



Artificial Intelligence for Drug Discovery

Landscape Overview
Q4 2022



www.deep-pharma.tech



Table of Contents

Report at a Glance	3
Introduction to AI in Drug Development	5
Notable Breakthrough in AI for Pharma	8
Application of AI for Advanced R&D	12
AI in Drug Development: Leaders	13
Selected Pharma AI Deals	16
AI in Drug Development: Geographical Coverage	19
Business Activity: Overview	24
Leading Companies by Amount and Stage of Funding	28
50 Leading Investors in Pharmaceutical AI	36
Big Pharma's Focus in AI	44
Selected Pharma AI Deals	47
AI in Pharma Publicly Traded Companies	56
AI for Advanced R&D: Applications and Use Cases	64
Computational Methods Used by the Most Advanced AI Companies	73
15 Notable R&D Use Cases of AI Application in Biopharma	77
Industry Developments Q1 2022 - Q4 2022	101
Selected Pharma AI Industry Developments	103
Key Takeaways	106
Overview of Deep Pharma Intelligence	111
Disclaimer	116

Introduction

This 115-page **"Artificial Intelligence for Drug Discovery Landscape Overview Q4 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 Q4 2022

Drug Repurposing

Preclinical Development

AI Companies - 700
Investors - 1400
Corporations - 100

End-to-end Drug Development

Clinical Development

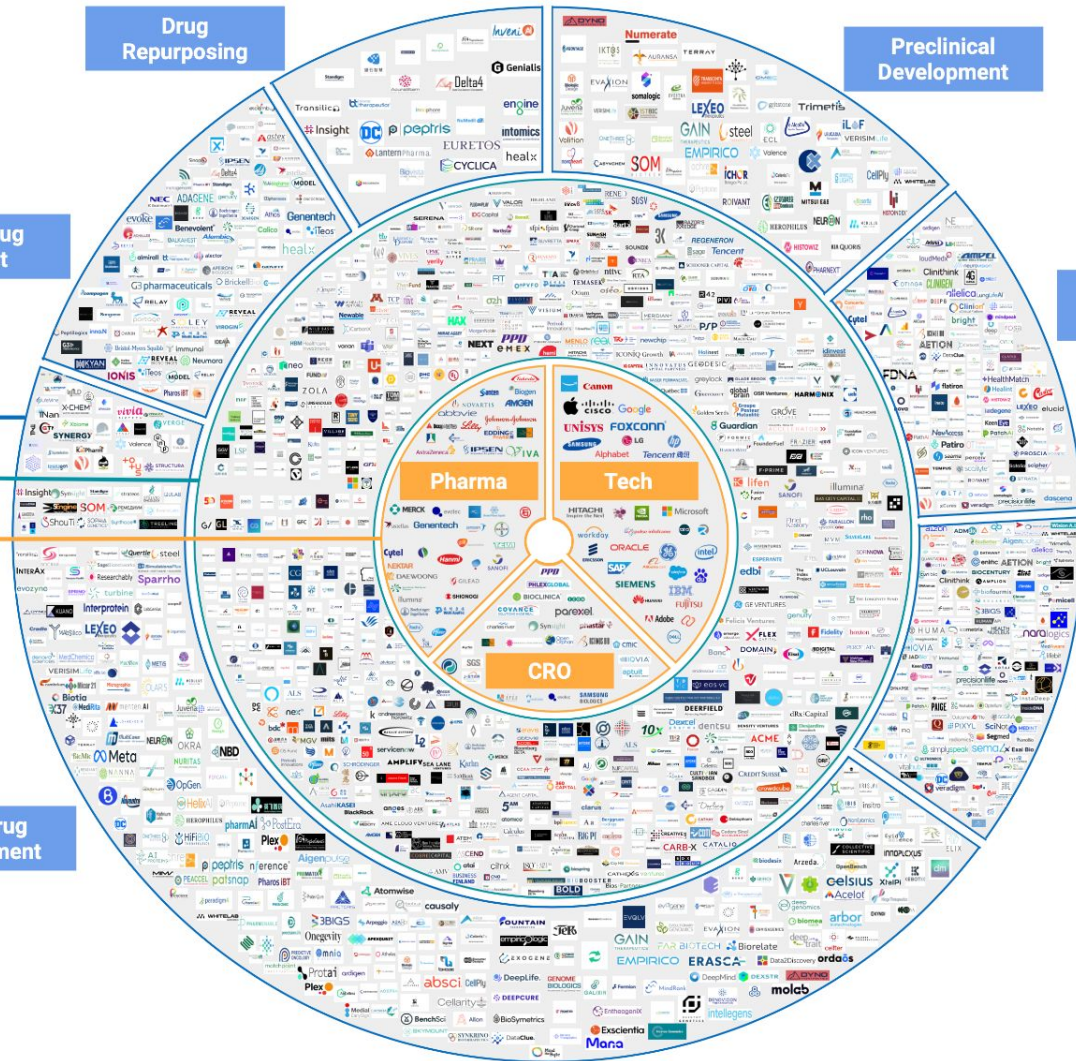
Companies

Investors

Corporations

Early Drug Development

Data Processing

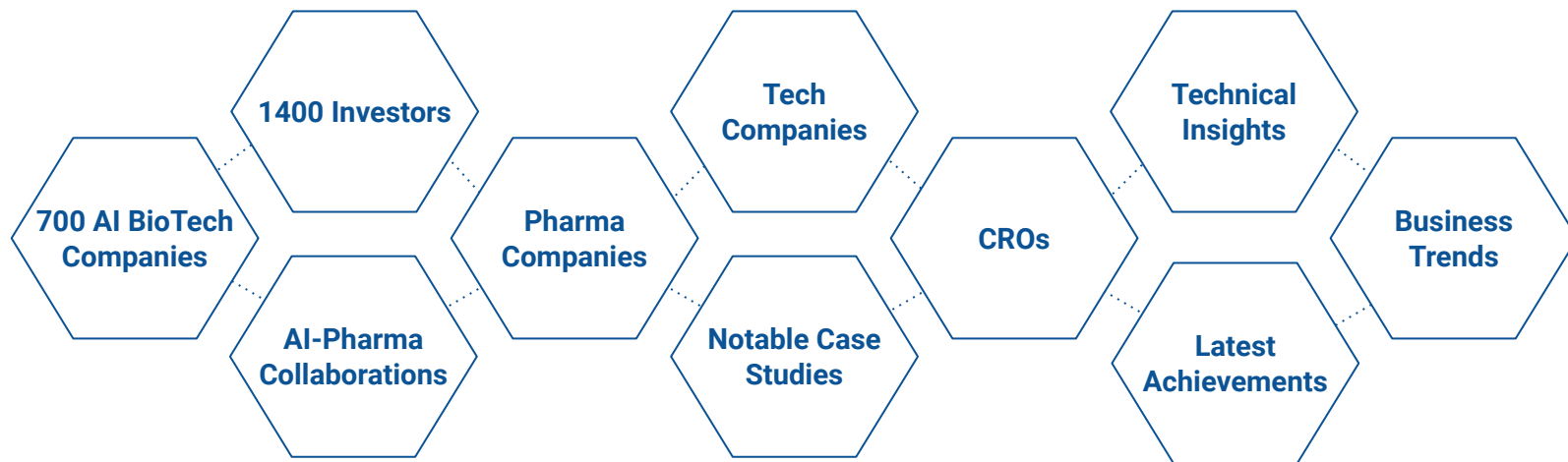


Report at a Glance

This **115-page “Artificial Intelligence for Drug Discovery Landscape Overview, Q4 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.

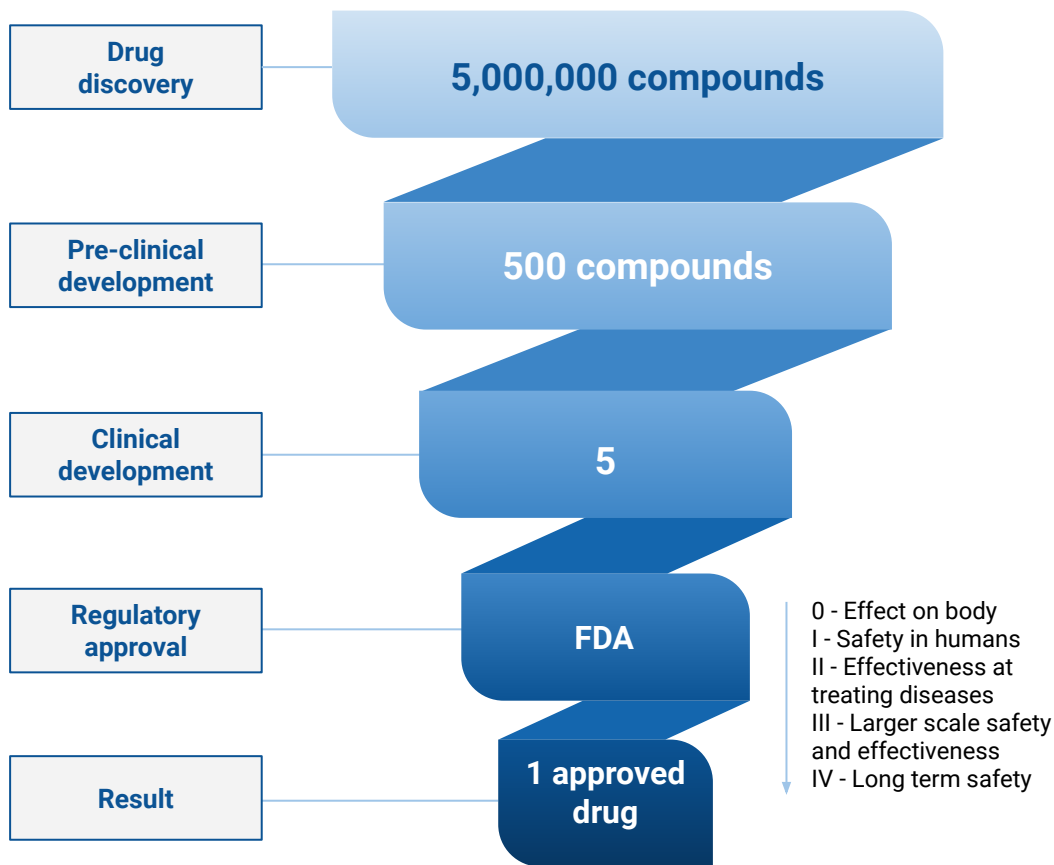
The main aim of this series of reports is to provide a comprehensive overview of the industry landscape in what pertains adoption of **AI in drug discovery, clinical research and other aspects of pharmaceutical R&D**. This overview highlights trends and insights in a form of **informative mind maps and 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.



Introduction to AI in Drug Development

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.)

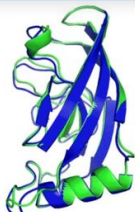
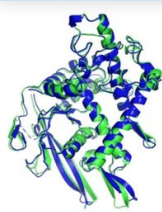
Notable Breakthroughs in AI for Pharma



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



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

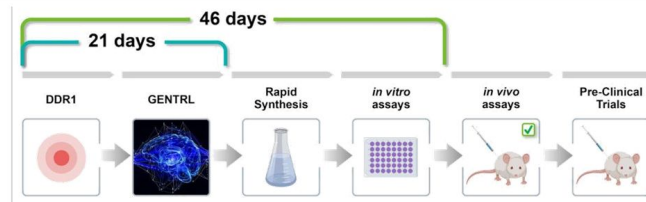


■ Experimental Result
■ Computational Prediction

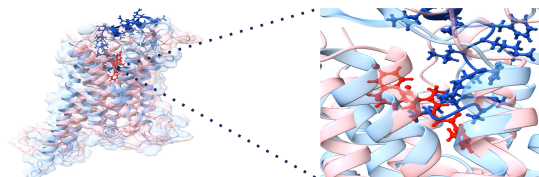


Insilico Medicine
英科智能

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



Peptilogics developed generative AI to predict peptides that bind to arbitrary proteins, even given only a protein's primary sequence, unlocking peptide drug design for established and novel targets.

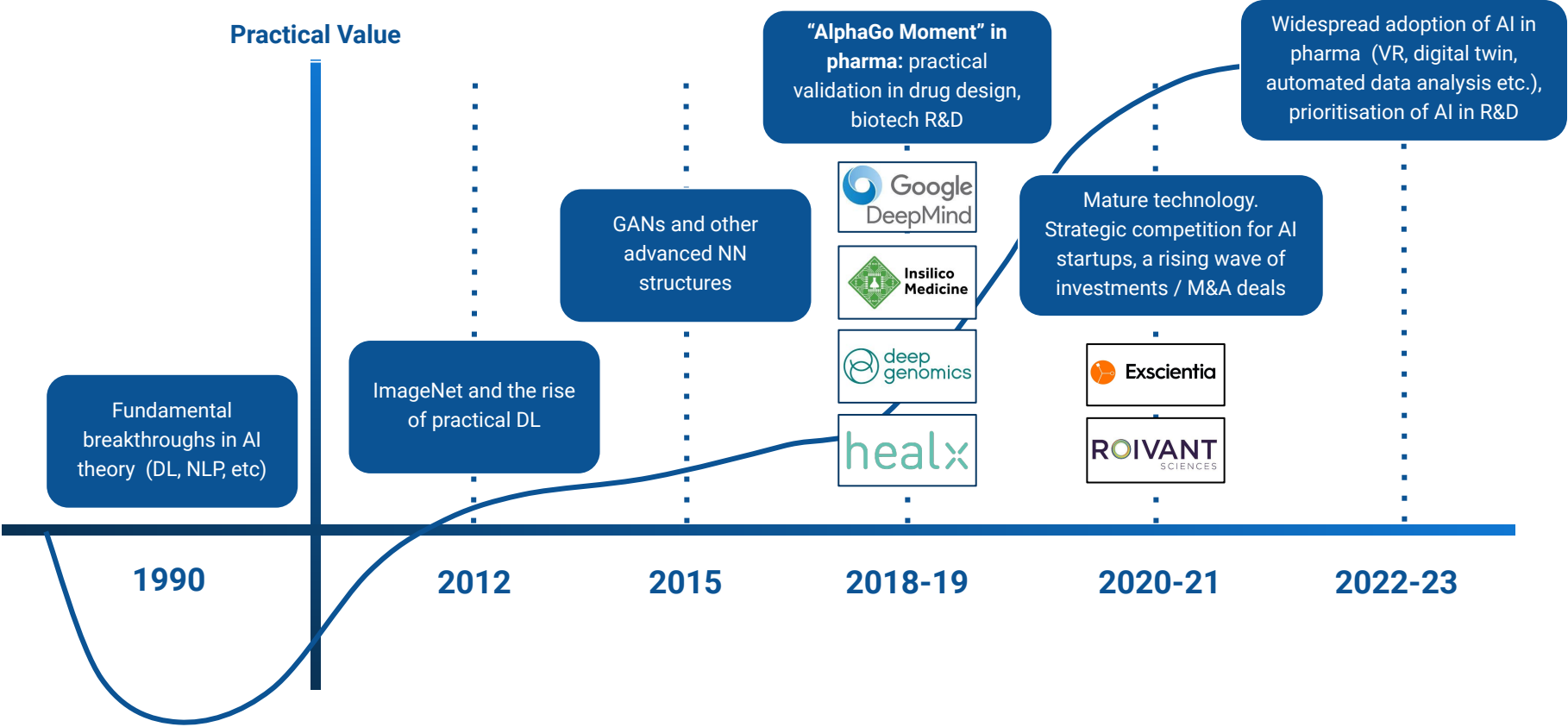


2019

2020

2021

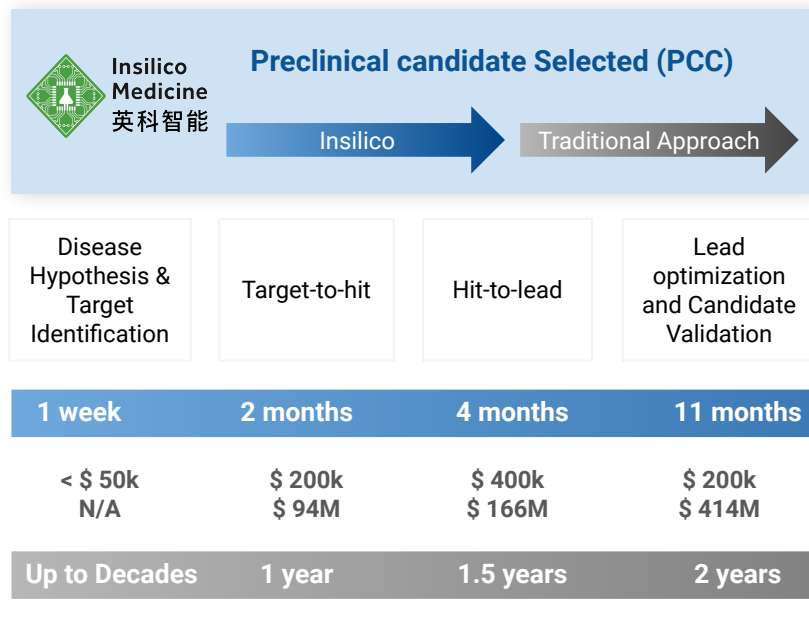
Pharma's "AlphaGo Moment"



Technological Advancements Defining the Market

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.

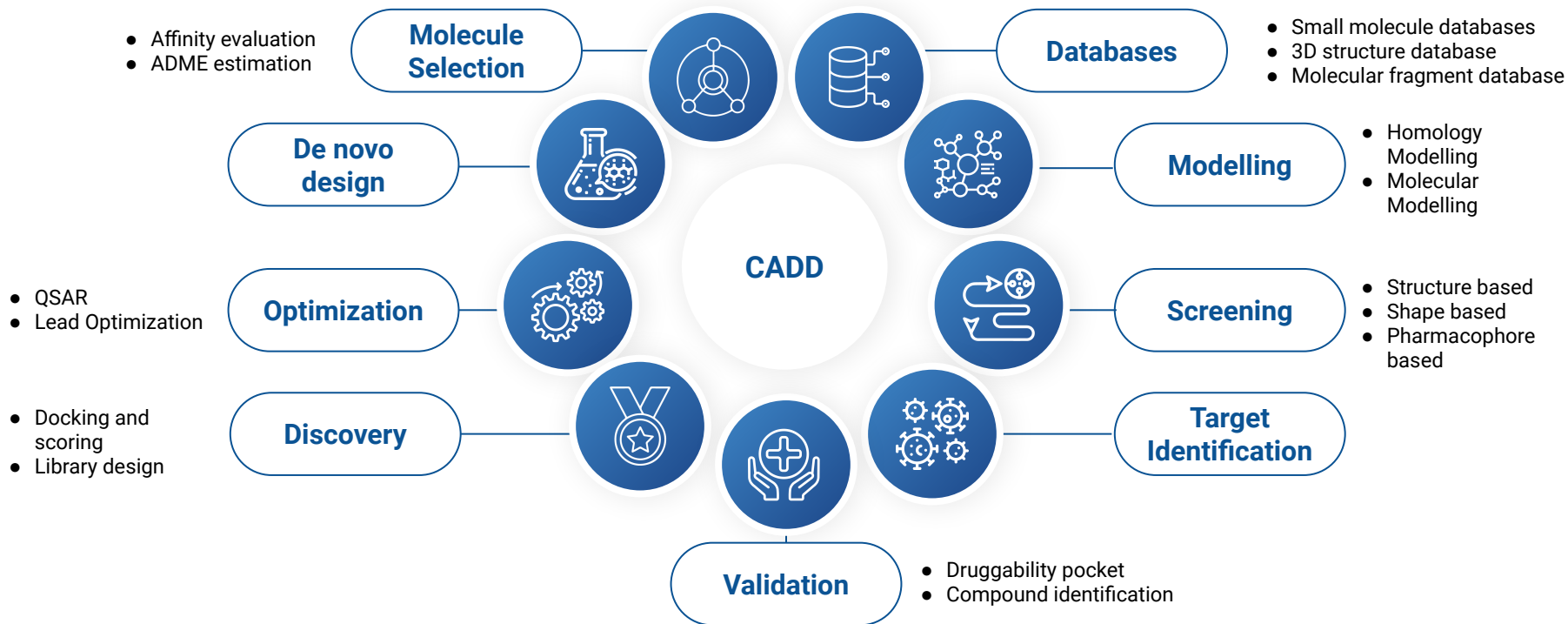
2021



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.

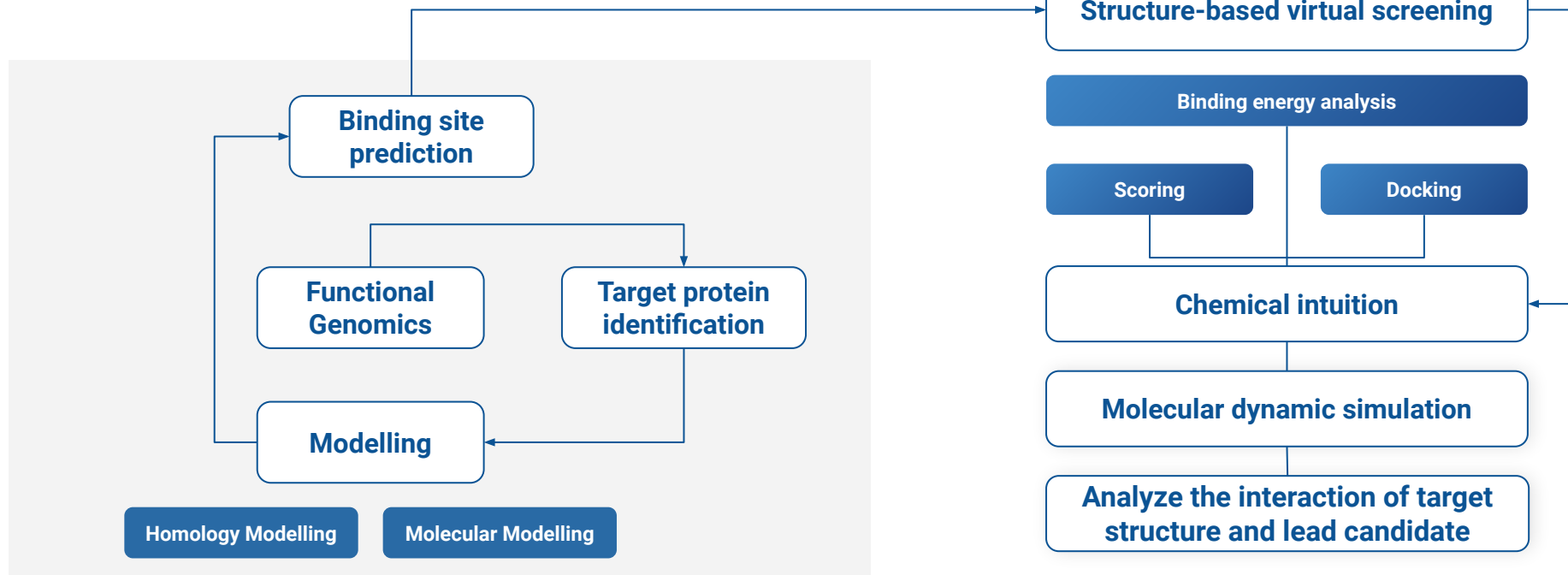
Computer-aided Drug Design

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.

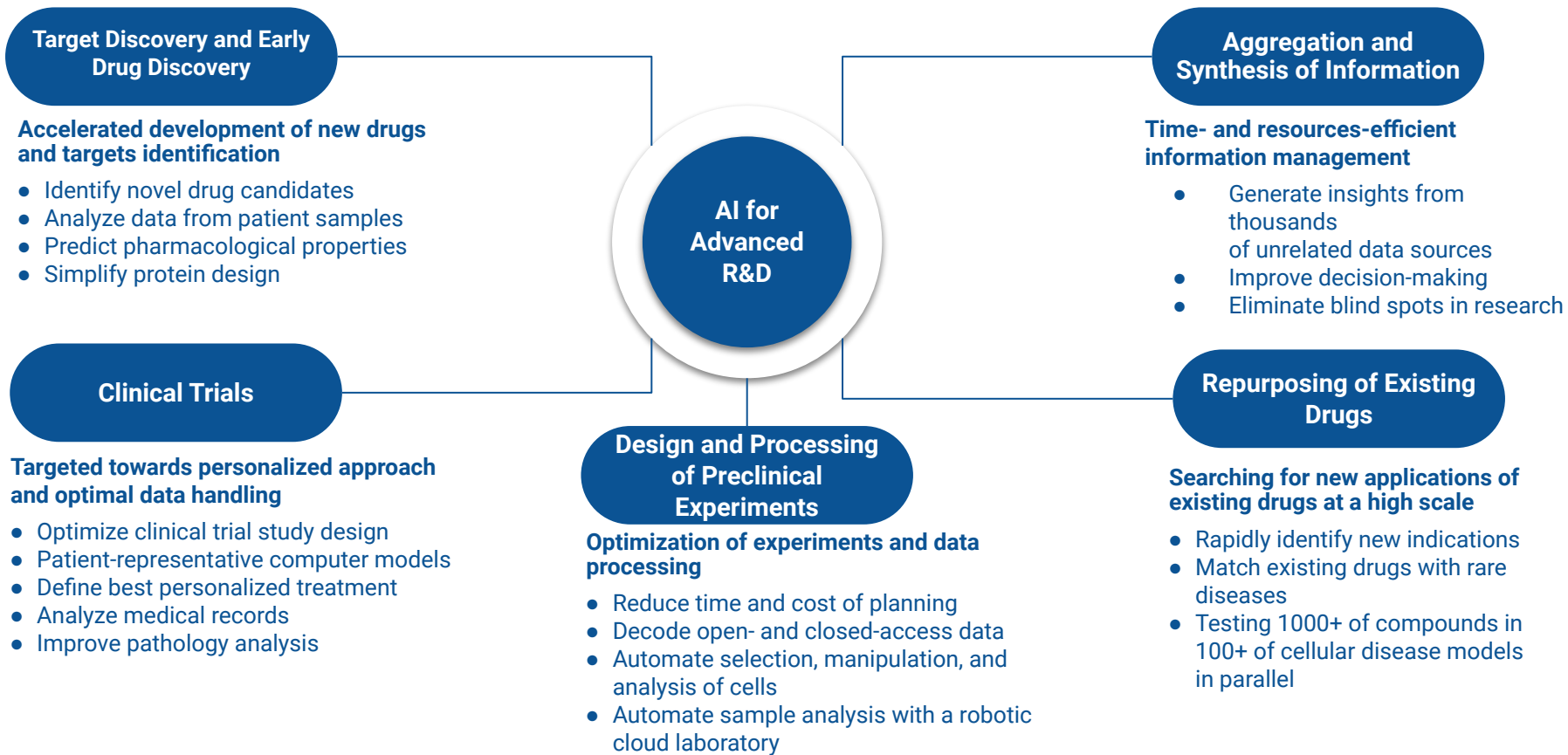


Computer-aided Drug Design

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.



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



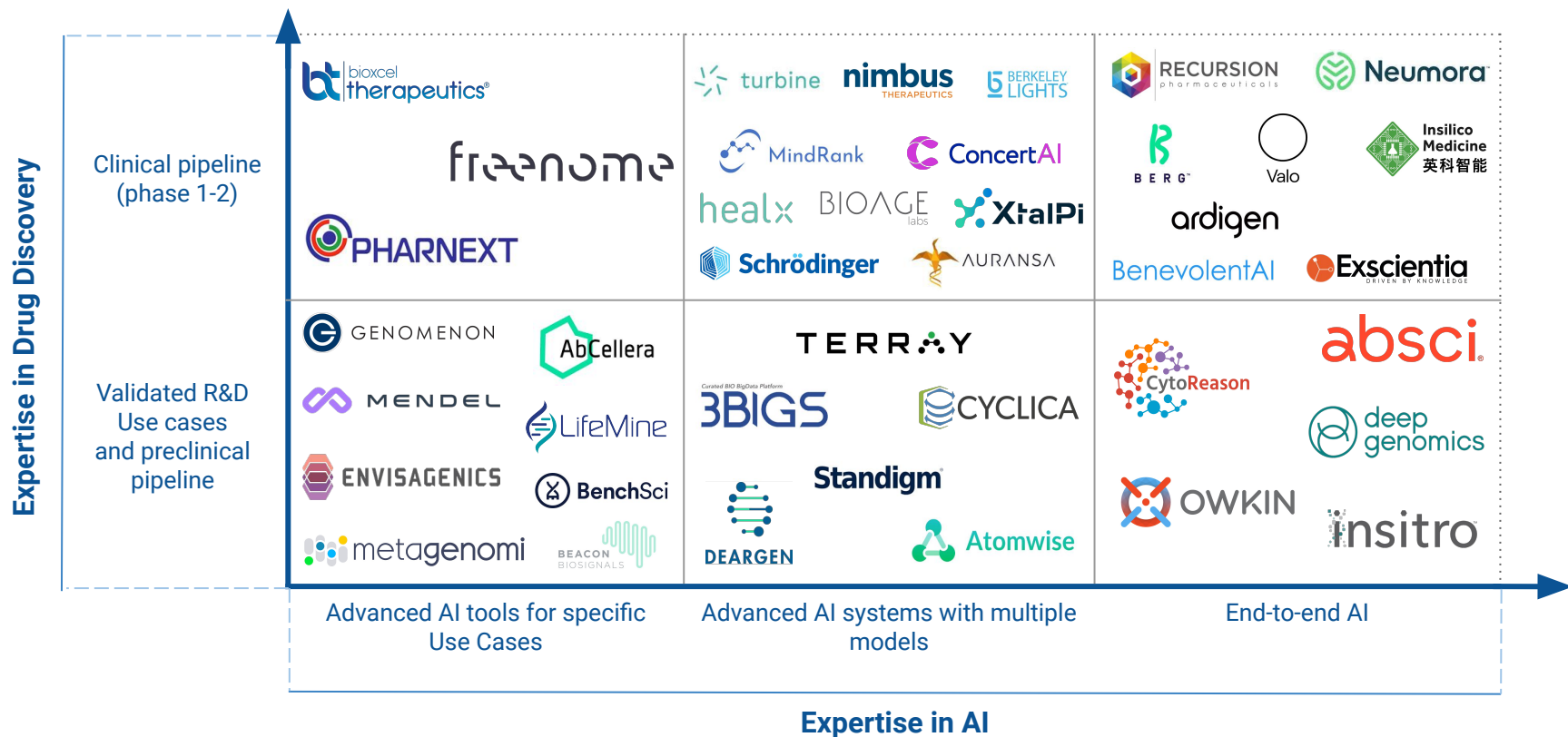
AI in Drug Development: Leaders

40 Leading Companies in AI for Drug Discovery Sector

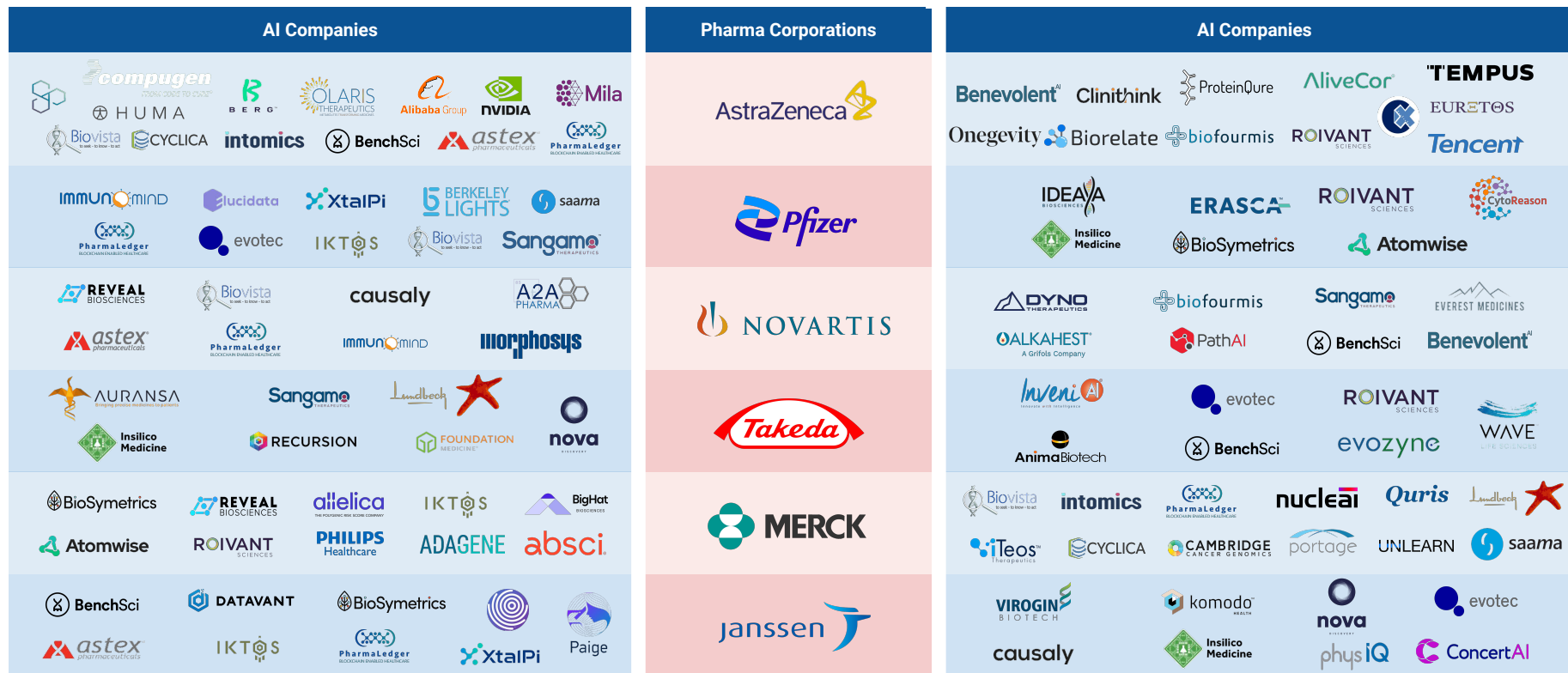
1	3BIGS
2	AbCellera
3	Absci
4	Ardigen
5	Atomwise
6	Auransa
7	Beacon Biosignals
8	BenchSci
9	Benevolent AI
10	Berg
11	Berkeley Lights
12	Bioage Labs
13	BioXcel Therapeutics
14	ConcertAI
15	Cyclica
16	CytoReason
17	Deargen
18	Deep Genomics
19	Envisagenics
20	Exscientia

21	Freenome
22	Genomenon
23	Healx
24	Insillico Medicine
25	Insitro
26	LifeMine Therapeutics
27	Mendel.ai
28	Metagenomi
29	MindRank AI
30	Neumora
31	Nimbus Therapeutics
32	Owkin
33	Pharnext
34	Recursion Pharmaceuticals
35	Schrodinger
36	Standigm
37	Terray Therapeutics
38	Turbine
39	Valo
40	XtalPi

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



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



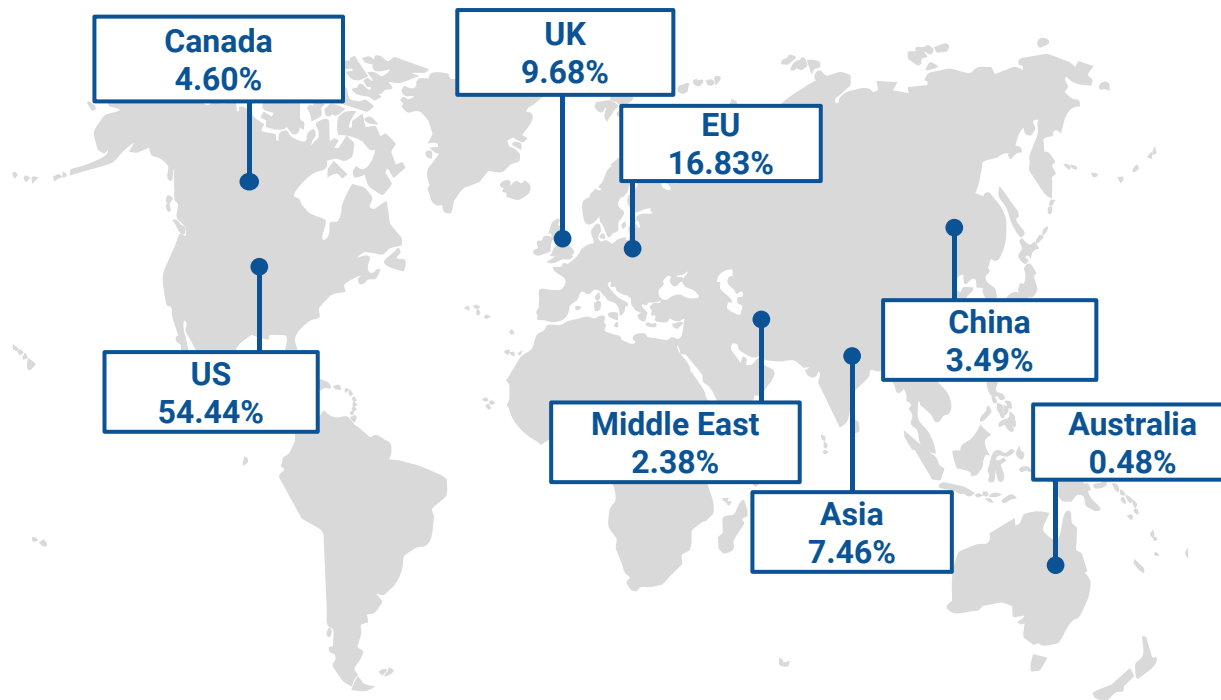
Note: the central column (red) defines the pharmaceutical corporations and side columns (blue) defines AI companies that have collaborations with pharma companies from the central column.

50 Leading Investors in AI for Drug Discovery Sector

1	Casdin Capital	18	Merck Global Health	35	AME Cloud Ventures
2	Y Combinator	19	RA Capital Management	36	Founders Fund
3	GV	20	Bill & Melinda Gates Foundation	37	OrbiMed
4	Creative Destruction Lab (CDL)	21	Foresite Capital	38	Lifeforce Capital
5	Perceptive Advisors	22	T. Rowe Price	39	Lilly Asia Ventures
6	Alexandria Venture Investments	23	Obvious Ventures	40	Polaris Partners
7	EASME	24	Lux Capital	41	Redmile Group
8	National Science Foundation	25	Alumni Ventures	42	DCVC Bio
9	MassChallenge	26	Section 32	43	New Enterprise Associates
10	Khosla Ventures	27	Sequoia Capital China	44	Tencent
11	Invus	28	8VC	45	WuXi AppTec
12	SoftBank Vision Fund	29	SOSV	46	Novo Holdings
13	Andreessen Horowitz	30	Felicis Ventures	47	Amplitude Venture Capital
14	ARCH Venture Partners	31	B Capital Group	48	Biotechnology Value Fund
15	ZhenFund	32	Amgen Ventures	49	Madrona
16	F-Prime Capital	33	Entrepreneur First	50	Logos Capital
17	General Catalyst	34	DCVC		

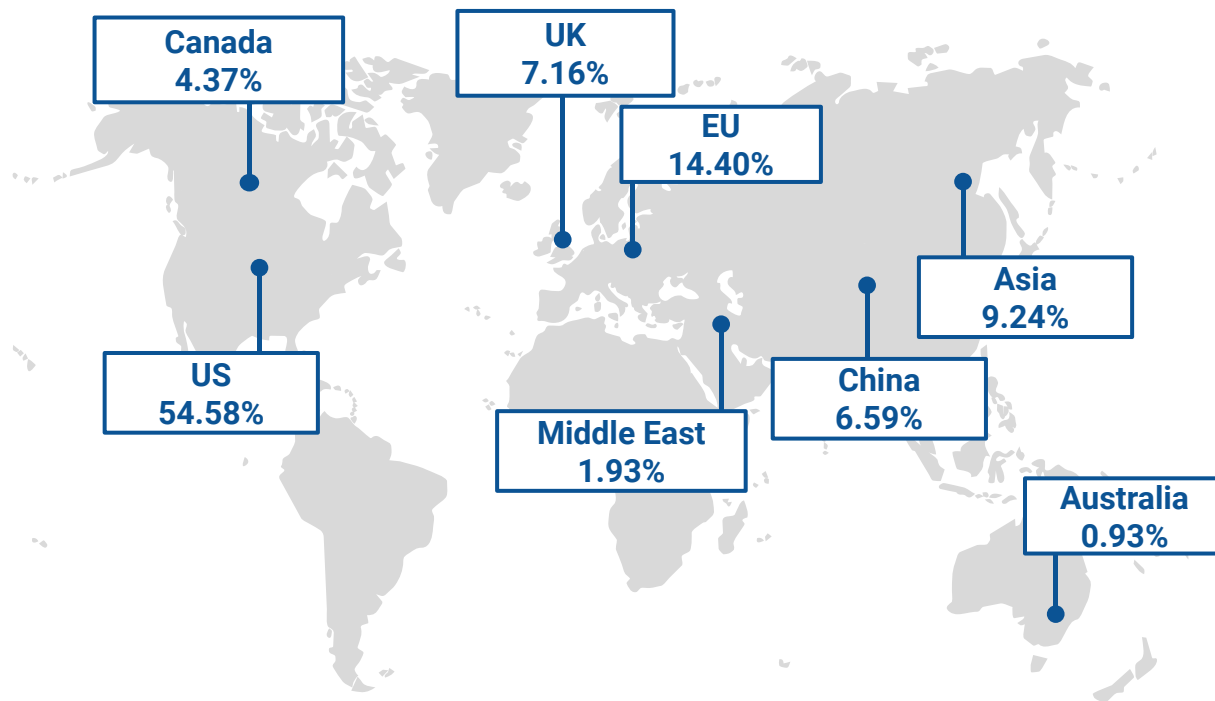
AI in Drug Development: Geographical Coverage

700 AI Companies: Regional Proportion



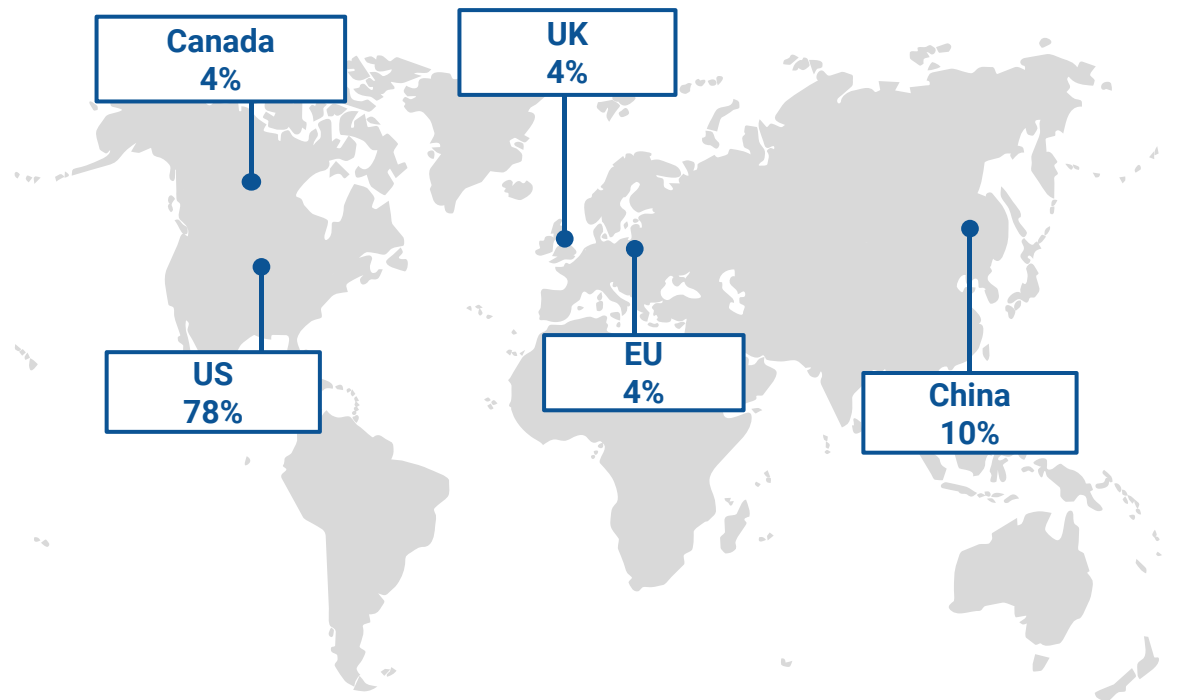
The US is still firmly in the lead regarding its proportion of AI for Drug Discovery companies. Interestingly, Asia and the Middle East continue to expand usage of AI technologies in the Pharmaceutical Industry. The ratio of companies that use AI for Drug Development in the UK and European countries 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.

1400 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 2022, we can observe significant growth of the number of investors in Asia, especially in China. The United States, Europe, China and UK 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 2022 we can observe significant growth of the number of investors in Asia, mainly in China. The USA, the UK, Canada, and EU remain to be leaders by the number of investors in AI in Pharma companies.

AI in the Global Context



Europe Actively Explores AI Applications for Drug Discovery

In Europe, the European Medicines Agency (EMA) has announced plans to use AI to improve the efficiency of its work, including the assessment of new drug applications. The UK's National Health Service (NHS) is also exploring the use of AI to improve patient care, including the development of personalized medicine.

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. The US Food and Drug Administration (FDA) has also established a program to explore the use of AI in regulatory science.

Asia Invest in AI in Drug Development Activity

In Asia, Japan and South Korea are also investing in AI for drug development. Japan's Ministry of Economy, Trade, and Industry has established a program to promote the development of AI-based drug discovery technologies, and South Korea is investing in AI research and development through its national program, "AI Korea."

China Plans to Become the World AI Leader by 2025

The National Development and Reform Commission, China's top economic planning body, has identified AI in the pharmaceutical industry as a key area for development under its "Made in China 2025" plan. This plan aims to make China a global leader in advanced manufacturing, including the development of AI-based technologies.

Business Activity: Overview

Business Activity

The business activity has been increasing in the pharmaceutical AI space over **Q1 2022 - Q4 2022**, judging by an increased number of transactions and partnership announcements in this period.

The most significant deals and collaborations in include:



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** 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 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** 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.

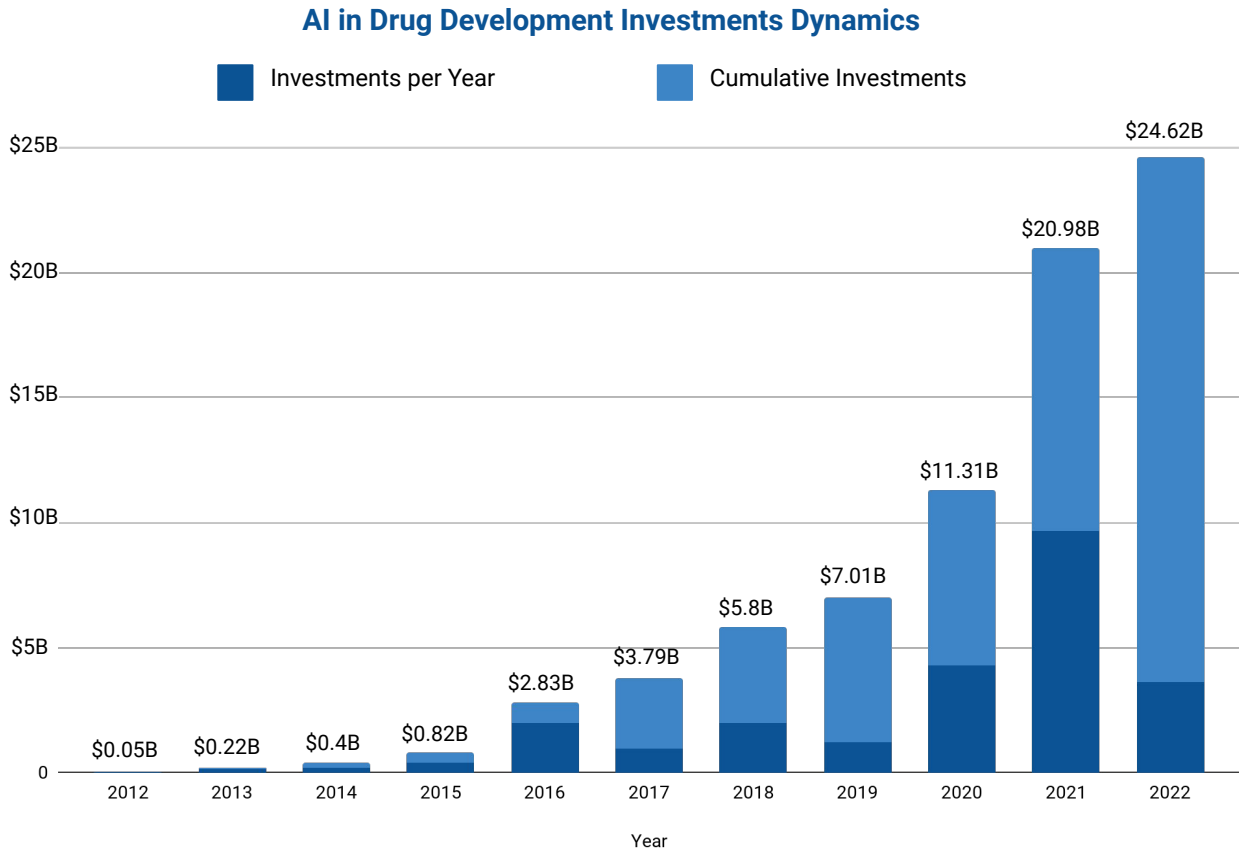


Microsoft and **Novo Nordisk** signed a contract to expedite the company's drug discovery process.



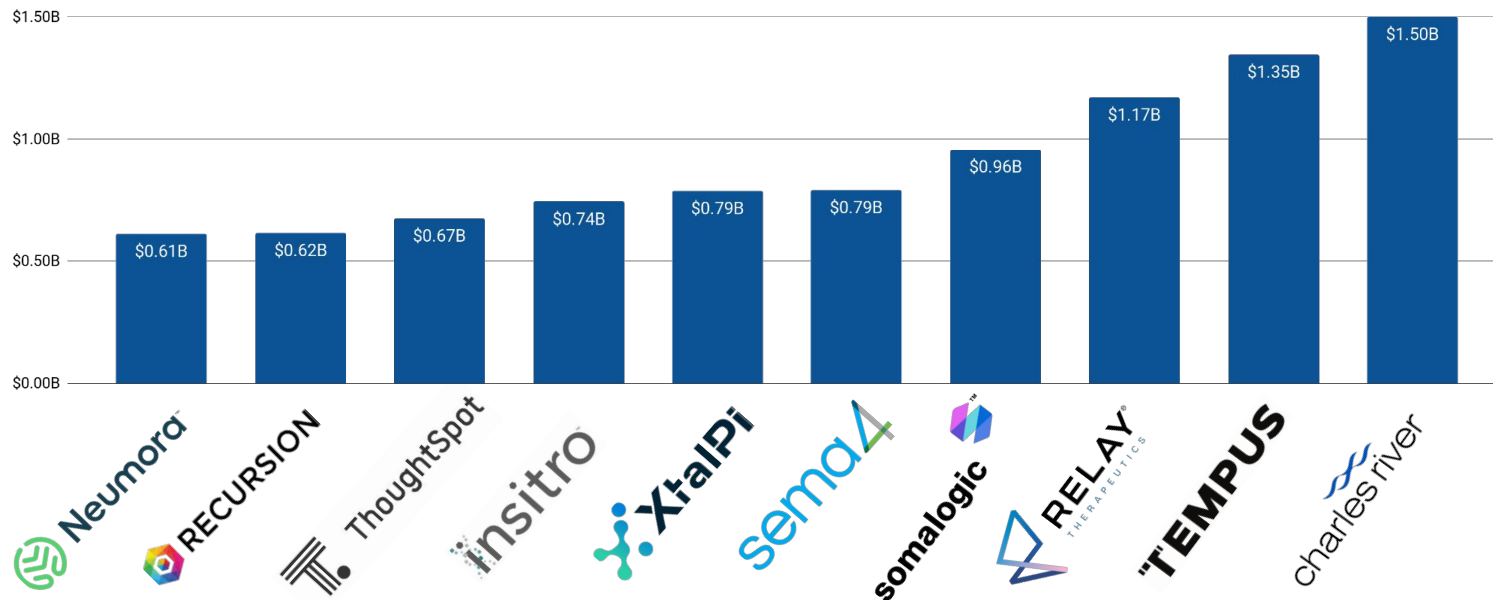
Roche announces **PathAI** collaboration for artificial intelligence-based digital pathology applications for improved patient care.

Dynamics of Investments in AI in Drug Development



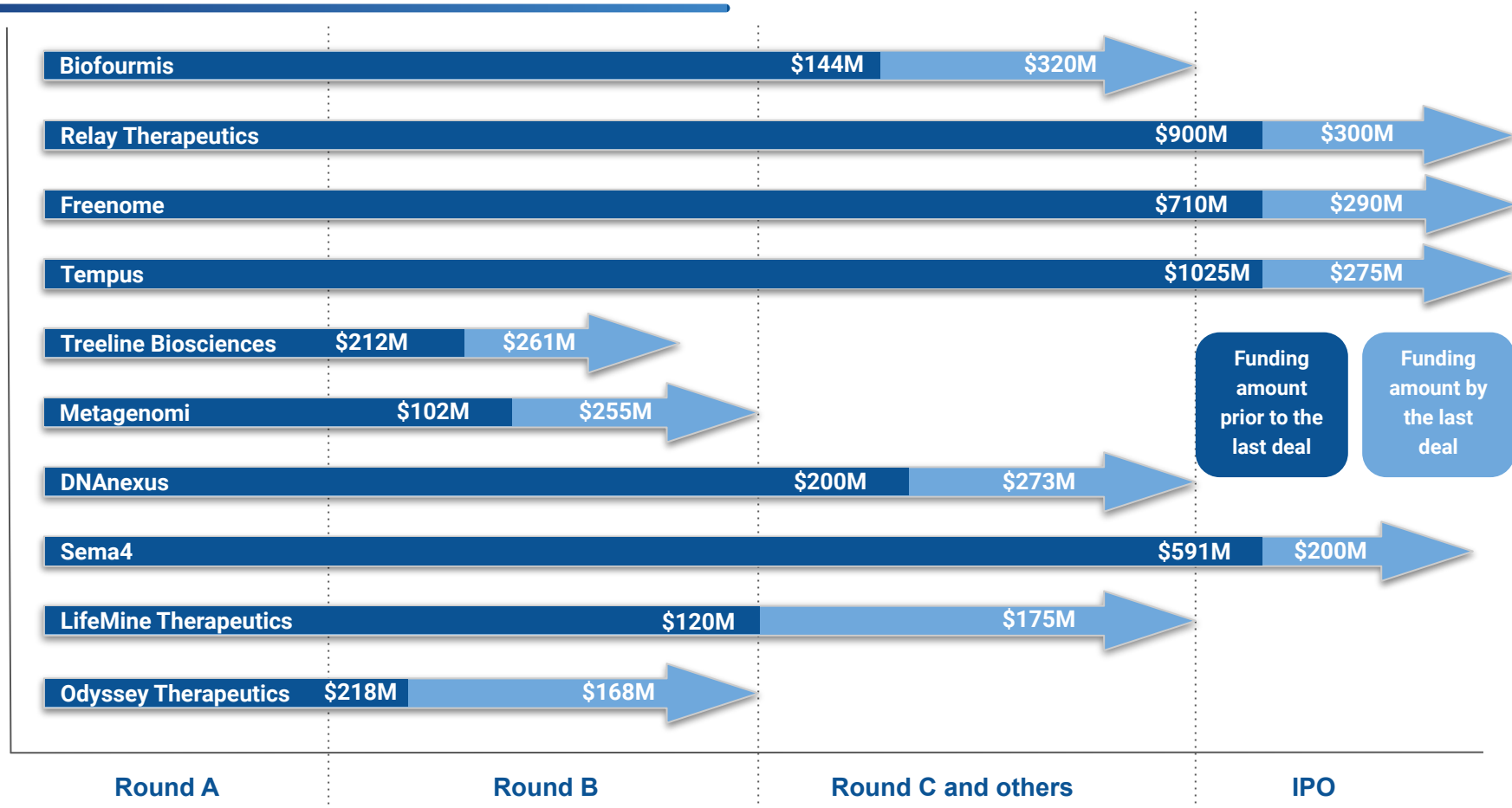
There has been a substantial increase in the amount of capital invested in AI-driven pharma companies **since 2015**. During the last nine years, the annual amount of investments in **700** companies has increased by almost **30 times** (to **\$24.62B** in total as of December 2022). The most rapid growth was in 2021, when the year investment in the AI in Drug Development companies was \$9.66B. We can suggest, that COVID-19 pandemic was the catalizator of this rapid growth. But because of the global economic recession, the investments in AI in Drug Development companies in 2022 are in 2.6 times smaller than in 2021 (\$3.63B to \$9.66B). On the December 2022, the total investments in AI in Drug Development companies are \$24.62B.

Top 10 AI in Pharma Companies by Total Investments in Q4 2022

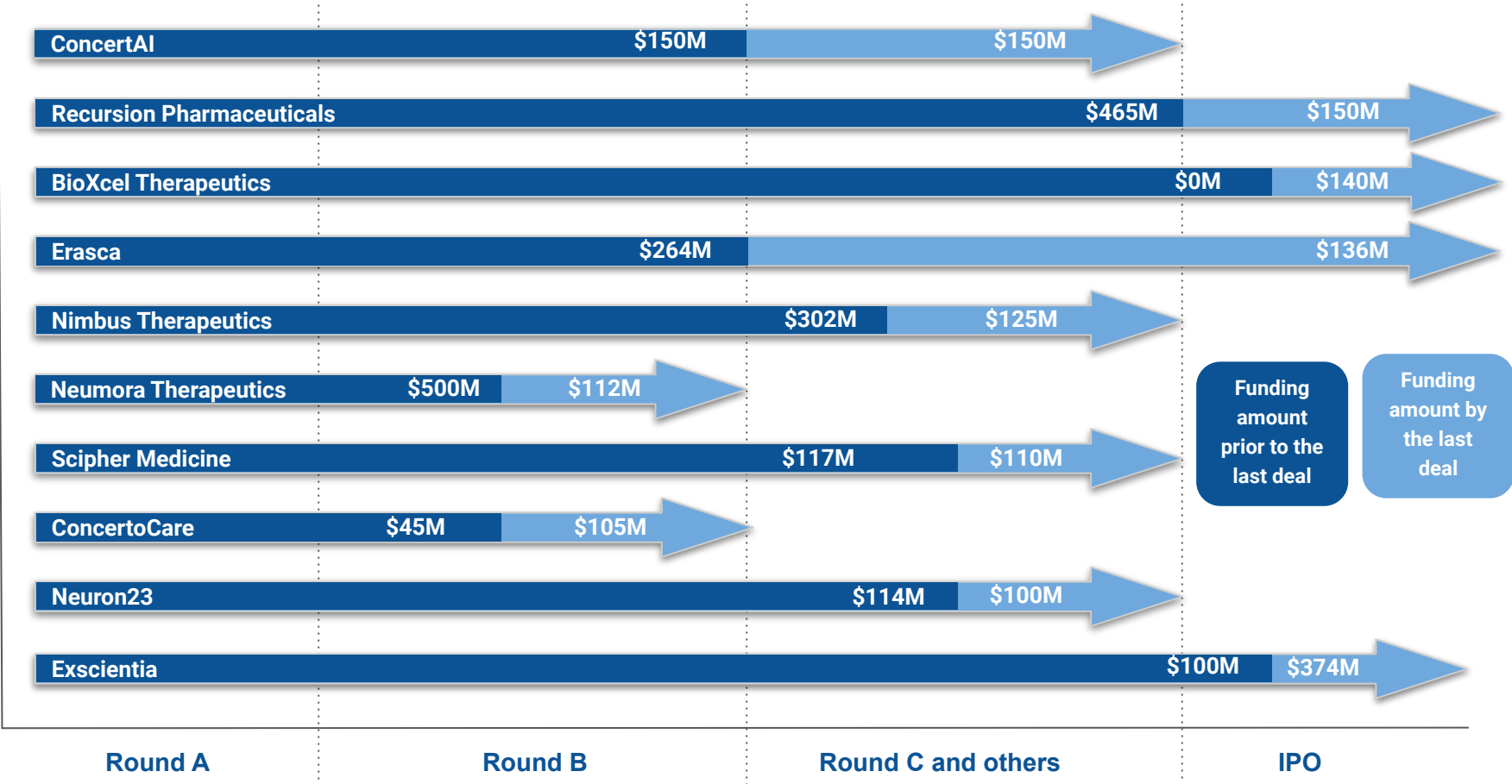


The chart shows the top 10 AI-driven drug discovery companies sorted by the **total funding** raised by the end of Q4 2022. **Charles River Laboratories**, an artificial intelligence-powered drug R&D company, is now at the top of the list. The company has the total funding raised to **\$1.48B**. **Tempus**, a technology company advancing precision medicine through the practical application of artificial intelligence in healthcare, could finance **\$1.35B** in capital market. **Relay Therapeutics**, **Somalogic** and **Sema4** are new companies due to late-stage mega-rounds **during the 2022**.

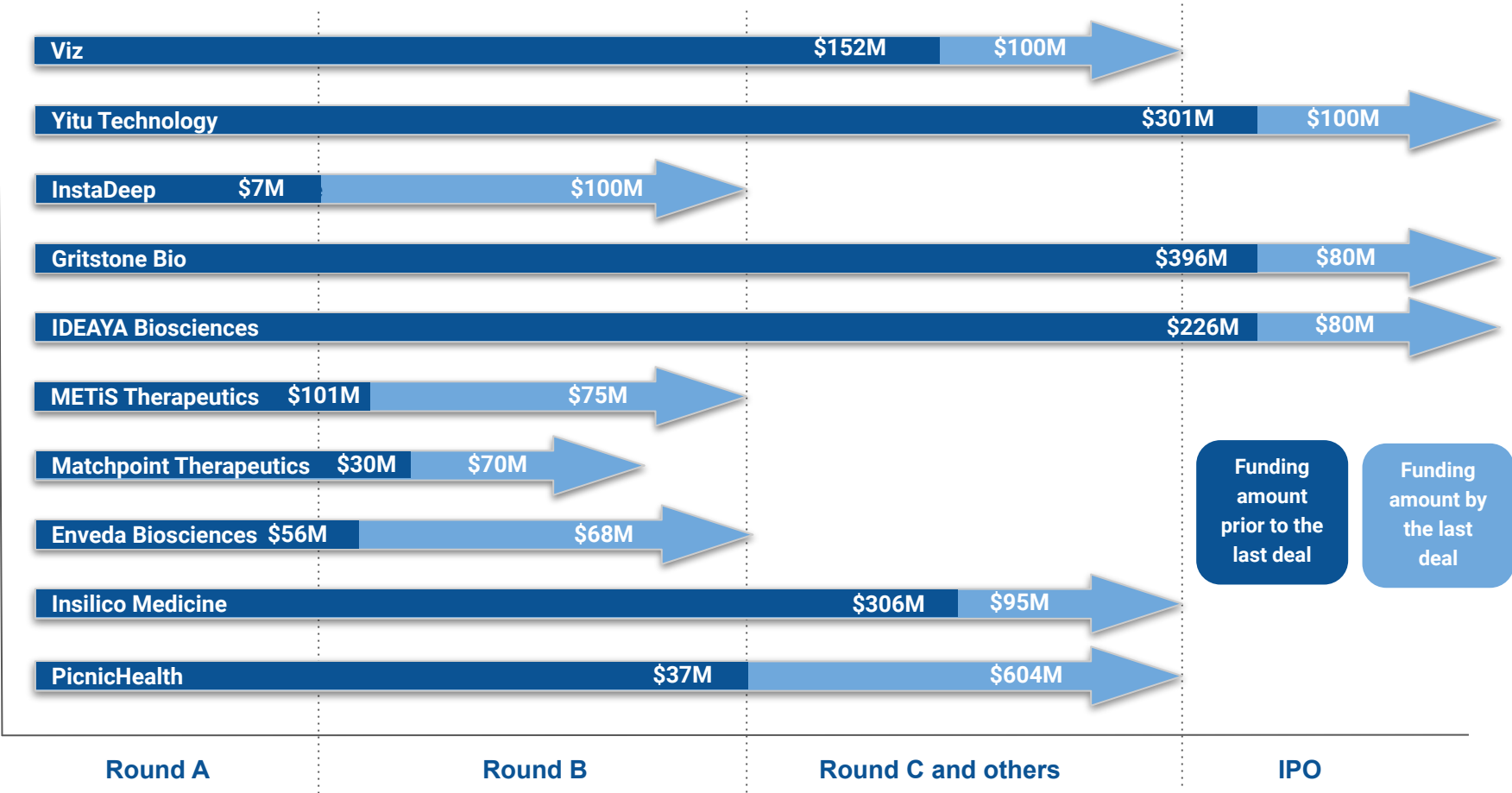
Leading Companies by Amount and Stage of Funding



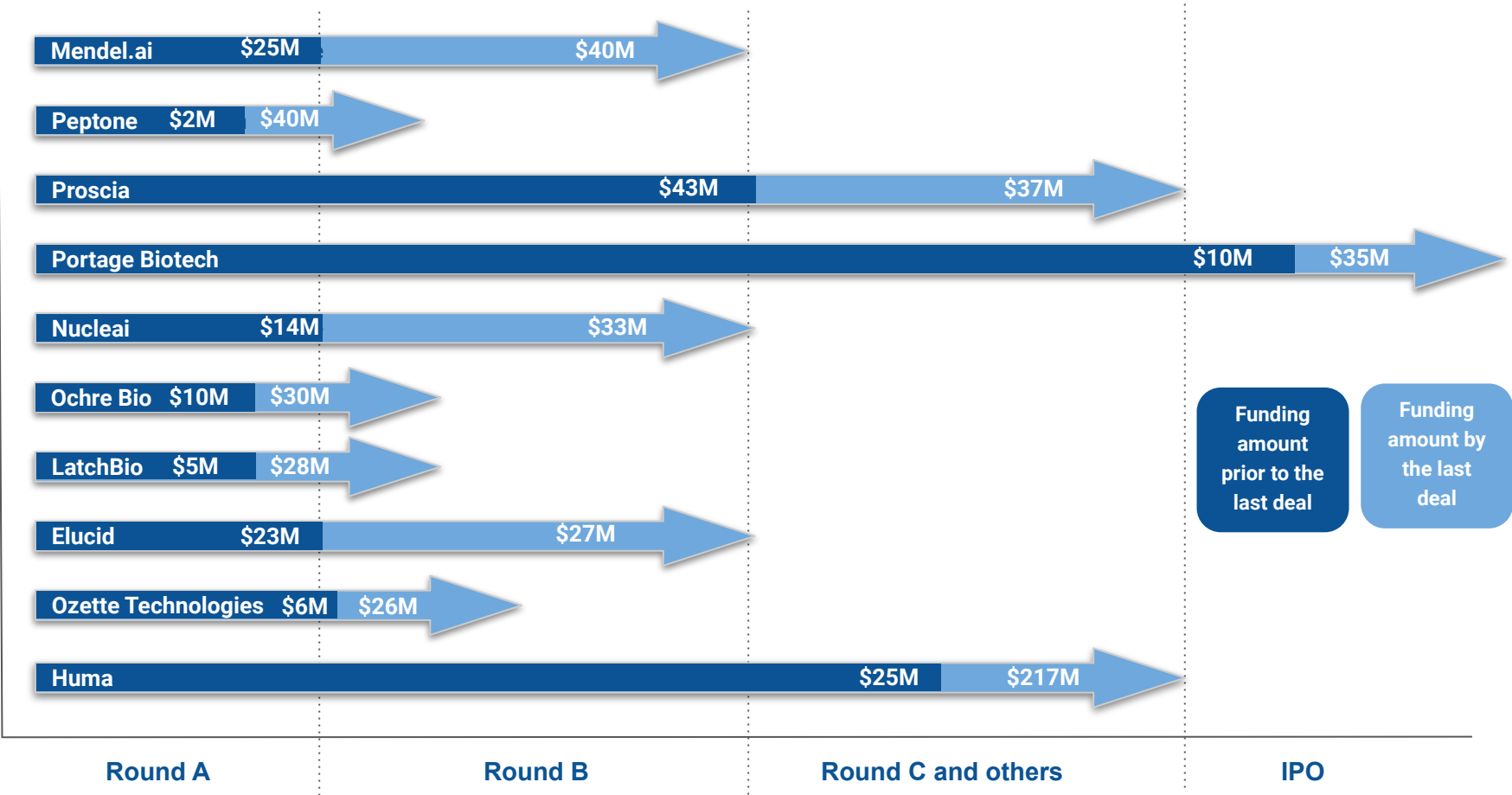
Leading Companies by Amount and Stage of Funding



Leading Companies by Amount and Stage of Funding

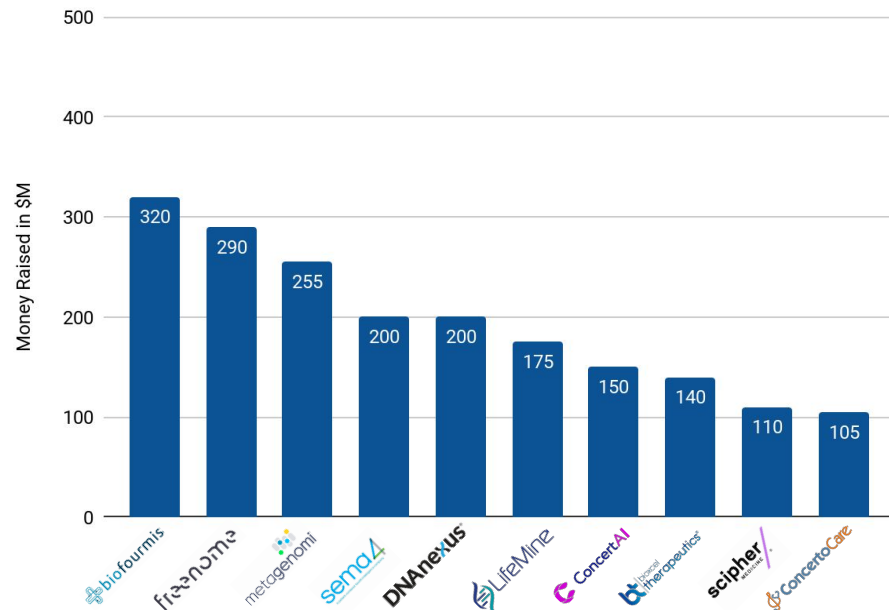


Leading Companies by Amount and Stage of Funding

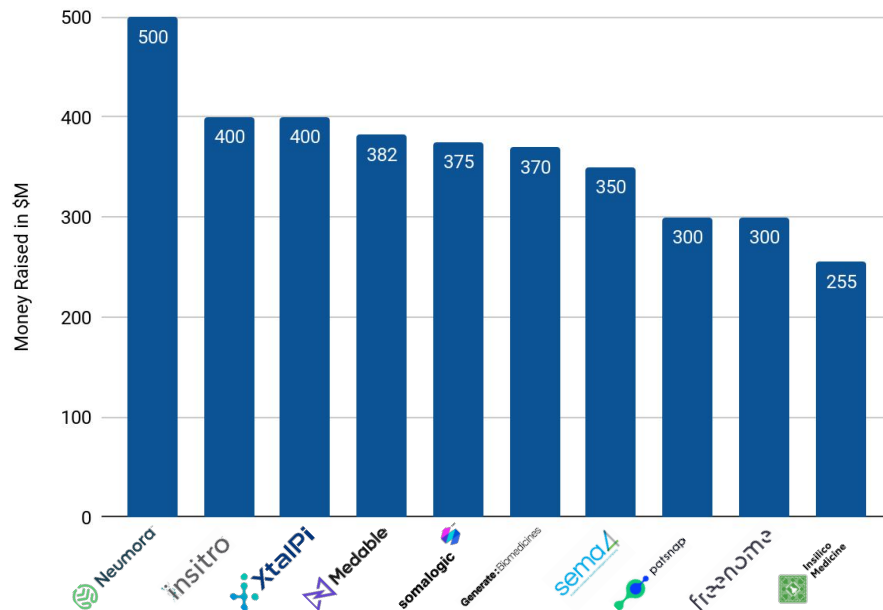


Top 10 Funded Companies in 2022 vs 2021

Top 10 Funded Companies in 2022



Top 10 Funded Companies in 2021



To visualise yearly trends, the charts represent the **top 10 funded companies in 2022 and 2021**. The observed central tendency is the decrease in investments in 2022 compared to 2021. The most significant raised investment in **2022** was in **Biofourmis** company, which raised **\$320M**, while in **2021**, **Neumora** raised **\$500M**. The **average investment in 2021** was **\$64.7M**, while in **2022**, it was **\$48.5M**. Additionally, the number of assets is two times smaller in 2022 (**75 investments in 2022 to 152 investments in 2021**).

Major Observations for 2022: Key Business Takeaways



Due to quickly growing proof of AI tech feasibility and innovation potential, big pharmaceutical companies and contract research organizations have been interested in collaborating with or utilizing the platforms of AI companies in the drug development process. These collaborations or platform usage can help speed up the drug development process and improve data analysis and decision-making. AstraZeneca is a leader in collaborations with AI companies, till the end of 2022 year, the company had more than 26 collaborations.



Big Pharmaceutical companies are very interested in the growth and development of AI companies. This interest can be observed not only in the high amount of collaboration between pharmaceutical companies and AI companies but also in the direct investments of big pharma in AI companies. In 2022, Roche invested \$290M in Freenome, Pfizer invested \$200M in Sema4, and Sanofi invested \$100M in Exscientia.



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).



The investment strategy changed in 2022. In 2021, the most significant investments came to innovative new companies with promising ideas, such as Neumora Therapeutics and Insitro, in both were invested \$400M in 2021. In 2022, investors preferred more mature companies with ready-to-go solutions or drugs that are already entered the latest phases of clinical trials, such as Biofurmus (\$320M) and Freenome (\$290M).

Major Observations for 2022: Key Business Takeaways



The global COVID-19 pandemic heated up the interest in BioTech and drug discovery sectors and catalysed AI development. During 2021, we have observed over 150 medium and large funding rounds for AI in Drug Development companies with an average investment of \$64.7M. In 2022, the interest in AI in drug development appeared to reach a plateau. In 2022, there were over 70 investments in AI in Drug Development companies with an average investment of \$48.5M.



In 2022, only **1 company that use AI for DD reached IPO status**. London-based Benevolent AI closed its IPO in April and raised \$292M. There is a huge recession comparing to 2021 year, when 10 companies reached IPO. The global downturn might be the reason for this.



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).



Despite the global downturn, the AI in Drug Development sector seems to be stable. Since the start of the 2022, the cumulative capitalization of publicly traded companies fell only by -3.1% and is **\$194,6B of cumulative capitalization as of end of December, 2022**.

AI in the Global Context



Europe Actively Explores AI Applications for Drug Discovery

In Europe, the European Medicines Agency (EMA) has announced plans to use AI to improve the efficiency of its work, including the assessment of new drug applications. The UK's National Health Service (NHS) is also exploring the use of AI to improve patient care, including the development of personalized medicine.

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. The US Food and Drug Administration (FDA) has also established a program to explore the use of AI in regulatory science.

Asia Invest in AI in Drug Development Activity

In Asia, Japan and South Korea are also investing in AI for drug development. Japan's Ministry of Economy, Trade, and Industry has established a program to promote the development of AI-based drug discovery technologies, and South Korea is investing in AI research and development through its national program, "AI Korea."

China Plans to Become the World AI Leader by 2025

The National Development and Reform Commission, China's top economic planning body, has identified AI in the pharmaceutical industry as a key area for development under its "Made in China 2025" plan. This plan aims to make China a global leader in advanced manufacturing, including the development of AI-based technologies.

50 Leading Investors in Pharmaceutical AI

50 Leading Investors in AI for Drug Discovery Sector

1	Casdin Capital	18	Merck Global Health	35	AME Cloud Ventures
2	Y Combinator	19	RA Capital Management	36	Founders Fund
3	GV	20	Bill & Melinda Gates Foundation	37	OrbiMed
4	Creative Destruction Lab (CDL)	21	Foresite Capital	38	Lifeforce Capital
5	Perceptive Advisors	22	T. Rowe Price	39	Lilly Asia Ventures
6	Alexandria Venture Investments	23	Obvious Ventures	40	Polaris Partners
7	EASME	24	Lux Capital	41	Redmile Group
8	National Science Foundation	25	Alumni Ventures	42	DCVC Bio
9	MassChallenge	26	Section 32	43	New Enterprise Associates
10	Khosla Ventures	27	Sequoia Capital China	44	Tencent
11	Invus	28	8VC	45	WuXi AppTec
12	SoftBank Vision Fund	29	SOSV	46	Novo Holdings
13	Andreessen Horowitz	30	Felicis Ventures	47	Amplitude Venture Capital
14	ARCH Venture Partners	31	B Capital Group	48	Biotechnology Value Fund
15	ZhenFund	32	Amgen Ventures	49	Madrona
16	F-Prime Capital	33	Entrepreneur First	50	Logos Capital
17	General Catalyst	34	DCVC		

Top-50 AI in Pharma Investors



San Francisco

BVC
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

Amgen Ventures
San Francisco, California, US

Redmile Group
San Francisco, California, US

Biotechnology Value Fund
San Francisco, California, US

Logos Capital
San Francisco, California, US

New York

OrbiMed
New York, New York, US

Bill & Melinda Gates Foundation
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

Lux Capital
New York, New York, US

Menlo Park

Andreessen Horowitz
Menlo Park, California, US

Felicit Ventures
Menlo Park, California, US

Khosla Ventures
Menlo Park, California, US

New Enterprise Associates
Menlo Park, California, US

Illinois

ARCH Venture Partners
Chicago, Illinois, 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

Massachusetts

MassChallenge
Boston, Massachusetts, US

RA Capital Management
Cambridge, Massachusetts, US

General Catalyst
Cambridge, Massachusetts, US

Polaris Partners
Boston, Massachusetts, US

F-Prime Capital
Cambridge, Massachusetts, US

Manhattan Beach

B Capital Group
Manhattan Beach, California, US



Other States

Merck Global Health Innovation Fund
Whitehouse, New Jersey, US

Alumni Ventures
Manchester, New Hampshire, US

SOSV
Princeton, New Jersey, US

National Science Foundation
Alexandria, Virginia, , US

T. Rowe Price
Baltimore, Maryland, US

Section 32
San Diego, California, US

Madrona
Seattle, Washington, US



Amplitude Venture Capital
Montréal, Quebec, Canada

Creative Destruction Lab (CDL)
Toronto, Canada



Novo Holdings
Hellerup, Hovedstaden, Denmark



Beijing

ZhenFund
Beijing, China

Sequoia Capital China
Beijing, China

Shanghai

WuXi AppTec
Shanghai, China

Lilly Asia Ventures
Shanghai, China

Tencent
Shenzhen, China













EASME
Brussels, Belgium













SoftBank Vision Fund
London, England, The UK

Entrepreneur First
London, England, The UK











Top-50 Investors in AI Companies

INVESTORS		INVESTMENTS OVERALL	AI FOR DRUG DISCOVERY COMPANIES	INVESTED IN
	Casdin Capital	202	27	Absci, Alector, Arzeda, Beacon Biosignals, Celsius Therapeutics, Exscientia, Gritstone Oncology, Fabric Genomics, Flatiron Health, Foundation Medicine, Lunit, Insitro, Paige, Recursion Pharmaceuticals, Relay Therapeutics, Sema4, ShouTi, SomaLogic, Treeline Biosciences, Character Biosciences, SomaLogic, Structure Therapeutics, Treeline Biosciences, Imagen Technologies, Exai Bio, Dyno Therapeutics
	Y Combinator	4,619	20	Arpeggio Bio, Athelas, Atomwise, CloudMedx, Coral Genomics, HistoWiz, iLabService, Menten AI, Notable Labs, Ochre Bio, PostEra, Reverie Labs, Segmed, Stratos, Verge Genomics, Nabla Bio, Darmiyan, Synkrino Biotherapeutics, Known Medicine, Gen1E Lifesciences
	GV	1,009	19	Alector, Arrakis Therapeutics, Celsius Therapeutics, DNAnexus, Gritstone Oncology, IDEAYA Biosciences, Insitro, Flatiron Health, Foundation Medicine, Owkin, Relay Therapeutics, Schrödinger, Strateos, Treeline Biosciences, Ultromics, ZappRx, Imagen Technologies, LifeMine Therapeutics, Dyno Therapeutics
	Creative Destruction Lab	744	15	OrganoTherapeutics, Epistemic AI, Altis Labs, NetraMark, biotx.ai, DeepCure, DeepLife, Entropica Labs, Kuano, Kyndi, Menten AI, ProteinQure, Winterlight Labs, Valence Discovery, Nostos Genomics
	Perceptive Advisors	223	15	Absci, Alector, Black Diamond Therapeutics, Champions Oncology, DNAnexus, Icosavax, IDEAYA Biosciences, Neuron23, Saama, Sema4, Soma Logic, Relay Therapeutics, Bodesix, Landos Biopharma, Achilles Therapeutics
	Alexandria Venture Investments	207	15	Arrakis Therapeutics, Celsius Therapeutics, Deep Genomics, GNS Healthcare, Gritstone Oncology, IDEAYA Biosciences, Immunai, Insitro, Fountain Therapeutics, LEXEO Therapeutics, Neuromora Therapeutics, Veralox Therapeutics, Matchpoint Therapeutics, Ozette Technologies, Terray Therapeutics
	EASME	3,680	14	Cytox, Optellum, Quibim, OmicX, Genialis, Acellera, Genome Biologics, Iris.ai, CellPly, MedAware, Castor, Mind the Byte, InterAx Biotech Ltd
	National Science Foundation	4,300	13	bioSyntagma, ADM Diagnostics, Strados Labs, Bioz, Cloud Pharmaceuticals, Data2Discovery Inc, TeselaGen, Nabla Bio, VeriSIM Life, Dascena, SplIntelx, VeriSIM Life, Canomiks
	MassChallenge	3,037	12	OrganoTherapeutics, Agamon, Simply Speak, Scaillyte, Strados Labs, ChemAlive sA, Vyasa Analytics, Neuroelectronics, Kintsugi, Clemedi, Canomiks, Therny
	Khosla Ventures	1,062	11	Arpeggio Bio, Atomwise, BIOAGE LABS, Fountain Therapeutics, Deep Genomics, Menten AI, Ochre Bio, Scipher Medicine, ThoughtSpot, Known Medicine, Gen1E Lifesciences











Top-50 Investors in AI Companies

	INVESTORS	INVESTMENTS OVERALL	AI FOR DRUG DISCOVERY COMPANIES	INVESTED IN
	Invus	180	10	Engine Biosciences, Recursion Pharmaceuticals, Erasca, Schrödinger, Valo Health, Black Diamond Therapeutics, ITEos Therapeutics, Neumora Therapeutics, LifeMine Therapeutics, Achilles Therapeutics
	SoftBank Vision Fund	409	10	Biofourmis, Datavant, Deep Genomics, Exscientia, Insitro, PatSnap, Relay Therapeutics, Roivant Sciences, XtalPi, Neuron23
	Andreessen Horowitz	1,322	10	Aria Pharmaceuticals, Asimow, BigHat Biosciences, BIOAGE LABS, Erasca, Flatiron HealthGenesis Therapeutics, Insitro, Freenome, Dyno Therapeutics
	ARCH Venture Partners	437	10	Arbor Biotechnologies, Generate Biomedicines, Glympse Bio, Erasca, Hangzhou Just Biotherapeutics (Just China), Insitro, Treeline Biosciences, Neumora Therapeutics, Vilya, LifeMine Therapeutics
	ZhenFund	765	9	AccutarBio, Deep Intelligent Pharma, HistoWiz, Spring Discovery, uBiome, Xbiome, XtalPi, Yitu Technology, Meliora Therapeutics
	F-Prime Capital	387	9	Adagene, BenchSci, Insilico Medicine, Notable, Neuromora Therapeutics, Owkin, Elucidata, Peptone, Castor
	General Catalyst	1,128	9	Athelas, Beacon Biosignals, PathAI, Spring Discovery, Swoop, ThoughtSpot, Odyssey Therapeutics, OM1, LatchBio
	Merck Global Health Innovation Fund	85	8	PathAI, Strata Oncology, PreciseDx, Antidote.me, Absci, OpGen, Turbine, Verge Genomics
	RA Capital Management	310	8	Everest Medicines, Freenome, Frontier Medicines, Bristol Myers Squibb, Icosavax, Nimbus Therapeutics, Wave Life Sciences, Achilles Therapeutics
	Bill & Melinda Gates Foundation	221	8	Atomwise, Evotec, Exscientia, Foundation Medicine, Novartis, Schrödinger, Takeda, Cyclica











Top-50 Investors in AI Companies

INVESTORS	INVESTMENTS OVERALL	AI FOR DRUG DISCOVERY COMPANIES	INVESTED IN
 B Capital Group	184	7	Aetion, Atomwise, Insilico Medicine, Notable Labs, HiFiBio, PicnicHealth, HotSpot Therapeutics
 Amgen Ventures	107	7	GNS Healthcare, Neumora Therapeutics, BigHat Biosciences, Celsius Therapeutics, Alector, Gandevea Therapeutics
 Entrepreneur First	370	7	DeepLife, Entropica Labs, Exogene, Sparrho, GTN, Ciference, Nostos Genomics
 DCVC	464	6	AbCellera Biologics, Asimov, Atomwise, Auransa, Strateos, Unlearn.AI
 AME Cloud Ventures	286	6	Asimov, Atomwise, Auransa, BigHat Biosciences, BIOAGE LABS, Molecule.one
 Founders Fund	820	6	AbCellera Biologics, Datavant, Emerald Cloud Lab, Notable Labs, Roivant Sciences, DeepMind
 OrbiMed	587	6	AbCellera, Alector, Erasca, Insilico Medicine, Treeline Biosciences, XtalPi
 Lifeforce Capital	53	6	Clover Therapeutics, Notable Labs, PostEra, TARA Biosystems, Verge Genomics, Character Biosciences
 Lilly Asia Ventures	167	6	Gritstone Oncology, Hangzhou Just Biotherapeutics (Just China), Insilico Medicine, ShouTi, Transcenta, Structure Therapeutics
 Polaris Partners	664	6	Freenome, OM1, Engine Biosciences, Alector, Neumora Therapeutics, Dyno Therapeutics

Top-50 Investors in AI Companies

INVESTORS	INVESTMENTS OVERALL	AI FOR DRUG DISCOVERY COMPANIES	INVESTED IN
 Redmile Group	150	6	Absci, Neuron23, Foundation Medicine, Wave Life Sciences, Gritstone bio, Achilles Therapeutics
 DCVC Bio	37	5	Empirico, Frontier Medicines, Totus Medicines, Unlearn.AI, X-37
 New Enterprise Associates	2,089	5	Aetion, Black Diamond Therapeutics, Champions Oncology, Tempus, Vertex Pharmaceuticals
 Tencent	732	5	Atomwise, Brainomix, iCarbonX, PatSnap, XtalPi
 WuXi AppTec	40	5	Arrakis Therapeutics, Verge Genomics, Schrödinger, Engine Biosciences, WuXi AppTec
 Novo Holdings	295	5	Evotec, Exscientia, Kebotix, Tempus, Metagenomi
 Amplitude Venture Capital	17	5	Imagia, Celsius Therapeutics, Deep Genomics, Valence Discovery, Gandevea Therapeutics
 Biotechnology Value Fund	47	5	Evotec, IDEAYA Biosciences, Nimbus Therapeutics, Relay Therapeutics, Gritstone bio
 Madrona	472	5	Ovation, Envisagenics, Ozette Technologies, Modulus Therapeutics, Terray Therapeutics
 Logos Capital	92	5	Freenome, OM1, Engine Biosciences, Alector, Neumora Therapeutics, Dyno Therapeutics

Top-50 Investors in AI Companies

INVESTORS	INVESTMENTS OVERALL	AI FOR DRUG DISCOVERY COMPANIES	INVESTED IN
 Foresite Capital	139	8	Aetion, Alector, DNAnexus, Generate Biomedicines, Insitro, Relay Therapeutics, Wave Life Sciences, Odyssey Therapeutics
 T. Rowe Price	311	8	Arbor Biotechnologies, Generate Biomedicines, Genesis Therapeutics, Insitro, Sema4, SomaLogic, Tempus, Odyssey Therapeutics
 Obvious Ventures	142	8	ConcertoCare, Inato, LabGenius, Medable, Recursion Pharmaceuticals, Gandeeva Therapeutics, Meliora Therapeutics, Dyno Therapeutics, Achilles Therapeutics
 Lux Capital	424	8	Alife, Auransa, LabGenius, Recursion Pharmaceuticals, Strateos, LatchBio, Gandeeva Therapeutics, Dyno Therapeutics
 Alumni Ventures	1,263	8	Scipher Medicine, Unlearn.AI, Notable Labs, Olaris, Strateos, Veralox Therapeutics, Verge Genomics, Juvena Therapeutics, Emerald Cloud Lab
 Section 32	102	8	Character Biosciences, Nucleai, BigHat Biosciences, Celsius Therapeutics, Verge Genomics, Glympse Bio, Alector, Exai Bio
 Sequoia Capital China	962	8	HiFiBio, METis Therapeutics, PatSnap, XtalPi, Adagene, Deep Intelligent Pharma, Transcenta, Exai Bio
 8VC	396	7	BigHat Biosciences, Coral Genomics, Immunai, Model Medicine, Notable, ProteinQure, Unlearn.AI
 SOSV	2,423	7	A2A Pharmaceuticals, Gatehouse Bio, Guided Clarity, Mendel.ai, Stelvio Therapeutics, Strados, Synthace
 Felicis Ventures	580	7	BIOAGE LABS, Genesis Therapeutics, Juvena Therapeutics, LabGenius, ProteinQure, Spring Discovery, PicnicHealth

Big Pharma's Focus on AI

AI and Pharma Collaborations in Q1 2022 - Q2 2022

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



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



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



Jan 2022

Feb 2022

Mar 2022

Apr 2022

May 2022

Jun 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



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



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.



AI and Pharma Collaborations in Q3 2022 - Q4 2022

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



Roche announces **PathAI** collaboration for artificial intelligence-based digital pathology applications for improved patient care.



Cyclica Inc and **SK Chemicals** announced an AI-driven drug discovery and development partnership to develop therapies across a range of disease areas.



Jul 2022

Aug 2022

Sep 2022

Oct 2022

Nov 2022

Dec 2022

Roche and **EarlySign** expand partnership to include AI-powered lung cancer diagnosis.



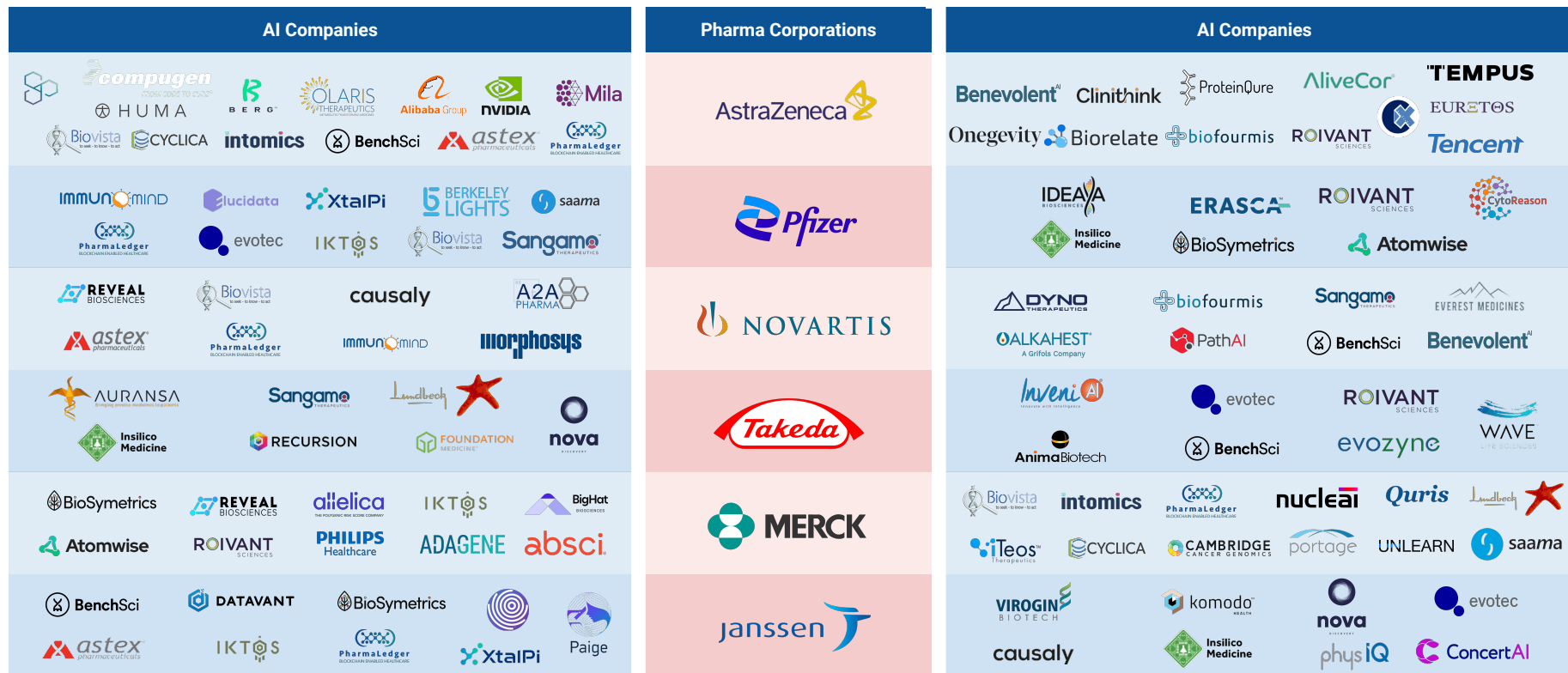
The AI partnership between **Bayer** and **Exscientia**, which saw the two parties search for cardiovascular and cancer targets came to an end.



Insilico Medicine signs strategic research collaboration with **Sanofi** worth up to **\$1.2B**. AI platform **Pharma.AI** will be used to advance drug development candidates for up to six new targets.



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



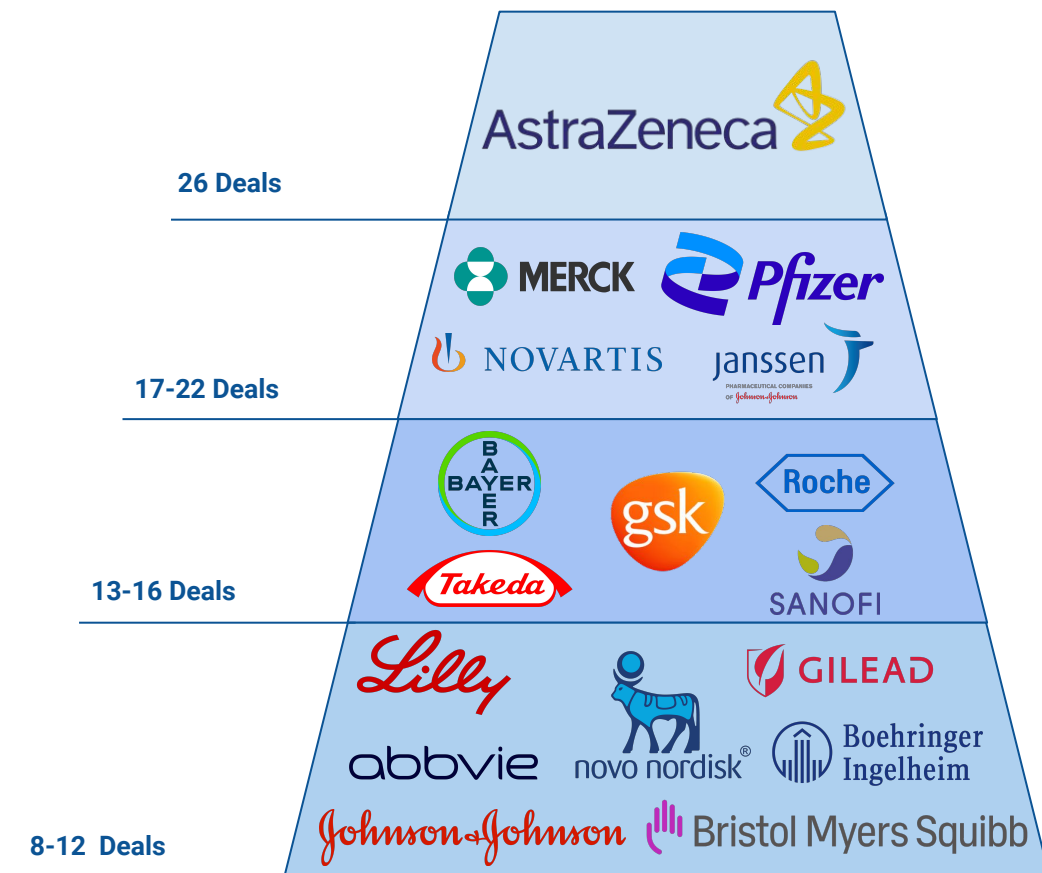
Note: the central column (red) defines the pharmaceutical corporations and side columns (blue) defines AI companies that have collaborations with pharma companies from the central column.

Big Pharmas' AI-focused partnerships till Q4 2022

In this report we have profiled **700 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 (**\$48.19B in HY 2020** against **\$126.4B in HY 2022**), 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.

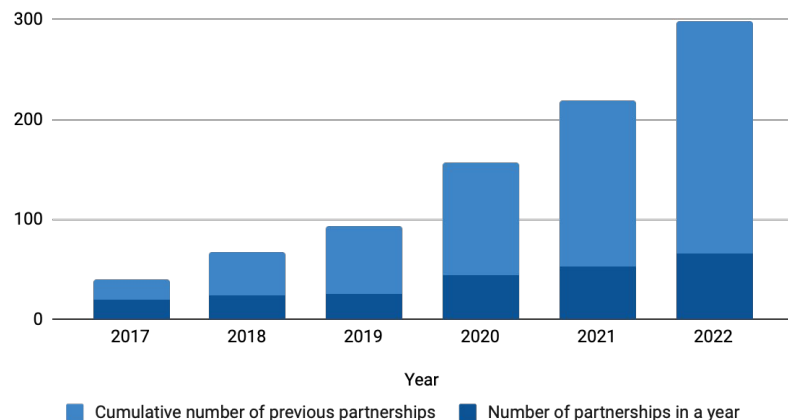
Some of the leading pharma executives increasingly see AI as not only a tool for lead identification, but also a more general tool to boost biology research and identify new biological targets and develop novel disease models.

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



A Growing Number of Collaborations Involving AI for Drug Discovery

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



The rising interest of the big pharma companies 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 2017, there has been an obvious shift in the perception from skepticism and cautious 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

Pharma Partners



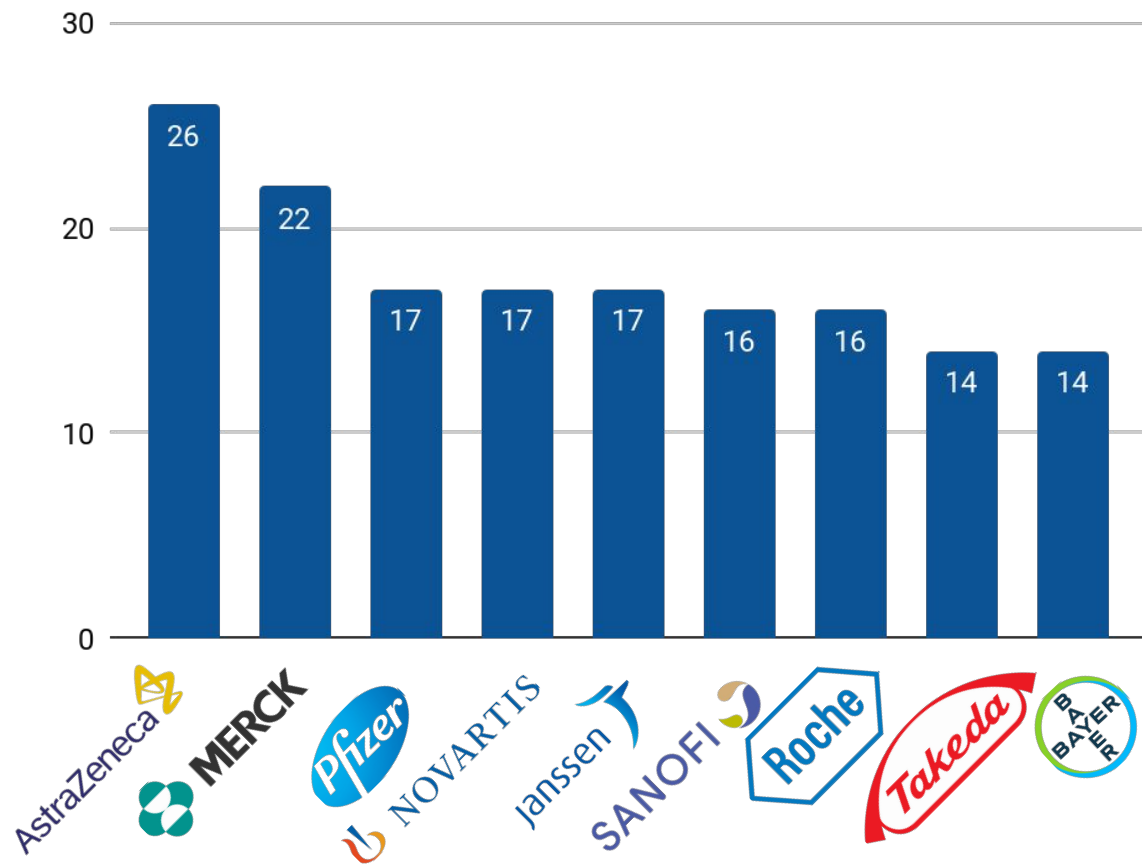
AI and Biotech Partners



Tech partners

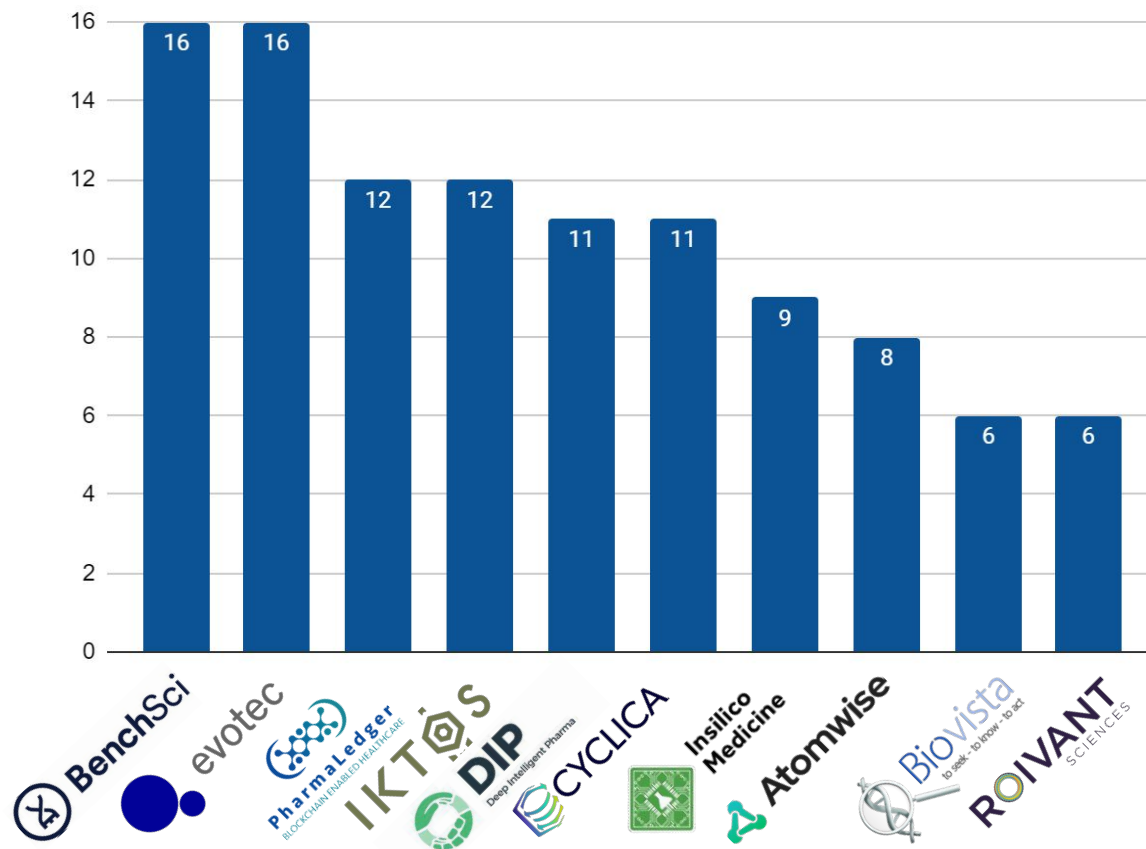


Leading Pharma Corporations by the Number of Pharma AI Deals in 2022



- 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 2022



- The leading AI players by the amount of major industry partnerships are **BenchSci**, **Evotec**, **PharmaLedger**, and **IKtos**.
- **The biggest number** of AI in Drug Discovery deals were conducted by **BenchSci and Evotec**.
- The companies are **early drug development** and **end-to-end**, AI-driven pharma-technology companies that accelerate drug development by proprietary **platform across biology, chemistry and clinical development**.
- All of the deals were categorized as the ones aiming at **saving costs and increasing operational efficiency** due to the character of the services provided.

Major Observations for 2022: Key Business Takeaways



Due to quickly growing proof of AI tech feasibility and innovation potential, big pharmaceutical companies and contract research organizations have been interested in collaborating with or utilizing the platforms of AI companies in the drug development process. These collaborations or platform usage can help speed up the drug development process and improve data analysis and decision-making. Astrazeneca is a leader in collaborations with AI companies, till the end of 2022 year, the company had more than 26 collaborations.



Big Pharmaceutical companies are very interested in the growth and development of AI companies. This interest can be observed not only in the high amount of collaboration between pharmaceutical companies and AI companies but also in the direct investments of big pharma in AI companies. In 2022, Roche invested \$290M in Freenome, Pfizer invested \$200M in Sema4, and Sanofi invested \$100M in Exscientia.



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).



The investment strategy changed in 2022. In 2021, the most significant investments came to innovative new companies with promising ideas, such as Neuromora Therapeutics and Insitro, in both were invested \$400M in 2021. In 2022, investors preferred more mature companies with ready-to-go solutions or drugs that are already entered the latest phases of clinical trials, such as Biofurmus (\$320M) and Freenome (\$290M).

Major Observations for 2022: Key Business Takeaways



The global COVID-19 pandemic heated up the interest in BioTech and drug discovery sectors and catalysed AI development. During 2021, we have observed over 150 medium and large funding rounds for AI in Drug Development companies with an average investment of \$64.7M. In 2022, the interest in AI in drug development appeared to reach a plateau. In 2022, there were over 70 investments in AI in Drug Development companies with an average investment of \$48.5M.



In 2022, only **1 company that use AI for DD reached IPO status**. London-based Benevolent AI closed its IPO in April and raised \$292M. There is a huge recession comparing to 2021 year, when 10 companies reached IPO. The global downturn might be the reason for this.



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).



Despite the global downturn, the AI in Drug Development sector seems to be stable. Since the start of the 2022, the cumulative capitalization of publicly traded companies fell only by -3.1% and is **\$194,6B of cumulative capitalization as of end of December, 2022**.

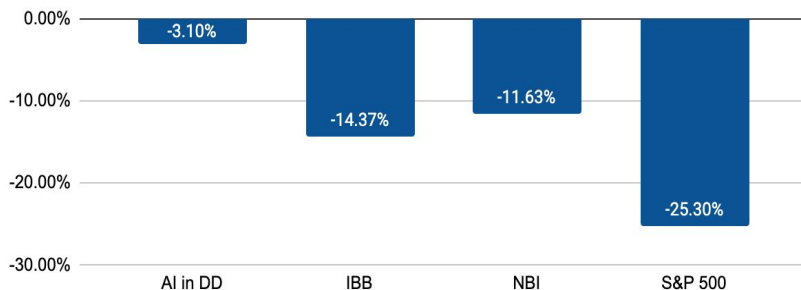
AI in Pharma Publicly Traded Companies

AI in Pharma Publicly Traded Companies

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



Market Capitalization Growth During 2022



Despite the crisis and high volatility, AI in Drug Development publicly traded companies **reached \$194,6B of cumulative capitalization as of December 24, 2022**. 42 AI in Drug Development companies were taken for this analysis, one of them Benelovent AI has closed its IPO in Q3 2022.

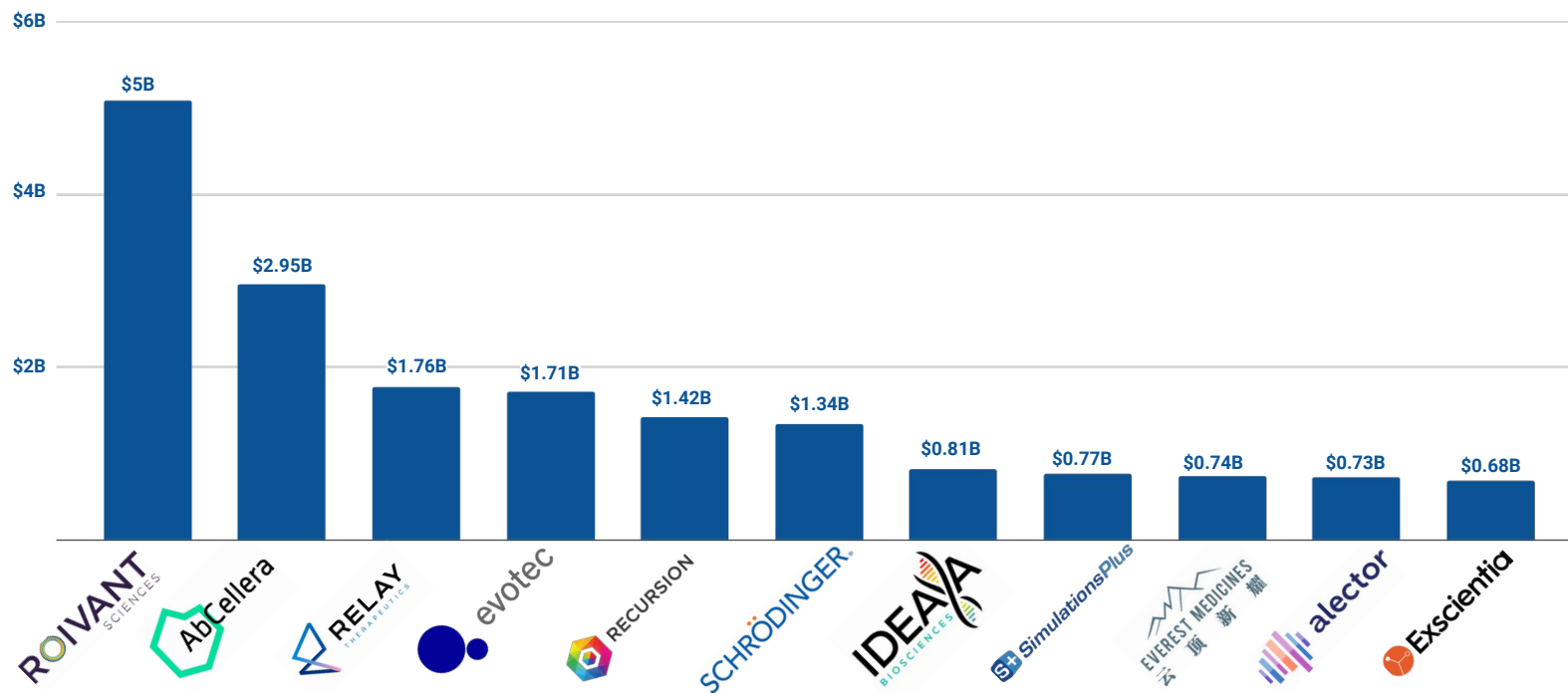
The largest companies by market capitalization are **Roivant Sciences, AbCellera and Relay Therapeutics**. The smallest market capitalization are in **Landos Biopharma, Evolutionary Genomics** and **OpGen Inc**.

Overall, the AI in drug development industry has demonstrated resilience and growth despite the challenges and uncertainties of the past year.

It's essential to measure the performance of publicly traded AI in Drug Development companies via comparison with significant market benchmarks such as iShares Biotechnology ETF (IBB), YTD NASDAQ Biotechnology Index (NBI), and S&P 500 gained solid.

Surprisingly, AI in the Drug development industry falls not so rapidly compared to the other benchmarks. The cumulative capitalization of publicly traded AI-in-DD companies went down only by -3.1%, while other indexes fell to -25.30%.

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 December 2022. **Roivant Science**, Switzerland-based healthcare company focused on applying technology to drug development. holds the first place with **\$5B** of market capitalization.

AI in Pharma IPOs in 2022

In Q2 2022, BenevolentAI 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.

BenevolentAI Stock



Ticker	Mean Daily Return	Volatility of Daily Returns	Growth after IPO	Capitalization, \$M
BAI	-0.50%	4.38%	-55.81%	\$205.9M

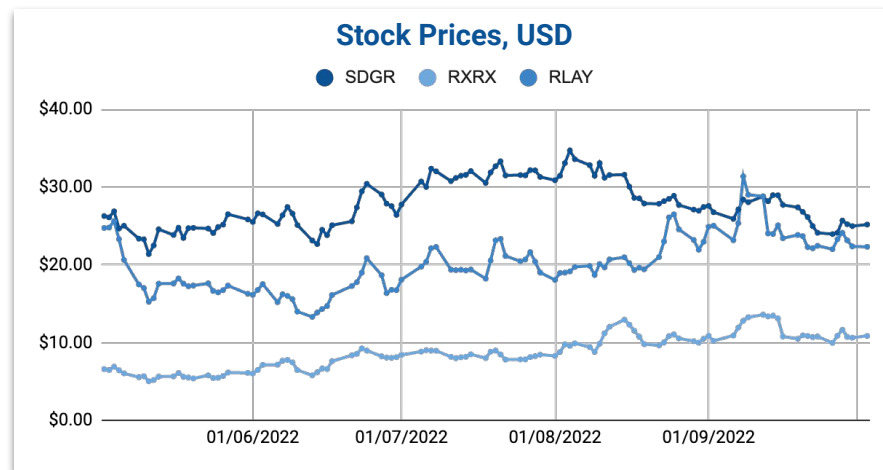
Benevolent's Platform™ is a powerful computational R&D platform. Scientists may query the data and disease networks inside the graph using Benevolent's range of exploratory and predictive AI tools. They can also ask biological queries, generate fresh insights, and prioritize ideas. In order to detect 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 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	25,18	-7.77X	-124.800
Recursion Pharmaceuticals	USA	208.5	17.07.2020	1.515	1355.2	19.00	10,87	-4.55X	-211.74
Relay Therapeutics	USA	520.0	16.07.2020	2.06	1736	20.00	22,32	-3.26X	-183,734

AI in Pharma Corporations Financials

Company	Capitalization \$M	Mean Daily Return	Volatility of Daily Returns	Estimated Monthly Return	IBB Beta	S&P 500 Beta	Enterprise Value (EV)	EBITDA	Gross Profit Margin	EV/EBITDA
AbCellera Biologics	\$2,955.4M	-0.04%	4.28%	-1.06%	0.1309	-0.0073	\$1,891.5M	\$353.9M	69.56%	5.35X
Alector	\$731.1M	-0.22%	4.67%	-5.42%	0.1792	0.0905	\$1.1M	\$132.2M	-56.73%	0.01X
BenevolentAI	\$205.9M	-0.50%	4.38%	-11.85%	-0.1794	0.0143	\$227.8M	-\$114.2M	100%	-2.00X
Berkeley Lights	\$155.32	-0.53%	6.97%	-11.57%	0.1124	0.0725	\$66.8M	-\$76.9M	68.78%	-0.87X
Everest Medicines	\$6,945.4M	-1.92%	15.20%	-0.02%	0.1949	0.1995	\$541.0M	-\$1,810.2M	64.75%	-0.30X
SOPHiA GENETICS	\$183.0M	-0.59%	6.18%	-13.84%	0.1456	0.1114	\$8.6M	-\$91.6M	63.07%	-0.09X

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

AI in Pharma Corporations Financials

Company	Capitalization \$M	Mean Daily Return	Volatility of Daily Returns	Estimated Monthly Return	IBB Beta	S&P 500 Beta	Enterprise Value (EV)	EBITDA	Gross Profit Margin	EV/EBITDA
Evotec	\$1,711.5M	-0.32%	3.36%	-7.02%	0.1812	0.1635	\$2,727.6M	\$54.1M	20.59%	50.38X
Exscientia	\$1,423.6M	-0.33%	6.53%	-9.68%	0.0927	0.1194	\$120.8M	-\$152.5M	-16.44%	-0.79X
Recursion Pharmaceuticals	\$1,765.1M	-0.17%	5.78%	-5.41%	0.1663	0.0179	\$1,074.8M	-\$236.1M	-587.95%	-4.55X
Relay Therapeutics	\$1,765.1M	-0.16%	5.51%	-3.11%	0.2032	0.0947	\$944.4M	-\$289.5M	-3102.77%	-3.26X
Renalytix AI	\$65.5M	-0.62%	6.69%	-13.15%	0.1664	0.1158	\$73.8M	-\$52.9M	25.80%	-1.40X
Roivant Sciences	\$5,085.2M	0.02%	4.74%	0.91%	0.1251	0.0246	\$6,355.4M	-	-985.88%	-
Schrödinger	\$1,343.5M	-0.16%	4.38%	-3.40%	0.0540	0.0975	\$1,064.2M	-\$136.9M	52.08%	-7.77X

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 for Advanced R&D: Applications and Use Cases

Notable AI Breakthroughs

Dec 2018

DeepMind built the **AlphaFold platform** to **predict 3D protein structures** that outperformed all other algorithms. AlphaFold won the **CASP13 competition**, where it could most accurately predict the shape for 25 of the 43 proteins without using previously solved proteins as templates.

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.

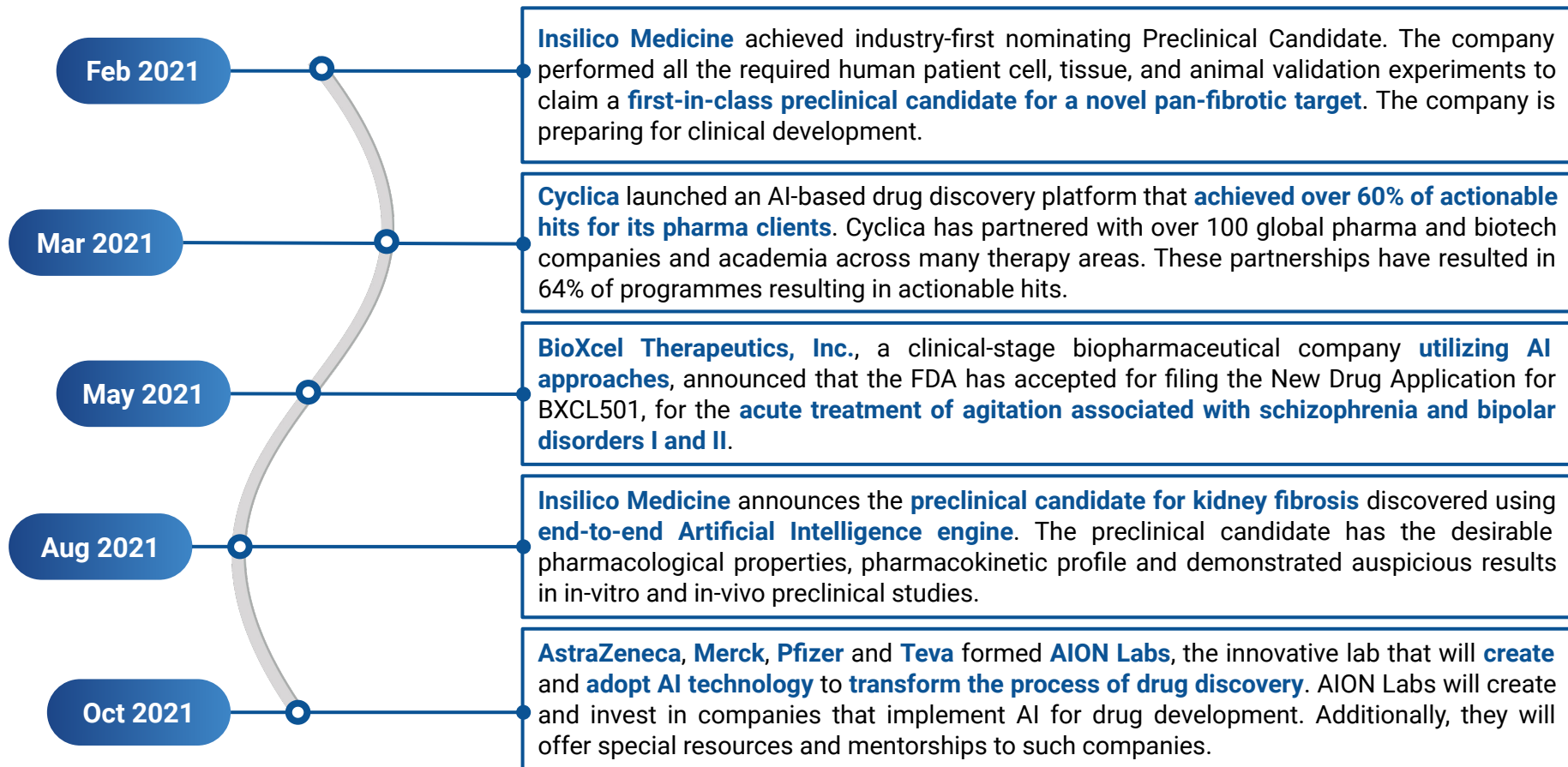
Sep 2020

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.

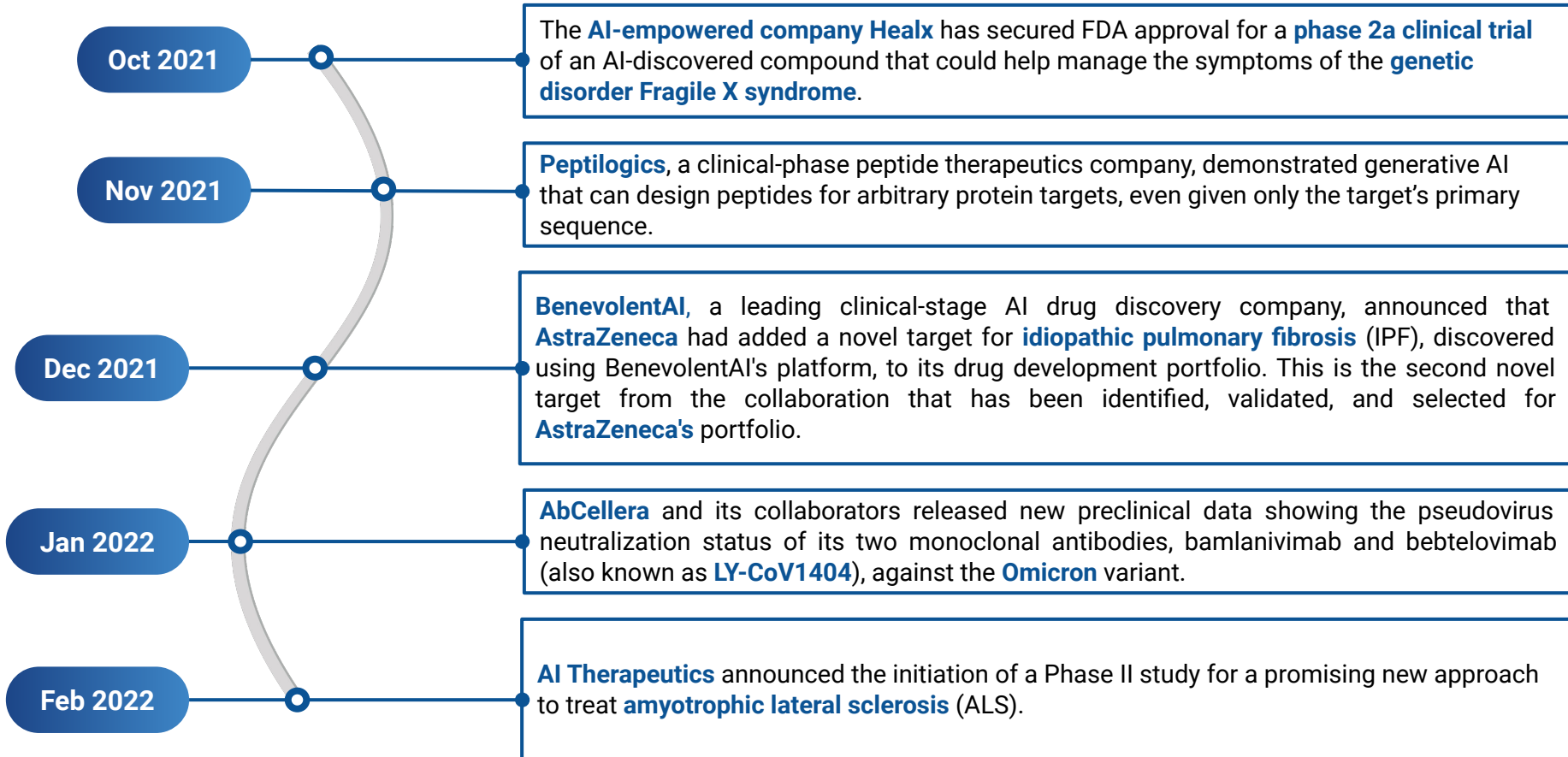
Sep 2020

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**.

Notable AI Breakthroughs



Notable AI Breakthroughs



Notable AI Breakthroughs

Mar 2022

The US FDA has officially approved **Niramai Health Analytix's** first product, which is used to provide an **innovative radiation-free, non-touch, accurate breast cancer screening solution**. A breast thermography tool aids medical professionals in reviewing, measuring, and analyzing thermally relevant indications in the breast region

Apr 2022

The purchase of **TARA Biosystems**, a biotech business focused on cardiovascular illness, by **Valo Health** has created the **first vertically integrated platform for the development of cardiovascular drugs**. The combination of TARA's unique human 3D tissue engineering technology and Valo's Opal Computational Platform™ allows Valo to revolutionize the research and development of drugs for cardiovascular diseases.

May 2022

The FDA has given Breakthrough Device Designation to **Anumana, Inc.**, an AI-driven health technology firm from **nference, Inc.**, for its **AI-enhanced, ECG-based Pulmonary Hypertension (PH) Early Detection Algorithm**. The algorithm is a precise, screening tool for earlier diagnosis of patients with pulmonary hypertension.

Jun 2022

Aizon wins the 2022 Artificial Intelligence **Breakthrough Awards** Program's "**Best AI-based Solution for Manufacturing**" Award.

Jul 2022

The FDA's gave **Biogen** and **Eisai's** follow-up to the Alzheimer's disease medication Aduhelm priority review status. The businesses are aiming for a quick assessment of their anti-amyloid medication lecanemab, which can replace the contentious Aduhelm.

Notable AI Breakthroughs

Oct 2022

Two additional novel **AI-generated targets** for chronic kidney disease and idiopathic pulmonary fibrosis discovered using the **Benevolent Platform™** selected to enter **AstraZeneca's** drug discovery portfolio.

Nov 2022

Amgen, Astellas, AstraZeneca, Bayer, Boehringer Ingelheim, GSK, Janssen, Merck, Novartis, and Servier all agreed to share drug discovery data through the **MELLODDY** platform, but not directly with each other or with Owkin. Substra is the software that made this possible. Instead, an **AI studied each dataset** the business had in turn to learn, retaining no actual data but a great deal of aggregate impressions.

Nov 2022

PatSnap, a global leader in innovation intelligence, launched **Eureka today**, an artificial intelligence (AI) powered solution that makes intellectual property (IP) **more accessible for Research and Development (R&D) engineers**. Eureka optimizes searches, technical insights, competitor monitoring, and collaboration for organizations.

Dec 2022

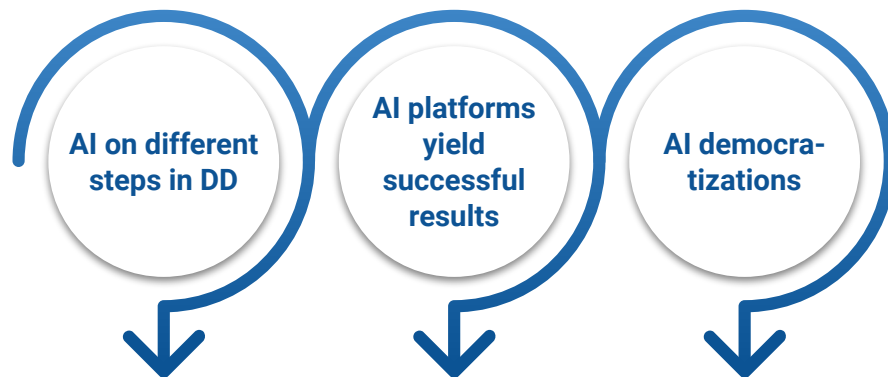
MindRank Announces U.S. FDA Clearance of IND Application for **MDR-001**, a Novel GLP-1 Receptor Agonist for the Treatment of **Type 2 Diabetes and Obesity**.

Dec 2022

Owkin is open sourcing **Substra**, its **Federated Learning (FL) software**, to allow researchers and developers to collaboratively train ML models without the data leaving its source.

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

There are several challenges and obstacles to the adoption of artificial intelligence (AI) in drug development. These include:

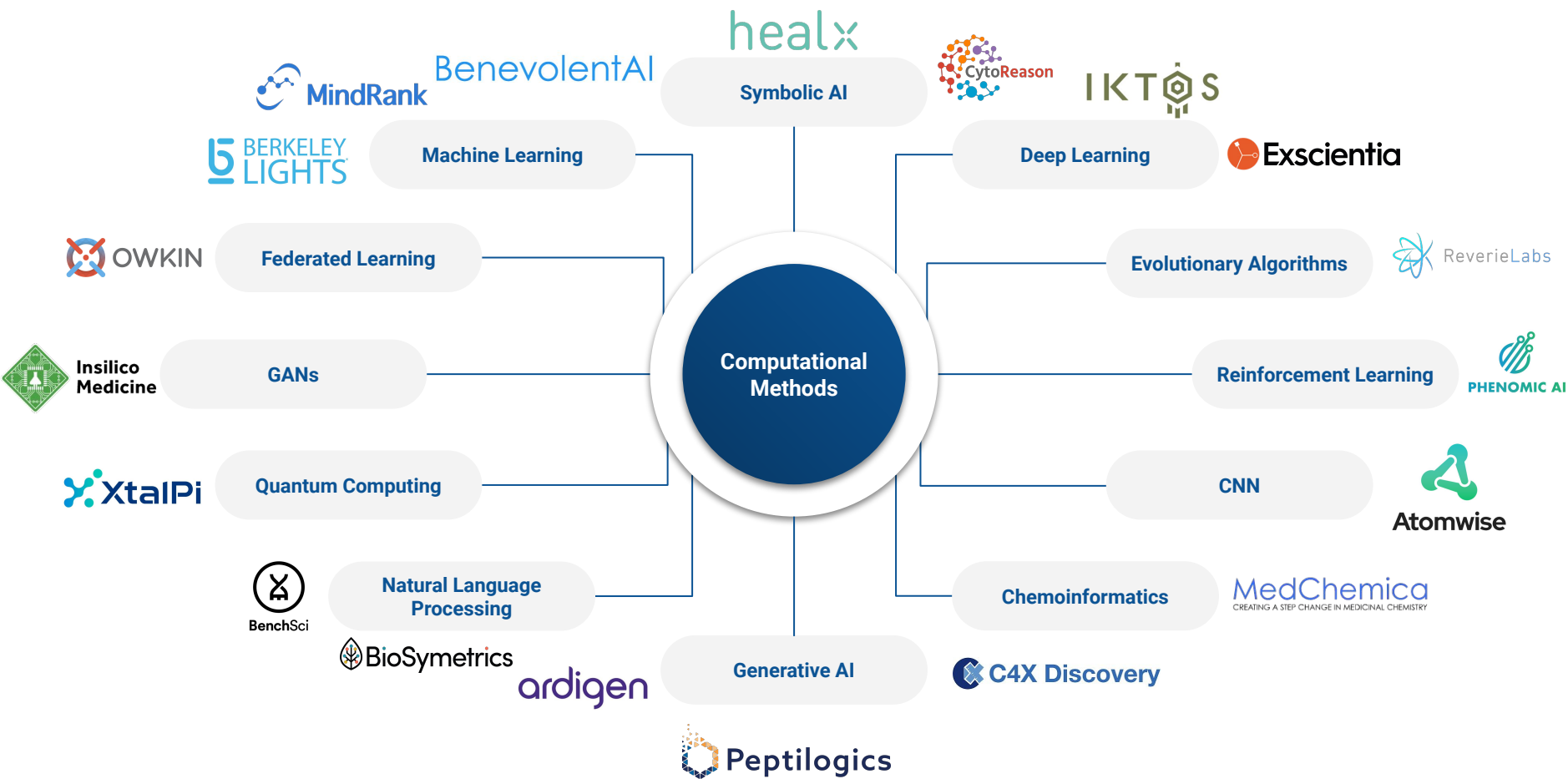
1. **Data quality and availability:** AI algorithms require large amounts of high-quality data to be effective. However, the pharmaceutical industry has historically struggled with data silos, which can make it difficult to access and integrate data from multiple sources.
2. **Regulation:** The regulatory environment for AI in drug development is still evolving. Regulators such as the US Food and Drug Administration (FDA) and the European Medicines Agency (EMA) are working to establish guidelines for the use of AI in drug development, but these are still in the early stages.
3. **Lack of understanding and expertise:** Many pharmaceutical companies and researchers may not have the necessary expertise in AI to effectively utilize it in drug development. This can make it difficult for these organizations to adopt and integrate AI into their processes.
4. **Ethical concerns:** There are also ethical concerns surrounding the use of AI in drug development, including issues related to bias in data and algorithms and the potential for AI to replace human decision-making.

AI in Biotech Challenges








Computational Methods Used by the Most Advanced AI Companies




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, Machine 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, NLP	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.
 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.
 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.

Computational Methods Used by the Most Advanced AI Companies

Companyz	Computational methods used	Technology Abstract
 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.
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.
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.

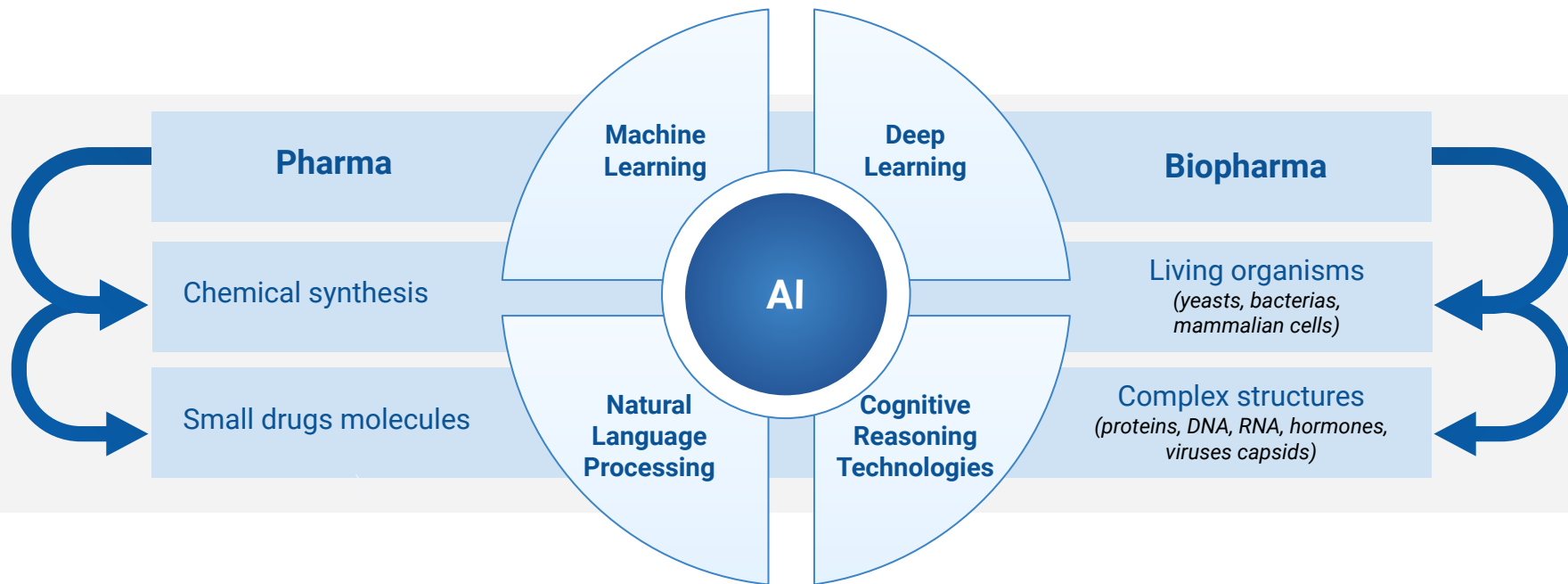
Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
 MindRank	Few-Shot Learning, Machine Learning, Deep Learning	MindRank aims to use machine learning to design and develop small molecule drugs with desirable preclinical efficacy and safety profiles.
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.
 Peptilogics	Generative AI, Deep learning, Bioinformatics, Cheminformatics, Computational biophysics, Quantum chemistry	Peptilogics' Nautilus platform combines generative AI, predictive models, computational biophysics, quantum chemistry , and purpose-built supercomputing to produce multiparameter-optimized leads for diverse targets and therapeutic areas.
 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	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

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

Biopharma utilizes living organisms (such as yeasts, bacteria, 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. 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:

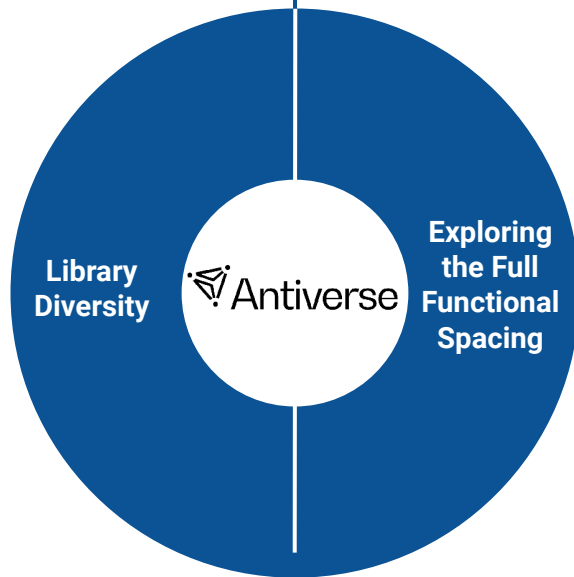
Antigen-antibody database



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

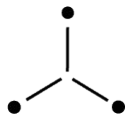
How Antiverse Engineers the Future of Drug Discovery



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.



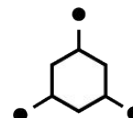
Target Selection

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.



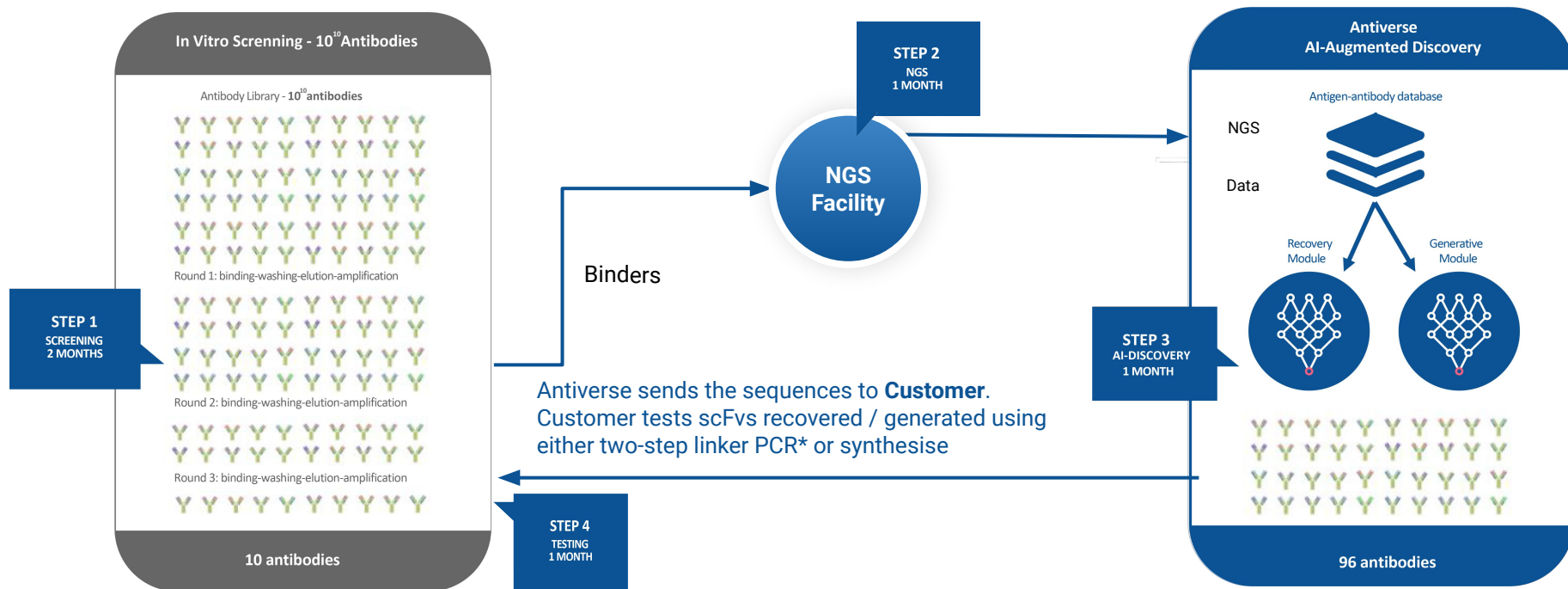
Binder Customisation

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

How Antiverse Uses AI in R&D

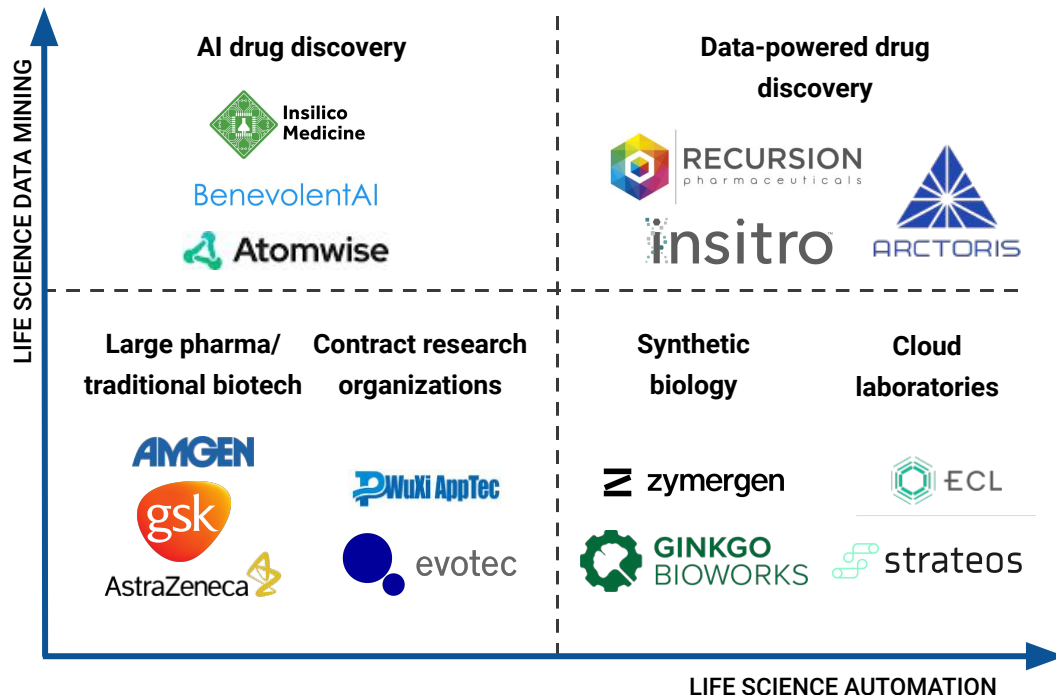


The **Antiverse AI-ADD** system found each and every cluster identified by other methods, plus more. These additional clusters contained rare and unique sequences.



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.



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.

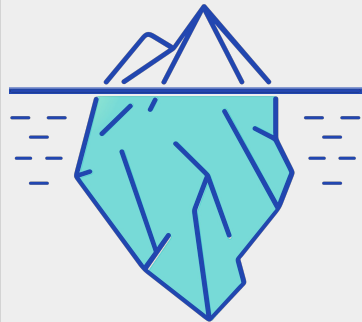
The **core thesis** of the company is that better data leads to better decisions, and that in order for drug discovery programs to develop and meet the next milestone faster and with higher chance of success, the underlying data must be rich, reliable, and reproducible. According to Arctoris, **the status 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

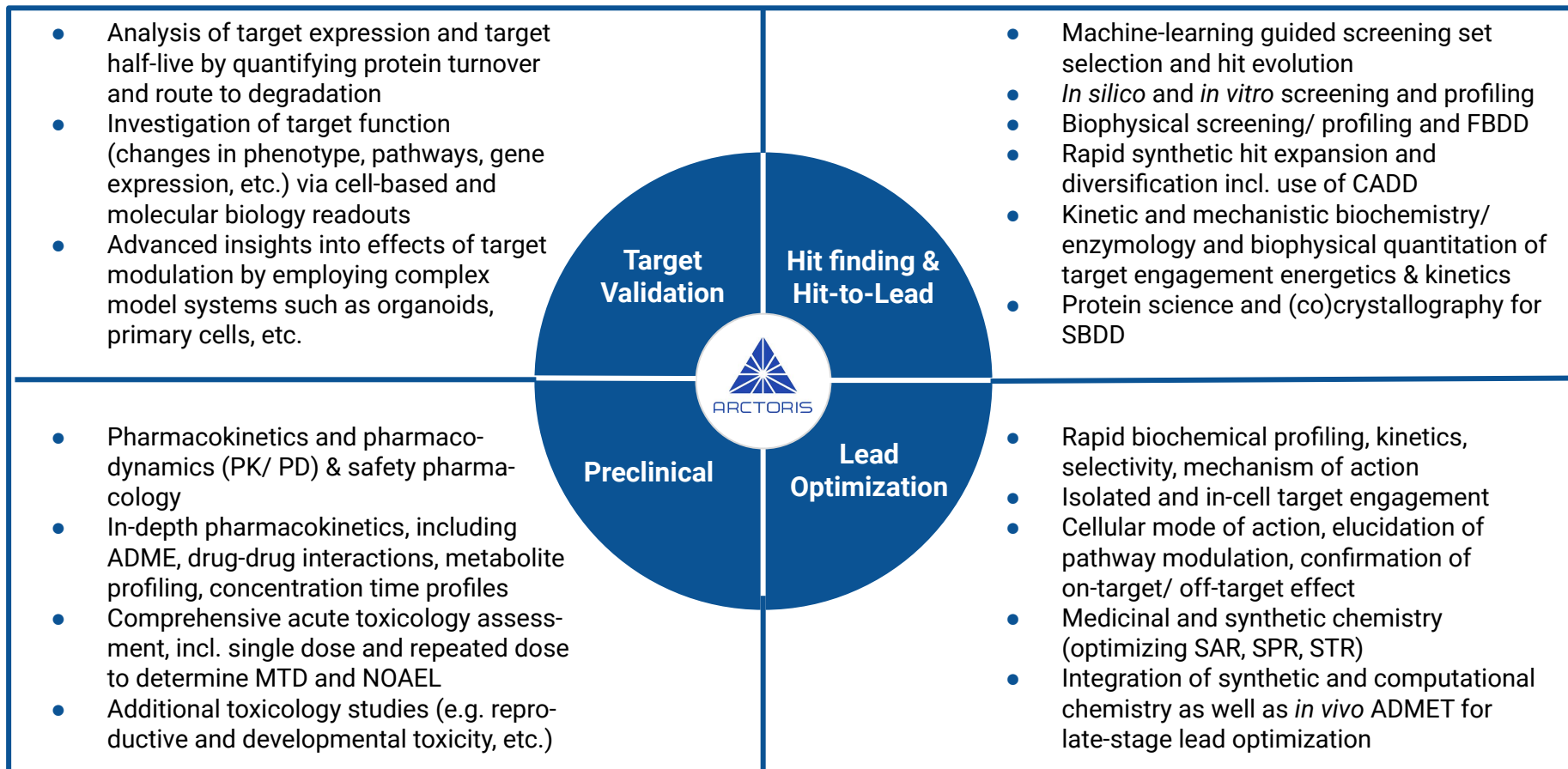
Both quality and speed are achieved by combining precision robotics with a unique data science platform and world-class drug discovery expertise from biotech and pharma veterans.

Arctoris tracks all experimental outputs in full depth, including the capture and analysis of extensive metadata – temperature, humidity, CO₂, 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.



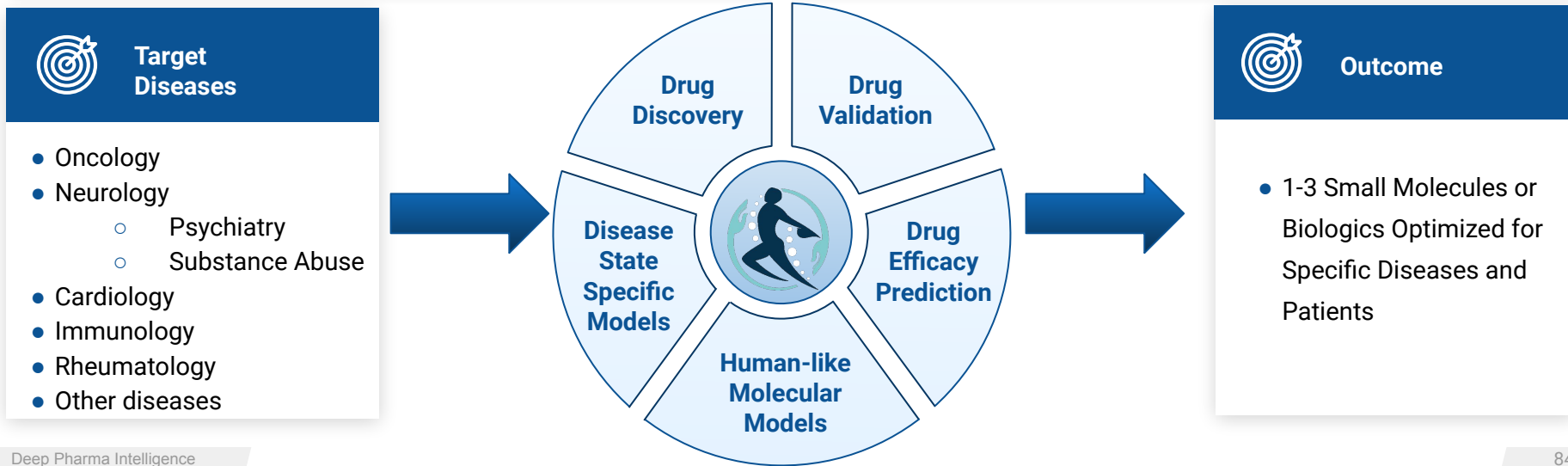
De-Risking and Accelerating Drug Discovery & Development for Improved Success in Biopharma. GATC Health



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.



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

6-9
months

Source &
Identity
Patient
Data

Rapid therapeutic
targeting



Automated
disease modeling



De-Novo therapeutic
assembly



Molecular
synthesis

Pre-clinical
Trials

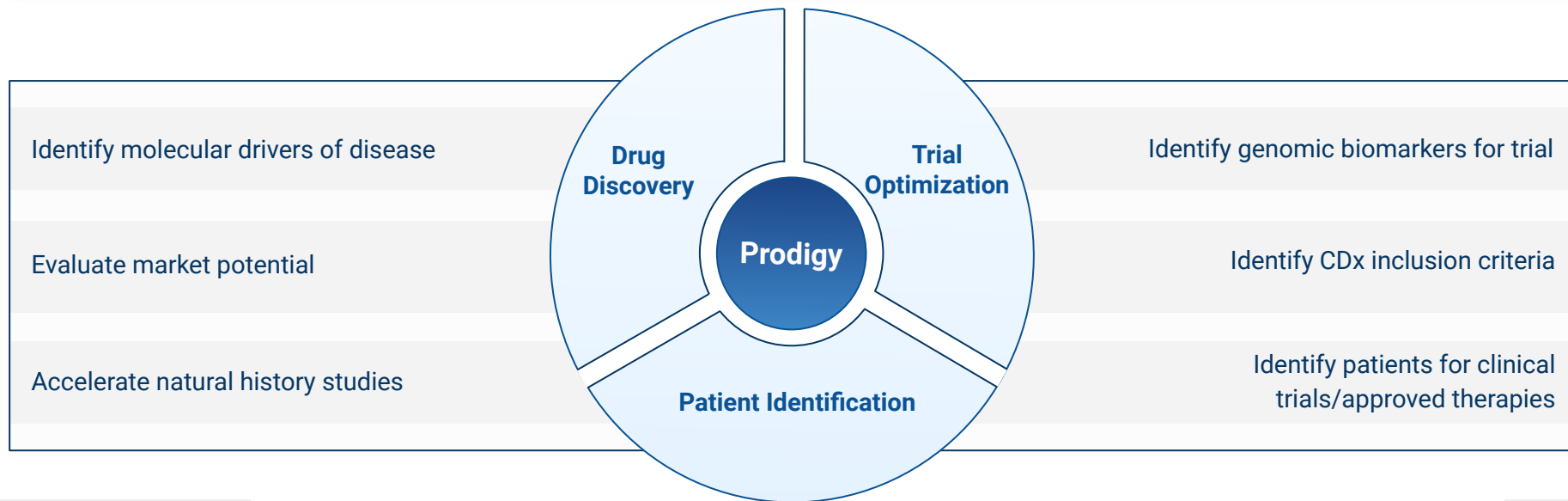
Most Innovative R&D Approaches of AI in Biopharma. Genomenon



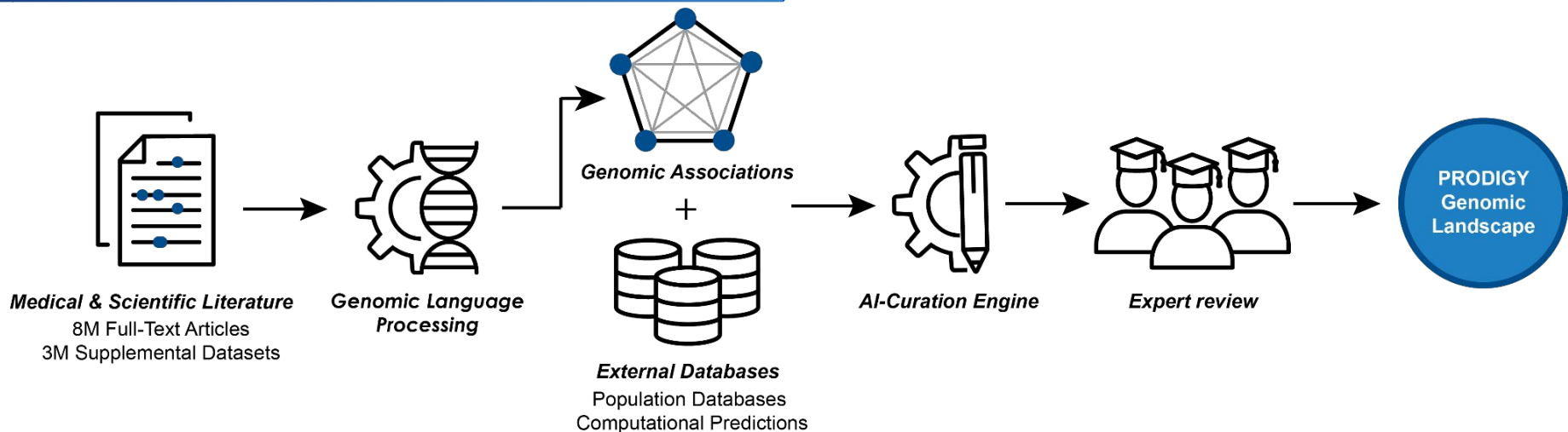
Genomenon is an AI-driven genomics company that organizes the world's genomic knowledge to accelerate the diagnosis and development of treatments for genetic disease.

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**.



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.

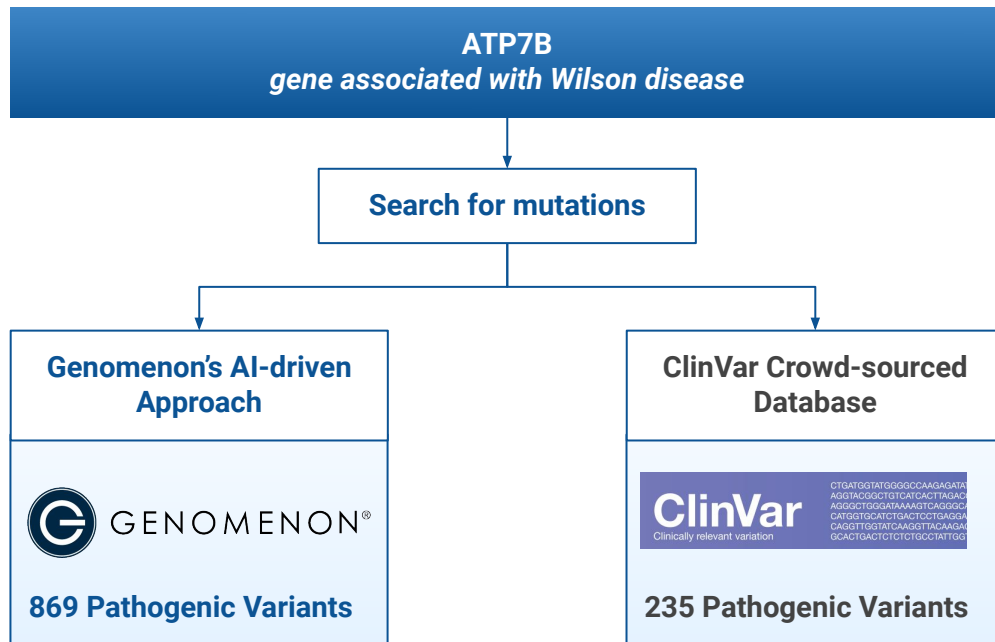
Genomic Language Processing (GLP) is a novel technology that systematically extracts and standardizes **genomic and clinical information** from the medical and scientific literature. Designed specifically to recognize this complex genomic information, GLP provides superior sensitivity compared to traditional 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**.



Genomenon's AI-driven approach identified 3.7x more evidence-supported, pathogenic/likely pathogenic variants for ATP7B than ClinVar.

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

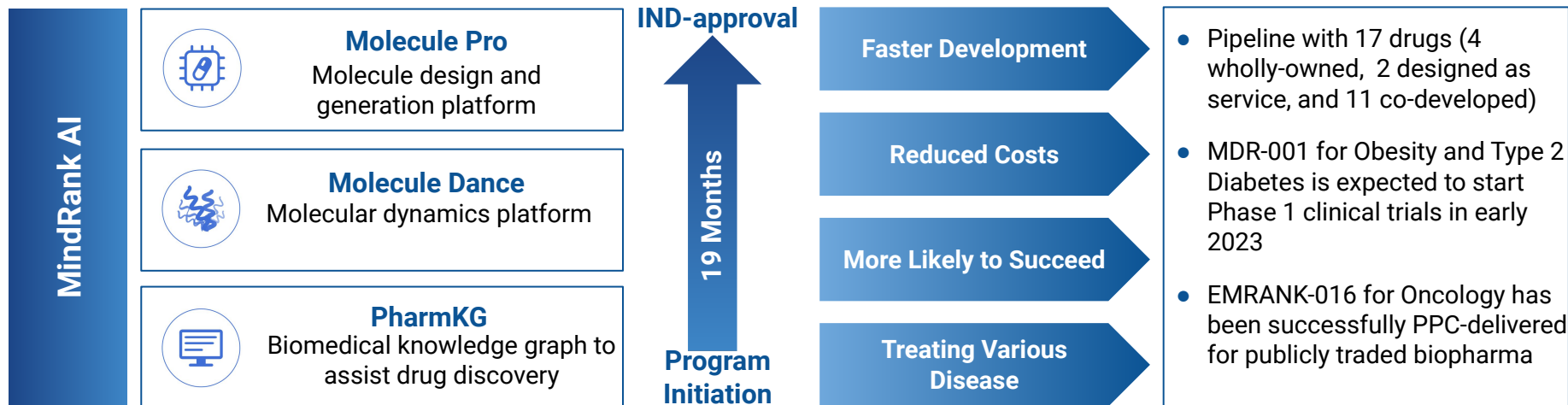
Most Innovative R&D Approaches of AI in Biopharma. MindRank AI



MindRank

MindRank AI is an artificial intelligence (AI)-empowered drug discovery company. By leveraging its proprietary AI platforms, the company aims to accelerate the drug discovery process and deliver small molecule drugs with desirable potency, efficacy and safety profiles. **Molecule Pro** is a molecule design and generation platform, **Molecule Dance** is a molecular dynamics platform to simulate protein movements, and **PharmKG** is a biomedical knowledge graph to assist with drug discovery.

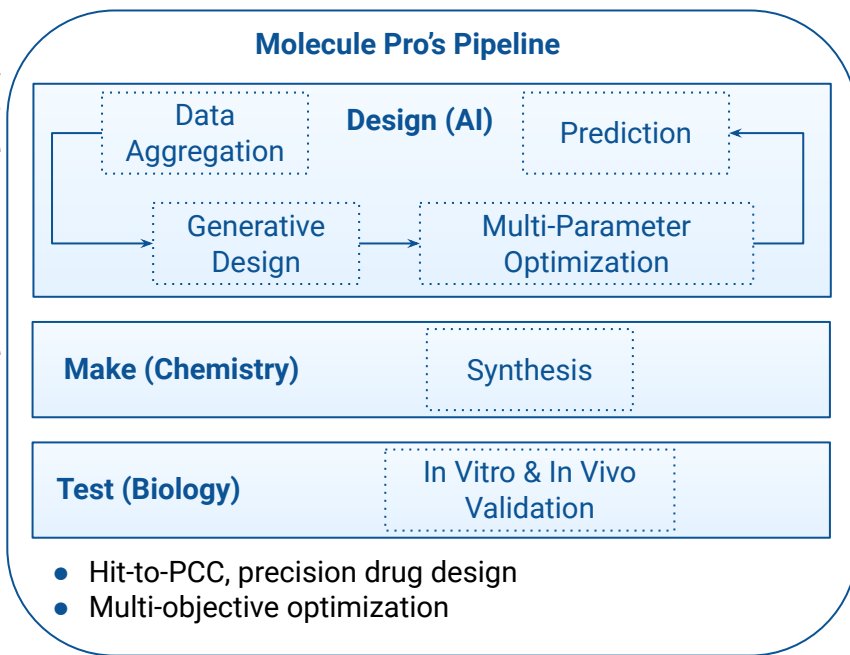
The company has a team of scientists with extensive experience in small molecule drugs R&D and technological innovation, and their proprietary AI solution has been recognized as one of the top AI breakthroughs in the biopharma industry.



How MindRank AI Transformed the Drug Development Process

- PharmKG** is a biomedical knowledge graph that helps to accelerate drug discovery by providing information about the relationships between diseases, genes, proteins, and small molecules. It can be used to generate potential targets hypothesis for drug development.
- Molecule Dance** is a molecular dynamics platform that performs docking /FEP and simulates the movements of proteins, helping to understand how proteins may interact with molecules and how they might be targeted by drugs. This information can be used to design and optimize small molecule drugs that are more likely to bind to the target proteins.
- Molecule Pro** is a platform for designing and generating small molecule drugs. It uses ML to generate molecules according to the pocket 3D structure and predict the ADME/T properties and PK of potential drug candidates, with the goal of identifying molecules that are more likely to be effective and successful in treating a specific disease.

- Target Discovery
 - Information Extraction
 - Customized project database construction
- Protein structure prediction & simulation
 - Docking and free energy perturbation (FEP)



PharmKG

Molecule Dance / Molecule Pro

Target Identification and Selection

Hit Discovery

Hit-to-Lead

Lead Optimization

Preclinical

IND-enabling

MDR-001: Completed in 19 Months

Key Advantages of MindRank AI

The company has obtained **US IND approval** for obesity and diabetes drug in **just 19 months** after the program initiation and successfully delivered an **oncology drug with best-in-class potential** to a public company.

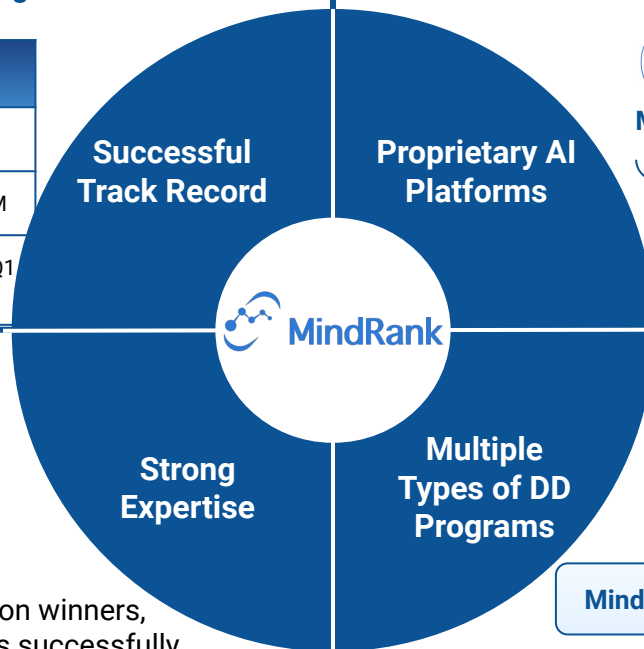
Drug	EMRANK-016	MDR-001
Target	Allosteric Inhibitor	GLP-1RA
Indication	Oncology	Obesity and T2DM
Status	PCC-delivered	Phase 1 starts in Q1 2023

The **company's team of scientists** has extensive experience in small molecule drugs R&D and technological innovation, which gives them a strong foundation for developing new drugs.

MindRank's Team:

- The team consist of global AI competition winners, experienced **medicinal chemist** who has successfully designed and developed drug on to the market and **biologists** who has discovered drug targets / pathways.

MindRank has **three proprietary AI platforms** that are designed to assist in the drug discovery process.



Molecule Pro



Molecule Dance



PharmKG

- Faster Drug Development
- Reducing Costs
-

The company is working on **different types of drug development** programs. This diversity could provide the company with multiple streams of revenue and increase their chances of success in the pharmaceutical market.

MindRank's Drug Development Programs

Proprietary Drugs

Design-as-Service


















Co-Developed Drugs

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**.

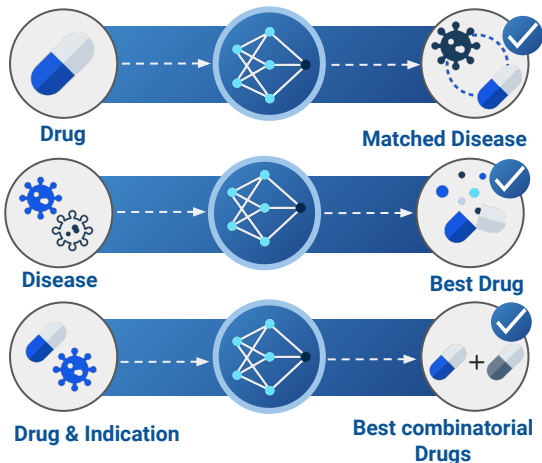
The company developed **ONCO AI Park** (**ONCOCROSS Artificial Intelligence Platform Ark**) - an Artificial Intelligence platform for drug development and predictions that includes several AI solutions.

<h3>Gene Expression Pattern Analysis</h3> <p>Instead of analyzing single target, single pathway, with single hypothesis, they analyse entire set of gene expression pattern</p>	<div>Traditional Approach</div> 	<div>Gene Expression Pattern Approach</div> 
<h3>Medically Curated Database</h3> <p>They have unrivalled quality transcriptome database that is curated by medical doctors and pharmacists at Oncocross</p>	<div> Patients 100,000+</div> <div> Chemicals 25,000+</div> <div> Cancer Prognosis 74,000+</div> <div> Disease Type 410+</div> <div> Cancer Types 42+</div>	
<h3>Pharmacophysiological & Pathophysiological Evidence Guided Drug-Disease Pairing</h3> <p>AI Platform performs comparative analysis at transcriptome levels of cells and human biopsy and blood samples</p>	<div>Pharmaco</div> <div>+</div> <div></div> <div>▶</div> <div></div> <div>▶</div> <div></div> <div>→</div> <div></div> <div>Patho</div> <div>+</div> <div></div> <div>▶</div> <div></div> <div>▶</div> <div></div> <div>→</div> <div></div>	

How ONCOCROSS Utilizes AI and Transcriptomics for Drug Development

RAPTOR AI™ (RNA 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-symmetry 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

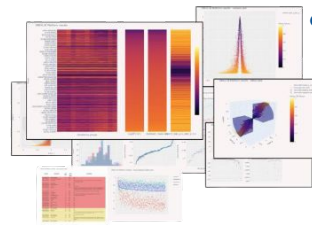
Rescue Drug

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-symmetry 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:

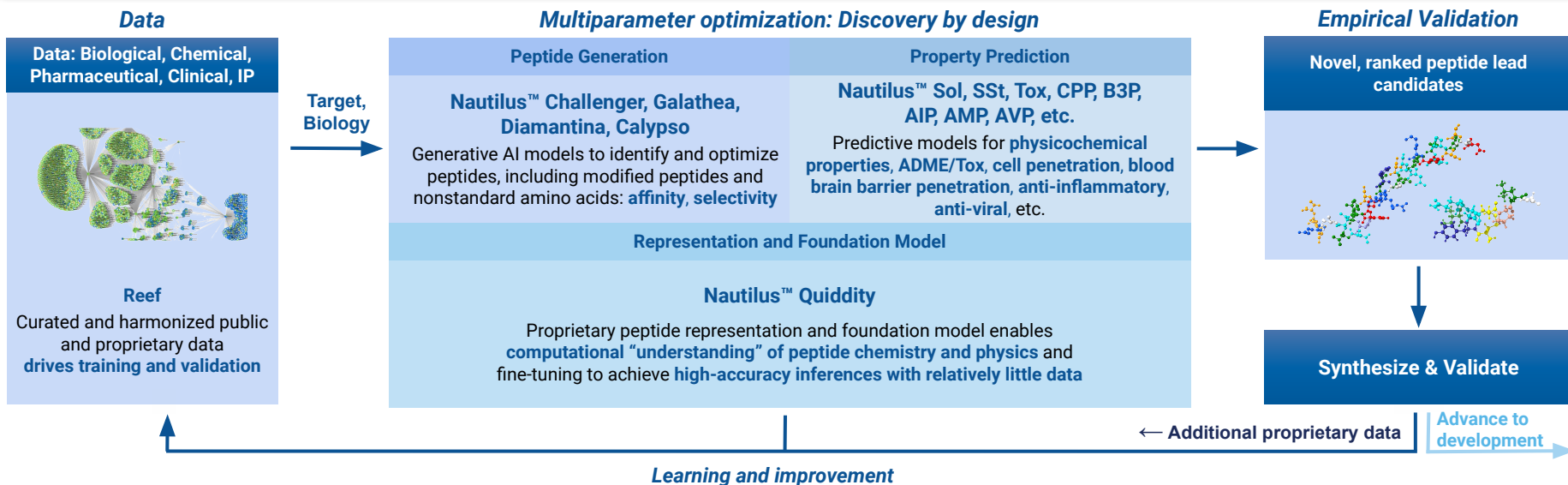
8	Internal pipelines
8	Partnered pipelines
1	Global clinical trial in Phase I
2	Phase IIa IND
1	Investigator initiated trial

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



Peptilogics engineers peptide therapeutic candidates to radically improve the treatment landscape for patients with life-threatening diseases. Uniting biological and pharmaceutical expertise, novel artificial intelligence algorithms, computational biology, and purpose-built supercomputing, Peptilogics is advancing an extensive therapeutic pipeline and accelerating discovery efforts at a pace and scale that was previously impossible.

Peptilogics' Nautilus™ platform combines **generative AI and a suite of predictive models** to produce **multiparameter-optimized leads** for a **broad range of targets and therapeutic areas**.



Nautilus™ is being used for: **internal programs, partnered programs, and focused peptide library generation**

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

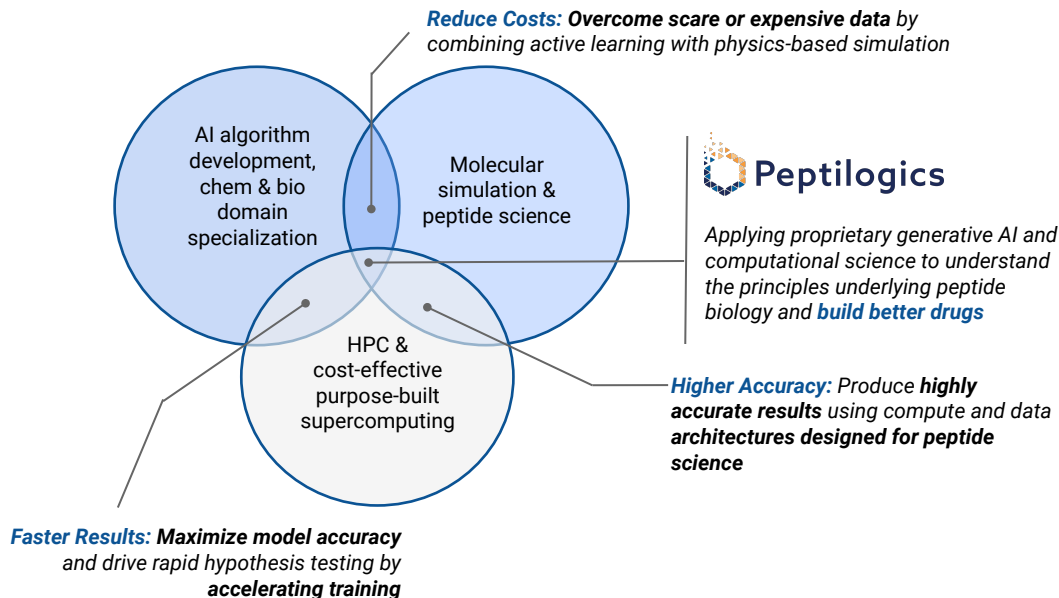


Peptides offer advantages over small molecules and biologics. Relative to small molecules, peptides can achieve higher selectivity and safety. Relative to biologics, peptides can more easily reach intracellular targets and cross the blood-brain barrier, and they can be manufactured at reasonable cost to broaden access. With Nautilus™, Peptilogics is enabling peptide generation including high diversity to explore novel chemical space.

Advantages of Nautilus™

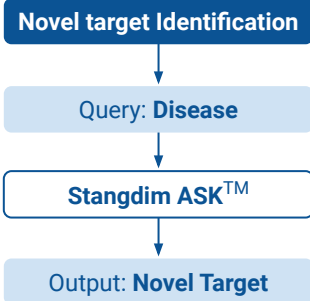
- **Go beyond just identifying binding hits:** encode an expanding list of pharmaceutical properties from the outset
- **Target-agnostic, therapeutic area-agnostic models** that can be applied to both **established and novel targets**
- **Access diverse chemical space** through proprietary algorithms and in-house, purpose-built supercomputing
- **Generate effective peptides in specific (tunable) size ranges and complexities**, including **nonstandard amino acids** and **cyclic and branched peptides**
- **Interpretable models** (where possible)
- **Validate peptide properties and provide rich data** for iterative learning through wet-lab synthesis and assays
- **Surpass high-throughput screening** through biologically informed, multiparameter design of pharmaceutical properties

Nautilus™ expands on principles demonstrated for the human-designed PLG0206, which is now in Ph1b.

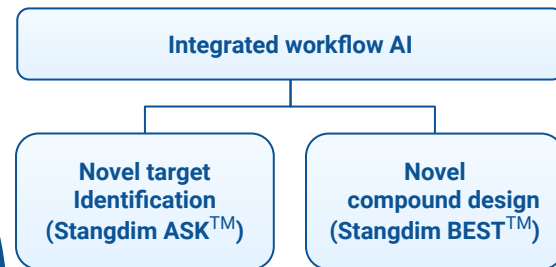


How Standigm Accelerates Drug Discovery using AI

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



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



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



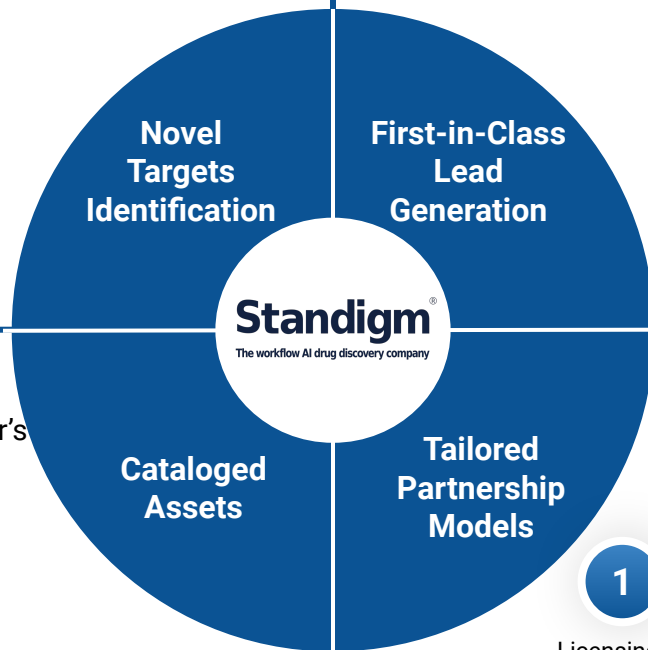
Parkinson's Disease



NASH

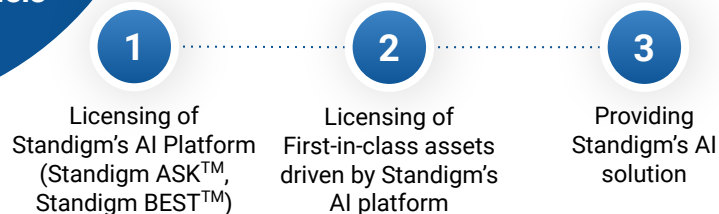


Mitochondrial Disease



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:



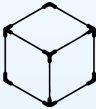
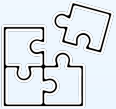
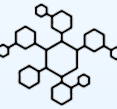

How Standigm Accelerates Drug Discovery using AI


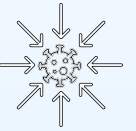
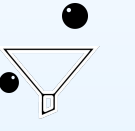

Standigm®

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.

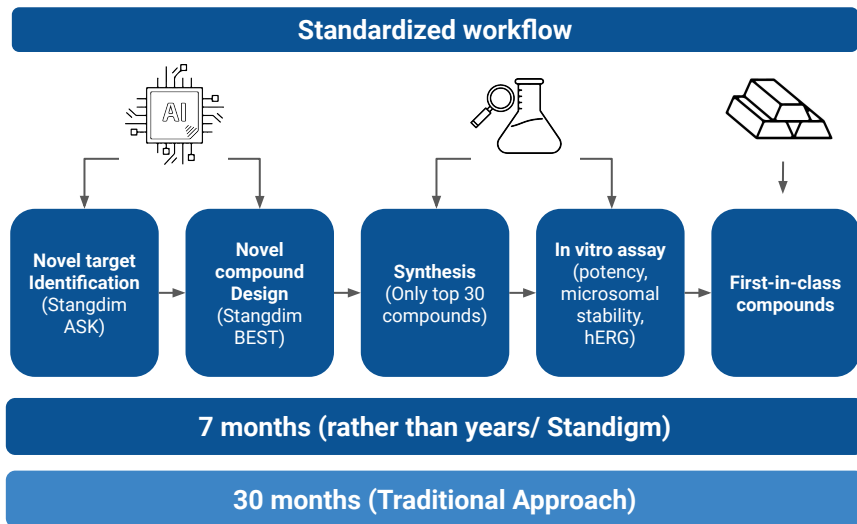
Standigm ASK™ is a customizable, AI-aided **drug target identification platform**, prioritizing disease-target relationships and providing evidence-based results through an interactive user interface.

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

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

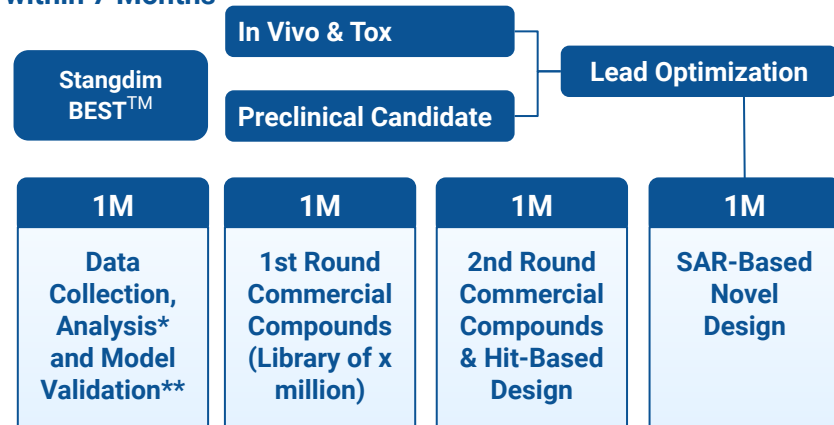
Standigm Releases First-in-Class Compounds within 7 Months



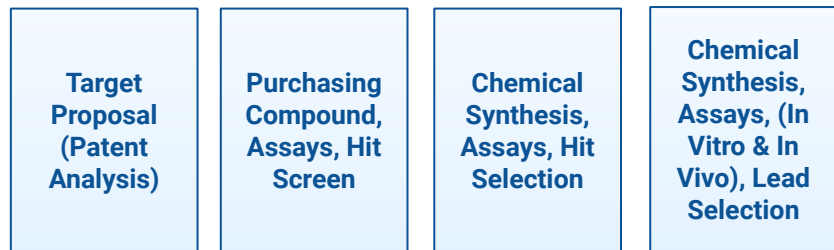
Featured Partners



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



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

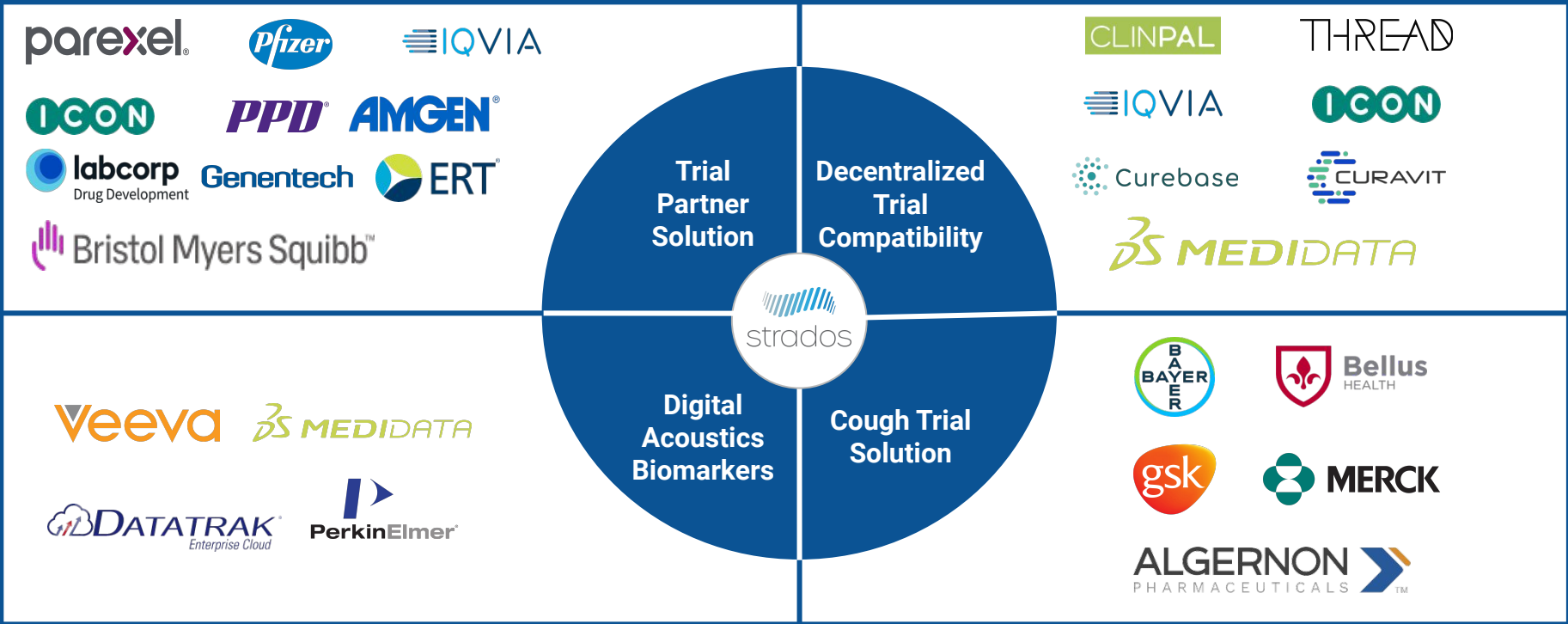


*Data Analysis – Binding site analysis using protein structure

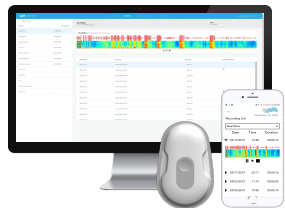
**Model Validation – Validation of activity prediction models: ChemMap-based, 2D structure QSAR-based, Simulation-based and Ensemble-based methods

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



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.

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.

**Data Collection
Capacity**

**Patient Privacy
& Security**

**Real-Time Data
Analysis**

**Patient
Centricity**

**Longitudinal
Lung Data**

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.

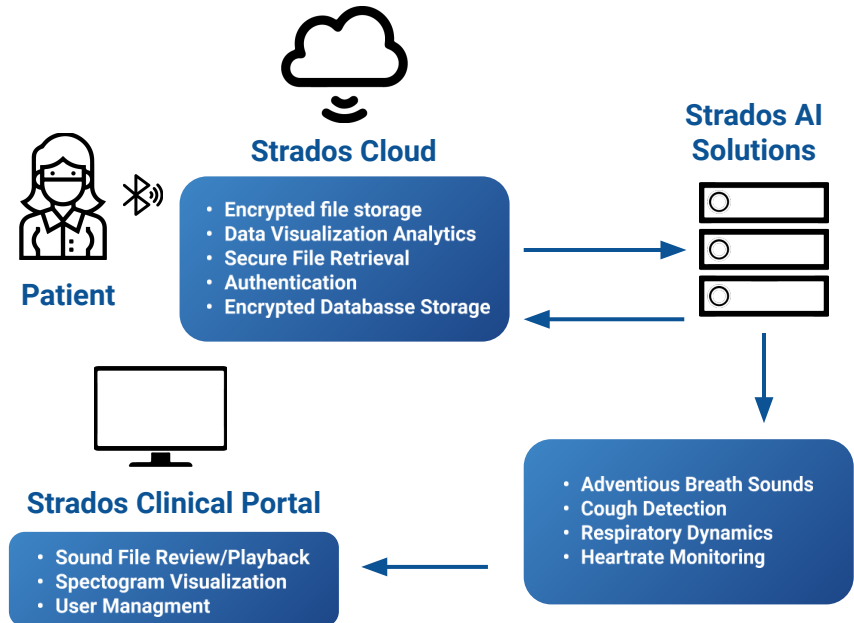
Today **Strados Labs** has a unique opportunity to stand as a leader in Respiratory Health: their clinically validated bioacoustic library of sounds and AI engine is the world's largest entirely hands-free, clinical-grade dataset enabling **Strados Labs** to be the standard bearer of acoustic digital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



Industry Developments Q1 2021- Q4 2022

Biggest Deals 2022

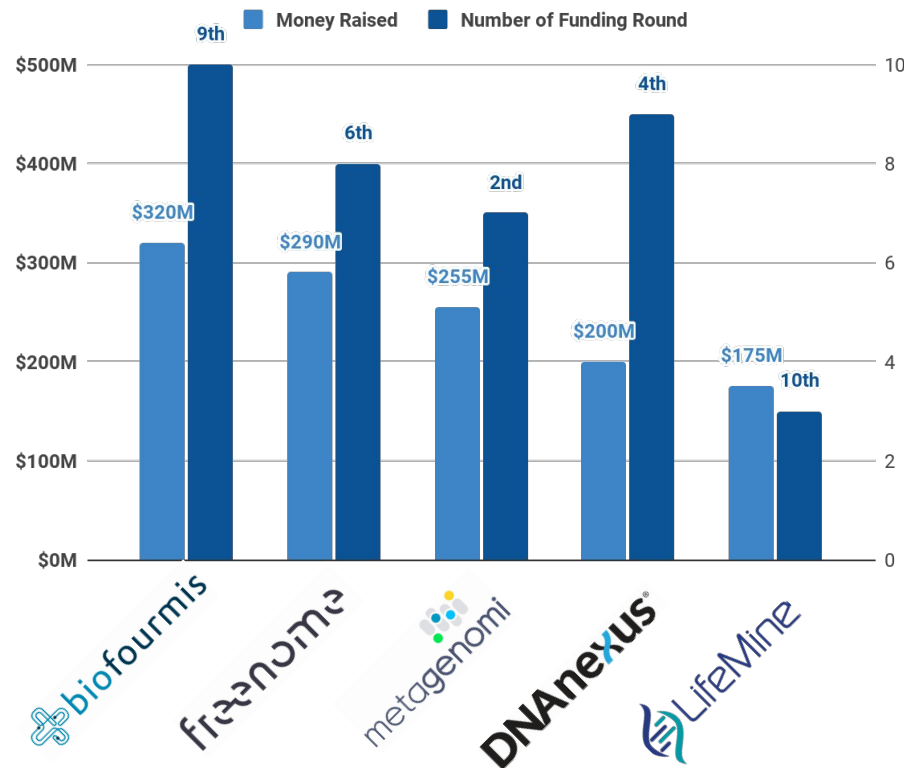
The total amount of VC funding in AI in drug development companies reached to \$26.5B in Q4 2022.

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.

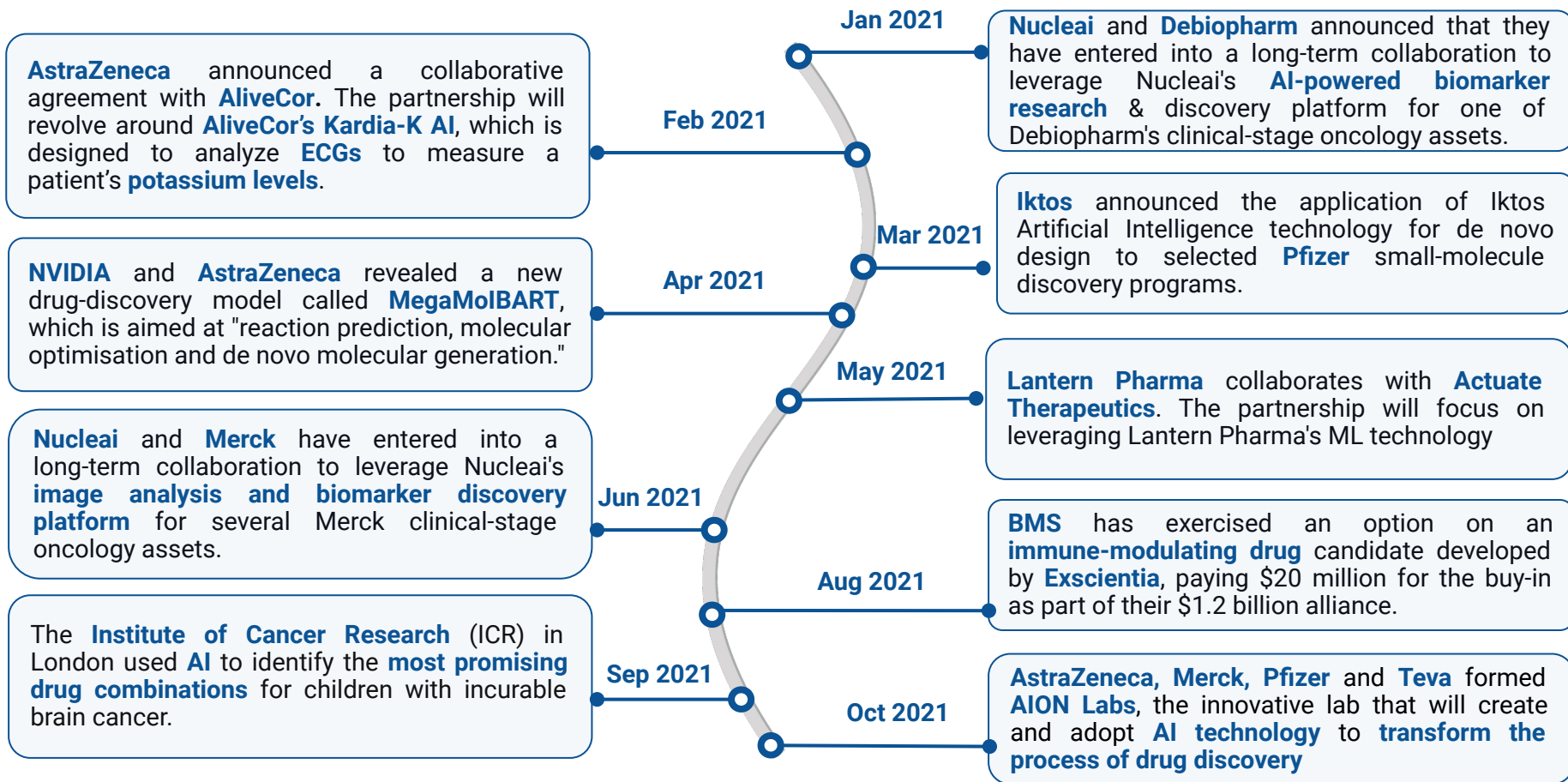
Top 5 highest fundings received the following companies:

1. **Biofourmis** with \$320 million (Series D)
2. **Freename** with \$290 million (Series D)
3. **Metagenomi** \$255 million (Series B)
4. **DNanexus** with \$200 million (Series H)
5. **LifeMine Therapeutics** with \$175 million (Series c)

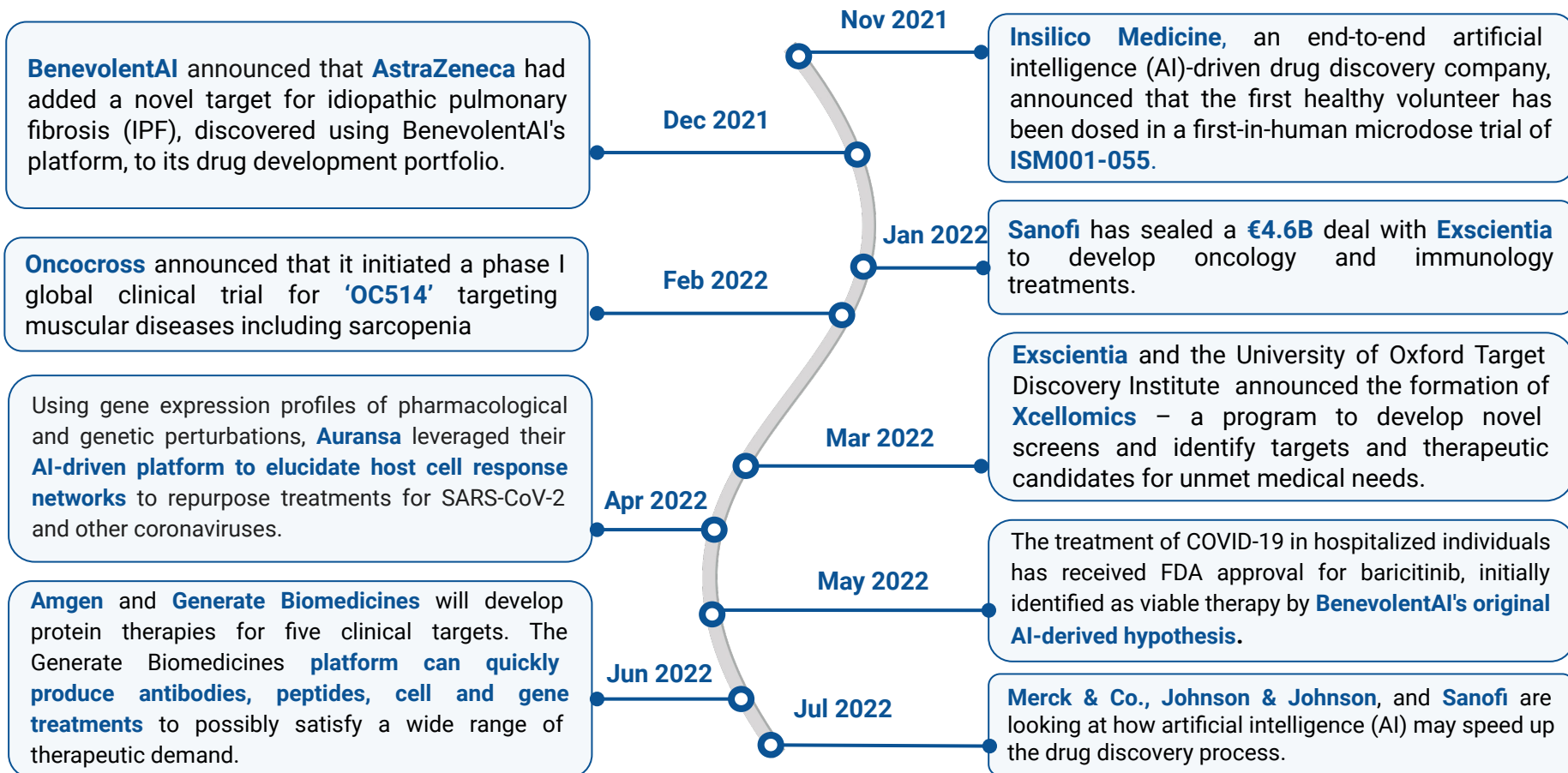
Biggest Funding 2022



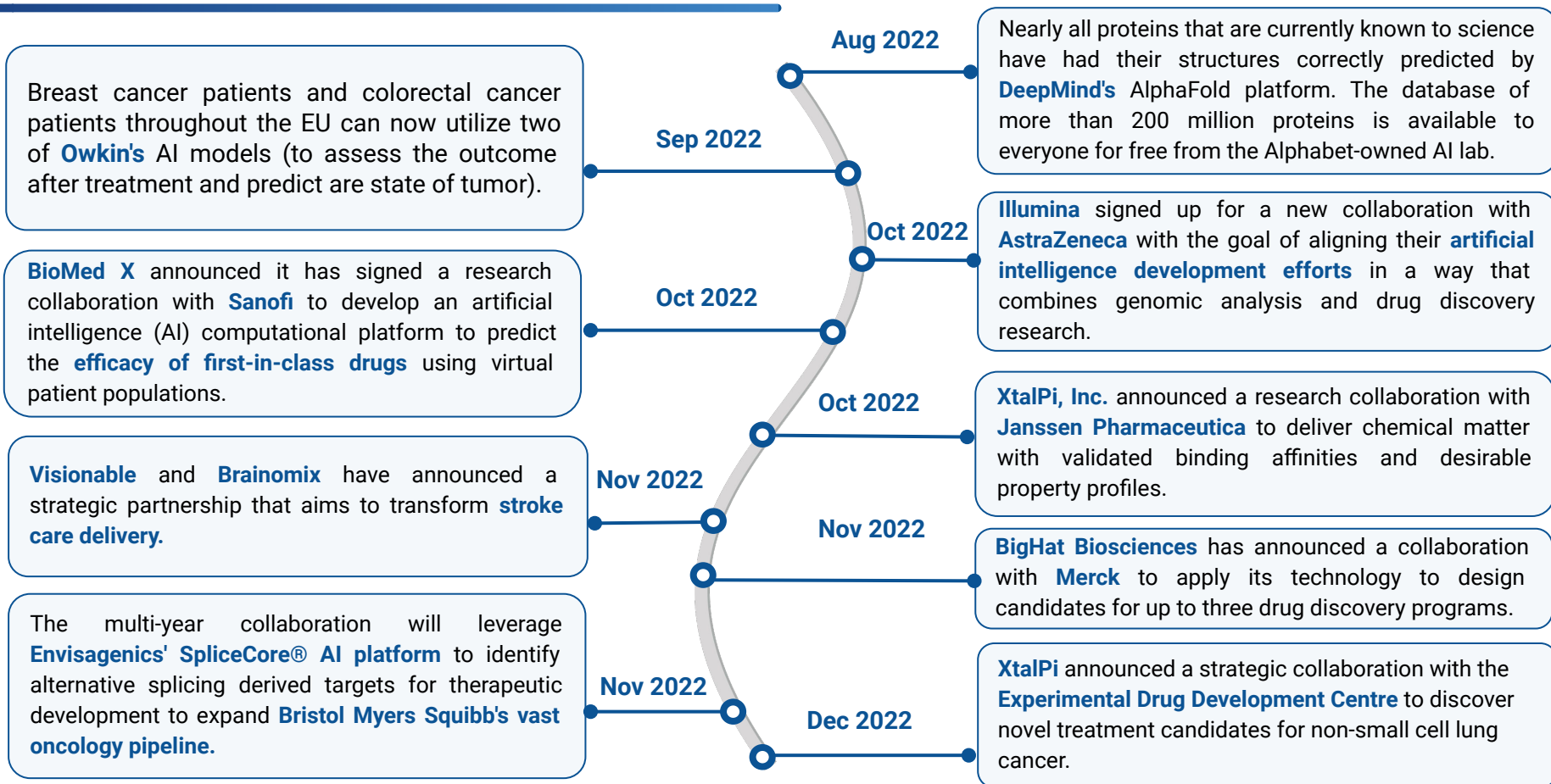
Selected Pharma AI Industry Developments 2022



Selected Pharma AI Industry Developments 2022



Selected Pharma AI Industry Developments 2022



Key Takeaways

Major Observations for 2022: Key Business Takeaways



Due to quickly growing proof of AI tech feasibility and innovation potential, big pharmaceutical companies and contract research organizations have been interested in collaborating with or utilizing the platforms of AI companies in the drug development process. These collaborations or platform usage can help speed up the drug development process and improve data analysis and decision-making. Astrazeneca is a leader in collaborations with AI companies, till the end of 2022 year, the company had more than 26 collaborations.



Big Pharmaceutical companies are very interested in the growth and development of AI companies. This interest can be observed not only in the high amount of collaboration between pharmaceutical companies and AI companies but also in the direct investments of big pharma in AI companies. In 2022, Roche invested \$290M in Freenome, Pfizer invested \$200M in Sema4, and Sanofi invested \$100M in Exscientia.



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).



The investment strategy changed in 2022. In 2021, the most significant investments came to innovative new companies with promising ideas, such as Neuromora Therapeutics and Insitro, in both were invested \$400M in 2021. In 2022, investors preferred more mature companies with ready-to-go solutions or drugs that are already entered the latest phases of clinical trials, such as Biofurmus (\$320M) and Freenome (\$290M).

Major Observations for 2022: Key Business Takeaways



The global COVID-19 pandemic heated up the interest in BioTech and drug discovery sectors and catalysed AI development. During 2021, we have observed over 150 medium and large funding rounds for AI in Drug Development companies with an average investment of \$64.7M. In 2022, the interest in AI in drug development appeared to reach a plateau. In 2022, there were over 70 investments in AI in Drug Development companies with an average investment of \$48.5M.



In 2022, only **1 company that use AI for DD reached IPO status**. London-based Benevolent AI closed its IPO in April and raised \$292M. There is a huge recession comparing to 2021 year, when 10 companies reached IPO. The global downturn might be the reason for this.



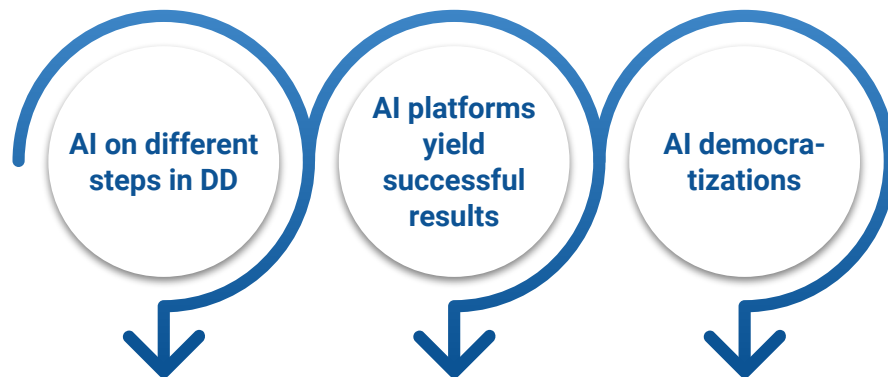
When some of the companies complete IPOs in the nearest future, it will attract a **significant number of non-biotech investors to enter the Life Sciences sector**. The prospects of this trend are already vivid: big tech companies enter partnerships with both innovative start-ups and pharma companies 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).



Despite the global downturn, the AI in Drug Development sector seems to be stable. Since the start of the 2022, the cumulative capitalization of publicly traded companies fell only by -3.1% and is **\$194,6B of cumulative capitalization as of end of December, 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

There are several challenges and obstacles to the adoption of artificial intelligence (AI) in drug development. These include:

1. **Data quality and availability:** AI algorithms require large amounts of high-quality data to be effective. However, the pharmaceutical industry has historically struggled with data silos, which can make it difficult to access and integrate data from multiple sources.
2. **Regulation:** The regulatory environment for AI in drug development is still evolving. Regulators such as the US Food and Drug Administration (FDA) and the European Medicines Agency (EMA) are working to establish guidelines for the use of AI in drug development, but these are still in the early stages.
3. **Lack of understanding and expertise:** Many pharmaceutical companies and researchers may not have the necessary expertise in AI to effectively utilize it in drug development. This can make it difficult for these organizations to adopt and integrate AI into their processes.
4. **Ethical concerns:** There are also ethical concerns surrounding the use of AI in drug development, including issues related to bias in data and algorithms and the potential for AI to replace human decision-making.

AI in Biotech Challenges



Overview of Deep Pharma Intelligence



Deep Pharma Intelligence – New Era in Pharma Analytics

Deep Pharma Intelligence (DPI), an analytical subsidiary of Deep Knowledge Group, is a highly specialised think tank in the area of BioTech innovation profiling, market intelligence, and BioTech development advisory. The company is dedicated to producing powerful data mining and visualisation systems, interactive analytics tools, and industry reports, offering deep technical insights, market intelligence, and strategic guidance in the high growth and significant opportunity areas.

DPI is Focusing on Three Key Activities:

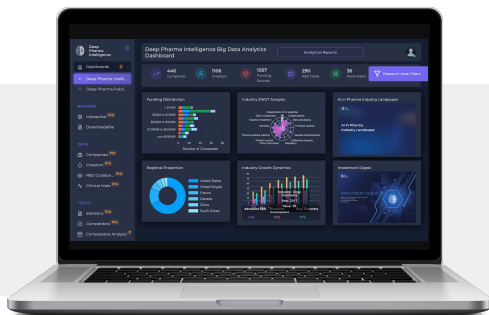
Conducting Market Intelligence

Producing regular **open-access** and **proprietary reports** on the emerging topics and trends in the pharmaceutical and healthcare industries. All reports are supported by our back-end analytics systems and tools that allow to receive fresh insights and updates about opportunities and risks.



Creating Big Data Analytical Dashboards

Building a comprehensive **Big Data Analytical Dashboard** (SaaS) as a one-stop-platform for all market and business intelligence operations our customers may need, including profiling thousands of companies, market signals and trends based on tens of millions of constantly updated data points.



Producing Scientific Content

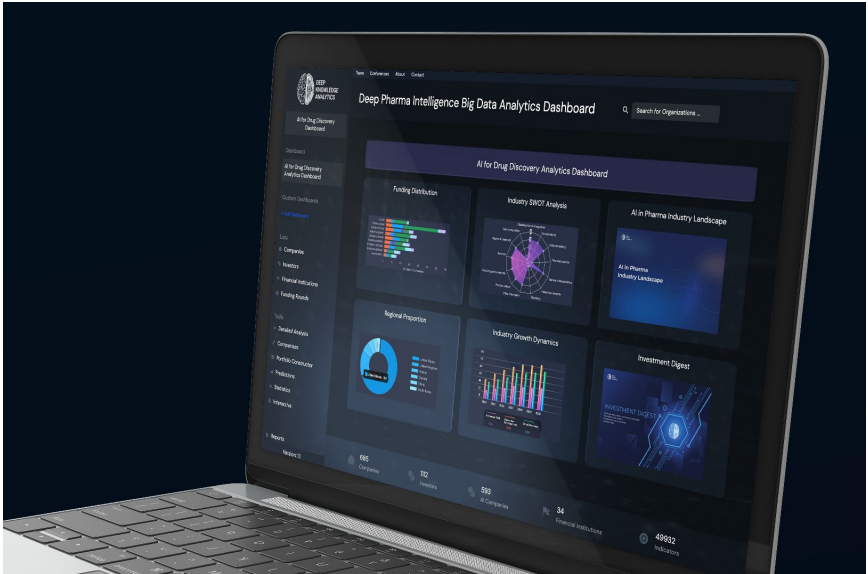
DPI provides a **full-cycle development of articles, scientific journals, and books**. We are ready to develop a detailed Requirement Specifications document, including layout of the journal, fully designed brand book, with example templates for each chapter.



AI in Drug Discovery Analytical Dashboard

AI in Drug Discovery Analytical Dashboard is a fundamental tool for strategic insights, opportunity evaluation, competitor profiling, and other purposes relevant to Pharma and BioTech decision-makers, life science investors, consulting companies, and regulatory agencies.

600	Companies
1,100	Investors
290	R&D Collaborations
120	Clinical Trials
170	Parameters of Automated SWOT Analysis



Market Intelligence Focus		
Automated SWOT Analysis	Stock Price Forecasting	Interactive Chart Builder
Automated Competitive Analysis	Financial Portfolio Constructor	Matching Tool for Investors

Comprehensive Market Intelligence

Deep Pharma Intelligence's proprietary services include **custom consulting projects based on the specific customer needs**, as well as a collection of preproduced 'ready-to-use' proprietary reports, developed by our research team and covering general trends and specific action ideas and strategy insights related to the most promising business prospects (e.g. new technologies, BioTech start-ups), M&A prospects (e.g. pipeline development targets), and strategic growth ideas (trends profiling, industry overviews, etc.).

Selected Open Access Reports



Artificial Intelligence for Drug Discovery Landscape Overview, Q3 2022 is an analytical report that aims to provide a comprehensive overview of the AI in drug discovery industry, clinical research, and other aspects of pharmaceutical R&D.



Epigenetic Drugs Q2 2022 report aims to provide a comprehensive overview of the current state of the epigenetic drugs market and research. The aim of this report is to provide insights into the diversity of possible epigenetic targets, mechanisms of their action in treating cancer and other diseases.



Landscape of Advanced Technology Companies in Pharmaceutical Industry Q4 2021 is an analytical report providing insights into the expansion of technology developers and vendors in the pharmaceutical space, as well as their increasing role in the pharmaceutical business.

Business Consulting Services

Deep Pharma Intelligence offers a comprehensive range of **consulting services**, including **market and competitor research, technology scouting and due diligence, investment landscape profiling, and comprehensive analytics support for investment decision-making.**

Investment Landscape Profiling

Identifying investment trends in the pharma, BioTech, medicine, healthcare, drug development technological space, investments risk profiling based on risk tolerance, risk capacity, and risk requirements.

Technology Scouting and Due Diligence

Identifying, locating, and evaluating existing or developing technologies, products, services, and emerging trends. The service includes business, science and technology, intellectual property (IP) profiling, and potential assessment.

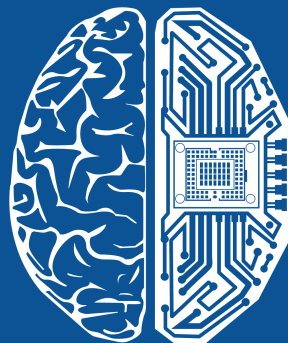
Market Research

Thorough market assessment within a specific industry in the field of pharma, BioTech, medicine, healthcare, drug development, AI, and others.

Competitor Research

Competitive analysis of companies, technologies, technological sectors, etc. Competitive analysis includes SWOT analysis and competitive profiling.





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

E-mail: info@deep-pharma.tech

Website: deep-pharma.tech

Deep Pharma Intelligence (DPI) Disclaimer

The information and opinions in this report were prepared by Deep Pharma Intelligence. The information herein is believed by DPI to be reliable but DPI makes no representation as to the accuracy or completeness of such information. There is no guarantee that the views and opinions expressed in this communication will come to pass. DPI may provide, may have provided or may seek to provide advisory services to one or more companies mentioned herein. In addition, employees of DPI may have purchased or may purchase securities in one or more companies mentioned in this report. Opinions, estimates and analyses in this report constitute the current judgment of the author as of the date of this report. They do not necessarily reflect the opinions of DPI and are subject to change without notice. DPI has no obligation to update, modify or amend this report or to otherwise notify a reader thereof in the event that any matter stated herein, or any opinion, estimate, forecast or analysis set forth herein, changes or subsequently becomes inaccurate. This report is provided for informational purposes only. It is not to be construed as an offer to buy or sell or a solicitation of an offer to buy or sell any financial instruments or to participate in any particular trading strategy in any jurisdiction.