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ARTIFICIAL INTELLIGENCE IN OPTIMIZATION OF PHARMACEUTICAL DEVELOPMENT AND PREDICTION OF DRUG STABILITY

Ensuring the stability of medicines is a critical stage of development that guarantees their safety and efficacy. Traditional tests according to ICH guidelines are long and resource-intensive, but the industry's digital transformation and the concept of "Smart Pharma" offer a transition to predictive *in silico modeling*. The use of artificial intelligence (AI) and machine learning enables us to detect nonlinear dependencies among the API structure, excipients, and external factors. The creation of "digital twins" of stability enables scientists to predict drug degradation at early stages, minimizing the number of experiments, optimizing costs, and implementing the Quality by Design (QbD) strategy, thereby significantly accelerating the market entry of innovative medicines.

The modern pharmaceutical industry is in the midst of a digital transformation. 2025 will be a watershed year for global medicine and pharmacy, with the integration

of AI transforming from an ancillary tool to a key technology in drug development (Сучасна фармація, 2026).

The use of machine learning algorithms can significantly reduce drug time-to-market and improve drug quality (Mak & Pichika, 2019).

The traditional trial-and-error method in pharmaceutical technology is being replaced by intelligent modeling. AI allows for the analysis of complex interactions between active pharmaceutical ingredients (APIs) and excipients (Yadav et al., 2025).

The use of neural networks helps predict the physicochemical properties of mixtures, enabling the creation of optimal dosage forms with a given bioavailability (Vora et al., 2023, 1916).

One of the most important achievements is the development of specialized web platforms for automating calculations. AI algorithms can predict the stability of extemporaneous and industrial pharmaceutical products by modeling degradation processes and predicting shelf life based on molecular structure analysis (Grigoryan et al., 2025).

AI is revolutionizing the early stages of pharmaceutical development by enabling virtual screening of millions of compounds, allowing the identification of high-accuracy potential candidate molecules and predicting their toxicity and pharmacokinetic profiles even before costly laboratory testing begins (Mak & Pichika, 2019).

AI technologies are being used to design innovative delivery systems, such as nanocarriers and microneedles. Modeling allows for fine-tuning of drug release parameters, ensuring targeted therapy and minimizing side effects. Although there is a huge scope for AI in drug delivery innovation and drug discovery, it still presents major limitations that ultimately require human intervention or intellectual interpretation of complex results. AI predictions are based on datasets, but interpreting the results, owing to the gray zone, requires human intervention to reach an appropriate conclusion. AI can experience issues with algorithmic bias in the processing of information for predictions and in the assessment of hypotheses. Moreover, it is not uncommon for docking

simulations to yield inactive molecules. Therefore, a critical analysis of these parameters still requires human involvement for effective decision-making and cross-verification to rule out system bias. Nevertheless, there is significant potential for AI applications, and thus extensive work can reduce the limitations associated with AI and make it more effective and reliable (Vora et al., 2023, 1916).

Furthermore, AI-powered personalized formulation development is becoming a cutting-edge use case. AI systems can be used to customize formulations that fit each patient's unique therapeutic response profile by combining pharmacogenomic data with physiological parameters unique to each patient. Off-the-shelf formulations frequently fall short in oncology, pediatrics, and rare diseases, where such customization may be especially helpful.

There is also significant promise in the convergence of AI with continuous manufacturing and PAT. PAT systems can incorporate predictive AI models to identify deviations, forecast batch failures, and adjust process parameters in real time. In addition to improving manufacturing efficiency, this degree of automation guarantees adherence to QbD guidelines.

Another avenue for the future is the creation of AI-enabled robotic labs, where humanoid robotic systems use real-time data and optimization feedback to develop formulations autonomously. It is anticipated that these systems will accelerate high-throughput screening of formulations and excipients, reducing development time and expense.

Despite these opportunities, it is important to carefully manage data privacy issues, regulatory gaps, and ethical concerns. To guarantee safety, openness, and reproducibility, regulatory agencies are expected to develop rules specifically for AI-assisted formulation tools (Yadav et al., 2025).

Therefore, the introduction of artificial intelligence and machine learning is fundamentally changing the pharmaceutical industry, replacing traditional trial-and-

error methods with predictive modeling and data-driven strategies. The use of complex algorithms enables rapid selection of excipients, prediction of formulation stability, and exploration of vast experimental space, significantly reducing development time and increasing the accuracy of product design. In addition to process optimization, AI contributes to the development of personalized medicine by enabling the formulation of dosage forms tailored to patients' pharmacogenomic profiles. Despite significant potential and gradual recognition by regulatory authorities, challenges remain, including data quality, the "black box" problem in algorithms, and the lack of validation standards. The future of the industry lies in the creation of autonomous systems using digital twins and robotics, which, through interdisciplinary collaboration, will usher in an era of highly efficient, patient-centered drug development.

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