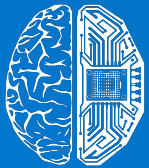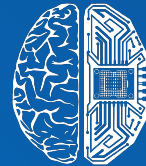# Artificial Intelligence for Drug Discovery 2023

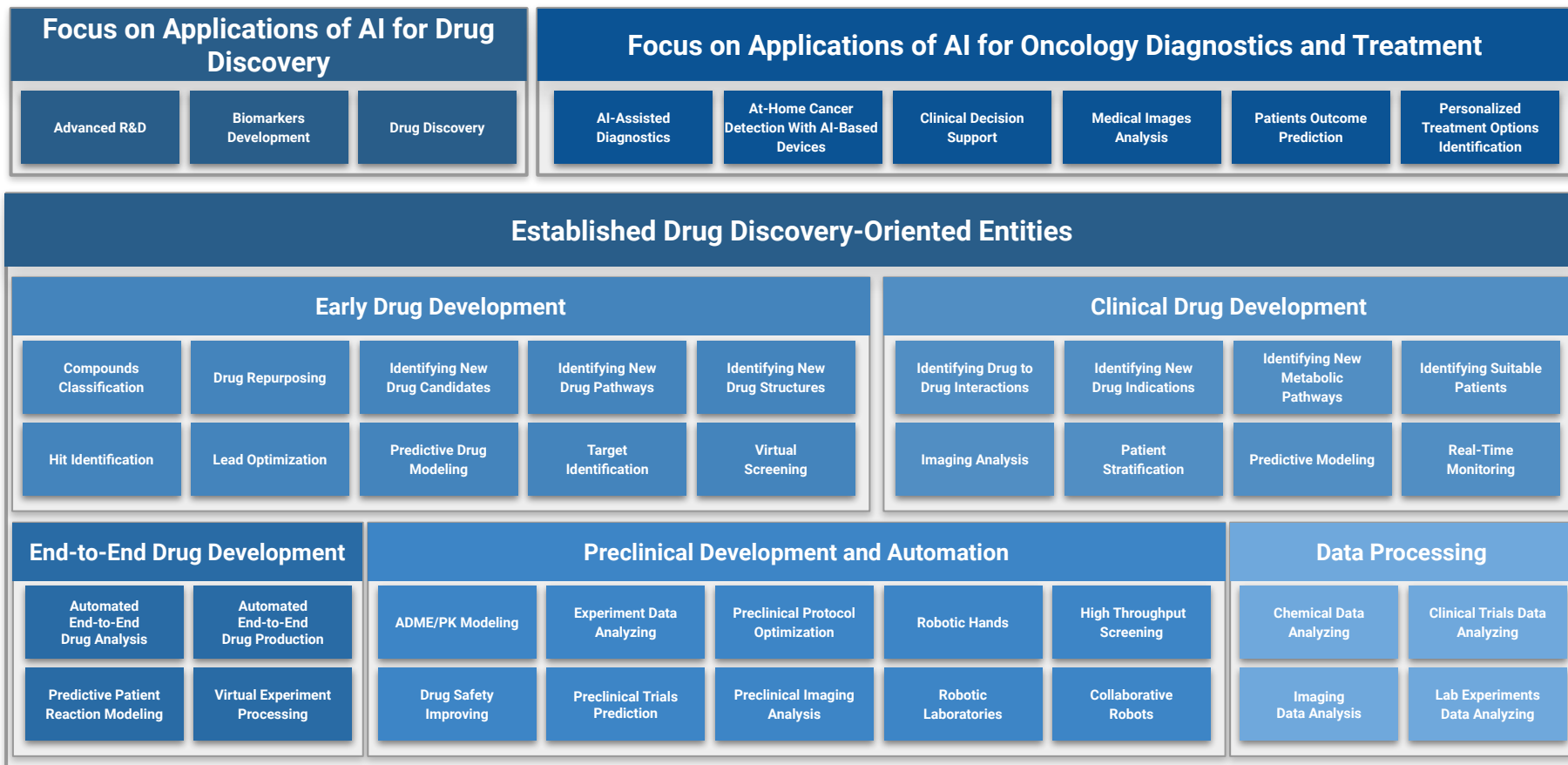## *Teaser*

Deep Pharma Intelligence

Deep Knowledge Group

Artificial Intelligence in Drug Discovery Analytical Framework

Focus on Applications of AI for Drug Discovery

Advanced R&D	Biomarkers Development	Drug Discovery

Focus on Applications of AI for Oncology Diagnostics and Treatment

AI-Assisted Diagnostics	At-Home Cancer Detection With AI-Based Devices	Clinical Decision Support	Medical Images Analysis	Patients Outcome Prediction	Personalized Treatment Options Identification

Established Drug Discovery-Oriented Entities

Early Drug Development

Compounds Classification	Drug Repurposing	Identifying New Drug Candidates	Identifying New Drug Pathways	Identifying New Drug Structures
Hit Identification	Lead Optimization	Predictive Drug Modeling	Target Identification	Virtual Screening

Clinical Drug Development

Identifying Drug to Drug Interactions	Identifying New Drug Indications	Identifying New Metabolic Pathways	Identifying Suitable Patients
Imaging Analysis	Patient Stratification	Predictive Modeling	Real-Time Monitoring

End-to-End Drug Development

Automated End-to-End Drug Analysis	Automated End-to-End Drug Production
Predictive Patient Reaction Modeling	Virtual Experiment Processing

Preclinical Development and Automation

ADME/PK Modeling	Experiment Data Analyzing	Preclinical Protocol Optimization	Robotic Hands	High Throughput Screening
Drug Safety Improving	Preclinical Trials Prediction	Preclinical Imaging Analysis	Robotic Laboratories	Collaborative Robots

Data Processing

Chemical Data Analyzing	Clinical Trials Data Analyzing
Imaging Data Analysis	Lab Experiments Data Analyzing

Pharma Efficiency: Challenges

Stage	Count
Drug discovery	5,000,000 compounds
Pre-clinical development	500 compounds
Clinical development	5
Regulatory approval	FDA
Result	1 approved drug

0 - Effect on body
I - Safety in humans
II - Effectiveness at treating diseases
III - Larger scale safety and effectiveness
IV - Long term safety

10 years + $2.6 bln = 1 new drug

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

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

The solution to this problem comes from three key strategies:
- evolution of business models towards more collaboration and pipeline diversification early
- **implementation of AI as a universal shift towards data-centric drug discovery**
- discovery of new therapeutic modalities (biologics, therapies, etc.)

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

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

AI for Advanced R&D

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

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

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

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

Notable Breakthroughs in AI for Pharma

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

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

2019

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

2020

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.

2021
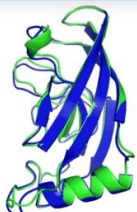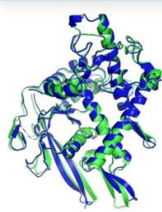
■ Experimental Result
■ Computational Prediction
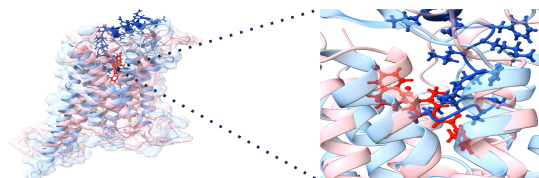
Dynamics of Investments in AI in Drug Development

AI in Drug Development Investments Dynamics

Legend:
- Investments per Year
- Cumulative Investments

Bar chart values by year:
- 2012: $0.33B
- 2013: $0.74B
- 2014: $1.4B
- 2015: $2.2B
- 2016: $5.6B
- 2017: $9.6B
- 2018: $14B
- 2019: $24.7B
- 2020: $31.4B
- 2021: $45.1B
- 2022: $59.3B
- 2023: $60.2B

X-axis: Year
Y-axis: $0.00B, $20.00B, $40.00B, $60.00B, $80.00B
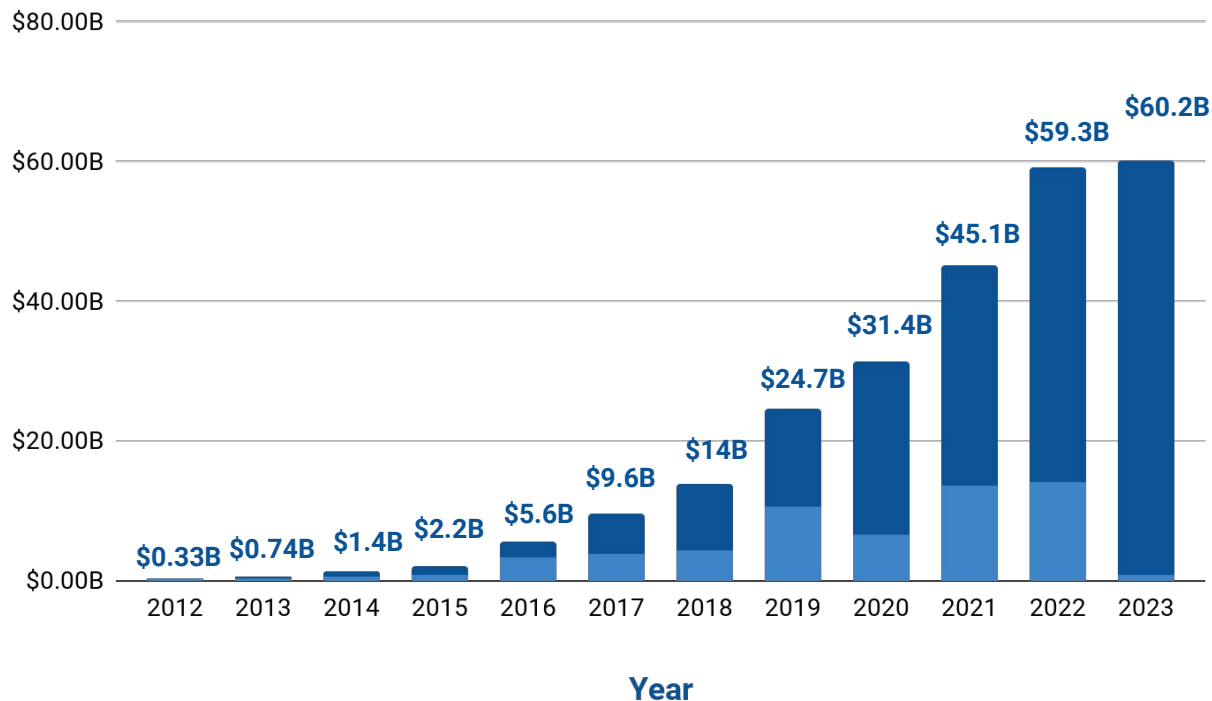
There has been a substantial increase in the amount of capital invested in AI-driven pharma companies **since 2015.** During the last 9 years, the annual amount of investments in **800** companies has increased **27 times** (to **$59.3B** in total as of December 2022). The most rapid growth was in 2021, when the year investment in the AI in Drug Development companies was $13.68B. 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 did not have these high growing increase in several times as in previous years ($14.18B in 2022 compared to $13.68B in 2021). On the March 2023, the total investments in AI in Drug Development companies are **$60.2B.**

Artificial Intelligence in Drug Discovery 2023

AI Companies - 950
Investors - 1,900
Corporations - 100

Drug Repurposing

Preclinical Development

End-to-end Drug Development

Clinical Development

AI Companies

Investors

Corporations

Pharma

Tech

CRO

Data Processing

Early Drug Development

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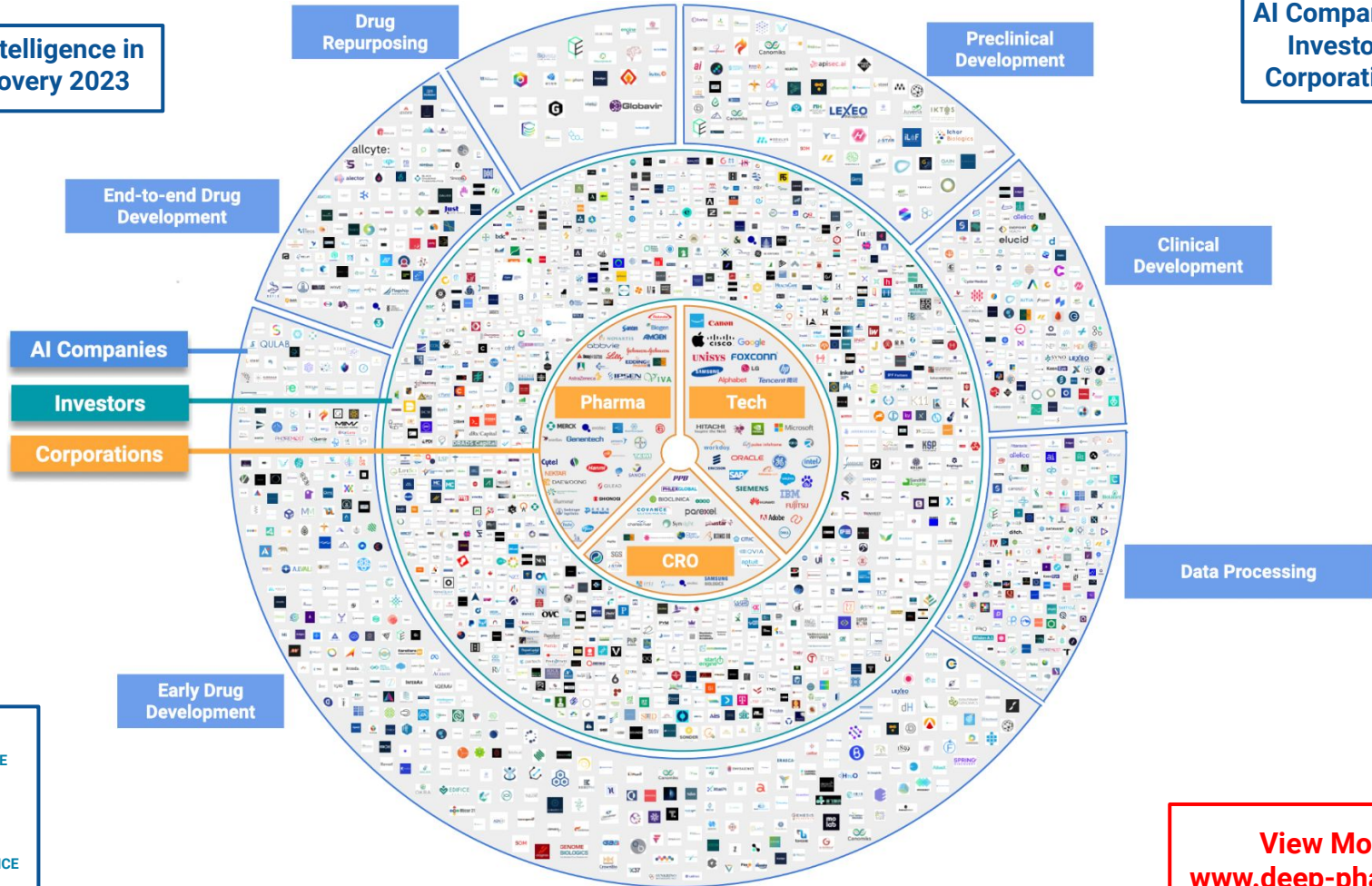
View More at www.deep-pharma.tech

900 AI Companies: Regional Proportion

Canada
4.6%

UK
10.0%

EU
17.1%

China
3.6%

US
53.3%

Middle East
2.5%

Australia
0.6%
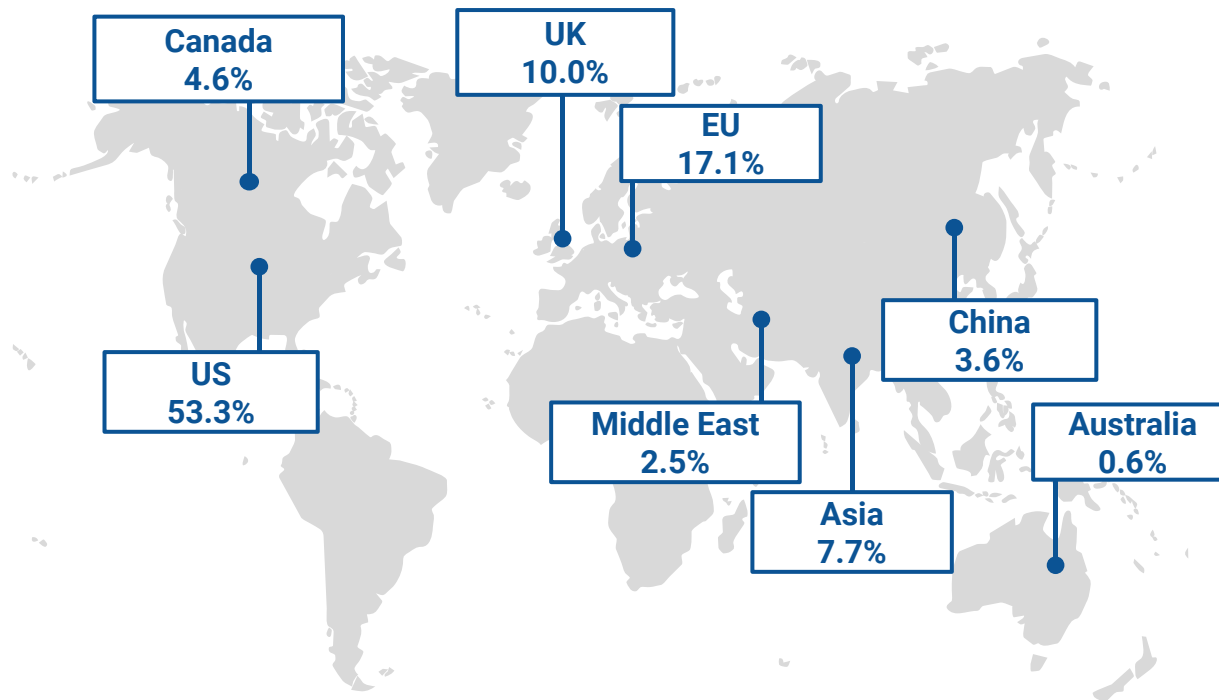
Asia
7.7%

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.

Comparison of Top-50 Leading AI for Drug Discovery Companies Expertise in Drug Discovery R&D

Expertise in Drug Discovery (vertical axis)

- Clinical pipeline (phase 1-2)
- Validated R&D Use cases and preclinical pipeline

Expertise in AI (horizontal axis)

- Advanced AI tools for specific Use Cases
- Advanced AI systems with multiple models
- End-to-end AI

Companies (clinical pipeline, advanced AI tools): bioxcel therapeutics, freenome, C4X Discovery Better, Safer, Faster, PHARNEXT, PathAI

Companies (clinical pipeline, advanced AI systems): MindRank, nimbus THERAPEUTICS, BERKELEY LIGHTS, Delta4, healx, ConcertAI, turbine, BIOAGE labs, XtalPi, Schrödinger, AURANSA

Companies (clinical pipeline, end-to-end AI): RECURSION pharmaceuticals, Neumora, BERG, Valo, Insilico Medicine 英科智能, ardigen, BenevolentAI, Exscientia DRIVEN BY KNOWLEDGE

Companies (validated R&D, advanced AI tools): GENOMENON, AbCellera, MENDEL, CloudPharmaceuticals, LifeMine, ReviveMed, ENVISAGENICS, BenchSci, metagenomi, BEACON BIOSIGNALS

Companies (validated R&D, advanced AI systems): TERRAY, Standigm, 3BIGS Curated BIO BigData Platform, CYCLICA, IKTOS Artificial Intelligence for new drug design, InveniAI Innovate with intelligence, DEARGEN, Atomwise

Companies (validated R&D, end-to-end AI): CytoReason, absci, deep genomics, OWKIN, insitro

Top-50 AI in Pharma Investors

San Francisco

8VC
San Francisco, California, US

Founders Fund
San Francisco, California, US

Foresite Capital
San Francisco, California, US

DCVC
San Francisco, California, US

Obvious Ventures
San Francisco, California, US

Lifeforce Capital
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

Manhattan Beach

B Capital Group
Manhattan Beach, 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

New Enterprise Associates
Menlo Park, California, US

Illinois

ARCH Venture Partners
Chicago, Illinois, US

Mountain View

Y Combinator
Mountain View, California, US

GV
Mountain View, California, US

Palo Alto

AME CLoud Ventures
Palo Alto, California, US

Alexandria Venture Investments
Pasadena, California, US

Massachusetts

MassChallenge
Boston, Massachusetts, US

RA Capital Management
Cambridge, Massachusetts, US

General Catalyst
Cambridge, Massachusetts, US

Polaris Partners
Boston, Massachusetts, US

F-Prime Capital
Cambridge, Massachusetts, US

Other States

Merck Global Health Innovation Fund
Whitehouse, New Jersey,US

Alumni Ventures
Manchester, New Hampshire, US

SOSV
Princeton, New Jersey, US

National Science Foundation
Alexandria, Virginia, , US

T. Rowe Price
Baltimore, Maryland, US

Section 32
San Diego, California, US

National Institutes of Health
Bethesda, Maryland, US

Techstars
Boulder, Colorado, US

Creative Destruction Lab (CDL)
Toronto, Canda

Venture Kick
Schlieren, Zurich, Switzerland

Beijing

ZhenFund
Beijing, China

Sequoia Capital China
Beijing, China

Shanghai

WuXi AppTec
Shanghai, China

Lilly Asia Ventures
Shanghai, China

5Y Capital
Shanghai, China

Tencent
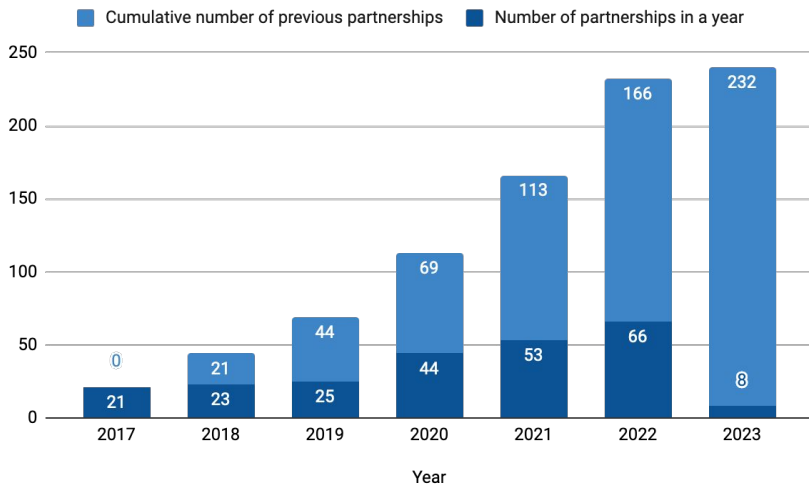Shenzhen, China

EASME
Brussels, Belgium

SoftBank Vision Fund
London, England, The UK

Entrepreneur First
London, England, The UK

A Growing Number of Collaborations Involving AI for Drug Discovery

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

Legend:
- Cumulative number of previous partnerships
- Number of partnerships in a year

Year	Number of partnerships in a year	Cumulative number of previous partnerships
2017	21	0
2018	23	21
2019	25	44
2020	44	69
2021	53	113
2022	66	166
2023	8	232

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

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

- a wave of proof-of-concept studies and research breakthroughs in a wide range of AI application use cases

- a number of commercial successes and successfully reached milestones, involving AI as a central element of research

- substantial advances in democratizing AI technology, where machine learning and deep learning algorithms become available at scale to non-AI experts

- decent increase in the overall understanding of AI "mechanics", due to increasing efforts in the education and professional development with a focus on AI-driven tools and approaches

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

Big Pharmas' AI-focused partnerships

In this report we have profiled **800 actively developing AI-driven biotech companies**. A steady growth in the AI for Drug Discovery sector can be observed in terms of substantially increased amount of investment capital pouring into the AI-driven biotech companies (**$48.19B in HY 2020** against **$126.4B in HY 2022**), the increasing number of **research partnerships between leading pharma organizations and AI-biotechs, and AI-technology** vendors, a continuing pipeline of industry developments, research breakthroughs, and proof of concept studies, as well as exploding attention of leading media and consulting companies to the topic of AI in Pharma and healthcare.

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

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

27 Deals

17-22 Deals

13-16 Deals

8-12 Deals
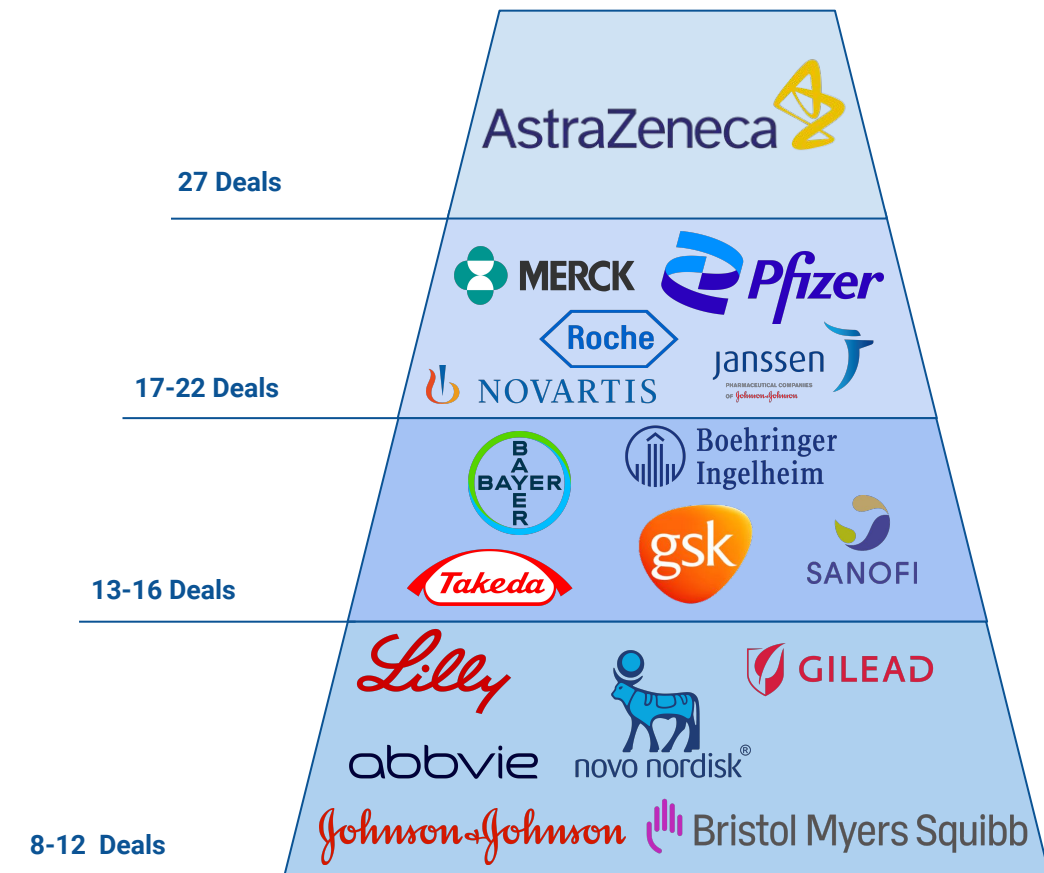
Selected Pharma AI Deals

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.

10 Most Recent Acquisitions of AI in Drug Discovery Companies

March 2023 — LexisNexis RISK SOLUTIONS → *undisclosed* → HUMAN API	**January 2023** — InstaDeep™ ← $440M ← BIONTECH
February 2023 — ENVISION PHARMA GROUP → *undisclosed* → OKRA	**January 2023** — VYASA ← $29M ← CERTARA
February 2023 — ZS → *undisclosed* → trials.ai	**December 2022** — nimbus THERAPEUTICS ← $4B ← Takeda
January 2023 — Paradigm → $200M → deep lens	**September 2022** — AMPLION ← *undisclosed* ← SCIENCE AND MEDICINE GROUP
January 2023 — CAMBRIDGE COGNITION → $7M → WINTERLIGHT	**June 2022** — PeerWell ← *undisclosed* ← BARDAVON HEALTH INNOVATIONS

Drug Candidates Designed by AI: Global

Disease	Drug	Phase I	Phase II	Phase III	Phase IV
Atopic dermatitis	BEN2293 🇬🇧		Benevolent		
COVID-19	Baricitinib 🇬🇧				Benevolent
Familial Adenomatous Polyposis	REC-4881 🇺🇸		(logo)		
Prostate cancer	BXCL701 🇺🇸		bioxcel therapeutics		
COVID-19	LY-CoV1404 🇨🇦				AbCellera
Cholangiocarcinoma	RLY-4008 🇺🇸		RELAY THERAPEUTICS		
Bipolar disorder	BXCL501 🇺🇸			bioxcel therapeutics	
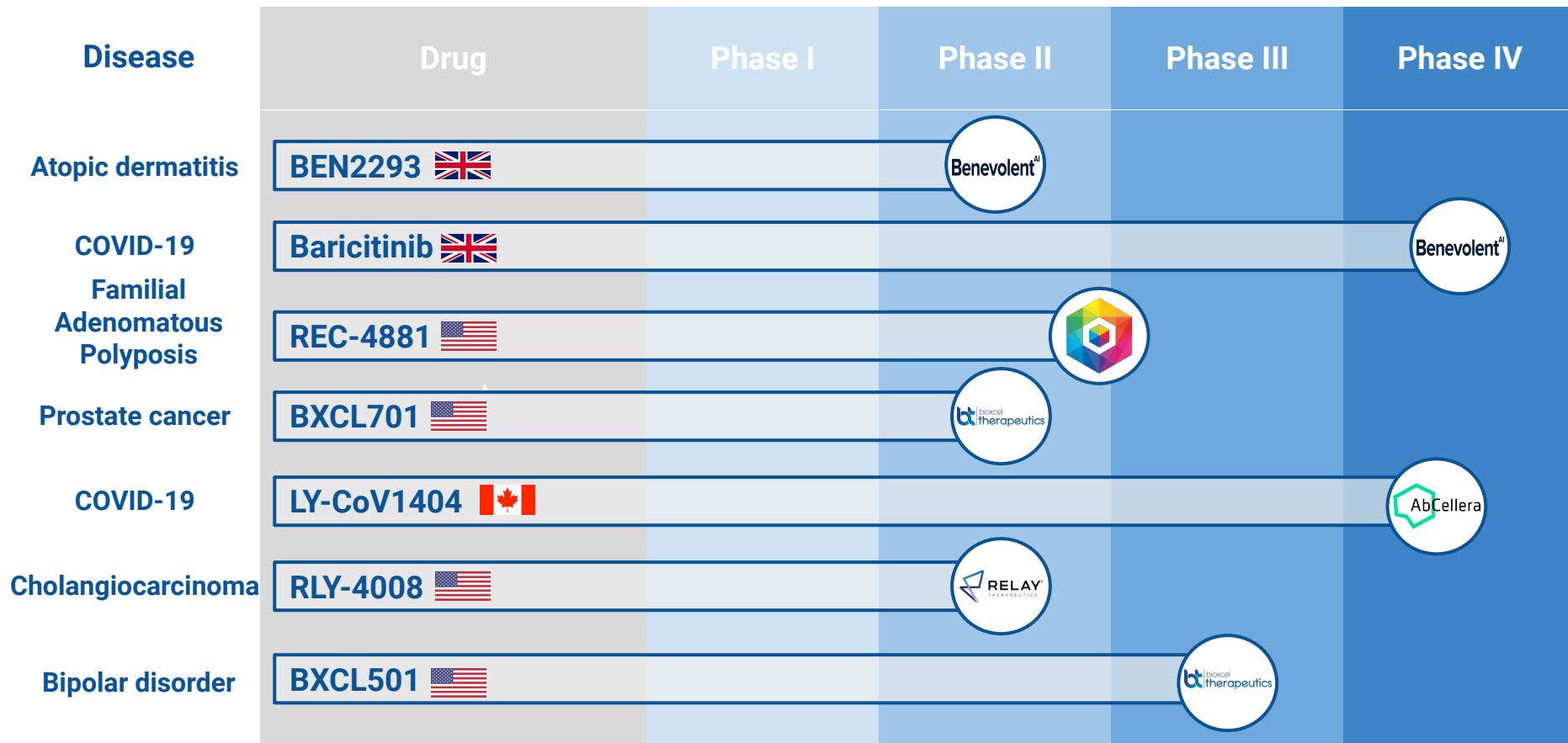
Leading Pharma Corporations by the Number of Pharma AI Deals

Bar chart values (number of deals):
- AstraZeneca: 27
- MERCK: 22
- Pfizer: 18
- NOVARTIS: 17
- Janssen: 17
- Roche: 17
- SANOFI: 16
- BAYER: 16
- Takeda: 14
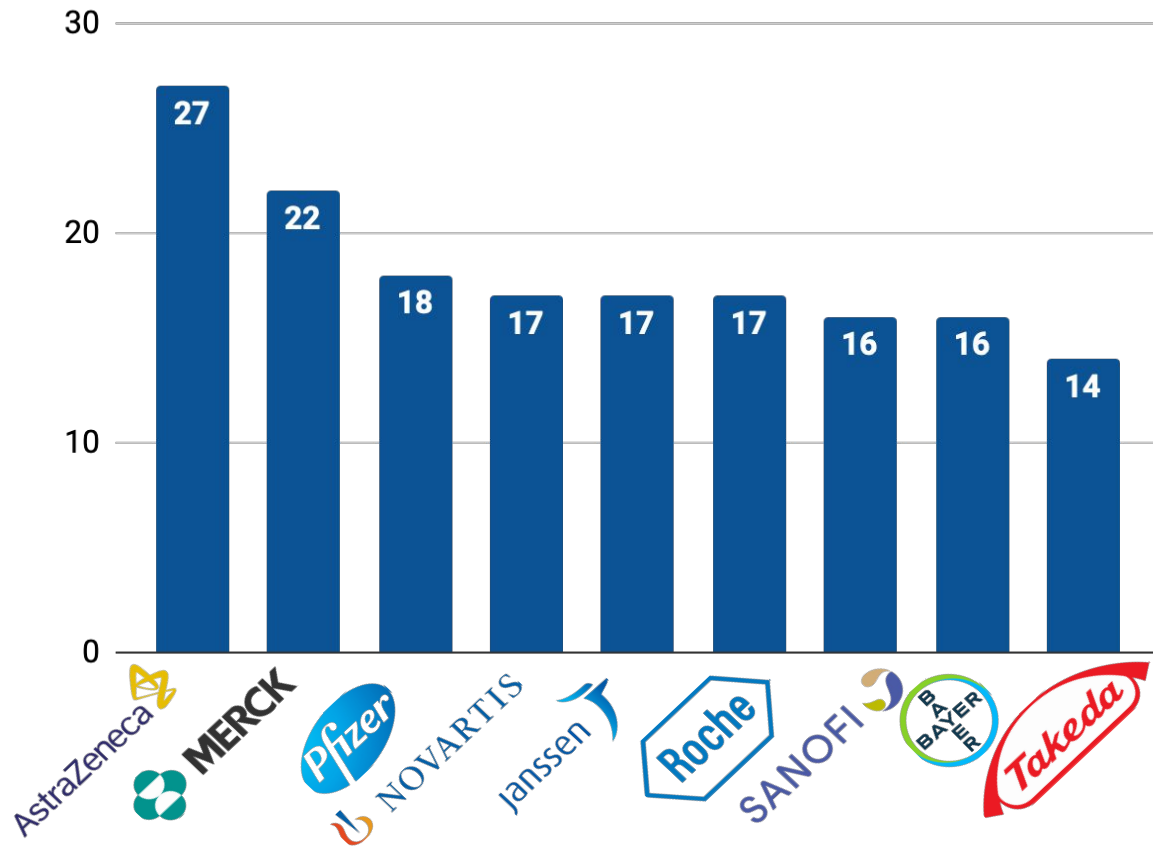
- The leading Pharma players by the amount of major industry partnerships are **AstraZeneca** and **Merck.**

- 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**.

Computational Methods Used by the Most Advanced AI Companies
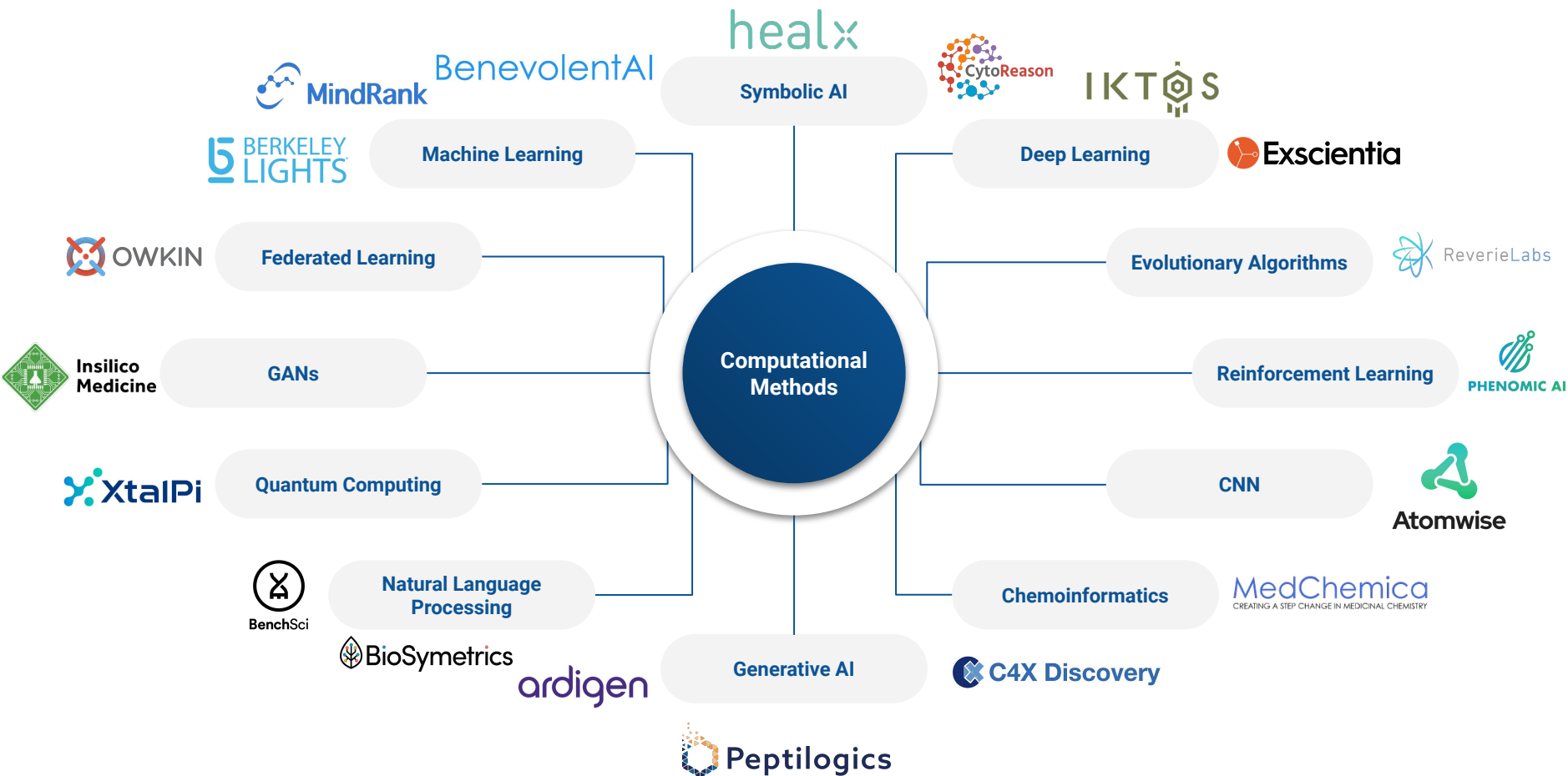
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550,000	**Companies**
50,000	**Investors**
52 million	**Data Points**
170	**Parameters of Automated SWOT Analysis**

Market Intelligence Focus

HealthTech	**DeepTech**	**BioTech**
Longevity	**GovTech**	**Philanthropy**

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Dashboards Constructor
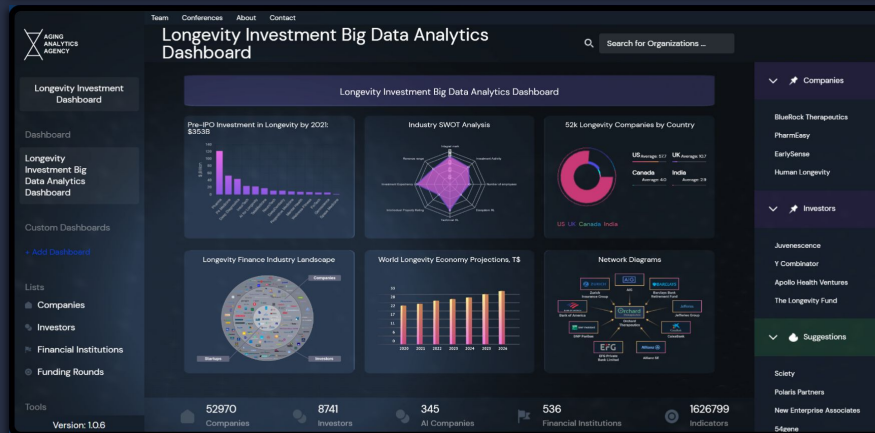
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