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Emerging role of Artificial Intelligence in High-Performance Liquid Chromatographic Analysis: A Mini Review

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Abstract: *High-performance liquid chromatography (HPLC) is one of the most widely employed analytical techniques for the qualitative and quantitative determination of compounds. Despite its exceptional sensitivity and reliability, conventional HPLC method development and data interpretation often require extensive experimental optimization, expert knowledge, and considerable time. Furthermore, peak detection, integration, and identification in chromatograms can be automated by artificial intelligence (AI) methods like machine learning and deep learning, allowing for quicker and more precise analysis of complicated datasets, resulting in the identification of compounds and the comprehension of complex reactions more quickly and creatively. From an economic perspective, these developments promote sustainable analytical chemistry and effective resource recovery. Moreover, AI can increase productivity and reduce the possibility of human error by automating chromatographic analysis. Additionally, AI has played a key role in enhanced analysis of complicated spectra in fields like spectroscopy and chromatography, as well as in handling heterogeneous data. This mini review discusses recent advancements in artificial intelligence and machine learning (ML) that enable scientists to address complex analytical challenges more effectively. It highlights the growing application of these technologies in chromatographic predictions, particularly in liquid chromatography method development. The present review further examines key AI-driven areas, including automated method development, retention time prediction, peak deconvolution, predictive maintenance, and intelligent data processing.*

Keywords: HPLC, Artificial Intelligence, Machine Learning, Retention Prediction

I. INTRODUCTION

High-Performance Liquid Chromatography (HPLC) is a versatile and powerful analytical technique widely employed to separate, detect, and quantify components of complex mixtures with high precision and accuracy [1]. HPLC has undergone significant advancements and seen great breakthroughs, including improvements in column design, detection technologies, and automation [2]. HPLC procedures include reversed-phase, normal-phase, size-exclusion, ion exchange, and affinity chromatography. The most often used method is reversed-phase HPLC, which is ideal for separating non-polar and slightly polar compounds. Normal-phase HPLC targets polar or moderately polar substances. Ion-exchange HPLC separates molecules according to their charge, whereas size-exclusion HPLC classifies them by molecular size, and affinity chromatography isolates components through particular binding interactions [3]. Reversed-

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phase chromatography typically uses C18 or C8 bonded silica columns, whereas normal-phase chromatography uses silica, alumina, or polar-bonded stationary phases. Ion-exchange chromatography uses stationary phases with charged groups, while size-exclusion chromatography uses porous polymeric or silica-based materials. Supercritical fluid chromatography (SFC) uses columns similar to HPLC, but tailored for supercritical CO_2 mobile phases [1]. Optimizing chromatographic conditions for optimal resolution includes adjusting pH and flow rate. Mobile phase composition, concentration, and temperature are crucial [4]. The use of retention prediction models in chromatography allows for faster and more accurate separation and identification during analysis [5].

Data collection and processing are increasingly software-driven. Modern chromatographic software uses advanced algorithms to achieve peak integration, baseline correction, noise filtering, and quantification. Standardizing integration parameters, such as slope sensitivity, peak threshold, and peak width, to reduce variability. Advanced spectral analysis software can deconvolute overlapping peaks, analyse peak purity, and identify compounds by linking chromatographic retention time to spectral libraries. Audit trails, secure data storage, and electronic signatures are all regulatory requirements that must be met in environments that follow GLP or GMP [6]. The ability of AI to handle diverse and complex data has been a watershed moment in its application in analytical chemistry. Historically, analysing such data required substantial knowledge and efforts. However, artificial intelligence (AI) systems can extract essential information fast and efficiently [7]. With improvements in AI and machine learning (ML), chromatographic platforms are becoming more intelligent and predictive, allowing for method optimization, spectrum data interpretation, and regulatory documentation assistance [8].

The use of AI in analytical chemistry, particularly in research requiring ML, has prompted serious issues about data security and privacy. The ultimate purpose of analytical chemistry is to verify that AI and machine learning models are robust, reliable, repeatable, and reproducible, as well as that they meet ethical and security criteria. This involves tackling the hazards connected with AI in data handling and maintaining high digital standards in research operations. There is also an increasing emphasis on green analytical chemistry, with a focus on miniaturized and solvent-free extraction processes, automation, and intelligent data processing and reporting systems. The literature study shows that research on artificial intelligence's involvement in HPLC is currently insufficient. By examining recent development in AI-driven methodologies, this article attempts to give a thorough understanding of how intelligent algorithms might improve the performance, efficiency and dependability of HPLC.

II. ARTIFICIAL INTELLIGENCE IN CHROMATOGRAPHY

The incorporation of AI with chromatographic procedures constitutes a substantial improvement in chemical and biochemical analysis. One of the key applications of AI in chromatography is data interpretation and analysis. ML methods, for example, are used to handle and interpret massive chromatographic datasets. They can detect patterns and correlations in complex data, making it easier to identify and quantify substances in samples [8].

III. AI-DRIVEN METHOD DEVELOPMENT

Traditional chromatographic method development often requires numerous iterative experiments involving adjustments to mobile phase composition, pH, column temperature, gradient profile, flow rate, and stationary phase selection. This trial-and-error approach is time-consuming, labour-intensive, and resource-intensive. AI techniques have emerged as powerful tools for accelerating and optimizing chromatographic method development. ML algorithms such as Artificial Neural Networks (ANNs), Random Forests (RFs), and Gaussian Process Models (GPMs) can analyse large historical datasets and predict optimal chromatographic conditions with minimal experimental effort [9-10].

These AI models are capable of identifying complex nonlinear relationships between chromatographic variables and analytical outcomes, including retention time, peak resolution, selectivity, and analysis time. By learning from previous experiments, AI algorithms can recommend experimental conditions that maximize method performance while reducing the number of required laboratory trials. This predictive capability significantly shortens method development timelines and lowers operational costs. Furthermore, AI-driven optimization strategies can be integrated with

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automated chromatographic systems to create closed-loop workflows. In such systems, experimental data are continuously collected, analysed, and fed back into the optimization algorithm, enabling real-time adjustment of chromatographic conditions. This approach facilitates the development of autonomous chromatography platforms capable of self-optimizing analytical methods with minimal human intervention. As a result, AI-driven method development improves efficiency, enhances method robustness, and supports the advancement of intelligent analytical laboratories [11-12].

IV. AI IN HPLC

Yash Raj Singh, et al. explored different AI and ML models, provided deep insights into fuzzy system with an ANN that maintained better accuracy and significant possibilities for chromatographic characteristics prediction in liquid chromatography over classical linear models. They also focus on the retention prediction of a target molecule applying QSRR (Quantitative structure retention relationship) methodology paired with an ANN, highlighting a more robust technique than the QSRR alone [13].

J. Abdul Basith, et al. examined the integration of AI techniques into HPLC impurity profiling, which covers theoretical underpinnings, data preparation, peak recognition, automated quantification, and future implications for regulatory compliance and pharmaceutical quality control. Conventional HPLC data interpretation relies mainly on manual analysis, making it time-consuming, operator-dependent, and prone to human mistake. Artificial Intelligence (AI) and Machine Learning (ML) have emerged as transformative techniques for automating chromatographic data analysis, enabling rapid and accurate impurity detection, identification, and quantification. Large chromatographic datasets may be processed effectively by AI algorithms, which can also recognize minute peak patterns, fix baseline drifts, and forecast retention behaviours in a variety of chromatographic scenarios [14].

Hayam Mahmoud Lotfy, et al. found even if AI is transforming analytical chemistry, but still its practical effectiveness in complex pharmaceutical separations has not yet been evaluated. In order to identify useful advantages and drawbacks, they compare an AI-powered HPLC method for amlodipine (AMD), hydrochlorothiazide (HYD), and candesartan (CND) with an empirically optimized method. For the In-Lab method, the linearity ranges were AMD (25.0–250.0 µg/mL), HYD (31.2–287.0 µg/mL), and CND (40.0–340.0 µg/mL); for the AI-HPLC method, linearity ranges were AMD (30.0–250.0 µg/mL), HYD (35.0–285.0 µg/mL), and CND (50.0–340.0 µg/mL). Both methods were verified for specificity, accuracy, and reliability in accordance with ICH criteria. The F-test and Student's t-test were used to statistically compare the acquired and reported results. In-Lab approach fared better in terms of sustainability than the AI-based approach since it used less solvent, generated less waste, and required less time for analysis [15].

A.G. Usman, et al. estimated the qualitative behaviour of thymoquinone (TQ) in HPLC method development in terms of retention properties, two distinct single non-linear models feedforward neural network (FFNN) and support vector machine (SVM) as well as a conventional linear regression model multi-linear regression (MLR) were used. The models' accuracy was assessed using four performance indices: correlation coefficient (R), mean square error (MSE), root mean square error (RMSE), and determination coefficient (R2). In order to take advantage of both the linear and non-linear characteristics of the models, hybrid models such as FFNN-MLR and SVM-MLR that integrate AI-based models and traditional MLR were proposed for the prediction of the bioactive compound in HPLC technique development. FFNN performed better than the other two models, according to the results derived from the predictive comparison of the individual models [16].

A.G. Usman, et al. predicted the retention time (tR) and peak area (PA) for iso-quercitrin using HPLC using three distinct nonlinear models, including artificial neural network (ANN), adaptive neuro-fuzzy inference system (ANFIS), and support vector machine (SVM), in addition to a classical linear model MLR. Relative mean square error (RMSE), mean square error (MSE), determination coefficient (DC), and correlation coefficient (CC) were used to assess the models' performance effectiveness. Results showed that the qualitative and quantitative features of the bioactive chemical predicted by all four models. Analysis of the data revealed that ANFIS is the best model for PA prediction,

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outperforming the other models. However, ANN demonstrated its value and became the most effective model for tR simulation [17].

M. Soner Bay, et al. created and verified two new HPLC techniques for the measurement of dolutegravir (DTG), lamivudine (3TC), and abacavir (ABA) in pharmaceutical formulations. AI engines like Copilot, ChatGPT 5.2, Gemini, and Perplexity were incorporated into the development of HPLC methods. The first technique, an isocratic HPLC, used an XBridge® C18 column and a mobile phase of acetonitrile: phosphate buffer (pH 3.5, 50:50 v/v) to quantify DTG and 3TC simultaneously, detection was carried out at 258 and 275 nm, respectively. Using methanol and TEA/TFA buffer (pH 3.15) as the mobile phase, the second technique, a gradient HPLC, allowed for the simultaneous measurement of DTG, 3TC, and ABA on a Spherisorb® ODS2 C18 column using 258, 278, 294 nm respectively. Excellent linearity was demonstrated by the extensive calibration ranges. The ICH Q2(R2) guidelines were followed in the validation of both methods [18].

Sara I. Aboras, et al. created and validated a strong and dependable HPLC–DAD (High- performance liquid chromatography with diode- array detection) method for the simultaneous measurement of ranolazine, diltiazem, and amlodipine a medication combination pertinent to the concurrent therapy of chronic angina and hypertension. Using the Multi-Color Assessment tool, the analytical performance and environmental impact were assessed and compared with other methods; the results showed an overall Whiteness Score of 64.8%, surpassing the other published methods. Using the Need, Quality, and Sustainability tool, the AI-optimized method's alignment with sustainability principles was evaluated and compared with traditional optimization. The findings show that the suggested method offers a dependable and ecologically friendly analytical technique for the simultaneous measurement of the investigated drug combination in pharmaceutical formulations with proven applicability in biological matrices [19]

S. I. Abba, et al. used three distinct data-driven algorithms to simulate the response surface for methyclothiazide (M) and amiloride (A), which are considered as (K'or k) modeling in HPLC, in which two nonlinear models (Artificial neural network (ANN) and Adaptive neuro-fuzzy inference system (ANFIS)) and a classical linear model (Multilinear regression analysis (MLR)). Five distinct performance efficiency criteria determination coefficients (R2), root mean square error (RMSE), correlation coefficient (R), mean square error (MSE), and mean absolute percentage error (MAPE) were used to assess the experimental and simulated outcomes. The overall results proved the reliability of artificial intelligence models ANN and ANFIS for simulation of response surface optimization method [20].

V. FUTURE PERSPECTIVE

Automation in chromatography is quickly developing, allowing for high-throughput and reproducible investigations. Robotic sample handling, automated injection systems, and integrated data analysis platforms enable faster sample processing while minimizing human error. Automated chromatography systems are increasingly commonplace in businesses that require large-scale testing and quality control, such as pharmaceuticals. Fully automated chromatography systems will continue to evolve, allowing forever more efficient operations in research and industrial applications. The use of AI and machine learning algorithms to predict and optimize chromatographic conditions will most likely transform the automation of these systems. Furthermore, fully integrated chromatographic systems that combine sample preparation, separation, and detection in a single platform would permit seamless, high-throughput operations.

VI. CONCLUSION

AI is rapidly transforming HPLC by enhancing method development, data processing, retention time prediction, peak detection, and overall analytical performance. Machine learning and deep learning algorithms have demonstrated remarkable capabilities in handling complex chromatographic datasets, identifying hidden patterns, and generating accurate predictive models. These technologies reduce experimental workload, improve method robustness, accelerate analytical workflows, and minimize human error. The integration of AI with automated chromatographic systems has further enabled the development of intelligent and self-optimizing analytical platforms capable of real-time decision-

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making and adaptive method optimization. In addition, AI-driven approaches have shown significant potential for improving peak resolution, compound identification, and quantitative analysis in increasingly complex analytical applications. Despite these advances, challenges related to data quality, model interpretability, standardization, regulatory acceptance, and cybersecurity must be addressed to ensure the reliable implementation of AI in routine analytical laboratories. Continued collaboration among analytical chemists, data scientists, software developers, and instrument manufacturers will be essential for overcoming these limitations. Overall, the convergence of AI and chromatographic science is driving a paradigm shift from conventional empirical approaches toward intelligent, predictive, and automated analytical systems. As computational techniques and analytical technologies continue to evolve, AI is expected to play an increasingly important role in shaping the future of HPLC and modern analytical chemistry.

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