ARTIFICIAL INTELLIGENCE TO EVALUATE DRUG DEVELOPMENT PROCESSES

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Information technology is changing the way medicines are developed and used. Developers, manufacturers, regulators, academic groups and other stakeholders are working to develop a common understanding of where and how specific innovations, such as artificial intelligence and machine learning, can best be used in the drug development process. The assessment procedure is the main tool for planning processes and managing software tools at the stages of the life cycle of the drug manufacturing process. The approach to assessing process properties should be defined by a documented assessment procedure and may depend on the class of assessment, taking into account its objectives. The article discusses the key role of artificial intelligence models for assessing the processes of creating medicinal products. The principles and approaches that provide a meaningful and consistent basis for assessing process quality characteristics based on objective process implementation data are discussed.

KEYWORDS

Neural network, AI/ML algorithms, pharmacokinetics, pharmacodynamics, drug product development, regulatory frameworks, process assessment, qualimetry

1 INTRODUCTION

Despite the hype and widespread use of artificial intelligence (AI) and machine learning (ML) (a subset of AI), the applicability of these universal tools to specific tasks in drug development remains largely unclear due to significant challenges, ethical issues, and risks [Ahmadi 2024]. AI is a highly interdisciplinary field. The interdisciplinary study and development of AI/ML systems aims to create computer systems capable of performing tasks that typically require intelligence. The concept of AI as a flow of input and output processes is shared by many AI researchers, and research into each stage of this process is ongoing. The drug development process is an iterative, continuous cycle of activities that is not strictly linear in nature. A review of the literature [Suriyaamporn 2024, Vidiyala 2025, Bumbaca 2025] recognises the potential of AI/ML to improve the development, improve the quality of manufacturing, and accelerate the delivery of safe and effective drugs, as well as personalised approaches to studying pharmacodynamic effects.

AI/ML systems that perform continuous learning change their behaviour during use, and therefore require special attention to ensure their responsible use [ISO/IEC 42001:2023]. Data-driven decision-making poses new challenges for data quality management in data analytics and machine learning-based artificial intelligence (AI) [ISO/IEC 5259-2:2024]. Certain AI features, such as the ability to continuously learn and improve or the lack of transparency or understandability, require different safeguards if they raise additional concerns compared to how the task would be performed traditionally. All factors change over time and therefore require review. Therefore, the AI governance system must be integrated with the organisation's processes and overall governance structure, including navigating the complex regulatory landscape of AI technologies and Good Manufacturing Practices (GMP) and Good Clinical Practices (GCP) [ISO/IEC 22989:2022].

Efforts are currently underway to explore the use of newer AI/model learning algorithms (e.g., artificial neural networks and tree-based models) for PK/PD modelling. For example, a recurrent neural network, a machine learning algorithm commonly used for time series data analysis, can be used to complement traditional PK/PD models in the area of analysing highly complex PK/PD data and potentially lead to improved accuracy for preclinical and clinical applications. Such a system should include clear internal standards and guidelines that prioritise accountability, transparency, and regulatory compliance [Tufail 2023]. By implementing best practices, organisations can create a robust governance structure that supports the responsible development and implementation of AI. There is a continuing need to ensure that potential risks associated with AI are assessed. In addition, there are security and privacy concerns when using such tools that need to be addressed, as companies are reluctant to provide sensitive, confidential information to train AI models [Cummings 2025]. Thus, the development and improvement of robust AI verification and monitoring structures to ensure compliance and safety.

The purpose of the study is to generalise the requirements for the creation, implementation, maintenance and continuous improvement of an AI/ML management system in the context of conducting an assessment of pharmacological research and development processes.

2 LITERATURE REVIEW

There are now fundamental principles that underpin drug development. The early stages of drug development typically rely on the initial identification of a suitable biological target for drug candidates. Emerging trends, such as the expansion of AI/ML, could significantly impact drug development in the future. As a starting point, the process of identifying biological targets and elucidating disease relationships can use AI/ML to analyse and synthesise large amounts of information from existing scientific studies, publications, and other data sources [Coskuner-Weber 2025]. The application of AI/ML in pharmaceuticals began in earnest in the late 1990s, when advances in machine learning and deep learning showed promise in drug development. Initially, AI/ML was used primarily to analyse data and identify potential drug targets. However, as algorithms became more sophisticated, the role of AI expanded to include compound screening, molecular design, and clinical trial design. The growing availability of genomic, transcriptomic, proteomic, and other data sources from healthy individuals and those with a specific disease of interest presents a significant opportunity for informed biological target selection [Niazi 2023a]. These datasets are often complex and come from diverse sources, which lend themselves well to AI/ML approaches [Niazi 2023b].

Building on existing validated data, AI/ML can be applied to analyse these large multi-omic and other datasets to gain insight into the potential structure and function of biological targets to predict their role in disease progression [Rosoff 2025]. Target

prioritisation is a critical step where AI/ML can help improve the efficiency and effectiveness of drug development, and it is important to confirm the role of the biological target in the disease under study through further studies. Artificial AI/ML approaches used to further elucidate drug-target interactions can also help predict drug classes that potentially interact with the same targets or have a similar mechanism of action, which can help predict the toxicity of a molecule based on specific known characteristics. This strategy can help guide drug repurposing efforts that could exploit previously characterised compounds. Drug repurposing efforts using AI/model learning could also potentially benefit from the increased availability of relevant RWD from various sources (e.g., electronic health records (EHRs), registries, and DHTs) to identify previously unknown drug effects on disease pathways [Mirakhori, 2025]. AI/ML can be applied to help predict the three-dimensional structure of target proteins, informing the chemical synthesis and potential effects of a drug candidate on the target, including prediction of affinity and potential toxicity. It is worth noting that caution should be exercised when using AI/ML in 3D structure prediction, as many proteins designed for pharmaceutical applications are codon-optimised (with many synonymous mutations), the effects of which on protein structure are still the subject of active research. Two main components help us understand the behaviour of drugs: the first is how drugs move in the body (pharmacokinetics [PK]), and the second is how drugs affect body functions (pharmacodynamics [PD]). Pharmacokinetics (PK) describes the duration of absorption, distribution, metabolism, and elimination of drugs. Pharmacodynamics (PD) examines the biological response of the body to drugs. Understanding both aspects of clinical pharmacology is an important part of drug development. When PK and PD are integrated into an AI/ML model, the model can describe how the effect of a drug will change over time when using a specific dosing regimen. Understanding both aspects of clinical pharmacology is an important part of drug development. Along with the development of computational tools and technologies, and the availability of modelling platforms, the use of physiologically based pharmacokinetic (PBPK) and physiologically based PK/PD (PBPK-PD) modelling is also increasing [Smiyan 2024]. Currently, efforts are underway to explore the use of emerging AI/ML algorithms (e.g., artificial neural network models) for PK/PD modelling [Qiu 2023]. In the comprehensive analysis of PK/PD data, the use of AI/ML can lead to increased accuracy for preclinical and clinical applications [Ouma 2024, Abdelrad 2025]. Although there are well-established clinical pharmacology studies with limited modifications in their design or application, the evolution of study design (adaptive/continuous designs, model-based adaptation) and methods for characterizing dose/exposure–response relationships (e.g., pharmacometrics, quantitative systems approaches, Bayesian approaches) have led to a new era of methodological applications and practices used in drug development [Lyu 2024, Kruse 2025].

Many regulatory authorities require a single, managed automated system to support AI/ML-based decision-making for drug development applications, which is a critical tool in a rapidly changing environment. To maximise the reproducibility, validity, and consistency of process assessments in drug development, it is necessary to document and update the evidence to support the assessments. The evidence is used in the form of assessment indicators, which are usually objectively demonstrated characteristics of the work results, practices, and resources associated with the relevant processes [Agrahari 2024]. The assessment should be conducted following the procedure established in the relevant documents [Rajput 2025]. The documented assessment procedure should ensure that the assessment objective is achieved and have an appropriate structure that ensures its rigorous and independent execution according to its intended purpose. The ISO/IEC 3300xx family of international standards provides a meaningful and consistent basis for assessing process quality characteristics based on objective data from the implementation of the processes. The use of AI/ML allows for increased decision-making validity in process assessments during drug development based on the principles and models of the ISO/IEC 3300xx family of international standards [ISO/IEC 33001:2015].

3 MATERIALS AND METHODS

In this study, AIs are considered from the perspective of the agent paradigm [ISO/IEC 42001:2023], since some artificial intelligence programs aim to simulate human intelligence and behavior (Fig. 1).

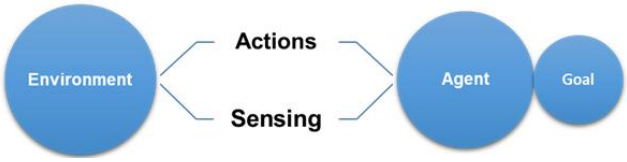

Figure 1. Paradigm of the agent

An AI agent interacts with its environment by performing actions that maximise its chances of successfully achieving its goals. Environments have different characteristics depending on the task at hand, and these characteristics affect the level of complexity of the problem. In this paradigm, several types of AI agents can be identified depending on their architecture [Kiranyaz 2021]:

– reflexive agents, which rely only on the current situation to choose an action;

– model-based agents, which rely on a model of their environment that allows them to consider the outcomes of the actions available to them;

– goal-oriented or utility agents, which rely on an internal utility function that allows them to choose actions that achieve goals and search for the most desirable ones among the goals;

– learning agents, which can collect information about their environment and learn to improve their performance.

Our view of the use of AI in pharmacology research is presented from the perspective of ensuring that the right patient receives the right drug at the right dose, at the right time. From this perspective, we highlight the importance of understanding and evaluating throughout the drug development lifecycle.

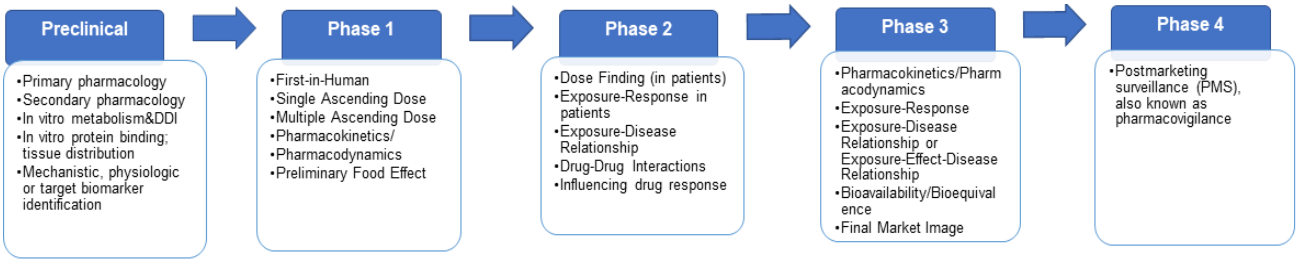

Figure 2. The drug development lifecycle

Figure 2 identifies the different stages of drug development. Not all of the studies listed are always necessary, and in fact, the physicochemical nature of the drug determines which studies are required for submission. Some studies can be cancelled if an adequate plan is developed, and sufficient information is collected during other studies.

Although any drug must be safe and effective to benefit the patient, this information is not available at the early stage of clinical development. Pharmacokinetic and pharmacodynamic data are tools for understanding the behaviour of a drug in the body and its interaction with the target. To obtain high-quality pharmacokinetic and pharmacodynamic data, it is key to properly assess the effectiveness of drug development processes.

The level of effectiveness of a process(s) is characterised by one or more properties that are formative dimensions of the process capability (Figure 3). Process properties are used in the design of process capabilities. Process properties are demonstrated by matching process quality outcomes, which are informative dimensions.

Figure 3. Formative and informative dimensions of process capabilities

We consider the process result as the result of successfully achieving the process goal, and the process quality result as the result of compliance with a certain process property. Process results and process property results can be characterised as an intermediate step in assigning a process quality rating. The concept of process capabilities does not provide the ability to measure anything other than the process capabilities formed by its properties. In this study, a process measurement system is defined that supports the assessment of process capabilities in accordance with the requirements of ISO/IEC 33003. This process measurement system provides a scheme that can be used to create a process capability assessment model.

Within this system, the measurement of process capabilities is based on a set of process properties. Each process property determines a measurable property of the process capabilities. The degree of process quality compliance is determined by a special rating scale. The level of process authority assessment is determined by the set of process property ratings presented in the process profile.

The compliance of one of the properties can be related to the compliance of another process property in the process measurement system.

The process measurement concept defined in this study forms a framework that [ISO/IEC 33001:2015]

a) facilitates self-assessment,

b) provides a basis for use in process improvement and process quality determination,

c) applies to all application domains and sizes of organisations,

d) produces a set of process attributes (capability) assessments (process profile), and

e) Derives the process capability level.

The study of the quality characteristics of processes during the life cycle of drug development was carried out using the ISO/IEC 33001: 2015 - ISO/IEC 33099 series of international standards [ISO/IEC 33001:2015], which define the requirements and resources needed for process assessment. For a process measurement system at life cycle stages based on the results of the analysis of quality process properties, it is proposed to use the measurement components at the process capability level in the form of an ordinal scale in ISO/IEC 33020. Process capability measurement systems are based on a set of process properties.

Within the framework of this process measurement system, a process property is a measurable property of the process capabilities. A process quality rating is a judgment about the degree of compliance with the quality of the assessed process. A process property is measured using an ordinal scale, the definition of which is given below.

Process capabilities were assessed using a six-digit ordinal scale. This scale allows for assessment from its lowest level (Incomplete) to its highest (Innovative) [ISO/IEC 33020:2019]:

– Process capability level “0”: Incomplete process.

– Process capability level “1”: Completed process.

– Process capability level “2”: Managed process.

– Process Capability Level “3”: Established process.

– Process Capability Level “4”: Predictable process.

– Process Capability Level “5”: Innovative process.

Process properties are measured using an ordinal scale, the definition of which is given as follows:

N – Not compliant: There is little or no evidence of compliance with the process property being assessed;

P – Partial compliance: There is some evidence of a method and some process quality compliance during its assessment; some aspects of the process property compliance may be unpredictable;

L – Significant compliance: There is evidence of a systematic method and significant process quality compliance during its assessment. Some deficiencies may be present in this property of the process being assessed;

F – Full compliance: There is evidence of a complete and systematic method and full process quality compliance during its assessment. There are no deficiencies in this quality of the process being assessed.

The ordinal scale below reflects the degree of compliance of the process quality in percentages:

N – does not comply: from 0 to 15% compliance:

P – partial compliance: from 15% to 50% compliance:

L – significant degree of compliance: from 50% to 85% compliance;

F – complete compliance: from 85% to 100% compliance.

The sensitivity of the process capability scale was tested during the tests. The studies included the use of agreement of ratings and internal consistency, both of which were assessed as acceptable [Dyadyura 2024].

The qualitative and quantitative properties of a process can be viewed as determinants or indices created by the observed measurements. The first type is called informative (effective) constructs or informative measurement models, and the second is called formative (conditional) models. The purpose of an informative measurement model is to measure a single property by taking several measurements, while a formative model attempts to summarise several properties in a single composite value [Chernobrovchenko 2022]. The decision rules for testing the specification of an informative or formative construct are given in Table 2. These rules can be applied to the qualitative properties of a process and its corresponding characteristics. These rules can be analysed by statistically testing the design specification.

The purpose of the informative measurement model is to measure a single property by taking multiple measurements, while the formative model attempts to summarise multiple properties into a single composite value. The determination is verified by statistical analysis [Valicek 2016].

Table 1. Decision rules for measuring the drug development lifecycle processes

Decision making rule	Informative measurement model	Formative measurement model
Measuring process properties	– Measuring defines process properties – Measuring has a common focus – Measurings are interchangeable – The content of the measurements is identical or similar – Excluding a measurement does not change the conceptual scope of the process – Measurements change in parallel with each other	– Measuring defines the properties of the construct – Measuring may not have a common direction – Measuring should not be interchangeable – The content of the measurements should not be identical or similar – Excluding a Measurements may change the conceptual scope of the construct – Measurements do not have to vary in parallel with each other
Direction of causality between process and measurements	Direction of causality - from process properties to complex measurements Changes made to a single measurement should not lead to a change in the process	Direction of causality - from measurements to process properties Changes made to the process should not lead to changes in measurements

4 RESULTS

This paper discusses models that can be used to determine the quality level of a process by summarizing measurement values (using a set of process property ratings. The relationship between process properties and their measurements is shown in Figure 4.

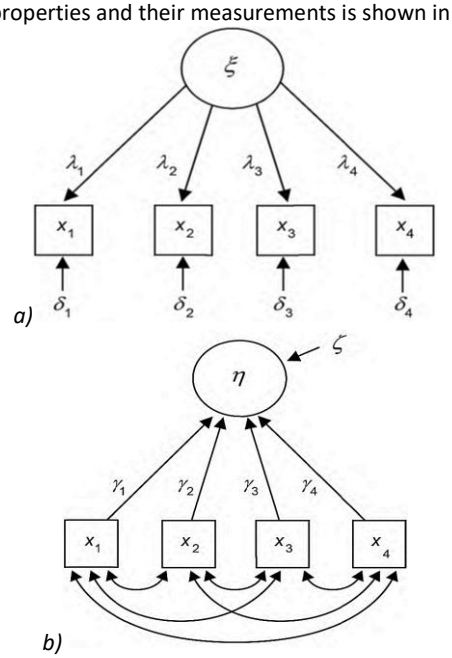

Figure 4. Measurement models: *a*) informative measurement model; *b)* Formative measurement model

The notations given in Figure 4:
– λ_i is loading parameter indicating the relationship between construct ξ and dimension x_i;
– δ_i is erroneous condition;
– γ is loading parameter of the x_i measurement;
– ζ is disturbing influence.

The direction of causal relationships has important consequences for the properties of the process in its context. If a process quality property is considered informative, the goal of actions should be to obtain natural advantages reflected in the process properties. Interventions that focus solely on specific properties of a process may divert resources from more important activities. Interventions in the formative design should be directed at specific areas related to process properties that represent the qualitative properties of the process [Panda 2020 & 2022]. In this case, improving one process property does not imply improving other dimensions. The decision rules for specifying designs are summarised in Table 1.

The relationships between process properties and their measurements are represented as an equation, where each measurement depends on a latent variable as follows

$$x_i = \lambda_i \cdot \xi + \delta_i, \quad (1)$$

Where x_i is informative measurement i, which depends on the hidden variable ξ; λ_i is a coefficient representing the expected impact of one unit of ξ in x_i; δ_i is the random error condition that represents the measurement error.

In the formative model shown in Figure 4b, the measurement values are considered as causes of process properties, and the process property is a composite variable formed or contributed by the combination of its measurements. The measurements characterise a set of clearly defined causes that are not interchangeable. Each measurement captures a specific aspect of the process properties [Dyadyura 2017, Pandová 2020, Sukhodub 2018 & 2019]. Thus, omitting a measurement may change the decision on the process properties, i.e., the process quality may be insufficiently substantiated. Since the measurements represent different facets of the process application area, they should not be too interrelated. Strong interrelations between the formative changes may affect the stability of the measurement coefficients and make it difficult to isolate the specific impact of individual measures on the process. The formative model can be represented as follows

$$\eta = \gamma_1 \cdot (\lambda_1 \cdot \xi + \delta_1) + \cdots + \gamma_i \cdot (\lambda_i \cdot \xi + \delta_i) + \zeta, \quad (1)$$

where η is a complex characteristic estimated by its formative measurement x_i ; γ_i is a coefficient indicating the influence of the measurement x_i on the latent variable η; ζ is a disturbance condition indicating the effect of missing measurements in the model on the variable η. The decision-making rules for the formative design are given in Table 1. The capability level achieved by a process is determined by the ratings of the properties of that process according to the process capability level model presented in Table 2.

A patient's response to a dose of a drug (ξ) is modelled. The effectiveness depends on the patient's "sensitivity" (latent variable). We want the neural network to infer this "sensitivity" based on other patient attributes (age, gender, genetics) and adjust the dose-response coefficient accordingly.

Input: [x_1 (dose), x_2 (age), x_3 (gender),…]

Neural Network (Encoder): Takes [x_1, x_2,…] and outputs the latent variable η (sensitivity).

Neural Network (Decoder/Coefficient Function): Takes η and outputs γ_1 (η) (the coefficient for the dose of x).

Prediction of η: $\eta = \gamma_1 \cdot x_1 + \gamma_2 \cdot x_2 + \gamma_3 \cdot x_3 + \zeta$.

Tools and libraries: PyTorch, TensorFlow, Keras: frameworks for building and training neural networks. Scikit-learn (for data preprocessing): normalization and scaling. Matplotlib, Seaborn, Plotly: for visualizing extracted relationships.

Table 2. Process Capability Level Ratings

Scale	Process properties	Assessment

Level 1	Process efficiency	Significant or complete
Level 2	Process efficiency Performance management. Process result management	Complete Significant or complete Significant or complete
Level 3	Process Performance Performance Management Process result management Process Definition Process Deployment	Complete Complete Complete Significant or complete Significant or complete
Level 4	Process Performance Performance Management Process Result Management Process Definition Process Deployment Quantitative Analysis Quantitative Control	Complete Complete Complete Complete Complete Significant or complete Significant or complete
Level 5	Process Performance Performance Management Process Result Management Process Definition Process Deployment Quantitative Analysis Quantitative Control Process Innovation Process Innovation Implementation	Complete Complete Complete Complete Complete Complete Complete Significant or complete Significant or complete

CONCLUSIONS

Artificial intelligence (AI) systems are being used by organisations of all types, sizes and purposes. These data are important for the development and functioning of SI systems.

The sphere of IT systems has a lot of vital data cycles that are analysed and considered for various purposes (for example, data availability, data analytics, data management, development and development of IT systems). Without a halal structure, all the different life cycles of data can be difficult to correctly interpret without prior knowledge, context and evidence. There is a clear risk that these numerical life cycles will not be properly stabilised. The effectiveness of the integration of artificial intelligence and machine learning in the development of human and clinical data is tried to be based on the content of the data and the creation of the care system with them, and correctly interpreting them. Improper collection or problems with the data can lead to poor results, which reinforces the need for rigorous testing and validation.

AI/ML can play a role in the analysis and interpretation of data collected through digital health technologies that are used in clinical research. AI/ML can also be used to speed up clinical trials and improve the efficiency of work.

The organisation is responsible for creating, implementing, maintaining, continuously improving and documenting the AI/ML management system, including the necessary processes and their interaction. The international standards of the ISO/IEC 330XX series examine clear characteristics of processes of any type, as well as establish capabilities before the development of process modification systems. These characteristics can be used to develop models for assessing processes at the stages of the life cycle of medicinal products. The results of the assessment can be used to enhance the process or to identify and manage the risks associated with AI/ML applications.

The results of the research make it possible to make recommendations for the development, promotion, support and continuous improvement of AI/ML artificial intelligence management systems in the context of pharmacological research and development.

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