



ARTIFICIAL INTELLIGENCE AND FORENSIC TOXICOLOGY: LEGAL CHALLENGES IN THE ADMISSIBILITY OF AI-ASSISTED TOXICOLOGICAL EVIDENCE IN INDIA

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Abstract:

Forensic toxicology occupies a pivotal place in the Indian criminal justice system, providing scientific answers to questions of poisoning, drug-facilitated crime, and cause of death. The discipline is now being reshaped by artificial intelligence (AI) and machine learning (ML) tools that promise faster compound identification, improved interpretation of mass-spectrometry data, and predictive modelling of toxicity. Yet Indian evidence law—rooted in Section 45 of the erstwhile Indian Evidence Act, 1872, and now Section 39 of the Bharatiya Sakshya Adhiniyam, 2023—was not designed with opaque, self-learning algorithms in mind. This paper examines how AI-assisted toxicological evidence fits within the Indian law of expert opinion and electronic evidence, drawing on comparative experience from the United States and the European Union, particularly the due-process controversies generated by proprietary risk-assessment algorithms such as COMPAS. It argues that the "black box" nature of many AI systems creates tension with foundational fair-trial guarantees—the right to cross-examine, the right to a reasoned judicial opinion, and the constitutional right to a fair investigation—and proposes a framework of algorithmic disclosure, human-in-the-loop verification, and judicial gatekeeping suited to Indian conditions.

Keywords: artificial intelligence, forensic toxicology, admissibility, expert evidence, Bharatiya Sakshya Adhiniyam, Section 45, due process, algorithmic transparency

1. Introduction

Forensic toxicology sits at the intersection of chemistry, pharmacology, and criminal law. Toxicologists are routinely called upon to determine whether a death was caused by poisoning, whether a driver was intoxicated, or whether a victim of sexual assault was drugged, and their conclusions frequently decide the outcome of a criminal trial. As instrumentation such as gas chromatography–mass spectrometry (GC–MS) and liquid chromatography–tandem mass spectrometry (LC–MS/MS) has become more sensitive, the volume and complexity of data generated in a single case has grown far beyond what a human analyst can manually parse. Artificial intelligence—including machine learning classifiers, deep neural networks, and increasingly generative AI and large language models—has stepped into this gap, offering to automate spectral matching, predict the toxicity of novel psychoactive substances, and even draft toxicology reports.

Recent scientific literature confirms that AI is already being used across the toxicological pipeline: natural-language-processing systems mine scientific literature to build knowledge bases, expert systems assist in rapid drug identification from biological samples, and machine-learning models interpret complex data such as drug interactions and biomarker patterns. Reviews of AI in new psychoactive substance (NPS) analysis likewise describe how machine learning is used to identify emerging drugs of abuse from spectral and chromatographic data. Parallel work on

machine-learning-enabled toxicity prediction demonstrates the use of both “black box” predictive algorithms and more interpretable models across categories such as organ-specific and carcinogenic toxicity.

This technological shift raises a legal question that Indian courts have not yet had to confront squarely: can the output of an AI system—whether a compound identification, a probability score, or a narrative report—be admitted as evidence, and if so, on what terms? This paper answers that question by situating AI-assisted toxicological evidence within India's expert-evidence framework, identifying the specific legal challenges that arise from algorithmic opacity, and drawing lessons from comparable controversies abroad.

2. AI in Forensic Toxicology: A Technical Overview

Before evaluating admissibility, it is necessary to understand what forensic AI systems actually do, because the legal characterisation of the evidence depends heavily on the underlying technology.

2.1 Categories of application

Contemporary literature identifies at least four broad categories of AI application in forensic toxicology. First, automated spectral interpretation, where machine-learning classifiers match unknown mass spectra against reference libraries faster and, proponents claim, more consistently than manual review. Second, predictive toxicology, in which models trained on chemical structure and biological assay data estimate the likely toxicity of novel or under-studied compounds, a task of growing importance given the rapid proliferation of new psychoactive substances that outpace conventional reference libraries. Third, postmortem interpretation, where AI models assist in accounting for postmortem redistribution—the phenomenon whereby drug concentrations change after death—thereby improving the accuracy of cause-of-death determinations. Fourth, natural-language and generative AI tools, used to draft or summarise toxicology reports and to mine scientific literature for interpretive context.

A recent comprehensive review of machine learning and optical imaging in pharmaceutical forensic toxicology stresses that, beyond raw technical performance, the deployment of such tools raises significant regulatory, ethical, and legal questions, and specifically highlights explainability, traceability, and data governance as prerequisites for legally defensible toxicological determinations. This technical observation maps directly onto the legal concerns discussed later in this paper.

2.2 The explainability problem

A recurring theme in the scientific literature is the trade-off between predictive accuracy and interpretability. Deep-learning models often outperform simpler statistical methods but function as “black boxes” whose internal decision logic is not transparent even to their developers. Techniques such as SHAP (SHapley Additive exPlanations) and LIME (Local Interpretable Model-agnostic Explanations) have been developed to approximate an explanation of a model's output after the fact, but these remain approximations rather than a true accounting of the model's reasoning. This distinction between a genuinely interpretable (“glass box”) system and a black box whose output is merely rationalised post hoc is central to the legal analysis that follows, because Indian evidence law has traditionally assumed that an expert can explain, and be cross-examined on, the basis of an opinion.

3. The Indian Framework for Expert and Scientific Evidence

3.1 Expert opinion under Section 45 of the Indian Evidence Act, 1872 and Section 39 of the Bharatiya Sakshya Adhiniyam, 2023

Indian law has long treated expert testimony as an exception to the general rule that witnesses may depose only to facts within their personal knowledge. Section 45 of the Indian Evidence Act, 1872 permitted courts to consider the opinion of persons “specially skilled” in matters of science, art, foreign law, or the identification of handwriting or finger impressions where the point in issue required such specialised knowledge. Toxicological findings—for instance, whether symptoms exhibited by a victim were consistent with a particular poison—fall squarely within this provision, and Section 46 of the 1872 Act separately made facts relevant if they supported or contradicted an expert's opinion, a provision of direct relevance to poisoning cases.

With effect from 1 July 2024, the Indian Evidence Act, 1872 has been replaced by the Bharatiya Sakshya Adhiniyam, 2023 (BSA). Section 39 of the BSA reproduces the substance of the old Section 45, recognising the relevance of opinions of persons specially skilled in science, art, or the identification of handwriting or finger or other impressions, while Section 40 preserves the corollary rule making corroborating or contradicting facts relevant in cases such as poisoning symptoms. Crucially, however, Indian courts have consistently held that expert opinion is only advisory: it assists but does not bind the court, and it is not conclusive proof by itself, requiring corroboration from other evidence in the case.

This “advisory, not conclusive” character of expert evidence is doctrinally significant for AI-assisted toxicology, because it means a court retains discretion to discount or reject an AI-generated finding—but that discretion can only be exercised meaningfully if the court understands enough about the tool to evaluate it, which is precisely what black-box systems make difficult.

3.2 Electronic and digital evidence: Section 65B and its successor

Because AI toxicological outputs are typically generated, stored, and transmitted electronically, they are also electronic records for evidentiary purposes and must satisfy India's stringent certification regime. The Supreme Court's decision in *Anvar P.V. v. P.K. Basheer* (2014) held that secondary electronic evidence is admissible only where it complies with the certificate requirement of Section 65B(4) of the Indian Evidence Act, overruling the earlier, more permissive position of *State (NCT of Delhi) v. Navjot Sandhu* (2005), which had allowed such evidence to be proved through ordinary secondary-evidence rules. The Court in *Anvar* held that Sections 65A and 65B constitute a complete code for electronic evidence, and that oral or other secondary evidence cannot substitute for the mandatory certificate.

The BSA carries this scheme forward and, in some respects, strengthens it. Section 63 of the BSA governs the admissibility of electronic records and now requires, in addition to the certificate signed by the person in charge of the relevant device, a certificate from an expert, formatted according to a prescribed two-part schedule (Part A completed by the party producing the record, Part B by the expert). Commentators have observed that this dual-certification requirement, while intended to enhance the reliability of digital evidence, presumes the ready availability of both institutional capacity and qualified experts—an assumption that is difficult to sustain given the acknowledged shortage of accredited personnel in India's Forensic Science Laboratories (FSLs). For AI-assisted toxicology, this raises a practical bottleneck: the “expert” required to certify an AI-generated report must be someone capable of vouching not merely for the integrity of the data but, implicitly, for the reliability of the algorithm that processed it—a competence that few current FSL personnel possess.

3.3 Absence of a dedicated reliability standard

Unlike the United States, where the *Daubert* standard (and its predecessor, *Frye*) requires trial judges to act as gatekeepers assessing the scientific validity, error rate, and peer acceptance of a methodology before admitting expert testimony, Indian law has no codified equivalent. Commentators note that, apart from the general expert-opinion provisions of the Evidence Act (now the BSA), there is no dedicated statute governing the admissibility of forensic

evidence, leaving courts to rely on precedent and the general discretion embedded in Sections 39–45 of the BSA. In *State of Himachal Pradesh v. Jai Lal*, the Supreme Court emphasised that an expert's opinion must rest on a reliable methodology and not on mere speculation—language that comes closest to a reliability threshold in Indian law—but this remains a general principle applied case-by-case rather than a structured admissibility test analogous to *Daubert*. The absence of a formal reliability filter is particularly consequential for AI evidence, where the "methodology" is often proprietary, statistically probabilistic, and resistant to the kind of first-principles explanation that Indian courts have historically expected of forensic experts.

4. Comparative Perspectives: Lessons from the United States and the European Union

4.1 The COMPAS controversy and the limits of “black box” tolerance

The most instructive comparative precedent is the Wisconsin Supreme Court's decision in *State v. Loomis* (2016), concerning the COMPAS recidivism-risk algorithm used at sentencing. The defendant argued that reliance on a proprietary algorithm whose internal workings were undisclosed—protected as a trade secret by its vendor, Northpointe—violated his due-process right to be sentenced on the basis of accurate and verifiable information. The Wisconsin Supreme Court rejected the challenge, reasoning that the algorithm was only one factor among many considered by the sentencing judge and that the defendant retained the ability to review and contest the *inputs* to the algorithm (his own criminal history and questionnaire responses) even though he could not examine the algorithm's internal logic. The court did require that judges receive a written advisement cautioning them about the tool's limitations, including its reliance on group-level data. The U.S. Supreme Court subsequently denied certiorari, leaving *Loomis* as the leading American precedent on algorithmic evidence.

Loomis has attracted sustained academic criticism. Legal scholarship analysing the decision argues that it mischaracterised a problem of output-contestability as a problem of input-verification, and that treating a private vendor's trade-secret interest as equivalent to the state's interest in fair administration of justice miscalibrated the due-process balancing exercise associated with *Mathews v. Eldridge*. Scholars have proposed tiered-disclosure frameworks under which the degree of algorithmic transparency required scales with the severity of the consequence the tool is used to determine—an approach with obvious relevance to toxicological evidence used to establish guilt in serious offences.

Broader empirical and doctrinal work on "black box" forensic technology—spanning DNA-mixture interpretation software, facial recognition, and recidivism tools—has challenged the assumption that opacity is the necessary price of accuracy, showing that interpretable ("glass box") models can in some domains match or exceed the performance of black-box alternatives while remaining auditable. This literature also documents a related evidentiary phenomenon: in a substantial majority of contested cases involving proprietary probabilistic genotyping software (such as TrueAllele), American courts have declined to compel disclosure of the underlying source code, illustrating how trade-secret claims can systematically limit a defendant's ability to test forensic algorithms regardless of the formal evidentiary standard applied.

4.2 Frye, Daubert, and Federal Rule of Evidence 702

More broadly, commentary on the U.S. position notes that existing standards—the *Frye* "general acceptance" test, the *Daubert* reliability factors, and Federal Rule of Evidence 702—already extend to algorithmic proof, but that the practical difficulty lies in applying a reliability inquiry to a methodology that is not accessible for independent scrutiny. Courts that admit AI-generated evidence without rigorous scrutiny of the underlying methodology risk compromising both the fairness of the individual trial and the broader legitimacy of forensic science, since routine judicial use of a

tool does not, by itself, establish that the tool is scientifically valid for the population or purpose to which it is being applied.

4.3 European and international regulatory responses

While a full survey of European law is beyond this paper's scope, the trajectory of EU policy—culminating in the EU Artificial Intelligence Act's risk-based classification of AI systems used in the administration of justice and law enforcement as "high-risk," triggering obligations of transparency, human oversight, and documentation—signals an emerging international consensus that forensic and judicial uses of AI warrant heightened, rather than ordinary, regulatory scrutiny. India's own policy documents have moved in a similar, if less binding, direction: NITI Aayog's National Strategy for Artificial Intelligence (2018) and its subsequent two-part Responsible AI approach papers (2021) articulate principles of transparency, accountability, and human oversight for AI deployment, including in the public sector, though these remain non-binding policy instruments rather than enforceable evidentiary standards.

5. Legal Challenges Specific to AI-Assisted Toxicological Evidence in India

5.1 The right to a fair trial and cross-examination

The centrepiece of the Indian adversarial system is the right to test evidence through cross-examination. When a toxicologist testifies that a biological sample tested positive for a substance using a conventional immunoassay or chromatographic method, defence counsel can meaningfully probe the calibration of the instrument, the chain of custody, and the analyst's qualifications. Where the finding is instead the output of a proprietary machine-learning classifier, counsel's ability to interrogate the *basis* of the opinion is sharply constrained: the algorithm's training data, feature weighting, and decision boundaries are typically commercial secrets, and even the testifying expert may be unable to explain why the model reached a particular conclusion rather than merely reporting that it did. This is the Indian analogue of the concern that animated the *Loomis* litigation, transposed from sentencing risk-scores to a substantive finding of fact—drug identification or cause of death—that can determine guilt itself.

5.2 Certification and the "expert" requirement under Section 63 BSA

As discussed in Section 3.2, the BSA's electronic-evidence regime requires an expert certificate as a precondition to admissibility. For AI-assisted toxicology reports, this raises an unresolved question: does the certifying "expert" need only vouch for the technical integrity of the electronic record (hash values, storage, and transmission), or must that person also be qualified to assess the validity of the underlying algorithm? Indian jurisprudence has not yet answered this question, and the shortage of FSL personnel trained in both toxicology and data science makes the more demanding interpretation difficult to operationalise in the near term.

5.3 The advisory-not-conclusive doctrine and judicial AI-literacy

Because Indian courts have consistently treated expert opinion as advisory rather than binding, a trial judge retains formal discretion to reject an AI-generated toxicological finding. In practice, however, meaningful exercise of that discretion presupposes some baseline understanding of the tool's reliability, error rate, and limitations—precisely the kind of understanding that the Wisconsin Supreme Court in *Loomis* found lacking among judges confronted with COMPAS, and that has been described in the literature as the "black box effect": confusion or disorientation among judicial actors when confronted with an opaque algorithmic system, followed by ad hoc adaptive responses rather than

principled scrutiny. Without structured judicial training or a codified reliability standard analogous to *Daubert*, Indian courts risk either uncritical deference to AI-generated findings because they appear scientifically authoritative, or inconsistent, ad hoc rejection that undermines legal certainty.

5.4 Privacy and bodily autonomy

Forensic toxicology inherently involves the analysis of bodily fluids and, increasingly, biometric and genomic data that AI systems can process, cross-reference, or infer from. The Supreme Court's recognition of privacy as a fundamental right under Article 21 in *Justice K.S. Puttaswamy v. Union of India* (2017) constrains the manner in which such sensitive personal data may be collected, stored, and processed by state agencies, including forensic laboratories deploying AI tools. Any AI system that aggregates toxicological data with other personal information—for instance, cross-referencing a suspect's toxicology results against pharmacy records or health databases—would need to satisfy the tests of legality, necessity, and proportionality articulated in *Puttaswamy*, an analysis Indian forensic policy has not yet systematically undertaken.

5.5 Algorithmic bias and population validity

Toxicological AI models are frequently trained on datasets drawn from non-Indian populations, raising the possibility that predictive thresholds calibrated on different demographic, dietary, or pharmacogenomic profiles may not transfer reliably to Indian subjects. The scientific literature on AI in toxicology explicitly flags data quality, accessibility, and algorithmic bias as unresolved challenges to regulatory acceptance, and this concern is amplified in a jurisdiction like India where locally validated datasets remain scarce. A finding that is statistically robust for the population on which a model was trained may carry a materially different, and unquantified, error rate when applied to an Indian defendant—an issue that current admissibility doctrine does not require litigants to probe.

5.6 Chain of custody in hybrid human–AI workflows

Traditional chain-of-custody doctrine assumes a linear, traceable sequence of human handlers. AI-assisted workflows introduce an additional, non-human link—the algorithm—that both reshapes the evidence (through processing, weighting, or interpretation) and cannot itself be examined about how it did so. Courts will need to determine whether the "chain" must now include documentation of model version, training data provenance, and any post-deployment updates to the algorithm, none of which is currently contemplated by Indian procedural law or FSL protocols.

6. Towards a Framework for Admissibility

Drawing on the preceding analysis, this paper proposes four elements for a workable Indian approach to AI-assisted toxicological evidence.

First, a graded reliability inquiry. Indian courts should develop, through judicial precedent or legislative rule-making, a structured reliability inquiry for algorithmic evidence—drawing selectively on *Daubert*-style factors such as testability, known error rate, and peer-reviewed validation—while remaining sensitive to the advisory character of expert opinion under Section 39 of the BSA. This need not import the entirety of American doctrine, but the absence of any structured test currently leaves reliability assessment almost entirely to the discretion of individual judges.

Second, mandatory algorithmic disclosure calibrated to consequence. Following the tiered-disclosure proposals developed in response to *Loomis*, disclosure obligations for AI toxicology tools could scale with the severity of the offence and the extent to which the AI output is determinative of guilt, rather than merely corroborative.

Third, a "glass box" preference in forensic procurement. Given evidence that interpretable models can rival black-box accuracy in several forensic domains, Indian FSLs and procurement policy should favour explainable AI systems—or, at minimum, require vendor-supplied SHAP/LIME-style explanations as a condition of deployment—so that certifying experts under Section 63 of the BSA can meaningfully discharge their certification function.

Fourth, judicial and expert capacity-building. Structured training for judges and forensic certifying experts on the statistical and computational basis of AI tools is a precondition for the advisory-opinion doctrine to function as intended; without it, the formal discretion Indian judges possess to discount unreliable expert evidence risks becoming illusory.

7. Conclusion

Artificial intelligence offers forensic toxicology genuine gains in speed, consistency, and analytical reach, particularly in identifying novel psychoactive substances and interpreting complex mass-spectrometric data. But Indian evidence law—built around Section 45 of the 1872 Act and now Section 39 of the Bharatiya Sakshya Adhiniyam, 2023, together with the electronic-evidence certification regime of Section 63—presupposes an expert who can explain, and be cross-examined on, the basis of an opinion. The comparative experience of *State v. Loomis* in the United States demonstrates how readily courts can default to deference when confronted with proprietary, opaque algorithms, and how difficult it is to unwind that deference once entrenched. India has an opportunity, while AI-assisted toxicology is still at an early stage of forensic deployment, to build reliability screening, disclosure obligations, and judicial AI-literacy into the admissibility framework before opacity becomes normalised. Doing so would allow the criminal justice system to capture the genuine scientific benefits of AI in forensic toxicology without compromising the constitutional guarantees of a fair trial, privacy, and reasoned judicial decision-making that the *Puttaswamy* and *Anvar* lines of authority have painstakingly established.

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