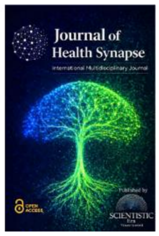
JOURNAL OF HEALTH SYNAPSE (JHS)
Peer Reviewed Refereed Open Access International Multidisciplinary Journal

Publisher: *Scientistic Era Private Limited*
Journal Hompage: *https://healthsynapse.org*



Artificial Intelligence in Forensic Toxicology: A Systematic Review of Emerging Trends, Analytical Techniques, and Future Directions

Himani Raj[a], Sneha Sagar[a], Mansi Negi[b*]

[a]*Department of Forensic Science, National Forensic Sciences University, Ponda, Goa 403401*
[b]*All India Institute of Ayurveda (AIIA), Government of India, New Delhi - 110076, India*

https://doi.org/
Received Date: 5 January 2026; **Revised Date:** 15 January 2026; **Accepted Dat**e: 25 January 2026; **Published Date:** 30 January 2026

ARTICLE INFO

Keywords:
Artificial Intelligence,
Machine Learning,
Forensic Toxicology,
Novel Psychoactive Substances,
Predictive Modeling,
Digital Forensics,
Legal Admissibility.

A B S T R A C T

An essential component of medico-legal investigations, forensic toxicology is being revolutionised by AI. Complex data generated by sophisticated analytical tools like LC-MS/MS and the ongoing appearance of new psychoactive substances (NPS) are two of the many obstacles that the sector must overcome. Machine learning (ML) and artificial intelligence (AI) are changing the face of toxicology by solving problems in areas like predictive toxicology, deconvolution of complicated datasets, AI-assisted spectral library curation, and the integration of multi-omics methods for thorough toxicological profiling. Artificial intelligence (AI)-powered plant toxin detection, postmortem drug redistribution modelling, pesticide categorisation, and NPS monitoring are some concrete examples. There are still a number of problems that need fixing with AI, such as the "black box" problem with algorithmic decision-making, limits on data quality and standardisation, and ethical and legal worries about the admissibility of evidence obtained from AI in court. Personalised toxicology, cloud-based platforms to increase accessibility, and federated learning for collaborative model creation are some of the promising new advancements in the near future. While artificial intelligence (AI) cannot fully replace forensic toxicologists, it is a valuable tool that can greatly improve their analytical accuracy, efficiency, and prediction powers. This, in turn, strengthens the credibility and value of forensic toxicology in the judicial system.

***Corresponding Author:**
Ms. Mansi Negi
All India Institute of Ayurveda (AIIA),
Government of India, New Delhi –
110076, India

I. Introduction

At the crossroads of science and law, forensic toxicology seeks to resolve basic concerns regarding the function of narcotics, poisons, and toxins in medico-legal proceedings [1]. Analytical tools like gas chromatography–mass spectrometry (GC–MS) and liquid chromatography– tandem mass spectrometry (LC–MS/MS) have long been the backbone of the field. These sensors collect very detailed and sensitive information, but they also produce massive datasets that are difficult to understand by hand [2, 3]. Hundreds of spectral peaks may be generated by a single HRMS run, with many of these peaks corresponding to undiscovered metabolites, environmental pollutants, or noise [4]. This data difficulty is made worse by the modern toxicological landscape. Numerous environmental contaminants, powerful plant poisons, and thousands of new psychoactive drugs (NPS) are currently challenges for forensic laboratories [5, 6]. Because they rely on reference standards that may not be available for novel or uncommon substances, traditional targeted screening approaches frequently fail to capture this "moving target" [7]. Because of this, forensic investigations become less efficient and have a smaller scope because there is a huge chasm between data collection and data interpretation.

Machine learning, a branch of artificial intelligence (AI), has recently arisen as a game-changing tool for closing this gap. Artificial intelligence (AI) is a system's capacity to read and learn from external inputs in order to adapt to new situations and accomplish predefined goals [8]. Forensic toxicologists may now use artificial intelligence algorithms to search through chromatographic and spectral data in ways that humans just cannot. These algorithms can detect minute patterns, accurately categorise new chemicals, and even forecast toxicological results [9, 10]. A proactive, data-driven science has replaced a reactive, reference-dependent practice, and this is the result.

The purpose of this review article is to give a critical and methodical analysis of the growing use of AI in forensic toxicology. In order to accomplish this, the article is structured around multiple primary goals. Initially, it will provide a systematic overview of the primary AI and ML techniques that are currently being used in the industry. Toxicology presents unique data kinds and challenges, such as spectral analysis and complicated pattern recognition. This introductory section will clarify important concepts like supervised and unsupervised learning, deep learning, and convolutional neural networks and how they relate to these problems. Using this groundwork in technology, the review will go on to describe the specific ways in which these AI approaches have been used in key areas of forensic toxicology. This encompasses an examination of how AI is facilitating the fast categorisation of pesticide mixtures, enhancing the interpretation of complex postmortem cases impacted by redistribution, and offering a proactive defence against the ongoing inflow of Novel Psychoactive Substances (NPS). By presenting these specific use-cases, the paper will synthesize the most significant emerging trends and practical implementations that are transitioning from research laboratories to casework.

In addition, the chapter takes a balanced and critical stance by thoroughly examining the present difficulties and constraints that come with this technological transition. The crucial subject of whether AI-derived evidence can be credibly presented in a court of law will be thoroughly examined, with an emphasis on the "black box" problem, data standardisation obstacles, and ethical-legal problems of responsibility that need to be addressed. The review will conclude with a prospective section that suggests specific avenues for further study and lays out the frameworks that will be required for the ethical, open, and efficient integration of AI. The ultimate goal is to chart a path where AI evolves from a novel research tool into a trusted, standardized, and indispensable component of forensic toxicology practice, thereby enhancing the pursuit of justice.

2. Artificial Intelligence and Machine Learning: A Primer for Toxicologists

An understanding of the fundamentals of the applicable AI approaches is necessary for comprehending the applications. The phrase "artificial intelligence" (AI) describes computer systems that are able to mimic human intelligence in some way. In machine learning, a branch of artificial intelligence, computers are able to "learn" from data automatically, rather than requiring constant programming [11]. The following are the primary toxicology-related learning paradigms, as shown in Figure 1:

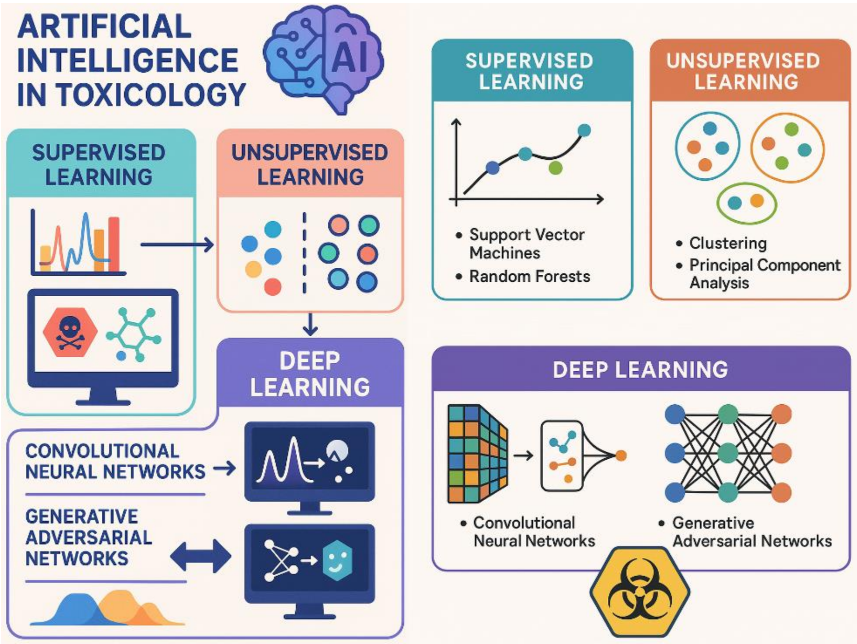


Figure 1: A Conceptual Taxonomy of Typical AI/ML Methods in Toxicology

• **Supervised Learning:** A labeled dataset, such as mass spectra with the compound's identity attached, is used to train the algorithm. It is capable of classifying novel, unidentified samples after training. Support Vector Machines (SVM) and Random Forests are popular algorithms that are very good at identifying spectra as either benign chemicals, metabolites, or poisons [12, 4].
• **Unsupervised Learning:** Applied to unlabeled data. The algorithm finds intrinsic structures or hidden patterns in the data. Principal Component Analysis (PCA) and clustering are useful methods for categorizing unknown chemicals according to spectral similarity or finding novel pharmacological classes [13,7].
• **Deep Learning (DL):** A more sophisticated type of machine learning that makes use of multi-layered artificial neural networks, or "deep" networks. These are especially effective when working with unstructured data.

- **Convolutional Neural Networks (CNNs):** Excel is useful for image analysis and can be used for pattern identification and deconvolution of overlapping peaks in 2D data, such as mass spectra or chromatograms [14, 15].
- **Generative Adversarial Networks (GANs):** can produce synthetic toxicological data (such as Tox-GAN), which is helpful for investigating the chemical space of possible toxins and supplementing small training datasets [16].

Table 1: Overview of Important AI/ML Methods in Forensic Toxicology

AI Technique	Learning Type	Primary Function	Example Application in Toxicology
Support Vector Machine (SVM)	Supervised	Classification & Regression	Classifying pesticide spectra in mixed matrices [4].
Random Forest	Supervised	Classification & Regression	Predicting toxicity of organic compounds [12].
Principal Component Analysis (PCA)	Unsupervised	Dimensionality Reduction & Clustering	Identifying patterns in postmortem biomarker data [13].
Convolutional Neural Network (CNN)	Deep Learning	Image & Pattern Recognition	Deconvoluting overlapping peaks in mass spectra; analyzing histopathology slides [14, 15].
Generative Adversarial Network (GAN)	Deep Learning	Data Generation & Augmentation	Creating synthetic toxicogenomics data (Tox-GAN) for model training [16].

3. Applications of AI in Forensic Toxicology: From Theory to Practice

From academic study to real-world casework, forensic toxicology is experiencing a transformation because to AI integration.

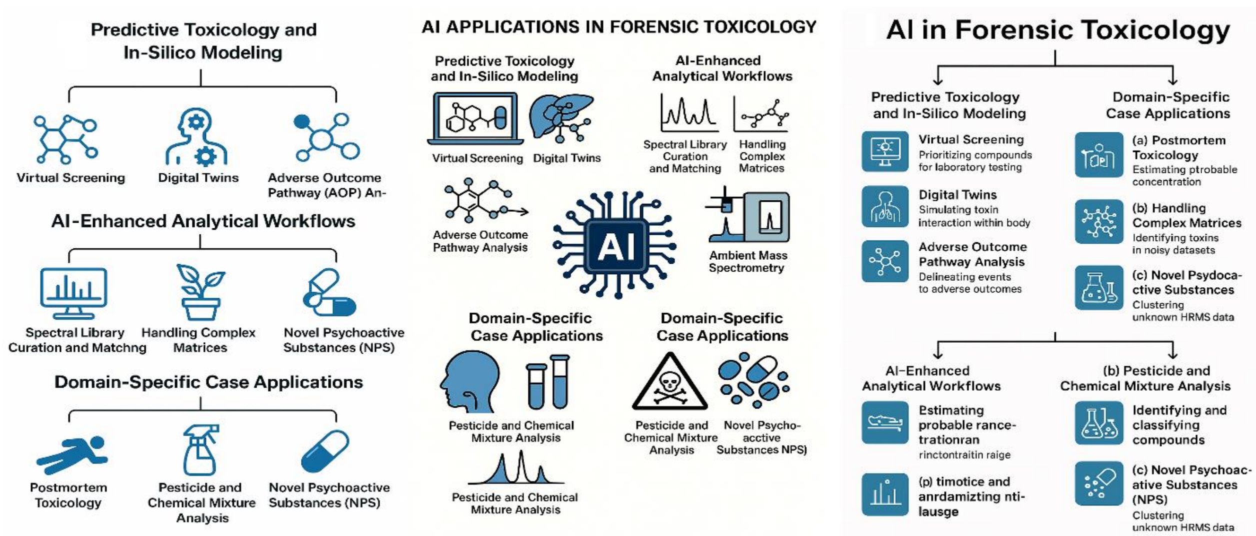


Fig. 2. An Overview of Artificial Intelligence Use in Forensic Toxicology

3.1. Predictive Toxicology and In-Silico Modeling

Predicting a substance's toxicity and metabolic destiny prior to physical testing is one of its main uses. Large datasets of chemical compounds, in vitro test findings, and established toxicological consequences can be used to train AI models [17, 18]. This makes it possible for:

- **Virtual Screening:** This method lowers expenses and eliminates animal testing by ranking substances for laboratory testing according to their anticipated toxicity [19].
- **Digital twins:** using artificial intelligence (AI)-driven virtual representations of biological systems, such as organs and metabolic pathways, to model how a new toxin interacts with the body and forecast lethal doses or metabolic breakdowns [20, 4].

- **Undesirable consequence Pathway (AOP) Analysis:** This method draws mechanistic insights by using artificial intelligence (AI) to outline the chain of events from a molecular initiating event to an undesirable consequence at the organism level [21].

3.2. AI-Enhanced Analytical Workflows

In order to increase the efficiency and precision of the analytical process, AI is being integrated directly into it.

- **Spectral Library Curation and Matching:** Manual curation is necessary for traditional spectrum libraries. Using deep learning to deconvolute overlapping peaks and AI to automate library updates, cleaner and more accurate identifications are achieved [22, 4].
- **Handling Complex Matrices:** In complex biological matrices, plant poisons (such as aconitine and abrin) are frequently detected at trace quantities. The distinctive fragmentation patterns of these uncommon pollutants can be detected using non-targeted HRMS screening in conjunction with ML models, even in datasets that are noisy, thus decreasing the need for scarce reference standards [23, 7].
- **Ambient Mass Spectrometry:** We use rapid sample triage techniques like DART-MS and paper-spray MS. They serve as a "front door" for mass spectrometry when combined with ML-assisted spectrum categorization, identifying possible positives for further study [24, 4].

3.3. Domain-Specific Case Applications

a) Postmortem Toxicology: Postmortem cases are more complicated because of factors like redistribution, degradation, and pH changes. Predicting probable concentration ranges in various fluids (blood, vitreous humor, etc.) requires AI/ML models trained on large datasets of postmortem cases to account for aspects like degradation and time since death. Researchers now have a structured quantitative baseline to work with, rather than relying on a single, potentially misleading, absolute statistic [25, 13].

b) Pesticide and Chemical Mixture Analysis: Pesticide combinations with overlapping chromatographic peaks are common in these cases. Rapid identification and classification of these substances, even in complicated biological or environmental samples, is possible with supervised ML models (e.g., SVM, Random Forest) that significantly decrease analysis time [4, 26].

c) Novel Psychoactive Substances (NPS): A lot is changing in the NPS world right now. AI provides a strong answer by way of:

- **Unsupervised Learning:** Using clustering to classify unknown HRMS data into recognized drug classes (e.g., nitazenes vs. fentanyl analogs) in the absence of reference standards [7].
- **Data-Centered Surveillance:** To identify new trends in drug usage, it is necessary to combine information from many sources, including toxicology labs, clinical entries, and wastewater-based epidemiology (WBE). A proactive "early-warning" system can be created by using ML models to forecast trends and transmit this intelligence back to labs [27, 28].

Table 2: A Survey of Artificial Intelligence Use in Various Fields of Forensic Toxicology

Domain	Key Challenge	AI Solution	Reported Benefit	Key Reference
Plant Toxins	Low concentration in complex matrices; lack of reference standards.	Non-targeted HRMS + ML for pattern recognition (e.g., CNN).	Identifies rare toxins without certified standards; suggests candidate identities with probability scores.	[7, 23]
Postmortem Toxicology	Postmortem redistribution and degradation affecting concentration accuracy.	ML models to estimate concentration boundaries based on decomposition stage and fluid type.	Provides a range of probable concentrations, stabilizing interpretation.	[25, 13]
Pesticides	Complex mixtures with overlapping chromatographic peaks.	Supervised learning (SVM, Random Forest) for spectral classification.	Rapid identification and classification in mixed samples; handles large-scale batch analysis.	[4, 26]
Novel Psychoactive Substances (NPS)	Rapidly evolving compounds absent from traditional libraries.	Unsupervised clustering of HRMS data; AI-driven surveillance from multiple data streams (e.g., WBE).	Enables proactive flagging of "suspect unknowns"; predicts emerging waves of NPS.	[7, 27, 28]
Toxicogenomics	Integrating large omics datasets for mechanistic insights.	AI models to integrate genomics, proteomics, and metabolomics data.	Provides a holistic view of toxicological mechanisms and identifies predictive biomarkers.	[29, 16]

4. Emerging Trends and Future Directions

Forensic toxicology AI is heading in the direction of more collaborative, individualized, and integrated systems.

- **Federated Learning:** Labs are hesitant to share critical patient information due to data privacy concerns. Through the use of federated learning, various labs can work together to train an AI model without actually sharing any data. Every lab does its own model training, and the only data that gets aggregated are the model changes. In doing so, a worldwide "collective intelligence" for toxicology is born, which evolves over time [30, 4].

- **Personalized Forensic Toxicology:** Beyond generalizations based on population averages, AI may now incorporate toxico-genomic, proteomic, and metabolic data to forecast a person's unique toxicity threshold. This could explain why two individuals experience different outcomes from the same exposure [31, 4].
- **Cloud-Based Toxicology Platforms:** Platforms on the cloud can provide sophisticated AI analysis as a service, making it accessible to everyone. By transferring raw data to a secure cloud service, which then returns standardized, court-ready reports, even labs with minimal resources might have access to state-of-the-art toxicology [4].
- **AI in Histopathology and Image Analysis**: Unlike conventional histopathology, AI-powered tissue slide analysis can identify microcellular alterations in the brain, kidneys, or liver that indicate certain toxic insults [15, 32].

5. Challenges, Limitations, and Ethical Considerations

The potential of artificial intelligence (AI) in forensic toxicology is exciting, but there are a lot of obstacles that need to be overcome before it can be used widely and trusted.

- **The "Black Box" Problem:** A lot of sophisticated AI models, especially DLSs, aren't very clear. They are good at making predictions, but they have a hard time explaining their reasoning. This is troublesome from a legal standpoint. For scientific evidence to be accepted in court, it must be clear, repeatable, and easy to grasp. The results drawn by AI can be contested by the opposing side using precedents such as Daubert or Frye [33, 34]. In order to get over this, it is essential to create "Explainable AI" (XAI).
- **Data Quality and Standardization:** AI models rely heavily on the quality of the data used to train them. Models will be inaccurate if the data is incomplete, biased, or not standardized. A significant obstacle to building universally robust AI tools is the variability in laboratory methods among institutions, which includes sample prep, equipment, and reporting thresholds [35, 36]. We must prioritize initiatives that aim to establish standardized standards and shared databases of the highest quality.
- **Legal Admissibility and Accountability:** Important concerns persist, such as: who is responsible in the event of an AI system's mistake—the programmer, the lab, or the specialist delivering the findings? The idea that an algorithm is perfect can also influence judges, a phenomenon called "automation bias." As previously stated[37,1], AI should always be portrayed as a tool to supplement human judgment rather than a replacement for it.
- **Ethical and Privacy Concerns:** Big datasets are needed to train AI models, and some of those datasets might contain private legal and medical records. To safeguard individual rights and uphold public trust, it is crucial to ensure that this data is anonymized, stored securely, and utilized ethically [38, 34].
- **Cost and Expertise:** There may be a "digital divide" in forensic capabilities if public-sector forensic laboratories are unable to implement sophisticated AI systems due to a lack of funding and specialist knowledge [1, 39].

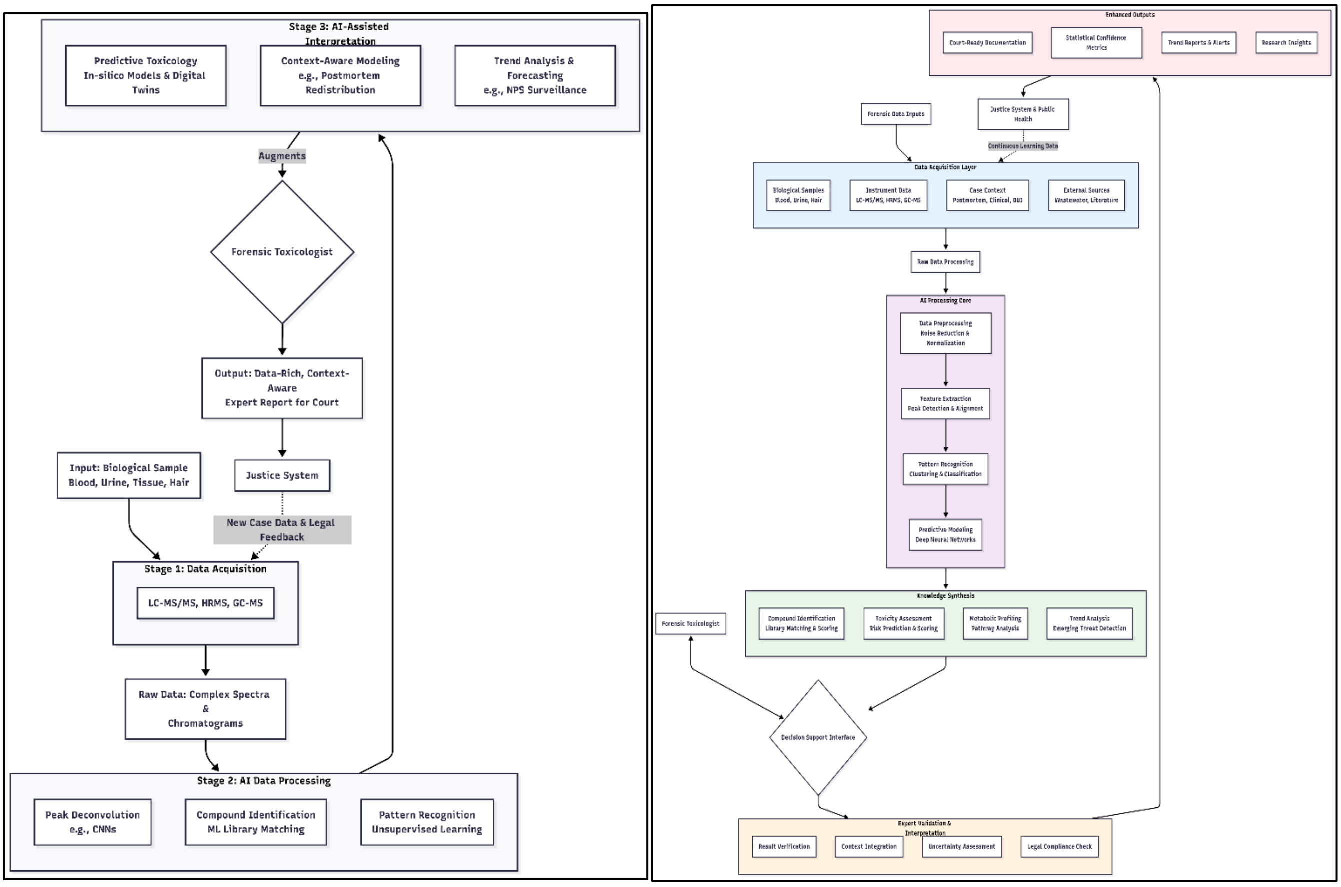
6. Framework Design and Implementation

6.1 Operational Workflow for AI-Assisted Toxicological Analysis

The Fig. 3 (a) is a simplified workflow in which AI plays a significant role beyond the initial data capture at every level.

- **Stage 1: Data Acquisition:** Advanced analytical tools such as Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) and High-Resolution Mass Spectrometry (HRMS) produce the major, intricate data from biological samples at this initial, foundational step [2, 4].
- **Stage 2: AI Data Processing:** At this point, AI starts to take over jobs that are too difficult for humans to do. In order to separate spectra with overlapping peaks, ML models, and CNNs in particular, use deconvolution. To identify compounds, supervised learning algorithms compare the cleaned spectra to databases that are constantly being updated with information curated by artificial intelligence. Finding new chemicals requires a combination of supervised and unsupervised learning methods, which search through data for patterns and classify unknown molecules [7, 14].
- **Stage 3: AI-Assisted Interpretation:** A new degree of insight is achieved by the processed data. Toxicology and substance behavior simulations are made possible by predictive models. Toxicological importance is estimated using case-specific context-aware models, like those for postmortem redistribution. In addition, by analyzing aggregated data trends, scientists might anticipate new drug dangers, allowing them to take a proactive rather than reactive approach [4, 25, 27].
- **The Augmented Toxicologist:** The AI systems' outputs should not be seen as a replacement for forensic toxicologists, but rather as an adjunct to their job, according to the process. Incorporating their own expertise, case background, and professional judgment, the expert incorporates the facts, patterns, and forecasts produced by the AI.
- **Iterative Feedback Loop (Dashed Line):** A well-developed AI system must have a feedback loop. To make sure the AI models learn and adapt over time, they are always being fine-tuned and validated with new case data and judicial system outcomes fed back into the workflow [30].

An expert report that is more data-rich, objective, and forensically robust is the result of an integrated workflow that uses AI to improve the entire process.



(a) **(b)**

Fig. 3 (a) (a) Implementing an AI-Assisted Toxicological Analysis Process (b) Intelligent Forensic Toxicology Decision-Support System Architecture

6.2 Architectural Design of the Integrated AI System

From multi-source data inputs via AI processing layers to expert-validated outputs—that is the hierarchical data flow depicted in Fig. 3 (b) for AI-augmented forensic toxicology. Data Acquisition deals with biological samples and instrumental data. The AI Processing Core handles feature extraction and pattern recognition. Knowledge Synthesis deals with compound identification and toxicity prediction. Human-AI Interaction handles expert validation and interpretation. Enhanced Outputs is where the system culminates. The system is able to learn and adapt thanks to a continuous feedback loop, which keeps forensic rigor high while improving analytical capabilities through organized human-AI collaboration. Sequential processing, bidirectional validation, adaptive learning, forensic compliance, and multi-source integration are the major features. While maintaining crucial human supervision and legal norms, this design shows how AI systematically augments traditional toxicological analysis.

6.3 A Proposed Mitigation Framework for Critical AI Implementation Challenges

An important part of this study is figuring out how to deal with the main problems with implementing clinical AI, which calls for a two-pronged approach including technological and governance measures, as shown in Figure 4. The following framework provides a summary of the main points: the difficulty in understanding complicated models (the "Black Box Problem"), the diversity of health records, and the lack of clarity regarding who is legally responsible for what. The suggested mitigation matrix combines legislative solutions with technical interventions like Explainable AI (XAI) tools and federated learning to solve them.

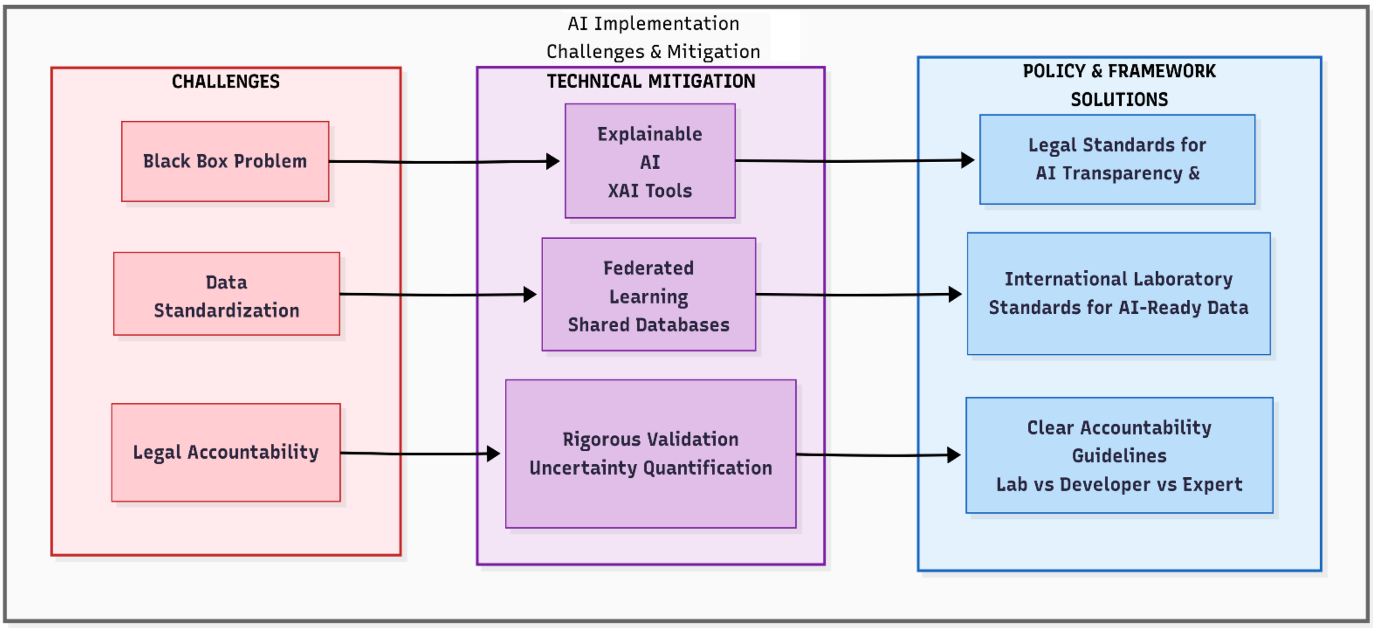


Fig. 4 A Roadmap for Successful AI Rollouts: Common Pitfalls and Their Solutions.

Some of these initiatives include creating worldwide laboratory standards for AI-ready data and establishing legal criteria for algorithmic transparency. In order to close accountability gaps and guarantee that strong legal and ethical frameworks back thorough technological validation, it is suggested that laboratories, software developers, and clinical experts all clearly define who is responsible for what. If artificial intelligence is to go from being a fresh concept in research to a trustworthy and dependable part of clinical practice, this integrated approach is crucial.

Conclusion

In this chapter, we have seen how the application of AI is propelling a radical rebalancing of forensic toxicology. The change from conventional approaches to AI-enhanced frameworks is not a small step; it signifies a sea change in the way the field operates. Machine learning's ability to deconvolute complicated spectral data, forecast the behavior of new psychoactive chemicals, and estimate postmortem redistribution gives contemporary toxicologists an unprecedented set of tools, as previously discussed. However, moving forward is hardly a walk in the park; it demands careful navigating of substantial obstacles. Researchers in this area need to tackle head-on the challenges of model interpretability, data foundational quality, and the inevitable legal scrutiny of their results. The key to success is a coordinated effort to develop systems that are open, strong, and can be defended in court. This can be achieved by interdisciplinary teams working together and following established standards. Therefore, the final vision does not involve replacement but rather a strong collaboration. It envisions a future where computational precision amplifies the toxicologist's expert judgment, guaranteeing that the pursuit of justice is guided by both deep data-driven insights and irreplaceable human expertise.

References

1. Wankhade, T. D., Ingale, S. W., Mohite, P. M., & Bankar, N. J. (2022). Artificial Intelligence in Forensic Medicine and Toxicology: The Future of Forensic Medicine. *Cureus*, 14(8), e28376.
2. Nasnodkar, S., Cinar, B., & Ness, S. (2023). Artificial Intelligence in Toxicology and Pharmacology. *Journal of Engineering Research and Reports*, 25(7), 192-206.
3. Shaki, F., Amirkhanloo, M., & Chahardori, M. (2025). The Future and Application of Artificial Intelligence in Toxicology. *Asia-Pacific Journal of Pharmacotherapy & Toxicology*.
4. Sisodia, N., & Dodiya, K. (2025). Artificial Intelligence in Forensic Toxic Science: Emerging Trends and Analytical Techniques. *International Journal for Research in Applied Science and Engineering Technology (IJRASET)*, 13(IX), 1571-1579.
5. Piraianu, A.-I., Fulga, A., Musat, C. L., Ciobotaru, O.-R., Poalelungi, D. G., Stamate, E., Ciobotaru, O., & Fulga, I. (2023). Enhancing the Evidence with Algorithms: How Artificial Intelligence Is Transforming Forensic Medicine. *Diagnostics*, 13(18), 2992.
6. Yadav, M., & Tiwari, A. (2017). Forensic toxicology and its relevance with criminal justice delivery system in India. *Forensic Res Criminol Int J*, 4(4), 122-128.
7. Lee, S. Y., Lee, S. T., Suh, S., Ko, B. J., & Oh, H. B. (2022). Revealing unknown controlled substances and new psychoactive substances using high-resolution LC-MS-MS machine learning models and the hybrid similarity search algorithm. *Journal of Analytical Toxicology*, 46(7), 732-742.
8. Kaplan, A., & Haenlein, M. (2019). Siri, Siri, in my hand: Who's the fairest in the land? On the interpretations, illustrations, and implications of artificial intelligence. *Business Horizons*, 62(1), 15-25.
9. Paul, D., Sanap, G., Shenoy, S., Kalyane, D., Kalia, K., & Tekade, R. K. (2021). Artificial intelligence in drug discovery and development. *Drug Discovery Today*,

26(1), 80-93.

10. Hasselgren, C., & Myatt, G. J. (2018). Computational toxicology and drug discovery. In *Computational Toxicology: Methods and Protocols* (pp. 233-244). Humana Press, New York, NY.
11. Russell, S. J., & Norvig, P. (2009). *Artificial Intelligence: A Modern Approach* (3rd ed.). Prentice Hall.
12. Wu, F., Zhang, X., Fang, Z., & Yu, X. (2023). Support Vector Machine-Based Global Classification Model of the Toxicity of Organic Compounds to Vibrio fischeri. *Molecules*, 28(6), 2703.
13. Notarstefano, V., et al. (2025). A new approach to assess post-mortem interval: A machine learning-assisted label-free ATR-FTIR analysis of human vitreous humor. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 327, 125326.
14. He, Q., et al. (2023). Dear-DIAXMBD: Deep Autoencoder Enables Deconvolution of Data-Independent Acquisition Proteomics. *Research*, 6, 0179.
15. Turner, O. C., et al. (2020). Society of toxicologic pathology digital pathology and image analysis special interest group article: opinion on the application of artificial intelligence and machine learning to digital toxicologic pathology. *Toxicologic Pathology*, 48(2), 277-294.
16. Yu, H., Ding, J., Shen, T., Liu, M., Li, Y., & Fiehn, O. (2025). MassCube improves accuracy for metabolomics data processing from raw files to phenotype classifiers. *Nature Communications*, 16(1), 1-15.
17. Jeong, J., & Choi, J. (2022). Artificial intelligence-based toxicity prediction of environmental chemicals: future directions for chemical management applications. *Environmental Science & Technology*, 56(12), 7532-7543.
18. Ciallella, H. L., & Zhu, H. (2019). Advancing computational toxicology in the big data era by artificial intelligence: data-driven and mechanism-driven modeling for chemical toxicity. *Chemical Research in Toxicology*, 32(4), 536-547.
19. Kavlock, R., & Dix, D. (2010). Computational toxicology as implemented by the US EPA: providing high throughput decision support tools for screening and assessing chemical exposure, hazard and risk. *Journal of Toxicology and Environmental Health, Part B*, 13(2-4), 197-217.
20. Gangwal, A., & Lavecchia, A. (2025). Artificial intelligence in preclinical research: enhancing digital twins and organ-on-chip to reduce animal testing. *Drug Discovery Today*, 30(5), 104360.
21. Burgoon, L. D. (2017). The AOPOntology: a semantic artificial intelligence tool for predictive toxicology. *Applied In Vitro Toxicology*, 3(3), 278-281.
22. Gasteiger, J. (2020). Chemistry in Times of Artificial Intelligence. *ChemPhysChem*, 21(20), 2233-2242.
23. Gaballah, M. H., et al. (2016). Simultaneous time course analysis of multiple markers based on DNA microarray in infected wound in skeletal muscle for wound aging. *Forensic Science International*, 266, 357-368.
24. Sisco, E., & Forbes, T. P. (2021). Forensic applications of DART-MS: A review of recent literature. *Forensic Chemistry*, 22, 100294.
25. Hachem, M., & Sharma, B. K. (2019). Artificial Intelligence in Prediction of Postmortem Interval (PMI) through Blood Biomarkers in Forensic Examination-A Concept. In *2019 Amity International Conference on Artificial Intelligence (AICAI)* (pp. 255-258). IEEE.
26. Wilton, D. J., Harrison, R. F., Willett, P., Delaney, J., Lawson, K., & Mullier, G. (2006). Virtual screening using binary kernel discrimination: analysis of pesticide data. *Journal of Chemical Information and Modeling*, 46(2), 471-477.
27. Di Giorgi, S., Pichini, S., Busardò, F. P., & Basile, G. (2025). Artificial intelligence in new psychoactive substances analysis: state-of-the-art and future perspectives. *Journal of Analytical Toxicology*.
28. Zissler, A., et al. (2021). Influencing factors on postmortem protein degradation for PMI estimation: A systematic review. *Diagnostics*, 11(7), 1146.
29. Shi, K., Lin, W., & Zhao, X. M. (2021). Identifying molecular biomarkers for diseases with machine learning based on integrative omics. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, 18(6), 2544-2555.
30. Antontsev, V., et al. (2021). A hybrid modeling approach for assessing mechanistic models of small molecule partitioning in vivo using a machine learning-integrated modeling platform. *Scientific Reports*, 11(1), 11143.
31. Mirza, B., Wang, W., Wang, J., Choi, H., Chung, N. C., & Ping, P. (2019). Machine learning and integrative analysis of biomedical big data. *Genes*, 10(2), 87.
32. Hosny, A., Parmar, C., Quackenbush, J., Schwartz, L. H., & Aerts, H. J. (2018). Artificial intelligence in radiology. *Nature Reviews Cancer*, 18(8), 500-510.
33. Helma, C. (2004). Data Mining and Knowledge Discovery in Predictive Toxicology. *SAR and QSAR in Environmental Research*, 15(5-6), 367-383.
34. Gerke, S., Minssen, T., & Cohen, G. (2020). Ethical and Legal Challenges of Artificial Intelligence-Driven Healthcare. In *Artificial Intelligence in Healthcare* (pp. 295-336). Academic Press.
35. Idakwo, G., Luttrell, J., Chen, M., Hong, H., Zhou, Z., Gong, P., & Zhang, C. (2018). A review on machine learning methods for in silico toxicity prediction. *Journal of Environmental Science and Health, Part C*, 36(4), 169-191.
36. Tan, H., Jin, J., Fang, C., Zhang, Y., Chang, B., Zhang, X., ... & Zhang, Q. (2023). Deep Learning in Environmental Toxicology: Current Progress and Open Challenges. *ACS ES&T Water*.
37. Chary, M. A., Manini, A. F., Boyer, E. W., & Burns, M. (2020). The role and promise of artificial intelligence in medical toxicology. *Journal of Medical Toxicology*, 16(4), 458-464.
38. Dilmaghani, S., Brust, M. R., Danoy, G., Cassagnes, N., Pecero, J., & Bouvry, P. (2019, December). Privacy and security of big data in AI systems: A research and standards perspective. In *2019 IEEE International Conference on Big Data (Big Data)* (pp. 5993-5994). IEEE.

39. Agrebi, S., & Larbi, A. (2020). Use of artificial intelligence in infectious diseases. In *Artificial Intelligence in Precision Health* (pp. 415-438). Academic Press.