



LAWFOYER INTERNATIONAL JOURNAL OF DOCTRINAL LEGAL RESEARCH

[ISSN: 2583-7753]

Volume 4 | Issue 3

2026

DOI: <https://doi.org/10.70183/lijdlr.2026.v04.269>

© 2026 LawFoyer International Journal of Doctrinal Legal Research

Follow this and additional research works at: www.lijdlr.com

Under the Platform of LawFoyer – www.lawfoyer.in

After careful consideration, the editorial board of LawFoyer International Journal of Doctrinal Legal Research has decided to publish this submission as part of the publication.

In case of any suggestions or complaints, kindly contact (info.lijdlr@gmail.com)

To submit your Manuscript for Publication in the LawFoyer International Journal of Doctrinal Legal Research, To submit your Manuscript [Click here](#)

ANALYSIS OF AI-ASSISTED FORENSIC TOXICOLOGY AND THE EVIDENTIARY CHALLENGES OF PROSECUTION IN POISONING CASES

Pooja S¹

I. ABSTRACT

Poisoning cases have their own evidentiary, mens rea, and causation issues to be established with reasonable certainty. These difficulties are more evident in cases concerning new psychoactive substances (NPS) and herbal poisonings such as Abrus precatorius and Nerium oleander, where detection is difficult, untimely, and often inconclusive. Standard toxicological methods cannot detect new chemicals or properly quantify herbal poisonings to prove their use with the intent to kill. This study will examine the potential of Artificial Intelligence (AI) in toxicological screenings in poisoning cases. AI models can detect and identify unknown substances and infer patterns. This study is crucial for examining whether such innovations could help fill the evidentiary gap in mens rea or raise any legal concerns regarding admissibility and reliability. In light of the merging nature between forensic science and criminal law, the paper suggests that there is much room for AI-assisted toxicology to strengthen the prosecution's case, yet whether this approach can legally be applied at the moment remains questionable. Moreover, if regulations remain unrigorous and judicial practices are lenient, it could prove less compelling than other cases in arguing for its viability. Ultimately, the author believes that an appropriate balance needs to be struck whereby the technological advancements align with the core tenets of criminal law. The study further undertakes a comparative analysis of regulatory approaches adopted in the United States, the European Union, the United Kingdom, and Australia to identify best practices governing AI-assisted forensic evidence. Based on these findings, it proposes legislative and procedural reforms for India, including clear admissibility standards, validation protocols, transparency requirements, and specialised regulatory oversight to ensure that AI-assisted forensic toxicology strengthens criminal investigations while safeguarding the rights of the accused.

¹ Student at Tamil Nadu Dr. Ambedkar Law University (India). Email ID: riteshraj2903@gmail.com

II. KEYWORDS

AI-assisted forensic toxicology; mens rea; evidentiary admissibility; poisoning prosecutions; Bharatiya Sakshya Adhiniyam.

III. INTRODUCTION

One of the most intricate and interconnected facets of criminal law and forensic science is the prosecution of poisoning cases, and a court decision is largely dependent on scientific evidence. In contrast to typical homicide, which frequently involves physical violence or eyewitness testimony, poisoning instances have concealed toxicity, delayed symptoms, and no direct evidence (i.e., indirect evidence), making the investigation considerably more difficult. Novel psychoactive drugs (NPS) and plant-derived poisons like *Abrus precatorius* and *Nerium oleander*, which are typically exceedingly difficult to detect due to their variable concentration, rapid metabolism, and difficulty in testing, further complicate this complexity.

From a doctrinal perspective, criminal liability for poisoning is predicated on three essential elements: the administration of poison, the direct causation of harm or death by the poison, and the presence of mens rea, or guilty intent. These pertain to culpable homicide and murder as delineated in Sections 100 and 101 of the Bharatiya Nyaya Sanhita (BNS) 2023², along with the specific offence of administering poison under Section 132. However, evidentiary limitations make it very hard to put these rules into practice, and scientific findings aren't always convincing or acceptable.

Sections 104 to 109 of the Bharatiya Sakshya Adhiniyam (BSA) of 2023³ set the burden of proof for these kinds of cases, and Section 39 lets expert opinions, like those of forensic toxicologists, be used as evidence. Expert testimony is very important for proving that toxic substances are present and how they affect people. But people have often questioned it because of problems with the methods used, the interpretation, and the time it took to report.⁴ When it comes to NPS and rare plant toxins,

² Bharatiya Nyaya Sanhita, No. 45 of 2023, §§ 100–101; 132

³ Bharatiya Sakshya Adhiniyam, No. 47 of 2023, §§ 39, 104–106.

⁴ Paul C. Giannelli, Edward J. Imwinkelried, Andrea L. Roth, Jane Campbell Moriarty and Valena E. Beety, *Scientific Evidence* § 1.03 (6th ed. 2020, LexisNexis/Matthew Bender, supp. 2022).

toxicological methods might not be able to find the substance at all. This creates gaps in the evidence that make the prosecution's case weaker and the defence's case of reasonable doubt stronger.

The creation of AI-assisted toxicological screening is a big step forward for forensic science. AI-powered systems that use machine learning and large chemical databases can find new compounds, predict their toxicity, and accelerate analysis in smart ways. These kinds of tools can change the way evidence is used in poisoning cases by making toxicological analysis more accurate and easier to understand. They may also make the reasoning behind *mens rea* stronger when there is no proof of intent.

But using AI in forensic toxicology also brings up difficult legal and moral issues.⁵ It is still not clear if AI-generated findings under Section 39 of the Bharatiya Sakshya Adhiniyam (BSA) of 2023⁶ can be used as evidence. There are worries about how clear, reliable, and fair the algorithms are. In addition to using these technologies, we need to think about how they fit with basic rules of criminal law, like the presumption of innocence, the right to a fair trial, and the need to prove guilt beyond a reasonable doubt. If algorithmic results are not used correctly, they could shift the balance of proof in a way that hurts the accused.

This paper aims to analyse the function of AI-assisted toxicological screening in addressing the evidentiary challenges associated with poisoning prosecutions. After looking into the problems with traditional toxicology, the legal requirements for criminal liability, and the possibilities of AI technologies. The paper also discusses what kind of legal structure we need to put in place so that AI-generated evidence can be used in court and to make sure that technology helps the criminal justice system instead of hurting it.

A. Problem Research

The prosecution of poisoning cases is challenged by significant evidentiary limitations, since conventional forensic toxicology is limited in its ability to identify

⁵ Cary Coglianese and David Lehr, *Regulating by Robot: Administrative Decision Making in the Machine-Learning Era*, 105 Geo. L.J. 1147 (2017).

⁶ Bharatiya Sakshya Adhiniyam, No. 47 of 2023, § 39, 104–06.

novel psychoactive substances (NPS) and plant-based poisons such as *Abrus precatorius* and *Nerium oleander*. Such limitations prevent a reasonable degree of certainty from being attached to the requisite *mens rea* and causation. Artificial Intelligence (AI) assisted toxicology provides state of the art capabilities in toxin detection, predictive analysis, and pattern recognition, however, there is still legal uncertainty regarding the admissibility, reliability, transparency, and evidentiary value of AI-generated forensic evidence under the Bharatiya Sakshya Adhiniyam, 2023. The lack of an all-encompassing legal and regulatory structure governing AI-assisted toxicological evidence creates a gap in the intersection of scientific innovation and the administration of criminal justice.

B. Aim of the Study

To critically examine the role of Artificial Intelligence-assisted forensic toxicology in overcoming evidentiary challenges in the prosecution of poisoning cases and to evaluate its admissibility, reliability, and legal implications under the Indian criminal justice system.

C. Objectives of the Study

1. To examine the limitations of conventional forensic toxicology in establishing causation and *mens rea* in poisoning cases.
2. To analyse the application of Artificial Intelligence-assisted toxicological screening in detecting novel psychoactive substances (NPS) and plant-derived poisons.
3. To evaluate the evidentiary value, reliability, and admissibility of AI-generated toxicological evidence under the Bharatiya Sakshya Adhiniyam, 2023.
4. To examine the statutory framework governing poisoning offences under the Bharatiya Nyaya Sanhita, Bharatiya Nagarik Suraksha Sanhita, and Bharatiya Sakshya Adhiniyam.
5. To undertake a comparative analysis of international legal frameworks governing AI-assisted forensic toxicology in jurisdictions such as the United States, the European Union, the United Kingdom, and Australia.

6. To propose legal and policy reforms for the effective regulation and admissibility of AI-assisted forensic toxicology in India.

D. Research Questions

1. To what extent do limitations in traditional toxicological methods affect the prosecution's ability to establish causation and mens rea in poisoning cases under the Bharatiya Nyaya Sanhita, 2023?
2. Can AI-assisted toxicological screening enhance evidentiary certainty in detecting novel psychoactive substances and plant toxins such as *Abrus precatorius* and *Nerium oleander*, thereby strengthening the chain of circumstantial evidence?
3. Whether AI-generated toxicological evidence can be admissible and reliable as expert opinion under Section 39 of the Bharatiya Sakshya Adhiniyam, 2023 (BSA)?

E. Research Hypotheses

1. The study argues that the inability of traditional forensic toxicology to detect new psychoactive substances and plant-derived poisons creates large evidentiary gaps in poisoning prosecutions, making it difficult for the prosecution to prove causation and mens rea beyond a reasonable doubt. It is further hypothesised that the use of Artificial Intelligence-assisted forensic toxicology will lead to improved accuracy of toxin detection, increased scientific reliability, strengthened circumstantial evidence chain and thus improve the efficiency of criminal prosecution in poisoning cases.
2. Moreover, the study further hypothesises that the absence of an overarching legal framework for the admissibility, reliability and regulation of AI-generated toxicological evidence creates uncertainty in its acceptance by the Indian courts. It is hoped that the advent of clear statutory standards, validation protocols and regulatory safeguards for AI-assisted forensic toxicology will increase judicial confidence, ensure procedural fairness and

promote the effective integration of AI-generated scientific evidence into the criminal justice system.

F. Research Methodology

This study utilizes a doctrinal (qualitative) approach because it analyzes the legal and evidential dimensions of the application of AI-assisted forensic toxicology for the prosecution of cases of poisoning. The research adopts an analytical and comparative approach to the study of the provisions, cases, and principles of criminal liability and the law of expert evidence and forensic science as contained in the Bharatiya Nyaya Sanhita, 2023, Bharatiya Sakshya Adhiniyam, 2023, Bharatiya Nagarik Suraksha Sanhita, 2023, the Narcotic Drugs and Psychotropic Substances Act, 1985, the Poisons Act, 1919, and other related laws. The study examines landmark decisions of the Supreme Court of India and of select foreign jurisdictions to evaluate the admissibility and evidential scope of AI-assisted forensic toxicology.

The research utilizes primary sources such as legislation, case law, governmental publications, and inter-governmental legal instruments, as well as secondary sources such as books, published articles, papers, law commission reports, forensic science publications, conference papers, and recognized online databases pertaining to artificial intelligence, forensic toxicology, criminal law, and evidence law. A comparative legal system approach has been adopted to examine the regulatory frameworks pertaining to AI-assisted forensic evidence in the United States, the European Union, the United Kingdom, and Australia. By means of critical legal analysis, the study intends to identify the gaps in the legal system of India and propose relevant legal, procedural, and policy recommendations to ensure the safe, effective, and legally sound application of AI-assisted forensic toxicology within the Indian criminal justice system.

IV. CONCEPTUAL FRAMEWORK

This study looks at where criminal law, forensic toxicology, evidence rules, and artificial intelligence all meet, especially when it comes to prosecuting poisoning cases. Poisoning is an act in criminal law where a person administers a toxic substance to another individual that can lead to injury or death. Poisoning is tricky in criminal law;

people usually commit it in secret, there's barely any clear evidence left behind, and you need science to figure out what really happened. In India, cases such as these fall mainly under the Bharatiya Nyaya Sanhita, 2023 (BNS). Establishing a charge of poisoning requires proof of both *actus reus* and *mens rea*, which may not always be easily achieved, as poisoning occurs clandestinely. There is also the Poisons Act of 1919⁷, which lets State Governments set rules for how people can possess, transport, sell, and distribute certain poisons. But it's mostly about prevention, not punishment.

Conditions required for establishing proof of a poisoning act include death occurring due to poisoning, the accused having possession of the poison, being in the position to administer the poison to the victim, and having a motive behind the act. Modern-day cases of poisoning can be challenging owing to substances such as novel psychoactive substances (NPS).

Novel Psychoactive Substances (NPS) are chemical substances that are used to avoid regulations regarding drugs. Laws such as the Narcotic Drugs and Psychotropic Substances Act of 1985⁸ provide control over several drugs. However, substances like NPS are often unregulated due to constantly changing chemical structures, thereby making it hard to prove *mens rea*.

However, there are no specific provisions for plant-based poisons like *Abrus precatorius* and *Nerium oleander* to be prohibited substances. There is an obvious evidence problem here. The prosecution must prove all such circumstances to prove their intention. It is often observed by the courts that mere possession of poison cannot be regarded as adequate unless there is a definite intention behind it. As observed in the case of *Anant Chintaman Lagu v. State of Bombay*,⁹ the conviction was justified despite the presence of strong evidence suggesting intentional poisoning. This case set a precedent that the conviction for the offence of poisoning would be valid even in the

⁷ The Poisons Act, 1919 (Act 12 of 1919).

⁸ Narcotic Drugs and Psychotropic Substances Act, 1985, § 8.

⁹ *Anant Chintaman Lagu v. State of Bombay*, AIR 1960 SC 500: (1960) 2 SCR 460 (Hidayatullah, Das and Sarkar JJ.).

absence of an identification of the poison in the post-mortem or chemical expert reports.

Moreover, Section 109 of the Bharatiya Sakshya Adhiniyam, 2023 (BSA)¹⁰ incorporates the doctrine relating to facts especially within the knowledge of a person. This provision may become relevant in poisoning cases committed in secluded settings, such as within a household, where the circumstances surrounding access to, possession of, or administration of the poison may be particularly within the knowledge of the accused. However, Section 109 does not relieve the prosecution of its primary burden to prove causation, administration of poison, and mens rea beyond reasonable doubt. Section 106 BSA, by contrast, concerns the general burden of proving a particular fact and should not be cited for the “special knowledge” doctrine. Thus, poisoning prosecutions present a dual evidentiary challenge: first, scientific uncertainty in identifying the poison, and second, legal difficulty in proving the mental element through a complete and reliable chain of circumstances.

V. THE HISTORICAL ORIGINS OF AI IN FORENSIC TOXICOLOGY

A. AI in Forensic Toxicology

The advent of artificial intelligence and its integration into forensic toxicology represent a gradual but revolutionary transition from manual chemical procedures to evidence-based and computer-generated decisions within criminal justice institutions. A chronological approach to the timeline of forensic toxicology reveals important events that had legal and scientific importance.

The first scientific basis for forensic toxicology was created in 1814, when Mathieu Orfila¹¹ became known as the founder of forensic toxicology due to his innovative approach to analysing poisons using chemical methods. The contribution made by Orfila became one of the milestones in the field of toxicology and helped establish toxicology as an essential method for gathering evidence in criminal cases.

¹⁰ Bharatiya Sakshya Adhiniyam, 2023, §§ 106, 109.

¹¹ Mathieu Joseph Bonaventure Orfila, *Traité des poisons tirés des règnes minéral, végétal et animal; ou toxicologie générale, considérée sous les rapports de la physiologie, de la pathologie et de la médecine légale* (Crochard, Paris, 1814).

The establishment of an association called TIAFT took place in London in 1963.¹² It became the starting point of globalisation, standardisation, and the dissemination of knowledge among forensic toxicologists and led to professionalisation at the international level.

Digitalisation of toxicology started in 1985, when TOXNET, the U.S. National Library of Medicine database dedicated to toxicological issues, was launched.¹³ This database became the first source of massive amounts of toxicological information available online.

In the latter part of the 1980s, early computational models like QSAR began using primitive neural networks to predict the toxicity of molecules, marking the start of the journey into computational toxicology, which involves the analysis of chemical properties through algorithms and not only experimentation.

During the 1990s, there came the emergence of expert systems used for the interpretation of GC-MS data, and they became the first attempt at computer assistance in identifying compounds. It was during this time that computers started helping forensic experts in their work.

The next great leap forward was made in 2007 when the ToxCast project was initiated by the U.S.¹⁴ Environmental Protection Agency, creating a huge dataset that could be used with machine learning to aid predictive toxicology, thus making AI more credible in science.

The popularisation of HRMS technologies circa 2010 resulted in an exponential surge in data production, which required machine learning tools due to data complexity and

¹² The International Association of Forensic Toxicologists (TIAFT), History of TIAFT, <https://tiaft.org/about/the-association/> (last visited 18 May 2026). [Founded in London, 21 April 1963.]

¹³ U.S. National Library of Medicine, TOXNET: Toxicology Data Network (established 1985, databases subsequently migrated to <https://www.nlm.nih.gov/toxicology>), <https://www.nlm.nih.gov> (last visited 18 May 2026).

¹⁴ U.S. Environmental Protection Agency, Toxicity ForeCaster (ToxCast) Program (launched 2007, Center for Computational Toxicology and Exposure), <https://www.epa.gov/comptox-tools/toxicity-forecasting-toxcast> (last visited 18 May 2026).

volume. Traditional analytical procedures proved to be incapable of coping with such massive amounts of information generated by HRMS.

From 2013 through 2016, machine learning approaches, including SVM and Random Forests, were successfully deployed in real-life forensics facilities. Such deployment could be regarded as the shift from artificial intelligence concepts to their application in practice for forensic toxicology purposes.

In 2018, the NPS Discovery programme launched in the USA, relying on the use of AI-assisted systems for the purposes of surveillance and novel psychoactive substances' identification. It could be considered the key moment in dealing with the challenges caused by constantly evolving illegal psychoactive substances in the context of regulation and forensics.

By 2022, the application of AI-assisted forensic toxicology in criminal courts had emerged in countries including Australia, the USA, and Germany. This milestone represents the move of the role of AI in forensic toxicology from the position of just analytical assistance to that of an evidence-based one.

Given the rising importance of AI in this field, TIAFT created the TTF1 AI Task Force in 2024, illustrating how international organisations are beginning to recognise the significance of AI in forensic toxicology, as well as the need for standardisation, validation, and proper ethics.

Finally, in 2024, the European Union adopted Regulation (EU) 2024/1689, commonly known as the Artificial Intelligence Act, which entered into force on 1 August 2024. The Act classifies certain AI systems used in law enforcement and evidentiary assessment as high-risk AI systems, thereby marking an important transition towards proactive regulation of AI technologies in criminal investigations. This development is significant for forensic AI because it emphasises compliance, documentation,

transparency, human oversight, and reliability in contexts where AI-generated evidence may affect fair-trial rights.¹⁵

This timeline shows how scientific and technological progress have been instrumental in transforming the field of forensic toxicology, advancing the field to the point where AI can be utilised. However, the rise of AI also brings legal implications regarding the use of AI evidence, which means that legal frameworks will become even more critical.

B. Role of AI in Toxicology: Technological Advancements

The incorporation of AI in toxicology marks a paradigm shift from a reactive approach to a predictive and data-intensive approach. With respect to poisonings like NPS and plant toxins, AI helps overcome the limitations posed by scientific factors, which have always served as poor evidence.

- 1. Detection and Identification of Toxins:** By leveraging machine learning on large chemical databases, AI systems can identify both known and unknown toxic substances. Contrary to traditional toxicology methods that depend on the use of reference standards, AI systems are capable of detecting structural analogues and new substances.¹⁶
- 2. Predictive toxicology and behaviour modelling:** Using predictive toxicology through artificial intelligence, the forensic specialist will be able to analyse and evaluate the behaviour of the poison inside the human body, taking into account all aspects of absorption, distribution, metabolism, and even the effects that lead to the death of the victim. The method can help predict the time when the poison was consumed by the victim and how it influenced their physiological condition. It will allow constructing a realistic

¹⁵ Regulation (EU) 2024/1689 of the European Parliament and of the Council of 13 June 2024 laying down harmonised rules on artificial intelligence (Artificial Intelligence Act), OJ L, 12 July 2024, entered into force 1 August 2024.

¹⁶ Andrew D. Maynard and Dana R. Fisher, Computational Toxicology, 45 Ann. Rev. Pharmacol. Toxicol. 123 (2005).

chronological sequence of events, which in turn will make it easier to prove causation.¹⁷

3. **Pattern recognition and data fusion:** The ability of artificial intelligence to analyse multiple sources of information, be it medical records, forensic lab results, environmental exposure, or even digital information like purchase behaviour and Internet activity, allows the system to make connections between the information that may have been difficult to discern otherwise. This helps in distinguishing cases of accidental poisoning from intentional acts of poisoning by highlighting connections that were previously unknown or overlooked.¹⁸
4. **Forensic Botany and Analysis of Natural Poisons:** In poisons obtained from plants, artificial intelligence-enabled forensic botany determines the precise type of plant used, extraction techniques, and the degree of its toxicity. This is essential in the case of *Abrus precatorius* and oleander, in which the effectiveness of the poison varies based on the preparation techniques. This could help establish whether the poison was applied in a prepared or concentrated manner, suggesting forethought and planning in advance, which are key characteristics of intent.
5. **Reduction of human error and subjectivity:** Forensic toxicology analysis is reliant on the expertise of the individuals involved, whose interpretation of results may differ from person to person. Artificial intelligence ensures that there is a standard way of analysing diagnoses and forensic evidence, thus minimising subjectivity and ensuring that results are reliable.¹⁹ AI makes forensic toxicology more than just forensic assistance and a primary evidence-gathering tool. AI is able to assist in filling in scientific holes that have existed for a long time in the investigation of poisonings.

¹⁷ OECD, *Artificial Intelligence in Society* (OECD Publishing, Paris, 2019).

¹⁸ National Institute of Standards and Technology, *Artificial Intelligence Risk Management Framework (AI RMF 1.0)*, NIST AI 100-1 (U.S. Department of Commerce, Gaithersburg, 2023).

¹⁹ National Institute of Standards and Technology, *Artificial Intelligence Risk Management Framework (AI RMF 1.0)*, NIST AI 100-1 (U.S. Department of Commerce, Gaithersburg, MD, 2023).

VI. INTERNATIONAL COMPARATIVE PERSPECTIVE

From the foregoing comparative analysis, that developed nations such as the US, EU, UK, and Australia have made arrangements to have a systematic approach in governing the introduction and assessment of AI-enabled forensic evidence, specifically in complicated poisoning cases. The above-listed countries have implemented systems of judicial gatekeeping, reliability criteria, mandatory disclosure laws, forensic testing certifications, and legislation measures such as analogue provisions to combat new substances.

A. The United States

The United States is home to the most advanced system of forensic evidence admissibility, which was based upon the precedent set by the case of *Daubert v. Merrell Dow Pharmaceuticals, Inc.*, 509 U.S. 579 (1993).²⁰ The Daubert Test (1993) creates a system through which the admissibility of expert scientific testimony can be evaluated in a systematic manner by making the trial judge the gatekeeper for such evidence. As the gatekeeper, the trial judge must evaluate not only the conclusions reached by the expert but also whether the scientific methodology used to arrive at those conclusions is valid.²¹ In evaluating this issue, the following factors play a crucial role: whether the theory is testable or falsifiable, whether there exists an error rate associated with the theory, and whether it has been peer-reviewed and accepted in the scientific community.²²

Significantly for AI toxicology, Rule 702 reads that the proponent must show that there is more than a fifty per cent probability that the requirements of Rule 702 have been met. The likelihood of establishing reliability is higher when the report contains a description of the methodology used and the limitations thereof. In terms of the Daubert standard, the revisions to the Federal Rules of Evidence in 2023 further emphasise that the party presenting expert testimony carries the responsibility of

²⁰ *Daubert v. Merrell Dow Pharmaceuticals, Inc.*, 509 U.S. 579 (1993) (Supreme Court of the United States, per Blackmun J.).

²¹ Controlled Substance Analogue Enforcement Act of 1986 (U.S.A.), 21 U.S.C. § 813.

²² Federal Rules of Evidence (U.S.A.), r. 702 (as amended 1 December 2023).

establishing its reliability. When it comes to cases involving homicides by means of new psychoactive substances (NPS), the U.S. courts have used the Daubert test to question the use of novel analytical technologies in such prosecutions. In such cases, it should be shown that: the testing error rate of the used AI model in relation to the library of NPS compounds; the peer-review of the method for LC-QTOF-MS analysis; and finally, the general acceptance of AI-assisted screening for suspect substances in the field of forensic toxicology. Proprietary databases utilised to evaluate the accuracy of these models are often not available to the public. The trade secret status of vendor algorithms can hamper peer review. Factors like model drift, training data, and environment can influence the testing error rates. Therefore, without sufficient validation, many AI programs fail to satisfy the Daubert criteria.

The Controlled Substance Analogue Enforcement Act of 1986, codified at 21 U.S.C. § 813, is an important legal safeguard because it permits a controlled substance analogue, when intended for human consumption, to be treated as a Schedule I controlled substance for purposes of federal law. This implies that even without an NPS being placed under scheduling when a murder takes place, the prosecution can rely on analogical scheduling, where the issue of mens rea becomes whether the defendant was aware that the substance caused effects analogous to those of a drug under scheduling. AI toxicology provides evidence of such an inference through structure and pharmacology.

B. European Union Approach

The European Union has developed the world's first complete set of rules concerning the use of artificial intelligence: The European Union formally adopted the AI Act in 2024, establishing the world's first comprehensive legal framework for the regulation of artificial intelligence. Its provisions are being implemented in phases according to the timetable prescribed under the Regulation. According to Annex III to the EU AI Act, an AI system intended to be used by or on behalf of law enforcement authorities in support of law enforcement authorities to assess the reliability of evidence during an investigation or prosecution of criminal offences constitutes a high-risk AI system. Also, any AI system intended to assess the likelihood of a natural person committing

crimes or being guilty of re-offending, or to determine personality traits or characteristics and past criminal behaviour, falls within the category of high-risk AI systems. High-risk AI systems must undergo numerous obligations before being placed on the market, such as providing detailed documentation on the system and its purpose to enable authorities to verify their compliance with all relevant regulations.²³

The implementation of obligations relating to high-risk AI systems under the EU AI Act is subject to the phased timetable currently applicable under European Union law. The compliance schedule has been updated following subsequent legislative developments, including the 2026 Digital Omnibus measures, and therefore should be understood in accordance with the latest regulatory framework. The AI Act in the European Union provides detailed obligations for high-risk AI systems, particularly where AI is deployed in law-enforcement, criminal-investigation, or evidentiary-assessment contexts. However, after the 2026 AI Omnibus amendments, the compliance date for Annex III stand-alone high-risk AI systems has been deferred to 2 December 2027. Accordingly, AI-assisted forensic toxicology tools used to assess the reliability of evidence in criminal investigations should be analysed as Annex III high-risk systems, subject to obligations relating to risk management, data governance, technical documentation, transparency, human oversight, accuracy, robustness, and post-market monitoring from the revised compliance date.

Where AI toxicology is used in poisoning cases, to either assess the evidence presented or to determine whether the accused was aware of their actions, the guidelines provide that the AI system must be documented and registered; undergo conformity assessment, provide human oversight measures, provide information regarding training data quality, and post-market monitoring. The application of AI technology that finds an NPS substance in the postmortem blood of an individual and makes inferences on mens rea qualifies as high risk.

²³ OECD, *Artificial Intelligence in Society* (OECD Publishing, Paris, 2019).

The EU model is based on the EU Charter of Fundamental Rights, which includes the right to a fair trial, presumption of innocence, and the right to an effective remedy. The courts of EU member states have relied on these rights when demanding that AI-produced forensic evidence be intelligible in terms comprehensible to the defendant and his/her counsel. The right to a fair trial might be violated by the introduction of unintelligible AI-generated forensic evidence. An algorithmic decision with its rationale incomprehensible to a person cannot be logically contested by him/her. The European Medicines Agency and the European Chemicals Agency have both approved the application of AI-driven toxicity predictions for regulatory filings, thus creating a reliable database of peer-reviewed AI toxicology methodologies that can be utilised in forensic cases.

C. The United Kingdom

The UK rules concerning the use of expert evidence in criminal cases are contained mainly in Part 19 of the Criminal Procedure Rules 2025.²⁴ The latest changes have been made to the rules of 2020, which have now been withdrawn. According to Rule 19.4, the report prepared by an expert in a case must contain certain facts that the court may rely upon to evaluate whether the expert opinion is admissible in a trial; it must state the expert's credentials and professional qualifications; and it should also include a statement declaring that the expert is aware of his or her duty to the court. If a party wishes to tender expert evidence into the trial, it shall serve with the report any information which comes to its knowledge and could potentially discredit the expert's opinion. Additionally, the party shall, if requested, provide the other side with copies of any examination or test used as a basis for forming the expert's opinion.

The Forensic Science Regulator (FSR)²⁵ of the UK, which operates under the authority of the Forensic Science Regulator Act of 2021, establishes standards for the provision and practice of forensic science. Codes of Practice made under the Forensic Science Regulator set standards in terms of laboratory accreditation to international

²⁴ Criminal Procedure Rules 2025, SI 2025/909 (UK), r. 19.4 (Content of Expert's Report) (in force 6 October 2025).

²⁵ Forensic Science Regulator Act 2021 (UK), c. 14 (Royal Assent 29 April 2021).

standards, such as ISO 17025, as well as validation of the analytical techniques utilised in forensic analysis, including those that rely on artificial intelligence. Parties introducing expert evidence should notify other parties of any matter that may undermine the reliability of their testimony, as well as any information that may affect the integrity of the expert giving the testimony.

The Streamlined Forensic Reporting system in the UK allows for graded reports by experts, where an SFR1 will summarise findings, while in case of any disagreement by the defence, an SFR2 will offer all the analysis of the report. As pointed out in 2005 by the Science and Technology Select Committee in the UK House of Commons in their recommendation for the creation of a Forensic Science Advisory Council for the regulation of forensic evidence in the UK: The lack of a standard protocol for validating scientific techniques before introducing them into legal proceedings is wholly unacceptable, and judges cannot assess scientific validity without scientific input.

The UK has traditionally followed a common law principle that presumes the reliability of computer outputs. The same principle was reaffirmed through statutes enacted in several common law countries, which provided that the output of any approved AI/ML system was presumed to be true unless otherwise contested. Under such circumstances, the scope for contesting the reliability of the said AI/ML system remained limited. However, the Horizon scandal by the UK's postal service demonstrated that the said principle was fraught with dangers, as it led to the prosecution of innocent persons owing to erroneous computer outputs.²⁶

It is necessary to highlight how the above learning can guide the use of AI in forensic toxicology. Presuming the reliability of any AI-generated report, particularly when issued by a laboratory that is approved by the government, can result in the undue acceptance of potentially defective reports. It is particularly pertinent in light of

²⁶ Criminal Procedure Rules 2025, SI 2025/909 (UK), r. 19.4 (in force 6 October 2025); Forensic Science Regulator Act 2021 (UK), c. 14 (Royal Assent 29 April 2021); Gary Edmond, Simon Cole, Emma Cunliffe and Andrew Roberts, *Admissibility Compared: The Reception of Incriminating Expert Evidence (i.e., Forensic Science) in Four Adversarial Jurisdictions*, 3 U. Denv. Crim. L. Rev. 31 (2013); Law Commission (UK), *Expert Evidence in Criminal Proceedings in England and Wales*, Law Com No 325 (The Stationery Office, London, 2011).

Section 329 of the BNSS, which provides for the admission of CFSL reports unless challenged.

D. Australia

The rule on the admissibility of expert evidence in Australia follows *Dasreef Pty Ltd v Hawchar* (2011) HCA 21, under which expert opinion must be based on specialised knowledge derived from training, study, or experience. Recent Australian poisoning prosecutions also demonstrate the practical importance of integrating toxicological, botanical, digital, and circumstantial evidence. In *DPP v Patterson* [2025] VSC 557, the Supreme Court of Victoria recorded that Erin Patterson was convicted of three counts of murder and one count of attempted murder after deliberately serving a meal containing death cap mushrooms. The case illustrates how complex poisoning prosecutions may depend on a combined evidentiary narrative rather than toxicology alone. However, the Patterson proceedings should be cited with caution: as of the current appeal listing, both the conviction appeal and the DPP's sentence appeal are listed before the Victorian Court of Appeal for hearing on 19–20 August 2026.

VII. EMERGENCE OF ARTIFICIAL INTELLIGENCE IN FORENSIC TOXICOLOGY IN INDIA

AI is starting to make its mark in forensic toxicology across India. And while there's still no nationwide, fully AI-powered system, more labs and universities are jumping in, especially since 2021. They've been exploring machine learning and other data-driven approaches, hoping to sharpen the accuracy and speed of toxicology investigations.

With more advanced tools like Gas Chromatography–Mass Spectrometry (GC-MS) and Liquid Chromatography–Mass Spectrometry (LC-MS) now common in forensic labs, AI is finding its place, too. These AI systems spot complex chemical patterns and help cut down on mistakes during toxicology tests. In India, there's a real push from both researchers and forensic institutions to modernise their labs with digital tech and smart systems. But right now, using AI in forensic toxicology here is mostly limited to

research, experiments, and a few pilot projects. It's still far from being standard practice everywhere.

A. Institutional Infrastructure in India

The principal institutional framework for forensic toxicology in India is represented by the Central Forensic Science Laboratories (CFSLS) working under the Directorate of Forensic Science Services (DFSS), Ministry of Home Affairs, Government of India.²⁷ On the instrumental front, Indian forensic toxicology laboratories currently use advanced analytical technologies like gas chromatography-mass spectrometry (GC-MS), liquid chromatography-tandem mass spectrometry (LC-MS/MS), high-resolution mass spectrometry, DNA profiling systems and automated firearms identification systems like IBIS.²⁸ While these are significant technical advances, it is important to note that they are data-intensive but not, in and of themselves, AI in the machine-learning sense; they are sophisticated detection tools that are operated and interpreted by human forensic experts. At this stage, the operationalisation of genuine AI integration into forensic toxicology workflows at Indian CFSLS is aspirational rather than operational.²⁹

B. Research and Academic Developments around AI Applications in Forensic Toxicology

Researchers at the All India Institute of Medical Sciences (AIIMS), Bibinagar, Hyderabad, have explored the role of AI in medico-legal autopsy, forensic toxicology and disaster victim identification.³⁰ In parallel, scholars associated with AIIMS institutions have separately examined applications of AI in the field of forensic

²⁷ Directorate of Forensic Science Services, Ministry of Home Affairs, Government of India, About DFSS, available at <http://dfs.nic.in> (last visited May 2026). See also Press Information Bureau, Ministry of Home Affairs, Government of India, 'Forensic Labs' (Rajya Sabha Written Reply by Minister of State, Shri Bandi Sanjay Kumar), PIB Release No. 2085688, available at <https://www.pib.gov.in/PressReleasePage.aspx?PRID=2085688> (last visited May 2026).

²⁸ Central Forensic Science Laboratory, Chandigarh, About CFSL Chandigarh, Directorate of Forensic Science Services, Ministry of Home Affairs, Government of India, available at <https://www.cfslchandigarh.gov.in> (last visited May 2026).

²⁹ Ibid. See further Directorate of Forensic Science Services, Ministry of Home Affairs, *supra* n. 33.

³⁰ Pragnesh Parmar, 'The Integration of Artificial Intelligence in Forensic Medicine and its Applications in Medico-Legal Autopsy, Forensic Toxicology, and Disaster Victim Identification' (2023) 8(4) International Journal of Forensic Sciences 1, DOI: 10.23880/ijfsc-16000331.

medicine and criminal investigation.³¹ Scholars at the Datta Meghe Institute of Medical Sciences, Nagpur, have published foundational work describing the potential of AI in the analysis of toxins, the collection of medico-legal samples from body cavities, the detection of pathological changes in organs, and the estimation of post-mortem intervals, all of which are directly relevant to poisoning and NDPS prosecutions.³²

The IP International Journal of Forensic Medicine and Toxicological Sciences (2024) has once again reviewed the use of AI in Indian forensic medicine and has underlined that AI delivers results with higher accuracy, efficiency, and cost-effectiveness compared to traditional methods, but has pointed out that its implementation is still in its early stages.³³ AI started gaining attention in forensic toxicology worldwide between 2018 and 2020. In India, though, conversations and research about using AI in this field really picked up steam in 2022. You can see this slow shift as part of India's push to modernise how they handle forensic investigations and boost the reliability of its criminal justice system.

VIII. ADMISSIBILITY OF AI ASSISTED TOXICOLOGY IN THE COURT OF LAW IN INDIA

The question of the admissibility of AI-assisted toxicology in India remains contentious. As per *Section 39 of the Bharatiya Sakshya Act, 2023*³⁴ and general principles of science and forensic toxicology, such evidence is relevant to the court to opine on a

³¹ Kumar S, Shah B, Shandil A, Kumar R and Singh G, 'Use of Artificial Intelligence in the Field of Forensic Medicine & Criminal Investigation: A Way Forward' (2024) 9(2) IP International Journal of Forensic Medicine and Toxicological Sciences 73, DOI: 10.18231/j.ijfmts.2024.014. See also Gajbhiye S et al., 'Application of Artificial Intelligence in the Field of Forensic Medicine' (2021) 21(4) Medico-legal Update 56 (authors affiliated with the Department of Forensic Medicine and Toxicology, All India Institute of Medical Sciences, Patna, Bihar).

³² Toshali D Wankhade, Sundeep W Ingale, Prakash M Mohite and Nandkishor J Bankar, 'Artificial Intelligence in Forensic Medicine and Toxicology: The Future of Forensic Medicine' (2022) 14(8) Cureus e28376, DOI: 10.7759/cureus.28376 (authors affiliated with Datta Meghe Medical College and Jawaharlal Nehru Medical College, Datta Meghe Institute of Medical Sciences, Nagpur and Wardha).

³³ Praveen Dixit, Udai Shankar Sinha, Rajeev Kumar, Mamta Kumari, Hitesh Chawla, Vikas Chandra and Aditya Anand, 'Digital Detectives: Exploring the Integration of Artificial Intelligence in Indian Forensic Medicine' (2024) 9(4) IP International Journal of Forensic Medicine and Toxicological Sciences 124, DOI: 10.18231/j.ijfmts.2024.026.

³⁴ Bharatiya Sakshya Adhiniyam, N.o. 47 of 2023, § 39.

field where specific knowledge is required. AI-assisted toxicology, as one of the tools used by forensic scientists, also follows the general principle of forensic toxicology and therefore requires a highly qualified human expert to present their opinion. The difficulty arises when the AI system is forced to act as a quasi-autonomous device, and therefore, the admissibility of this type of analysis cannot equate to expert evidence.

And the issue of admissibility of AI outputs also falls under Section 63 of Bharatiya Sakshya Adhiniyam, 2023 (BSA),³⁵ dealing with electronic records. This calls for the necessity to have the system certified, and the integrity and reliability of data and procedures through which the output was generated.³⁶

Cases like *Anvar P.V. v. P.K. Basheer*³⁷ have made it clear that for electronic evidence to be considered valid, it needs to be fully compliant with Section 65B of IEA (now Section 63 of BSA), and similarly, for technical evidence to be used as an aid to proving a case, it needs to satisfy particular criteria. The same thing can be said about the use of AI-generated forensic evidence, as highlighted by the Supreme Court case of *Arjun Panditrao Khotkar v. Kailash Kushanrao Gorantyal*.³⁸

AI will be viewed as merely a tool to assist with analysis, but not an independent source of evidence whose results must be confirmed through conventional forensic techniques and expert testimonies in court. This approach complies with the conservative nature of the Indian court system when working with innovative technologies.

In general, AI toxicology will significantly increase the accuracy of evidence and allow such evidence to be admitted into court; however, it will be possible only if this takes place within the framework of the applicable laws and fair proceedings in the judicial system.

³⁵ Bharatiya Sakshya Adhiniyam, No. 47 of 2023, § 63.

³⁶ Information Technology Act, 2000, § 85B.

³⁷ *Anvar P.V. v. P.K. Basheer*, (2014) 10 SCC 473 (Lodha CJ, Kurian Joseph and Nariman JJ., 18 September 2014).

³⁸ *Arjun Panditrao Khotkar v. Kailash Kushanrao Gorantyal*, (2020) 7 SCC 1 (Nariman, Ravindra Bhat and Ramasubramanian JJ., 14 July 2020).

IX. THE STATUTORY ARCHITECTURE GOVERNING POISON OFFENCES IN INDIA

A. Indian Penal Code, 1860 (IPC) / Bharatiya Nyaya Sanhita, 2023 (BNS)

The BNS provides a hierarchical scheme of offences involving poison that is aligned with varying levels of mens rea:

Section 280 BNS provides for penalties for negligence in dealing with a poisonous substance, concerning risking human lives or causing injury. Culpable homicide, which may include causing death through the use of a poisonous substance, is provided under Section 100 of the Bharatiya Nyaya Sanhita (BNS) 2023. Murder, including death through the use of a poisonous substance with the intention of killing, is mentioned in Section 101 of BNS. Section 106 of the Bharatiya Nyaya Sanhita (BNS) provides for causing death through rash or negligent acts of poisoning. Under Section 118(1) of the Bharatiya Nyaya Sanhita (BNS), the injury inflicted through poison becomes more serious in nature, thus deserving severe punishments. Section 123 of BNS penalises anyone who uses poison or any kind of stupefying, intoxicating, or unhealthy substance to cause injuries.³⁹

The importance of the statutory hierarchy cannot be overstated. The distinction between liability for rash or negligent acts causing death, culpable homicide not amounting to murder, and murder by poison depends primarily on the mental element proved by the prosecution. Where poisoning is accompanied by the requisite intention or knowledge for murder, liability may arise under Sections 101 and 103 of the Bharatiya Nyaya Sanhita, 2023; where the case falls short of murder but amounts to culpable homicide, Section 105 may apply. Thus, forensic evidence regarding causation, administration of poison, and the accused's mental state may substantially influence the classification of the offence.

B. Reporting Obligations and Procedural Law (Cr.PC/ BNSS)

³⁹ Bharatiya Nyaya Sanhita, 2023, §§ 100–101, 106, 118, 123.

Sections 174 to 176 of the Code of Criminal Procedure, 1973 (Section 194-196 of BNSS) lay out how police and magistrates handle investigations into suspicious, unnatural, or custodial deaths. The law makes sure evidence, especially in cases like poisoning, is properly collected, stored, and examined. Things like inquest reports, witness statements, and toxicology tests are key to figuring out why someone died, what caused it, and whether there was any criminal intent. Under Section 37 of BNSS 2023,⁴⁰ all cases of homicidal poisoning, whether confirmed or suspected, have to be reported compulsorily to the police. Not doing so makes one liable under Section 203 of the Bharatiya Nyaya Sanhita (BNS).

In addition to the existing statutory framework, India has taken significant steps towards regulating artificial intelligence through policy-based governance initiatives. The Ministry of Electronics and Information Technology (MeitY) issued the AI Governance Guidelines in November 2025 to promote the responsible, transparent, safe, and accountable development and deployment of AI systems. Although these guidelines do not presently constitute binding legislation, they provide an important policy framework emphasising fairness, transparency, human oversight, privacy protection, accountability, and risk-based governance. In the context of AI-assisted forensic toxicology, these principles support the need for validated AI models, explainable decision-making, proper documentation, and human supervision to ensure that AI-generated forensic evidence satisfies the requirements of fairness and reliability in criminal proceedings.

X. EVIDENTIARY CHALLENGES

A. The Mens Rea Proof Burden on Prosecution

The prosecution often has trouble reliably identifying and proving the nature and effects of the poisoning agent when trying to prove mens rea beyond a reasonable doubt. This makes it harder to use evidence to infer intent. It is the position of the Supreme Court that, as the prosecution bears the burden of proving that the crime

⁴⁰ Bharatiya Nyaya Sanhita, 2023 (BNS)

was committed by the accused, the prosecution also bears the burden of proof throughout the trial.⁴¹

When figuring out if a crime is culpable homicide under Section 100 of the Bharatiya Nyaya Sanhita (BNS), 2023 (which is the same as Section 299 IPC), or murder under Section 101 BNS (which is the same as Section 300 IPC), the elements of intention and knowledge are very important. In poisoning cases, this evaluation is especially intricate due to the lack of direct evidence, such as a weapon, observable injuries, or eyewitnesses, necessitating dependence on circumstantial and scientific evidence. In cases involving plant alkaloids or novel psychoactive substances (NPS), the challenge lies not in the substance's impossibility, but in the complexity of definitively identifying it and determining its lethal effects and dosage.⁴² This is by far the most crucial aspect, and the toughest one too, as it is very hard to prove mens rea in poisoning cases. In the case of *Anant Chintaman Lagu v. State of Bombay*,⁴³ the conviction was upheld since the prosecution proved that the accused had engaged in a series of deliberate acts, such as preparing and administering the poison.

The opposite happens when intention cannot be proven. The Supreme Court has always said that if the prosecution can't prove the key parts of Section 101 BNS, especially mens rea, beyond a reasonable doubt, the crime can't be called murder. Instead, it might be culpable homicide not amounting to murder under Section 100 BNS. This, however, does not mean that the person will be automatically found not guilty or that the outcome is already known. If the prosecution can't prove beyond a reasonable doubt what kind of poison it was, how it was given, and how deadly it was, it creates reasonable doubt.

⁴¹ David H. Kaye, David E. Bernstein, et al., *The New Wigmore: A Treatise on Evidence: Expert Evidence* (Wolters Kluwer Law & Business, Austin, 2nd edn., 2011).

⁴² Ryan Calo, "Artificial Intelligence Policy: A Primer and Roadmap" 51 UC Davis L. Rev. 399 (2017); Frank Pasquale, *The Black Box Society: The Secret Algorithms That Control Money and Information* 3–27 (Harvard University Press, Cambridge, MA, 2015); OECD, *Artificial Intelligence in Society* (OECD Publishing, Paris, 2019).

⁴³ *Anant Chintaman Lagu v. State of Bombay*, AIR 1960 SC 500.

B. Admissibility Of AI-Generated Toxicology Evidence Under the BSA, 2023

The Bharatiya Sakshya Adhiniyam (BSA) 2023 is the principal legislation providing for the legal rules that govern AI-generated toxicology reports as admissible in courts. Though this Act makes significant improvements by updating the Indian law with the modern concept of admissible electronic documents, it lacks any concrete guidelines regarding AI-generated outputs.

In addition, the IT Act 2000, specifically Section 85B and Section 63 of BSA, creates a presumption of trustworthiness of secure electronic documents and allows certified digital evidence to be admitted in court. However, it fails to solve critical problems related to biased algorithms, non-explainability, and accountability associated with errors in such AI technologies. Thus, there remains room for improvement as far as AI-related issues are concerned.

C. Forensic And Procedural Limitations

The forensic infrastructure in India is plagued by a number of serious deficiencies that hinder the effectiveness of toxicology evidence in the investigation of crimes. Such deficiencies include delayed reporting of chemical test results, inadequate use of modern forensic toxicology methodologies, and a lack of databases on new drugs like Novel Psychoactive Substances (NPS). Besides this, there are certain procedural issues, including inappropriate collection of samples, poor preservation of evidence, and chain-of-custody problems that have undermined the value of forensic evidence. Any negligence on the part of the investigators can jeopardise the entire process.

D. The Expert Witness Framework and AI Under Section 39 BSA

According to Section 39 of the Bharatiya Sakshya Adhiniyam (BSA), 2023, expert opinion is considered as evidence. AI can provide help to experts, but their findings should always be clear, comprehensible, testable, and understandable during judicial proceedings.

AI-assisted results can never serve as independent evidence and require expert witnesses who can justify the methodology used for analysis and the validity of conclusions. At the same time, in case an expert witness cannot explain how he

worked with an AI system because of its opacity, this will have a negative impact on his or her testimony.

Finally, the findings obtained with the help of AI are debatable because of their lack of transparency and verifiability. In view of the fact that judges and lawyers might not possess technological expertise in terms of complex algorithms and computer analysis, their failure to understand the mechanism by which the AI identified a substance would hardly undermine the results, but certainly create some doubts.

E. The Absence of a Forensic Reliability Standard

India does not yet have a binding forensic-specific reliability standard for the admissibility of AI-generated toxicological evidence comparable to Rule 702 of the United States Federal Rules of Evidence or the Daubert framework. However, it would be inaccurate to state that India has no AI governance framework at all. The Ministry of Electronics and Information Technology released the India AI Governance Guidelines in November 2025 as a soft-law, sector-agnostic framework based on seven guiding principles, including trust, people-first development, fairness and equity, accountability, explainability, and safety. These Guidelines recognise the need for risk-based governance, institutional oversight, and sectoral adaptation of existing legal frameworks. Nevertheless, because they are non-binding and do not prescribe courtroom admissibility tests, validation thresholds, error-rate disclosure, laboratory accreditation norms, or defence-access safeguards for forensic AI systems, a specific evidentiary reliability standard remains necessary for AI-assisted forensic toxicology.

XI. CHAIN OF CUSTODY FOR DIGITAL ANALYTICAL DATA

The traditional chain of custody rules in India involve ensuring the safety of evidence collected at the crime scene until analysed. However, the new concept of AI-assisted toxicology calls for an additional safeguard of ensuring the integrity of analytical results, which cannot be achieved by the existing legal instruments.

The process of performing AI-assisted toxicology involves using raw data obtained via mass spectrometry, followed by the processing of these data and matching them against databases. In each of these steps, there may appear data manipulation,

corruption, or malfunction. Although, as required by Section 63(4) of the Bharatiya Sakshya Adhiniyam (BSA),⁴⁴ 2023, all pieces of electronic evidence must be certified; in some cases, it may become rather difficult.

However, it becomes complex while working with cloud-stored data, AI-generated reports, and blockchains. CCTV footage stored on a private server may fail to qualify even if it clearly proves the guilt of the accused due to a lack of proper documentation.

This holds true with even more conviction when it comes to AI toxicology: If the files containing the mass spectrometry data had been stored in the cloud hosted by a private lab and the analysis had taken place via an AI system running on a commercial license and without any publicly available algorithm, then it would be practically impossible to provide the certificate required under Section 63(4).⁴⁵

In such circumstances, especially when the data is stored in third-party servers and analysed using AI-based systems that are commercially licensed but lack transparency, adhering to certification standards can prove to be difficult from a legal perspective. Thus, questions arise as to the evidentiary nature of such toxicology reports rather than making them inadmissible.

A. The Expert Witness Appearance Exemption Under Section 330, BNSS 2023

As per Section 330 of the Bharatiya Nagarik Suraksha Sanhita, 2023, certain expert reports shall be admissible without the appearance of the expert himself in the Court unless the Court or the opposite party requests their appearance. In this way, certain expert reports which have not been challenged will be admissible as evidence even without being put to the test of cross-examination.⁴⁶

The above provision would affect the presentation of AI-based toxicology evidence. Reports made by such experts may not require an appearance in case there is no challenge by the defence to the report. On the other hand, should there be an objection

⁴⁴ Bharatiya Sakshya Adhiniyam, N.o. 47 Of 2023, § 63(4).

⁴⁵ Bharatiya Sakshya Adhiniyam, No. 47 of 2023, § 63(4).

⁴⁶ Bharatiya Nagarik Suraksha Sanhita, No. 46 of 2023, § 330.

from the defence, then the expert himself will have to come and explain how he came up with his conclusions using the AI-based techniques.

B. The NPS Legislative Gap

The NDPS Act, 1985, still acts as the main legal framework in India when dealing with offences involving substances, but this Act is reactionary due to the nature of the scheduling system under this Act, because regulation occurs once there is a specific notification about the particular substance. In cases under the NDPS Act, courts can presume culpability of the offender where he/she dealt with a scheduled substance, thereby providing evidence to the prosecution. Thus, it is difficult to provide evidence on intention and knowledge in cases involving new substances, as they will be beyond the legal jurisdiction. This situation allows manufacturers of synthetic drugs to use regulatory arbitrage to design such substances.

Whereas other countries, such as the US, adopt an “analogue” approach, whereby substances similar in composition or effects to regulated substances are deemed as prohibited substances.

This poses several challenges for the prosecution in the case. So, it will be difficult for the prosecution to prove that the substance is indeed illegal since it is not captured under the current law. Secondly, the prosecution must demonstrate beyond any reasonable doubt that the accused was aware of the harmfulness or toxicity of the drug without relying on any statutory presumption. This means that the burden of proof in establishing the guilty mind of the accused would be very difficult because there will be no statute supporting the prosecution’s claim.

C. Plant Poisons and the Absence of a Specific Regulatory Framework

Some commonly encountered poisonous plants in India are Datura (*Datura stramonium*/metel), oleander (*Nerium oleander*), aconite (*Aconitum* species), strychnos (*Nux vomica*), yellow oleander (*Cascabela thevetia*), and calotropis. These drugs do not find mention in any of the schedules of the NDPS Act; therefore, their regulation is minimal.⁴⁷ The Poisons Act, 1919, provides for certain regulations

⁴⁷ The Poisons Act, 1919 (Act 12 of 1919).

regarding the import and sale of poisons, but there is no provision for criminality of their usage within this act. As a result, cases where plant-based drugs have been used as poison depend upon sections about culpable homicide from the criminal code. This poses an important issue from a forensic point of view, since routine toxicology screens may not be able to identify and quantify the presence of certain alkaloids obtained from plants.

D. Infrastructural And Geographic Inequality in Forensic Capacity

The legal issue that arises in relation to AI-assisted toxicology cannot be divorced from the forensic reality of the Indian forensic system. The use of AI-assisted toxicology analysis in India is restricted to the CFSs in Hyderabad, Chandigarh, and Kolkata and perhaps a small number of academic/private labs. It must be pointed out that the state FSLs are limited to outdated GC-MS machines, insufficient reference databases, and absolutely no AI at all.

Thus, there is a clear legal issue raised by this scenario, as the quality of the toxicology evidence available to a Sessions Court will depend on the state where the crime took place. In one instance, for example, a homicide carried out via plant alkaloids in Tamil Nadu would get AI-assisted analysis from the CFS. The same case in a remote part of another state might be subjected to chemical colour tests and only a generic conclusion of "death caused by poisoning." Such a scenario is likely to be detrimental to the existing problem in the system of personnel shortage and inadequate forensic infrastructure.

E. Judicial Competence, Training, And the Risk of AI Over-Reliance

The first and foremost issue related to the application of AI in toxicology is that courts have to comprehend the complicated technicalities involved in scientific evidence and algorithms. They need to analyse the technical elements of the AI system, its error rate, the validity of the outcomes produced by the system, and the technical concepts such as post-mortem redistribution or probabilities of statistics. But the point is that they are extremely specialised scientific questions and require a technical understanding that courts do not possess at all.

It is a real practical dilemma. Courts, confronted with scientific evidence of such complexity, would have to rely excessively on the evidence since it appears to be scientific and objective. Alternatively, they could simply dismiss it as being too complicated for comprehension.

Most AI systems work as a 'black box' where it is difficult to understand the underlying logic or working principles of the technology. Thus, it may be tough for the judiciary to determine whether a specific conclusion drawn from an AI analysis is reliable or valid. Hence, the primary concern is not related to the use of AI per se, but rather the ability of the judicial system to analyse such scientific evidence and determine its reliability.

XII. SUGGESTIONS AND RECOMMENDATIONS

The present study identifies significant legal and procedural challenges in the use of Artificial Intelligence (AI)-assisted forensic toxicology in poisoning prosecutions. To address these challenges, the following recommendations are proposed:

1. Build a Forensic-AI Framework upon the MeitY AI Governance Guidelines:

India should not proceed on the assumption that there is no AI governance baseline. The India AI Governance Guidelines, 2025 already provide a soft-law foundation for responsible AI through principles such as trust, fairness, accountability, explainability, safety, and human-centric governance. However, because these Guidelines are sector-agnostic and non-binding, they should be supplemented by a forensic-specific legal and procedural framework governing the development, validation, admissibility, and courtroom use of AI-assisted forensic evidence. Such a framework should translate the MeitY principles into enforceable forensic standards on algorithmic validation, technical documentation, error-rate disclosure, independent audit, laboratory accreditation, human expert certification, chain of custody, and the accused's right to meaningfully challenge AI-generated evidence.

2. Introduce Scientific Reliability Standards for AI Evidence: Building on the MeitY Guidelines' emphasis on accountable, understandable, and safe AI, Indian courts and lawmakers should adopt statutory or procedural standards

requiring AI-assisted forensic evidence to satisfy scientific criteria before admission. These should include independent validation, peer review, known or reasonably ascertainable error rates, reproducibility, model-performance documentation, data-quality assessment, and general acceptance within the forensic toxicology community. This would convert India's general AI governance principles into a legally usable reliability test for criminal trials.

3. **Amend the Bharatiya Sakshya Adhiniyam, 2023:** The Bharatiya Sakshya Adhiniyam should be amended to expressly recognise AI-assisted forensic reports as a specialised form of expert evidence while mandating that such evidence be supported by qualified human experts. The legislation should also require disclosure of the AI system's methodology, validation process, limitations, and accuracy to ensure transparency during judicial proceedings.
4. **Strengthen Certification of Electronic and AI-Generated Evidence:** Clear procedural guidelines should be framed under Section 63 of the Bharatiya Sakshya Adhiniyam, 2023, for preserving, certifying, and authenticating AI-generated toxicological reports and digital forensic data. These guidelines should safeguard the integrity of electronic evidence and maintain an unbroken chain of custody throughout the investigative process.
5. **Develop a National AI-Based Toxicology Database:** The Government should establish a centralised national toxicological database containing validated information on novel psychoactive substances, plant-derived poisons, synthetic drugs, and toxicological profiles. Such a database would improve AI model accuracy, facilitate uniform forensic analysis, and assist investigators in identifying emerging toxic substances.
6. **Modernise Forensic Toxicology Laboratories:** Central and State Forensic Science Laboratories should be equipped with advanced analytical technologies integrated with AI-based screening systems capable of detecting novel psychoactive substances and plant toxins. Standardisation of laboratory protocols across India would improve consistency, reliability, and scientific accuracy.

- 7. Capacity Building and Specialised Training:** Continuous training programmes should be organised for judges, prosecutors, defence counsel, investigating officers, forensic scientists, and laboratory personnel regarding AI-assisted forensic technologies, digital evidence, algorithmic decision-making, and evidentiary standards. Improved technical understanding would enable courts to assess AI-generated evidence more effectively.
- 8. Ensure Human Oversight in AI Decision-Making:** AI-assisted toxicological analysis should function only as a decision-support tool. Final forensic conclusions should always be reviewed, interpreted, and certified by qualified forensic toxicologists to prevent over-reliance on automated systems and to preserve judicial confidence in scientific evidence.
- 9. Create Sector-Specific Oversight under the National AI Governance Architecture:** Consistent with the MeitY Guidelines' institutional approach, forensic AI should be supervised through a sector-specific mechanism involving MeitY, the Ministry of Home Affairs, DFSS, forensic science laboratories, legal experts, toxicologists, and AI specialists. This body should evaluate, certify, periodically audit, and monitor AI systems used in forensic investigations. It should also develop forensic-AI standards for validation, model updates, incident reporting, bias testing, audit trails, and courtroom disclosure. Such an approach would preserve India's sector-led AI governance model while addressing the heightened due-process risks of criminal proceedings.
- 10. Promote Research and International Collaboration:** Universities, forensic institutions, and government agencies should encourage interdisciplinary research on AI-assisted forensic toxicology through collaborative projects with international forensic organisations. Such cooperation would facilitate technology transfer, standardisation, and the development of globally accepted best practices.
- 11. Address the Legislative Gap Relating to Novel Psychoactive Substances (NPS):** The NDPS Act should be amended to include analogue provisions or generic scheduling mechanisms capable of regulating newly emerging

psychoactive substances. This would reduce evidentiary difficulties in proving criminal liability where newly developed substances are involved.

12. Formulate National Standard Operating Procedures (SOPs): Uniform SOPs should be developed for AI-assisted toxicological examinations, covering sample collection, laboratory analysis, algorithm validation, report preparation, data storage, cybersecurity, and courtroom presentation. Standardised procedures would ensure consistency, enhance evidentiary reliability, and reduce procedural disputes during criminal trials.

Collectively, these recommendations seek to bridge the gap between technological innovation and criminal justice by ensuring that AI-assisted forensic toxicology strengthens the prosecution of poisoning cases while safeguarding the rights of the accused, maintaining scientific reliability, and upholding the constitutional principles of fairness, transparency, and due process.

XIII. CONCLUSION

AI has been a driving force of advancement in many areas of science and technology, including forensic toxicology. By developing powerful methods to detect, identify, and analyse toxic compounds, AI has helped create more sophisticated and reliable investigative techniques. In the investigation and prosecution of causes related to poisoning, accurate identification of poisonings, proof of cause-and-effect relationships, and proving intent are necessary for the successful conviction of accused. However, many current traditional forensic toxicology methods are insufficient for testing a diverse range of new synthetic and plant-derived psychoactive drugs and poisons because new synthetic molecules can be synthesised rapidly, used in very low amounts, metabolised by human beings and for which reference standards do not exist, resulting in major scientific shortcomings that hinder their successful inclusion into cases by the prosecution.

The current paper indicates that the field of AI-assisted forensic toxicology can largely remedy many of the difficulties of finding conclusive evidence. By applying AI technologies such as machine learning algorithms, predictive toxicology, high-resolution mass spectrometry data and pattern recognition methods, investigators can

increase accuracy, speed and efficiency when carrying out analyses of toxicological information. AI technologies will allow toxicological evidence to provide even greater weight to a chain of circumstantial evidence used in cases of poisoning by, for instance, identifying unknown substances, foreseeing toxic effects, and reconstructing timeline of poisonings and integrating diverse data into an investigation. Therefore, AI can be used to raise quality of forensic information provided before the criminal courts, which supports decisions to be more objective. However, while technology is advancing, the legal difficulties in using AI-powered forensic evidence to investigate cases of poisoning may still be overcome only if new legislation is put into practice.

The Bharatiya Sakshya Adhiniyam 2023 has made great progress in recognizing expert opinion and digital evidence. But it fails to adequately provide guidance for using AI-powered investigative tools and to determine the quality and certification standards required for evidence derived from them. Key challenges in terms of algorithmic transparency, explainability, reliability, certification, human supervision and intervention, accountability, chain of custody of analytical data, and algorithmic bias remain unresolved in Indian legal framework.

Over-reliance on the results produced by algorithms is in risk of harming justice and constitutional rights of defendants. This comparative analysis showed that some of the leading jurisdictions have formulated coherent policies on AI-enabled forensic investigations. For example, in the United States, the scientific reliability is evaluated through the Daubert standard and Rule 702 of the Federal Rules of Evidence; while in the European Union, the recently published AI Act designates AI-powered forensic tools as high-risk technologies subject to compliance procedures. In Australia and the UK, measures for better judicial review and standardisation of expert accreditation are enforced.

It is clear that AI implementation should not be done only at the expense of procedural safeguard; therefore, this policy review recommends that India also should introduce a specific legal framework to govern use of AI-powered forensic technologies. Our criminal investigation agencies face infrastructural challenges as well: lack of well-equipped labs, fewer trained experts, no centralised AI-driven toxicological data sets

and varying lab protocols between centre and state. These challenges limit the application of forensic AI tools. This, in turn, necessitates coordinated investment in AI technologies, research capacity, infrastructure development, training for scientists, and interdisciplinary research on the subject matter by lawyers, scientists, and computer scientists.

Legislative amendments should address scientific standardisation of AI technologies, clarity of explanation, and the standards for using algorithms, certifications of digital evidence, independent certification and human oversight on the AI-generated data to address the legal shortcomings of the current framework.

AI-assisted investigations should enhance professional opinions and not replace toxicologists or judicial interpretation of the evidence. Last but not the least, poisoning cases have been complicated by a range of novel psychoactive compounds and naturally derived toxins that are beyond current regulatory coverage and for which conventional diagnostic approaches are often inefficient. The new drugs and poisons require an overhaul of current Narcotic drugs and intoxicating substances Act, and equivalent laws regulating plant poisons. Moreover, to keep up with these rapidly changing criminal methodologies, forensic laboratories need to develop and integrate AI-powered analytical tools.

XIV. REFERENCES

A. Primary Sources

1. Bharatiya Nyaya Sanhita, No. 45 of 2023.
2. Bharatiya Sakshya Adhiniyam, No. 47 of 2023.
3. Bharatiya Nagarik Suraksha Sanhita, No. 46 of 2023.
4. Narcotic Drugs and Psychotropic Substances Act, 1985.
5. Information Technology Act, 2000.
6. Poisons Act, 1919.
7. Regulation (EU) 2024/1689 (Artificial Intelligence Act).
8. Federal Rules of Evidence (United States), Rule 702.
9. Criminal Procedure Rules 2025 (United Kingdom).
10. Forensic Science Regulator Act 2021 (United Kingdom).

B. Cases

1. Anant Chintaman Lagu v. State of Bombay, AIR 1960 SC 500.
2. Anvar P.V. v. P.K. Basheer, (2014) 10 SCC 473.
3. Arjun Panditrao Khotkar v. Kailash Kushanrao Gorantyal, (2020) 7 SCC 1.
4. Daubert v. Merrell Dow Pharmaceuticals, Inc., 509 U.S. 579 (1993).
5. Dasreef Pty Ltd v. Hawchar, (2011) HCA 21.
6. Lang v. The Queen, (2012) HCA 16.

C. Books

1. Paul C. Giannelli et al., Scientific Evidence (6th ed., LexisNexis, 2020).
2. David H. Kaye et al., The New Wigmore: A Treatise on Evidence – Expert Evidence (2nd ed., Wolters Kluwer, 2011).
3. Frank Pasquale, The Black Box Society: The Secret Algorithms That Control Money and Information (Harvard University Press, 2015).
4. OECD, Artificial Intelligence in Society (OECD Publishing, 2019).
5. Journal Articles
6. Cary Coglianese & David Lehr, "Regulating by Robot: Administrative Decision Making in the Machine-Learning Era", 105 Georgetown Law Journal 1147 (2017).
7. Andrew D. Maynard & Dana R. Fisher, "Computational Toxicology", 45 Annual Review of Pharmacology and Toxicology 123 (2005).
8. Toshali D. Wankhade et al., "Artificial Intelligence in Forensic Medicine and Toxicology: The Future of Forensic Medicine", Cureus (2022).
9. Pragnesh Parmar, "The Integration of Artificial Intelligence in Forensic Medicine and its Applications in Medico-Legal Autopsy, Forensic Toxicology and Disaster Victim Identification", International Journal of Forensic Sciences (2023).
10. Praveen Dixit et al., "Digital Detectives: Exploring the Integration of Artificial Intelligence in Indian Forensic Medicine", IP International Journal of Forensic Medicine and Toxicological Sciences (2024).

D. Reports and Online Sources

1. National Institute of Standards and Technology (NIST), Artificial Intelligence Risk Management Framework (AI RMF 1.0) (2023).
2. Directorate of Forensic Science Services, Ministry of Home Affairs, Government of India.
3. U.S. Environmental Protection Agency, ToxCast Program.
4. International Association of Forensic Toxicologists (TIAFT).
5. Central Forensic Science Laboratories (CFSL), India.