

In Silico Modeling and Artificial Intelligence: FDA Regulatory Navigation

The international regulatory environment for drug approvals is diverse, but generally considers the use of computational simulations and predictions to be of value to drug makers throughout the discovery and development lifecycle. In the United States, the FDA has acknowledged that model-informed drug development (MIDD) approaches can be used to support decisions on whether, when, and how to conduct certain pharmacology studies, and to support dosing recommendations in product labeling, among other applications. The use of Artificial Intelligence and Machine Learning techniques has also been recognized as increasingly playing a key role in drug discovery and development.

Data and analysis derived from these approaches are acceptable within submissions for new drug and biologics applications The presence of this data has supported [hundreds of applications](#), as well as clinical trial design and specific regulatory approval decisions.

FDA Policy and Guidance on use of MIDD and AI in Regulatory Submissions

[Considerations for the Use of Artificial Intelligence To Support Regulatory Decision-Making for Drug and Biological Products](#)

January 2025

The FDA's draft guidance on the use of Artificial Intelligence (AI) to support regulatory decision-making for drugs and biologics provides recommendations for how sponsors can use AI-generated data across nonclinical, clinical, postmarketing, and manufacturing settings (excluding discovery and internal efficiency uses) to inform decisions on product safety, effectiveness, and quality. Central to the guidance is a risk-based credibility assessment framework—a structured seven-step process to define the context of use, assess model risk, and document evidence to ensure AI models are reliable for their intended purpose. The FDA emphasizes ongoing life cycle management to monitor model performance over time and encourages early engagement with the Agency to align on expectations, reinforcing the importance of transparency, rigor, and trust in applying AI within regulated drug development.



[M15 General Principles for Model-Informed Drug Development](#)

December 2024

The FDA's draft guidance "M15 General Principles for Model-Informed Drug Development"—prepared under the International Council for Harmonisation (ICH)—offers foundational, non-binding recommendations to foster a harmonized, multidisciplinary approach to model-informed drug development (MIDD). It provides guidance on planning MIDD strategies, evaluating models, documenting supporting evidence, and introduces a harmonized framework for assessing MIDD-generated data. The goal is to improve consistency and transparency in the use and regulatory evaluation of MIDD across geographic regions, ultimately advancing drug development efficiency and decision-making processes



[50 shades of AI in regulatory science](#)

June 2024

This document, co-authored by VeriSIM Life CSO Dr. Szczepan Baran and Dr. Weida Tong, Director of Division of Bioinformatics and Biostatistics for FDA, emphasizes the need for tailored regulatory measures to accommodate AI's diverse roles, ensuring AI enhances rather than complicates regulatory processes. [Learn More](#)



[PDUFA Reauthorization Performance Goals and Procedures Fiscal Years 2023 Through 2027](#)

This document, referred to as the “goal letter,” “represents the product of FDA’s discussions with the regulated industry and public stakeholders, as mandated by Congress. The performance and procedural goals and other commitments specified in this letter apply to aspects of the human drug review program that are important for facilitating timely access to safe, effective, and innovative new medicines for patients.” The document outlines the FDA’s intent to continue building on the success of MIDD and exploring the benefits AI can add to solving drug development challenges.



[Survey of AI-based Approaches to Generating MIDD Assets Across the Drug Development Continuum](#)

July 2023

VeriSIM Life Founder & CEO Dr. Jo Vashney was quoted as a subject matter expert in this article from The AAPS Journal. This review details the potential of the use of AI in model-informed drug development and encourages organizations to embrace/adopt AI as a way of evolving traditional methods.



“
An AI/ML-based approach to MIDD has the potential to transform regulatory science and the current drug development paradigm, optimize information value, and increase candidate and eventually product confidence with respect to safety and efficacy.

”

[Survey of AI-based Approaches to Generating MIDD Assets Across the Drug Development Continuum](#), July 2023

[Discussion Paper: Using Artificial Intelligence & Machine Learning in the Development of Drug & Biological Products](#)

May 2023

This paper was released by the FDA in order to address the developing landscape of AI in MIDD and to request input from industry experts. VeriSIM Life responded to this paper with guidance that we provided based on the principles we used to create our computational drug development platform, [BIOiSIM](#). [Read more](#) about our response to the FDA.



[FDA Modernization Act 2.0](#)

Sep 2022

([signed into law](#) December 2022)

This legislation was critical in acknowledging the benefit of, and approving the usage of AI in model-informed drug development. Passed at the end of 2022, it authorizes sponsors of novel drugs to make use of

Read our response to this legislation [here](#).



“
Authorizes certain alternatives to animal testing, including cell-based assays and computer models, to obtain an exemption from the Food and Drug Administration to investigate the safety and effectiveness of a drug.

”

FDA Modernization Act 2.0

[Select Examples of MIDD Approaches to Support Regulatory Decision-making](#)

May 2022

This is a list of examples of model-informed drug development approaches that support recent regulatory action.



[Physiologically Based Pharmacokinetic Analyses — Format and Content Guidance for Industry](#)

August 2018

This resource informs the structure and standardization of computational analysis. The FDA writes, “This guidance outlines the recommended format and content for a sponsor or applicant to submit physiologically based pharmacokinetic (PBPK) analyses to the FDA to support applications including, but not limited to, investigational new drug applications (INDs), new drug applications (NDAs), biologics license applications (BLAs), or abbreviated new drug applications (ANDAs).” [Learn more](#) about how BIOiSIM’s reporting was built to be in compliance with this guideline.

