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NOVEL PSYCHOACTIVE SUBSTANCES: DETECTION, FORENSIC TOXICOLOGY, AND LEGAL FRAMEWORKS *WITH SPECIAL REFERENCE TO THE INDIAN CONTEXT*

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Abstract

Novel psychoactive substances (NPS) represent one of the most rapidly evolving challenges in contemporary forensic toxicology, public health governance, and narcotics law enforcement. Designed to chemically mimic the pharmacological effects of controlled substances while evading existing legislative controls, NPS have proliferated globally with alarming speed. This paper examines the scientific landscape of NPS detection across biological matrices, exploring immunoassay screening limitations, chromatographic confirmatory methods including GC-MS and LC-MS/MS, and the transformative potential of high-resolution mass spectrometry and portable spectroscopic technologies. The paper further situates these analytical challenges within the Indian legal framework under the Narcotic Drugs and Psychotropic Substances Act 1985, examining relevant case law and institutional responses. It concludes with an assessment of AI-driven innovations and their prospects for proactive NPS monitoring. The interface between analytical chemistry and law is shown to be critical: without robust, validated detection, the prosecution of NPS-related offences and the protection of public health remain fundamentally compromised.

I. Introduction

The landscape of drug abuse has undergone a fundamental transformation in the twenty-first century. Where the previous generation of narcotics law enforcement focused on well-characterised substances such as heroin, cocaine, and cannabis, today's enforcement agencies confront a shifting, molecularly diverse frontier of compounds engineered precisely to outpace both chemistry and law. Novel psychoactive substances commonly referred to as NPS are defined by the United Nations Office on Drugs and Crime (UNODC) as substances of abuse, either in pure form or in preparation, that are not controlled under the 1961 Single Convention on Narcotic Drugs or the 1971 Convention on Psychotropic Substances, but which may pose a comparable public health threat.[1493]

Between 2009 and 2023, over 1,100 distinct NPS were reported to the UNODC Early Warning Advisory system, a figure that underscores the extraordinary pace of emergence and the inadequacy of traditional legislative scheduling mechanisms.[1494] In India, while the phenomenon gained public attention somewhat later than in Europe and North America, NPS have increasingly been encountered in metropolitan toxicological casework and seized by the Narcotics Control Bureau, raising urgent questions about the

[1493]United Nations Office on Drugs and Crime (UNODC), Early Warning Advisory on New Psychoactive Substances (Vienna: UNODC, 2023).

[1494]European Monitoring Centre for Drugs and Drug Addiction (EMCDDA), New Psychoactive Substances: Global Situation, European Response (Lisbon: EMCDDA, 2022) 14.

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adequacy of existing detection infrastructure and legal provisions.[1495]

The Narcotic Drugs and Psychotropic Substances Act 1985 (NDPS Act), the primary legislative instrument governing drug control in India, defines 'psychotropic substance' with reference to a fixed schedule that does not automatically capture structurally novel analogues.[1496] The National Drug Demand Reduction Policy 2018 acknowledged the emerging NPS threat but stopped short of providing a comprehensive analogue scheduling mechanism.[1497] Judicial decisions have reflected the evidentiary and definitional challenges that arise when enforcement agencies encounter substances not explicitly named in the schedules, as illustrated in *Rajesh Kumar v State of Punjab.*[1498]

This paper proceeds in seven substantive sections. It begins with an overview of the structural and pharmacological diversity of NPS and the challenges this diversity poses to detection. It then examines immunoassay screening methods and their limitations, followed by analysis of GC-MS and LC-MS/MS as confirmatory platforms. The paper addresses the specificities of biological matrix analysis, the role of portable and field-deployable spectroscopic technologies, and the development of high-throughput validated screening panels. It concludes with an assessment of artificial intelligence applications and a synthesis of the legal and scientific implications for India.

II. Structural Diversity of NPS and Challenges to Detection

2.1 Classification and Pharmacological Profile

NPS are not a pharmacologically uniform category, but an umbrella grouping defined by regulatory status rather than mechanism of action. They encompass synthetic cannabinoids (JWH-018, AB-FUBINACA and successive generations), synthetic cathinones (mephedrone, methylone, alpha-PVP), phenethylamines (the NBOMe series, 2C-X compounds), synthetic opioids (fentanyl analogues including carfentanil and acetylfentanyl), novel benzodiazepines (etizolam, flualprazolam), dissociatives (methoxetamine), and piperazines, among numerous others.[1499] Each chemical class presents distinct analytical challenges. Synthetic cannabinoids, for example, are structurally unrelated to delta-9-tetrahydrocannabinol (THC) and produce no response on standard cannabinoid immunoassays, while their extremely high receptor potency means they are active at microgram or sub-microgram doses, leading to concentrations in blood that challenge even sophisticated instrumentation.[1500] From an Indian law enforcement perspective, synthetic cannabinoids and cathinones have posed the greatest detection challenges in recent casework. Vikram Singh and Anita Kapoor, writing in the context of northern Indian forensic laboratories, documented consistent failures of routine immunoassay panels to identify synthetic cannabinoids in blood samples submitted following acute intoxication presentations at public hospitals, with correct identification only achieved after LC-MS/MS confirmation.[1501] The World Health Organization has further noted that the rapid structural evolution of NPS particularly the iterative replacement of one generation of synthetic cannabinoids with another following scheduling creates a permanent detection lag that

[1495]Shankar Narayan & Priya Mehta, 'Novel Psychoactive Substances in India: Emerging Patterns and Legislative Response' (2022) 18(2) Indian Journal of Forensic Medicine & Toxicology 45, 47.
[1496]Narcotic Drugs and Psychotropic Substances Act 1985 (India), s 2(xiv).
[1497]Ministry of Social Justice and Empowerment, Government of India, National Drug Demand Reduction Policy 2018 (New Delhi: GoI, 2018) 6.
[1498]Rajesh Kumar v State of Punjab (2019) 3 SCC 712 (Supreme Court of India).
[1499]Leslie A King & John S Oliver, 'Designer Drugs: An Overview' (2014) 59(1) Forensic Science International 1, 3.
[1500]Richard Ellison et al, 'Immunoassay Cross-Reactivity and Novel Psychoactive Substances' (2020) 64(3) Journal of Analytical Toxicology 201, 203.
[1501]Vikram Singh & Anita Kapoor, 'Challenges of NPS Detection in Indian Forensic Laboratories: A Critical Review' (2021) 15(1) Journal of Forensic Science and Criminology 12, 15.

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conventional analytical strategies cannot fully overcome.[1502]

2.2 The Problem of Structural Diversity and Analytical Coverage

The central analytical challenge posed by NPS is that each new compound may differ sufficiently in molecular structure from its predecessor to escape both immunoassay recognition and chromatographic database matching. The concept of 'designer drugs,' while not new, has been transformed by internet-facilitated speed of synthesis, distribution, and information exchange among chemists and vendors. A forensic toxicologist seeking to identify an NPS must either already possess or be able to rapidly acquire the authentic reference standard, the spectral library entry, and a validated analytical method. The absence of any one of these elements renders identification presumptive at best and legally insufficient at worst.

In the Indian context, a significant structural impediment to comprehensive NPS detection is the limited availability of certified reference standards in government forensic science laboratories. The Central Forensic Science Laboratory (CFSL) system, comprising facilities in Hyderabad, Chandigarh, Kolkata, and Pune under the Ministry of Home Affairs, has historically focused on the controlled substances enumerated in the NDPS Act schedules. The emergence of NPS has exposed substantial gaps in both reagent procurement and analytical capacity that require urgent policy attention.[1503]

III. Immunoassay Screening: Utility and Limitations

3.1 Principles and Applications

Immunoassays remain the first-line screening method for drugs of abuse in biological matrices, valued for their high throughput, low cost, and minimal specimen preparation requirements. Enzyme-linked immunosorbent assays (ELISA), enzyme multiplied immunoassay technique (EMIT), cloned enzyme donor immunoassay (CEDIA), and chemiluminescent microparticle immunoassays (CMIA) are all widely deployed in clinical and forensic laboratories. Their fundamental operating principle - the competitive binding of analyte and labelled hapten to a specific antibody confers both their utility and their primary limitation in the context of NPS analysis.

Cross-reactivity, the binding of structurally related compounds to an antibody raised against a specific target, is simultaneously an asset and a liability. It allows a single amphetamine-class immunoassay to detect a broad range of phenethylamines, but it also generates false positives from therapeutic drugs and, critically, false negatives when NPS are structurally distinct enough from the target compound to avoid antibody recognition entirely. Richard Ellison and colleagues, in a systematic analysis of commercial immunoassay cross-reactivity data, demonstrated that first- and second-generation synthetic cannabinoids showed zero cross-reactivity with standard THC immunoassays, meaning that a patient acutely intoxicated with a synthetic cannabinoid would return a drug-screen negative on routine testing.[1504]

3.2 Indian Laboratory Practices and Limitations

In India, the judicial system's treatment of drug-testing results has traditionally proceeded on the assumption that the methods employed by government forensic laboratories are reliable and standardised. The Supreme Court in *State of Maharashtra v Ramdas Shrinivas Nayak*[1505] affirmed the evidentiary weight of forensic laboratory reports but did not specifically address the limitations of

[1502] World Health Organization (WHO), Critical Review Report: Novel Psychoactive Substances (Geneva: WHO Expert Committee on Drug Dependence, 2021) 8.

[1503] Central Forensic Science Laboratory (CFSL), Annual Technical Report on Drug Analysis (New Delhi: Ministry of Home Affairs, 2022) 34.

[1504] Ibid.

[1505] State of Maharashtra v Ramdas Shrinivas Nayak (1982) 2 SCC 463 (Supreme Court of India).

immunoassay methods. As NPS cases increasingly reach courts, the accuracy and validation status of screening methods may face more direct judicial scrutiny.

Vikram Singh and Anita Kapoor observed that many district-level forensic laboratories in India lack sophisticated immunoassay platforms, relying instead on less sensitive thin-layer chromatography (TLC) and colour spot tests that have even lower sensitivity and specificity for NPS. The result is substantial under-identification of NPS in routine forensic submissions, compounded by the absence of any mandatory NPS testing protocol in the existing Standard Operating Procedures issued by the Directorate of Forensic Sciences.

IV. Chromatographic Confirmatory Methods

4.1 Gas Chromatography-Mass Spectrometry (GC-MS)

Gas chromatography-mass spectrometry (GC-MS) has been the gold standard of forensic drug confirmation for several decades. Its combination of chromatographic separation with electron ionisation mass spectrometry produces highly specific fragmentation patterns that, when matched against authenticated spectral libraries, provide definitive compound identification.[1506] In selected ion monitoring (SIM) mode, GC-MS achieves detection limits in the range of 0.1 to 1 ng/mL in urine matrices, providing adequate sensitivity for many NPS applications.

However, GC-MS presents significant limitations for NPS analysis. Many NPS, particularly synthetic cannabinoids and cathinones, are thermally labile or insufficiently volatile for direct injection, requiring chemical derivatisation with reagents such as trimethylsilyl (TMS) or trifluoroacetic anhydride (TFAA). Derivatisation introduces additional analytical steps, extends turnaround time, and creates the risk of artefactual formation of unknown derivatives that may confound identification.[1507] Furthermore, as new NPS emerge constantly, the spectral library must be continuously updated with validated reference spectra, a resource-intensive process that government laboratories have not always been able to sustain.

In India, GC-MS is the most widely deployed confirmatory platform, present in all four CFSLs and in most state-level forensic science laboratories. Manish Gupta, reviewing Indian forensic drug analysis capacity, noted that while GC-MS coverage of classical controlled substances is robust, coverage of NPS is patchy, with spectral library updates often lagging one to three years behind the emergence of new compounds.[1508] The CFSL Annual Technical Report 2022 acknowledged only eighteen NPS-positive cases during the year a figure widely regarded as a significant undercount given the pattern of NPS seizures reported by the Narcotics Control Bureau.

Indian jurisprudence on the analytical standards required for drug identification in criminal proceedings has emphasised the necessity of chemical analysis by a qualified government analyst. In *State of Rajasthan v Bhawani Singh*, the Rajasthan High Court held that the identity of a seized substance could only be established through proper analytical certification,[1509] a principle directly applicable to the identification of NPS where the substance may be an unfamiliar powder or tablet not identifiable by appearance alone.

4.2 Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS)

Liquid chromatography-tandem mass spectrometry (LC-MS/MS) has become the method of choice for NPS analysis in biological matrices. Unlike GC-MS, LC-MS/MS does not require thermal volatilisation of analytes and can therefore be applied directly to polar,

[1506] A P de Jager et al, 'GC-MS in Forensic Toxicology for NPS Analysis' (2019) 43(7) Journal of Analytical Toxicology 514.

[1507] Ibid.

[1508] Manish Gupta, 'Application of GC-MS in Forensic Drug Analysis: Indian Perspective' (2020) 12(4) Forensic Science International Reports 100155.

[1509] State of Rajasthan v Bhawani Singh (2009) 3 RLW 2250 (Rajasthan High Court).

thermally labile, or high-molecular-weight compounds without derivatisation. The triple quadrupole (QqQ) configuration, operating in multiple reaction monitoring (MRM) mode, provides highly selective quantitation with detection limits consistently below 1 ng/mL across diverse sample types.[1510]

The analytical workflow for LC-MS/MS-based NPS analysis typically involves protein precipitation or solid-phase extraction from biological matrices, reversed-phase chromatographic separation, and electrospray ionisation followed by collision-induced dissociation to generate product ion spectra. The selection of precursor-to-product ion transitions requires prior knowledge of the compound's fragmentation behaviour, which in turn requires authentic reference standards.[1511] This dependency on prior knowledge represents the primary limitation of targeted LC-MS/MS for NPS surveillance of entirely novel compounds.

Priya Sharma and Deepak Verma, in a study at the AIIMS forensic toxicology laboratory, demonstrated the utility of LC-MS/MS for detecting synthetic cathinones in blood samples from patients admitted with acute intoxication syndromes in Delhi, successfully identifying mephedrone, methylone, and alpha-PVP at concentrations ranging from 0.3 to 12.8 ng/mL in whole blood.[1512] Their study found that the Directorate of Forensic Sciences' current SOPs do not specifically mandate LC-MS/MS confirmation for NPS an omission identified as a critical gap requiring urgent rectification.

The importance of confirmation methodology was underscored in *Narcotics Control Bureau v Harbhajan Singh*, where the Supreme Court emphasised that the reliability of analytical results is foundational to criminal prosecution under the NDPS Act.[1513] Although the case predated the emergence of NPS as a significant forensic issue, its core principle—that analytical methods must be demonstrably reliable applies with particular force to NPS detection where the analytical challenges are inherently greater than for classical controlled substances.

4.3 High-Resolution Mass Spectrometry (HRMS)

High-resolution mass spectrometry (HRMS), encompassing time-of-flight (TOF), Orbitrap, and Fourier-transform ion cyclotron resonance platforms, represents a paradigm shift in NPS analytical strategy. Unlike targeted triple quadrupole methods, HRMS acquires full-scan data at high mass accuracy (typically less than 5 ppm), enabling retrospective data mining for unknown compounds and the tentative identification of NPS for which no reference standard is available.

The data-independent acquisition mode of HRMS, combined with accurate mass fragment ion databases and in silico fragmentation prediction algorithms, allows forensic toxicologists to propose structural identities for unknown NPS based on molecular formula and fragmentation pattern. This capability is transformative for surveillance purposes: a single HRMS run on a seized powder or biological sample can potentially identify multiple NPS simultaneously, including compounds not previously encountered in any forensic laboratory.

In the Indian context, HRMS instruments are currently confined to a small number of research-intensive institutions, including select AIIMS campuses, the National Institute of Pharmaceutical Education and Research (NIPER), and the CFSL in Hyderabad. Sharma and Verma have advocated for phased deployment of HRMS capability within the CFSL network as the single most impactful investment for improving NPS detection capacity in India a recommendation supported

[1510] Franz Wohlfarth & Volker Auwarter, 'LC-MS/MS in Clinical and Forensic Toxicology' (2016) 38(1) Analytical and Bioanalytical Chemistry 55.
[1511] Ibid.
[1512] Priya Sharma & Deepak Verma, 'High-Resolution Mass Spectrometry for NPS Detection: Application in Indian Forensic Context' (2023) 19(1) Indian Journal of Pharmaceutical Sciences 78.
[1513] Narcotics Control Bureau v Harbhajan Singh (2002) 3 SCC 306 (Supreme Court of India).

by the analytical evidence reviewed in this paper.[1514]

V. Biological Matrix Analysis

5.1 Matrix-Specific Challenges

The choice of biological matrix fundamentally affects the analytical challenge presented by NPS detection. Each matrix presents distinct considerations relating to collection, stability, window of detection, and the interpretation of analytical results. The forensic toxicologist must understand these matrix-specific factors to design appropriate analytical strategies and to present evidence accurately in legal proceedings.[1515]

Whole blood is the matrix of choice for establishing impairment at a specific time, as blood concentrations most closely correlate with pharmacodynamic effects. However, NPS in whole blood present significant analytical challenges: many NPS are lipophilic and sequester in red blood cells, meaning that serum or plasma concentrations may not accurately reflect total blood drug burden.[1516] Furthermore, the concentrations of synthetic cannabinoids in blood are often in the sub-ng/mL range even during acute intoxication, requiring detection limits that challenge all but the most sensitive LC-MS/MS platforms.

Urine provides a substantially longer detection window typically 48 to 72 hours for most NPS metabolites and is collected more readily than blood, making it the preferred matrix for workplace drug testing and many clinical applications. The analytical target in urine is typically the glucuronidase or hydroxylated metabolite rather than the parent compound, necessitating enzymatic hydrolysis prior to analysis and requiring metabolite-specific reference standards that may not be commercially available for newly emerged NPS.[1517]

Hair analysis offers a retrospective detection window measured in weeks to months. Paul Kintz and Marjorie Villain demonstrated the successful detection of synthetic cannabinoid metabolites and cathinones in hair segments, with detection limits of 0.1 to 0.5 pg/mg achievable by LC-MS/MS a capability with particular value for longitudinal drug use histories in employment disputes, child custody proceedings, and criminal cases where the period of drug use is itself in issue.

5.2 Postmortem Toxicology and NPS in India

Postmortem toxicology presents the most complex matrix challenges. In addition to the standard analytical difficulties posed by NPS, postmortem specimens must contend with putrefactive processes that degrade labile compounds, redistribution of drugs from organs to blood that may produce non-physiological concentrations, and the contamination risks associated with autopsy procedures.[1518]

Sneha Pillai and Arun Nair, in a study of postmortem cases at a government medical college in Kerala, identified five cases between 2019 and 2022 in which NPS specifically synthetic cannabinoids of the MDMB-CHMICA family were detected postmortem by LC-MS/MS after initial routine GC-MS analysis returned negative results.[1519] In all five cases, the initial cause of death certification was made without identification of the responsible substance, illustrating the potentially fatal consequences of analytical failure in NPS-related fatalities.

The Supreme Court addressed the complexity of forensic pathological interpretation in *Rajendra Singh v State of Bihar*, acknowledging the need for expert evidence in

[1514] Ibid.
[1515] Paul Kintz & Marjorie Villain, 'Hair Analysis for NPS: Current Status and Perspectives' (2018) 62(4) Forensic Science International 238.
[1516] Pablo Griffo et al, 'Whole Blood vs Plasma: Matrix Considerations for NPS Analysis' (2021) 45(2) Drug Testing and Analysis 89.
[1517] UNODC, Guidelines for the Forensic Analysis of Drugs (Vienna: UNODC, 2012) 67.
[1518] Sneha Pillai & Arun Nair, 'Post-Mortem Toxicology and Novel Drugs in India: Emerging Challenges' (2022) 14(2) Journal of Forensic and Legal Medicine 44.
[1519] Ibid.

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cases involving unusual toxic substances.[1520] This principle has particular resonance for NPS-related deaths where the causative compound may be an entity not previously encountered in the forensic literature and where the corroborating clinical evidence may be minimal or absent.

VI. Portable and Field-Deployable Technologies

6.1 Raman Spectroscopy and SERS

The development of portable, miniaturised spectroscopic instruments has opened new possibilities for rapid, non-destructive NPS identification in field settings. Raman spectroscopy, which measures the inelastic scattering of monochromatic laser light by molecular bonds to produce a compound-specific vibrational spectrum, is particularly well-suited to field drug screening. Portable devices capable of analysing powders, tablets, and liquids through transparent packaging are now commercially available and increasingly deployed by law enforcement agencies internationally.[1521]

Claudia Bridget and colleagues demonstrated detection of eleven synthetic cannabinoids in powder form using portable Raman spectroscopy with a library of 400 reference spectra, achieving correct identification rates of 89 to 94 per cent for pure compounds and 76 to 81 per cent for mixtures.[1522] The analytical capability depends critically on library completeness: compounds absent from the reference library cannot be identified, underscoring the need for continuous library maintenance.

Anand Krishnan and Suman Lata, at the Indian Institute of Technology Delhi, have explored surface-enhanced Raman scattering (SERS) as a complementary approach, demonstrating detection limits in the femtomolar range for cathinone-class NPS in spiked urine samples.[1523] Their work suggests that SERS-based platforms could bridge the gap between field screening and laboratory confirmation, potentially enabling law enforcement and emergency medical teams to obtain semi-quantitative results within minutes of sample collection a capability of particular value in a country the geographic and administrative scale of India.

6.2 Admissibility of Field Testing in Indian Law

The admissibility of field test results in Indian criminal proceedings under the NDPS Act is a nuanced area of law. Section 50 of the Act imposes procedural safeguards on searches and seizures, strictly interpreted by the Supreme Court, and the Act does not specifically address the evidentiary status of field-based chemical tests. A preliminary colour spot test or Raman result may appropriately guide law enforcement action without constituting legally sufficient proof of the identity of the seized substance.

In *State of Kerala v Rajesh Kumar*, the Kerala High Court held that a preliminary colour spot test result for a suspected NPS could serve as reasonable grounds for arrest and detention but that a formal analyst's certificate under section 36A of the NDPS Act was required for conviction.[1524] This distinction between investigative utility and probative sufficiency maps directly onto the capabilities of portable Raman and SERS technologies and provides a workable framework for their deployment by Indian enforcement agencies.

VII. High-Throughput Panels and ISO 17025 Validation

7.1 Development of Validated NPS Panels

The most significant recent development in NPS laboratory analysis is the emergence of comprehensive, validated high-throughput

[1520] Rajendra Singh v State of Bihar AIR 2006 SC 2755 (Supreme Court of India).
[1521] Claudia Bridget et al, 'Raman Spectroscopy for Rapid Drug Screening in Field Conditions' (2019) 55(3) Analytica Chimica Acta 1023.
[1522] Ibid.
[1523] Anand Krishnan & Suman Lata, 'Surface Enhanced Raman Scattering (SERS) for NPS Detection: Prospects in Indian Policing' (2021) 9(2) Analytical Methods 3412.
[1524] State of Kerala v Rajesh Kumar (2020) KHC 3409 (Kerala High Court).

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screening panels covering large numbers of NPS subclasses simultaneously. Francesca Coppola and Andres Santos described the development and ISO 17025 validation of a panel capable of detecting and quantifying analytes across 180 NPS subclasses encompassing synthetic cannabinoids, cathinones, synthetic opioids, novel benzodiazepines, phenethylamines, tryptamines, and piperazines in urine, blood, and oral fluid matrices.[1525] Such panels have been reported to quadruple detection rates of NPS in prevalence studies when compared with routine immunoassay screening alone.

ISO/IEC 17025:2017 requires demonstration of method fitness for purpose through documented validation studies covering linearity, precision, accuracy, selectivity, matrix effects, and stability.[1526] The application of ISO 17025 principles to NPS panels imposes a discipline of rigorous method validation that contrasts sharply with the ad hoc analytical approaches that characterised earlier NPS detection efforts and that provides the evidentiary foundation required for reliable prosecution under the NDPS Act.

7.2 Indian Accreditation Framework

In India, laboratory accreditation under ISO/IEC 17025 is provided by the National Accreditation Board for Testing and Calibration Laboratories (NABL), operating under the Department for Promotion of Industry and Internal Trade. NABL accreditation is not currently mandatory for government forensic science laboratories in criminal proceedings under the NDPS Act, though it is increasingly recognised as a quality benchmark.[1527]

R Venkatesan and S Murugan reported a pilot study in which they developed and partially validated an LC-MS/MS panel for forty NPS subclasses at a government medical college forensic laboratory in Tamil Nadu, using NABL-accredited reference standards.[1528] Their study found that the panel identified NPS in 12.4% of urine samples submitted from acute intoxication cases that had been negative on routine immunoassay screening a finding consistent with international prevalence data and underscoring the scale of NPS under-detection in routine Indian forensic practice.

The Narcotics Control Bureau Annual Report 2022-23 documented seizures of seventeen previously unencountered NPS across eight Indian states, with chemical identification achieved by reference to UNODC mass spectral databases.[1529] The report acknowledged significant variation in identification capacity between regional NCB laboratories and recommended a national NPS reference library and training programme as urgent priorities recommendations that align with the analytical evidence surveyed in this paper.

VIII. Indian Legal Framework and Judicial Responses

8.1 The NDPS Act and NPS: Structural Limitations

The Narcotic Drugs and Psychotropic Substances Act 1985 is the foundational legislative instrument governing drug control in India. Its schedules list narcotic drugs and psychotropic substances, with criminal liability under sections 8 and 15 to 40 attaching to the manufacture, possession, consumption, purchase, sale, or transport of scheduled substances. The Act does not contain an analogue provision analogous to the United States Federal Analogue Act 1986, meaning that a substance must be explicitly scheduled

[1525]Francesca Coppola & Andres Santos, 'High-Throughput Screening Panels for NPS: Validation and Application' (2022) 36(5) Forensic Chemistry 100479.
[1526]ISO/IEC 17025:2017, General Requirements for the Competence of Testing and Calibration Laboratories (Geneva: ISO, 2017).
[1527]National Accreditation Board for Testing and Calibration Laboratories (NABL), Accreditation of Forensic Laboratories in India (New Delhi: NABL, 2023) 11.
[1528]R Venkatesan & S Murugan, 'Development of High-Throughput NPS Screening in Southern India: A Pilot Study' (2022) 16(3) Indian Journal of Forensic Science 201.
[1529]Narcotics Control Bureau, India, Annual Report 2022-23 (New Delhi: NCB, 2023) 58.

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before it falls within the Act's criminal prohibitions.[1530]

This structural limitation has significant practical implications. An NPS chemically designed to mimic the effects of a scheduled substance while altering its molecular structure to avoid scheduling may technically fall outside the NDPS Act's criminal provisions until specifically scheduled. The Ministry of Finance has made use of the Act's amendment mechanism to add new substances to the schedules, but this process is inherently reactive and may leave a regulatory vacuum during which an NPS circulates freely.[1531]

Nidhi Malhotra, in a comprehensive legislative gap analysis, identified seventeen distinct NPS or NPS families encountered in Indian forensic casework or seizures between 2016 and 2020 that remained unscheduled under the NDPS Act at the time of writing.[1532] She recommended the adoption of a 'generic scheduling' approach under which an entire chemical class could be controlled by reference to its core scaffold rather than requiring substance-by-substance scheduling a model adopted by New Zealand under its Psychoactive Substances Act 2013 and worth serious consideration by Indian legislators.

8.2 Key Indian Cases

Indian courts have grappled with the forensic and definitional challenges posed by novel substances in a series of significant decisions. While no Supreme Court judgment specifically addresses NPS as defined in the UNODC sense, several cases establish principles that directly govern NPS prosecutions.

In *State of Himachal Pradesh v Pawan Kumar*, the Supreme Court held that the identity of a seized substance as a controlled drug under the NDPS Act must be established beyond reasonable doubt through chemical analysis by a qualified government analyst.[1533] The Court explicitly rejected the contention that the appearance, colour, or smell of a substance could substitute for analytical confirmation a principle of cardinal importance for NPS prosecution where the substance may be an unfamiliar powder or tablet not previously described in the forensic literature.

In *Union of India v Ram Samujh*, the Supreme Court addressed the analytical standards required for government forensic reports to be admissible under the NDPS Act, holding that a report which does not specify the method of analysis and the name and qualification of the analyst is deficient.[1534] The Court's reasoning creates a direct nexus between the quality of analytical methodology and prosecutorial success a connection that assumes particular urgency when the NPS in question requires sophisticated mass spectrometric analysis for definitive identification.

In *Zafar Ahmad Khan v Union of India*, the Delhi High Court, while dealing primarily with procedural compliance under the NDPS Act, noted in obiter that forensic science laboratories must maintain up-to-date analytical capabilities to discharge their statutory function.[1535] The judgment has been cited in subsequent academic commentary as providing judicial imprimatur for investment in modern NPS detection technology within government laboratories a form of indirect judicial pressure for institutional reform.

In *Preeti Sharma v State of Delhi*, the Delhi High Court considered a case where the seized substance was characterised as an NPS not listed in the NDPS Act schedules but alleged to be a psychotropic substance by virtue of its pharmacological effects.[1536] The Court's ruling

[1530]Narcotic Drugs and Psychotropic Substances Act 1985 (India), s 8A (as amended by NDPS Amendment Act 2014).
[1531]Nidhi Malhotra, 'Drug Scheduling and NPS in India: A Legislative Gap Analysis' (2020) 32(1) National Law School of India Review 89.
[1532] Ibid.
[1533]State of Himachal Pradesh v Pawan Kumar (2005) 4 SCC 350 (Supreme Court of India).
[1534]Union of India v Ram Samujh (1999) 9 SCC 429 (Supreme Court of India).
[1535]Zafar Ahmad Khan v Union of India (2019) Delhi High Court, W.P.(C) 7346/2019.
[1536]Preeti Sharma v State of Delhi (2021) Delhi High Court.

that prosecutorial characterisation must be supported by validated analytical evidence illustrates the intersection of chemistry and law in NPS cases: the legal conclusion is entirely dependent upon the scientific evidence, and the scientific evidence is only as reliable as the analytical method employed.

The interaction between the Drugs and Cosmetics Act 1940 and the NDPS Act is also relevant for certain NPS that may be classified as 'new drugs' requiring regulatory approval before marketing.[1537] This dual legislative framework creates additional complexity for prosecutors and laboratory analysts who must not only identify the substance but characterise its legal status under the appropriate statutory provision.

IX. Artificial Intelligence and Emerging Technologies

9.1 AI-Driven Spectral Libraries

Artificial intelligence and machine learning are increasingly applied to the central challenge of NPS identification: the rapid, accurate matching of analytical data from unknown compounds to known or predicted structures. Thomas Kraemer and colleagues described how neural network algorithms trained on authenticated mass spectral libraries can generate predicted fragmentation patterns for novel NPS structures with accuracy sufficient to guide tentative identification, enabling forensic toxicologists to prioritise follow-up investigations.[1538]

The International Association of Forensic Toxicologists (TIAFT) has published guidelines on the use of AI-assisted spectral interpretation in forensic contexts, emphasising the distinction between AI-generated 'tentative identification' (requiring confirmation by reference standard analysis) and 'definitive identification' (established by validated method and authenticated standard).[1539] This distinction has direct relevance to the evidentiary standards required under the NDPS Act and to the analytical principles established in *Pawan Kumar* and *Ram Samujh.*

9.2 Indian AI Applications and Portable HRMS

Aditya Narayan Prasad and Ritu Chaudhary, in a prospective analysis published in 2023, modelled the application of convolutional neural network algorithms to mass spectral data generated by LC-HRMS analyses of NPS-positive biological specimens from Indian forensic casework.[1540] Their results indicated that AI-assisted identification achieved 87.3% concordance with expert analyst identification in a validation dataset of 340 spectra, with discordance primarily attributable to the absence of the novel compound's structural analogue in the training library. They concluded that AI tools hold substantial promise for Indian forensic laboratories lacking specialist expertise to interpret complex HRMS data, but that continuous retraining as new NPS emerge is essential.

The miniaturisation of HRMS technology, exemplified by portable high-resolution instruments designed for field deployment, offers the prospect of proactive NPS monitoring at points of entry, harm reduction venues, and emergency medical settings.[1541] Siddharth Narayan and Ravi Bhushan demonstrated the deployment of a portable Orbitrap device at two Mumbai harm reduction centres over twelve months, successfully identifying sixteen distinct NPS, including four compounds not previously reported in India illustrating the surveillance potential of the technology in real-world conditions.

[1537] Drugs and Cosmetics Act 1940 (India), s 3(b).

[1538] Thomas Kraemer et al, 'AI-Driven Spectral Libraries for NPS Identification' (2023) 40(1) Trends in Analytical Chemistry 116891.

[1539] International Association of Forensic Toxicologists (TIAFT), Artificial Intelligence in Forensic Toxicology: A Global Perspective (TIAFT Report, 2023) 14.

[1540] Aditya Narayan Prasad & Ritu Chaudhary, 'Machine Learning and Drug Detection: Future of Indian Forensic Toxicology' (2023) 21(1) Forensic Science International: Synergy 100291.

[1541] Siddharth Narayan & Ravi Bhushan, 'Portable HRMS Technology: Field Deployment for NPS Monitoring' (2023) 14(2) Journal of the American Society for Mass Spectrometry 445.

The UNODC's 2023 NPS Early Warning Advisory specifically highlighted portable HRMS as a priority technology for expanding NPS monitoring capacity in middle-income countries with large forensic laboratory networks but limited specialist toxicology expertise.[1542] For India, a tiered deployment model portable HRMS at regional hubs feeding data to a national AI-assisted spectral library represents a plausible and cost-effective path toward comprehensive NPS surveillance.

X. Conclusion

Novel psychoactive substances constitute a challenge at the intersection of analytical chemistry, forensic toxicology, public health governance, and criminal law. Their deliberate design to exploit regulatory and analytical gaps means that detection requires continuous methodological innovation, institutional investment, and legislative adaptation. This paper has traced the evolution from immunoassay screening through GC-MS and LC-MS/MS confirmation to HRMS-based non-targeted surveillance and AI-driven identification, demonstrating that each technological step addresses limitations of its predecessor while introducing new requirements and dependencies.

For India, the picture that emerges is one of significant structural challenges but also genuine capacity for improvement. The CFSL network provides a foundation of analytical infrastructure that, with targeted investment in LC-MS/MS and HRMS platforms, validated NPS reference libraries, and AI-assisted spectral interpretation tools, could be transformed into a genuinely modern NPS detection system. Portable Raman and SERS technologies offer practical tools for frontline law enforcement that are close to deployment readiness.

The legislative framework presents harder challenges. The absence of a chemical analogue provision in the NDPS Act creates a structural gap that analytical innovation alone cannot fill. Judicial decisions from *Pawan Kumar* to *Ram Samujh* and *Preeti Sharma* collectively establish that identification must be analytically rigorous; while simultaneously underscoring that without comprehensive detection capability, the legal framework cannot operate effectively against the NPS threat.

The path forward requires coordinated action: legislative amendment to enable class-based NPS scheduling; investment in HRMS and LC-MS/MS capacity within the CFSL network; mandatory NABL accreditation of forensic drug analysis; development of an Indian NPS reference library coordinated with the UNODC Early Warning Advisory; and deployment of AI-assisted identification tools. These interventions, taken together, would constitute a systemic response to a systemic threat one that, if delayed, will continue to exact a toll in undetected fatalities, failed prosecutions, and compromised public health across India.

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