



JAGIELLONIAN UNIVERSITY
MEDICAL COLLEGE
IN KRAKOW

AI/ML for pharmaceutical sciences – an industrial perspective

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AI/ML in pharmaceutical applications

- Why AI/ML
- Discovery
- Development
- Manufacturing
- Post-marketing surveillance
- Regulatory



Generated with Gemini

- Hard vs. soft computing
- Traceability
- Transparency
- Regulated environments
- Industrial term: validation

Public Assessment Report

Scientific discussion

Ibuprofen Healthypharm liquid caps 400 mg,
soft capsules
(ibuprofen)

This module reflects the scientific discussion for the approval of Ibuprofen Healthypharm liquid caps. The procedure was finalised at 9 March 2022. For information on changes after this date please refer to the 'steps taken after finalisation' at the end of this PAR.

AI/ML in pharmaceutical applications | why AI/ML

- Hard vs. soft computing
- Traceability
- Transparency
- Regulated environments
- Industrial term: validation

**FDA** U.S. FOOD & DRUG
ADMINISTRATION

Proposed Regulatory Framework for Modifications to Artificial Intelligence/Machine Learning (AI/ML)-Based Software as a Medical Device (SaMD)

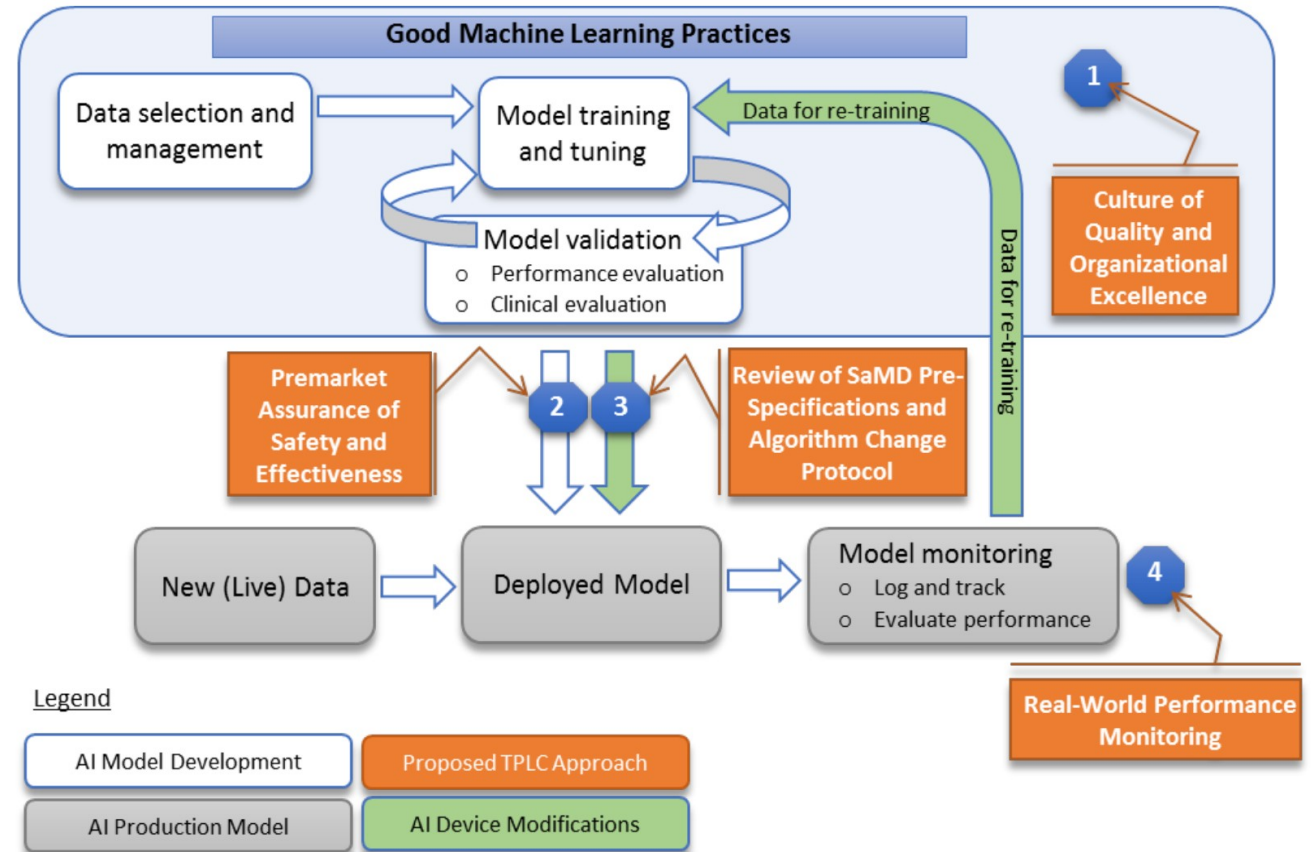
Discussion Paper and Request for Feedback



The diagram illustrates the components of AI/ML-based Software as a Medical Device (SaMD). It features a central cluster of eight hexagonal icons, each representing a different function: Pattern Recognition (magnifying glass over a brain), Artificial Intelligence (circuit board with 'AI'), Machine Learning (hand pointing at a glowing hexagon), Automation (gears), Data Mining (magnifying glass over binary code), Problem Solving (crosses and arrows), Neural Networks (neural network diagram), and Algorithm (flowchart). The background of the diagram shows a person's hand interacting with a digital interface.

AI/ML in pharmaceutical applications | why AI/ML

- Hard vs. soft computing
- Traceability
- Transparency
- Regulated environments
- Industrial term: validation



AI/ML in pharmaceutical applications | Discovery

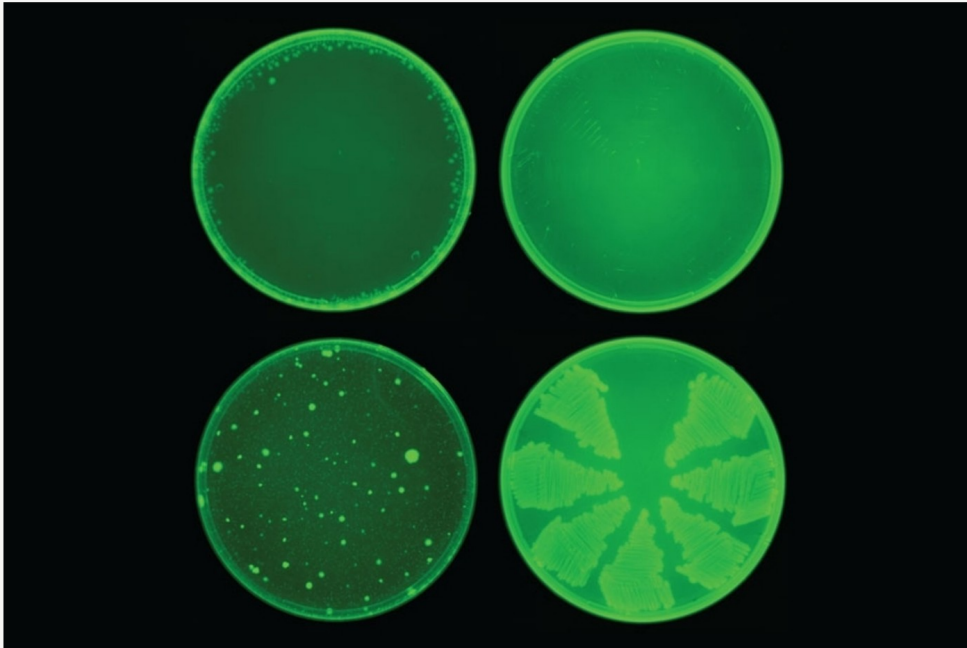
MIT News
ON CAMPUS AND AROUND THE WORLD

SUBSCRIBE

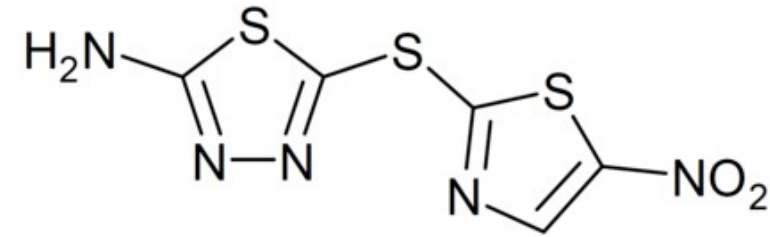
Artificial intelligence yields new antibiotic

A deep-learning model identifies a powerful new drug that can kill many species of antibiotic-resistant bacteria.

Anne Trafton | MIT News Office
February 20, 2020



Halicin



From Wikipedia: “... Halicin (SU-3327) is a chemical compound that acts as an **inhibitor of the enzyme** c-Jun N-terminal kinase (JNK). Originally, it was researched for the treatment of **diabetes** ...”

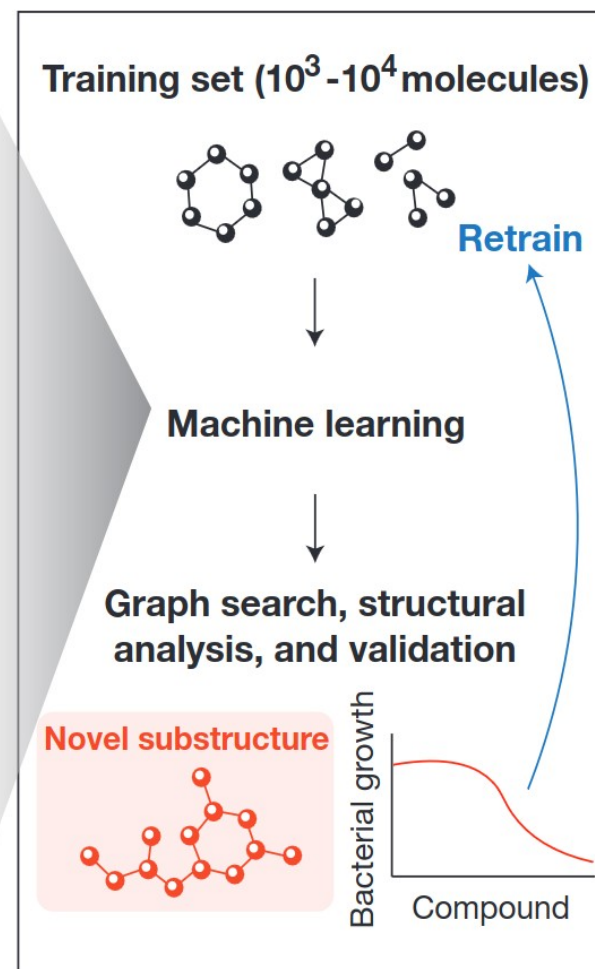
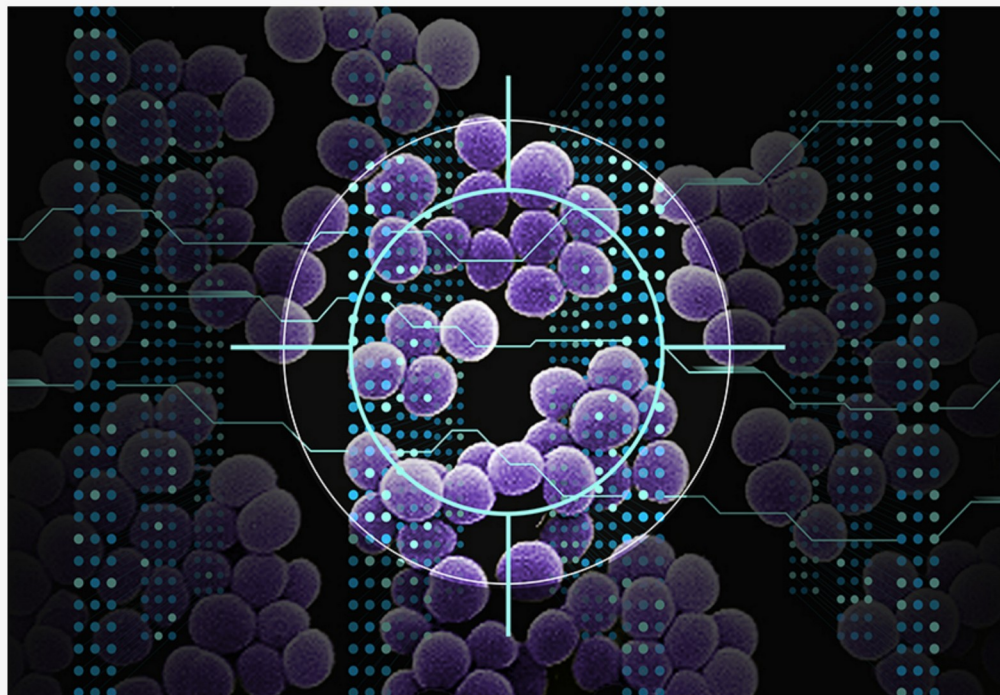
drugs repurposing

AI/ML in pharmaceutical applications | Discovery

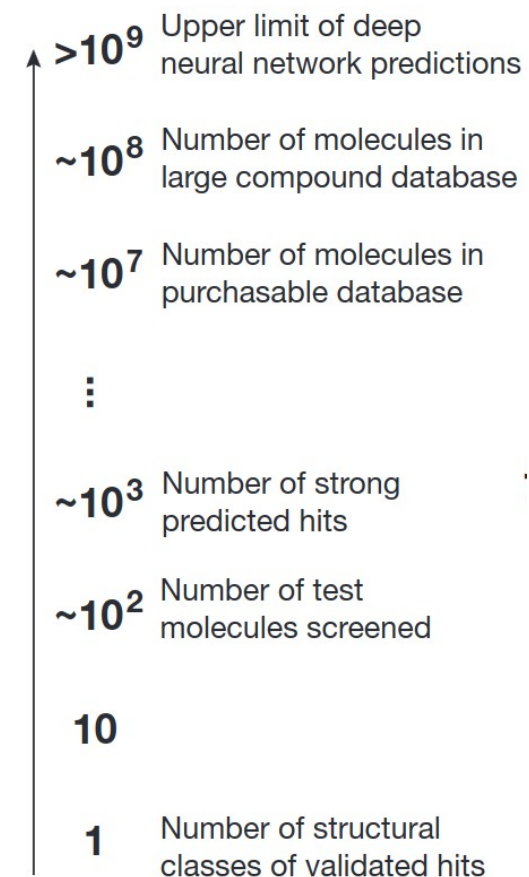
Using AI, MIT researchers identify a new class of antibiotic candidates

These compounds can kill methicillin-resistant *Staphylococcus aureus* (MRSA), a bacterium that causes deadly infections.

Anne Trafton | MIT News
December 20, 2023



Chemical landscape



AI/ML in pharmaceutical applications | Discovery

ANTIMICROBIAL RESISTANCE INTERDISCIPLINARY RESEARCH GROUP (AMR IRG)

A Singapore-MIT initiative creating solutions to address AMR

The AMR IRG is a translational research and entrepreneurship program that tackles the growing threat of antimicrobial resistance.

By leveraging talent and convergent technologies across Singapore and MIT together, we aim to tackle AMR head-on by developing multiple innovative and disruptive approaches to identify, respond to, and treat drug-resistant microbial infections. Through strong scientific and clinical collaborations, our goal is to provide transformative, holistic solutions for Singapore and the world.

OUR WORK

ABOUT AMR

The AMR IRG is funded by the National Research Foundation Singapore under its Campus for Research Excellence and Technological Enterprise (CREATE) program.

<https://amr.smart.mit.edu/>

MIT News
ON CAMPUS AND AROUND THE WORLD

 [SUBSCRIBE](#)

Using generative AI, researchers design compounds that can kill drug-resistant bacteria

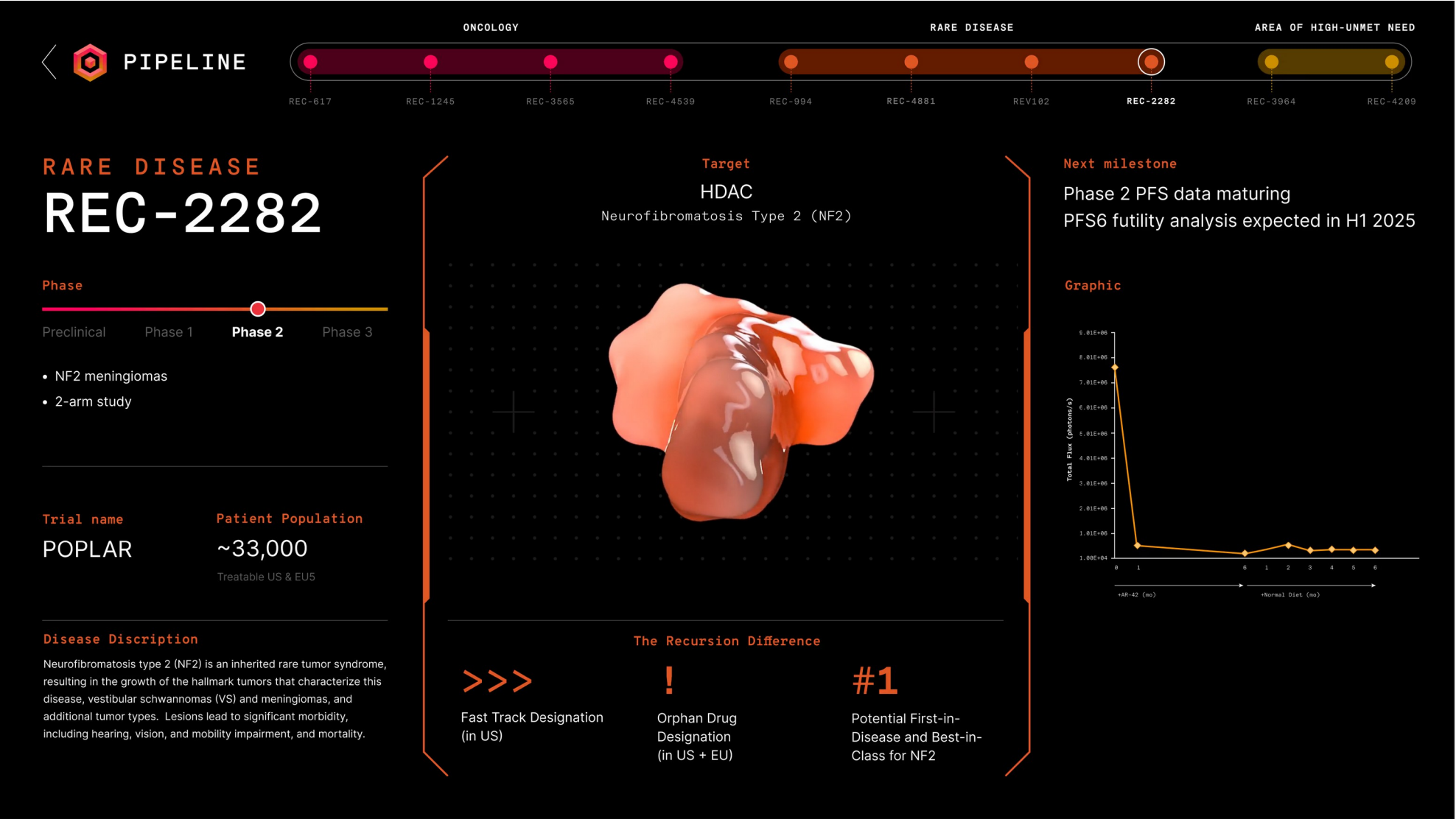
The team used two different AI approaches to design novel antibiotics, including one that showed promise against MRSA.

Anne Trafton | MIT News
August 14, 2025

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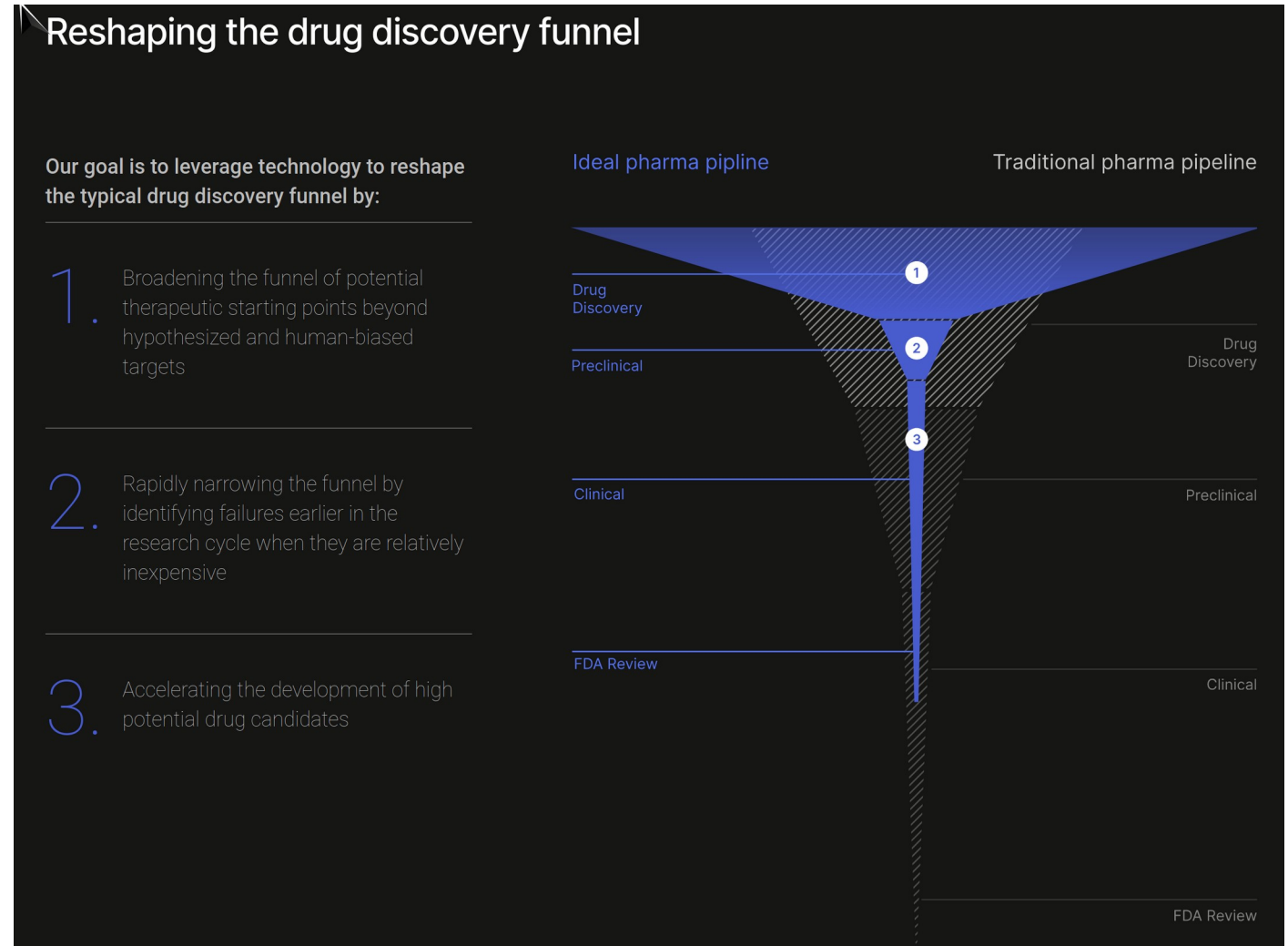
<https://news.mit.edu/2025/using-generative-ai-researchers-design-compounds-kill-drug-resistant-bacteria-0814>

AI/ML in pharmaceutical applications | Discovery



AI/ML in pharmaceutical applications | Discovery

- Data first
- Automated labs
- Standardized data
- Petabytes of data
- Scalability



AI/ML in pharmaceutical applications | Discovery



Integrated wet lab & dry lab

In silico predictions are validated in our own wet laboratories, and repeated, creating a mutually reinforcing cycle of learning. Predictions that validate experimentally are advanced rapidly and reinforce our learning. Predictions that do not validate experimentally generate valuable data that test our understanding and can be used to retrain or reweight the algorithms to improve future predictions. This iterative process of prediction and validation is a key element of successful machine learning over complex datasets.



Unconstrained by human bias

Human bias is often a major threat to the drug discovery process. As humans, we are limited in the size and scale of data we can interpret and are prone to seeing the data that suits us and justifies our hypothesis. Our machine learning tools are designed to extract insights from foundational biological datasets that are too complex for human interpretation, minimizing human bias and identifying relationships that traditional drug discovery approaches may miss.



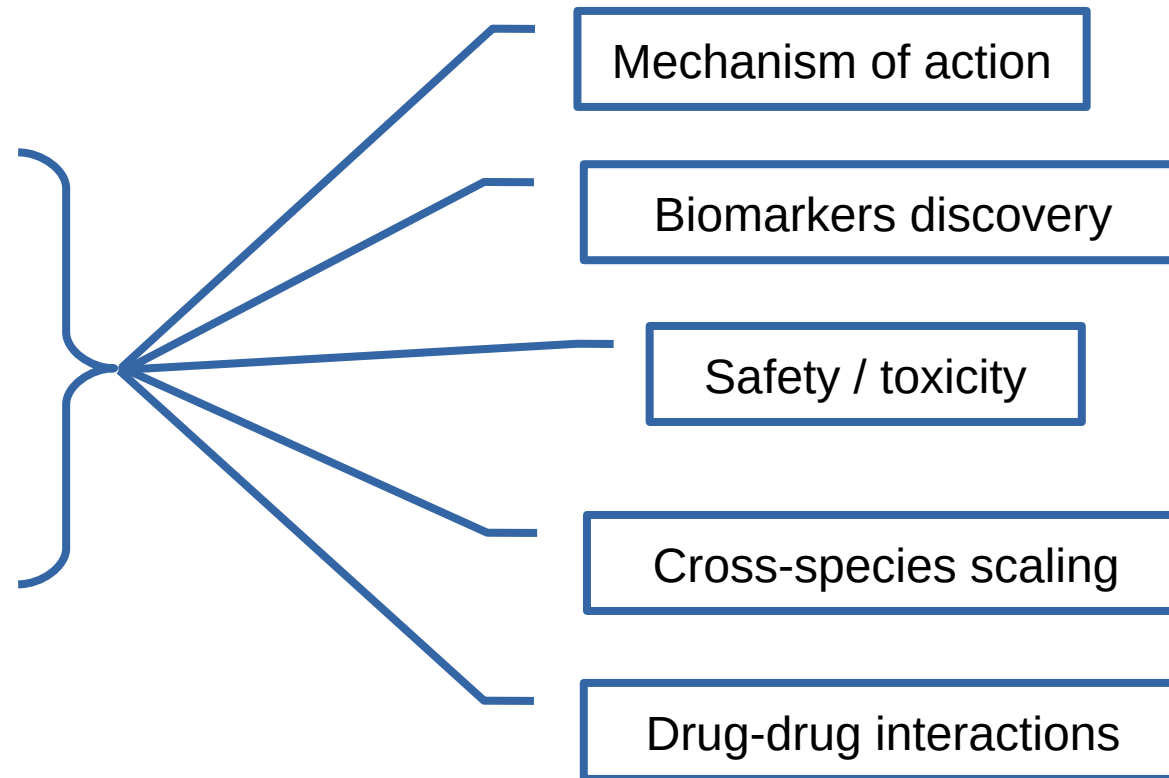
Scale, scale, and scale again

Since 2017, we have approximately doubled the capacity of our phenomics platform each year and currently generate up to nine million images or 80 terabytes of new data to the Recursion Data Universe per week across 1.5 million experiments.

Data is the first step

- Non-clinical (preclinical)

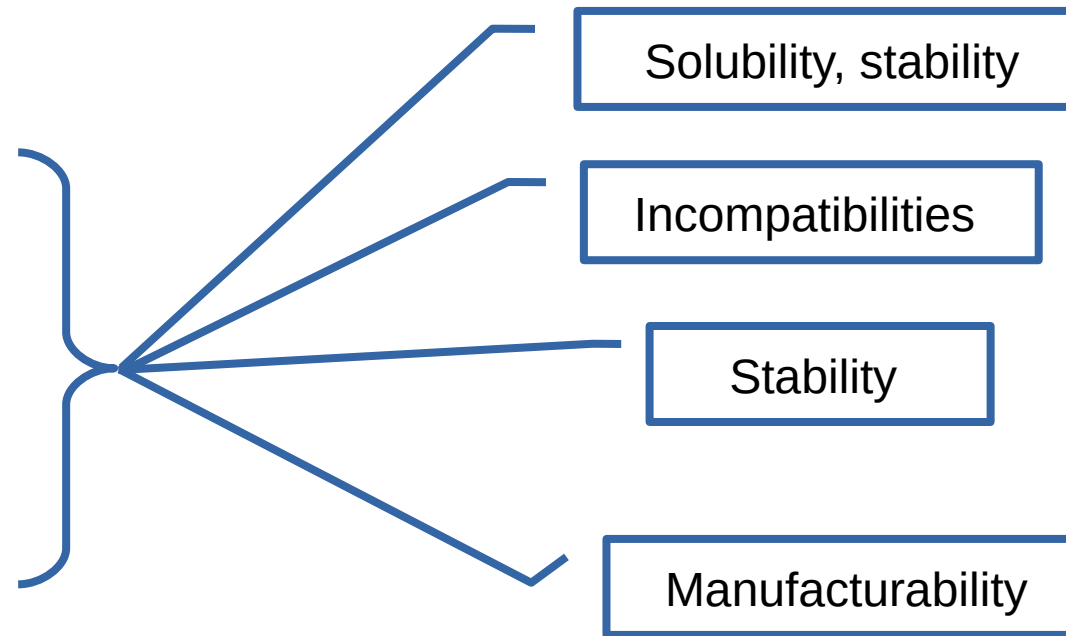
- Proteomics
- Metabolomics
- Genomics



AI MODEL

- Non-clinical (preformulation)

- phys/chem
- API
- excipients



AI MODEL

AI/ML in pharmaceutical applications | Development

- Clinical (clinical trials)
 - subjects recruitment
 - data analysis
 - documentation management / development

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7 z 198

Protocol No. BA14101334
Project No. BA14101334-01

PPD

PROTOCOL

<u>PROTOCOL TITLE:</u>	Single dose oral bioequivalence study of Darunavir film-coated Tablets 600 mg and 'PREZISTA' (Darunavir Ethanolate) film-coated Tablets 600 mg with co-administration of 'NORVIR'® (Ritonavir) film-coated Tablets 100 mg in healthy adult human subjects under fed conditions.
<u>STUDY DESIGN:</u>	An open label, randomized, two-period, two-treatment, two-sequence, crossover, balanced, single dose oral bioequivalence study.
<u>INVESTIGATIONAL PRODUCTS:</u>	<ul style="list-style-type: none">• <i>Test Product (T):</i> Darunavir film-coated Tablets 600 mg – Manufactured by: Mylan Laboratories Limited, F-4 & F-12, MIDC, Malegaon, Sinnar-422 113, Nashik District, Maharashtra State, India.• <i>Reference Product (R):</i> 'PREZISTA' (Darunavir Ethanolate) film-coated Tablets 600 mg – Marketing authorisation holder: Janssen-Cilag International NV, Turnhoutseweg 30, B-2340 Beerse, Belgium.• <i>Concomitant medication:</i> 'NORVIR'® (Ritonavir) film-coated Tablets 100 mg - Marketing authorisation holder: AbbVie Ltd, Maidenhead, SL6 4XE, United Kingdom.
<u>REGION OF SUBMISSION:</u>	European member states
<u>PROTOCOL VERSION NO.</u> 00	<u>SUPERSEDES VERSION NO.</u> None
<u>PROTOCOL DATE:</u> June 11, 2014	<u>SUPERSEDES DATE:</u> NA

- Digitization of industrial processes
- Industry 4.0
- Continuous manufacturing
- Process Analytical Technologies
- Quality by Design
- Regulatory

INTERNATIONAL CONFERENCE ON HARMONISATION OF TECHNICAL
REQUIREMENTS FOR REGISTRATION OF PHARMACEUTICALS FOR HUMAN USE

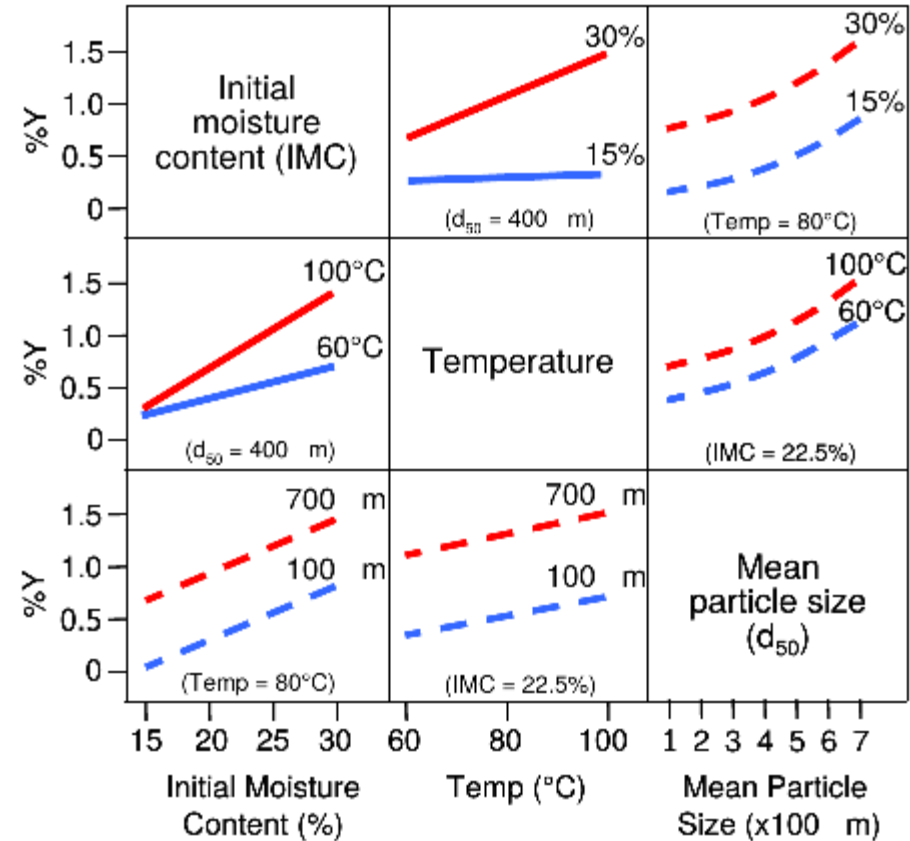
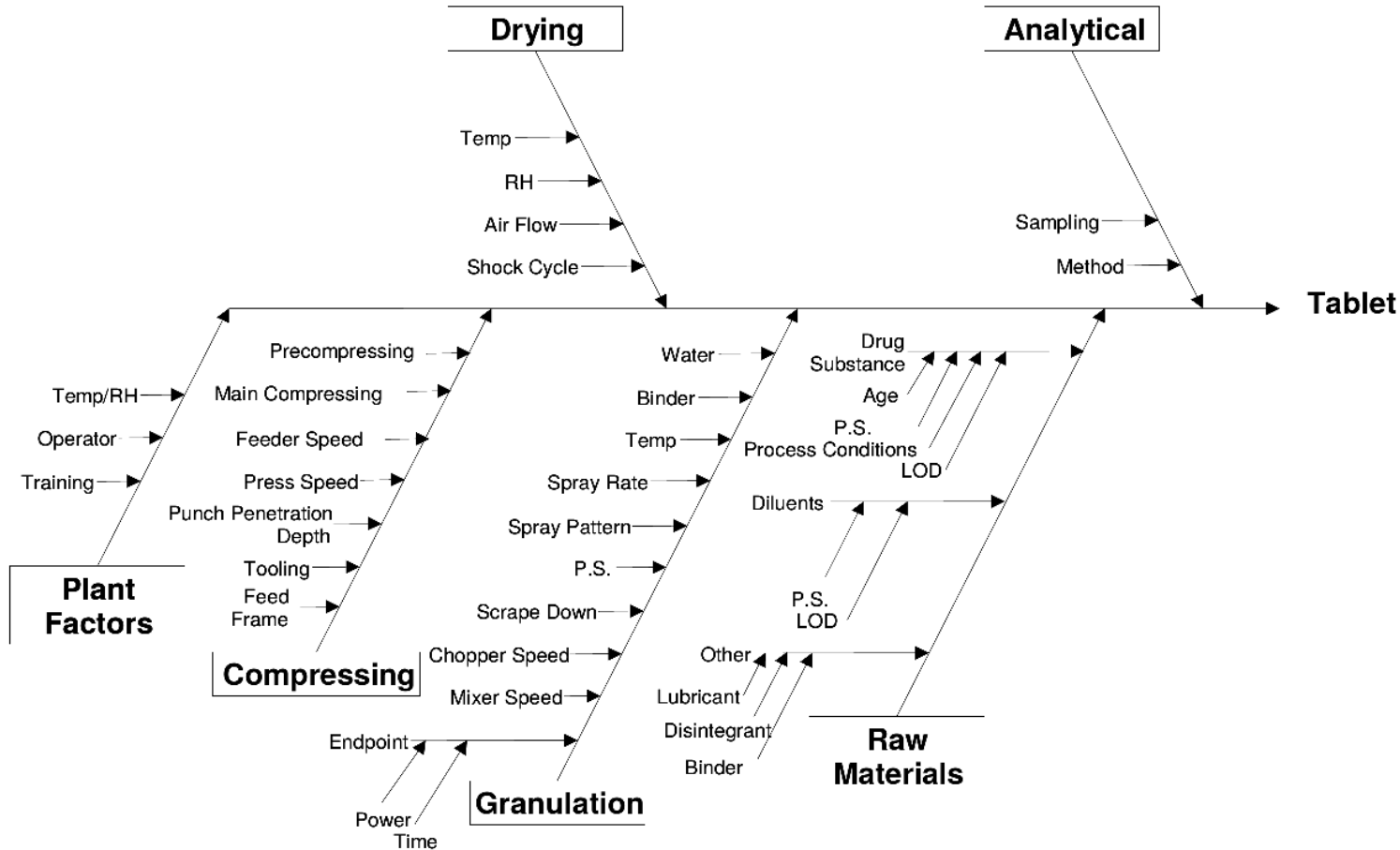
ICH HARMONISED TRIPARTITE GUIDELINE

PHARMACEUTICAL DEVELOPMENT
Q8(R2)

Current Step 4 version
dated August 2009

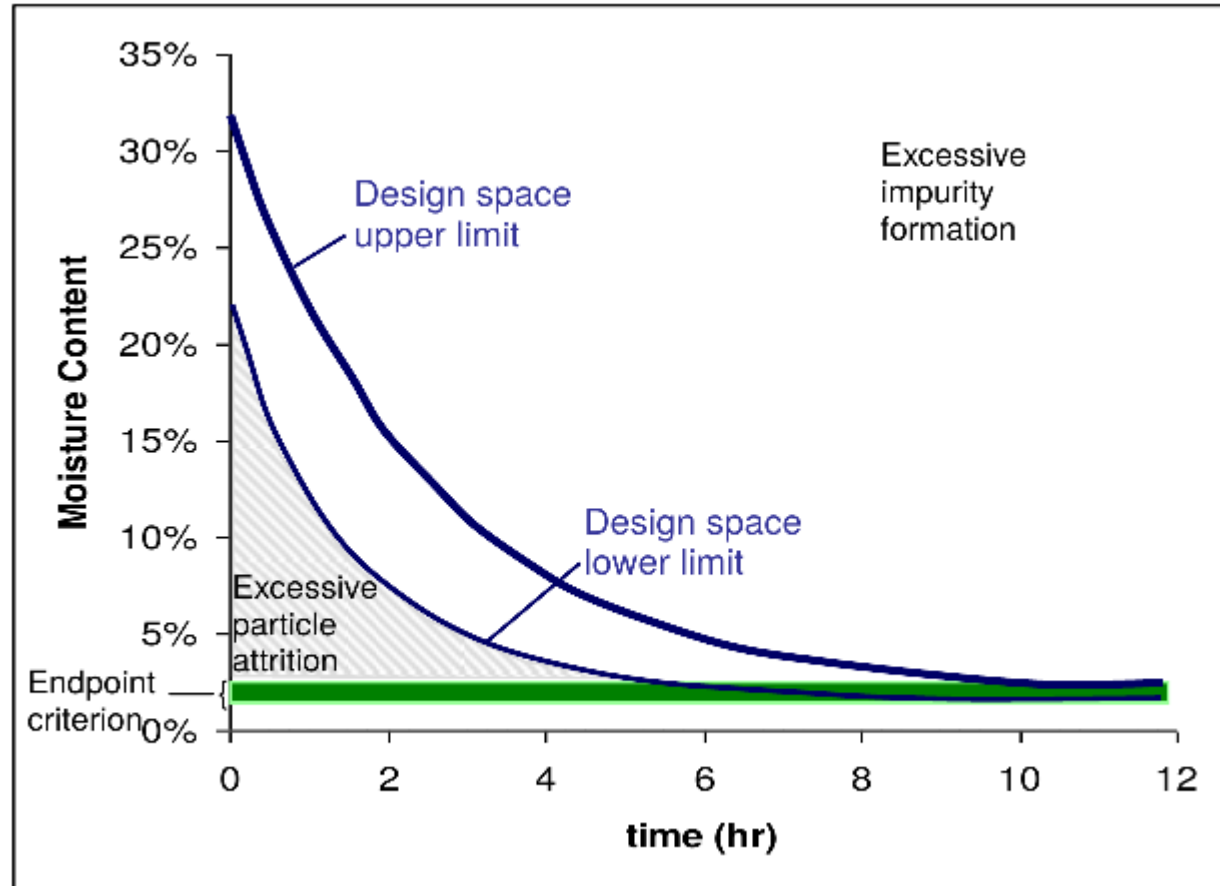
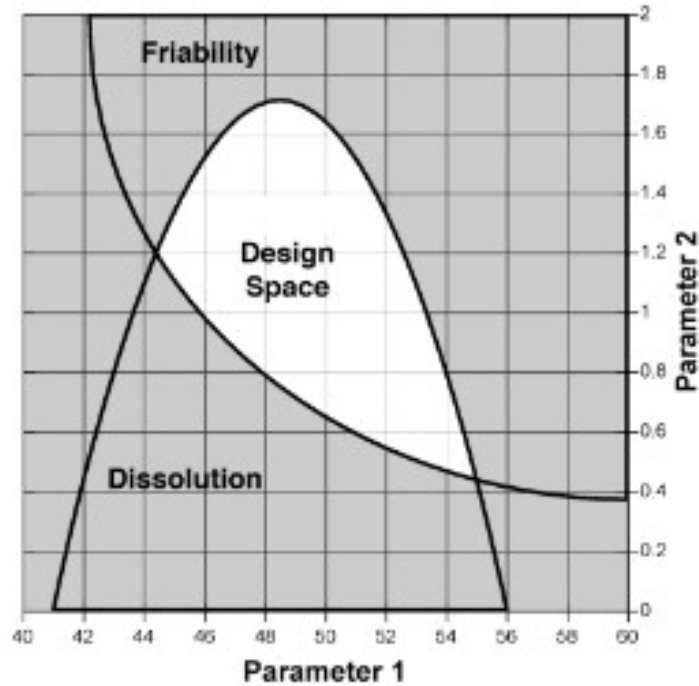
This Guideline has been developed by the appropriate ICH Expert Working Group and has been subject to consultation by the regulatory parties, in accordance with the ICH Process. At Step 4 of the Process the final draft is recommended for adoption to the regulatory bodies of the European Union, Japan and USA.

AI/ML in pharmaceutical applications | Manufacturing



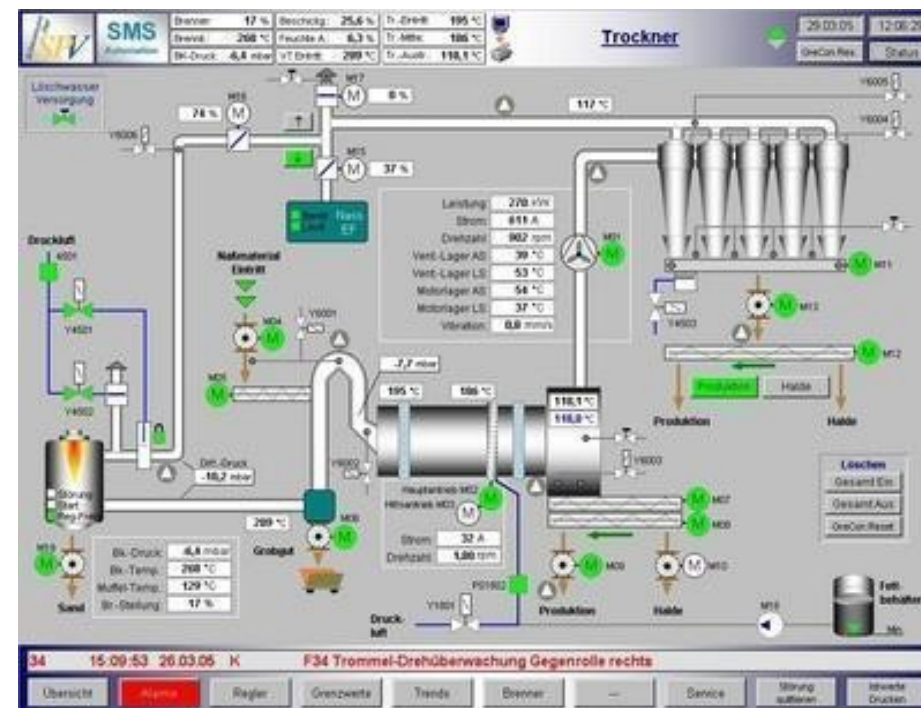
vendor&site-related: individual model required

AI/ML in pharmaceutical applications | Manufacturing



Required!

AI/ML in pharmaceutical applications | Manufacturing



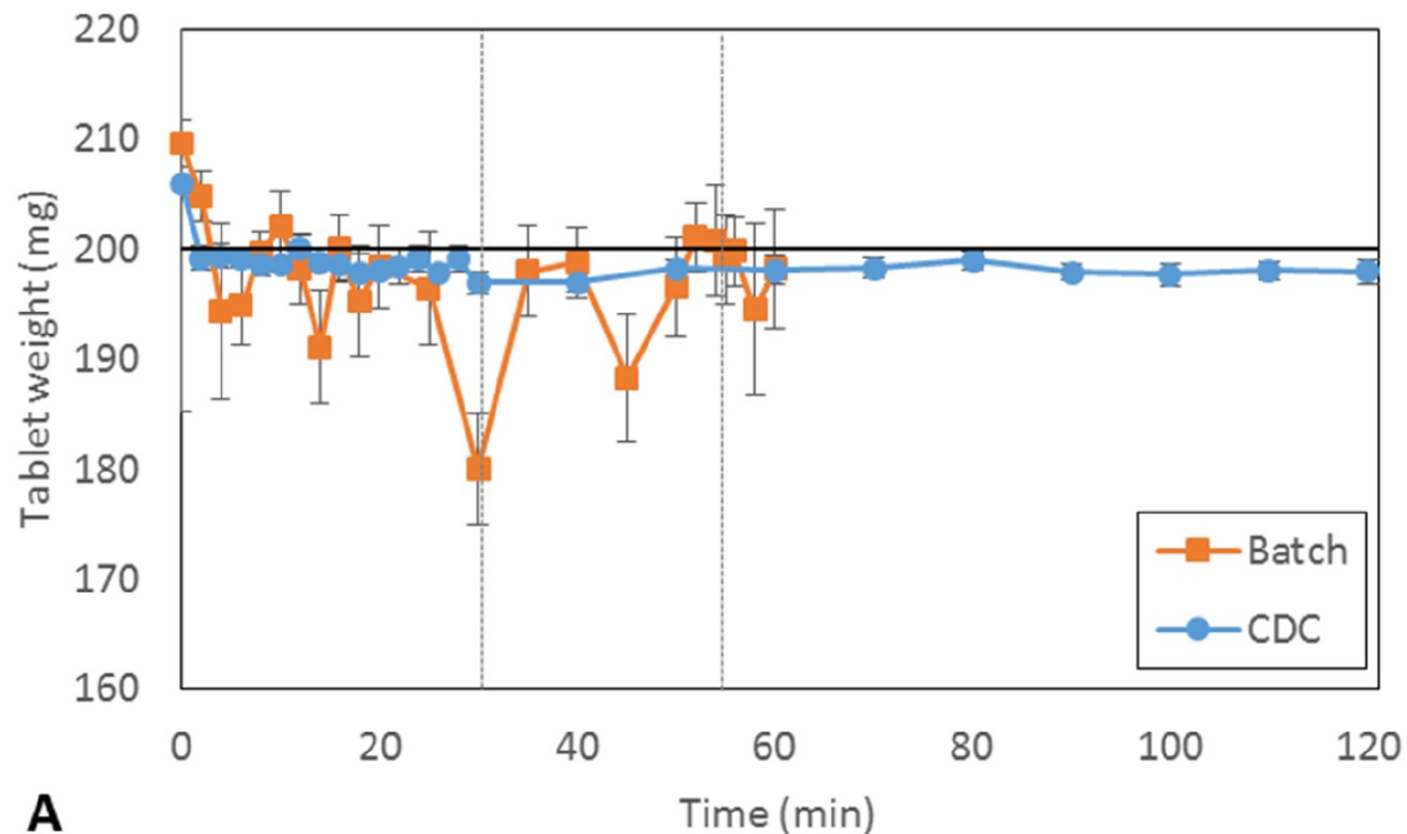
the source of data

AI/ML in pharmaceutical applications | Manufacturing



the source of data (PAT)

AI/ML in pharmaceutical applications | Manufacturing



Comparison between integrated continuous direct compression line and batch processing - The effect of raw material properties. Karttunen AP, Wikström H, Tajarobi P, Fransson M, Sparén A, Marucci M, Ketolainen J, Folestad S, Korhonen O, Abrahmsén-Alami S. Eur J Pharm Sci. 2019 May 15;133:40-53. doi: 10.1016/j.ejps.2019.03.001

Critical Quality Attribute (CQA):

A physical, chemical, biological or microbiological property or characteristic that should be within an appropriate limit, range, or distribution to ensure the desired product quality.

Critical Process Parameter (CPP):

A process parameter whose variability has an impact on a critical quality attribute and therefore should be monitored or controlled to ensure the process produces the desired quality.

Quality Target Product Profile (QTPP):

A prospective summary of the quality characteristics of a drug product that ideally will be achieved to ensure the desired quality, taking into account safety and efficacy of the drug product.

AI/ML in pharmaceutical applications | Manufacturing

The screenshot shows the Quotient Sciences website. The header includes the Quotient Sciences logo, the tagline 'Molecule to cure. Fast.™', and navigation links: About, News, Events, Blog, Careers, Volunteer for a Clinical Trial, and a search icon. Below the header is a dark blue navigation bar with links for Integrated Programs, Services, Solutions, Resources, and a Contact button. The main content area has a blue background with the seminar title 'Seminar: Accelerating Formulation Development with AI' and the location/date 'San Antonio, United States | 11 November 2025'. Below this is a breadcrumb trail: Home > Events > Seminar: Accelerating Formulation Development with AI. The 'Overview' section describes the seminar as an exclusive breakfast event exploring AI in formulation development. To the right, there is a 'Register' section with a 'Register now' button and a 'Location' section listing the Grand Hyatt San Antonio River Walk.

Quotient Sciences
Molecule to cure. Fast.™

About News Events Blog Careers Volunteer for a Clinical Trial

Integrated Programs Services Solutions Resources Contact

Seminar: Accelerating Formulation Development with AI

San Antonio, United States | 11 November 2025

Home > Events > Seminar: Accelerating Formulation Development with AI

Overview

Join Quotient Sciences and Intrepid Labs for an exclusive breakfast seminar exploring how artificial intelligence (AI) is transforming formulation development. Learn how AI platforms are helping reduce development timelines, optimising formulation strategies and improving predictability of clinical performance.

Register Register now

Location Grand Hyatt San Antonio River Walk
600 E Market St, TX 78205
San Antonio, United States

- active learning
- tailored models
- AI-based platform

<https://www.quotientosciences.com/events/seminar-accelerating-formulation-development-ai>

AI/ML in pharmaceutical applications | Regulatory

CENTER FOR DRUG EVALUATION AND RESEARCH

FY 2024

GDUFA SCIENCE AND
RESEARCH REPORT

Generic drugs

CHAPTER 8: DATA ANALYTICS & ARTIFICIAL INTELLIGENCE



Generic drugs

ChatGPT to support the development of PSGs. In a proof-of-concept study, ChatGPT was employed to generate a summary of food effect information by analyzing publicly available new drug application (NDA) review documents available at Drugs@FDA. This study serves as an important milestone in exploring the feasibility of using LLMs to aid regulatory assessments

Large Language Models to Support BE Evaluation

LLMs to assist FDA reviewers in their critical work {...} interactive **expert system** trained on publicly available FDA data and relevant publications to quickly respond to queries and summarize complex study information.

ML-CFD-DEM Based Reduced Order Models (ROM) to Quantify Variability in Inhalers, Drugs, and Users for Evaluating Comparability of Generic ODP Complex Products: **ML to overcome certain limitations associated with computational fluid dynamics.**

AI/ML in pharmaceutical applications | Pharmacovigilance

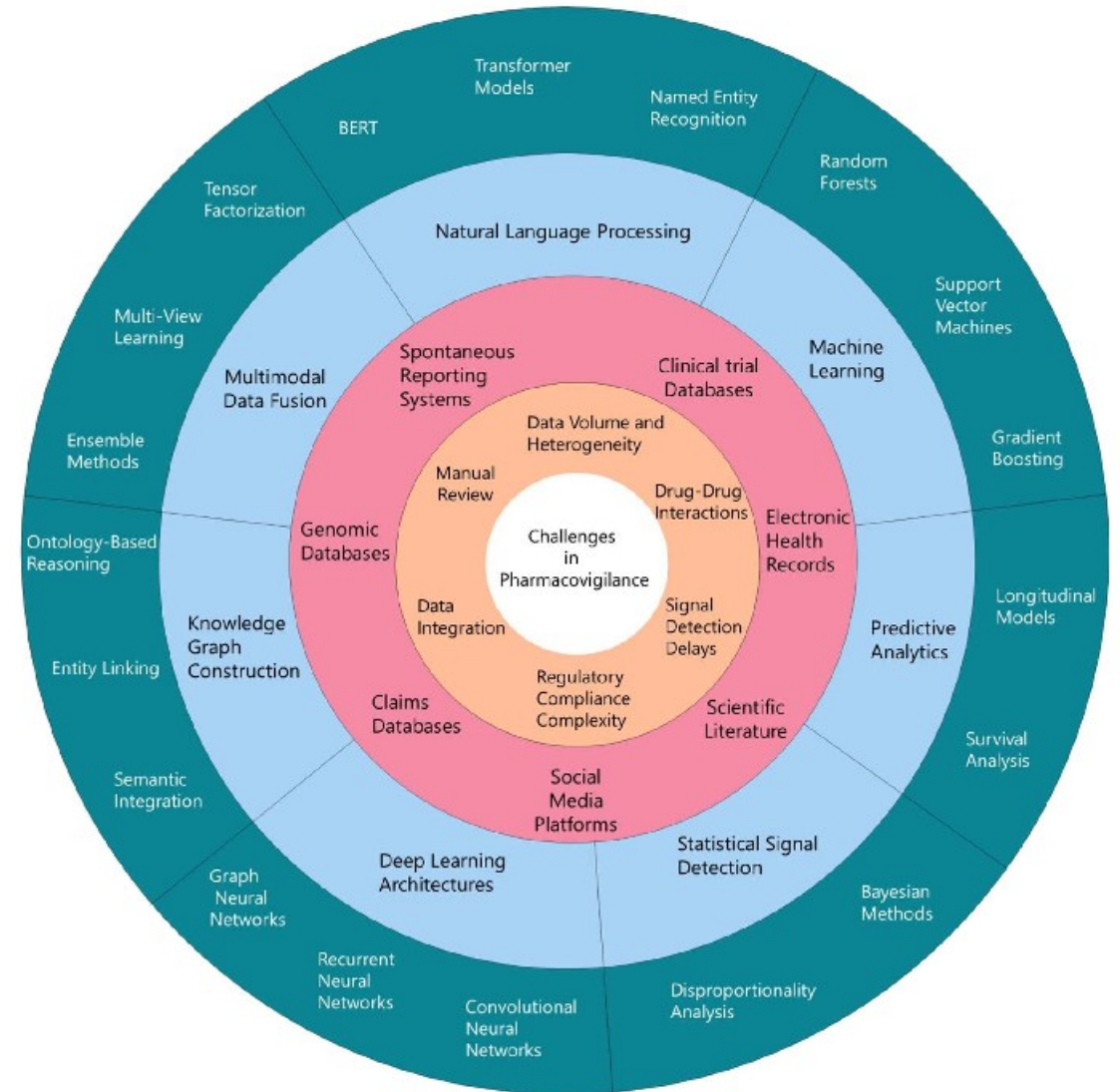
- Medical data monitoring
- Deep research mode
- Web-scrapping

THERAPEUTIC ADVANCES in
Drug Safety

Artificial intelligence in pharmacovigilance: advancing drug safety monitoring and regulatory integration

Ankit Nagar , Joga Gobburu and Alok Chakravarty

<https://doi.org/10.1177/20420986251361435>

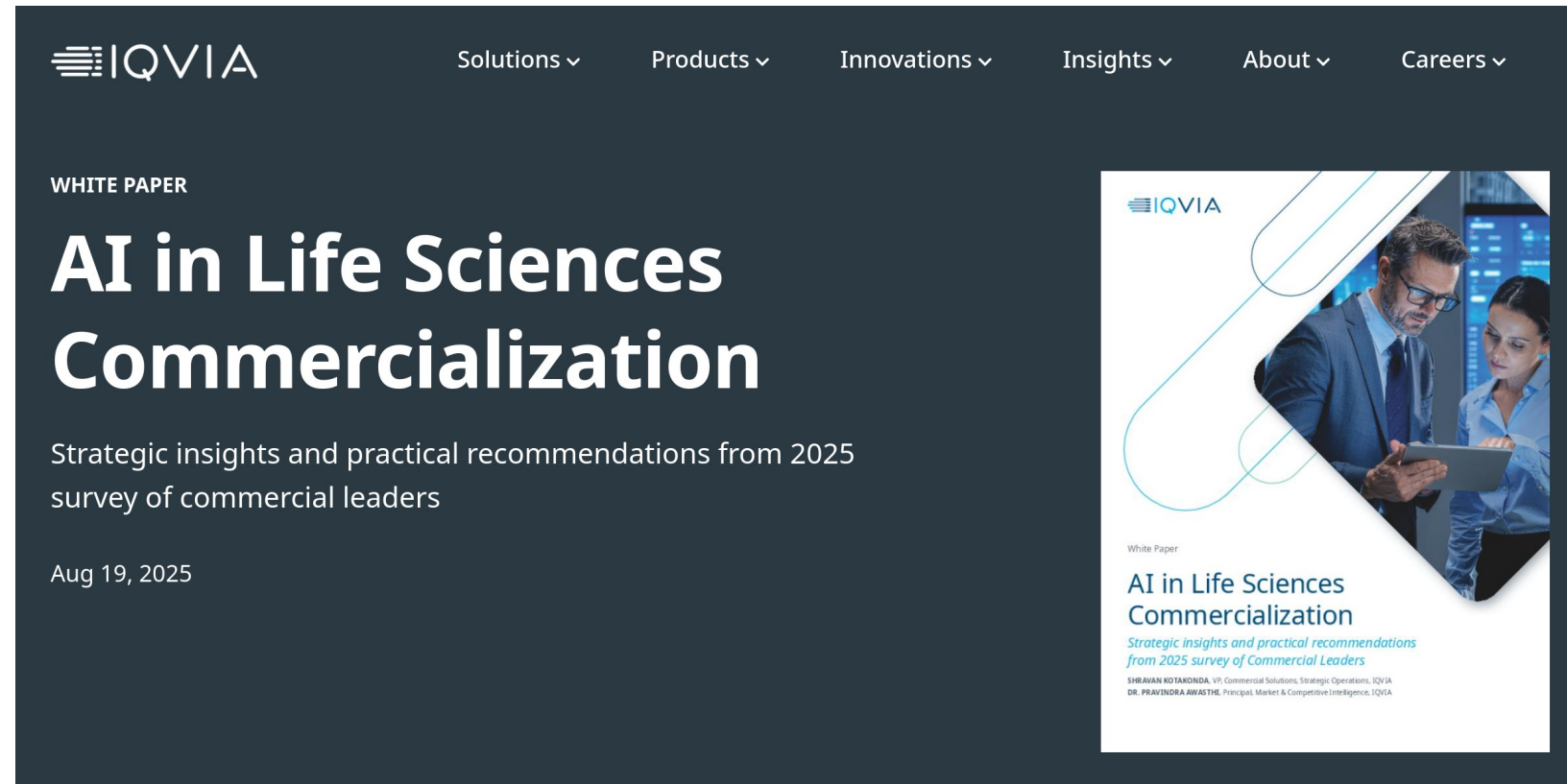


Real cases

WHITE PAPER

AI is no longer experimental, it's essential

Discover how leading life sciences companies around the world are embedding AI into their commercial strategies to drive meaningful results. This white paper reveals insights from 100+ senior leaders, including where AI is delivering ROI, what's holding teams back, and how to move from ambition to execution.



The screenshot displays the IQVIA website's header with navigation links: Solutions, Products, Innovations, Insights, About, and Careers. The main content area features a white paper titled "AI in Life Sciences Commercialization" with the subtitle "Strategic insights and practical recommendations from 2025 survey of commercial leaders" and a date of "Aug 19, 2025". To the right, a thumbnail of the white paper cover is shown, featuring the IQVIA logo, the title, subtitle, and authors: Shrawan Kotakonda, VP, Commercial Solutions, Strategic Operations, IQVIA, and Dr. Pravendra Awasthi, Principal, Market & Competitive Intelligence, IQVIA. The cover image depicts two professionals in business attire reviewing a tablet.

<https://www.iqvia.com>



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