



## Integrating chemistry disciplines with artificial intelligence

Nadia Kh. Radhi <sup>a</sup> , Qabeela Q. Thabit <sup>\*b</sup>

<sup>a</sup>Department of Pharmaceutical chemistry, College of Pharmacy, University of Basrah, Basrah, Iraq

<sup>b</sup>Basrah Education Directorate, Ministry of Education, Basrah, Iraq

Email: [nadia.khalid@uobasrah.edu.iq](mailto:nadia.khalid@uobasrah.edu.iq), [qabeelaqassim@basrahaoe.iq](mailto:qabeelaqassim@basrahaoe.iq)

### ABSTRACT

The tremendous development in the field of artificial intelligence (AI) is impacting all areas of scientific research, especially applied sciences. It has connected disciplines, leaving no field of science untouched in one way or another. Chemistry has been particularly affected, with AI permeating all areas of chemistry—organic, inorganic, physical, analytical, and biological—in addition to linking chemistry research with other sciences. AI tools have been used extensively in recent years, especially the last decade, to find solutions, discover or predict the outcomes of reactions, develop pharmaceuticals, conduct chemical synthesis, and in materials science. They offer a more effective alternative to traditional methods. It seems we are witnessing significant and clear progress in scientific research, industry, and applied fields, reflecting the results and analysis of the data we provide as fuel for AI algorithms. In this research study, we present the smart face of chemistry specializations, or in other words, we highlighted the advancements in chemistry fields supported by modern smart tools and methods.

**Keywords:** Artificial Intelligence, chemistry disciplines, deep learning, machine learning, database training-based, Analytic, Biochemistry, predictive learning, and modern computational chemistry.

Received: 03/07/2026

Accepted: 09/09/2026

Published: 30/09/2026

### Introduction

It is no secret that chemistry is a central and vital science, interacting with virtually every aspect of life, from the smallest to the largest, and has been based for thousands of years on practical research methods. These methods rely on experimentation and discovery, which consume resources, effort, and time, and are subject to logical deductions based on the results of experiments. This presents challenges for researchers in their assigned fields. The emergence of artificial intelligence and its integration into the field of chemistry marked the beginning of a leap forward, expanding and facilitating research in all chemistry disciplines[1,2].

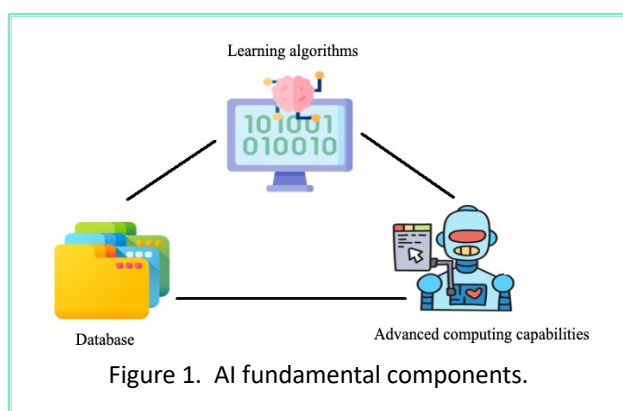
Today's research methods rely on predictive research based on the use of training models, testing, and training optimization. For this purpose, algorithms have been employed, including machine learning algorithms, deep learning algorithms, and algorithms that use both methods [3-5]. The choice of algorithm depends on the database used. Modern research methods also require data from reputable scientific institutions and academies responsible for preparing this data with high professionalism. Moreover, this data is also subjected to multiple processing methods, which have been provided by special programs and applications that are capable of carrying out these tasks [6-8].

Like other sciences, chemistry needs development and to benefit from what is produced or made available from modern research methods and tools, including software, applications, and artificial intelligence algorithms in its various general specializations, such as analytical [9,10], biological[11], inorganic[12], organic[13], industrial[14], physical[15], and nano-chemistry [16-18]and its sub-branches. Recently, a new specialization has emerged that integrates simulation, analysis, and deduction programs with the science of chemistry in all its aforementioned branches. In fact, it is a simulation of chemical processes, calculation of reactions, and analysis of the main components and statistical significance. The convergence of efforts has led to the specialization of a new field in chemistry, which is called computational chemistry [19,20].

### Artificial intelligence and Basic components

With the tremendous advancements in computer science applications, scientific fields have been evolving alongside artificial intelligence in ways unlike anything seen before. What distinguishes computer science and its software is that it has experienced a qualitative leap in the last two decades. Unlike other sciences that took hundreds of years to develop to reach their current state, it has expanded significantly, giving rise to what is known

as artificial intelligence (AI) [21,22]. This field has swept across all other sciences and disciplines in just a few years, becoming so vast that it is now virtually ubiquitous in science and life. AI came to solve the problem of programming, so programming has been thinking since it was created in the fifties of the last century and developed in the nineties. It has solved many of the problems that companies, institutions, and businesses face and provided great services. It is known that the entry of the computer into scientific fields facilitated calculations and data storage, but the machine executes certain decisions that are known in advance without having a role in decision-making. Many applications have appeared in all fields, entertainment, scientific, industrial, religious, commercial, economic, and so on, so that there is hardly a field that is devoid of a large number of applications, whether on mobile, desktop computer, laptop, Web Development, and so on [23-25]. The crisis facing computer scientists was that these applications were merely programs designed to be directed and incapable of making decisions. In other words, the application simply executes instructions it already knows without any intervention or thought; it is not an intelligent application. The dream of scientists was to make computers and their applications capable of thinking, analyzing data, drawing conclusions, and making decisions about people. This was the initial spark that led to what is now called artificial intelligence[26,27]. Today, intelligence is based on three fundamental components, and it is incomplete without all three as explained in Figure 1:



1. Database
2. Learning algorithms (Artificial Intelligence algorithms)
3. Advanced computing capabilities[28].

## 1.Database

One of the most prominent factors driving the remarkable progress in artificial intelligence is the availability of a reliable database. Educational, health, commercial, and economic institutions have actively contributed to this research field by providing various types of data. Sometimes the data requires significant effort to process before commencing any work or training, while other times it is organized and requires minimal effort and time. Artificial intelligence has provided an important tool for addressing any flaws in the data structure. This includes ensuring that no data is missing from the database, that values are not significantly different, and other methods for correcting any errors in the data used. Generally, data can be categorized into two types, as follows [29-32]:

### 1- Structure Data.

This refers to organized data where each piece of information has a specific name or classification, whether it's a description of the information, its size, percentage, or logical value. There are many examples, such as a data table containing the symptoms of influenza in a group of people, a record listing stock market prices, or a record of the number of visitors to the Amazon website, from which country they come, their interests, the time they spend there, and whether they are only browsing or shopping, and so on.

### 2- Unstructured Data.

This data is essentially unorganized and lacks a specific name or classification; there are no column headings, such as "Sound to be understood," "Images to be interpreted," or "Videos to be analyzed."

## 2. Artificial Intelligence Algorithms

### Artificial Intelligence Types

Artificial intelligence tools have led to a significant leap in research and scientific innovation, particularly in the last twenty-five years. Virtually every research field now utilizes AI algorithms, which were previously considered

pure science fiction. This has begun in sectors such as education, finance, economics, agriculture, industry, health, the environment, space, and countless others. AI has become an indispensable part of our lives. When we talk about the education sector, we mean it has permeated every aspect of research, teaching, and the acquisition of research skills. Naturally, the widespread use of artificial intelligence in applications and devices has contributed to the services it provides, including impactful research facilities at the level of research formulation and practical application of rigorous scientific research, with the latter utilizing helpful tools. Artificial intelligence (AI) is divided into two main categories. The first category is based on AI capabilities. The second category is based on the function AI provides. Figure 2 illustrates the different types of AI in detail [33-35].

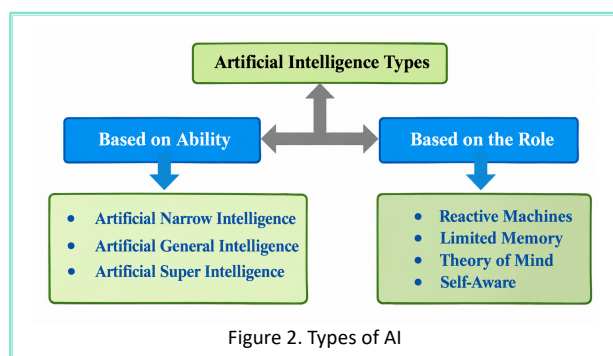


Figure 2. Types of AI

## Artificial Intelligence Branches

Artificial intelligence (AI) branches are divided into sub-branches according to their applications, the type and volume of data they process, their training and learning methods, and other criteria. Figure 3 illustrates these branches. It's worth noting that there is a primary classification of work in AI based on its operational mechanism: supervised training and unsupervised training. Among the most prominent branches in research fields are machine learning and deep learning, which we will focus on due to their close connection to chemical research compared to other branches [34,28].

## Machine Learning Concept

Machine learning is a major branch of artificial intelligence. Its concept relies on a mathematical

relationship between inputs and outputs, and it's typically used to train data organized into tables.

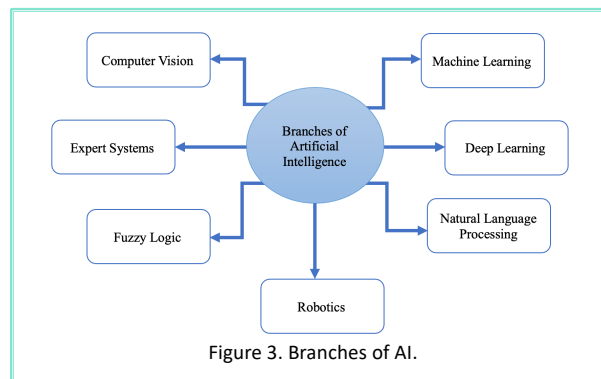


Figure 3. Branches of AI.

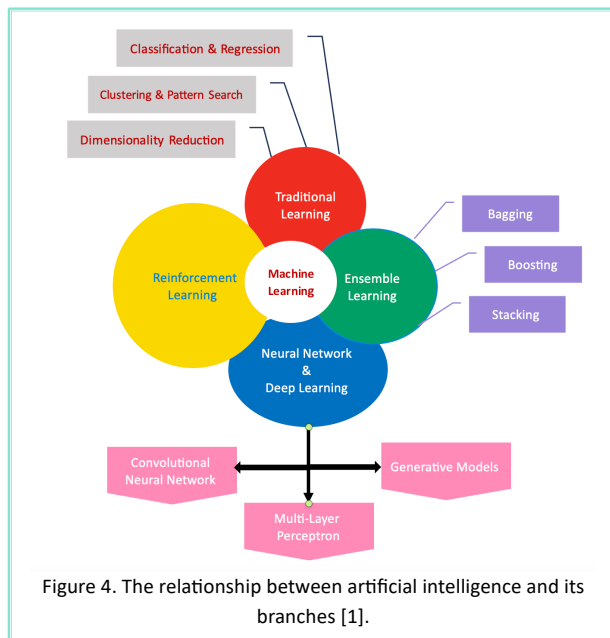
However, this doesn't preclude its use for training other types of data, such as images, audio, videos, and more. The name comes from the fact that this type of algorithm trains the machine to function similarly to a human. The idea is based on providing data as input and teaching it the outputs resulting from each input scenario. This principle is applied until high accuracy is achieved over time. Afterward, the algorithm is fed only inputs and asked to predict the corresponding outputs. In fact, all other branches have developed from the basic concept of machine learning, which relies on analytical and statistical methods for processing the data used [36,37].

## Deep Learning Concept

Deep learning is an advanced level of one of the branches of machine learning. In other words, it is based on machine learning but relies on deep neural networks to reach the desired results. Professor Andrew Engi is considered one of the pioneers of machine learning and deep learning, and he uses it in all areas of machine learning such as regression, classification, reinforcement, supervised, and unsupervised. Due to the number of hidden middle layers of neural networks that are trained in this type of learning, it naturally requires more powerful and faster hardware and enormous computing power, as we mentioned before [34,38,39]. The construction of this network contains multiple neural layers. Professor Andrew mentioned a beautiful analogy for deep learning, comparing it to a rocket engine, and its fuel is the data used. Both must be large in size, high



in power, and efficient in effectiveness. The relationship between artificial intelligence and its branches can be represented as Figure 4.



In summary, what we need here is a brilliant algorithm and a massive database. This is the foundation of deep learning, which rests on two essential pillars, neither of which can be dispensed with: a powerful algorithm and huge datasets. There are three main types of deep learning, depending on the type of input and processing data[39,40]]:

- Deep Neural Network DNN
- Convolved Neural Network CNN
- Recurrent Neural Network RNN

As we explained earlier, the term "deep" comes from its composition of dozens of layers of neural networks. The term "learning" itself originates from machine learning. A comparison between machine learning and deep learning can be made as shown in the Table 1 below [17,37,38,39,41]:

## The Science of Chemistry and its Branches

Chemistry is the science concerned with the chemical changes in matter, including its composition, structure, properties, and the transformations that occur between substances during chemical reactions. It studies the transformations that take place in matter. Chemistry involves delving into the smallest element of matter and studying it: atoms, or the building blocks of matter. These atoms, through specific reactions, produce molecules, which are defined as groups of atoms linked together by specific chemical bonds, resulting in energy changes. Since ancient times, researchers have dedicated themselves to experimentation and repeated trials to arrive at sound conclusions based on the obtained results. Like other sciences, chemistry has benefited from artificial intelligence tools, which have permeated all fields [42].

**Table 1:** A comparison between machine learning and deep learning

| Different Face                            | Machine Learning                                                                                     | Deep Learning                                                                                                                                                                     |
|-------------------------------------------|------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Calculation operations and execution time | Smaller and less                                                                                     | Bigger and longer than machine learning                                                                                                                                           |
| Data                                      | Data is often structured data SD, ordered, organized, and tabulated.                                 | Data is often unstructured (UD), and while it may be structured, this is very rare. For example, images, audio, handwriting, and videos can contain tens of millions of features. |
| Quantity of data                          | It is sufficient to provide a certain amount of data, and any further increase in data is pointless. | It benefits from enormous amounts of data.                                                                                                                                        |
| Number of rows                            | It is reasonable                                                                                     | It would be enormous                                                                                                                                                              |
| Input\output                              | SD\SD (Number or information)                                                                        | UD-SD\ UD-SD Audio, image, video, text                                                                                                                                            |

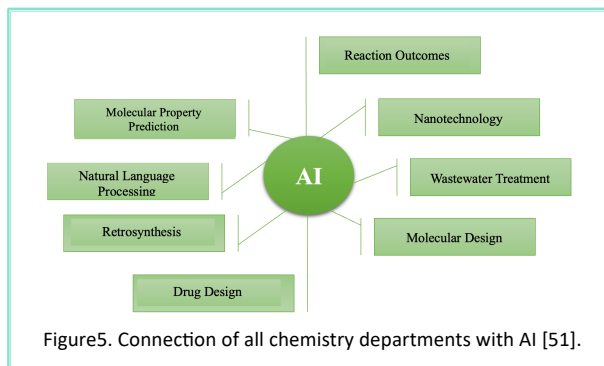


For example, the medical field has used machine learning and deep learning techniques for the early detection of various diseases, including COVID-19[43], which has been the subject of extensive scientific research since the 2020 pandemic, as it is a critical research topic addressing a disease that threatened humanity and resulted in very high mortality rates. Furthermore, numerous research studies have analyzed patient data for the early detection of various types of cancer, such as breast[38] and lung[44] cancer, as well as for detecting tuberculosis, chest or respiratory infections[44], infectious diseases[46], thyroid disorders[47], diabetes[37], stroke[39], and all other diseases. In the industrial sector, work in this area has been extensive, for example, in detecting rust in iron and metals in oil pipelines and large containers [48]. In agriculture, it is used to assess crop quality [49].

In the field of cybersecurity, researchers have also worked on employing algorithms to detect and protect against vulnerabilities and threats, because the method of artificial intelligence is to analyze a huge and large dataset and study it well to reach the correct conclusions, as well as to detect and prevent phishing, which may be a site, person, application, or link, and to provide protection and security to confidential information and to beware of misleading, fake, and deceptive websites[36,50].

Studies in chemistry have benefited greatly from artificial intelligence. Traditional methods, which relied solely on laboratory experiments and repeated procedures, were time-consuming, laborious, and resource-intensive. However, learning and training tools have introduced an analytical approach and a study methodology focused on data analysis. This approach leads to results that are often relevant to practical experiments, such as identifying resulting compounds or executing equations and performing calculations using intelligent simulations. These simulations are also subject to experimentation and testing, but this time electronically[9,10]. Furthermore, the emerging field of computational chemistry has taken on the responsibility of simulating all aspects of laboratory work through

advanced smart applications [19,20]. Today, all branches of chemistry have adopted a new application in their experiments: the smart field, which relies on data input and the generation of research results. Figure 5 illustrates the connection of all chemistry departments and specializations to artificial intelligence.



## Integrating Chemistry Disciplines with Artificial Intelligence

Calculations of chemical compounds and related matters are very difficult, sometimes even impossible, especially with regard to chemical calculations of biological data. Therefore, a structured and stable model for calculations is necessary, involving two important steps. First, molecular indicators are used to represent the complete molecular structure. Then, a series of pairs known as molecular indicators are used, representing the core of the compound, to arrive at a reliable mathematical model that can later be used to predict previously unknown properties and characteristics of other compounds and molecules. This is known in chemistry as the link between quantitative structure and property [13,15].

### 1-Analytical Chemistry:

Descriptive chemistry, a major branch of chemistry, describes chemical substances and compounds that may be collected from food samples, archaeological finds, medicinal plants, urine, or explosives. These substances are often analyzed using various methods, such as descriptive analysis, spectroscopy, or chromatography. The resulting data constitutes a vast amount of chemical

information, but without organization and structuring, the work becomes a waste of time, resources, and effort, ultimately wasting the researcher's time and energy. However, the emergence of artificial intelligence tools has made it possible and easy to organize, structure, refine, and filter data, utilizing it in diverse ways. This allows researchers to achieve fruitful and accurate results that enhance their laboratory work and provide valuable background information for future researchers, enabling them to work with less effort, time, and cost. This is what advanced artificial intelligence has adopted in research, particularly across all branches of chemistry, with analytical chemistry in particular benefiting from numerous machine learning and deep learning experiments. The table below lists some of these experiments, which are too numerous to list entirely [10,52].

Therefore, chemistry based on description and analysis is analytical chemistry, a major branch of chemistry concerned with the quantitative and qualitative determination of the elements and compounds that make up a specific substance under analysis, and identifying its components. Like other branches, this branch is divided according to the methods and techniques used, the most important of which are gravimetric, thermal, and volumetric analysis[53]. Figure 6 explains AI techniques and analytical chemistry.

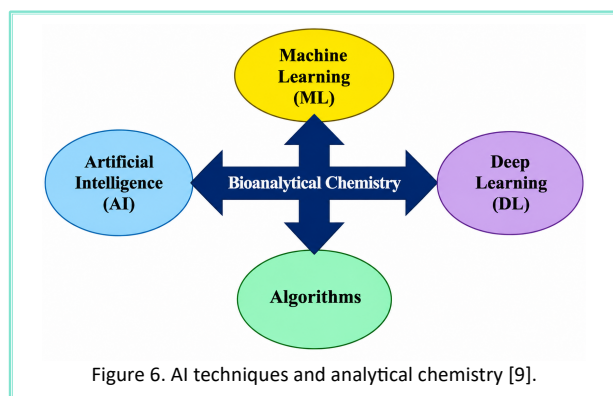


Figure 6. AI techniques and analytical chemistry [9].

Analytical chemistry, like other branches of chemistry and other fields of scientific research, has turned particularly and intensively in the last decade to the use

of artificial intelligence (AI) with most of its tools, from algorithms and applications to data of all kinds, from simple databases in the form of sorted tables to massive datasets. This has brought about a radical and significant scientific change in research, conclusions, and results, with excellent performance and high efficiency achieved by researchers in this field. Quantitative, descriptive, and qualitative analysis is no longer limited to the practical laboratory aspect. Work in the fields of artificial intelligence is distributed across various disciplines of analytical chemistry, including machine learning algorithms such as K-Nearest Neighbor (KNN), neural networks (NN), and random forest(RF), as well as in the field of analysis, inference, and statistics such as principle component analysis (PCA)[54]. Deep learning has also been used extensively in analytical chemistry research for example, convolution neural network (CNN)[55] , recurrent neural network (RNN), such as long short-term memory( LSTM)[54]. Figure 7 illustrates the use of artificial intelligence methods in all disciplines of analytical chemistry, which we will list as follows:

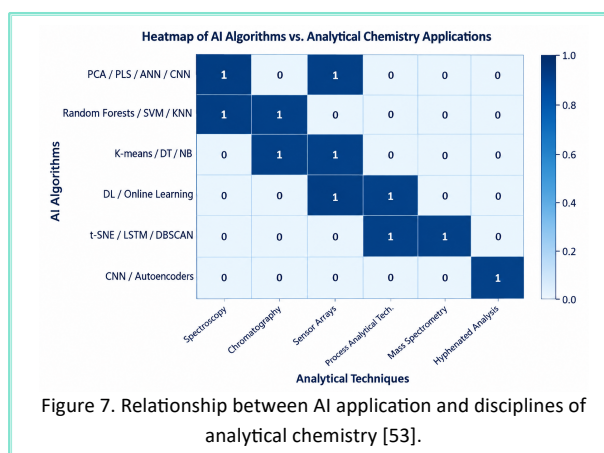


Figure 7. Relationship between AI application and disciplines of analytical chemistry [53].

Chromatography implemented by an artificial intelligence technique: Chromatographic analysis is an excellent method in analytical chemistry for separating mixtures in solution and identifying the constituent compounds of those mixtures. The analysis depends on several factors, including the affinity of the mixture in two different phases, the distribution coefficient, and the adsorption capacity. To perform analyses using more



modern methods characterized by speed, efficiency, and quality, numerous and diverse machine learning models have been employed. These models, with their almost limitless algorithms, are used to analyze and develop databases of any type, size, or subject matter, process the data algorithmically, and achieve results of high accuracy and performance. The purposes of this approach are varied, including focusing on developing high-performance liquid chromatography (HPLC) methods for analyzing compounds such as amlodipine (AMD), candesartan (CND), and hydrochlorothiazide (HYD)[56,57].

Generally, mixtures are separated using the quantum chromatography method with machine learning algorithms to improve upon traditional separation methods and identify their components. Examples support vector machine ensemble (SVM) of such techniques include [insert examples here]. The objectives of this type of study are optimally achieved: peak detection, results analysis, prediction of retention time, optimization of the gravitational amplitude, and phase testing. The use of deep learning algorithms is a crucial step in obtaining high accuracy without distortion, identifying the basic components in a less complex and less costly way in terms of time, effort, and resources, and obtaining a model that can be considered a better set of results to which researchers can refer. This is something that traditional separation methods cannot achieve [9,10,58].

## 2- Bio-Chemistry:

Biochemistry is the science concerned with studying the chemical components of living matter and the chemical changes that occur within it. It encompasses all the interactions of a living organism throughout its life cycle, from birth to death, and includes all living organisms, both animals and plants. It has several sub-disciplines and is divided into two main branches:

- Descriptive Biochemistry: This branch focuses on the precise structure of biological matter.

- Kinematic Biochemistry: This branch deals with the metabolic processes and chemical changes that occur in living systems.[59]

**Biochemistry** The molecules of living matter are primarily composed of oxygen, nitrogen, hydrogen, sulfur, and phosphorus atoms. These atoms combine to form smaller biomolecules (fatty acids, amino acids, sugars, nucleotides, purines, pyrimidines), which in turn contribute to the formation of larger biomolecules (lipids, proteins, nucleic acids, glycogen, starch). These larger molecules then form the cell, the basic building block of a living organism, composed of carbohydrates, proteins, lipids, salts, and water. Biochemistry focuses on the study of: biochemical compounds and their relationship to diseases; the role of enzymes in biochemical reactions; energy production through metabolic processes; and the qualitative and quantitative composition of cells through their chemical structure [60].

One of the fields that has witnessed significant and remarkable advancements is biochemistry, which has utilized machine learning, deep learning, and all available artificial intelligence tools and applications. These technologies offer substantial advantages to researchers in this field, enabling the development and modernization of research in both results and methodologies. This represents an innovative approach to advancing the methodology employed in pharmaceutical fields[60].

Previously, research relied on lengthy waiting periods for laboratory results, adding to the researcher's burden and the challenges of material availability and cost. Furthermore, smart tools have distinguished themselves by entering a crucial area: drug discovery [11].

Innovation in this vital and sensitive field is not limited to discovery; smart algorithms also enhance results and can be further developed in research directions. Here, the researcher is not restricted to specific outcomes but has the ability to predict and achieve results by employing



these smart tools. The expansion of work towards processing, cleaning, organizing, and structuring databases of all types provides encouragement and motivation to delve into applications. Systematic intelligent search techniques have been developed to expand the researcher's scope, contributing significantly to the prediction of protein structures [61].

This has resulted in accurate and rapid classifications, and the discovery, analysis, and study of compounds, as well as performing all related calculations, has become very easy and straightforward. Furthermore, modern artificial intelligence models have provided a precise organizational framework for laboratory information management systems. Previously, these systems were not as effective in terms of accuracy, speed, and organized direction. In advanced modern information systems operating according to intelligent algorithms, information is stored correctly and automatically, with alerts or notifications sent to all laboratories whose work may depend on this information and data. This data can also be retrieved and used in statistical analysis models for components and in questionnaires, which are the basis of most research today related to health and the environment [59,60].

### 3- Inorganic Chemistry:

Inorganic chemistry is a vast and diverse field, encompassing more than one specialization. It includes all elements, starting from organic chemistry—specifically the chemistry of carbon in its bonds with oxygen, nitrogen, hydrogen, halogens, and countless other elements—to physical chemistry, which studies the quantitative behavior and physical properties of matter. It also studies a wider range of materials, such as atomic gases, extended-structured solids, air-sensitive compounds, hydrolyzable compounds, compounds soluble in other organic solvents, and compounds soluble in inorganic solvents. Inorganic materials are classified into:

- 1- All elements
- 2- Ionic compounds
- 3- Molecular compounds

4- Polymers. This means that inorganic chemistry encompasses a diverse range of materials, thus requiring extensive study. This makes it difficult for inorganic chemists to determine the properties and reactions of materials with varying structural and reactivity characteristics. Therefore, it is essential to focus on:

- 1- Synthesis methods of all types and names
- 2- Treatment and characterization techniques for inorganic compounds

To explain the existence of inorganic materials, we need aspects of physical chemistry to describe their behavior. Inorganic compounds are used as medicines, fuels, dyes, catalysts, and in many other applications [62].

Intelligent learning models and the features available in their smart tools have revolutionized the field of inorganic chemistry, across its various types and methods, leading to rapid development and highly accurate results. These models utilize large databases within the framework of intelligent algorithms capable of processing, cleaning, and zeroing out all errors, while focusing on normalization. Following this, the analysis and deduction phase begins. Analysis involves several approaches, such as dividing the data into clusters and selecting the optimal result from each cluster, or dividing it into groups based on their similarity. A crucial point that prevents oversampling is ensuring realistic accuracy within the data sample. The final stage involves inference and the presentation of results [12].

### 4- Organic Chemistry:

Organic compounds can be obtained from living organisms through the vital energy present within their tissues; this is known as the "vital energy theory." In short, they are compounds containing carbon atoms in addition to hydrogen and oxygen. Later, a scientist succeeded in synthesizing them in the laboratory by creating urea through the chemical reaction between ammonium chloride and silver cyanide.

Later, another scientist succeeded in preparing acetic acid from carbon, oxygen, and hydrogen, the basic elements of acetic acid. Following this, another scientist prepared methane and acetylene gases, leading to the realization that organic compounds could be prepared



experimentally, rather than relying solely on theory. Organic compounds are divided into two groups [63]:

1- Hydrocarbons, which consist of two elements: carbon and hydrogen, and include alkanes, alkenes, and aromatic compounds.

2- Hydrocarbon derivatives, in which the hydrogen atom is replaced by an atom or atomic group called a functional group. Examples include aldehydes, ketones, carboxylic acids, ethers, alcohols, and amines.

The uses of organic compounds are wide-ranging. However, it has been shown that some organic compounds are more toxic than previously thought. Some contribute to the destruction of the ozone layer, which protects life from the harmful effects of ultraviolet radiation, while others are carcinogenic [64].

Organic chemistry, like other chemical disciplines, has witnessed significant expansion and advancement, particularly in its experiments and studies. Online platforms have emerged, operating efficiently at any time, to perform reactions and calculations, providing products, weights, and bonds in mere seconds. Furthermore, the ability to predict reactions in advance has become highly reliable. Artificial intelligence models possess the capacity to train a large dataset, continuously and rigorously, until they achieve highly accurate results. This ensures researchers obtain efficient models, which can then be tested to verify accuracy and efficiency. Algorithms can then be used to predict synthesis patterns, providing a comprehensive inventory of the environmental conditions, materials, and supplies required for each reaction. This is in addition to the automation of laboratories facilitated by AI applications, enabling the prediction of reaction paths and products, and providing insights into reverse synthesis pathways and directions [13,63,64].

## 5- Physical Chemistry:

Physical chemistry deals with the properties, composition, and structure of matter (whether elements or compounds), the reactions and transformations it undergoes, and the energy released (exothermic

reactions) or absorbed (endothermic reactions). It explains chemical phenomena using the fundamental laws of physics. It focuses on the quantitative description of matter and energy, explaining how molecular structure and motion govern chemical behavior. This science provides a theoretical foundation for understanding chemical reactions, phase changes, and the properties of materials. Key areas of physical chemistry include thermodynamics, reaction kinetics, quantum mechanics, electrochemistry, and molecular spectroscopy. These concepts enable scientists to predict the likelihood of a reaction, calculate energy changes, and analyze the stability of chemical systems. Physical chemistry also plays a vital role in industrial processes, environmental analysis, pharmaceutical research, and materials development. The importance of measurement in physical chemistry: Measurement is a cornerstone of experimental and theoretical studies in physical chemistry, allowing scientists to determine numerical values for physical properties by comparing them to agreed-upon standards. Without precise measurement, scientific observations cannot be verified or reproduced. Common physical quantities—such as mass, temperature, volume, and time—must be measured using standardized units. Consistent measurement practices ensure data reliability and allow for meaningful comparisons of experimental results across different laboratories and disciplines. The International System of Units (SI): The SI provides a unified framework for scientific measurements worldwide, ensuring clarity, consistency, and accuracy in the exchange of experimental information in base units. Physical chemistry, as a discipline, has expanded and developed by integrating it with available artificial intelligence methods, approaches, and tools, particularly those used for research and scientific purposes. Studying the nature of matter is now possible through massive databases, which are fed into intelligent algorithms that rigorously analyze its features, characteristics, properties, and all influencing factors. Furthermore, exploring the type of chemical reaction a substance undergoes, determining whether it is energy-releasing or energy-gathering, has become easier and more



accessible with the application of machine learning or deep learning tools. The study of the kinetic nature of molecules and their resulting structures has also been enhanced by research using intelligent tools. In addition, the various types of unit conversion systems have been provided with modern tools, making it a field of in-depth specialization through efficient and purposeful scientific research, exploration, and inquiry[15,66].

### Conclusion:

The widespread adoption and rapid development of artificial intelligence tools have significantly altered many fields and impacted our daily lives. Applications operating within the context of artificial intelligence have entered every aspect of our lives, from the smallest tools related to our daily lives to the largest in industrial fields. This has enriched scientific research fields and integrated them with these modern applications. It is now commonplace for every discipline to conduct experiments, deduce results, analyze data, or implement reactions and methodologies using AI. This is a particularly effective contribution to the various branches of chemistry, as AI has facilitated and simplified processes. Much more awaits us given the rapid advancements in these software programs. Furthermore, a new field of study, computational chemistry, is emerging, though still relatively new. Efforts will be combined to develop it according to the ever-evolving standards, constantly updated with the continuous advancements in AI technologies and their integration with various branches of chemistry. It is worth mentioning our work plan in this area: we plan to:

1. Expand the use of smart scientific research tools.
2. Integrate all chemistry disciplines with computational chemistry.
3. Expand and develop chemistry research within the framework of the new methodology.

### References

[1] Karthikeyan, A., & Priyakumar, U. D. (2021). Artificial intelligence: machine learning for chemical sciences.

Journal of Chemical Sciences, 134(1), 2. <https://doi.org/10.1007/s12039-021-01995-2>.

[2] Khulbe, M., Goel, S., Sharma, R., Bargujar, S., & Kathuria, A. (2022). AI's role in enhancing the capabilities of Chemists. Zenodo (CERN European Organization for Nuclear Research). <https://doi.org/10.5281/zenodo.7461655>.

[3] Lee, T., Natalwala, J., Chapple, V., & Liu, Y. (2023). A brief history of artificial intelligence embryo selection: from black-box to glass-box. Human Reproduction, 39(2), 285–292. <https://doi.org/10.1093/humrep/dead254>.

[4] Tabassi, E. (2023). Artificial Intelligence Risk Management Framework (AI RMF 1.0). <https://doi.org/10.6028/nist.ai.100-1>.

[5] Peng, C., Van Doorn, J., Eggers, F., & Wieringa, J. E. (2022). The effect of required warmth on consumer acceptance of artificial intelligence in service: The moderating role of AI-human collaboration. International Journal of Information Management, 66, 102533. <https://doi.org/10.1016/j.ijinfomgt.2022.102533>.

[6] Ntoutsis, E., Fafalios, P., Gadiraju, U., Iosifidis, V., Nejd, W., Vidal, M., Ruggieri, S., Turini, F., Papadopoulos, S., Krasanakis, E., Kompatsiaris, I., Kinder-Kurlanda, K., Wagner, C., Karimi, F., Fernandez, M., Alani, H., Berendt, B., Kruegel, T., Heinze, C., . . . Staab, S. (2020). Bias in data-driven artificial intelligence systems—An introductory survey. Wiley Interdisciplinary Reviews Data Mining and Knowledge Discovery, 10(3). <https://doi.org/10.1002/widm.1356>.

[7] Kitsios, F., & Kamariotou, M. (2021). Artificial Intelligence and Business Strategy towards Digital Transformation: A Research Agenda. Sustainability, 13(4), 2025. <https://doi.org/10.3390/su13042025>.

[8] Fang, B., Yu, J., Chen, Z., Osman, A. I., Farghali, M., Ihara, I., Hamza, E. H., Rooney, D. W., & Yap, P. (2023).



- Artificial intelligence for waste management in smart cities: a review. *Environmental Chemistry Letters*, 21(4), 1959–1989. <https://doi.org/10.1007/s10311-023-01604-3>.
- [9] Garugu, S. (2025). Artificial Intelligence in Bioanalytical Chemistry: A Review of Algorithms, Applications, And Future Prospects. *Journal of Applied Bioanalysis*, 661–667. <https://doi.org/10.53555/jab.v11i4.410>.
- [10] Nowak, P. M. (2026). Artificial Intelligence in Analytical Chemistry: Towards yet Undiscovered opportunities. *Analytical Chemistry*, 98(8), 5843–5853. <https://doi.org/10.1021/acs.analchem.5c06840>.
- [11] Alizadehsani, R., Oyelere, S. S., Hussain, S., Jagatheesaperumal, S. K., Calixto, R. R., Rahouti, M., Roshanzamir, M., & De Albuquerque, V. H. C. (2024). Explainable Artificial Intelligence for Drug Discovery and Development: A Comprehensive survey. *IEEE Access*, 12, 35796–35812. <https://doi.org/10.1109/access.2024.3373195>.
- [12] Ward, L., Agrawal, A., Choudhary, A., & Wolverton, C. (2016). A general-purpose machine learning framework for predicting properties of inorganic materials. *Npj Computational Materials*, 2(1). <https://doi.org/10.1038/npjcompumats.2016.28>.
- [13] Li, T., Song, W., Chen, N., Wang, Q., Gao, F., Xing, Y., Wu, S., Song, C., Li, J., Liu, Y., Li, S., Wu, C., & Zhang, Z. (2025). The Artificial Intelligence-Driven Intelligent Laboratory for Organic Chemistry Synthesis. *Applied Sciences*, 15(13), 7387. <https://doi.org/10.3390/app15137387>.
- [14] Choudhary, K., DeCost, B., Chen, C., Jain, A., Tavazza, F., Cohn, R., Park, C. W., Choudhary, A., Agrawal, A., Billinge, S. J. L., Holm, E., Ong, S. P., & Wolverton, C. (2022). Recent advances and applications of deep learning methods in materials science. *Npj Computational Materials*, 8(1). <https://doi.org/10.1038/s41524-022-00734-6>.
- [15] Prezhdo, O. V. (2020). Advancing Physical Chemistry with Machine Learning. *The Journal of Physical Chemistry Letters*, 11(22), 9656–9658. <https://doi.org/10.1021/acs.jpclett.0c03130>.
- [16] Del Bosque, A., Fernández-Arias, P., & Vergara, D. (2026). Machine learning for nanomaterial discovery and design. *Machine Learning and Knowledge Extraction*, 8(1), 10. <https://doi.org/10.3390/make8010010>.
- [17] Jia, Y., Hou, X., Wang, Z., & Hu, X. (2021). Machine learning boosts the design and discovery of nanomaterials. *ACS Sustainable Chemistry & Engineering*, 9(18), 6130–6147. <https://doi.org/10.1021/acssuschemeng.1c00483>.
- [18] Baduge, S. K., Thilakarathna, S., Perera, J. S., Arashpour, M., Sharafi, P., Teodosio, B., Shringi, A., & Mendis, P. (2022). Artificial intelligence and smart vision for building and construction 4.0: Machine and deep learning methods and applications. *Automation in Construction*, 141, 104440. <https://doi.org/10.1016/j.autcon.2022.104440>.
- [19] Kasar, H. M. A., Abd, Z. N. B., Khnyab, Z. S. J., & Jofan, A. S. M. (2024). Inorganic Chemistry: Principles of structure and reactivity. In Bright Sky Publications eBooks. <https://doi.org/10.62906/bs.book.181>.
- [20] Alzubaidi, L., Zhang, J., Humaidi, A. J., Al-Dujaili, A., Duan, Y., Al-Shamma, O., Santamaría, J., Fadhel, M. A., Al-Amidie, M., & Farhan, L. (2021). Review of deep learning: concepts, CNN architectures, challenges, applications, future directions. *Journal of Big Data*, 8(1), 53. <https://doi.org/10.1186/s40537-021-00444-8>.
- [21] Nguyen, A., Ngo, H. N., Hong, Y., Dang, B., & Nguyen, B. T. (2022). Ethical principles for artificial intelligence in education. *Education and Information Technologies*,



- 28(4), 4221–4241. <https://doi.org/10.1007/s10639-022-11316-w>.
- [22] Glover, F. (1986). Future paths for integer programming and links to artificial intelligence. *Computers & Operations Research*, 13(5), 533–549. [https://doi.org/10.1016/0305-0548\(86\)90048-1](https://doi.org/10.1016/0305-0548(86)90048-1).
- [23] Kumar, A., Balasubramanian, S., Byeon, H., & Manerkar, G. V. (1995). Artificial intelligence: a modern approach. *Choice Reviews Online*, 33(03), 33–1577. <https://doi.org/10.5860/choice.33-1577>.
- [24] Weiß, G. (2000). Multiagent Systems: A modern approach to distributed artificial intelligence. In *Medical Entomology and Zoology*. <http://ci.nii.ac.jp/ncid/BA40989172>.
- [25] Huang, M., & Rust, R. T. (2018). Artificial intelligence in service. *Journal of Service Research*, 21(2), 155–172. <https://doi.org/10.1177/1094670517752459>.
- [26] Alowais, S. A., Alghamdi, S. S., Alsuhebany, N., Alqahtani, T., Alshaya, A. I., Almohareb, S. N., Aldairem, A., Alrashed, M., Saleh, K. B., Badreldin, H. A., Yami, M. S. A., Harbi, S. A., & Albekairy, A. M. (2023). Revolutionizing healthcare: the role of artificial intelligence in clinical practice. *BMC Medical Education*, 23(1), 689. <https://doi.org/10.1186/s12909-023-04698-z>.
- [27] Haenlein, M., & Kaplan, A. (2019). A Brief History of artificial intelligence: on the past, present, and future of artificial intelligence. *California Management Review*, 61(4), 5–14. <https://doi.org/10.1177/0008125619864925>.
- [28] Wang, P. (2019). On defining artificial intelligence. *Journal of Artificial General Intelligence*, 10(2), 1–37. <https://doi.org/10.2478/jagi-2019-0002>.
- [29] Allen, E. J., St-Yves, G., Wu, Y., Breedlove, J. L., Prince, J. S., Dowdle, L. T., Nau, M., Caron, B., Pestilli, F., Charest, I., Hutchinson, J. B., Naselaris, T., & Kay, K. (2021). A massive 7T fMRI dataset to bridge cognitive neuroscience and artificial intelligence. *Nature Neuroscience*, 25(1), 116–126. <https://doi.org/10.1038/s41593-021-00962-x>.
- [30] Chen, L., Wang, P., Dong, H., Shi, F., Han, J., Guo, Y., Childs, P. R., Xiao, J., & Wu, C. (2019). An artificial intelligence-based data-driven approach for design ideation. *Journal of Visual Communication and Image Representation*, 61, 10–22. <https://doi.org/10.1016/j.jvcir.2019.02.009>.
- [31] Pachouly, J., Ahirrao, S., Kotecha, K., Selvachandran, G., & Abraham, A. (2022). A systematic literature review on software defect prediction using artificial intelligence: Datasets, Data Validation Methods, Approaches, and Tools. *Engineering Applications of Artificial Intelligence*, 111, 104773. <https://doi.org/10.1016/j.engappai.2022.104773>.
- [32] Zhou, X., Chai, C., Li, G., & Sun, J. (2020). Database meets Artificial Intelligence: a survey. *IEEE Transactions on Knowledge and Data Engineering*, 34(3), 1096–1116. <https://doi.org/10.1109/tkde.2020.2994641>.
- [33] Mariani, M. M., Machado, I., & Nambisan, S. (2022). Types of innovation and artificial intelligence: A systematic quantitative literature review and research agenda. *Journal of Business Research*, 155, 113364. <https://doi.org/10.1016/j.jbusres.2022.113364>.
- [34] Janiesch, C., Zschech, P., & Heinrich, K. (2021). Machine learning and deep learning. *Electronic Markets*, 31(3), 685–695. <https://doi.org/10.1007/s12525-021-00475-2>.
- [35] Sjödin, D., Parida, V., Palmié, M., & Wincent, J. (2021). How AI capabilities enable business model innovation: Scaling AI through co-evolutionary processes and feedback loops. *Journal of Business Research*, 134, 574–587. <https://doi.org/10.1016/j.jbusres.2021.05.009>.



- [36] Thabit, Q. Q., Alkhafaji M. K. and Issa, B. A. (2025). Phishing Website Detection Based on Data Tuning Methods with PCA of Multidimensional Features by Machine Learning Algorithms. *Journal of Information Systems Engineering & Management*, 10(41s), 598–610. <https://doi.org/10.52783/jisem.v10i41s.7978>
- [37] Thabit, Q. Q., Fahad, T. O., & Dawood, A. I. (2022). Detecting Diabetes Using Machine Learning Algorithms. 2022 Iraqi International Conference on Communication & Information Technologies (IICCIT-2022), Basrah University, Basrah, Iraq, 131–136. <https://doi.org/10.1109/iiccit55816.2022.10010408>.
- [38] Thabit, Q. Q. (2023). Deep Learning and Machine Learning for Improving Breast Cancer Detection. *Engineering and Technology Journal*, 8(12), 3156–3163. DOI: 10.47191/etj/v8i12.06.
- [39] Thabit, Q. Q., Dawood, A. I., & Issa, B. A. (2024). Early prediction of stroke based on deep learning and machine learning by applying medical imaging and tabular data. *Mathematical Modelling and Engineering Problems*, 11(12), 3499–3508. <https://doi.org/10.18280/mmep.111228>.
- [40] Liu, H., & Lang, B. (2019). Machine Learning and Deep Learning Methods for Intrusion Detection Systems: A Survey. *Applied Sciences*, 9(20), 4396. <https://doi.org/10.3390/app9204396>.
- [41] Thabit, Q. Q. (2026). Driver fatigue monitoring system using an artificial intelligence algorithm model. *Australian Journal of Engineering and Innovative Technology*, 8(3), 305–311. <https://doi.org/10.34104/ajeit.026.03050311>.
- [42] Shaw, J., Rudzicz, F., Jamieson, T., & Goldfarb, A. (2019). Artificial intelligence and the implementation challenge. *Journal of Medical Internet Research*, 21(7), e13659. <https://doi.org/10.2196/13659>.
- [43] Jamshidi, M., Lalbakhsh, A., Talla, J., Peroutka, Z., Hadjilooei, F., Lalbakhsh, P., Jamshidi, M., La Spada, L., Mirmozafari, M., Dehghani, M., Sabet, A., Roshani, S., Roshani, S., Bayat-Makou, N., Mohamadzade, B., Malek, Z., Jamshidi, A., Kiani, S., Hashemi-Dezaki, H., & Mohyuddin, W. (2020). Artificial Intelligence and COVID-19: Deep learning approaches for diagnosis and treatment. *IEEE Access*, 8, 109581–109595. <https://doi.org/10.1109/access.2020.3001973>.
- [44] Wani, N. A., Kumar, R., & Bedi, J. (2023). Deep X-plainer: An interpretable deep learning based approach for lung cancer detection using explainable artificial intelligence. *Computer Methods and Programs in Biomedicine*, 243, 107879. <https://doi.org/10.1016/j.cmpb.2023.107879>.
- [45] Thabit, Q. Q., Issa, B. A. & Dawood, A. I. (2025). Detection of Pneumonia by Combining Transfer Learning Models with Data Regularization Based on Deep Learning Methods. In book: *Proceedings of Data Analytics and Management*, 129–145. DOI: 10.1007/978-981-96-3358-6\_11.
- [46] Agrebi, S., & Larbi, A. (2020). Use of artificial intelligence in infectious diseases. In Elsevier eBooks (pp. 415–438). <https://doi.org/10.1016/b978-0-12-817133-2.00018-5>.
- [47] Dawood, A. I., Thabit, Q. Q. & Fahad, T. O. (2023). Thyroid Disease Prediction with Machine Learning Algorithms. *Eurasian Research Bulletin*, 18, 229–237.
- [48] Imran, M. M. H., Jamaludin, S., Ayob, A. F. M., Ali, A. a. I. M., Ahmad, S. Z. a. S., Akhbar, M. F. A., Suhrab, M. I. R., Zainal, N., Norzeli, S. M., & Mohamed, S. B. (2023). Application of artificial intelligence in marine corrosion prediction and detection. *Journal of Marine Science and Engineering*, 11(2), 256. <https://doi.org/10.3390/jmse11020256>.
- [49] Mohanty, S. P., Hughes, D. P., & Salathé, M. (2016). Using deep learning for Image-Based plant disease



- detection. *Frontiers in Plant Science*, 7, 1419. <https://doi.org/10.3389/fpls.2016.01419>.
- [50] Jada, I., & Mayayise, T. O. (2023). The impact of artificial intelligence on organisational cyber security: An outcome of a systematic literature review. *Data and Information Management*, 8(2), 100063. <https://doi.org/10.1016/j.dim.2023.100063>.
- [51] Choudhary, N., Bharti, R., & Sharma, R. (2021). Role of artificial intelligence in chemistry. *Materials Today Proceedings*, 48, 1527–1533. <https://doi.org/10.1016/j.matpr.2021.09.428>.
- [52] Advanced Techniques of Analytical Chemistry: Volume 1. (2022). In BENTHAM SCIENCE PUBLISHERS eBooks. <https://doi.org/10.2174/97898150502331220101>.
- [53] Lotfy, H. M., Obaydo, R. H., & Mouhamed, A. A. (2025). GLANCE visualization for smart analytical chemistry methods: Artificial intelligence for spectrophotometric determination of solifenacin-mirabegron combination. *Sustainable Chemistry and Pharmacy*, 47, 102159. <https://doi.org/10.1016/j.scp.2025.102159>.
- [54] Yasir F. Mahmood. (2026). Digital Transformation in Analytical Chemistry: A Literature Review on the Integration of Artificial Intelligence and Big Data Technologies in Modern Chemical Analysis. *Dijlah Journal of Engineering Science (DJES)*, 3(1), 173-180. ID.121.
- [55] M. Hamed Mozaffari and Li-Lin Tay, (2021). Convolutional Neural Networks for Raman Spectral Analysis of Chemical Mixtures. Conference: 2021 5th SLAAI International Conference on Artificial Intelligence (SLAAI-ICAI). DOI: 10.1109/SLAAI-ICAI54477.2021.9664686.
- [56] Shrivastava, A. (2025). Chromatography and artificial intelligence. *International Journal of Newgen Research in Pharmacy & Healthcare*, 98–103. <https://doi.org/10.61554/ijnrph.v3i2.2025.196>.
- [57] Lotfy, H. M., Erk, N., Genc, A. A., Obaydo, R. H., & Tiris, G. (2025). Artificial intelligence in chromatography: Greenness and performance evaluation of AI-predicted and in-lab optimized HPLC methods for simultaneous separation of amlodipine, hydrochlorothiazide, and candesartan. *Talanta Open*, 11, 100473. <https://doi.org/10.1016/j.talo.2025.100473>.
- [58] Ghali, U. M., Usman, A. G., Chellube, Z. M., Degm, M. a. A., Hoti, K., Umar, H., & Abba, S. I. (2020). Advanced chromatographic technique for performance simulation of anti-Alzheimer agent: an ensemble machine learning approach. *SN Applied Sciences*, 2(11). <https://doi.org/10.1007/s42452-020-03690-2>.
- [59] Loertscher, J., Green, D., Lewis, J. E., Lin, S., & Minderhout, V. (2014). Identification of threshold concepts for biochemistry. *CBE—Life Sciences Education*, 13(3), 516–528. <https://doi.org/10.1187/cbe.14-04-0066>.
- [60] Al-Ani, R. M. (2025). Application of artificial intelligence in biochemistry. *Mağallaṭ ‘ulūm Al-rāfidayn*, 34(3), 42–49. <https://doi.org/10.33899/rjs.2025.189205>.
- [61] Gligorijević, V., Renfrew, P. D., Kosciolk, T., Leman, J. K., Berenberg, D., Vatanen, T., Chandler, C., Taylor, B. C., Fisk, I. M., Vlamakis, H., Xavier, R. J., Knight, R., Cho, K., & Bonneau, R. (2021). Structure-based protein function prediction using graph convolutional networks. *Nature Communications*, 12(1), 3168. <https://doi.org/10.1038/s41467-021-23303-9>.
- [62] Introduction to modern inorganic chemistry (6th edition). (2004). *Open Chemistry*, 2(1), 276–277. <https://doi.org/10.2478/bf02476196>.
- [63] Ali, R. S. a. E., Meng, J., Khan, M. E. I., & Jiang, X. (2024). Machine learning advancements in organic



synthesis: A focused exploration of artificial intelligence applications in chemistry. Artificial Intelligence Chemistry, 2(1), 100049.  
<https://doi.org/10.1016/j.aichem.2024.100049>.

[64] Sayed, J. (2026). AI-enhanced organic chemistry: Emerging tools and computational strategies. Global Trends in Science and Technology, 36.  
<https://doi.org/10.70445/gtst.2.1.2026.36-52>.

[65] Seiffert, S. (2023). Physical chemistry of polymers.  
<https://doi.org/10.1515/9783110713268>.

[66] Prezhdo, O. V. (2020). Advancing Physical Chemistry with Machine Learning. The Journal of Physical Chemistry Letters, 11(22), 9656–9658.  
<https://doi.org/10.1021/acs.jpclett.0c03130>.