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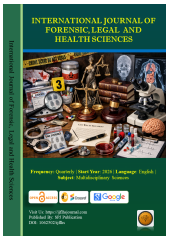

Review Article

Artificial Intelligence in Forensic Toxicology: A Systematic Review

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ABSTRACT

Artificial Intelligence (AI) is increasingly transforming the analytical and investigative landscape of forensic toxicology. Traditional toxicological workflows rely on gas/liquid chromatography-mass spectrometry (GC-MS/LC-MS), manual interpretation, and expert judgment face mounting challenges from data complexity, novel psychoactive substances (NPS), and throughput demands. This systematic review synthesizes evidence from 17 primary studies (2019–2026) to map how AI and machine learning (ML) are integrated across the forensic toxicology pipeline, spanning novel psychoactive substance identification, predictive toxicology and risk assessment, postmortem interval (PMI) estimation, and laboratory workflow automation. A structured literature search was conducted across PubMed, Scopus, Web of Science, and Google Scholar using predefined MeSH and keyword terms. Studies were screened using PRISMA guidelines. Seventeen studies were included based on defined eligibility criteria covering original research, systematic reviews, and comprehensive narrative reviews on AI applications in forensic and analytical toxicology. Across domains, AI and ML methods including deep generative models, convolutional and artificial neural networks, random forests, and explainable AI frameworks has consistently improved analytical sensitivity, processing speed, and detection of previously unidentifiable substances, while highlighting persistent challenges around dataset standardization, model generalizability, and forensic/legal admissibility.

Keywords: Artificial Intelligence, Gas/Liquid Chromatography-Mass Spectrometry, Analytical Toxicology, Psychoactive Substance

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INTRODUCTION

Artificial intelligence (AI) has become one of the most influential technologies in modern science and is increasingly being applied in forensic science and forensic toxicology. AI refers to computer systems that can perform tasks such as pattern recognition, classification, prediction, and decision-making, which traditionally require human intelligence. Machine learning (ML) and deep learning (DL), two important branches of AI, are particularly useful for analysing large and complex datasets generated during forensic investigations. Their ability to identify hidden patterns and make accurate predictions has opened new possibilities for improving forensic analysis and laboratory workflows. [1,2] Forensic science applies scientific principles to support criminal and civil investigations through disciplines such as forensic pathology, toxicology, anthropology, and digital forensics. The integration of AI into these fields has improved the speed, accuracy, and consistency of forensic investigations. AI-based systems can assist in biometric identification, crime scene reconstruction, digital evidence analysis, and automated interpretation of forensic data, thereby reducing manual effort and enhancing decision-making. [2] Forensic toxicology focuses on the detection, identification, and interpretation of drugs, poisons, alcohol, and their metabolites in biological specimens to provide scientific evidence in medico-legal investigations. Advanced analytical techniques, including liquid chromatography–tandem mass spectrometry (LC–MS/MS) and high-resolution mass spectrometry (HRMS), generate large volumes of complex data that require detailed interpretation. Conventional analytical workflows are often labour-intensive, time-consuming, and susceptible to human

error, creating a growing need for intelligent computational approaches. [2,3] The rapid emergence of new psychoactive substances (NPS) has further complicated forensic toxicological analysis. More than 1,100 NPS have been reported worldwide over the past decade, many of which are identified before certified reference standards or spectral libraries become available. This situation limits the effectiveness of conventional reference-based analytical methods and highlights the need for alternative strategies capable of recognising unknown compounds. AI-based models can analyse complex toxicological datasets, detect subtle analytical patterns, predict toxicological outcomes, and support the identification of previously unreported substances with greater efficiency than traditional approaches. [3–5] Machine learning algorithms have demonstrated considerable potential in interpreting high-dimensional data generated by chromatographic and mass spectrometric techniques. These models improve the sensitivity and specificity of compound identification while reducing analysis time. In addition to substance detection, AI has also been successfully applied to predictive toxicology, toxicity assessment, and postmortem interval (PMI) estimation using metabolomic, microbiomic, and spectroscopic datasets. Such applications illustrate the growing role of AI in supporting forensic decision-making and improving the accuracy of toxicological investigations. [4–7]

MATERIALS AND METHODS

Review Design and Protocol: This review was conducted following the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) 2020 guidelines to ensure a transparent and systematic approach to the identification, selection, and reporting of relevant literature. A predefined review protocol outlining the objectives, eligibility criteria, search strategy, data extraction process, and quality assessment methods was established before the literature search and data extraction.
Eligibility Criteria: Studies were selected according to the PICOS (Population, Intervention, Comparator, Outcome, and Study Design) framework (Table-1)

Table 1. PICOS Framework

PICOS Component	Eligibility Criteria
Population (P)	Studies involving forensic toxicology, analytical toxicology laboratories, medicolegal investigations, postmortem toxicology, or computational toxicology applications.
Intervention (I)	Application of artificial intelligence techniques, including machine learning, deep learning, neural networks, natural language processing, generative AI, or other AI-based computational models.
Comparator (C)	Conventional analytical methods, including GC–MS, LC–MS/MS, immunoassays, manual expert interpretation, or studies without a comparator where appropriate.
Outcomes (O)	Analytical performance, identification accuracy, processing efficiency, detection of novel psychoactive substances, predictive capability, implementation feasibility, or ethical and legal considerations.
Study Design (S)	Original research articles, systematic reviews, scoping reviews, and comprehensive narrative reviews published in English. Conference abstracts, editorials, letters, case reports, book chapters, and non-English publications were excluded.

Literature Search Strategy: A comprehensive literature search was performed using PubMed/MEDLINE, Scopus, Web of Science Core Collection, and Google Scholar. Publications published between January 2019 and March 2026 were considered eligible. The search strategy combined Medical Subject Headings (MeSH) and free-text keywords using Boolean operators. The principal search string was as follows: ("Artificial Intelligence" OR "Machine Learning" OR "Deep Learning" OR "Neural Network") AND ("Forensic Toxicology" OR "Analytical Toxicology" OR "Forensic Chemistry" OR "Postmortem Toxicology") AND ("Drug Detection" OR "Substance Identification" OR "Novel Psychoactive Substances" OR "Predictive Toxicology" OR "Toxicokinetics") Reference lists of eligible publications were also manually screened to identify additional relevant studies that were not retrieved during the electronic database search.
Study Selection: All retrieved records were imported into a systematic review management platform for screening. Duplicate records were removed before the screening process. Two sequential screening stages were performed: (i) title and abstract screening and (ii) full-text assessment based on the predefined eligibility criteria. Studies meeting all inclusion criteria were included in the final review. The study selection process is illustrated in the PRISMA 2020 flow diagram (Figure 1).
Data Extraction: Data were extracted independently using a standardized data extraction form. The extracted information included the first author, publication year, country of origin, study design, AI methodology employed, forensic toxicology application, biological specimen or analytical platform, principal findings, reported performance metrics, study limitations, and ethical or regulatory considerations. Any discrepancies during data extraction were resolved through discussion and consensus.
Quality Assessment: The methodological quality of the included studies was assessed according to their study design. Narrative review articles were evaluated using the Scale for the Assessment of Narrative Review Articles (SANRA), whereas original empirical studies were assessed using the Mixed Methods Appraisal Tool (MMAT). Each study was evaluated for clarity of

objectives, methodological rigor, quality of data, transparency of reporting, and discussion of study limitations. Based on the overall assessment, studies were categorized as high quality (✓✓), moderate quality (△), or low quality (✗).

RESULTS

The systematic literature search identified 9,290 records from four electronic databases (PubMed/MEDLINE, Scopus, Web of Science, and Google Scholar). After removing duplicate records, 5,700 unique articles remained for title and abstract screening. A total of 5,650 studies were excluded because they did not meet the predefined eligibility criteria. The full texts of the remaining 50 articles were assessed for eligibility, of which 33 studies were excluded due to reasons including lack of relevance to forensic toxicology, insufficient methodological information, duplicate publication, or failure to satisfy the inclusion criteria. Ultimately, 17 studies were included in the qualitative synthesis. The complete study selection process is presented in the PRISMA 2020 flow diagram (Figure 1).

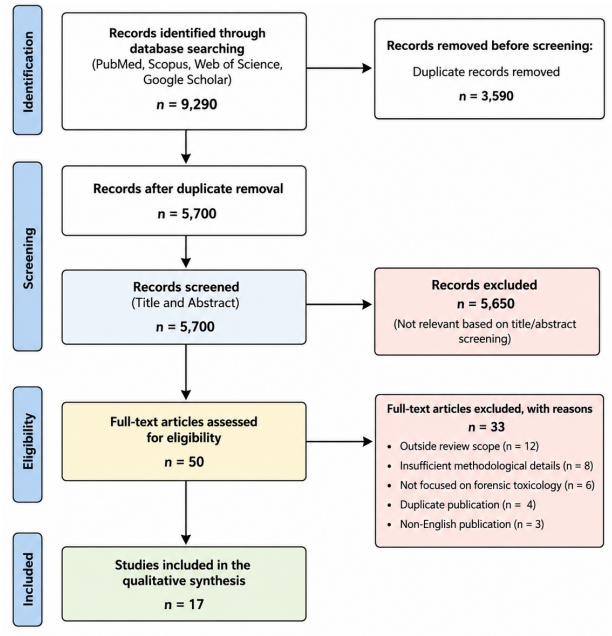

Figure 1. PRISMA 2020 flow diagram illustrating the study identification, screening, eligibility assessment, and inclusion process for the systematic review.

Artificial Intelligence for Novel Psychoactive Substance Identification: Among the included studies, the identification of novel psychoactive substances (NPS) represented the most extensively investigated application of artificial intelligence. Multiple studies demonstrated that deep learning and machine learning algorithms substantially improve the identification of emerging psychoactive compounds that lack certified reference standards or spectral library information. Skinnider et al. developed the DarkNPS framework, a recurrent neural network capable of predicting the molecular structures of unknown psychoactive substances directly from mass spectrometric data. The model achieved approximately 51% top-1 prediction accuracy and 86% top-10 accuracy, highlighting its ability to predict emerging designer drugs before their inclusion in conventional databases. Similarly, Lin et al. introduced the PS2MS deep-learning platform, which generated plausible structural analogues of NPS and accurately predicted their corresponding mass spectra, enabling successful identification of synthetic cathinone derivatives in forensic samples. Wong et al. evaluated several supervised machine learning models, including artificial neural networks (ANN), convolutional neural networks (CNN), and balanced random forest (BRF), for automated classification of GC–MS spectra. Among these algorithms, the balanced random forest model demonstrated the highest classification performance with a macro-F1 score of approximately 0.90. In addition, Jurowski and Krośniak employed quantitative structure–activity relationship (QSAR) modelling to predict the toxicological characteristics of the emerging synthetic opioid AP-238, demonstrating that AI can estimate toxicological properties even in the absence of experimental laboratory data.

Artificial Intelligence in Predictive Toxicology: Predictive toxicology emerged as another major area of AI application. Several studies reported the successful use of machine learning and deep learning algorithms for toxicity prediction, toxicokinetic modelling, and chemical risk assessment. Lin and Chou demonstrated that AI-assisted physiologically based pharmacokinetic (PBPK) models improved dose-response modelling and toxicokinetic simulations compared with conventional computational approaches. However, the authors noted that the generalizability of these models across different populations and chemical classes remains a challenge. Similarly, Almalki et al. reported that AI significantly accelerated high-throughput toxicity screening while reducing dependence on conventional animal testing. Despite these advantages, the review identified several challenges, including algorithmic bias, limited model transparency, data privacy concerns, and the absence of standardized regulatory guidelines for AI implementation. Teunis et al. further emphasized that open-access databases, standardized validation protocols, and collaborative data-sharing initiatives are essential for ensuring the reproducibility and regulatory acceptance of AI-based toxicological risk assessment.

Artificial Intelligence for Postmortem Interval Estimation: Postmortem interval (PMI) estimation represented another rapidly expanding area of AI research. Machine learning algorithms demonstrated superior capability in modelling complex biological datasets generated from metabolomics, microbiome sequencing, biochemical analysis, and medical imaging. Sharma et al., through a systematic review of eighteen studies, reported that regression algorithms, random forest models, and neural networks consistently provided more accurate and reproducible PMI estimates than conventional methods based solely on physical postmortem changes. Magnusson

et al. developed a feedforward neural network using metabolomic profiles obtained from 4,876 forensic blood samples. The model achieved a mean absolute prediction error of 1.45 days while maintaining excellent performance during external validation. Likewise, Cui et al. applied random forest regression to gravesoil microbiome sequencing data and achieved a mean absolute error of 1.27 days over a 36-day decomposition period, identifying several bacterial taxa as potential biomarkers for PMI estimation.

Artificial Intelligence for Forensic Toxicology Workflow Automation: Several review articles described the integration of AI throughout the forensic toxicology workflow. Reported applications included automated interpretation of toxicological findings, high-resolution mass spectrometry data processing, natural language processing for laboratory reporting, laboratory information management systems, and automated unknown-compound screening. Collectively, these studies demonstrated that AI improves analytical efficiency by reducing manual data processing, shortening turnaround time, enhancing analytical consistency, and increasing the accuracy of pattern recognition. AI-assisted workflows also facilitated automated spectral interpretation and supported decision-making during forensic investigations.

DISCUSSION

The findings of this review demonstrate that artificial intelligence (AI) is increasingly transforming forensic toxicology by improving analytical accuracy, efficiency, and decision-making across multiple stages of forensic investigations. Among the identified applications, the detection and identification of novel psychoactive substances (NPS) represents the most advanced and well-validated area. Deep learning, machine learning, and generative AI models have shown remarkable capability in predicting molecular structures and interpreting mass spectrometric data, even when certified reference standards or spectral libraries are unavailable. Such approaches provide an effective solution for the rapid identification of emerging designer drugs, addressing one of the most significant challenges faced by modern forensic laboratories. Another important application identified in this review is postmortem interval (PMI) estimation. Machine learning models developed using metabolomic, microbiome, biochemical, and imaging datasets consistently demonstrated greater accuracy than conventional PMI estimation methods based on physical postmortem changes. The reviewed studies suggest that AI-based predictive models are capable of reducing estimation errors while providing more objective and reproducible results. These findings indicate that AI has considerable potential to improve medico-legal investigations, particularly in cases where traditional PMI indicators become unreliable during advanced decomposition. [8-11]

Artificial intelligence has also demonstrated promising applications in predictive toxicology and toxicological risk assessment. AI-assisted physiologically based pharmacokinetic (PBPK) models, quantitative structure–activity relationship (QSAR) modelling, and deep learning algorithms have improved toxicity prediction, chemical risk assessment, and dose-response modelling. Furthermore, these computational approaches have the potential to reduce reliance on animal experiments while accelerating toxicological screening. However, most of the available evidence originates from pharmaceutical or regulatory toxicology rather than routine forensic casework, limiting its direct applicability to forensic investigations. Beyond analytical applications, AI is increasingly being integrated into the overall forensic toxicology workflow. Automated spectral interpretation, high-resolution mass spectrometry data analysis, laboratory information management, natural language processing, and decision-support systems have collectively improved laboratory efficiency by reducing manual interpretation, minimizing turnaround time, and enhancing analytical consistency. [12-17] These developments suggest that AI will become an important component of future forensic laboratory practice. Despite these encouraging developments, several challenges remain before AI can be routinely implemented in accredited forensic laboratories. Most studies were conducted using relatively small and heterogeneous datasets, limiting the generalizability of the developed models. Many AI algorithms also function as "black-box" systems, making their predictions difficult to interpret and raising concerns regarding transparency, reproducibility, and legal admissibility in judicial proceedings. In addition, the absence of standardized validation protocols, regulatory guidelines, and internationally accepted quality assurance frameworks continues to hinder widespread implementation. Addressing these issues through explainable AI (XAI), external multicentre validation, standardized datasets, and forensic-specific regulatory standards will be essential for the successful integration of AI into forensic toxicology. The summary of all included study mentioned in Table-2.

Table 2. Summary of studies included in the systematic review of AI applications in forensic toxicology.

Sl. No	Authors (Year)	Title (Abbreviated)	Study Design/Sample	AI Technique	Key Findings	Limitations
1	Wankhade et al. (2022)	AI in Forensic Medicine & Toxicology	Narrative review	ML, imaging AI, pattern recognition systems, predictive analytics for autopsy interpretation and toxicological screening.	AI improved diagnostic accuracy in autopsy analysis, toxic substance identification, postmortem interval estimation, and forensic imaging	The review lacked empirical validation studies and relied mainly on descriptive discussions. Real-world implementation and standardized forensic datasets were limited.

					interpretation. Machine learning reduced human error and enhanced efficiency in toxicological investigations.	
2	Jhatam (2025)	Digital Forensic Chemistry	Systematic review	ML, DL, automated spectral analysis, predictive toxicology models, AI-assisted chemical profiling.	AI enabled automated substance detection, rapid interpretation of chromatographic and spectrometric data, and predictive identification of toxic compounds.	Most findings were theoretical and lacked laboratory-based validation. Limited discussion on algorithm performance and forensic admissibility of AI-generated evidence.
3	Marinelli et al. (2026)	AI and ML in Forensic Toxicology	Narrative review	ML, DL, AI-assisted bioanalytical systems, predictive toxicodynamic models, spectral interpretation algorithms, automated interpretation software.	AI enhanced bioanalysis, toxicodynamics, metabolite prediction, and interpretation of toxicological findings, supporting forensic decision-making with improved objectivity and consistency.	Limited availability of validated datasets, data scarcity, and lack of explainable AI models restricted model reliability, reproducibility, and legal admissibility.
4	Swan et al. (2025)	AI-HRMS Screening for Unknown Substances	Method development	Machine learning integrated with High-Resolution Mass Spectrometry (HRMS), automated spectral deconvolution,	AI significantly improved screening efficiency for unknown substances and novel	High data complexity and variability in HRMS datasets affected reproducibility and interpretability of results.

				compound recognition algorithms.	psychoactive compounds. Automated analysis reduced turnaround time and increased detection sensitivity.	
5	Lin & Chou (2022)	AI in Toxicological Sciences	Narrative review	Physiologically based pharmacokinetic (PBPK) modelling, predictive toxicity/dose-response models.	AI-supported predictive models enhanced toxicity prediction, dose-response analysis, and simulation of toxicokinetic processes. PBPK models improved risk assessment and chemical safety evaluation.	Predictive models showed limited generalizability across different populations, chemicals, and biological conditions.
6	Almalki et al. (2024)	AI in Toxicology	Narrative review	ML, DL, high-throughput screening systems, AI-assisted toxicity prediction, data integration techniques.	AI improved analytical efficiency, accelerated toxicity screening, reduced dependence on animal testing, and enhanced interpretation of toxicological data.	Ethical concerns, algorithmic bias, data privacy issues, and lack of regulatory frameworks were major barriers to implementation.
7	Grafinger et al. (2026)	Machine Learning in Forensic Toxicology Workflows	Narrative review	Machine learning algorithms, chemometric modeling, predictive analytics,	Machine learning improved forensic toxicology workflows through	Small and heterogeneous datasets limited model generalizability. Few real-world validation

				automated classification systems.	automated classification of toxic substances, pattern recognition, and enhanced interpretation of analytical data.	studies were available.
8	Pasin et al. (2025)	AI and NLP in Toxicology Workflow Automation	Narrative review	Machine learning, Natural Language Processing (NLP), workflow automation systems, AI-driven data management.	AI and NLP automated toxicology workflows, facilitated data extraction from forensic databases, and improved analytical processing efficiency and laboratory productivity.	Validation and standardization issues remained unresolved, limiting large-scale implementation and cross-laboratory consistency.
9	Skinnider et al. (2021)	DarkNPS: Deep Generative Model for NPS Structure Elucidation	Method development (MS-based)	Deep generative (recurrent neural network) model trained on known NPS structures to predict unidentified designer-drug structures from mass spectra.	DarkNPS elucidated the exact structure of unidentified NPS with ~51% top-1 accuracy and ~86% top-10 accuracy, enabling de novo structure prediction ahead of substances reaching reference databases.	Performance depends on the size and diversity of the training structural library; accuracy decreases for structurally novel scaffolds outside prior chemical space.
10	Jurowski & Krośniak (2024)	In Silico Toxicity Prediction of AP-238 (NPS)	In silico/QSAR study	In silico/computational toxicology (QSAR-based) modelling of toxicity endpoints for a newly identified psychoactive substance.	The in silico approach predicted key toxicity endpoints for AP-238 in the absence of empirical toxicological data, supporting rapid clinical and forensic risk triage for emerging NPS.	In silico predictions require empirical (in vivo/in vitro) confirmation; applicability domain limitations restrict extrapolation to structurally dissimilar substances.
11	Ketsekioulafis et al. (2024)	AI in Forensic Sciences: Systematic Review	Systematic review	Survey of ML/DL applications across forensic subdisciplines (identification, cause-of-death estimation, PMI, toxicology, imaging).	AI applications improved accuracy and reproducibility across multiple forensic domains, including toxicological screening and postmortem interval estimation.	Heterogeneity of included study designs and AI methods limited direct comparability; forensic-specific validation and legal admissibility remain unresolved.
12	Wong et al. (2023)	GC-MS Based Machine Learning Screening of Unknown NPS	Method development (n = 891 GC-MS spectra)	Supervised ML classifiers — artificial neural network (ANN), convolutional neural network (CNN), and balanced random forest (BRF).	ML classifiers effectively screened seven NPS/compound classes (cathinones, cannabinoids, phenethylamines, piperazines, tryptamines, fentanyl-type, and unrelated compounds) using GC-MS data alone, with balanced random forest achieving the best	Model performance depends on the representativeness of the training spectral library; classification of entirely novel structural classes remains challenging.

					performance (macro-F1 ≈ 0.9).	
13	Sharma, Diksha, Bhute & Bastia (2022)	AI/ML for Postmortem Interval Prediction: Systematic Review	Systematic review (18 studies)	Survey of supervised and unsupervised ML models (e.g., regression, random forest, neural networks) applied to PMI estimation using microbiome, biochemical, and imaging data.	ML models displayed high accuracy and precision for PMI prediction across preclinical and clinical studies, outperforming traditional physical-sign-based estimation in several contexts.	Ethical, legal, and practical barriers to real-world implementation persist; limited number of AI-trained forensic researchers and computational complexity were noted as key barriers.
14	Magnusson et al. (2026)	Human Metabolome and Machine Learning for PMI Prediction	Retrospective cohort (n = 4,876; validation n = 512)	Feedforward neural network trained on femoral blood metabolomic profiles from routine toxicological screening.	The neural network predicted PMI with a mean/median absolute error of 1.45/1.03 days, outperforming six other ML architectures, and retained accuracy (1.78/1.29 days) on an independent, cross-platform validation set.	Model trained on a single population/laboratory context; broader multi-site validation is needed before forensic casework adoption.
15	Cui et al. (2022)	Gravesoil Microbiome and Random Forest for PMI Prediction	Experimental/field study	Random forest regression applied to gravesoil microbiome community sequencing data.	The random forest model predicted PMI with a mean absolute error of 1.27 days within a 36-day decomposition window and identified 18 informative bacterial taxa as biomarkers.	Findings are specific to soil/environmental conditions studied; generalizability across climates, soil types, and burial contexts requires further validation.
16	Lin, Chien, Wang, Wang, Yang, Tseng & Hung (2024)	PS2MS: Deep Learning Prediction System for NPS Identification	Method development	Deep learning (NEIMS/DeepEI-based spectrum prediction) combined with a synthetic NPS structure/fingerprint database and integrated similarity metrics.	PS2MS successfully identified cathinone derivatives in real forensic evidence specimens by predicting mass spectra for enumerated candidate NPS structures when no reference spectrum existed.	Effectiveness is bounded by the completeness of the enumerated derivative database; computationally intensive for very large candidate structure sets.
17	Teunis, Luechtefeld & Hartung (2025)	AI and Open Science for Toxicological Risk Assessment	Editorial/perspective	Discussion of AI-enabled new approach methodologies (NAMs), open data, and validation frameworks for computational toxicology.	The authors argue that combining AI with open science practices can accelerate validated, reproducible toxicological risk assessment and reduce reliance on animal testing.	As an editorial/perspective piece, it does not present original empirical validation data; recommendations require empirical testing across toxicology subfields.

LIMITATIONS

This review has several limitations. First, only 17 studies fulfilled the predefined eligibility criteria, reflecting the relatively recent development of AI applications specifically within forensic toxicology. Second, considerable heterogeneity existed among the included studies regarding AI methodologies, analytical platforms, study designs, and reported outcome measures, preventing quantitative meta-analysis. Third, most published studies focused on algorithm development or proof-of-concept investigations rather than validation using routine forensic casework. Finally, because AI technologies continue to

evolve rapidly, recently published studies may not have been captured within the selected search period.

CHALLENGES AND FUTURE PERSPECTIVES

Despite the encouraging findings, the reviewed studies consistently identified several limitations that currently restrict the routine implementation of AI in accredited forensic laboratories. Most AI models have been developed using relatively small and heterogeneous datasets, limiting their external validity. In addition, many algorithms function as "black-box" models, making their decision-making processes difficult to interpret, thereby raising concerns regarding explainability and legal admissibility in judicial proceedings. Other commonly reported challenges included insufficient external validation using real forensic casework, lack of standardized reporting guidelines, concerns regarding algorithmic bias, data privacy, and the absence of internationally accepted regulatory frameworks governing AI applications in forensic science. Overall, the evidence indicates that artificial intelligence has considerable potential to transform forensic toxicology through improved identification of novel psychoactive substances, enhanced predictive toxicology, more accurate postmortem interval estimation, and automation of laboratory workflows. Nevertheless, further multicentre validation studies, standardized datasets, transparent AI models, and comprehensive regulatory guidelines are required before these technologies can be routinely implemented in forensic practice.

CONCLUSION

Artificial intelligence is rapidly emerging as a valuable tool in forensic toxicology, with applications spanning novel psychoactive substance identification, predictive toxicology, postmortem interval estimation, and laboratory workflow automation. The reviewed evidence demonstrates that machine learning and deep learning models can improve analytical accuracy, enhance pattern recognition, accelerate data interpretation, and support forensic decision-making beyond the capabilities of conventional analytical approaches. Nevertheless, current evidence remains largely based on experimental research and narrative reviews rather than large-scale validation in accredited forensic laboratories. Future research should prioritize multicentre validation studies, development of transparent and explainable AI models, standardized reporting guidelines, and robust regulatory frameworks to ensure the scientific reliability and legal admissibility of AI-assisted forensic evidence. Successful integration of these advances will strengthen forensic toxicology practice and contribute to more accurate, efficient, and evidence-based medico-legal investigations.

DECLARATIONS

Ethics Approval and Consent to Participate: This study is a systematic review of previously published literature and did not involve human participants, animals, or the collection of primary biological samples. Therefore, ethical approval and informed consent were not required.

Availability of Data and Materials: All data analysed during this study were obtained from published literature and are included within this manuscript. Additional information is available from the corresponding author upon reasonable request.

Conflict of Interest: The authors declare that they have no competing interests.

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