius, chemical reactivity, electron negativity, electron affinity, etc. These various patterns determine the underlying properties of the molecules, furthermore these heuristic models were built from the combination of the scientist's expertise, creativity and simplified physical imagery. Artificial Intelligence most especially Machine learning, are committed to recognizing and learning these patterns [1].

Machine learning techniques is gradually replacing these heuristic approach due to the increase amount of data which is primarily available via high through-put *ab initio* computations and advances in machine learning methods that are available through open source software [2]. Deep Learning is a technique under machine learning which can be used to solve various problems in Chemistry such as the description of soft matter behaviour, identification and classification of compounds, etc. [3].

The amount and quality of chemical data which has been generated by experiments and simulations have established a bridge between computation, experiment, theory, and simulation. The aim of this review is to analyse in a critical and concise way the relevant contributions which has been done in recent times in various areas of chemistry and in the development of chemistry using various Artificial Intelligence Techniques such as Chemometrics, Deep Learning and Machine Learning.

II. DEEP LEARNING, MACHINE LEARNING, DEEP CHEMISTRY

According to Goh *et al.,* [4], Deep learning (DL) is a branch of machine learning that is growing speedily, it deals with complex learning and extrapolation tasks and is supported by a broad range of open-source code, Chemistry literature, and datasets. DL has the ability to expedite chemical reactions, solve critical analytical uncertainties, reduce costs and resources, model compound properties and reactions, etc. However, there are challenges to be overcome such as the lack of standardization of chemical data, production of accurate chemical information and clean data.
Most DL algorithms are mainly based on artificial neural networks and Deep Neural Networks (DNNs). DNNs are designed to function like the brain, with information passing through a sequence of interconnected nodes that imitate neurons. They are important for research in various fields of the chemical sciences [5].

DL algorithms has made it possible to simulate and identify countless numbers of compounds in a safe, economical and sustainable manner, therefore, DL algorithms are gaining a lot of interest in the enhancement of discoveries in pharmaceutical, medicinal and environmental chemistry [6]. It is also an innovative source of new perspectives and cost effective.

Cova and Pais [7] stated that researchers are investigating the possibilities of using machine learning for data collection by computations and experimental measurements. Data mining is a technique for analyzing large data to find and link related correlations between different properties of chemicals and materials. The advancement of software and the continuous growth of chemical data in databases such as Protein data bank and PubChem has aided the increase in Machine learning and deep learning applications in Chemistry such as Quantitative structure-activity relationship (QSAR), drug discovery, materials design, protein structure prediction, quantum chemistry, etc.

Chemical reactions are vital in chemistry, however the issues associated with chemical reactions such as the discovery of novel reactions, optimization of conditions and the selection of reactions provide numerous opportunities to use Machine Learning. A reaction often consists of a series of elementary steps, it can be considered to be the conversion of starting materials to a major product. A reaction procedure including temperature, isolation and purification, order and speed of addition, etc. play vital roles which are often not characterized or put into consideration. This means that Quantitative structure-activity relationship

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(QSAR) – which is a modelling chemical reaction, multiple reactants, rection conditions, products, varying amounts of additional compounds e.g., reagents, solvents, catalysts and additives need to be put into consideration [8].

Reactions usually have multi-molecular problems, in order to overcome this challenge an encoding software which has all the information of the specific compound in the reaction or not can be applied [9]. However, encoding all components may not be necessary but the major focus of the reaction should be changed. During the course of the reaction, all atoms and bonds that were either modified, added or removed will be characterized, hence, they will be recognized using atom-to-atom mapping of reactants and products. It is vital to keep in mind that these reaction rules do not describe the reaction mechanism but they analyse the different (dis)connections the molecules and the bonds present.

III. Analysis of Spectral Data via Chemometrics, Machine Learning, and Deep Learning Methods

According to Houhou and Bocklitz [10], in chemical analysis, data generation is more effective when it is combined with the best tools for analysing the data that was collected. The techniques for analyzing chemical data depend on the sample and the task, however it is vital that pre-analysis are evaluated in the chemical data notwithstanding the task. It is common to have distortions of data when retrieving chemical data using various measurement techniques. These distortions are referred to as artifacts and they arise due to the nature of the sample or from the measuring devices. The removal or suppression of artifacts leads to the enhancement of data and is vital for the analysis of data to produce meaningful results.

Spectroscopic measurements such as X-ray spectroscopy, nuclear magnetic resonance (NMR), mass spectroscopy (MS), vibrational spectroscopy etc, generate profiles with high dimensions which have a great value of information, and can be harnessed through machine learning, deep learning and chemometrics methods. These techniques are aimed at determining the sample's fundamental chemical properties with greater precision and accuracy.

A. Mass Spectroscopy (MS)

Mass spectroscopy (MS) is an analytical technique that is used to measure the mass of charge ratio of molecules in any given sample. It is also used to determine and analyze a sample to discover the unknown compounds in a sample, determination and structure elucidation of the chemical properties of different molecules. The basic concept deals with the breaking of compounds and molecules into fragments and charged species respectively. These fragments and charged species are finally focused on a detector according to their mass and charge ratio to count the number of ions and the resulting data is plotted as a graph according to their various masses.

Gas chromatography-mass spectrometry (GC-MS) analysis creates charged fragmented particles for each analyzed molecule, causing the sample deconvolution and peak alignment extremely difficult. Duan *et al.,* [11] developed a new software, QPMASS (a parallel peak alignment and quantification software), to analyze GC-MS data on a large scale. They implemented parallel computing with an advanced dynamic programming approach to tackle the issue of sample deconvolution and peak alignment. Li *et al.,* [12] developed a software that can identify and improve the reliability and sensitivity in peptides. They combined deep learning predictions of the peptide features with other peptide features to rescore peptide-spectrum matches. The results showed increase in the reliability and sensitivity of the data that was predicted of MHC-binding peptides.

B. Nuclear Magnetic Resonance (NMR)

Nuclear magnetic resonance (NMR) is an approach that is used to determine the chemical and physical properties of the atoms in a molecule by exploiting the magnetic properties of the atomic nuclei. It is difficult to make conclusions or interpret the spectra of an NMR analysis without the use of Chemometric methods. Zhao *et al.,* [13] applied a chemometric method on ^{1}H NMR spectra to provide extensive report on the changes that occurred during the Danshen extract. They used this technique to analyze the effects of the multistep processing on the chemical changes. Marion Marion et al. [14] created a new method for simultaneous dimensionality reduction and variable clustering called adaptive clustering around latent variables (AdaCLV). This method was used to analyze NMR spectra and can be used to find possible biomarkers.

C. X-ray Spectroscopy

X-ray spectroscopy is a spectroscopic technique that is used to characterize materials by the excitation of the molecules to emit the characteristics wavelength of the elements available in the sample. The emitted wavelength is used to determine the specific elements present in the sample. Machine learning, Chemometrics and deep learning techniques are important in addressing some practical issues in spectroscopy. Mullaliu *et al.,* [15] investigated the electrochemical activity in manganese hexacyanoferrate (MnHCF) by varying the ion content in the interstitial spaces. They combined X-ray absorption spectroscopy and a Multivariate Curve Resolution Alternating Least Squares (MCR-ALS) to analyze the modifications that occurred during the Li insertion and Na release structurally and electronically. It was observed that at the Fe site, the rate of the absorption of water affects the reaction dynamics.

D. Vibrational Spectroscopy

Vibrational spectroscopy also referred to as Infrared (IR) spectroscopy, it analyses the infrared region of an electromagnetic spectrum. Vibrational Spectroscopy is a non-destructive technique that measures the vibrational energies of the unique chemical bonds of the molecules in a sample. This vibrational energy gives the compound a unique identity, which can be used for the identification and characterization of compounds, for the determination of complex structures and the detection of contaminants. Raman spectroscopy and Infrared absorption are the two types of vibrational spectroscopy, the challenge with vibrational spectroscopy is that it needs extensive data

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processing to obtain relevant information from spectra. Akpolat *et al.,* [16] investigated the pattern recognition techniques by using a handheld Raman spectroscopic device to classify and quantify various types of tomato carotenoids samples with different carotenoids. Artificial neural network (ANN), Soft independent modeling of class analogy (SIMCA), and partial least squares regression (PLSR) were used to analyze the resulting spectra for classification and quantification purposes. Zafar and Hong [17] used a functional near-infrared spectroscopy (fNIRS) as a new approach to monitor the oxyhemoglobin changes produced by neuronal activations. They used a kernel-based recursive least squares (KRLS) algorithm with a Gaussian kernel to minimize the amount of time used to detect the time in fNIRS signals from the neuronal activation. KRLS was able to estimate the changes in oxyhemoglobin and deoxyhemoglobin and it showed the best performance.

IV. Artificial Intelligence for the Analysis of Spectral Data

Machine Learning, Deep Learning, Chemometrics are some of the Artificial Intelligence techniques that can be used to analyze chemical image data. They can analyze the various images and structures of a sample ranging from grayscale image to hyperspectral images and provide vital information on their spatial and spectroscopic data.

A. Two-dimensional (2D) chromatography

A chromatographic technique that provides information on the chemical composition of a sample, by combining two different chromatographic columns in sequence and injecting a fraction from the first column to the second column is the 2D chromatographic technique. As a result, the peaks that were not separated in the first column was separated in the second column [10]. Huygens *et al.,* [18] compared three algorithms which are genetic algorithms (GA), covariance matrix adaptation-evolution strategy (CMA-ES) and evolution strategies (ES), to a plain grid search for the enhancement of searches in 1D and 2D chromatography techniques. The results demonstrated notable enhancement, particularly in terms of the number of search runs required to obtain a given separation quality. In the huge search run number limit, the ES and GA performance followed a hyperbolic law.

Nagai et al., [19] discovered a biomarker of hepatocellular carcinoma (HCC) in the human liver by using multivariate analysis methods such as Principal Component Analysis (PCA) and orthogonal partial least square discriminant analysis (OPLS-DA). Ultrahigh-performance liquid chromatography/quadrupole time-of-flight mass spectroscopy (UHPLC/QTOFMS) instrument equipped with a mixed-mode column was used to extract the data. From the results, it could be seen that global metabolomics/metabolic profiling (G-Met) method can be used to identify the novel biomarkers.

B. Atomic Force Microscopy (AFM)

Atomic Force Microscopy (AFM) also referred to as Scanning Force Microscopy (SFM) is a high-resolution microscopy technique that enables the nanoscale characterization of various material properties such as magnetic, electrical, and mechanical properties. It is a high-resolution imaging technique where a small probe with a sharp tip is scanned back and forth in a controlled manner across a sample to measure its surface.

To address the issue of the required time for the oscillating tip to reach a steady-state motion in AFM imaging, Javazm and Pishkenari [20] suggested a new imaging technique based on an artificial intelligence-based algorithm. Several artificial intelligence-based methods were investigated, including radial basis function neural networks, adaptive neural fuzzy inference system networks, and multi-layer perceptron, to see if artificial intelligence techniques could directly assess surface topography. In terms of surface features estimation, the results showed that the multilayer perceptron outperformed the other strategies.

C. Electron Microscopy (EM)

Electron microscopy (EM) is a microscopy technique that creates the image of a sample via an electron beam. Due to the higher energy of the electrons which is greater than that of visible light, Electron Microscope has a far higher resolution than a light microscope. Electron microscopy can be used to examine the microstructure of a variety of biological and inorganic objects, as well as to get morphologic and crystallographic data.

One of the challenges in electron microscopy (EM) imaging was resolved via some artificial intelligence-based techniques as discussed by Yu et al., [21]. There are some limitations when traditional image recognition technique such as the scanning electron microscopy (SEM) is used for imaging, these are the inability to obtain the complete pore space characteristics in images and the poor segmentation and low accuracy of results. The authors used an artificial intelligence-based semantic image segmentation technique to examine pore characteristics and investigate the link between microscopic pore characteristics and macroscopic permeability parameters of sandstone in SEM images. The findings revealed that deep learning can effectively recognize images and can be used to process microscopic images automatically.

V. Improving Computational and Quantum Chemistry using ML

Computational and Quantum chemistry are a branch of chemistry that has been immensely boosted by the advances in machine learning. Kang *et al.,* [22] used an Extreme Learning Machine (ELM) algorithm to predict the refractive index of ionic liquids on quantum chemistry calculations. A model was designed using a stepwise regression algorithm and R^2 and AARD% values of 0.841% and 0.855% respectively to perform quantum chemistry calculations on numerous ionic liquids to obtain their structures and descriptors. The results showed that ionic liquid anions significantly affected the predicition of the refractive index when compared with the cations. Furthermore, with the use of the ELM algorithms, better performances were achieved.

Brockherde et al., [23] used a ML algorithm to understand the atomic interactions within a molecule, this was used in pharmaceuticals for the determination of the behaviour of molecules and the design of new molecules to enhance the performance of emerging energetic materials, such as battery technologies, solar cells, and digital displays.

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VI. Planning and Predicting Reactions and Routes

Machine Learning technique has been used to answer some practical questions in Organic Chemistry such as the estimation of the precise rate, yield and time of a reaction, prediction of the major or minor product of a reaction, identification of the optimal conditions e.g., catalyst, temperature, reactants, etc., and the most appropriate method of synthesis for a specific compound. The backbone of organic chemistry is retrosynthesis and reaction prediction. Retrosynthesis is a method for synthesizing tiny organic compounds in which the target molecules are broken down recursively into smaller precursors. The findings gained from this approach are often insufficient; nevertheless, rule-based procedures have been widely used to solve both reaction prediction and retrosynthesis computationally [24].

VII. Analytical Chemistry and Catalysis with ML

In analytical chemistry, many statistical studies combined with ML approaches have been used to classify mass spectra, NMR, or IR using assessments on accessible substances. In catalytic processes, machine learning is utilized to forecast unexpected reactive events or relevant mechanistic insights. Researchers have developed tools for predicting catalytic components and dynamics using machine learning. Durand and Fey [25] examined the identification and prediction of ligands for metal-catalyzed coupling reactions in order to build a synthetic method that is both cost-effective and environmentally friendly, with the potential to be expanded into a pharmaceutically relevant system.

The application of machine learning has opened up new possibilities for identifying catalysts utilizing efficient methods that avoid the requirement for high-throughput screening and reduce the number of compounds and materials that exhibit the desired properties and can be experimentally validated. Inverse design, for example, can be used to control catalytic activity by changing the first and second coordination spheres of the catalyst binding site (e.g., functionality of catalytic cofactors in enzymes) [26].

VIII. Applicatioms of ML for Risk Management and Environmental Protection

A. Estimation Of Minimum Ignition Energy Of Explosive Chemicalsan and The Heat Of Detonation Of Aromatic Energetic Compound Using ML

Minimum Ignition Energy (MIE) is the smallest energy required by a combustible compound to successfully catch fire. It is the main parameter that is used to predict the possibility of igniting explosives and for indicating the sensitivity of a combustible compound. It is vital in the risk assessments of accidental explosions in industries and for aviation safety. MIE is important while handling and characterizing hazardous chemical explosives in the laboratory. Although MIE is very significant, it is expensive, time consuming and its experimental determination is very risky due to the challenges with the interpretation of data, errors in measurements or wrong assumptions of values, [27]. Owolabi et al., [28] employed a hybridization of the gravitational search algorithm (GSA) and support vector regression (SVR) to estimate MIE with a small number of descriptors, such as the compound's molecular weight and the quantity of Carbon and Hydrogen atoms. Using a hybrid support vector regression and gravitational search algorithm, they were able to estimate the MIE of sixty-one chemical compounds while avoiding experimental difficulty and maintaining precision.

The heat of detonation (HD) is a quantitative method of analysis that is used to determine the amount of energy of organic energetic substances, it is also used to evaluate the detonation performance of explosives. Furthermore, HD demonstrates the amount of energy available for mechanical activity and examines the potential damage to the environment. It is important in the determination of the explosives performance parameters such as detonation pressure and velocity which is necessary for the optimum performance of the explosives without causing environmental disasters.

Adeyemo et al., [29] used a technique that combined support vector regression (SVR) and gravitational search algorithm (GSA) to estimate the heat of detonation of thirty energetic aromatic compounds. This method demonstrated the importance of quickly estimating the HD of organic energetic compounds without sacrificing experimental precision.

Conclusion

Artificial intelligence-based techniques such as machine learning, Chemometrics and deep learning have been combined with spectroscopic measurements in Chemistry for the analysis of data has yielded promising application results in various fields of chemistry. This review paper examined recent research and applications of artificial intelligence-based techniques for specific spectroscopic measurements, imaging approaches such as NMR, MS, vibrational spectroscopy, X-ray, AFM, EM, and 2D chromatography, as well as the advancement of computational and quantum chemistry and reaction route prediction. These strategies have made it possible to solve chemical problems that are difficult to express and explain using traditional methods.

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