

Artificial Intelligence for Drug Discovery

Landscape Overview Q4 2022





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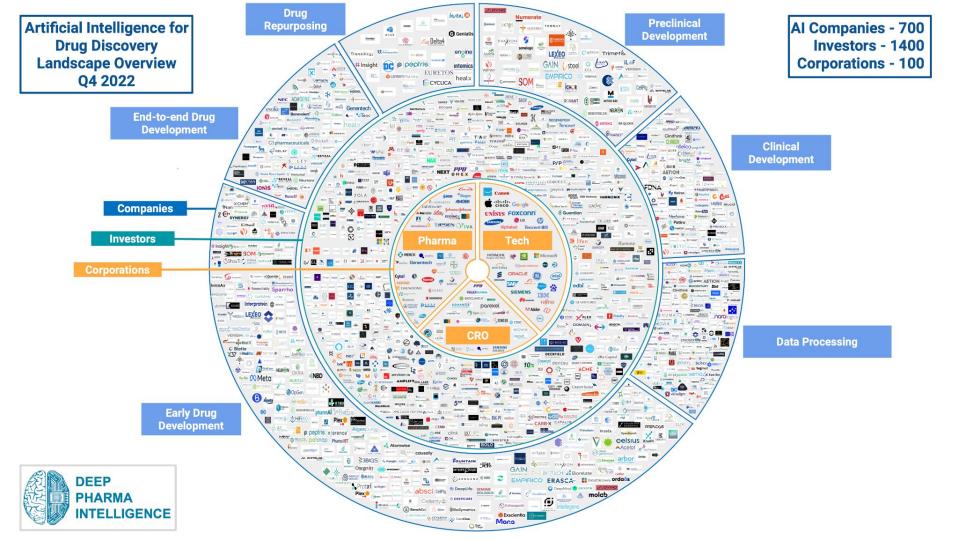
Introduction

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 Al 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 Al investment and business development activities. The listings of Al-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 Al applications and research achievements.

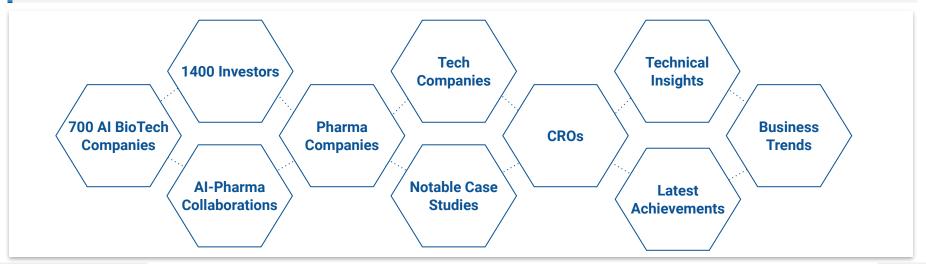


Report at a Glance

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 Al 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 Al application and research.

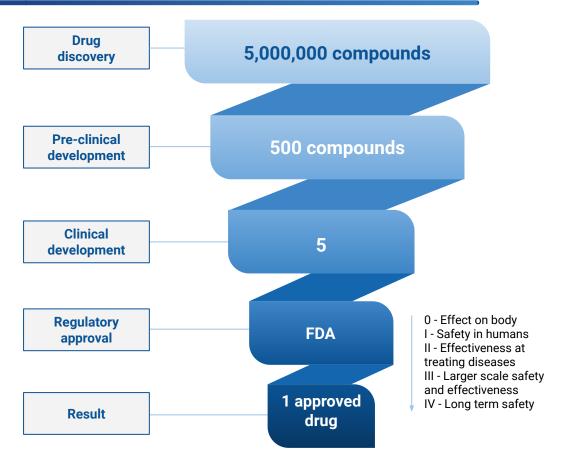


Introduction to AI in Drug Development





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 Al 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 Al-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.

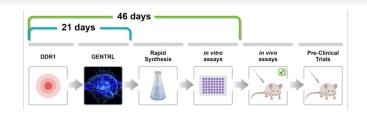




Experimental ResultComputational Prediction

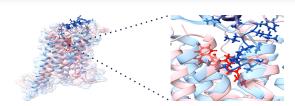


Insilico Medicine applied generative adversarial network-based system GENTRL for rapid identification of potent DDR1 Kinase inhibitors within 21 days.

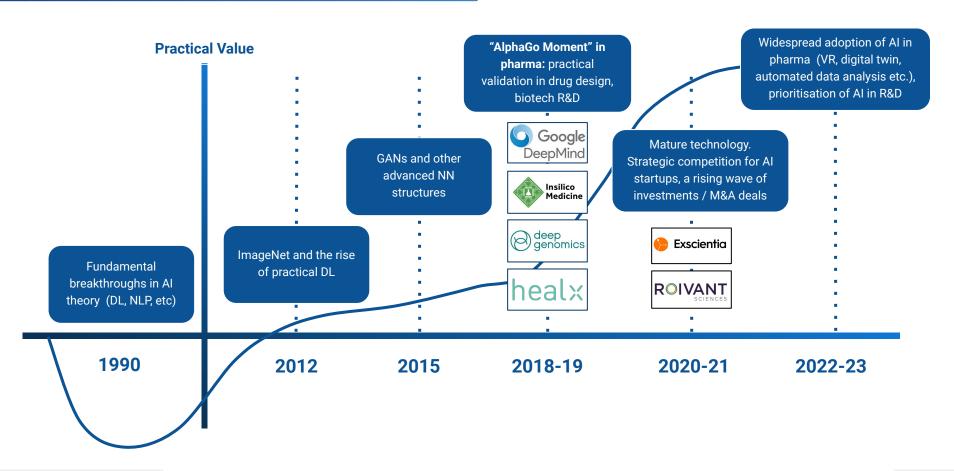




Peptilogics developed generative AI to predict peptides that bind to arbitrary proteins, even given only a protein's primary sequence, unlocking peptide drug design for established and novel targets.



Pharma's "AlphaGo Moment"



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



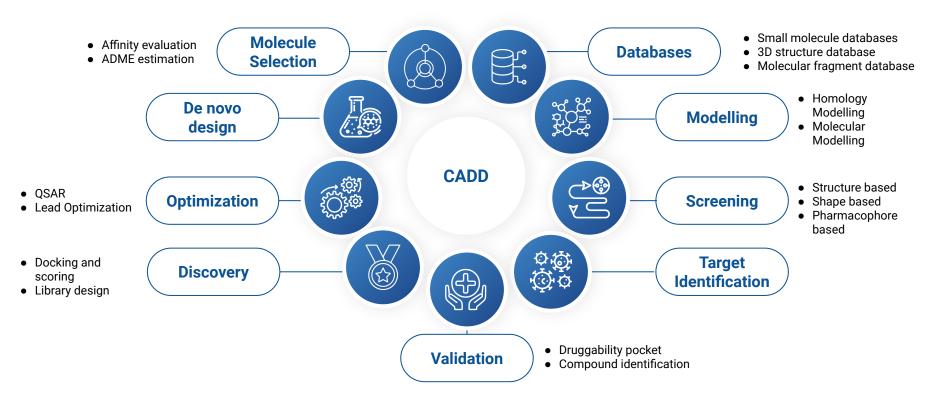
When optimizing ISM001, Insilico managed to achieve increased solubility, good ADME properties, and no sign of CYP inhibition — with retained nanomolar potency. Interestingly, the optimized compounds also showed nanomolar potency against nine other targets related to fibrosis. The efficacy and a good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

1 week	2 months	4 months	11 months	Phase 1	Phase 2	Phase 3	Submission to launch
< \$ 50k N/A	\$ 200k \$ 94M	\$ 400k \$ 166M	\$ 200k \$ 414M				
Up to Decades	1 year	1.5 years	2 years	Phase 1	Phase 2	Phase 3	Submission to launch

Deep Pharma Intelligence Source: Insilico Medicine

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 Small molecule databases has established novel platforms that mostly have a similar structure for testing drug candidates. The **Databases** usage of AI can simplify and facilitate the drug 3D structure databases design from filtering datasets for appropriate compounds to advanced lead modification and in Molecular fragment databases silico testings. Structure-based virtual screening Binding energy analysis **Binding site** prediction **Docking** Scoring **Functional Target protein Chemical intuition Genomics** identification **Molecular dynamic simulation** Modelling **Analyze the interaction of target** structure and lead candidate **Homology Modelling Molecular Modelling**

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

Target Discovery and Early Drug Discovery

Accelerated development of new drugs and targets identification

- Identify novel drug candidates
- Analyze data from patient samples
- Predict pharmacological properties
- Simplify protein design

Clinical Trials

Targeted towards personalized approach and optimal data handling

- Optimize clinical trial study design
- Patient-representative computer models
- Define best personalized treatment
- Analyze medical records
- Improve pathology analysis

Al for Advanced R&D

Design and Processing of Preclinical Experiments

Optimization of experiments and data processing

- Reduce time and cost of planning
- Decode open- and closed-access data
- Automate selection, manipulation, and analysis of cells
- Automate sample analysis with a robotic cloud laboratory

Aggregation and Synthesis of Information

Time- and resources-efficient information management

- Generate insights from thousands of unrelated data sources
- Improve decision-making
- Eliminate blind spots in research

Repurposing of Existing
Drugs

Searching for new applications of existing drugs at a high scale

- Rapidly identify new indications
- Match existing drugs with rare diseases
- Testing 1000+ of compounds in 100+ of cellular disease models in parallel

Al in Drug Development: Leaders

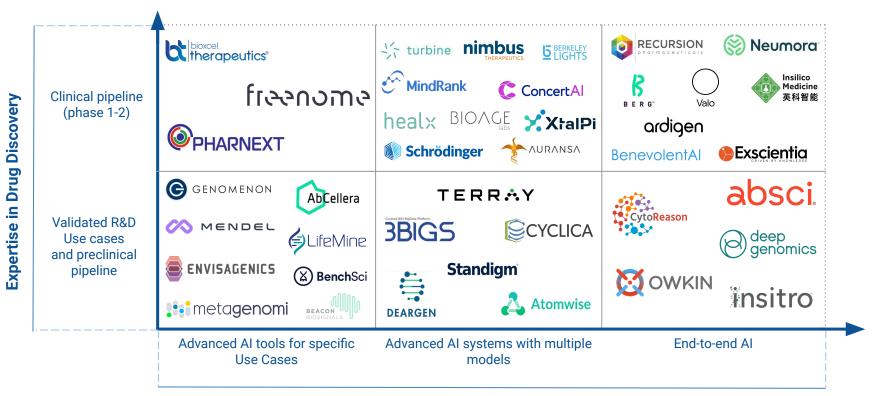




40 Leading Companies in AI for Drug Discovery Sector

1	3BIGS	21	Freenome
2	AbCellera	22	Genomenon
3	Absci	23	Healx
4	Ardigen	24	Insillico Medicine
5	Atomwise	25	Insitro
6	Auransa	26	LifeMine Therapeutics
7	Beacon Biosignals	27	Mendel.ai
8	BenchSci	28	Metagenomi
9	Benevolent Al	29	MindRank Al
10	Berg	30	Neumora
11	Berkeley Lights	31	Nimbus Therapeutics
12	Bioage Labs	32	Owkin
13	BioXcel Therapeutics	33	Pharnext
14	ConcertAl	34	Recursion Pharmaceuticals
15	Cyclica	35	Schrodinger
16	CytoReason	36	Standigm
17	Deargen	37	Terray Therapeutics
18	Deep Genomics	38	Turbine
19	Envisagenics	39	Valo
20	Exscientia	40	XtalPi

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



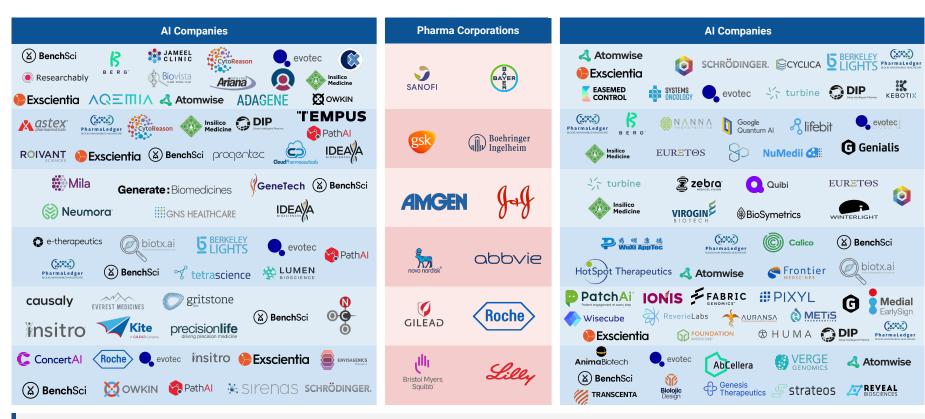
Expertise in Al

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



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50 Leading Investors in AI for Drug Discovery Sector

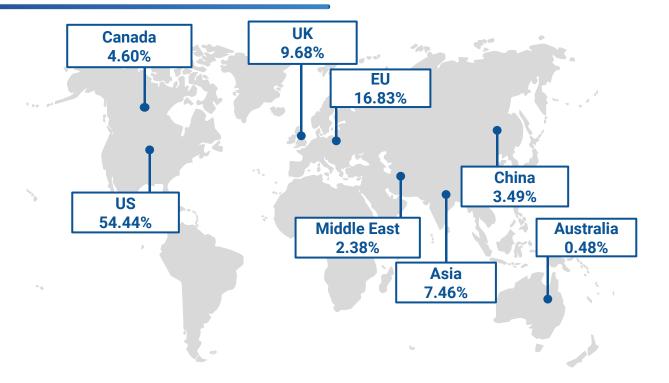
1	Casdin Capital	18	Merck Global Health	35	AME Cloud Ventures
2	Y Combinator	19	RA Capital Management	36	Founders Fund
3	GV	20	Bill & Melinda Gates Foundation	37	OrbiMed
4	Creative Destruction Lab (CDL)	21	Foresite Capital	38	Lifeforce Capital
5	Perceptive Advisors	22	T. Rowe Price	39	Lilly Asia Ventures
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		

Al in Drug Development: Geographical Coverage



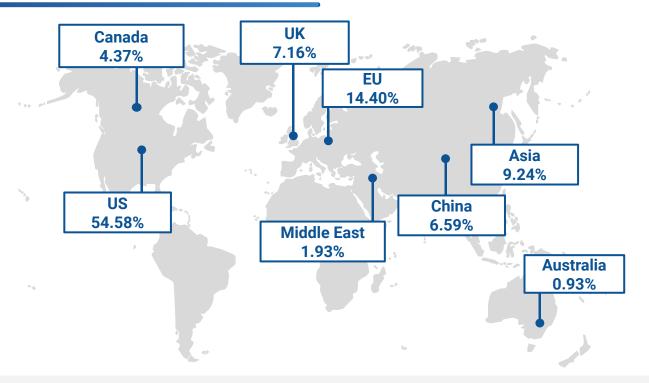


700 AI Companies: Regional Proportion



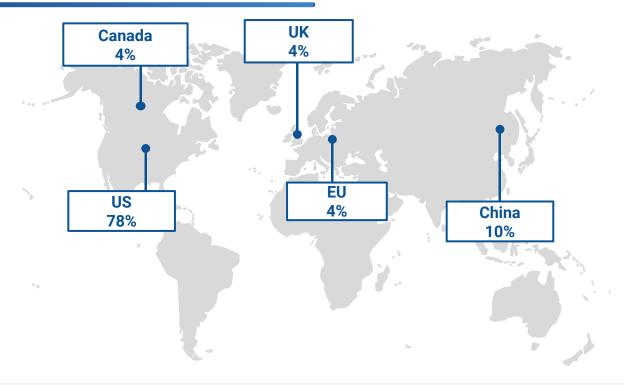
The US is still firmly in the lead regarding its proportion of AI for Drug Discovery companies. Interestingly, Asia and the Middle East continue to expand usage of AI technologies in the Pharmaceutical Industry. The ratio of companies that use AI for Drug Development in the UK and European countries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

Al in the Global Context

Europe Actively Explores Al Applications for Drug Discovery

In Europe, the European Medicines Agency (EMA) has announced plans to use Al 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 Al 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 Al 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.

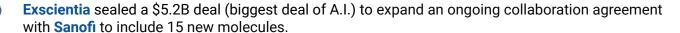


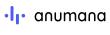


Amgen - Mila partnership that permits Amgen to expand its knowledge of Al and deep learning by interacting and engaging with experts in Mila's unique ecosystem.











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.





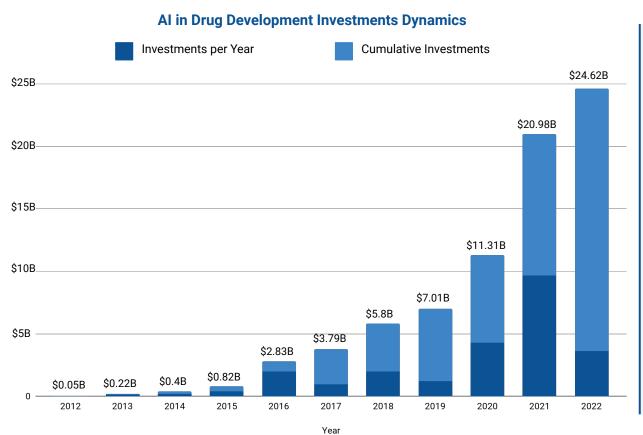
Microsoft and Novo Nordisk signed a contract to expedite the company's drug discovery process.





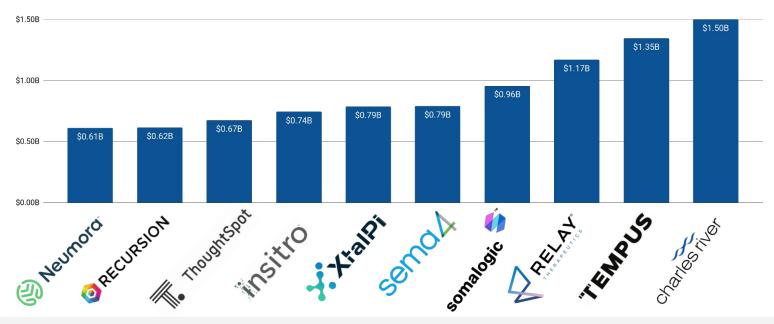
Roche announces PathAl collaboration for artificial intelligence-based digital pathology applications for improved patient care.

Dynamics of Investments in AI in Drug Development

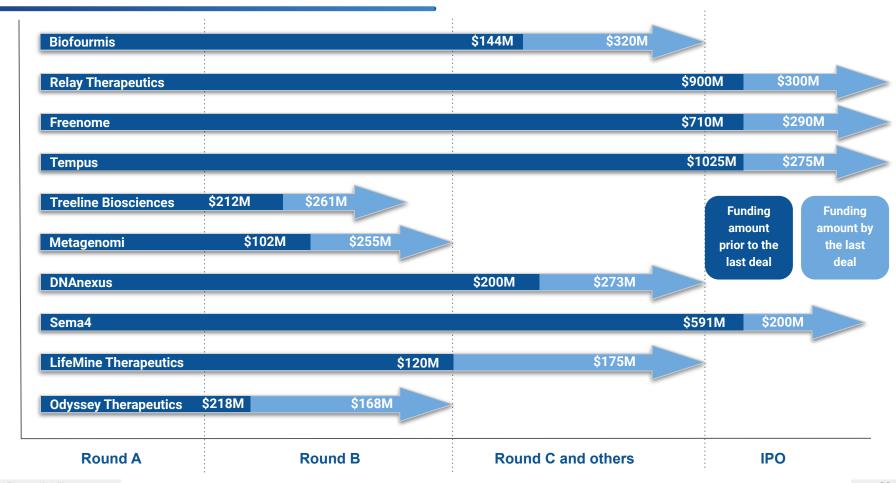


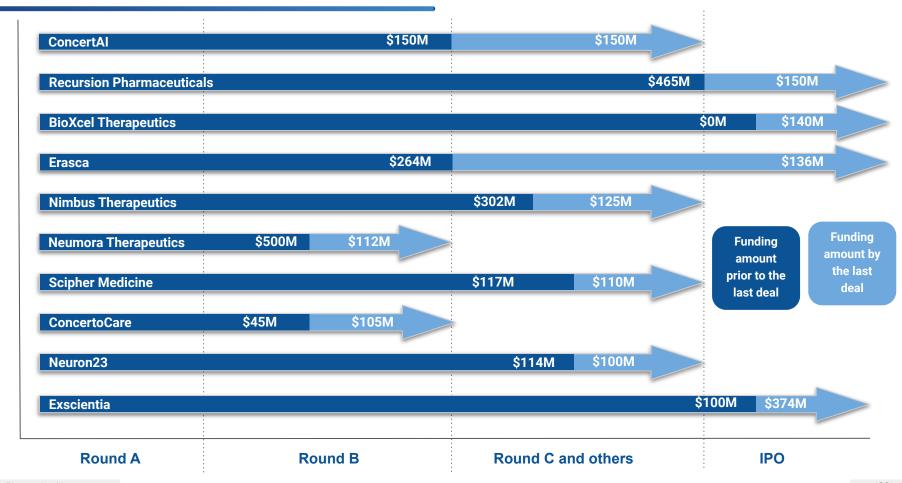
There has been a substantial increase in the amount of capital invested in Al-driven pharma companies since 2015. During the last nine years, the annual amount of investments in 700 companies has increased by almost 30 times (to \$24.62B in total as of December 2022). The most rapid growth was in 2021, when the year investment in the AI in Drug Development companies was \$9.66B. We can suggest, that COVID-19 pandemia 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.

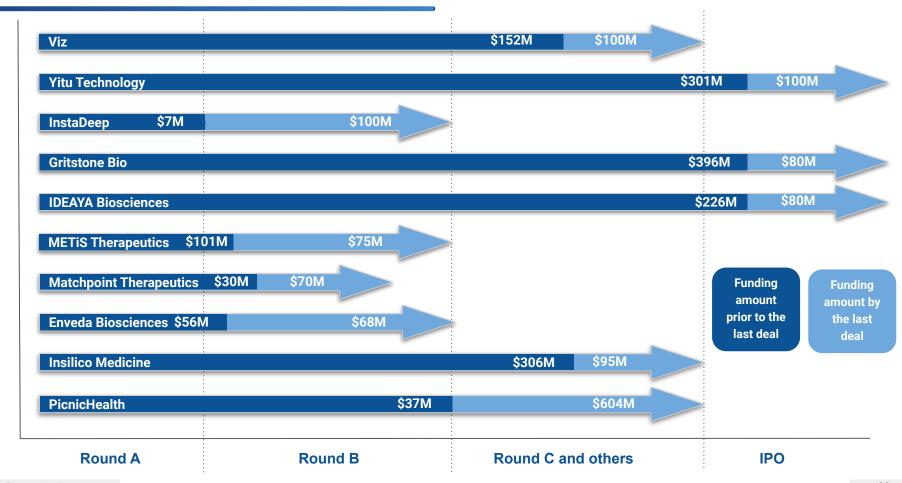
Top 10 Al in Pharma Companies by Total Investments in Q4 2022

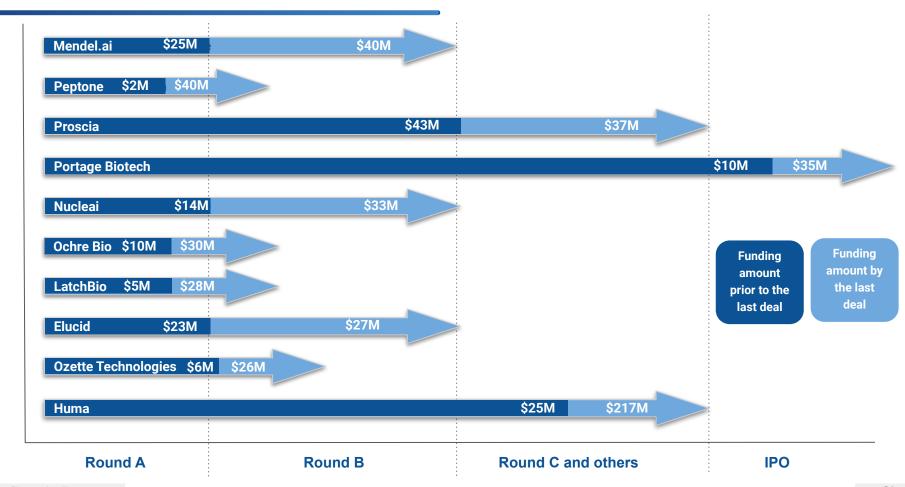


The chart shows the top 10 Al-driven drug discovery companies sorted by the **total funding** raised by the end of Q4 2022. **Charles River Laboratories**, an artificial intelligence-powered drug R&D company, is now at the top of the list. The company has the total funding raised to \$1.48B. **Tempus**, 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**.



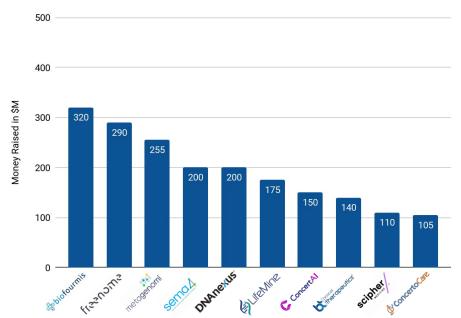




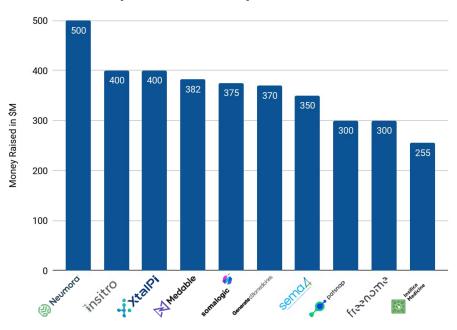


Top 10 Funded Companies in 2022 vs 2021

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 Al development. During 2021, we have observed over 150 medium and large funding rounds for Al in Drug Development companies with an average investment of \$64.7M. In 2022, the interest in Al in drug development appeared to reach a plateau. In 2022, there were over 70 investments in Al 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.

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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
1		10	WEICK GIODAI FIERIUI	33	
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 Al in Pharma Investors



San Francisco



San Francisco California LIS



Founders Fund San Francisco, California, US



Foresite Capital San Francisco, California, US



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



Felicis Ventures Menlo Park, California, US



Khosla Ventures Menlo Park, California, US

NEA

New Enterprise Associates Menlo Park, California, US

Illinois



ARCH Venture Partners Chicago, Illinois, US

Mountain View



Y Combinator Mountain View, California, US



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 Jersev. US



National Science Foundation Alexandria, Virginia, , US



T. Rowe Price Baltimore, Maryland, US



Section 32 San Diego, California,



Madrona Seattle, Washington,







Creative Destruction Lab (CDL) Toronto, Canda



Novo Holdings Hellerup, Hovedstaden,

Denmark



Beijing

ZhenFund ZhenFund Beijing, China



Seguoia Capital China Beijing, China

Shanghai

WuXi AppTec Shanghai, China



Lilly Asia Ventures Shandhai, China



Shenzhen, China



EASME Brussels, Belgium



SoftBank Vision Fund London, England, The UK



Entrepreneur First C London, England, The UK

	INVESTORS	INVESTMENTS OVERALL	AI FOR DRUG DISCOVERY COMPANIES	INVESTED IN
© CASDIN	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
Υ	Y Combinator	4,619	20	Arpeggio Bio, Athelas, Atomwise, CloudMedx, Coral Genomics, HistoWiz, iLabService, Menten Al, Notable Labs, Ochre Bio, PostEra, Reverie Labs, Segmed, Stratos, Verge Genomics, Nabla Bio, Darmiyan, Synkrino Biotherapeutics, Known Medicine, Gen1E Lifesciences
G/	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 9	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	Perceptive Advisors	223	15	Absci, Alector, Black Diamond Therapeutics, Champions Oncology, DNAnexus, Icosavax, IDEAYA Biosciences, Neuron23, Saama, Sema4, Soma Logic, Relay Therapeutics, Biodesix, Landos Biopharma, Achilles Therapeutics
ALEXANDRIA	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	EASME	3,680	14	Cytox, Optellum, Quibim, OmicX, Genialis, Acellera, Genome Biologics, Iris.ai, CellPly, MedAware, Castor, Mind the Byte, InterAx Biotech Ltd
NSI	National Science Foundation	4,300	13	bioSyntagma, ADM Diagnostics, Strados Labs, Bioz, Cloud Pharmaceuticals, Data2Discovery Inc, TeselaGen, Nabla Bio, VeriSIM Life, Dascena, SpIntellx, VeriSIM Life, Canomiks
MC MAGSCHALLENGE SWIZERLAND	MassChallenge	3,037	12	OrganoTherapeutics, Agamon, Simply Speak, Scailyte, Strados Labs, ChemAlive sA, Vyasa Analytics, Neuroelectrics, Kintsugi, Clemedi, Canomiks, Thermy
khosla ventures	Khosla Ventures	1,062	11	Arpeggio Bio, Atomwise, BIOAGE LABS, Fountain Therapeutics, Deep Genomics, Menten Al, Ochre Bio, Scipher Medicine, ThoughtSpot, Known Medicine, Gen1E Lifesciences

	INVESTORS	INVESTMENTS OVERALL	AI FOR DRUG DISCOVERY COMPANIES	INVESTED IN
INVUS	Invus	180	10	Engine Biosciences, Recursion Pharmaceuticals, Erasca, Schrödinger, Valo Health, Black Diamond Therapeutics, ITeos Therapeutics, Neumora Therapeutics, LifeMine Therapeutics, Achilles Therapeutics
SoftBank	SoftBank Vision Fund	409	10	Biofourmis, Datavant, Deep Genomics, Exscientia, Insitro, PatSnap, Relay Therapeutics, Roivant Sciences, XtalPi, Neuron23
a16z	Andreessen Horowitz	1,322	10	Aria Pharmaceuticals, Asimow, BigHat Biosciences, BIOAGE LABS, Erasca, Flatiron HealthGenesis Therapeutics, Insitro, Freenome, Dyno Therapeutics
ARCH VENTURE FARTNEAS	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	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
<u>©</u>	General Catalyst	1,128	9	Athelas, Beacon Biosignals, PathAl, Spring Discovery, Swoop, ThoughtSpot, Odyssey Therapeutics, OM1, LatchBio
(E) Global Starith Innovation	Merck Global Health Innovation Fund	85	8	PathAl, Strata Oncology, PreciseDx, Antidote.me, Absci, OpGen, Turbine, Verge Genomics
ra capital	RA Capital Management	310	8	Everest Medicines, Freenome, Frontier Medicines, Bristol Myers Squibb, Icosavax, Nimbus Therapeutics, Wave Life Sciences, Achilles Therapeutics
BILLO MEZINEM GALLS //www.inse	Bill & Melinda Gates Foundation	221	8	Atomwise, Evotec, Exscientia, Foundation Medicine, Novartis, Schrödinger, Takeda, Cyclica

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

	INVESTORS	INVESTMENTS OVERALL	AI FOR DRUG DISCOVERY COMPANIES	INVESTED IN
Red mile Group	Redmile Group	150	6	Absci, Neuron23, Foundation Medicine, Wave Life Sciences, Gritstone bio, Achilles Therapeutics
Bio	DCVC Bio	37	5	Empirico, Frontier Medicines, Totus Medicines, Unlearn.AI, X-37
NEA Em	New Enterprise Associates	2,089	5	Aetion, Black Diamond Therapeutics, Champions Oncology, Tempus, Vertex Pharmaceuticals
Tencent #M	Tencent	732	5	Atomwise, Brainomix, iCarbonX, PatSnap, XtalPi
P 6 4 2 2 WILLI AppToc	WuXi AppTec	40	5	Arrakis Therapeutics, Verge Genomics, Schrödinger, Engine Biosciences, WuXi AppTec
novo holdings	Novo Holdings	295	5	Evotec, Exscientia, Kebotix, Tempus, Metagenomi
A MPLITUDE	Amplitude Venture Capital	17	5	Imagia, Celsius Therapeutics, Deep Genomics, Valence Discovery, Gandeeva Therapeutics
BVF	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	Logos Capital	92	5	Freenome, OM1, Engine Biosciences, Alector, Neumora Therapeutics, Dyno Therapeutics

	INVESTORS	INVESTMENTS OVERALL	AI FOR DRUG DISCOVERY COMPANIES	INVESTED IN
FORESITE CAPITAL	Foresite Capital	139	8	Aetion, Alector, DNAnexus, Generate Biomedicines, Insitro, Relay Therapeutics, Wave Life Sciences, Odyssey Therapeutics
GER.	T. Rowe Price	311	8	Arbor Biotechnologies, Generate Biomedicines, Genesis Therapeutics, Insitro, Sema4, SomaLogic, Tempus, Odyssey Therapeutics
OBVIOUS	Obvious Ventures	142	8	ConcertoCare, Inato, LabGenius, Medable, Recursion Pharmaceuticals, Gandeeva Therapeutics, Meliora Therapeutics, Dyno Therapeutics, Achilles Therapeutics
LUX	Lux Capital	424	8	Alife, Auransa, LabGenius, Recursion Pharmaceuticals, Strateos, LatchBio, Gandeeva Therapeutics, Dyno Therapeutics
	Alumni Ventures	1,263	8	Scipher Medicine, Unlearn.Al, Notable Labs, Olaris, Strateos, Veralox Therapeutics, Verge Genomics, Juvena Therapeutics, Emerald Cloud Lab
SECTION 32	Section 32	102	8	Character Biosciences, Nucleai, BigHat Biosciences, Celsius Therapeutics, Verge Genomics, Glympse Bio, Alector, Exai Bio
延移資本	Sequoia Capital China	962	8	HiFiBiO, METiS Therapeutics, PatSnap, XtalPi, Adagene, Deep Intelligent Pharma, Transcenta, Exai Bio
8VC	8VC	396	7	BigHat Biosciences, Coral Genomics, Immunai, Model Medicine, Notable, ProteinQure, Unlearn.Al
SUSV	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 Al





Al 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



evozyne

AstraZeneca obtains a second pulmonary fibrosis target with a partnership with BenevolentAl



Benevolent^A

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
Al driven platform



Generate: Biomedicines

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.





Al 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.



Atomwise SANOFI

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





Cyclica Inc and SK Chemicals announced an Al-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 Al-powered lung cancer diagnosis.





The Al 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. Al platform Pharma.AI will be used to advance drug development candidates for up to six new targets.



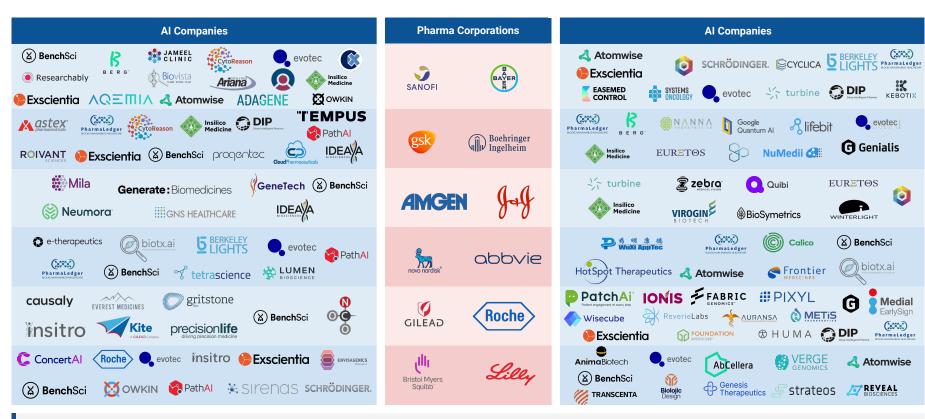


Selected Pharma AI Deals



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



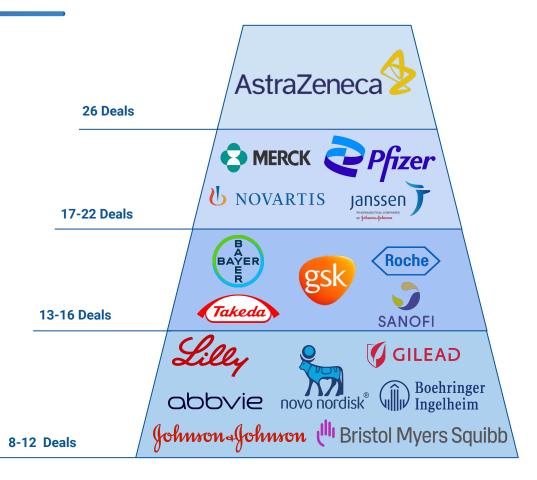
Note: the central column (red) defines the pharmaceutical corporations and side columns (blue) defines AI companies that have collaborations with pharma companies from the central column.

Big Pharmas' Al-focused partnerships till Q4 2022

this report we have profiled 700 actively developing Al-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 Al-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 Al-biotechs, and Al-technology vendors. a continuing pipeline industry of 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.

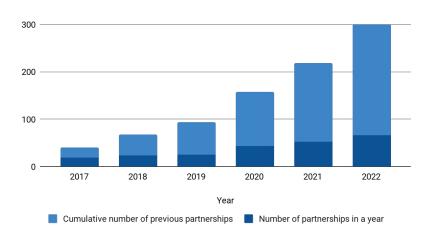
Some of the leading pharma executives increasingly see Al as not only a tool for lead identification, but also a more general tool to boost biology research and identify new biological targets and develop novel disease models.

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 Al Companies over the last 6 years



The rising interest of the big pharma companies towards Al-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.

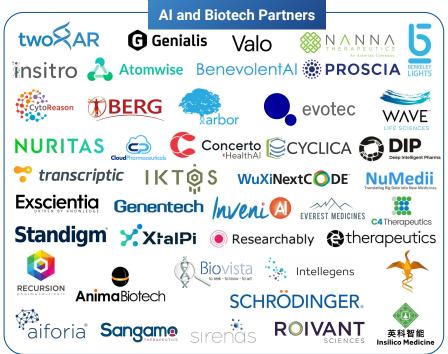
Summarizing industry observations over the last five years, we can observe a fundamental shift in perception of top executives at leading pharmaceutical organizations about the need of advanced AI technologies. Since 2017, there has been an obvious shift in the perception from skepticism and cuasious interest, all the way to a realization of a strategic role AI has to play in the emerging "data-centric" model of innovation. This change in perception was underpinned by a number of factors:

- a wave of proof-of-concept studies and research breakthroughs in a wide range of Al 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 Al-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 Al-drug design, and other aspects of data mining and analytics.

Corporation and Al-companies Participating in the Pharma Al Deals































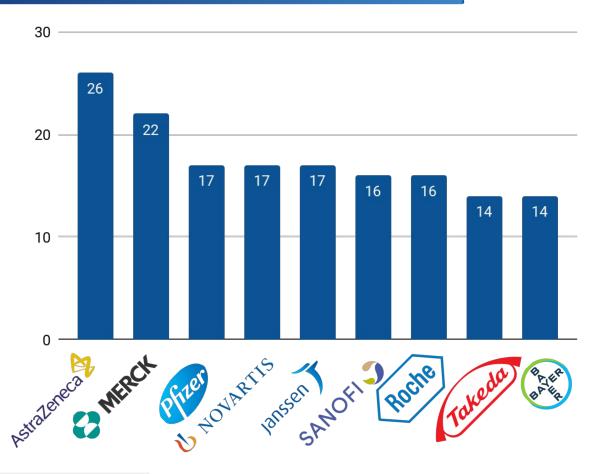








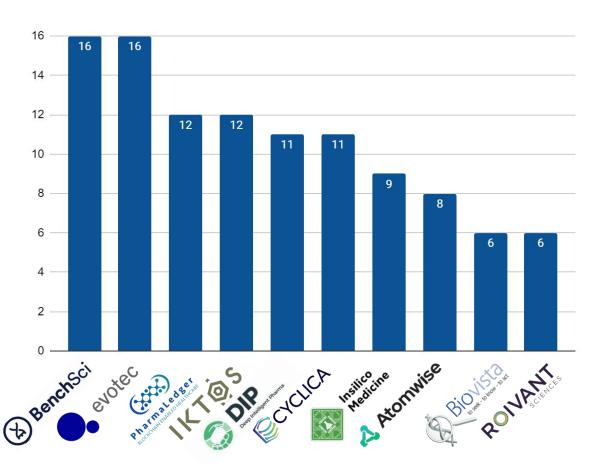
Leading Pharma Corporations by the Number of Pharma AI Deals in 2022



- 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 Al and Tech Partners by Number of Major Pharma Al Deals in 2022



- The leading Al 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, Al-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 Al development. During 2021, we have observed over 150 medium and large funding rounds for Al in Drug Development companies with an average investment of \$64.7M. In 2022, the interest in Al in drug development appeared to reach a plateau. In 2022, there were over 70 investments in Al 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.

Al in Pharma Publicly Traded Companies





AI in Pharma Publicly Traded Companies

Cumulative Capitalization of Publicly Traded Al-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.

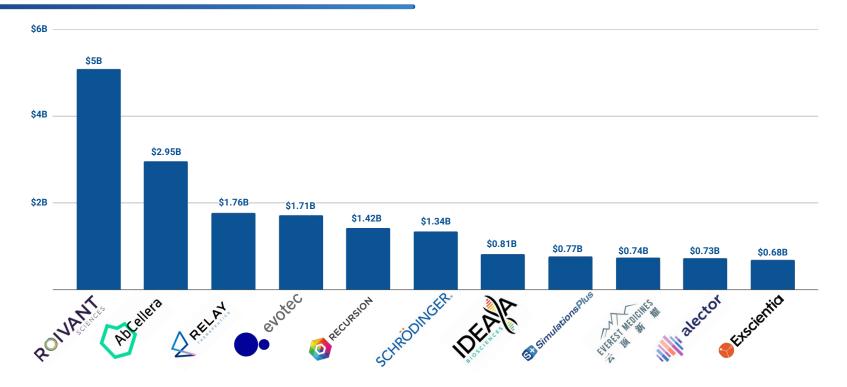
The largest companies by market capitalization are **Roivant Sciences**, **AbCellera and Relay Therapeutics**. The smallest market capitalization are in **Landos Biopharma**, **Evolutionary Genomics** and **OpGen Inc**.

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%.

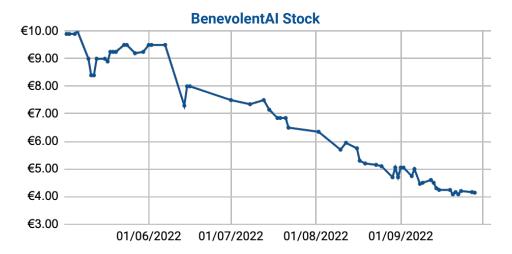
Top-10 Al-Driven Publicly Traded Pharma Companies by Market Capitalization in 2022



The chart presents the **Top-10 Al-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.

Al in Pharma IPOs in 2022

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



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

Benevolent's PlatformTM is a powerful computational R&D platform. Scientists may query the data and disease networks inside the graph using Benevolent's range of exploratory and predictive Al 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 BenevolentAl 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 Pharmaceutica	ls USA	208.5	17.07.2020	1.515	1355.2	19.00	10,87	-4.55X	-211.74
Relay Therapeu	ics USA	520.0	16.07.2020	2.06	1736	20.00	22,32	-3.26X	-183,734

Al 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%		-5.42%	0.1792	0.0905	\$1.1M	\$132.2M	-56.73%	0.01X
BenevolentAl	\$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		\$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	-\$1,810.2 M	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 Al-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 Al-driven pharma market segment is more volatile.

The distribution of the returns in the segment of Al-driven pharma companies is right-skewed, which differentiates it from the vast majority of stock indices and segments

Large
Medium
Low

Al 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%		-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%		0.1194	\$120.8M	-\$152.5M	-16.44%	-0.79X
Recursion Pharmaceuti- cals	\$1,765.1M	-0.17%	5.78%	-5.41%	0.1663		\$1,074.8M	-\$236.1M	-587.95%	-4.55X
Relay Therapeutics	\$1,765.1M	-0.16%		-3.11%	0.2032	0.0947	\$944.4M	-\$289.5M	-3102.77%	-3.26X
Renalytix Al	\$65.5M	-0.62%	6.69%		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		\$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.

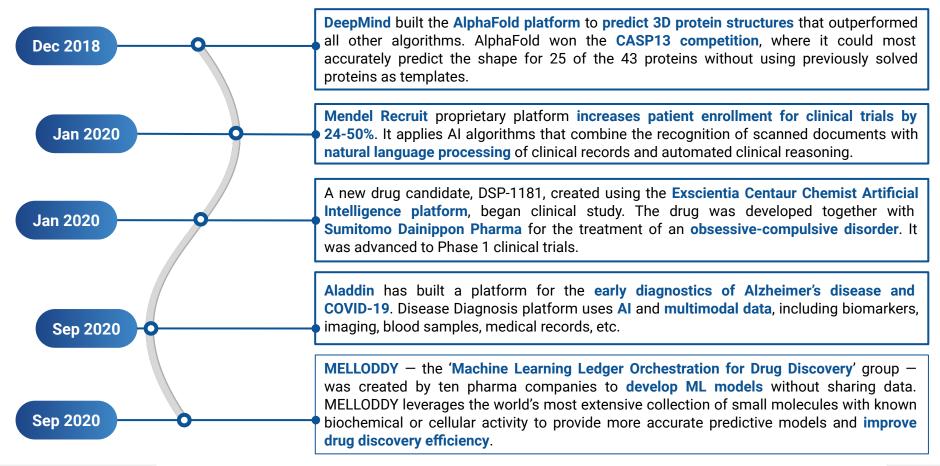
Selling shares to investors allows them to maintain their cash burn ratios on an acceptable levels.

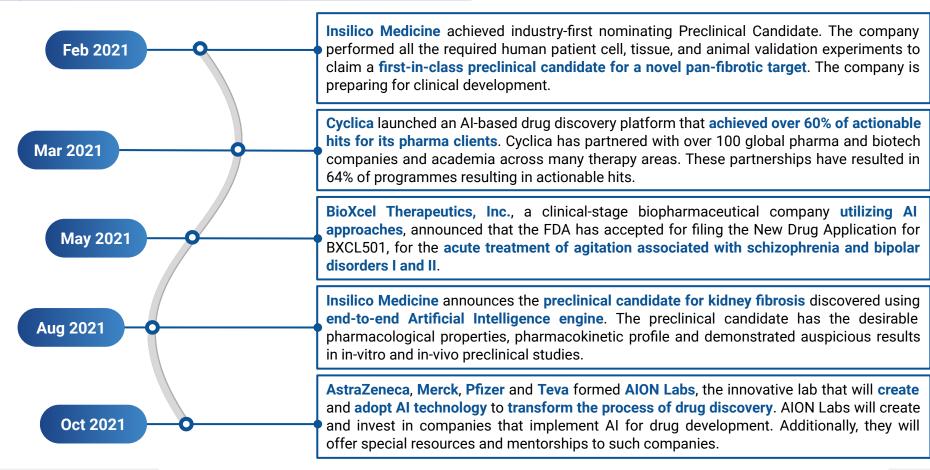
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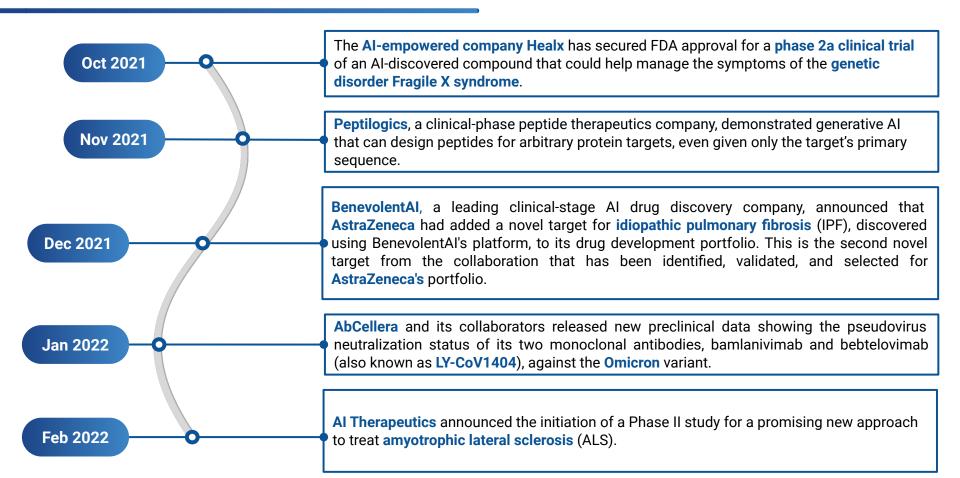
Al for Advanced R&D: Applications and Use Cases

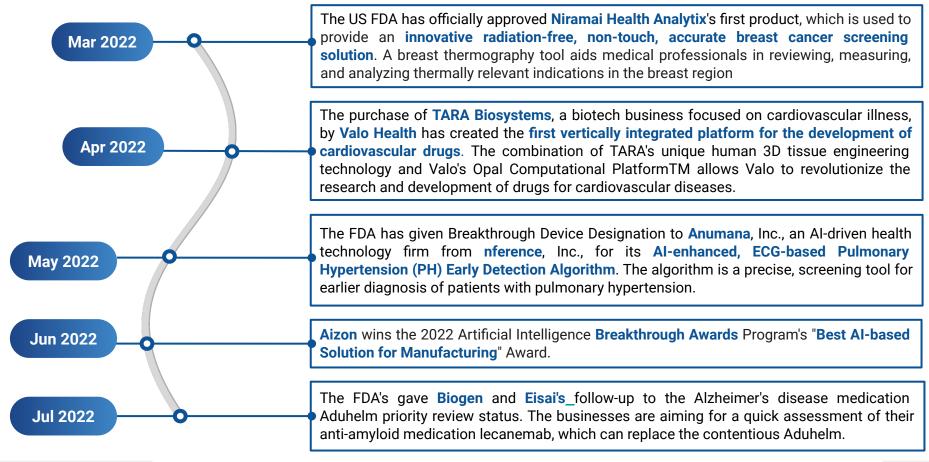


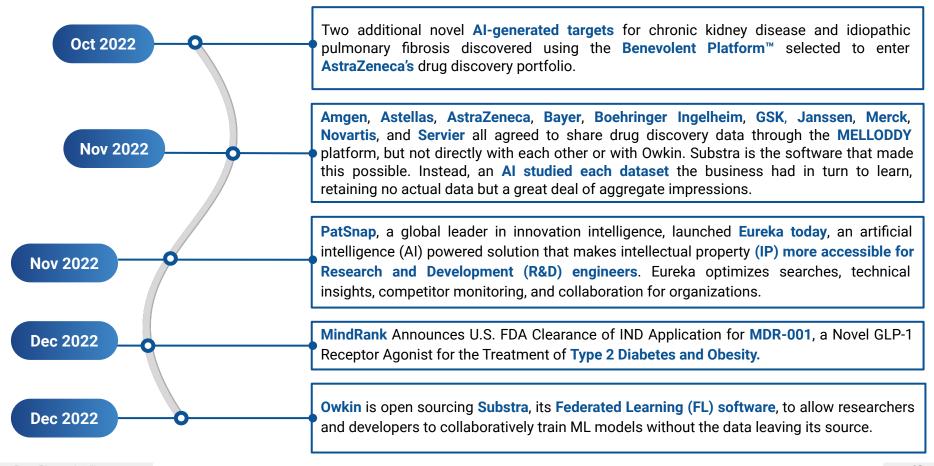






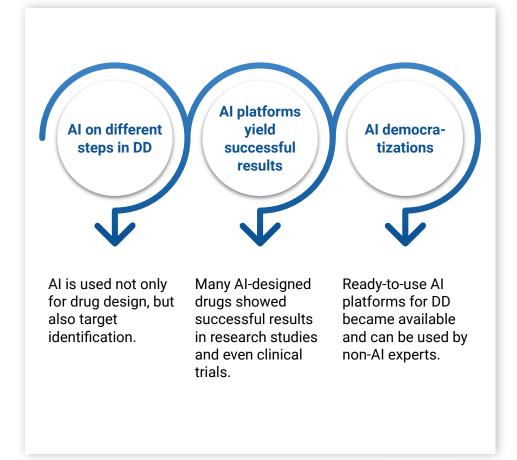






Key Technology Takeaways

- Al 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 Al in drug discovery, alongside with data mining from unstructured data, like text (using natural language processing, NLP).
- 2. There is a considerable trend for "Al 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 Al-pipeline building platforms (for example, KNIME). This is among key factors in the acceleration of Al adoption by the pharmaceutical organizations where a non-Al 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 Al-based drug design platforms.



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:** All 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.

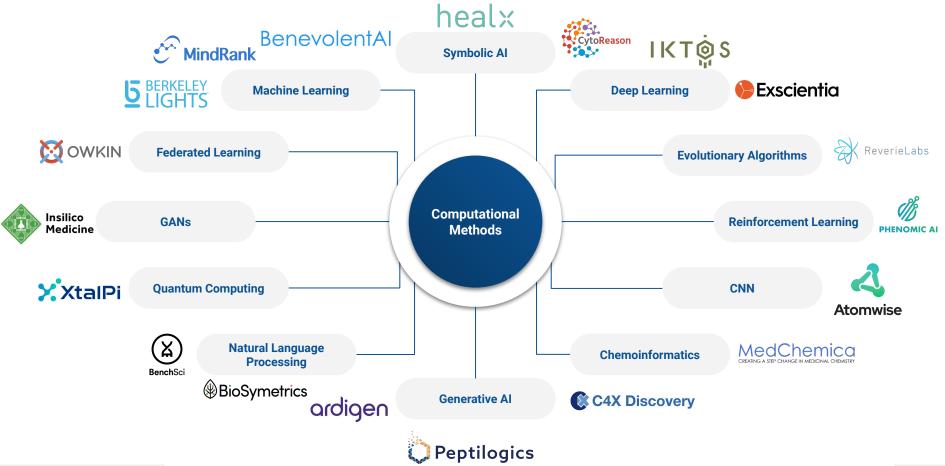


Computational Methods Used by the Most Advanced Al Companies





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.
BenevolentAl	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 Al platform uses natural language processing to extract disease knowledge from published sources and to complement biomedical databases and proprietary, curated data.
IKTĠS	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 Al Application in Biopharma

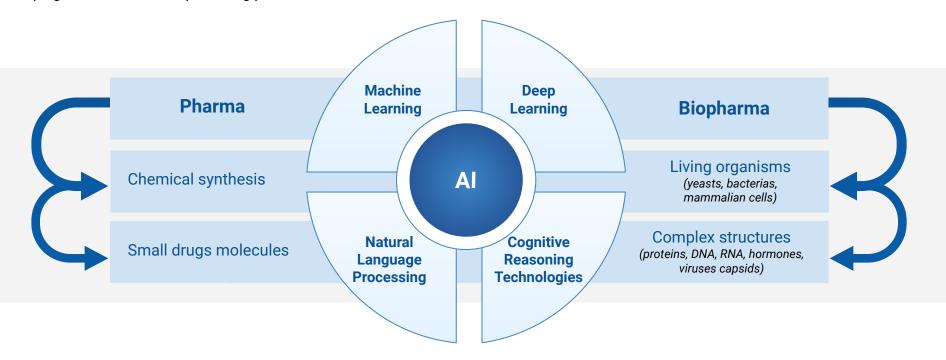






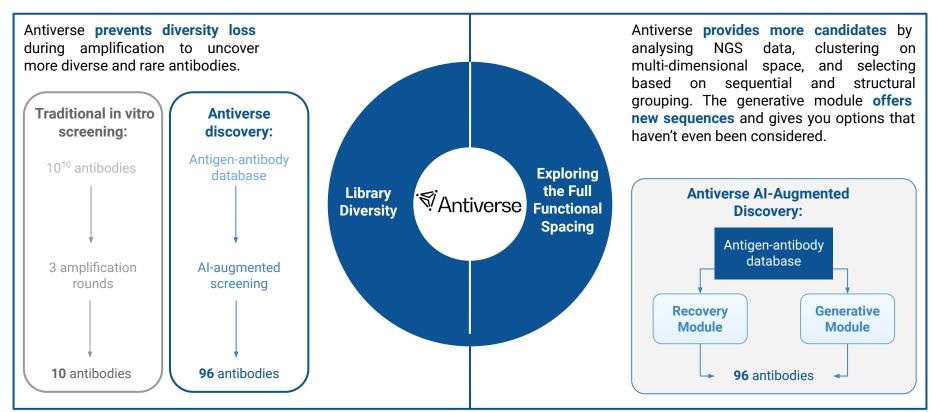
Introduction to Most Innovative R&D Approaches of AI in Biopharma

Biopharma utilizes living organisms (such as yeasts, bacterias, and mammalian cells) which are capable to produce complexly structured products such as proteins, hormones, RNA and DNA products, and virus capsids. Whereas Pharma relies on a classical chemical synthesis producing small drug molecules. However, both industries may benefit from Al-driven applications. To develop new small drug molecules or biologically-derived products, Al-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.



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 Al-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 **Al-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.



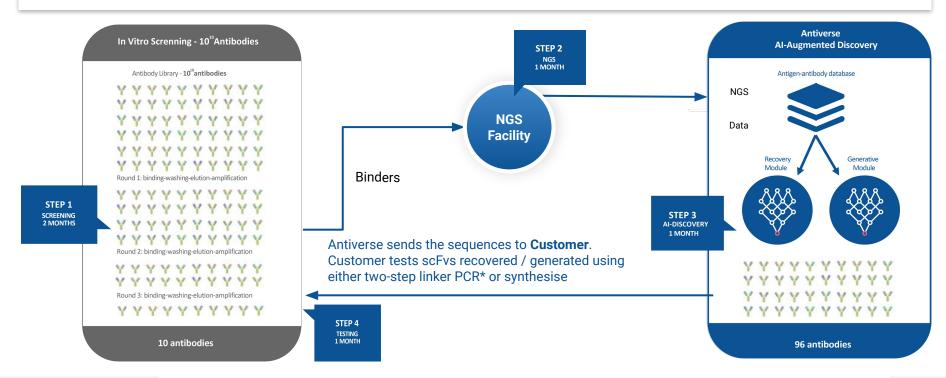
Binder Customisation

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

How Antiverse Uses AI in R&D

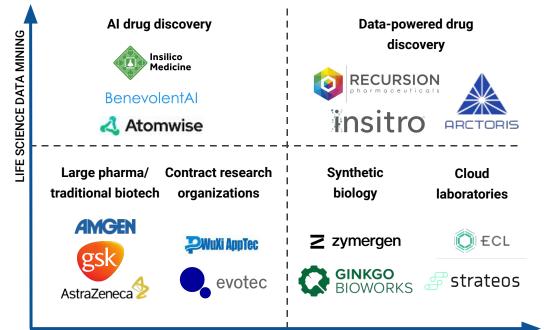


The **Antiverse Al-ADD** system found each and every cluster identified by other methods, plus more. These additional clusters contained rare and unique sequences.



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**.

LIFE SCIENCE AUTOMATION

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

The greatest challenge in Al-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.

Target

Validation

- Analysis of target expression and target half-live by quantifying protein turnover and route to degradation
- Investigation of target function (changes in phenotype, pathways, gene expression, etc.) via cell-based and molecular biology readouts
- Advanced insights into effects of target modulation by employing complex model systems such as organoids, primary cells, etc.
- Pharmacokinetics and pharmacodynamics (PK/ PD) & safety pharmacology
- In-depth pharmacokinetics, including ADME, drug-drug interactions, metabolite profiling, concentration time profiles
- Comprehensive acute toxicology assessment, incl. single dose and repeated dose to determine MTD and NOAEL
- Additional toxicology studies (e.g. reproductive and developmental toxicity, etc.)

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



Hit finding &

Hit-to-Lead

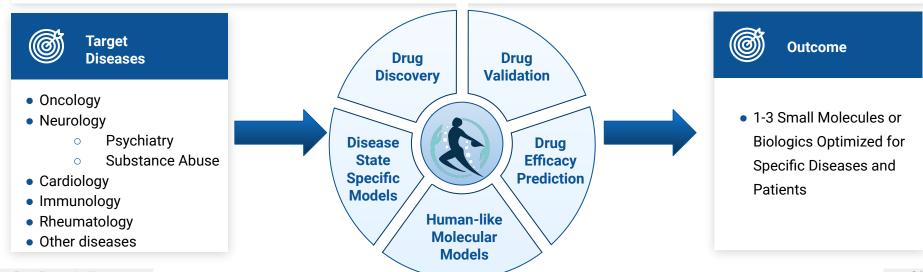
- Rapid biochemical profiling, kinetics, selectivity, mechanism of action
- Isolated and in-cell target engagement
 - Cellular mode of action, elucidation of pathway modulation, confirmation of on-target/ off-target effect
- Medicinal and synthetic chemistry (optimizing SAR, SPR, STR)
- Integration of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

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



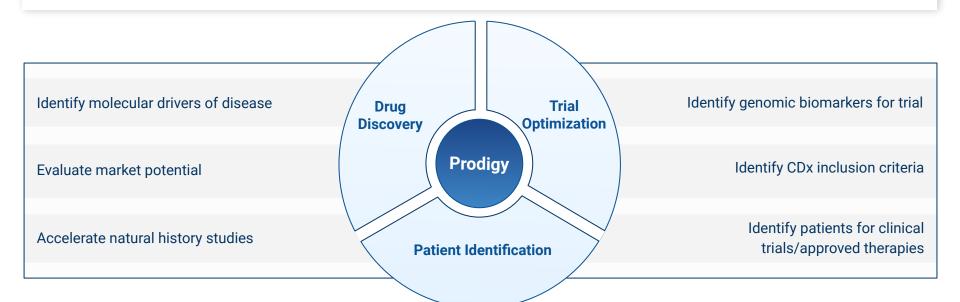
Most Innovative R&D Approaches of AI in Biopharma. Genomenon



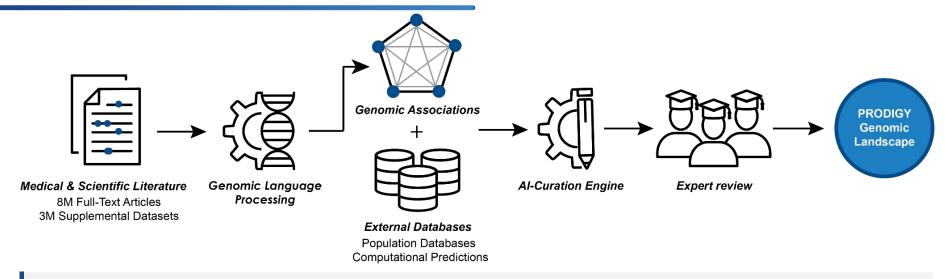
Genomenon is an Al-driven genomics company that organizes the world's genomic knowledge to accelerate the diagnosis and development of treatments for genetic disease.

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 **Al-assisted curation engine** that expedites manual review of the data indexed by GLP.

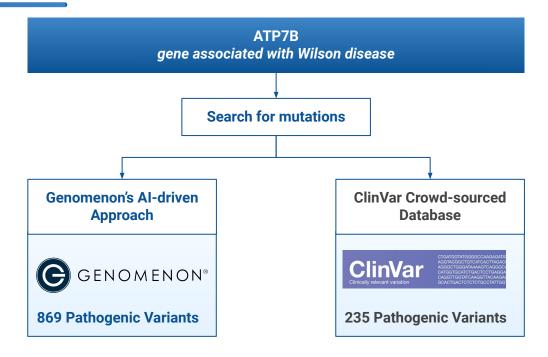
Genomic Language Processing (GLP) is a novel technology that systematically extracts and standardizes **genomic and clinical information** from the medical and scientific literature. Designed specifically to recognize this complex genomic information, GLP provides superior sensitivity compared to traditional 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 Al technology to help accelerate the genetic diagnosis for rare disease patients. Genomenon's novel combination of Al-powered Genomic Language Processing and expert review identified significantly more pathogenic variants associated with Wilson disease.

Genomenon's Al-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 Al-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 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 molecule 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.

MindRank Al



Molecule Pro

Molecule design and generation platform



Molecule Dance

Molecular dynamics platform



PharmKG

Biomedical knowledge graph to assist drug discovery



Faster Development

Reduced Costs

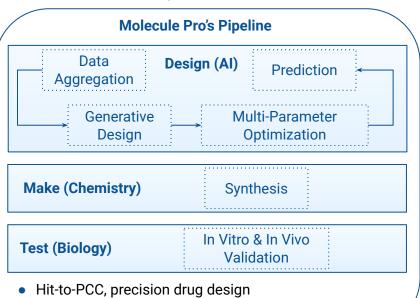
More Likely to Succeed

Treating Various
Disease

- Pipeline with 17 drugs (4 wholly-owned, 2 designed as service, and 11 co-developed)
- MDR-001 for Obesity and Type 2
 Diabetes is expected to start
 Phase 1 clinical trials in early
 2023
- EMRANK-016 for Oncology has been successfully PPC-delivered for publicly traded biopharma

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

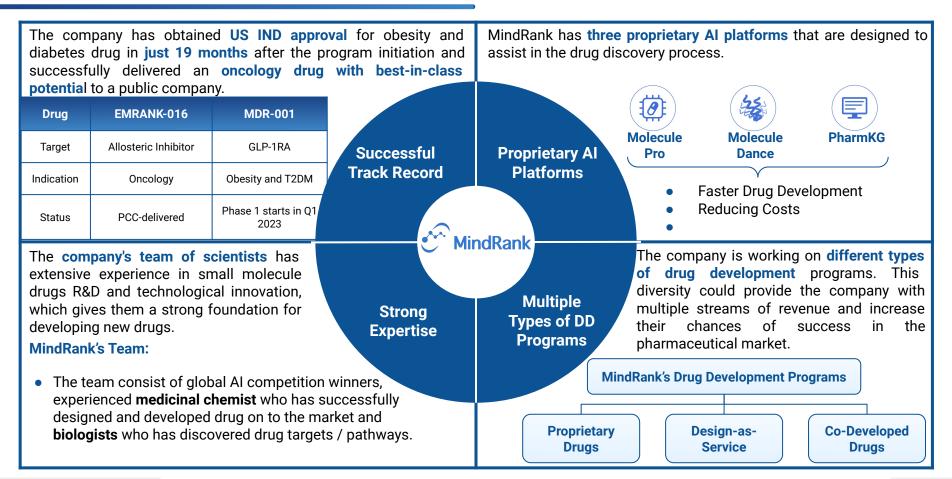
Lead Optimization

Multi-objective optimization

Preclinical

IND-enabling

Key Advantages of MindRank Al



How ONCOCROSS Utilizes AI and Transcriptomics for Drug Development

ONCOCROSS

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

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

Traditional Approach **Gene Expression Pattern Approach Gene Expression Pattern Analysis** Instead of analyzing single target, single pathway, with single hypothesis, they analyse entire set of gene expression pattern **Medically Curated Database** They have unrivalled quality transcriptome database that is **Patients** Chemicals **Cancer Prognosis Disease Type Cancer Types** curated by medical doctors and pharmacists at Oncocross 100.000+ 25,000+ 74.000+ 410+ 42+

Pharmacophysiological & Pathophysiological Evidence Guided Drug-Disease Pairing

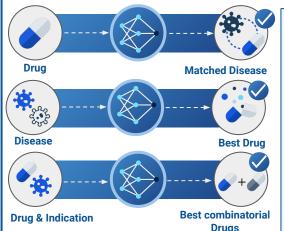
Al Platform performs comparative analysis at transcriptome levels of cells and human biopsy and blood samples



How ONCOCROSS Utilizes AI and Transcriptomics for Drug Development

RAPTOR AI™ (RNA expression-based Anti-symmetrical Pairing Tool for On-demand Response AI) is transcriptome-based disease and drug-screening platform.

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



RAPTOR AI™ solution

Indication Expansion

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

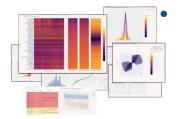
Rescue Drug

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

Combination

predict a partnering drug that can improve the efficacy

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



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

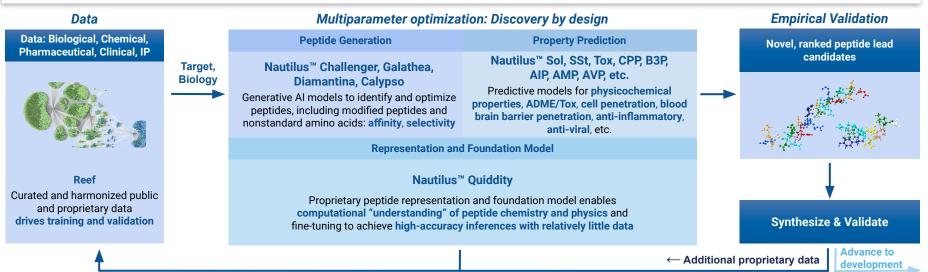
- Scoring anti-symmetricity with integrating various cell line-based experimental results via cell-tissue similarity. Cell-tissue similarity-based integration method is necessary for accurate prediction, as drug effect data are derived by cell line, and disease effect data are from human tissue.
- The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



Learning and improvement

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

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

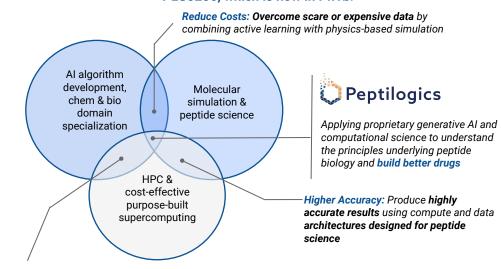


Peptides offer advantages over small molecules and biologics. Relative to small molecules, peptides can achieve higher selectivity and safety. Relative to biologics, peptides can more easily reach intracellular targets and cross the blood-brain barrier, and they can be manufactured at reasonable cost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

Advantages of Nautilus™

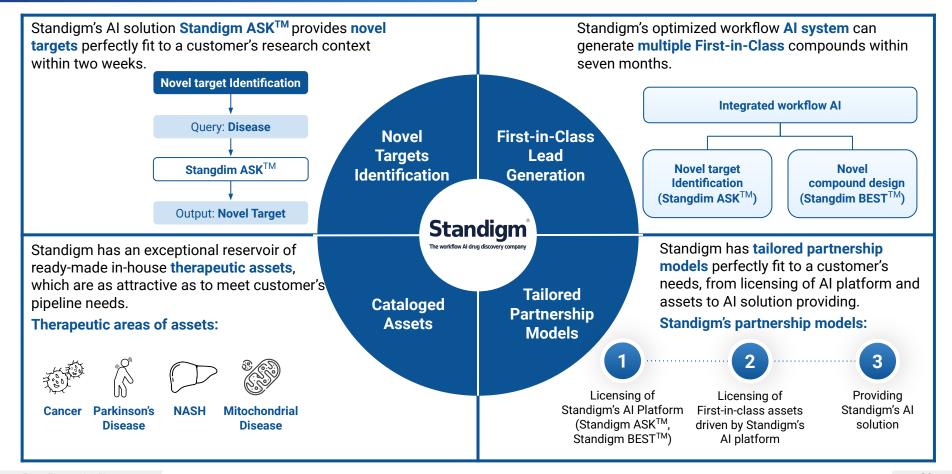
- Go beyond just identifying binding hits: encode an expanding list of pharmaceutical properties from the outset
- Target-agnostic, therapeutic area-agnostic models that can be applied to both established and novel targets
- Access diverse chemical space through proprietary algorithms and in-house, purpose-built 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.



Faster Results: Maximize model accuracy and drive rapid hypothesis testing by accelerating training

How Standigm Accelerates Drug Discovery using Al



How Standigm Accelerates Drug Discovery using Al

Standigm[®]

Standigm is a workflow Al-driven drug discovery company headquartered in Seoul, South Korea and subsidiarized in Cambridge, UK. Standigm has proprietary Al platforms encompassing novel **target identification to compound design**, to generate commercially valuable drug pipelines. The company has established an early-stage drug discovery workflow Al 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 Al technology. One of the company's pipelines is expected to enter a pre-clinical stage in 4Q 2021.

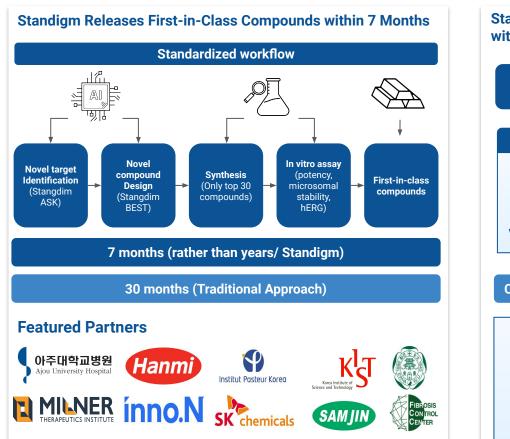
Standigm BESTTM is a novel **compound generation platform**, which can investigate lead compounds whenever target or ligand information is lacking or enough.

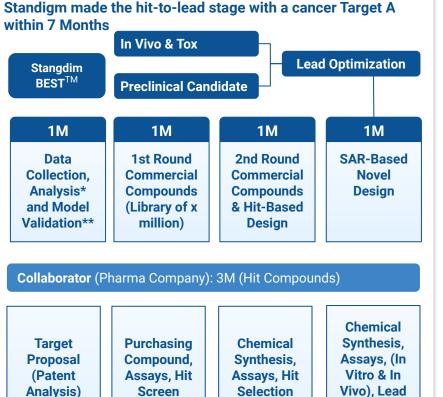
Database	Hit ID	Hit to Lead	Lead Optimization
Deep learning chemical space	Securing activity	Securing novelty	Druggability optimization
150-dimensional vector space which learned various compound properties	Accurate prediction of binding	New scaffold with various structures	Mainly-based substructural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

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

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

How Standigm Accelerates Drug Discovery using Al

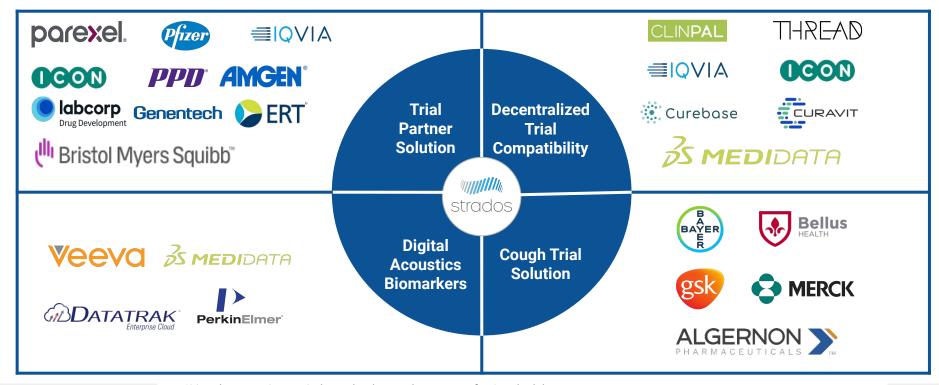




Selection

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

How Strados Labs Uses AI in R&D?

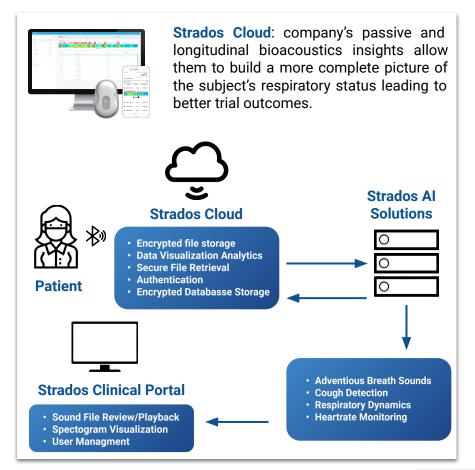


The Strados Respiratory Management Solution is the world's first FDA-cleared lung sound platform with a proprietary wireless biosensor, RESP, that is passive, patient-friendly, and clinically validated to acquire lung sounds in the real world.

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.



Industry Developments Q1 2021- Q4 2022





Biggest Deals 2022

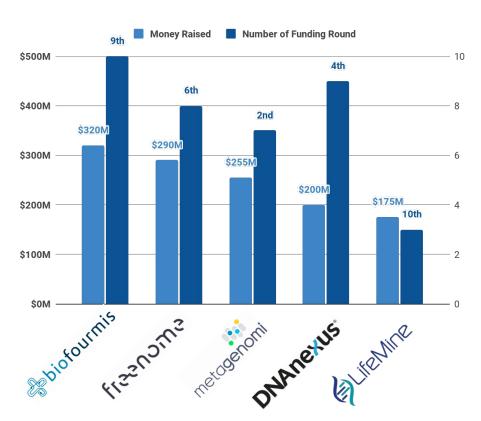
The total amount of VC funding in AI in drug development companies reached to \$26.5B in Q4 2022.

There is an increasing number of late-stage mega-rounds including hundreds of millions. The apparent trend is sector consolidation, where a number of Al-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 Al technology, making Al 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. Freenome 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



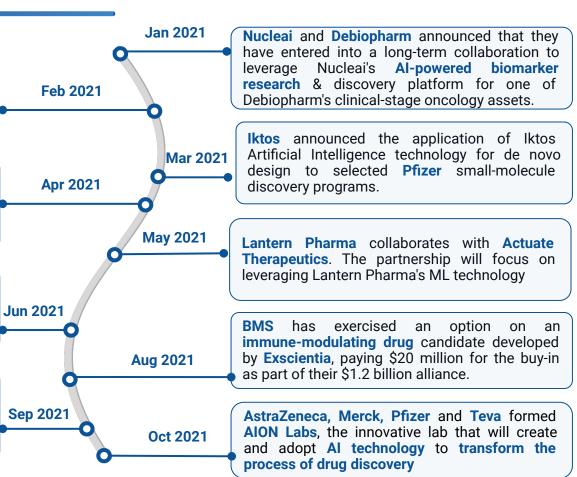
Selected Pharma AI Industry Developments 2022

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

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

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

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



Selected Pharma AI Industry Developments 2022

BenevolentAl announced that **AstraZeneca** had added a novel target for idiopathic pulmonary fibrosis (IPF), discovered using BenevolentAl's platform, to its drug development portfolio.

Oncocross announced that it initiated a phase I global clinical trial for 'OC514' targeting muscular diseases including sarcopenia

Using gene expression profiles of pharmacological and genetic perturbations, **Auransa** leveraged their **Al-driven platform to elucidate host cell response networks** to repurpose treatments for SARS-CoV-2 and other coronaviruses.

Amgen and Generate Biomedicines will develop protein therapies for five clinical targets. The Generate Biomedicines platform can quickly produce antibodies, peptides, cell and gene treatments to possibly satisfy a wide range of therapeutic demand.

Dec 2021

Insilico Medicine, an end-to-end artificial intelligence (AI)-driven drug discovery company, announced that the first healthy volunteer has been dosed in a first-in-human microdose trial of ISM001-055.

Sanofi has sealed a €4.6B deal with Exscientia to develop oncology and immunology treatments.

Exscientia and the University of Oxford Target Discovery Institute announced the formation of Xcellomics – a program to develop novel screens and identify targets and therapeutic candidates for unmet medical needs.

The treatment of COVID-19 in hospitalized individuals has received FDA approval for baricitinib, initially identified as viable therapy by **BenevolentAl's original Al-derived hypothesis.**

Merck & Co., Johnson & Johnson, and Sanofi are looking at how artificial intelligence (AI) may speed up the drug discovery process.

Deep Pharma Intelligence

Apr 2022

Jun 2022

Mar 2022

May 2022

Jul 2022

Selected Pharma AI Industry Developments 2022

Breast cancer patients and colorectal cancer patients throughout the EU can now utilize two of Owkin's Al models (to assess the outcome after treatment and predict are state of tumor).

BioMed X announced it has signed a research collaboration with Sanofi to develop an artificial intelligence (AI) computational platform to predict the efficacy of first-in-class drugs using virtual patient populations.

Visionable and Brainomix have announced a strategic partnership that aims to transform stroke care delivery.

The Envisagenics' SpliceCore® Al platform to identify alternative splicing derived targets for therapeutic development to expand Bristol Myers Squibb's vast oncology pipeline.

Nearly all proteins that are currently known to science have had their structures correctly predicted by DeepMind's AlphaFold platform. The database of more than 200 million proteins is available to everyone for free from the Alphabet-owned AI lab.

Illumina signed up for a new collaboration with AstraZeneca with the goal of aligning their artificial intelligence development efforts in a way that combines genomic analysis and drug discovery research.

XtalPi. Inc. announced a research collaboration with Janssen Pharmaceutica to deliver chemical matter with validated binding affinities and desirable property profiles.

BigHat Biosciences has announced a collaboration with Merck to apply its technology to design candidates for up to three drug discovery programs.

Experimental Drug Development Centre to discover novel treatment candidates for non-small cell lung cancer.

multi-year collaboration will leverage **XtalPi** announced a strategic collaboration with the Nov 2022 **Dec 2022**

Sep 2022

Oct 2022

Nov 2022

Aug 2022

Oct 2022

Oct 2022

Nov 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 Al development. During 2021, we have observed over 150 medium and large funding rounds for Al in Drug Development companies with an average investment of \$64.7M. In 2022, the interest in Al in drug development appeared to reach a plateau. In 2022, there were over 70 investments in Al 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.



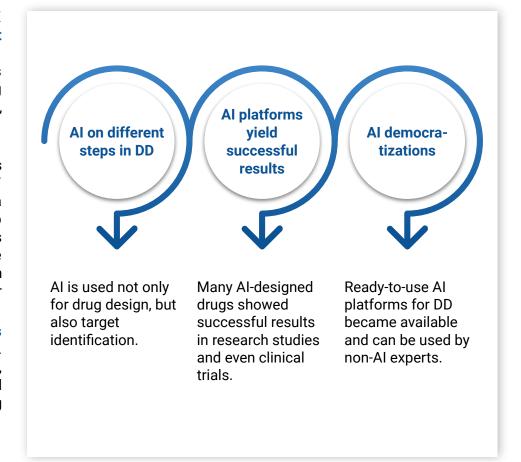
When some of the companies complete IPOs in the nearest future, it will attract a **significant number of non-biotech investors to enter the Life Sciences sector**. The prospects of this trend are already vivid: big tech companies enter partnerships with both innovative start-ups and pharma companies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

- Al 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 Al in drug discovery, alongside with data mining from unstructured data, like text (using natural language processing, NLP).
- 2. There is a considerable trend for "Al 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 Al-pipeline building platforms (for example, KNIME). This is among key factors in the acceleration of Al adoption by the pharmaceutical organizations where a non-Al 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 Al-based drug design platforms.



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:** All 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.
- 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.



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

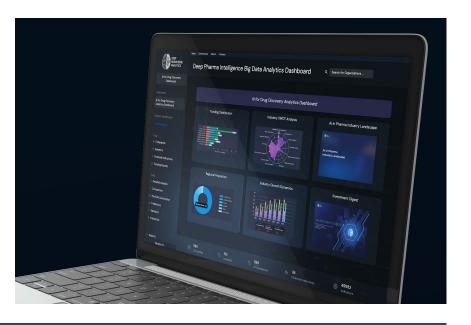
DPI provides a **full-cycle development of articles, scientific journals, and books**. We are ready to develop a detailed Requirement Specifications document, including layout of the journal, fully designed brand book, with example templates for each chapter.



Al in Drug Discovery Analytical Dashboard

Al 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.

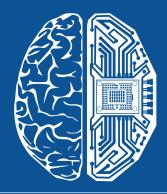
Market Research

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

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