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Artificial Intelligence for Drug Discovery

Landscape Overview
Q3 2022

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Introduction

This 135-page **"Artificial Intelligence for Drug Discovery Landscape Overview Q3 2022"** report represents the eleventh issue of market analytics focused on the Artificial Intelligence (AI) application in the pharmaceutical research industry.

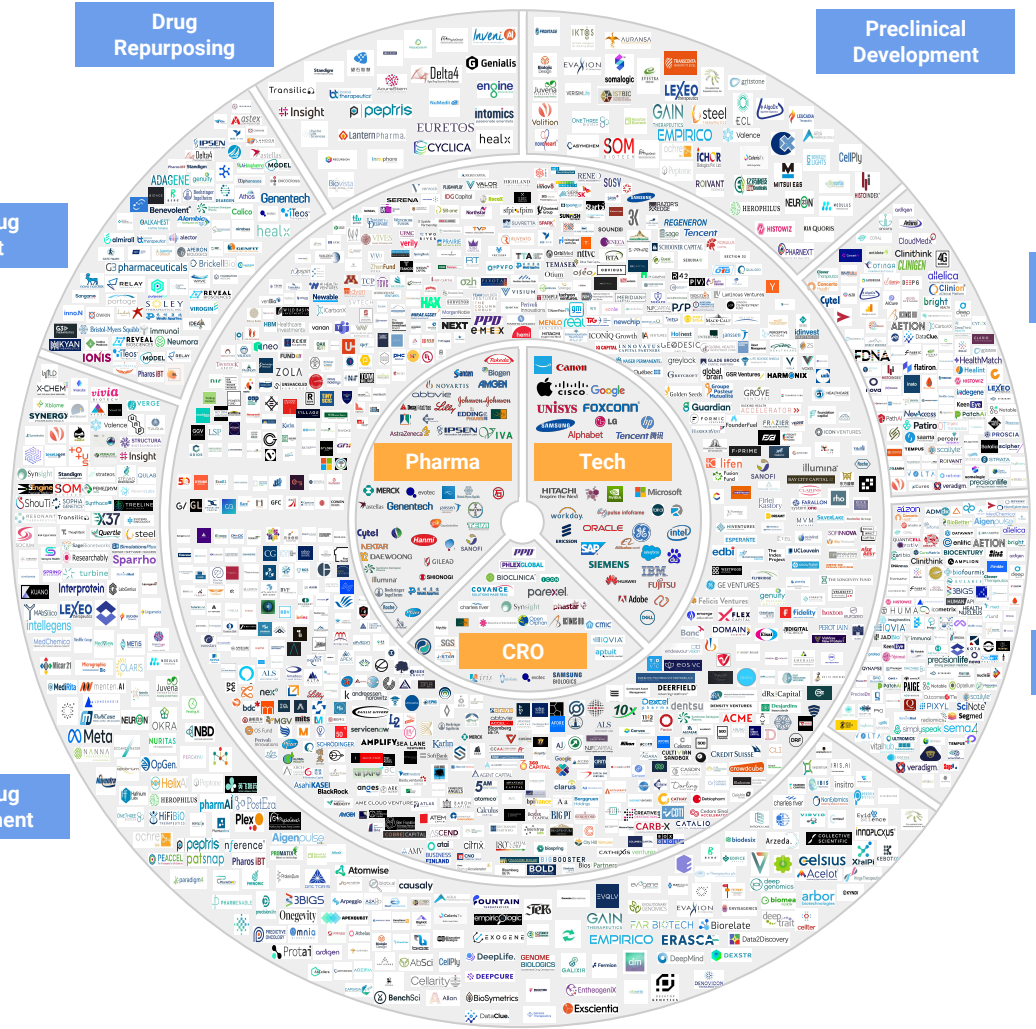
The primary goal of this series of reports is to give a complete picture of the industry environment in terms of AI usage in drug discovery, clinical research, and other elements of pharmaceutical research and development. This overview highlights recent trends and insights in the form of helpful mind maps and infographics and gauges the performance of prominent players who shape the industry's space and relationships. It can help the reader comprehend what is going on in the sector and potentially predict what will happen next.

Since the last edition, data has been significantly updated to reflect the fast-paced market dynamics and an overall increase in pharmaceutical AI investment and business development activities. The listings of AI-biotech businesses, biotech investors, and pharmaceutical organizations have been expanded to reflect the pharmaceutical industry's rising interest in sophisticated data analytics technology.

Alongside investment and business trends, the report also provides technical insights into some of the latest AI applications and research achievements.

Artificial Intelligence for Drug Discovery Landscape Overview Q3 2022

AI Companies - 600
Investors - 1200
Corporations - 100



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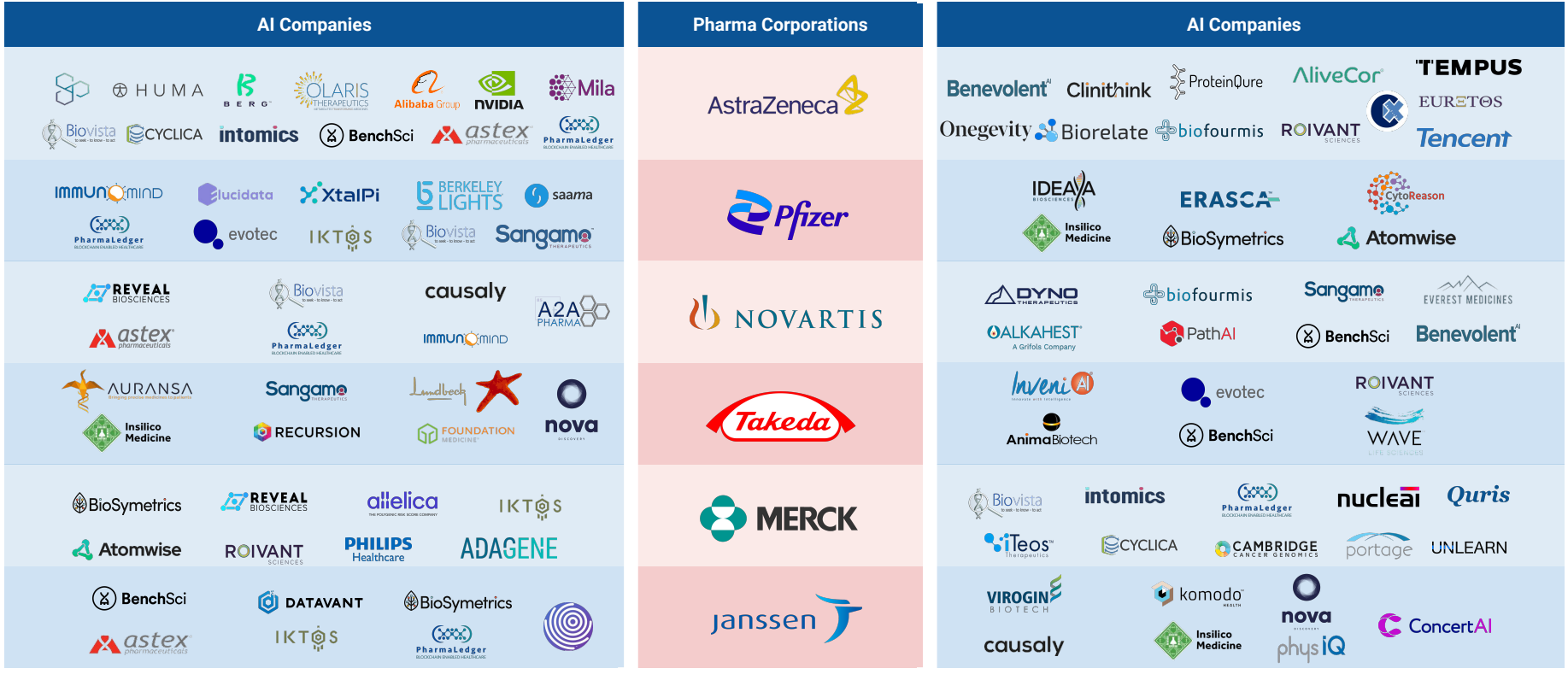
Selected Pharma AI Deals



Note: the central column (red) defines the pharmaceutical corporations and side columns (blue) defines AI companies that have collaborations with pharma companies from the central column.

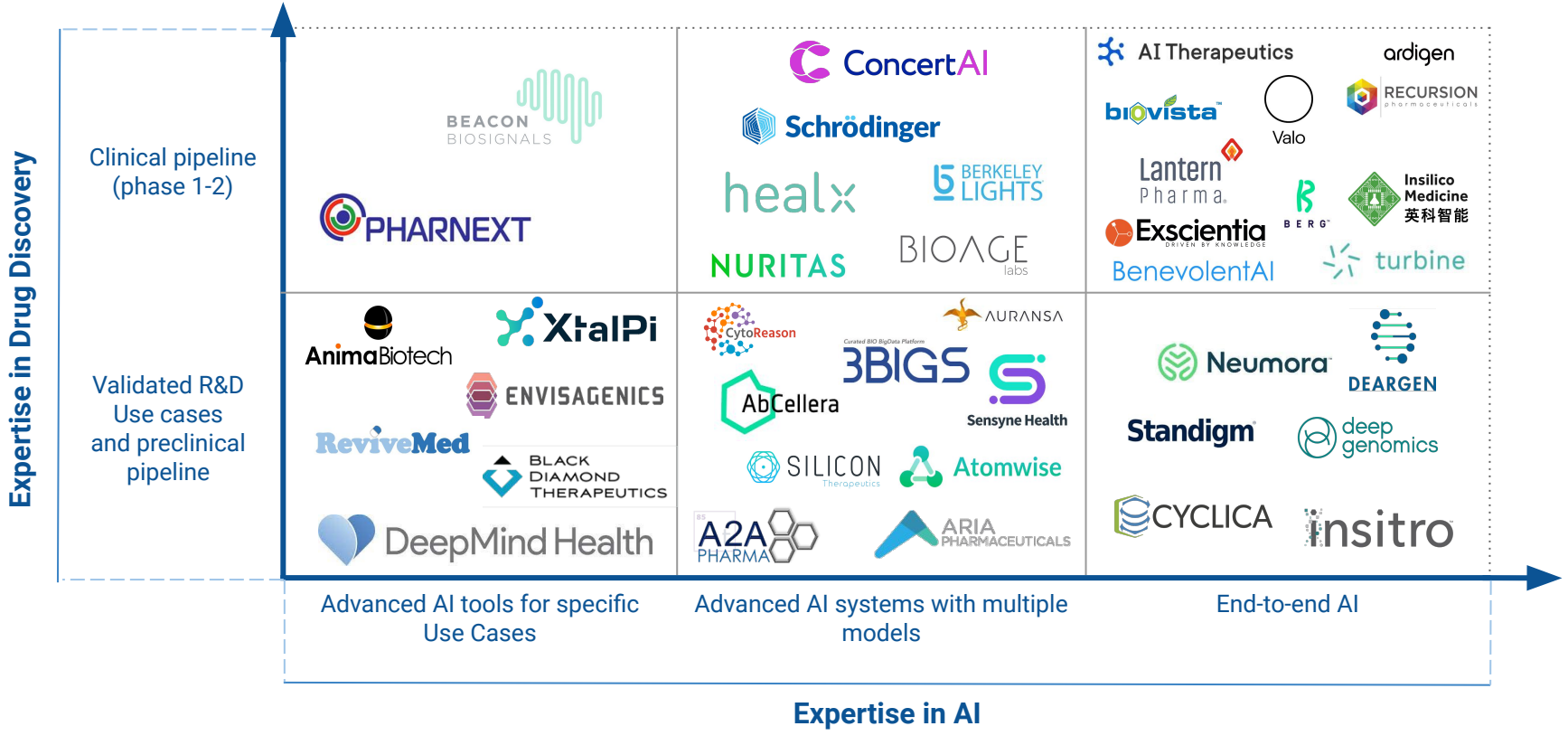
Selected Pharma AI Deals

Note: the central column (red) defines the pharmaceutical corporations and side columns (blue) defines AI companies that have collaborations with pharma companies from the central column.

40 Leading Companies in AI for Drug Discovery Sector

1	3BIGS
2	A2APharma
3	AbCellera
4	AI Therapeutics
5	AnimaBiotech
6	Ardigen
7	AriaPharmaceuticals
8	Atomwise
9	Auransa
10	Beacon Biosignals
11	Benevolent AI
12	Berg
13	Berkeley Lights
14	Bioage Labs
15	Biovista
16	Black Diamond Therapeutics
17	ConcertAI
18	Cyclica
19	CytoReason
20	Deargen
21	DeepGenomics
22	DeepMindHealth
23	Envisagenics
24	Exscientia
25	Healx
26	Insillico Medicine
27	Insitro
28	Lantern Pharma
29	Neumora
30	Nuritas
31	Pharnext
32	Recursion
33	ReviveMed
34	Schrodinger
35	SensyneHealth
36	Silicon
37	Standigm
38	Turbine
39	Valo
40	XtalPi

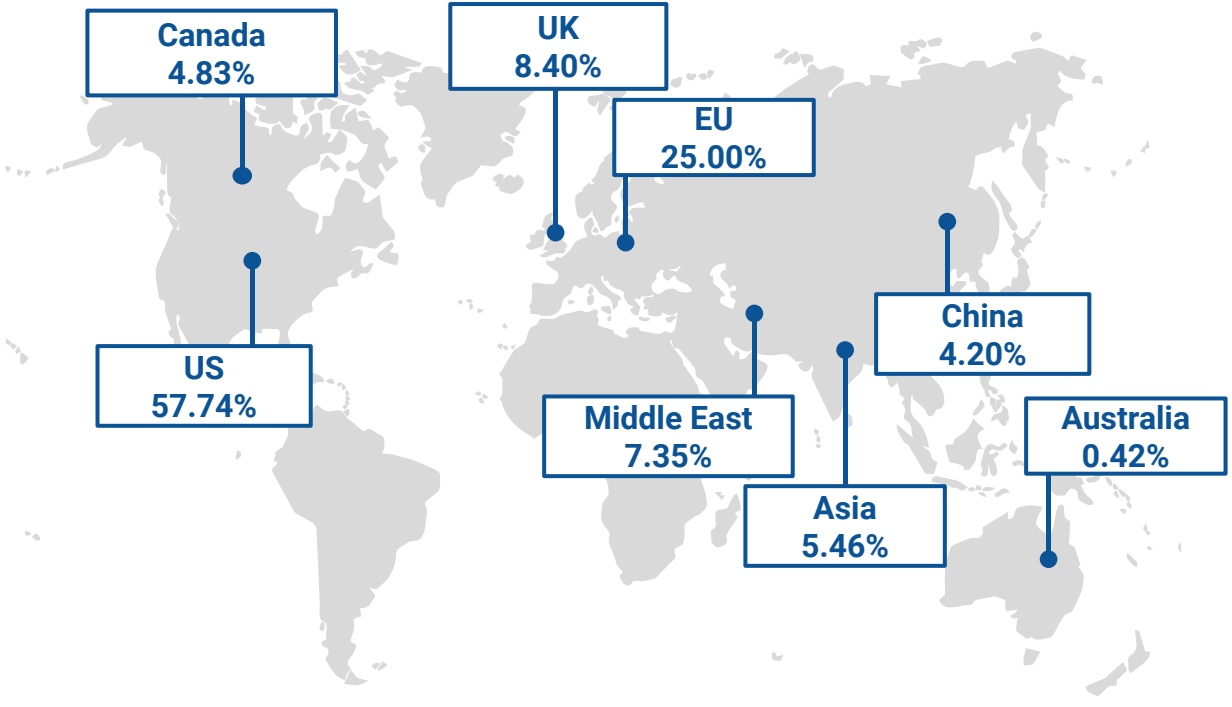
Comparison of Top-40 Leading AI for Drug Discovery Companies Expertise in Drug Discovery R&D



50 Leading Investors in AI for Drug Discovery Sector

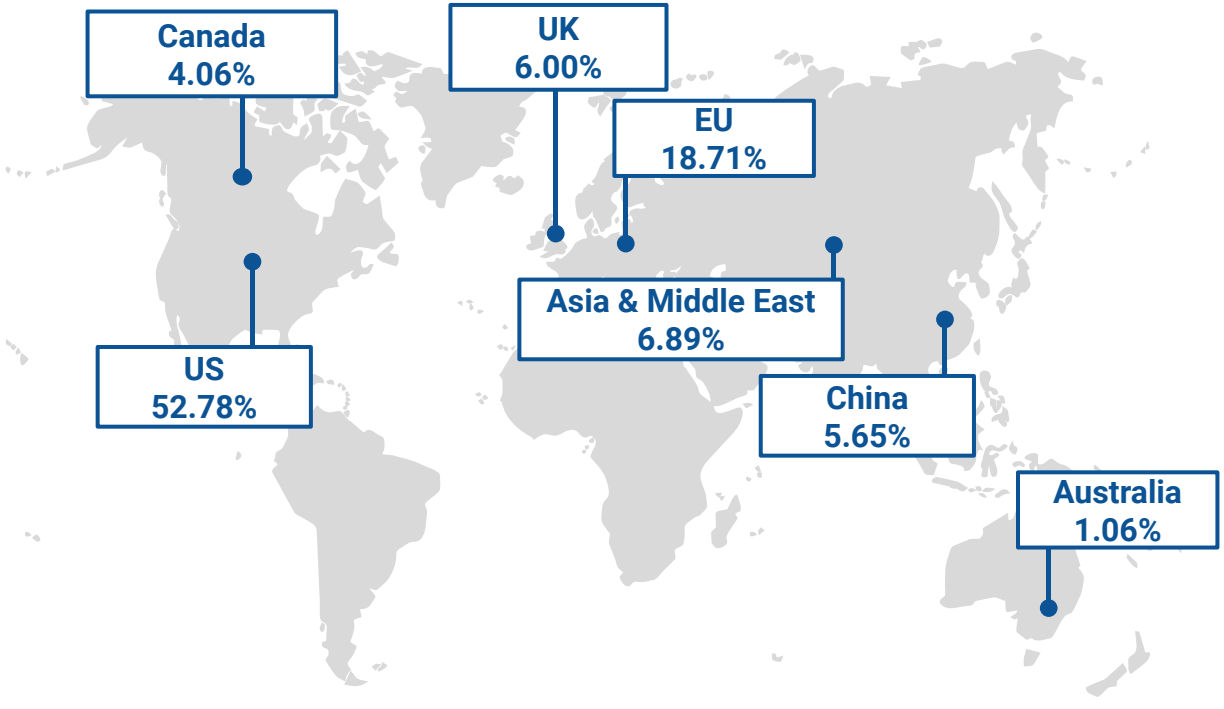
1	Casdin Capital
2	Creative Destruction Lab (CDL)
3	SOSV
4	National Science Foundation
5	GV
6	Y Combinator
7	Perceptive Advisors
8	Alexandria Venture Investments
9	Sequoia Capital China
10	RA Capital Management
11	Merck Global Health
12	Alumni Ventures
13	Khosla Ventures
14	Foresite Capital
15	8VC
16	DCVC Bio
17	National Institute of Health
18	EASME - EU Executive Agency
19	MassChallenge
20	T.Rowe Price
21	SoftBank Vision Fund
22	Invus
23	Deerfield
24	F-Prime Capital
25	Redmile Group
26	DCVC Bio
27	Founders Fund
28	IndieBio
29	Fidelity Management
30	Surveyor Capital
31	Temasek Holding
32	Cormorant Asset Management
33	5Y Capital
34	Northpond Ventures
35	Obvious Ventures
36	Andreessen Horowitz
37	Section 32
38	Lux Capital
39	AME Cloud Ventures
40	Eight Roads Ventures
41	Lifeforce Capital
42	Felicis Ventures
43	BlackRock
44	Foresite Capital
45	Janus Henderson Investors
46	Tencent
47	ARCH Venture Partners
48	Novo Holdings
49	Flagship Pioneering
50	Biotechnology Value Fund

600 AI Companies: Regional Proportion



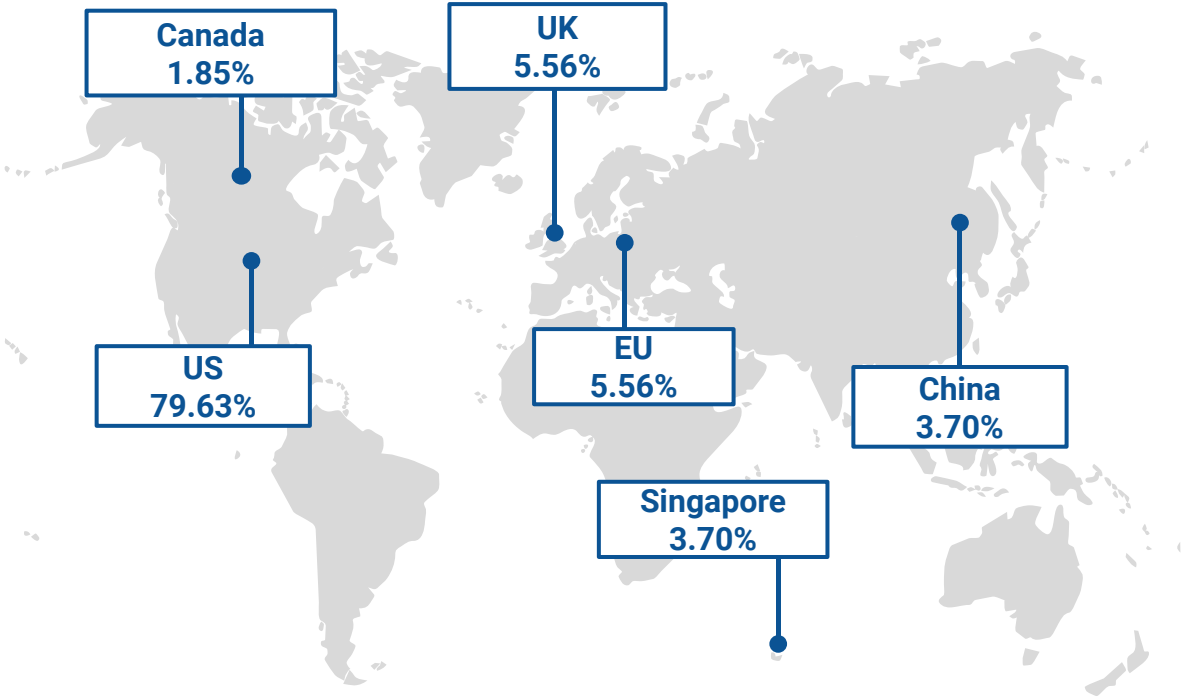
The US is still firmly in the lead regarding its proportion of AI for Drug Discovery companies. Interestingly, Asia and the Middle East continue to expand usage of AI technologies in the Pharmaceutical Industry. The ratio of companies that use AI for Drug Development in the UK and European countries is decreasing compared to the Asian market. The Asia-Pacific region continues to aggressively increase the number of AI for Drug Discovery Companies, particularly in China, and this tendency will probably maintain.

1120 Investors: Regional Proportion



The United States continues to lead the rest of the world in terms of artificial intelligence for companies and funds that invest in Drug Discovery. This is reasonable, given that more than a half of the world's AI for Drug Discovery companies have their headquarters in USA. Comparing with previous periods of 2021, we can observe significant growth of the number of investors in China, as well as in US as Europe. Thus, together with UK these regions are leaders by the number of investors in AI in Drug Discovery companies.

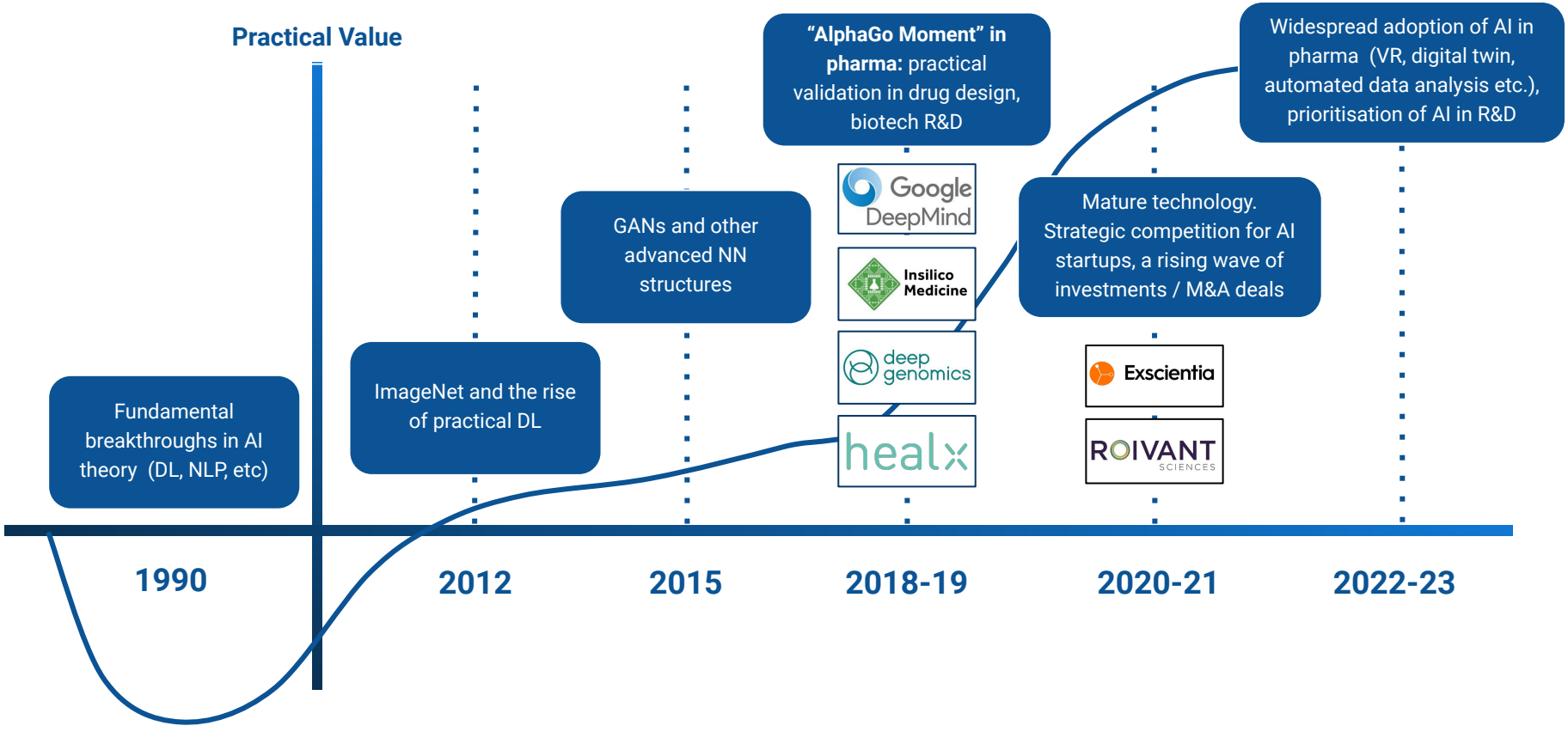
50 Leading Investors: Regional Proportion



The United States continues to lead the rest of the world in terms of artificial intelligence for companies and funds that invest in Drug Discovery. This is reasonable, given that more than a half of the world's AI for Drug Discovery companies have their headquarters in USA. During 2021 we can observe significant growth of the number of investors in Asia, mainly in China, Hong Kong and Singapore. The USA, the UK, and EU remain to be leaders by the number of investors in AI in Pharma companies.

Sources: *Investment Digest AI in Pharma*

Pharma's “AlphaGo Moment”



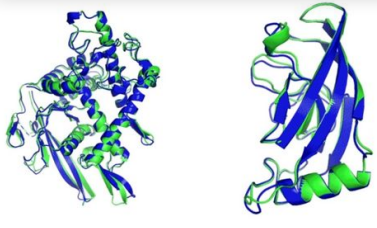
Notable Breakthroughs in AI for Pharma

2019

Deep Genomics AI-driven platform predicted novel target and oligonucleotide candidate for Wilson disease in under 18 months.

2020

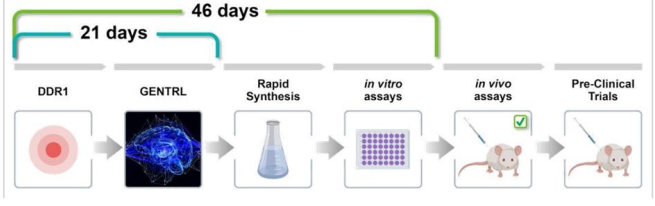
DeepMind's AlfaFold learns to predict protein's 3D shape from its amino-acid sequence, a 50 year-old grand challenge in biology.



Experimental Result
Computational Prediction

2021

Insilico Medicine applied generative adversarial network-based system GENTRL for rapid identification of potent DDR1 Kinase inhibitors within 21 days.



The University of Washington has developed a deep learning model, "**RoseTTAFold**", that calculates protein structure on a single gaming computer within 10 minutes.

Technological Advancements Defining the Market

2021

Insilico Medicine achieved industry-first fully AI-based Preclinical Candidate. Initial hypothesis was build via DNN analysis of omics and clinical datasets of patients. After that company used its AI PandaOmics engine for target discovery, analyzing all relevant data, including patents and research publications with NLP algorithms. In the next step Insilico has applied its generative chemistry module (Chemistry42) in order to design a library of small molecules that bind to the novel intracellular target revealed by PandaOmics. The series of novel small molecules generated by Chemistry42 showed promising on target inhibition. One particular hit ISM001 demonstrated activity with nanomolar (nM) IC50 values.

When optimizing ISM001, Insilico managed to achieve increased solubility, good ADME properties, and no sign of CYP inhibition — with retained nanomolar potency. Interestingly, the optimized compounds also showed nanomolar potency against nine other targets related to fibrosis. The efficacy and a good safety of the molecule led to its nomination as a pre-clinical drug candidate in December 2020 for IND-enabling studies. The phase I clinical trial for the novel drug candidate is planned for December 2021.

Disease Hypothesis & Target Identification	Target-to-hit	Hit-to-lead	Lead optimization and Candidate Validation
1 week	2 months	4 months	11 months
< $ 50k N/A	$ 200k $ 94M	$ 400k $ 166M	$ 200k $ 414M
Up to Decades	1 year	1.5 years	2 years

Phase 1 → Phase 2 → Phase 3 → Submission to launch

Phase 1 → Phase 2 → Phase 3 → Submission to launch

Source: *Insilico Medicine*

Executive Summary

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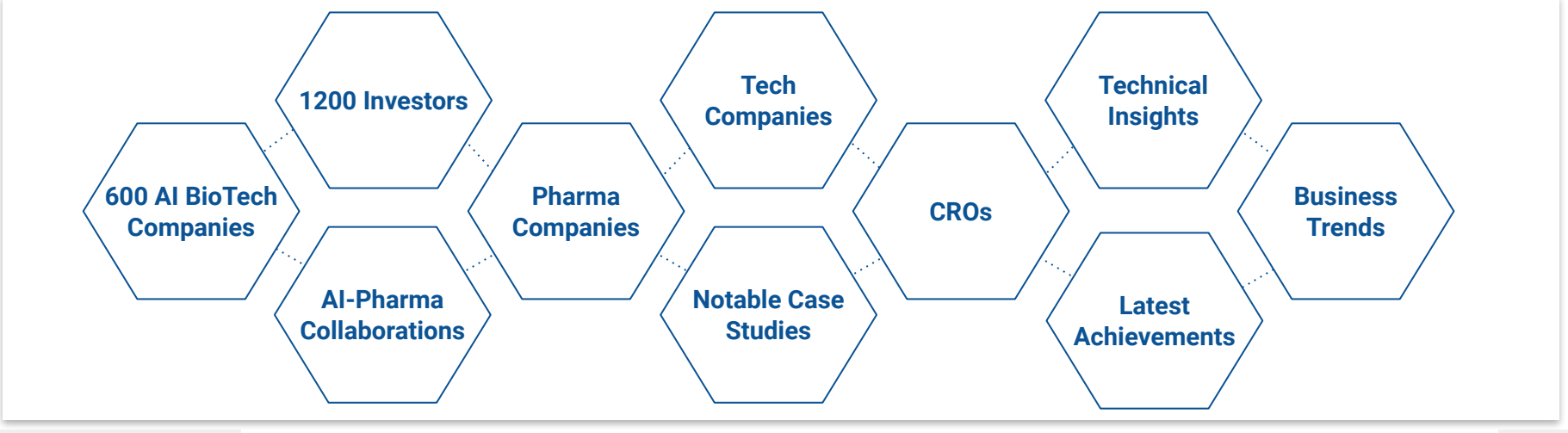
Report at a Glance

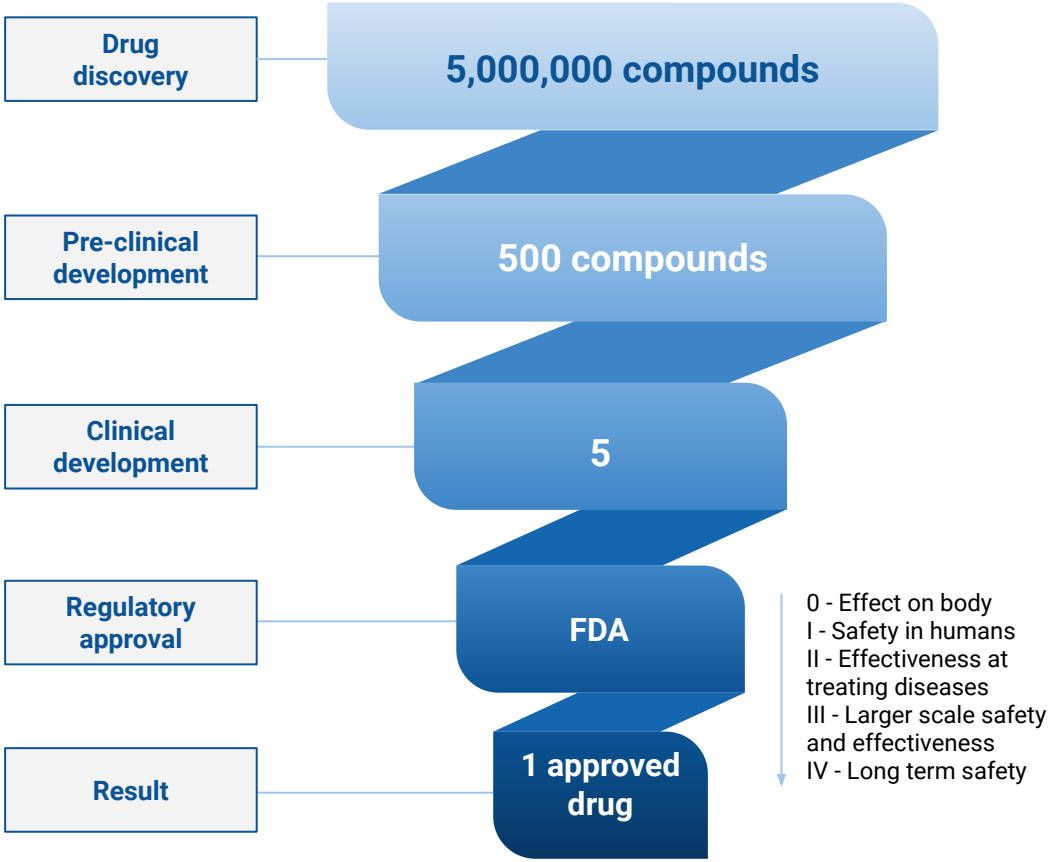
This **135-page** "**Artificial Intelligence for Drug Discovery Landscape Overview, Q3 2022**" report marks the installment in a series of reports on the topic of the Artificial Intelligence (AI) application in pharmaceutical research industry that DPI have been producing since 2017.

The main aim of this series of reports is to provide a comprehensive overview of the industry landscape in what pertains adoption of **AI in drug discovery, clinical research and other aspects of pharmaceutical R&D**. This overview highlights trends and insights in a form of **informative mind maps and infographics** as well as benchmarks the performance of key players that form the space and relations within the industry. This is an overview analysis to help the reader understand what is happening in the industry nowadays and possibly give an idea of what is coming next.

Alongside investment and business trends, the report also provides technical insights into some of the latest achievements in the AI application and research.



Pharma Efficiency: Challenges



10 years + $2.6 bln = 1 new drug

It takes on average over 10 years to bring a new drug to market. As of 2014, according to Tufts Center for the Study of Drug Development (CSDD), the cost of developing a new prescription drug that gains market approval is approximately $2.6 billion. This is a 145% increase, correcting for inflation, compared to the same report made in 2003.

The pharmaceutical industry is in a terminal decline, and the returns on new drugs that do get to market do not justify the massive investments that Pharma currently puts into R&D anymore.

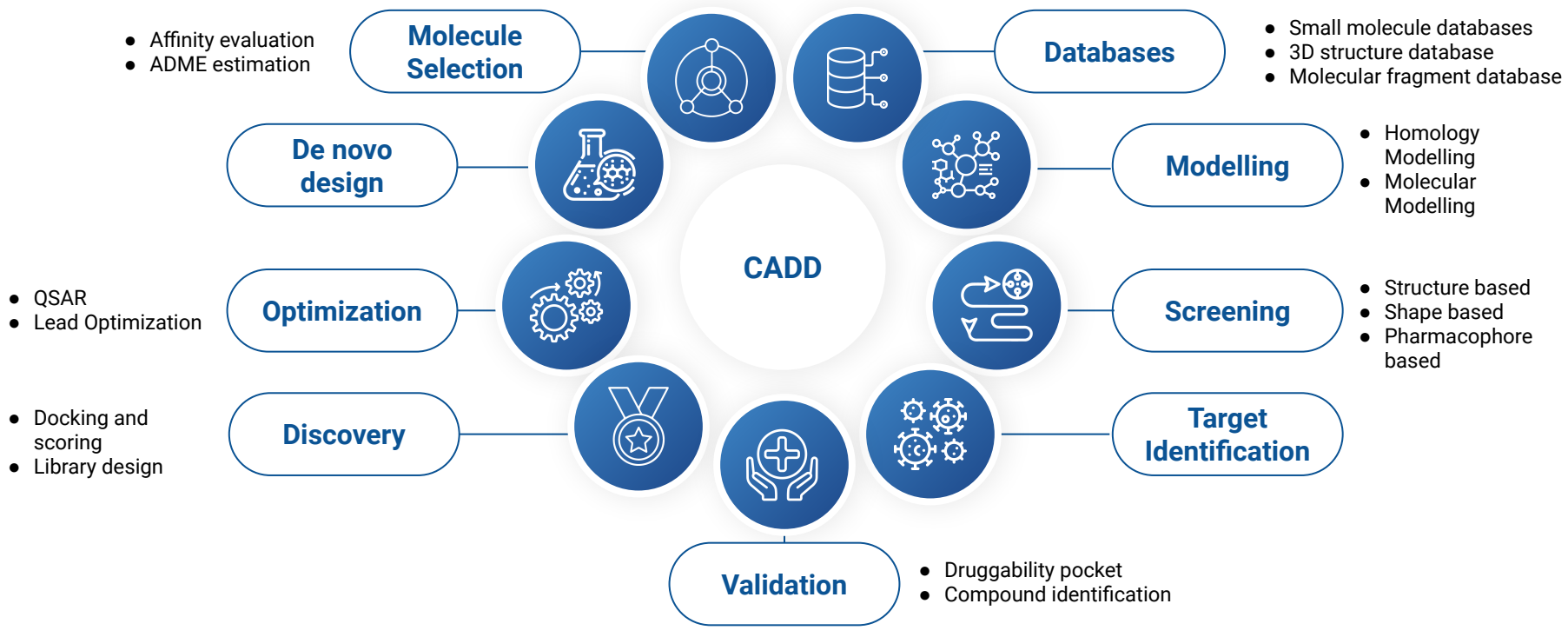
The solution to this problem comes from three key strategies:

- evolution of business models towards more collaboration and pipeline diversification early
- implementation of AI as a universal shift towards data-centric drug discovery
- discovery of new therapeutic modalities (biologics, therapies, etc.)

Source: *Conflict of Interest in Medical Research, Education, and Practice*, *medinicenet.com*

Computer-aided Drug Design

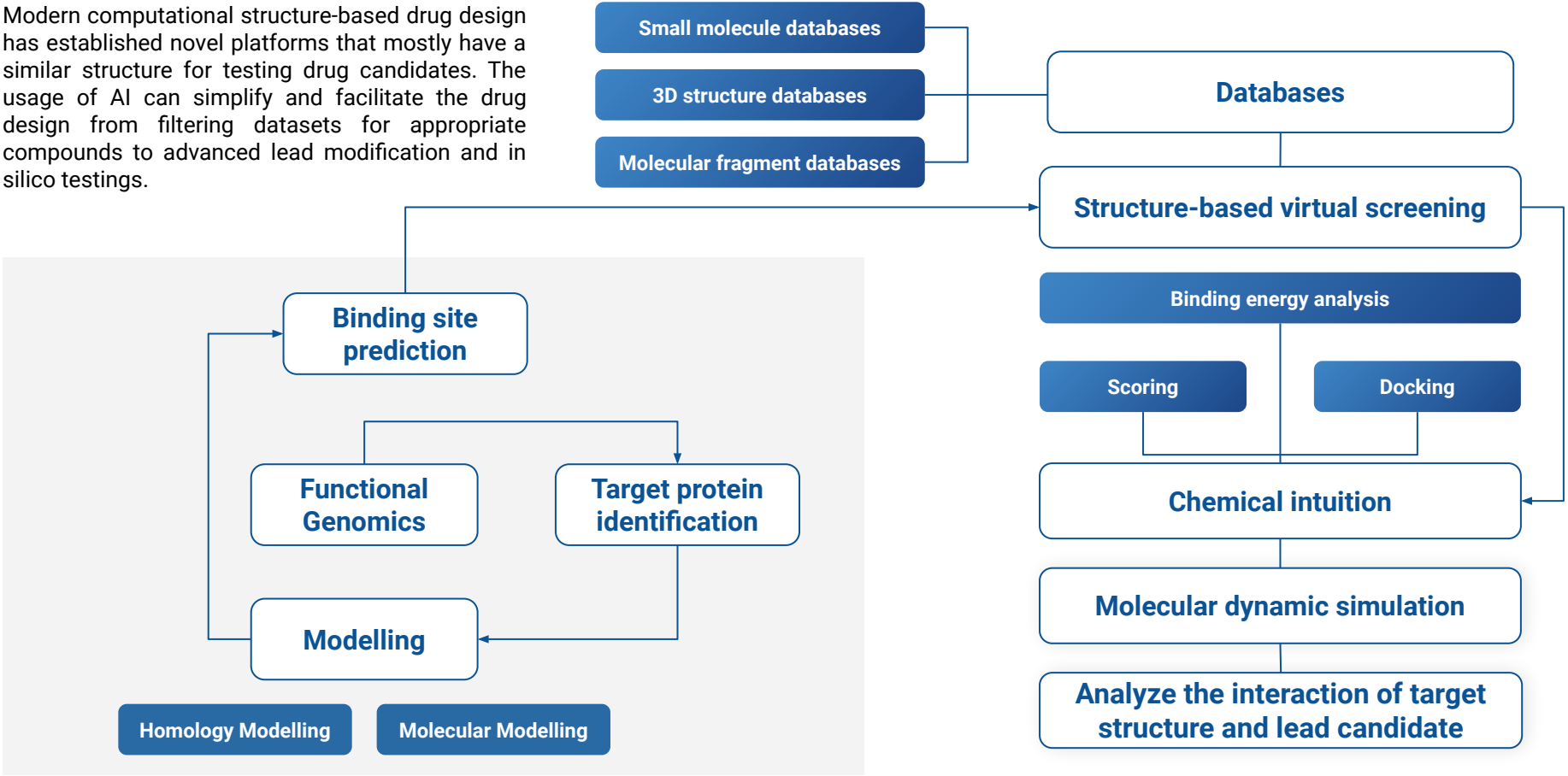
Today's task for the pharma industry is to create a cheap and effective solution for drug development, companies apply various computational methods to reach that goal. **Computer-aided drug design (CADD)** is a modern computational technique used in the drug discovery process to identify and develop a potential lead. CADD includes computational chemistry, molecular modeling, molecular design and rational drug design.



Sources: *Advantages of Structure-Based Drug Design Approaches in Neurological Disorders.*

Computer-aided Drug Design

Modern computational structure-based drug design has established novel platforms that mostly have a similar structure for testing drug candidates. The usage of AI can simplify and facilitate the drug design from filtering datasets for appropriate compounds to advanced lead modification and in silico testings.



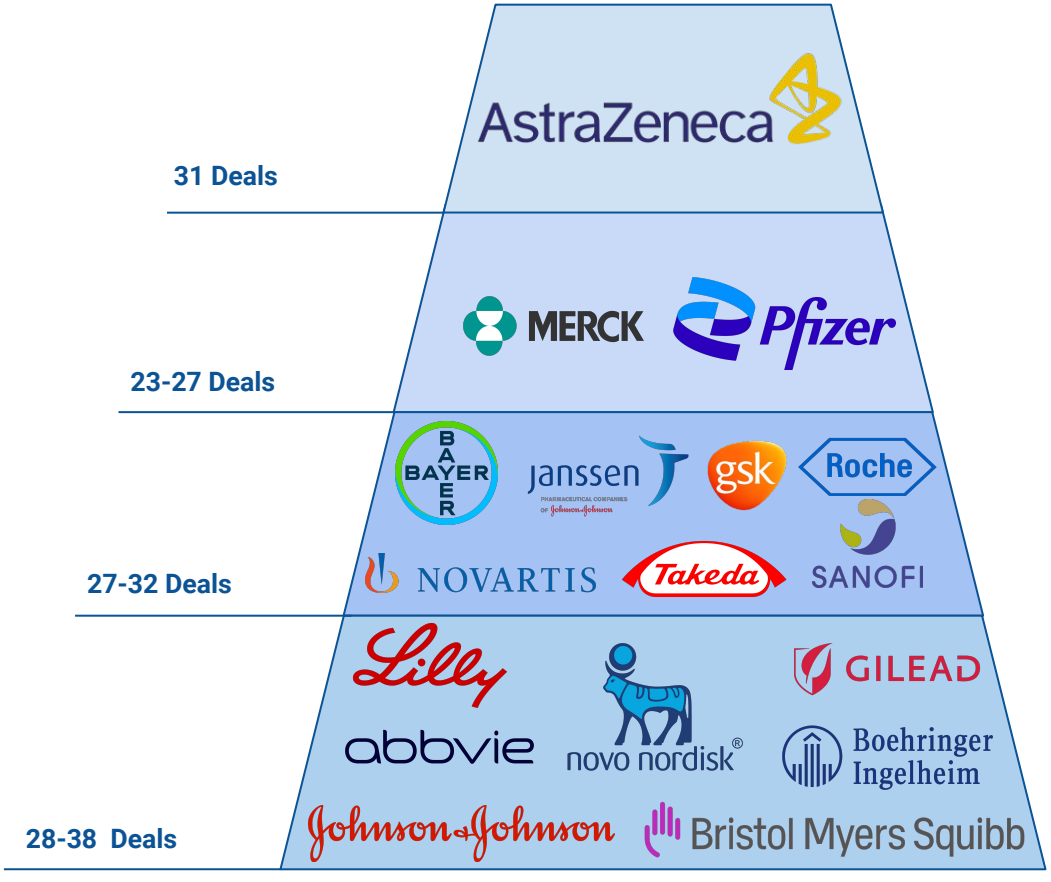
Sources: *Advantages of Structure-Based Drug Design Approaches in Neurological Disorders.*

Big Pharmas' AI-focused partnerships till Q3 2022

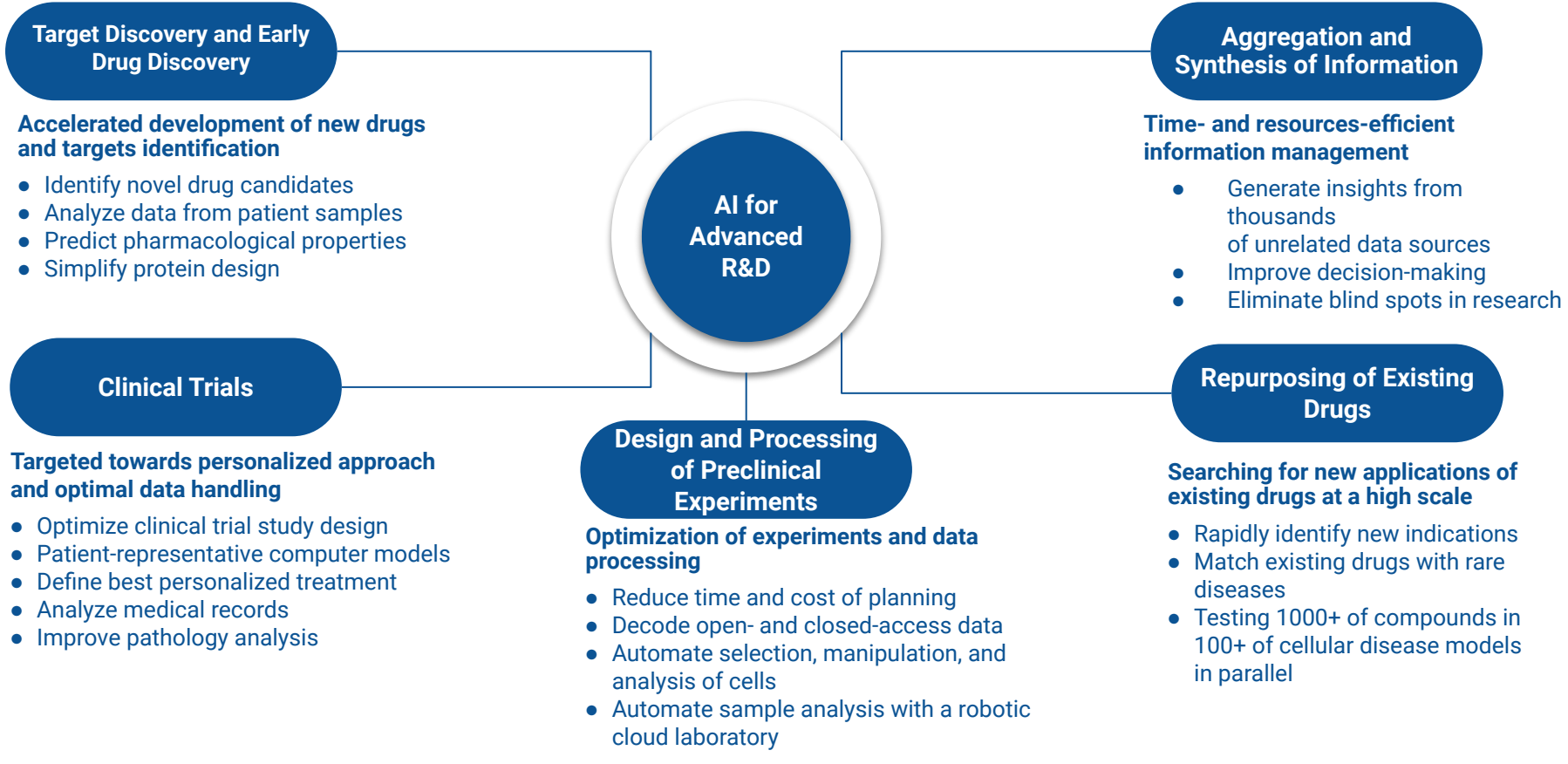
In this report we have profiled **600 actively developing AI-driven biotech companies**. A steady growth in the AI for Drug Discovery sector can be observed in terms of substantially increased amount of investment capital pouring into the AI-driven biotech companies (**$2.28B in HY 2020** against **$2.93B in HY 2021**), the increasing number of **research partnerships between leading pharma organizations and AI-biotechs, and AI-technology** vendors, a continuing pipeline of industry developments, research breakthroughs, and proof of concept studies, as well as exploding attention of leading media and consulting companies to the topic of AI in Pharma and healthcare.

Some of the leading pharma executives increasingly see AI as not only a tool for lead identification, but also a more general tool to boost biology research and identify new biological targets and develop novel disease models.

The main focus of AI research for today is still on small molecules as a therapeutic modality.



Application of AI for Advanced R&D to Address Pharma Efficiency Challenges



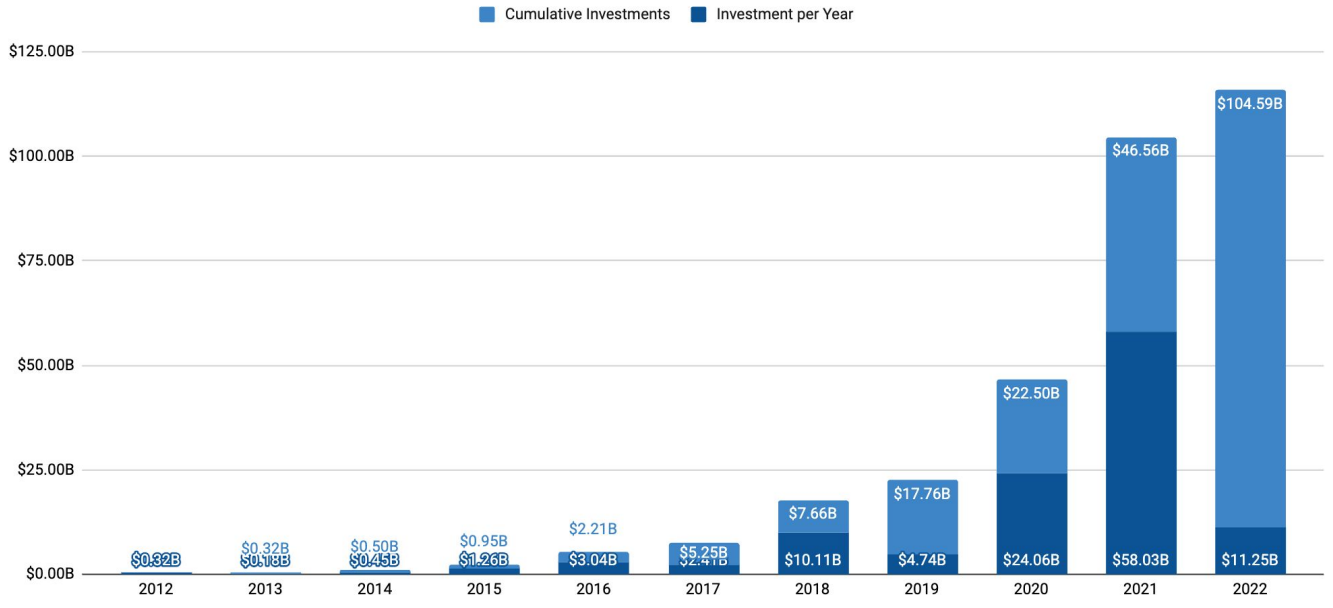
Business Activity

The business activity has been increasing in the pharmaceutical AI space over **Q1 2022 - Q3 2022**, judging by an increased number of transactions and partnership announcements in this period.

The most significant deals and collaborations in include:

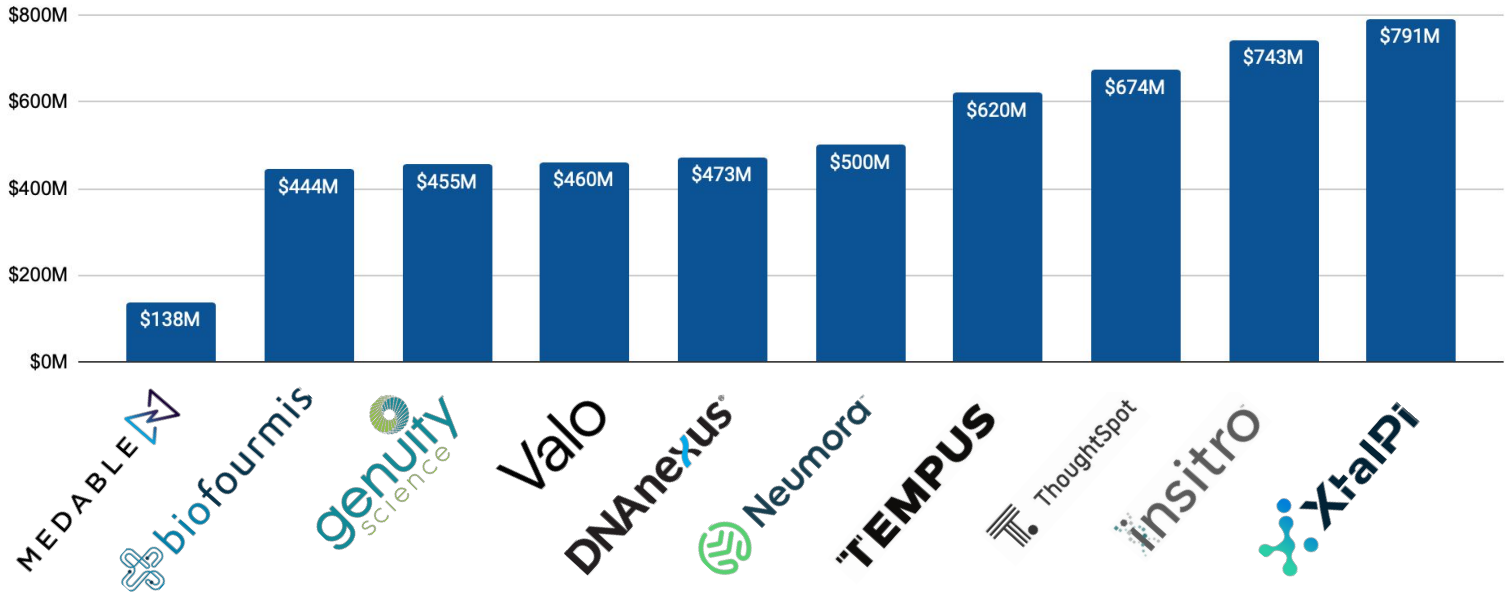
insitro, CASDIN CAPITAL, CPP INVESTMENT BOARD	**Insitro** has raised $400M for machine learning-powered drug discovery efforts. The financing was led by the **Canada Pension Plan Investment Board** with additional backing from **Andreessen Horowitz**, **Casdin Capital**
Valo, KDT KOCH DISRUPTIVE TECHNOLOGIES	**Valo Health** announced the final closing of its Series B at $300M, including a $110 million investment from Koch Disruptive Technologies (KDT). This brings the overall funding of Valo to over $450M to accelerate the creation of life-changing drugs
AMGEN, Mila	**Amgen** — **Mila** partnership that permits Amgen to expand its knowledge of AI and deep learning by interacting and engaging with experts in Mila's unique ecosystem
Exscientia, SANOFI	**Exscientia** sealed a $5.2B deal (biggest deal of A.I.) to expand an ongoing collaboration agreement with **Sanofi** to include 15 new molecules.
anumana, Janssen, MAYO CLINIC	**Anumana**, **Janssen** and **Mayo Clinic** have developed ECG-based Pulmonary Hypertension (PH) Early Detection Algorithm which will help doctors identify pulmonary hypertension early, a condition that is progressive and life-threatening.
novo nordisk, Microsoft	**Microsoft** and **Novo Nordisk** signed a contract to expedite the company's drug discovery process.

Dynamics of Investments in AI in Drug Development



There has been a substantial increase in the amount of capital invested in AI-driven pharma companies **since 2014.** During the last seven years, the annual amount of investments in **600** companies has increased by almost **52 times** (to **$115.84B** in total as of October 2022). In 2021, the flow of investments increased by **143%** compared to the previous year. The estimated amount of investments in the AI in Pharma sub-sector of the Longevity industry has increased in **2.5** times in 2021 compared to 2020 which identifies strong investors' (foremost VCs) interest in this field regardless of risks.

Top 10 AI in Pharma Companies by Total Investments in Q2-Q3 2022



The chart shows the top 10 AI-driven drug discovery companies sorted by the **total funding** raised by the end of Q3 2022. **XtalPi**, an artificial intelligence-powered drug R&D company, is now at the top of the list. Having completed the business combination with **Excelra**, **XtalPi** has the total funding raised to **$791M**. Insitro, american company utilizing ML drug discovery, could finance **$743M** in capital market. Tempus, Insitro and ThoughtSpot are new companies due to late-stage mega-rounds during the 2021.

Major Observations for Q2-Q3 2022: Key Business Takeaways

The segment of pharmaceutical AI continues consolidation with the increasing number of later stage mega-rounds, including XtalPi, Neuromora Therapeutics and Insitro (both $400M), Medable and Biofourmis (both $304M), Insilico Medicine ($255M), and DNAnexus and Genuity Science (both $200M). The AI start-up pack is clear leaders with significant resources, financial leverage, technical edge, and laggards with fewer finances, technology, and scientific assets. Besides, there is one company that received IPO status recently: Benevolent AI .

The pharmaceutical AI business is "heating up", becoming a profitable area for expert biotech investors as well as investor groups looking to diversify their portfolios with high-risk/high-reward firms. A growing number of proof-of-concept breakthroughs confirm that AI technology has matured enough to provide tangible value to pharma and contract research organizations (CROs).

Due to quickly growing proof of AI tech feasibility and innovation potential, **big pharma** and **contract research organizations are actively competing for AI collaborations**. **Amgen** and **Generate Biomedicines** will team together to find and develop protein therapies for five clinical targets using a variety of treatment methods and therapeutic regions. **Cyclica** has announced 10 new academic partnerships. With its new agreements, Cyclica hopes to **equip academia academics with AI-enhanced drug development platforms and hasten the process**.

Major Observations for Q2-Q3 2022: Key Business Takeaways

The global COVID-19 pandemic prolongs the rise of **the overall biotech and drug discovery sectors.** During 2021 we have observed over 100 medium and large funding rounds for biotech and drug design companies, especially those focused on antiviral therapies and vaccines.

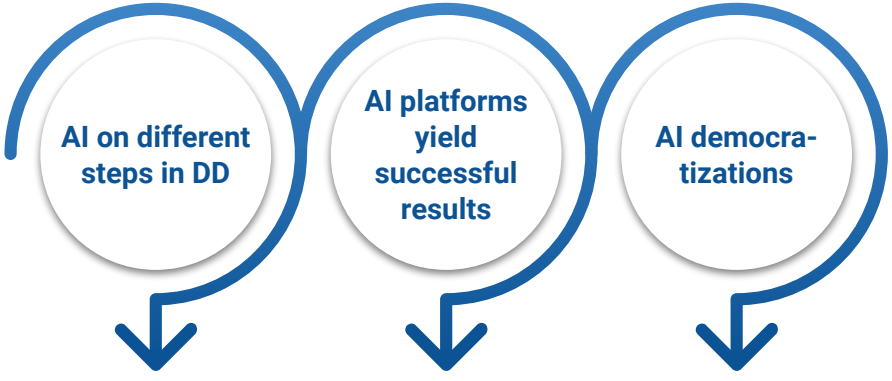
In Q2-3 2022, **1 company that use AI for DD reached IPO status**. London-based Benevolent AI closed its IPO in April and raised $292M. The vast majority of companies started gaining IPO status after 2018, marked by a growth of 136.0% during the last four years and we expect this trend growth to continue.

When some of the companies complete IPOs in the nearest future, it will attract a **significant number of non-biotech investors to enter the Life Sciences sector**. The prospects of this trend are already vivid: big tech companies enter partnerships with both innovative start-ups and pharma companies to consolidate resources, mainly in personalized medicine, cell and gene therapy, and molecule prediction software. Some of these companies even open subsidiaries harvesting AI in Drug Design (like Isomorphic Labs from Google).

The growing industry traction, reflected in the increasing number of R&D partnerships between big pharma and CROs with AI startups, is a sign that the market is maturing for rapid increase in M&A activity in the nearest future. Because of the crisis AI-in-Drug Development publicly traded companies fell to **$85,7B of cumulative capitalization as of October 3rd, 2022**.

Key Technology Takeaways

1. AI is regarded by some top executives at big pharma (**GSK and others**) as **a tool to uncover not only new molecules, but also new targets**. Ability of deep neural networks to build ontologies from multimodal data (e.g. "omics" data) is believed to be among the most disruptive areas for AI in drug discovery, alongside with data mining from unstructured data, like text (using natural language processing, NLP).
2. There is **a considerable trend for "AI democratization"** where various machine learning/deep learning technologies become available in pre-trained, pre-configured "of-the-shelf" formats, or in relatively ready-to-use formats — via cloud-based models, frameworks, and drag-and-drop AI-pipeline building platforms (for example, KNIME). This is among key factors in the acceleration of AI adoption by the pharmaceutical organizations — where a non-AI experts can potentially use fairly advanced data analytics tools for their research.
3. **Proof-of-concept projects keep yielding successful results** in research studies, and in the commercial partnerships alike. For example, companies like Recursion Pharmaceuticals, Insilico Medicine, Deep Genomics, and Exscientia achieved important research milestones using their AI-based drug design platforms.



AI is used not only for drug design, but also target identification.

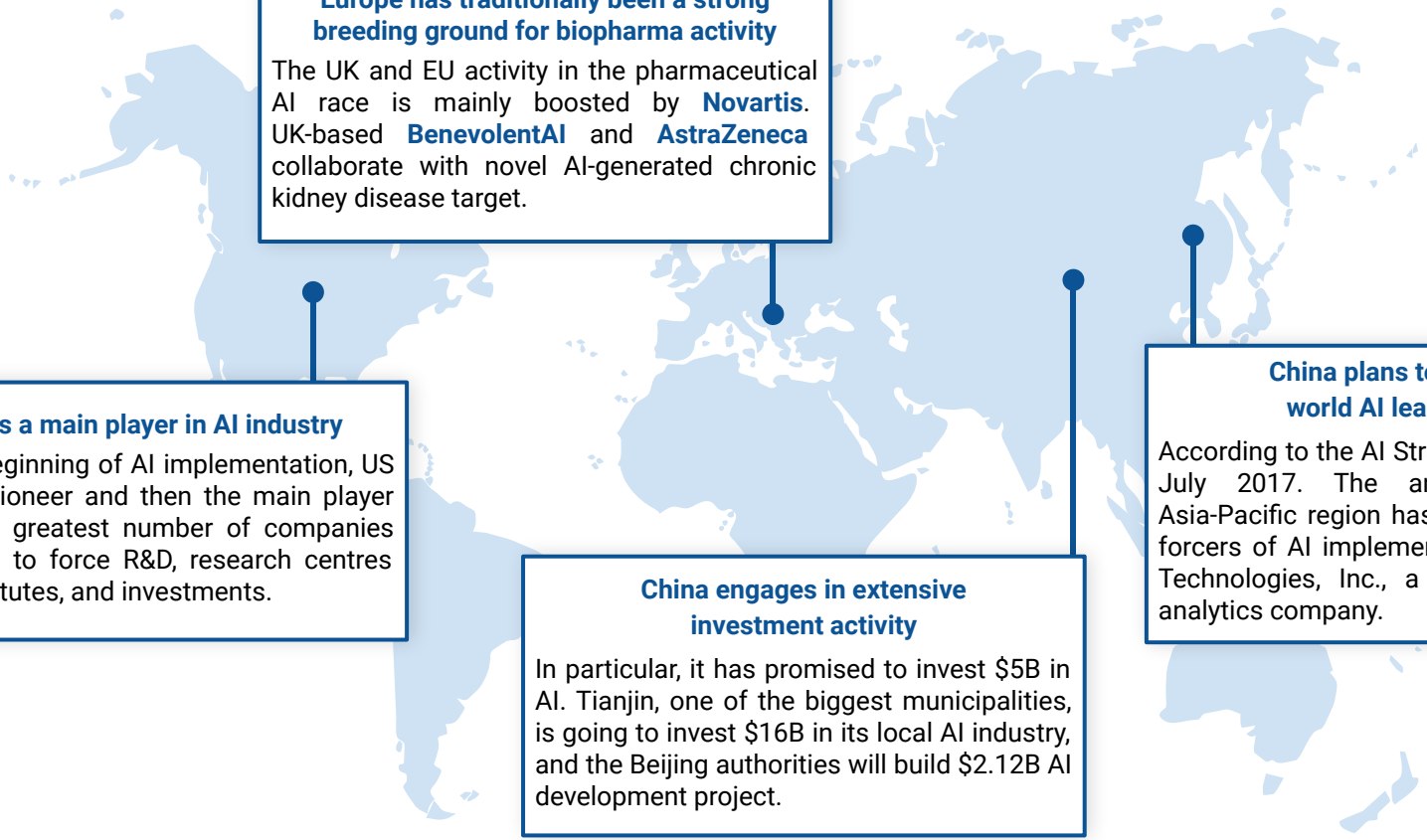
Many AI-designed drugs showed successful results in research studies and even clinical trials.

Ready-to-use AI platforms for DD became available and can be used by non-AI experts.

Obstacles That Still Remain

1. **Global shortage of AI talent** continues to be a serious challenge for the biopharma industry, repeating the trend from our previous reports. While big pharmaceutical companies invest substantial capital in recruitment of AI specialists, still the majority of them are acquired by large tech corporations (Google, Amazon, Alibaba, Tencent, Baidu etc.) However, a growing wave of specialized university programs and courses, geared towards data science and AI application, is projected to address this issue to certain extent in the coming years.
2. **Lack of available quality data is still a challenge for the unleashing full potential of deep learning technologies.** Numerous variations of deep learning (DL) are believed to be the most lucrative area of AI for applications such as drug discovery and clinical research. The key challenge is that DL algorithms are "data-greedy", while big data in biotech is not always well-versed for modeling, or is inaccessible due to privacy reasons.
3. **Ethical, legal, and regulatory issues for AI adoption in the pharmaceutical sciences.** This set of challenges is related to the previous point, but also includes other questions — AI explainability, patentability of AI-generated results, non-optimal regulations in various countries, slowing down the progress and adoption of AI technologies in general, and in the pharmaceutical industry in particular.

AI in the Global Context



Europe has traditionally been a strong breeding ground for biopharma activity

The UK and EU activity in the pharmaceutical AI race is mainly boosted by **Novartis**. UK-based **BenevolentAI** and **AstraZeneca** collaborate with novel AI-generated chronic kidney disease target.

US is a main player in AI industry

In the beginning of AI implementation, US was a pioneer and then the main player with the greatest number of companies using AI to force R&D, research centres and institutes, and investments.

China engages in extensive investment activity

In particular, it has promised to invest $5B in AI. Tianjin, one of the biggest municipalities, is going to invest $16B in its local AI industry, and the Beijing authorities will build $2.12B AI development project.

China plans to become the world AI leader by 2030

According to the AI Strategic Plan released in July 2017. The analysis of the the Asia-Pacific region has shown that the main forcers of AI implementation include Saama Technologies, Inc., a leading clinical data analytics company.

Business Activity: Overview

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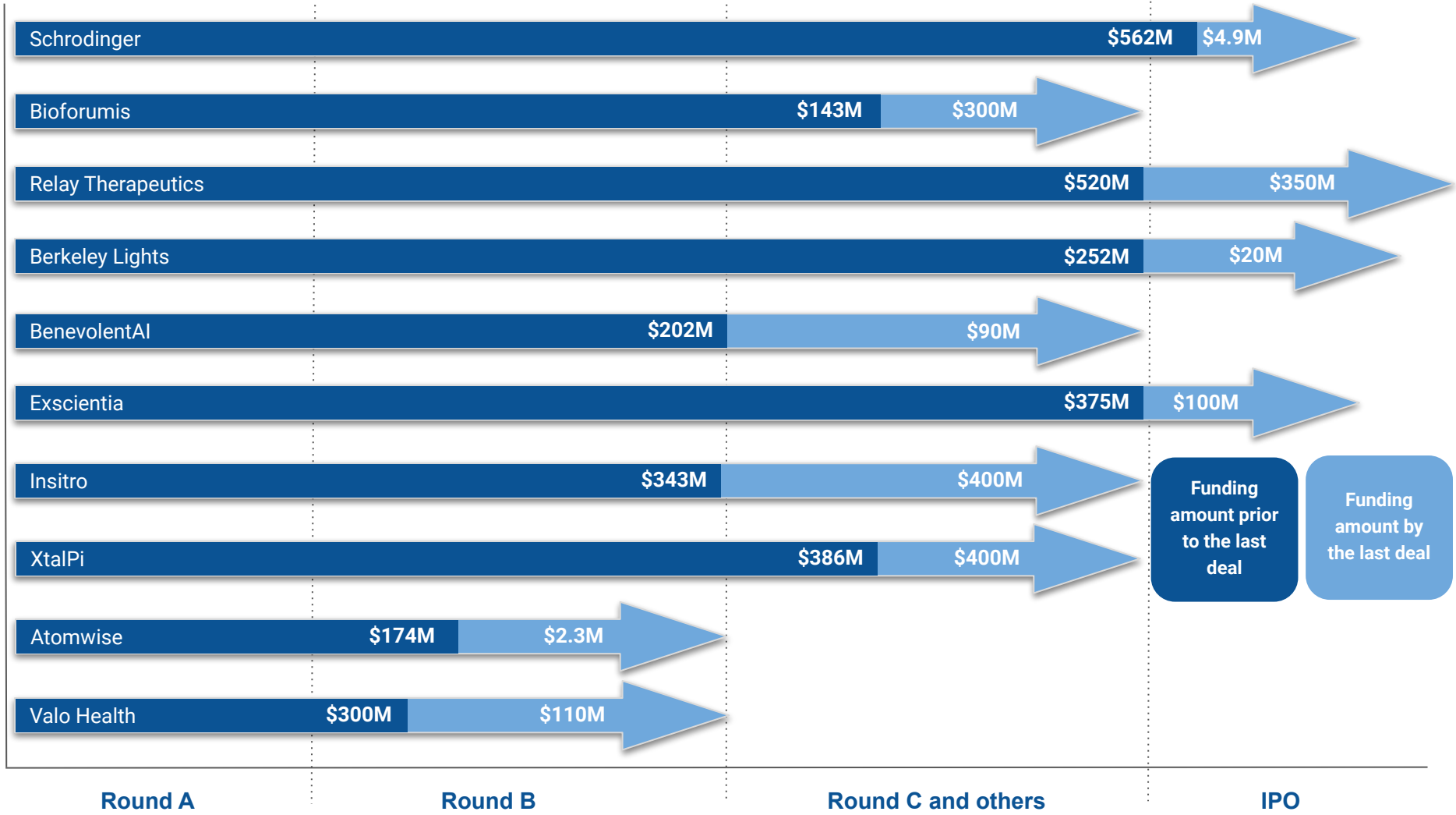
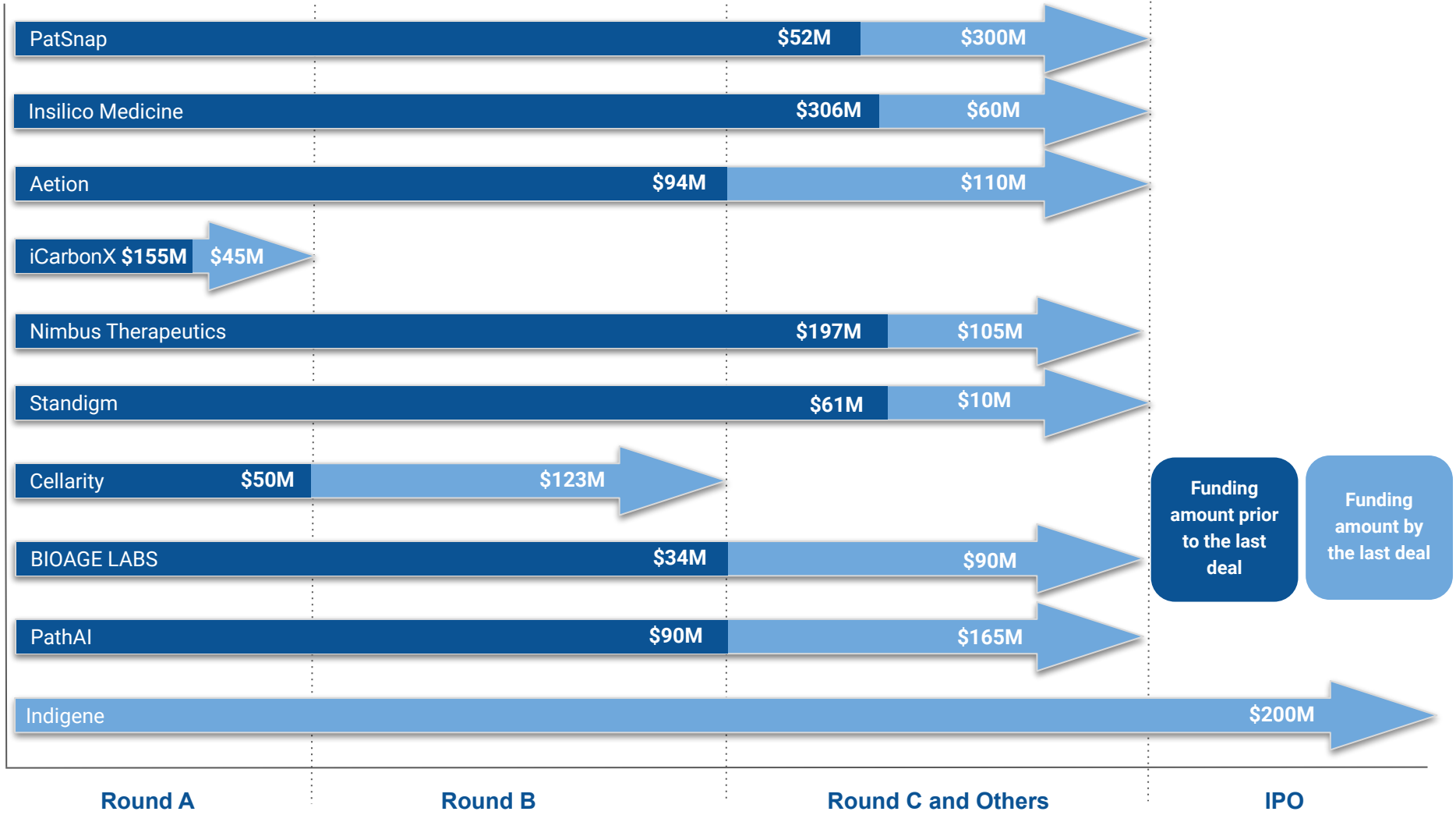

Schrodinger
$562M
$4.9M
Bioforumis
$143M
$300M
Relay Therapeutics
$520M
$350M
Berkeley Lights
$252M
$20M
BenevolentAI
$202M
$90M
Exscientia
$375M
$100M
Insitro
$343M
$400M
XtalPi
$386M
$400M
Atomwise
$174M
$2.3M
Valo Health
$300M
$110M
Funding amount prior to the last deal
Funding amount by the last deal
Round A
Round B
Round C and others
IPO


PatSnap
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Aetion
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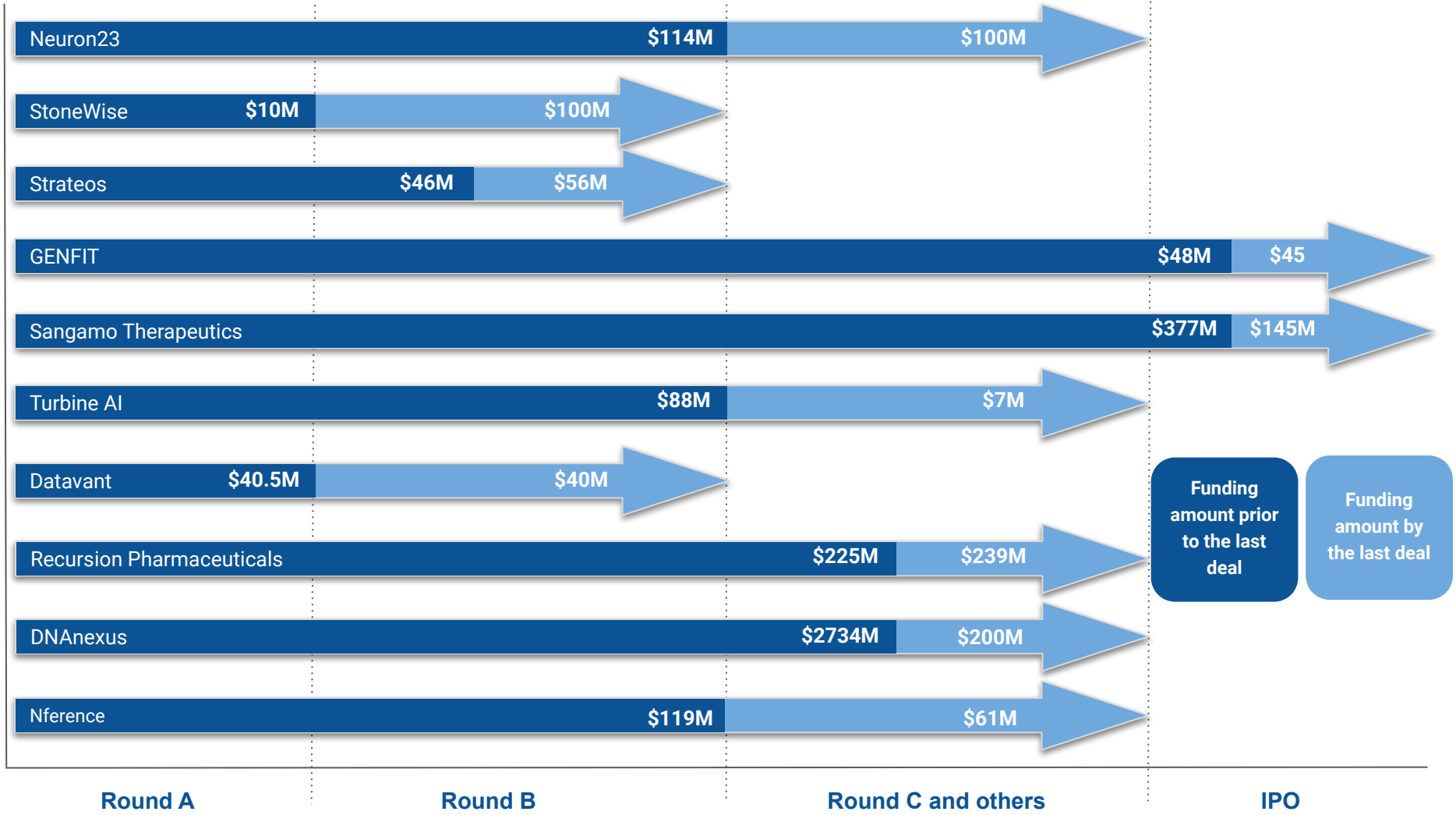
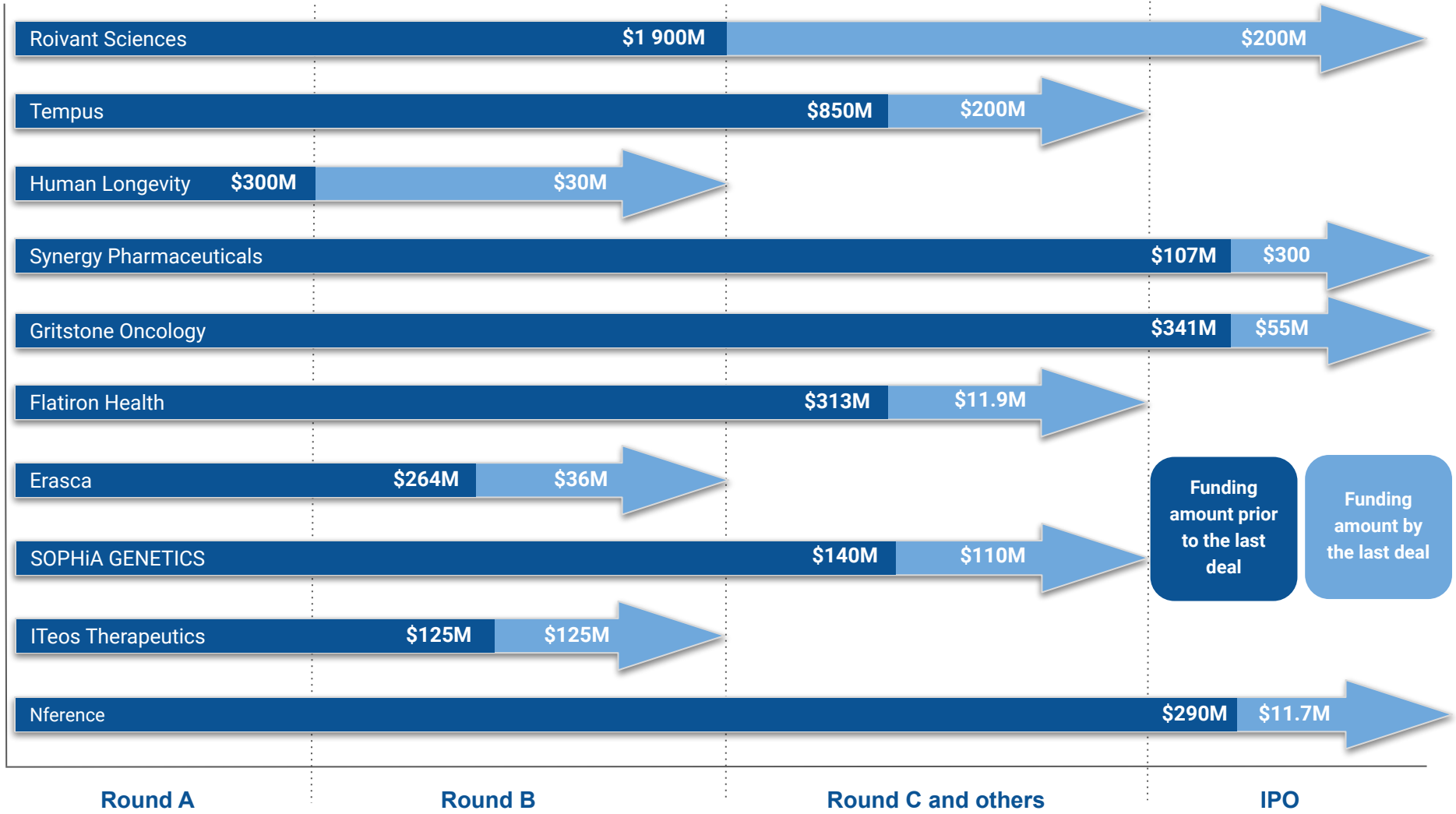
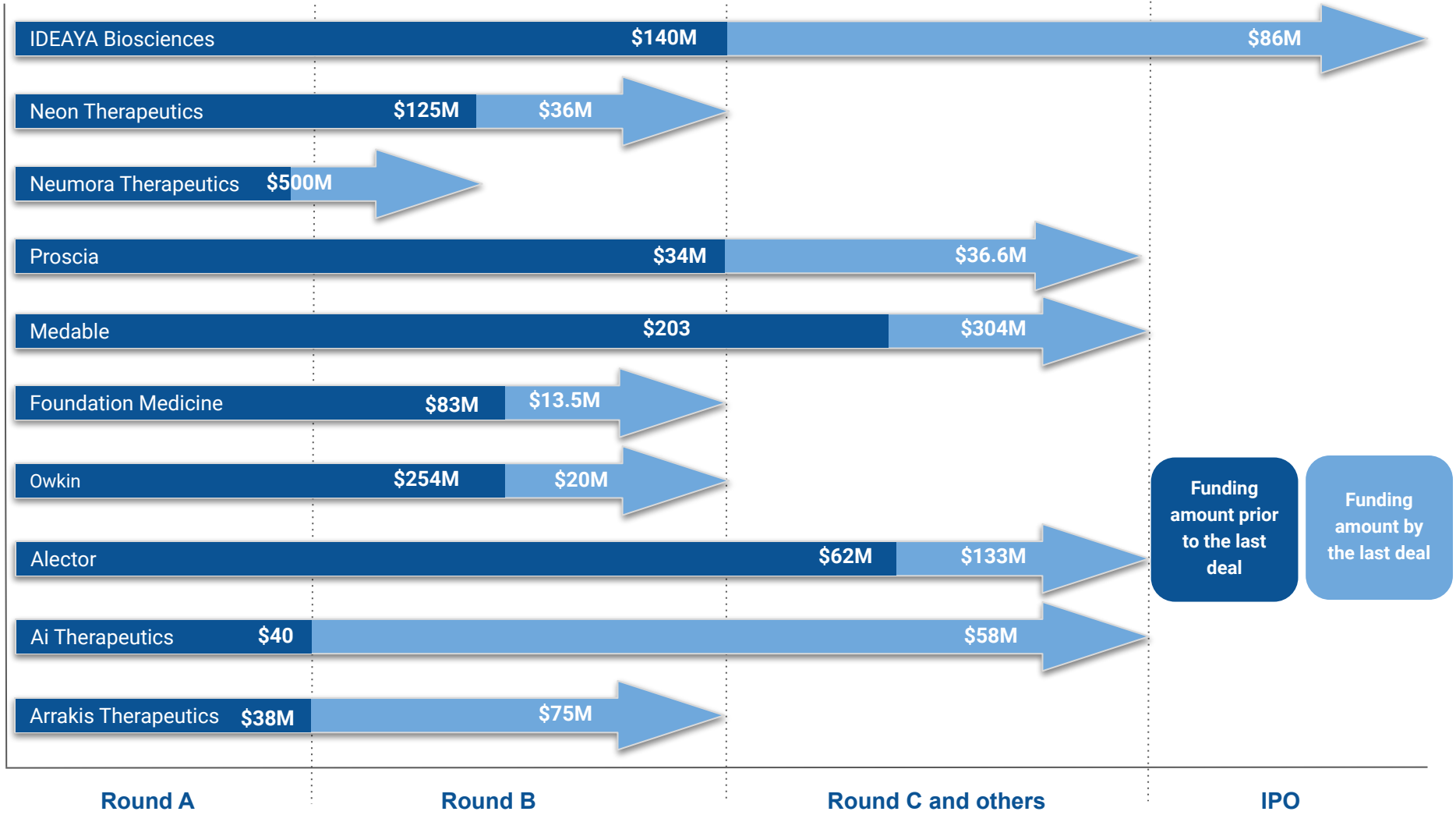
$110M
iCarbonX $155M
$45M
Nimbus Therapeutics
$197M
$105M
Standigm
$61M
$10M
Cellarity
$50M
$123M
BIOAGE LABS
$34M
$90M
PathAI
$90M
$165M
Indigene
$200M
Funding amount prior to the last deal
Funding amount by the last deal
Round A
Round B
Round C and Others
IPO


Neuron23
$114M
$100M
StoneWise
$10M
$100M
Strateos
$46M
$56M
GENFIT
$48M
$45
Sangamo Therapeutics
$377M
$145M
Turbine AI
$88M
$7M
Datavant
$40.5M
$40M
Recursion Pharmaceuticals
$225M
$239M
DNAnexus
$2734M
$200M
Nference
$119M
$61M
Funding amount prior to the last deal
Funding amount by the last deal
Round A
Round B
Round C and others
IPO


Roivant Sciences
$1 900M
$200M
Tempus
$850M
$200M
Human Longevity
$300M
$30M
Synergy Pharmaceuticals
$107M
$300
Gritstone Oncology
$341M
$55M
Flatiron Health
$313M
$11.9M
Erasca
$264M
$36M
SOPHiA GENETICS
$140M
$110M
ITeos Therapeutics
$125M
$125M
Nference
$290M
$11.7M
Funding amount prior to the last deal
Funding amount by the last deal
Round A
Round B
Round C and others
IPO


IDEAYA Biosciences
$140M
$86M
Neon Therapeutics
$125M
$36M
Neumora Therapeutics
$500M
Proscia
$34M
$36.6M
Medable
$203
$304M
Foundation Medicine
$83M
$13.5M
Owkin
$254M
$20M
Alector
$62M
$133M
Ai Therapeutics
$40
$58M
Arrakis Therapeutics
$38M
$75M
Funding amount prior to the last deal
Funding amount by the last deal
Round A
Round B
Round C and others
IPO

50 Leading Investors in Pharmaceutical AI

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50 Leading Investors in AI for Drug Discovery Sector

1	Casdin Capital
2	Creative Destruction Lab (CDL)
3	SOSV
4	National Science Foundation
5	GV
6	Y Combinator
7	Perceptive Advisors
8	Alexandria Venture Investments
9	Sequoia Capital China
10	RA Capital Management
11	Merck Global Health
12	Alumni Ventures
13	Khosla Ventures
14	Foresite Capital
15	8VC
16	DCVC Bio
17	National Institute of Health
18	EASME - EU Executive Agency
19	MassChallenge
20	T.Rowe Price
21	SoftBank Vision Fund
22	Invus
23	Deerfield
24	F-Prime Capital
25	Redmile Group
26	DCVC Bio
27	Founders Fund
28	IndieBio
29	Fidelity Management
30	Surveyor Capital
31	Temasek Holding
32	Cormorant Asset Management
33	5Y Capital
34	Northpond Ventures
35	Obvious Ventures
36	Andreessen Horowitz
37	Section 32
38	Lux Capital
39	AME Cloud Ventures
40	Eight Roads Ventures
41	Lifeforce Capital
42	Felicis Ventures
43	BlackRock
44	Foresite Capital
45	Janus Henderson Investors
46	Tencent
47	ARCH Venture Partners
48	Novo Holdings
49	Flagship Pioneering
50	Biotechnology Value Fund

Top-50 AI in Pharma Investors

San Francisco

- **8VC** — San Francisco, California, US
- **Founders Fund** — San Francisco, California, US
- **Foresite Capital** — San Francisco, California, US
- **DCVC** — San Francisco, California, US
- **Alexandria Venture** — San Francisco, California, US
- **Obvious Ventures** — San Francisco, California, US
- **Lifeforce Capital** — San Francisco, California, US
- **DCVC Bio** — San Francisco, California, US

Mountain View

- **Y Combinator** — Mountain View, California, US
- **GV** — Mountain View, California, US

Palo Alto

- **AME CLoud Ventures** — Palo Alto, California, US
- **Alexandria Venture Investments** — Pasadena, California, US

New York

- **OrbiMed** — New York, New York, US
- **Bristol-Myers Squibb** — New York, New York, US
- **Perceptive Advisors** — New York, New York, US
- **Invus** — New York, New York, US
- **Casdin Capital** — New York, New York, US

Maryland

- **National Institute of Health** — Maryland, US
- **Northpond Ventures** — Maryland, US

Menlo Park

- **Andreessen Horowitz** — Menlo Park, California, US
- **Felicis Ventures** — Menlo Park, California, US
- **Khosla Ventures** — Menlo Park, California, US

Illinois

- **Deerfield Capital** — Rosamond Ridge, Illinois, US
- **ARCH Venture Partners** — Chicago, Illinois, US

Other States

- **Altitude Life Science Ventures** — Washington, US
- **Lili Ventures** — Indianapolis, Indiana, US
- **SOSV** — Princeton, New Jersey, US
- **National Science Foundation** — Alexandria, Virginia, , US
- **T. Rowe Price** — Baltimore, Maryland, US

Massachusetts

- **MassChallenge** — Boston, Massachusetts, US
- **RA Capital Management** — Cambridge, Massachusetts, US
- **Cormorant Asset Management** — Boston, Massachusetts, US
- **Third Rock Ventures** — Boston, Massachusetts, US
- **F-Prime Capital** — Cambridge, Massachusetts, US

Manhattan Beach

- **B Capital Group** — Manhattan Beach, California, US

Switzerland

- **HBM Healthcare Investments AG** — Zug, Switzerland
- **Roche** — Basel, Switzerland

Denmark

- **Novo Holdings** — Hellerup, Hovedstaden, Denmark

Singapore

- **EDBI** — Singapore, Central Region
- **Temasek** — Singapore, Central Region

Canada

- **Creative Destruction Lab (CDL)** — Toronto, Canda

United Kingdom

- **SoftBank Vision Fund** — London, England, The UK
- **Counterpoint Global** — London, England, The UK
- **Baillie Gifford** — Edinburgh, Edinburgh, The UK
- **Janus Henderson Investors** — London, England, The UK

Beijing

- **ZhenFund** — Beijing, China
- **Sequoia Capital China** — Beijing, China

Shanghai

- **5Y Capital** — Shanghai, China
- **Lilly Asia Ventures** — Shanghai, China
- **Ping An Bank** — Shenzhen, China
- **Tencent** — Shenzhen, China
- **GT Healthcare Capital Partners** — Central, Hong Kong Island, Hong Kong

Top-50 Investors in AI Companies

INVESTORS	AI FOR DRUG DISCOVERY COMPANIES	HEADQUARTERS LOCATION	INVESTED IN
Casdin Capital	19	USA	Absci, Alector, Arzeda, Beacon Biosignals, Celsius Therapeutics, Clover Therapeutics, Exscientia, Gritstone Oncology, Fabric Genomics, Flatiron Health, Foundation Medicine, Lunit, Insitro, Paige, Recursion Pharmaceuticals, Relay Therapeutics, Sema4, ShouTi, SomaLogic, Treeline Biosciences
Creative Destruction Lab (CDL)	15	Canada	Biotx.ai, DeepCure, DeepLife, Entropica Labs, Epistemic AI, Juvena Therapeutics, Kyndi, Kuano, Menten AI, NetraMark,OrganoTherapeutics, ProteinQure, Winterlight Labs, Valence Discovery
SOSV	14	USA	A2A Pharmaceuticals, Gatehouse Bio, Guided Clarity, Mendel.ai, Stelvio Therapeutics, Strados, Synthace
National Science Foundation	14	USA	bioSyntagma, ADM Diagnostic, Bioz, Cloud Pharmaceutical, Data2Doscovery, Strados Labs, VeriSIM Life, TeselaGen,
GV	13	USA	DNAnexus, Flatiron Health, Foundation Medicine, IDEAYA Bioscience, insitro, Owkin, Schrödinger, Relay Therapeutics, Ultromics, Celsius Therapeutics, Alector,
Y Combinator	12	USA	HistoWiz, iLab Service, Menten AI, Reverie Labs, Segmed, Arpeggio Bio, Athelas, Atomwise, CloudMedx, Coral Genomics
Perceptive Advisors	11	USA	Absci, Alector, Black Diamond Therapeutics, Champions Oncology, DNAnexus, Icosavax, IDEAYA Biosciences, Neuron23, Saama, Sema4, Soma Logic, Relay Therapeutics
Alexandria Venture Investments	11	USA	Arrakis Therapeutics, Celsius Therapeutics, Deep Genomics, GNS Healthcare, Gritstone Oncology, IDEAYA Biosciences, Immunai, Insitro, Fountain Therapeutics, LEXEO Therapeutics, Neuromora Therapeutics, Veralox Therapeutics
Sequoia Capital China	10	China	METiS Therapeutics, PatSnap, Transcenta, XtalPi, Adagene, Athelas, Biofourmis, Deep Intelligent Pharma, HiFiBiO, Genuity Bio
RA Capital Management	9	USA	Nimbus Therapeutics, Wave Life Sciences, Bristol Myers Squibb, Xbiome, Everest Medicines, Freenome, Frontier Medicines, Icosavax

Top-50 Investors in AI Companies

INVESTORS	AI FOR DRUG DISCOVERY COMPANIES	HEADQUARTERS LOCATION	INVESTED IN
Merck Global Health	9	USA	OpGen, PathAI, PreciseDx, Strata Oncology, Verge Genomics, Absci, Antidote.me
Alumni Ventures	9	USA	Emerald Cloud Lab, Notable Labs, Olaris, Scipher Medicine, Strateos, Unlearn.AI, Veralox Therapeutics, Verge Genomics
Khosla Ventures	8	USA	Arpeggio Bio, Atomwise, BIOAGE LABS, Fountain Therapeutics, Deep Genomics, Menten AI, Ochre Bio, Scipher Medicine, ThoughtSpot
Foresite Capital	8	USA	Aetion, DNAnexus, Insitro, Relay Therapeutics, Wave Life Sciences
8VC	8	USA	BigHat Biosciences, Coral Genomics, Immunai, Model Medicine, Notable, ProteinQure, Unlearn.AI
DCVC Bio	8	USA	Empirico, Frontier Medicines, Totus Medicines, Unlearn.AI, X-37
National Institute of Health	8	USA	Imaginostics, PostEra, Sangamo Therapeutics, SEngine Precision Medicine, Simulations Plus, Virvio, bioSyntagma, Coral Genomics
EASME - EU Executive Agency for SMEs	8	USA	Quibim, Acellera, CellPly, Cytox, Genome Biologics, Genialis
MassChallenge	8	USA	Scailyte, Simply Speak, Strados Labs, Vyasa Analytics, ChemAlive sA, Agamon, OrganoTherapeutics
T.Rowe Price	7	USA	Arbor Biotechnologies, Generate Biomedicines, Genesis Therapeutics, Insitro, Sema4, SomaLogic, Tempus

Top-50 Investors in AI Companies

INVESTORS	AI FOR DRUG DISCOVERY COMPANIES	HEADQUARTERS LOCATION	INVESTED IN
SoftBank Vision Fund	7	UK	Biofourmis, Datavant, Deep Genomics, Exscientia, Insitro, PatSnap, Relay Therapeutics, Roivant Sciences, XtalPi
Invus	7	USA	Valo Health, Black Diamond Therapeutics,Engine Biosciences, Erasca, ITeos Therapeutics, Neumora Therapeutics, Schrödinger
Deerfield	7	USA	Sema4, Strata Oncology, Alector, ConcertoCare, Foundation Medicine, Frontier Medicines, Insilico Medicine, Schrödinger
F-Prime Capital	7	USA	BenchSci, Neumora Therapeutics, Notable, Owkin, Peptone, Adagene
Redmile Group	7	USA	Foundation Medicine, Gritstone Oncology, Neuron23, Wave Life Sciences, Absci
DCVC Bio	7	USA	Empirico, Frontier Medicines, Totus Medicines, Unlearn.AI, X-37
Founders Fund	7	USA	AbCellera Biologics, Datavant, Emerald Cloud Lab, Notable Labs, Roivant Sciences, DeepMind
IndieBio	7	USA	Gatehouse Bio, Guided Clarity, Stelvio Therapeutics, A2A Pharmaceuticals
Fidelity Management	6	USA	Roivant Sciences, Sema4, Wave Life Sciences, Absci, Deep Genomics, Generate Biomedicines,
Surveyor Capital	6	USA	ShouTi, Arbor Biotechnologies, Icosavax, Neumora Therapeutics, Neuron23, Nimbus Therapeutics

Top-50 Investors in AI Companies

INVESTORS	AI FOR DRUG DISCOVERY COMPANIES	HEADQUARTERS LOCATION	INVESTED IN
Temasek Holding	6	Singapore	Transcenta, BenevolentAI, Genuity Science, Glympse Bio, Insitro
Cormorant Asset Management	6	Switzerland	Strata Oncology, Wave Life Sciences, Biomea Fusion, Erasca, Icosavax
5Y Capital	6	China	Xbiome, XtalPi, AliveX Biotech, Galixir, METiS Therapeutics
Northpond Ventures	6	USA	Deep Lens, DNAnexus, Outcomes4Me, Scipher Medicine, Totus Medicines
Obvious Ventures	6	USA	LabGenius, Medable, Recursion Pharmaceuticals, ConcertoCare, Inato
Andreessen Horowitz	6	USA	Aria Pharmaceuticals, Asimov, BigHat Biosciences, BIOAGE LABS, Freenome
Section 32	6	USA	Character Biosciences, Glympse Bio, Nucleai, Verge Genomics,Alector
Lux Capital	6	USA	Alife, Auransa, LabGenius, Recursion Pharmaceuticals, Strateos
AME Cloud Ventures	6	USA	Asimov, Atomwise, Auransa, BigHat Biosciences, BIOAGE LABS
Eight Roads Ventures	6	UK	Owkin, ShouTi, WuXi AppTec, Adagene

Top-50 Investors in AI Companies

INVESTORS	AI FOR DRUG DISCOVERY COMPANIES	HEADQUARTERS LOCATION	INVESTED IN
Lifeforce Capital	6	USA	PostEra, TARA Biosystems, Verge Genomics, Character Bioscience
Felicis Ventures	6	USA	Juvena Therapeutics, LabGenius, ProteinQure, Spring Discovery
BlackRock	5	USA	Verge Genomics, Cellarity, Exscientia, Insitro, Sema4
Foresite Capital	5	USA	Wave Life Sciences, Aetion, DNAnexus, Insitro, Relay Therapeutics
Janus Henderson Investors	5	USA	Everest Medicines, LEXEO Therapeutics, ShouTi, SomaLogic
Tencent	5	China	Atomwise, Brainomix, iCarbonX, PatSnap, XtalPi
ARCH Venture Partners	5	USA	Arbor Biotechnologies, Erasca, Generate Biomedicines, Glympse Bio
Novo Holdings	5	Denmark	Kebotix, Tempus, Evotec, Exscientia,
Flagship Pioneering	5	USA	Valo Health, Cellarity, Generate Biomedicines,
Biotechnology Value Fund	5	USA	Evotec, Gritstone Oncology, IDEAYA Biosciences, Nimbus Therapeutics

Big Pharma’s Focus on AI

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AI and Pharma Collaborations in Q2 2022 - Q3 2022

Bayer, Aalto and **HUS** expanded collaboration to apply artificial intelligence to support clinical drug trials

HUS Helsinki University Hospital · Aalto University · BAYER

Elix announced a research partnership with **Shionogi** on the validating retrosynthetic analysis utilizing data from Shionogi.

ELIX · SHIONOGI

AstraZeneca obtains a second pulmonary fibrosis target with a partnership with **BenevolentAI**

AstraZeneca · Benevolent AI

Sanofi focuses on using **Atomwise's** AtomNet platform to conduct small molecule research on up to five therapeutic targets.

Atomwise · SANOFI

Jan 2022 | Feb 2022 | Mar 2022 | Apr 2022 | May 2022 | Jun 2022 | Aug 2022 | Sep 2022

Amgen collaborated with **Generate Biomedicines** to create protein therapeutics for five clinical targets. **Amgen** will pay potentially up to **$1.9 billion** in this collaboration for a novel AI driven platform

AMGEN · Generate:Biomedicines

Takeda and **Evozyne** will create novel gene therapies for up to four rare disease targets. The deal worth up to **$400 million**

Takeda · evozyne

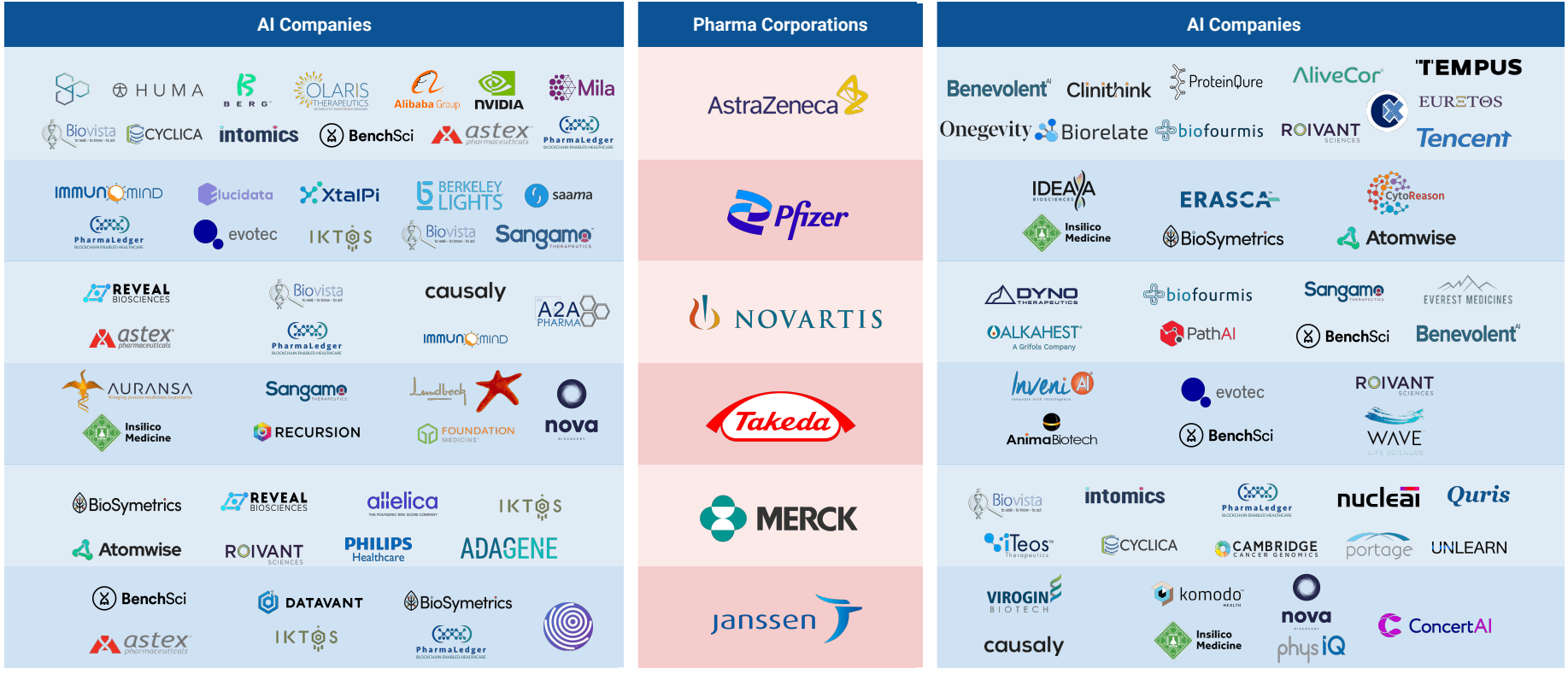
Aqemia and **Sanofi** will work together on a number of initiatives in cancer, a major therapeutic area for Sanofi, to design and find new medicines.

SANOFI · AQEMIA

The AI partnership between **Bayer** and **Exscientia**, which saw the two parties search for cardiovascular and cancer targets came to an end.

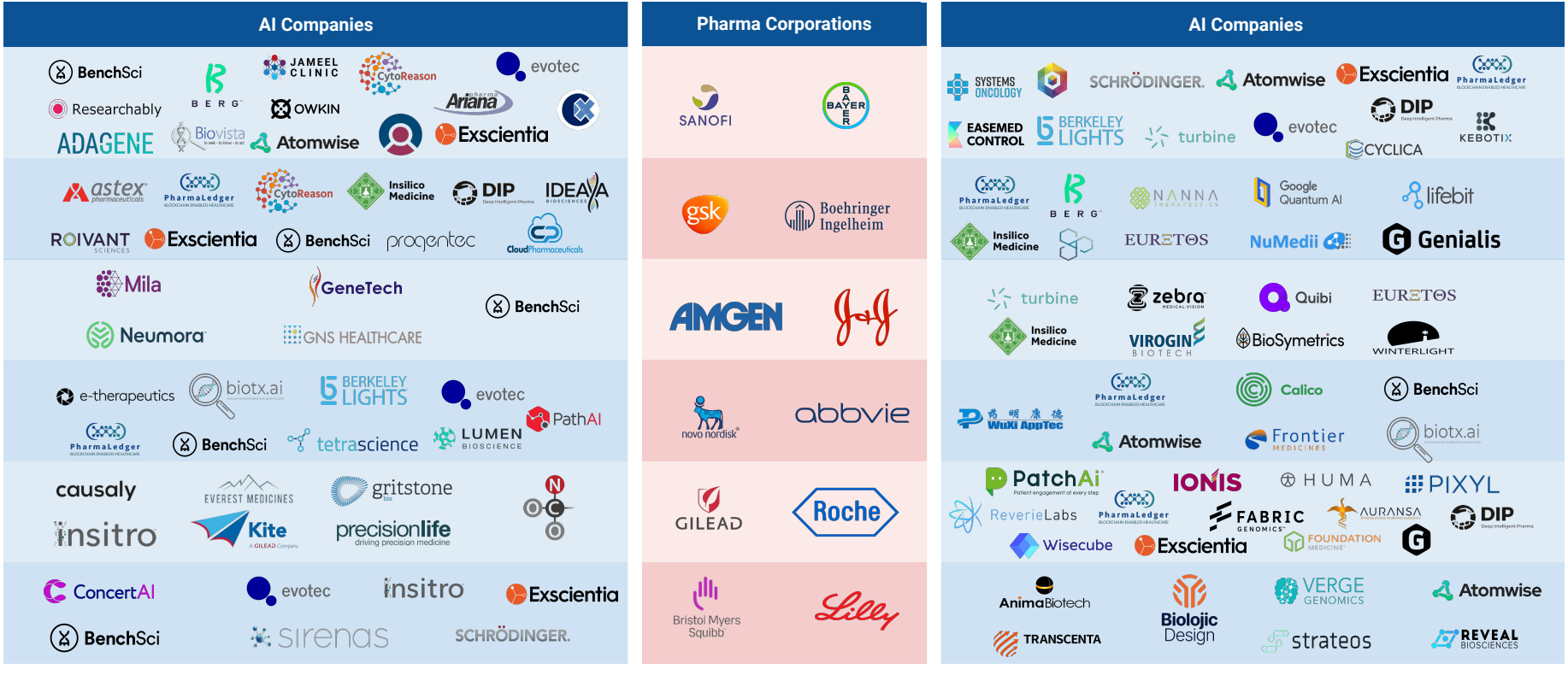
Exscientia · BAYER

Selected Pharma AI Deals



Note: the central column (red) defines the pharmaceutical corporations and side columns (blue) defines AI companies that have collaborations with pharma companies from the central column.

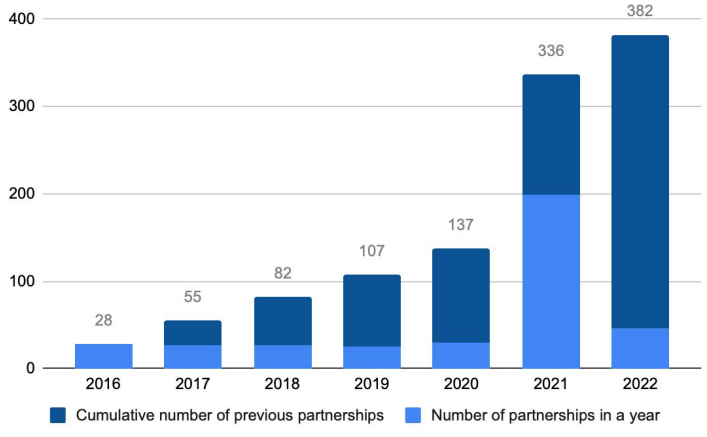
Selected Pharma AI Deals



Note: the central column (red) defines the pharmaceutical corporations and side columns (blue) defines AI companies that have collaborations with pharma companies from the central column.

A Growing Number of Collaborations Involving AI for Drug Discovery

Increasing number of partnerships between Pharma and AI Companies over the last 6 years



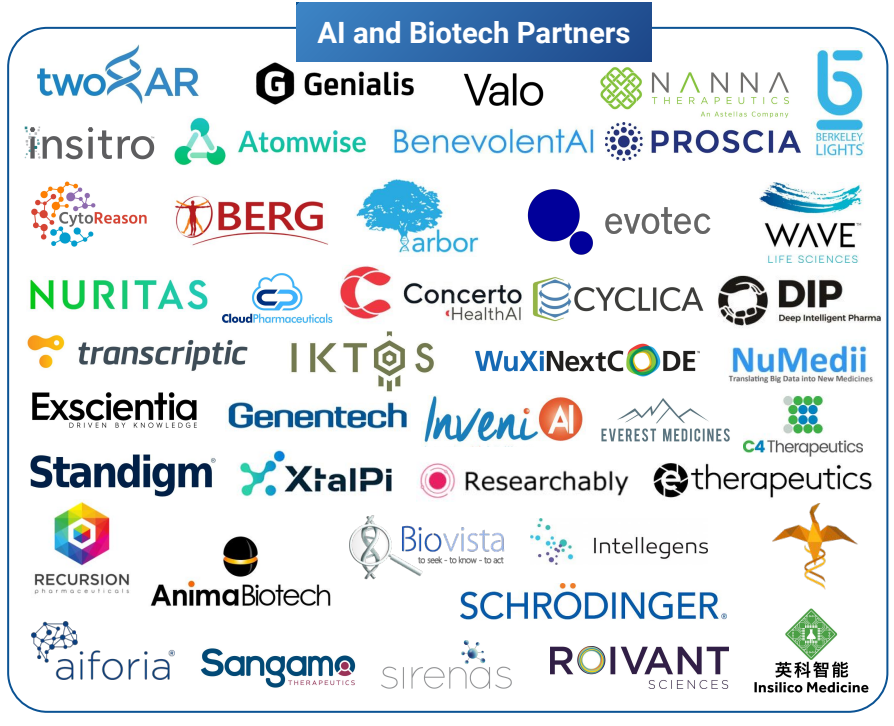
The rising interest of leading pharma and contract research organizations towards AI-driven biotech startups is a major driver for the area to become more attractive for investors, since the industry is becoming well-suited for successful exit strategies in future.

Summarizing industry observations over the last five years, we can observe a fundamental shift in perception of top executives at leading pharmaceutical organizations about the need of advanced AI technologies. Since 2015, there has been an obvious shift in the perception from skepticism and cuasious interest, all the way to a realization of a strategic role AI has to play in the emerging “data-centric” model of innovation. This change in perception was underpinned by a number of factors:

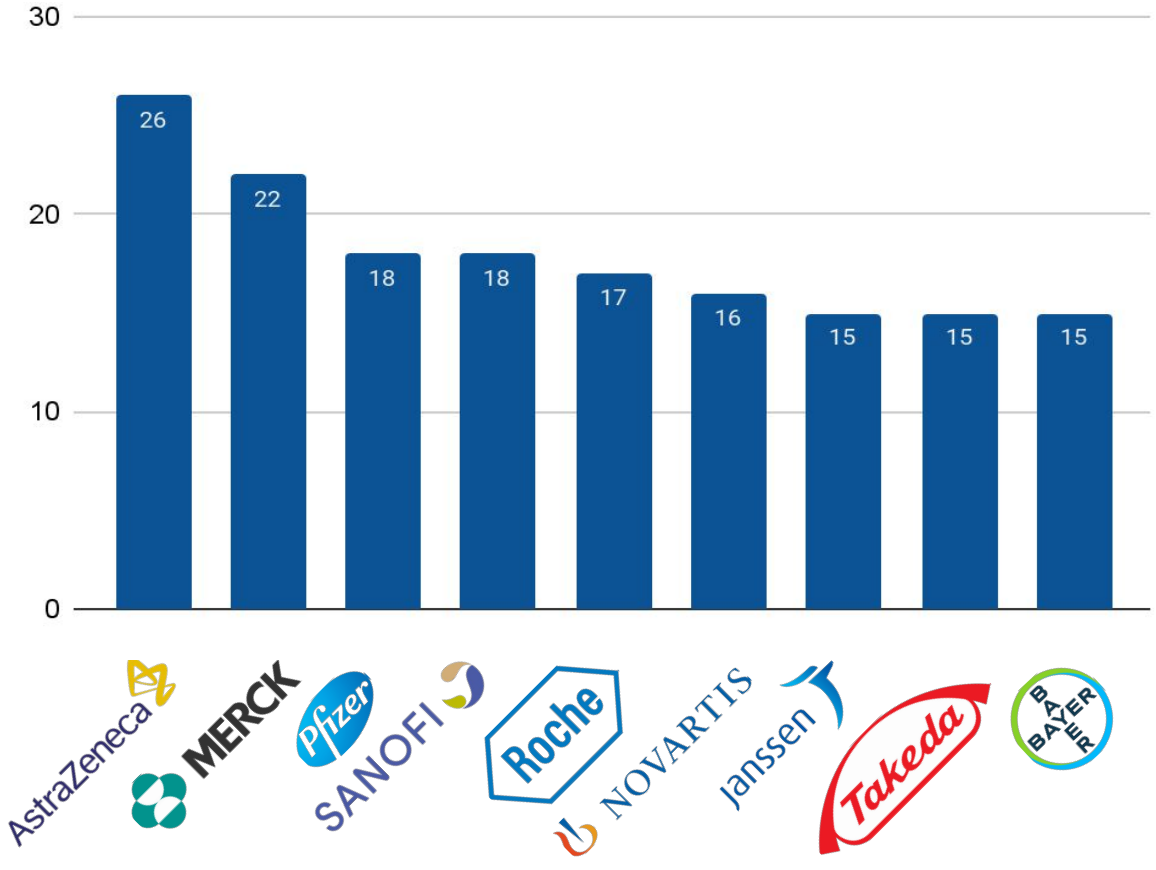
- a wave of proof-of-concept studies and research breakthroughs in a wide range of AI application use cases
- a number of commercial successes and successfully reached milestones, involving AI as a central element of research
- substantial advances in democratizing AI technology, where machine learning and deep learning algorithms become available at scale to non-AI experts
- decent increase in the overall understanding of AI “mechanics”, due to increasing efforts in the education and professional development with a focus on AI-driven tools and approaches

Pharmaceutical companies of all sizes start competing for AI-expertise, talent, and partnerships. In this report we summarize some of the most high-profile such collaborations, involving top-20 pharma giants. Even though, we can see a clear uprising trend in the number of collaborations, focused on AI-drug design, and other aspects of data mining and analytics.

Corporation and AI-companies Participating in the Pharma AI Deals

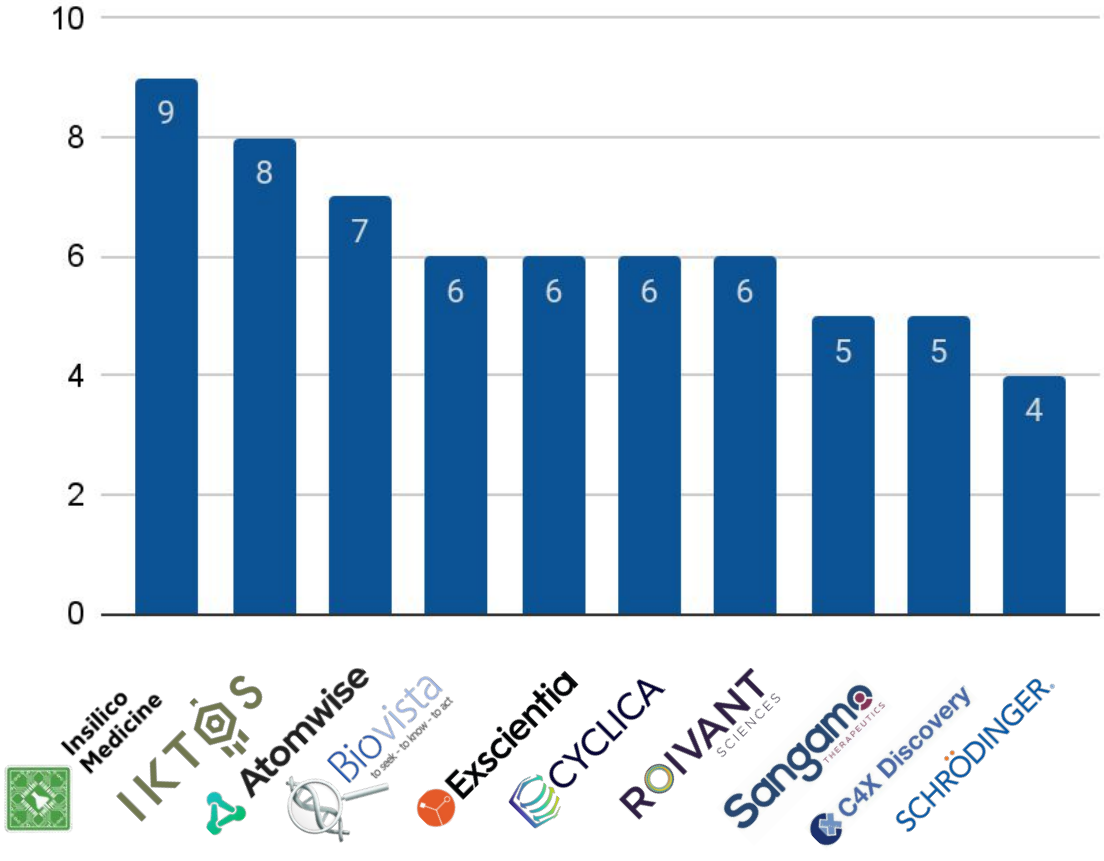


Leading Pharma Corporations by the Number of Pharma AI Deals in Q3 2022



- The leading Pharma players by the amount of major industry partnerships are **AstraZeneca** and **Merck**.
- These companies demonstrate increasing commitment to probing the grounds in the AI space — by investing into internal programs, as well as partnering with external AI vendors to pilot programs in drug discovery and other research areas.
- The most common type of deals are **true partnerships** and **saving the costs deals**.
- The leading big pharma brands are increasingly open to partnerships with AI startups and corporations to get competitive edge, and mitigate **the problem of declining R&D efficiency**.

Top-10 AI and Tech Partners by Number of Major Pharma AI Deals in 2021 - Q3 2022



- The leading AI players by the amount of major industry partnerships are **Insilico Medicine, IKTOS and Atomwise.**
- **The biggest number** of AI in Drug Discovery deals was conducted by **Insilico Medicine**.
- The company is an **end-to-end**, AI-driven pharma-technology company that accelerates drug development by proprietary **platform across biology, chemistry and clinical development**.
- All of the deals concluded with this company were categorized as the ones aiming at **saving costs and increasing operational efficiency** due to the character of the services provided.

AI in Pharma Publicly Traded Companies

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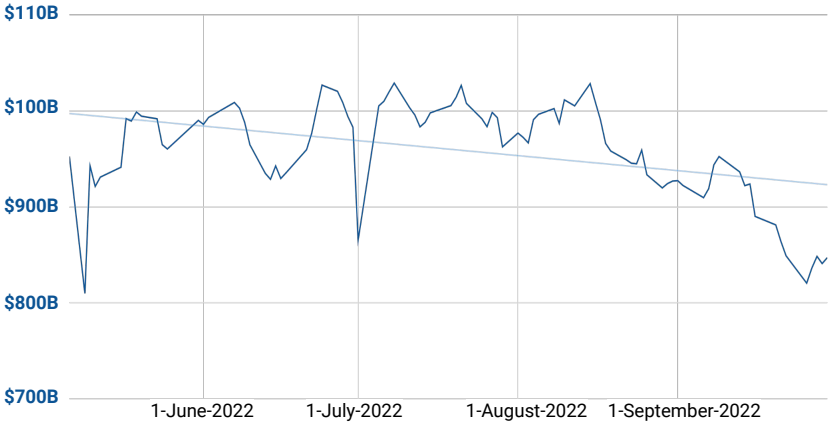
AI in Pharma Publicly Traded Companies

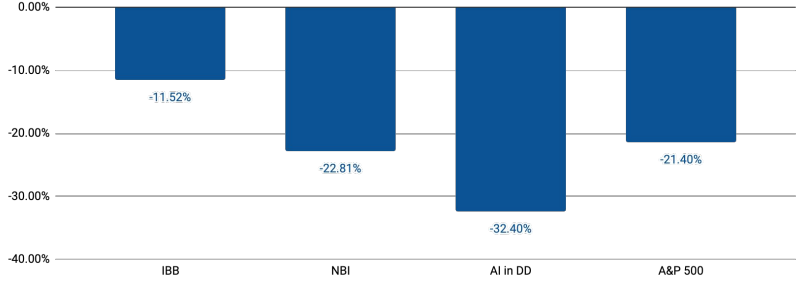
Cumulative Capitalization of Publicly Traded AI-in-Drug Development Companies, Q2-Q3 2022, $ Billion



Despite the crisis and high volatility, AI-in-Pharma publicly traded companies present growth **reaching $85,7B of cumulative capitalization as of October 3, 2022**. About 50 AI in Drug Development companies were taken for this analysis, one of them Benelovent AI has closed its IPO in Q3 2022.

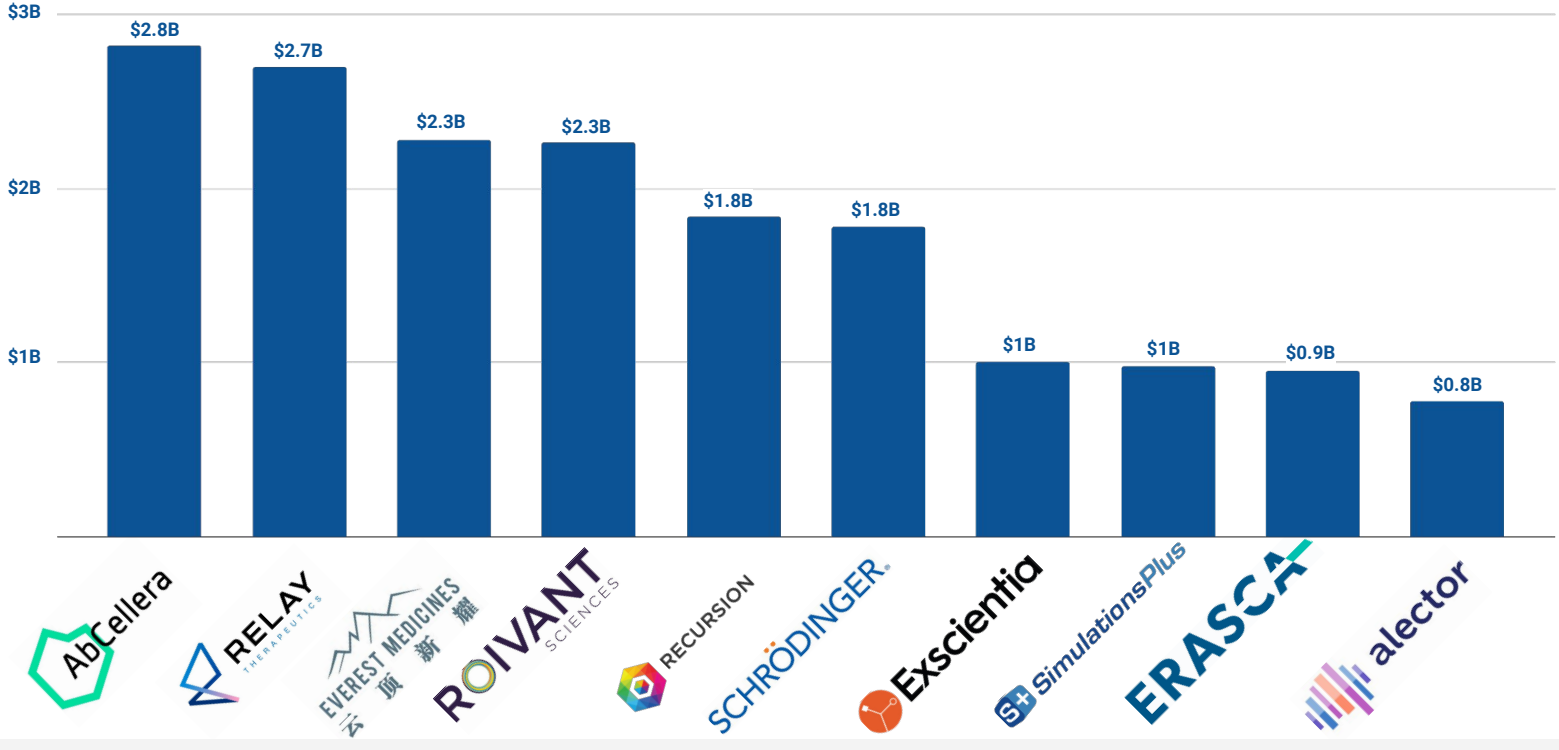
The largest companies by market capitalization are **Evotec, AbCellera and Relay Therapeutics.** The smallest market capitalization are in **Pharnext SA**, **Deepmatter Group** and **OpGen Inc**.

Market Capitalization Growth During Q2-Q3 2022



It's essential to measure the performance of publicly traded AI in Drug Development companies via comparison with major market benchmarks such as IBB, NBI and S&P 500. Because of the crisis, the cumulative market capitalization dynamics of AI in Pharma corporations are losing to YTD NASDAQ Biotechnology Index (NBI), iShares Biotechnology ETF (IBB), and S&P 500 gained solid.

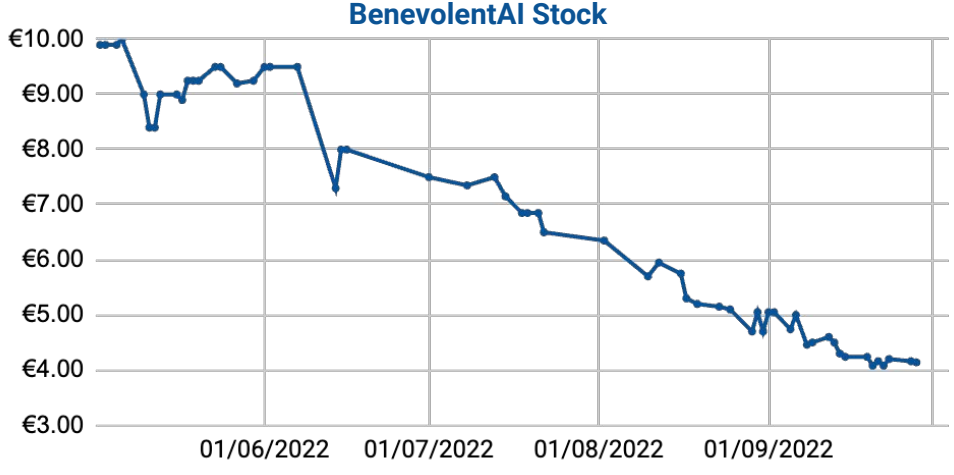
Top-10 AI-Driven Publicly Traded Pharma Companies by Market Capitalization in 2022



The chart presents the **Top-10 AI-driven drug discovery** public companies arranged by market capitalization as of end of September 2022. **AbCellera,** British Columbia-based biotechnology firm that researches and develops human antibodies holds the first place with **$2.8B** of market capitalization.

AI in Pharma IPOs in Q2 - Q3 2022

In Q2 2022, BeneloventAI has successfully closed IPO. The IPO took place in the UK. The company has beta smaller than 1 (although positive), which means that AI in pharma stock prices move following the general market, yet the degree of such “movements” is lower. Major adverse market events in 2020-2022 did not significantly affect AI in pharma sector. The industry’s features remain to play a designative role in the overall market volatility.



Ticker	Mean Daily Return	Volatility of Daily Returns	Growth after IPO	Capitalization, $M
BAI	-0.55%	3.27%	-30.81%	779.9M

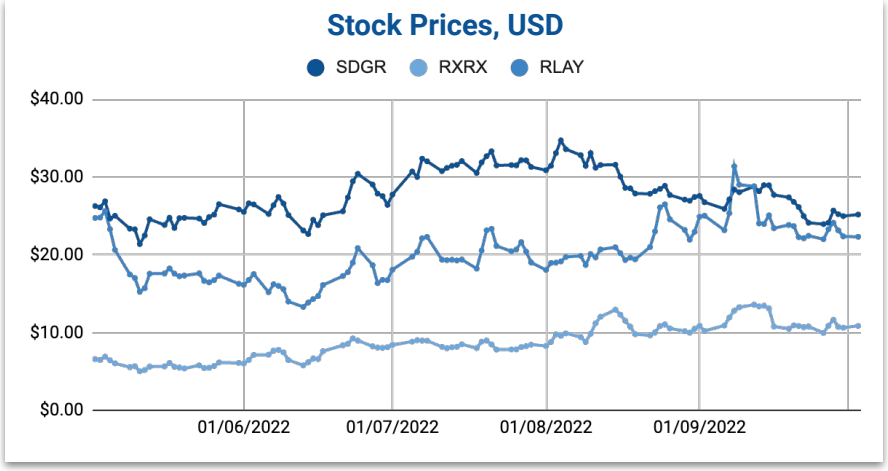
Benevolent’s PlatformTM is a powerful computational R&D platform. Scientists may query the data and disease networks inside the graph using Benevolent's range of exploratory and predictive AI tools. They can also ask biological queries, generate fresh insights, and prioritize ideas. In order to detect dysregulated pathways and processes and visualize the major distinctions between health and sickness, this enables researchers to target the most effective therapeutic approaches.

The graph on the left depicts a comparative performance of BenevolentAI on Euronext Amsterdam starting 25.04.2022.

Top AI in Pharma Best-Promising Companies in Q2-Q3 2022

Schrödinger, **Recursion Pharmaceuticals** and **Relay Therapeutics** constitute the group of promising companies selected for analysis. They are new to the market (their IPOs closed in 2020). Therefore, their future might change significantly. Moreover, they have decent multi-target pipelines of novel therapeutics to address unmet medical needs. The companies are expected to translate their proprietary insights and technical solutions into effective therapeutics.

Currently, the companies have a firm market position and thus receive high expectations from investors.



Name	Country	Funding Amount, $M	IPO Date	Capitalization, $B	Valuation at IPO, $M	IPO Share Price, $	Current Share Price, $	EV/ EBITDA	Net Income, $M
Schrödinger	USA	562.3	02.05.2020	2.24	819	17.00	31.45	-15.74	-134.800
Recursion Pharmaceuticals	USA	208.5	17.07.2020	1.515	1355.2	19.00	8.81	-4.60	-211.74
Relay Therapeutics	USA	520.0	16.07.2020	2.06	1736	20.00	18.95	-4.80	-383,734

AI in Pharma Corporations Financials

Company	Capitalization, $M	Mean Daily Return	Volatility of Daily Returns	Estimated Monthly Return	Actual Monthly Return	IBB Beta	S&P 500 Beta	Total Funding Amount, $M	Operating Margin	EV/EBITDA	Net Income, $M
Gritstone Oncology	247.564	-0.09%	5.87%	8,78%	24.54%	0.51	9	396	-713.26%	--0.36	--111,921
Lantern Pharma	59.13	-0.25%	4.31%	5.32%	-7.05%	1.08	1.32	68.70	0.00%	0.67	-14.03
Alector	1078	0.24%	4.18%	5.77%	-2.66%	N/A	1.34	194.50	11.95%	-5.06	-28.78
Relay Therapeutics	2144	-0.06%	5.27%	5.67%	-3.13%	1.48	1.34	520.00	-10,056.81%	-4.79	-383,734
Schrödinger	2391	-0.17%	4.16%	10.51%	13.03%	1.13	1.14	567.20	-79.25%	-16.85	-134,804
Sensyne Health	790	-0.83%	15.44%	2.75%	135%	1.59	0.87	37.25	-450.76%	0.23	-34,834
Berkeley Lights	356	-0.61%	6.63%	-6.76%	-9.52%	1.59	N/A	272.60	-88.44%	-3.39	-77,715

AI in Pharma corporations tend to be more volatile than average publicly traded company. For most of the corporations, daily returns are positive and abnormal compared to the market. More volatile stocks are usually characterized by higher betas (both calculated for IBB index and for S&P 500). AI in Pharma segment is definitely a segment of growth stocks with the investors focused on the prospects of the companies rather than on the dividends.

Large
Medium
Low

AI in Pharma Corporations Financials

Company	Capitalization, $M	Mean Daily Return	Volatility of Daily Returns	Estimated Monthly Return	Actual Monthly Return	IBB Beta	S&P 500 Beta	Total Funding Amount, $M	Operating Margin	EV/EBITDA	Net Income, $M
Biodesix	110	-0.22%	6.89%	-10.85%	82.91%	N?A	1.43	289.70	-162.47%	-2.46	-51,784
C4X discovery	78	-0.01%	3.18%	12.75%	28.91%	0.14	0.18	8.71	-120.92%	-7.71	-4,721
DeepMatter Group	4.63	-0.72%	7.47%	-5.89%	-11.54%	1.22	0.37	N/A	-323.44%	-1.54	-3,026
eTherapeutics	108	-0.01 %	4.32%	14.72%	26.25%	0.35	0.97	98.50	-2,006.29 %	-8.73	-8,070
GenFit	231.14	0.16%	4.93%	14.68%	31.92%	1.32	0.83	93.69	37.71%	0.33	67,25
Biomea Fusion	347.09	0.13%	6.54%	-14.26%	-2.13%	N?A	0.32	56.00	0.00%	-2.86	-60,940

Market capitalization of some AI in Pharma corporations (such as Schrödinger) exceeds **$6B** whereas other companies are priced in the range of dozens of millions of dollars - the difference in the valuation is immense. There is no strong correlation between operating margin or net income and market capitalization - the valuation of the corporations still being unprofitable can exceed billion of dollars.
Selling shares to investors allows them to maintain their cash burn ratios on an acceptable levels.

Large
Medium
Low

AI in Pharma Corporations Financials

Company	Capitalization, $M	Mean Daily Return	Volatility of Daily Returns	Estimated Monthly Return	Actual Monthly Return	IBB Beta	S&P 500 Beta	Total Funding Amount, $M	Operating Margin	EV/EBITDA	Net Income, $M
BioXcel Therapeutics	459.24	-0.04%	5.49%	-5.89%	8.13%	1.18	1.03	N/A	0.00%	-1.95	-112,027
Evolutionary Genomics	4.63	-0.06%	4.51%	6.44%	0.00%	-0.06	-0.07	1.5	0.00%	-4.81	-3,090
IDEAYA Biosciences	608.192	-0.10%	3.92%	2.48%	8.68%	1.36	1.47	226.10	-172.69%	-6.49	-56,839
ITeos Therapeutics	968.484	0.12%	4.04%	8.42%	29.24%	1.50	0.73	249.74	77.35%	0.29	297,637
Recursion Pharmaceuticals	1737	-0.29%	5.87%	5.56%	8.47%	N?A	1.22	465.38	-1,608.40 %	-5.74	-211,741
Sangamo Therapeutics	814.076	-0.19%	4.08%	7.98%	2.14%	1.40	1.14	93.20	-157.09%	-2.62	-176,330
Renalytix AI	98.31	-0.79%	5.63%	1.66%	5.580%	1.69	1.05	76.40	-1,922.86 %	-0.37	-46,2
Evaxion Biotech	73.408	0.00%	8.05%	12.58%	33.18%	N?A	0.96	17.00	0.00	-1.89	-26,230

Market capitalization growth of AI-driven Pharma corporations exceeds that of the entire market and general BioTech Industry indices represented as S&P 500 index and IBB, respectively. The difference is that compared to the general market, the AI-driven pharma market segment is more volatile. The distribution of the returns in the segment of AI-driven pharma companies is right-skewed, which differentiates it from the vast majority of stock indices and segments.

Large
Medium
Low

Top Publicly Traded Companies Related to AI-Pharma

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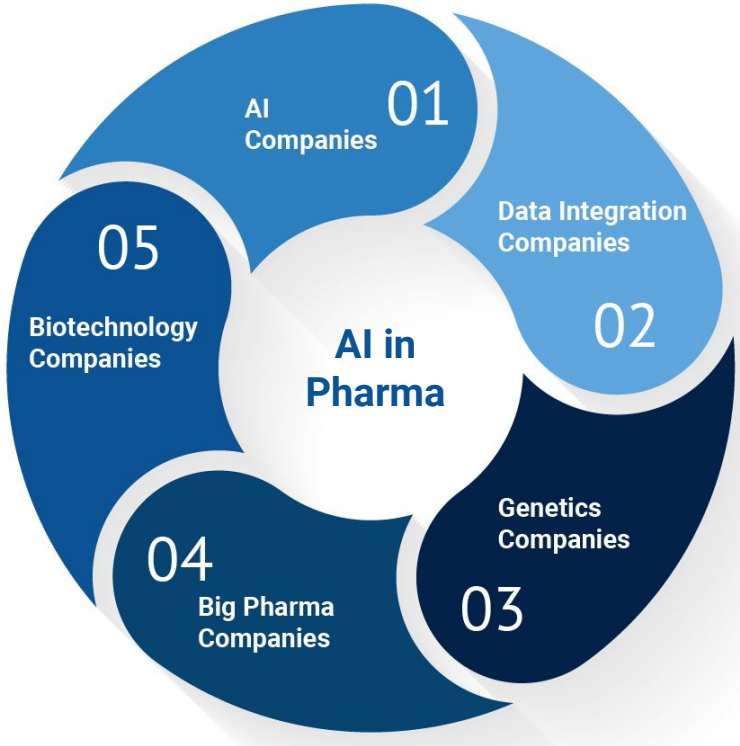
Companies Related to AI-Pharma

AI in pharma sector is an integral part of the contemporary pharmaceutical industry. AI-Pharma sector, defined broadly, is not limited to AI companies, but includes also pharma, tech, chemistry corporations, and CROs that are engaged in collaborations with AI startups, including but not limited to: Mergers & Acquisitions, scientific researches, partnerships, and so on. Hence the companies chosen are better to be described as AI-related or AI-aiming than AI-based solely.

The number of new partnerships between pharma companies and AI companies is ever increasing across the whole industry. On the one hand, AI-focused companies may spend a few years developing all software and tools which pharma companies do not have. On the other hand, large companies, mainly public ones, have solid understanding of their science, extensive experience in the industry and regulatory field, and they are ready to share the risk.

In this chapter we introduce the list of top corporations related to AI-Pharma that were selected based on the analysis of their R&D, financials, and collaborations with the most promising and advanced AI-Pharma startups.



Publicly Traded Companies Related to AI-Pharma

Cumulative Capitalization of Publicly Traded Companies Related to AI-Pharma, Q2-Q3 2022, $ Billions

Driven to some extent by the COVID-19 pandemic, publicly traded companies related to AI-Pharma demonstrated significant growth, **reaching $14.13T** industry capitalization as of the end of Q3 2022. Investors' interest is being shifted towards industries of this nature.

We see significant potential for **Artificial Intelligence** in the Pharmaceutical Industry. The **Expected Compound Annual Growth Rate** for this is market is projected to be **around 40% over the next 3 years**. The Biotechnology Industry is poised to witness a quantum leap soon, mainly because of the impact of Artificial Intelligence on biomedicine R&D. Many transactions are being announced, including Parexel's **acquisition for $8.5B**, that indicates growing awareness of the disruptive potential in this sector for ones having the right means for participation. COVID-19 will continue to push valuations and M&A activity in the sector.

Top 10 Publicly Traded AI-Pharma Related Companies by Market Capitalization in 2022

The chart represents the top-10 public companies that ended up in our portfolios according to their market capitalization. **Johnson and Johnson, NVIDIA and Eli Lilly** top our list, accounting **50.5%** of the capitalization of all companies included. During the last year and a half period of pandemic, AstraZeneca has being raised the capitalization by more than **10 times**, reaching **$172B.**

Top Publicly Traded Companies Related to AI-Pharma

Roche Holding (RHHBY) — Roche Holding AG offers pharmaceutical products for treating anemia, cancer, cardiovascular, central nervous system, dermatology, hepatitis B and C, HIV/AIDS, inflammatory, autoimmune and other diseases. The company widely implements data-driven solutions, for example Roche has acquired Viewics, Inc. Viewics focuses on business analytics for laboratories, taking data from a variety of sources and extracting it to make faster data-driven decisions in operating processes in the labs.

Novo Nordisk (NVO) — Novo Nordisk is a healthcare company, engages in the research, development, manufacture, and marketing of pharmaceutical products worldwide. It operates in two segments, Diabetes and Obesity care, and Biopharm. Novo Nordisk actively implements different AI in Pharma solutions, its foundation awards DKK 138 million under its new data science and artificial intelligence initiative.

Astrazeneca (AZN) — Astrazeneca discovers, develops, manufactures, and commercializes prescription medicines in the areas of oncology, cardiovascular, renal and metabolism, respiratory, infection, neuroscience, and gastroenterology worldwide. Astrazeneca uses advancing genomics research with AI and big data, AI is already being embedded across companies R&D both for research and experiment optimization.

AbbVie (ABBV) — AbbVie is one of the so-called Big Pharma companies. The company uses AI not only for direct development but also for its own enhancement: Abbelfish Machine Translation and AbbVie Search are built for accelerating and scaling the work of the company' researchers, reducing the time it takes to discover and deliver transformative medicines and therapies for patients.

Top Publicly Traded Companies Related to AI-Pharma

Berkeley Lights (BLI) — Berkeley Lights is a leading Digital Cell Biology company focused on enabling and accelerating the rapid development and commercialization of biotherapeutics and other cell-based products for the customers. Besides 2 unique optofluidics system, Berkeley Lights is known for antibody discovery and cell lines development that definitely requires the usage of AI-powered algorithms and technical solutions.

DeepMatter Group (DMTR) — DeepMatter Group Plc operates as a big data and analysis company. It offers DigitalGlassware platform to deliver applications resulting in optimized chemicals, materials, and formulations in various areas, such as pharmaceutical research, fine chemicals, scientific publications, and teaching. The company develops and commercialises cheminformatics software to handle, store, and retrieve chemical structures and reactions for application in pharma; and tools for the production of synthesis planning and reaction prediction solutions, as well as engages in the automatic extraction of scientific information from text and images.

Pharmaceutical Product Development (PPD) — Pharmaceutical Product Development is another big CRO company. PPD ended up in our portfolio for a great reason, collaborating with Happy Life Tech for AI support, the company aims to create Data Science-driven Clinical Research Solutions in China to enhance global drug development.

Charles River Laboratories (CRL) — Charles River Laboratories is a well-known Contract Research Organization (CRO) specializing in research and drug development. CRL uses the AtomNet™ platform, which is a deep convolutional neural network created for structure-based drug discovery. The company also works with the Valence Discovery Platform for Hit-to-Lead acceleration and optimization and provides all research services considering these platforms.

Top Publicly Traded Companies Related to AI-Pharma

Agilent (A) — Agilent is one of the biggest Biotech companies providing technical solutions for the Pharmaceutical industry. Lots of company' technical solutions already have built-in or support different type of AI algorithms. Also, Agilent and Visiopharm co-promote advanced digital Precision Pathology Solutions.

Thermo Fisher Scientific (TMO) — Thermo Fisher is another, even bigger, Biotech company that is specializing in technical solutions, providing also a wide range of other services. "The connected Lab" is a good example of AI-enhanced services providing by the company, creating solutions for enhanced in-Lab performance via AI-based info-gathering and analysis. AI-based processing tools are now also available in Thermo Scientific Amira-Avizo Software and PerGeos Software.

Johnson and Johnson (JNJ) — Johnson and Johnson is considered o be among the TOP-3 biggest Pharmaceutical companies in the world, therefore not only implementation but also investing in AI in Pharma is provided by the company. In 2020, J&J announced an investment in Datavant Holdings, which is working to help healthcare organizations unite data across institutions to enhance medical research and patient care. Another JJI partner, Aetion Inc., analyzes electronic medical records, insurance claims, patient registries and lab results to generate healthcare-related decisions.

Almirall (ALM) — Almirall is a leading skin-health focused global pharmaceutical company, that has some recent collaborations with Iktos for the creation of generative modelling AI technology for quick identification of molecules with multiple bioactivity and drug-like criteria.

AI for Advanced R&D: Applications and Use Cases

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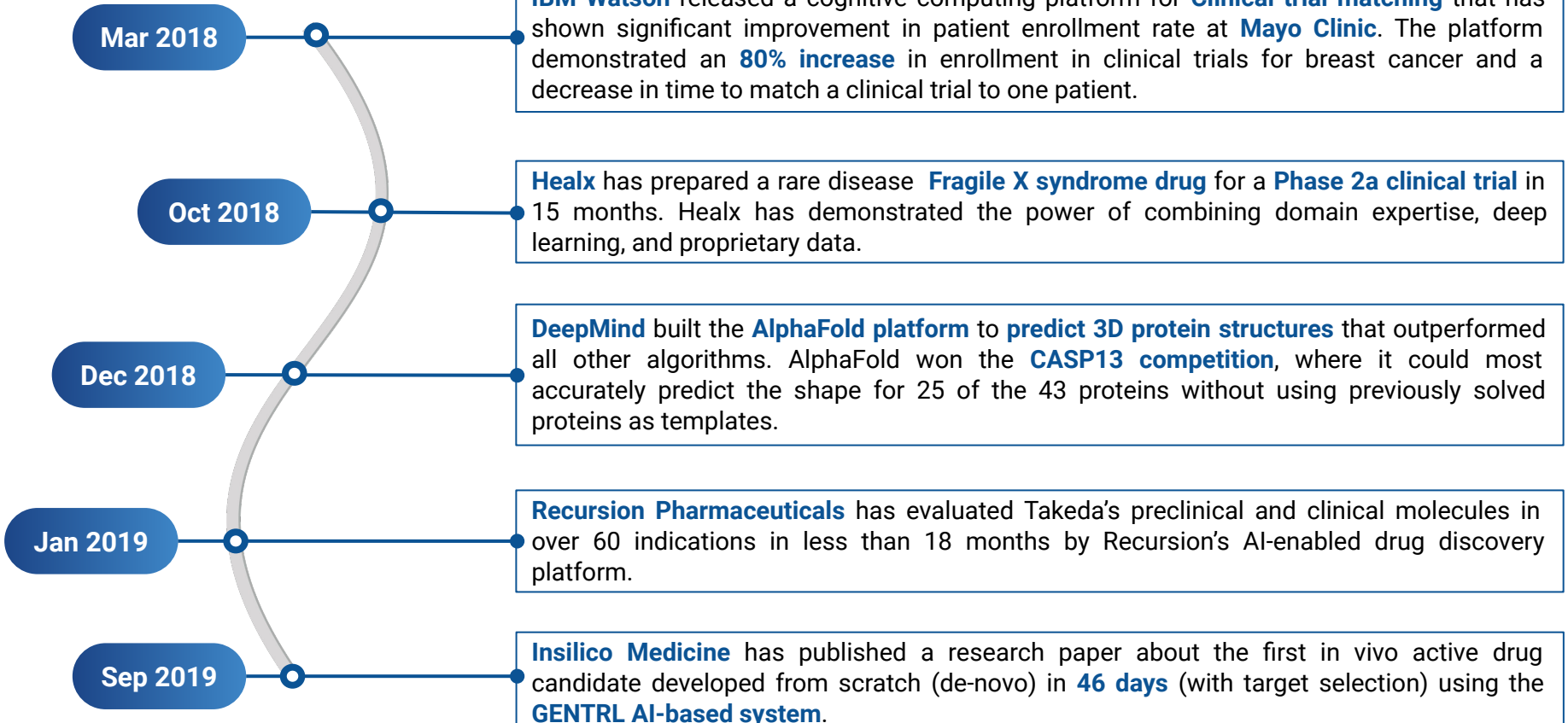
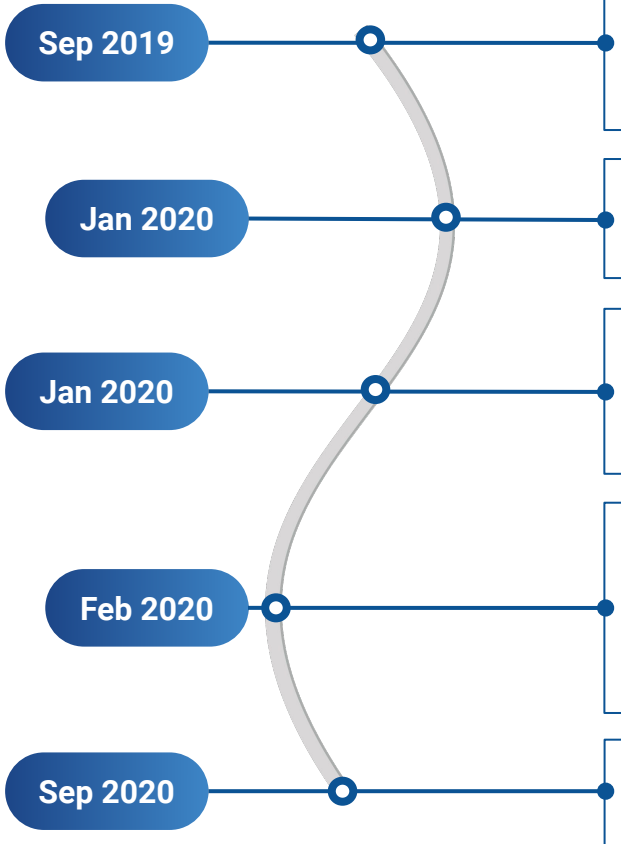
Notable AI Breakthroughs



Notable AI Breakthroughs



Sep 2019

Deep Genomics created a DG12P1 drug in 18 months using an **AI-augmented drug design**. It is an **antisense oligonucleotide therapy** to treat **rare Wilson disease**. Deed Genomics platform screened over 2,400 diseases and over 100,000 mutations to predict and confirm the precise disease-causing mechanism of the mutation Met645Arg.

Jan 2020

Mendel Recruit proprietary platform **increases patient enrollment for clinical trials by 24-50%**. It applies AI algorithms that combine the recognition of scanned documents with **natural language processing** of clinical records and automated clinical reasoning.

Jan 2020

A new drug candidate, DSP-1181, created using the **Exscientia Centaur Chemist Artificial Intelligence platform**, began clinical study. The drug was developed together with **Sumitomo Dainippon Pharma** for the treatment of an **obsessive-compulsive disorder**. It was advanced to Phase 1 clinical trials.

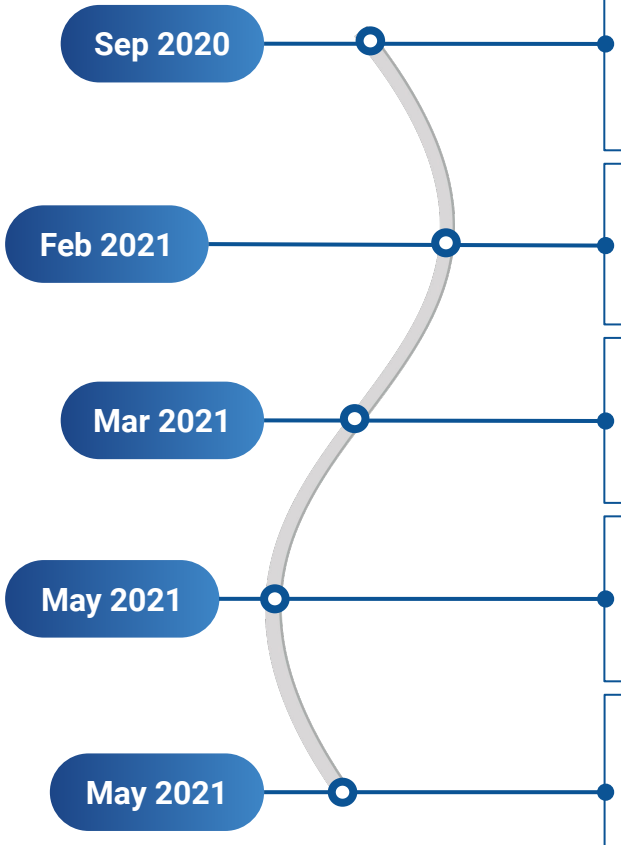
Feb 2020

Scientists from **MIT** discovered **halicin** — **a new super powerful antibiotic capable of killing 35 of the world's most problematic disease-causing bacteria**, including multiresistant strains. The model applied was able to screen more than a hundred million chemical compounds and pick out potential antibiotics that kill bacteria using different mechanisms than existing drugs.

Sep 2020

Aladdin has built a platform for the **early diagnostics of Alzheimer's disease and COVID-19**. Disease Diagnosis platform uses **AI** and **multimodal data**, including biomarkers, imaging, blood samples, medical records, etc.

Notable AI Breakthroughs



Sep 2020

MELLODDY — the '**Machine Learning Ledger Orchestration for Drug Discovery**' group — was created by ten pharma companies to **develop ML models** without sharing data. MELLODDY leverages the world's most extensive collection of small molecules with known biochemical or cellular activity to provide more accurate predictive models and **improve drug discovery efficiency**.

Feb 2021

Insilico Medicine achieved industry-first nominating Preclinical Candidate. The company performed all the required human patient cell, tissue, and animal validation experiments to claim a **first-in-class preclinical candidate for a novel pan-fibrotic target**. The company is preparing for clinical development.

Mar 2021

Cyclica launched an AI-based drug discovery platform that **achieved over 60% of actionable hits for its pharma clients**. Cyclica has partnered with over 100 global pharma and biotech companies and academia across many therapy areas. These partnerships have resulted in 64% of programmes resulting in actionable hits.

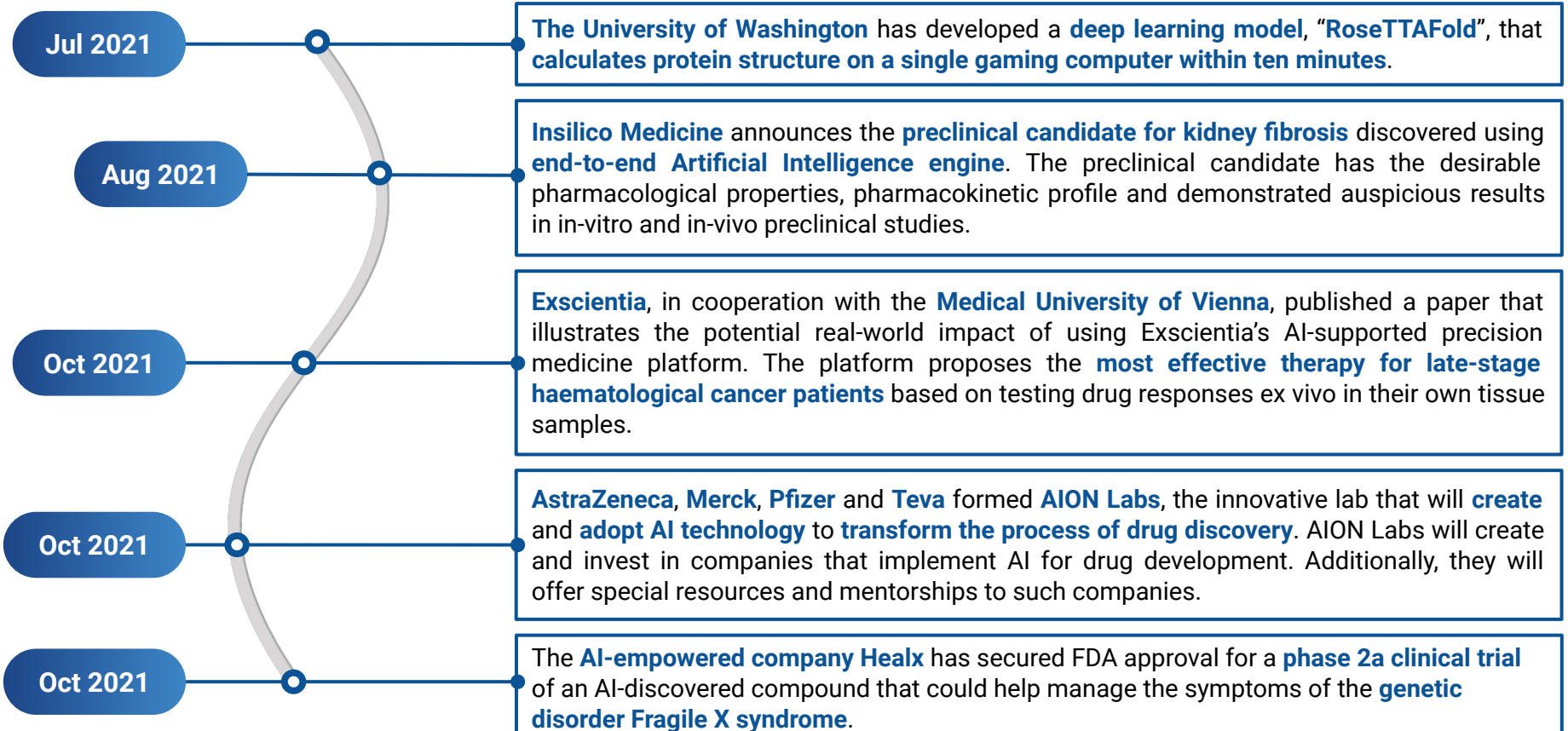
May 2021

BioXcel Therapeutics, Inc., a clinical-stage biopharmaceutical company **utilizing AI approaches**, announced that the FDA has accepted for filing the New Drug Application for BXCL501, for the **acute treatment of agitation associated with schizophrenia and bipolar disorders I and II**.

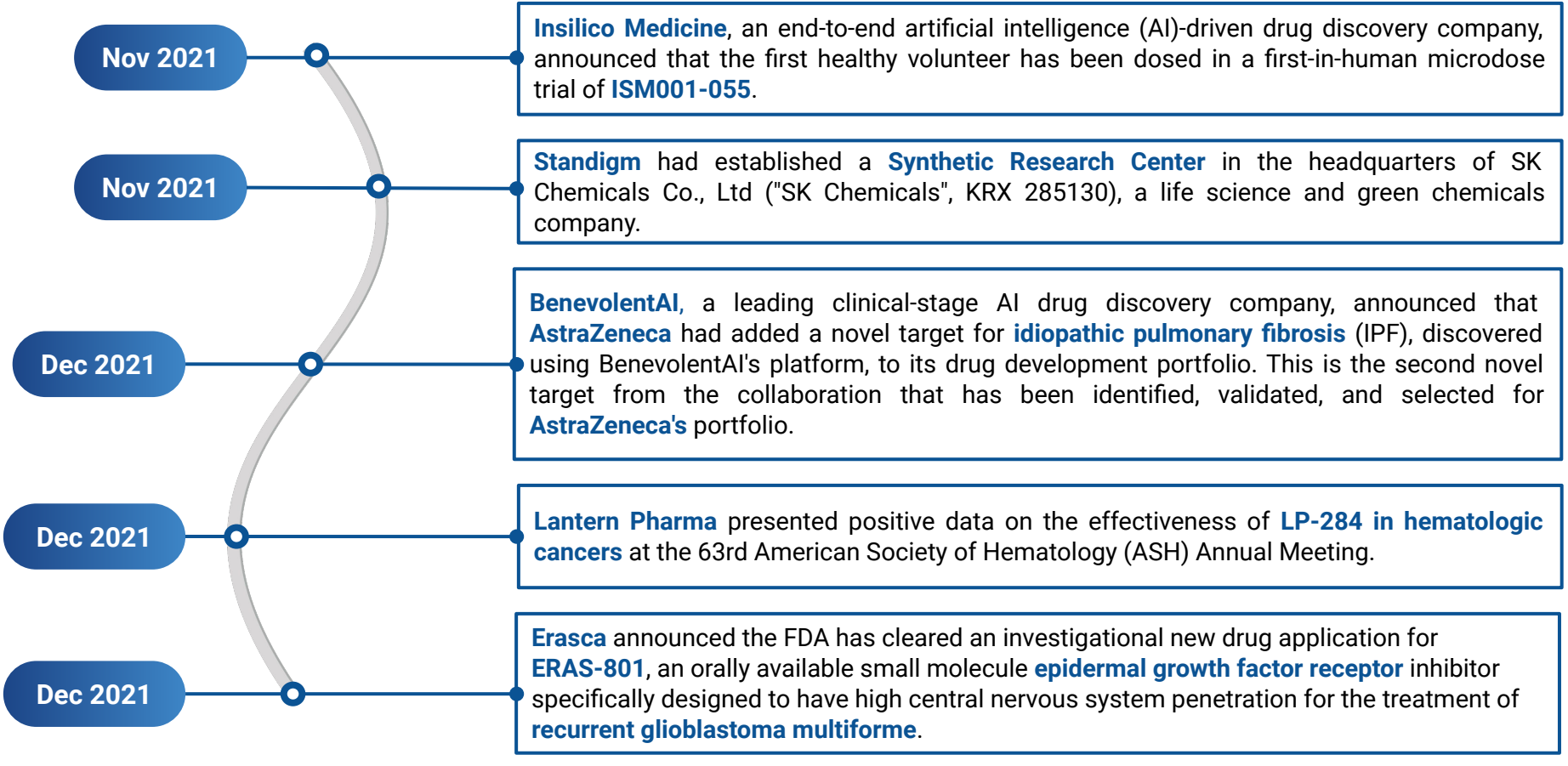
May 2021

Using its AI technology, **Exscientia** designed an **Alzheimer's disease drug candidate** who has **entered Phase I clinical testing**. The AI-designed drug candidate will be assessed for improved antipsychotic effects associated with Alzheimer's psychosis, in addition to improvements in behavioural and psychological symptoms of dementia

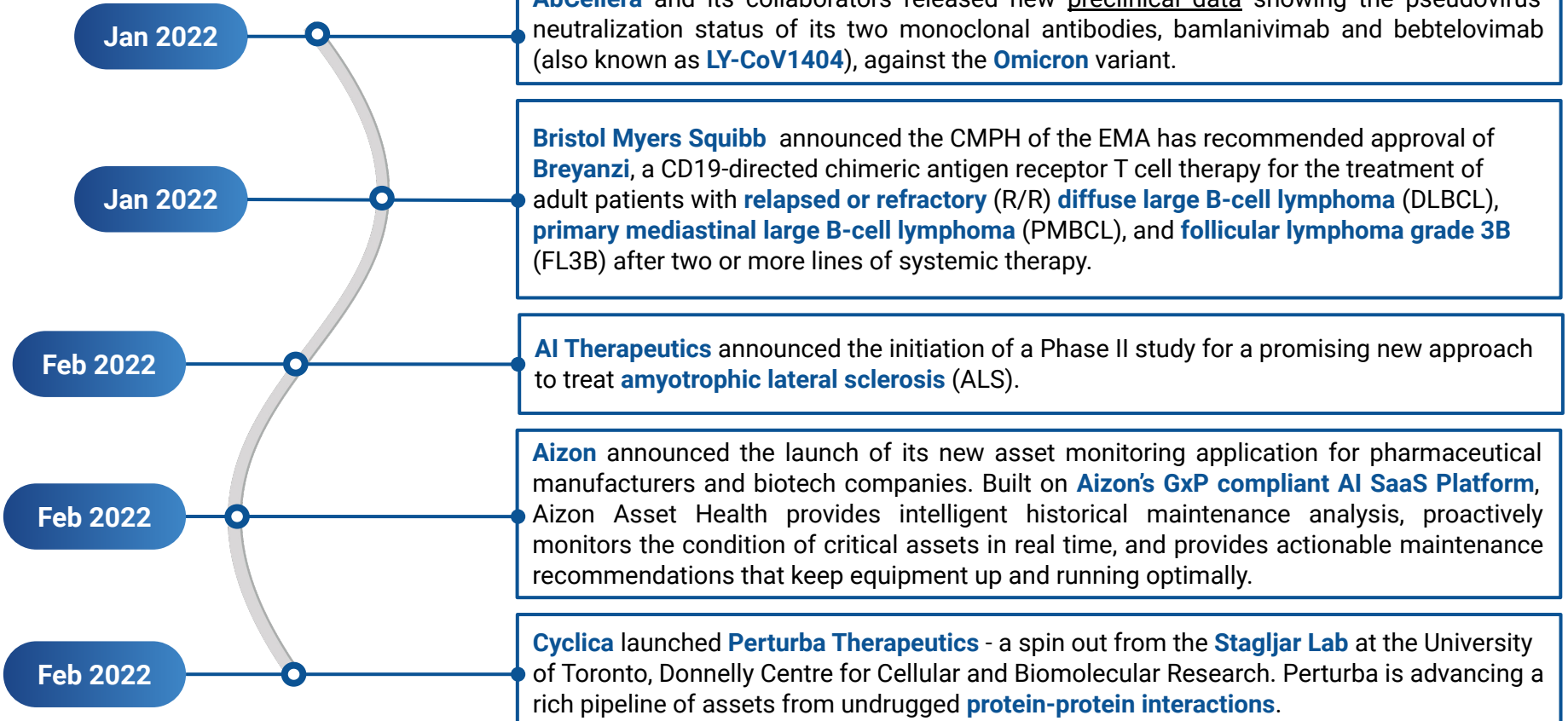
Notable AI Breakthroughs



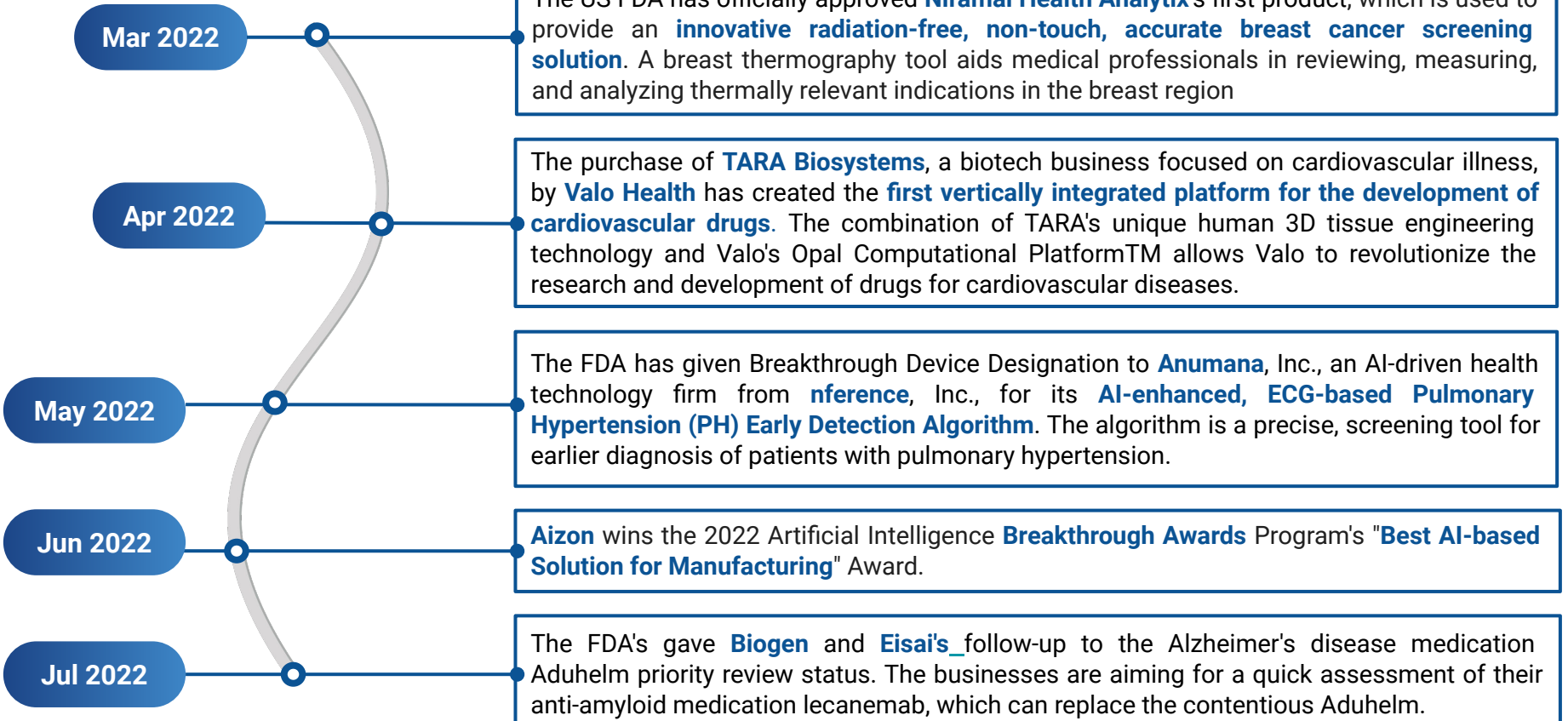
Notable AI Breakthroughs



Notable AI Breakthroughs



Notable AI Breakthroughs



Computational Methods Used by the Most Advanced AI Companies

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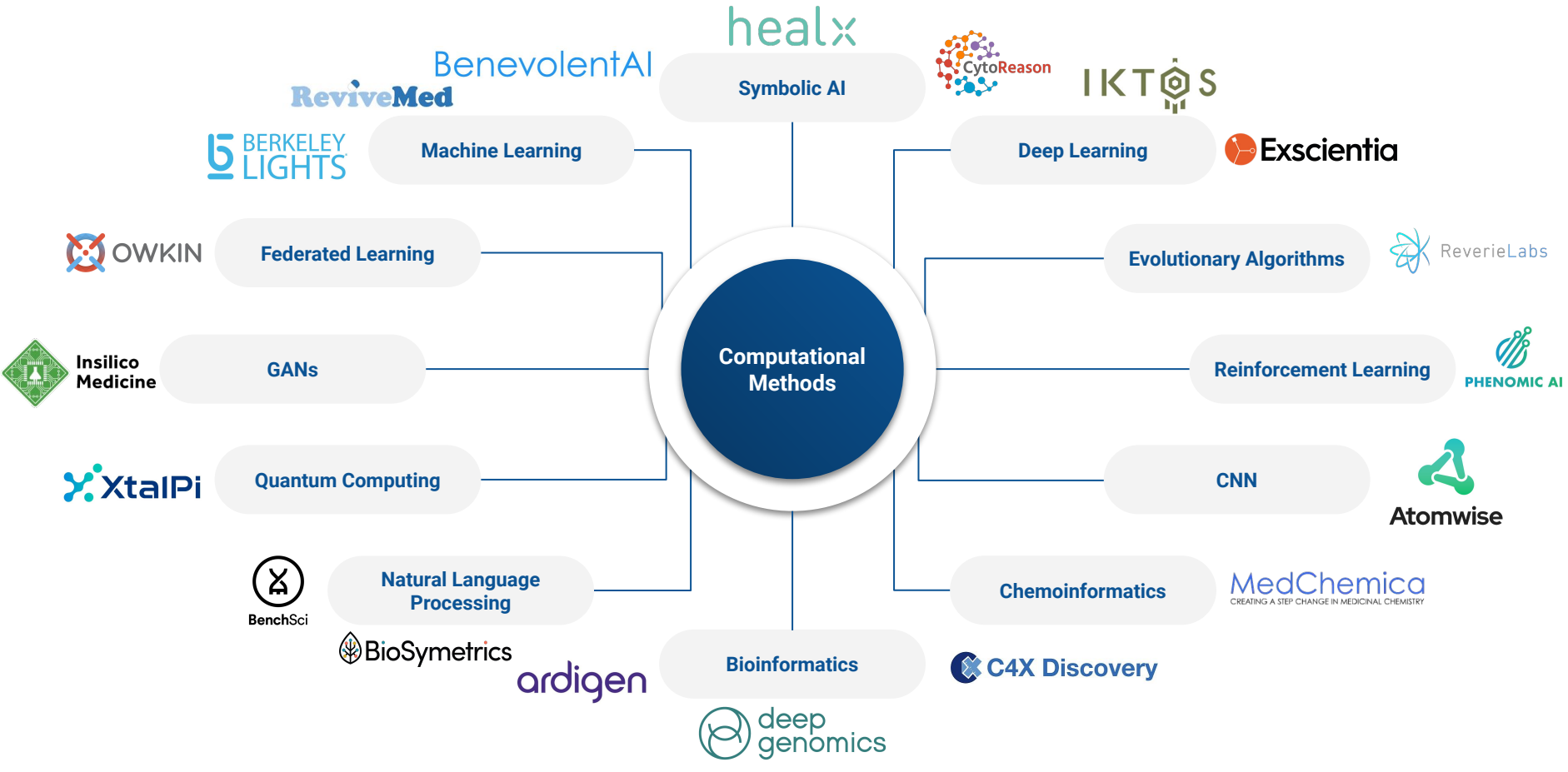
Computational Methods Used by the Most Advanced AI Companies



Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
ardigen	**Bioinformatics, Deep Learning, NLP**	**Ardigen** is active in the field of **laboratory information management systems**, **biological and clinical data analysis**, **Big Data integration**, as well as **custom application development**.
Atomwise	**Machine Learning, Deep Learning (Convolutional neural networks), chemoinformatics**	**AtomNet** is the first drug discovery algorithm to use a **deep convolutional neural network**. It has already explored questions in cancer, neurological diseases, antivirals, antiparasitics, and antibiotics.
BenchSci	**NLP, Deep Learning, Machine Learning**	**Decodes open- and closed-access data on reagents** such as antibodies and **present published figures** with actionable insights.
BenevolentAI	**Machine Learning, Deep Learning, symbolic AI, chemoinformatics**	Evolved from text mining and semantic linking into **knowledge graphs** to tackle complex multifactorial diseases, identify novel targets, small molecule drug discovery and patient stratification.
BERG	**Machine Learning, Deep Learning, bioinformatics**	**Analyze data from patient samples** in both healthy and diseased states to generate novel biomarkers and therapeutic targets.
BERKELEY LIGHTS	**Machine Learning, bioinformatics**	**Automate selection, manipulation, and analysis of cells**. Allows researchers to: Expedite development of cell lines and automate manufacturing of cellular therapeutics.

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
BioSymetrics	NLP, Deep Learning, Machine Learning	**Process raw phenotypic, imaging, drug, and genomic data sets**. Allows researchers to integrate rapid analytics and machine learning capabilities into existing business processes.
bioz	NLP, Deep Learning, Machine Learning	**Bioz** has developed a **search engine for Life Sciences community** using natural language processing and machine learning technology to scan hundreds of millions of pages of complex and unstructured scientific papers on the web.
bioxcel therapeutics	Machine Learning, Deep Learning, chemoinformatics	**Bioxcel Corporation** is a biopharmaceutical company pioneering the **application of artificial intelligence and big data analytics** integrated with drug development expertise.
C4X Discovery	Machine Learning, Deep Learning, chemoinformatics, bioinformatics	**C4X** innovative **DNA-based target identification platform (Taxonomy3(R))** utilises human genetic datasets to identify novel patient-specific targets.
CelerisTx	Deep Learning, Bioinformatics	It is a **deep learning company** that uses innovative, computer-based methods to degrade undruggable targets and validate lead drug candidates in automated lab
CytoReason	Machine Learning, Deep Learning, symbolic AI, chemoinformatics, bioinformatics	**CytoReason's** access to unmatched proprietary and public data, combined with cutting-edge machine learning technologies, **creates their unique biological models of disease, tissue and drug.**

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
Data4Cure	**Machine Learning, Deep Learning, NLP**	**The Data4Cure** platform's modular architecture allows independent system components to **handle integration and advanced analysis of heterogeneous data types** spanning molecular, phenotypic and clinical data, both structured and unstructured.
deep genomics	**Machine Learning, Deep Learning, bioinformatics**	**Deep Genomics** is using **artificial intelligence** to build a new universe of life-saving genetic therapies.
DESKTOP GENETICS	**Bioinformatics, Machine Learning**	**Desktop Genetics** is team of **genome editing experts, bioinformaticians and data scientists,** driven by the real-world impact of CRISPR technology. Their core technology, DESKGEN AI, was trained on the largest database of genome editing data in the world.
ENVISAGENICS	**Machine Learning, Deep Learning, high-performance computing**	**Envisagenics'** SpliceCore platform integrates proprietary **machine learning algorithms, high performance computing, and RNA-splicing analytics** to identify disease-specific alternatively spliced RNA that will function as therapeutic targets.
EURETOS	**Machine Learning, Deep Learning, bioinformatics**	**Euretos** provides direct access to the cloud based discovery platform via user friendly application and also allows **integration of company proprietary data and public data in a secure environment.**
Exscientia	**Machine Learning, Deep Learning, bioinformatics, chemoinformatics**	The company uses ML for **predicting ADME, novelty, synthetic accessibility, pharmacology of molecules.**

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
Genialis	**Machine Learning, Deep Learning**	**Blending computational biology and AI-based methods**, Genialis merges and models data at the intersection of clinical and translational medicine.
GNS HEALTHCARE	**Machine Learning, Deep Learning**	**GNS Healthcare** AI technology **integrates and transforms a wide variety of patient data types into in silico patients** which reveal the complex system of interactions underlying disease progression and drug response.
healx	**Machine Learning, NLP, symbolic AI, chemoinformatics, bioinformatics**	**Healx** AI platform uses **natural language processing** to extract disease knowledge from published sources and to complement biomedical databases and proprietary, curated data.
IKTOS	**Machine Learning, Deep Learning, cheminformatics**	**Iktos** has invented and is developing a technology based on **DL for ligand-based de novo drug design**, focusing on multi parametric optimization (MPO)
Insilico Medicine	**Deep Learning, GANs, GANs + Reinforcement Learning, symbolic AI, Machine Learning, chemoinformatics, bioinformatics**	**Comprehensive DL pipeline**. Biology: **Signaling pathways, DNNs for target ID and HTS analysis.** Chemistry: **GANs-RL for novel molecule generation.**
KYNDI	**NLP, Deep Learning, Machine Learning**	**Kyndi** provides **leading artificial intelligence software** that can analyze long-form text and find actionable insights in a smarter, faster, and more explainable way.

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
MedChemica CREATING A STEP CHANGE IN MEDICINAL CHEMISTRY	**Machine Learning, chemoinformatics**	With a huge experience in **Lead Generation, Lead Optimisation and method development** the goal of the company is to accelerate the progress of our clients programmes.
nference®	**NLP, Deep Learning**	**nferX** uses state-of-the-art **Neural Networks for real-time, automated extraction of knowledge** from the commercial, scientific, and regulatory body of literature.
NuMedii	**Big data analytics; Deep Learning, Machine Learning**	**Discover connections between drugs and diseases at a systems level** by analyzing of millions of raw human, biological, pharmacological, and clinical data points.
NURITAS	**Deep Learning, Bioinformatics**	**Predict the therapeutic potential of food-derived bioactive peptides**. Allows researchers to: cost-effectively develop highly targeted treatments for specific diseases from natural food sources.
OWKIN	**Machine Learning, Federated Learning**	**Owkin** combines the **expertise in biology** and **machine learning** to fuel precision medicine. Owkin facilitates access to real-world data by therapeutic area through its data connect service.
Peptone	**Deep Learning (TensorFlow + Keras base)**	World's first **protein database** specifically for Deep Learning and AI applications **with full Keras™ and Tensorflow™ integration.**

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
PHENOMIC AI	Deep Learning, Reinforcement Learning	**Phenomic predicts which cells will survive chemotherapy** and **identifies compounds that selectively target** these resistant cells. It will then develop the compounds and bring them to market.
ProteinQure	Quantum Computing, Reinforcement Learning, Chemoinformatics	**ProteinQure** is combining quantum computing, reinforcement learning, and atomistic simulations to **design protein drugs.** They can design p**eptide-based therapeutics** and explore **protein structures** without crystal structures.
ReverieLabs	Evolutionary algorithms, Machine Learning	**ML-based structure based predictive models f**or potency and ADMET/PK properties of small molecules.
ReviveMed	Machine Learning, Deep Learning	**ReviveMed's** platform enables the **rapid, high-throughput, and cost-effective application of metabolic data** to discover new disease mechanisms for drug discovery and, simultaneously metabolomic biomarkers to identify which patients stand to benefit by targeting the disease mechanism.
STRUCTURA BIOTECHNOLOGY	Machine Learning (stochastic gradient descent and branch-and-bound maximum likelihood optimization)	**The cryoSPARC System™** enables high-throughput structure discovery of **proteins and molecular complexes** from cryo-EM data with help of machine learning.
XtalPi	Quantum physics; Machine Learning	**XtalPi's ID4** platform provides accurate predictions on the **physiochemical and pharmaceutical properties of small-molecule candidates for drug design, solid-form selection,** and other critical aspects of drug development.

15 Notable R&D Use Cases of AI Application in Biopharma

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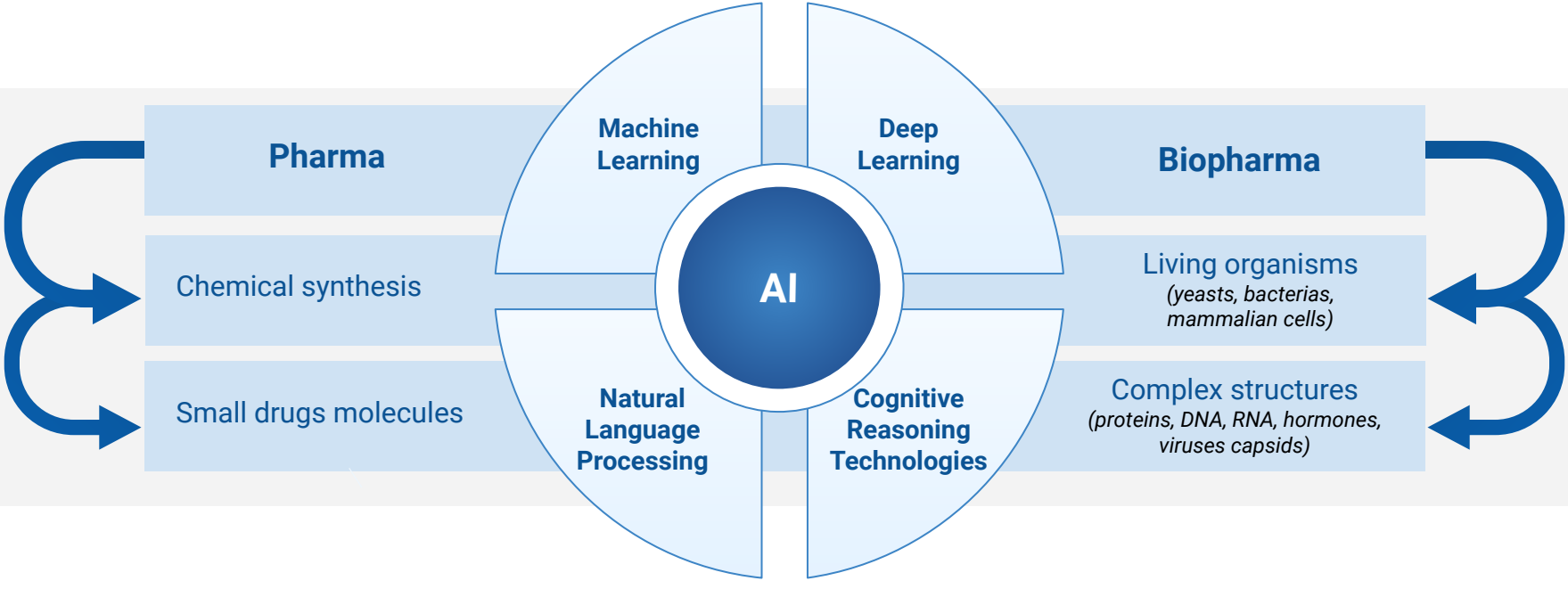
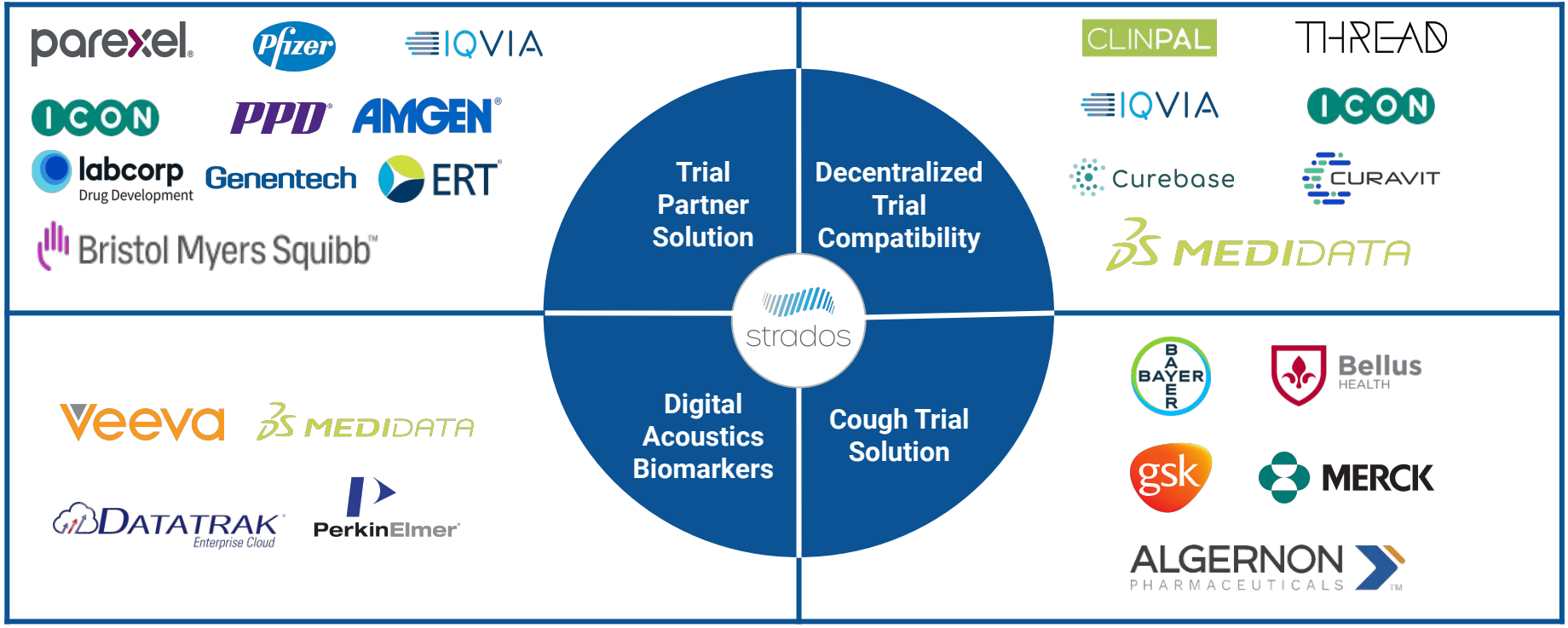
Introduction to Most Innovative R&D Approaches of AI in Biopharma

Biopharma utilizes living organisms (such as yeasts, bacterias, and mammalian cells) which are capable to produce complexly structured products such as proteins, hormones, RNA and DNA products, and virus capsids. Whereas Pharma relies on a classical chemical synthesis producing small drug molecules. However, both industries may benefit from AI-driven applications. To develop new small drug molecules or biologically-derived products, AI-driven data processing serves as a tool that allows minimising time consuming biological testings while helping to select the most promising products to test.



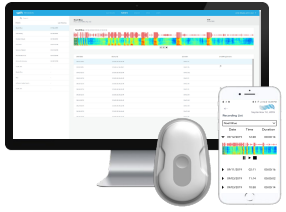
Most Innovative R&D Approaches of AI in Biopharma. Strados Labs

Strados Labs enters the Pharma and Life Science market with a **Respiratory Management Solution** that includes the only FDA-cleared, RESP biosensor which acquires lung sound acoustics wireless and hands-free, making it a perfect fit for clinical research to measure patient response to new drugs by objectively collecting coughs and other lung sounds discreetly, comfortably, and securely in a streamlined way, while having access to data for post-processing and analysis.



*Listed companies are industry leaders and prospects for Stradoslabs

How Strados Labs Uses AI in R&D?



Strados Labs — a respiratory management solution, which brings innovation at the intersection of lung biomarkers, patient centricity, and machine learning. The industry of life sciences can largely benefit from the enhancement of pulmonary care monitoring capabilities provided by Strados Labs to gain insight into patient drug response by analysis of longitudinal lung acoustics.

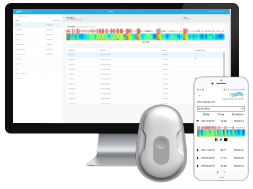
Data Collection Capacity	Patient Privacy & Security	Real-Time Data Analysis	Patient Centricity	Longitudinal Lung Data
220 hours of continuous data collection without patient intervention of objective lung sounds and respiratory dynamics while having access to data for post-processing and analysis.	Noise cancellation is applied to enhance the signal to noise ratio and eliminate speech discernibility while being HIPAA compliant with an end to end encryption.	Data collected via RESP is uploaded automatically to the Strados Cloud to allow assessment of recordings timely with identification of adventitious breath sounds including respiratory dynamics with ML algorithms.	Wireless, non invasive biosensor that monitors, records and stores every lung sound. That translates into longer wear times and an astounding 99.59% patient compliance.	Identification of wheeze, cough, and CABS detection gives the objective measurement of these changes over time on a patient and population basis with an ability to differentiate cough types in addition to frequency.

How Strados Labs Uses AI in R&D?

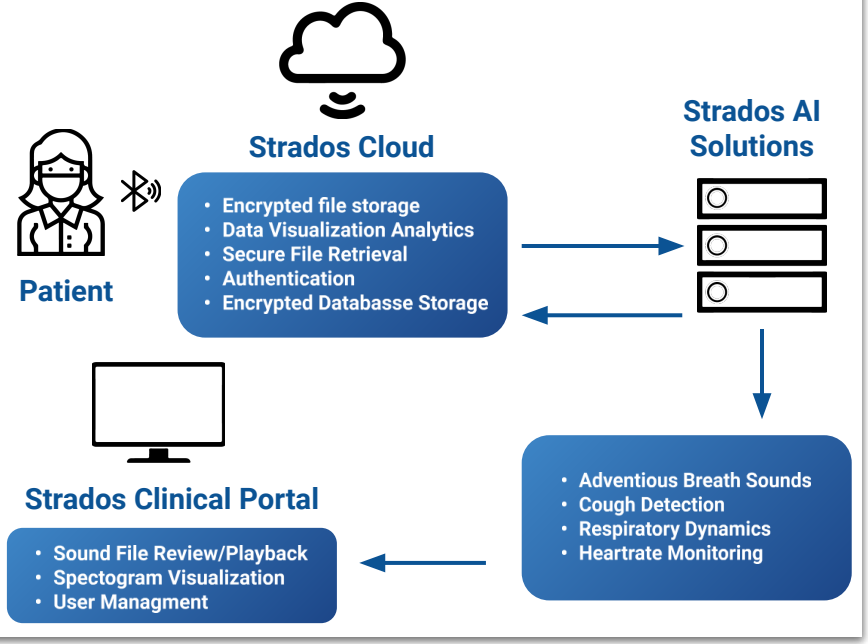
The **Strados Respiratory Management Solution** is the world's first FDA-cleared lung sound platform with a proprietary wireless biosensor, **RESP**, that is passive, patient-friendly, and clinically validated to acquire lung sounds in the real world.

Today **Strados Labs** has a unique opportunity to stand as a leader in Respiratory Health: their clinically validated bioacoustic library of sounds and AI engine is the world's largest entirely hands-free, clinical-grade dataset enabling **Strados Labs** to be the standard bearer of acoustic digital biomarkers for clinical research and respiratory care globally.

For instance, **Strados Labs RESP** fits perfectly into decentralized trials allowing remote patient access by unlocking lung sound data and putting it into the hands of the entire research team via the cloud. Making decentralized respiratory trials scalable and able to develop entirely new insights about respiratory status without episodic patient interaction.



Strados Cloud: company's passive and longitudinal bioacoustics insights allow them to build a more complete picture of the subject's respiratory status leading to better trial outcomes.



How Standigm Accelerates Drug Discovery using AI

Standigm's AI solution **Standigm ASK™** provides **novel targets** perfectly fit to a customer's research context within two weeks.

- **Novel target Identification**
- Query: **Disease**
- **Stangdim ASK™**
- Output: **Novel Target**

Standigm's optimized workflow **AI system** can generate **multiple First-in-Class** compounds within seven months.

- **Integrated workflow AI**
  - **Novel target Identification (Stangdim ASK™)**
  - **Novel compound design (Stangdim BEST™)**

Novel Targets Identification

First-in-Class Lead Generation

Standigm
The workflow AI drug discovery company

Cataloged Assets

Tailored Partnership Models

Standigm has an exceptional reservoir of ready-made in-house **therapeutic assets**, which are as attractive as to meet customer's pipeline needs.

Therapeutic areas of assets:


Cancer


Parkinson's Disease


NASH


Mitochondrial Disease

Standigm has **tailored partnership models** perfectly fit to a customer's needs, from licensing of AI platform and assets to AI solution providing.

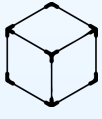
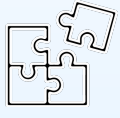
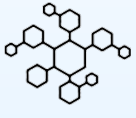
Standigm's partnership models:

1. Licensing of Standigm's AI Platform (Standigm ASK™, Standigm BEST™)
2. Licensing of First-in-class assets driven by Standigm's AI platform
3. Providing Standigm's AI solution

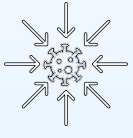
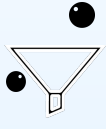
How Standigm Accelerates Drug Discovery using AI

Standigm is a workflow AI-driven drug discovery company headquartered in Seoul, South Korea and subsidiarized in Cambridge, UK. Standigm has proprietary AI platforms encompassing novel **target identification to compound design**, to generate commercially valuable drug pipelines. The company has established an early-stage drug discovery workflow AI to generate First-in-Class lead compounds within seven months. o date, Standigm is running 42 in-house or collaborative pipelines for drug discovery using the workflow AI technology. One of the company's pipelines is expected to enter a pre-clinical stage in 4Q 2021.

Standigm BEST™ is a novel **compound generation platform**, which can investigate lead compounds whenever target or ligand information is lacking or enough.

Database	Hit ID	Hit to Lead	Lead Optimization
			
Deep learning chemical space	**Securing activity**	**Securing novelty**	**Druggability optimization**
150-dimensional vector space which learned various compound properties	Accurate prediction of binding	New scaffold with various structures	Mainly-based substructural variation 3D-based druggability prediction

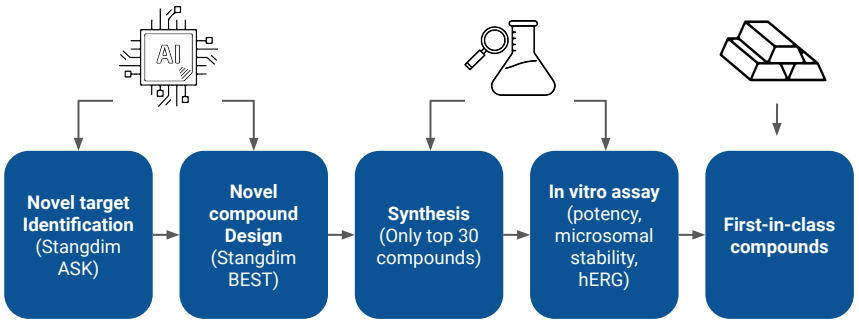
Standigm ASK™ is a customizable, AI-aided **drug target identification platform**, prioritizing disease-target relationships and providing evidence-based results through an interactive user interface.

Graph DB	Prioritization Algorithm	Multi Filters	Novel Target Selection
			
Biomap (Knowledge + Omics)	**Target prioritization based on disease-target-association scores**	**Screening attractive target's with multi filters**	**Novel Target Selection**

How Standigm Accelerates Drug Discovery using AI

Standigm Releases First-in-Class Compounds within 7 Months

Standardized workflow



7 months (rather than years/ Standigm)

30 months (Traditional Approach)

Featured Partners

아주대학교병원 Ajou University Hospital · Hanmi · Institut Pasteur Korea · KIST Korea Institute of Science and Technology · MILNER THERAPEUTICS INSTITUTE · inno.N · SK chemicals · SAMJIN · Fibrosis Control Center

Standigm made the hit-to-lead stage with a cancer Target A within 7 Months

Standgim BEST™ → **In Vivo & Tox** / **Preclinical Candidate** → **Lead Optimization**

1M	1M	1M	1M
Data Collection, Analysis* and Model Validation**	1st Round Commercial Compounds (Library of x million)	2nd Round Commercial Compounds & Hit-Based Design	SAR-Based Novel Design

Collaborator (Pharma Company): 3M (Hit Compounds)

Target Proposal (Patent Analysis)	Purchasing Compound, Assays, Hit Screen	Chemical Synthesis, Assays, Hit Selection	Chemical Synthesis, Assays, (In Vitro & In Vivo), Lead Selection

*Data Analysis – Binding site analysis using protein structure
**Model Validation – Validation of activity prediction models: ChemMap-based, 2D structure QSAR-based, Simulation-based and Ensemble-based methods

Most Innovative R&D Approaches of AI in Biopharma. Antiverse

Antiverse is a new type of antibody discovery company accelerating drug development. The Antiverse platform exists at the intersection of structural biology, machine learning and medicine to enable breakthroughs to happen more quickly and cost-effectively.

Antiverse **prevents diversity loss** during amplification to uncover more diverse and rare antibodies.

Traditional in vitro screening:

10^{10} antibodies

↓

3 amplification rounds

↓

10 antibodies

Antiverse discovery:

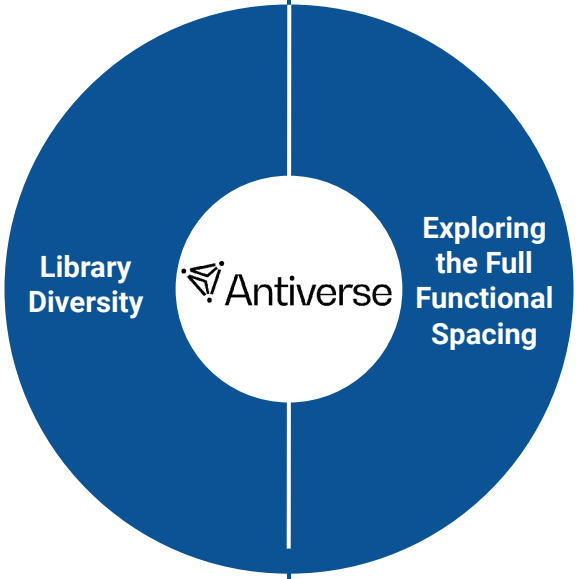
Antigen-antibody database

↓

AI-augmented screening

↓

96 antibodies



Antiverse **provides more candidates** by analysing NGS data, clustering on multi-dimensional space, and selecting based on sequential and structural grouping. The generative module **offers new sequences** and gives you options that haven't even been considered.

Antiverse AI-Augmented Discovery:

Antigen-antibody database

Recovery Module

Generative Module

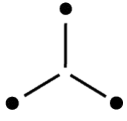
96 antibodies

How Antiverse Engineers the Future of Drug Discovery

Antiverse is recognized as one of the top biotech startups in the UK with our antibody discovery service already in use by big pharma. The main feature of the company is **10x Diversity with AI-Augmented Drug Discovery**.

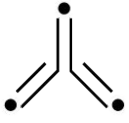
Existing antibody discovery methods are well-developed and often effective at discovering binders. But when there is a need to find the best possible candidate, or when finding a suitable candidate is hard with current methods, the options are **limited** and often **costly**.

Antiverse uses **next-generation sequencing (NGS)** to extract more data from existing workloads. The **AI-Augmented Drug Discovery platform** and trained models analyse the statistics gained from thousands of experiments. These outputs are compared against known data in order to select best candidates.



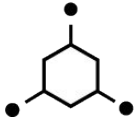
Target Selection

Antiverse provides targeted options in order to focus on testing safely once there are too many antibody-antigen binding options.



Binder Recovery

Antiverse can help to find sufficient potential binders that can be missed by conventional methods.



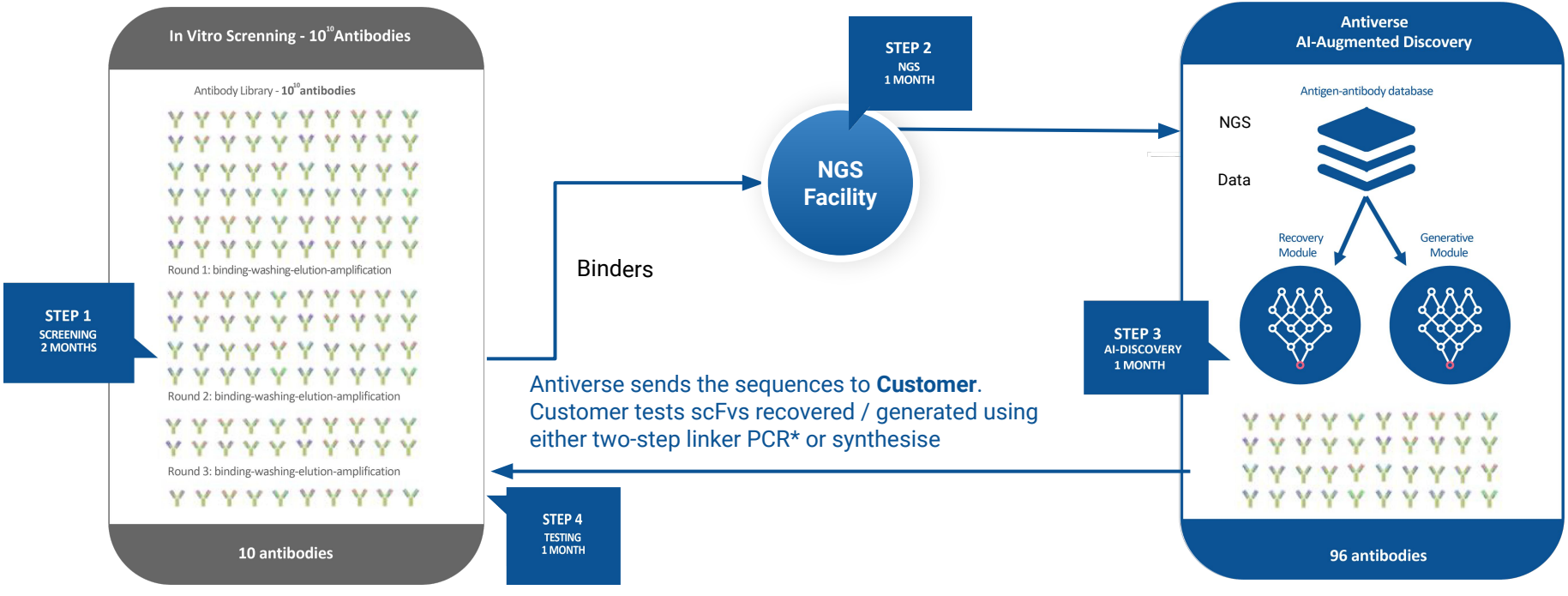
Binder Customisation

Antiverse can generate new binder variants that will be sufficient for clients purposes.

How Antiverse Uses AI in R&D

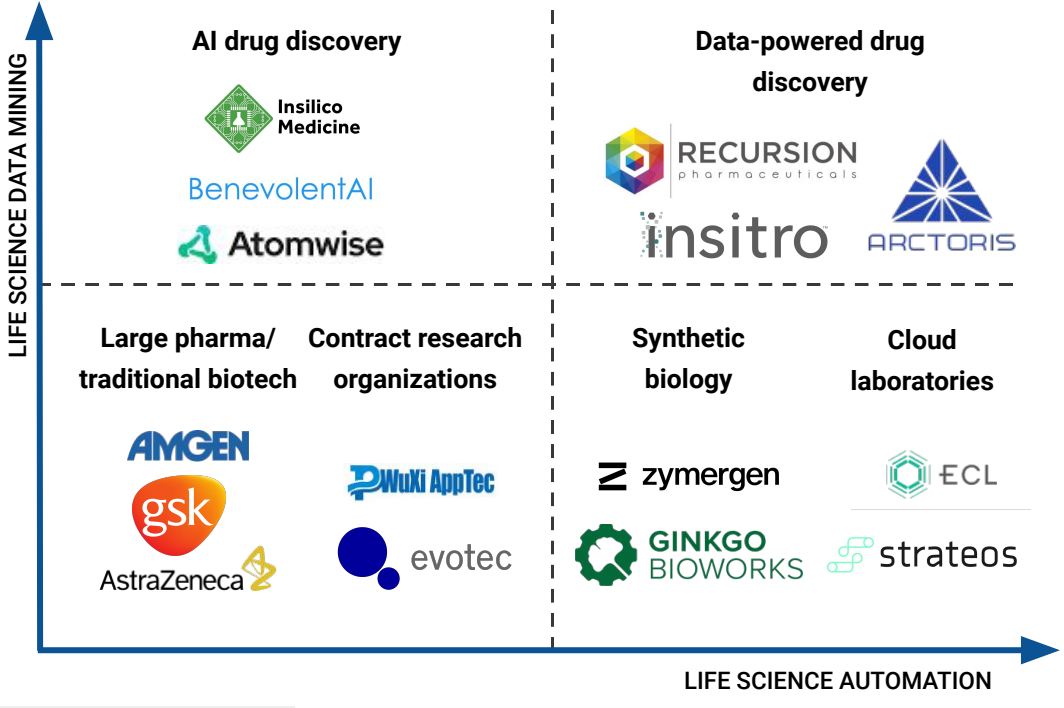
Antiverse

The **Antiverse AI-ADD** system found each and every cluster identified by other methods, plus more. These additional clusters contained rare and unique sequences.



The Drug Discovery Ecosystem is Evolving Rapidly - And Data is at the Core.

Drug discovery is undergoing massive and rapid change - the rise of Artificial Intelligence and Machine Learning for Drug Discovery and the evolution of robotics-centric companies in the biomedical research space has enabled a new generation of companies to emerge: **data-powered drug discovery companies** that combine automation and data science.



Arctoris is one of them: a biotech platform company with operations in Oxford, Boston, and Singapore, leveraging its **fully automated platform** for drug discovery.

ARCTORIS

The company was founded by an oncologist and a medicinal/ synthetic chemist, with the goal to accelerate the discovery and development of new therapies by harnessing the power of technology and combining it with deep industry expertise.

The **core thesis** of the company is that better data leads to better decisions, and that in order for drug discovery programs to develop and meet the next milestone faster and with higher chance of success, the underlying data must be rich, reliable, and reproducible. According to Arctoris, **the status quo is no longer enough**: in order to develop the best drugs, industry leaders have to rethink how they can improve their decision-making, powered by better data.

Having developed a suite of proprietary technologies across robotics and data science/ AI/ ML, Arctoris is a leader in this **new and rapidly evolving field**.

How Do Robotics and AI/ ML Synergize in Drug Discovery?

The greatest challenge in AI-driven and ML-powered drug discovery is access to well structured, fully annotated, reproducible and robust data. **Arctoris** leverages the power of robotics to generate vast amounts of **ML-ready data that enable better decisions** - thereby significantly accelerating timelines from target to hit, lead, and candidate.

INDUSTRY-STANDARD DATA GENERATION & PROCESSING

- Widespread lack of reproducibility
- Unclear reagent and cell line provenance
- Inconsistent use of methods & protocols
- Human error & variability
- Only collection of high-level results data
- Highly fragmented file & storage systems

ARCTORIS-ENABLED DATA GENERATION & PROCESSING

- Strict adherence to automated protocols
- Fully verified reagents and cell lines with complete audit trails
- Reproducible results data in standardized structure
- Additional collection of rich research meta-data
- Secure & convenient data storage & access
- Advanced assay performance monitoring

Both quality and speed are achieved by combining precision robotics with a unique data science platform and world-class drug discovery expertise from biotech and pharma veterans.

Arctoris tracks all experimental outputs in full depth, including the capture and analysis of extensive metadata – temperature, humidity, CO_2, reagent provenance and batch ID among many others. At the same time, the platform enables automated QA/ QC processing, applying statistical tools to ensure full reliability and validity of all results.

Thereby, **Arctoris** ensures **superior data to be generated in accelerated timeframes**, leading to better decisions taken earlier - in human-powered but especially in AI/ ML-driven programs, thanks to training of AI models with the best possible data.

Taken together, **Arctoris** has developed a **unique technology platform** based on robotics and data science that powers drug discovery programs both in the company's internal pipeline and in partnerships with biotech and pharma companies worldwide.

The Arctoris Platform: Leveraging Robotics & Data Science from Target to Candidate.

- Analysis of target expression and target half-live by quantifying protein turnover and route to degradation
- Investigation of target function (changes in phenotype, pathways, gene expression, etc.) via cell-based and molecular biology readouts
- Advanced insights into effects of target modulation by employing complex model systems such as organoids, primary cells, etc.

- Machine-learning guided screening set selection and hit evolution
- *In silico* and *in vitro* screening and profiling
- Biophysical screening/ profiling and FBDD
- Rapid synthetic hit expansion and diversification incl. use of CADD
- Kinetic and mechanistic biochemistry/ enzymology and biophysical quantitation of target engagement energetics & kinetics
- Protein science and (co)crystallography for SBDD

- Pharmacokinetics and pharmaco-dynamics (PK/ PD) & safety pharma-cology
- In-depth pharmacokinetics, including ADME, drug-drug interactions, metabolite profiling, concentration time profiles
- Comprehensive acute toxicology assess-ment, incl. single dose and repeated dose to determine MTD and NOAEL
- Additional toxicology studies (e.g. repro-ductive and developmental toxicity, etc.)

- Rapid biochemical profiling, kinetics, selectivity, mechanism of action
- Isolated and in-cell target engagement
- Cellular mode of action, elucidation of pathway modulation, confirmation of on-target/ off-target effect
- Medicinal and synthetic chemistry (optimizing SAR, SPR, STR)
- Integration of synthetic and computational chemistry as well as *in vivo* ADMET for late-stage lead optimization

Most Innovative R&D Approaches of AI in Biopharma. Genomenon

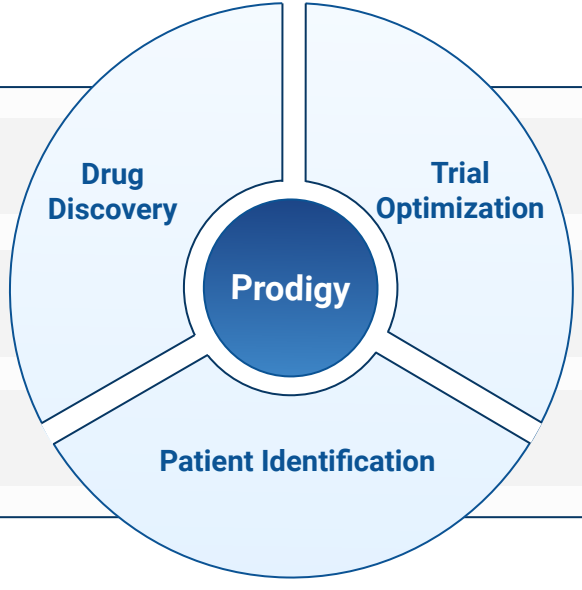
GENOMENON®
AI-DRIVEN GENOMICS

Genomenon is an AI-driven genomics company that organizes the world's genomic knowledge to accelerate the diagnosis and development of treatments for genetic disease.

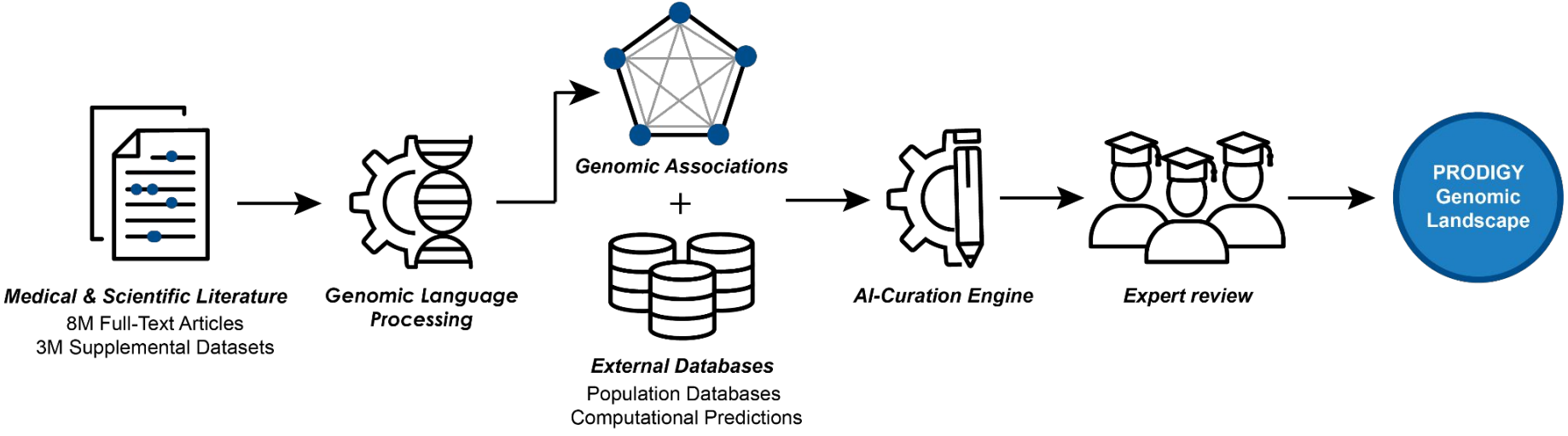
Genomenon's **Prodigy™** Genomic Landscapes deliver a profound understanding of the genetic drivers and clinical attributes of any genetic disease and support the entire drug development process, from discovery to commercialization.

Genomenon's main focus therapeutic areas are **rare diseases**, **genetic diseases**, and **hereditary** and **somatic cancers.**

Identify molecular drivers of disease	**Drug Discovery**	Identify genomic biomarkers for trial
Evaluate market potential	**Prodigy**	Identify CDx inclusion criteria
Accelerate natural history studies	**Patient Identification**	Identify patients for clinical trials/approved therapies



How Genomenon Uses AI in R&D



Genomenon's **Prodigy™ Genomic Landscapes** use a unique combination of proprietary **Genomic Language Processing (GLP)** and **expert, scientific review** to provide an evidence-based foundation for all stages of the drug development process. These landscapes can be completed at the disease, gene, variant, or patient level, and are maximally comprehensive as a result of GLP. Genomic Landscapes are also rapidly produced using an **AI-assisted curation engine** that expedites manual review of the data indexed by GLP.

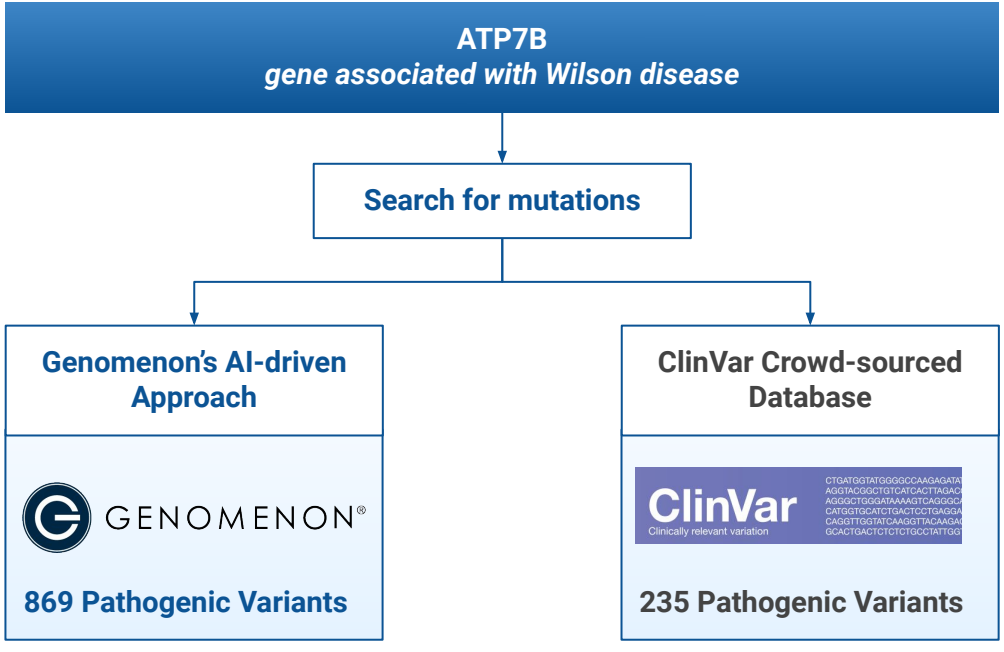
Genomic Language Processing (GLP) is a novel technology that systematically extracts and standardizes **genomic and clinical information** from the medical and scientific literature. Designed specifically to recognize this complex genomic information, GLP provides superior sensitivity compared to traditional methods, finding more variants and subsequently, more patients. **Genomenon's database**, built using GLP, currently contains over **14.8 million variants, 8.8 million full-text articles, and 3 million supplemental datasets**.

How Genomenon Uses AI in R&D

In collaboration with **Alexion**, AstraZeneca's Rare Disease group, **Genomenon applied its AI technology to help accelerate the genetic diagnosis for rare disease patients**. Genomenon's novel combination of AI-powered Genomic Language Processing and expert review **identified significantly more pathogenic variants associated with Wilson disease**.

Genomenon's AI-driven approach **identified 3.7x more evidence-supported, pathogenic/likely pathogenic variants for ATP7B** – a gene associated with Wilson disease – **compared to the crowd-sourced database, ClinVar**. This significantly expands the resources available to healthcare providers to make more informed diagnostic decisions.

With greater adoption of Mastermind, we predict that the substantial increase in the number of known, disease-causing variants **will improve the diagnosis of people living with Wilson disease by improving the ability to interpret genetic testing results**.



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We predict that this **will improve the diagnosis of people living with Wilson disease** by improving the ability to interpret genetic testing results.

De-Risking and Accelerating Drug Discovery & Development for Improved Success in Biopharma. GATC Health

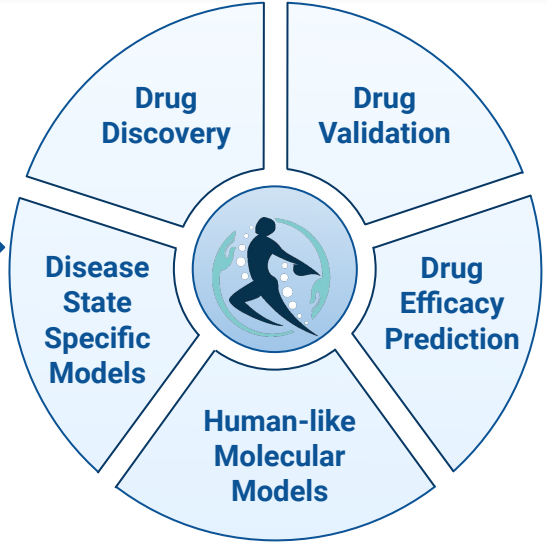
GATC Health

GATC Health has an unprecedented technology that will lower costs and accelerate the drug discovery and development process to create better and safer drugs, faster. The company delivers highly efficient services for pharma companies reducing the risk in the drug discovery process. GATC Health develops **an end-to-end drug development cutting-edge AI-based platform** with capabilities that include: earlier disease detection, identification of the disease biology, creation of new drug and therapeutic solutions, simulation of in-silico clinical trials and providing a feedback loop for in-vitro and in-vivo testing.

GATC's Platform combines massive volumes of disease-specific data and proprietary AI solutions to replicate human biology's billions of interactions for rapidly and accurately discovering and validating novel drugs. This is a revolutionary approach to drug discovery that can address nearly any condition, disease or disorder; while drastically improving costs, efficiency and time for clinical development.

Target Diseases

- Oncology
- Neurology
  - Psychiatry
  - Substance Abuse
- Cardiology
- Immunology
- Rheumatology
- Other diseases



Outcome

- 1-3 Small Molecules or Biologics Optimized for Specific Diseases and Patients

How GATC Health Uses AI in R&D

Diagnostic Biomarker Discovery

- Diagnostic biomarkers are discovered on a dataset.
- Biomarkers are mathematically assessed for causal and effect impacts.
- Validated causal biomarkers and pathways are simulated and evaluated by AI-assisted database models and human expertise.
- A final set of treatment targets emerges.

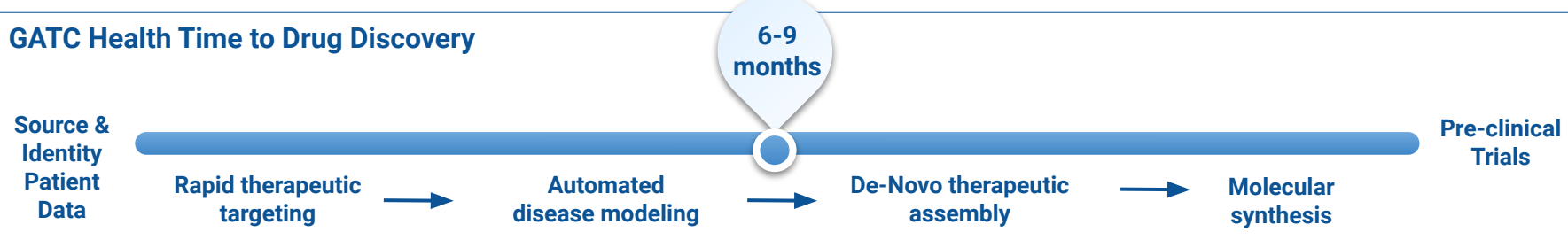
Drug Compound Discovery

- Identifies the causal relationship between the biomarkers and the disease to illuminate insights into the disease.
- AI-assisted compound discovery is used to produce a set of novel treatment compounds.
- The targets and compounds are prioritized and documented for pre-clinical testing.

Pre-Clinical De-Risking of Drug

- Develop new therapeutics using in-silico and in-vivo clinical studies with more comprehensive analysis.
- Ensure higher levels of success as the drug progresses through FDA trials.
- Eliminate majority of the risk and cost associated with treating the disease.

GATC Health Time to Drug Discovery

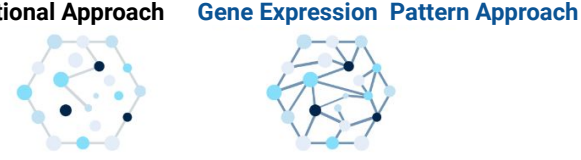


How ONCOCROSS Utilizes AI and Transcriptomics for Drug Development

Oncocross, a leading biotech company in Korea, utilizes an **AI platform** to identify new disease indications for new drug candidates or existing drugs based on a **transcriptome database** and is collaborating with leading global/Korean pharmaceutical companies and hospitals. The company strives to develop treatments for intractable and rare diseases both in the **oncology** and **non-oncology space**.

The company developed **ONCO AI PArk** (**ONCO**CROSS **A**rtificial **I**ntelligence **P**latform **A**rk) - an Artificial Intelligence platform for drug development and predictions that includes several AI solutions.

Gene Expression Pattern Analysis
Instead of analyzing single target, single pathway, with single hypothesis, they analyse entire set of gene expression pattern



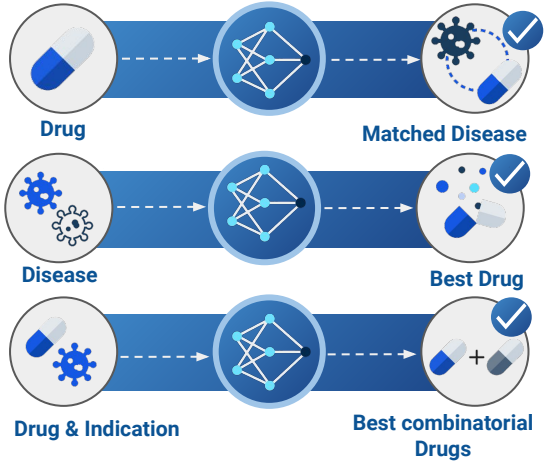
Medically Curated Database
They have unrivalled quality transcriptome database that is curated by medical doctors and pharmacists at Oncocross

Pharmacophysiological & Pathophysiological Evidence Guided Drug-Disease Pairing
AI Platform performs comparative analysis at transcriptome levels of cells and human biopsy and blood samples

How ONCOCROSS Utilizes AI and Transcriptomics for Drug Development

RAPTOR AI™ (**R**NA expression-based **A**nti-symmetrical **P**airing **T**ool for **O**n-demand **R**esponse **AI**) is transcriptome-based disease and drug-screening platform.

- Scoring anti-symmetricity of diseases and drugs using various algorithms, and integrating them to search optimal disease or drug.



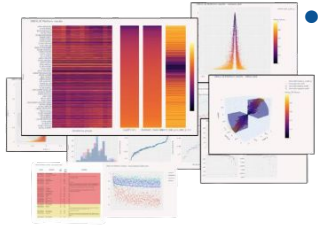
RAPTOR AI™ solution

Indication Expansion
predict additional indication of a clinical stage drug candidate in Phase I, II or III

Rescue Drug
predict the optimal indication of a drug candidate that has failed in Phase II or III

Combination
predict a partnering drug that can improve the efficacy

- Database with hundreds of disease cohorts and tens of thousands of chemical data.



- The platform has accurate gene expression alteration scoring system for drug or disease. Comparative analysis is performed at the transcriptome level to predict the optimal drug-disease pair.

- Scoring anti-symmetricity with integrating various cell line-based experimental results via cell-tissue similarity. Cell-tissue similarity-based integration method is necessary for accurate prediction, as drug effect data are derived by cell line, and disease effect data are from human tissue.
- The company has validated internally and in partnership:

8	Internal pipelines
8	Partnered pipelines
1	Global clinical trial in Phase I
2	Phase IIa IND
1	Investigator initiated trial

Industry Developments 2020- Q3 2022

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Biggest Deals Q1 2021 - Q1 2022

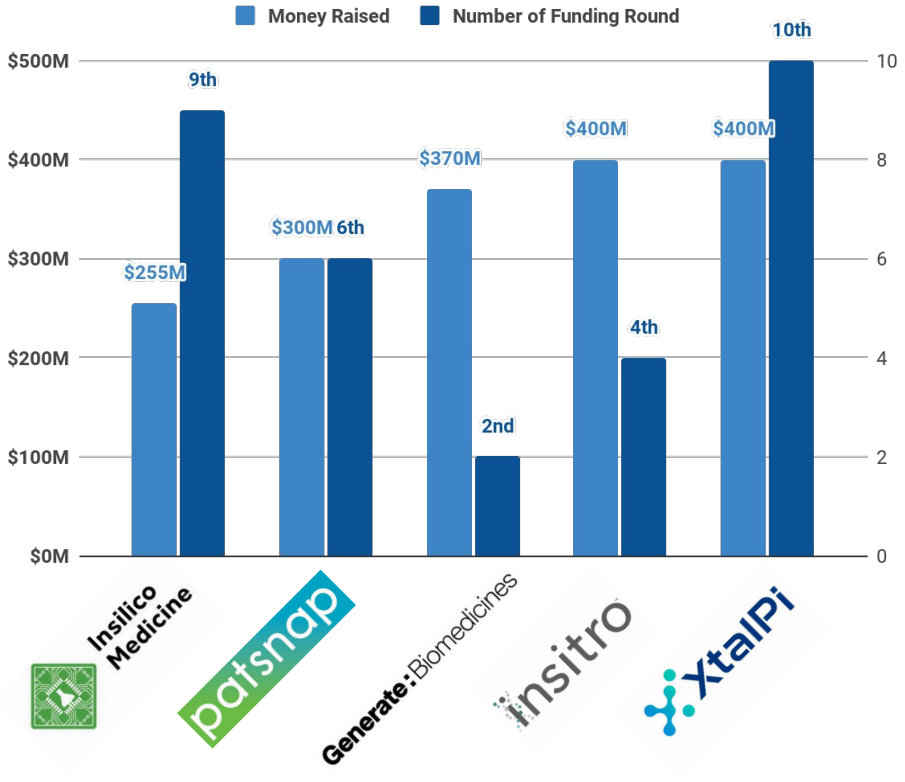
The total amount of VC funding in AI-biotech startups increased during Q1 of 2022 approaching a total of $12B.

There is an increasing number of late-stage mega-rounds including hundreds of millions. The apparent trend is sector consolidation, where a number of AI-startups have achieved substantial leadership and grown in resources and technology. An important driver of growth for the sector is a substantial shift in Big Pharma's interest in AI technology, making AI an important integral part in the research and implementation areas.

Top 5 highest fundings received the following companies:

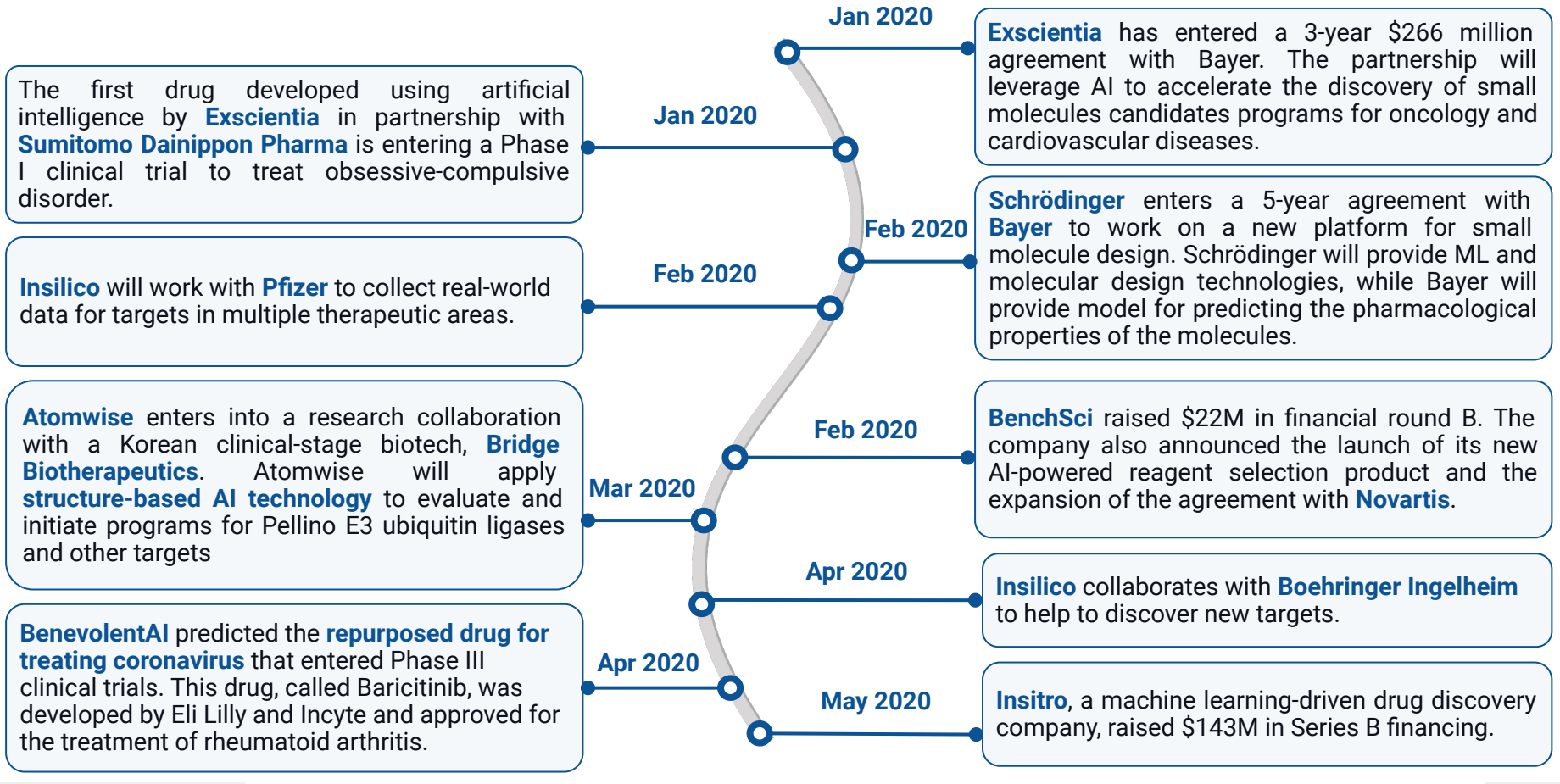
1. **Insitro** with $400 million (Series C)
2. **XtalPi** with $400 million (Series D)
3. **Generate Biomedicines** $370 million (Series B)
4. **PatSnap** with $300 million (Series E)
5. **Insilico Medicine** with $255 million (Series C)

Biggest Funding in Q1 2021 - Q1 2022



Sources: *Investment Digest AI in Pharma*

Selected Pharma AI Industry Developments Q1 2020 — Q2 2022



Selected Pharma AI Industry Developments Q1 2020 — Q1 2022

Jun 2020

Cyclica secured $17M in financing round B. This start-up developed two platforms — Ligand Design and Ligand Express that predict molecular properties using deep learning technology.

Jul 2020

Lantern Pharma prepares for the start of **Phase II** and **Phase I clinical trials** of its two anti-cancer drug candidates. Both drug candidates were created using the RADR® **AI platform**.

Jul 2020

Global Open Science project **COVID Moonshot** was launched by the international consortium of industrial and academic partners, including AI-driven startup **PostEra**.

Aug 2020

IBM introduced a new cloud platform — **RoboRXN**, a free AI-enabled chemical service for the prediction of molecule interactions and the discovery of new drugs. The platform will be primarily used to **discover compounds against coronavirus proteins**.

Aug 2020

Atomwise raised $123M in a round B led by **B Capital Group** and **Sanabil Investments**.

Sep 2020

Insilico Medicine is launching a new target and drug discovery platform **Pandomics.**

Sep 2020

Exscientia teams up with **Huadong Medicine** for the **small molecules oncology program**. The project focuses on DNA damage repair and investigates the transcription control of DNA damage response genes, which disruption leads to mutation accumulations.

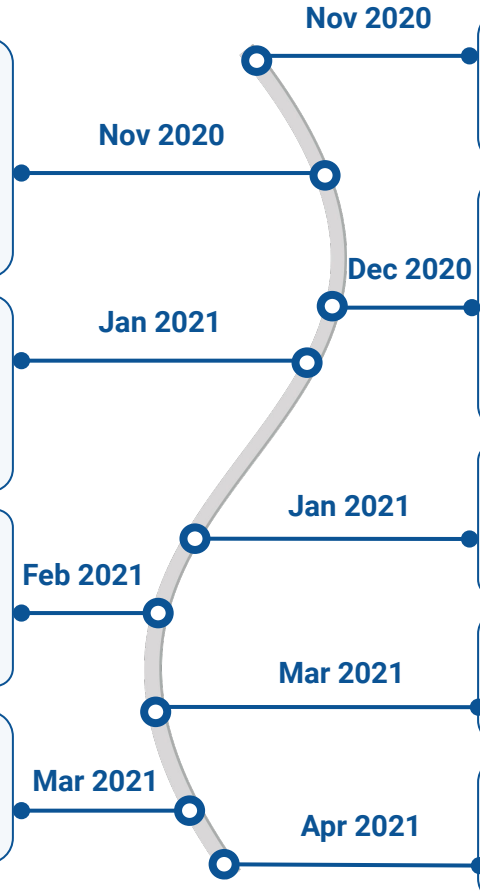
Oct 2020

Nvidia has entered into a partnership with **GlaxoSmithKline (GSK)** and its AI group to discover drugs and vaccines.

Oct 2020

Taisho Pharmaceutical and **Insilico** have entered into a research collaboration to identify **novel therapeutics against aging**.

Selected Pharma AI Industry Developments Q1 2020 — Q1 2022



Nov 2020

Schrödinger has announced a discovery collaboration with **BMS** to discover, develop, and commercialize therapeutics in multiple disease areas.

Nov 2020

BioMarin and **Deep Genomics** have announced a partnership on **AI rare disease drug discovery**. Deep Genomics will provide its AI drug discovery platform to identify and validate targets and leads. At the same time, BioMarin will be responsible for preclinical and clinical development.

Dec 2020

Insilico partnered with **APRINOIA** on **AI-powered neurodegenerative drug discovery**. The partnership aimed to utilise Insilico's generative AI technology to accelerate the discovery of compounds targeting abnormal proteins in the brain associated with neurodegenerative diseases.

Jan 2021

Nucleai and **Debiopharm** announced that they have entered into a long-term collaboration to leverage Nucleai's **AI-powered biomarker research** & discovery platform for one of Debiopharm's clinical-stage oncology assets.

Jan 2021

The **Jameel Clinic** and **Sanofi** announced collaboration on the development and application of AI to revolutionize healthcare and advance impactful and effective drug development.

Feb 2021

AstraZeneca announced a collaborative agreement with **AliveCor.** The partnership will revolve around **AliveCor's Kardia-K AI**, which is designed to analyze **ECGs** to measure a patient's **potassium levels**.

Mar 2021

Iktos announced the application of Iktos Artificial Intelligence technology for de novo design to selected **Pfizer** small-molecule discovery programs.

Mar 2021

Amgen announced that it has entered into a multi-year partnership with **Mila** – Quebec Artificial Intelligence Institute.

Apr 2021

NVIDIA and **AstraZeneca** revealed a new drug-discovery model called **MegaMolBART**, which is aimed at "reaction prediction, molecular optimisation and de novo molecular generation."

Selected Pharma AI Industry Developments Q1 2020 — Q1 2022

Apr 2021

NVIDIA announced a strategic partnership with **Schrödinger** to **expand speed and accuracy of Schrödinger's computational drug discovery platform** and enable rapid, accurate evaluation of billions of molecules for the potential development of therapeutics.

May 2021

Lantern Pharma collaborates with **Actuate Therapeutics**. The partnership will focus on leveraging Lantern Pharma's ML technology, large-scale oncology datasets, and the AI platform to accelerate critical aspects of **Actuate's 9-ING-41 drug candidate**.

Jun 2021

CytoReason announced the initiation of a project with **Sanofi**. This project aims to gain clarity on the heterogeneity of **asthma** patients.

Jun 2021

Nucleai and **Merck** have entered into a long-term collaboration to leverage Nucleai's **image analysis and biomarker discovery platform** for several Merck clinical-stage oncology assets.

Jul 2021

Eli Lilly has entered a three-year partnership with biotech company **Verge Genomics** to research and create new drugs to treat **amyotrophic lateral sclerosis (ALS)**

Aug 2021

Insilico Medicine in collaboration with **4B Technologies** aims to find a cure for **amyotrophic lateral sclerosis** (**ALS**).

Aug 2021

BMS has exercised an option on an **immune-modulating drug** candidate developed by **Exscientia**, paying $20 million for the buy-in as part of their $1.2 billion alliance.

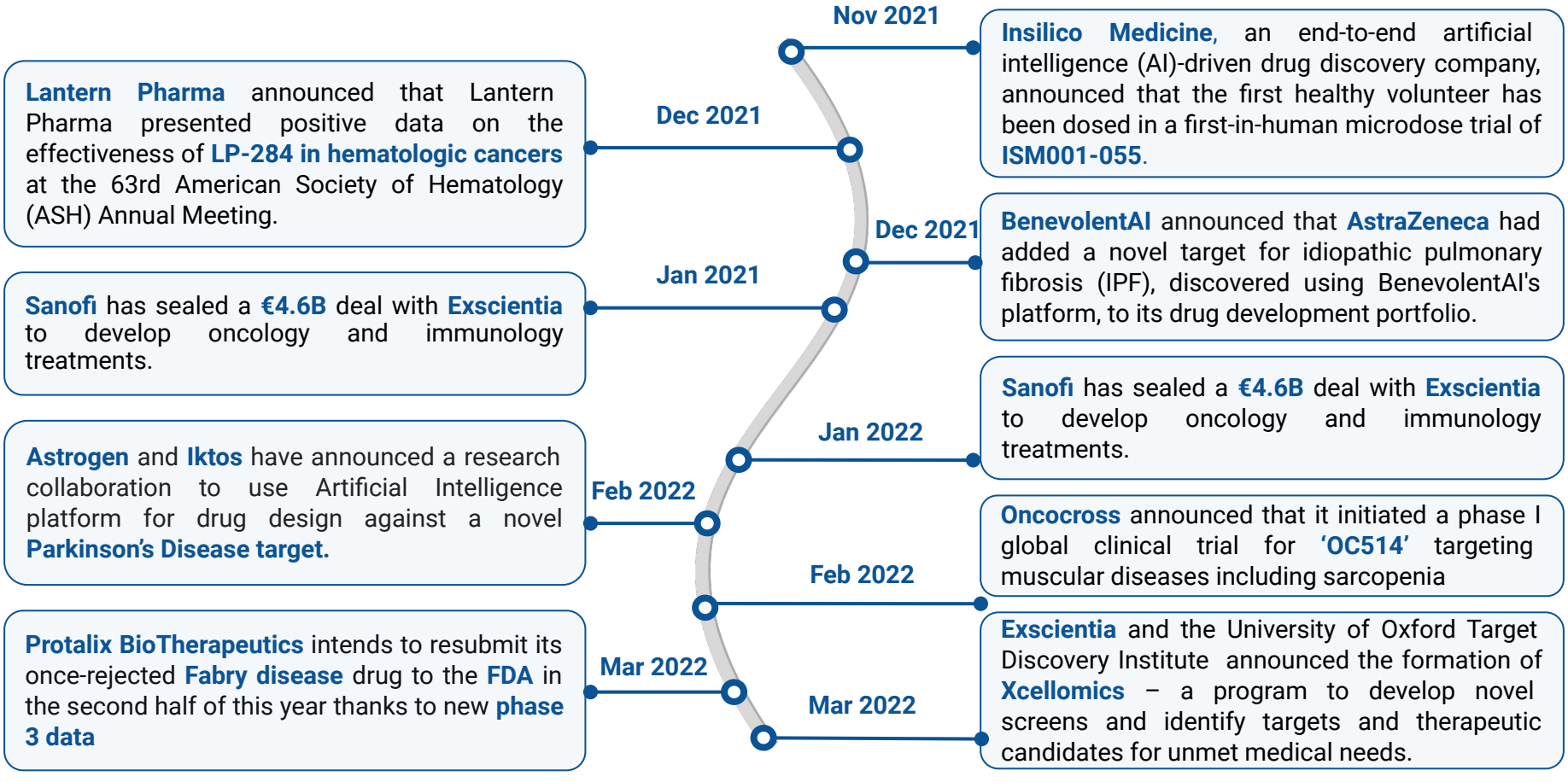
Sep 2021

The **Institute of Cancer Research** (ICR) in London used **AI** to identify the **most promising drug combinations** for children with incurable brain cancer.

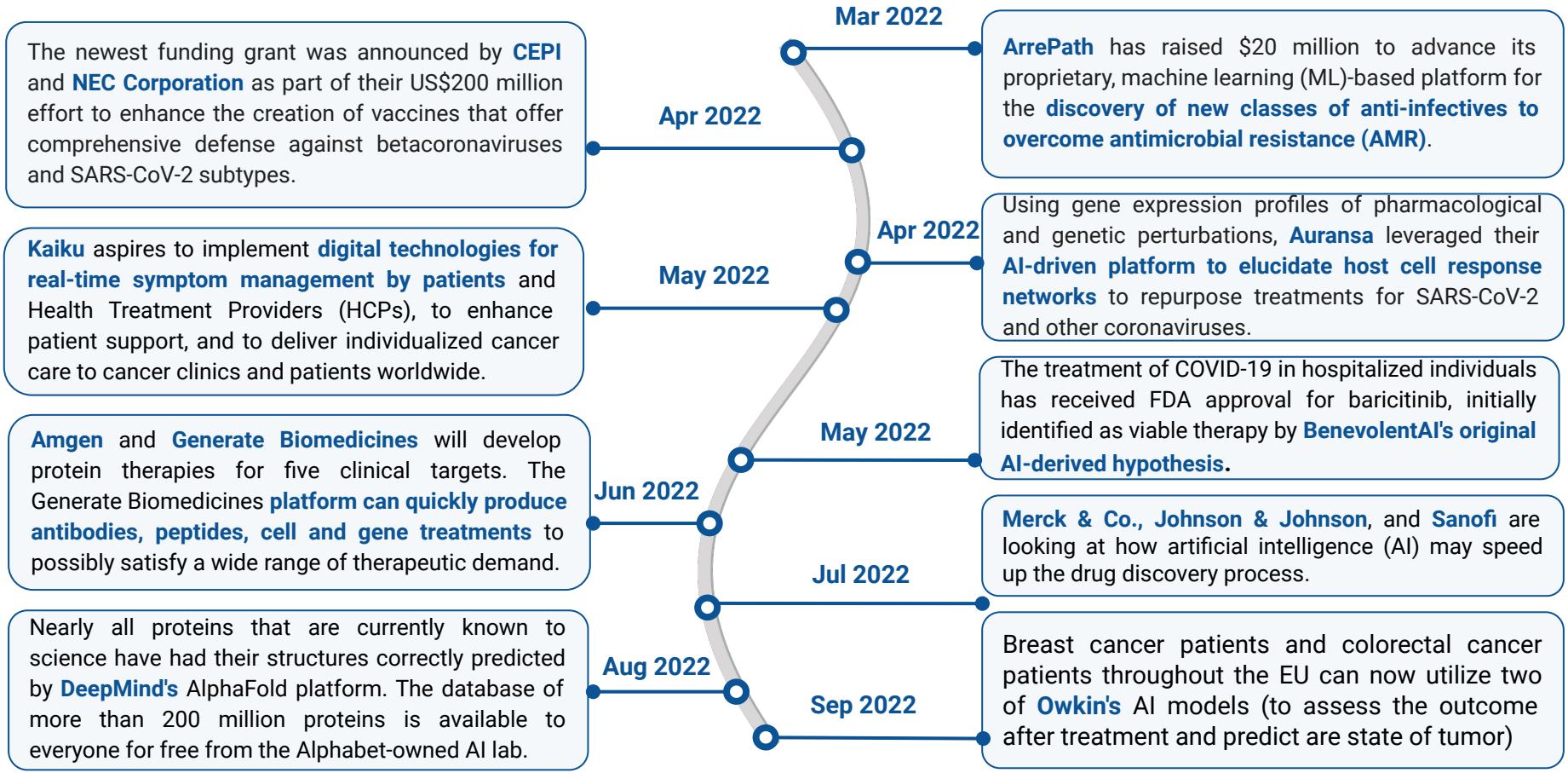
Oct 2021

AstraZeneca, Merck, Pfizer and **Teva** formed **AION Labs**, the innovative lab that will create and adopt **AI technology** to **transform the process of drug discovery**

Selected Pharma AI Industry Developments Q1 2020 — Q1 2022



Selected Pharma AI Industry Developments Q1 2020 – Q3 2022



Key Takeaways

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Major Observations for Q2-Q3 2022: Key Business Takeaways

The segment of pharmaceutical AI continues consolidation with the increasing number of later stage mega-rounds, including XtalPi and Insitro (both $400M), Generate Biomedicines ($370M), Exscientia and Insilico Medicine (both $255M), and Arbor Biotechnologies ($215M). The AI start-up pack is clear leaders with significant resources, financial leverage, technical edge, and laggards with fewer finances, technology, and scientific assets. Notably, the BioTech business adopts a new robust trend of taking firms public through SPACs (SPACs). Recently, Roivant Sciences, an AI-driven firm, exited through SPAC. Roivant's consolidated cash position will be about $2.5B on September 30, 2021.

The pharmaceutical AI business is "heating up", becoming a profitable area for expert biotech investors as well as investor groups looking to diversify their portfolios with high-risk/high-reward firms. The total amount invested in AI in Pharma in 2021 has quadrupled from $4,7B to $12,73B. A growing number of proof-of-concept breakthroughs confirm that AI technology has matured enough to provide tangible value to pharma and contract research organizations (CROs).

Due to quickly growing proof of AI tech feasibility and innovation potential, big pharma and **contract research organizations are actively competing for AI collaborations**. Valo Health started partnership with Charles River Laboratories to accelerate preclinical drug discovery using Valo's small molecule Drug Discovery platform. Exscientia has signed a research collaboration with Sanofi and received an investment of $100M to develop potential drug candidates for cancer and immune-mediated diseases.

Major Observations for Q2-Q3 2022: Key Business Takeaways

The global COVID-19 pandemic prolongs the rise of **the overall biotech and drug discovery sectors.** During 2021 we have observed over 100 medium and large funding rounds for biotech and drug design companies, especially those focused on antiviral therapies and vaccines.

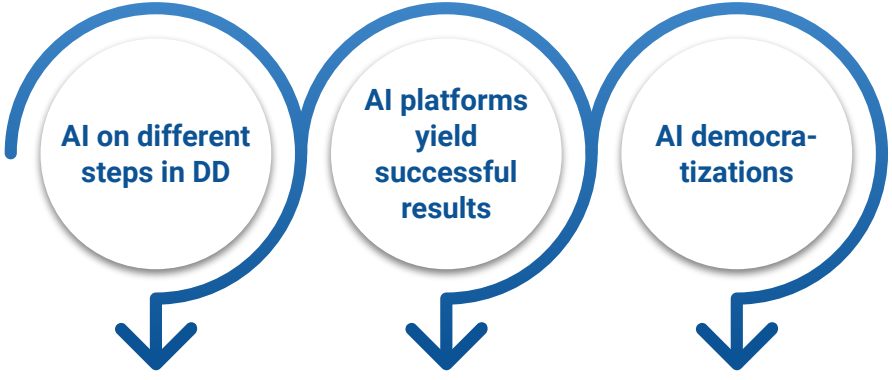
In Q2-3 2022, **1 company that use AI for DD reached IPO status**. London-based Benevolent AI closed its IPO in April and raised $292M. The vast majority of companies started gaining IPO status after 2018, marked by a growth of 136.0% during the last four years and we expect this trend growth to continue.

When some of the companies complete IPOs in the nearest future, it will attract a **significant number of non-biotech investors to enter the Life Sciences sector**. The prospects of this trend are already vivid: big tech companies enter partnerships with both innovative start-ups and pharma companies to consolidate resources, mainly in personalized medicine, cell and gene therapy, and molecule prediction software. Some of these companies even open subsidiaries harvesting AI in Drug Design (like Isomorphic Labs from Google).

The growing industry traction, reflected in the increasing number of R&D partnerships between big pharma and CROs with AI startups, is a sign that the market is maturing for rapid increase in M&A activity in the nearest future. Because of the crisis AI-in-Drug Development publicly traded companies fell to **$85,7B of cumulative capitalization as of October 3rd, 2022**.

Key Technology Takeaways

1. AI is regarded by some top executives at big pharma (**GSK and others**) as **a tool to uncover not only new molecules, but also new targets**. Ability of deep neural networks to build ontologies from multimodal data (e.g. "omics" data) is believed to be among the most disruptive areas for AI in drug discovery, alongside with data mining from unstructured data, like text (using natural language processing, NLP).
2. There is **a considerable trend for "AI democratization"** where various machine learning/deep learning technologies become available in pre-trained, pre-configured "of-the-shelf" formats, or in relatively ready-to-use formats — via cloud-based models, frameworks, and drag-and-drop AI-pipeline building platforms (for example, KNIME). This is among key factors in the acceleration of AI adoption by the pharmaceutical organizations — where a non-AI experts can potentially use fairly advanced data analytics tools for their research.
3. **Proof-of-concept projects keep yielding successful results** in research studies, and in the commercial partnerships alike. For example, companies like Recursion Pharmaceuticals, Insilico Medicine, Deep Genomics, and Exscientia achieved important research milestones using their AI-based drug design platforms.



Ai is used not only for drug design, but also target identification.

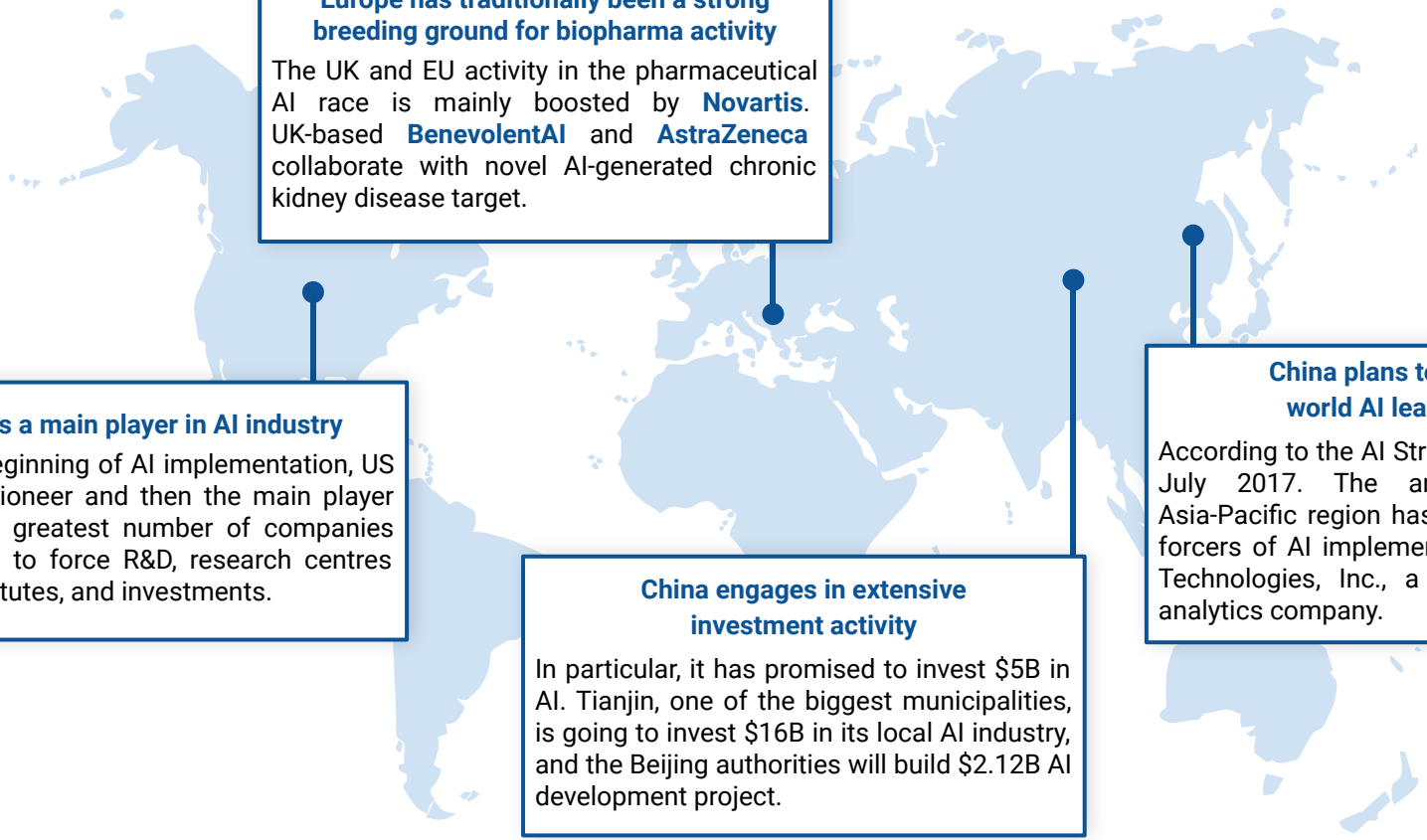
Many AI-designed drugs showed successful results in research studies and even clinical trials.

Ready-to-use AI platforms for DD became available and can be used by non-AI experts.

Obstacles That Still Remain

1. **Global shortage of AI talent** continues to be a serious challenge for the biopharma industry, repeating the trend from our previous reports. While big pharmaceutical companies invest substantial capital in recruitment of AI specialists, still the majority of them are acquired by large tech corporations (Google, Amazon, Alibaba, Tencent, Baidu etc.) However, a growing wave of specialized university programs and courses, geared towards data science and AI application, is projected to address this issue to certain extent in the coming years.
2. **Lack of available quality data is still a challenge for the unleashing full potential of deep learning technologies.** Numerous variations of deep learning (DL) are believed to be the most lucrative area of AI for applications such as drug discovery and clinical research. The key challenge is that DL algorithms are "data-greedy", while big data in biotech is not always well-versed for modeling, or is inaccessible due to privacy reasons.
3. **Ethical, legal, and regulatory issues for AI adoption in the pharmaceutical sciences.** This set of challenges is related to the previous point, but also includes other questions — AI explainability, patentability of AI-generated results, non-optimal regulations in various countries, slowing down the progress and adoption of AI technologies in general, and in the pharmaceutical industry in particular.

AI in the Global Context



Europe has traditionally been a strong breeding ground for biopharma activity

The UK and EU activity in the pharmaceutical AI race is mainly boosted by **Novartis**. UK-based **BenevolentAI** and **AstraZeneca** collaborate with novel AI-generated chronic kidney disease target.

US is a main player in AI industry

In the beginning of AI implementation, US was a pioneer and then the main player with the greatest number of companies using AI to force R&D, research centres and institutes, and investments.

China engages in extensive investment activity

In particular, it has promised to invest $5B in AI. Tianjin, one of the biggest municipalities, is going to invest $16B in its local AI industry, and the Beijing authorities will build $2.12B AI development project.

China plans to become the world AI leader by 2030

According to the AI Strategic Plan released in July 2017. The analysis of the the Asia-Pacific region has shown that the main forcers of AI implementation include Saama Technologies, Inc., a leading clinical data analytics company.

Cancer Vaccines - Another Prospective Direction in Pharma

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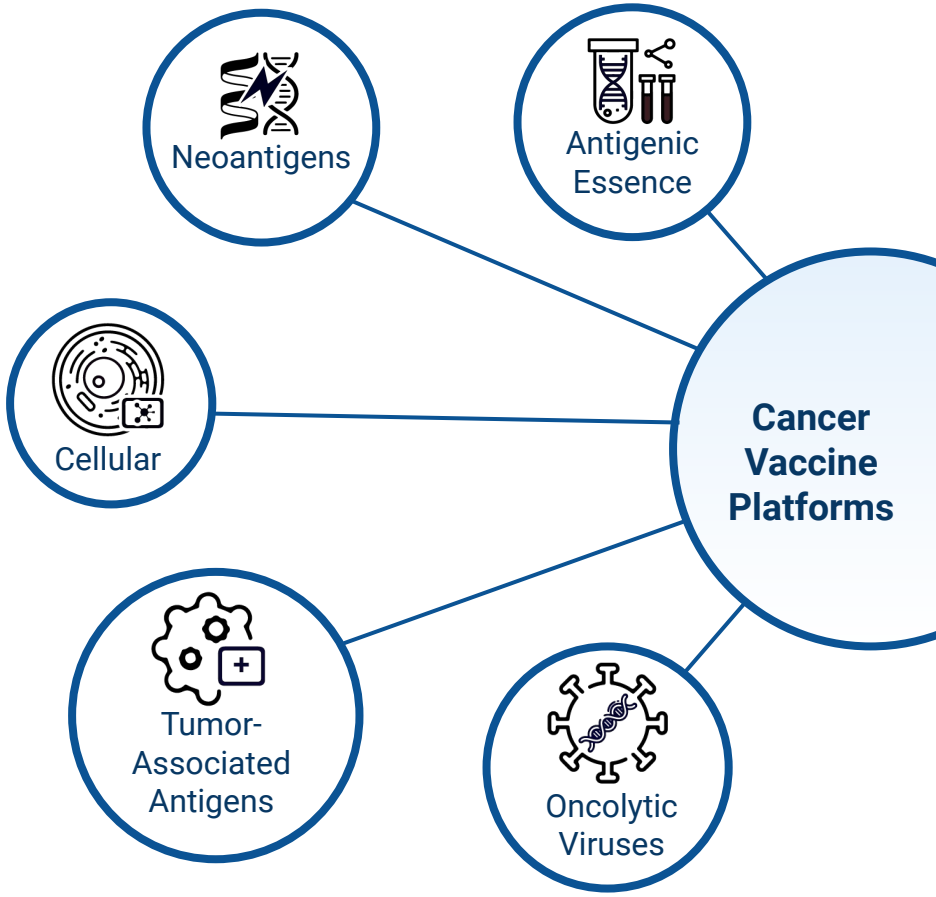
What is a Cancer Vaccine?

The most powerful weapon against malignancies can be hidden inside the host human body and it is called **immune system**. Cancer mechanisms usually trick our immune system but a proper therapy can turn our immunity back against the tumor.

That's the very aim of **cancer vaccination — to activate host immunity cells to destroy the tumour cells.**

There are multiple platforms developed to obtain cancer vaccines, in this report we are going to discuss 5 of such platforms, which serve as a basement for vaccines creation.

Some of these cancer vaccine platforms overlap and evolve out of each other while still have some unique distinguishable features which was a reason for suggested classification.



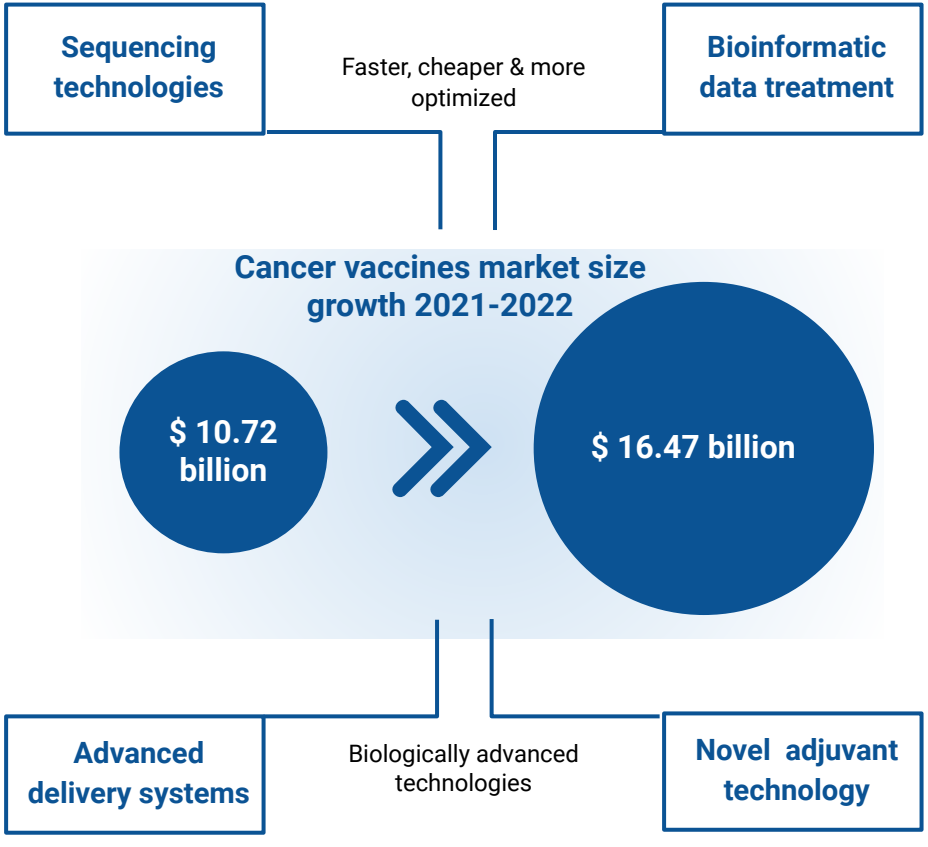
Cancer Vaccine Industry

At first, cancer vaccines didn't succeed: the enthusiasm and interest towards this technology dropped after seeing the high level of adverse effects versus low efficacy.

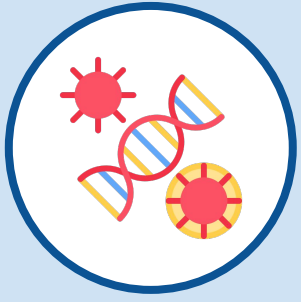
However, with the development of **sequencing technologies**, innovative **delivery systems, bioinformatic data treatment strategies** and vaccine **adjuvants** — cancer vaccines have more and more prominent chances to become deeply integrated into the market.

In 2021 the **market size** of cancer vaccines was estimated as 10.72 billion US$ and it was reached to **16.47 billion US$ in 2022.**

Considering this tendency, it is reasonable to say that cancer vaccines start forming a **separate branch of industry.**



Intro: Where is Cancer Vaccination Right Now?



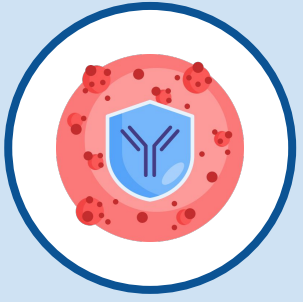
We learnt how to target tumors through their unique mutations - **neoantigens**

To prevent **tumour escape** we need to target multiple antigens on the tumour cell

cytotoxic CD8+ T-cells

We targeted **cytotoxic CD8+ T-cells** to kill the cancer cells

We need to engage **both CD8+ and memory CD4+ T-cells** to prolongate the effect

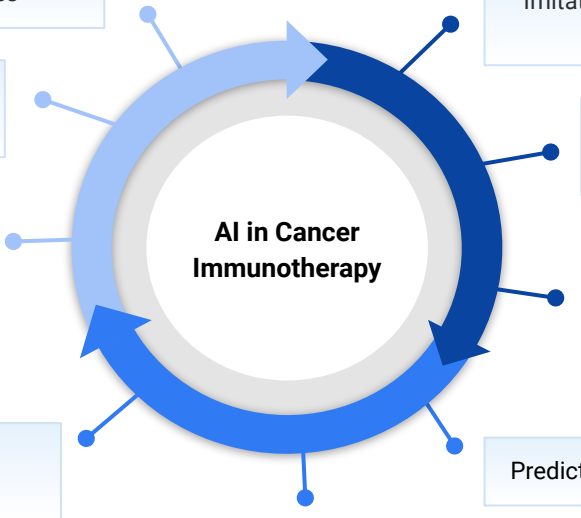


We found out that the **tumour lysates** can activate the immune response to cancer

Off-tumor effects became a severe reason for the damage so scientists are working to decrease them

Applying Artificial Intelligence For Cancer Immunotherapy

In the quest for **computer-assisted cancer vaccines development**, AI has remarkably advanced as a technique. Although the technology is still distant from being widely used in clinical practice, it has the potential to expand the functional roles in immunotherapy response when clinical data and improved AI methodologies are developed. We anticipate a bright future where AI will probably change the way cancer immunotherapy is done and eventually enhance patient safety and healthcare quality.



- Design of oncolytic viruses
- Identification and selection of TAA antigens for each cancer type
- Portray gene methylation and mutation landscapes in cancer
- Characterization of tumor-immine microenvironment
- Multi-omics Data Integration
- Prediction of immunotherapy response
- Developing of AI-based medical imaging biomarkers for patient selection and outcome prediction
- Identification and selection of TSA antigens for each cancer
- Imitation the behavior of tumor growth in dendritic cell-based immunotherapy

Level of Cancer Vaccine Innovation of 30 Leading Companies in Drug Discovery Sector

Innovative Approach

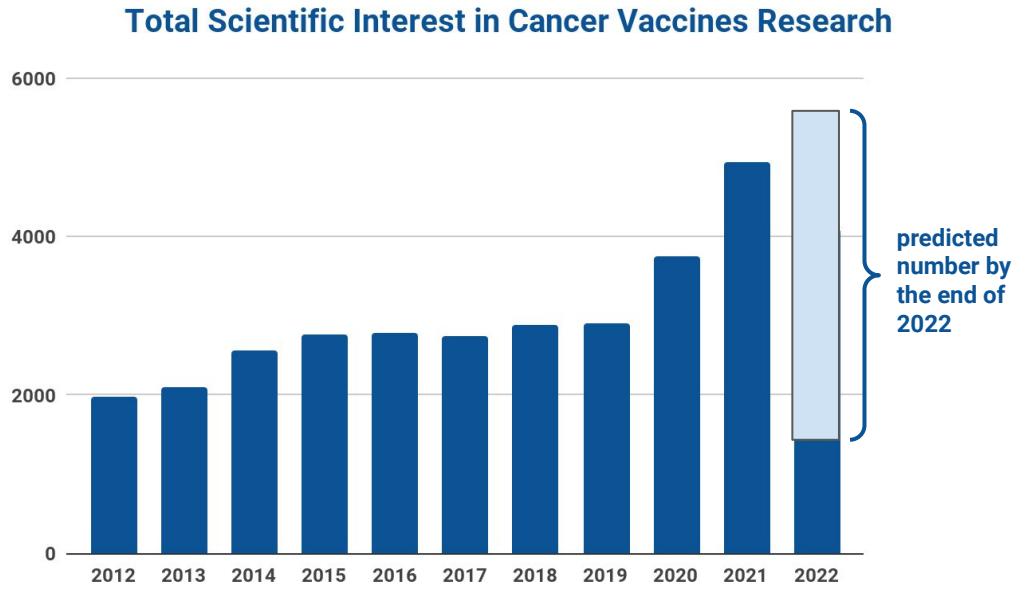
1	Biobohemia
2	AiVita Biomedical
3	Gradalis
4	Editas Medicine
5	Genocea Biosciences (NASDAQ:GNCA)
6	Gritstone Oncology (NASDAQ:GRTS)
7	Heat Biologics (NASDAQ:HTBX)
8	NexImmune (NASDAQ:NEXI)
9	Oxford Vacmedix
10	IO Biotech
11	Scancell Holdings (LSE:SCLP)
12	Sorrento Therapeutics (NASDAQ:SRNE)
13	Ionis Pharma (NASDAQ:IONS)
14	Rubius Therapeutics (NASDAQ:RUBY)
15	Arrowhead Pharmaceuticals (NASDAQ:ARWR)

Classic Approach

1	Agenus Inc. (NASDAQ:AGEN)
2	AstraZeneca (NSE:ASTRAZEN)
3	BioNTech (NASDAQ:BNTX)
4	CureVac (NASDAQ:CVAC)
5	Vaccitech
6	Enochian Biosciences (NASDAQ:ENOB)
7	Immunomic Therapeutics
8	Inovio Pharmaceuticals (NASDAQ:INO)
9	GlaxoSmithKline (NYSE:GSK)
10	Moderna Therapeutics (NASDAQ:MRNA)
11	Northwest Biotherapeutics (OTC:NWBO)
12	OncoPep
13	Gilead Sciences
14	PsiOxus Therapeutics
15	Nykode Therapeutics

Methodology: database creation followed by the detailed analysis of every individual use case by the quantitative and qualitative features such as: cancer vaccine category; complexity and development possibilities of the technology; number of similar products on the market/development pipelines; novelty of the product; addressment of the unmet needs etc.

Key Takeaways



The graph demonstrates the growing number of publications mentioning cancer vaccines by year. Over a decade the annual publishing grew more than 2.5 fold and is expected to continue increasing.

The interest in cancer vaccination is continually growing and is currently experiencing an outburst in 2021. This mature field of immunotherapy requires **novel approaches and revitalization solutions.**

The most actively developing platform right now is **neoantigens platform,** which we observe from analysing the lead products of big pharmaceutical companies.

The most **prominent research vectors** in the field of cancer vaccines are aimed at **enhancement of immunogenicity** while reducing a non-targeted damage of healthy cells, targeting **multiple antigens** and developing an **universal vaccine** for a broad spectrum of malignancies.

Sources — PubMed Database

Neoantigen Platform: Overview

Neoantigens represent a large platform in cancer vaccines fied and generally in tumor immunotherapy.

Neoantigens include antigens produced by **tumor viruses** integrated into the genome and antigens originated by **mutant proteins,** which are abundantly expressed specifically in cancer cells and have strong immunogenicity and tumor heterogeneity.

Currently a **considerable number of neoantigens** have been discovered, which are unique to tumor cells and are not affected by immune tolerance mechanism.

Neoantigens

Shared

Common across different cancer patients and not present in the normal genome

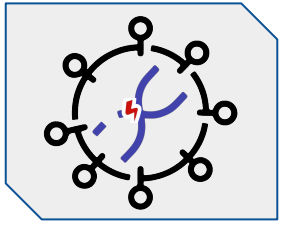
Shared neoantigens that are highly immunogenic have the potential to be screened for use as broad-spectrum therapeutic cancer vaccines for patients with the same mutated gene.

Private

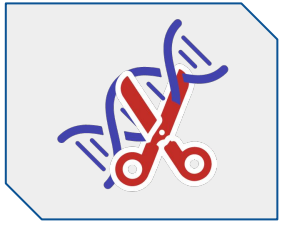
Unique to most neoantigens and completely different from patient to patient

Personalized neoantigen preparation drug can only be specifically targeted to each patient, that is, personalized therapy

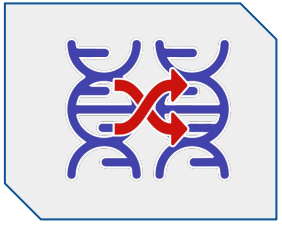
Viral infection



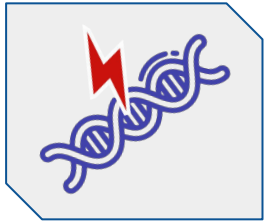
Alternative splicing



Gene rearrangement



Protein coding sequence mutation



Zhang et al., Frontiers in Immunology (2021)

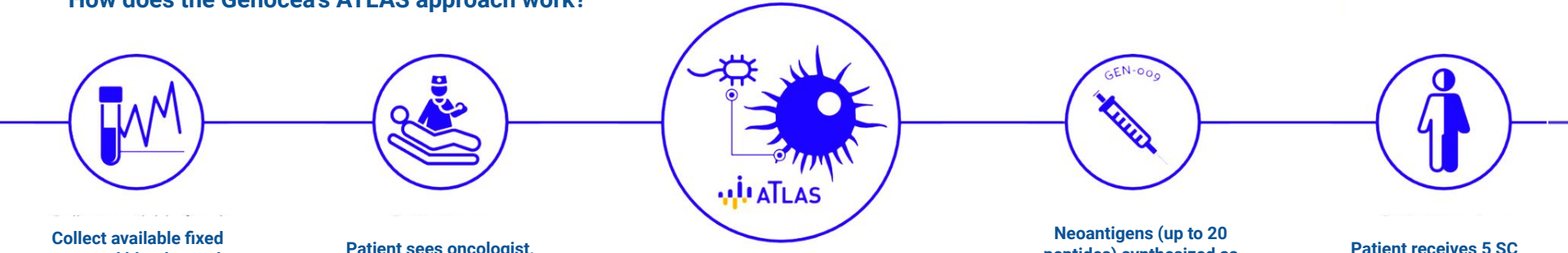
Neoantigen Platform: Key Player

Genocea Biosciences greatly focuses in the **antigen selection** for the best tumor targeting and destruction, which lies at the very basement of the ATLAS platform.

GEN-009 is a neoantigen vaccine candidate in a Phase 1/2a clinical trial to treat a variety of solid tumors. ATLAS identifies neoantigens optimized both to **patients' T cell responses and their tumors**, underscoring the advantages of the technology for neoantigen selection.

Other vaccine candidate **GEN-011** belong to the class of **adoptive T cell therapy**. GEN-011 Neoantigen-activated Peripheral T cells (NPTs) are peripheral blood T cells activated by the ATLAS-identified patient-specific neoantigens and expanded to create a **customized therapeutic.**

How does the Genocea's ATLAS approach work?



Collect available fixed tumor and blood sample, send for sequencing

Patient sees oncologist, begins SoC ICI

Inhibigens and neoantigens identified by ATLAS

Neoantigens (up to 20 peptides) synthesized as peptides and formulated with Poly-ICLC

Patient receives 5 SC doses over 6 months

Sources — Genocea Pipeline

Tumor-Associated Antigens Platform: Overview

Tumor-Associated Antigens (TAA) are self-proteins that are abnormally expressed by cancer cells.

It means they are **present both in healthy and cancer cells** and differ just by the level of exposure or presentation by cell.

This makes TAA slightly easier to discover compared to neoantigens, but at the same time TAA might cause **peripheral tolerability issues** in patients, lack of T-cell activation and collateral damage.

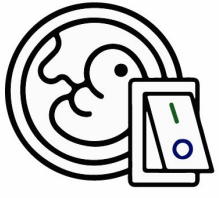
Even though TAA are used for the currently well-developed **CAR-T** technology, they still remain to be challengeable for cancer vaccines development.

Tumor-Associated Antigens

Overexpressed proteins

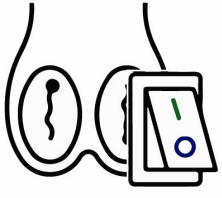
Detected both on healthy and cancer cells of human body but due to the **higher amount at malignant cells** their detection will be preferable

Differentiation antigens



Differentiation factors are meant to be present at cells only **during the early development** and are saved only in small subset of cells in developed body

Cancer testis antigens



Are not supposed to be present in healthy adult somatic tissues but are expressed in **testicles in male germ cells**

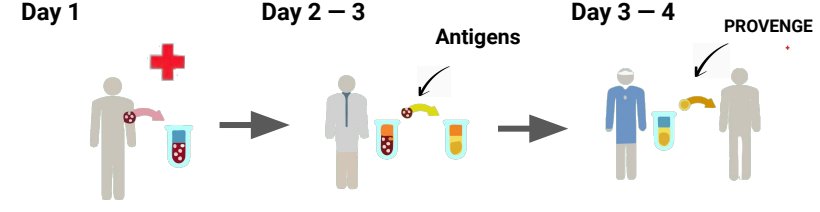
Tumor-Associated Antigens Platform: Development Milestones

Cancer immunotherapy field experienced at least two significant breakthroughs connected with **tumor-associated antigens platform:**

- Promising approval of **Provenge cancer vaccine** (sipuleucel-T) by FDA for the treatment of prostatic cancer, which used tumor-associated antigen as a target
- Development and approval of multiple **CAR-T therapies** which are based on targeting of TAA

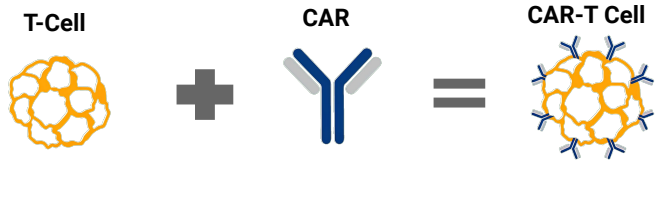
Dendreon

2010 - first FDA approved cancer vaccine



NOVARTIS Kite Pharma

2017 - first FDA approved CAR-T

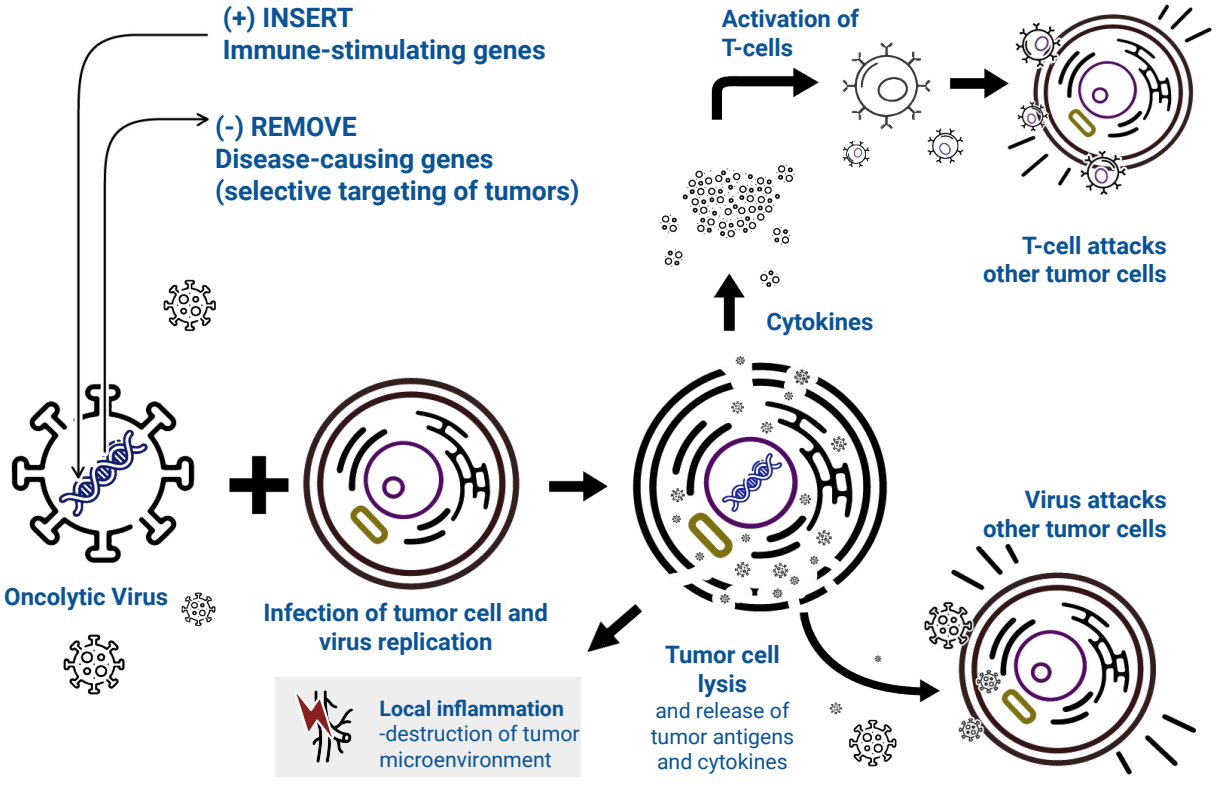


Oncolytic Viruses Platform: Overview

Oncolytic virotherapy is based on the property of some viruses to infect the cells and induce the cell lysis.

In case of cancer vaccination these viruses are **modified to target cancer cells** and enhance the immune response to completely destroy the tumor.

Oncolytic viruses cancer vaccines platform is greatly based on the neoantigens and tumor-associated antigens platforms, since the viruses and "taught" to target such antigens on the cancer cells. But due to the drastic uniqueness of the mechanism of action of such vaccines it is fair enough to separate them from other molecular and cellular cancer vaccines.



Cancer Vaccines Report

This 90--page “Cancer Vaccine Industry Landscape Overview Q3 2022” aims to provide a comprehensive overview of the current state of the cancer vaccines market and research. Along with the five high-impact cancer vaccine platforms, we provide an overview of cancer vaccine delivery systems within a human body, which tends to be the focus of the last advances in the field of cancer vaccination R&D.

The current release includes insights about **200 cancer vaccine companies** and **450 investors.**

Learn more: **https://www.deep-pharma.tech/cancer-vaccines-q3-2022**

Overview of Proprietary Analytics by Deep Pharma Intelligence

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Overview of Proprietary Analytics by Deep Pharma Intelligence

Deep Pharma Intelligence (DPI) is a strategic partner to the leading Life Science organizations, investment institutions (VC funds, investment banks), and governments across the globe — in matters related to investments, strategic positioning, and policy development in the areas of pharmaceutical and biotech research, and healthcare tech.

While Deep Pharma Intelligence is regularly producing open industry reports covering high-growth sectors in the Life Sciences, including artificial intelligence (AI), digital health, and new therapies, some of the more in-depth research is only available to our clients and strategic partners under the "**Proprietary Analytics**" category.

Our range of proprietary services includes custom consulting projects, based on the specific customer needs, as well as a collection of pre-produced "ready-to-use" proprietary reports, produced by our research team, covering general trends and specific action ideas and strategy insights related to the most promising investment prospects (e.g. new technologies, biotech startups), M&A prospects (e.g. pipeline development targets), and strategic growth ideas (trends profiling, industry overviews etc).

Services:

- Investment landscape profiling, identifying investment ideas in the biotech/healthcare tech space
- Preliminary due-diligence (business, science and technology, intellectual property (IP) profiling, freedom of operation assessment, legal assessment etc)
- Comprehensive due-diligence (deep business, science and technology assessment, IP and legal assessment, growth potential assessment etc)
- Infringement analysis of technology (i.e. If you plan to partner or invest in a data-analytics biotechs, or AI-development vendors, it is essential to understand their technological assets, both in terms of innovation potential and in terms of legal protection and non-infringement risk management)
- SWOT analysis of companies and technological sectors, competitive profiling
- Industry profiling and growth strategy development for top-tier companies and governments.

Overview of Proprietary Analytics by Deep Pharma Intelligence

Proprietary Reports

There are a few 40+ page reports delivering practical answers to these specific questions in order to optimize the short and long-term strategies of biopharma corporations and other institutions related to the industry, with a newly updated edition being released each quarter, incrementally increasing the precision, practicality and actionability of its technological and financial analysis.

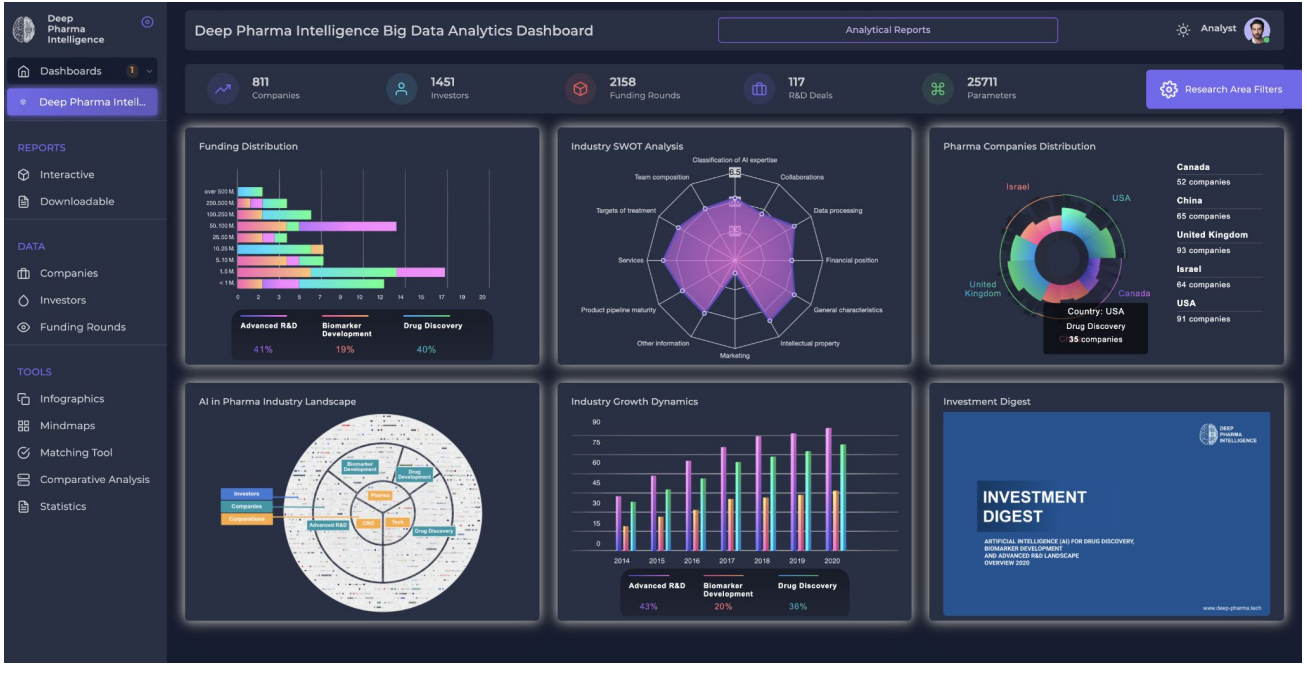
Our reports are supported by our rapidly developing data mining engine, data visualization platform and analytics dashboards.

The value our reports can deliver:

- Deep analysis of the deal-making prospects in the biotech and healthcare tech space, identification of top mini-trends and larger tendencies in innovations and technology adoption (e.g. AI, blockchain, eHealth tech, longevity biomarkers, new therapeutics and therapies etc.)
- Tangible forecasts on the 3-5 years horizon, providing an overview of future scenarios of the development of various technologies in the pharma industry
- Practical guides for adopting various technological solutions and best practises, vendor profiling and contract research strategy building
- Analysis of key market players in the emerging and high-growth areas of the pharmaceutical and biotech industries.

The parties who gain early access to these reports will have deep expertise on how their strategic agendas can be optimized in order to leverage novel research, new technologies, and emerging market opportunities, and stay competitive in a rapidly-changing technological environment, and taking into account shifting global priorities and trends.

Deep Pharma Intelligence: Analytical Dashboard



Our company is building a sophisticated cloud-based engine for advanced market and business intelligence in the pharmaceutical and healthcare industries. It includes data mining engine, infrastructure for expert data curation, and advanced visualization dashboards, including mindmaps, knowledge graphs, and 3-dimensional visualizations.

Visit our dashboard to learn more: **www.platform.dkv.global/dashboards/ai-for-drug-discovery**

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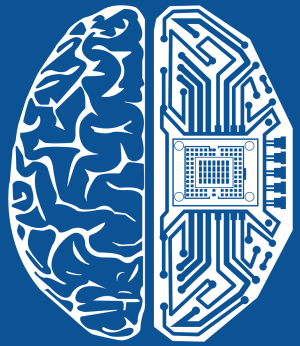

Link to the Report: www.deep-pharma.tech/ai-in-dd-q3-2022-subscribe

E-mail: info@deep-pharma.tech | **Website: deep-pharma.tech**