Artificial intelligence in pharmacy ecosystems: opportunities and challenges for Iran

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PHARMD PHD

TABRIZ UNIVERSITY OF MEDICAL SCIENCES

دانشگاه علوم پزشکی
و خدمات بهداشتی درمانی تبریز

To be discussed

Computational drug discovery and development

VS

Pharmacointeligence

What is not new

Computational Drug Discovery and Development

Europe PMC Funders Group
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110 Years of the Meyer–Overton Rule: Predicting Membrane Permeability of Gases and Other Small Compounds

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Abstract

The transport of gaseous compounds across biological membranes is essential in all forms of life. Although it was generally accepted that gases freely penetrate the lipid matrix of biological membranes, a number of studies challenged this doctrine as they found biological membranes to have extremely low gas-permeability values. These observations led to the identification of several membrane-embedded “gas” channels, which facilitate the transport of biological active gases, such as carbon dioxide, nitric oxide, and ammonia. However, some of these findings are in contrast to the well-established solubility–diffusion model (also known as the Meyer–Overton rule), which predicts membrane permeabilities from the molecule's oil–water partition coefficient. Herein, we discuss recently reported violations of the Meyer–Overton rule for small molecules, including carboxylic acids and gases, and show that Meyer and Overton continue to rule.

Keywords

electrochemical microscopy; gas transport; membranes; Meyer–Overtone rule; unstirred layers

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1. Introduction

110 years ago, Meyer and Overton established a simple rule to predict membrane permeabilities.[1,2] This rule does not account for transport processes, mediated by membrane carriers, channels or pumps, which were not known at that time, and it ignores inhomogeneities, such as rafts,[3] which may exist in the biological membrane. The rule works fine for all molecules that merely cross the lipid matrix by simple diffusion.

According to this rule, the transmembrane flux density, J, of a membrane-permeating molecule can be predicted if its partition coefficient, K_p, from the aqueous phase into the organic phase, is known. Therefore, Fick's law of diffusion has to be rewritten as Equation (1) (compare also Figure 1):

$$J=-D_M\frac{dc_m}{dx}=-D_M\frac{c_{1m}-c_{2m}}{d}$$
$$J=P_M(c_{2w}-c_{1w}) \quad \text{with} \quad P_M\equiv\frac{K_pD_M}{d} \qquad (1)$$

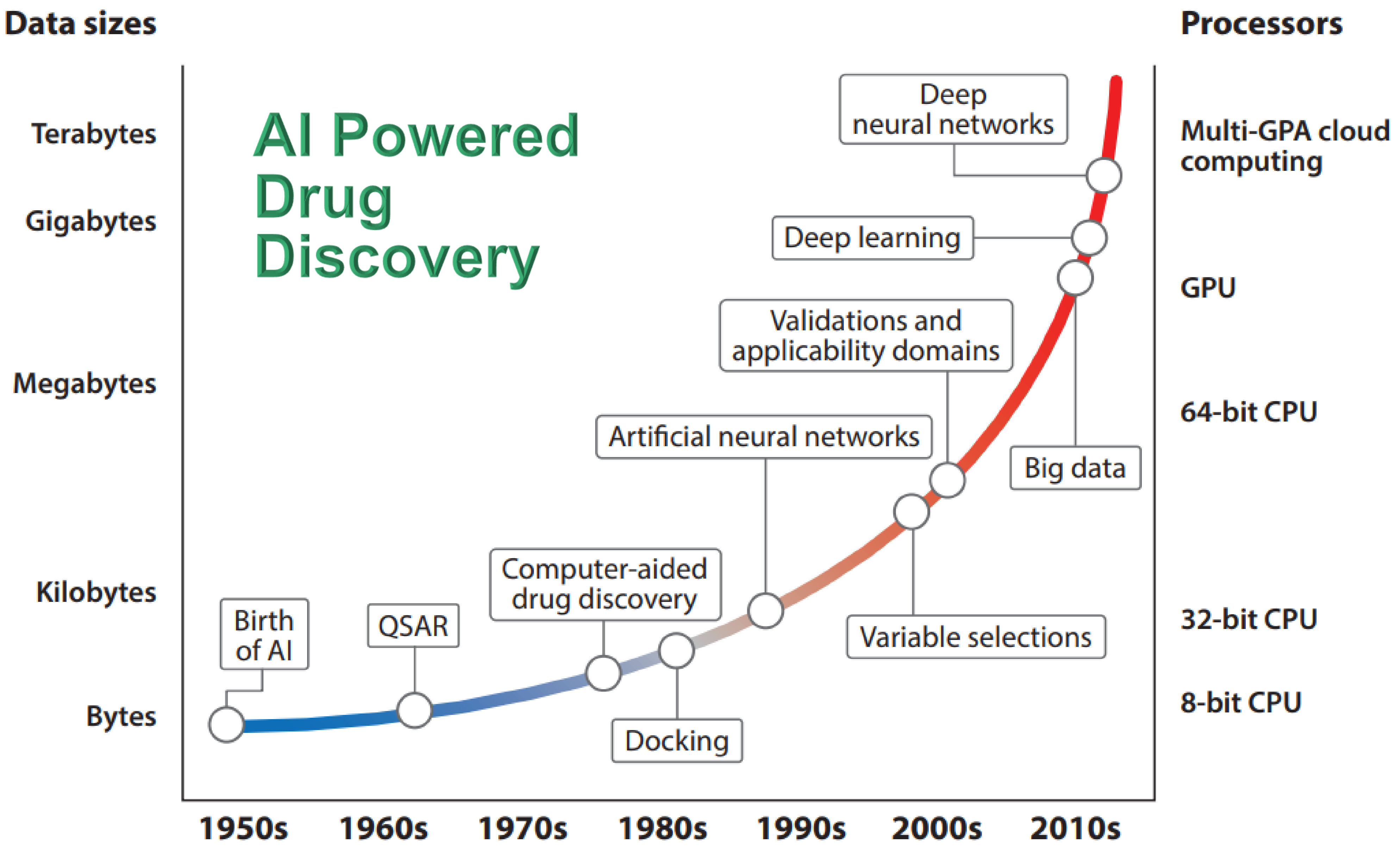
where D_M, c_{1m}, c_{2m}, c_{1w}, c_{2w}, x, and d are the diffusivity within the organic phase, the concentration of the permeating molecule within the membrane at the first and second interfaces—and their aqueous concentrations at the first and second interfaces—the distance from the first interface, and the membrane thickness, respectively. The term membrane permeability, P_M, is defined based on Equation (1).

What was going on in the Pharmacy faculty of Tabriz university of medical sciences

- Prediction of physicochemical properties of drugs using SVM, ANN, Classification methods etc
- Feature selection using GA based methods, clustering algorithms, etc
- Image analysis for the quantification of experimental results using CNN
- Drug effect prediction using supervised and unsupervised methods
- Drug-target interaction studies using molecular modeling methods
- Target discovery using various ML methods based on fingerprint similarity search methods
- Drug repurposing
- Solvent Design based on the combination of molecular modeling and machin learning methods
- Cryopreservation medium design (combined MD and ML)
- Biomaterial design
- Formulation Design
- Integration of chemometrics with biological evaluations
- Fine tuning and Rag of LLMs for the database generation

Using MATLAB, Knime, Python

But not based on a systematic strategic planning


Data sizes
Processors
AI Powered Drug Discovery
Terabytes
Gigabytes
Megabytes
Kilobytes
Bytes
Multi-GPA cloud computing
GPU
64-bit CPU
32-bit CPU
8-bit CPU
Deep neural networks
Deep learning
Validations and applicability domains
Artificial neural networks
Big data
Computer-aided drug discovery
Birth of AI
QSAR
Variable selections
Docking
1950s
1960s
1970s
1980s
1990s
2000s
2010s

What's not new and whats new?

Era	Key Technologies	Before (What We Had)	After (What Is New or Improved)
Pre-2000s	- Basic computational tools	- Manual drug discovery and design (e.g., trial-and-error methods).	- Early computational chemistry tools (e.g., molecular modeling).
	- Early QSAR models	- Limited data storage and processing capabilities.	- Basic predictive models for drug properties (e.g., solubility, toxicity).
		- Paper-based clinical trial records and regulatory submissions.	- Early electronic data capture (EDC) systems for clinical trials.

What's not new and whats new?

Era	Key Technologies	Before (What We Had)	After (What Is New or Improved)
2000s–2010s	- High-performance computing (HPC)	- Reliance on small datasets and limited computational power.	- HPC enabled faster molecular simulations and virtual screening.
	- Early machine learning (ML)	- Manual analysis of adverse events and pharmacovigilance data.	- ML models for predicting drug-target interactions and ADME properties.
	- Electronic Health Records (EHRs)	- Limited patient data integration for personalized medicine.	- EHRs enabled better patient data management and analysis.
		- Manual quality control in drug manufacturing.	- Early automation in manufacturing (e.g., robotic dispensing).

What's not new and whats new?

Era	Key Technologies	Before (What We Had)	After (What Is New or Improved)
2010s–2020s	- Cloud computing	- On-premise data storage and limited scalability.	- Cloud computing enabled real-time data sharing, collaboration, and scalable analytics.
	- IoT and sensors	- Manual monitoring of manufacturing processes and supply chains.	- IoT enabled real-time monitoring of production lines and supply chain logistics.
	- Advanced ML and deep learning	- Limited ability to analyze unstructured data (e.g., scientific literature, social media).	- Deep learning models improved image analysis (e.g., defect detection) and NLP for literature mining.
		- Limited transparency in drug supply chains.	- Early blockchain pilots for supply chain traceability.

What's not new and whats new?

Era	Key Technologies	Before (What We Had)	After (What Is New or Improved)
2020s–Present	- Large Language Models (LLMs)	- Manual literature reviews and regulatory document preparation.	- LLMs automate literature analysis, regulatory submissions, and patient communication.
	- Blockchain and smart contracts	- Limited data security and traceability in clinical trials and supply chains.	- Blockchain ensures tamper-proof records for clinical trials, supply chains, and compliance.
	- Quantum computing (early stages)	- Limited ability to solve complex molecular simulations.	- Quantum computing promises breakthroughs in molecular modeling and drug discovery.
	- Edge computing	- Centralized data processing with latency issues.	- Edge computing enables real-time data processing at the source (e.g., IoT devices in manufacturing).
	- Generative AI	- Limited ability to generate novel drug candidates.	- Generative AI designs new molecules and optimizes drug formulations.
	- Digital twins	- Limited ability to simulate and optimize manufacturing processes.	- Digital twins enable virtual simulations of production lines for optimization.

Already AI leads to?

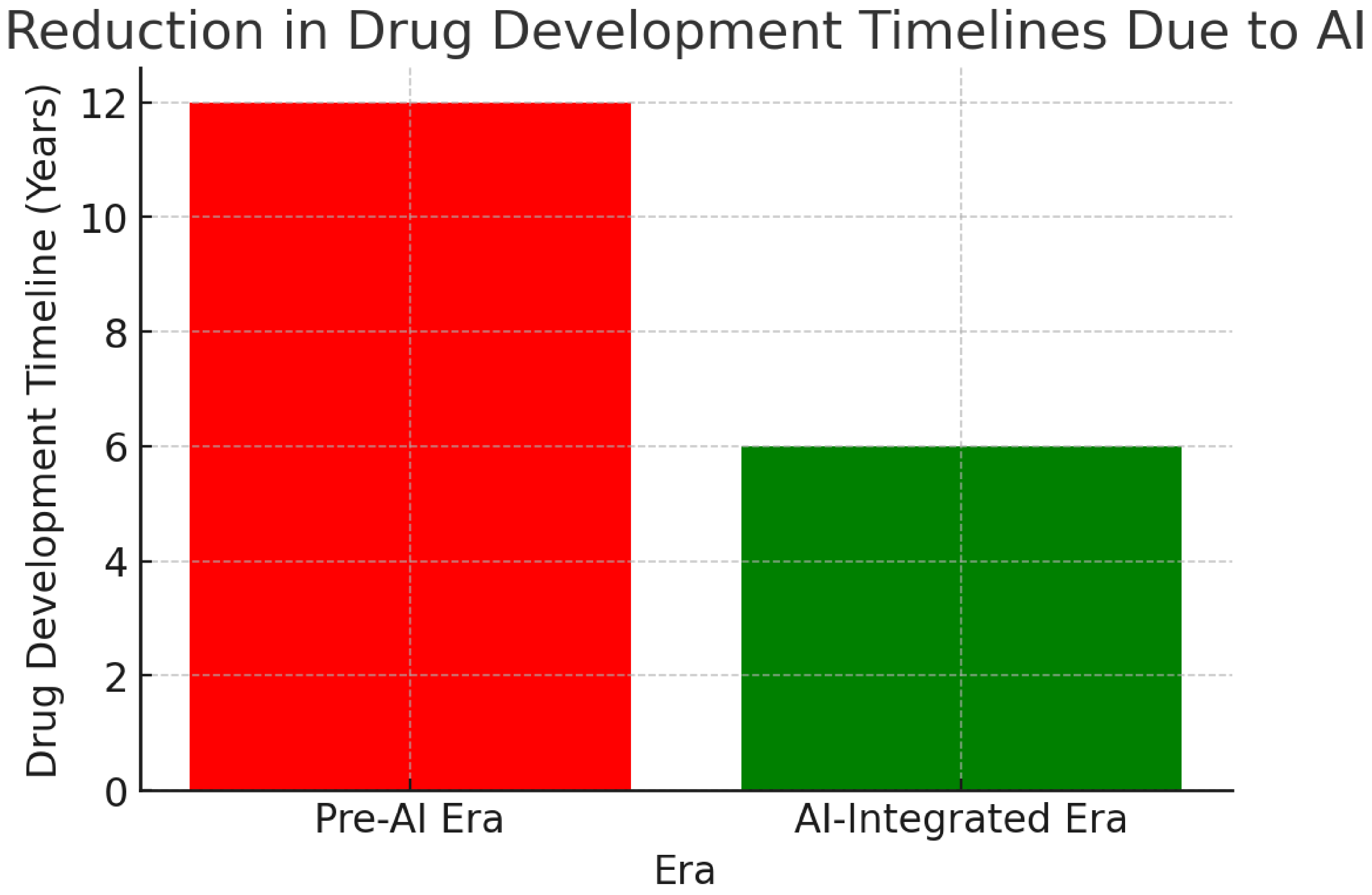
Faster drug development!

This happens because of the nature of the drug discovery!

Drug discovery is a learning process rather than a making process!

*****AI learns faster than human?*****

Why?


Reduction in Drug Development Timelines Due to AI
Drug Development Timeline (Years)
12
10
8
6
4
2
0
Pre-AI Era
AI-Integrated Era
Era

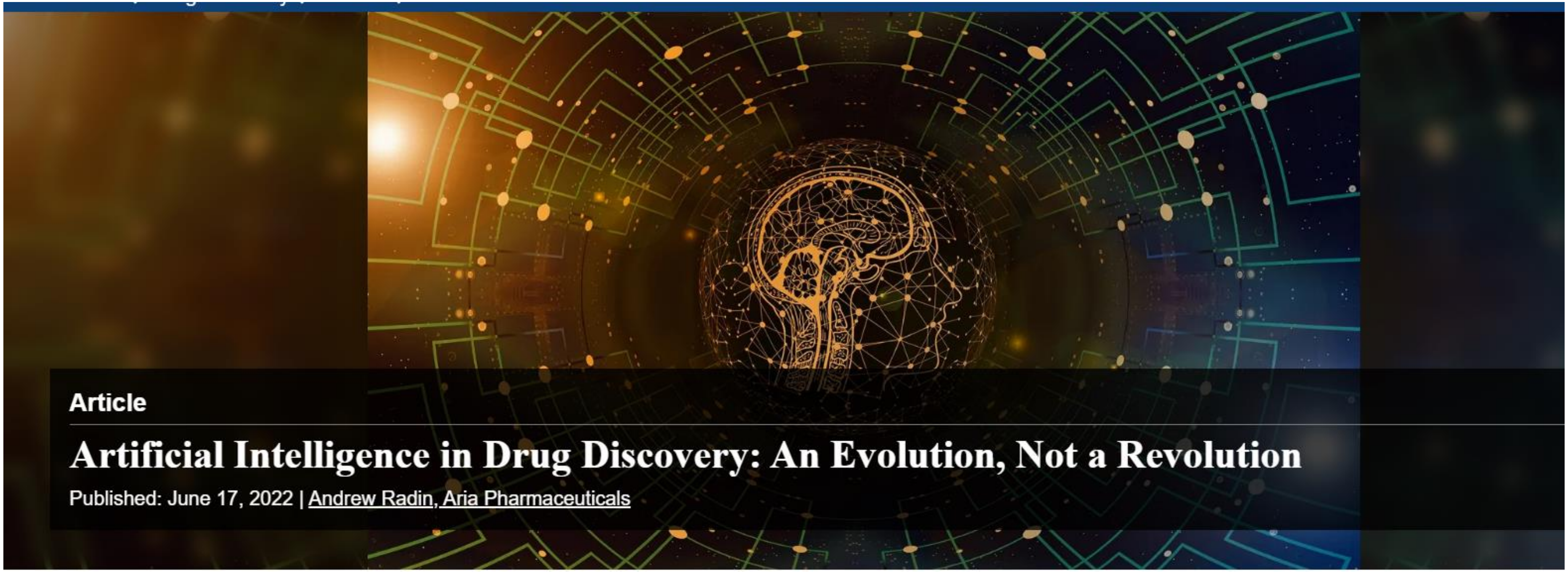
deepseek

AI learns faster than human!

Aspect	DeepSeek-V3	GPT (e.g., GPT-4)	Humans
Speed of Learning	Can process and learn from massive datasets in seconds or minutes.	Similar to DeepSeek-V3; learns quickly from large datasets.	Learning is slower, as it requires time to read, understand, and practice.
Retention	Instantly retains information without forgetting (unless data is overwritten).	Same as DeepSeek-V3; retains information perfectly unless retrained.	May forget information over time without reinforcement.
Scalability	Can learn from billions of data points simultaneously.	Same as DeepSeek-V3; highly scalable with large datasets.	Limited by cognitive capacity and focus.
Contextual Understanding	Struggles with nuanced or abstract concepts without explicit training.	Better than DeepSeek-V3 at understanding context but still limited.	Excels at understanding context, emotions, and abstract ideas.
Adaptability	Requires retraining or updates to adapt to new information.	Similar to DeepSeek-V3; requires updates for new knowledge.	Can adapt and learn dynamically from real-world experiences.

AI learns faster than human!

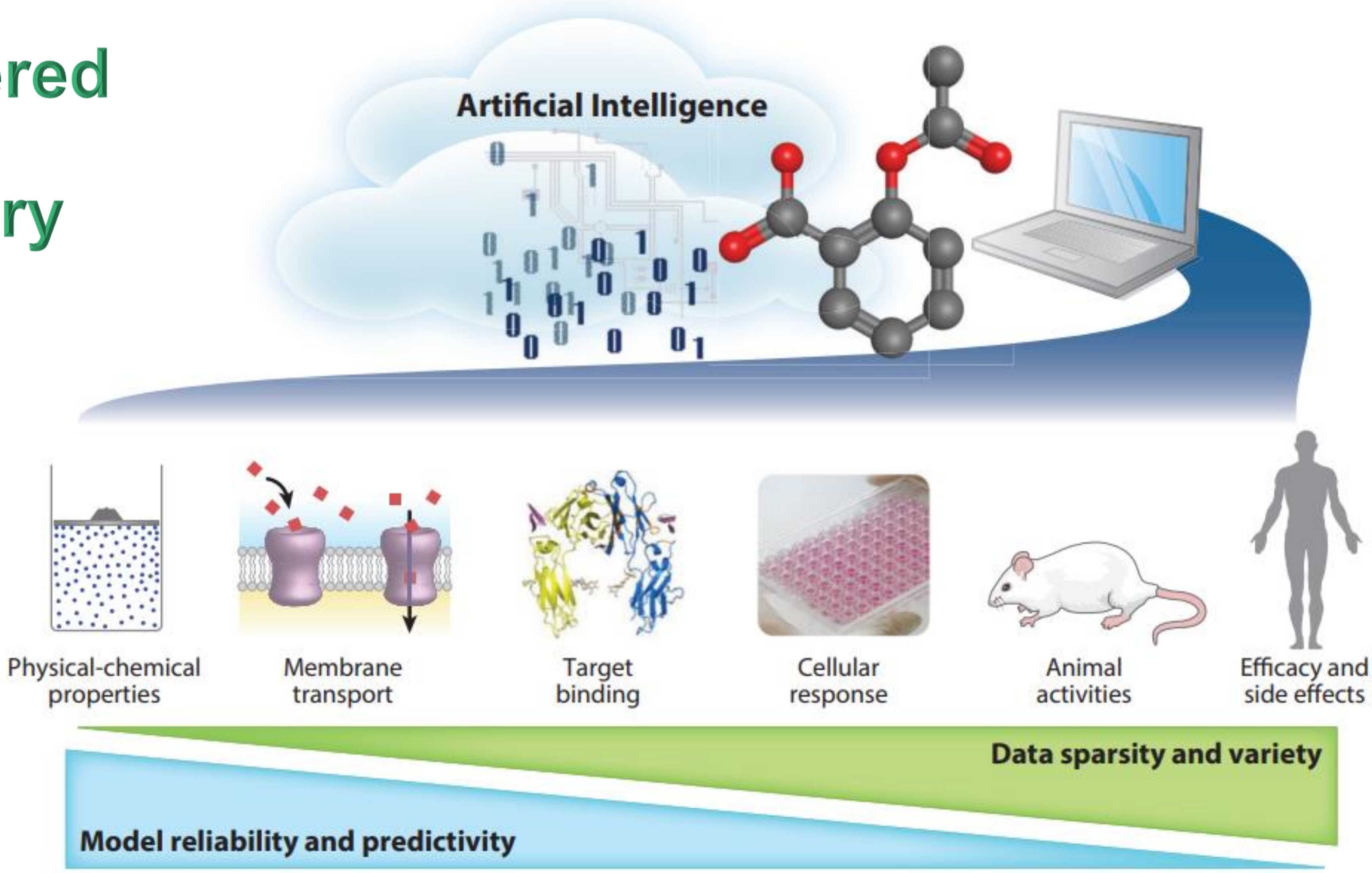
Aspect	DeepSeek-V3	GPT (e.g., GPT-4)	Humans
Energy Efficiency	Requires significant computational resources for training.	Similar to DeepSeek-V3; computationally intensive.	Learns efficiently with minimal energy compared to AI systems.
Creativity	Limited to patterns in training data; struggles with true creativity.	More creative than DeepSeek-V3 but still bound by training data.	Highly creative, capable of original thought and innovation.
Real-Time Learning	Cannot learn in real-time; requires retraining.	Same as DeepSeek-V3; no real-time learning capability.	Can learn and adapt in real-time from experiences.
Emotional Intelligence	Lacks emotional understanding and empathy.	Simulates empathy but lacks genuine emotional intelligence.	Excels at emotional understanding and empathy.
Generalization	Performs well within trained domains but struggles with unfamiliar tasks.	Better at generalization than DeepSeek-V3 but still limited.	Can generalize knowledge across diverse and unfamiliar situations.


Article

Artificial Intelligence in Drug Discovery: An Evolution, Not a Revolution

Published: June 17, 2022 | Andrew Radin, Aria Pharmaceuticals

AI Powered Drug Discovery



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REVIEWS

ELSEVIER

Artificial intelligence in drug discovery: what is realistic, what are illusions? Part 1: Ways to make an impact, and why we are not there yet

Reviews • INFORMATICS

Andreas Bender[1,2] and Isidro Cortés-Ciriano[3]

Ligand or Drug?

Applications of AI in Pharmacy

- ✓ **Clinical Pharmacy Practice**
- ✓ **Community Pharmacy Practice**
- ✓ **Pharmacy Education and Research**
- ✓ **Drug Discovery and Development**

World 2: uphill battle for autonomy—AI as a double-edged sword

In stark contrast, the second world portrays a dystopian reality where pharmacists find themselves grappling with systemic challenges that hinder their professional autonomy. Despite technological advancements elsewhere, pharmacists are burdened by archaic regulations, administrative red tape, and a lack of recognition for their expertise. The promise of provider status remains elusive, as pharmacists are relegated to the periphery of patient care teams.

The aftermath of the DIR fee apocalypse has left pharmacies grappling with closures, unable to adapt to the seismic shifts in the healthcare landscape. Vertical integration, driven by AI, robotics, and drone delivery, has paved the way for corporate giants to dominate dispensing. Pharmacists and technicians, once pillars of patient care, are now relegated to the sidelines, merely performing prescription verifications duties in the few states where that final human check is still required by law.

AI, a tool that could have empowered pharmacists, has paradoxically become a force that displaced them. The relentless march of technology has left many pharmacists seeking refuge in niche roles around AI at large corporations, leveraging their unique knowledge of gene therapies, precision medicine, 3D printing, and digital therapeutics. Others have ventured into entirely different industries. The resilient rebels, akin to dwindling bookstores of the early 00's, struggle on, but hope for a resurgence remains elusive. The autonomy pharmacists once enjoyed has been eroded, overshadowed by the pervasive influence of AI-driven corporate medication fulfillment.

As we peer into these two contrasting worlds of pharmacy practice in 2037, we are confronted with the stark reality that

fession at the forefront of patient care, actively shaping the future of health care in America.

Conversely, the second world serves as a cautionary tale, reminding us of the perils of complacency and resistance to change. The uphill battle for autonomy and recognition in this dystopian reality underscores the importance of advocacy, innovation, and a collective commitment to advancing the profession.

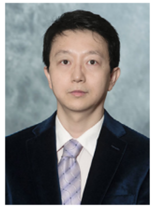
The choice is ours. Will we engage with AI to usher in a future where pharmacists play a central role in health care, or will we allow outdated systems and inertia to consign us to a reality where the potential of pharmacy remains untapped? The answer lies in our actions today, as we lay the foundation for pharmacy practice in 2037 and beyond.

Samm Anderegg, PharmD, MS, Chief Executive Officer, DocStation, Austin, TX, E-mail: samm@docstation.co.

Role of artificial intelligence in pharmaceutical health care

APhA—APRS

Artificial Intelligence (AI) is a branch of science that focuses on the development of intelligent computer programs capable of mimicking human cognitive processes.[1] It leverages this technology to conduct more precise analyses and achieve meaningful interpretations. From this viewpoint, AI integrates a range of statistical models and computational intelligence techniques.



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education and pharmaceutical research. However, there are some key challenges that need to be addressed with AI in terms of possible opportunities and application of AI in these various areas. For instance, how to use AI in small data sets such as primary data while ensure data quality, how to ensure accurate AI estimates and prediction in socially disadvantaged populations, and how it can help and enhance pharmacists' daily practice more efficiently.

Advanced AI technologies are poised to revolutionize clinical pharmacy practice, seamlessly integrating, and enhancing pharmacists' roles in health care teams, particularly in hospital settings.[3] These AI-driven platforms facilitate real-time communication between pharmacists and clinicians, providing updates on patient medications, potential drug-drug interactions, and dosage recommendations based on integrated patient data. This elevates the role of pharmacists in ensuring patient safety and therapeutic effectiveness. AI's ability to process vast patient data and clinical guidelines aids in recommending suitable drug therapies and dosages.[4] AI also contributes significantly to quality improvement by identifying patterns in medication errors and adverse reactions, thereby informing quality improvement strategies.[5]

Additionally, AI is set to transform community pharmacy practice, significantly impacting areas beyond primary responsibilities of pharmacists. First, AI significantly improves supply chain management in pharmacy. It employs algorithms to analyze extensive data, helping predict the demand for different medications and optimize inventory of pharmacies.[6] Second, AI can greatly enhance Automated Dispensing Systems (ADS) in pharmacies by increasing accuracy and precision in dispensing medications, learning from past errors, and utilizing machine learning algorithms for

Challenges in AI Integration

- **Data Quality and Availability:**
  - AI methods require large, high-quality datasets; limited or inconsistent data can affect accuracy and reliability.
- **Ethical Considerations:**
  - Concerns about fairness and bias, especially if training data is unrepresentative, potentially leading to unequal treatment access.
- **Regulatory Compliance:**
  - Ensuring AI applications adhere to existing laws and regulations governing pharmacy practice to maintain patient safety and privacy.

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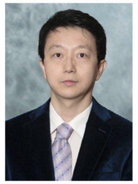

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DATA is the main player

Public data resources for the marketed drugs and their effects in human subjects

Datasets for adverse drug reactions (ADR):

DrugBank, SIDER, OFFSIDES and TWO SIDES

Datasets for Drug induced Liver Injury:

DILIrank

Data, Representation and Benchmark Platforms

Category	Database	Description	Applications
Chemical Databases	PubChem	Provides chemical structures, properties, and biological activities of small molecules.	Drug discovery, QSAR modeling, virtual screening.
	ChEMBL	A manually curated database of bioactive molecules with drug-like properties.	Predictive modeling for drug discovery and development.
	DrugBank	Comprehensive resource with detailed drug and drug target data.	Drug-target interaction prediction, drug repurposing.
	ZINC Database	A free database of commercially available compounds for virtual screening.	AI-driven drug design, virtual screening.
	BindingDB	Database of measured binding affinities for drug-target interactions.	Training datasets for molecular docking, binding prediction.
Genomic Databases	Ensembl	Genome browser providing annotated genomic data for multiple species.	Genomics-based AI model development.
	TCGA	Contains genomic and clinical data from various cancer types.	AI models in cancer research, personalized medicine.
	GTEx	Dataset of human gene expression and regulation across tissues.	AI models for transcriptomics, gene expression analysis.
Protein Databases	Human Protein Atlas	Provides information on protein expression in tissues and cells.	AI models in biomarker identification, proteomics.
	PDB	Repository of 3D structural data of proteins, nucleic acids, and complexes.	AI models for protein-ligand interaction prediction.

Data, Representation and Benchmark Platforms

Category	Database	Description	Applications
Pharmacology Databases	PharmGKB	Information on the impact of genetic variation on drug response.	Pharmacogenomics, personalized medicine AI models.
	IUPHAR/BPS Guide to Pharmacology	Detailed information on drug targets and associated pharmacological data.	AI-based target identification.
Clinical Databases	MIMIC-III/MIMIC-IV	Critical care database with de-identified health data for patients.	AI models for clinical decision support, EHR data analysis.
	ClinicalTrials.gov	Registry and results database of clinical trials.	AI-based clinical trial analysis, prediction models.
Literature Databases	PubMed	Literature database with millions of biomedical research articles.	Text-mining, NLP model development.
Pathway Databases	KEGG	Integrates information on genes, pathways, drugs, and diseases.	AI models for pathway and drug-disease association analysis.
	Open Targets	Information linking targets with diseases using evidence from genetics and omics.	Target identification, drug repurposing models.

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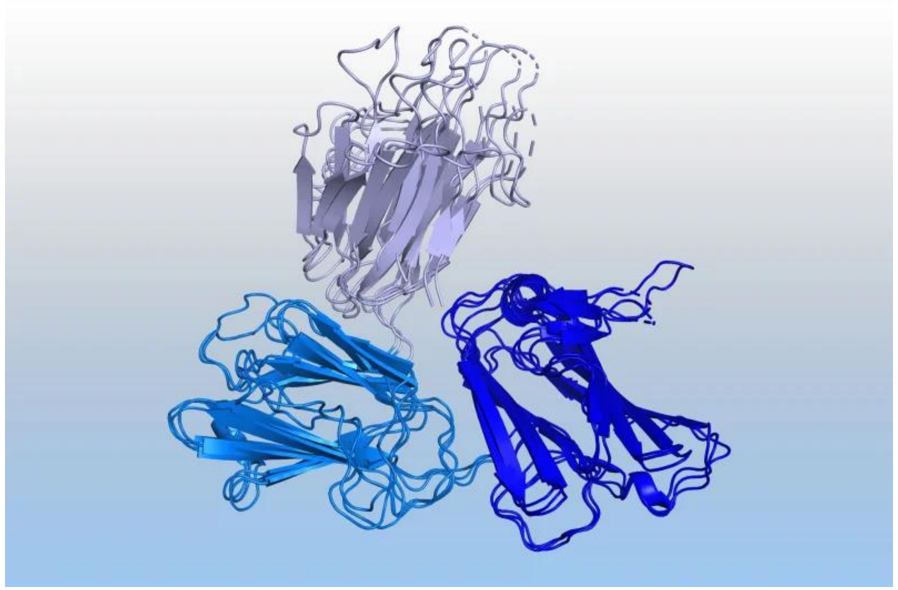
Chemical Entities Databases	CHEBI	Information on small molecules and metabolites.	AI models for metabolomics, drug design.
	PANDA	Database integrating pathway and annotation data.	AI models for pathway analysis, annotation.
Toxicology Databases	TOX21	Data on the toxicity of chemicals for AI model development.	Predictive toxicology modeling.
	ToxCast	Provides high-throughput screening data for environmental chemicals.	AI models for chemical toxicity prediction.
AI Model Training Datasets	Kaggle Datasets	A wide variety of datasets for AI research, including healthcare and pharma.	Training and testing machine learning models.
	Open ML	Collaborative platform for sharing datasets and models.	Developing AI/ML models across domains.

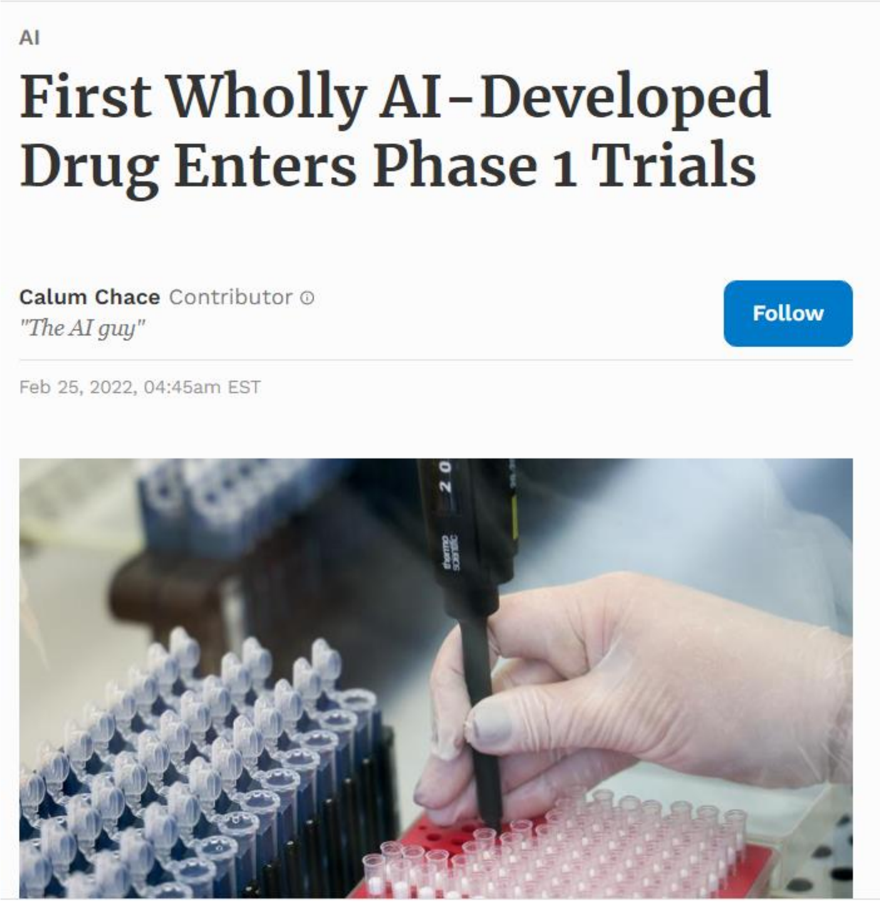
AI in complex drug discovery

Google's Deepmind AI system **AlphaFold** has found a solution to how proteins fold into their 3D structure, which may create new opportunities in structure based drug design.



Protein Pfs48/45, a crucial part of the malaria parasite that eluded scientists until DeepMind's AlphaFold was able to predict its 3D structure

ISM001 055



AI

First Wholly AI-Developed Drug Enters Phase 1 Trials

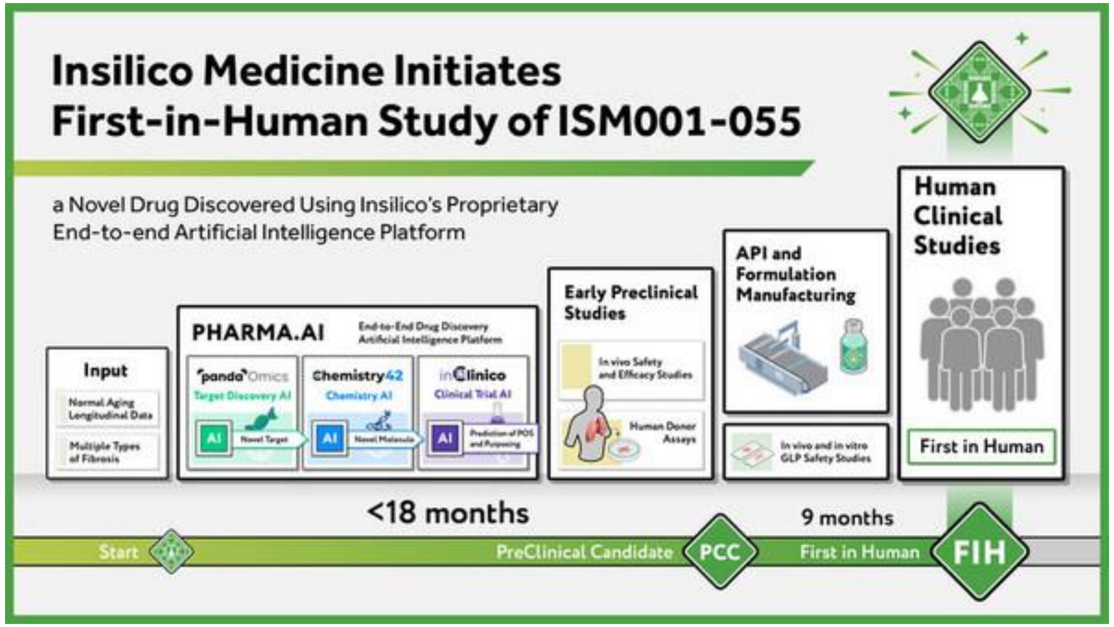
Calum Chace Contributor
"The AI guy"

Follow

Feb 25, 2022, 04:45am EST

In April of 2022, the German biotechnology company Evotec announced a phase 1 clinical trial on a new **anticancer molecule.**

The candidate was created in partnership with **Exscientia,** a company based in Oxford, UK, that applies artificial intelligence (AI) techniques to small molecule drug discovery.



AI and Automation

A robot scientist

Its name is **Adam**

Created by **Professor Ross King**

The first robot to design, perform, and interpret a series of scientific experiments leading to a new discovery.

He discovered the encoding genes of yeast enzymes

https://singularityhub.com/2010/03/16/adam the robot scientist makes its first discovery/

What Professor king is doing now?

“I will recruit a couple of postdocs, an assistant professor and 2-3 PhD students. We need people familiar with **biology** and **laboratory automation, artificial intelligence and machine learning**.

I’m also bringing **my last generation robot, Eve,** from Manchester.

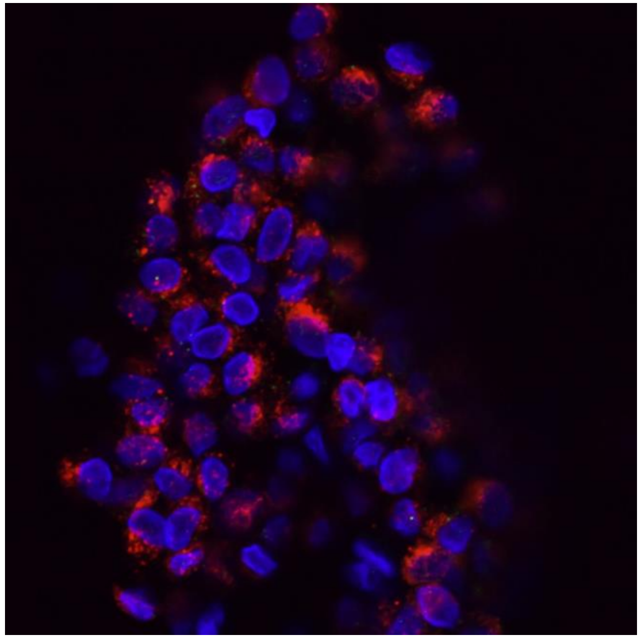
She was developed for **studying neglected tropical diseases** such as Malaria, African sleeping sickness etc.

AI and Research

By combining automated text analysis with 'Eve' – a computer/robotic system that uses AI, **researchers found that just a third of the results of a cohort of research papers in breast cancer cell biology were fully reproducible.**

"It's quite shocking how big of an issue reproducibility is in science, and it's going to need a complete overhaul in the way that a lot of science is done,"

"We think that machines have a key role to play in helping to fix it."



April 2022

https://wasp sweden.org/robot scientist eve illuminates reproducibility in breast cancer research/

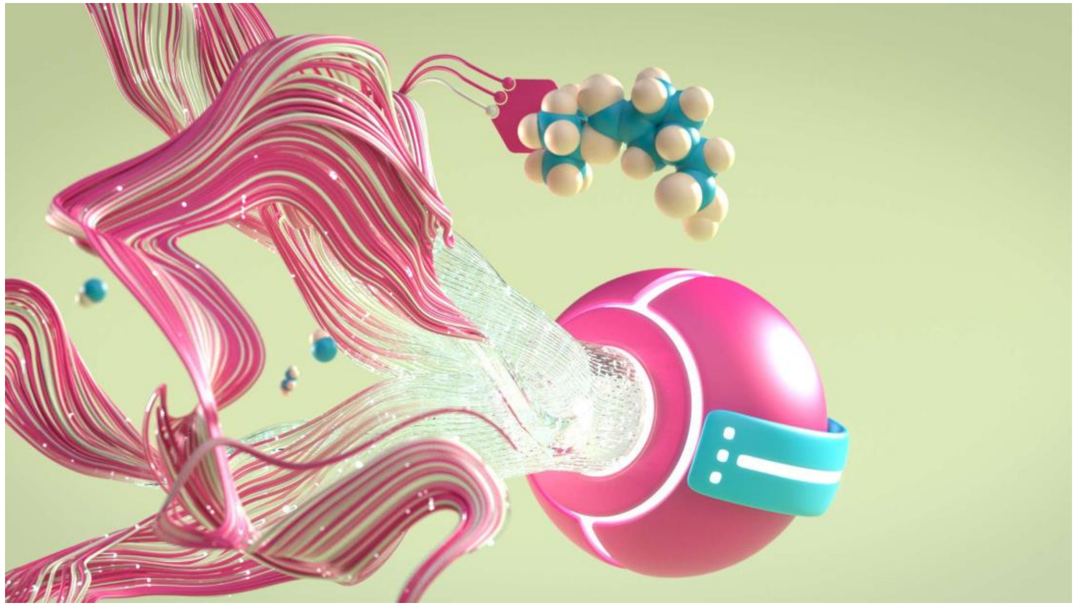
What's happening in the industry and regulatory side?

Organization	AI Integration Initiatives	Source
Novo Nordisk	Collaborating with AI startups in India to enhance drug safety data management and streamline document processing.	https://economictimes.indiatimes.com/industry/healthcare/biotech/pharmaceuticals/wegovy-maker-novo-nordisk-bets-big-on-talent-ai-partnerships-in-india/articleshow/114148019.cms?from=mdr
AION Labs	Formed by AstraZeneca, Merck KGaA, Pfizer, and Teva, in partnership with Amazon Web Services, to foster AI-driven drug discovery startups.	https://aionlabs.com/
Verily Life Sciences	Pivoting towards AI by offering tech infrastructure to support AI model and app development for healthcare companies.	https://verily.com/
U.S. Food and Drug Administration (FDA)	Recognizing the increased use of AI throughout the drug development process and across a range of therapeutic areas.	https://www.fda.gov/news-events/press-announcements/fda-proposes-framework-advance-credibility-ai-models-used-drug-and-biological-product-submissions
European Medicines Agency (EMA)	Exploring AI applications to enhance regulatory processes and improve efficiency in evaluating medicinal products.	https://www.scilife.io/

Big pharma is using AI and machine learning in drug discovery and development to save lives

While the healthcare industry is rapidly adopting digital tech, **the pharma industry is lagging on digital maturity,** and any measures **even early movers are taking** to catch up are patchworked due to a **lack of strategy** and **digital focused leadership.**

Digiceuticals!



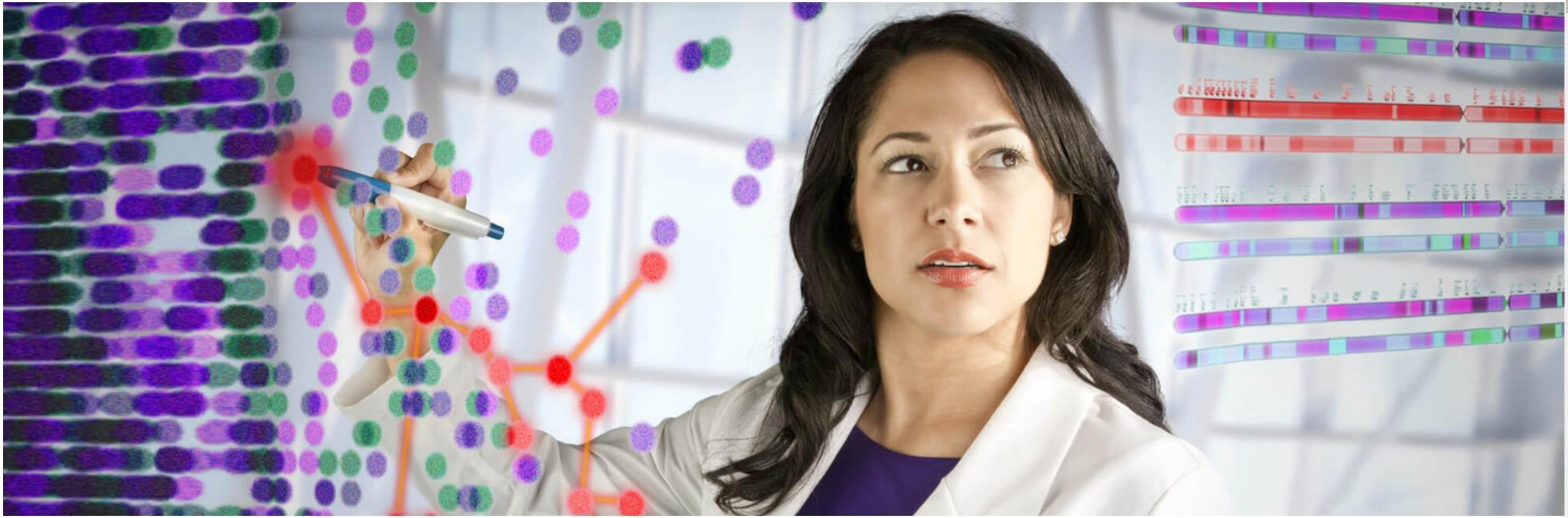
Pfizer

Documentation and regulatory

"We used to focus on **storing and searching data**," "Now we need to concentrate on **true mining of our data for recommendations**."

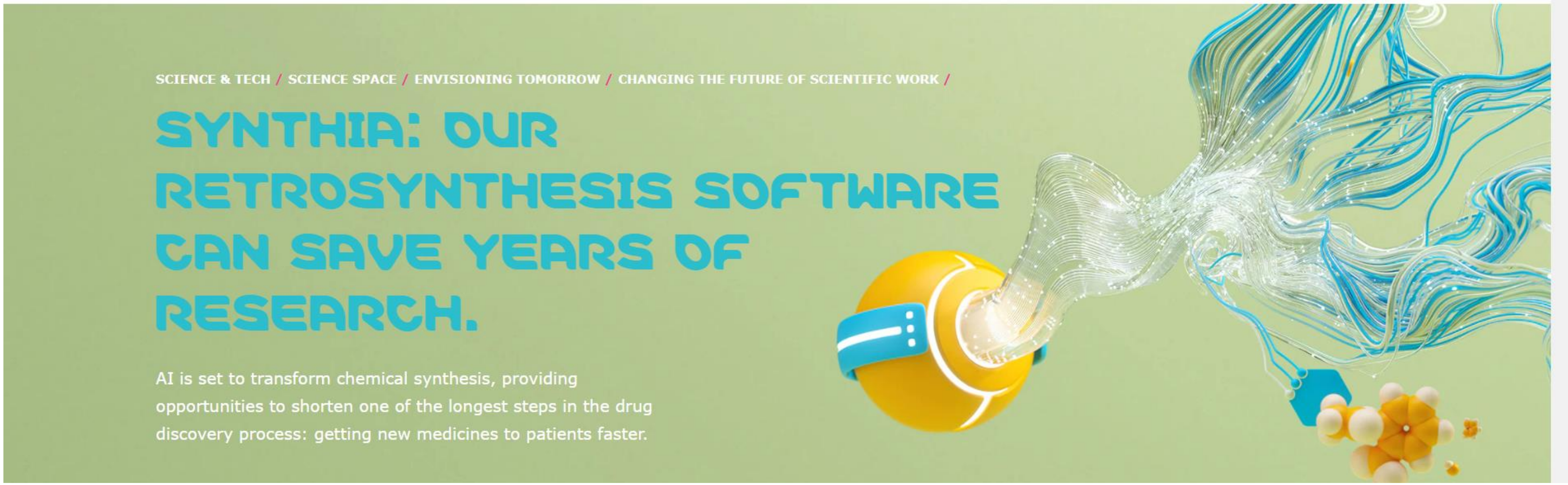
"In the future we believe that AI may help us predict what queries regulators are likely to come back with,"

Boris Braylyan



Data Doctors: How Biostatisticians Play a Critical Role in Discovering and Developing Medicine

Pfizer



MERCK

Despite decades of research this is still a long, laborious procedure – and is a key bottleneck for advancing new medicines to the clinic.

But recent advances in AI based software offer unprecedented new opportunities to help speed up this stage of drug discovery and get effective drugs to patients, faster.

Everyone is talking about artificial intelligence (AI) – in the media, at conferences and in product brochures.

Yet the technology is still in its infancy. Applications that would have been dismissed as science fiction not long ago could become reality within a

MERCK

Big pharma and AI companies collaboration

Company	Year	AI Integration Area	Initiative	Details
Pfizer	2021	Drug Discovery	Collaboration with IBM Watson	Utilized IBM Watson's AI capabilities to accelerate immuno-oncology drug discovery, enhancing the identification of promising drug candidates.
Exscientia	2021	Drug Discovery	AI-Designed Drug Development	Developed the world's first AI-designed drug, which entered clinical trials within 12 months, demonstrating AI's potential to expedite drug development timelines.
Novartis	2021	Manufacturing	AI Integration in Manufacturing	Employed AI to **optimize manufacturing processes**, enabling real-time monitoring and improving production quality.
Gilead Sciences, Novartis, Johnson & Johnson, Bristol Myers Squibb	2024	Manufacturing	CAR-T Therapy Manufacturing Optimization	Worked to reduce manufacturing turnaround times for CAR-T therapies, personalized cancer treatments, from 37 days in 2017 to approximately 14 days, with potential future reductions to around a week.
CSL	2024	Personalized Pharmacotherapy	AI Initiatives for Drug Development	Leveraged AI to expedite drug development and devise more personalized, effective treatments for serious diseases, including cancer.
AION Labs (AstraZeneca, Merck KGaA, Pfizer, Teva)	2021	Drug Discovery	AI-Powered Antibody Discovery	Launched ventures like DenovAI and TenAces Biosciences to focus on AI-powered antibody discovery and molecular glue therapies, contributing to personalized medicine advancements.

Big pharma and AI companies collaboration

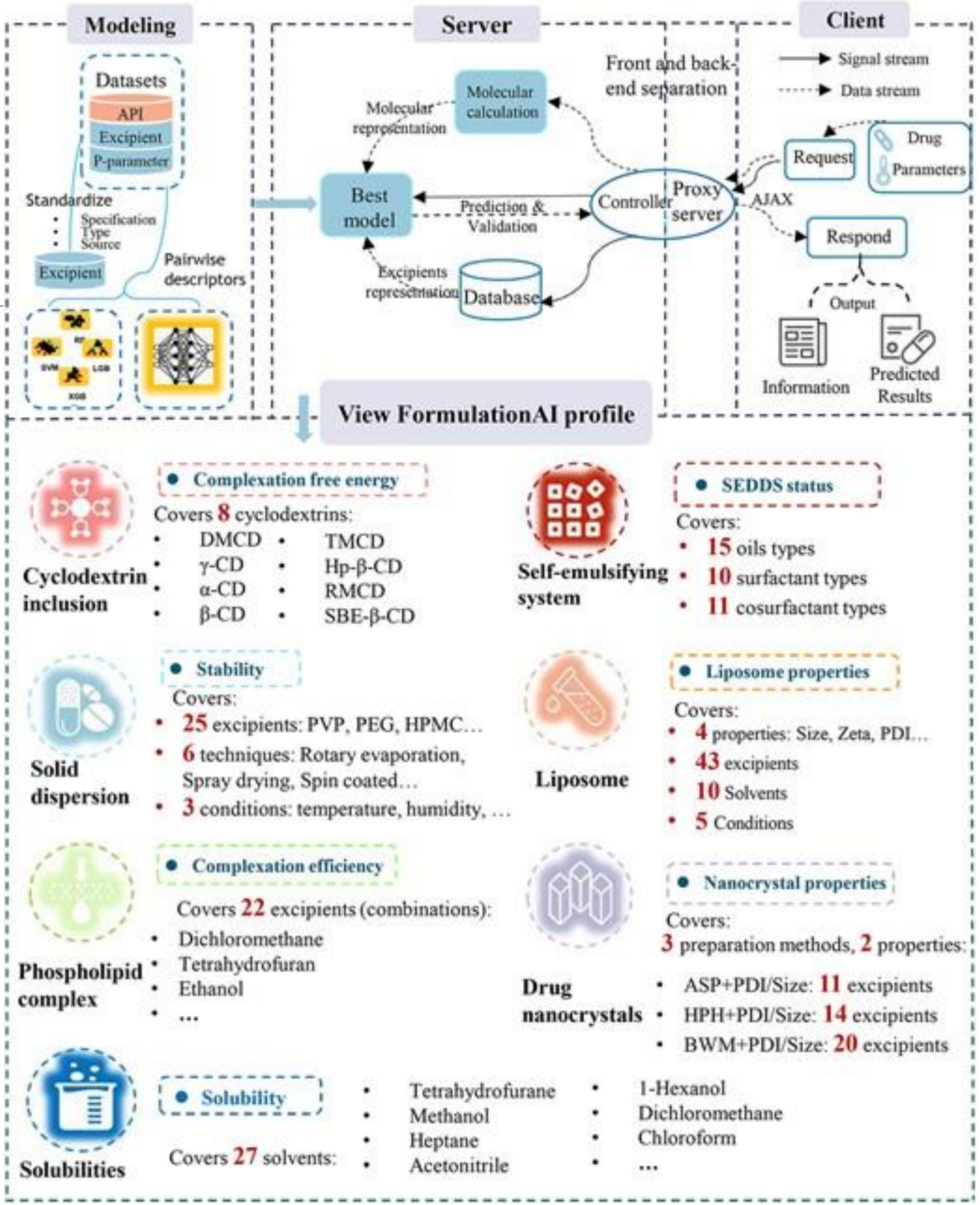
Company	Date	Headline
Schrödinger	February 2020	Drug discovery software company closes $232 million IPO backed by Bill Gates and David Shaw.
Insitro	May 2020	Insitro raises $143 million in Series B funding, to help drive its machine learning-based drug discovery approaches further.
AbCellera	May 2020	AbCellera raises $105 million in Series B funding round to expand its antibody drug discovery platform.
Relay Therapeutics	July 2020	Relay Therapeutics, which focuses on understanding protein motion to design drug candidates, closes $400 million IPO.
Atomwise	August 2020	Sanabil Investments co-leads $123 million Series B funding round for Atomwise to support the development of its molecule identification software.
Recursion Pharmaceuticals	September 2020	Recursion Pharmaceuticals, which is applying machine learning to cellular imaging data, raises $239 million in Series D financing round led by Bayer's investment department Leaps. Other investors include Casdin Capital, Samsara BioCapital, Baillie Gifford and Lux Capital.
XtalPi	September 2020	More than a dozen investment companies raise $318 million in Series C round for start-up XtalPi, which is applying quantum physics with AI to discover drug candidates.
AbCellera	December 2020	AbCellera closes its IPO at $556 million.
Cellarity	February 2021	Cellarity raises $123 million in Series B funding for its drug discovery approach based on modulating cellular behaviors.
Valo Health	March 2021	Valo Health, which is developing its Opal computational drug discovery and development platform, raises $110 million to add to its $190 million raised in January 2021 for its Series B funding round.
Insitro	March 2021	Insitro raises $400 million in Series C financing led by Canada Pension Plan Investment Board.
Exscientia	March 2021	Exscientia completes $100 million Series C financing, with investors including Evotec, Bristol Myers Squibb and GT Healthcare.
Recursion Pharmaceuticals	April 2021	Recursion completes $436 million IPO.
Exscientia	April 2021	Exscientia secures additional $225 million in a series D round led by SoftBank Vision Fund 2.

AI in Drug Formulation design

FormulationAI

Orion

Shrodinger



AI in Drug Formulation design

FormulationDT

we introduce FormulationDT, the first data-driven and knowledge-guided artificial intelligence (AI) platform for rational formulation strategy design

ELSEVIER
Journal of Controlled Release
Volume 378, 10 February 2025, Pages 619-636

AI-directed formulation strategy design initiates rational drug development

Nannan Wang [a], Jie Dong [b], Defang Ouyang [a c]

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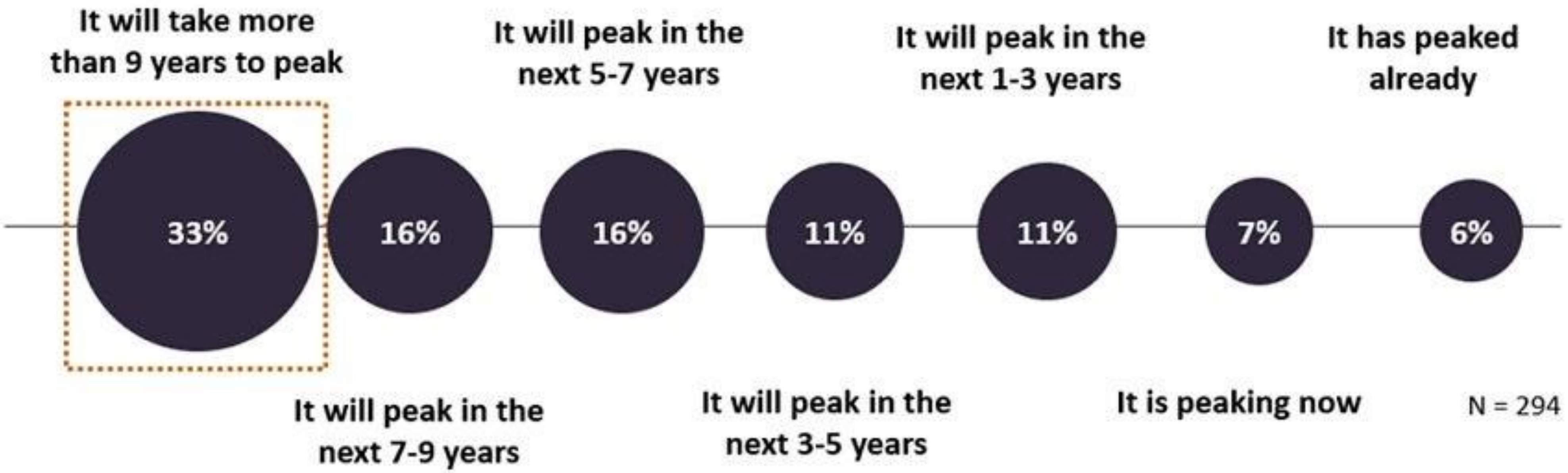
Current landscape

It will take years for AI use to peak in drug discovery and development process

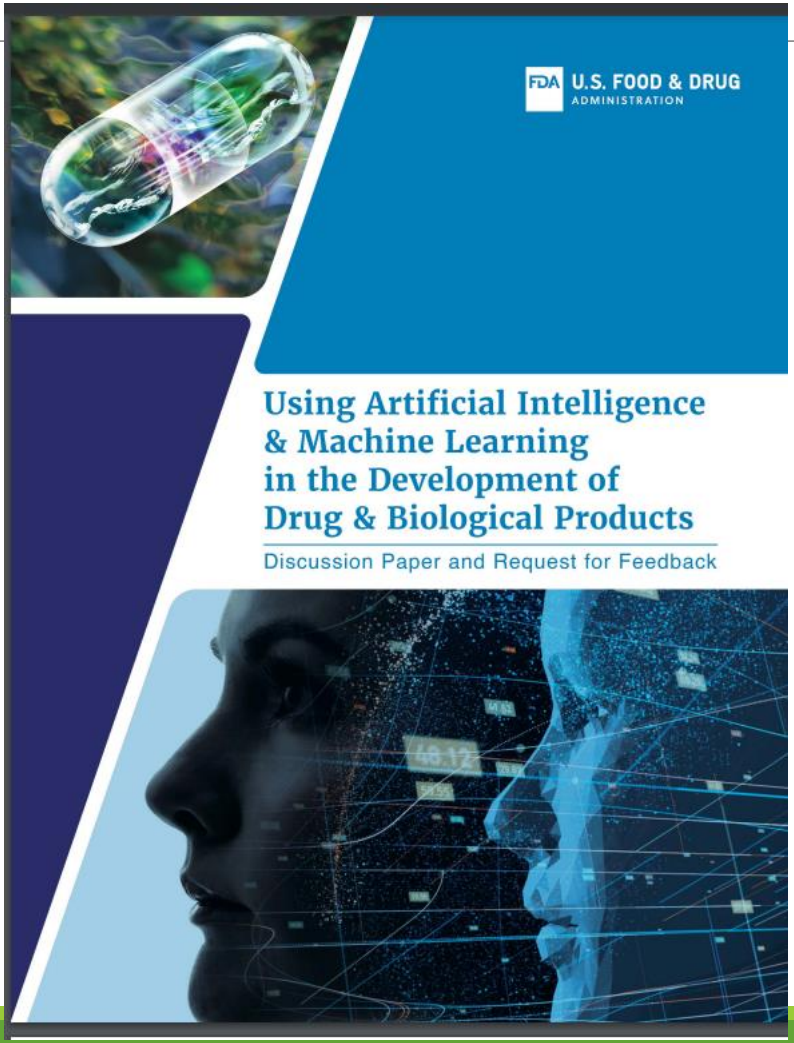
While AI is already being used to enhance drug discovery and development, it is still in the infancy stage.

Figure 1: Time Needed for the Use of AI to Peak in Drug Discovery and Development Process



Q: When do you think the use of artificial intelligence in drug discovery and development process will reach its peak in pharmaceutical industry?
Note: Percentages are rounded to nearest 0 decimal places.
Source: GlobalData

AI and FDA


U.S. FOOD & DRUG
ADMINISTRATION
Using Artificial Intelligence
& Machine Learning
in the Development of
Drug & Biological Products
Discussion Paper and Request for Feedback

How is artificial intelligence used in regulatory affairs?

AI tools can be applied to automate regulatory processes such as:

- administrative work,
- dossier filling,
- data extraction,
- auditing,
- the implementation of regulations,
- and quality management.

AI creates process links and reduces complexity, resulting in a more efficient management system.

What is FDA's perspective on the use of AI/ML in drug development?

FDA is committed to **ensuring that drugs are safe and effective** while **facilitating innovations** in their development.

FDA has accelerated its efforts to create an agile **regulatory ecosystem** that can **facilitate innovation** while **safeguarding public health**.

AI/ML will **undoubtedly play a critical role in drug development**, and FDA plans to **develop and adopt a flexible risk-based regulatory framework that promotes innovation** and protects patient safety.

What is FDA's perspective on the use of AI/ML in drug development?

FDA's Center for **Drug Evaluation and Research (CDER),** in collaboration with the **Center for Biologics Evaluation and Research (CBER)** and the **Center for Devices and Radiological Health (CDRH)**, issued an **initial discussion paper** to communicate with a range of stakeholders and to explore **relevant considerations for the use of AI/ML in the development of drugs and biological products.**

Year	Title	Key Points
2019	Proposed Regulatory Framework for Modifications to AI/ML-Based Software as a Medical Device (SaMD)	Introduced a potential approach to premarket review for AI/ML-driven software modifications, emphasizing the need for a tailored regulatory framework.
2021	Artificial Intelligence/Machine Learning (AI/ML)-Based Software as a Medical Device Action Plan	Detailed the FDA's approach to advancing oversight of AI/ML-based medical software, focusing on Good Machine Learning Practices (GMLP) and real-world performance monitoring.
2023	Discussion Paper: Artificial Intelligence in Drug Manufacturing	Explored AI/ML applications in drug manufacturing to enhance efficiency and product quality; sought stakeholder feedback to inform future regulatory policies.
2023	Discussion Paper: Using AI & ML in the Development of Drug & Biological Products	Discussed AI/ML use in drug and biological product development, including clinical trial design and data analysis; invited public comment to shape regulatory considerations.
2024	**Good Machine Learning Practice Guiding Principles**	Developed in collaboration with Health Canada and the UK's MHRA, these principles aim to promote safe, effective, and high-quality AI/ML-enabled medical devices.

2025

FDA U.S. FOOD & DRUG ADMINISTRATION

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Artificial Intelligence and Machine Learning (AI/ML)-Enabled Medical Devices

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Software as a Medical Device (SaMD)

Your Clinical Decision Support Software: Is It a Medical Device?

Artificial Intelligence and Machine Learning (AI/ML)-Enabled Medical Devices

Artificial Intelligence and

October 19, 2023 update: 171 Artificial Intelligence and Machine Learning (AI/ML)-Enabled Medical Devices were added to the list below. Of those newly added to the list, 155 are devices with final decision dates between August 1, 2022, and July 30, 2023, and 16 are devices from prior periods identified through a refinement of methods used to generate this list.

As technology continues to advance every aspect of health care, software incorporating artificial intelligence (AI), and specifically the subset of AI known as machine learning (ML), has become an important part of an increasing number of medical devices. One of the greatest potential benefits of AI/ML resides in its ability to create new and important

Content current as of:
12/06/2023

Regulated Product(s)
Medical Devices

FDA U.S. FOOD & DRUG ADMINISTRATION

Artificial Intelligence and Machine Learning (AI/ML) for Drug Development

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Artificial Intelligence and Machine Learning for Drug Development

What is Artificial Intelligence and Machine Learning?

Artificial Intelligence (AI) and Machine Learning (ML) can be described as a branch of computer science, statistics, and engineering that uses algorithms or models to perform tasks and exhibit behaviors such as learning, making decisions, and making predictions. ML is considered a subset of AI that allows models to be developed by training algorithms through analysis of data, without models being explicitly programmed.

What role is AI/ML playing in drug development?

FDA recognizes the increased use of AI/ML throughout the drug development life cycle

U.S. FOOD & DRUG ADMINISTRATION

Digital Health Technologies (DHTs) for Drug Development

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Science and Research Special Topics

Digital Health Technologies

Advancing Regulatory Science

Artificial Intelligence and Machine Learning for Drug Development

Digital health technologies (DHTs) offer many potential benefits in the development of medical products, including drugs. Advances in DHTs, including electronic sensors, computing platforms and information technology, provide new opportunities to obtain clinical trial data directly from patients. Portable DHTs that may be worn, implanted, ingested, or placed in the environment allow real-time collection of data from trial participants in their homes or at locations remote from clinical trial sites. Potential advantages of these DHTs include the ability to:

- make continuous or frequent measurements of clinical features
- record or measure novel clinical features that could not be captured during traditional study visits
- decentralize clinical trial activities by obtaining clinical data from study participants remotely

ADMINISTRATION

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Real-World Evidence

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Real-World Evidence

Center for Biologics Evaluation and Research & Center for Drug Evaluation and Research Real-World Evidence

FDA has a long history of using what we currently call real-world data (RWD) and real-world evidence (RWE) to monitor and evaluate the postmarket safety of approved drugs. RWE has also been used historically to support effectiveness, but on a more limited basis. Advances in the availability and analysis of RWD have increased the potential for generating robust RWE to support FDA regulatory decisions.

FDA is committed to realizing the full potential of fit-for-purpose RWD to generate RWE that will advance the development of therapeutic products and strengthen regulatory oversight of medical products across their lifecycle.

Definitions

Real-world data are data relating to patient health status and/or the delivery of health care routinely collected from a variety of sources. Examples of RWD include data derived from electronic health records, medical claims data, data from product or disease

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FDA-approved A.I.-based algorithms

+ Submit a new item here

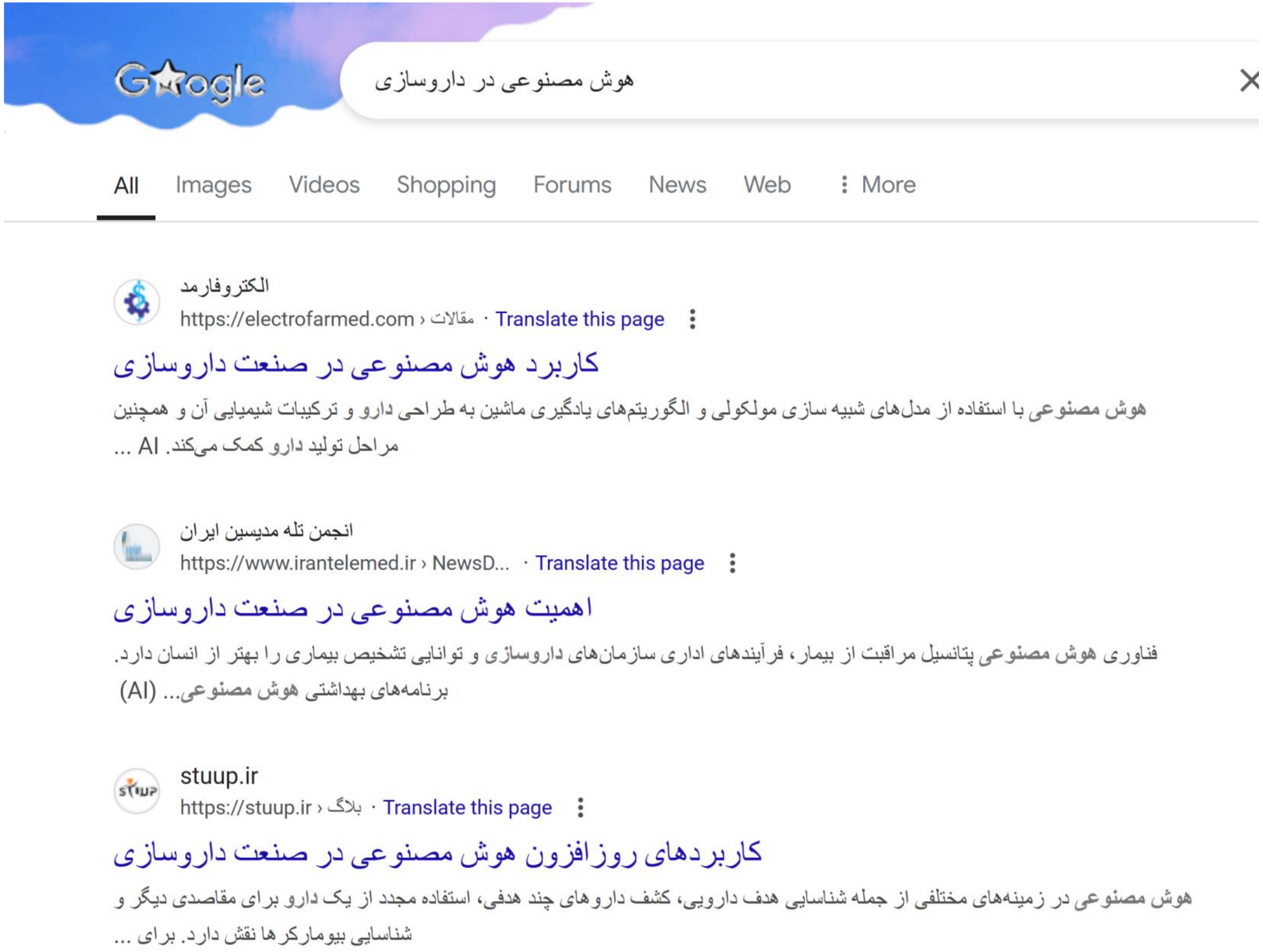
Type to filter data...

Name of device or algorithm	Name of parent company	Short description	FDA approval number	Type of FDA approval	Mention of A.I. in announcement	If no mention of A.I. in FDA announcement	Date	Medical specialty	Secondary medical specialty
Arterys Cardio DL	Arterys Inc	software analyzing cardiovascular images from MR	K163253	510(k) premarket notification	deep learning		2016 11	Radiology	Cardiology
EnsoSleep	EnsoData, Inc	diagnosis of sleep disorders	K162627	510(k) premarket notification	automated algorithm		2017 03	Neurology	
Arterys Oncology DL	Arterys Inc	medical diagnostic application	K173542	510(k) premarket notification	deep learning		2017 11	Radiology	Oncology
Idx	IDx LLC	detection of diabetic retinopathy	DEN180001	de novo pathway	A.I.		2018 01	Ophthalmology	

Date of Final Decision	Submission Number	Device	Company	Panel (Lead)	Primary Product Code
07/27/2023	K231195	Brainomix 360 Triage ICH	Brainomix Limited	Radiology	QAS
07/26/2023	K231038	Global Hypoperfusion Index (GHI) Algorithm	Edwards Lifesciences, LLC	Cardiovascular	QNL
07/25/2023	K223473	ME-APDS™; MAGENTIQ-COLO™	Magentiq Eye LTD	Gastroenterology/Urology	QNP
07/25/2023	K230365	Sonio Detect	Sonio	Radiology	IYN
07/25/2023	K230913	ANDI	Imeka Solutions, Inc.	Radiology	QIH
07/24/2023	K223347	UltraSight AI Guidance	UltraSight Inc	Radiology	QJU
07/21/2023	K230150	OptimMRI	RebrAIn, SAS	Radiology	QIH
07/21/2023	K223288	Cranial Navigation, Navigation Software Cranial, Navigation Software Craniofacial, Cranial EM System, Automatic Registration iMRI	Brainlab AG	Neurology	HAW
07/21/2023	K231173	Irregular Rhythm Notification Feature (IRNF)	Apple Inc.	Cardiovascular	QDB
07/20/2023	K230039	uOmnispace	Shanghai United Imaging Healthcare Co., Ltd.	Radiology	QIH

There are now more than 692 market-cleared artificial intelligence (AI) medical algorithms available in the United States, according to the U.S. Food and Drug Administration (FDA) as of July 30, 2023.

What is going on in Iran



What is going on in Iran

متاسفانه هیچ اطلاعاتی در مورد
مصوبه های احتمالی، کمیته های
راهبری، مقررات مرتبط با
مستندسازی دیتا، در جستجوی گوگل
و اخبار یافت نشد.

What's going **around** Iran?

Strategic planning,

systematic acts

and

relevant collaborations with AI companies!

Opportunities for Leveraging Artificial Intelligence in Iran's Pharmaceutical Ecosystem

Drug Research and Development

- Designing new drugs using machine learning models.
- Modeling diseases and predicting drug effects.
- Simulating drug effects on the human body.

Drug Manufacturing

- Optimizing production processes.
- Enhancing drug quality control.
- Designing and analyzing clinical trials.
- Predicting and preventing production-related issues.

Pharmacy and Healthcare Services

- Managing existing drugs with demand forecasting and supply optimization.
- Advanced drug counseling and patient consultation.
- Monitoring and preventing drug interactions and adverse effects.

Thanks for your attention

Share your comments:

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