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Editorial Office Address

Department of Forensic Medicine & Toxicology, Third Floor, Mortuary Building, Lokmanya Tilak Municipal Medical College & LTMG Hospital, Sion, Mumbai, Maharashtra, India. Pin-400 022. Email id: mlameditor@gmail.com Phone: 022-68660000/ +91-9423016325.



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Review Article

Leveraging AI for Clinical and Toxicological Profiling of New Psychoactive Substances

Veenakirthika Seetharaman^a, Rajkumar Krishnan Vasanthi^b, Kumaraswamy Dabburu^c, Ramanya Gayathri Muraliram^d, Lubna Khondker^e, Shanthi Balasubramanian^f, Pichandy Muthuprasanna^g, Abhijit Dutta^{h*}

^aProfessor, Faculty of Physiotherapy, Dr. M.G.R Educational and Research Institute, Deemed to be University, Chennai, Tamil Nadu, India, 600095, Orcid ID- 0000-0003-3790-9579, ^bFaculty of Health and Life Sciences, INTI International University, Nilai, Negeri Sembilan, Malaysia, 71800, Orcid ID- 0000-0001-6866-8224, ^cProfessor of Pharmacology, University: Bridgetown International University, Barbados, USA, BB14022, Orcid ID- 0009-0004-7226-0538. ^dAssistant Professor, School of Law, SASTRA Deemed to be University, Thanjavur, Tamil Nadu, India, 613401, Orcid ID- 0000-0001-5748-9570. ^eAssociate Professor, Dept of Dermatology and Venereology, Bangladesh Medical University(BMU), Dhaka, Bangladesh, Orcid ID-0000-0002-7186-3749. ^fProfessor and HOD, Dept of Biochemistry, Sree Balaji medical college and hospital, Tamil Nadu, India, 600044, Orcid ID- 0000-0002-7435-5985. ^gProfessor, Department of Pharmaceutical Biotechnology, Surya School of Pharmacy, Vikiravandi, Villupuram Dt. Tamil Nadu, India, 605652, Orcid ID- 0000-0001-5907-6649. ^hDean and Professor, Royal School of Medical and Allied Sciences, The Assam Royal Global University, Betkuchi, Guwahati, Assam, India, 781035, Orcid ID- 0000-0002-0055-6696.

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Abstract

Background: Artificial intelligence (AI) is an important tool for dealing with the growing problem of new psychoactive substances (NPSs). AI can predict how chemicals will behave, create new psychoactive frameworks, and assist forensic labs in identifying drugs that have not been recognized but can be detected by advanced machine learning (ML), deep neural networks, and generative algorithms. Generative models such as Dark-NPS and STNGS have demonstrated efficacy in producing libraries of potential NPS analogs, thereby enhancing proactive detection and management. **Objective:** To explore AI's role in predicting, detecting, and regulating new psychoactive substances while ensuring ethical and legal compliance. **Discussion:** AI-driven quantitative structure-activity relationship (QSAR) modeling and predictive analytics facilitate the evaluation of pharmacological efficacy, toxicity, and metabolic stability, thereby supporting drug research and regulatory decision-making. Policymakers in the EU and the US are realizing that there needs to be a flexible law for AI-generated drugs that affect the mind. **Conclusion:** To ensure AI is used correctly in the NPS domain, we need a multidisciplinary approach that includes data science, toxicology, chemistry, and legal frameworks. This helps us find a balance between innovation and public safety.

1. Introduction

Psychoactive substances are chemical compounds that act on the central nervous system to perception observation, mood, cognition, or behavior. NPS are newly emerging compounds

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***Corresponding author:** Dr. Abhijit Dutta, Dean and Professor, Royal School of Medical and Allied Sciences, The Assam Royal Global University, Betkuchi, Guwahati, Assam, India. E-mail: duttapapa2025@gmail.com

designed to produce similar effects to controlled drugs while often evading regulatory classification. AI has rapidly become an important tool for solving the NPS problem. QSAR algorithms and deep learning (DL) can explore large biological spaces to identify candidates with a strong interest in therapeutic goals or a high level of harmfulness before synthesis.¹ NPS are a heterogeneous collection of compounds often marketed as "legal" substitutes for traditional controlled narcotics, including heroin, cocaine, amphetamines, and benzodiazepines. The word may be seen as rather misleading, since several chemicals have subsequently been included in the roster of scheduled drugs at both national and international levels. The "legality" of these substances remains a primary appeal for users. Although several drugs are now regulated, some remain unscheduled, undiscovered, and unidentified. The primary motivations for using NPS are the asserted attributes of "safety" and "natural origin" by the provider, both of which have contributed to a remarkable surge in the appeal of NPS, despite being marketed as "safe" or labeled "not for human consumption," these chemicals pose significant health hazards, requiring a comprehensive understanding of their pharmacokinetic and pharmacodynamic characteristics for effective prevention. NPSs are also referred to as upscale drugs or exploration compounds. More than 850 NPSs were being watched in Europe, and about two NPSs were sent out every week. Globally, more than 1,200 NPSs were recorded.²

These chemicals come in many different types, and most of them have not been through safety tests. Many NPSs were linked to major health problems and even death, which was a threat to public health. Regulatory authorities have struggled to keep up with the NPS problem. The use of AI in the domain of innovative psychoactive drugs is a classic double-edged sword. AI provides robust answers to methodical and forensic experiments: it may expedite drug discovery effectively, assist forensic laboratories in outpacing traffickers, and deliver insights into the extensive biochemical landscape of psychoactive that were formerly unattainable for humans.³ AI models do not get biased, so they can constantly look for strange patterns in data streams like mass spectra and social media signals. In medical chemistry, this could be beneficial (for instance, finding new pain relievers with less potential for addiction). In illegal drug markets, it could get around current rules by

bringing in drugs that do not fit into traditional structural categories. When legislators find out about new chemicals, they often make them illegal.⁴ The present review aims to critically examine AI applications in the prediction, detection, and regulation of NPS, with emphasis on analytical toxicology, forensic identification, regulatory challenges and future research directions.

2. Discussion

AI Generative Models

Generative models are designed to create new molecular structures by analyzing how existing substances behave and using that information to predict the behavior of new substances. The Dark-NPS methodology is a new way to look at NPSs.⁵ By sampling this model, researchers developed a substantial collection of probable NPS like structures, referred to as structural "priors," which might aid in identifying unknown designer drugs. The Smart Technology-Enabled Novel Generation Systems (STNGS) framework, devised by Liu and co-authors⁶, represents an AI-driven system for NPS prediction and evaluation. This framework provides a scaffold-based molecular generator, equipped with a multifaceted recording system to evaluate the generated compounds.

As a replacement for employing unfocused generation techniques, STNGS emphasizes established core scaffolds typical in natural products. It utilizes a transformer-based neural network, which includes a T-scaffold encoder-decoder and a Mol-GPT module, to produce analogs based on these scaffolds. Current AI models for molecular generation and prediction employ varied architectures, each with distinct advantages. Graph neural networks (GNNs) represent molecules as graphs containing atoms and bonds, allowing direct learning of structural relationships and chemical topology. These models are particularly effective for forecasting molecular properties and receptor interactions. In contrast, SMILES-based transformer models treat molecular structures as sequential strings and apply natural language processing techniques to generate novel compounds or predict chemical properties.⁷ While SMILES-based methods enable efficient large-scale generation, they may produce syntactically valid but chemically impractical molecules. Hybrid approaches combining graph-based representations with sequence-based learning have also been explored to improve analytical accuracy and chemical validity. Generative models are subjective to biases in training

datasets, which may limit chemical diversity and lead to over-representation of known structural classes. The dual-use nature of such technologies also raises concerns regarding the potential generation of harmful or toxic compounds without adequate safeguards.

AI-Based QSAR Modeling

QSAR is a computational method widely used in pharmacology, leveraging arithmetical and ML models to forecast biological actions based on chemical structure descriptors. QSAR modeling relies on the removal of molecular descriptors that numerically represent chemical structure and physicochemical properties. Common descriptor categories include constitutional descriptors (molecular weight, atom counts), topological descriptors (connectivity indices), electronic descriptors (charge distribution, polarizability), and physicochemical properties such as lipophilicity and hydrogen bonding capacity.⁸ More progressive approaches incorporate 3D structural descriptors, pharmacophore features, and molecular fingerprints. The choice of descriptors suggestively influences model performance and interpretability, and inappropriate descriptor selection may lead to dismissal, model variability, or reduced predictive accuracy. Similarly, Floresta⁹ and co-authors introduced a multi QSAR modeling method aimed specifically at predicting μ -opioid receptor (μ -OR) binding similarities for newly synthesized fentanyl analogs. AI algorithms are being employed to predict additional attributes essential for NPSs. ML techniques are being harnessed to forecast the metabolic stability and toxicity of novel analogs, a critical aspect given that some NPSs can function as prodrugs or generate harmful metabolites.¹⁰ AI predictive models can forecast chromatographic retaining times or mass spectrometry fragmentation arrangements, enhancing analytical detection capabilities. Workflow of QSAR-Based Prediction is NPSs shown in [figure 01](#). Virtual docking, paired with ML scoring, is also pragmatic for forecasting which new psychoactive analogs are likely to stimulate the serotonin 5-HT_{2A} receptor, a determinant in distinguishing genuine psychedelic compounds from potentially therapeutic or inert analogs.¹¹

Despite the capable predictive performance of QSAR models, several limitations must be considered. QSAR models are highly dependent on the quality and diversity of training datasets and limited chemical space coverage may restrict their applicability to NPS

with uncommon structures. Excessive model fitting remains a major concern, particularly when models are trained on small datasets or large numbers of molecular descriptors. Internal validation alone may overrate predictive performance and external validation using independent datasets is critical to ensure generalizability. The applicability domain of QSAR models must be clearly defined, as estimates outside this domain may lead to unpredictable estimates of biological activity or toxicity.

AI-Based Automated NPS Synthesis

AI is significantly advancing the development of NPSs through the creation of AI-driven retrosynthetic planning tools. These tools can propose synthetic pathways for new chemicals, potentially optimizing the laboratory synthesis of NPS analogs. Innovations in computerized synthesis might lead to the rapid production of AI-designed psychotropic substances for further evaluation.¹² This capability allows for feasible synthesis designs to be identified within minutes when integrated into an AI-generated NPS framework. These same AI techniques can be beneficial for reputable laboratories, enabling them to swiftly produce reference materials for new NPSs, which is critical for analytical and toxicological assessments. The revolution in NPS creation and preliminary assessment, driven by AI methodologies ranging from DL generative models to predictive QSAR and property models, transforms the landscape. Instead of reacting to the emergence of new drugs, scientists and regulators can proactively investigate potential NPSs that may be created. AI technology can build virtual libraries of analogs and predict their potency or hazard levels, thus assisting in the prioritization of properties for synthesis, preparation, and observation of the most concerning applicants.

AI-Based Mass Spectrophotometry for NPS

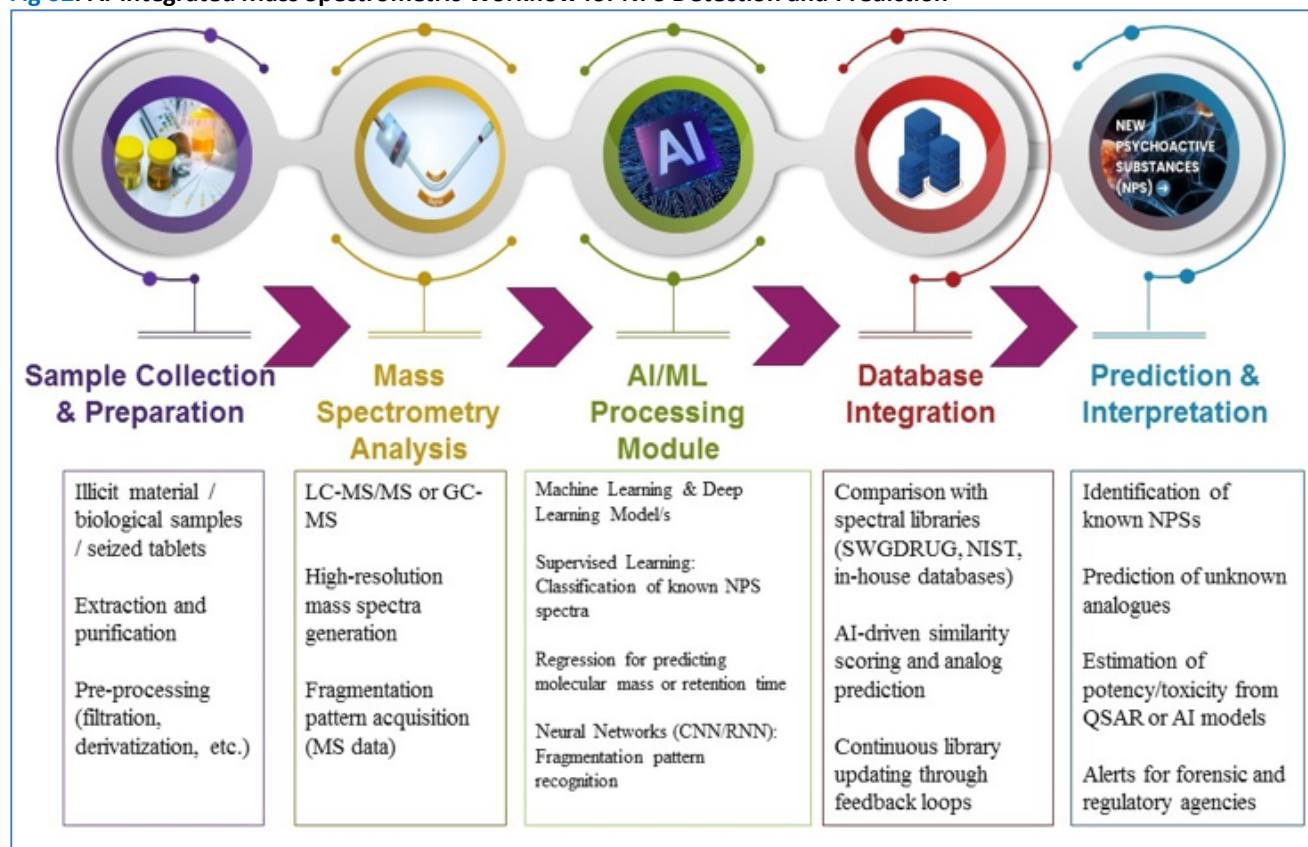
The exploration of NPSs presents significant challenges, particularly due to the lack of available reference spectra for newly discovered compounds. Innovative advancements in AI and ML have developed as powerful tools for overcoming these challenges. The progress of DL models that can directly forecast mass spectrometry/mass spectrometry (MS/MS) spectra of organic compounds based on their structures.¹³ The authors also compiled an extensive database containing approximately 8.8 million potential NPS structures, informed by the "Dark-NPS" library and additional combinatorial inventories, each linked to its

anticipated spectra. Methodologies like Competitive Fragmentation Modeling (CFM) have demonstrated effectiveness in predicting fragmentation pathways and their intensities.¹⁴

Figure 01: Workflow of QSAR-Based Prediction in NPSs



Fig 02: AI-Integrated Mass Spectrometric Workflow for NPS Detection and Prediction



AI further aids in spectral matching, wherein unidentified spectra are aligned against databases of known spectra to ascertain potential matches. In practical applications, Tian¹⁵ and co-authors have combined Shifted-Excitation Raman Difference Spectroscopy (SERDS) with ML to facilitate rapid on-

site identification of NPSs. By employing SERDS to curate fluorescence-free Raman spectra of samples and subsequently applying support vector machines (SVMs), their enhanced SVM model has achieved over 97% accuracy in classifying unknown substances into distinct drug families, such as fentanyl analogs,

amphetamine-type stimulants, or synthetic cannabinoids.¹⁶ AI-Integrated Mass Spectrometric Workflow for NPS Detection and Prediction, shown in [figure 2](#). This integrated computational-analytical framework supports forensic chemists and regulatory authorities in rapidly identifying emerging NPSs, estimating toxicity or abuse potential, and guiding effective law enforcement responses. AI-assisted mass spectrometry has significantly improved NPS detection; several analytical trials remain. Predictive models may produce false positive or false negative identifications, mainly when analyzing structurally novel compounds outside the model's training distribution. Indecision quantification is often limited in current operations, which may affect the certainty in forensic interpretation. Performance depends heavily on the quality of spectral databases and reference libraries and incomplete datasets may reduce identification accuracy. These limitations highlight the need for standardized validation procedures and cautious interpretation of AI-assisted results in forensic settings.

Explainable AI and Model Interpretability in NPS Research

The application of AI in forensic and governing contexts requires model transparency. Explainable AI (XAI) techniques aim to clarify how predictive models generate outputs, thereby increasing trust and supporting decision-making in legal and clinical environments. Methods such as feature importance analysis, SHAP (Shapley Additive Explanations), and attention-based conception enable identification of structural features responsible for expected biological activity or toxicity. In QSAR modeling, transparency allows researchers to identify key molecular descriptors influencing receptor binding or pharmacological effects. Model transparency is particularly important for forensic toxicology, where AI-generated forecasts may influence regulatory classification or legal evidence. Lack of transparency in "black-box" models remains a significant challenge and future research should order interpretable architectures and standardized explanation methods to ensure responsibility and regulatory acceptance.¹⁷

Governance and Legal Perspectives On AI-Driven Psychoactive Compound Development

The convergence of AI, NPSs, and drug policy introduces complex legal and supervisory challenges, particularly within the European Union (EU) and the United States (USA). In the EU, the management of NPSs is coordinated through an initial cautionary

system functioned by the European Monitoring Center for Drugs and Drug Addiction. At present, no law exists to prohibit the public dissemination of procreative models that may be used to produce NPSs or other hazardous substances. In the USA, the regulatory landscape for NPSs is primarily governed by the **Controlled Substances Act** and the **Controlled Substances Analog Enforcement Act of 1986**¹⁸, which empowers authorities to classify substances that are "substantially similar" to existing controlled drugs. Both areas are gradually strengthening their rules to find a balance between rapid regulatory responses and the risks associated with faster AI-driven drug synthesis.

a. AI Regulatory Frameworks for High-Risk Systems

The rising use of AI in drug discovery and forensic analysis has prompted the development of regulatory frameworks addressing high-risk AI applications. The European Union has introduced the EU AI Act, which categorizes AI tools used in forensic toxicology or drug prediction may fall within this high-risk classification, requiring transparency, human oversight and rigorous concert evaluation.¹⁹ Such frameworks highlight data quality, accountability, and traceability of AI decisions, which are particularly relevant for AI-assisted identification or prediction of NPS. Traditional drug control policies primarily rely on structure-based scheduling, where substances are regulated based on structural similarity to known controlled drugs.²⁰ AI-assisted prediction of receptor required and pharmacodynamic effects may support such effect-based regulation by enabling early identification of harmful compounds. A hybrid regulatory strategy combining structural and functional evaluation may therefore provide more effective control of emerging AI-generated psychoactive substances.

b. Liability and Responsibility in AI-Generated Molecules

The use of AI systems capable of generating novel psychoactive compounds raises multiple questions regarding legal liability. Responsibility may extend to developers of AI algorithms, providers of training datasets, or users who apply predictive tools for illegal purposes. The absence of clear legal frameworks creates uncertainty regarding accountability when AI-generated molecular designs contribute to public health risks or illegal drug production. Starting liability standards for AI-assisted drug design remains a significant policy challenge and requires clear guidelines defining originator

responsibility, user responsibility and institutional oversight.

c. Regulation of Predictive Modeling and Dual-Use Concerns

AI-based predictive modeling of psychoactive compounds presents a dual-use problem, as the same technologies that assist forensic laboratories and public health authorities may also enable the design of illegal substances. This raises policy questions regarding whether access to predictive models, generative algorithms, or chemical libraries should be restricted.²¹ While open scientific research promotes innovation and public safety alertness, unrestricted distribution of models capable of generating highly important compounds may increase the risk of misuse. Balancing scientific openness with security deliberations remains a key challenge for regulators and research institutions.

1. 3. Regulatory Challenges and Ethical Considerations

AI applications in the calculation and generation of NPS raise concerns related to dual-use research, where technologies planned for beneficial purposes may also be misused. Governance frameworks for dual-use research emphasize risk mitigation, institutional error and responsible distribution of sensitive findings. International policy discussions highlight the need for ethical review mechanisms, organized data sharing and observation of high-risk research outputs. Several risk qualification approaches have been proposed to reduce potential misuse of AI systems capable of predicting or generating psychoactive compounds. Monitoring usage patterns, incorporating safety filters to prevent the generation of risky compounds, and establishing institutional review procedures for high-risk research may further decrease misuse. Such safeguards can help balance scientific openness with public health and security considerations. AI algorithms may generate dangerous or unstable chemicals if not meticulously regulated, and insufficient or inconsistent data often constrain the predicted accuracy for NPSs.²²⁻²⁴

Responsible organization of AI in forensic and pharmaceutical research requires adherence to principles of transparency, accountability, equality. International enterprises, including guidelines proposed by the OECD and regulatory efforts within the European Union, emphasize reliable AI systems that ensure data integrity, model dependability and explainability. In forensic toxicology, responsible AI implementation is particularly important because

predictive outputs may influence clinical decisions, regulatory classification, or legal proceedings. Creating standardized governance frameworks and ethical guidelines will be essential to ensure safe and accountable use of AI technologies in the study of NPS.

4. Prospective Outlook

Advancements in generative AI within the field of NPS are increasingly directed toward the creation of models capable of designing unique molecular scaffolds with targeted psychoactive effects. Future investigations are anticipated to integrate multi-parametric optimization, assessing not only psychoactive potency but also toxicity, metabolic stability, and other pharmacokinetic parameters to generate comprehensive “risk” or “danger” scores.²⁵ Such outputs could significantly aid both drug developers and regulatory authorities in evaluating potential threats. At the same time, policymakers might push for the use of predictive modeling platforms to predict when new NPS will appear and help with proactive control strategies. Because NPS proliferation happens across borders, effective implementation will depend on countries working together and sharing data. It is also very important to consider the ethical issues that arise when using AI in this field.²⁶⁻²⁸ To stop abuse and allow responsible innovation, there needs to be oversight similar to high-risk biological research.

5. Limitations of AI in NPS Research

Despite rapid advancements, AI-based approaches for NPS prediction and detection face several limits. Model performance is strongly reliant on data quality, dataset representativeness and validation policies. Many studies report high predictive accuracy without adequate external validation or reproducibility evaluation. Algorithmic bias, uncertainty in predictions and lack of standardized evaluation metrics may affect forensic dependability. Transparency of DL models remains limited, which poses challenges for legal and regulatory acceptance of AI-generated evidence. Addressing these limitations requires improved data sharing, standardized benchmarking procedures and transparent validation frameworks. Consistent QSAR model development requires rigorous validation procedures to ensure analytical performance. Common approaches include k-fold cross-validation, leave-one-out validation and external validation using independent datasets.²⁹ Cross-validation helps evaluate a model and detect overfitting, while

external validation provides stronger evidence of predictive dependability for novel compounds. The limited availability of diverse NPS datasets often constrains healthy validation, which may affect model reproducibility and applicability in forensic practice.

2. 6. Conclusion

AI is renovating the field of NPS through advancements in the design, estimation, and identification of new chemical compounds. Mass spectrometry, predominantly in ML, improves the speed and accuracy of NPS identification, addressing substantial challenges in forensic science. The growth of AI necessitates a reevaluation of regulatory strategies, as prevailing policies in the EU and the USA need to adapt to the evolving landscape of illegal drugs.

Future efforts must emphasize emerging specialized AI models for NPS, refining data sharing, and fostering interdisciplinary association to validate AI predictions. Policymakers, scientists, and ethicists must engage in ongoing dialogue to ensure that advancing laws reflect current scientific empathy and uphold principles of ethical and accountable AI use. There is a perilous need for training practitioners in forensic labs to interpret AI outputs precisely.

Finally, while AI delivers powerful tools to address the complexities of the designer drug market, cautious oversight is vital to stabilize its benefits against potential risks, ensuring we stay ahead in combating substance abuse. Future work should arrange interpretable AI models and standardized validation frameworks to support forensic and regulatory adoption.

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