

Insilico Medicine

Využitie umelej inteligencie vo vývoji liekov

April 30th, 2025





COGNEXA 2019 - 2020 Cognexa (Slovak Al company)



Ján Szöllös, MBA

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- 2013 Big Data in Drug R&D
- 2014 Al in Drug R&D
- 2017 Al Disruptors competition

2020 - 2025 Insilico Medicine (Global TechBio pioneer company)



Agenda

- 1. What's the situation with AI in drug discovery and development?
- 2. What are shortcomings?
- 3. What are the opportunities?
- 4. Who's already making the impact?
- 5. How is Insilico Medicine changing the drug discovery?
- 6. Al & Robotics marriage made in heaven?

Forbes

INNOVATION > AI

AI Hype Or AI Hope: When Will AI Disrupt The Pharmaceutical Industry?

By <u>Alex Zhavoronkov, PhD</u>, Former Contributor. (i) Expert in AI for healthcare and longevity bi... • for COGNITIVE WORLD

Apr 30, 2020, 03:56pm EDT

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In the past decade or so, artificial intelligence has gone from the pages of science fiction novels to a very real power that has disrupted — or threatens to disrupt — nearly every process on earth. AI helps our cars, aircraft, and spacecraft navigate, offers you movie suggestions on Netflix, and facilitates dozens of other disruptions, both grand and mundane.

Why, then, has the pharmaceutical industry — an industry which, literally, has life and death in its hands — shown, relatively speaking, almost no sign of disruption, despite ready access to computers and computer tools, such as AI? Experts suggest that the pharmaceutical industry remains one of the most inefficient industries, a last holdout against technological

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FEATURES A.I.

Will AI ever cure cancer? The multibillion-dollar race to bring the first AIdiscovered drug to market

BY ERIKA FRY April 3, 2025 at 6:00 AM EDT

HYPE?

REALITY?



WHERE ARE WE NOW?



How to improve R&D productivity: the pharmaceutical industry's grand challenge (Paul, et.al)



https://www.nature.com/articles/nrd3078

Nature Reviews | Drug Discovery

Simplified and updated



ρ (TS)	80%	75%	85%	69%	54%	34%		
Cycle time (years)	1.0	1.5	2.0	1.0	1.5	2.5		
Cost per launch (capitalized), \$ Millions	\$94	\$166	\$414	\$150	\$273	\$319		

Discovery

Development

Modified from Paul et al, How to improve R&D productivity: the pharmaceutical industry's grand challenge. Nature Reviews Drug Discovery, 2010



Development cost in 2010 ~\$1.9B In 2013: \$2.6**B**

Sales and marketing



Why 90% of clinical drug development fails and how to improve it?

https://pmc.ncbi.nlm.nih.gov/articles/PMC9293739/

- 1. Lack of clinical efficacy (40%–50%)

- 1. Lack of commercial needs and poor

Key facts about drug discovery and development

We need:

- Drug discovery is too risky
 (95%+ failure rate for discovery programs).
- 2. Failures are very expensive.
- Insufficient understanding of disease biology results in target selection with low Biological Relevance.

- 1. New and better therapeutics targets.
- 2. Better and safer molecules that are cheap to
 - produce.
- 3. Better Biomarker selection strategies.
- 4. Shorter and cheaper development cycles.
- 4. It take 10-12 years to deliver a new drug from program inception to the market launch.
- 5. Most 'low hanging fruit' has been already collected.

THE EMERGENCE OF TECHBIO



Algorithms: The New Age of Al



https://www.biopharmatrend.com/ai-drug-discovery-pipeline-2024/

THE NOBEL PRIZE

Nobel Prize in Chemistry 2024

Summary

Laureates

David Baker

Demis Hassabis

John Jumper

Prize announcement

Press release

Popular information

Advanced information

Award ceremony video

Award ceremony speech

Share this





9 October 2024

The Royal Swedish Academy of Sciences has 2024

with one half to

David Baker University of Washington, Seattle, WA, USA Howard Hughes Medical Institute, USA

"for computational protein design"

and the other half jointly to

Demis Hassabis Google DeepMind, London, UK

John Jumper Google DeepMind, London, UK

"for protein structure prediction"

THE NOBEL PRIZE

Nobel Prize in Physics 2024 Summary Laureates John J. Hopfield **Geoffrey Hinton** Prize announcement Press release Popular information Advanced information Award ceremony video Award ceremony speech

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Nobel prizes for **Chemistry** and **Physics** were awarded to AI pioneers in 2024!



© Nobel Prize Outreach. Photo: Nanaka Adachi John J. Hopfield Prize share: 1/2

© Nobel Prize Outreach. Photo: Clément Morin **Geoffrey Hinton** Prize share: 1/2

The Nobel Prize in Physics 2024 was awarded jointly to John J. Hopfield and Geoffrey Hinton "for foundational discoveries and inventions that enable machine learning with artificial neural networks"







Q

The dawn of the TechBio

























AI/ML Deals with Life Sciences Companies Deals with value >\$200Mn in 2024

Source: IQVIA Pharma Deals, Jan 2025.

Drug discovery 5 deals \$5,492 M	Isomorphic Laboratories 🕂 🔏	Small Molecules	\$1,745 M
	Isomorphic Laboratories + U NC	VARTIS Small Molecules	\$1,238 M
	Generate: Biomedicines 🕂 🔱 NO	OVARTIS Protein	\$1,065 M
	ochrebi	oehringer Regenerative ngelheim medicines	\$1,035 M
	🛆 Genetic Leap 🕂 🔏	Oligonucleotide	\$409 M
Drug design 5 deals \$3,161 M		AAV Vectors	\$1,050 M
		stol Myers Molecular Glues	\$674 M
	VNabla Bio + AstraZena	Protein	\$550 M
	Stemline + 🚸	Insilico Medicine Small Molecules	\$512 M
	👔 Biolojic Design 🕂 树	CRCK Antibody	\$375 M
Target identification 2 deals \$1,058 M	BIONGE 🕂 🔥	NOVARTIS	\$550 M
	C RELATION + 5	SK	\$508 M

As of June 2023, more than **\$18 billion** had poured into some 200 "AI-first" biotechs, and by January 2024, at least **75 drugs** or vaccines from those companies had entered clinical trials, according to Boston Consulting Group.

Citeline, a pharmaceutical market research firm, meanwhile, has counted 446 financing rounds totaling **\$30.6 billion** in the AI-driven life sciences space since 2020.

Biotechs are applying AI and machine learning to drug development, potentially creating dozens of new medicines and a **\$50 billion** market over the next decade (published in 2022).

https://www.bcg.com/publications/2023/unlocking-the-potential-of-ai-in-drug-discovery https://www.morganstanley.com/ideas/ai-drug-discovery?utm_source=chatgpt.com

TechBio already making impact

For instance, companies like Insilico Medicine, Recursion, and Exscientia have compressed the discovery phase from the industrystandard 2.5 to 4 years (40-50 months) down to 9 to 18 months in some cases.

According to a recently published benchmark, Insilico Medicine averages **12-18 months** per program, testing only **60-200 molecules**, while Recursion advances candidates in **18 months** with fewer than 200 molecules per program.

Exscientia, which merged with Recursion, claims to have shortened its timeline from four to five years to just **12 to 18 months**, screening **150-250 molecules** — a notable contrast to traditional methods that sometimes require testing 3,000-5,000 molecules per program.





New Yorku. O novinke informoval portál CNBC.

THERAPEUTIC TARGET DISCOVERY





The Landscape of **AI-discovered Drug Candidates** and Targets

The indicated data are for March 2025 *

Data includes both in-house and partner programs, data is NOT exhaustive, it reflects only information disclosed by companies on their websites.



Schrodinger

https://www.biopharmatrend.com/

https://www.TechLifeSci.com



https://www.biopharmatrend.com/ai-drug-discovery-pipeline-2024/



panda Omics OMICs Research and Target Identification



Sophisticated AI tool enables the system's biology platform to address challenges in target discovery, biomarker identification, and computational repurposing

Core Features

- Target Identification and Evaluation
- OMICs Data Analysis
- Pathway Analysis
- Target Attention and Trend Prediction
- Gene-disease Association Prediction



Version 4.0 New Features

- ChatPandaGPT Large Language Model for Target Discovery
- Indication Prioritization
- Transformer-based knowledge graph
- Cross-dataset Comparison and Data harmonization
- Genetic Data and Evidence Exploration

PandaOmics allows scientists to quickly and easily pick the Best Target for their organization with their data

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Contact us

GENERATIVE CHEMISTRY





Structure-based drug discovery

"Flow chart for structure based drug design" by Laozhengzz, via Wikimedia Commons (CC BY-SA (30)



Structure Based Rational Drug Design



Unlock the power of Novel Biologics Engineering with Al

Select the type of biologic and define your goal ΑΙ **Biologics** Proteins Antibodies Nanobodies **Workflows** Generation Affinity Optimization Properties ~~ Screening





First Al-discovered & Al-designed molecule is here!







INSILICO MEDICINE'S PHARMA.AI PLATFORM POWERS DRUG R&D ACCELERATION AND COST REDUCTION



Traditional Approach – 4.5 Years

TNIK Discovery and Development



Multiple Pilots and Projects with Pharmaceutical companies

IMPACT OF AI ON CLINICAL TRIALS







How successful are AI-discovered drugs in clinical trials? A first analysis and emerging lessons.

https://www.sciencedirect.com/science/article/pii/S135964462400134X?via%3Dihub





Al is cutting costs, speeding up processes, and boosting success rates across 12 use cases in clinical development.

Value drivers from AI and AI effects on clinical development

Cost efficiency Improved speed Increase possibility of success

Protocol co-developer

25% faster protocol approval 30–50% fewer amendments

- *One click" real-world evidence and historical trial summaries
- Protocol synopsis drafting
- Automated protocol quality

control

Site management copilot

50% fewer deviations 20% higher principal investigator satisfaction

- Site next-best-action engine-personalized principal investigator engagement
- Next-generation risk-based site monitoring

9

Regulatory intelligence engine

30% faster responses 50% fewer regulatory affairs (RA) follow-ups

- RA360 informed by RA responses, advisory committee insight
- Intelligent health assessment guestionnaire response
- Competitive label monitoring

Randomized control trial optimizer

10-20% cost efficiency 20-30% net present value increase.

- 5-10% trial acceleration
- Subpopulation and inclusion/exclusion criteria recommendations
- Endpoint recommendations
- Portfolio co-positioning on novel and existing mechanism of action

n

Patient trial companion

30% lower dropout rate 20% increase in patient satisfaction

 Patient-facing Al companion (conversational Al, alerts, trial Q&A)

3

Study start-up engine

10-20% faster enrollment 30% faster activation

- Al-based site selection Feasibility copilot
- Informed consent form auto-generator
- Site initiation visit material localization

30% cost efficiency

- case report from auto-generator (based on digital protocol)
- patient data
- Al-based smart data cleaning and guery engine

Postmarket regulatory /pharmacovigilance 30%+ cost efficiency

- Annual report auto-drafting
- Routine adverse-event
- report auto-drafting Label drafting/translations
- Signal management
- Al-powered signal detection and assessment

12

Indication-finding engine New high probability of success disease areas, with 100% preclinical validation

- Indication identification and prioritization for existing and novel mechanism of action
- Quantification of biological relevance by indication

(myTomorrows, TrialGPT)

dossiers?

clinical-development-with-artificial-intelligence#/

Development/

10 Major submission content writer 40% faster

2x fewer quality control issues 50% cost efficiency

- Clinical study report auto-drafting
- Routine tables, listings, and figures generation
- Auto quality control
- Safety and Health Economics and Outcomes Research insights driven by real-world evidence engine

Smart data management

70%+ fewer manual gueries

- One-click database creator
- Single source of truth for all

Biostats builder 30-50% cost efficiency

(A&O

 Standard statistical analysis (eg, efficacy, safety, chemistry, manufacturing, controls, population pharmacokinetics)

Trial performance copilot

10-20% faster enrollment

(alerts, conversational Al,

Predictive trial trajectory

with explanatory drivers

Study team companion

20% cost efficiency

 Auto-database build /guality control

- Advancements in Patient Recruitment and Study Design
- **Clinical Trial Data Management Solution Update**
- **Clinical Trial Management Systems (CTMS)**
- Generative AI to auto-generate entire regulatory
- **New Al Models: The Rise of the Clinical Agents**
- **New Partnerships and Ecosystem Growth**

https://www.mckinsey.com/industries/life-sciences/our-insights/unlocking-peak-operational-performance-in-

https://insights.citeline.com/PS147786/FDAs-CDER-Is-Fostering-Use-Of-Artificial-Intelligence-In-Drug-



Insilico Medicine

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https://www.youtube.com/watch?v=J_Z-xfmcY6U





Combine Pharma.Al with Data Generation – Lab-in-the-Loop



Six functional robotics modules For the rapid generation of reproducible and accurate data



Sample Intake

SIQC

Sample pretreatment (Tissue, blood, plasma)

Sample QC (mycoplasma, bacteria and fungi)

PE Envision plate reading



Compound Management CMS

Compound dissolving Compound reformatting Cherry-picking Serial dilutions

Cell Culture CC

Automated cell culture **CRISPR** screening

High Throughput Screening

HTS

Cell-based HTS

Cell-panel sensitivity

Combination screening

Biochemical-based HTS

ADP-Glo, HTRF, TR-FRET, et al





High Content Imaging

Image

Cell painting assays Immunofluorescence **ELISA**



Next-Generation Sequencing

NGS

WES

Standard mRNAseq

HTS-mRNAseq

Methylation seq (RRBS)



"I don't think we're yet at the technological level where any of us should expect these models to go cure cancer on their own. We will get there, I think. Yes. But for now, I think this can help researchers be much more productive in what they do."

Sam Altman, CEO, Open Al

""This is such a fun time for you guys... I'm jealous. You might be within a click or two away from really being able to understand the meaning of life.""

Jensen Huang, CEO, Nvidia

GLOBAL PRESENCE GLOBAL PARTNERSHIPS

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