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Machine learning in analytical chemistry: From synthesis of nanostructures to their applications in luminescence sensing

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ABSTRACT

Over the past decade, the wide-scale adoption of artificial intelligence (AI) and machine learning (ML) has transformed the landscape of scientific research and development, which extends their influence across various scientific disciplines. Analytical chemistry has benefited significantly from these advances, with ML techniques proving to be valuable tools for researchers involved in the design, synthesis, and optimization of nanomaterials, as well as for the development of sensing platforms and data analysis for the detection of diverse analytes. In this review, we survey the practical applications of ML in the development of luminescent sensing approaches by analyzing recent publications on the synthesis of luminescent nanomaterials and ML-assisted electrochemiluminescence, fluorescence, and chemi- and bio-luminescent sensors. Our analysis illustrates how ML techniques can enhance the efficiency, sensitivity, and selectivity of luminescent sensing platforms, thereby paving the way for future innovations in this field.

1. Introduction

Since Frank Rosenblatt, the psychologist from Cornell University, created "perceptron" in 1957 [1], the prototype of artificial neural networks (ANN) and machine learning (ML) has gained an unimaginable amount of attention worldwide. "Perceptron" was fabricated in such a way to be able to receive visual inputs and then generate outputs like labels and categorize them properly. Machine learning, a branch of artificial intelligence (AI), can be defined as a computational science focusing on the development of algorithms for the analysis and interpretation of patterns, enabling the computer to learn, reason, and decide based on the data provided with, without any human interventions, similar to a human brain [2,3]. Using machine learning, the user feeds the computer an immeasurable amount of data, with which the computer makes decisions after proper analysis of the data. To further improve the decision making process, the user can identify errors and pursue to make corrections in the process [4].

Deep learning (DL) is a sub-category of ML with algorithms based on artificial neural networks which attempt to simulate the behavior of the human brain [5]. ML and DL are the basis of AI-driven applications in the design and development of "smart" technologies; from the ubiquitous smartphones, to smart homes and smart cities. Scientific research in various fields, including engineering [6,7], chemistry [8], biochemistry [9], pharmacology [10,11], biotechnology [12,13], medicine [14,15], etc. have also been impacted by the vast spread of ML. Analytical and bio-analytical chemistry, the science of separation, detection and quantification of chemical and biochemical molecules have also not been impervious to the widespread impact of AI and ML [16,17]. Every day, more and more studies focused on the implementation of ML algorithms in the detection and sensing of molecules and biomolecules for environmental monitoring [18,19], food safety and health control [20], and also the diagnosis of complex diseases such as neurological disorders [21] and cancers [22], are being published. The implementation of ML and especially DL algorithms to chemical and biochemical sensors, devices which measure a particular analyte by converting a physical or chemical attribute of that to a measurable signal proportional to its concentration, can pave the way toward the development of on-site detection of environmental and food pollutants and point-of-care (POC) testing and diagnosis of medical conditions [23,24], which is the ultimate goal of bioanalytical chemistry.

In this review, we explore the implementations of ML in bioanalytical research and sensing. First, we will briefly introduce the

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concept of ML and explain some general terms, followed by investigating how ML can benefit analytical chemistry. We will then discuss the implementation of ML technics in recent studies on luminescent sensors and biosensors. ML implementation in the synthesis of nanomaterials for luminescence sensing approached will be discussed, followed by recent studies on sensor development based on fluorescence, chemi- and bioluminescence and electrochemiluminescence approaches with the aid of ML algorithms. The limitations and future perspective of ML-assisted luminescence sensors will thus be examined.

1.1. The concept of ML

Simply, machine learning is made up of three sections: I) the algorithm which is the core of the decision-making process, II) variables that formulate the decision, and III) the known data and base knowledge that train the algorithm. The created model is firstly fed with parameter data that have known results. The algorithms are then run until they can develop a predictive model with answers which are agreeable with the answer of the known data.

Machine learning is often classified 4 approaches; I) supervised-, II) unsupervised-, III) semi-supervised-, and IV) reinforcement-learning. In supervised learning, the user feeds algorithms with specified training data and defines the variables that the algorithm needs for correlations assessment. In the case of unsupervised learning the algorithms are trained on unlabeled data in search of meaningful correlations between them. Here both the training data and the output of the algorithm are predetermined. Semi-supervised learning can be defined as a mixture of the previous two where the algorithm is fed mostly with labeled data; however, the model is also permitted to study the data on its own and develop a self-understanding of the data. When it comes to reinforcement training, the user desires the machine to go through a multi-step process with defined boundaries. The user arranges the algorithm to accomplish a task and gives it positive and negative signs as it tries to complete the mission. Depending on the type of the problem faced, each of the 4 approaches can be adapted to address the issue. However, most of the problems in the bioanalysis realm are solved using supervised learning [25,26].

In supervised modeling the user trains the algorithm with both classified inputs and preferred outputs. This type of machine learning can be adapted when researchers want a binary classification (e.g., dividing the data into two groups), multi-class classification (e.g., choosing between more than two answers), regression modeling (e.g., predicting values), and in the case of ensemble learning (where the answer is obtained from a combination of multiple machine learning models that provide a higher accuracy). The main purpose of supervised machine learning models is to advance a model (i.e., function) that can predict the responses based on the input values (e.g., vectors, images, graphs, etc.) [27,28]. The function model can be chosen from a variety of function families (e.g., kernel methods, random decision forests, neural networks). The model function can be defined as follows:

$$y(\mathscr{X}) = f(\mathscr{X}, W) \quad (1)$$

where the model depends on the parameter W. Using the input training data, the model will study different choices for W to finally determine the best W that would describe the relationship between x and y in the best possible way considering a loss function which is the measurement of how well the outputs match the data [25].

One main concern in the development of machine learning algorithms which persists is the identification of when a model has learnt a significant pattern between the data and when the pattern is somehow fake. One example can be overfitting in regressions where the model introduces structures that were not existent in the initial training sets. This problem is much bolder in cases where the data sets are too small or too noisy. To ensure that no overfitting has taken place, a process called cross-validation is of utter importance. Using cross-validation, the user intermittently alters the definitions of training and test data to ensure a suitable error measure exists [26,29].

1.2. ML in analytical chemistry

The enhancement of computer capabilities throughout the years and the increasing size of the data sets have dramatically shifted the key factors of data procurement and model training. Regarding how ML can be beneficial in luminescent sensors, here specifically, in the synthesis of nanostructures and the sensing applications, researchers can categorize them to where there can hardly be found a pattern or none at all, to surpass the limits, and speed up the data analysis. When researchers carry out experiments across a wide range of materials and study their outcomes aiming to understand what the reason behind the observed phenomenon is, machine learning can assist them with finding rare patterns [30,31]. While observing novel phenomena, researchers can come up with speculations and hypotheses and generalize them for other circumstances as well, neglecting the fact that there might not exist a linear relationship. Using machine learning models like neural networks, a scientist can see the outcomes previously unknown [32,33]. Developed machine learning models are orders of magnitude faster in data analysis than whichever method used for their training sets' data curation.

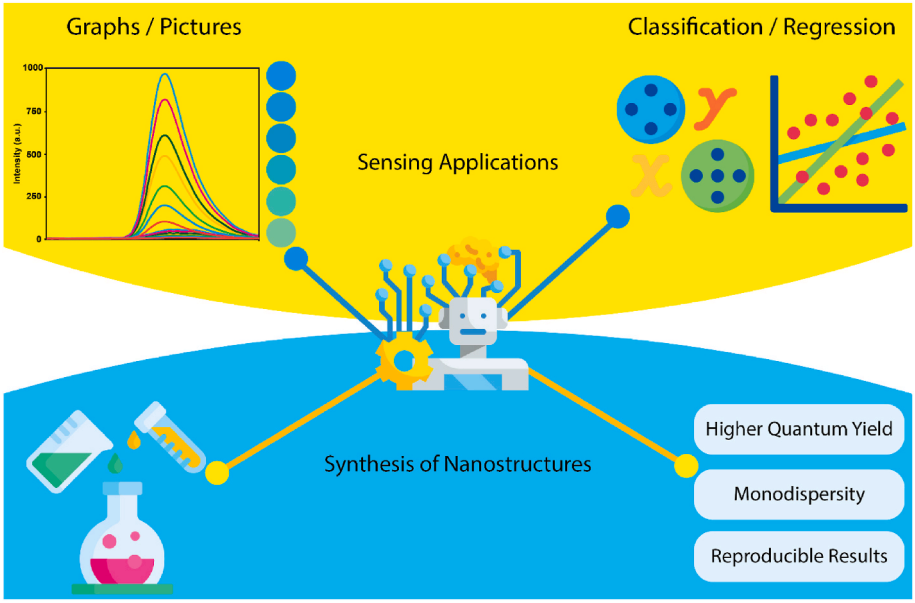
These days, prediction of material properties before their actual lab synthesis has become very important and hence has proposed some significant challenges. This problem has been previously addressed with the help of an expert or through numerous trials and errors. Since the supervision of an expert is not possible at all times and through-out the world, and the cost of trials and errors can sometimes not be affordable [34], hence, ML models trained via the data inputs of experts in that field, can come in very handy, eliminate extensive laborious and costly trial-and-error experiments and guide scientists toward the synthesis of structures with desired features [35–37].

Another huge challenge that an analytical chemist is likely to face is the analysis of large data sets. In the field of sensing, finding linear relationships and patterns between the input data is one great concern [38]. If the input data are images particularly, since they have numerous features (e.g., RGB, HSV, LAB, contrast, entropy, homogeneity, etc.), it would be somewhat impossible to investigate all these parameters in search of a pattern, unless using machine learning models. One may not find a pattern using each of the features alone, but learning algorithms can be trained on a combination of these features to distinguish meaningful patterns [39,40]. In array sensing, researchers are also faced with complex data, in which ML can be used to discern patterns for multi-class classification [41].

2. ML in nanostructure synthesis

The synthesis process of nanomaterials includes time-consuming and costly laboratory experiments in order to attain the structures with desired features. For this, researchers are incorporating computer-assisted methods to develop more effective chemical synthesis routes to accelerate the design process of novel nanostructures and the optimization of current materials [42,43]. Contrary to first principle simulation methods, which require deep understanding of the domain of interest, ML technics can be trained to learn from past experiments, both successful and unsuccessful, and guide the future synthesis procedures. Besides increasing the speed of material design, this data-driven screening process can effectively save time and money, and also reduce the chemical waste produced in the synthesis and optimization process of novel luminescent materials (Scheme 1) [44–46].

Luminescent materials, described as materials with the ability to emit light (besides thermal radiation) after being excited by stimulus such as UV radiation, as in fluorescence and phosphorescence; chemical reactions, as in chemiluminescence; applied potential, as in electrochemiluminescence; etc. [47]. Due to their efficiency, accuracy, and



Scheme 1. Schematic illustration of ML in sensing and synthesis applications.

simplicity, luminescent materials have been the focus of numerous research studies for their application in chemical and bioanalytical sensing [48,49]. For applications in sensing, luminescent materials need to possess certain features including chemical and physical stability in extreme conditions, insensitivity towards undesired quenching, and the ability to respond to the sought-after analyte [50].

Although natural luminescent materials are available, nanotechnology has enabled the design of numerous luminescent nanostructures including quantum dots, carbon and graphene dots, metal-organic frameworks (MOFs), covalent-organic frameworks (COFs), nanoclusters, up-conversion nanoparticles (UCNPs), etc. Furthermore, there have numerous attempts in the development of nanostructures which, when combined with luminescent systems, enhance various aspects of the system including the emission intensity, the color of the emitted light, the photostability of the system, etc. As the design of the ideal nanostructure for this purpose can be time-consuming, numerous research studies have been reported on the implementation of ML algorithms in the design and development of luminescent systems [51–53]. In this section we will examine recent published reports on the implementation of ML in the synthesis and optimization of various kinds of luminescent materials.

2.1. Carbon dots

Carbon dots (CDs), are among the favorable luminescent nanomaterials highly suited for sensing applications due to merits including rapid response, feasible functionalization, tunable emission coupled with a wide excitation range, high photostability and lower toxicity compared to organic fluorophores and heavy metal containing quantum dots [54,55]. Currently, there are two main synthesis routes for CDs including the hydrothermal method and the bottom-up solvo-thermal approach. Quantum yield (QY), defined as the ability of a compound to convert the photons absorbed to emitted light, is considered as a viable parameter to assess luminescent nanomaterials [56]. As numerous parameters might be effective in QY, optimizing it through the traditional synthesis procedures would include assessing one reaction parameter while the rest are kept fixed, and thus the correlation of reaction parameters cannot be evaluated.

In a recent study reported in 2020 by Han et al., a machine learning approach was implemented in the hydrothermal synthesis of CDs to analyze the relationship between various parameters and experimental outcomes to attain green-emitting CDs with high QY. For this study, different combinations of five parameters including reaction temperature, reaction time, precursor mass, ramp rate and EDA volume were investigated through 391 reactions and the respective QY for each experiment was recorded. Thus, machine learning regression models based on XGBoost regressor (XGBoost-R), multilayer perceptron regressor (MLP-R), support vector machine regressor (SVM-R), and Gaussian process regressor (GP-R) were developed to correlate the experiment parameters with the quantum yield. XGBoost-R was able to develop the best model for this purpose (Fig. 1A). The results showed that the volume of EDA had the most significant role in the QY of CDs, followed by the precursor mass and reaction temperature, respectively. Using the two most determining factors, meaning EDA volume and precursor mass, a series of predictions were done using the modal in order to optimize the synthesis procedure. It was shown that the EDA volume of 10–50 μL promoted the synthesis of CDs with high QY regardless of the precursor mass, whereas higher EDA volumes of 60–90 μL only resulted in high QYs in the presence of a large precursor mass and higher volumes of over 100 μL had an adverse effect on QY. These findings were experimentally tested to achieve CDs with QYs of 39.3%. This study successfully shows the feasibility and effectiveness of ML algorithms in synthesis [57].

Inspired by ML techniques, another study attempted to investigate the relations between numerous synthesis parameters with multiple photoluminescence properties of CDs. For this, first, 270 multi-color CDs were produced in the laboratory under different conditions and their photoluminescence features including the QY, maximum emission wavelength and stokes shift was calculated. The synthesis parameters investigated include the precursor type (*p*-phenylenediamine and urea or *p*-phenylenediamine and citric acid), precursor ratio, temperature, reaction time, and solvent (water, ethanol, and N, N-dimethylformamide). Various ML algorithms including Extreme Gradient Boosting (XGBoost), Random Forest (RF), Light Gradient Boosting Machine (LGBM), Ridge Regression (Ridge), Least Absolute Shrinkage and Selection Operator (LASSO), and Support Vector Regression (SVR) were used and compared in terms of Mean Absolute Error (MAE) and coefficient of determination (R^2). The RF model was witnessed to have the best performance among others. How each reaction parameter influenced the three investigated photoluminescence properties was also further evaluated. It was seen that the maximum emission wavelength was mainly impacted by the solvent, as it can control the carbonization

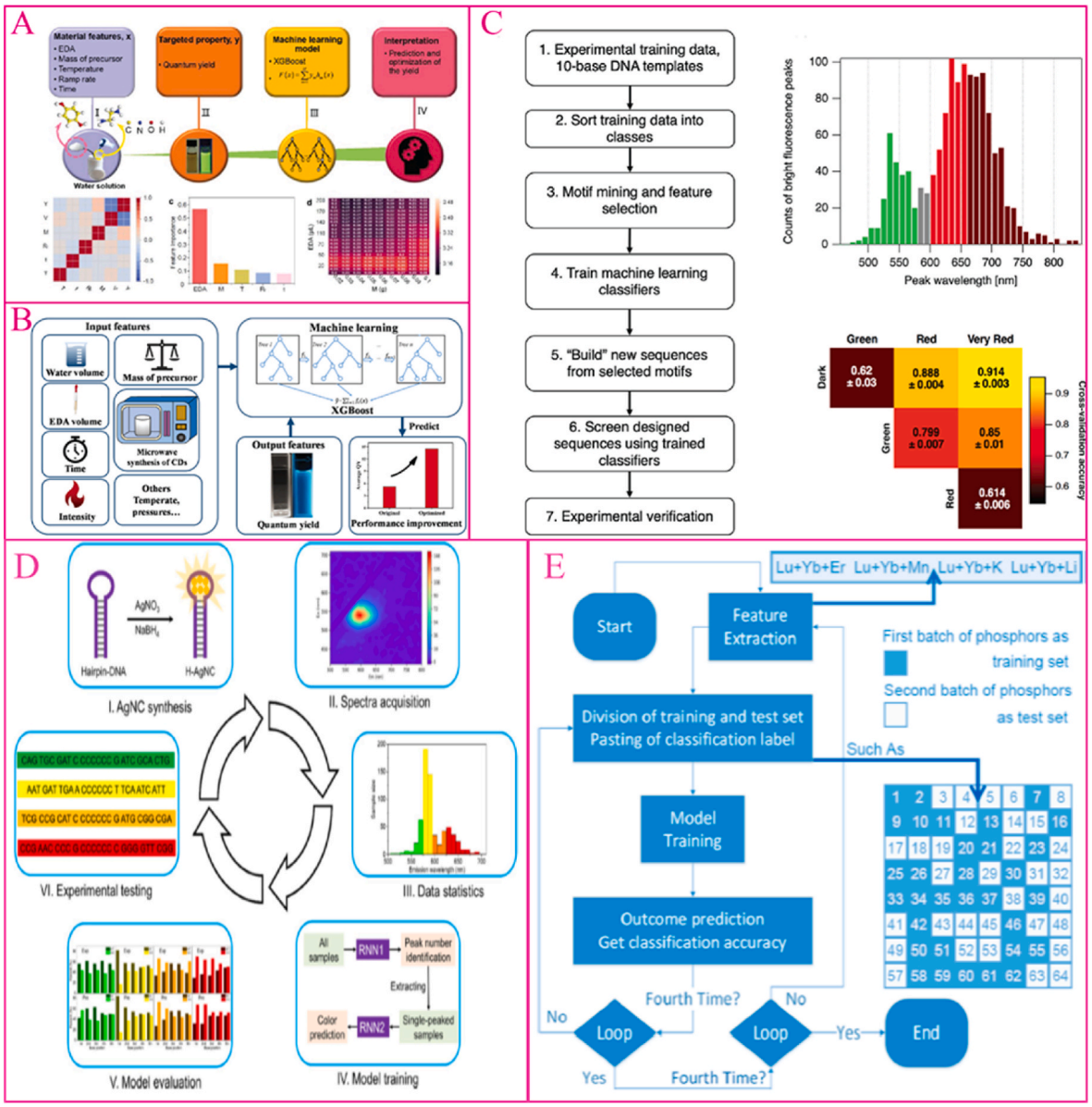


Fig. 1. Machine learning-assisted synthesis of luminescent nanomaterials including (A) green-emitting carbon dots [57], (B) carbon dots with elevated quantum yield [59], (C) DNA-stabilized AgNCs [76], (D) the workflow of a ML-guided AgNC synthesis process based on hairpin DNA using neural network model to optimize numerous factors [78], and (E) a diagram of the SVM-based method used to optimize the synthesis of up-conversion luminescent phosphors [85]. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

and dehydration process of the precursor. Furthermore, the precursor ratio was seen to have the largest impact on the fluorescence QY since this ratio affects the polymerization, dehydration, carbonization, and passivation processes of the CD formation. The stokes shift was also seen to be mainly influenced by the precursor type [58]. This research is an excellent example of how ML strategies can pave the way to rationally designing the synthesis routes for nanomaterials. A similar study was performed in which an ML approach was implemented to optimize the synthesis of CDs via the microwave method in order to attain CDs with higher QY. A model based on the XGBoost algorithm using five features including mass of precursor, EDA volume, water volume, microwave intensity and Microwave time was developed, through which optimization of CD synthesis was done and a 15.7% improvement of the QY was attained (Fig. 1B). The optimal CDs were then used to detect H_2O_2 residues on teeth with high sensitivity and a detection limit of 0.12 M [59]. Other recent studies on ML-guided carbon dot synthesis have aimed at producing CDs with high intensity and tunable emission at room temperature using an XGBoost model [60], increasing the efficiency of red-emitting CDs [61], generating a predictive model to investigate the impact of synthesis parameters and make accurate predictions on the emission color of the resulting CDs based on ANN [62]. As can be seen, ML can aid the synthesis of CDs with desired characteristics and help investigate the impact of various precursors on the ultimate outcome. Through ML-guided synthesis, CDs with desired FL colors and enhanced emission and QY can be generated. More importantly, ML can significantly help reduce the cost of synthesis optimization by eliminating the need to numerous experiments.

2.2. *Quantum dots*

Colloidal quantum dots (CQDs) are semiconducting nanocrystals with a maximum size of 20 nm with size-tunable bandgaps with high applications in light emission and electroluminescence devices. Attaining CQDs with high monodispersity is an important factor in reducing

noise-to-signal ratios in luminescence sensors [63]. Recent research was performed in order to optimize the synthesis of CQDs with high monodispersity by investigating the parameter space, meaning the number and range of parameters investigate in the optimization of a synthesis process, using machine learning algorithms in order to predict which synthesis route will provide CQDs with desired properties [64]. A dataset of various synthesis parameters including the oleylamine (OLA) volume, the volume of PbOA2 and bis(trimethylsilyl) sulfide ((TMS)2S) as the precursors, the concentration of PbCl2 as a chloride and the temperature. Within a particular wavelength, the peak/value ratio and the half-width at half-maximum (hwhm), calculated from the peak/-value, were used to interpret the monodispersity. Contrary to other ML techniques, Bayesian models are able to provide a range of possible prediction values, and if the prediction proves to be incorrect, the collected data can be used to correct the model in that region. Thus, the researchers used a Bayesian neural network with 8 parameter synthesis inputs. In this study it was seen that OLA improved the size range and monodispersity of the PbS CQD. Through ML, the researchers were able to explore higher Pb:S ratios and a larger parameter space than that feasible through laboratory experimentation alone.

Another recent study has aimed at generating a prediction model based on data accumulated from publication for the prediction of characteristics including absorption, emission and diameter of indium phosphide quantum dots (InP QDs). The results of this study were used to generate a web application for the prediction of synthesis outcomes on InP QDs [65]. Again, we can see that ML can ease the optimization of QDs with specific characteristic through eliminating the need for numerous experiments and enabling the investigation of a wider range of parameters on synthesis outcomes.

2.3. Nobel metal nanoclusters

Nobel metal nanoclusters (NCs), which consist of fewer than 150 metal atoms and a size of less than 10 nm, are regarded as the link between atoms and nanoparticles as they display molecular-like features including discrete electronic states and size-dependent photoluminescence resulting from result of an inter-band transition and an intra-band HOMO-LUMO transition [66,67]. The size and structure of NCs is a determining factor in their light-emitting properties. Generally, these clusters are made of a shell of ligands which stabilize several to one hundred metal atoms in the centers. Thus, a molecular formula of [MnLm]q, in which n, m, and q are the number of metal atoms, ligand molecules, and the net charge in a single NC [68,69]. The properties of NCs can be immensely varied by fluctuation in the values of n, m, and q. Therefore, it is highly desirable to attain clusters with atomic precision through a synthesis procedure.

As gold nanoclusters are among the most studied NCs [70], in a recent study [71], researchers attempted to develop a deep learning framework to accelerate the synthesis of atomically precise AuNCs through studying the relationship between reaction conductions and molecular properties on the monodispersity of the final product. In this research, a very diverse dataset gathered from synthesis procedures in various studies, of 54 examples labeled as 1 for atomically precise and 0 for non-atomically precise, was used. 17 basic descriptors were used to represent the synthesis data including 5 reaction condition descriptors (ligand concentration, $HAuCl_4$ concentration, reducing agent concentration, reducing reaction temperature, pH) and 12 descriptors for key reaction components (the solvent dielectric constant, the solubility of ligand in corresponding solvent, the redox potential of the reducing agent, and 9 features to describe the ligand including the charge potential, hydrogen donor number, hydrogen acceptor number, aromatic or aliphatic, molecular weight, rotatable bonds number, complexity, topological polar surface area, and xlogP3). Pertaining the different attributes, 2 datasets were developed to train the model; the first a full dataset of 54 examples, and the second one with just 35 examples of the aqueous synthesis samples generating Au25NCs. The second dataset was used to gain chemical insight into the parameters effective on synthesis, especially how pH and ligand-to-Au molar ratio can impact atomic precision. Six different ML algorithms were tested on the first dataset and the siamese neural networks (SNN) stacked with graph convolutional neural networks (GCNN) on top of it generated the most precise classification model. It was seen that when ML algorithms are combined with GCNN, they have elevated performance which can be due to the ability of the GCNN algorithm to provide incorporate molecular structure information and use it as a feature vector in any other model. As deep learning methods like GCNN + SNN are considered like a black box, meaning the process of decision making with these models is not shown and they are impervious to detailed examination, a "model of the model" was also developed using the synthetic data provided from the deep learning method to train a decision tree in order to gain detailed chemical insight into the synthetic route for atomically precise Au25NCs in aqueous phase. The developed tree showed that in the aqueous phase, the use of aliphatic ligands is more likely to result in atomically precise Au NCs in comparison with aromatic ligands. The ligand-to-molar ratio was also found to be critical. This study is an excellent example of how ML-guided synthesis can accelerate the process in attaining luminescent materials with desired features.

DNA-stabilized silver nanoclusters, which are partially oxidized clusters of 10–30 silver atoms stabilized by 1–2 DNA oligomers are another group of favorable clusters used in sensing. It has been reported that silver nanoclusters can be stabilized by single-stranded DNA leading to a variety of sequence-selected sized and visible to near-IR emission, which can generate tunable fluorophores. Although much research has been devoted to optimizing the synthesis of AgNCs, there still remains a poor understanding of the impact of the DNA sequence on the properties of the final clusters. Though it has been witnessed that cytosine (C) and guanine (G) show a greater affinity toward silver ions than the other bases, all four bases can ultimately affect the properties of the clusters [72–75]. Recent research was also focused on employing machine learning to develop a model to predict the colors of AgNCs based on the template DNA sequence. A database of 10-base DNA sequences and the motifs present in each of the sequences was used to train an ML classifier and uncover how certain motifs correlate to fluorescence emission and others do not. This information was then used to further develop an ML model to classify the relationship between the fluorescence color of the clusters produced and the DNA (Fig. 1C). The results of the ML models were then used to investigate how the color-related motifs can be used to generate sequences ranging from 8 to 16 bases which can result in desired clusters with fluorescence emissions around 600–660. It was shown that with the aid of a machine learning method, DNA base patterns could be applied to other sequence lengths and AgNCs with 99%–154% increased intensity in the desired emission range could be synthesized [76].

Similarly, regarding AgNCs, a study was performed in which the chemical features of DNA sequences which reflect aspects of DNA−silver interactions in the crystal structures were used to develop ML models to discover AgNCs with near-infrared emission. First, the database was divided into color classes as Green, Red, Far Red, NIR, and Dark (those without emission) classes. Thus, an SVM model was trained using feature vectors with information on adjacent motifs to the silver atoms as well as non-adjacent nucleobase patterns. The model was also experimentally validated and displayed strong predictive precision with applicability to synthesize near-IR AgNCs [77].

DNA-stabilized AgNCs were the focus of another study in which a deep learning model based on recurrent neural networks (RNNs) was generated to predict the FL properties of AgNCs templated with hairpin-DNA structures. The hairpin stem sequence along with other synthesis parameters were used to train the RNN model emission peak and FL color of the resulting AgNCs. Accuracies of over 80% were attained in this experiment [78]. As can be seen, numerous factors are influential in the final outcome of NCs with precise atomic numbers, desired emission color and high QYs, including various precursors and ligands for

stabilization. ML-guided synthesis of NCs can accelerate the optimization and generation of desired NCs by helping to explore various parameters more efficiently. Through ML, the effect of different ligands including nucleic acids and proteins, various salts (silver, gold, and copper), various reducing agents, etc. can simultaneously be analyzed, whereas through solely experimental technics, this vast range of parameter investigation is almost impossible.

2.4. Metal halides

Zero-dimensional (0D) metal halides have recently attracted great attention as luminescent materials. Due to numerous advantageous features including high QY, tunable emission over a wide range and high absorption coefficient, they are gaining increased attention for applications in luminescent sensing platforms [79]. Although many metal halides with high QY have been successfully discovered, other halides with were seen to display low QYs without a satisfactory explanation. Thus, it is important in investigate the factors affecting the QY of 0D metal halides in order to accelerate the discovery and synthesis of novel luminescent materials [80]. In an attempt to understand the influential factors on QY, a recent study relied on machine learning to investigate how structural features related to high QY [81]. For this, a dataset of 3 0D metal halides was generated and structural parameters including the average length of the M-X bonds (M = Pb^{2+}, Sn^{2+}, Sb^{3+}, and Bi^{3+}) as "d (M−X) average", MXn distortion, the shortest distance between two M ions as "d (M … M)", and the local symmetry of M site. First, principle component analysis (PCA) was used to evaluate how the selected features correlate with the QY. It was seen that increased d (M … M) had the biggest impact on improved QY. A model using random forests (RF) was then developed to estimate the QY of the metal halides with a mean absolute error (MAE) of 15 ± 5% after 5-fold cross-validation. Several new metal halides were further tested using this method and good agreement was seen between the actual QYs and the compared ones. Although less investigated compared to other luminescent materials, it is clear that ML can also help optimize the synthesis of metal halides to generate more enhanced luminescence.

2.5. Up-conversion nanoparticles

Conventional photoluminescence probes require excitation through UV illumination, which are known as down-conversion luminescence. Recently, photoluminescence compound which are excited through the absorption of near-IR light, known as up-conversion luminescence (UCL), are attracting attention as potential sensing and imaging compounds because the near-IR light is absorbed less by tissues and displays lower auto-fluorescence [82]. Despite its merits, the application of up-conversion luminescence can be hindered by its low efficiency and insufficient intensity. Thus, methods such as adjusting the crystal shape and size, metal co-doping, implementing a core-shell structure, and coupling the process with surface plasmon resonance have been investigated to overcome this problem [83,84]. In a recent study, ML algorithms were employed to increase the UCL intensity and efficiency with the aim of discovering optimized phosphors modulated with K/Li/Mn metals to enhance their red UCL emission [85]. First, the researchers used the genetic algorithm (GA) to optimize the synthesis of the up-conversion phosphors over four generations of 16 tests by optimizing the proportion of six synthetic elements (Lu, Yb, Er, Mn, K, and Li). It was witnessed that the third-generation phosphors had the highest intensity and efficiency. They also investigated how single and multiple doping of elements impacts the up-conversion intensity to find that the increasing of the K + Li + Mn sensitizers first increases the intensity leading to a decrease. An SVM algorithm was employed to verify the reliability of the genetic algorithm by synthesizing all the previous four generations of phosphor for a second time with the same elemental compositions (Fig. 1D). The intensity of the phosphors was recorded and used for comparison with the previous batch to find that there was no significant difference in the fluorescence intensities of the two batches. As can be seen, ML can help with overcoming current limitations hindering the use of up-conversion materials.

We can evidently conclude that implementing ML in synthesis of novel luminescent materials and optimizing previously discovered materials has numerous benefits. Firstly, ML can intensely accelerate the search and optimization of luminescent materials. Furthermore, through ML, a vaster range of parameters can simultaneously be investigated; and also, numerous outcomes can be optimized. ML can also enable the investigation of extreme conditions on synthesis outcomes, which may not be possible to feasibly explore through traditional experimental methods. Also, as the need for numerous laboratory experimentation is reduced through the implementation of ML, the cost for the discovery and optimization of luminescent materials also significantly decreases.

3. ML-assisted luminescence sensing

Sensors and biosensors, based on the produces signal, can be divided into optical, physical and electrochemical. Optical sensors detect and quantify analytes based on interactions leading to photon signals in the visible, ultraviolet, or infra-red region. Luminescent sensing methods are a subset of optical methods based on the emission of light by specific molecules which have previously been excited. These methods include fluorescence, chemiluminescence, bioluminescence, electrochemiluminescence, etc. Possessing many advantages, including simplicity, high sensitivity, feasible set-up and their possibility to turn to portable sensors, luminescence strategies are among the most prevalent methods for detection and diagnosis purposes. The signals of luminescent sensors can be read in spectral terms or through capturing images. Both methods generate noisy, complex data, which can highly benefit from ML analysis (Scheme 1).

The advance of cameras and especially smartphone cameras has brought into focus the possibility of image-based sensing for both qualitative and quantitative target measurements. Luminescent signals can be translated into numeric data in various color spaces including RGB (Red-Green-Blue), HSV (Hue-Saturation- Value), and L*a*b* (Lightness, Green-Red, Blue-Yellow) and used to analyze the presence and concentration of an analyte [86,87]. Although many sensing platforms have been developed which solely depend on image processing technics, these methods can often be unreliable as they are highly dependent on camera optics, meaning the kind of lens and camera settings chosen for photographing, and illumination conditions. Different cameras and smartphone cameras have different lenses with various strengths, which can lead to slight differences when photographing the same object. Thus, solely relying on image processing technics might not lead to universal results which can be duplicated with other cameras and smartphones. Incorporating ML algorithms with image processing technics can help eliminate the effects of cameras and environmental conditions. Furthermore, through ML, researchers can investigate numerous image features simultaneously including both color attributes and texture features and extract meaningful patterns from them, which might otherwise not be possible.

In this section, recent studies on ML implementation in fluorescence, chemi- and bio-luminescence and electrochemiluminescence sensing approaches, based on spectral or image-based data, will be discussed.

3.1. Electrochemiluminescence

Electrogenerated chemiluminescence is the generation of light by an electrochemical reaction. ECL is a detection method capable of an almost noise-free detection of the target molecule that also benefits from high sensitivity and specificity [88,89]. ECL-based detection can be categorized into two main groups signal-on and signal-off sensing formats [90,91]. In recent years, ECL-based detection systems have been vastly developed with the ultimate aim of device miniaturization [92,93]. In doing so, most of the ECL signals are recorded as images using

smartphone cameras. The intensity of light in the pictures is proportional to the concentration of the target [94,95]. Thus, machine learning can be employed to better analyze the images and find more sustainable patterns between them in reaching the ultimate goal of impeccable detection.

The healthcare industry is one of the major fields where ECL-based detections are used. The ultra-high sensitivity and specificity of ECL-based assays are the main reason behind their usage [96]. Reaching reliable, stable, affordable, and most important of all, user-friendly assays for the healthcare management of patients is what researchers have worked on for decades, and ML-assisted ECL seems to be a potential answer to it. Investigation into most of the disease cases has revealed that a great portion of these cases could have been better managed had the situation been diagnosed earlier. This early detection is often relied on the detection of the related biomarkers in body fluids [97,98].

A recent study was performed in which a closed bipolar ECL sensor was fabricated for the detection of glucose, lactate, and choline [99]. The ECL signals in a luminol-H_2O_2 system were recorded and a series of ML techniques (Linear Regression, Huber Regression, Random Sample Consensus (RANSAC), Theil-Sen, Support Vector Machine Regression, k-Nearest Neighbor, Decision Trees, and Random Forests) were employed for the analysis and validation of the data and the ranking of the best fitting curve. Employing the combination of ECL and ML led to a linear range of 0.05–3 mM, 0.1–4 mM, and 0.0007–1 mM for glucose, lactate, and choline, respectively (Fig. 2A). It was seen that ensemble methods including Decision Trees and Random Forests were able to produce better models with the least error.

Long considered a good antibiotic in the food industry and an antiseptic in treating human skin infections, nitrofurazone is now banned from further usage as it has been found to have detrimental effects on human health [100,101]. In an attempt to detect this carcinogen, Liu and colleagues [102] developed a portable MIP-ECL system that featured Ag^{+}@UiO-66-NH_2/$CsPbBr_3$ as the ECL luminophore. To fabricate the molecularly imprinted membrane, nitrofurazone was

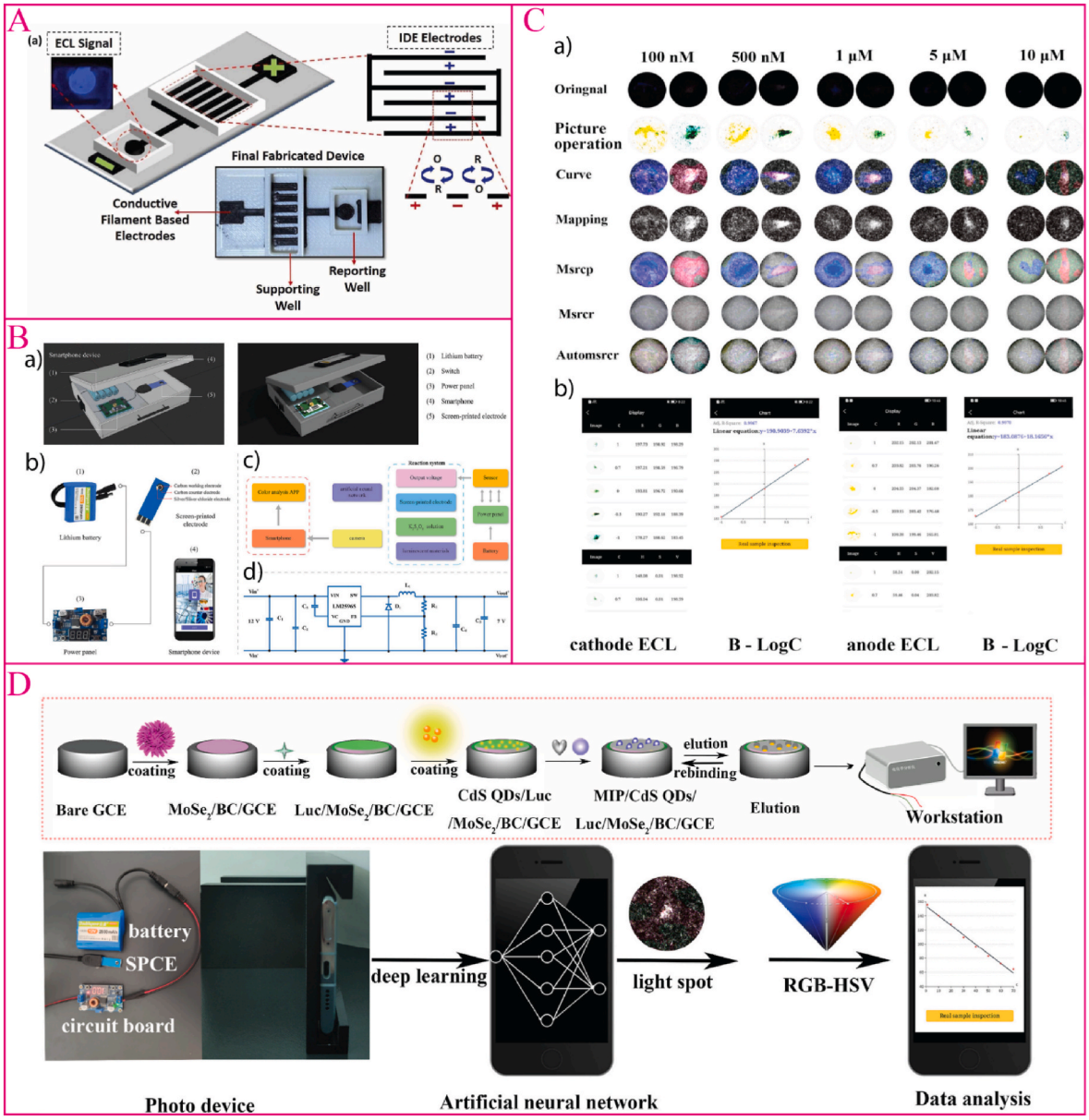


Fig. 2. ML in ECL-based assays. (A) ML-assisted ECL BPE for glucose, lactate, and choline detection [99]; (B) ECL-based NFZ detection with the help of ANN [102]; (C) ECL detection of 2,4-D using with the help of convolutional neural networks [106]; (D) Detection of furosemide using a smartphone-based ECL with the help of ANN [108].

electrochemically polymerized. The ECL signals were recorded using a smartphone camera and artificial neural networks (ANN) were developed to analyze the image features. Under the optimal conditions, NFZ was detected in a linear range of 0.5 nM–100 μM with a LOD of 0.09 nM (Fig. 2B).

Another previously-used pesticide is the synthetic plant hormone called 2,4-Dichlorophenoxyacetic acid (2,4-D). The hormone has long been used in the regulation of plant growth and metabolism and in keeping fruits and vegetables fresh [103,104]. The pesticide is found to be harmful to both human health and environment due to low biodegradation and water solubility [105]. A molecularly imprinted ECL system was developed by the team of Wang to detect the pesticide [106]. The ratiometric ECL system featured luminol-H_2O_2 as the anodic luminophore and Te–CdS@Mn_3O_4 as the cathodic one. Electrochemical polymerization of 2,4-D was used for the fabrication of the 2,4-D-MIP. The ECL system is suppressed both on the anodic and cathodic sites with the prevention of hydrogen peroxide binding to luminol and an increase in the resistance of the cathodic site. ECL signals were recorded by a smartphone camera and convolutional neural networks (CNNs) were applied to analyze the images. A wide linear range of 1 nM–100 μM with a LOD of 0.63 nM for 2,4-D was achieved (Fig. 2C).

In an attempt to detect furosemide (FSM), which is a diuretic agent used in the treatment of congestive heart failure and edema [107], Zhang et al. developed a smartphone-based MIP-ECL platform assisted by deep learning techniques to detect the molecule of interest [108]. The developed platform benefitted from an ECL-RET mechanism using lucigenin as the donor and CdS QDs as acceptor luminophores in a persulfate system. The smartphone-recorded ECL signals were analyzed using convolutional neural networks enabling the analysis of non-linear data and batch processing of the captured images. Here, FSM was detected in a wide linear range of 0.010 μM–100 μM with a LOD of 4 nM (Fig. 2D).

The new acute respiratory syndrome coronavirus 2 (SARS-CoV-2) outbreak posed a serious global health threat and generated a great, immediate need for rapid detection devices [109]. Recently our team developed a ML-assisted ECL immunosensor for the detection of SARS-CoV-2 [97]. Going through the sensors fabricated for this purpose we felt the need for a more comprehensible result readout than the more common forms of PFU or g mL^{-1} so that the target audience that are the normal not trained people could use. We figured that since almost everyone has somehow been associated with the disease and its appropriate gold standard testing (RT-PCR), it would be more sensible to report the results as RT-PCR CT values. A signal-on sandwich immunoassay was developed featuring an anti-S2 antibody immobilized on the sensor surface to capture the virus and an anti-M antibody modified nanocomposite as the ECL reporter. The signals were recorded using a smartphone camera and the images were analyzed using artificial neural networks (ANNs). Upon the application of ML, we were able to detect

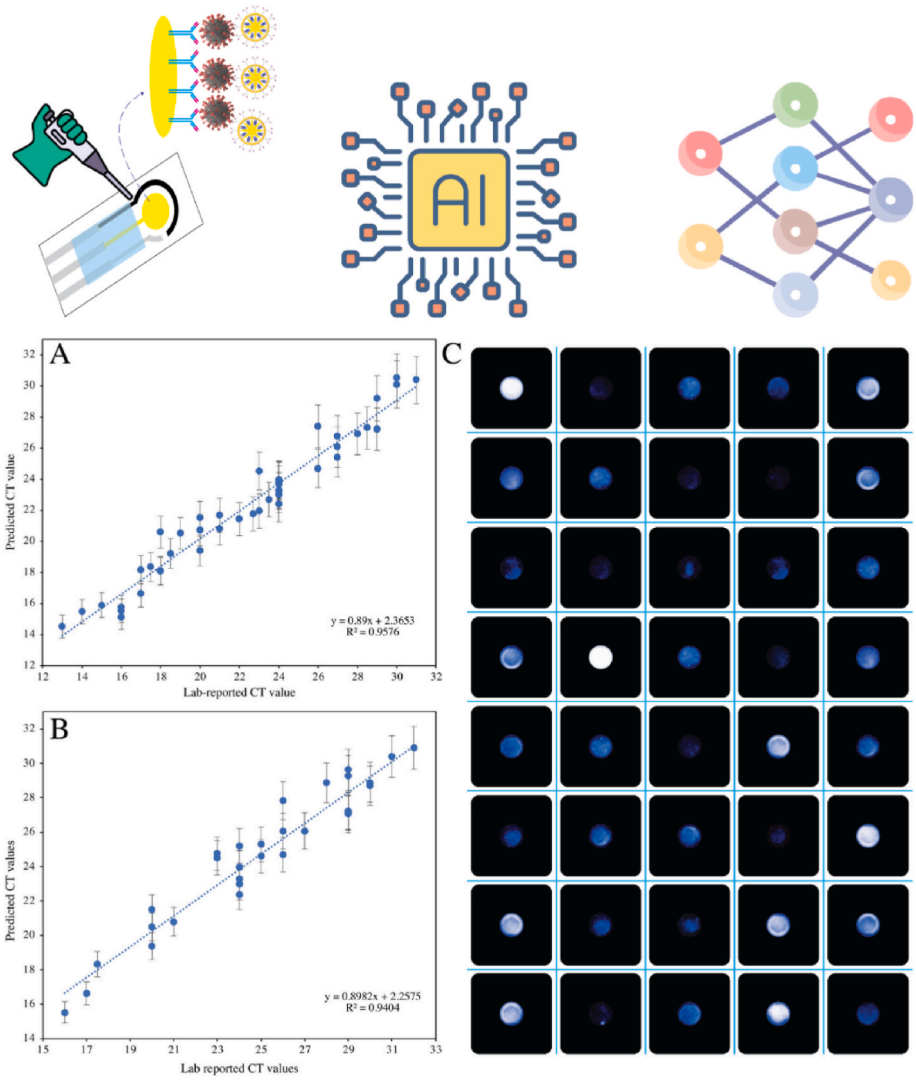


Fig. 3. Detection of COVID-19 using ML-assisted ECL immunoassays [97].

the virus in a linear range of 16–32 (reported as RT-PCR CT values) with a LOD as low as 10^{-12} g mL^{-1} (Fig. 3).

Although ECL is endowed with numerous advantages, biosensors that rely on bioreceptors such as antibodies and aptamers are faced with some limitations including stability and shelf-life problems. ML can help tackle these problems by identifying unknown interdependencies between biomarkers and signals and automating the analysis process [110]. ML-assisted ECL sensors show great potential for POC testing with enhanced performance and accuracy.

3.2. Fluorescence

Fluorescence (FL) is a form of luminescence in which the emission of light is a result of the excitation of a fluorophore through the absorption of electromagnetic energy. The emitted light generally has a longer wavelength and lower energy compared to the absorbed light [111,112]. FL sensing is a result of the interaction between the analyte and the fluorophore which can lead to various changes including the quenching of the emission, increased emission intensity, a shift in the emission wavelength, changes in the fluorescence lifetime, or fluorescence resonance energy transfer (FRET) [49,113,114]. The two major advantages of FL are its rapid signal response and simplicity, which have made this approach among the most favorable for analytical research. Although many analytes might possess innate FL properties, there is a wide range of fluorophores to choose from to label those without natural FL including organic fluorophores (rhodamine, fluorescein, cyanine, and coumarin) [115] and numerous nanomaterials with FL properties [116] which have so far been reported including nanoparticles [117], metal nanoclusters [67,74,118], quantum dots [119,120], carbon and graphene dots [121–123], metal organic frame works (MOFs) [124–126], up-conversion nanoparticles (UCNPs) [127,128], etc. As previously discussed, these nanomaterials provide numerous advantages including lower toxicity, feasible functionalization, wider emission range, etc.

ML can be used to analyze the raw FL data, in order to categorize the sensing signals, reduce signal noise which is a main problem with FL detection, and also to investigate if the signal is correct [59,129]. ML-based FL detection can be carried out using either spectral data or data derived from images [130]. The latter can be done with the aid of smartphone cameras, which can in turn pave the way for point-of-care (POC) testing. In this section, we will analyze the recent published reports on ML-based FL sensing platforms. As the articles in this area are plenty and various, we have divided this section based on data acquisition methods into images-based and spectra-based.

3.2.1. FL image-based detection

Smartphone-assisted ML-based FL sensing is highly applicable for environment monitoring and food safety control as it can pave the way to on-site evaluation in remote places with minimal laboratory facilities [87,131,132]. In an attempt to detect tetracycline (TC), our team developed an ML-assisted sensing platform using red-emitting bimetallic Au/Ag nanoclusters stabilized with BSA to precisely predict the TC concentrations in milk and water samples (Fig. 4). BSA is known to interact with TC, and this interaction in the bimetallic NCs leads to the shift in their emission color from red to yellow. TC concentrations ranging from 50 to 3000 μg L^{-1} in both water and milk samples were tested for their interaction with the BSA-stabilized NCs and the color change from red to yellow was captured using four various smartphone cameras in order to minimize the effect of camera optics. The captured images were then analyzed and 16 different features including R, G, B, mean RGB, mean grey, H, S, V, L*, a*, b*, entropy, contrast, correlation, homogeneity, and STD were extracted from each image to generate a comprehensive dataset. Five ML models were developed for both the milk samples and the water samples. It was witnessed that the ensemble method of bagging was best able to develop a model to predict the TC

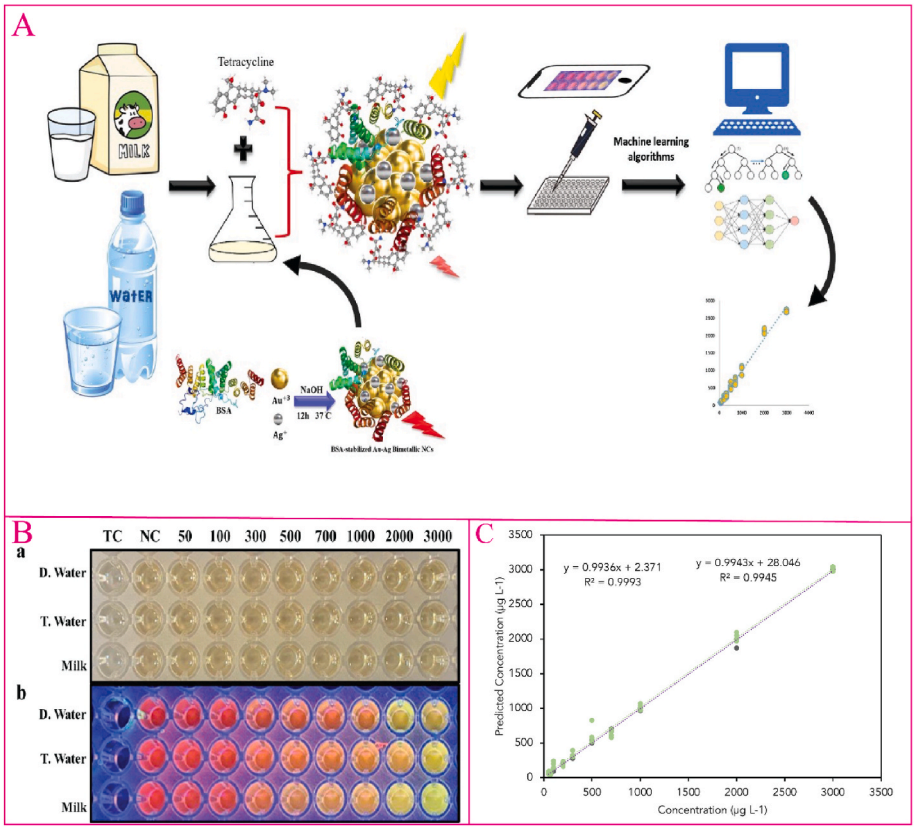


Fig. 4. ML-assisted sensing approach based on BSA-bimetallic nanoclusters and image-driven data for the detection and quantification of tetracycline in milk and water [133].

concentrations; the bagging and artificial neural networks developed the best model for water samples with $R^2 = 0.994$ and NRMSE = 0.078 and the bagging and decision trees model had the highest performance for milk sample with $R^2 = 0.999$, NRMSE = 0.027. The developed model for milk was further used to assess the TC content of various store purchased milk samples; for which it also showed acceptable recovery [133]. The interaction between BSA and TC was also exploited in another ML-assisted sensing platform developed using blue-emitting carbon dots and red fluorescent-emitting BSA-stabilized CuNCs. A trichromatic system was combined with a smartphone WeChat applet with the ability to extract color information and predict TC concentrations based on a deep learning model [134].

A recent study was done in which azodicarbonamide (ADA), as an adulterant in flour, and glutathione (GSH) were detected using a smartphone-based ratiometric FL approach based on blue emitting biomass-derived carbon dots (BCDs) and yellow emitting 2,3-diaminophenazine (OxOPD). Silver ions are able to oxidize OPD to OxOPD, which in turn quenches the FL intensity of the BCDs through FRET. The presence of GSH inhibits this process through chelating the silver ions, whereas the presence of ADA can again reverse this inhibition as it can oxidize GSH to GSSG. The intensity ratios of BCDs/OxOPDs can be used to quantify GSH and ADA. A WeChat applet, developed based on convolution neural networks, deep learning, and simple image processing, was used to find the linear relationship between RGB and HSV values with the concentrations of the analytes [135]. In another attempt, ML-based technics were coupled with dual-emission molecularly imprinted polymers, using two FL probes, namely SiO_2 coatings on red-emitting CdSe/ZnS quantum dots (r-SiO_2@QDs) on the inner layers and blue-emitting nitrogen-doped graphene quantum dots (N-GQDS) on the surface, to detect pretilachlor, a pesticide, in fish and water samples (Fig. 5A) Increased concentrations of pretilachlor led to the quenching of the blue emission of the GQDs, whereas the red emission was not altered. This led to changes in the fluorescence emission which were captured using a digital camera. The RGB values were then extracted and used as the input data for a random forests (RF) model to predict the concentrations of the pretilachlor. The recovery of the developed RF model for fish and river water samples was respectively 92.2–107.6% and 84.2–108.2%, which shows the high performance of the designed platform for the prediction of analyte concentrations [136].

Besides food and environmental monitoring, image-based ML-assisted sensing is attracting much attention in medical diagnosis as it can pave the way to POC testing. In one study, a smart-phone based method coupled with deep learning technics was used to identify the population of natural killer (NK) cells, which are known to be correlated with numerous diseases from basic inflammatory responses to complex illnesses such as cancer, through CD56 and inflammatory cytokine IL-2. A two-compartment paper microfluidic chip with fluorescent nanoparticles coated with antibodies against IL-2 and CD56 was used; one for the measurement of NK cells and IL-2 through a smartphone-captured video of the flow velocity of the blood samples; another for the separation of two NK cell populations (CD56dim and CD56bright). ML techniques based on smartphone image analysis was used to develop a predictive model based on random forests for the differentiation of NK cells with 89% accuracy [137]. ML algorithms were also used with CRISPR fluorescent approach for the diagnosis of SARS-CoV-2 (Fig. 5B). In this approach, smartphones were used for capturing images, which were subsequently analyzed in the HSV color-space to calculated the FL intensity. A logistic regression model was built based on the FL intensity to classify the images into positive and negative samples to determine the probability of infection [138].

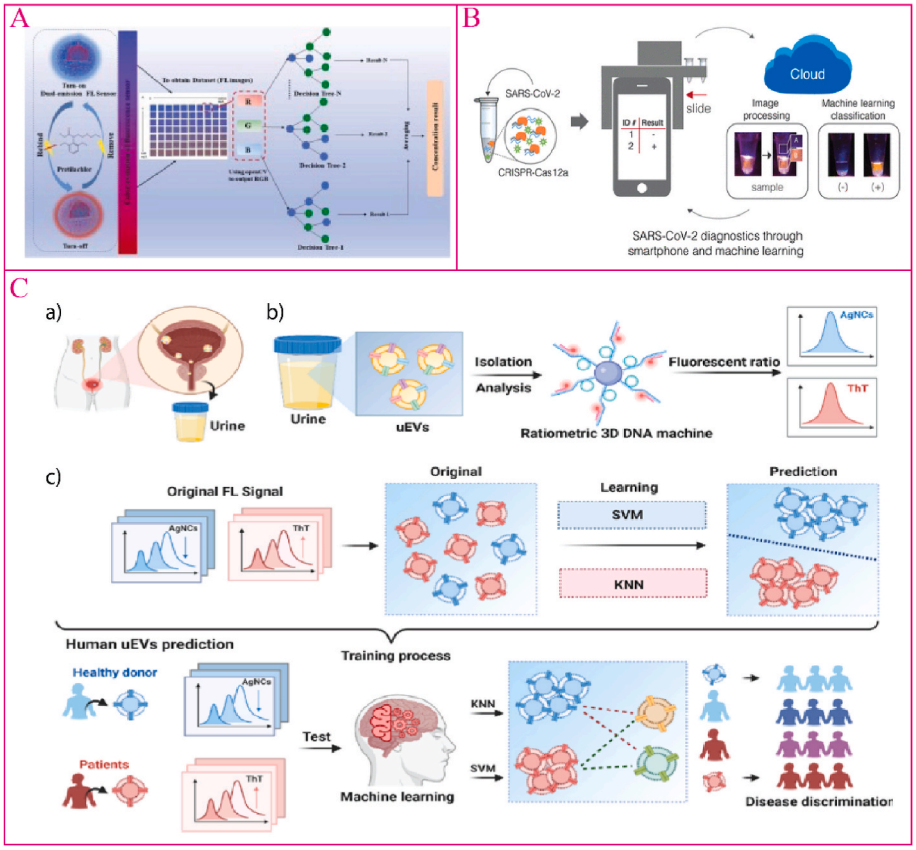


Fig. 5. (A) An ML-assisted fluorescent sensor for the detection of pretilachlor based on RBG data and a random forests algorithm [136], (B) A CRISPR fluorescent approach for the detection of SARS-CoV-2 based on smartphone captured images and logistic regression model [138], and (C) A machine learning-based method for distinguishing biomarkers present on urinary extracellular vesicles based on SVM and KNN for the detection of urinary diseases [146].

Although many reports on ML-assisted image-based classification on performed via feature extraction from images, with the advance of deep learning algorithms, development of learning models that can be trained on images has become easier and more efficient. Although prior to learning, raw images need to be pre-processed which can include adjusting the image size, segmentation, re-orientation of the images and even filtering the colors. The required pre-processing highly depends on the nature of the images captured and also the chosen algorithm for learning; for instance, the convolutional neural networks, among the mostly used ML algorithms for learning based on images, work through developing fully connected layers which require images of the same size and orientation. Furthermore, pre-processing of images can reduce the learning time and result in more accurate predictions. In an attempt to perform learning using images as input data, cancer diagnosis and monitoring were pursued based on the label-free detection and characterization of circulating tumor cells (CTCs). In this report convolutional neural networks, as a powerful image classification algorithm, were used to classify bright field microscopy images of blood samples containing WBCs and CTCs. High classification accuracy of about 88.6% and 97% was achieved for images from patient blood and cultured cells, respectively [139]. Deep learning was employed in order to investigate the inhibition of the transcription of DNA to RNA by anticancer drugs by a fluorescence image-based method. Two successive models based on deep convolutional neural networks were developed to detect cell nuclei and monitor cell death and also to classify the captured images. The approach applied in this study presents a simpler, more cost-efficient method to monitor the impact of anticancer drugs on tumors [140].

Overall, implementing ML in image-based FL sensing methods can help overcome many of the current limitations. As images are generally prone to ambient illumination conditions, camera optics and photography settings, a sensor developed solely based on image processing might not be able to be expanded to other situations using various cameras. Through ML, models can be developed using numerous cameras which can in turn eliminate the limitations mentioned. Furthermore, data collected from images may not always be linear, and thus cannot be feasibly discerned using regular methods. ML is a powerful tool to extract patterns from non-linear data, and thus can help overcome this problem. Also, using ML various color spaces and image features can simultaneously be used for pattern discernment, which will lead to more precise outcomes. It is evident that ML can benefit image-based FL sensing in many aspects and, with the aid of smartphones, can pave the way for POC diagnosis and on-site sensors.

3.2.2. FL spectra-based detection

Given the global explosion of smart-phones in our technology-driven time and the immense improvement in smart-phone cameras, image-driven data based on either FL microscopy or photographed images are attracting more attention in ML-aided FL sensing as they can pave the way for POC testing, but spectral data can provide more sensitive and reliable results especially when detecting small amounts of an analyte [141]. This is because small alterations in FL emission can be easily detected using FL spectrometers, whereas these changes may not display themselves in images [142,143]. Furthermore, camera optics can impact the data extracted from images to some extent, thus rendering spectral data more reliable. For these reasons, many researchers prefer to rely on spectral data.

Deep learning technics were used to detect copper ions (Cu^{2+}) concentrations in recent research. The sensing platform was an Eu(III) functionalized PI hydrogel film (Eu-1) used for the consecutive detection of two analytes: spermine (Spm) and Cu^{2+}. The sensing platform initially reacts with Spm, generating a red FL signal. Cu^{2+} will then interact with the Eu-1@Spm with high selectivity to quench the red signal. Back-propagation neural networks (BPNN), as a deep learning method, was used to predict the concentration of Cu^{2+} based on the Eu-1@Spm sensing platform. The model was made of three layers; the first containing the I/I0 values as the input information, the second is a hidden layer of five neurons, and the third is the output layer which included various Cu^{2+} concentrations represented by six neurons. Through numerous iterations and by adjusting the weights, the researchers were able to decrease the MSE to 0, attaining highly perfect concentration predictions [144].

The Support Vector Machines (SVM), a highly popular algorithm in binary classification, was implemented for the detection of aflatoxin B in almonds in a recent ML-based sensor. Spectra of almond samples under excitation at 375 nm were gathered and the Area Under the Receiving Operating Characteristic (ROC) Curve (AUC) score was calculated for each in order to develop the dataset. The mentioned dataset was employed to train an SVM model with Radial Basis Function kernel for the classification of contaminated (labeled as 1) and safe (labeled as 0) almond samples. After validation using a testing dataset, results of 95% accuracy and 5% false negative rate were achieved [145].

In an attempt to develop a sensing platform for the early diagnosis of urinary diseases including cancers of the urinary tract, a ratiometric 3D DNA machine was coupled with ML algorithms to distinguish the biomarkers present on urinary extracellular vesicles (uEVs). The DNA machine sensing system consists of an aptamer-walker hybridization complex, with specific aptamers against the uEVs biomarkers including CD63, CEA, EpCAM, MUC1, and PSA (Fig. 5C). Upon the interaction of the biomarkers with the aptamers, the walker strand, which is complementary to a portion of the anchor strand, is released which in turn generates the ratiometric FL intensity signal changes. The cascade of interactions after the release of the walking strand ultimately results in the decrease in the FL intensity of the DNA-stabilized AgNCs and the formation of a ThT-G-quadruplex which enhances the FL intensity of ThT. The spectral data from the uEVs and the ration of the FL intensity of the ThT and AgNCs were used to develop models based on KNN and SVM algorithms for binary classification of samples into healthy and disease types, and also to further distinguish the diseases (including bladder cancer, kidney stones, and renal cysts) based on a combination of biomarker responses. Using both algorithms, classification of individuals to diseases and healthy was done with 100% accuracy; and the discrimination of disease types was done with precision of 86.1% [146]. This report perfectly shows the ability of ML algorithms to discern patterns from heterogeneous information generated from multibiomarker-based diagnosis, and thus aid in the development of more precise diagnostic devices for the detection of complex conditions.

Overall, ML-guided FL sensing has proven to show enhanced performance and accuracy and overcome various limitations. FL generally creates noisy data and can be easily influenced by ambient conditions including pH, temperature, etc. Through generating large datasets and implementing ML for pattern extraction, the hindering effect of these problems can be reduced, leading to the enhancement of the detection performance. Also, through incorporating ML with FL sensors, multiplex recognition of biomarkers and analytes can be done with higher precision. To conclude, FL sensors, both image-based and spectra-based, can immensely benefit from the implementation of ML to enhance sensor performance to detect and diagnose various conditions.

3.3. Chemi- and bio-luminescence

Chemiluminescence (CL), in which a chemical reaction provides the required energy for the excitation of molecules, leading to the emission of light upon relaxation, overcomes many of the problems faced in FL including the scattering of light and high background noise as there is no need for an external source of excitation [147,148]. Due to some limitations, including a high blank signal, interference of other oxidants (O_2, OCl^-, O_2^-), and quenchers present in samples, the capabilities of CL have not yet been fully exploited [149,150].

In an attempt to profile the phenolic compounds in wines, Kazak et al. developed a CL-based machine learning-assisted assay [151]. The lack of antioxidants in food is known to cause weakened immunity of the body and might even lead to chronic diseases. CL is regarded as the most

standardized method in for the determination of antioxidant properties of food. With the help of neural network regression models (NNRMs) they were able to detect 5 μmol dm^{-3} to 2 mol dm^{-3} (Fig. 6A).

Bioluminescence (BL), as a subset of CL, is a process in which certain organisms including the ubiquitously known fireflies, and also some marine creatures, certain species of fungi and bacteria produce and emit light as a result of a reaction catalyzed by the enzyme luciferase. In this reaction, a light-emitting molecule named luciferin reacts with oxygen to produce oxyluciferin and energy in the form of light [152,153]. Numerous luciferin and luciferase from various sources have been yet discovered and paired for analytical sensing purposes [154–156]. The advent of genetic engineering and molecular biology has also enabled the production of recombinant bacteria possessing the necessary components of bioluminescence for the design of portable whole-cell biosensors [157,158]. Although BL has many undisputable advantages including high detectability resulting from the absence of a background signal and the requirement of low analyte concentration and high sensitivity because of the turnover of the enzymatic reaction catalyzed by luciferase, it has remained among the least explored luminescence strategies because of its dependence of advanced molecular biology technics which enable the large-scale production of recombinant enzymes [159]. ML-aided BL detection has not been as explored as other strategies, albeit recently the number of research papers in this area is increasing.

A whole-cell sensing array based on fifteen genetically modified *Escherichia coli* strains, each harboring a plasmid containing a bioluminescence reporter system, was recently reported for the detection and characterization of antibiotic compounds (Fig. 6B). Varied BL patterns were observed in the presence of each antibiotic, which was processed into four different indices, including ratio to blank, time normalization, strain normalization, and omnibus index, and used to train a Multiclass Decision Forest (MDF). After 3 h, an accuracy of 65% for compound detection and 90% for class classification was attained. The MDF model showed an accuracy of over 70% in the classification of eight antibiotics at concentrations from 125 ppb to 1000 ppb. The trained ML model was also able to successfully categorize unknown antibiotics based on data from previously known samples [160]. Through this approach and with the aid of ML, facile and rapid identification and categorization of antibiotics can be pursued.

Other works report an NAD(P)H:FMN-oxidoreductase-luciferase bacterial bioluminescent system was used to evaluate the presence of three water contaminants including 1,4-benzoquinone, copper sulfate and 1,3-dihydroxybenzene with multilayer perceptrons. As a result of the various interactions made with this system, different kinetics of light emission arose which were used as input data for training the multilayer perceptron model with 61 inputs neurons, 3 hidden layers and 3 output neurons. This approach shows great performance and could be implemented for rapid detection of contaminants [161].

Although the published studies on ML-assisted CL and BL detection are limited, we have here presented some examples to illustrate the potential of this approach in sensing and biosensing.

3.4. Sensor arrays

Array-based sensing endows numerous advantages which include high accuracy, selectivity and the ability to simultaneously a selection of analytes; thus, these approaches have emerged as a powerful tool for the detection of chemically diverse analytes and in multiplex sensing studies. Instead of relying on specific "lock and key" interactions based on target capturing using molecules like antibodies and aptamers, sensor arrays mimic the mammalian gustatory and olfactory systems by relying on a series of selective elements that can be used to interact with various analytes generating different patterns [162–165]. These patterns are thus analyzed by pattern detection methods in order to discern meaning fingerprints, specific for each analyte. These methods generate large amounts of data and meticulous pattern recognition is of utmost importance in array-based approaches. Although chemometrics methods such as PCA and LDA have immensely been used for pattern recognition in array-based sensing and proven to be effective in many cases [166–168], they are faced with limitations hindering the accurate identification of fingerprints when dealing with linearly inseparable datasets [169,170]. Chemometrics is the discipline that uses mathematical statistical methods to analyze multivariate data, instrumental or not, and mainly answer linear problems. It can be considered as a subset of machine learning that generally performs well on linear data [171]. ML algorithms have a wide variety and are able to deal with both linear and nonlinear data effectively, and thus have proven to be more reliable in distinguishing meaningful patterns in array-based approaches [172]. In this section, we will review some of the most recently published studies on the incorporation of ML algorithms in FL and ECL sensor arrays.

3.4.1. FL sensor arrays

Numerous reports have been published on the development of FL sensor arrays; the data collected from which is of a higher dimension and requires complex analysis for pattern recognition. ML algorithms are highly implemented in array-based FL sensors to translate the data into understandable patterns in order to discern each analyte [41,170,173,174]. Recent research was performed in which a dual channel sensing array was developed to distinguish four different kinds of tetracycline (TC), including tetracycline (TC), oxytetracycline (OTC), doxycycline (DOX), and metacycline (MTC) based on the LDA and SVM algorithm. Two carbon dots were synthesized using quinaldine red, as QR-CDs with blue emission, and cetylpyridinium chloride, as CPC-CDs with yellow

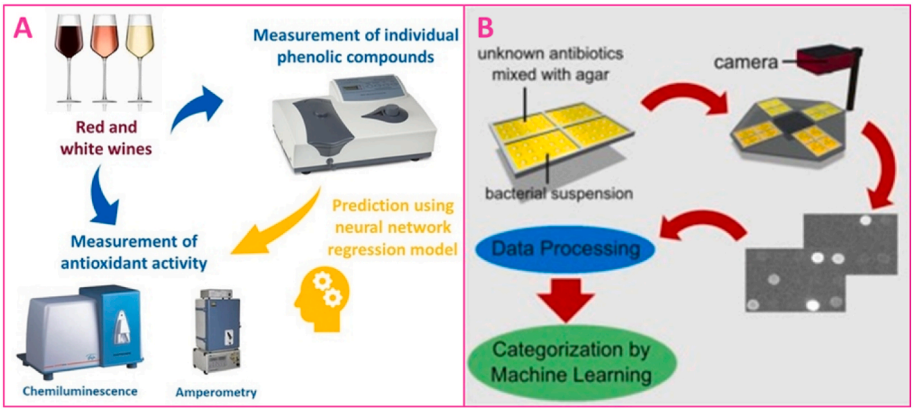


Fig. 6. Examples of ML-assisted CL and BL sensors; (A) a chemiluminescence sensing platforms coupled with neural networks for the detection of phenolic compounds in wine [151], and (B) a bioluminescence sensor coupled with decision trees for the classification of antibiotics [160].

emission. As a result of the inner filter effect and due to appropriate overlapping of the absorption spectra of the TCs and the excitation spectra of the two CDs, FL quenching of the CDs occurred as the analyte interacted with the fluorophores. Variations in the FL intensity of the CDs before and after interaction with the analytes, as I/I0, were used to develop a pattern for each of the TCs at the concentration of 1.0 μM. The approach showed high selectivity and sensitivity and was able to distinguish TCs in complex unknown samples including water and milk with an accuracy of 100%, providing an effective approach for antibiotic monitoring in the environment [175]. In another sensor array developed for the discrimination of aminoglycoside antibiotics (amikacin, kanamycin, streptomycin, gentamycin, tobramycin, and neomycin), ML algorithms were employed to discern meaningful patterns for each antibiotic (Fig. 7A). Three commercially available fluorophores were used in this sensing platform including 2, 3-Naphthalenedicarboxaldehyde (NDA) to investigate the amino information, (alizarin red-S)-(diphenylborinic acid 2-aminoethyl ester) (ARS-DPBA) for the hydroxyl information and sulforhodamine B (SRB) for the anionic or cationic charging. A dataset based on features extracted from the 8496 fluoromoetric images was developed to train two deep learning models (convolutional neural networks (CNN) and multilayer perceptron (MLP)) and eight ML algorithms (naïve Bayes, LDA, logistic regression, decision trees, random forest, SVM, K-nearest neighbors, extreme gradient boosting), and it was concluded that the CNN model had the highest efficiency in fingerprint pattern discernment with an accuracy of 100% [176]. Another study was reported on the discernment of various antibiotics, a nine-channel fluorescence array was developed using carbon nanoparticles (CNPs) using different precursors and various surface functional groups. The array was used to detect six different antibiotics, each from a different class, including ampicillin, ciprofloxacin, kanamycin, sulphamethoxazole, tetracycline, and trimethoprim. Fluorescence variations resulting from the interaction of the antibiotics with the CNPs were captured using images and transformed to CMYK values (C: cyan, M: magenta, Y: yellow, and K: key) to generate a dataset used for analysis with seven different machine learning algorithms. Among the tested algorithms, Multilayer Perceptron (MLP) showed the highest performance with 82% accuracy [177]. These studies show the outstanding power of ML algorithms once coupled with array-based sensing platforms for environmental monitoring, which can pave the way to on-site detection of environmental, agricultural, and food contaminants, even in remote, underdeveloped places.

Proteins play a vital role in numerous biological and physiological functions and fluctuations in their concentration can lead to various abnormalities and diseases. Furthermore, in many complex diseases, such as cardiovascular diseases, neurodegenerative problems, liver cirrhosis, etc. various proteins are involved; changes in all of which need to be detected for precise disease diagnosis. Thus, array-based sensing platforms and chemical nose strategies designed for protein detection are of high importance [178]. CDs were also used to develop a sensor array for the detection of eight different proteins. CDs with five different surface functionalities, including S-CDs with carboxylic acid and hydroxyl groups, G-CDs with higher carboxylic acid groups, Z-CDs with a zwitterionic surface, C-CDs with a hydrophobic surface, and P-CDs with monophosphate surface groups, were used which can interact with biological protein at a concentration of 100 nM leading to different patterns in the fluorescence intensity of the CDs after their interaction with each analyte. LDA and various ML algorithms were employed to discern meaningful models from the pattern of interactions, and it was seen that ML algorithms such as gradient boosted trees, which could

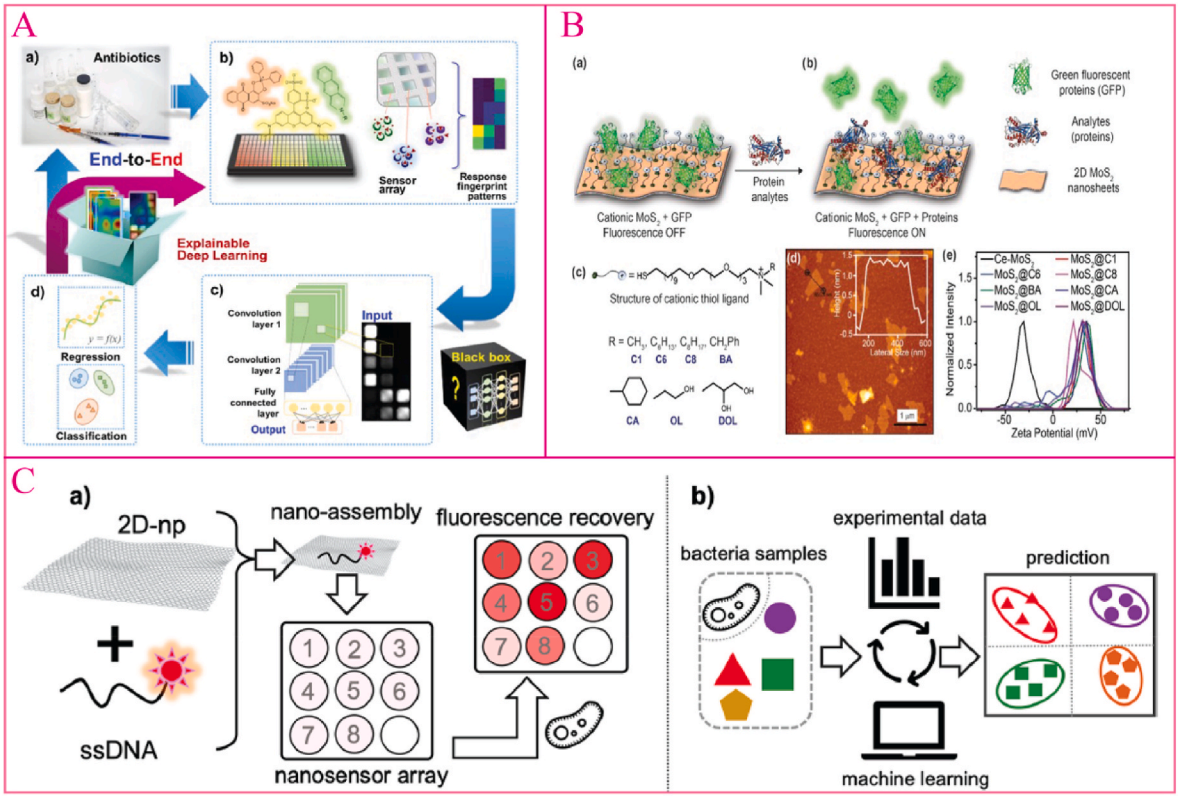


Fig. 7. Examples of ML-assisted fluorescent sensor arrays (A) for the discrimination of aminoglycoside antibiotics based on features extracted from images [176], (B) for distinguishing proteins based on a two-dimensional platform with MoS_2 nanosheets with seven different functionalities as the receptor and green fluorescent protein (GFP) [180], and (C) for the multiplex detection of bacteria using dimensional (2D) nanoparticles including nanographene oxide, MoS_2, and WS_2 along with fluorescently labeled random short single-stranded DNAs [182]. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

deliver a model with 100% accuracy, could analyze the data more efficiently [179]. Another study on the detection of proteins was reported in which a sensor array using two-dimensional platform with MoS_2 nanosheets with seven different functionalities as the receptor and green fluorescent protein (GFP) as the signal transducer was developed. Fifteen various proteins at a concentration of 50 nM were detected through their interaction with the various functionalities of the MoS_2 nanosheets and the subsequent quenching of the GFP emission (Fig. 7B). Various ML algorithms were also compared with each other and also with LDA, and it was concluded that although LDA can sufficiently analyze smaller less complicated datasets, ML algorithms like neural networks are more efficient in discerning nuances in larger, more complex datasets [180]. Another study developed an ML-assisted FL sensing array based on MOFs for the detection of post-neurosurgical meningitis (PNM) based on the comprehensive analysis of proteins, biomolecules and cells in the cerebrospinal fluid. The FL signal change was processed with two ML algorithms, including k-nearest neighbors (k-NNs) and artificial neural networks (ANNs). Based on various strategies, discrimination confidences of around 80%–100% was achieved for the biomolecules, proteins and cells. The sensing array was ultimately used to diagnose PNM patients to three classes including normal, mild and severe and an accuracy of 88.7% was attained [181]. These examples display the impact ML can have on smart, array-based diagnosis of complex dieses requiring the detection of multiple analytes.

Rapid detection of pathogens remains a challenge to date as most gold standard methods, which include cell culture and PCR methods, are highly time-consuming and require special laboratory facilities. In attempt to develop point-of-care testing for pathogen detection, many researchers are exploring ML-assisted array-based chemical tongue/nose platforms. In an attempt to develop ML-based FL sensing, a nanosensor platform using 2-dimensional (2D) nanoparticles including nanographene oxide, MoS_2, and WS_2 along with fluorescently labeled random short single-stranded DNAs (ssDNA) were used. The 2D nanoparticles are able to absorb the ssDNA strands, and in turn quench the FL of the labels. The interaction of bacterial lysates with the ssDNA strands can release them from the 2D nanoparticles, hence leading to the recovery of their FL emission. The FL recovery signals were used to train numerous ML algorithms including Logistic Regression (LR), Support Vector Machines (SVM), k-Nearest Neighbor (kNN), Random Forests (RF), Decision Tree (DT), Ridge, Gradient Boosting (GB), and Multilayer Perceptron (MLP) (Fig. 7C). MLP was seen to deliver the most accurate classification model with 90% accuracy. Furthermore, it was seen that this array-based approach could also effectively distinguish untreated wild-type *E. coli* strains from those undergone antimicrobial treatment [182]. A similar approach based on 2D-nanomaterials and FAM labeled ssDNA sequences was used in other research for the detection of bacteria with the aid of ML. Eight different pathogenic strains were distinguished based on the FL signal change with an accuracy of 97.9% [170].

As can be seen, ML can play a significant role the pattern recognition from the complex data extracted from FL sensing arrays. Compared to chemometrics methods, ML algorithms are much stronger with the ability to discern patterns from both linear and non-linear data.

3.4.2. ECL sensor arrays

ECL possesses numerous advantages over other detection methods, i.e., high sensitivity and selectivity toward the analyte and high control over the reaction leading to outstanding reproducibility. Additionally, as the ECL is endowed with high control over emission location as the produced light is only seen in vicinity to the electrode surface, the detection of multiple analytes is facilitated through using various electrodes [183,184]. Besides the traditional luminophores, such as ruthernium (II) complexes and Ru $(bpy)_3^{2+}$, recently various luminescent nanomaterials have been employed in ECL systems, leading to the rapid development of various ECL emitters and detection systems for multiplex ECL sensing [185,186]. Though not as explored as FL sensor arrays, ML-assisted ECL arrays are also becoming increasingly popular with analytical chemists. In this section we will briefly review some recent studies on ML-guided ECL sensing arrays.

A recent study by Guo et al. has reported an ECL immunoarray for diagnosis of acute myocardinal infarction (AMI) based on the simultaneous detection of copeptin, h-FABP, and cTnI concentrations. A single electrode array microchip was developed using immune-gold nano-assemblies attached to the surface of the microchip. The immune-gold nano-assemblies were attained through combining Cu^{2+}/cysteine complexes with gold nanoparticles functionalized with chitosan and antibodies. Using a highly sensitive imaging system, coupled with image analysis, the intensities were extracted and used to train an SVM model (Fig. 8). The model was able to distinguish AMI from non-AMI patients with 100% accuracy, which was substantially higher than the gold standard cardiac troponin T (cTnT) method [41]. This study shows how using machine learning, highly sensitive ECL arrays can be developed to simultaneously detect numerous biomarkers involved in complex diseases for precise diagnosis.

These examples shed light on the significant role of machine learning in array-based sensing. As previously mentioned, arrays generate highly complex data, and thus need to be coupled with strong pattern recognition methods. ML and multi-class classification models can provide such methods to accurately extract meaningful patterns and develop accurate prediction. Using ML-assisted sensing arrays, the diagnosis of complex diseases, such as cancers, neurodegenerative disorders, etc. with rely on the precise detection of multiple biomarkers can become more feasible. Furthermore, the development of on-site detection devices for the recognition of numerous food and environmental pollutants can be possible through arrays combined with ML.

4. Future challenges and perspectives

Although machine learning (ML) has become increasingly prevalent in the field of analytical chemistry, there is still significant potential for further development and expansion of its applications. As previously mentioned, ML algorithms rely heavily on input data, meaning that they require a large and diverse set of data to function effectively. However, the practicality of collecting and maintaining such datasets can present a significant challenge in terms of both time and resources. Furthermore, not all analytical chemists possess the knowledge or skills required to fully leverage the benefits of ML techniques, which can hinder their adoption and integration into everyday research practices. Another major limitation is device manufacturing and the implementation of smart technologies within sensing platforms. These issues can majorly impact the widespread adoption of ML-assisted biosensors in analytical chemistry.

Despite these challenges, there are clear advantages to using ML in analytical chemistry, including the ability to obtain more accurate and reliable results in less time. To maximize the potential benefits of ML, user-friendly software and tools must be developed that can be readily adopted by researchers with varying levels of experience and expertise. Moreover, it is essential to recognize that ML is not always the best solution for every analytical chemistry problem. Traditional regression tools and other simpler analytical methods may be more appropriate in cases where the data is straightforward and easy to interpret [187].

Looking ahead, there is great potential for continued growth and advancement in the field of ML in analytical chemistry, with the ultimate goal of reducing errors and improving overall accuracy and efficiency in data analysis [188]. One area in which ML can be especially beneficial, is with the development of POC testing. Currently, POC testing suffers from low accuracy and reliability in many cases. ML, especially when integrated with smartphone applications, can overcome these limitations and help advance POC sensing devices. Furthermore, wearable sensors, which are used to monitor human conditions from biological fluids (e.g., sweat, tears, and saliva), can also be combined with ML technics for advanced health monitoring [189]. The ultimate goal of these devices is to monitor numerous biomarkers and human

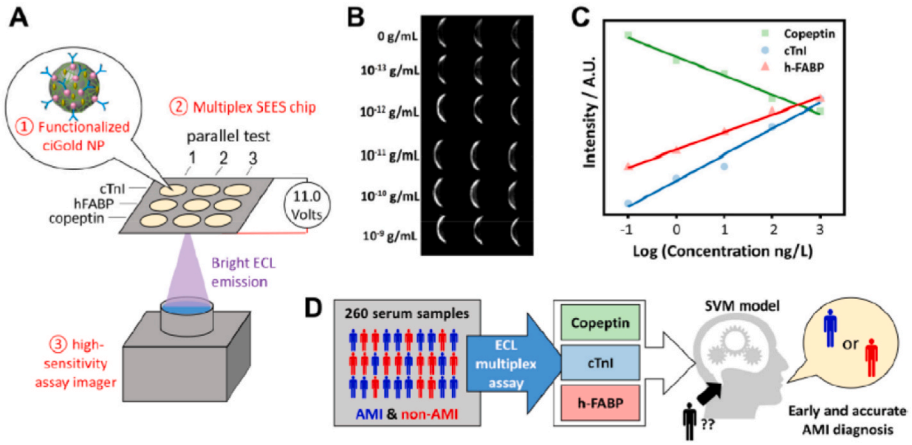


Fig. 8. An ML-assisted ECL sensor array (A) the ECL immunoarray based on immune-gold nano-assemblies coupled with an imaging system, (B) the raw ECL images attained, (C) the corresponding calibration curves for each of the three biomarkers (copeptin, h-FABP, and cTnI), and (D) the overall workflow of the ECL immunoassay used for the detection of acute myocardial infarction using SVM [41]. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

conditions using a series of small sensing networks. ML can aid with pattern recognition and multiplex detection in these devices to ultimately generate POC and wearable sensors with the ability to continuously and precisely monitor various human conditions. Moreover, ML-assisted sensing platforms can also pave the way for onsite monitoring of environmental and food pollutants [190]. ML help with the detection of multiple food and environmental analytes to develop smart devices to control health threatening compounds in remote places with limited access to advances laboratory facilities.

To conclude, we have tried to show the benefits of implementing ML with luminescent biosensors in this review, both in the synthesis of luminescent nanomaterials and sensor development. It is evident that ML-assisted biosensing has numerous advantages, especially relating to image-based analysis and multiplex detection. With the widespread adoption of smart technologies in numerous aspects of everyday life, doubtlessly analytical and bioanalytical chemistry will also move in the direction of developing smart, POC sensors with the ultimate aim of continuous, precise health and environment monitoring.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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References

[1] F. Rosenblatt, The perceptron: a probabilistic model for information storage and organization in the brain, Psychol. Rev. 65 (1958) 386–408, https://doi.org/10.1037/H0042519.
[2] ACM: Digital Library: Communications of the ACM, (n.d.). https://dl.acm.org/doi/fullHtml/10.1145/319382.319388 (accessed July 29, 2023).
[3] P. Puthongkham, S. Wirojsaengthong, A. Suea-Ngam, Machine learning and chemometrics for electrochemical sensors: moving forward to the future of analytical chemistry, Analyst 146 (2021) 6351–6364, https://doi.org/10.1039/D1AN01148K.
[4] M.I. Jordan, T.M. Mitchell, Machine learning: trends, perspectives, and prospects, Science 349 (2015) 255–260, https://doi.org/10.1126/SCIENCE.AAA8415/ASSET/AB2EF18A-576D-464D-B1B6-1301159EE29A/ASSETS/GRAPHIC/349_255_F5.JPEG, 1979.
[5] A. Mathew, P. Amudha, S. Sivakumari, Deep learning techniques: an overview, Adv. Intell. Syst. Comput. 1141 (2021) 599–608, https://doi.org/10.1007/978-981-15-3383-9_54/COVER.
[6] Y. Reich, Machine learning techniques for civil engineering problems, Comput. Aided Civ. Infrastruct. Eng. 12 (1997) 295–310, https://doi.org/10.1111/0885-9507.00065.
[7] D. Rangel-Martinez, K.D.P. Nigam, L.A. Ricardez-Sandoval, Machine learning on sustainable energy: a review and outlook on renewable energy systems, catalysis, smart grid and energy storage, Chem. Eng. Res. Des. 174 (2021) 414–441, https://doi.org/10.1016/J.CHERD.2021.08.013.
[8] J. Wei, X. Chu, X.Y. Sun, K. Xu, H.X. Deng, J. Chen, Z. Wei, M. Lei, Machine learning in materials science, InfoMat 1 (2019) 338–358, https://doi.org/10.1002/INF2.12028.
[9] X. Pan, J. Yang, R. Van, E. Epifanovsky, J. Ho, J. Huang, J. Pu, Y. Mei, K. Nam, Y. Shao, Machine-learning-assisted free energy simulation of solution-phase and enzyme reactions, J. Chem. Theor. Comput. (2021), https://doi.org/10.1021/ACS.JCTC.1C00565/SUPPL_FILE/CT1C00565_SI_001.PDF.
[10] R. Burbidge, M. Trotter, B. Buxton, S. Holden, Drug design by machine learning: support vector machines for pharmaceutical data analysis, Comput. Chem. 26 (2001) 5–14, https://doi.org/10.1016/S0097-8485(01)00094-8.
[11] M. Staszak, K. Staszak, K. Wieszczycka, A. Bajek, K. Roszkowski, B. Tylkowski, Machine learning in drug design: use of artificial intelligence to explore the chemical structure–biological activity relationship, Wiley Interdiscip. Rev. Comput. Mol. Sci. 12 (2022) e1568, https://doi.org/10.1002/WCMS.1568.
[12] M. Mousavizadegan, H. Mohabatkar, An Evaluation on Different Machine Learning Algorithms for Classification and Prediction of Antifungal Peptides, (n.d.).
[13] M. Mousavizadegan, H. Mohabatkar, Computational Prediction of Antifungal Peptides via Chou's PseAAC and SVM, 16, 2018, https://doi.org/10.1142/S0219720018500166, 10.1142/S0219720018500166.
[14] A. Holzinger, Trends in interactive knowledge discovery for personalized medicine: cognitive science meets machine learning, IEEE Intellig. Inf. Bull. 15 (2014) 6–14. https://graz.elsevierpure.com/en/publications/trends-in-interactive-knowledge-discovery-for-personalized-medici (accessed July 29, 2023).
[15] D. Komura, S. Ishikawa, Machine learning approaches for pathologic diagnosis, Virchows Arch. 475 (2019) 131–138, https://doi.org/10.1007/S00428-019-02594-W/FIGURES/3.
[16] B. Debus, H. Parastar, P. Harrington, D. Kirsanov, Deep learning in analytical chemistry, TrAC, Trends Anal. Chem. 145 (2021), 116459, https://doi.org/10.1016/J.TRAC.2021.116459.
[17] Y.C. Huang, H.H. Chung, E.P. Dutkiewicz, C.L. Chen, H.Y. Hsieh, B.R. Chen, M. Y. Wang, C.C. Hsu, Predicting breast cancer by paper spray ion mobility spectrometry mass spectrometry and machine learning, Anal. Chem. 92 (2020) 1653–1657, https://doi.org/10.1021/ACS.ANALCHEM.9B03966/ASSET/IMAGES/LARGE/AC9B03966_0004.JPEG.
[18] M. Zhu, J. Wang, X. Yang, Y. Zhang, L. Zhang, H. Ren, B. Wu, L. Ye, A review of the application of machine learning in water quality evaluation, Eco-Environ. Health 1 (2022) 107–116, https://doi.org/10.1016/J.EEHL.2022.06.001.
[19] Z.M. Yaseen, An insight into machine learning models era in simulating soil, water bodies and adsorption heavy metals: review, challenges and solutions, Chemosphere 277 (2021), 130126, https://doi.org/10.1016/J.CHEMOSPHERE.2021.130126.
[20] A.M. Jiménez-Carvelo, A. González-Casado, M.G. Bagur-González, L. Cuadros-Rodríguez, Alternative data mining/machine learning methods for the analytical evaluation of food quality and authenticity – a review, Food Res. Int. 122 (2019) 25–39, https://doi.org/10.1016/J.FOODRES.2019.03.063.
[21] Y. Asim, B. Raza, A.K. Malik, S. Rathore, L. Hussain, M.A.M. Iftikhar, A multi-modal, multi-atlas-based approach for Alzheimer detection via machine learning, Int. J. Imag. Syst. Technol. 28 (2018) 113–123, https://doi.org/10.1002/IMA.22263.
[22] R. Ramos-Pollán, M.A. Guevara-López, C. Suárez-Ortega, G. Díaz-Herrero, J. M. Franco-Valiente, M. Rubio-Del-Solar, N. González-De-Posada, M.A.P. Vaz, J. Loureiro, I. Ramos, Discovering mammography-based machine learning classifiers for breast cancer diagnosis, J. Med. Syst. 36 (2012) 2259–2269, https://doi.org/10.1007/S10916-011-9693-2/FIGURES/4.

[23] Z.S. Ballard, H.A. Joung, A. Goncharov, J. Liang, K. Nugroho, D. Di Carlo, O. B. Garner, A. Ozcan, Deep learning-enabled point-of-care sensing using multiplexed paper-based sensors, Npj Digit. Med. 3 (2020) 1–8, https://doi.org/10.1038/s41746-020-0274-y, 2020 3:1.
[24] A.R. Porras, K. Rosenbaum, C. Tor-Diez, M. Summar, M.G. Linguraru, Development and evaluation of a machine learning-based point-of-care screening tool for genetic syndromes in children: a multinational retrospective study, Lancet Digit. Health 3 (2021) e635, https://doi.org/10.1016/S2589-7500(21)00137-0, e643.
[25] A.L. Fradkov, Early history of machine learning, IFAC-PapersOnLine 53 (2020) 1385–1390, https://doi.org/10.1016/J.IFACOL.2020.12.1888.
[26] N. Artrith, K.T. Butler, F.X. Coudert, S. Han, O. Isayev, A. Jain, A. Walsh, Best practices in machine learning for chemistry, Nat. Chem. 13 (2021) 505–508, https://doi.org/10.1038/s41557-021-00716-z, 2021 13:6.
[27] M. Münch, C. Raab, M. Biehl, F.M. Schleif, Data-driven supervised learning for life science data, Front. Appl. Math. Stat. 6 (2020), 553000, https://doi.org/10.3389/FAMS.2020.553000/BIBTEX.
[28] S. Sharma, G. Singh, M. Sharma, A comprehensive review and analysis of supervised-learning and soft computing techniques for stress diagnosis in humans, Comput. Biol. Med. 134 (2021), 104450, https://doi.org/10.1016/J.COMPBIOMED.2021.104450.
[29] Z. Xiong, Y. Cui, Z. Liu, Y. Zhao, M. Hu, J. Hu, Evaluating explorative prediction power of machine learning algorithms for materials discovery using k-fold forward cross-validation, Comput. Mater. Sci. 171 (2020), 109203, https://doi.org/10.1016/J.COMMATSCI.2019.109203.
[30] D.E. Jones, H. Ghandehari, J.C. Facelli, A review of the applications of data mining and machine learning for the prediction of biomedical properties of nanoparticles, Comput. Methods Progr. Biomed. 132 (2016) 93–103, https://doi.org/10.1016/J.CMPB.2016.04.025.
[31] N. Dordević, J.S. Beckwith, M. Yarema, O. Yarema, A. Rosspeintner, N. Yazdani, J. Leuthold, E. Vauthey, V. Wood, Machine learning for analysis of time-resolved luminescence data, ACS Photonics 5 (2018) 4888–4895, https://doi.org/10.1021/ACSPHOTONICS.8B01047/SUPPL_FILE/PH8B01047_SI_001.PDF.
[32] M. Jalali-Heravi, Neural networks in analytical chemistry, Methods Mol. Biol. 458 (2008) 81–121, https://doi.org/10.1007/978-1-60327-101-1_6/COVER.
[33] R.M. Balabin, E.I. Lomakina, Support vector machine regression (SVR/LS-SVM)—an alternative to neural networks (ANN) for analytical chemistry? Comparison of nonlinear methods on near infrared (NIR) spectroscopy data, Analyst 136 (2011) 1703–1712, https://doi.org/10.1039/C0AN00387E.
[34] Y. Zhuo, J. Brgoch, Opportunities for next-generation luminescent materials through artificial intelligence, J. Phys. Chem. Lett. 12 (2021) 764–772, 10.1021/ACS.JPCLETT.0C03203/ASSET/IMAGES/LARGE/JZ0C03203_0005.JPEG.
[35] S. Li, R.-J. Xie, Critical review—data-driven discovery of novel phosphors, ECS J. Solid State Sci. Technol. 9 (2020), 016013, https://doi.org/10.1149/2.0192001JSS/XML.
[36] Y. Zhuo, A.M. Tehrani, J. Brgoch, A new era of inorganic materials discovery powered by data science, RSC Theor. Comput. Chem. Ser. (2020) 311–339, https://doi.org/10.1039/9781839160233-00311, 2020-January.
[37] Y. Zhuo, A. Mansouri Tehrani, A.O. Oliynyk, A.C. Duke, J. Brgoch, Identifying an efficient, thermally robust inorganic phosphor host via machine learning, Nat. Commun. 9 (2018) 1–10, https://doi.org/10.1038/s41467-018-06625-z, 2018 9:1.
[38] G. Camps-Valls, Machine Learning in Remote Sensing Dataprocessing, Machine Learning for Signal Processing XIX - Proceedings of the 2009 IEEE Signal Processing Society Workshop, 2009, https://doi.org/10.1109/MLSP.2009.5306233. MLSP 2009.
[39] M.E. Solmaz, A.Y. Mutlu, G. Alankus, V. Kılıç, A. Bayram, N. Horzum, Quantifying colorimetric tests using a smartphone app based on machine learning classifiers, Sensor. Actuator. B Chem. 255 (2018) 1967–1973, https://doi.org/10.1016/J.SNB.2017.08.220.
[40] M. Kashif, K.R. Malik, S. Jabbar, J. Chaudhry, Application of Machine Learning and Image Processing for Detection of Breast Cancer, Innovation in Health Informatics: A Smart Healthcare Primer, 2020, pp. 145–162, https://doi.org/10.1016/B978-0-12-819043-2.00006-X.
[41] M. Guo, D. Du, J. Wang, Y. Ma, D. Yang, M.A. Haghighatbin, J. Shu, W. Nie, R. Zhang, Z. Bian, L. Wang, Z.J. Smith, H. Cui, Three-biomarker joint strategy for early and accurate diagnosis of acute myocardial infarction via a multiplex electrochemiluminescence immunoarray coupled with robust machine learning, Chem. Biomed. Imag. 1 (2023) 179–185, https://doi.org/10.1021/CBMI.3C00035.
[42] S. Szymkuć, E.P. Gajewska, T. Klucznik, K. Molga, P. Dittwald, M. Startek, M. Bajczyk, B.A. Grzybowski, Computer-assisted synthetic planning: the end of the beginning, Angew. Chem. Int. Ed. 55 (2016) 5904–5937, https://doi.org/10.1002/ANIE.201506101.
[43] S.V. Ley, D.E. Fitzpatrick, R.J. Ingham, R.M. Myers, Organic synthesis: march of the machines, Angew. Chem. Int. Ed. 54 (2015) 3449–3464, https://doi.org/10.1002/ANIE.201410744.
[44] C.W. Coley, R. Barzilay, T.S. Jaakkola, W.H. Green, K.F. Jensen, Prediction of organic reaction outcomes using machine learning, ACS Cent. Sci. 3 (2017) 434–443, https://doi.org/10.1021/ACSCENTSCI.7B00064/ASSET/IMAGES/OC-2017-00064K_M003.GIF.
[45] O.A. von Lilienfeld, K. Burke, Retrospective on a decade of machine learning for chemical discovery, Nat. Commun. 11 (2020) 1–4, https://doi.org/10.1038/s41467-020-18556-9, 2020 11:1.
[46] T. Le, V.C. Epa, F.R. Burden, D.A. Winkler, Quantitative structure-property relationship modeling of diverse materials properties, Chem. Rev. 112 (2012) 2889–2919, https://doi.org/10.1021/CR200066H/SUPPL_FILE/CR200066H_SI_001.PDF.
[47] G. Blasse, B.C. Grabmaier, A general introduction to luminescent materials, Luminescent Mater. (1994) 1–9, https://doi.org/10.1007/978-3-642-79017-1_1.
[48] M.J.P. Leiner, Luminescence chemical sensors for biomedical applications: scope and limitations, Anal. Chim. Acta 255 (1991) 209–222, https://doi.org/10.1016/0003-2670(91)80049-Y.
[49] M. Mousavizadegan, A. Alaei, M. Hosseini, Optical Detection of Targets for Food Quality Assessment, Nanosensing and Bioanalytical Technologies in Food Quality Control, 2022, pp. 109–128, https://doi.org/10.1007/978-981-16-7029-9_5/COVER.
[50] Y. Zhang, S. Yuan, G. Day, X. Wang, X. Yang, H.C. Zhou, Luminescent sensors based on metal-organic frameworks, Coord. Chem. Rev. 354 (2018) 28–45, https://doi.org/10.1016/J.CCR.2017.06.007.
[51] M. Wang, T. Wang, P. Cai, X. Chen, Nanomaterials discovery and design through machine learning, Small Methods 3 (2019), 1900025, https://doi.org/10.1002/SMTD.201900025.
[52] J. Timoshenko, D. Lu, Y. Lin, A.I. Frenkel, Supervised machine-learning-based determination of three-dimensional structure of metallic nanoparticles, J. Phys. Chem. Lett. 8 (2017) 5091–5098, https://doi.org/10.1021/ACS.JPCLETT.7B02364/SUPPL_FILE/JZ7B02364_SI_001.PDF.
[53] A.M. Hiszpanski, B. Gallagher, K. Chellappan, P. Li, S. Liu, H. Kim, J. Han, B. Kailkhura, D.J. Buttler, T.Y.J. Han, Nanomaterial synthesis insights from machine learning of scientific articles by extracting, structuring, and visualizing knowledge, J. Chem. Inf. Model. 60 (2020) 2876–2887, https://doi.org/10.1021/ACS.JCIM.0C00199/SUPPL_FILE/CI0C00199_SI_002.PDF.
[54] Y.P. Sun, B. Zhou, Y. Lin, W. Wang, K.A.S. Fernando, P. Pathak, M.J. Meziani, B. A. Harruff, X. Wang, H. Wang, P.G. Luo, H. Yang, M.E. Kose, B. Chen, L.M. Veca, S.Y. Xie, Quantum-sized carbon dots for bright and colorful photoluminescence, J. Am. Chem. Soc. 128 (2006) 7756–7757, https://doi.org/10.1021/JA062677D/SUPPL_FILE/JA062677DSI20060417_112943.PDF.
[55] S. Behzadifar, A. Bagheri Pebdeni, M. Hosseini, J. Mohammadnejad, A new ratiometric fluorescent detection of Glucose-6-phosphate dehydrogenase enzyme based on dually emitting carbon dots and silver nanoparticles, Microchem. J. 182 (2022), 107947, https://doi.org/10.1016/J.MICROC.2022.107947.
[56] M. Kurian, A. Paul, Recent trends in the use of green sources for carbon dot synthesis–A short review, Carbon Trends 3 (2021), 100032, https://doi.org/10.1016/J.CARTRE.2021.100032.
[57] Y. Han, B. Tang, L. Wang, H. Bao, Y. Lu, C. Guan, L. Zhang, M. Le, Z. Liu, M. Wu, Machine-learning-driven synthesis of carbon dots with enhanced quantum yields, ACS Nano 14 (2020) 14761–14768, https://doi.org/10.1021/ACSNANO.0C01899/SUPPL_FILE/NN0C01899_SI_001.PDF.
[58] J. Chen, J.B. Luo, M.Y. Hu, J. Zhou, C.Z. Huang, H. Liu, Controlled synthesis of multicolor carbon dots assisted by machine learning, Adv. Funct. Mater. 33 (2023), 2210095, https://doi.org/10.1002/ADFM.202210095.
[59] Q. Xu, Y. Tang, P. Zhu, W. Zhang, Y. Zhang, O.S. Solis, T.S. Hu, J. Wang, Machine learning guided microwave-assisted quantum dot synthesis and an indication of residual H2O2 in human teeth, Nanoscale 14 (2022) 13771–13778, https://doi.org/10.1039/D2NR03718A.
[60] Q. Hong, X.Y. Wang, Y.T. Gao, J. Lv, B. Bin Chen, D.W. Li, R.C. Qian, Customized carbon dots with predictable optical properties synthesized at room temperature guided by machine learning, Chem. Mater. 34 (2022) 998–1009, https://doi.org/10.1021/ACS.CHEMMATER.1C03220/SUPPL_FILE/CM1C03220_SI_002.XLSX.
[61] J.B. Luo, J. Chen, H. Liu, C.Z. Huang, J. Zhou, High-efficiency synthesis of red carbon dots using machine learning, Chem. Commun. 58 (2022) 9014–9017, https://doi.org/10.1039/D2CC03473E.
[62] R.D. Senanayake, X. Yao, C.E. Froehlich, M.S. Cahill, T.R. Sheldon, M. McIntire, C.L. Haynes, R. Hernandez, Machine learning-assisted carbon dot synthesis: prediction of emission color and wavelength, J. Chem. Inf. Model. 62 (2022) 5918–5928, https://doi.org/10.1021/ACS.JCIM.2C01007/SUPPL_FILE/CI2C01007_SI_001.PDF.
[63] F.Y. Ramírez-Castillo, A. Loera-Muro, M. Jacques, P. Garneau, F.J. Avelar-González, J. Harel, A.L. Guerrero-Barrera, Waterborne pathogens: detection methods and challenges, Pathogens 4 (2015) 307–334, https://doi.org/10.3390/PATHOGENS4020307.
[64] O. Voznyy, L. Levina, J.Z. Fan, M. Askerka, A. Jain, M.J. Choi, O. Ouellette, P. Todorović, L.K. Sagar, E.H. Sargent, Machine learning accelerates discovery of optimal colloidal quantum dot synthesis, ACS Nano 13 (2019) 11122–11128, https://doi.org/10.1021/ACSNANO.9B03864/SUPPL_FILE/NN9B03864_SI_002.ZIP.
[65] H.A. Nguyen, F.Y. Dou, N. Park, S. Wu, H. Sarsito, B. Diakubama, H. Larson, E. Nishiwaki, M. Homer, M. Cash, B.M. Cossairt, Predicting indium phosphide quantum dot properties from synthetic procedures using machine learning, Chem. Mater. 34 (2022) 6296–6311, https://doi.org/10.1021/ACS.CHEMMATER.2C00640/SUPPL_FILE/CM2C00640_SI_001.PDF.
[66] J.P. Wilcoxon, B.L. Abrams, Synthesis, structure and properties of metal nanoclusters, Chem. Soc. Rev. 35 (2006) 1162–1194, https://doi.org/10.1039/B517312B.
[67] A. Bagheri Pebdeni, M. Mousavizadegan, M. Hosseini, Sensitive detection of S. Aureus using aptamer- and vancomycin -copper nanoclusters as dual recognition strategy, Food Chem. 361 (2021), 130137, https://doi.org/10.1016/J.FOODCHEM.2021.130137.
[68] Y.S. Borghei, M. Hosseini, M.R. Ganjali, H. Ju, Colorimetric and energy transfer based fluorometric turn-on method for determination of microRNA using silver nanoclusters and gold nanoparticles, Microchim. Acta 185 (2018) 1–9, https://doi.org/10.1007/S00604-018-2825-3/METRICS.

[69] Y. Negishi, K. Nobusada, T. Tsukuda, Glutathione-protected gold clusters revisited: bridging the gap between gold(I)-thiolate complexes and thiolate-protected gold nanocrystals, J. Am. Chem. Soc. 127 (2005) 5261–5270, https://doi.org/10.1021/JA042218H/SUPPL_FILE/JA042218HSI20050208_094656.PDF.

[70] H. Jia, L. Yang, X. Dong, L. Zhou, Q. Wei, H. Ju, Cysteine modification of glutathione-stabilized Au nanoclusters to red-shift and enhance the electrochemiluminescence for sensitive bioanalysis, Anal. Chem. 94 (2022) 2313–2320, https://doi.org/10.1021/ACS.ANALCHEM.1C05047/SUPPL_FILE/AC1C05047_SI_001.PDF.

[71] J. Li, T. Chen, K. Lim, L. Chen, S.A. Khan, J. Xie, X. Wang, Deep learning accelerated gold nanocluster synthesis, Adv. Intell. Syst. 1 (2019), 1900029, https://doi.org/10.1002/AISY.201900029.

[72] H.A. Kermani, M. Hosseini, M. Dadmehr, M.R. Ganjali, Rapid restriction enzyme free detection of DNA methyltransferase activity based on DNA-templated silver nanoclusters, Anal. Bioanal. Chem. 408 (2016) 4311–4318, https://doi.org/10.1007/S00216-016-9522-Z/METRICS.

[73] M. Hosseini, A. Akbari, M.R. Ganjali, M. Dadmehr, A.H. Rezayan, A novel label-free microRNA-155 detection on the basis of fluorescent silver nanoclusters, J. Fluoresc. 25 (2015) 925–929, https://doi.org/10.1007/S10895-015-1574-5/METRICS.

[74] M. Dadmehr, M. Hosseini, S. Hosseinkhani, M. Reza Ganjali, R. Sheikhnejad, Label free colorimetric and fluorimetric direct detection of methylated DNA based on silver nanoclusters for cancer early diagnosis, Biosens. Bioelectron. 73 (2015) 108–113, https://doi.org/10.1016/J.BIOS.2015.05.062.

[75] Y.P. Xie, Y.L. Shen, G.X. Duan, J. Han, L.P. Zhang, X. Lu, Silver nanoclusters: synthesis, structures and photoluminescence, Mater. Chem. Front. 4 (2020) 2205–2222, https://doi.org/10.1039/D0QM00117A.

[76] S.M. Copp, S.M. Swasey, A. Gorovits, P. Bogdanov, E.G. Gwinn, General approach for machine learning-aided design of DNA-stabilized silver clusters, Chem. Mater. 32 (2020) 430–437, https://doi.org/10.1021/ACS.CHEMMATER.9B04040/SUPPL_FILE/CM9B04040_SI_001.PDF.

[77] P. Mastracco, A. Gonzàlez-Rosell, J. Evans, P. Bogdanov, S.M. Copp, Chemistry-informed machine learning enables discovery of DNA-stabilized silver nanoclusters with near-infrared fluorescence, ACS Nano 16 (2022) 16322–16331, https://doi.org/10.1021/ACSNANO.2C05390/SUPPL_FILE/NN2C05390_SI_003.XLSX.

[78] F. Zhai, Y. Guan, Y. Li, S. Chen, R. He, Predicting the fluorescence properties of hairpin-DNA-templated silver nanoclusters via deep learning, ACS Appl. Nano Mater. 5 (2022) 9615–9624, https://doi.org/10.1021/ACSANM.2C01827/SUPPL_FILE/AN2C01827_SI_001.PDF.

[79] M. Aamir, M. Shahiduzzaman, T. Taima, J. Akhtar, J.M. Nunzi, It is an all-rounder! On the development of metal halide perovskite-based fluorescent sensors and radiation detectors, Adv. Opt. Mater. 9 (2021), 2101276, https://doi.org/10.1002/ADOM.202101276.

[80] M. Li, Z. Xia, Recent progress of zero-dimensional luminescent metal halides, Chem. Soc. Rev. 50 (2021) 2626–2662, https://doi.org/10.1039/D0CS00779J.

[81] M.S. Molokeev, B. Su, A.S. Aleksandrovsky, N.N. Golovnev, M.E. Plyaskin, Z. Xia, Machine learning analysis and discovery of zero-dimensional ns2 metal halides toward enhanced photoluminescence quantum yield, Chem. Mater. 34 (2022) 537–546, https://doi.org/10.1021/ACS.CHEMMATER.1C02725/SUPPL_FILE/CM1C02725_SI_004.ZIP.

[82] F. Wang, D. Banerjee, Y. Liu, X. Chen, X. Liu, Upconversion nanoparticles in biological labeling, imaging, and therapy, Analyst 135 (2010) 1839–1854, https://doi.org/10.1039/C0AN00144A.

[83] C. Homann, L. Krukewitt, F. Frenzel, B. Grauel, C. Würth, U. Resch-Genger, M. Haase, NaYF4:Yb,Er/NaYF4 core/shell nanocrystals with high upconversion luminescence quantum yield, Angew. Chem. Int. Ed. 57 (2018) 8765–8769, https://doi.org/10.1002/ANIE.201803083.

[84] J. Shen, G. Chen, T.Y. Ohulchanskyy, S.J. Kesseli, S. Buchholz, Z. Li, P.N. Prasad, G. Han, J. Shen, S.J. Kesseli, S. Buchholz, G. Han, G. Chen, T.Y. Ohulchanskyy, P. N. Prasad, Z. Li, Tunable near infrared to ultraviolet upconversion luminescence enhancement in (α-NaYF4:Yb,Tm)/CaF2 core/shell nanoparticles for in situ real-time recorded biocompatible photoactivation, Small 9 (2013) 3213–3217, https://doi.org/10.1002/SMLL.201300234.

[85] F. Yang, Y. Wang, X. Jiang, B. Lin, R. Lv, Optimized multimetal sensitized phosphor for enhanced red up-conversion luminescence by machine learning, ACS Comb. Sci. 22 (2020) 285–296, https://doi.org/10.1021/ACSCOMBSCI.0C00035/SUPPL_FILE/CO0C00035_SI_001.PDF.

[86] M. Rezazadeh, S. Seidi, M. Lid, S. Pedersen-Bjergaard, Y. Yamini, The modern role of smartphones in analytical chemistry, TrAC, Trends Anal. Chem. 118 (2019) 548–555, https://doi.org/10.1016/J.TRAC.2019.06.019.

[87] J.L.D. Nelis, A.S. Tsagkaris, M.J. Dillon, J. Hajslova, C.T. Elliott, Smartphone-based optical assays in the food safety field, TrAC, Trends Anal. Chem. 129 (2020), 115934, https://doi.org/10.1016/J.TRAC.2020.115934.

[88] Q. Zhao, J. Xue, X. Ren, D. Fan, X. Kuang, Y. Li, Q. Wei, H. Ju, Competitive electrochemiluminescence aptasensor based on the Ru(II) derivative utilizing intramolecular ECL emission for E2 detection, Sensor. Actuator. B Chem. 348 (2021), 130717, https://doi.org/10.1016/J.SNB.2021.130717.

[89] X. Dong, Y. Du, G. Zhao, W. Cao, D. Fan, X. Kuang, Q. Wei, H. Ju, Dual-signal electrochemiluminescence immunosensor for Neuron-specific enolase detection based on “dual-potential” emitter Ru(bpy)32+ functionalized zinc-based metal-organic frameworks, Biosens. Bioelectron. 192 (2021), 113505, https://doi.org/10.1016/J.BIOS.2021.113505.

[90] A. Firoozbakhtian, N. Sojic, G. Xu, M. Hosseini, Electrochemiluminescence sensors in bioanalysis, in: Encyclopedia of Sensors and Biosensors, Elsevier, 2023, pp. 317–340, https://doi.org/10.1016/B978-0-12-822548-6.00147-3.

[91] Y. Chen, S. Zhou, L. Li, J. jie Zhu, Nanomaterials-based sensitive electrochemiluminescence biosensing, Nano Today 12 (2017) 98–115, https://doi.org/10.1016/J.NANTOD.2016.12.013.

[92] X. Shao, X. Song, X. Liu, L. Yan, L. Liu, D. Fan, Q. Wei, H. Ju, A dual signal-amplified electrochemiluminescence immunosensor based on core-shell CeO2-Au@Pt nanosphere for procalcitonin detection, Microchim. Acta 188 (2021) 1–9, https://doi.org/10.1007/S00604-021-04988-7/TABLES/1.

[93] L. Zhao, M. Wang, X. Song, X. Liu, H. Ju, H. Ai, Q. Wei, D. Wu, Annihilation luminescent Eu-MOF as a near-infrared electrochemiluminescence probe for trace detection of trenbolone, Chem. Eng. J. 434 (2022), 134691, https://doi.org/10.1016/J.CEJ.2022.134691.

[94] W. Gao, M. Saqib, L. Qi, W. Zhang, G. Xu, Recent advances in electrochemiluminescence devices for point-of-care testing, Curr. Opin. Electrochem. 3 (2017) 4–10, https://doi.org/10.1016/J.COELEC.2017.03.003.

[95] M. Bhaiyya, P.K. Pattnaik, S. Goel, A brief review on miniaturized electrochemiluminescence devices: from fabrication to applications, Curr. Opin. Electrochem. 30 (2021), 100800, https://doi.org/10.1016/J.COELEC.2021.100800.

[96] B. Mohan, S. Kumar, V. Kumar, T. Jiao, H.K. Sharma, Q. Chen, Electrochemiluminescence metal-organic frameworks biosensing materials for detecting cancer biomarkers, TrAC, Trends Anal. Chem. 157 (2022), 116735, https://doi.org/10.1016/J.TRAC.2022.116735.

[97] A. Firoozbakhtian, M. Hosseini, M.N. Sheikholeslami, F. Salehnia, G. Xu, H. Rabbani, E. Sobhanie, Detection of COVID-19: a smartphone-based machine-learning-assisted ECL immunoassay approach with the ability of RT-PCR CT value prediction, Anal. Chem. 94 (2022) 16361–16368, https://doi.org/10.1021/ACS.ANALCHEM.2C03502/SUPPL_FILE/AC2C03502_SI_001.PDF.

[98] Y. Fu, Q. Ma, Recent developments in electrochemiluminescence nanosensors for cancer diagnosis applications, Nanoscale 12 (2020) 13879–13898, https://doi.org/10.1039/D0NR02844D.

[99] S.K. Srivastava, M. Bhaiyya, S. Dudala, C. Hota, S. Goel, A machine learning approach for electrochemiluminescence based point of care testing device to detect multiple biomarkers, Sens. Actuators A Phys. 350 (2023), 114135, https://doi.org/10.1016/J.SNA.2022.114135.

[100] V.K. Gupta, R. Jain, K. Radhapyari, N. Jadon, S. Agarwal, Voltammetric techniques for the assay of pharmaceuticals-A review, (n.d.). https://doi.org/10.1016/j.ab.2010.09.027.

[101] A. Gupta, N.K. Upadhyay, S. Parthasarathy, C. Rajagopal, P.K. Roy, Nitrofurazone-loaded PVA–PEG semi-IPN for application as hydrogel dressing for normal and burn wounds, J. Appl. Polym. Sci. 128 (2013) 4031–4039, https://doi.org/10.1002/APP.38594.

[102] T. Liu, J. He, Z. Lu, M. Sun, M. Wu, X. Wang, Y. Jiang, P. Zou, H. Rao, Y. Wang, A visual electrochemiluminescence molecularly imprinted sensor with Ag+@UiO-66-NH2 decorated CsPbBr3 perovskite based on smartphone for point-of-care detection of nitrofurazone, Chem. Eng. J. 429 (2022), 132462, https://doi.org/10.1016/J.CEJ.2021.132462.

[103] G.H. Dao, G.X. Wu, X.X. Wang, L.L. Zhuang, T.Y. Zhang, H.Y. Hu, Enhanced growth and fatty acid accumulation of microalgae Scenedesmus sp. LX1 by two types of auxin, Bioresour. Technol. 247 (2018) 561–567, https://doi.org/10.1016/J.BIORTECH.2017.09.079.

[104] C. Palma-Bautista, H.E. Cruz-Hipólito, R. Alcántara-de la Cruz, J.G. Vázquez-García, M. Yanniccari, R. De Prado, Comparison of premix glyphosate and 2,4-D formulation and direct tank mixture for control of Conyza canadensis and Epilobium ciliatum, Environ. Pollut. 281 (2021), 117013, https://doi.org/10.1016/J.ENVPOL.2021.117013.

[105] M.K. Silver, J. Shao, M. Li, C. Ji, M. Chen, Y. Xia, B. Lozoff, J.D. Meeker, Prenatal exposure to the herbicide 2,4-D is associated with deficits in auditory processing during infancy, Environ. Res. 172 (2019) 486–494, https://doi.org/10.1016/J.ENVRES.2019.02.046.

[106] Z. Lu, S. Dai, T. Liu, J. Yang, M. Sun, C. Wu, G.H. Su, X. Wang, H. Rao, H. Yin, X. Zhou, J. Ye, Y. Wang, Machine learning-assisted Te–CdS@Mn3O4 nano-enzyme induced self-enhanced molecularly imprinted ratiometric electrochemiluminescence sensor with smartphone for portable and visual monitoring of 2,4-D, Biosens. Bioelectron. 222 (2023), 114996, https://doi.org/10.1016/J.BIOS.2022.114996.

[107] Y. Wang, J. Cheng, X. Liu, F. Ding, P. Zou, X. Wang, Q. Zhao, H. Rao, C3N4 nanosheets/metal-organic framework wrapped with molecularly imprinted polymer sensor: fabrication, characterization, and electrochemical detection of furosemide, ACS Sustain. Chem. Eng. 6 (2018) 16847–16858, https://doi.org/10.1021/ACSSUSCHEMENG.8B04179/SUPPL_FILE/SC8B04179_SI_001.PDF.

[108] Y. Zhang, Y. Cui, M. Sun, T. Wang, T. Liu, X. Dai, P. Zou, Y. Zhao, X. Wang, Y. Wang, M. Zhou, G. Su, C. Wu, H. Yin, H. Rao, Z. Lu, Deep learning-assisted smartphone-based molecularly imprinted electrochemiluminescence detection sensing platform: protable device and visual monitoring furosemide, Biosens. Bioelectron. 209 (2022), 114262, https://doi.org/10.1016/J.BIOS.2022.114262.

[109] M. Hosseini, E. Sobhanie, F. Salehnia, G. Xu, H. Rabbani, M. Naghavi Sheikholeslami, A. Firoozbakhtian, N. Sadeghi, M. Hossein Farajollah, M. Reza Ganjali, H. Vosough, Development of sandwich electrochemiluminescence immunosensor for COVID-19 diagnosis by SARS-CoV-2 spike protein detection based on Au@BSA-luminol nanocomposites, Bioelectrochemistry 147 (2022), 108161, https://doi.org/10.1016/J.BIOELECHEM.2022.108161.

[110] K.C. Suresh, R. Prabha, N. Hemavathy, S. Sivarajeswari, D. Gokulakrishnan, M. Jagadeesh kumar, A machine learning approach for human breath diagnosis

with soft sensors, Comput. Electr. Eng. 100 (2022), 107945, https://doi.org/10.1016/J.COMPELECENG.2022.107945.
[111] R.A. Mathies, K. Peck, L. Stryer, Optimization of high-sensitivity fluorescence detection, Anal. Chem. 62 (1990) 1786–1791, https://doi.org/10.1021/AC00216A012/ASSET/AC00216A012.FP.PNG_V03.
[112] N. Li, W. Zhang, Y. Li, J.M. Lin, Analysis of cellular biomolecules and behaviors using microfluidic chip and fluorescence method, TrAC, Trends Anal. Chem. 117 (2019) 200–214, https://doi.org/10.1016/J.TRAC.2019.05.029.
[113] F. Bazzi, B. Ebrahimi-Hoseinzadeh, E.A. Sangachin, M. Hosseini, The integration of hybridization chain reaction (HCR) with fluorogenic silver nanoclusters (AgNCs) in an aggregation induced emission (AIE)-based nanosensor for sex determination and its forensic application, Microchem. J. 185 (2023), 108188, https://doi.org/10.1016/J.MICROC.2022.108188.
[114] A.B. Pebdeni, M. Hosseini, A. Barkhordari, Smart fluorescence aptasensor using nanofiber functionalized with carbon quantum dot for specific detection of pathogenic bacteria in the wound, Talanta 246 (2022), 123454, https://doi.org/10.1016/J.TALANTA.2022.123454.
[115] X. Fei, Y. Gu, Progress in modifications and applications of fluorescent dye probe, Prog. Nat. Sci. 19 (2009) 1–7, https://doi.org/10.1016/J.PNSC.2008.06.004.
[116] J. Yao, M. Yang, Y. Duan, Chemistry, biology, and medicine of fluorescent nanomaterials and related systems: new insights into biosensing, bioimaging, genomics, diagnostics, and therapy, Chem. Rev. 114 (2014) 6130–6178, https://doi.org/10.1021/CR200359P/ASSET/IMAGES/CR200359P.SOCIAL.JPEG_V03.
[117] M.J. Ruedas-Rama, J.D. Walters, A. Orte, E.A.H. Hall, Fluorescent nanoparticles for intracellular sensing: a review, Anal. Chim. Acta 751 (2012) 1–23, https://doi.org/10.1016/J.ACA.2012.09.025.
[118] Z. Dehghani, M. Hosseini, J. Mohammadnejad, A fluorescence nanobiosensor for detection of Campylobacter jejuni DNA in milk based on Au/Ag bimetallic nanoclusters, J. Food Meas. Char. 13 (2019) 1797–1804, https://doi.org/10.1007/S11694-019-00098-4/METRICS.
[119] S. Han, L. Yang, Z. Wen, S. Chu, M. Wang, Z. Wang, C. Jiang, A dual-response ratiometric fluorescent sensor by europium-doped CdTe quantum dots for visual and colorimetric detection of tetracycline, J. Hazard Mater. 398 (2020), 122894, https://doi.org/10.1016/J.JHAZMAT.2020.122894.
[120] U. Resch-Genger, M. Grabolle, S. Cavaliere-Jaricot, R. Nitschke, T. Nann, Quantum dots versus organic dyes as fluorescent labels, Nat. Methods 5 (2008) 763–775, https://doi.org/10.1038/nmeth.1248, 2008 5:9.
[121] F. Nemati, R. Zare-Dorabei, M. Hosseini, M.R. Ganjali, Fluorescence turn-on sensing of thiamine based on Arginine – functionalized graphene quantum dots (Arg-GQDs): central composite design for process optimization, Sens. Actuator. B Chem. 255 (2018) 2078–2085, https://doi.org/10.1016/J.SNB.2017.09.009.
[122] F. Nemati, M. Hosseini, R. Zare-Dorabei, F. Salehnia, M.R. Ganjali, Fluorescent turn on sensing of Caffeine in food sample based on sulfur-doped carbon quantum dots and optimization of process parameters through response surface methodology, Sens. Actuator. B Chem. 273 (2018) 25–34, https://doi.org/10.1016/J.SNB.2018.05.163.
[123] S.Y. Lim, W. Shen, Z. Gao, Carbon quantum dots and their applications, Chem. Soc. Rev. 44 (2014) 362–381, https://doi.org/10.1039/C4CS00269E.
[124] Z. Pinar Gumus, M. Soylak, Metal organic frameworks as nanomaterials for analysis of toxic metals in food and environmental applications, TrAC, Trends Anal. Chem. 143 (2021), 116417, https://doi.org/10.1016/J.TRAC.2021.116417.
[125] E. Mirsadoughi, A.B. Pebdeni, M. Hosseini, Sensitive colorimetric aptasensor based on peroxidase-like activity of ZrPr-MOF to detect Salmonella Typhimurium in water and milk, Food Control 146 (2023), 109500, https://doi.org/10.1016/J.FOODCONT.2022.109500.
[126] H.C.J. Zhou, S. Kitagawa, Metal–organic frameworks (MOFs), Chem. Soc. Rev. 43 (2014) 5415–5418, https://doi.org/10.1039/C4CS90059F.
[127] L.Y. Ang, M.E. Lim, L.C. Ong, Y. Zhang, Applications of Upconversion Nanoparticles in Imaging, Detection and Therapy, 6, 2011, pp. 1273–1288, https://doi.org/10.2217/NNM.11.108, 10.2217/Nnm.11.108.
[128] K. Li, E. Hong, B. Wang, Z. Wang, L. Zhang, R. Hu, B. Wang, Advances in the application of upconversion nanoparticles for detecting and treating cancers, Photodiagnosis Photodyn. Ther. 25 (2019) 177–192, https://doi.org/10.1016/J.PDPDT.2018.12.007.
[129] I. Barra, S.M. Haefele, R. Sakrabani, F. Kebede, Soil spectroscopy with the use of chemometrics, machine learning and pre-processing techniques in soil diagnosis: recent advances–A review, TrAC, Trends Anal. Chem. 135 (2021), 116166, https://doi.org/10.1016/J.TRAC.2020.116166.
[130] M.G. Madden, T. Howley, A machine learning application for classification of chemical spectra, in: Applications and Innovations in Intelligent Systems XVI - proceedings of AI 2008, the 28th SGAI International Conference on Innovative Techniques and Applications of Artificial Intelligence, 2009, pp. 77–90, https://doi.org/10.1007/978-1-84882-215-3_6/COVER.
[131] R. Sivakumar, N.Y. Lee, Recent progress in smartphone-based techniques for food safety and the detection of heavy metal ions in environmental water, Chemosphere 275 (2021), 130096, https://doi.org/10.1016/J.CHEMOSPHERE.2021.130096.
[132] A. Frydrych, K. Jurowski, Portable X-ray fluorescence (pXRF) as a powerful and trending analytical tool for in situ food samples analysis: a comprehensive review of application - State of the art, TrAC, Trends Anal. Chem. 166 (2023), 117165, https://doi.org/10.1016/J.TRAC.2023.117165.
[133] M. Mousavizadegan, M. Hosseini, M.N. Sheikholeslami, Y. Hamidipanah, M. Reza Ganjali, Smartphone image analysis-based fluorescence detection of tetracycline using machine learning, Food Chem. 403 (2023), 134364, https://doi.org/10.1016/J.FOODCHEM.2022.134364.
[134] Z. Lu, S. Chen, M. Chen, H. Ma, T. Wang, T. Liu, J. Yin, M. Sun, C. Wu, G. Su, X. Dai, X. Wang, Y. Wang, H. Yin, X. Zhou, Y. Shen, H. Rao, Trichromatic ratiometric fluorescent sensor based on machine learning and smartphone for visual and portable monitoring of tetracycline antibiotics, Chem. Eng. J. 454 (2023), 140492, https://doi.org/10.1016/J.CEJ.2022.140492.
[135] T. Liu, S. Chen, K. Ruan, S. Zhang, K. He, J. Li, M. Chen, J. Yin, M. Sun, X. Wang, Y. Wang, Z. Lu, H. Rao, A handheld multifunctional smartphone platform integrated with 3D printing portable device: on-site evaluation for glutathione and azodicarbonamide with machine learning, J. Hazard Mater. 426 (2022), 128091, https://doi.org/10.1016/J.JHAZMAT.2021.128091.
[136] C. Liu, J. Liao, Y. Zheng, Y. Chen, H. Liu, X. Shi, Random forest algorithm-enhanced dual-emission molecularly imprinted fluorescence sensing method for rapid detection of pretilachlor in fish and water samples, J. Hazard Mater. 439 (2022), 129591, https://doi.org/10.1016/J.JHAZMAT.2022.129591.
[137] R. Zenhausern, A.S. Day, B. Safavinia, S. Han, P.E. Rudy, Y.W. Won, J.Y. Yoon, Natural killer cell detection, quantification, and subpopulation identification on paper microfluidic cell chromatography using smartphone-based machine learning classification, Biosens. Bioelectron. 200 (2022), 113916, https://doi.org/10.1016/J.BIOS.2021.113916.
[138] A. Samacoits, P. Nimsamer, O. Mayuramart, N. Chantaravisoot, P. Sitthi-Amorn, C. Nakhakes, L. Luangkamchorn, P. Tongcham, U. Zahm, S. Suphanpayak, N. Padungwattanachoke, N. Leelarthaphin, H. Huayhongthong, T. Pisitkun, S. Payungporn, P. Hannanta-Anan, Machine learning-driven and smartphone-based fluorescence detection for CRISPR diagnostic of SARS-CoV-2, ACS Omega 6 (2021) 2727–2733, https://doi.org/10.1021/ACSOMEGA.0C04929/SUPPL_FILE/AO0C04929_SI_003.ZIP.
[139] S. Wang, Y. Zhou, X. Qin, S. Nair, X. Huang, Y. Liu, Label-free detection of rare circulating tumor cells by image analysis and machine learning, Sci. Rep. 10 (2020) 1–10, https://doi.org/10.1038/s41598-020-69056-1, 2020 10:1.
[140] A. Sauvat, G. Cerrato, J. Humeau, M. Leduc, O. Kepp, G. Kroemer, High-throughput label-free detection of DNA-to-RNA transcription inhibition using brightfield microscopy and deep neural networks, Comput. Biol. Med. 133 (2021), 104371, https://doi.org/10.1016/J.COMPBIOMED.2021.104371.
[141] Y. Yang, Y. Chen, J. Guo, H. Liu, H. Ju, A Pore-Forming Protein-Induced Surface-Enhanced Raman Spectroscopic Strategy for Dynamic Tracing of Cell Membrane Repair, 2021, https://doi.org/10.1016/j.isci.2021.102980.
[142] T. Howley, M.G. Madden, M.-L. O'Connell, A.G. Ryder, The Effect of Principal Component Analysis on Machine Learning Accuracy with High Dimensional Spectral Data, Applications and Innovations in Intelligent Systems XIII, 2006, pp. 209–222, https://doi.org/10.1007/1-84628-224-1_16.
[143] D. Wang, M. Zhang, Z. Zhang, J. Li, H. Gao, F. Zhang, X. Chen, Machine learning-based multifunctional optical spectrum analysis technique, IEEE Access 7 (2019) 19726–19737, https://doi.org/10.1109/ACCESS.2019.2895409.
[144] X. Quan, B. Yan, Eu(III) functionalized crystalline polyimide hydrogel film as a multifunctional platform for consecutive sensing of spermine and copper ions, ACS Appl. Mater. Interfaces 14 (2022) 49072–49081, https://doi.org/10.1021/ACSAMI.2C12822/SUPPL_FILE/AM2C12822_SI_001.PDF.
[145] F.R. Bertani, L. Businaro, L. Gambacorta, A. Mencattini, D. Brenda, D. Di Giuseppe, A. De Ninno, M. Solfrizzo, E. Martinelli, A. Gerardino, Optical detection of aflatoxins B in grained almonds using fluorescence spectroscopy and machine learning algorithms, Food Control 112 (2020), 107073, https://doi.org/10.1016/J.FOODCONT.2019.107073.
[146] N. Wu, X.Y. Zhang, J. Xia, X. Li, T. Yang, J.H. Wang, Ratiometric 3D DNA machine combined with machine learning algorithm for ultrasensitive and high-precision screening of early urinary diseases, ACS Nano 15 (2021) 19522–19534, https://doi.org/10.1021/ACSNANO.1C06429.
[147] C. Dodeigne, L. Thunus, R. Lejeune, Chemiluminescence as diagnostic tool. A review, Talanta 51 (2000) 415–439, https://doi.org/10.1016/S0039-9140(99)00294-5.
[148] L.J. Kricka, Clinical applications of chemiluminescence, Anal. Chim. Acta 500 (2003) 279–286, https://doi.org/10.1016/S0003-2670(03)00809-2.
[149] N. Barnett, P. Francis, Chemiluminescence: Liquid-phase, articles/journal_contribution/Chemiluminescence_liquid-phase/20569734/1 (accessed July 30, 2023), 2005.
[150] A. Firoozbakhtian, M. Hosseini, Chemiluminescence sensors in bioanalysis, in: Encyclopedia of Sensors and Biosensors, Elsevier, 2023, pp. 341–356, https://doi.org/10.1016/B978-0-12-822548-6.00148-5.
[151] A. Kazak, Y. Plugatar, J. Johnson, Y. Grishin, P. Chetyrbok, V. Korzin, P. Kaur, T. Kokodey, The use of machine learning for comparative analysis of amperometric and chemiluminescent methods for determining antioxidant activity and determining the phenolic profile of wines, Appl. Syst. Innov. 5 (2022) 104, https://doi.org/10.3390/asi5050104.
[152] A.J. Syed, J.C. Anderson, Applications of bioluminescence in biotechnology and beyond, Chem. Soc. Rev. 50 (2021) 5668–5705, https://doi.org/10.1039/D0CS01492C.
[153] A.C. Love, J.A. Prescher, Seeing (and using) the light: recent developments in bioluminescence technology, Cell Chem. Biol. 27 (2020) 904–920, https://doi.org/10.1016/j.chembiol.2020.07.022.
[154] M.A. Paley, J.A. Prescher, Bioluminescence: a versatile technique for imaging cellular and molecular features, Medchemcomm 5 (2014) 255–267, https://doi.org/10.1039/C3MD00288H.
[155] Y. Oba, C.V. Stevani, A.G. Oliveira, A.S. Tsarkova, T.V. Chepurnykh, I. V. Yampolsky, Selected least studied but not forgotten bioluminescent systems, Photochem. Photobiol. 93 (2017) 405–415, https://doi.org/10.1111/PHP.12704.

[156] V.R. Viviani, The origin, diversity, and structure function relationships of insect luciferases, Cell. Mol. Life Sci. 59 (2002) 1833–1850, https://doi.org/10.1007/PL00012509/METRICS.
[157] G. Cheol Gil, R.J. Mitchell, S. Tai Chang, M. Bock Gu, A biosensor for the detection of gas toxicity using a recombinant bioluminescent bacterium, Biosens. Bioelectron. 15 (2000) 23–30, https://doi.org/10.1016/S0956-5663(99)00074-3.
[158] S.H. Choi, M.B. Gu, A portable toxicity biosensor using freeze-dried recombinant bioluminescent bacteria, Biosens. Bioelectron. 17 (2002) 433–440, https://doi.org/10.1016/S0956-5663(01)00303-7.
[159] A. Roda, M. Guardigli, E. Michelini, M. Mirasoli, Bioluminescence in analytical chemistry and in vivo imaging, TrAC, Trends Anal. Chem. 28 (2009) 307–322, https://doi.org/10.1016/J.TRAC.2008.11.015.
[160] W.C. Huang, C.D. Wei, S. Belkin, T.H. Hsieh, J.Y. Cheng, Machine-learning assisted antibiotic detection and categorization using a bacterial sensor array, Sens. Actuator. B Chem. 355 (2022), 131257, https://doi.org/10.1016/J.SNB.2021.131257.
[161] I.A. Denisov, Luciferase-based bioassay for rapid pollutants detection and classification by means of multilayer artificial neural networks, Sens. Actuator. B Chem. 242 (2017) 653–657, https://doi.org/10.1016/J.SNB.2016.11.071.
[162] Y. Geng, W.J. Peveler, V.M. Rotello, Array-based "chemical nose" sensing in diagnostics and drug discovery, Angew. Chem. Int. Ed. 58 (2019) 5190–5200, https://doi.org/10.1002/ANIE.201809607.
[163] Y. Vlasov, A. Legin, Non-selective chemical sensors in analytical chemistry: from "electronic nose" to "electronic tongue", Fresenius' J. Anal. Chem. 361 (1998) 255–260, https://doi.org/10.1007/S002160050875/METRICS.
[164] X. Zhu, T. Li, X. Hai, S. Bi, A nanozyme-based colorimetric sensor array as electronic tongue for thiols discrimination and disease identification, Biosens. Bioelectron. 213 (2022), 114438, https://doi.org/10.1016/J.BIOS.2022.114438.
[165] T. Li, X. Zhu, X. Hai, S. Bi, X. Zhang, Recent progress in sensor arrays: from construction principles of sensing elements to applications, ACS Sens. 8 (2023) 994–1016, 10.1021/ACSSENSORS.2C02596/ASSET/IMAGES/MEDIUM/SE2C02596_0009.GIF.
[166] W. Cuypers, P.A. Lieberzeit, Combining two selection principles: sensor arrays based on both biomimetic recognition and chemometrics, Front. Chem. 6 (2018), 379036, https://doi.org/10.3389/FCHEM.2018.00268/BIBTEX.
[167] T. Minami, N.A. Esipenko, B. Zhang, L. Isaacs, P. Anzenbacher, "Turn-on" fluorescent sensor array for basic amino acids in water, Chem. Commun. 50 (2013) 61–63, https://doi.org/10.1039/C3CC47416J.
[168] L. Moreno, A. Merlos, N. Abramova, C. Jiménez, A. Bratov, Multi-sensor array used as an "electronic tongue" for mineral water analysis, Sens. Actuator. B Chem. 116 (2006) 130–134, https://doi.org/10.1016/J.SNB.2005.12.063.
[169] A. Biancolillo, F. Marini, Chemometric methods for spectroscopy-based pharmaceutical analysis, Front. Chem. 6 (2018), 412780, https://doi.org/10.3389/FCHEM.2018.00576/BIBTEX.
[170] Z. Li, Y. Jiang, S. Tang, H. Zou, W. Wang, G. Qi, H. Zhang, K. Jin, Y. Wang, H. Chen, L. Zhang, X. Qu, 2D nanomaterial sensing array using machine learning for differential profiling of pathogenic microbial taxonomic identification, Microchim. Acta 189 (2022) 1–14, https://doi.org/10.1007/S00604-022-05368-5/FIGURES/4.
[171] H.P. Wang, P. Chen, J.W. Dai, D. Liu, J.Y. Li, Y.P. Xu, X.L. Chu, Recent advances of chemometric calibration methods in modern spectroscopy: algorithms, strategy, and related issues, TrAC, Trends Anal. Chem. 153 (2022), 116648, https://doi.org/10.1016/J.TRAC.2022.116648.
[172] V. Schroeder, E.D. Evans, Y.C.M. Wu, C.C.A. Voll, B.R. McDonald, S. Savagatrup, T.M. Swager, Chemiresistive sensor array and machine learning classification of food, ACS Sens. 4 (2019) 2101–2108, https://doi.org/10.1021/ACSSENSORS.9B00825/SUPPL_FILE/SE9B00825_SI_001.PDF.
[173] F. Cui, Y. Yue, Y. Zhang, Z. Zhang, H.S. Zhou, Advancing biosensors with machine learning, ACS Sens. 5 (2020) 3346–3364, https://doi.org/10.1021/ACSSENSORS.0C01424/ASSET/IMAGES/MEDIUM/SE0C01424_0010.GIF.
[174] M.X. Liu, H. Zhang, X.W. Zhang, S. Chen, Y.L. Yu, J.H. Wang, Nanozyme sensor array plus solvent-mediated signal amplification strategy for ultrasensitive ratiometric fluorescence detection of exosomal proteins and cancer identification, Anal. Chem. (2020), https://doi.org/10.1021/ACS.ANALCHEM.1C02010/SUPPL_FILE/AC1C02010_SI_001.PDF, 93–93.
[175] Z. Xu, Z. Wang, M. Liu, B. Yan, X. Ren, Z. Gao, Machine learning assisted dual-channel carbon quantum dots-based fluorescence sensor array for detection of tetracyclines, Spectrochim. Acta Mol. Biomol. Spectrosc. 232 (2020), 118147, https://doi.org/10.1016/J.SAA.2020.118147.
[176] X. Tan, Y. Liang, Y. Ye, Z. Liu, J. Meng, F. Li, Explainable deep learning-assisted fluorescence discrimination for aminoglycoside antibiotic identification, Anal. Chem. 94 (2022) 829–836, https://doi.org/10.1021/ACS.ANALCHEM.1C03508/SUPPL_FILE/AC1C03508_SI_001.PDF.
[177] S. Mandal, D. Paul, S. Saha, P. Das, Multi-layer perceptron for detection of different class antibiotics from visual fluorescence response of a carbon nanoparticle-based multichannel array sensor, Sensor. Actuator. B Chem. 360 (2022), 131660, https://doi.org/10.1016/J.SNB.2022.131660.
[178] P. Behera, M. De, Nano-graphene oxide based multichannel sensor arrays towards sensing of protein mixtures, Chem. Asian J. 14 (2019) 553–560, https://doi.org/10.1002/ASIA.201801756.
[179] S. Pandit, T. Banerjee, I. Srivastava, S. Nie, D. Pan, Machine learning-assisted array-based biomolecular sensing using surface-functionalized carbon dots, ACS Sens. 4 (2019) 2730–2737, https://doi.org/10.1021/ACSSENSORS.9B01227/SUPPL_FILE/SE9B01227_SI_001.PDF.
[180] P. Behera, K.K. Singh, S. Pandit, D. Saha, D.K. Saini, M. De, Machine learning-assisted array-based detection of proteins in serum using functionalized MoS2Nanosheets and green fluorescent protein conjugates, ACS Appl. Nano Mater. 4 (2021) 3843–3851, https://doi.org/10.1021/ACSANM.1C00244/SUPPL_FILE/AN1C00244_SI_002.TXT.
[181] R. Xie, X. Song, H. Chen, P. Lin, S. Guo, Z. Zhuang, Y. Chen, W. Zhao, P. Zhao, H. Long, J. Tao, Intelligent clinical lab for the diagnosis of post-neurosurgical meningitis based on machine-learning-aided cerebrospinal fluid analysis, Anal. Chem. 94 (2022) 15720–15728, https://doi.org/10.1021/ACS.ANALCHEM.2C03154/SUPPL_FILE/AC2C03154_SI_001.PDF.
[182] N. Nandu, C.W. Smith, T.B. Uyar, Y.S. Chen, M.J. Kachwala, M. He, M.V. Yigit, Machine-learning single-stranded DNA nanoparticles for bacterial analysis, ACS Appl. Nano Mater. 3 (2020) 11709–11714, https://doi.org/10.1021/ACSANM.0C03001/SUPPL_FILE/AN0C03001_SI_001.PDF.
[183] M.S. Wu, Z. Liu, H.W. Shi, H.Y. Chen, J.J. Xu, Visual electrochemiluminescence detection of cancer biomarkers on a closed bipolar electrode array chip, Anal. Chem. 87 (2015) 530–537, https://doi.org/10.1021/AC502989F/SUPPL_FILE/AC502989F_SI_001.PDF.
[184] A.M. Spehar-Délèze, R. Gransee, S. Martinez-Montequin, D. Bejarano-Nosas, S. Dulay, S. Julich, H. Tomaso, C.K. O'Sullivan, Electrochemiluminescence dna sensor array for multiplex detection of biowarfare agents, Anal. Bioanal. Chem. 407 (2015) 6657–6667, https://doi.org/10.1007/S00216-015-8831-Y/FIGURES/6.
[185] W. Lv, H. Ye, Z. Yuan, X. Liu, X. Chen, W. Yang, Recent advances in electrochemiluminescence-based simultaneous detection of multiple targets, TrAC, Trends Anal. Chem. 123 (2020), 115767, https://doi.org/10.1016/J.TRAC.2019.115767.
[186] Y.Z. Wang, C.H. Xu, W. Zhao, Q.Y. Guan, H.Y. Chen, J.J. Xu, Bipolar electrode based multicolor electrochemiluminescence biosensor, Anal. Chem. 89 (2017) 8050–8056, https://doi.org/10.1021/ACS.ANALCHEM.7B01494/SUPPL_FILE/AC7B01494_SI_001.PDF.
[187] P. Mishra, D. Passos, F. Marini, J. Xu, J.M. Amigo, A.A. Gowen, J.J. Jansen, A. Biancolillo, J.M. Roger, D.N. Rutledge, A. Nordon, Deep learning for near-infrared spectral data modelling: hypes and benefits, TrAC, Trends Anal. Chem. 157 (2022), 116804, https://doi.org/10.1016/J.TRAC.2022.116804.
[188] F. Lussier, V. Thibault, B. Charron, G.Q. Wallace, J.F. Masson, Deep learning and artificial intelligence methods for Raman and surface-enhanced Raman scattering, TrAC, Trends Anal. Chem. 124 (2020), 115796, https://doi.org/10.1016/J.TRAC.2019.115796.
[189] A.M.V. Mohan, V. Rajendran, R.K. Mishra, M. Jayaraman, Recent advances and perspectives in sweat based wearable electrochemical sensors, TrAC, Trends Anal. Chem. 131 (2020), 116024, https://doi.org/10.1016/J.TRAC.2020.116024.
[190] Y. Shang, X. Xiang, Q. Ye, Q. Wu, J. Zhang, J.M. Lin, Advances in nanomaterial-based microfluidic platforms for on-site detection of foodborne bacteria, TrAC, Trends Anal. Chem. 147 (2022), 116509, https://doi.org/10.1016/J.TRAC.2021.116509.

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