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

AI/ML in pharmaceutical applications | why AI/ML

- 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)

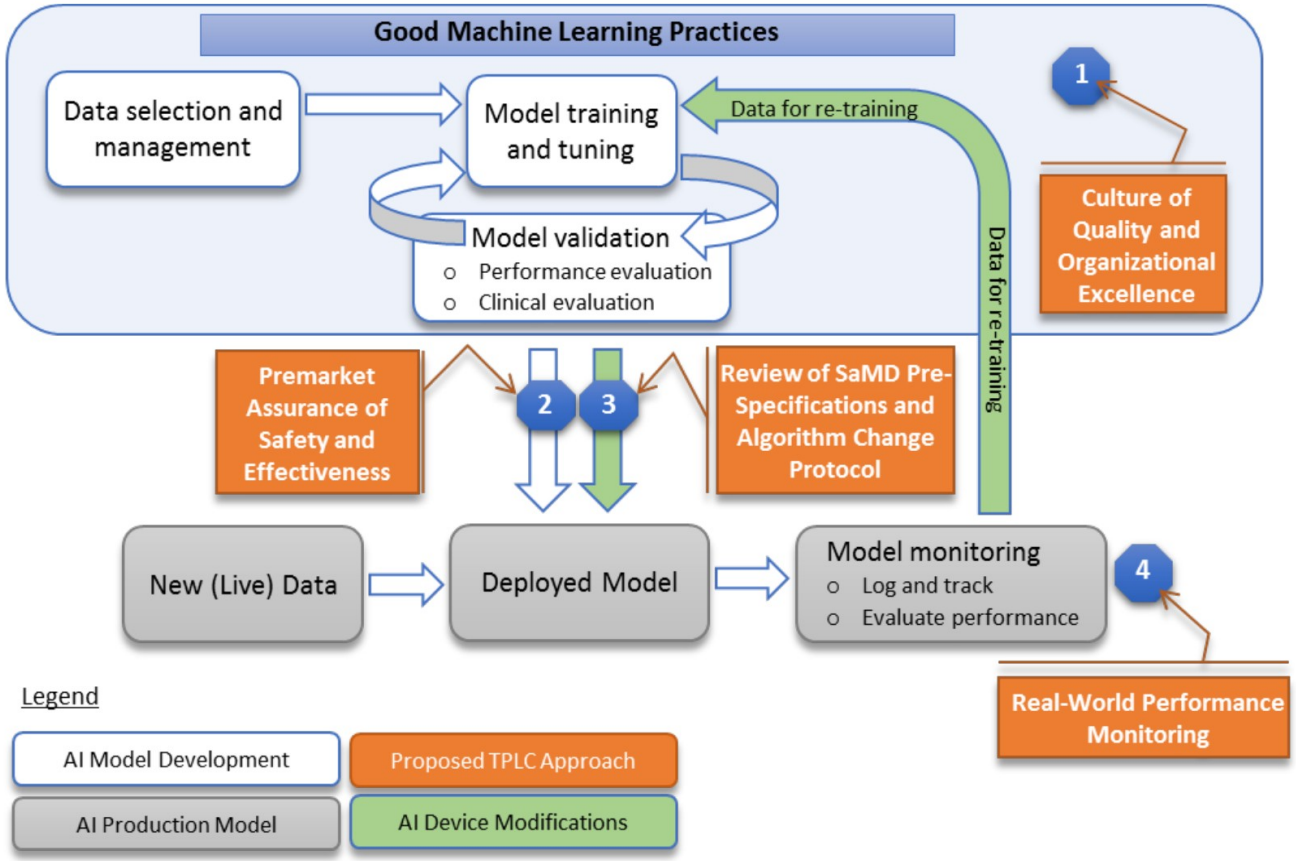
This module reflects the scientific discussion for the approval of Ibuprofen Healthypharm liquid caps. The procedure was finalised at 9 March 2022. For information on changes after this date please refer to the 'steps taken after finalisation' at the end of this PAR.

AI/ML in pharmaceutical applications | why AI/ML

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

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

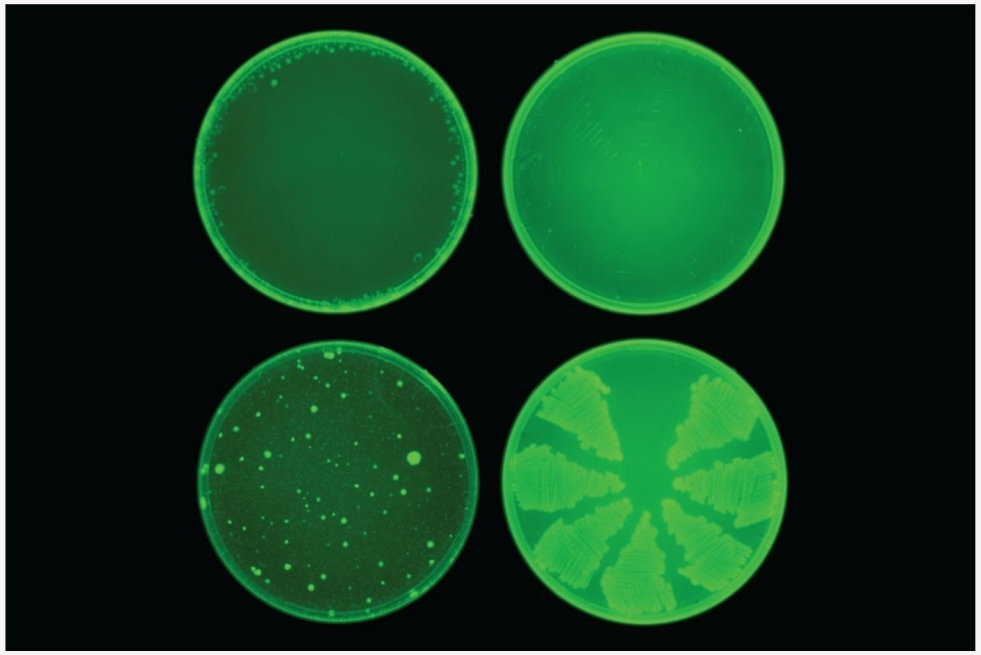
MIT News
ON CAMPUS AND AROUND THE WORLD

SUBSCRIBE

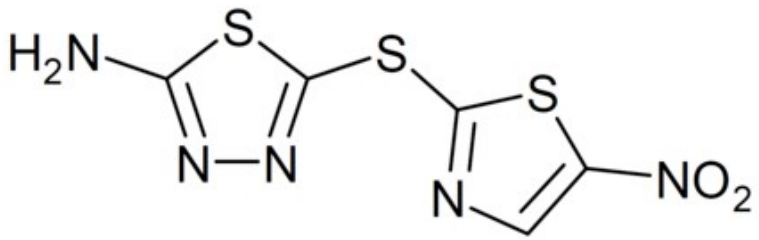
Artificial intelligence yields new antibiotic

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** ..."

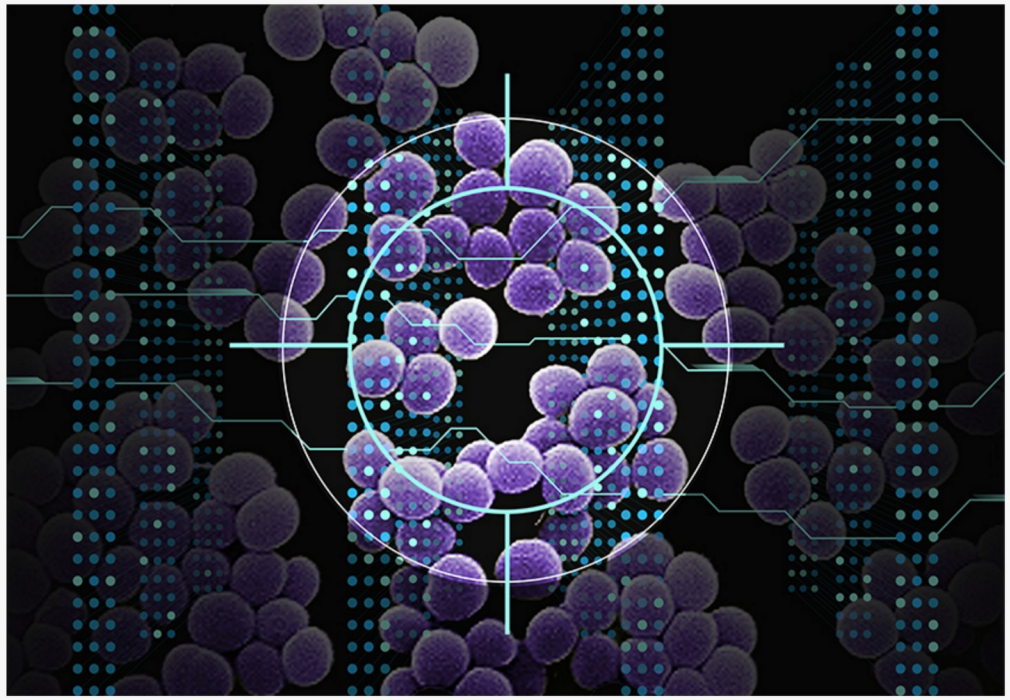
drugs repurposing

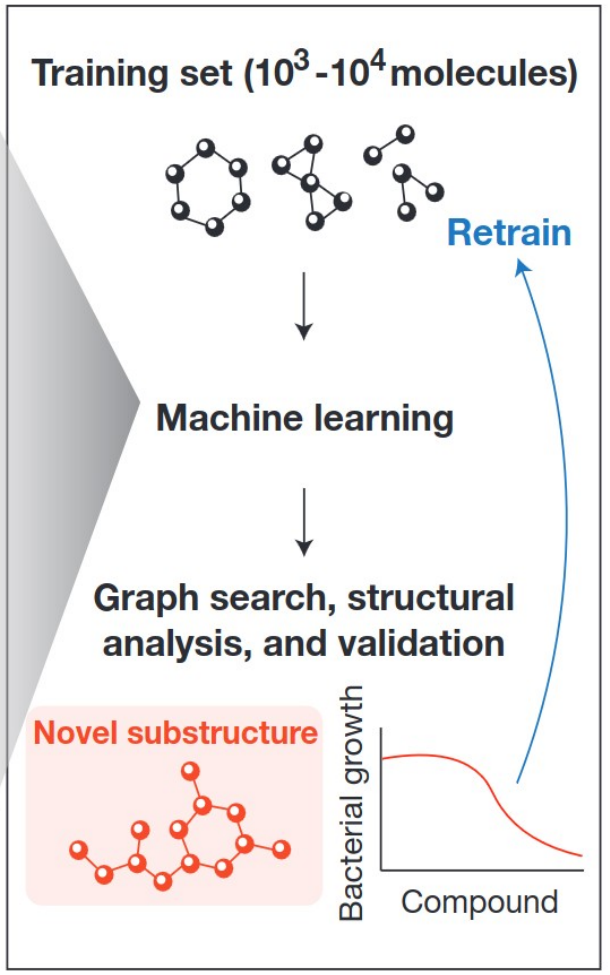
AI/ML in pharmaceutical applications | Discovery

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

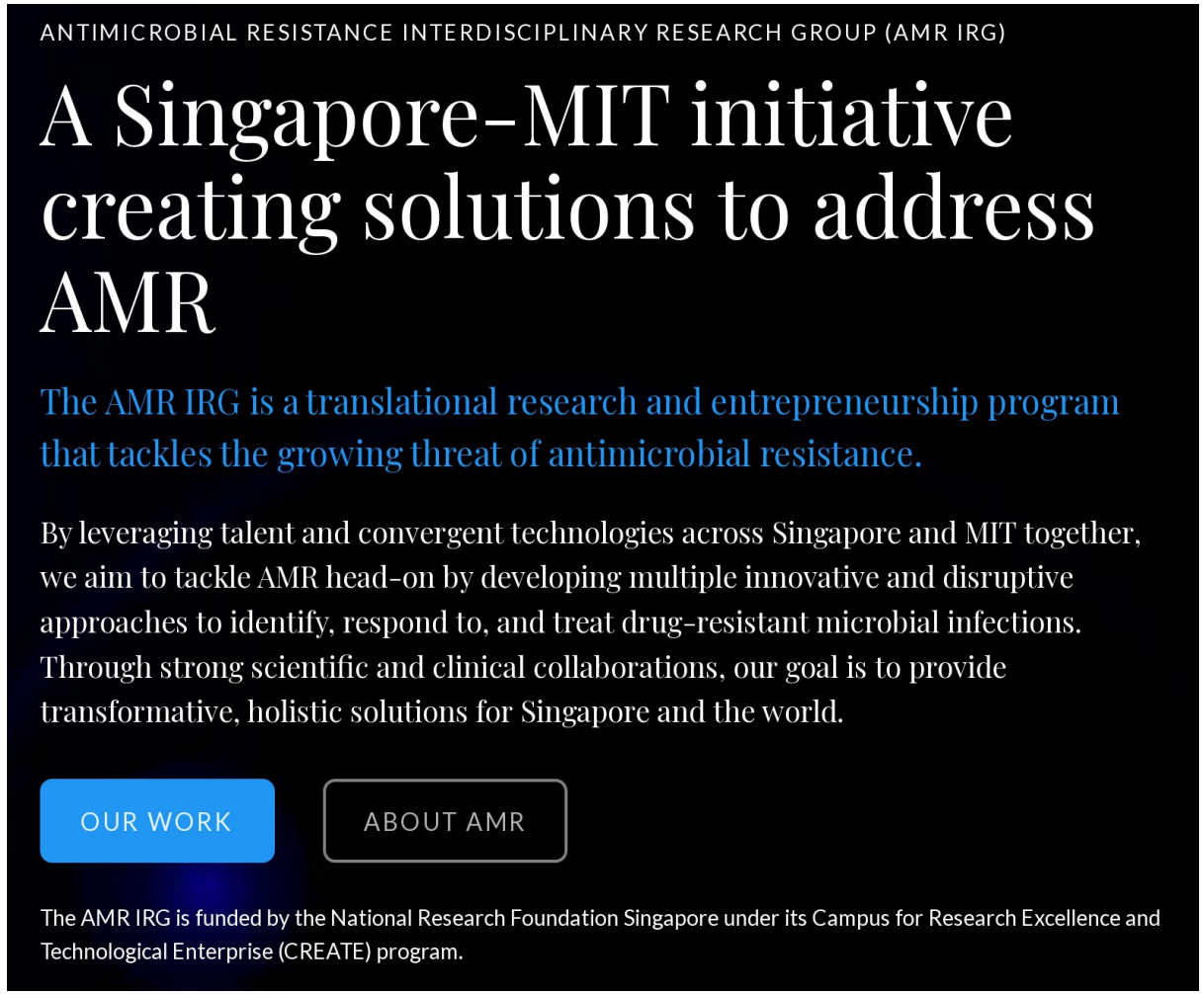




Chemical landscape

- $>10^9$ Upper limit of deep neural network predictions
- $\sim10^8$ Number of molecules in large compound database
- $\sim10^7$ Number of molecules in purchasable database
- ⋮
- $\sim10^3$ Number of strong predicted hits
- $\sim10^2$ Number of test molecules screened
- 10
- 1 Number of structural classes of validated hits

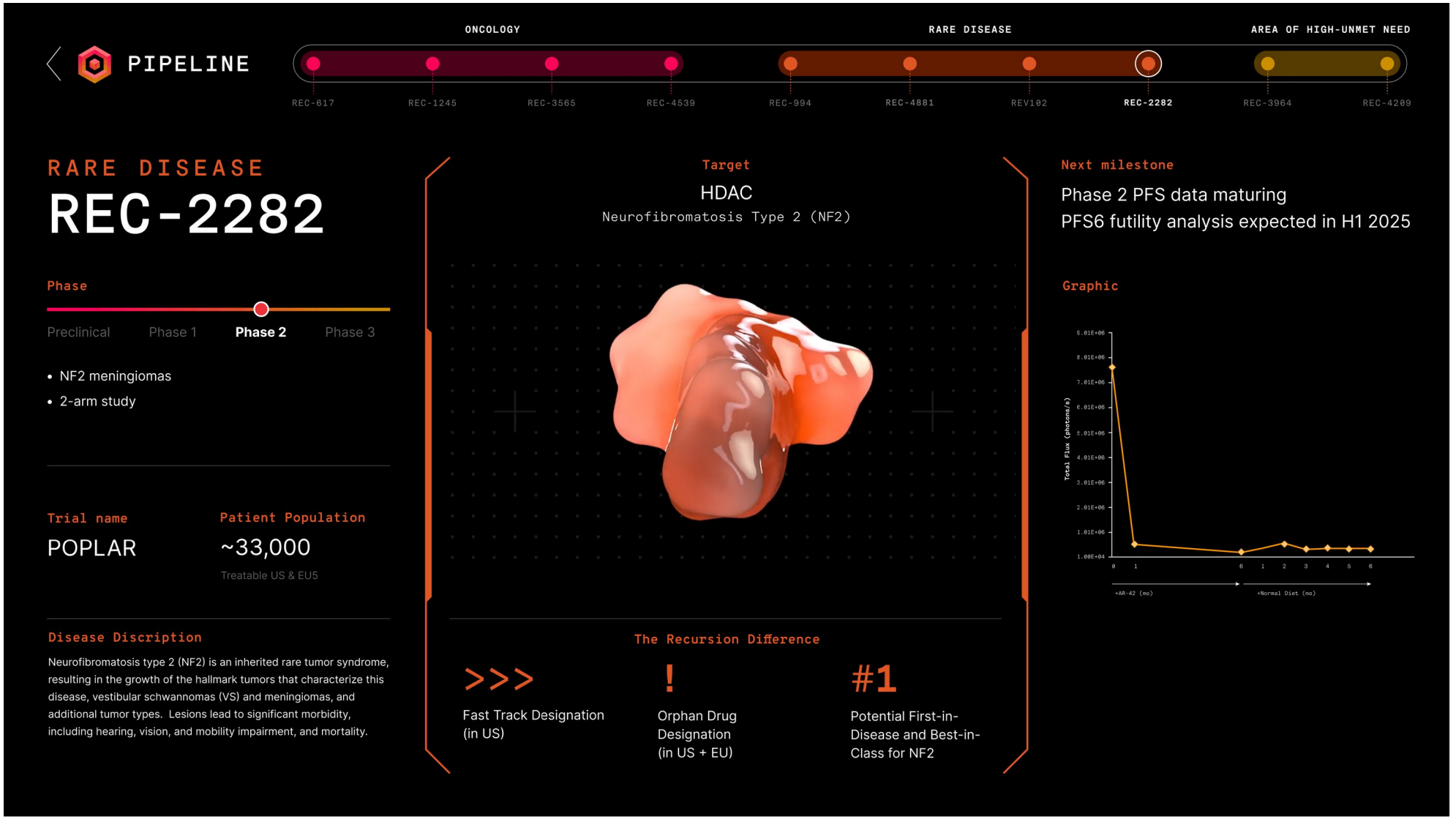
AI/ML in pharmaceutical applications | Discovery



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

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

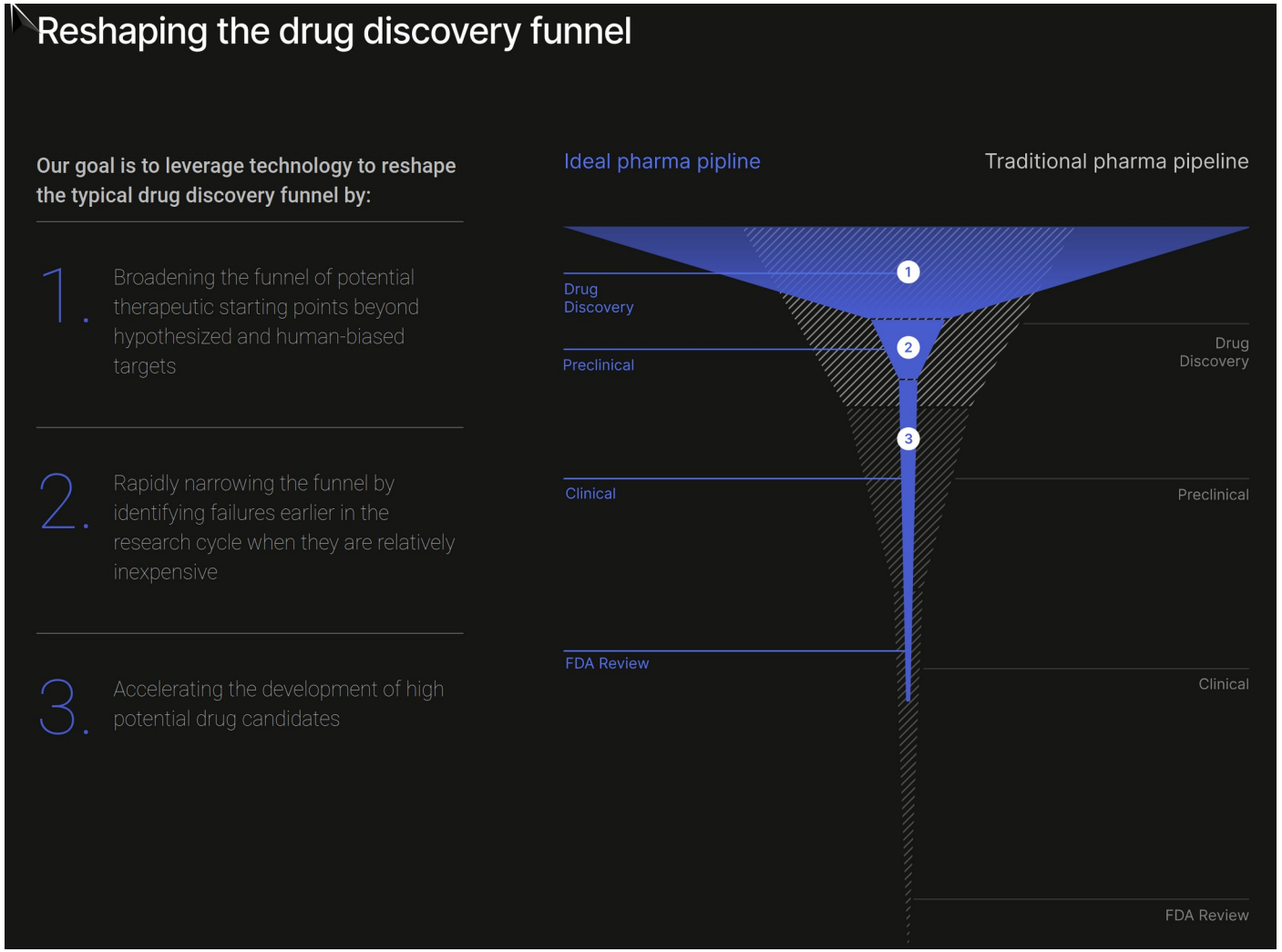
AI/ML in pharmaceutical applications | Discovery



https://www.recursion.com/

AI/ML in pharmaceutical applications | Discovery

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



https://www.recursion.com/

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.

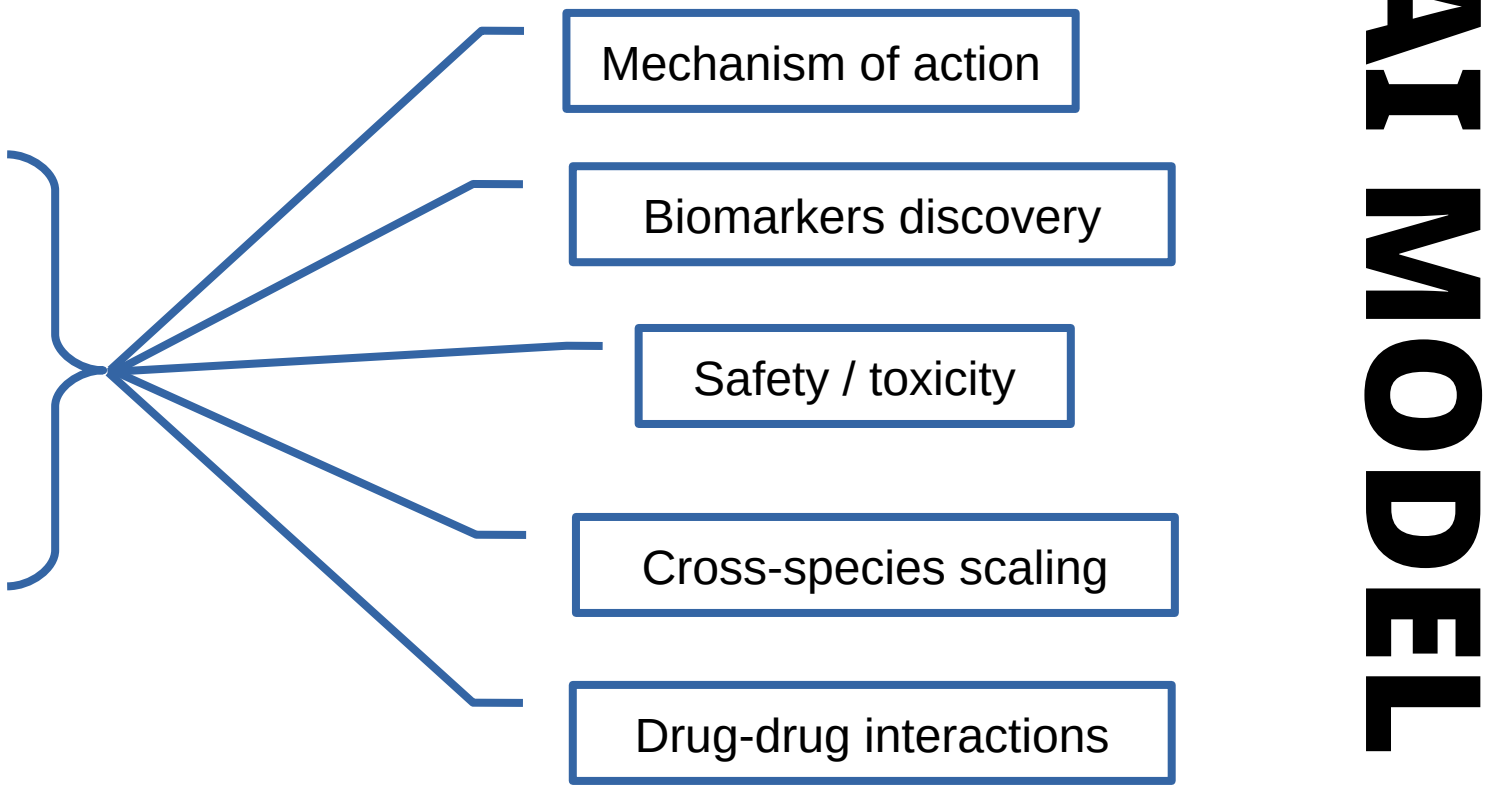
Scale, scale, and scale again

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

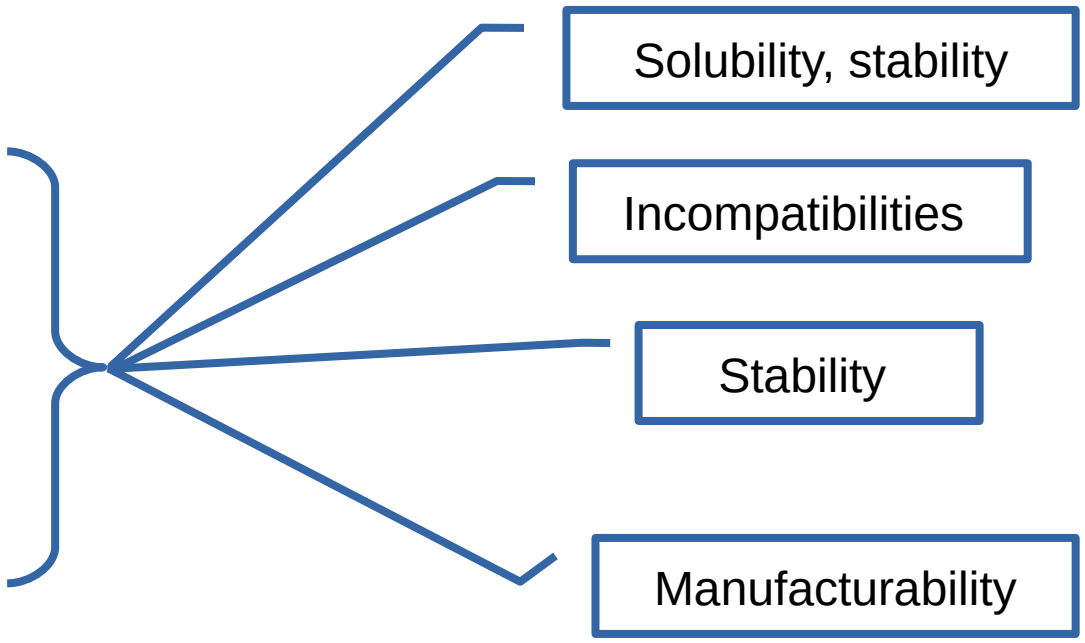
AI/ML in pharmaceutical applications | Development

- Non-clinical (preclinical)
  - Proteomics
  - Metabolomics
  - Genomics



AI/ML in pharmaceutical applications | Development

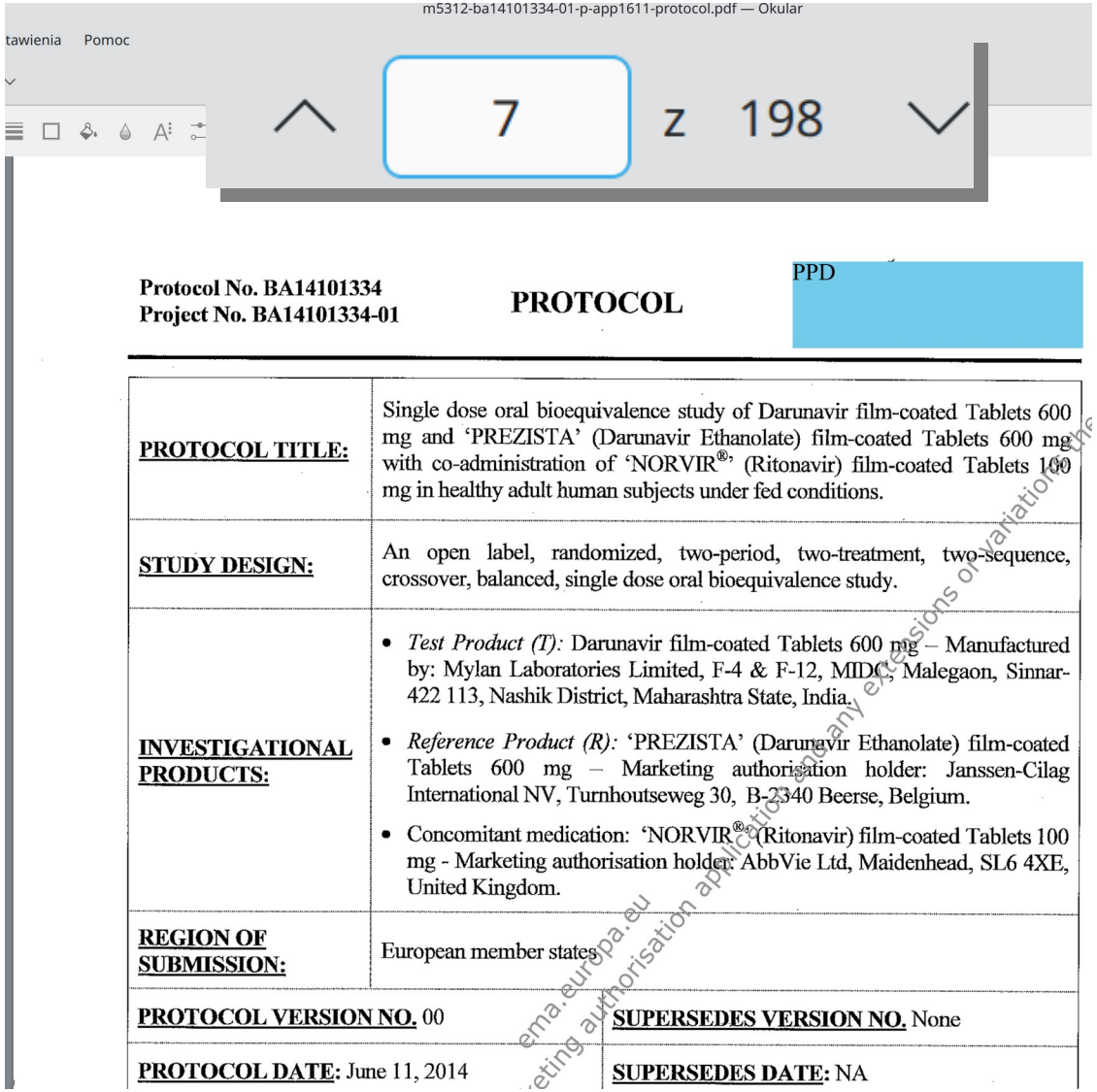
- Non-clinical (preformulation)
  - phys/chem
  - API
  - excipients



AI MODEL

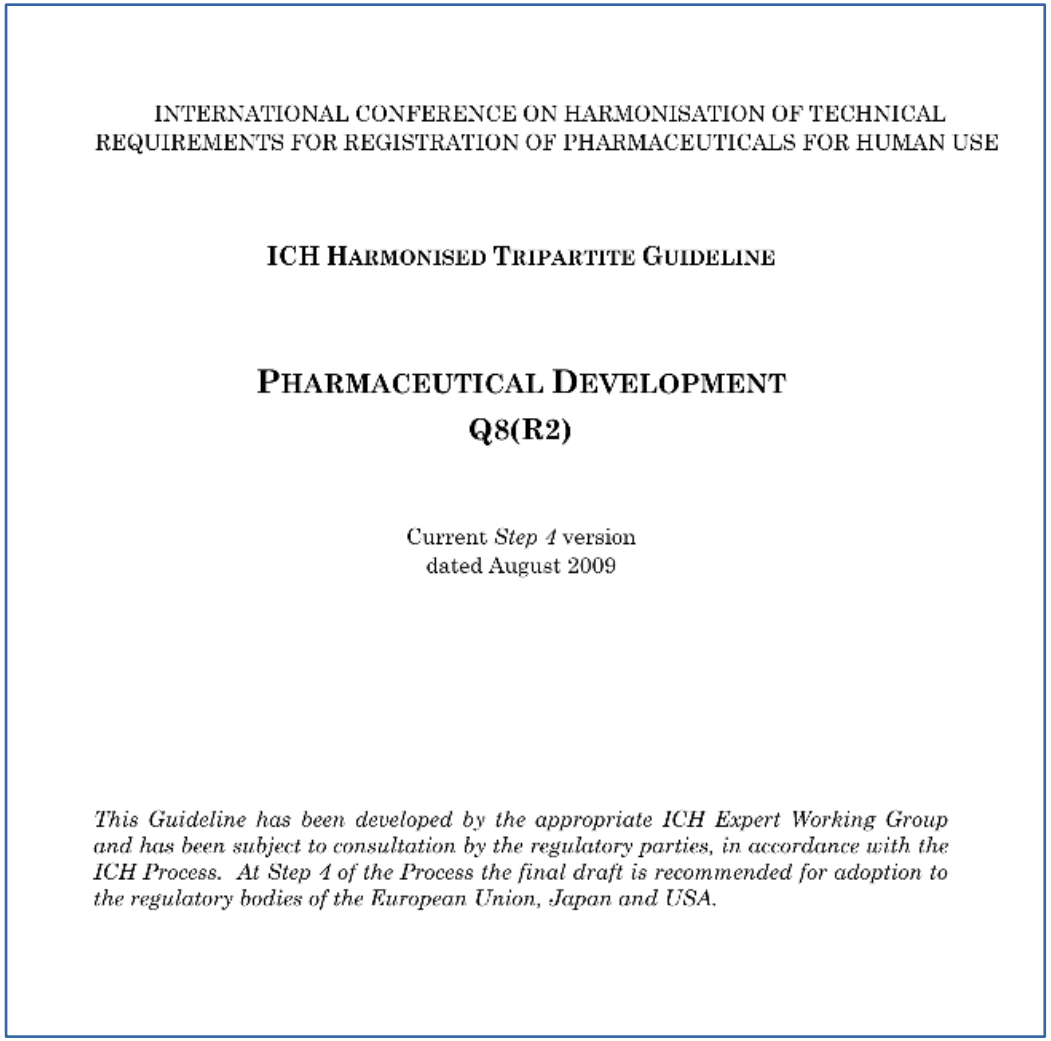
AI/ML in pharmaceutical applications | Development

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



AI/ML in pharmaceutical applications | Manufacturing

- 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

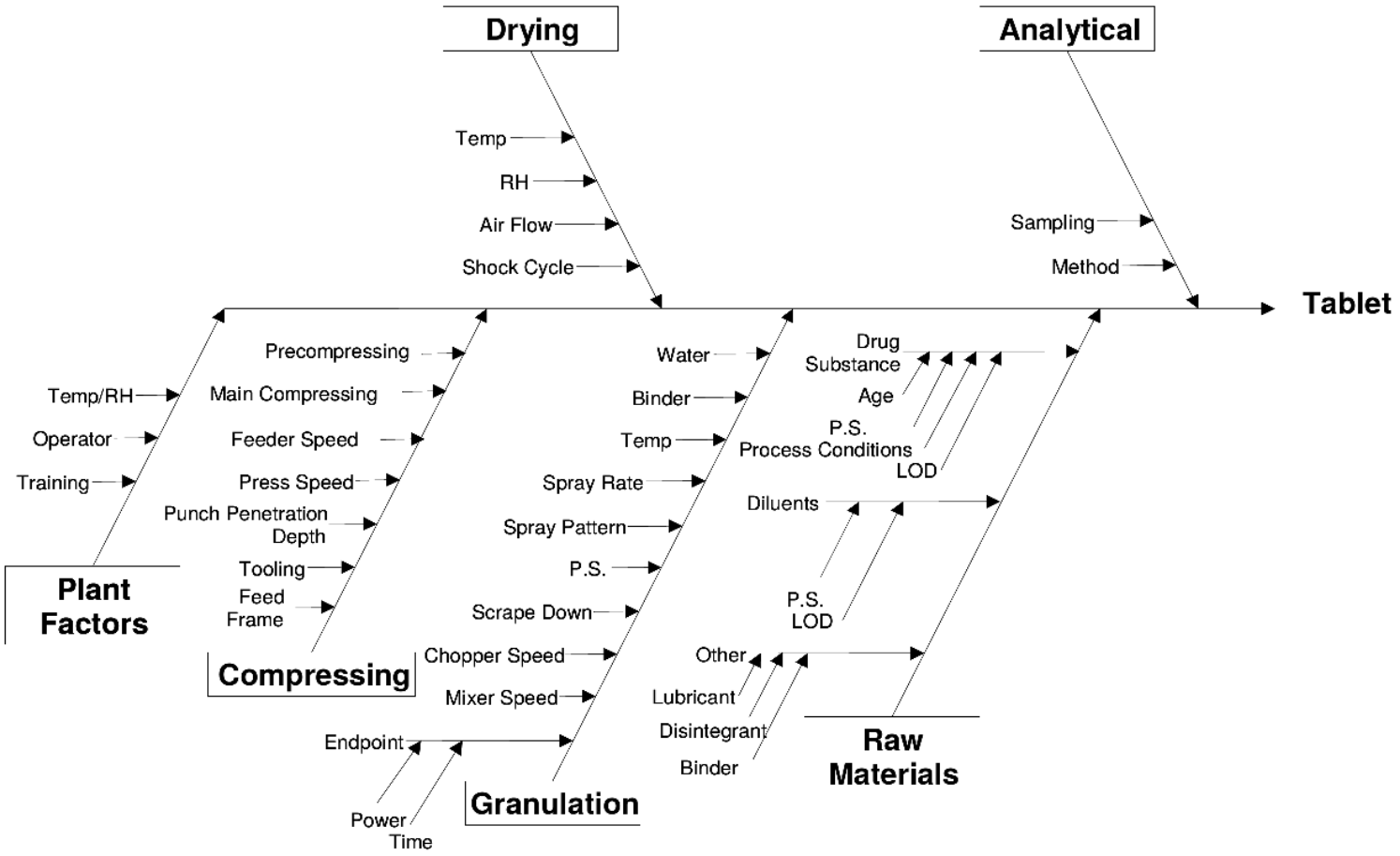
ICH HARMONISED TRIPARTITE GUIDELINE

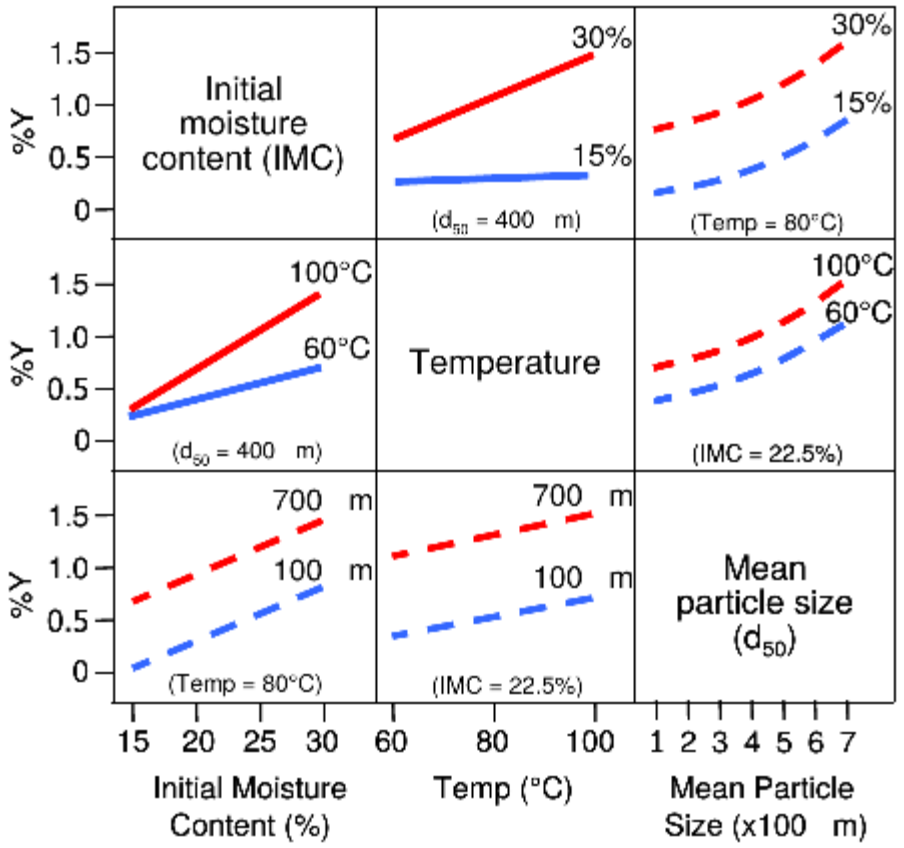
PHARMACEUTICAL DEVELOPMENT
Q8(R2)

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.

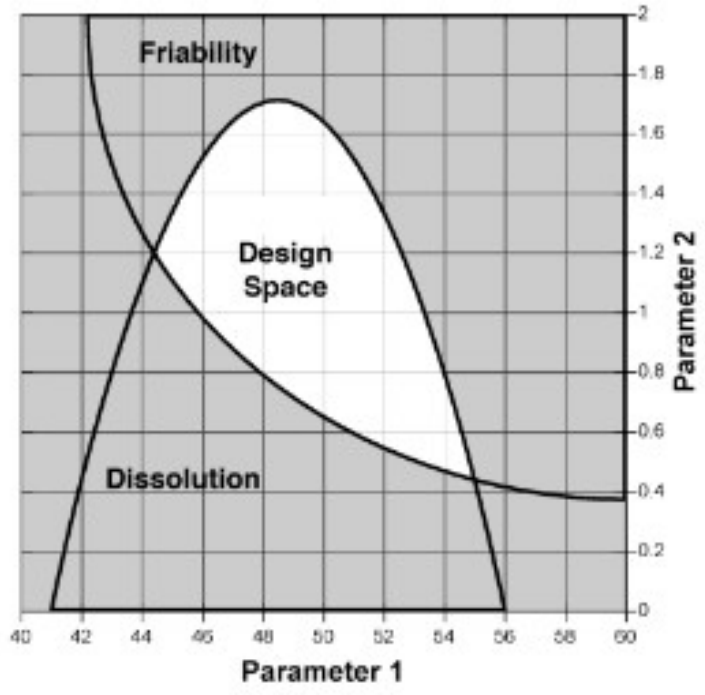
AI/ML in pharmaceutical applications | Manufacturing

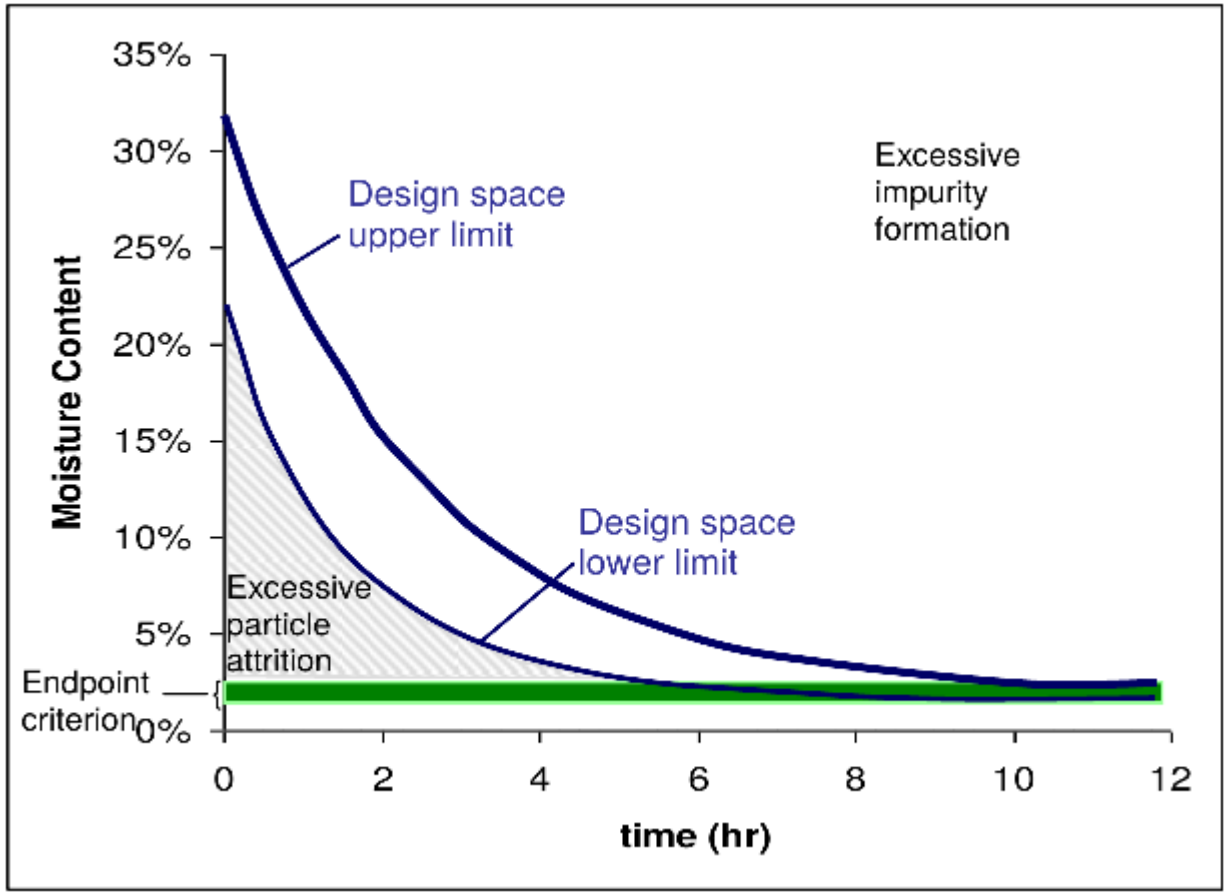




vendor&site-related: individual model required

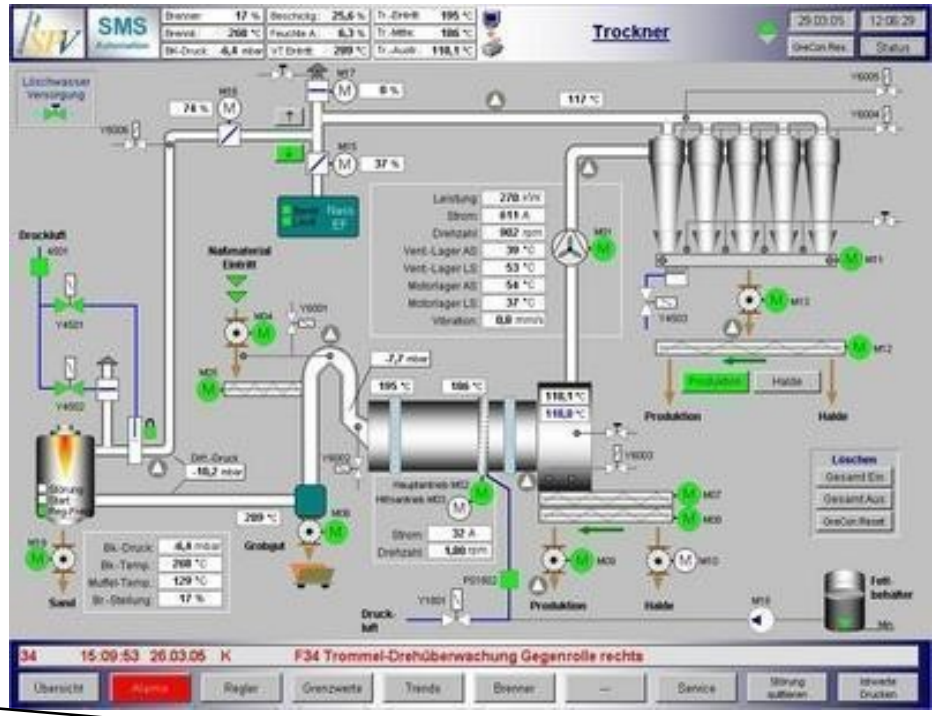
AI/ML in pharmaceutical applications | Manufacturing





Required!

AI/ML in pharmaceutical applications | Manufacturing

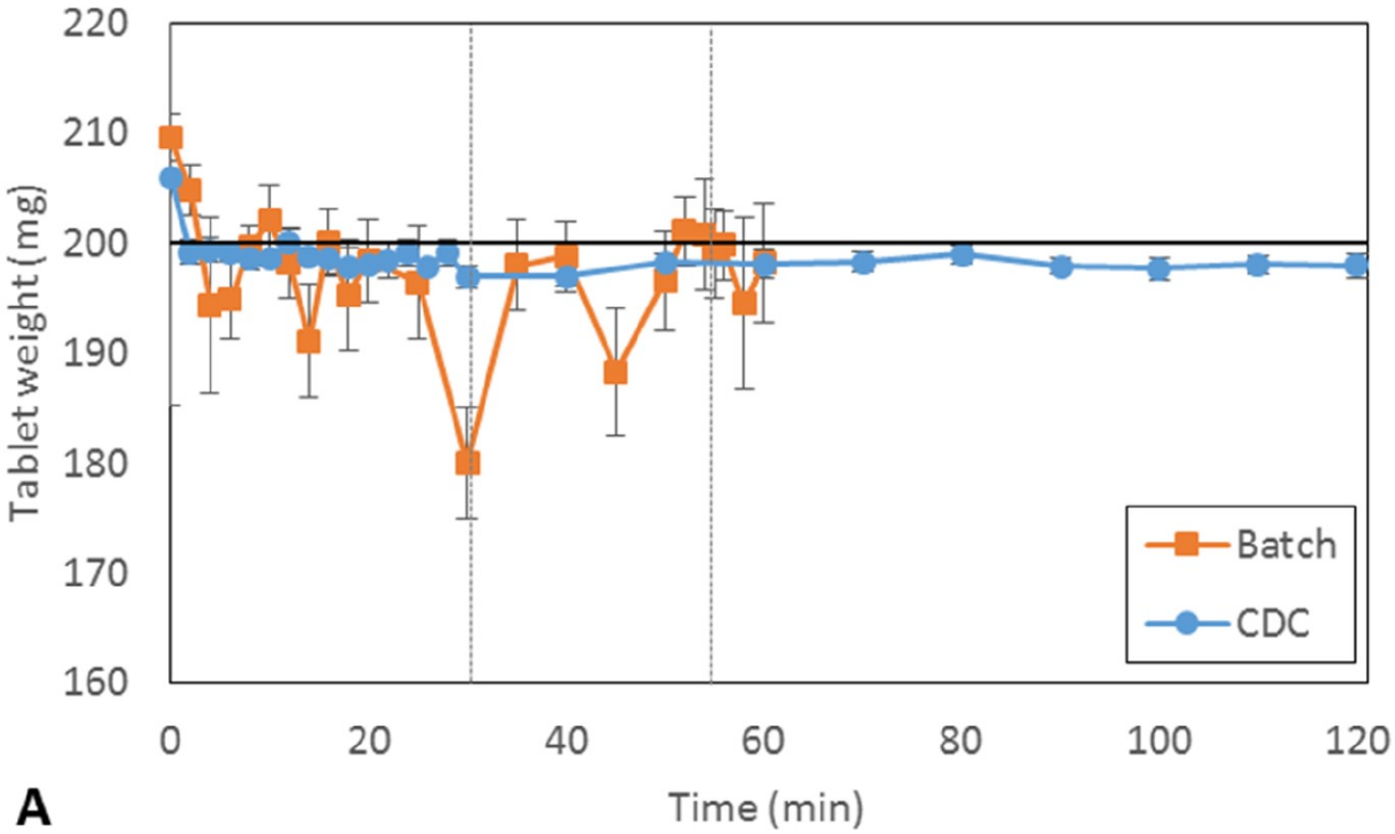


the source of data

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

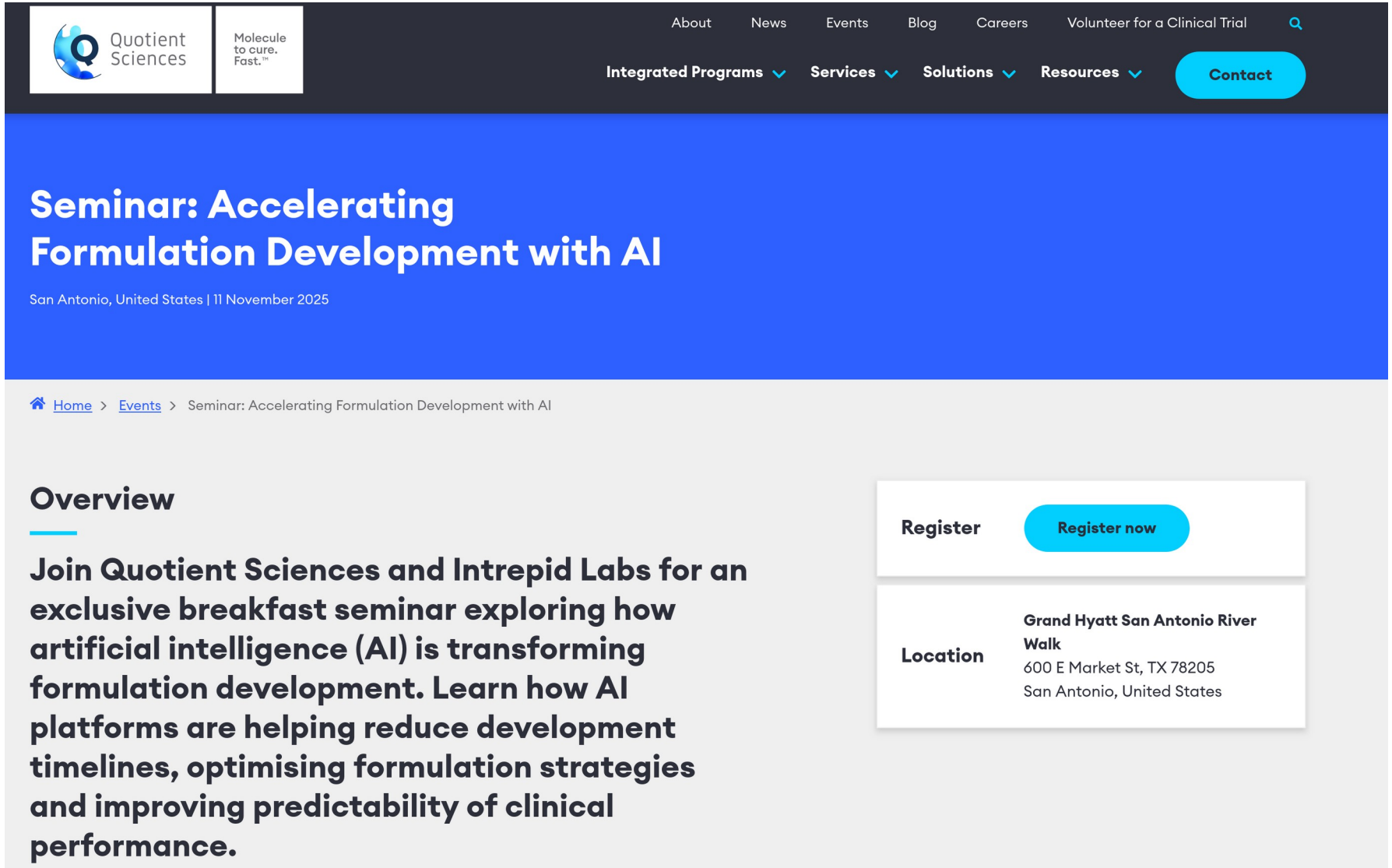
AI/ML in pharmaceutical applications | Manufacturing

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



https://www.quotientsciences.com/events/seminar-accelerating-formulation-development-ai

- active learning
- tailored models
- AI-based platform

AI/ML in pharmaceutical applications | Regulatory

CENTER FOR DRUG EVALUATION AND RESEARCH

FY 2024

GDUFA SCIENCE AND RESEARCH REPORT

Generic drugs

AI/ML in pharmaceutical applications | Regulatory

CENTER FOR DRUG EVALUATION AND RESEARCH

FY 2024
GDUFA SCIENCE AND RESEARCH REPORT

Generic drugs

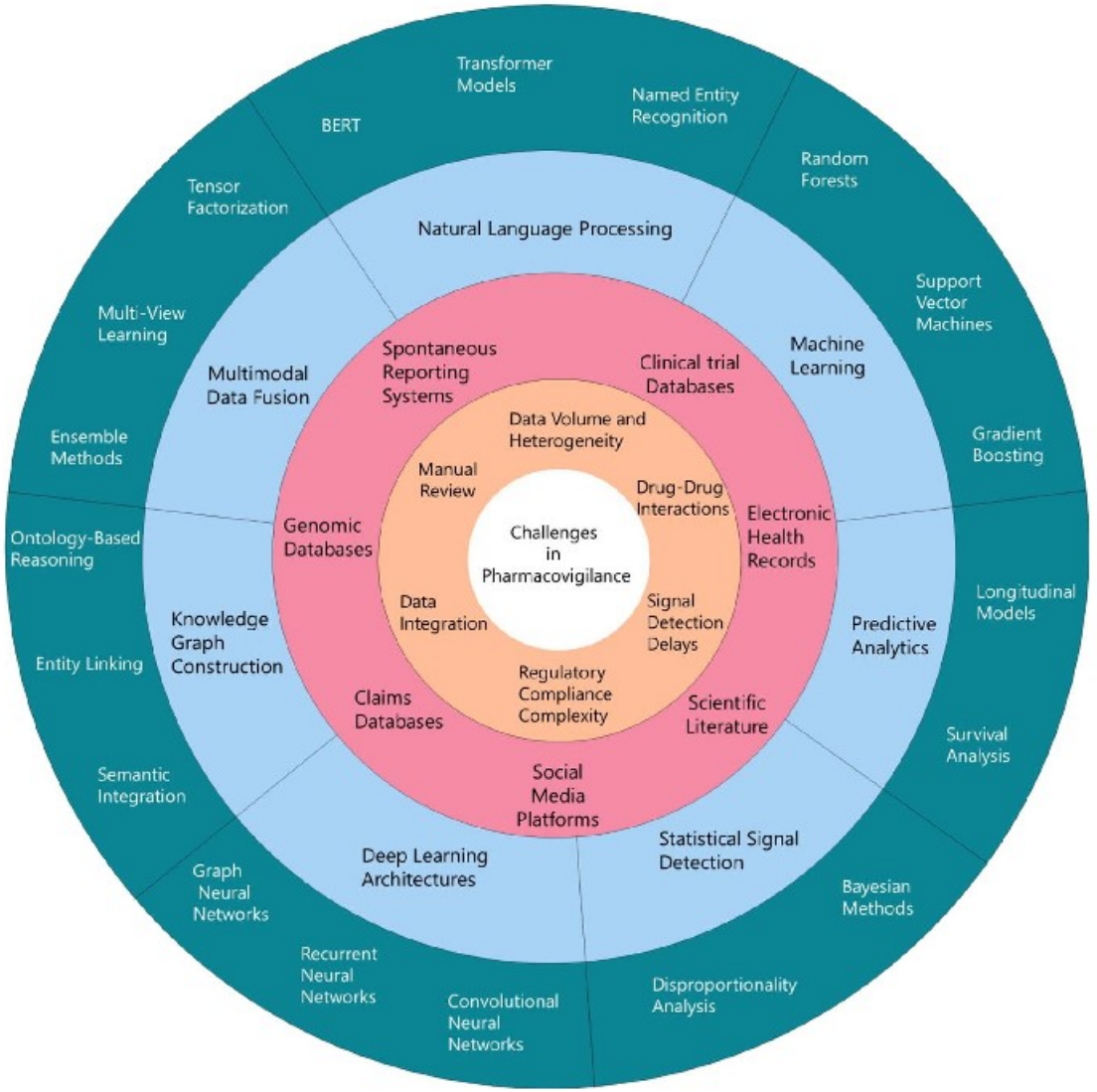
ChatGPT to support the development of PSGs. In a proof-of-concept study, ChatGPT was employed to generate a summary of food effect information by analyzing publicly available new drug application (NDA) review documents available at Drugs@FDA. This study serves as an important milestone in exploring the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

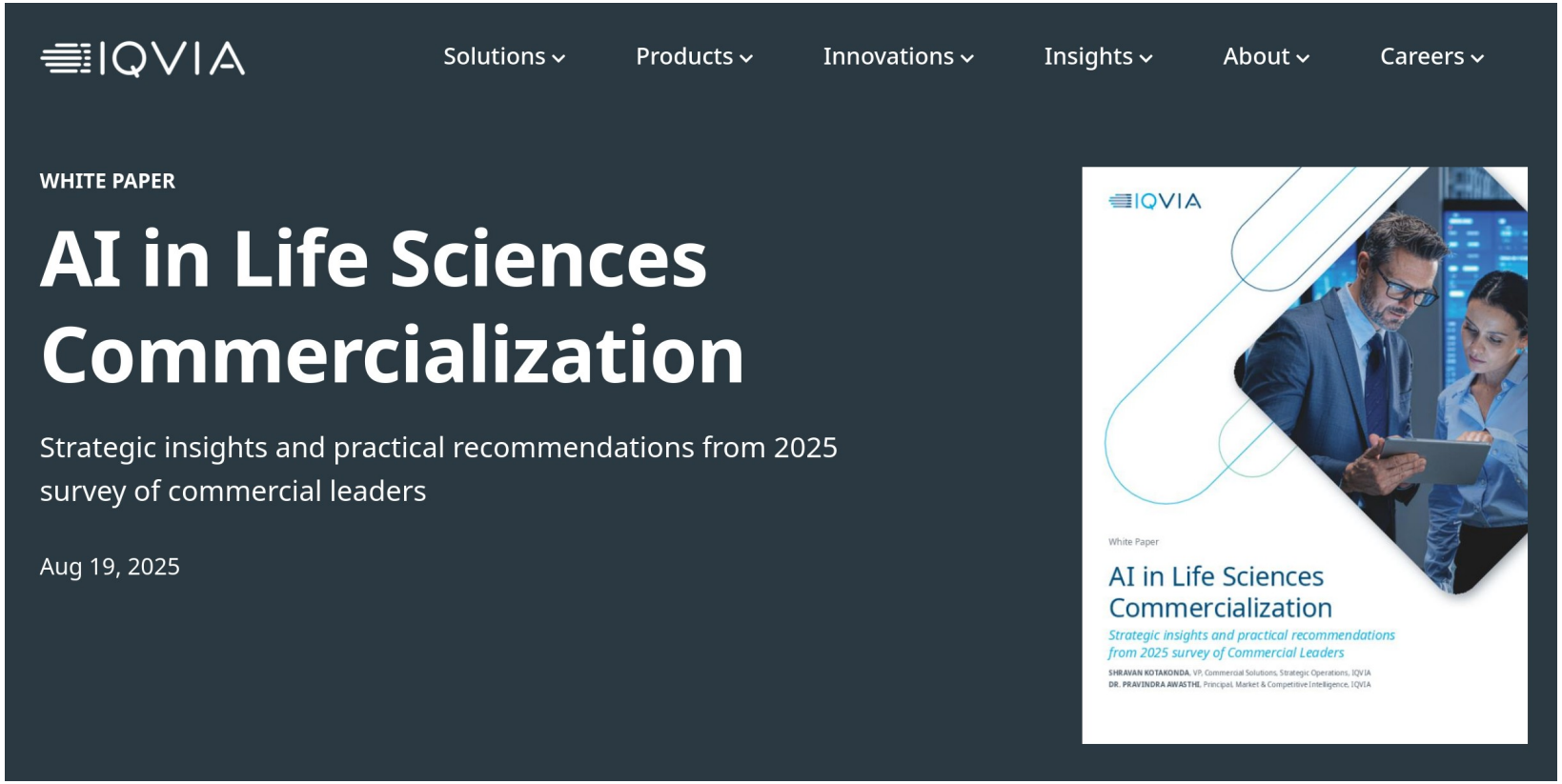
https://doi.org/10.1177/20420986251361435

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.



https://www.iqvia.com

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