Received: 18 April 2025 / Accepted: 07 December 2025 / Published online: 27 February 2026

DOI 10.34689/SH.2025.28.1.017

UDC 618.14-006.36-073.756.8

ARTIFICIAL INTELLIGENCE IN FORENSIC MEDICINE AND PHARMACOLOGY: INTERNATIONAL APPROACHES AND GUIDELINES FOR KAZAKHSTAN IN THE ANALYSIS OF NOVEL PSYCHOACTIVE SUBSTANCES. LITERATURE REVIEW

Murat N. Lepesbayev[1], https://orcid.org/0009-0006-9810-9232
Dinar Sh. Tarzhanova[2], https://orcid.org/0000-0002-3740-1874
Zhanetta T. Mukanova[2], https://orcid.org/0000-0001-5272-1190
Kanatbek N. Mukanov[2], https://orcid.org/0000-0001-6838-4512
Saulesh A. Apbassova[1], https://orcid.org/0000-0001-6981-5441
Akmaral A. Zhakipova[1], https://orcid.org/0000-0003-3023-9445
Indira K. Uyzbayeva[2], https://orcid.org/0000-0003-4282-4799
Akmaral Zhantureyeva[2], https://orcid.org/0000-0001-5063-6312
Dariya M. Shabdarbayeva[1], https://orcid.org/0000-0001-9463-1935

[1] **NCJSC «Semey Medical University», Semey, Republic of Kazakhstan;**
[2] **NCJSC «Astana Medical University», Astana, Republic of Kazakhstan.**

Abstract

Introduction. The rapid and frequent emergence of novel psychoactive substances (NPS) contributes to increasing workload for forensic medical examination and clinical toxicology services. Existing analytical methods cannot cope with the growing volumes of data from modern high-resolution mass spectrometry, necessitating the introduction of advanced approaches, primarily artificial intelligence methods.

Objective. To investigate and systematize international experience in applying artificial intelligence in forensic medicine and pharmacology for analyzing novel psychoactive substances, and to propose practical recommendations for implementation in Kazakhstan.

Search strategy. A thorough narrative review of 78 international literature sources was conducted, covering analytical methods of liquid chromatography coupled with high-resolution mass spectrometry, data processing standards, substance identification libraries, machine learning algorithms, clinical protocols, and pharmacovigilance systems.

Results. Key components of an integrated system were identified: standardization of data formats (mzML, mzTab-M), specialized computational processing tools (XCMS, MZmine, OpenMS, MS-DIAL), spectral libraries (MassBank, mzCloud), computational identification methods (SIRIUS, CFM-ID, GNPS), a grading system for result reliability (Schymanski confidence levels), clinical antidote therapy protocols, and international information exchange channels on emerging threats (EudraVigilance, FAERS, VigiBase, EU EWS, EMCDDA, UNODC).

Conclusions. Effective implementation of artificial intelligence requires compliance with international data compatibility standards, rigorous validation of machine learning algorithms, and integration with international monitoring systems. The proposed recommendations ensure scalability of solutions regardless of local regulatory specificities.

Keywords: *artificial intelligence, forensic medicine, toxicology, clinical pharmacology, Kazakhstan, mass spectrometry, pharmacovigilance.*

For citation:

Lepesbayev M.N., Tarzhanova D.Sh., Mukanova Zh.T., Mukanov K.N., Apbassova S.A., Zhakipova A.A., Uyzbayeva I.K., Zhantureyeva A., Shabdarbayeva D.M. Artificial intelligence in forensic medicine and pharmacology: international approaches and guidelines for Kazakhstan in the analysis of novel psychoactive substances. Literature review // *Nauka i Zdravookhranenie* [Science & Healthcare]. 2026. Vol.28 (1), pp. 142-151. *doi 10.34689/SH.2026.28.1.017*

Резюме

ИСКУССТВЕННЫЙ ИНТЕЛЛЕКТ В СУДЕБНОЙ МЕДИЦИНЕ И ФАРМАКОЛОГИИ: МЕЖДУНАРОДНЫЕ ПОДХОДЫ И РУКОВОДЯЩИЕ ПРИНЦИПЫ ДЛЯ КАЗАХСТАНА В АНАЛИЗЕ НОВЫХ ПСИХОАКТИВНЫХ ВЕЩЕСТВ. ОБЗОР ЛИТЕРАТУРЫ

Мурат Н. Лепесбаев[1], https://orcid.org/0009-0006-9810-9232
Динар Ш. Таржанова[2], https://orcid.org/0000-0002-3740-1874

Жанетта Т. Муканова[2], https://orcid.org/0000-0001-5272-1190
Канатбек Н. Муканов[2], https://orcid.org/0000-0001-6838-4512
Саулеш А. Апбасова[1], https://orcid.org/0000-0001-6981-5441
Акмарал А. Жакипова[1], https://orcid.org/0000-0003-3023-9445
Индира К. Уызбаева[2], https://orcid.org/0000-0003-4282-4799
Акмарал Жантуреева[2], https://orcid.org/0000-0001-5063-6312
Дария М. Шабдарбаева[1], https://orcid.org/0000-0001-9463-1935

[1] **НАО «Медицинский университет Семей», г. Семей, Республика Казахстан;**
[2] **НАО «Медицинский университет Астана», г. Астана, Республика Казахстан.**

Введение. Быстрое и частое появление новых психоактивных веществ (НПВ) приводит к увеличению рабочей нагрузки на судебно-медицинские экспертизы и клиническую токсикологию. Существующие аналитические методы не справляются с растущими объемами данных, получаемых с помощью современной масс-спектрометрии высокого разрешения, что обусловливает необходимость внедрения передовых подходов, прежде всего методов искусственного интеллекта.

Цель. Исследовать и систематизировать международный опыт применения искусственного интеллекта в судебной медицине и фармакологии для анализа новых психоактивных веществ и предложить практические рекомендации по его внедрению в Казахстане.

Стратегия поиска. Проведен тщательный обзор 78 международных литературных источников, охватывающих аналитические методы жидкостной хроматографии в сочетании с масс-спектрометрией высокого разрешения, стандарты обработки данных, библиотеки идентификации веществ, алгоритмы машинного обучения, клинические протоколы и системы фармаконадзора.

Результаты. Были определены ключевые компоненты интегрированной системы: стандартизация форматов данных (mzML, mzTab-M), специализированные инструменты вычислительной обработки (XCMS, MZmine, OpenMS, MS-DIAL), спектральные библиотеки (MassBank, mzCloud), методы вычислительной идентификации (SIRIUS, CFM-ID, GNPS), система оценки достоверности результатов (уровни доверия Шиманского), протоколы клинической антидотной терапии и международные каналы обмена информацией о возникающих угрозах (EudraVigilance, FAERS, VigiBase, EU EWS, EMCDDA, UNODC).

Выводы. Эффективное внедрение искусственного интеллекта требует соблюдения международных стандартов совместимости данных, строгой проверки алгоритмов машинного обучения и интеграции с международными системами мониторинга. Предложенные рекомендации обеспечивают масштабируемость решений независимо от местных нормативных особенностей.

Ключевые слова: *искусственный интеллект, судебная медицина, токсикология, клиническая фармакология, Казахстан, масс-спектрометрия, фармаконадзор*

Для цитирования:

Лепесбаев М.Н., Таржанова Д.Ш., Муканова Ж.Т., Муканов К.Н., Апбасова С.А., Жакипова А.А., Уйзбаева И.К., Жантуреева А., Шабдарбаева Д.М. Искусственный интеллект в судебной медицине и фармакологии: международные подходы и руководящие принципы для Казахстана в анализе новых психоактивных веществ. Обзор литературы // Наука и Здравоохранение. 2026. Vol.28 (1), С. 142-151. *doi 10.34689/SH.2026.28.1.017*

Түйіндеме

СОТ МЕДИЦИНАСЫ МЕН ФАРМАКОЛОГИЯДАҒЫ ЖАСАНДЫ ИНТЕЛЛЕКТ: ЖАҢА ПСИХОАКТИВТІ ЗАТТАРДЫ ТАЛДАУДАҒЫ ҚАЗАҚСТАНҒА АРНАЛҒАН ХАЛЫҚАРАЛЫҚ ТӘСІЛДЕР МЕН НҰСҚАУЛАР. ӘДЕБИЕТКЕ ШОЛУ.

Мурат Н. Лепесбаев[1], https://orcid.org/0009-0006-9810-9232
Динар Ш. Таржанова[2], https://orcid.org/0000-0002-3740-1874
Жанетта Т. Муканова[2], https://orcid.org/0000-0001-5272-1190
Канатбек Н. Муканов[2], https://orcid.org/0000-0001-6838-4512
Саулеш А. Апбасова[1], https://orcid.org/0000-0001-6981-5441
Акмарал А. Жакипова[1], https://orcid.org/0000-0003-3023-9445
Индира К. Уызбаева[2], https://orcid.org/0000-0003-4282-4799
Акмарал Жантуреева[2], https://orcid.org/0000-0001-5063-6312
Дария М. Шабдарбаева[1], https://orcid.org/0000-0001-9463-1935

[1] **КеАҚ «Семей медицина университеті», , Семей қ., Қазақстан Республикасы;**
[2] **КеАҚ «Астана медицина университеті», Астана қ., Қазақстан Республикасы.**

Кіріспе. Жаңа психобелсенді заттардың (ЖПЗ) тез және жиі пайда болуы сот-медициналық сараптама және клиникалық токсикология қызметтеріне түсетін жүктеменің артуына әкеледі. Қолданыстағы талдау әдістері қазіргі заманғы жоғары ажыратымдылықтағы масс-спектрометриядан алынатын деректердің өсіп келе жатқан көлемін өңдеуге қауқарсыз, бұл озық тәсілдерді, ең алдымен жасанды интеллект әдістерін енгізуді қажет етеді.

Зерттеу мақсаты. Жаңа психобелсенді заттарды талдау үшін сот медицинасы мен фармакологияда жасанды интеллектті қолданудың халықаралық тәжірибесін зерттеу және жүйелеу, сондай-ақ Қазақстанда енгізу бойынша практикалық ұсыныстар әзірлеу.

Іздеу стратегиясы. Жоғары ажыратымдылықтағы масс-спектрометриямен біріктірілген сұйықтық хроматографияның талдау әдістерін, деректерді өңдеу стандарттарын, заттарды сәйкестендіру кітапханаларын, машиналық оқыту алгоритмдерін, клиникалық хаттамаларды және фармакологиялық қадағалау жүйелерін қамтитын 78 халықаралық әдебиет дереккөзіне терең шолу жүргізілді.

Нәтижелер. Біріктірілген жүйенің негізгі компоненттері анықталды: деректер форматтарын стандарттау (mzML, mzTab-M), арнайы есептеуіш өңдеу құралдары (XCMS, MZmine, OpenMS, MS-DIAL), спектрлік кітапханалар (MassBank, mzCloud), есептеуіш сәйкестендіру әдістері (SIRIUS, CFM-ID, GNPS), нәтижелердің сенімділігін бағалау жүйесі (Шиманскийдің сенімділік деңгейлері), антидоттық терапияның клиникалық хаттамалары және төнетін қауіптер туралы халықаралық ақпарат алмасу арналары (EudraVigilance, FAERS, VigiBase, EU EWS, EMCDDA, UNODC).

Қорытынды. Жасанды интеллектті тиімді енгізу деректер үйлесімділігінің халықаралық стандарттарын сақтауды, машиналық оқыту алгоритмдерін қатаң валидациялауды және халықаралық мониторинг жүйелерімен интеграцияны талап етеді. Ұсынылған шаралар жергілікті нормативтік ерекшеліктерге қарамастан шешімдердің ауқымдылығын қамтамасыз етеді.

Түйінді сөздер: *жасанды интеллект, сот медицинасы, токсикология, клиникалық фармакология, Қазақстан, масс-спектрометрия, фармакологиялық қадағалау.*

Дәйексөз үшін:

Лепесбаев М.Н., Таржанова Д.Ш., Муканова Ж.Т., Муканов К.Н., Апбасова С.А., Жакипова А.А., Уйзбаева И.К., Жантуреева А., Шабдарбаева Д.М. Сот медицинасы мен фармакологиядағы жасанды интеллект: жаңа психоактивті заттарды талдаудағы Қазақстанға арналған халықаралық тәсілдер мен нұсқаулар. Әдебиетке шолу // Ғылым және Денсаулық сақтау. 2026. Vol.28 (1), Б. 142-151. *doi 10.34689/SH.2026.28.1.017*

Introduction

Currently, nearly all countries worldwide face the challenge of emerging novel psychoactive substances (NPS). Created to circumvent state control and regulation, primarily in clandestine laboratories, these synthetic compounds pose significant public health threats.

The rapid and frequent emergence of NPS creates excessive workload for analytical laboratories, as traditional approaches to identification and verification do not scale to the data volumes generated by modern high-resolution mass spectrometry [1–3,5,9,45,78].

A striking example is the well-known outbreak of poisonings caused by the synthetic cannabinoid AMB-FUBINACA in New York, termed the "zombie epidemic" due to characteristic neurological symptoms in affected individuals. Similarly, a series of intoxications with acrylfentanyl (STRIDA project, Sweden) highlighted the role of advanced liquid chromatography protocols with **high-resolution mass spectrometry (LC-HRMS)** in poisoning investigations. The emergence of notazene derivatives, including isotonitazene, required adaptation of quantitative analysis methods and metabolite detection approaches.

It is well-established that analytical toxicology primarily relies on **LC-HRMS methods**, which allow separation of complex substance mixtures and precise determination of molecular mass with high accuracy. However, the volume of generated data is enormous, and traditional manual processing becomes nearly impossible. Therefore, the conjunction of forensic medicine and pharmacology requires standardized data and artificial intelligence methods for processing growing volumes of analytical information. **Artificial intelligence**, including machine learning and automatic data analysis methods, offers solutions to these problems through automation of identification processes, prediction of toxicological properties of new compounds, and integration of various information sources.

International experience demonstrates that the most effective systems are built on principles of open standards, enabling different laboratories and countries to exchange data and work collaboratively on solving common problems [11–13,31–33,70–73].

The objective of this review is to systematize international approaches to applying artificial intelligence in forensic medicine and pharmacology when working with novel psychoactive substances, and to formulate universal guidelines for implementing these technologies in Kazakhstan.

Search strategy. A narrative review of sources with thematic synthesis was conducted, covering the period from 2000 to 2024. Key methodological and review publications were analyzed covering data standards, software tools, identification methods, machine learning algorithms and validation, clinical toxicology, and surveillance systems.

The narrative approach enabled not only presentation of factual data but also analysis of development trends, identification of knowledge gaps, and formulation of practical recommendations. In contrast to systematic reviews focusing primarily on specific research questions, the narrative review allowed broader coverage of issues and integration of knowledge from various disciplines.

Particular attention was given to material relevance to novel psychoactive substances, analytical toxicology, and artificial intelligence applications in medicine. Publications in peer-reviewed scientific journals indexed in leading international databases were included: those indexed in Scopus (47.1%), PubMed (30.5%), and others from international agencies, databases, official guidelines, and monographs.

To ensure comprehensive coverage, sources were grouped into the following main thematic areas:

1. Publications on LC-HRMS analytical methods, data processing standards, and specialized software.
2. Sources on chemical compound identification methods, including spectral libraries and computational approaches.
3. Applications of artificial intelligence and machine learning in toxicology.
4. Publications on clinical aspects of toxicology, including antidote therapy and risk management.
5. Materials on pharmacovigilance systems and early warning of emerging threats.
6. Sources addressing ethical aspects of artificial intelligence application in medicine and corresponding international standards.

Results

I. Capabilities and Limitations of Modern Mass Spectrometry

The foundational method for laboratory diagnosis of NPS is LC-HRMS combined with tandem mass spectrometry (LC-HRMS/MS). As widely recognized, this principle is based on separation of biological sample components in a liquid chromatograph followed by analysis of each component in a mass spectrometer. Their highest sensitivity (nanograms per milliliter) enables detection of minute quantities of substances in biological samples [5,39,61].

The practical significance is confirmed by real clinical cases, particularly analysis of acrylfentanyl poisonings and other designer fentanyls within the STRIDA project, which analyzed numerous cases including fatal outcomes; rapid identification was critical [28]. Investigation of isotonitazene demonstrated the need for developing specialized approaches not only for quantification of the substance itself but also for detecting its metabolites in the organism [39].

Development of metabolome profiling using LC-HRMS expands capabilities for characterizing unknown compounds through detailed analysis of their biological transformation products. Contemporary reviews of designer drug metabolism emphasize the particular importance of Phase II biotransformation reactions, during which conjugates with glucuronic acid and other endogenous molecules form [31,44,57,60,75].

II. Data Standards and Ecosystem: Foundation for Integration

Effective work with large volumes of mass spectrometric data requires unified approaches to storage, processing, and exchange among different laboratories and countries. Analysis reproducibility and interoperability are ensured through open data formats **mzML and mzTab-M**, as well as a developed software ecosystem for processing [31–33,42,50,53,57,60,68].

The mzML format is the internationally accepted standard for mass spectrometric data exchange, ensuring compatibility between instruments from different manufacturers and various data analysis software packages. It is based on extensible markup language (XML) and includes not only spectral data but also complete information about analysis parameters [31,42].

MzTab-M is a complementary standard specifically developed for exchanging quantitative results from metabolomics studies and adapted for work with NPS [31].

MZmine 2 as a software platform provides a modular system for processing mass spectrometric data through a graphical interface with automation capabilities. An alternative approach is implemented in the OpenMS system, an open-source platform oriented toward command-line operation and integration into automated data processing pipelines [50].

The XCMS tool remains among the most cited solutions for metabolite profiling with integrated statistical analysis capabilities for comparing differences between sample groups [57].

The specialized MS-DIAL system focuses on deconvolution of data-independent analysis across the entire ion stream (DIA MS/MS) — a mode of fragment spectrum collection without selection of individual precursors [60,68].

The International Chemical Identifier (InChI) provides a unified method for representing molecular structures independent of data source or software used [29] .

The Chemical Entities of Biological Interest Database (ChEBI) provides a controlled vocabulary of small molecules with hierarchical classification [11,27,29]

The Medical Subject Headings (MeSH) system ensures standardized indexing of toxicological literature [40].

Large-scale databases play a key role in information integration about chemical compounds. Thus, **the DrugBank database** contains detailed structural and pharmacological information about drugs [29,74] .

The Human Metabolome Database (HMDB) focuses on endogenous metabolites and their transformation products [11,50,75]. **The 2023 update of the PubChem database** included over 110 million chemical compounds with search capabilities by structural similarity and biological activity [11,38,50,74].

III. Identification of Unknown Compounds: From Libraries to Computational Methods

Determination of NPS typically begins with comparing experimentally obtained mass spectra to reference spectra collected in specialized libraries. Leading spectral libraries **MassBank and mzCloud** represent two different models of organizing such resources. MassBank functions as an open public repository, enabling researchers from different countries to exchange mass spectral data [32,73]. However, library search capabilities are somewhat limited by the availability of reference spectra for specific compounds. For NPS that initially lack reference standards, corresponding computational approaches to identification are necessary. **The SIRIUS 4 system** is a rapid tool for converting tandem mass spectra into structural information about metabolites through detailed analysis of characteristic molecular fragmentation patterns. This approach is complemented by methods for systematic classification of unknown metabolites that combine high-resolution mass spectrometry data with information from nuclear magnetic resonance spectroscopy [11]

The CFM-ID 4.0 platform implements an alternative approach based on predicting fragmentation patterns for known chemical structures and subsequent comparison of predicted spectra with experimental data. The web version of CFM-ID makes these complex computational capabilities accessible to researchers without requiring local installation of specialized software [70,71].

Molecular network mapping, implemented **in the GNPS system**, opens fundamentally new possibilities. It reveals connections between different chemical compounds through analysis of the similarity of their fragmentation spectra, which is particularly valuable for characterizing series of structurally related NPS analogs [11,32,44,50,73]. A critically important aspect of any identification system is transparent communication of the degree of confidence in obtained results. Agreed transmission of identification results at the reporting level is achieved through the Schymanski confidence level scale. This system distinguishes results from Level 1, corresponding to confirmation of identification by a reference standard, to Level 5, based solely on exact molecular mass [54] .

IV. Artificial Intelligence and Toxicity Prediction: Possibilities and Limitations

The use of machine learning (ML) and quantitative structure-activity relationship (QSAR) methods — computational models linking molecular structure to biological activity — represents one of the most promising approaches for assessing potential toxicity of NPS before detailed experimental study. However, such application is justified only with proper algorithm validation and clear understanding of their explanatory limitations [20–22,24–25,55,58].

Contemporary deep learning models demonstrate significant progress in predicting various aspects of chemical compound toxicity, though serious problems persist with result interpretability and models' ability to generalize to fundamentally new classes of compounds.

An experimental basis for developing and validating predictive models is provided by large-scale high-throughput screening systems ToxCast and Tox21. The ToxCast program [21,52] includes over a thousand different in vitro biological assays for assessing potential effects of chemical compounds on living systems. The U.S. federal Tox21 program expands these capabilities through full automation of the testing process and tight integration with existing chemical structure databases [21,58].

Validation methods for machine learning algorithms acquire particular importance in the context of predictive modeling. Traditional cross-validation approaches based on random data splitting into training and test sets can give inflated model quality estimates. The time-split validation method provides more realistic assessment of models' ability to predict properties of truly new compounds [55].

In parallel with technical achievements, understanding grows of fundamental limitations in contemporary approaches to explainable artificial intelligence in medical applications. Critical analysis of this field indicates [24] that many contemporary methods of "explaining" machine learning model decisions do not provide true understanding of underlying mechanisms and may create a dangerous illusion of transparency [22,34,35].

V. Ethical Aspects of Artificial Intelligence Application

These issues are regulated by a developing system of international standards. The **ISO/IEC 23053:2022** standard establishes framework principles for artificial intelligence systems using machine learning, including requirements for documentation, testing, and quality monitoring [34].

For developing artificial intelligence in society, an ethical system is used — the International Ethical System **AI4People**. It emphasizes the need to balance encouragement of innovation with ensuring responsible use of technologies [22].

VI. Clinical Toxicology: Protocols and Antidotes

Practical application of analytical identification results for NPS in clinical practice requires clear action protocols, especially in acute poisoning situations. Management tactics for patients with suspected opioid intoxication include immediate assessment of respiratory status and readiness to administer the specific antidote **naloxone**, while routine flumazenil use should be avoided in suspected mixed poisonings, and in all cases careful **electrocardiographic monitoring** is necessary [2,3,10,28,49,56,76].

It is well-known that the American College of Medical Toxicology **(ACMT)** — the professional organization of toxicologists in the United States — is a leading authority in clinical toxicology worldwide. Its recommendations are used by toxicology centers and emergency departments in virtually all countries, including protocols for managing new psychoactive substance poisonings. The ACMT statement on **flumazenil** application emphasizes potential risks of its use in polyintoxication. Benzodiazepine combination with tricyclic antidepressants is particularly dangerous, as sedative effect reversal by flumazenil can lead to development of severe seizures [2,56].

To prevent dangerous cardiac arrhythmias, systematic **QT interval** monitoring on electrocardiography is required for all persons with suspected NPS intoxication. Many synthetic cannabinoids and stimulants have the ability to block potassium channels in cardiac muscle cells, potentially leading to life-threatening **arrhythmias** even at relatively low blood concentrations [10].

The World Health Organization (WHO) emphasizes the critical importance of **immediate** naloxone application at the slightest suspicion of opioid intoxication. Due to synthesis of highly potent opioids such as **carfentanil** and various fentanyl analogs, significantly **higher doses** of antidote or repeated administration may be required to achieve clinical effect [3,28].

A comprehensive approach to managing patients with NPS intoxication requires tight integration of analytical toxicology data obtained by high-resolution mass spectrometry with clinical protocols in real time. This means the need to create information systems capable of automatically matching laboratory analysis results with recommended treatment protocols [10,49,56,76].

VII. Surveillance Systems and Early Warning: International Experience

To reduce the adverse consequences of NPS use, coordinated international cooperation and information exchange on identified risks is critically necessary. International pharmacovigilance systems enable signal exchange on new NPS risks through specialized databases EudraVigilance, FAERS, and VigiBase [20,26].

EudraVigilance functions as the European database of suspected adverse drug reactions and includes special modules for analyzing signals related to NPS. The system allows collecting reports of adverse reactions from healthcare professionals and patients and applying statistical methods to identify unusual patterns [13].

FAERS (FDA Adverse Event Reporting System) — the American system for registering adverse reactions — provides detailed methodological guidance for analyzing spontaneous reports [23].

VigiBase (WHO Global ICSR database) — the WHO database contains the largest international collection of adverse reaction reports and serves as the basis for international drug safety monitoring [67].

The European Union Early Warning System on new psychoactive substances ensures operative information exchange among European Union member states. Operational guidelines of this system clearly define risk assessment criteria and procedures for notifying of emerging threats. The system includes not only exchange of information on new chemical structures but also data on clinical cases, toxicological research results, and effectiveness of various treatment approaches [17].

EMCDDA — the European Centre for Drugs and Drug Addiction, in assessing NPS risks, prepares reports representing comprehensive systematic analysis of all possible toxicological and pharmacological data for making informed regulatory decisions. These reports serve as models for developing national risk assessment systems [14,15,16].

UNODC — the United Nations Office on Drugs and Crime's programs on NPS include a broad range of initiatives: from developing guidelines for testing biological samples to providing technical support to laboratories in developing countries and creating international early warning systems. The Synthetic Drugs and Research Analysis and Monitoring Programme (SMART) coordinates international efforts to monitor NPS [61–66].

An interesting approach to epidemiological surveillance of NPS use is wastewater analysis, which allows assessing the scale of use of various substances at the level of entire cities or regions. Research covering the period from 2019 to 2024 demonstrates the capabilities of monitoring drug use trends through systematic analysis of samples from treatment facilities of major cities [6,16].

Discussion

International experience demonstrates a clear sequence of interconnected elements of a successful system for working with NPS: standardized data formats create the foundation for interoperability, specialized processing tools ensure efficient work with large volumes of information, spectral libraries and computational identification methods allow determining unknown compounds, a system of confidence levels ensures result transparency, and integration with surveillance systems and clinical protocols completes the chain from laboratory analysis to practical action [31–33,42,54,70–73].

The possibility of standardizing data formats through implementing open standards mzML and mzTab-M forms a fundamental foundation for collaborative work among laboratories of different countries and integration of results from equipment of various manufacturers. This approach significantly reduces barriers to international cooperation and allows small laboratories to utilize developments from leading research centers [44,47].

The combination of traditional library search with contemporary computational identification methods substantially expands analytical capabilities beyond available reference standards [11–13,32,46,70–73]. This is particularly important in the context of NPS, for which, by definition, no commercially available reference samples exist. The Schymanski confidence level system ensures transparent communication of identification result limitations among analysts and clinical specialists [54].

Overall, the following strengths of the contemporary approach to NPS problems can be identified:

- technical maturity of analytical methods;
- wide availability of commercial and open data processing tools;
- established international information exchange standards;
- growing capabilities of machine learning methods for predicting properties of new compounds.

Thus, it can be assumed that today the international scientific community has created a solid foundation for coordinated response to threats associated with NPS [61–67].

At the same time, we cannot ignore the weaknesses of contemporary approaches. In particular, these include: uneven quality of spectral libraries for the newest psychoactive substances, as the process of creating and curating high-quality spectral data requires significant resources; limitations of machine learning model interpretability, which create risks of misapplying results in clinical context. There is also uneven access to contemporary analytical equipment among different regions of the world, which significantly restricts possibilities for coordinated international efforts [20–22].

Nevertheless, the main risks include high dependence on input data quality, meaning errors can propagate through the entire analysis system. The need for continuous algorithm validation as new compound classes emerge creates ongoing operational burden. Potential interpretation errors from insufficient understanding of computational method limitations can lead to incorrect clinical decisions [24–25].

Effective risk management requires implementing clear validation protocols, creating comprehensive audit trails for all machine learning-based decisions, and regular monitoring of data quality at all process stages [34–35,55,58]. International artificial intelligence standards provide useful framework principles but require careful adaptation to specific toxicology application requirements [22,34–35].

PRACTICAL GUIDELINES FOR KAZAKHSTAN

Artificial intelligence increasingly becomes the basis for qualitative advancement in identification, monitoring, and risk prediction for novel psychoactive substances. Machine learning systems based on HRMS data arrays are capable of automatically recognizing unique spectral "fingerprints" of substances, modeling their fragmentation, and proposing structural candidates without access to expensive standards. Deep neural networks and analysis algorithms build molecular networks, revealing hidden connections among compounds, while anomaly detection algorithms in ECG streams predict dangerous arrhythmias long before clinical manifestations. AI models, supported by multi-task cross-validation and continuous drift monitoring, provide high accuracy, reproducibility, and adaptability to the constantly changing NPS landscape, becoming an integral partner to forensic pathologists and pharmacologists.

The guidelines offered below are universal in nature and can be adapted without requiring changes to regulatory requirements. Successful artificial intelligence implementation in forensic medicine and pharmacology requires a phased approach, beginning with basic data infrastructure elements and gradually expanding to full integration with international monitoring systems [31–33,42,50,53,57,60,70–73].

Data and Reporting: adoption of mzML formats for mass spectra and mzTab-M for summary tables, mandatory marking of confidence level per Schymanski. This will ensure compatibility with international data exchange systems and create a foundation for transparent result communication among laboratories and clinical specialists.

Tools: use of standard XCMS/MZmine/OpenMS/MS-DIAL pipeline for primary data processing, then integration with MassBank/mzCloud for library search, followed by SIRIUS/CFM-ID for computational identification and GNPS for molecular network mapping; fixation of software versions and analysis parameters [11–13,31–33,42,46,50,53,57,60,70–73]. Priority should be given to open solutions to minimize licensing costs and ensure long-term sustainability.

Clinical: maintaining readiness for immediate naloxone administration in suspected opioid intoxication, exercising caution with flumazenil in mixed poisonings, systematic QT-interval monitoring to prevent torsade de pointes. Creating systems for integrating high-resolution mass spectrometry analytical data with clinical decision-making processes in real time is critically important.

Surveillance: establishing technical channels for exchanging aggregated data with EudraVigilance/FAERS/VigiBase and early warning systems EU EWS/EMCDDA/UNODC [13–19,61–67]. Such integration does not require immediate regulatory status changes but provides access to international early warning signals and creates opportunities to contribute to international monitoring of emerging threats.

Artificial Intelligence and Machine Learning: application of validation with time-split data division, maintenance of comprehensive audit trails for all machine learning-based decisions, systematic monitoring of data quality and model drift, careful documentation of limitations and uncertainty sources for each model used [20–22,24–25,55,58]. Particular attention should be given to result interpretability for clinical application and clear communication of confidence levels to all system users.

Limitations

Local regulatory acts and data of the Republic of Kazakhstan were deliberately not considered; proposed guidelines are universal in nature and derived from international practices presented in sources [1–78].

Conclusions

International experience shows that effective artificial intelligence integration in forensic medicine and pharmacology when working with NPS is achieved through sequential implementation of standardized data formats, use of proven information processing tools, and a clear system for grading identification result reliability. Key success elements are mzML and mzTab-M formats ensuring data compatibility, mature software ecosystem for analysis, and transparent confidence level system for communicating results [31–33,42,50,53,54,57,60,70–73].

Minimum conditions for successful implementation include access to high-resolution mass spectrometry equipment, systematic mastery of basic open data processing tool stack, comprehensive staff training in interpreting computational identification results, and formation of reliable information exchange channels with international monitoring systems [11–13,31–33,50,53,57,60]. These elements create a foundation for effective participation in coordinated international efforts against NPS threats.

Implementation effectiveness can be measured through several key indicators, including reduction of time for identifying unknown compounds from hours to minutes, improvement of analytical method sensitivity and specificity, substantial reduction in time to initiating adequate antidote therapy in clinical settings, and enhanced quality of integration with international early warning signals [2,10,49,56,76; 13–19,61–67]. These measurable results provide clear benchmarks for assessing progress and continuous system improvement.

Long-term implementation success depends on commitment to continuous validation of machine learning algorithms as new classes of psychoactive substances emerge, sustained efforts to maintain and improve spectral library quality, and continuous development of staff competencies in interpreting computational toxicology results [20–22,24–25,32,46,54,55,58]. Investments in these areas ensure sustainability and continued system effectiveness in the rapidly evolving NPS landscape.

The proposed guidelines ensure solution scalability and compatibility with international standards while requiring minimal local regulatory framework modifications, making them practical and achievable for implementation in various regulatory environments [34–35].

Acknowledgements

The authors express gratitude to the international community of researchers and developers who created an open ecosystem of tools for mass spectrometry and toxicology, providing an accessible technological foundation for implementing artificial intelligence methods in forensic medicine practice.

Funding

This research was conducted without dedicated funding.

Author contributions

All authors contributed equally to developing the research concept, analyzing the literature, and preparing the manuscript.

Conflict of interest

The authors declare no conflict of interest.

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Contact information:

Murat N. Lepesbayev - Assistant of the Department of Pathological Anatomy and Forensic Medicine named after Professor Yu.V. Pruglo, forensic physician of the highest category; Postal address: Republic of Kazakhstan, Semey city, Abay street, 103, https://orcid.org/0009-0006-9810-9232; E-mail: king87ml@gmail.com; Phone +77021222911

Dinar Sh. Tarzhanova – Candidate of Medical Sciences, Head of the Department of General Pharmacology at the Medical University of Astana; Postal address: Republic of Kazakhstan, Astana city, Postal address: Republic of Kazakhstan, Astana city, Saryarka Avenue 33, https://orcid.org/0000-0002-3740-1874; E-mail: dinar.tsh@gmail.com; Phone +77019991257

Zhanetta T. Mukanova - Candidate of Medical Sciences, Associate Professor of the Department of Otorhinolaryngology, Astana Medical University; Postal address: Republic of Kazakhstan, Astana city, Beybitshilik street 49a, https://orcid.org/0000-0001-5272-1190; E-mail: zhanetta2000@mail.ru; Phone +7 7015141133

Kanatbek N. Mukanov – Doctor of Medical Sciences, Professor of the Department of Pharmacology, Astana Medical University; Postal address: Republic of Kazakhstan, Astana city, Saryarka Avenue 33, https://orcid.org/0000-0001-6838-4512; E-mail: mkn36@mail.ru; Phone + 7 7011113440

Saulesh A. Apbassova - Candidate of Medical Sciences, Associate Professor, Head of the Department of Pathological Anatomy and Forensic Medicine named after Professor Yu.V. Pruglo; Postal address: Republic of Kazakhstan, Semey city, Abay street, 103, https://orcid.org/0000-0001-6981-5441, E-mail: apbasova65@mail.ru; Phone +7079196975

Akmaral A. Zhakipova - Candidate of Medical SciencesAssistant of the Department of Pathological Anatomy and Forensic Medicine named after Professor Yu.V. Pruglo, forensic physician of the highest category; Postal address: Republic of Kazakhstan, Semey city, Abay street, 103, https://orcid.org/0000-0003-3023-9445, E-mail: zhakipova_akmaral@mail.ru; Phone +77081681858

Indira K. Uyzbayeva – Master of Medical Sciences, Senior Lecturer at the Department of General Pharmacology at the Medical University of Astana; Postal address: Republic of Kazakhstan, Astana city, Saryarka Avenue 33, https://orcid.org/0000-0003-4282-4799; E-mail: indirauyzbayeva@yandex.kz; Phone +77014036676

Akmaral Zhantureyeva - Candidate of Medical Sciences, Associate Professor of the Department of General Pharmacology at the Medical University of Astana; Postal address: Republic of Kazakhstan, Astana city, Saryarka Avenue 33, https://orcid.org/0000-0001-5063-6312; E-mail: zhantureeva.a@amu.kz; Phone +77011509277

Dariya M. Shabdarbayeva - Doctor of Medical Sciences, Full Professor, Vice-Rector for Science at Semey Medical University; Semey city, Abay street, 103, https://orcid.org/0000-0001-9463-1935, E-mail: dariya.kz@bk.ru; Phone +77472506108

Corresponding author:

Kanatbek N. Mukanov – Doctor of Medical Sciences, Professor of the Department of Pharmacology, Astana Medical University; https://orcid.org/0000-0001-6838-4512;

Postal address: Republic of Kazakhstan, Astana city, Saryarka Avenue 33,

E-mail: mkn36@mail.ru;

Phone + 7 7011113440