AI

**FOR DRUG DISCOVERY,
BIOMARKER DEVELOPMENT
AND ADVANCED R&D LANDSCAPE
OVERVIEW 2020**

AI Startups - 240
Corporations -   90
R&D Centers -   35
Investors - 600

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Introduction

This 130-page "AI for Drug Discovery, Biomarker Development and Advanced R&D Landscape Overview 2020" report marks the ninth installment in a series of reports on the topic of the Artificial Intelligence (AI) application in pharmaceutical research industry that DKA Pharma Division have been producing since 2017.

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

Substantial updates has been introduced since the previous edition, which highlight fast-pacing industry dynamics, and overall growth of investment and business development activity in the area of pharmaceutical AI. The lists of AI-biotech companies, biotech investors, and pharma organizations have been expanded to include new entities, and a new list of leading contract research organizations (CROs) has been added to outline the growing interest of contract research industry in the advanced data analytics technologies. We have also revisited data and chapters from the last edition, and reflected on the changes that occured ever since.

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

AI for Drug Discovery, Biomarker Development and Advanced R&D Landscape / 2020

AI Companies - 240
Investors - 600
Corporations - 90

Preclinical Development

Clinical Development

End-to-end Drug Development

Drug Repurposing

AI Companies

Investors

Corporations

Early And Preclinical Drug Development

Early drug development

Pharma

Tech

CRO

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AI for Drug Discovery, Biomarker Development and Advanced R&D Landscape / 2020

AI Companies - 240
Investors - 600
Corporations - 90

Asia
Canada
EU
China
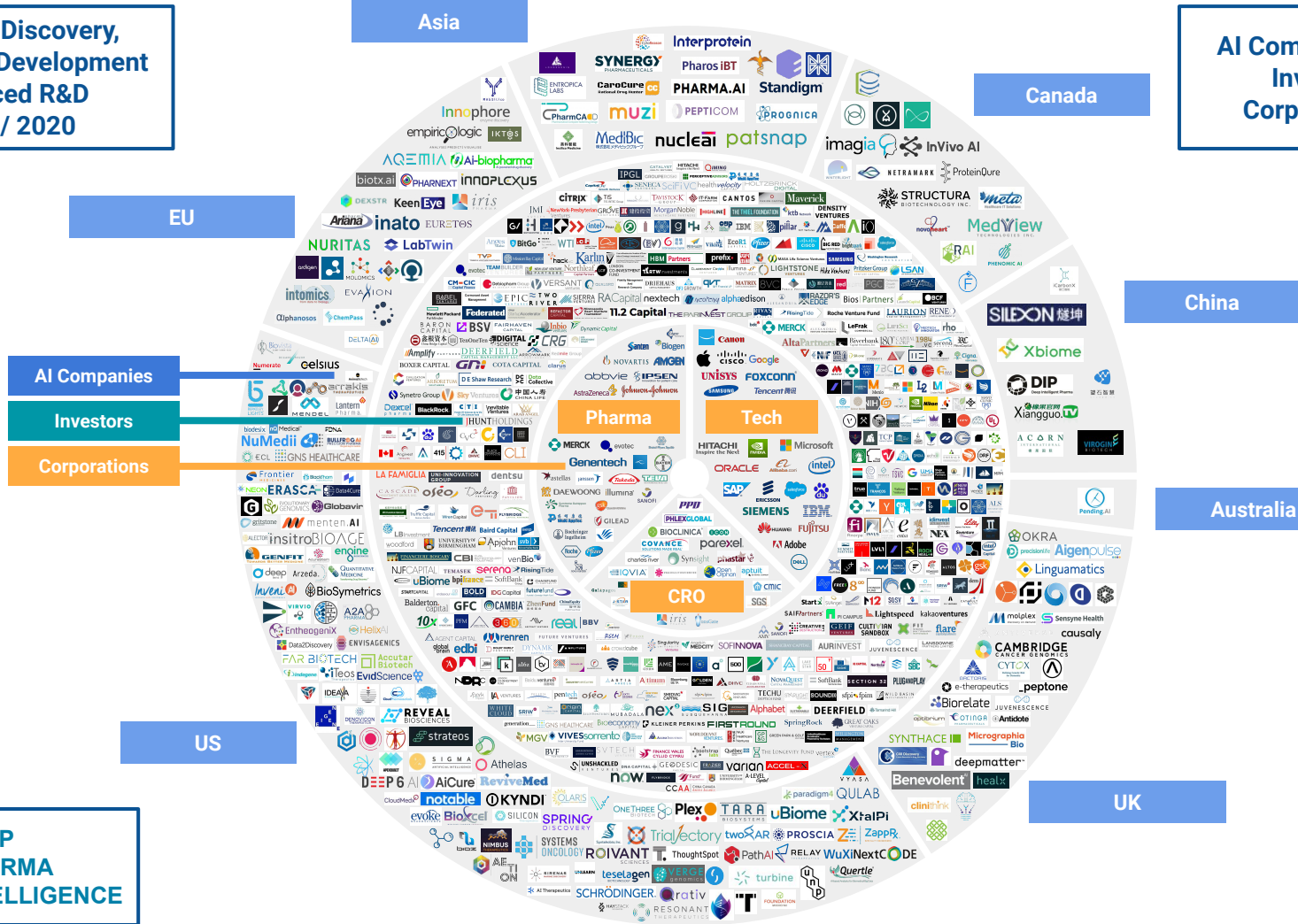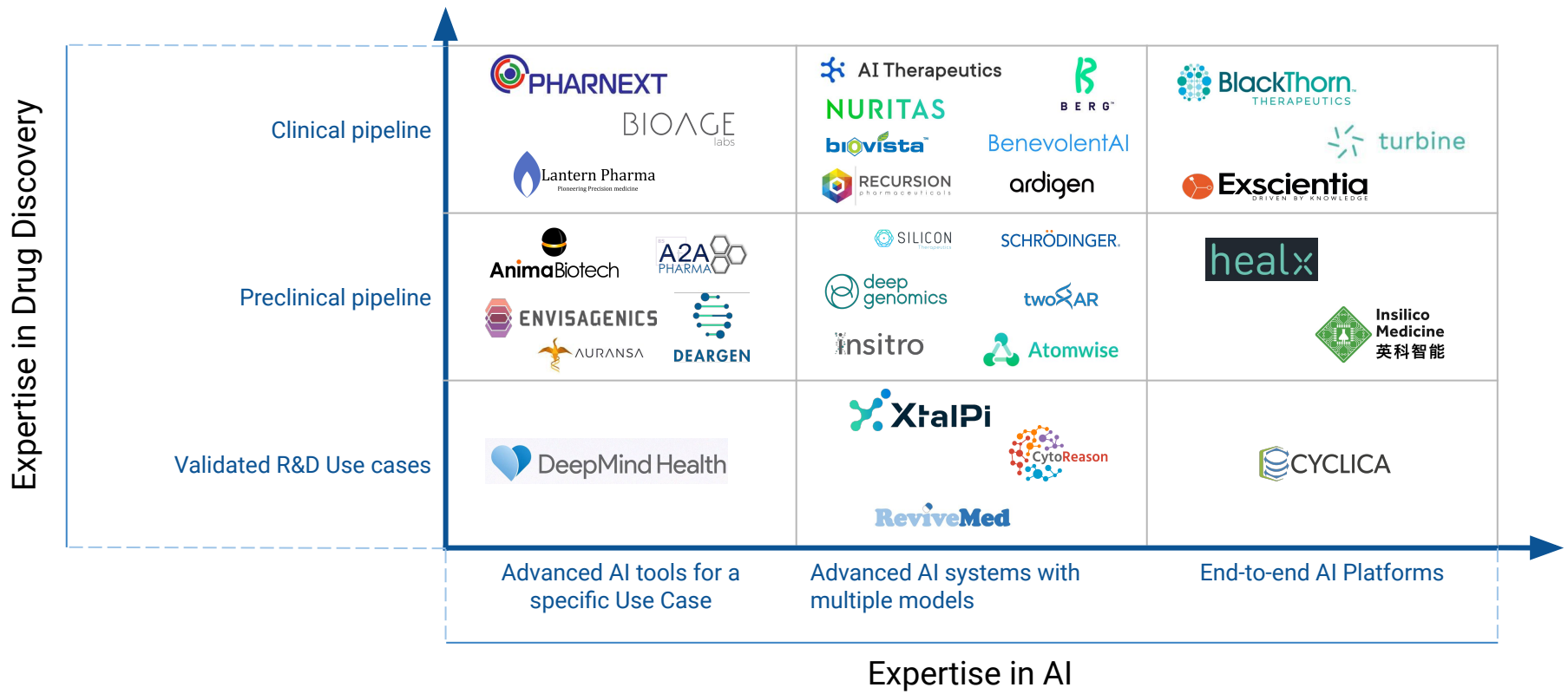Australia
US
UK

AI Companies
Investors
Corporations

Pharma
Tech
CRO

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Pharma AI Deals Structure 2020

Comparison of Top-32 Leading AI for Drug Discovery Companies Expertise in Drug Discovery R&D / AI

30 Leading Companies in AI for Drug Discovery Sector

1	A2A Pharma		16	DeepMind Health
2	AI Therapeutics		17	Envisagenics
3	Anima Biotech		18	Exscientia
4	Ardigen		19	healx
5	Atomwise		20	Insilico Medicine
6	Auransa		21	Insitro
7	BenevolentAI		22	Lantern Pharma
8	Berg		23	Nuritas
9	Bioage		24	Pharnext
10	biovista		25	Recursion Pharmaceuticals
11	BlackThorn Therapeutics		26	ReviveMed
12	Cyclica		27	Silicon Therapeutics
13	CytoReason		28	Turbine.AI
14	Deargen		29	twoXAR
15	Deep Genomics		30	XtalPi

240 AI Companies: Regional Proportion

Canada 6.7%
UK 14.2%
EU 13.4%
US 54.4%
China 2.5%
Australia 0.4%
Asia 8.4%
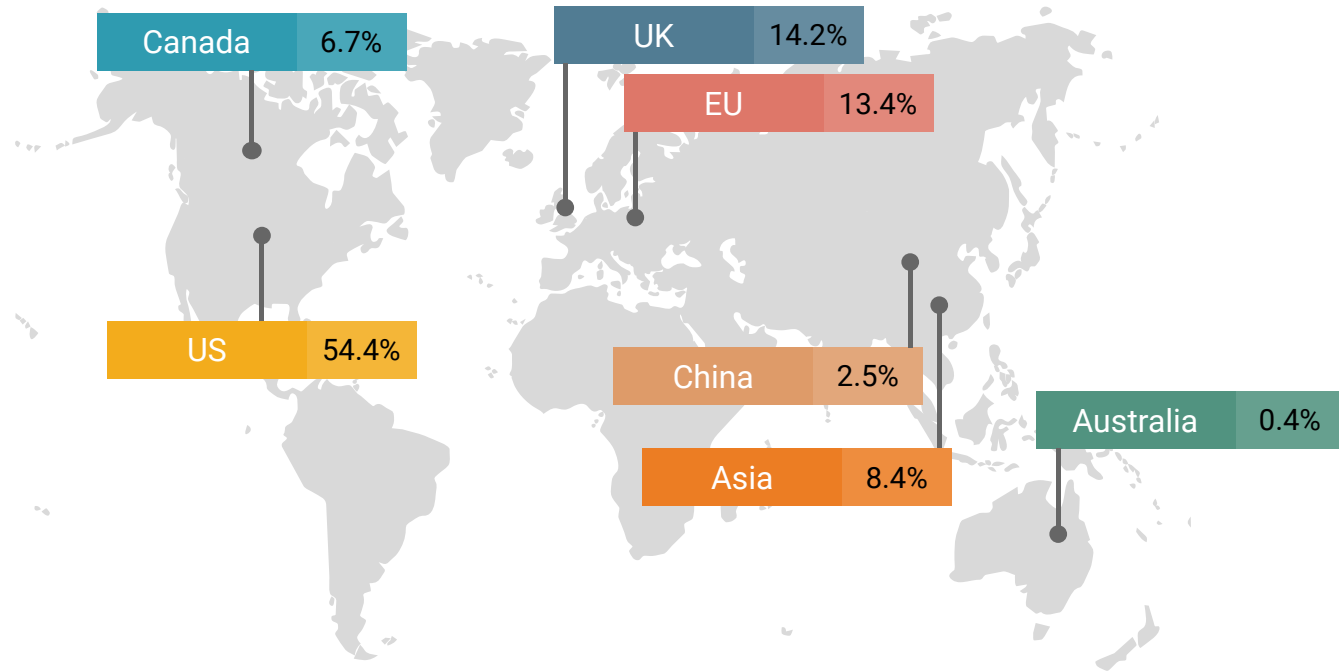
The US is still firmly in the lead in terms of its proportion of AI for Drug Discovery companies. Interestingly, Asia currently has the fifth-lowest proportion of AI for Drug Discovery companies. However, Asia-Pacific region has begun to aggressively increase its activity in the space in terms of investments into foreign companies (largely US-based companies), and we expect to see an increase in the number of AI for Drug Discovery Companies located in the Asia-Pacific region generally, and in China particularly.

600 Investors: Regional Proportion

Region	Proportion
Canada	2.53%
UK	8.75%
EU	13.5%
US	64.9%
Asia	8.92%
China	1.35%
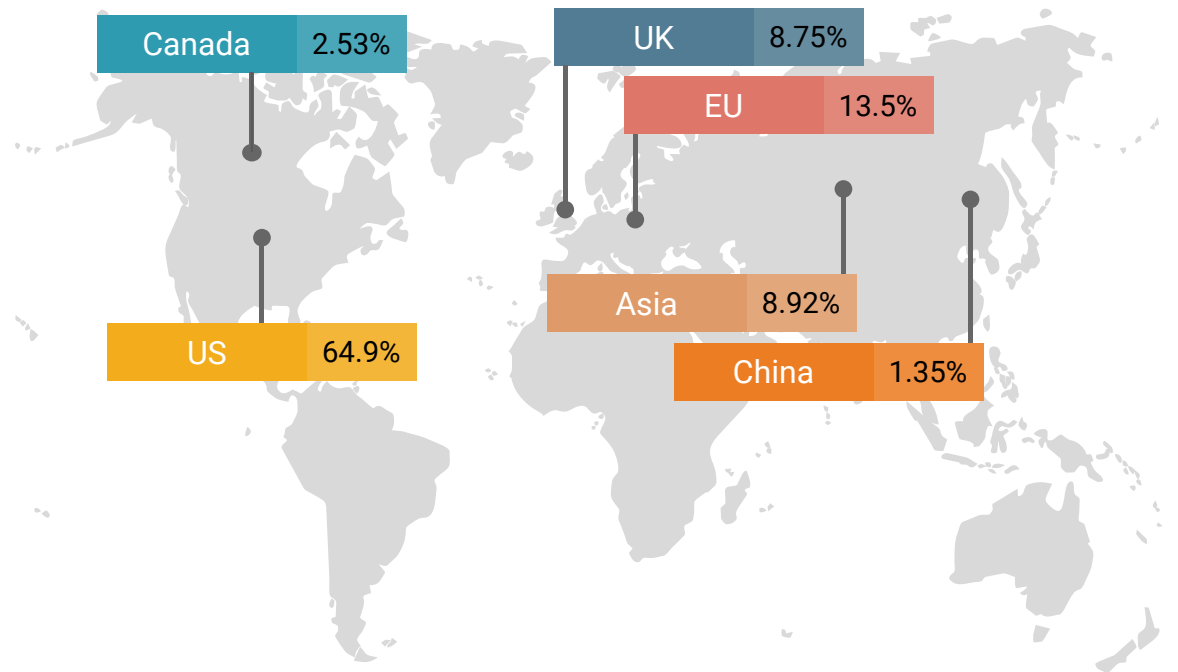
The United States continues to lead the rest of the world in terms of artificial intelligence for companies and funds that invest in Drug Discovery. This is reasonable, given that more than a half of the world's AI for Drug Discovery companies have their headquarters in USA. Comparing with previous periods of 2020, we can observe significant growth of the number of investors in the USA and EU. Thus, together with UK these regions are leaders by the number of investors in AI in Drug Discovery companies.

20 CROs: Regional Proportion

UK 10%

EU 30%

US 55%
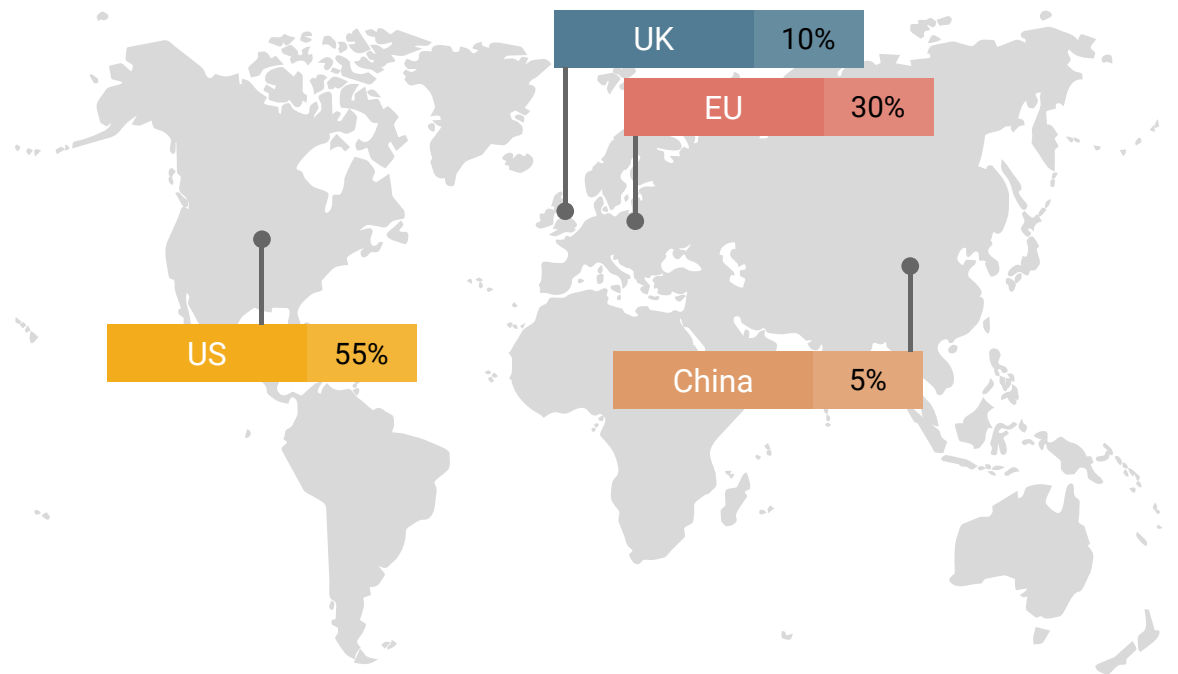
China 5%

The United States leads the AI race on the level of Contract Research Organizations as well, with 55% of CROs being based in the US. It is followed by the European Union with around 30%. The other 10% have their headquarters in the UK. China represents only 5% of the AI-interested CROs, which would probably increase in the following years due to Chinese strategy on AI implementation and large investments in the AI industry.

35 Leading R&D Centers: Regional Proportion

Region	Proportion
UK	8.6%
EU	31.4%
US	37.1%
China	5.7%
Asia	17.2%
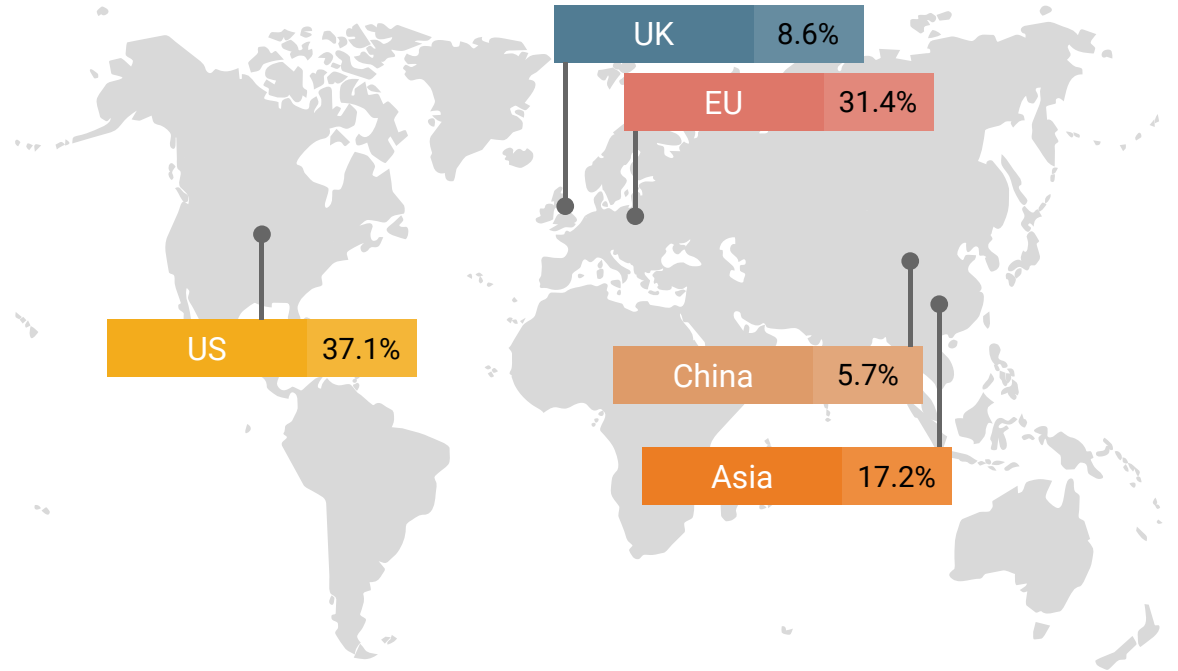
Following the trend from our previous reports the map indicates that the US leads the world in terms of the number of R&D Centers focused on AI for Drug Discovery. This is sensible within the context of the recent increase in the number of investors that invest in AI for Drug Discovery space within the territory of United States. The same trend can be observed in European Union as it demonstrates second biggest figure of investors' part in the world that results in second biggest share of Leading R&D Centers.

30 Pharma Corporations Applying Advanced AI in Healthcare and Drug Discovery

UK	7%
Switzerland	7%
EU	23%
US	40%
Asia	23%
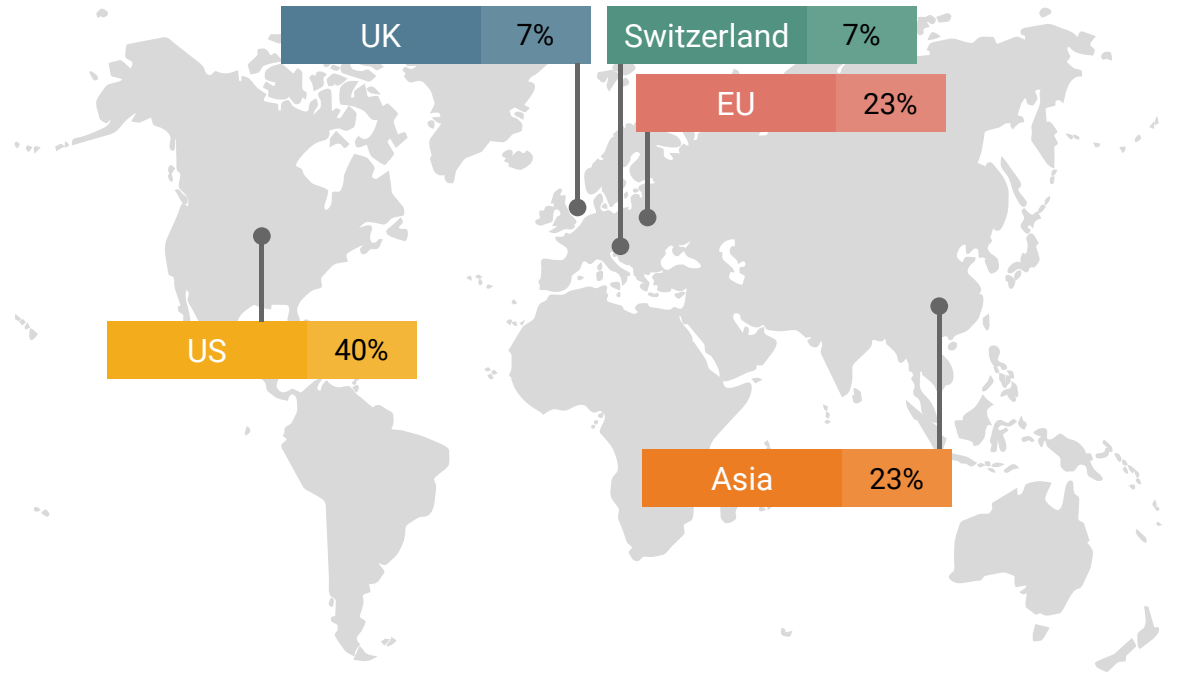
The industry is seeing an increasing level of regional diversification. Whereas historically the US has dominated the AI for Drug Discovery race in terms of the number of AI companies, the volume of investments and number of industry specialized conferences, in 2019 we are seeing an increased level of activity from the UK, Switzerland and China.

40 Leading Tech and Chemical Corporations: Regional Proportion

Region	%
Switzerland	5%
EU	20%
US	45%
China	10%
Asia	20%
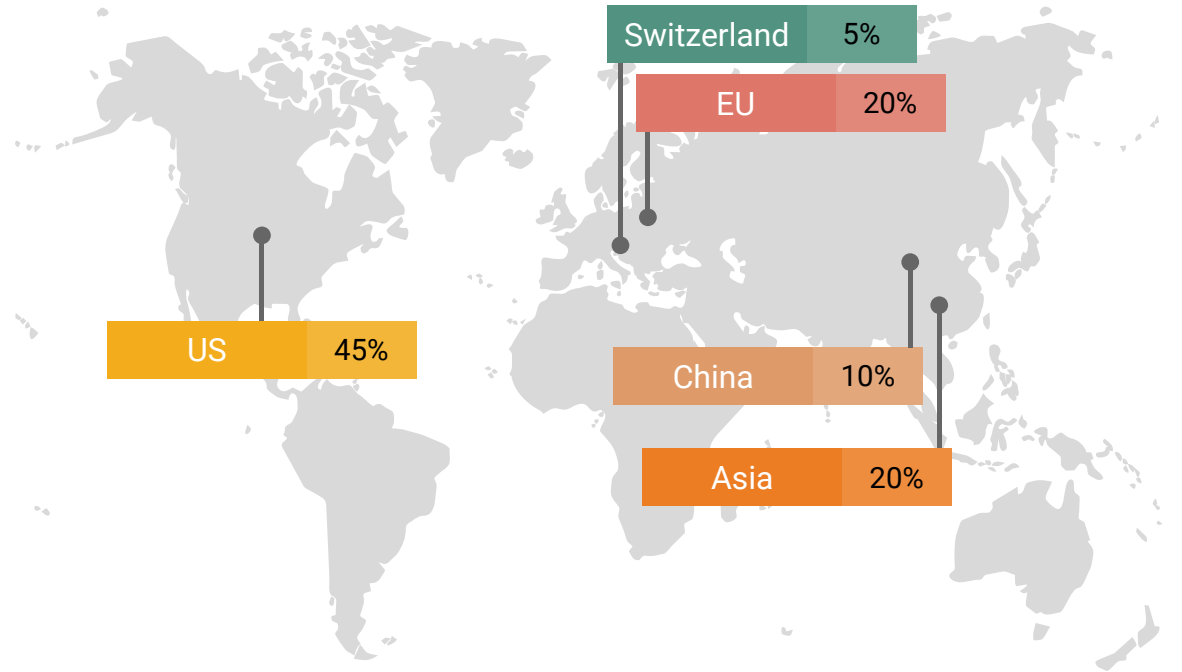
The US is the leader according to the number of tech corporations applying advanced AI in healthcare and drug discovery. EU leads the world in terms of the number of Chemical Corporations. The second biggest figure can be observed in Asia while the US is in the third place. This is sensible within the context of the recent increase in the chemical industry in EU that overweight the US and Asian markets of chemical substances and related products. A lot of these chemical corporations are participating in cooperations and partnerships that are aimed at drug discovery and are related to pharmaceutical issues.

Executive Summary

This Report at a Glance

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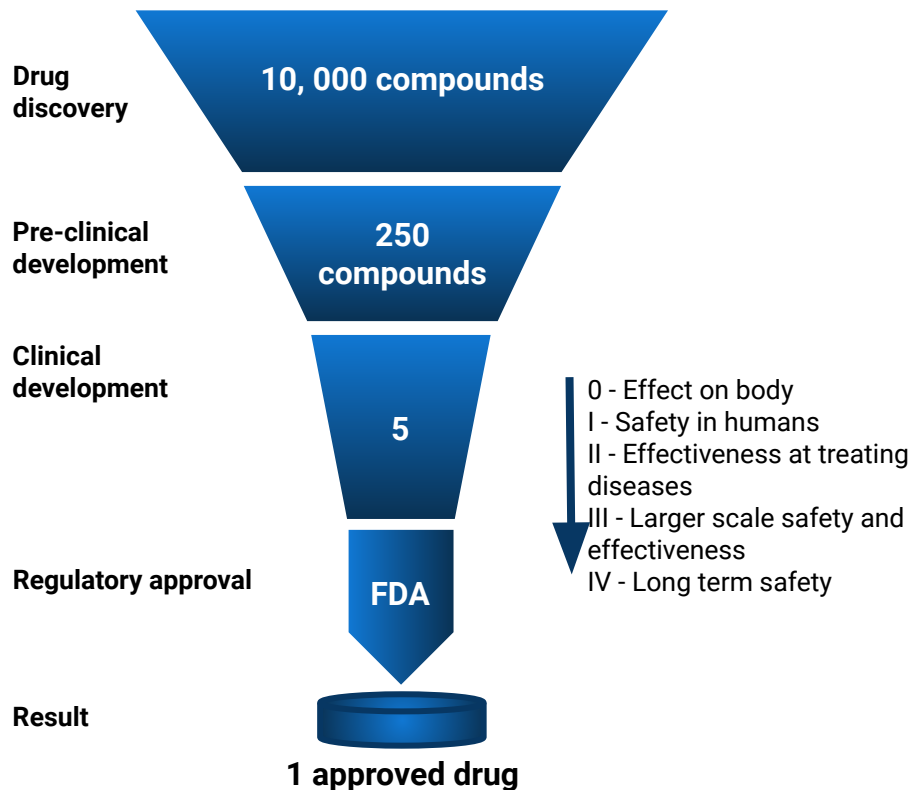
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Alongside investment and business trends, the report also provides technical insights into some of the latest achievements in the AI application and research.

This report has been put together taking into account the unprecedented global COVID19 pandemics, which substantially impacted every industry on the planet, pharma and biotech not being an exception. Quite expectedly, COVID19 brought about quite a few opportunities for the drug makers and vaccine developers and in general, it catalyzed more rapid progress in the pharmaceutical AI space as well. Not only a lot of AI-assisted drug repurposing programs have been launched in first half of 2020, but also the research environment has become more collaborative, with lots of open science project, and numerous companies opening free access to their platforms. However, COVID19 also created major challenges for the pharma industry, such as disruptions in clinical trials and regular research projects and lab workflows. However, our findings related to COVID19 impact on the biotech investment landscape will be presented in the upcoming report, dedicated specifically to this issue.

Pharma Efficiency: **Challenges**

Drug discovery
10, 000 compounds

Pre-clinical development
250 compounds

Clinical development
5

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

Regulatory approval
FDA

Result
1 approved drug

Source: Endpoints News | ePharmacology

> **> 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 145% increase, correcting for inflation, comparing 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)**

The pharmaceutical AI sector is "heating up"

In this report we have profiled 240 actively developing AI-driven biotech startups, adding some 40 companies since our 2019 edition. A steady growth in the "AI for Drug Discovery sector" can be observed in terms of substantially increased amount of venture capital pouring into the AI-driven biotech startups (around $1.9B in 2020 alone, so far), 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 alos 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.

Big Pharmas active in AI-focused partnerships

8 Deals

7 Deals

6 Deals

4 Deals

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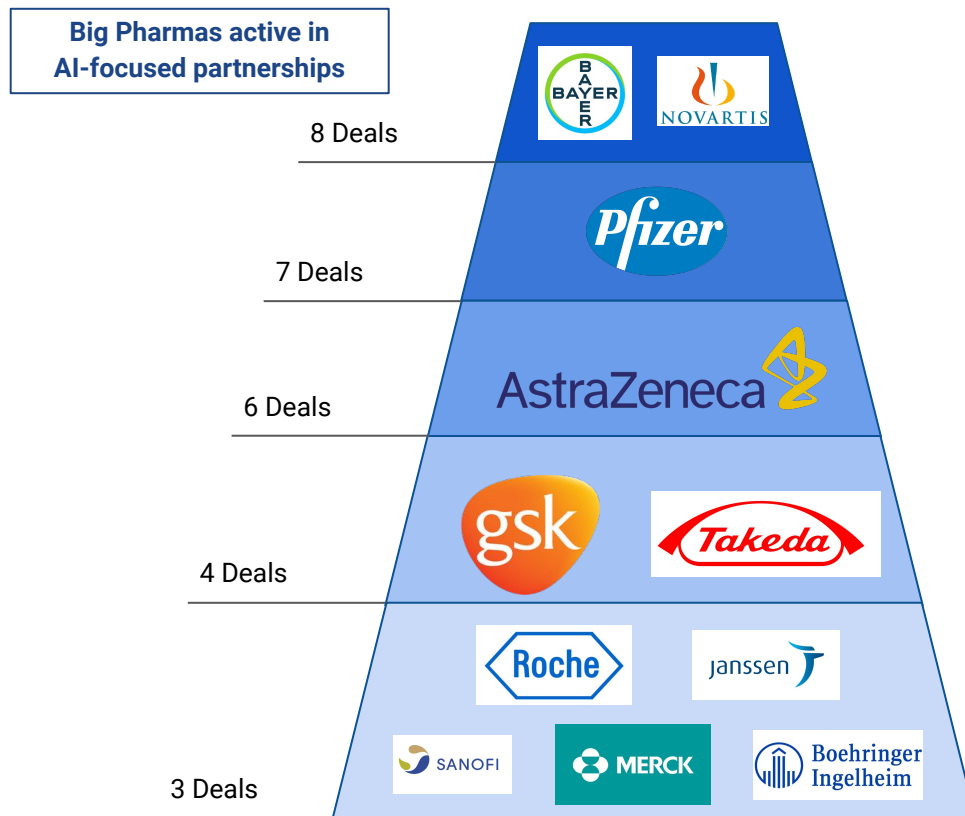
Application of AI for Advanced R&D to Address Pharma Efficiency Challenges

Target Discovery and Early Drug Discovery

- Analyze data sets, form hypotheses and generate novel insights
- Identify novel drug candidates
- Analyze data from patient samples in both healthy and diseased states to generate novel biomarkers and therapeutic targets
- Predict binding affinity and other pharmacological properties of molecules
- Allow filtering for drug-like properties of molecules
- Reduce complexity in protein design

Clinical Trials

- Optimize clinical trial study design
- Transform diverse streams of biomedical and healthcare data into computer models representative of individual patients
- Deliver personalized medicine at scale by revealing optimal health interventions for individual patients
- Analyze medical records to find patients for clinical trials
- Automate matching cancer patients to clinical trials through personal medical history and genetic analysis
- Improve pathology analysis
- Identify patients that would benefit from novel therapies

Design and Processing of Preclinical Experiments

- Reduce time, money, and uncertainty in planning experiments
- Decode open- and closed-access data on reagents and get actionable insights
- Automate selection, manipulation, and analysis of cells
- Expedite development of cell lines and automate manufacturing of cellular therapeutics
- Automate sample analysis with a robotic cloud laboratory

Repurposing of Existing Drugs

- Rapidly identify new indications for many known drugs
- Match existing drugs with rare diseases
- Conduct experimental biology at scale by testing 1000+ of compounds on 100+ of cellular disease models in parallel
- Generate novel biomarkers and therapeutic targets

Aggregation and Synthesis of Information

- Extract knowledge from literature
- Generate insights from thousands of unrelated data sources
- Improve decision-making
- Eliminate blind spots in research
- Identify competitive whitespace

Business Activity

The business activity has been increasing in the pharmaceutical AI space over 2020, judging by an increased number of transactions and partnership announcements in this period.

The most significant deals and collaborations in 2020 include:

- **XtalPi** — **SoftBank Vision Fund 2**, **PICC Capital**, and **MorningSide Venture Capital**: XtalPi has raised $319M in funding round C. The funding will be used for the further development of XtalPi's Intelligent Digital Drug Discovery and Development (ID4) platform.

- **AstraZeneca** intends to open AI and drug research centers in **China** and make a $1 billion capital infusion into Chinese biotech innovations.

- **Exscientia** — **Bayer**: Exscientia has entered a 3-year $266 million agreement with Bayer. The partnership will leverage AI to accelerate the discovery of small molecules candidates programs for oncology and cardiovascular diseases.

- **Schrödinger** — **Bayer**: Schrödinger has entered a 5-year agreement with Bayer to work on a new virtual platform for small molecules design, which will be able to design and screen synthetically feasible compounds.

- **Schrödinger** — **Google Cloud**: Schrödinger enters a 3-year collaboration with Google Cloud to leverage the supercomputer power for speeding up Schrödinger's molecular modeling platform.

- **Boehringer Ingelheim** — **BERG**: Boehringer Ingelheim partners with BERG to investigate inflammatory diseases, particularly inflammatory bowel disease and Crohn's disease, find the causes, develop new biomarkers, targets, and new drugs.

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

- **Insitro** — **Andreessen Horowitz**, **Canada Pension Plan Investment Board**: insitro, a machine learning-driven drug discovery company, has raised $143 million in Series B financing. The investment will be used to further develop the company's technology and automation.

Partnerships like these provide a huge effect on Pharma industry and are needed in case if a company intends to become a leader in the ongoing competition.

Major Observations for 2020: **Key Business Takeaways**

1. **The segment of pharmaceutical AI continues consolidation** with the increasing number of later stage mega-rounds, including those of Insitro (), Recursion Pharmaceuticals, XtalPi and others. The AI startups pack is clearly differentiating into the leaders, who developed substantial resources, financial leverage, and technological advantage, and others lagging behind -- companies with less resources or less mature technology and scientific assets. The latter are usually focused on narrow therapeutic or technological niches, and are following service-oriented business models.

2. **Pharmaceutical AI sector is "heating up",** and becomes a lucrative area for specialized biotech investors as well as investor organizations just entering the pharma space with a goal of including high-risk/high-return companies in their investment portfolios. This is backed by several observations, including an overall increasing investment activity in this sector in 2020, the increasing rush among leading pharma and contract research organizations (CROs) to compete for partnerships with AI-driven companies, and the increasing amount of proof-of-concept breakthroughs, confirming that AI technology has achieved substantial maturity to be able to bring tangible value for drug discovery -- far beyond a simple optimization gain.

3. **Big pharma and contract research organizations increasingly compete for AI partnerships**, and continue building in-house AI workflows -- driven by rapidly emerging evidence of the AI tech feasibility and innovation potential. A number of highly notable proof-of-concept results has been announced in 2019-2020.

4. **COVID-19 pandemics appears to be a positive catalyst for the acceleration of the AI adoption** by the pharmaceutical organizations. This is primarily stipulated by the necessity to rapidly process vast amounts of data, and come up with innovations under strict deadlines. Therefore, this urgency pushed companies and investors into more opportunistic projects than ever before.

Key Technology Takeaways

1. AI is regarded by some top executives at big pharma (<u>GSK and others</u>) as **a tool to uncover not only new molecules, but also new targets**. Ability of deep neural networks to build ontologies from multimodal data (e.g. "omics" data) is believed to be among the most disruptive areas for AI in drug discovery, alongside with data mining from unstructured data, like text (using natural language processing, NLP).

2. There is **a considerable trend for "AI democratization"** where various machine learning/deep learning technologies become available in pre-trained, pre-configured "of-the-shelf" formats, or in relatively ready-to-use formats -- via cloud-based models, frameworks, and drag-and-drop AI-pipeline building platforms (for example, KNIME). This is among key factors in the acceleration of AI adoption by the pharmaceutical organizations -- where a non-AI experts can potentially use fairly advanced data analytics tools for their research.

3. **Proof-of-concept projects keep yielding successful results** -- in research studies, and in the commercial partnerships alike. For example, companies like Recursion Pharmaceuticals and Exscientia achieved important research milestones using their AI-based drug design platforms.

Obstacles That Still Remain

1. **Global shortage of AI talent** continues to be a serious challenge for the biopharma industry, repeating the trend from our previous reports. While big pharmaceutical companies invest substantial capital in recruitment of AI specialists, still the majority of them are acquired by large tech corporations (Google, Amazon, Alibaba, Tencent, Baidu etc.) However, a growing wave of specialized university programs and courses, geared towards data science and AI application, is projected to address this issue to certain extent in the coming years.

2. **Lack of available quality data is still a challenge for the unleashing full potential of deep learning technologies.** Numerous variations of deep learning (DL) are believed to be the most lucrative area of AI for applications such as drug discovery and clinical research. The key challenge is that DL algorithms are "data-greedy", while big data in biotech is not always well-versed for modeling, or is inaccessible due to privacy reasons.

3. **Ethical, legal, and regulatory issues for AI adoption in the pharmaceutical sciences.** This set of challenges is related to the previous point, but also includes other questions -- AI explainability, patentability of AI-generated results, non-optimal regulations in various countries, slowing down the progress and adoption of AI technologies in general, and in the pharmaceutical industry in particular.

AI in the global context

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. However, we observe the increased level of the UK and EU activity through big corporations that use AI to reorganise drug discovery and in launching government initiatives. It is also important to note a great increase in activity from the Asia-Pacific region generally, and particular from China — AI superpower.

China engages in extensive investment activity. In particular, it has promised to invest $5 billion in AI. Tianjin, one of the biggest municipalities, is going to invest $16 billion in its local AI industry, and the Beijing authorities will build $2.12 billion AI development project. China also has at least ten privately owned AI startups valued at more than US$1 billion. Moreover, China has been heavily investing in biotech R&D, although lately a serious decrease in Chinese investment in US biotech startups has been observed which can be explained by the trade conflicts between the US and China.

China plans to become the world AI leader by 2030, according to the AI Strategic Plan released in July 2017. The analysis of the the Asia-Pacific region has shown that the main forcers of AI implementation include Saama Technologies, Inc., a leading clinical data analytics company. It has announced a collaboration with researchers at the Tufts Center for the Study of Drug Development to ascertain how biopharmaceutical companies optimize automation and information technologies, including machine learning and neural networks, to support the research and development of new therapeutics. Moreover, XtalPi provides a huge number of talent to work with machine learning, create drug discovery and development applications that predict the properties of small molecules. Another innovators of Asian AI industry are Cytlimic and Fujitsu that offer software for predicting how well compounds will bind with each other and proteins.

Europe has traditionally been a strong breeding ground for biopharma activity, with some recent large valuations and mega deals. The UK and EU activity in the pharmaceutical AI race is mainly boosted by Novartis that announced an important step in reimagining medicine by founding the Novartis AI innovation lab and by selecting Microsoft Corp. as its strategic AI and data-science partner for this effort. Furthermore, GlaxoSmithKline has announced a few deals with companies such as Exscientia, Insilico Medicine, Insilico Biotechnology to use new computer modelling systems. BenevolentAI, a global leader in the application of AI for scientific innovation, also has several high-profile research collaborations, including AstraZeneca, and licensed in a group of drugs to develop from Janssen in 2016. This all demonstrate that Pharma is increasingly turning to AI to transform the drug discovery process.

Pharmaceutical AI Sector is "Heating Up":

Top 50 AI for Drug Discovery Investors

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Investment landscape at a glance (Q4 2019 — 2020)

The total amount of VC funding in AI-biotech startups increased in 2020 (as of November) by around 23%, compared to 2019, approaching a total of $1.9B, which is also more than in 2015, 2016 and 2017 combined.
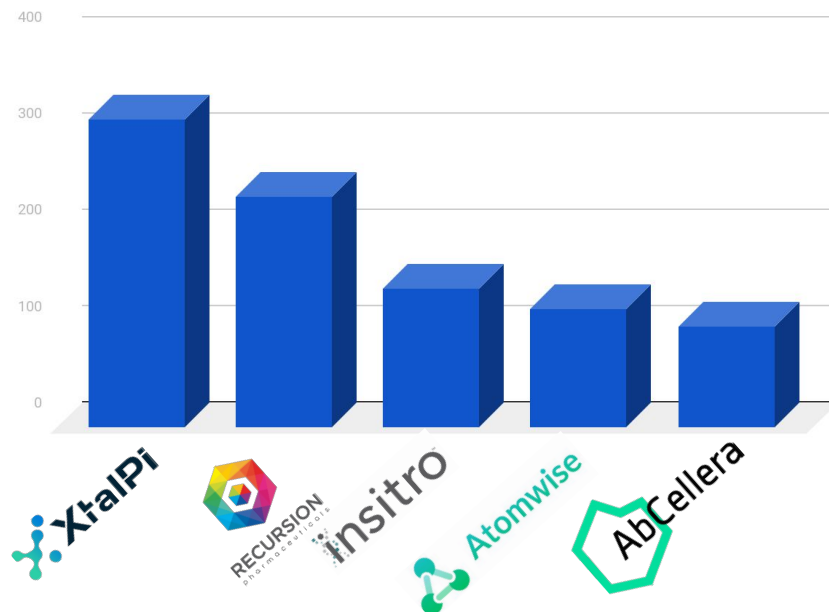
There is an increasing number of late-stage mega-rounds (e.g. B, C), including hundreds of millions. The apparent trend is sector consolidation, where a number of AI-startups have achieved substantial leadership and grown in resources and technology, while others have lagged behind and had to focus on niche service-oriented segments of drug discovery. Several AI startups also went out of business.

Some of the major deals included:

- insitro with their $143 million (Series B);
- XtalPi with $319 million (Series C);
- Atomwise with $123 million (Series B);
- Recursion Pharmaceuticals with $239 million (series D);
- AbCellera with the sum of $105 million (Series B).

An important driver of growth for the sector is a substantial shift in Big Pharma's interest in AI technology from "nice to try" to "strategically important". Such increasing market demand will drive more exits in future, and is important for heating up the investor's interest in this sector.

Top 5 Investment Deals in 2020 (in million US dollars)

50 Leading Investors in AI for Drug Discovery Sector

#	Investor	#	Investor
1	GV	16	Third Rock Ventures
2	Casdin Capital	17	ZhenFund
3	Creative Destruction Lab	18	500 Startups
4	Y Combinator	19	Bill & Melinda Gates Foundation
5	Alexandria Venture	20	Celgene
6	WuXi AppTec	21	Data Collective DCVC
7	Andreessen Horowitz	22	F-Prime Capital
8	EASME - EU Executive Agency for SMEs	23	Foresite Capital
9	Lilly Asia Ventures	24	Founders Fund
10	OS Fund	25	Inovia Capital
11	AME Cloud Ventures	26	Intel Capital
12	ARCH Venture Partners	27	Khosla Ventures
13	Felicis Ventures	28	Perceptive Advisors
14	National Institutes of Health	29	SoftBank Vision Fund
15	StartX (Stanford-StartX Fund)	30	UK Innovation & Science Seed Fund

50 Leading Investors in AI for Drug Discovery Sector

31	8VC
32	Alexandria Real Estate Equities
33	Vertex Ventures
34	Atlas Venture
35	Baidu Ventures
36	Baillie Gifford
37	General Catalyst
38	IA Ventures
39	Johnson & Johnson Innovation
40	Luminous Ventures

41	Mubadala Capital | Ventures US
42	Nextech Invest
43	Obvious Ventures
44	Qiming Venture Partners
45	RA Capital Management
46	Refactor Capital
47	Sequoia Capital
48	SOSV
49	Tencent Holdings
50	Two Sigma Ventures

Top-50 AI for Drug Discovery Investors

Alexandria Real Estate Equities
Pasadena, California, US

Intel Capital
Santa Clara, California, US

Refactor Capital
Burlingame, California, US

Other

Sequoia Capital
Menlo Park, California, US

Andreessen Horowitz
Menlo Park, California, US

Felicis Ventures
Menlo Park, California, US

Khosla Ventures
Menlo Park, California, US

Menlo Park

California

Palo Alto

StartX
Palo Alto, California, US

AME CLoud Ventures
Palo Alto, California, US

Vertex Ventures
Palo Alto, California, US

Mountain View

Y Combinator
Mountain View, California, US

GV
Mountain View, California, US

8VC
San Francisco, California, US

Founders Fund
San Francisco, California, US

Foresite Capital
San Francisco, California, US

500 Startups
San Francisco, California, US

Alexandria Venture
San Francisco, California, US

Obvious Ventures
San Francisco, California, US

Data Collective DCVC
San Francisco, California, US

Mubadala Capital | Ventures US
San Francisco, California, US

San Francisco

United States

Illinois

OS Fund
Park Ridge, Illinois, US

ARCH Venture Partners
Chicago, Illinois, US

Perceptive Advisors
New York, New York, US

IA Ventures
New York, New York, US

Two Sigma Ventures
New York, New York, US

Casdin Capital
New York, New York, US

New York

Other States

Bill & Melinda Gates Foundation
Seattle, Washington, US

Lili Ventures
Indianapolis, Indiana, US

SOSV
Princeton, New Jersey, US

Celgene
Summit, New Jersey, US

National Institutes of Health
Bethesda, Maryland, US

Johnson & Johnson Innovation
New Brunswick, New Jersey, US

Canada

Inovia Capital
Montréal, Quebec, Canada

Creative Destruction Lab
Toronto, Ontario, Canada

China

Tencent Holdings
Shenzhen, China

Beijing

ZhenFund
Beijing, China

Baidu Ventures
Beijing, China

Shanghai

WuXi AppTec
Shanghai, China

Lilly Asia Ventures
Shanghai, China

Qiming Venture Partners
Shanghai, China

Belgium

EASME - EU Executive Agency for SMEs
Brussels, Brussels Hoofdstedelijk Gewest, Belgium

Switzerland

Nextech Invest
Zürich, Zurich, Switzerland

Massachusetts

Atlas Venture
Cambridge, Massachusetts, US

General Catalyst
Cambridge, Massachusetts, US

SR One
Cambridge, Massachusetts, US

Third Rock Ventures
Boston, Massachusetts, US

F-Prime Capital
Cambridge, Massachusetts, US

RA Capital Management
Boston, Massachusetts, US

United Kingdom

SoftBank Vision Fund
London, England, United Kingdom

Amadeus Capital Partners
London, England, United Kingdom

Baillie Gifford
Edinburgh, Edinburgh, United Kingdom

UK Innovation & Science Seed Fund
Harwell, Oxfordshire, United Kingdom

Luminous Ventures
London, England, United Kingdom

Dynamics of Investments (in millions of USD per year)

Year	Investment
2014	219.5
2015	342.2
2016	665.8
2017	772.9
2018	1343.3
2019	1415.3
2020 (up to 1st December)	1835.5
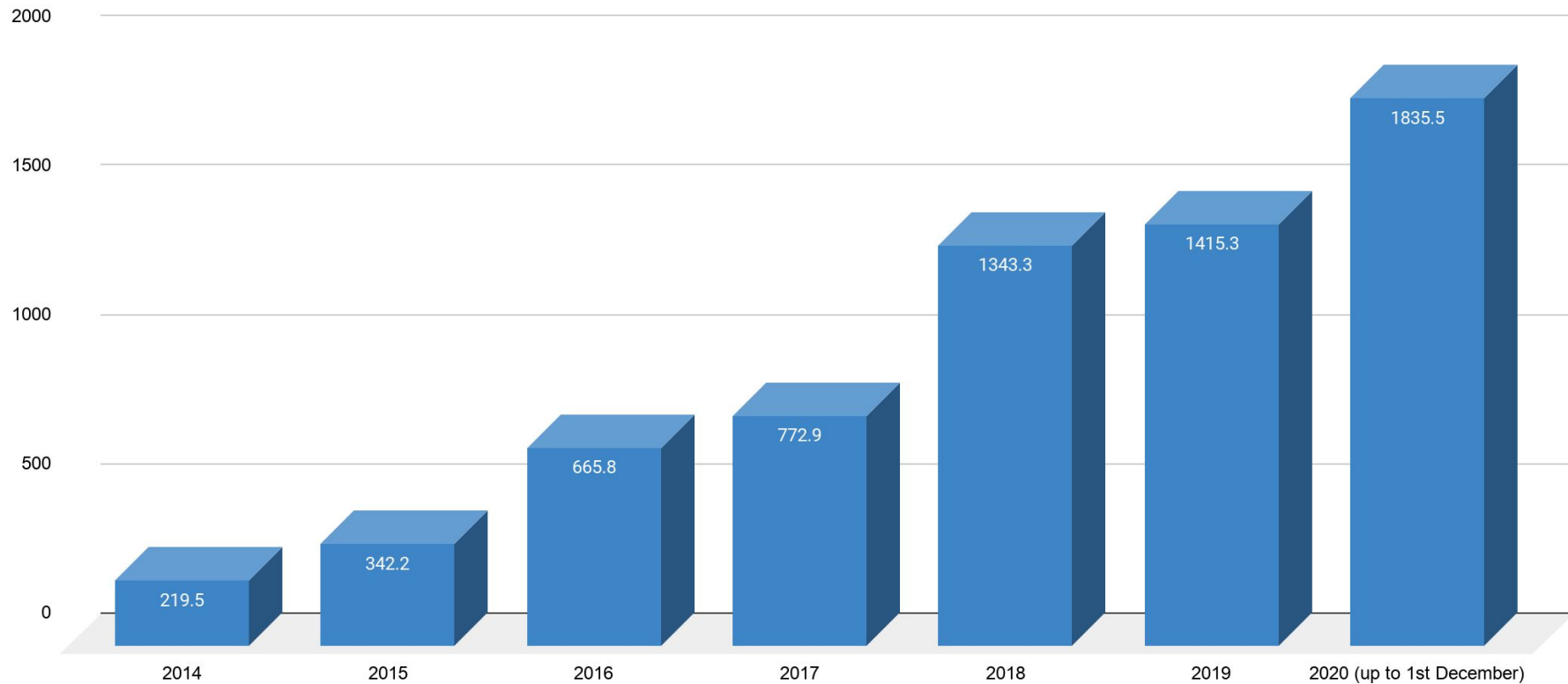
Source: BioPharmaTrend

50 Leading Investors
AI in Drug Discovery (Part 1)

Portfolios of leading biotech investors include startups from the list of Top 30

Other AI Companies
Investors
Top-30 AI Companies
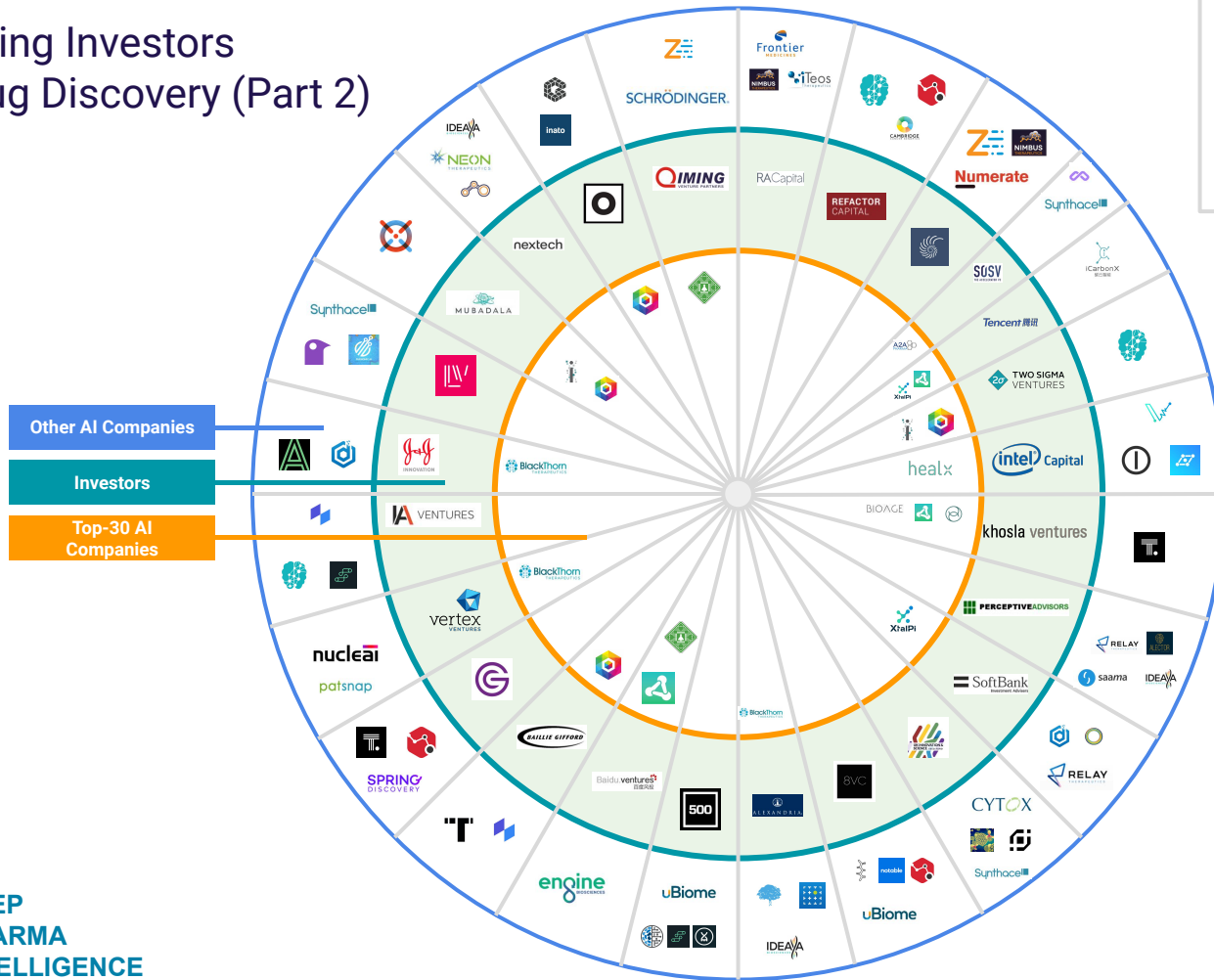
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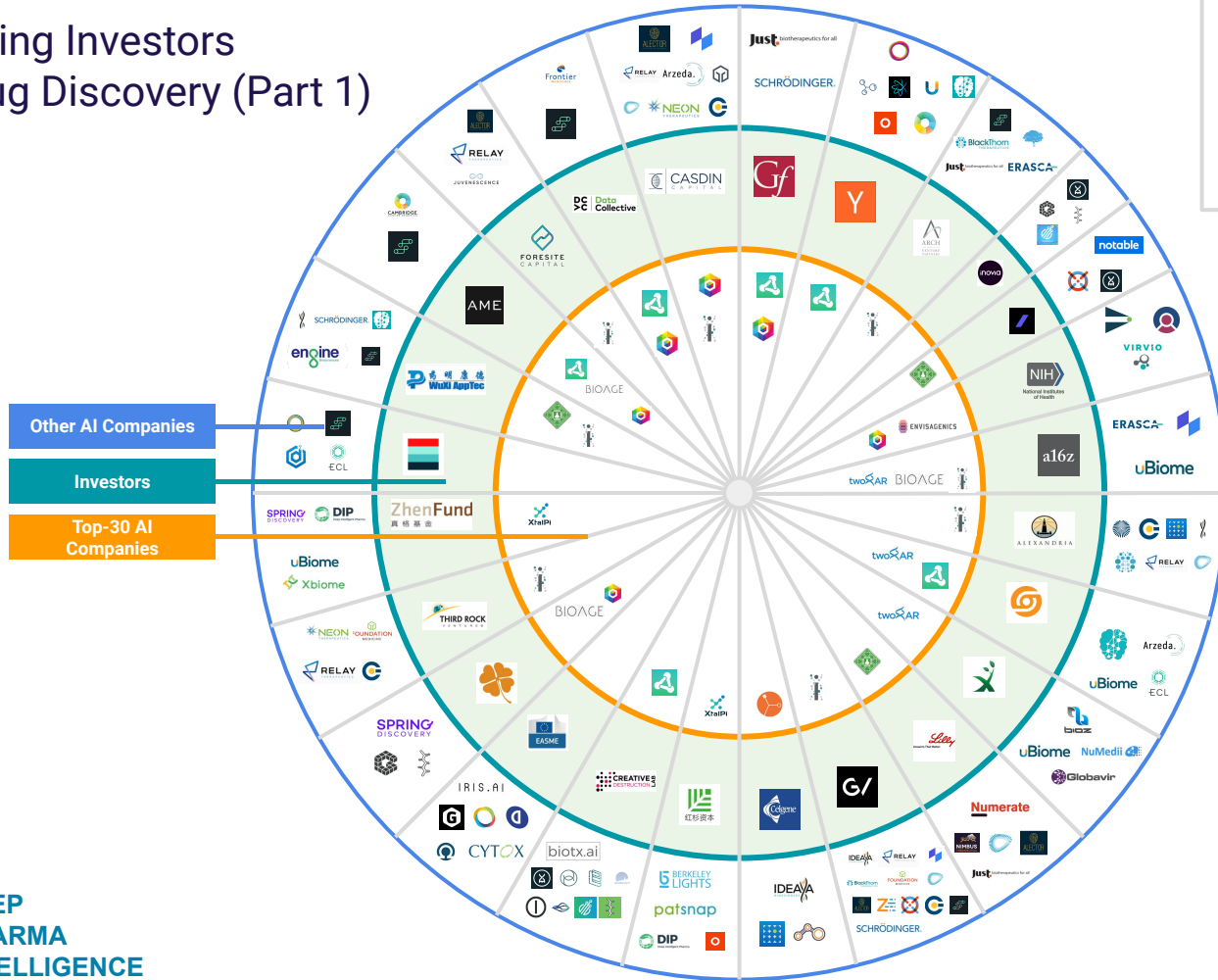
50 Leading Investors
AI in Drug Discovery (Part 2)

Portfolios of leading biotech investors include startups from the list of Top 30

Other AI Companies

Investors

Top-30 AI Companies

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Top-50 Investors in AI Companies

INVESTORS		AI Companies	Investments overall	
GV		13 AI for Drug Discovery Companies	24	Alector, BlackThorn Therapeutics, Celsius Therapeutics, Flatiron Health, Foundation Medicine, Gritstone Oncology, Ideaya Biosciences, Insitro, Relay Therapeutics, Owkin, Schrödinger, Strateos, ZappRx
Casdin Capital		10 AI for Drug Discovery Companies	11	Alector, Arzeda, Celsius Therapeutics, Flatiron Health, Foundation Medicine, Gritstone Oncology, Insitro, Neon Therapeutics, Recursion Pharmaceuticals, Relay Therapeutics
Creative Destruction Lab		10 AI for Drug Discovery Companies	10	Atomwise, BenchSci, Biotx.ai, Deep Genomics, Entropica Labs, Kyndi, NetraMark, Phenomic AI, ProteinQure, WinterLight Labs
Y Combinator		9 AI for Drug Discovery Companies	14	Athelas, Atomwise, Cambridge Cancer Genomics, CloudMedX, PostEra, Reverie Labs, Strateos, uBiome, Verge Genomics
Alexandria Venture		8 AI for Drug Discovery Companies	11	Relay Therapeutics, TARA Biosystems, BlackThorn Therapeutics, Celsius Therapeutics, GNS Healthcare, Gritstone Oncology, Ideaya Biosciences, Insitro
WuXi AppTec		7 AI for Drug Discovery Companies	8	Engine Biosciences, Insilico Medicine, Insitro, Schrödinger, Strateos, Verge Genomics, Ideaya Biosciences
Andreessen Horowitz		6 AI for Drug Discovery Companies	9	BioAge Labs, Erasca, Flatiron Health, Insitro, TwoXAR, uBiome
EASME - EU Executive Agency for SMEs		6 AI for Drug Discovery Companies	6	Accutar Biotech, Cytox, Genialis, Iris.ai, Mind the Byte, omicX
Lilly Asia Ventures		6 AI for Drug Discovery Companies	9	Alector, Gritstone Oncology, Insilico Medicine, Just Biotherapeutics, Nimbus Therapeutics, Numerate
OS Fund		6 AI for Drug Discovery Companies	9	Arzeda, Atomwise, Emerald Cloud Lab, TwoXAR, uBiome, Verge Genomics

Top-50 Investors in AI Companies

INVESTORS	AI Companies	Investments overall	
AME Cloud Ventures	5 AI for Drug Discovery Companies	**11**	Atomwise, BioAge Labs, Cambridge Cancer Genomics, Recursion Pharmaceuticals, Strateos
ARCH Venture Partners	5 AI for Drug Discovery Companies	**10**	Arbor Biotechnologies, BlackThorn Therapeutics, Erasca, Insitro, Just Biotherapeutics
Felicis Ventures	5 AI for Drug Discovery Companies	**10**	BioAge Labs, LabGenius, ProteinQure, Recursion Pharmaceuticals, Spring Discovery
National Institutes of Health	5 AI for Drug Discovery Companies	**6**	Envisagenics, Recursion Pharmaceuticals, Sangamo BioSciences, SEngine Precision Medicine, Virvio
StartX (Stanford-StartX Fund)	5 AI for Drug Discovery Companies	**7**	Bioz, Globavir Biosciences, NuMedii, TwoXAR, uBiome
Third Rock Ventures	5 AI for Drug Discovery Companies	**11**	Celsius Therapeutics, Foundation Medicine, Insitro, Neon Therapeutics, Relay Therapeutics
ZhenFund	5 AI for Drug Discovery Companies	**8**	Deep Intelligent Pharma, Spring Discovery, uBiome, Xbiome, XtalPi
Sequoia Capital China	5 AI for Drug Discovery Companies	**8**	Athelas, Berkeley Lights, Deep Intelligent Pharma, PatSnap, XtalPi
Bill & Melinda Gates Foundation	4 AI for Drug Discovery Companies	**5**	Atomwise, Just Biotherapeutics, Recursion Pharmaceuticals, Schrödinger
Celgene	4 AI for Drug Discovery Companies	**5**	Arrakis Therapeutics, Exscientia, GNS Healthcare, Ideaya Biosciences

Top-50 Investors in AI Companies

| INVESTORS	AI Companies	Investments overall	
Data Collective DCVC	4 AI for Drug Discovery Companies	**12**	Atomwise, Frontier Medicines, Recursion Pharmaceuticals, Strateos
F-Prime Capital	4 AI for Drug Discovery Companies	**5**	BenchSci, Insilico Medicine, Notable, Owkin
Foresite Capital	4 AI for Drug Discovery Companies	**10**	Alector, Insitro, Juvenescence AI, Relay Therapeutics
Founders Fund	4 AI for Drug Discovery Companies	**6**	Datavant, Emerald Cloud Lab, Roivant Sciences, Strateos
Inovia Capital	4 AI for Drug Discovery Companies	**7**	BenchSci, LabGenius, Phenomic AI, ProteinQure
Intel Capital	4 AI for Drug Discovery Companies	**4**	Healx, Kyndi, Reveal Biosciences, VERISIM Life
Khosla Ventures	4 AI for Drug Discovery Companies	**8**	Atomwise, BioAge Labs, Deep Genomics, ThoughtSpot
Perceptive Advisors	4 AI for Drug Discovery Companies	**4**	Alector, Ideaya Biosciences, Relay Therapeutics, Saama
SoftBank Vision Fund	4 AI for Drug Discovery Companies	**5**	Datavant, Relay Therapeutics, Roivant Sciences, XtalPi
UK Innovation & Science Seed Fund	4 AI for Drug Discovery Companies	**6**	Antiverse, Cytox, Desktop Genetics, Synthace

Top-50 Investors in AI Companies

INVESTORS		AI Companies	Investments overall	
8VC		4 AI for Drug Discovery Companies	6	Notable, PathAI, ProteinQure, uBiome
Alexandria Real Estate Equities		4 AI for Drug Discovery Companies	5	Arbor Biotechnologies, BlackThorn Therapeutics, GNS Healthcare, Ideaya Biosciences
500 Startups		4 AI for Drug Discovery Companies	5	Massive Bio, Strateos, uBiome, BenchSci
Baidu Ventures		3 AI for Drug Discovery Companies	4	Atomwise, Engine Biosciences, Insilico Medicine
Baillie Gifford		3 AI for Drug Discovery Companies	5	Flatiron Health, Recursion Pharmaceuticals, Tempus
General Catalyst		3 AI for Drug Discovery Companies	6	PathAI, Spring Discovery, ThoughtSpot
Vertex Ventures		3 AI for Drug Discovery Companies	6	Nuclei, PatSnap, BlackThorn Therapeutics
IA Ventures		3 AI for Drug Discovery Companies	4	Flatiron Health, Strateos, Verge Genomics
Johnson & Johnson Innovation		3 AI for Drug Discovery Companies	4	Aetion, BlackThorn Therapeutics, Datavant
Luminous Ventures		3 AI for Drug Discovery Companies	4	Phenomic AI, Sparrho, Synthace

Top-50 Investors in AI Companies

INVESTORS		AI Companies	Investments overall	
Mubadala Capital | Ventures US		3 AI for Drug Discovery Companies	5	Insitro, Owkin, Recursion Pharmaceuticals
Nextech Invest		3 AI for Drug Discovery Companies	4	Arrakis Therapeutics, Ideaya Biosciences, Neon Therapeutics
Obvious Ventures		3 AI for Drug Discovery Companies	8	Inato, LabGenius, Recursion Pharmaceuticals
Qiming Venture Partners		3 AI for Drug Discovery Companies	3	Insilico Medicine, Schrödinger, ZappRx
RA Capital Management		3 AI for Drug Discovery Companies	3	Frontier Medicines, iTeos Therapeutics, Nimbus Therapeutics
Refactor Capital		3 AI for Drug Discovery Companies	4	Cambridge Cancer Genomics, PathAI, Verge Genomics
Atlas Venture		3 AI for Drug Discovery Companies	9	Nimbus Therapeutics, Numerate, ZappRx
SOSV		3 AI for Drug Discovery Companies	10	A2A Pharmaceuticals, MendelAI, Synthace
Tencent Holdings		3 AI for Drug Discovery Companies	6	Atomwise, iCarbonX, XtalPi
Two Sigma Ventures		3 AI for Drug Discovery Companies	5	Recursion Pharmaceuticals, Verge Genomics, Antiverse

AI for Drug Discovery Market Timeline

The first AI approaches

- The first scalable AI approaches for Drug Discovery and Advanced R&D were developed and several industry players with forward-thinking executives started launching pilot collaborations and making small investments.
- However, only few market players believed in the technology.

2013-2015

Criticism

- Because AI is still a young approach within the life sciences, many pilot projects failed, creating a lot of criticism towards the use of deep learning for Drug Discovery and Advanced R&D.
- Since then the race for the acquisition of the best, AI startups began.
- Testing of the technology began.

2016-2017

Market cap growth

- Capitalization of the industry was continuously growing.
- Many bets of early investors appeared to be justified.
- Over the next several years, we can expect to see VC firms and subsidiary funds focused exclusively on the AI for Drug Discovery subsector, and funds that invest in a maximally-diverse number of AI for Drug Discovery companies.

2018

Transition from quantity to quality

- It is going to be an important milestone in transitioning from the quantity of AI-related collaborations, investments, and M&As to qualitative gains — first practical validations of previously conducted research might be appearing during this year.
- Competition for the most successful pharma AI companies will increase drastically.

2019

Intensive competition

- Pretty much all big players in pharma industry are concerned with AI adoption, the tech has become a strategic priority, among other things.

2020-2021

Pharma AI Deals

A growing number of collaborations involving AI for drug discovery

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

- a wave of proof-of-concept studies and research breakthroughs in a wide range of AI application use cases;
- a number of commercial successes and successfully reached milestones, involving AI as a central element of research
- substantial advances in democratizing AI technology, where machine learning and deep learning algorithms become available at scale to non-AI experts.
- substantial 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.

Increasing of number of partnerhips between Pharma and AI Companies over the last 5 years
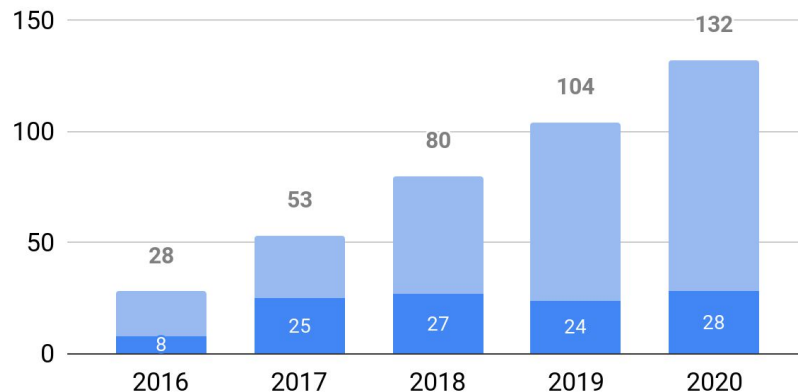
The rising interest of leading pharma and contract research organizations towards AI-driven biotech startups is a major driver for the area to become more attractive for investors, since the industry is becoming well-suited for successful exit strategies in future.

Corporation and AI-companies Participating in the Pharma AI Deals

Top 10 Leading Corporations by The Number of Major Pharma AI Deals
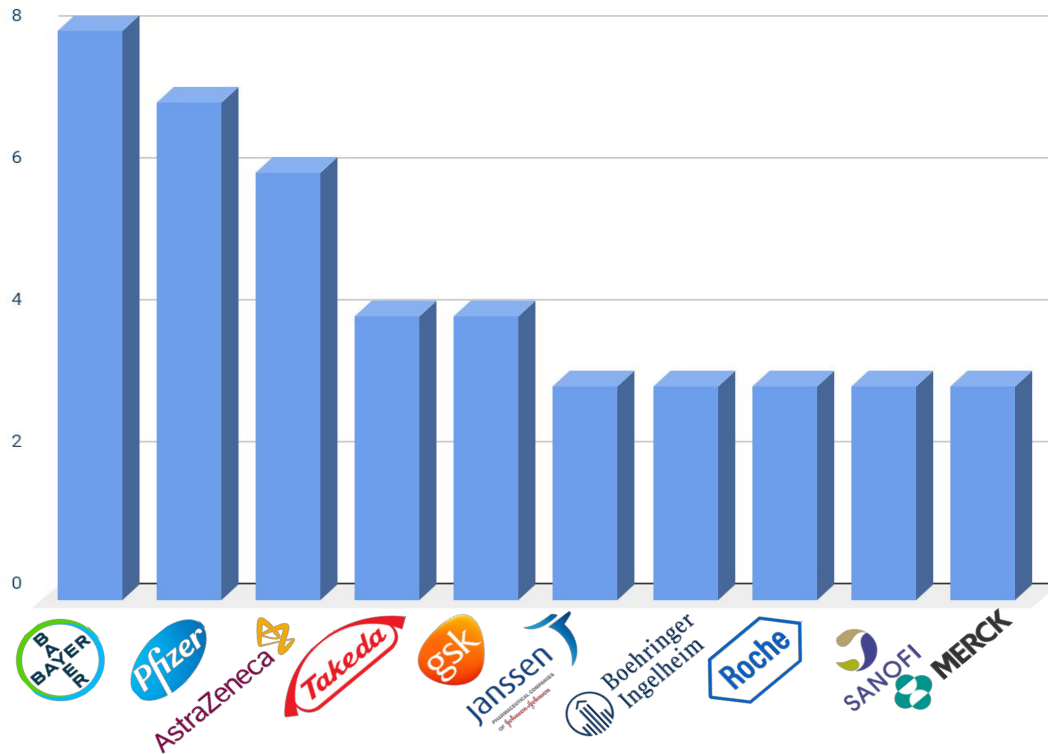
Top AI and Tech Partners by the Number of Pharma AI Deals
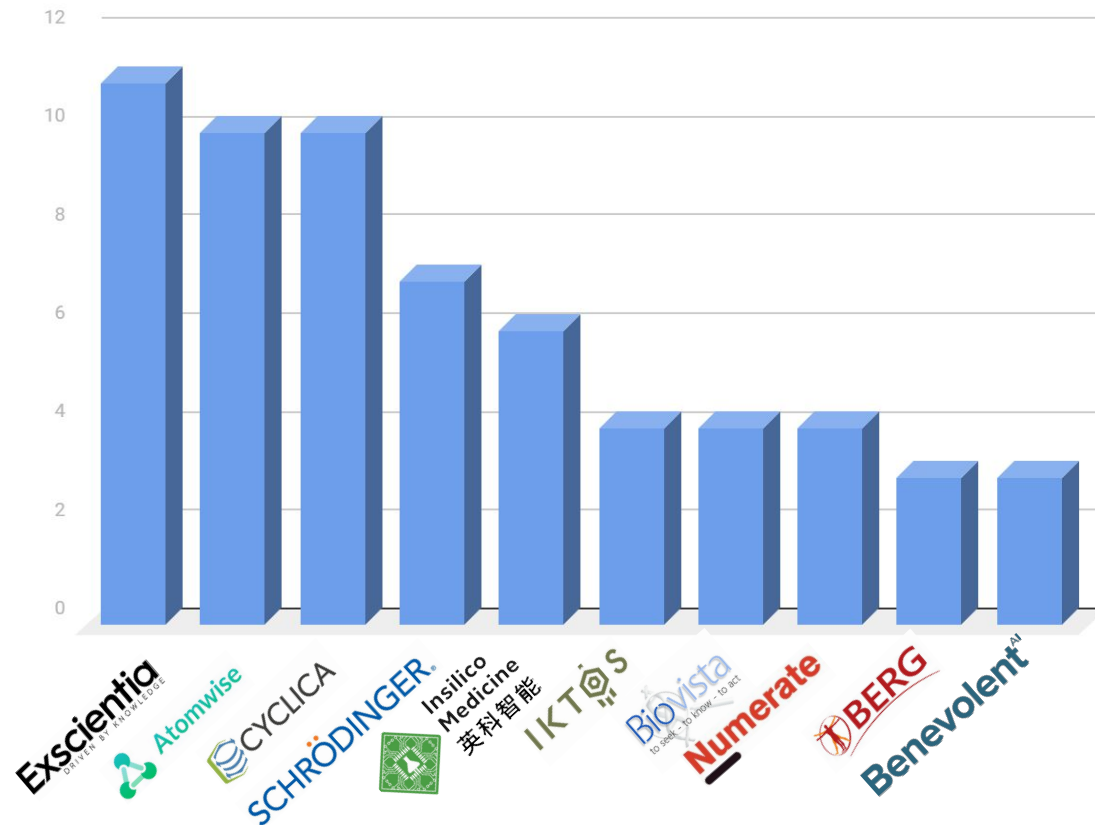
Implications

The biggest number of AI in Drug Discovery deals was conducted by **Exscientia**.

The company engages in **small molecule drug discovery, selective single target molecules, bispecific small molecules, and phenotypic drug design.**

All of the deals concluded with this company were categorized as the ones aiming at **saving costs and increasing operational efficiency** due to the character of the services provided.

Top AI Breakthroughs 2018-2020

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Notable AI Breakthroughs

March, 2018

IBM Watson released a cognitive computing platform for Clinical trial matching that has shown significant improvement in patient enrollment rate at **Mayo Clinic**. Since its implementation in the Mayo clinic in 2016, the platform demonstrated an 80% increase in enrollment in clinical trials for breast cancer. The platform also significantly reduced the time to match a clinical trial to one patient.

October, 2018

Healx has prepared a rare disease drug for a Phase 2a clinical trial in 15 months. Healx has demonstrated the power of combining domain expertise, deep learning, and proprietary data. As a result, the company implemented a scalable platform for drug discovery — Healnet. The drug was created for the of Fragile X syndrome. It tooks 15 month to conduct lead discovery, preclinical validation, and submitting a publication.

December, 2018

DeepMind built AlphaFold platform to predict 3D protein structure that outperformed all other algorithms. AlphaFold won the CASP13 competition. AlphaFold was able to most accurately predict the shape for 25 of the 43 proteins from scratch without using previously solved proteins as templates. AlphaFold uses two methods based on deep neural networks: one is trained to predict the distances between pairs of certain amino acids, and the other estimates the possible angles of chemical bonds between them.

January, 2019

Recursion Pharmaceuticals has announced progress in its collaboration with **Takeda.** Recursion has evaluated Takeda's preclinical and clinical molecules in over 60 indications in less than 18 month. New drug candidates were identified for 15 indications. Recursion's AI-enabled drug discovery platform combines massive biological data generation at scale with state-of-the-art machine learning that can draw meaning from millions of microscopy images generated in Recursion's laboratory with Takeda's compounds.

Top AI Breakthroughs

September, 2019

1. **Insilico Medicine** has published a research paper about the first in vivo active drug candidate developed from scratch (de-novo) using GENTRL system. GENTRL system is a modular drug design platform based on generative adversarial networks (GANs) and other machine learning methods. A new candidate has been developed staggeringly quickly: in 46 days, including target selection.

2. **Deep Genomics** created DG12P1 drug using an AI-augmented drug design. It is an antisense oligonucleotide therapy designed via their platform **AI Workbench** to treat rare Wilson disease, leading to copper accumulation in the liver, brain and other vital organs. The discovery took under 18 month from the concept to an actual clinical trials-ready drug candidate, which is way faster compared to classical approaches. Deed Genomics platform screened over 2,400 diseases and over 100,000 pathogenic mutations. It predicted and confirmed the precise disease-causing mechanism of the mutation Met645Arg. Then it identified 12 lead candidate molecules.

January, 2020

1. **Mendel** Recruit proprietary platform could increase patient enrollment for clinical trials by 24-50%. Mendel Recruit platform was applied retroactively to two completed oncology clinical studies and one that failed to recruit patients at a clinical trial site. Using the Mendel.ai platform resulted in a 24-50% increase over the standard practice in the number of patients correctly identified as potentially eligible. Mendel applied AI algorithms that combine the recognition of scanned documents with natural language understanding of clinical records and automated clinical reasoning.

2. A new drug candidate, DSP-1181, created using **Exscientia** Centaur Chemist Artificial Intelligence platform began clinical study. The drug was developed together with **Sumitomo Dainippon Pharma** for the treatment of obsessive-compulsive disorder, it was advanced to Phase 1 clinical trials. Less than 12 months was spent to complete the exploratory research phase when it typically takes 4.5 years.

Top AI Breakthroughs

February, 2020

Scientists from **MIT** discovered halicin — a new super powerful antibiotic capable to kill 35 the world's most problematic disease-causing bacteria, including multiresistant strains. In experiments with E. coli, this bacteria didn't develop resistance during 30 days. The model applied was able to screen more than a hundred million chemical compounds in a matter of a day, and is designed to pick out potential antibiotics that kill bacteria using different mechanisms than those of existing drugs.

September, 2020

1. **Aladdin** has built a platform for the early diagnostics of Alzheimer's disease and COVID-19. The company is building biomedical knowledge graphs — PharmaKG — around age-related disease to reveal mechanisms and potential drugs by uncovering key relationships between disease, genes, chemical compounds and drugs. Disease Diagnosis platform uses AI and multimodal data, including biomarkers, imaging, blood samples, medical records, ect.

2. **MELLODDY** — the 'Machine Learning Ledger Orchestration for Drug Discovery' group — was created by ten pharma companies to jointly develop ML models without sharing data. MELLODDY leverages the world's largest collection of small molecules with known biochemical or cellular activity to provide more accurate predictive models and improve drug discovery efficiency. MELLODDY is trying to achieve this by creating a flexible, scalable, and secure framework for federated and privacy-preserving machine learning that can train and evaluate predictive models related to drug discovery.

Computational Methods Used by the Most Advanced AI Companies

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Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
Ardigen	Bioinformatics, Deep Learning, NLP	Ardigen is a Polish bioinformatics company, part of the Selvita Group. The company is active in the field of laboratory information management systems, biological and clinical data analysis, Big Data integration, as well as custom application development. Through its know-how, experience and products, Ardigen supports the life science and healthcare industries in executing the idea of personalized medicine. Ardigen employs world-class specialists in the field of bioinformatics, biotechnology, mathematics, statistics and computer science.
Atomwise	Machine Learning, Deep Learning (Convolutional neural networks), cheminformatics	AtomNet is the first drug discovery algorithm to use a deep convolutional neural network. It excels at understanding complex concepts as a combination of smaller and smaller pieces of information. AtomNet has been predicting new potential treatments for two years. 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. It allows researchers to: reduce time, money, and uncertainty in planning experiments.
BenevolentAI	Machine Learning, Deep Learning, symbolic AI, cheminformatics	Evolved from text mining and semantic linking into knowledge graphs. Recent small efforts into DL and computational chemistry mostly for PR.

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
Berg	Machine Learning, Deep Learning, bioinformatics	Analyze data from patient samples in both healthy and diseased states to generate novel biomarkers and therapeutic targets. Allows researchers to: Generate therapeutic targets from biological data in an unbiased way, and implement personalized medicine at scale.
Berkeley Lights	Machine Learning, bioinformatics	Automate selection, manipulation, and analysis of cells. Allows researchers to: Expedite development of cell lines and automate manufacturing of cellular therapeutics
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 to improve care, enhance discoveries, gain insight into business, and enable fast data-driven decisions.
Bioz	NLP, Deep Learning, Machine Learning	Bioz has developed a search engine for Life Sciences community using natural language processing and machine learning technology to scan hundreds of millions of pages of complex and unstructured scientific papers on the web. Then it helps summarize the information into usable visualized format.
Euretos	Machine Learning, Deep Learning, bioinformatics	Euretos provides direct access to the cloud based discovery platform via user friendly application. It also allows API Integration of the discovery platform in user's company's IT environment/workflows, as well as Integration of company proprietary data and public data in a secure environment.

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
Exscientia	Machine Learning, Deep Learning, bioinformatics, cheminformatics	ML for predicting ADME, novelty, synthetic accessibility, pharmacology of molecules. Single and multi-target prediction.
Iktos	Machine Learning, Deep Learning, cheminformatics	Iktos has invented and is developing a 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, cheminformatics, bioinformatics	Comprehensive DL pipeline. Biology: Signaling pathways, DNNs for target ID and HTS analysis. Chemistry: GANs-RL for novel molecule generation.
Kyndi	NLP, Deep Learning, Machine Learning	Explainable AI
MedChemica	Machine Learning, cheminformatics	Molecular design and analysis. With over 40 years of drug hunting experience across all major target classes in 6 disease areas both in Lead Generation, Lead Optimisation and method development our goal is to accelerate the progress of our clients programmes.
nference	NLP, Deep Learning	nferX uses state-of-the-art Neural Networks (shallow and deep learning models) for real-time, automated extraction of knowledge from the commercial, scientific, and regulatory body of literature.

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
NuMedii	Big data analytics; Deep Learning, Machine Learning	Discover connections between drugs and diseases at a systems level by analyzing hundreds of millions of raw human, biological, pharmacological, and clinical data points. Allows researchers to: find drug candidates and biomarkers predictive of efficacy for diseases.
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.
Peptone	Deep Learning (TensorFlow + Keras base)	World's first protein database specifically for Deep Learning and AI applications with full Keras™ and Tensorflow™ integration.
Phenomic AI	Deep Learning, Reinforcement Learning	Phenomic predicts which cells will survive chemotherapy and identifies compounds that selectively target these resistant cells. It will then develop the compounds and bring them to market. The prediction requires the use of cell imaging technology, which is where the AI comes in.
ProteinQure	Quantum Computing, Reinforcement Learning, cheminformatics	ProteinQure is combining quantum computing, reinforcement learning, and atomistic simulations to design novel protein drugs. Using this mix of technologies they model essential processes, such as protein folding, and the underlying physics of interactions between biomolecules. Using their proprietary algorithms and external supercomputing resources, ProteinQure can design small peptide-based therapeutics (including cyclic peptides), and explore protein structures without known crystal structures.

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
Quantitative Medicine	Active Learning, Machine Learning, quantum computing	CoRE™ is a dynamic and comprehensive in silico predictive modeling platform for constructing, assessing, validating and deploying exceedingly accurate predictive models to efficiently guide the testing process and solve complex drug discovery optimization problems. CoRE™ applies cutting edge machine learning techniques from three complementary informatics technologies: Supervised Learning, Transfer Learning and Active Learning.
Reverie Labs	Evolutionary algorithms, Machine Learning	ML-based structure based predictive models for potency and ADMET/PK properties of small molecules
ReviveMed	Machine Learning, Deep Learning	ReviveMed's platform for the first time enables the rapid, high-throughput, and cost-effective application of metabolic data to discover new disease mechanisms for drug discovery and, simultaneously metabolomic biomarkers to identify which patients stand to benefit by targeting the disease mechanism.
Structura Biotechnology	Machine Learning (stochastic gradient descent and branch-and-bound maximum likelihood optimization)	The cryoSPARC System™ enables high-throughput structure discovery of proteins and molecular complexes from cryo-EM data with help of machine learning.
XtalPi	Quantum physics; Machine Learning	XtalPi's ID4 platform provides accurate predictions on the physiochemical and pharmaceutical properties of small-molecule candidates for drug design, solid-form selection, and other critical aspects of drug development.

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
BioXcel	Machine Learning, Deep Learning, cheminformatics	Bioxcel Corporation is a biopharmaceutical company pioneering the application of artificial intelligence and big data analytics integrated with drug development expertise.
C4X discovery	Machine Learning, Deep Learning, cheminformatics, bioinformatics	C4X innovative DNA-based target identification platform (Taxonomy3(R)) utilises human genetic datasets to identify novel patient-specific targets leading to greater discovery productivity and increased probability of clinical success. This is complemented by C4XD's novel drug design platform which comprises two innovative chemistry technologies, Conformetrix and Molplex, that combine 4D molecular shape analyses (based on experimental data) with best-in-class computational chemistry.
CytoReason	Machine Learning, Deep Learning, symbolic AI, cheminformatics, bioinformatics	CytoReason turns human clinical data into clear biology, to deliver data-driven target discovery and drug development. 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.
Deep Genomics	Machine Learning, Deep Learning, bioinformatics	Deep Genomics is using artificial intelligence to build a new universe of life-saving genetic therapies.

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
Desktop Genetics	Bioinformatics, Machine Learning	Desktop Genetics is a recognised leader in genome editing technology, staffed by dedicated team of genome editing experts, bioinformaticians and data scientists, driven by the real-world impact of CRISPR technology. Their core technology, DESKGEN AI, was trained on the largest database of genome editing data in the world.
C4X discovery	Machine Learning, Deep Learning, cheminformatics, bioinformatics	C4X innovative DNA-based target identification platform (Taxonomy3(R)) utilises human genetic datasets to identify novel patient-specific targets leading to greater discovery productivity and increased probability of clinical success. This is complemented by C4XD's novel drug design platform which comprises two innovative chemistry technologies, Conformetrix and Molplex, that combine 4D molecular shape analyses (based on experimental data) with best-in-class computational chemistry.
Data4Cure	Machine Learning, Deep Learning, NLP	The Data4Cure platform's modular architecture allows independent system components to handle integration and advanced analysis of heterogeneous data types spanning molecular, phenotypic and clinical data, both structured and unstructured. Data are mapped to a dynamic biomedical ontology allowing cross-referencing and joint analyses across thousands of datasets and millions of publications.
Envisagenics	Machine Learning, Deep Learning, high-performance computing	Envisagenics' SpliceCore platform integrates proprietary machine learning algorithms, high performance computing, and RNA-splicing analytics to identify disease-specific alternatively spliced RNA that will function as therapeutic targets.

Computational Methods Used by the Most Advanced AI Companies

Company	Computational methods used	Technology Abstract
Genialis	Machine Learning, Deep Learning	Blending computational biology and AI-based methods, Genialis merges and models data at the intersection of clinical and translational medicine.
GNS Healthcare	Machine Learning, Deep Learning	GNS Healthcare AI technology integrates and transforms a wide variety of patient data types into in silico patients which reveal the complex system of interactions underlying disease progression and drug response.
Healx	Machine Learning, NLP, symbolic AI, cheminformatics, bioinformatics	Healx AI platform uses natural language processing (NLP) to extract disease knowledge from published sources and to complement biomedical databases and proprietary, curated data. The data is integrated in the form of the largest, rare disease-focused Knowledge Graph. It shows prioritised hidden and novel connections between drugs and diseases when explored by expert pharmacologists and biologists.

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

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

The industry of AI in Biopharma continues to grow after a long period of skepsis, which is reflected in ongoing flow of investments and increase in the number of collaborations between pharmaceutical corporations and AI companies in 2020 compared to 2019 and previous years. The difference between Pharma and Biopharma fields is that biopharma medicines and drug products are manufactured in living organisms like bacteria, yeast and mammalian cells. The prefix "bio" refers to how drugs are produced. Biopharma is the subset of drugs produced by biological methods. Pharmaceutical drugs cover biological means as well as chemical synthesis.

The Biopharma industry's growth dynamics is largely influenced by the more active participation of largest pharmaceutical corporations in the AI-related investment and research collaborations. Despite some Pharma corporations still being critical about AI applications, the volume of research, number of scientific publications in the field of AI in Biopharma, and research collaborations between pharma companies and AI-expertise vendors are rapidly increasing.

Research in AI is facing challenges today, but the demand for the ML/AI technologies, as well as for ML/AI talent, is growing in pharmaceutical and healthcare industries and driving the formation of a new interdisciplinary field — data-driven drug discovery/healthcare. The overall success of all the companies in the industry depends strongly on the presence of highly skilled interdisciplinary leaders. It will be crucial to hire top AI experts, especially for Big Pharma companies that are fighting to survive.

Trending and most innovative R&D approaches of top AI in Biopharma companies include application of:

Machine Learning

Deep Learning

Natural Language Processing

Cognitive Reasoning Technologies

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

AbbVie is a global, research-based biopharmaceutical company formed in 2013 following separation from Abbott. The company's mission is to use its expertise, dedicated people and unique approach to innovation to develop and market advanced therapies that address some of the world's most complex and serious diseases.

There is not much information about use of artificial intelligence in drug discovery by AbbVie. But it does have a confidential project listed with Atomwise. Also, in September 2016, together with its partner AiCure, AbbVie announced how its AI-based patient monitoring platform improved adherence in an AbbVie phase 2 schizophrenia trial.

Main focus areas:

- Alzheimer's Disease
- Schizophrenia
- Parkinson's Disease
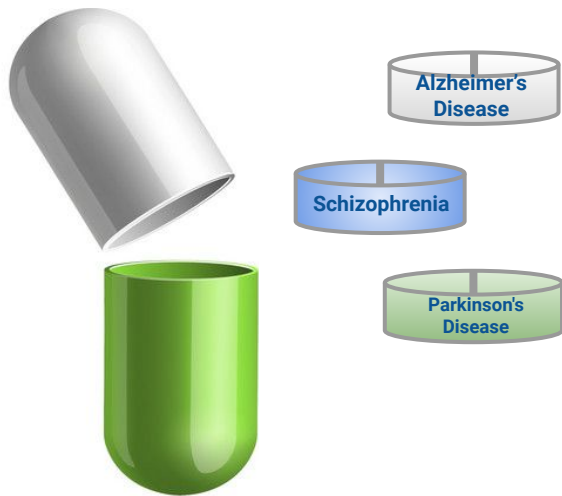
The way AI is used:

- to visually confirm medication ingestion;
- to increase medication adherence in patients;
- to use data to assess effectiveness of treatment.

Cooperation:

- AiCure
- Mission Therapeutics

Source

Crunchbase
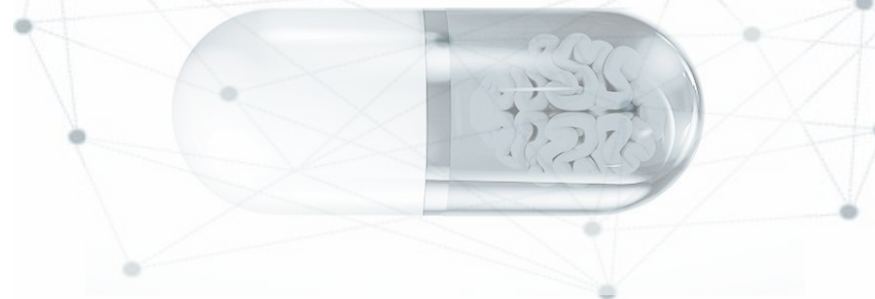
How **Abbvie** Uses AI in R&D?

abbvie

Abbvie and Mission Therapeutics collaboration is aimed at developing DUB inhibitors that promise to treat two currently incurable conditions, Parkinson's and Alzheimer's diseases. With over 50 million Americans struggling Alzheimer's and dementia, this AI partnership will bring treatment closer and hope for many.

1. Abbvie in cooperation with another AI-specialized company AiCure, a clinically-validated artificial intelligence company that visually confirms medication ingestion on smartphones, announced that study results presented during the International Society for CNS Clinical Trials and Methodology (ISCTM) Scientific Sessions confirm that use of the AiCure Platform significantly increases medication adherence in patients with schizophrenia, as measured by drug concentration levels.

Subjects of the investigation were enrolled and randomized to placebo or ABT-126	**Subjects were dosed once daily (QD) 25, 50, or 75mg ABT-126 or matching placebo, as 3 capsules in the morning for 24 weeks**	**Subjects were monitored either by AiCure or by modified Directly Observed Therapy (mDOT) at least 3 times per week**	**Adherence was measured by review of returned study drug blister and scheduled pharmacokinetic sampling**

2. The sub-study was part of a larger Phase 2, multicenter, randomized, double-blind, placebo-controlled, dose-ranging, parallel-group, study in nonsmoking subjects with schizophrenia who were clinically stable. Subjects were enrolled and randomized to placebo or ABT-126. The AiCure platform was introduced in 10 of 31 US sites; subjects were monitored either by AiCure or by modified Directly Observed Therapy (mDOT) at least 3 times per week. In addition, adherence was measured by review of returned study drug blister and scheduled pharmacokinetic sampling.

3. Results: cumulative adherence, measured by study drug concentrations above the LLOQ (minimum required therapeutic level), were higher through 24 weeks for subjects monitored using the AiCure platform (89.7%) compared with subjects monitored using mDOT (71.9%). This research adds to the growing body of scientific evidence showing the advantages of using AI to increase statistical power and reduce sample size in clinical trials, thereby decreasing costs and accelerating drug development.

Source

AiCure	Blog.Benchsci	Healthcare Weekly

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

AstraZeneca is a global, science-led biopharmaceutical company, whose innovative medicines are used by millions of patients worldwide. Jim Weatherall, Vice President in AstraZeneca, said that data science and AI has the potential to transform the way they develop new medicines – turning yesterday's science fiction into today's reality with the aim of enabling the translation of innovative science into life-changing medicines.

AstraZeneca uses AI to combine information from multiple sources in order to draw more accurate conclusions than if science literature was analysed by hand. AI also has the potential to find patterns in these graphs revealing previously unexplored hypotheses.

Main focus areas:

Kidney Disease

Fibrosis
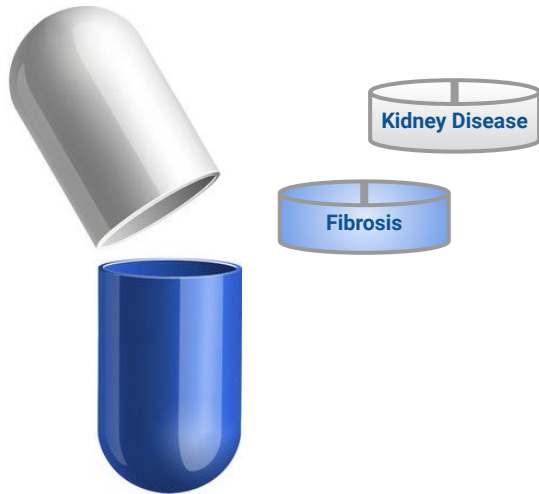
The way AI is used:

- to build disease understanding through knowledge graphs to integrate genomic, disease, drug and safety information;
- to identify new targets for novel medicines;
- for fast, accurate image analysis.

Cooperation:

- Schrödinger

Source

AstraZeneca

How **AstraZeneca** Uses AI in R&D?

AstraZeneca focuses on the discovery, development and commercialisation of prescription medicines, primarily for the treatment of diseases in three therapy areas - Oncology, Cardiovascular, Renal & Metabolism and Respiratory. The company has turned to AI to cut development costs by improving the efficiency of repetitive tasks and engendering better-informed decision.

1. The knowledge graphs are used to give scientists the information they need about genes, proteins, diseases and compounds and how they relate to each other. Using AI to combine information from multiple sources, they hope to draw more accurate conclusions than if researchers analysed science literature by hand. AI also has the potential to find patterns in these graphs revealing previously unexplored hypotheses. The company's knowledge graphs integrate:

Genomic	Disease	Drug	Safety

Researchers can ask key questions to help identify and prioritise drug targets
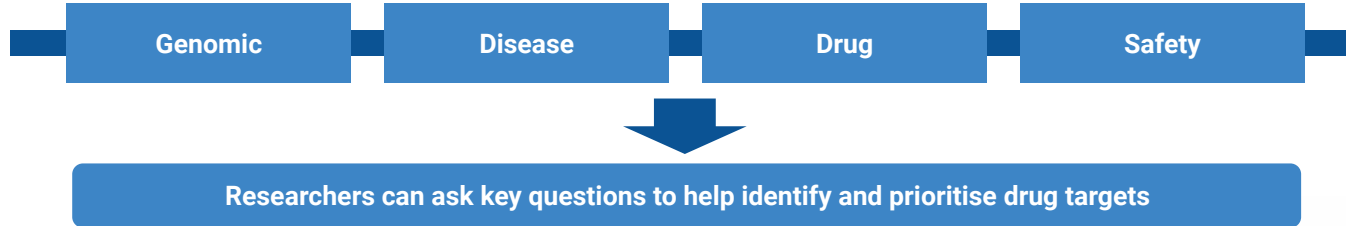
2. Discovering a potential drug molecule requires several years of detailed scientific research. AI is enabling us to rapidly generate novel ideas for molecules to make and rank these ideas using predictions based on large data sets available to us. Having identified promising molecules, the next step is to synthesise the molecules in the laboratory. AI is starting to help here too – the science of synthesis prediction is rapidly evolving and scientist will soon be able to use AI to help deduce the best way to make a molecule in the shortest time.

3. AI systems are trained to assist pathologists in analysing samples accurately and more effortlessly. This has the potential to cut analysis time by over 30%. For one of their AI systems, they implemented an approach inspired from how some self-driving cars understand their environment. They trained the AI system to score tumour cells and immune cells for a biomarker, called PD-L1, which has potential to help inform immunotherapy-based treatment decisions for bladder cancer.

Source | AstraZeneca | TechCrunch

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

Amgen is one of the world's leading biotechnology companies committed to unlocking the potential of biology for patients suffering from serious illnesses by discovering, developing, manufacturing and delivering innovative human therapeutics. This approach begins by using tools like advanced human genetics to unravel the complexities of disease and understand the fundamentals of human biology.

AI is but one of a series of emerging digital capabilities Amgen is advancing to improve how they do a whole host of activities across the company — from drug discovery and patient identification to optimized interactions with physicians. Other technologies that company is leveraging include digital automation, natural language processing, advanced analytics.

Main focus areas:

Cardiovascular Diseases

Osteoporosis
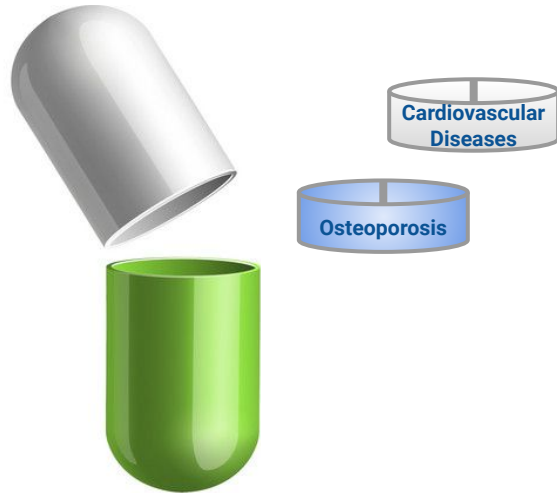
The way AI is used:

- to boost the accuracy of risk predictions;
- to provide personalized approach to patient care;
- to support compliance via real-time answers with accuracy, consistency;
- to use data to determine the most effective treatment.

Cooperation:

- Owkin

Source

Wired

How **Amgen** Uses AI in R&D?

Amgen is piloting a process using AI that has the potential to greatly enhance its ability to find patterns in manufacturing deviations and to prevent their recurrence. The AI tool will replace a manual, labor-intensive process with one that can look across large data sets and find correlations between obscure signals and events which the previous system could have missed.

1. While large company manufactures, purifies, and packages biotech drugs, a huge amount of diverse data is generated, not all of which is digitized. The focus of Amgen is the application of data science specifically in quality operations, using a data science process:

Ask an interesting question → Get the data → Explore the data → Model the data → Visualise the results
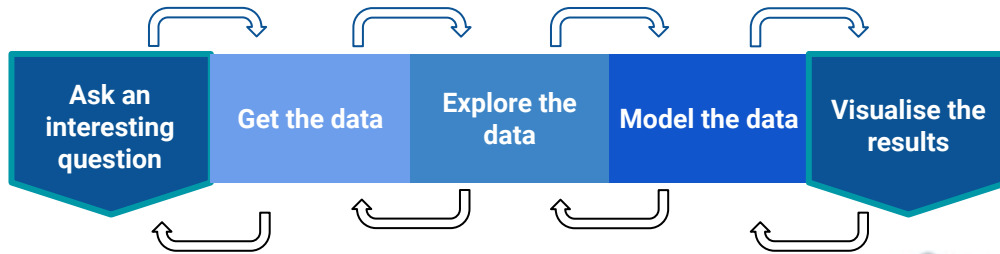
Quality data sciences creates solutions that unlock and leverage data. These solutions will efficiently provide insights and intelligence for the Quality Operation. This involves:

1) Ensuring data access; **2) Application of appropriate analysis methods to unlock information; 3) Meaningful visualisation**

2. Amgen have created a project team to look for a system algorithm that could replicate and perhaps improve upon the manual process. The goal was to think big but start small and build a product that could be deployed across the manufacturing network. Using an **agile development approach** and **natural language processing (NLP)** tools, the team developed a consistent algorithm that was able to reasonably replicate the manual process.

NLP is described as an AI technology that turns text into numbers, which can be read by a computer and used to identify similar records. Each record has a series of numbers associated with it that can be analyzed to create similarity scores. The records can then be clustered together. Those clusters can then be given to an subject matter expert, who can decide if there is trending and if action should be taken. Feedback can then be given to the algorithm, which can be adjusted.

Source

Wired	Pharmaceutical Online

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

BAI

BenevolentAI is the global leader in the application of AI for scientific innovation. The company's aim is to accelerate the journey from inventive ideas to medicines for patients by developing AI to generate new treatments for some of the world's 8,000 untreated diseases. BenevolentAI integrates AI technologies at every step of the drug discovery process: from early discovery to late stage clinical development.

The company has developed the Benevolent Platform™ — a leading computational and experimental discovery platform that allows our scientists to find new ways to treat disease and personalise medicines to patients. The Benevolent Platform™ focuses on three key areas: Target Identification, Molecular Design and Precision Medicine.

Main focus areas:

Kidney Disease

Cancer

Fibrosis

Parkinson's Disease
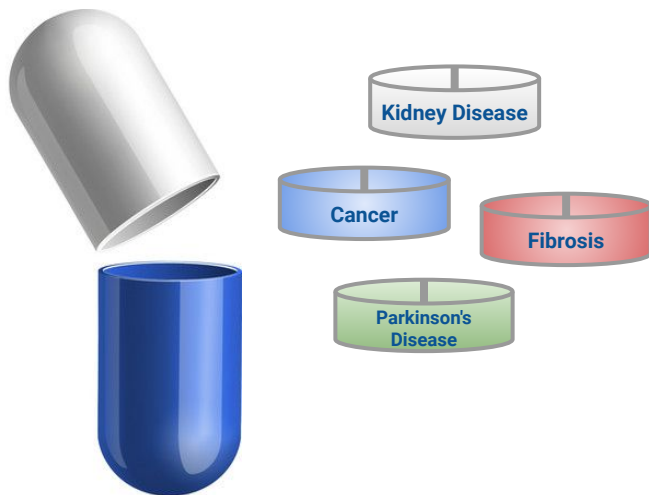
The way AI is used:

- to force the discovery of drug patterns;
- to collect more diverse data;
- to identificate specific target;
- in molecular design;
- in patient stratification.

Cooperation:

- Neuropore Therapies
- Novartis
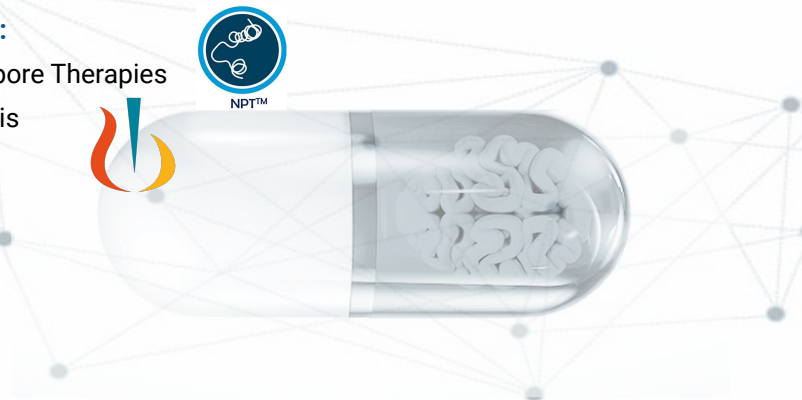
Source | Wired | Benevolent.ai

How **BenevolentAI** Uses AI in R&D?

BAI

The Benevolent Platform™ of computational and experimental technologies and processes draws on vast quantities of mined and inferred biomedical data and is built and used by their world-class scientists, researchers, and technologists, working side-by-side, to improve and accelerate every steps of the drug discovery process.

1. BenevolentAI uses AI to mine and analyse biomedical information, from clinical trials data to academic papers. The company's approach:

- **AI-Augmented molecular design**
- **Hypothesis generation and target identification**
- **Patient stratification for better clinical trials**
- **Benevolent Knowledge Graph including algorithmically derived knowledge**

AI
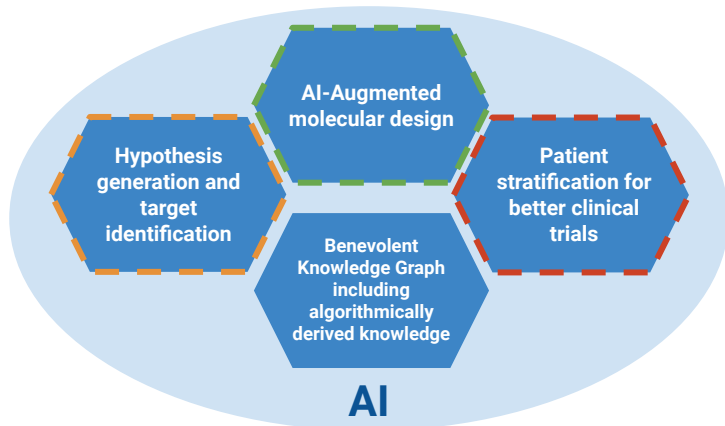
2. BenevolentAI has spent the last five years developing a knowledge pipeline that pulls data from various structured and unstructured biomedical data sources and **curates and standardizes this knowledge via a data fabric**.

This is fed into our proprietary **knowledge graph** which extracts and contextualises the relevant information.

The knowledge graph is made up of a vast number of contextualised, machine curated relationships between diseases, genes, drugs and with over 20 types of biomedical entities.

3. Relation inference AI models help to predict **potential non-obvious disease targets** that may be overlooked. Their specific expression based models help to identify proteins, genes that express differently in a disease and healthy cell.

4. By leveraging advanced AI, the *EvoChem* product designs de novo compounds based on multiparametric optimisations with a scoring function that factors in all the properties the company is seeking to optimise for that molecule.

5. Company applies ML models to identify patient groups by the molecular signature of their disease and design, allowing to run faster clinical trials.

Source | Wired | Benevolent.ai |

Most Innovative R&D Approaches of AI in Biopharma. **Boehringer Ingelheim**

Boehringer Ingelheim Boehringer Ingelheim is one of the world's largest pharmaceutical companies, and the largest private one. The company's key areas of interest are: respiratory diseases, metabolism, immunology, oncology and diseases of the central nervous system.

The focus of the company's AI-related activity is in doing so is on diseases for which no satisfactory treatment option exists to date. The company therefore concentrates on developing innovative therapies that can extend patients' lives. In animal health, Boehringer Ingelheim stands for advanced prevention.

Main focus areas:

- Alzheimer's Disease
- ALS
- Schizophrenia
- Parkinson's Disease
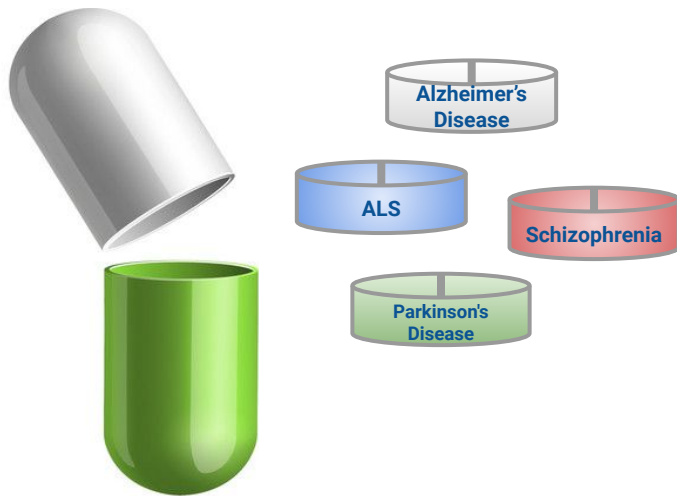
The way AI is used:

- to boost the efficiency speed;
- to reduce the time needed to discover a new drug;
- to improve the quality of discovered drugs and molecules.

Cooperation:

- Bactevo
- Bi X

Source | Boehringer

How **Boehringer Ingelheim** Uses AI in R&D?

Boehringer Ingelheim

Boehringer Ingelheim has partnered with UK-based AI tech company Bactevo to speed up its drug discovery efforts. In this collaboration, Boehringer will leverage Bactevo's AI-powered platform – Totally Integrated Medicines Engine platform (TIME) – to boost the efficiency, speed, and quality of drug discovery from small molecule lead compounds. As a result they obtain the reduction of time to take drugs to market for treatment of conditions caused by defects in mitochondrial function. It essentially brings together the powerful drug research experience at Boehringer and state of the art TIME drug discovery platform to discover new medicines for ALS, Parkinson's disease and Alzheimer's disease.

1. With the founding of BI X as independent subsidiary Boehringer Ingelheim will focus on breakthrough innovative digital solutions in healthcare from idea to pilot. The start-up will work closely together with all three business units of the company - Human Pharma, Animal Health and Biopharmaceuticals. It will provide a platform for collaborating with specialists in the field of data science, agile software development and user experience design.

2. BI X will develop prototypes for new products and solutions and test them together with the company's business units in pilot phases. The business units will then use the successfully developed new products and solutions themselves and bring them to the market. This approach is to ensure that knowledge and experience accrued at BI X are being quickly integrated into the digital lab's parent house.

3. Analytical algorithms in audio tools can lead to advances in the earlier diagnosis of diseases in humans and animals. SoundTalks, an audio monitoring system for the early detection of respiratory diseases, is currently being tested in livestock farming. In humans as well, faster treatment can slow or even halt the progression of a disease – which is essential, particularly for central nervous system disorders. Intelligent speech recognition software – via smartphone, for example – will be able to analyze speech patterns, recognize risks, and thereby contribute to a reliable diagnosis and effective therapy.
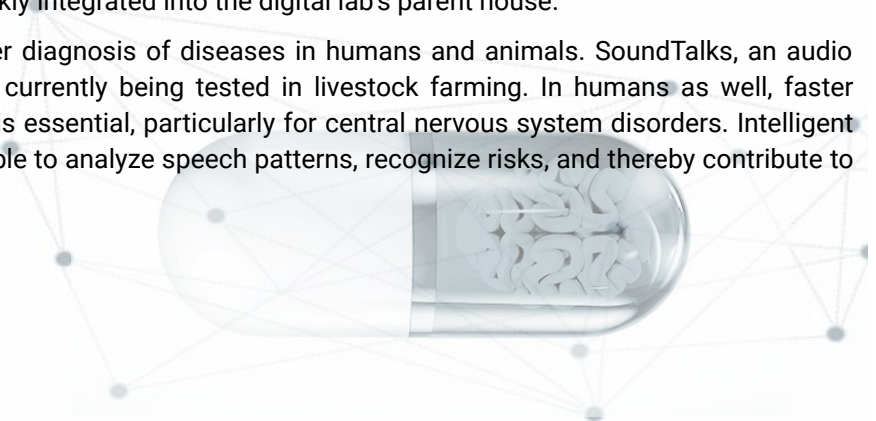
Source | eHealth News | pmlive

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

Their vision as a company is to build a major biopharmaceutical corporation while focusing on the discovery, the development, and the commercialization of products for the treatment of cancer and other severe, immune, inflammatory conditions. There are more than 300 clinical trials at medical centers using compounds from Celgene. The company is transforming pharmacovigilance (PV) to drive the new era of patient safety.

Pharmacovigilance detects, assesses, and prevents adverse events (AEs) and other drug-related problems by collecting, evaluating, and acting upon AEs. The value of using AI methodologies in PV is compelling; however, as PV is highly regulated, acceptability will require assurances of quality, consistency, and standardization.

Main focus areas:

- Autoimmunity
- Cancer
- Pharmacovigilance
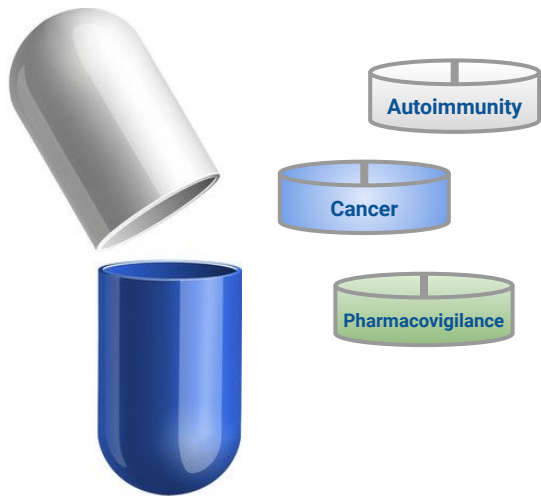
The way AI is used:

- to speed up the discovery of drug candidates for for cancer and autoimmune diseases;
- to identify and standardize PV knowledge elements;
- to develop, review and validate cognitive services;
- to increase operational efficiency, consistency, quality of data collection, and signal detection.

Cooperation:

- GNS Healthcare

Source Springer
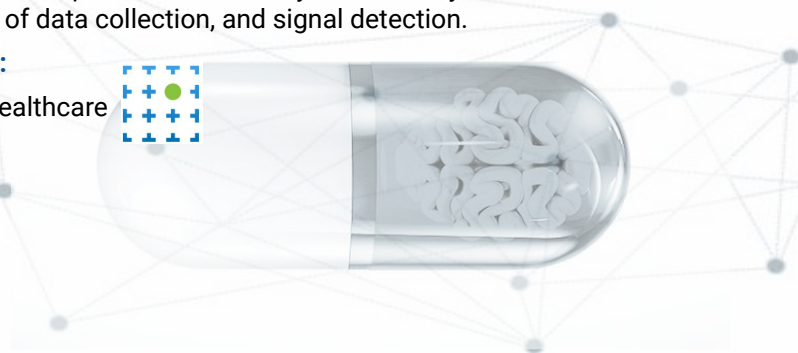
How **Celgene** Uses AI in R&D?

Celgene force boost AI implementation in drug discovery particularly machine learning and deep learning. Machine learning involves computing techniques that analyze vast amounts of data to find understanding that might be too abstract and time consuming for humans. Deep learning takes that even further, using code that attempts to mimic the brain's ability to recognize patterns in unstructured data.

1. In the past, researchers relied on imperfect image-processing algorithms to analyze cancer cells, and then they corrected them by hand. With tens of thousands of cells, this required a huge expenditure of time and effort. But using deep learning, images can be processed almost instantaneously with much better results. For these analyses use:

Amazon SageMaker machine-learning platform

Apache MXNet deep-learning framework

Virtually analyzing the biological impact of a potential drug

Toxicology prediction

*without putting live patients (or even lab rats) at risk
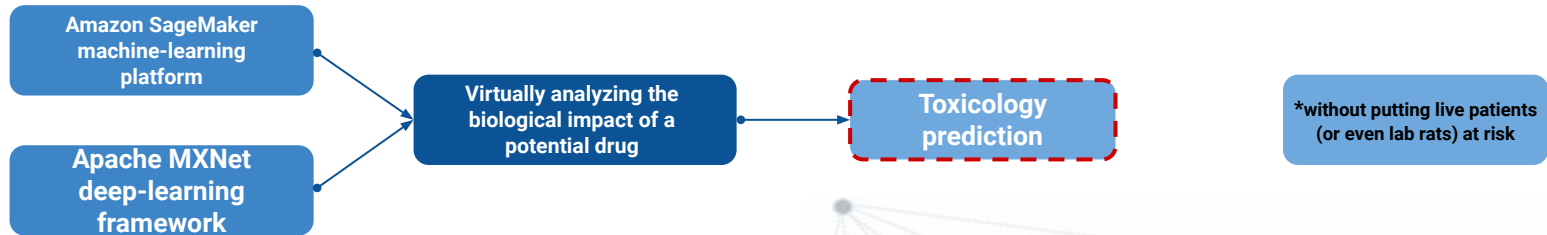
2. Pharmaceutical research revolves heavily around exceedingly complex algorithms to predict how certain compounds will interact with the human body. To this end, Celgene uses high-performance **Amazon EC2 P3** instances powered by NVIDIA Tesla V100 Tensor Core GPUs (graphics processing units) to process the complexity. These NVIDIA GPUs have thousands of cores that accelerate the training of machine-learning models (which can, for instance, test the effectiveness of a drug at faster and more accurate rates). The results have been game changing: **A model that once took two months to train can now be trained in four hours**.

3. AI is used to identify areas across the pharmacovigilance (PV) value chain that can be augmented by cognitive service solutions using the methodologies of contextual analysis and cognitive load theory. It will also provide a framework of how to validate these PV cognitive services leveraging the acceptable quality limit approach.

Source

| Springer | Labiotech | AWS Amazon |

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

GlaxoSmithKline has 3 global businesses - Pharmaceuticals, Vaccines, Consumer Healthcare - that research, develop and manufacture innovative pharmaceutical medicines, vaccines and consumer healthcare products. Their R&D approach focuses on science related to the immune system, use of genetics and advanced technologies.

GlaxoSmithKline has many deals with different companies such as Exscientia, Insilico Medicine, Insilico Biotechnology to use new computer modelling systems to bring differentiated, high-quality and needed healthcare products.

Main focus areas:

Vaccines

Immune System
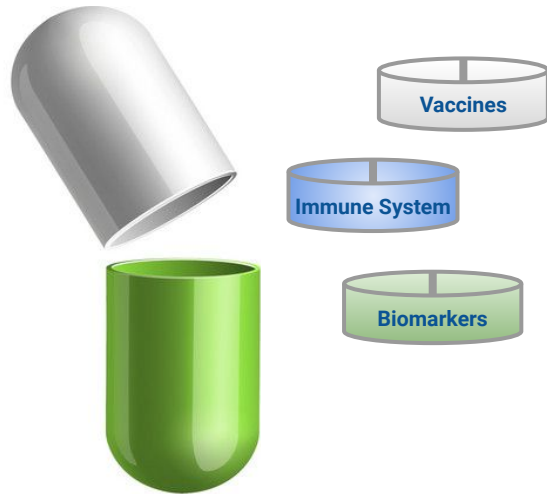
Biomarkers

The way AI is used:

- to improve the discovery of drugs, biomarkers, and new vaccines;

- to interpret and understand genetics and genomic data;

- to understand the effect of interventions on diseases.

Cooperation:

- Exscientia

- Insilico Medicine

Source GSK

How **GSK** Uses AI in R&D?

The goal of GSK is to achieve a sustainable flow of meaningful new treatments, utilising modalities such as small molecules, antibodies, antibody drug conjugates and cells, either alone or in combination. Their research focuses on science related to the immune system and human genetics, while leveraging advanced technologies including functional genomics, AI and machine learning.

1. According to the GSK and Exscientia collaboration, AI enabled platform will be applied and combined with the expertise of GSK, in order to discover novel and selective small molecules for up to 10 disease-related targets, nominated by GSK across multiple therapeutic areas.

2. GSK evaluates Insilico Medicine technology in the identification of novel biological targets and pathways of interest to GSK to enhance its drug discovery process.

3. GSK uses Insilico' Biotechnology technology platform to analyse predictive simulations of cell responses. As a result an almost unlimited number of scenarios will be generated and utilized to significantly reduce the number of experiments necessary during bioprocess development. This has the potential to cut down the time taken to research Vaccine manufacturing processes and could therefore speed up the time-to-market for candidate Vaccines in GSK's research portfolio.

Insilico's technology is built around Insilico Cells™:

| Genome-based mechanistic network models of common host organisms | → | Models are refined and calibrated | → | Models become individualized representation of the specific cells in silico | → | Simulation of cells behavior in a bioprocess |
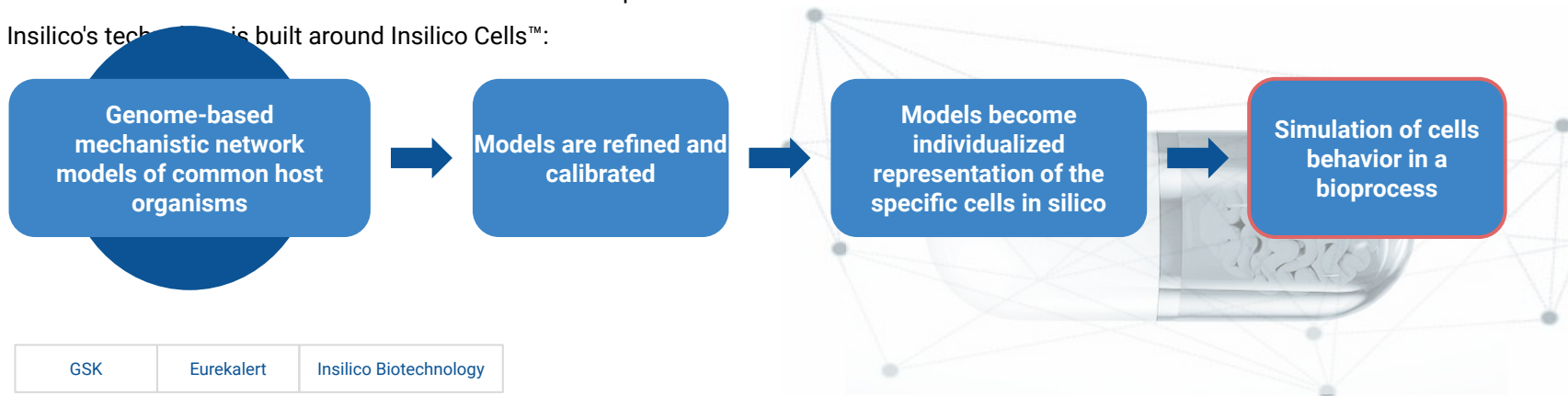
Source

| GSK | Eurekalert | Insilico Biotechnology |

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

Gilead is focused on developing and delivering medications that advance the treatment of life-threatening diseases. The commercial success of their products provides them with the resources to generate new clinical data defining their profiles and supports their development of new therapeutic advancements. As they bring new products into clinical development, their goal remains the same – to discover, develop and commercialize therapeutics that advance patient care.

In spring 2019 Gilead and insitro announced that the companies have entered into a strategic collaboration to discover and develop therapies for patients with nonalcoholic steatohepatitis (NASH).

Main focus areas:

Nonalcoholic Steatohepatitis
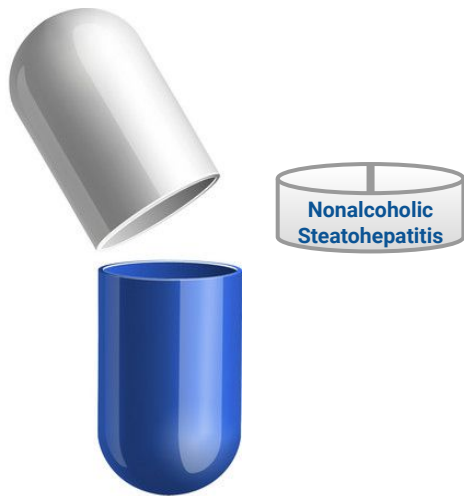
The way AI is used:

- to create disease model;
- to discover new targets that influence disease progression and regression.

Cooperation:

- insitro **insitro**

Source   Gilead
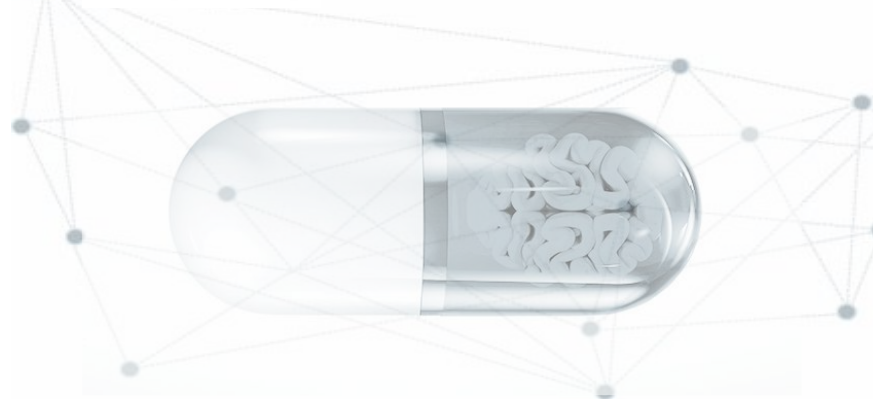
How **Gilead** Uses AI in R&D?

According to John McHutchison, the company's Head of Research and Development, Gilead is committed to researching and developing treatments for patients living with NASH, particularly those with advanced fibrosis who have the greatest unmet need. Gilead is able to utilize deep learning to explore the scientific underpinnings of the biology and clinical spectrum of NASH, with the goal of accelerating the development of highly effective treatment options for patients with this disease.

1. The startup's insitro Human platform combines AI with human genetics and genomic data to provide insights into the disease's makeup and progression, propose forms of treatment and predict patient responses to those therapies. With that information, Gilead is planning to chemically develop up to five of the proposed treatments for NASH.

2. By generating high-throughput, functional genomic data sets that align with patient data, and interpreting those data via novel machine learning methods, insitro builds predictive models that can accelerate target selection and the design of effective therapeutics. The company is building a high-throughput bio-data factory based on state-of-the-art technologies from bioengineering, allowing the creation of large data sets that enable cutting edge machine learning methods to be brought to bear on key bottlenecks in drug development.

Gilead datasets from patients and preclinical trials **+** Insitro IHS platform → Data interpretation with machine learning methods → Predictive model → Target 1, Target 2, Target 3, Target 4, Target 5 → Design of new drugs & therapeutics
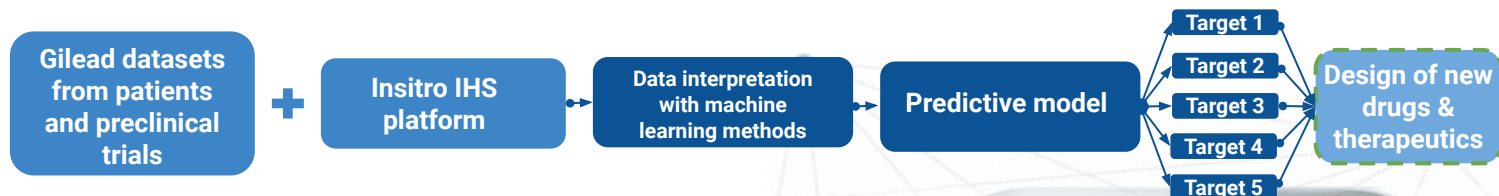
3. The insitro Human (ISH) platform applies machine learning, human genetics and functional genomics to generate and optimize unique in vitro models and drive therapeutic discovery and development. The ISH platform provides insights into disease progression, suggest candidate targets, and predict patient responses to potential therapeutic interventions. Gilead can advance up to five targets identified through this collaboration and is responsible for chemistry and development against these targets.

Source

Wire	GEN	Beckershospitalreview

Most Innovative R&D Approaches of AI in Biopharma. **Insilico Medicine**
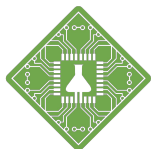
Insilico Medicine, Inc. is a bioinformatics company located at the Emerging Technology Centers at the Johns Hopkins University Eastern campus in Baltimore. It utilizes advances in genomics, big data analysis and deep learning for in silico drug discovery and drug repurposing for age-related diseases. The company pursues internal drug discovery programs and geroprotector discovery and provides services to pharmaceutical companies.

Combining genomics, big data analysis, and deep learning, the company has been using artificial intelligence algorithms to potentially discover the next world-changing drug.

Main focus areas:

- Alzheimer's Disease
- Sarcopenia
- Cancer
- Parkinson's Disease
- Fibrosis
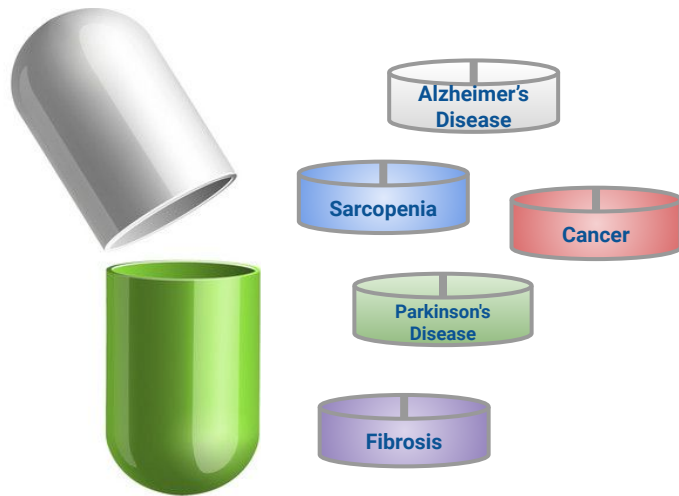
The way AI is used:

- to cheaper and faster discover of drug molecules;
- to imagine new molecules with drug-like properties;
- to find new drug candidates, biological targets and molecules;
- to validate the targets, using novel chemistry.

Cooperation:

- BioTime
- Juvenescence AI Limited
- Bitfury

BIOTIME

JUVENESCENCE.AI

Bitfury
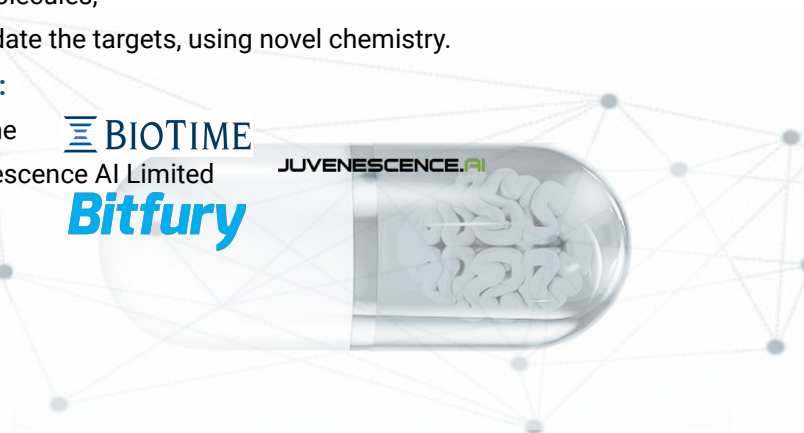
Source | Eurekalert | Insilico

How **Insilico Medicine** Uses AI in R&D?
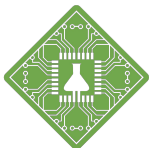
Next-generation AI developed by Insilico Medicine can be used to validate, assess and improve the quality of biological samples as well as learn using large volumes of heterogeneous data without human intervention. Multiple new methodologies including the feature importance, deep feature selection and deep pathway analysis among the others can provide the biologically-relevant interpretation of the inner workings of the AI systems.

1. Since 2016, Insilico Medicine researchers have been working to get GANs (Generative Adversarial Networks consisting of two distinct neural networks) to "imagine" new molecules with drug-like properties. In 2017, they combined this with another type of groundbreaking A.I. in the form of Reinforcement Learning. Reinforcement Learning is built around the notion of A.I. agents which use trial-and-error to maximize some kind of reward.

Nominated Target → GENTRL → Rapid synthesis → *in vitro* assays → *in vivo* assays → Pre-clinical Trials
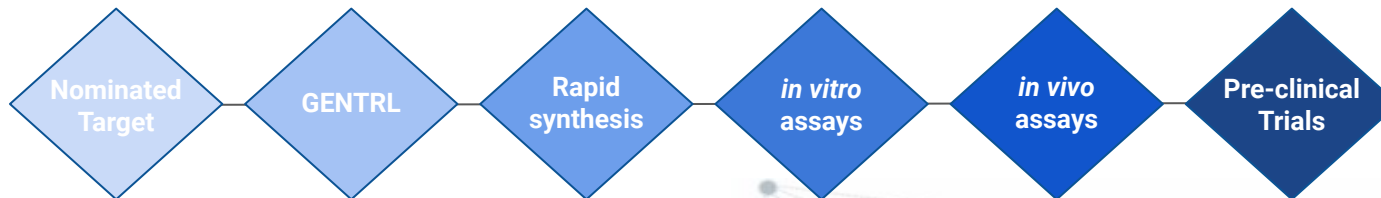
2. Insilico Medicine has developed GENTRL (Generative Tensorial Reinforcement Learning), a new artificial intelligence system for drug discovery that dramatically accelerates the process from years to days (from 3 years to 21 days before first synthesis and trials). In the industry's first successful experimental validation of such AI technology for drug discovery in cells and animals, Insilico successfully tested the technology by creating a series of entirely new molecules capable of combating disorders like fibrosis.

3. The system bucks the standard brute-force approach for AI drug development, which involves screening millions of potential molecular structures looking for a viable fit, in favor of a creative AI algorithm that can imagine potential protein structures based on existing research and certain preprogrammed design criteria. Insilico's system initially produced 30,000 possible designs, which the research team whittled down to six that were synthesized in the lab, with one design eventually tested on mice to promising results.

Source

Biospace	Digital Trends	Business Insider

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

NURITAS

Nuritas is revolutionising the discovery of novel, natural and scientifically proven active ingredients that can manage and improve human health. The company's disruptive computational approach to discovery uses artificial intelligence and genomics to, for the first time ever, rapidly and efficiently predict and then provide access to the most health-benefiting components hidden within food, called bioactive peptides.

Their bioactive peptides provide patented innovative solutions to companies needing new therapeutic options to deal with significant unmet medical needs. The Bioactive Peptides they discover have the potential to offer new and innovative treatments for many of the illnesses that are becoming more prevalent as the world population continues to expand and age.

Main focus areas:

Inflammation

Skin Diseases
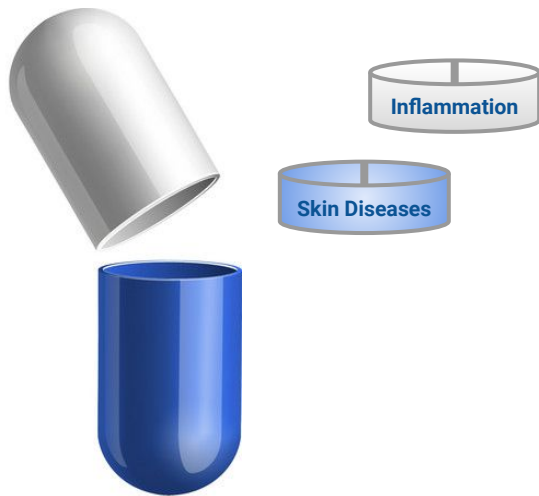
The way AI is used:

- to target, predict and unlock novel bioactive peptides;
- to deliver highly specific, efficient and life-changing health solutions;

Cooperation:

- BASF

◻∎BASF
We create chemistry

Source   Nuritas

How **Nuritas** Uses AI in R&D?

NURITAS

At Nuritas, they recognise the vast untapped potential that exists in naturally occurring Bioactive Peptides. Their unique discovery platform targets, predicts and unlocks these natural ingredients to provide new solutions and opportunities for their partners across a wide range of application areas. Together with their partners, they are changing the lives of billions of people worldwide.

1. They begin the discovery process by precisely defining the health condition and targets they wish to modulate. They then use proprietary search tools to identify the characteristics specific to their area of focus. The most up-to-date academic and scientific knowledge is used to maximise the efficiency and effectiveness of prediction algorithms.

Defining of targets to modulate → **Identifying the key characteristics of the focus area** → **Predicting the bioactive peptides' effect using deep learning algorithms** → **Unlocking peptides from food source**

BENEFITS
- Naturally Sourced Ingredients
- High Speed Prediction
- Sustainability
- Targeted Approach
- Product Differentiation
- Cost Effective Innovation
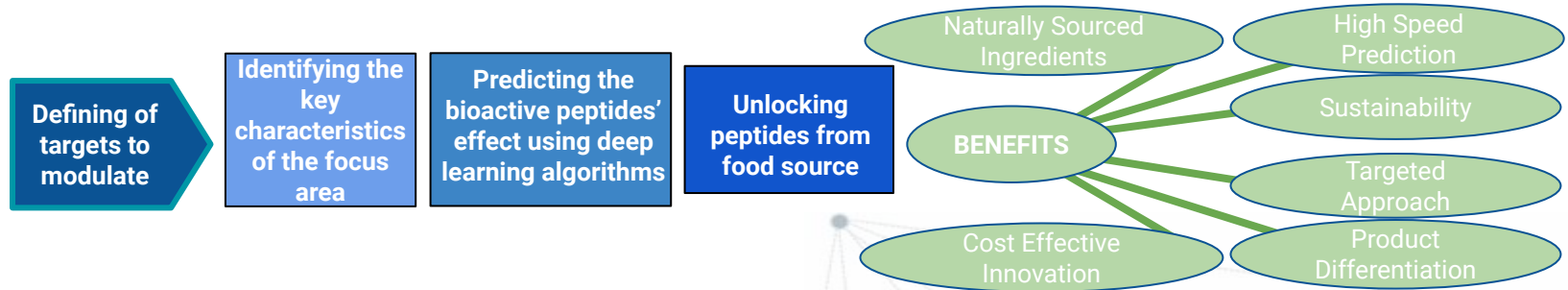
2. Having begun the discovery process as above, Nuritas takes advantage of multiple proprietary AI algorithms, including deep learning. Using these, they are now uniquely able to predict which novel food-derived bioactive peptides deliver the pre-determined effect that they are seeking. This cuts out many thousands of hours of trial and error.

3. After targeting and predicting high potential Bioactive Peptides, Nuritas unlocks them from within the food source for their pre-defined therapeutic use.

4. Their library of plant and animal derived Bioactive Peptides have gone through hundreds of millions of years of selective evolution to become the most potent repairers, healers and protectors.

Source | Nuritas

Most Innovative R&D Approaches of AI in Biopharma. **Novo Nordisk**

Novo Nordisk is a global healthcare company with more than 95 years of innovation and leadership in diabetes care. This heritage has given us experience and capabilities that also enable us to help people defeat other serious chronic diseases: haemophilia, growth disorders and obesity. At Novo Nordisk, they are driving change to defeat diabetes and other serious chronic diseases.

Novo Nordisk cooperates with e-Therapeutics to use its AI-based drug discovery technology to find new therapies for type 2 diabetes. e-Therapeutics uses a suite of powerful computational tools to augment and interrogate the vast amount of biological information currently available in both public and private databases.

Main focus areas:

Type 2 Diabetes
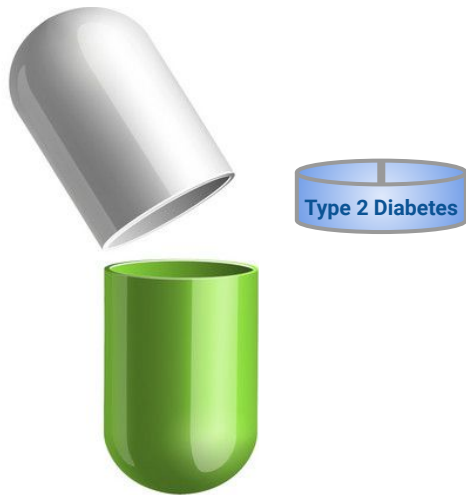
The way AI is used:

- to identify novel intervention strategies;
- to find new biological pathways and compounds;
- tease out previously unknown disease processes and pathways;
- to form the basis for new therapies.

Cooperation:

- e-Therapeutics

Source   Pharma Forum

How **Novo Nordisk** Uses AI in R&D?

The company said this approach more realistically reflects the true complexity of disease with its multiple and often interconnected cellular pathways. Novo Nordisk already has a research centre in Oxford, where visiting researchers are working with Oxford University academics to advance development of therapies for type 2 diabetes.

1. Using techniques such as machine learning and state of the art data analysis, e-Therapeutics creates and analyses network models of disease to identify likely proteins that could be disrupted to treat diseases. Company's scientists use AI to improve and accelerate active pharmaceutical ingredient (API) and drug product (DP) designs of new peptides and biologics. They have access to advanced state-of-the-art protein modelling software and are applying data science tools and prediction models to a variety of biological and chemical data, including high-throughput analytical data and images.

AI-related research department structure		
Modelling scientists	Data scientists	Data engineers
Modelling of molecules and proteins in order to create better and more stable drugs	Understanding and applying of complex machine learning algorithms	Ensuring that entire working infrastructure is as agile and stable as possible
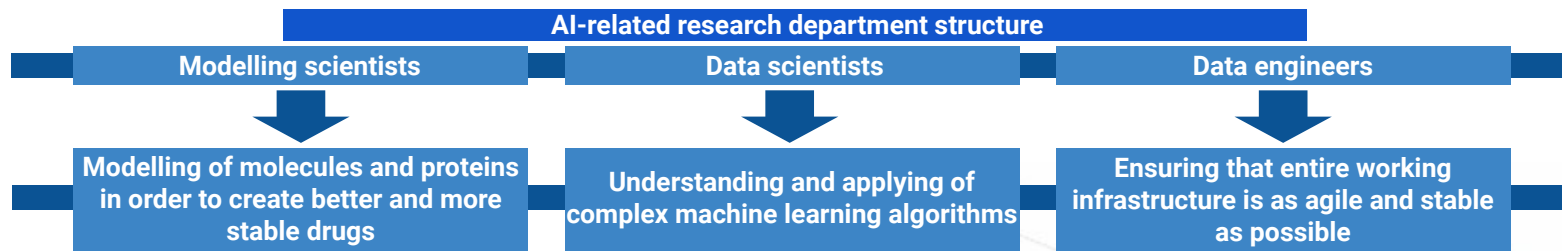
2. Novo Nordisk is the first pharma partner to sign up to use the GAIN platform, which taps into genome-wide association study (GWAS) data to find mutations in DNA linked to disease traits and – according to the UK company – bridges the gap between genetic susceptibility and disease mechanism. While many gene variants discovered using GWAS studies often don't map to a plausible biological mechanism, e-Therapeutics says its "network biology" approach can improve the hit rate.

3. Using GAINs, the company will be able to interrogate genomics data from patients with complex, polygenic disease and shed new light on important and novel biological pathways for particular groups of patients.

Source

Novo Nordisk	Pharma Forum

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

Pfizer is a leading research-based biopharmaceutical company. They apply science and their global resources to deliver innovative therapies that extend and significantly improve lives. The company's products are the results of 1500 scientists overseeing more than 500,000 lab tests and over 36 clinical trials before the first prescription.

Pfizer in late 2016 announced a collaboration that will utilize IBM Watson for Drug Discovery. Pfizer is using IBM's AI technology on its immuno-oncology research, a strategy of using a body's immune system to help fight cancer. Based on their research, this appears to be one of the first significant uses of Watson for drug discovery.

Main focus areas:

Hematologic Malignancies

Cancer

Menopause
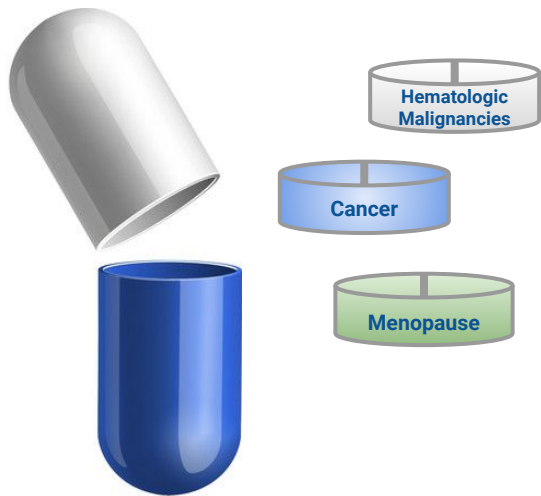
The way AI is used:

- to uncover new information or insights related to patient needs;
- to analyze massive volumes of disparate data sources, including licensed and publicly available data;
- to discover new drug targets and alternative drug indications.

Cooperation:

- IBM Watson

IBM **Watson**

Source

Pfizer

How **Pfizer** Uses AI in R&D?

Pfizer is among the healthcare companies investing heavily in AI and teamed with IBM Watson to identify better targets for cancer during the discovery phase and Concerto HealthAI to to apply real-world datasets and artificial intelligence techniques to develop new and more precise treatment options for patients with solid tumors and hematologic malignancies.

1. Pfizer is one of the first organizations worldwide to deploy Watson for Drug Discovery, and the first to customize the cloud-based cognitive tool:

Machine learning

Natural language processing

Cognitive reasoning technologies
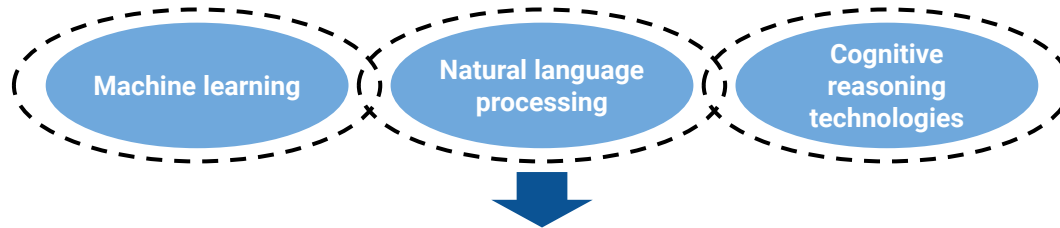
Supporting the identification of new drug targets, combination therapies for study, and patient selection strategies in immuno-oncology

2. Pfizer uses newly launched Watson for Drug Discovery, a cloud-based offering that aims to help life sciences researchers discover new drug targets and alternative drug indications. The average researcher reads between 200 and 300 articles in a given year 2, while Watson for Drug Discovery has ingested 25 million Medline abstracts, more than 1 million full-text medical journal articles, 4 million patents and is regularly updated. Watson for Drug Discovery can be augmented with an organization's private data such as lab reports and can help researchers look across disparate data sets to surface relationships and reveal hidden patterns through dynamic visualizations.

3. AI systems are used in progressive ways to analyze data, to uncover new information or insights related to patient needs.

Source

| Pfizer | Medtechdive | Pfizer |

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

Roche

To intensify it`s on healthcare, Roche divests two businesses: fragrances and flavours, and vitamins and fine chemicals. As a research-driven company committed to innovation, the Group's Pharmaceuticals and Diagnostics Divisions supply products spanning the healthcare spectrum, from the early detection and prevention of disease to diagnosis and treatment.

Sensors, wearables, IOT, blockchain, high performance compute, Machine Learning and Deep Learning are drivers and enables of digital transformation of Roche`s entire Pharma value chain. AI is expected to have a dramatic impact on medicine that Roche provides.

Main focus areas:

- Asthma
- Diabetic Macular Edema
- Cancer
- Diabetes
- Neurodegenerative Diseases
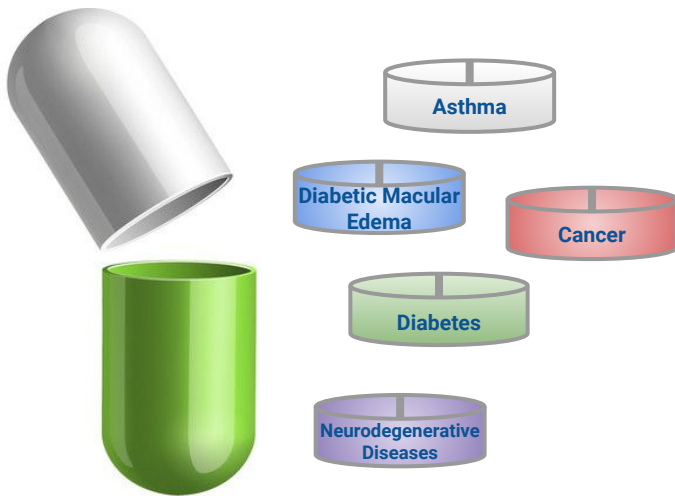
The way AI is used:

- to improve the ability to diagnose disease;
- to select the best treatments for individual patients;
- to De novo compound design;
- to better target selection.

Cooperation:

- Owkin **OWKIN**

Source — Roche
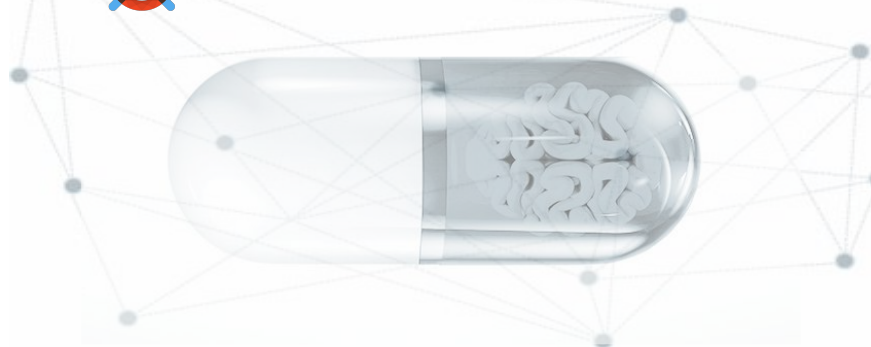
How **Roche** Uses AI in R&D?

With the advent of more sophisticated digital technologies, personalised healthcare is entering a new phase, expanding from companion diagnostics to a more complex, holistic view of patient health generated from a wide variety of data sources. Combining and standardising data, using AI and algorithms to make sense of it all, enhance the way Roche can develop and bring medicines to patients in a much more targeted fashion.

1. Examples of transformative digital use cases across different areas, modalities and pipeline phases:

Machine Learning	Deep Learning	AI and Wearables
Molecule discovery and optimization	Deep image analysis in Ophthalmology	Digital biomarkers in Neuroscience
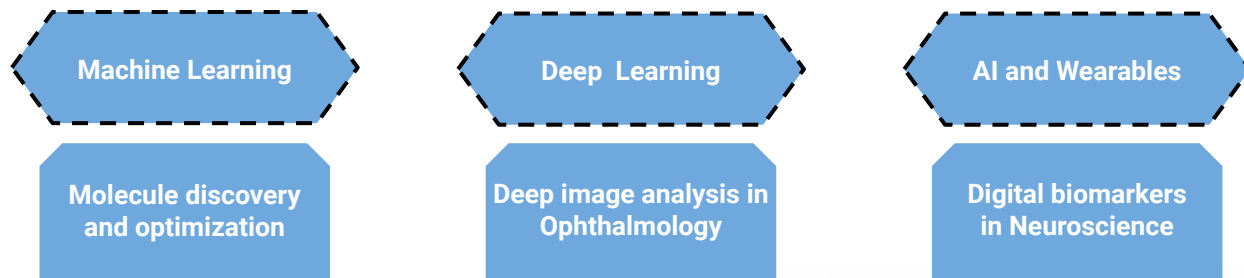
2. AI could revolutionise the way ophthalmologists diagnose diabetic macular edema (DME), a complication of diabetes that causes a thickening of the retina that can lead to irreversible blindness if left untreated. The best way to prevent DME is through regular eye exams that use a technique called colour fundus photography (CFP) and optical coherence tomography (OCT). The company's researchers use deep learning to teach computers how to estimate macular thickness from CFP images, making DME diagnosis easier, so they gave their computers a large set of CFP and OCT data from participants in two large DME clinical trials to train on.

The deep learning system examined a total of 17,997 CFP images from ~700 patients and compared them with corresponding OCT thickness measurements. Deep learning could even do a reliable job of predicting the actual OCT measurement of the macula's thickness from a CFP image if it was of sufficient quality.

Source | Roche | Roche

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

Sanofi is a healthcare company engaged in the research, development, manufacturing, and marketing of innovative therapeutic solutions. It covers areas such as diabetes solutions, human vaccines, innovative drugs, consumer healthcare, etc. Its products includes prescriptions and over-the-counter drugs for thrombosis, cardiovascular disease, diabetes, central nervous system disorders, oncology and internal medicine, vaccines.

Sanofi and Google apply artificial intelligence (AI) across diverse datasets to better forecast sales and inform marketing and supply chain efforts. Using AI will take into account real-time information as well as geographic, logistic and manufacturing constraints to help the accuracy of these complex activities.

Main focus areas:

- Diabetes
- Cancer
- Pneumonia
- Central Nervous System
- Heart Diseases
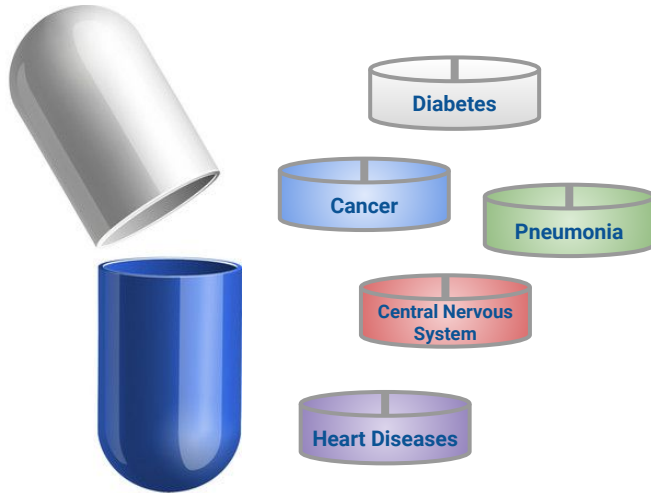
The way AI is used:

- to provide remote connection between patients and doctors;
- to diagnose diseases at early stage;
- to decentralize clinical trials;
- to improve marketing strategies.

Cooperation:

- Google

Source

Crunchbase
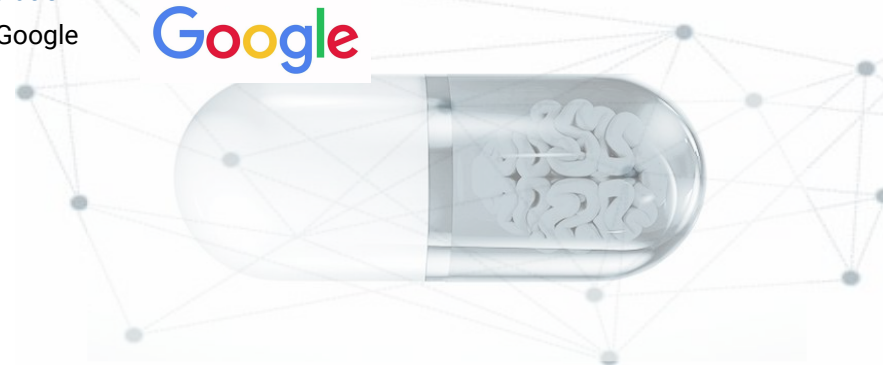
How **Sanofi** Uses AI in R&D?

Big data and a better understanding of the human genome are also providing medical professionals with better tools to make faster, more accurate diagnoses and deliver more personalized treatments. Large, multinational databases of clinical data called patient registries can also play a key role in the study of rare diseases. Additionally, Sanofi IT will be modernizing its infrastructure by migrating some existing business applications to Google Cloud Platform (GCP).

Mouthlab

1. MouthLab is a single, noninvasive device that measures more than 10 different health indicators in less than a minute. The AI-powered system uses the patient's mouth and hand to measure in real-time vital health signs typically monitored at the doctor's office, including respiratory rate, pulse, electrocardiogram, blood oxygen saturation, temperature, blood pressure, and several lung functions. In addition, the device connects to the cloud, so patient data is accessible in real time to physicians and caregivers. By making this data easily available, Sanofi aims to reduce hospitalizations, patient costs and risks.

Wavy Assistant

2. Wavy Assistant delivers continuous real-time heart health monitoring using voice and AI solutions. After a patient's data is collected and analyzed, Wavy can provide advice tailored to that individual. Our heart health monitoring solution uses a smart home speaker as its main user interface, which allows customers to interact with their heart health easily through a natural conversation instead of a mobile app. If the system detects something is wrong, Wavy instantly sends an emergency signal to designated doctors, friends and family. It can also trigger an immediate alert during emergency situations. Almost all heart attacks and strokes happen at home and most of the damage occurs because the emergency services are called too late.

LIFEdata

3. LIFEdata is an intuitive, easy to use AI platform that automates personally tailored conversational experiences across all channels. In terms of user experience, healthcare is no different than any other industry.

Source   Sanofi

How **Sanofi** Uses AI in R&D?

SANOFI

ChatbotPack.com

4. Computers that understand humans through text and voice are Sanofi's solution for healthcare with many applications. Voice technologies are used to detect, e.g. flu—or a general decline in condition—before it gets worse (e.g. pneumonia). A device in the elderly person's home can analyze changes in a person's voice and detect symptoms early on. It helps homecare and home nurses to detect their patients' illness before they need hospital care.

Mentalab

5. Mentalab combines a wearable patch that can measure electrocardiogram biosignals continuously, with a cloud-based analysis service to diagnose and monitor cardiac and respiratory conditions. The patch can be applied by patients directly, and worn throughout their daily activities, while data is transmitted and analyzed seamlessly. In site-less clinical trials, this solution can increase patient engagement and participation rates.

NeuroAdvise

6. NeuroAdvise is a clinical decision support tool available as a mobile application that helps physicians make better clinical decisions. Our system can archive all demographic and clinical patient-related information in a classified manner. Data is currently stored without patient identity according to time and date. NeuroAdvise algorithms are simulations of a clinician's mental diagnostic process and most of the important diagnostic factors are included in its comprehensive database. It only takes a few seconds for the user to access the list of differential diagnosis, which are sorted in order of probability and unique for each patient. The system is flexible with unlimited capacity for adding new symptoms, disorders and diagnostic tests.

CART

7. A ring-design cardio tracker, or CART, can provide continuous monitoring of vital signs in real-world clinical trials and can be worn easily in daily life.

Source | Sanofi

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

Teva is investing in both original biologic medicines and in biosimilars (highly similar versions to specific innovator biologics) to help patients around the world. We are focusing on treatments for the central nervous system, respiratory conditions, and in the field of oncology. Teva uses the help of AI for development of 'Single device location-algorithm pair' for optimal treatment of impaired mobility resulting from ageing and chronic disease as well as for digital technology, including body worn sensors.

In cooperation with IBM Research, Teva focuses on two key healthcare areas: the discovery of new treatment options and improving chronic disease management.

Main focus areas:

- Migraine
- Cancer
- Asthma
- Central Nervous System

The way AI is used:

- to improve chronic disease management;
- to discover new treatment options;
- to repurpose already existing drugs.

Cooperation:
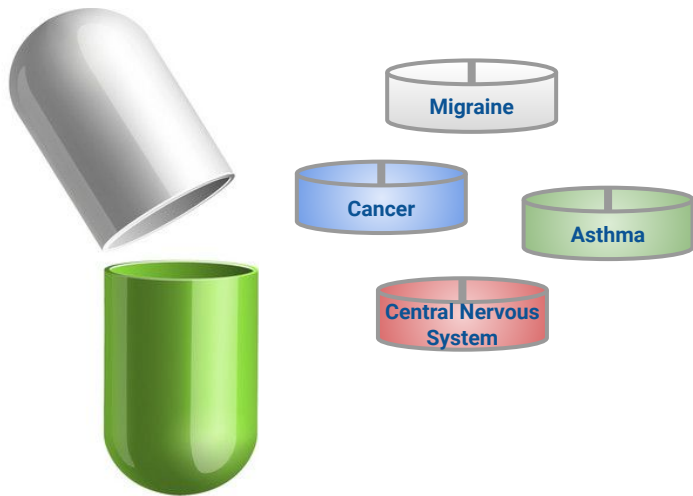
- IBM Research

Source

Startuphub	7wdata

How **Teva** Uses AI in R&D?

In cooperation with IBM Research, Teva focuses on two key healthcare areas: the discovery of new treatment options and improving chronic disease management. Teva's AI projects are based on the IBM Watson Health Cloud, that is a health-data enabled platform-as-a-service which is designed to help healthcare organizations derive individualized insights and obtain a more complete picture of the many factors that can affect people's health based on machine learning.

1. Teva has chosen the IBM Watson Health Cloud as a preferred global technology platform and managed to build solutions designed to help millions of individuals worldwide with complex and chronic conditions such as asthma, pain, migraine and neurodegenerative diseases. In addition, a joint Teva-IBM Research team will deploy Big Data and machine learning technology to create disease models and advanced therapeutic solutions.

2. Watson is a groundbreaking cognitive computing platform that represents a new era of computing based on its ability to interact in natural language, process vast amounts of Big Data to uncover patterns and insights, and learn from each interaction. The Watson Health Cloud provides an open development platform for physicians, researchers, insurers and companies focused on creating health and wellness solutions.

3. IBM's Global Business Services works closely with a Teva Analytics team to assess the data and the analytics model requirements for the Real World Evidence e-health solution.

4. By building on the Watson Health Cloud, Teva is in a unique position to put the best information and insights in the hands of physicians, care teams and patients, to empower treatment optimization for individuals and populations across the spectrum of acute and chronic conditions. Watson provides Teva with better insights, real-time feedback and options for clinicians to consider to improve patient care.
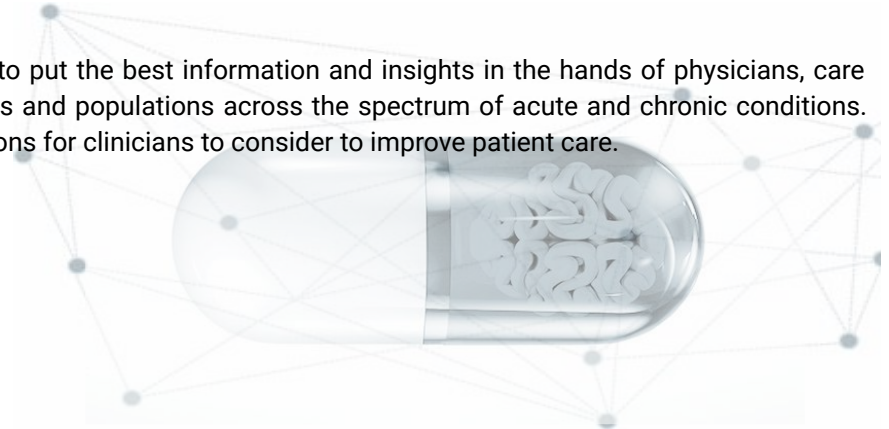
Source

7wdata	Teva

Most Innovative R&D Approaches of AI in Biopharma. **Recursion Pharmaceuticals**

Recursion Pharmaceuticals is a digital biology company, which applies AI for the development of its drug discovery platform and pipeline.

The company is Reengineering drug discovery by taking a target-agnostic approach that combines automation, machine learning and **the world's largest biological image dataset** with a highly cross-functional team to discover transformative new treatments.

The company currently has 4 clinical stage programs and 6 preclinical candidates in its pipeline.

Main focus areas:

- Genetic Disease
- Immunology
- Inflammation
- Infectious Disease
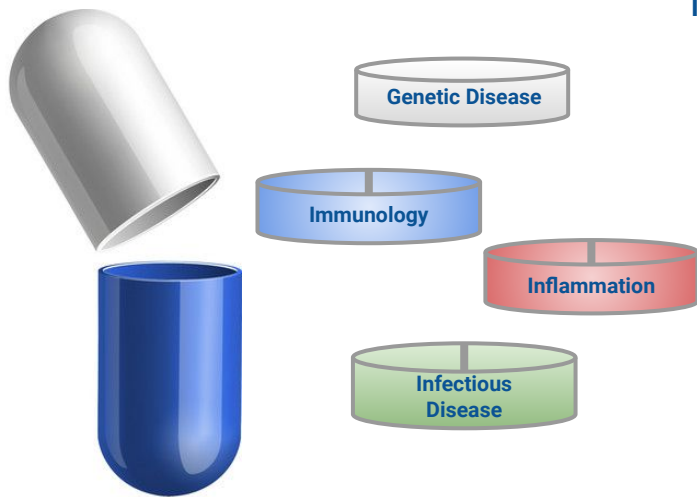
The way AI is used:

- for imaging analyses;
- to select and design chemical compounds (ReChem);
- to plan large, complex experiments (ReScreen);
- to screen hundreds of thousands of drug compounds and cellular disease models (ReScreenRun);
- to create digital mathematical signatures, or Phenoprints (ReRun);
- to compute the effectiveness of each drug compound in their assays, as well as any unintended effects (ReAnalyze);
- to model drug compound relationships (RePredict).

How **Recursion Pharmaceuticals** Uses AI in R&D?

The Recursion Pharmaceuticals' platform is a continuous, iterative loop of "biology and bits" which combines wet lab biology experiments that are executed automatically with machine learning algorithms computing the results in a cloud.

The Recursion drug discovery platform is based on five million images of human cells every week requires built-for-purpose components

Analyse & Predict

Design Experiment

Run workflow
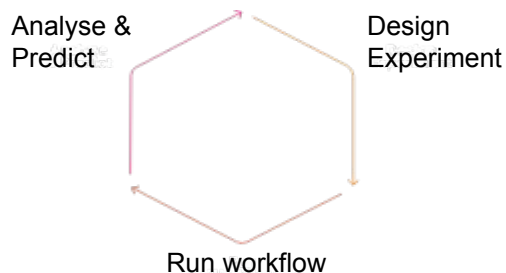
To generate its datasets Recursion Pharmaceuticals is primarily focused on:

Data reliability and relatability

By generating its own quality-controlled data, fit-for-the purpose of machine learning, Recursion is minimizing data noise to be able to ensure comparability of data.

Generalized assay framework for broad biology:

The technology is based on the principle of inducing the disease states and screening of various cell types together with healthy cells using fluorescent microscopy. By applying different substances, it's possible to detect signals of potential drug-like molecules which return diseased cells to a healthy state, as well as potential side-effects.

Scale and scale again through automation and innovation:

Recursion's software engineers, screening technicians and data scientists work closely to create a platform which allow to decrease the costs of drug discovery process. Recursion is trying to automatize as much part of workflow as possible.
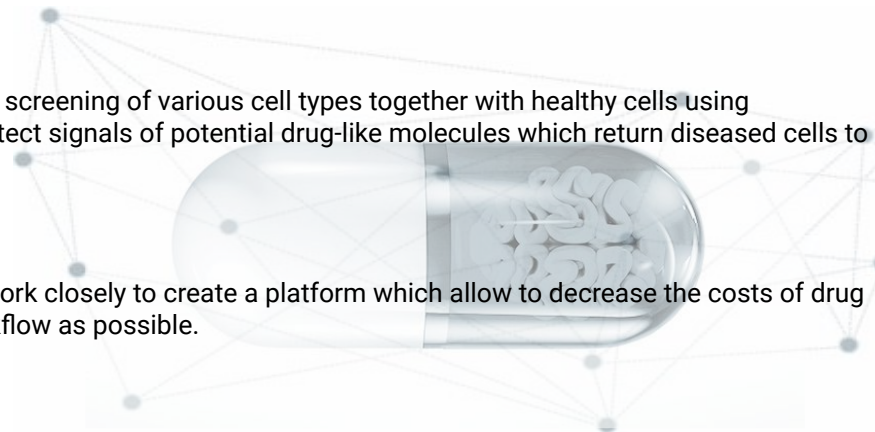
Most Innovative R&D Approaches of AI in Biopharma. **OWKIN**

Owkin is a predictive analytics company that was founded based on the belief that medical research must be collaborative, inclusive and protect privacy. Today, Owkin is building a global research network leveraging federated learning that brings data scientists, physicians, researchers and pharmaceutical companies together on a research platform that ensures data security and privacy.

Owkin is developing AI tools for medical researches to give patients access to safer and more effective therapies.

Main focus areas:

Oncology

Immunology

Cardiovascular Diseases
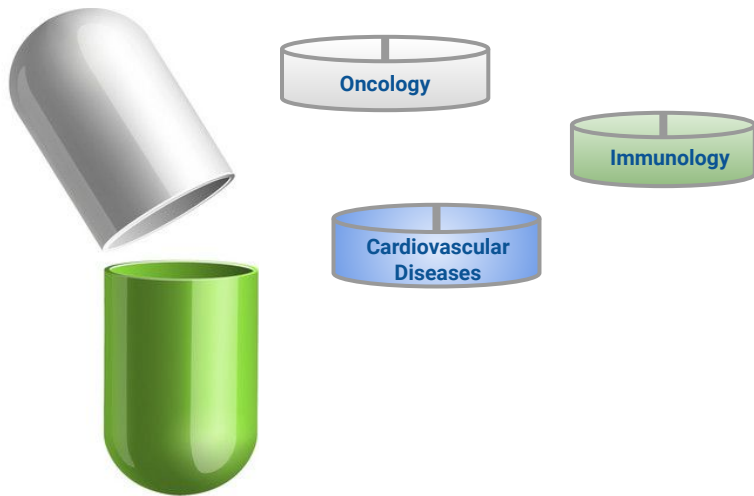
The way AI is used:

- to understand why drug efficacy varies from patient to patient;

- to enhance the drug development process;

- to identify the best drug for the right patient to improve treatment outcomes.
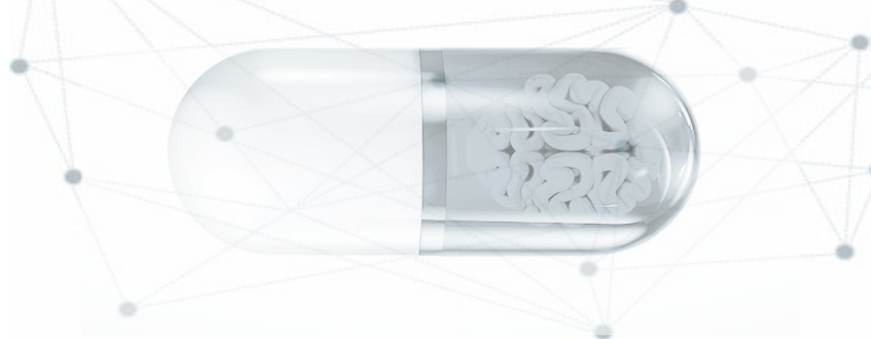
How **Owkin** Uses AI in R&D?

Owkin has created a unique research platform, and a portfolio of AI models and solutions.

The **Owkin Loop** is the heart of the Owkin Research Platform: it connects medical researchers with high-quality datasets from leading academic research centers around the globe. Owkin Loop is powered by the two main components of Owkin's Software Stack: **Owkin Studio**, their machine learning platform, and **Owkin Connect**, their **federated learning** framework.

Owkin AI models

Owkin created a catalog of 30 live diseases models and has 40 additional models in the pipeline.These models differ from traditional black box models because they are built using interpreted AI, which allows the company to move further in research and identify biomarkers responsible for predictions. The discovery of new multimodal biomarkers is essential to identify new biological targets, optimize the design of clinical trials using patients subgroups, and identify patients eligible for a particular treatments.

Data Enrichment Models
Designed for translational researchers and pathologists, these models link histology to molecular markers.

Outcome Prediction Models
Designed for translational researchers, development executives, and commercial staff, these models can be implemented throughout the clinical drug development process to improve clinical trial design and evaluation, and to optimize product strategy.

Patient Identification Models
Designed for commercial and precision medicine leaders, these models help identify patients who will benefit from a particular treatment.
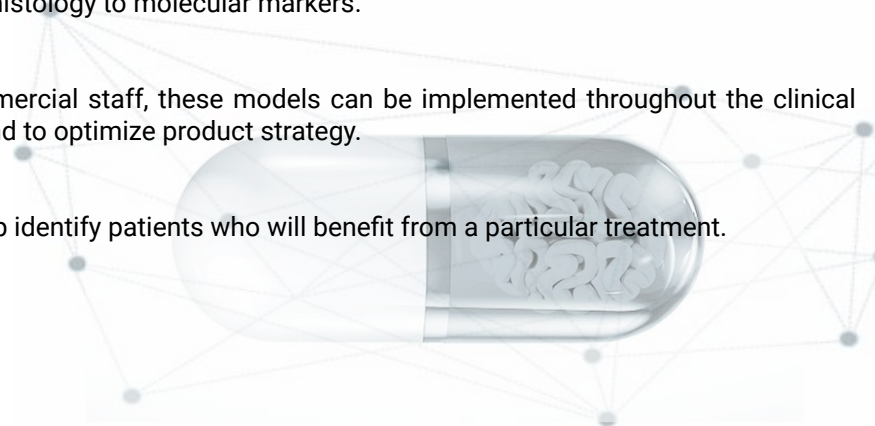
Most Innovative R&D Approaches of AI in Biopharma. **Deep Genomics**

Deep Genomics is using artificial intelligence to build a new universe of life-saving genetic therapies. The company has trained AI algorithms to better understand and search new drug targets in human genomic sequences, specifically those that have been deemed "undruggable," as well as to design new Antisense Oligonucleotides (ASOs) drugs.

Main focus areas:

Metabolic Disease (Wilson Disease)

Genetic Disease

Ophthalmologic Disease
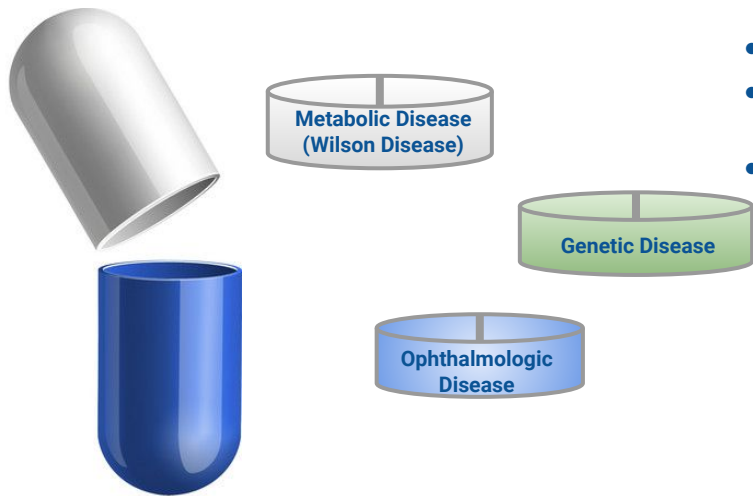
The way AI is used:

- to find drug candidates (ASOs) with desirable properties;
- to predict molecular phenotypes alterations, such as transcription, splicing, translation and protein binding;
- to produce On-target and genome-wide off-target effect data, cell viability data and animal toxicity data.
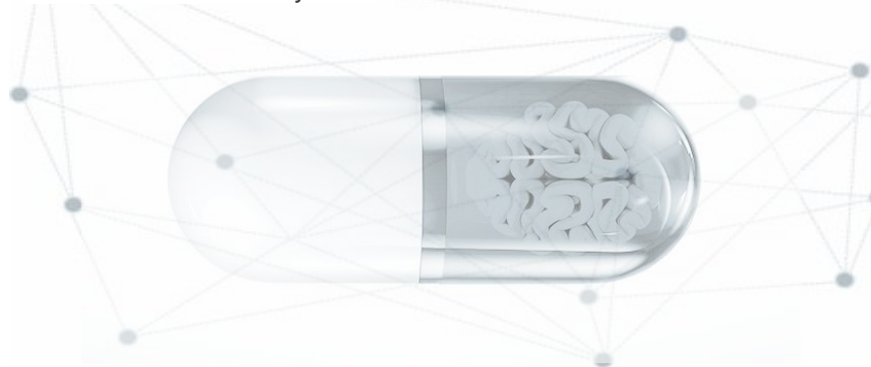
How **Deep Genomics** Uses AI in R&D?

Deep Genomics use its AI Workbench to rapidly discover and develop genetic therapies, and to do so with a increasing success rate.

Genetic Medicines. Deep Genomics' AI Workbench enables them to efficiently find drugs with desired properties. The company is focussing on the development and marketing of antisense oligonucleotide therapies that target the disrupted genes that cause diseases at the level of RNA or DNA. Deep Genomics is predicting altered molecular phenotypes, such as transcription, splicing, translation and protein binding that may caused genetic diseases.

The **Deep Genomics platform** is able to produce On-target and genome-wide off-target effect data, cell viability data and animal toxicity data for every compound. They also collect data related to biomarkers. All data is processed using feedback loops.

The **Deep Genomics' research works** have appeared in Science, Nature, Nature Genetics, Nature Medicine, Nature Methods, Proceedings of the IEEE, NIPS, Bioinformatics, RECOMB and ISMB.

Project Saturn has proved the utility of Deep Genomics' AI platform

In Project Saturn, the Deep Genomics' team was using their platform to evaluate over 69 billion oligonucleotide molecules against 1 million targets *in silico*, to generate a library of 1000 compounds that were experimentally verified to manipulate cell biology as had intended.
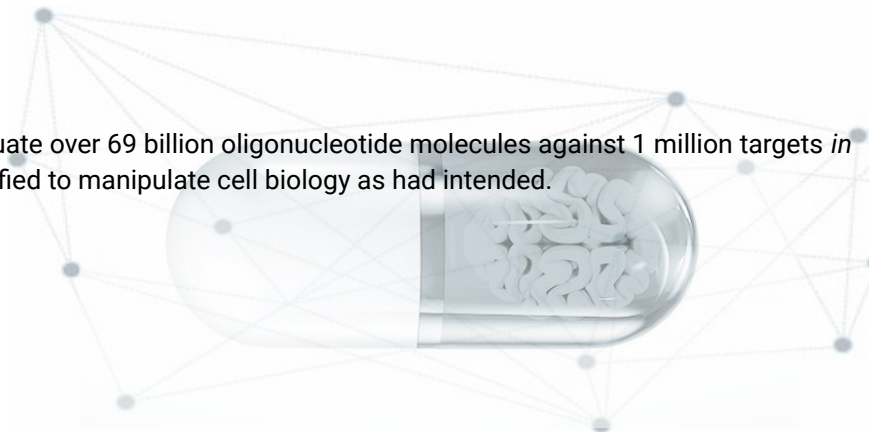
Most Innovative R&D Approaches of AI in Biopharma. **AI Therapeutics**

AI Therapeutics is an AI-driven company with a unique ability to match drugs according to indications and prosecute through clinical development. AI Therapeutics' revolutionary approach to drug discovery and development has led to clinical trials of three drugs.

Main focus areas:

Rare Disease

Cancer
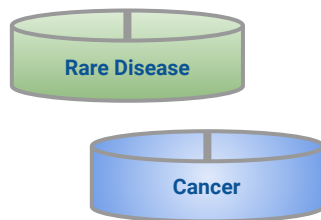
Drugs currently in **clinical trials** target:

- Lymphangioleiomyomatosis;
- B-cell non-Hodgkin lymphoma;
- acute myeloid leukemia;
- amyotrophic lateral sclerosis;
- facial angiofibroma;
- COVID-19

The way AI is used:

- to precisely match drugs to diseases;
- to identify the best care for individual patients.

AI Therapeutics has developed a new Guardian Angel™ artificial intelligence algorithm that has learned to predict new therapies for diseases with unprecedented accuracy. Guardian Angel ™ combines public and proprietary data and is designed to search for drugs for any indication.

Industry Developments 2020

Biggest Investment Deals of Q4 2019 — 2020

Some of the major investment deals included:

- insitro with their $143 million (Series B);

- XtalPi with $319 million (Series C);

- Atomwise with $123 million (Series B);

- Recursion Pharmaceuticals with $239 million (series D);

- AbCellera with the sum of $105 million (Series B).

If AI companies provide more evidence and successful studies demonstrating the functionality and value of their solutions, especially regarding the COVID-19 crisis, investors and pharma partners will probably consider increasing the number and sums of the investment deals in the future.

Additionally, the growing biotechnology industry is expected to provide growth opportunities for AI companies in terms of collaborations and partnerships.

Top 5 Investment Deals in 2020 (in million US dollars)
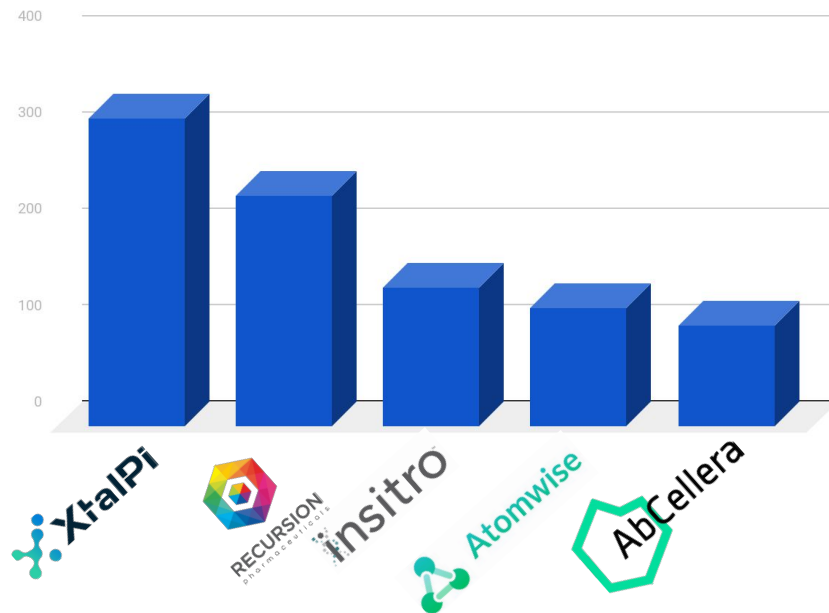
Industry Developments Q4 2019 — 2020

NOV 2019

- AI start-up, **Deep6**, secured $17 Million from **Point72 Ventures** to accelerate patient recruitment. According to the Forbes, the Deep6's AI-powered platform is valued at $50 million and is able to find patient for the clinical trial in minutes, whereas this process usually takes months. Deep6 applies natural language processing to extract data from electronic medical records, pathology reports, physicians notes, and other documentation.

- **AstraZeneca** intends to open AI and drug research centers in China and make a $1 billion capital infusion into Chinese biotech innovations. The global R&D center will be opened in Shanghai, where research will be focused on diseases prevalent in China. China is already the second market for AstraZeneca after the United States, and sales in China continue to grow.

DEC 2019

- **Page** raised $45 M to accelerate cancer research. The round was led by **Healthcare Venture Partners**, with the participation of previous investor **Breyer Capital**, **Kenan Turnacioglu**, and others. Page's artificial intelligence technology for mapping cancer pathology was developed by Dr. Thomas Fuchs, also known as the "father of computational biology." The company also has access to the repository of 25 million pathology slides owned by the Memorial Sloan Kettering Cancer Center, which is the perfect material to feed the AI engine.

JAN

- **Exscientia** has entered a 3-year $266 million agreement with Bayer. The partnership will leverage AI to accelerate the discovery of small molecules candidates programs for oncology and cardiovascular diseases.

- The first drug developed using artificial intelligence by **Exscientia** in partnership with **Sumitomo Dainippon Pharma** is entering Phase I clinical trial for the treatment of the obsessive-compulsive disorder. The drug, called DSP-1181, was discovered using Exscientia proprietary Centaur Chemist technology. The clinical trials will start in Japan, and Sumitomo Dainippon Pharma will add DSP-1181 to its psychiatry and neurology pipeline.

- **Deep Genomics**, a Toronto-based start-up, raised $40M in Series B funding round. The round was led by **Future Ventures** with the participation of **Amplitude Ventures**, **Khosla Ventures**, **Magnetic Ventures**, and **True Ventures**. The Deep Genomics software, Saturn, is used to identify and better understand drug targets, especially ones that are thought to be undruggable. The company hopes two programs will be advanced to the IND application in 2020.

Industry Developments Q4 2019 — 2020

- **Schrödinger** enters a 5-year agreement with **Bayer** to work on a new virtual platform for small molecules design, which will be able to design and screen synthetically feasible compounds. The collaboration will be built on Schrödinger's machine learning and molecular design technologies, while Bayer will provide in silico model for predicting the pharmacological properties of the molecules.

- **Insilico** will work with **Pfizer** to collect real-world-data for targets in multiple therapeutic areas.

FEB

- **Schrödinger**, a chemical software company, raised $232M in IPO. Several drug candidates that are currently developing by the pharmaceutical companies were discovered using Schrödinger's software. In the future, the company will focus on the expanding of its software applications and bringing up new customers. The company is also developing its own pipeline for oncological indications.

- Scientists from **MIT** discovered one the most powerful antibiotic known to date using Artificial Intelligence. The algorithm was trained on 2500 existing antibiotics and was able to screen more than one hundred million molecules in several days. This is an absolute breakthrough in antibiotic discovery, the area that is now facing the problem of multi-resistance of bacteria strains. The new antibiotic, called halicin, was able to kill 35 types of potentially deadly bacteria.

- **Lunit**, a Korean start-up, has raised $26M in its series C funding led by Korea's **Shinhan Investment**, followed by **InterVest**, **IMM Investment**, **Kakao Ventures**, and China's **Legend Capital** of Lenovo Group. With the new funding, Lunit plans to increase the global sales of its AI products — Lunit INSIGHT CXR for analyzing chest X-rays images and Lunit INSIGHT MMG for mammography. Additionally, the fund will support the development of the AI tool for analyzing cancer pathological tissue slides — Lunit SCOPE.

- **BenchSci** raised $22 million in financial round B, bringing the company to $45 million of total funding. Besides raising a new round, the company announced the launch of its new AI-powered reagent selection product and the expansion of the agreement with **Novartis**. Another BenchSci's product, AI-Assisted Antibody Selection, uses AI to search for data on published antibodies and can select antibodies in 30 seconds instead of 12 weeks. The fund will help BenchSci to develop its products and accelerate drug testing.

- **Qure.ai** has secured $16 million from **Sequoia Capital India** and Singapore-based **MassMutual Ventures Southeast Asia**. Qure.ai is artificial intelligence provider of automated interpretation of radiology images: X-rays, CTs, and MRI scans.

Industry Developments Q4 2019 — 2020

MAR

— **Atomwise** enters into a research collaboration with a Korean clinical-stage biotech **Bridge Biotherapeutics**. Atomwise will apply structure-based AI technology to evaluate and initiate programs for Pellino E3 ubiquitin ligases and other targets.

— **Alibaba Cloud** launched a series of AI solutions to help fight the coronavirus infection. The three of them are available for free for research institutes and medical specialists worldwide. The solutions were created by the joint work of **Alibaba Cloud**, **Alibaba DAMO Academy**, and **DingTalk**. These include Epidemic Prediction Solution, CT Image Analytics Solution, Genome Sequencing for Coronavirus Diagnostic Solution, and Elastic High-Performance Computing (E-HPC) Solution for Life Sciences. The last was built especially for Computational and AI-driven drug discovery, as well as for other life science applications, and has been applying by 20 research groups in China.

— **Schrödinger** enters a 3-year collaboration with **Google Cloud** to leverage the supercomputer power for speeding up Schrödinger's molecular modeling platform. Schrödinger has ambitious plans to hire thousands of professors to be able to run simulations for billion compounds per week. The agreement is following Schrödinger's IPO last month, where the company raised $232 million. The purpose of this collaboration is targeting DNA damage response pathways and related cancers with small molecules. The company has plans to start IND-enabling, preclinical studies in 2021.

— **Reverie Labs** enters a multi-target partnership with **Roche** to discover next-generation kinase inhibitors. The company will apply its expertise to screen, generate hits, and perform hit-to-lead optimization together with scientists at Roche and **Genentech**. The kinases are perfect objects to drain ML models, as there is a lot of published data about them.

APR

— **BenevolentAI** predicted the repurposed drug for treating coronavirus, that entered Phase III clinical trials. This drug, called Baricitinib, was developed by **Eli Lilly** and **Incyte** and approved for the treatment of rheumatoid arthritis under the "Olumiant" name. Benevolent claims that it took only 1,5 hours to run it's AI algorithms and 3 days of manual work to predict this molecule.

— **Insilico** collaborates with **Boehringer Ingelheim** to help to discover new targets within the Boehringer's Research Beyond Borders initiative, created to expand areas and the geographies of the company's drug discovery collaborations. Insilico will provide its generative models and machine learning programs and give access to its new Pandomic platform to facilitate visualization of omics data connected to signaling pathways and disease profiling.

Industry Developments Q4 2019 — 2020

MAY

- **insitro**, a machine learning-driven drug discovery company, raised $143 million in Series B financing. The round was led by **Andreessen Horowitz**, with the participation of the **Canada Pension Plan Investment Board** (CPP Investments) and other funds. The investment will be used to further develop the company's technology and automation, which allows the in-house generation of a massive amount of biological data to train algorithms and built predictive disease models. The company also plans to advanced biomarker development and personalized therapeutics.

- **AbCellera** received $105 Million Series B Financing from **OrbiMed**, **DCVC Bio**, and an investor syndicate that includes **Viking Global Investors**, **Peter Thiel**, **Founders Fund**, **Eli Lilly**, **University of Minnesota**, and **Presight Capital**. By applying AI, AbCellera is transforming the area of antibody discovery. The investments will be used to improve and expand their technology creating new tools and to develop new therapeutic modalities. AbCellera successfully developed 55 drug candidates, including targeting GPCRs and ion channels.

- **Exscientia** has raised $60M in financial round C. The round was led by **Novo Holdings**, **Evotec**, **Bristol Myers Squibb**, and **GT Healthcare Capital**. Proceeds will be used to expand the company's drug discovery pipeline and to built "full-stack" capabilities. Additionally, Exscientia plans to expand its presence to the USA market. The company is also involved in the coronavirus pandemic fight, as it partnered with **Calibr** and **Diamond Light Source** to develop an anti-Sars-Cov-2 treatment.

- **Boehringer Ingelheim** partners with **BERG** to investigate inflammatory diseases, particularly inflammatory bowel disease and Crohn's disease, find the causes, develop new biomarkers, targets, and new drugs. BERG CEO Niven Narain emphasizes that it is a biology company that has wet lab facilities for data generation, applies a mathematical approach distinct from machine learning, and has 2 drugs in companies portfolio that have been advanced to the clinic.

- **Immunai** has raised $20M in a seed round from **Viola Group** and **TLV Partners** to map the entire immune system. The startup combines machine-learning and single-cell technologies to map immune cells and their functions. The technology was developed to profile immune cells from blood samples, support biomarker discovery, and investigate the cellular response to the cancer immunotherapies. This research will help to improve immunotherapies, as even a slight variation in immunotherapies can bring to dramatically different patient responses.

Industry Developments Q4 2019 — 2020

— **Owkin** raised $18 M in Series A financing. The investment was made by **Mubadala Capital** and **Bpifrance**, through the bank's **Large Venture** fund. The company will continue to develop its platform aimed to make the drug discovery process more collaborative. The platform utilizes imaging, genomic, and clinical data and connects researchers from industry and academia, clinicians, and other players.

— **Cyclica** secured $17M in financing round B from **Drive Capital** with the participation of **Chiesi Farmaceutici**, **GreenSky Capital**, and members of Cyclica's management team. This Toronto-based start-up developed two platforms — Ligand Design and Ligand Express that predict molecular properties via applying deep learning technology.

— **Google** partners with a fresh start-up, **ZebiAI**, to launch Chemome initiative. Previously, Google and X-Chem demonstrated a new approach for finding biologically active compounds — a combination of DNA encoded libraries screening technology and virtual screening using a graph convolutional neural network developed by Google.

— **Yale School of Medicine** and **AI therapeutics** launched Phase II clinical trials of a new anti-Sars-Cov-2 drug "LAM-002A". The drug, also called apilimod, has been shown to prevent the virus from entering cells. Previously LAM-002A proved safety for the treatment of lymphoma and autoimmune diseases, and it is being repurposed for coronavirus treatment after AI Therapeutics screened about 13,000 existing drugs against two strains of Sars-Cov-2. The study results were published in Nature.

— **Lantern Pharma** announced an agreement with leading contract manufacturing companies to prepare for the start of Phase II and Phase I clinical trials of its two anti-cancer drug candidates. The first candidate - LP-300, that was developed against non-small cell lung cancer among never-smoker, is entering the Phase II clinical trial stage. The second candidate, LP-184, developed to treat a specific type of solid tumor and glioblastoma multiforme, is anticipated to enter Phase I stage at the end of 2021 or in early 2022. Latent hopes that annual sales of this drug will be accounted for $3.5 billion USD by 2025. Both drug candidates were created using RADR® A.I. platform, which combines ML methods, genomics, and computational biology to unveil drugs MoA and discover biomarkers for precision oncology.

— Global Open Science project **COVID Moonshot** was launched by the international consortium of industrial and academic partners, including AI-driven startup **PostEra**. The goal of this initiative is to create novel anti-COVID drugs, including attempts to block SARS-Cov-2 main protease. The project is managed by PostEra, the start-up that applies AI to prioritize ideas and find optimal synthesis routes.

Industry Developments Q4 2019 — 2020

— **Atomwise** raised $123 million in a round B of financing led by **B Capital Group** and **Sanabil Investments**, also including **DCVC**, **BV**, **Tencent**, **Y Combinator**, **Dolby Family Ventures**, **AME Cloud Ventures**, and 2 top insurance companies. The investment will be used to start the company's own drug discovery pipeline, extend the market, and develop new partnerships with pharmaceutical companies.

— **IBM** introduced a new cloud platform — **RoboRXN**, which is a free AI-enabled chemical service for the prediction of molecule interactions and the discovery of new drugs. The platform will be primarily used to discover compounds against coronavirus proteins. RoboRXN combines artificial intelligence, cloud technologies, and automation for organic chemistry. Additionally, new organic reactions might be discovered using the platform. The platform can work remotely and analyze commands copied from literature by chemists.

— Chinese tech giant **Baidu** plots an AI-baked drug discovery startup, looking for investors to collectively infuse $2B in. The start-up is planned to be a standalone company, but not Baidu's subsidiary. Baidu has previously invested in other AI startups — Atomwise, Insilico, and Polaris Biology.

— **XtalPi**, a Chinese pharmaceutical tech company, has raised $319M in funding round C, which was led by **SoftBank Vision Fund 2**, **PICC Capital**, and Chinese firm **MorningSide Venture Capital**. The funding will be used for the further development of XtalPi's Intelligent Digital Drug Discovery and Development (ID4) platform, which combines artificial intelligence, quantum mechanics, and high-performance cloud computing algorithms to predict activities of small molecule drug candidates, solid-form selection, and other critical aspects of drug development.

— **Recursion Pharmaceuticals** raises $239M in series D funding round. This includes $50 million from **Bayer**'s investment arm **Leaps** and funds from **Casdin Capital**, **Baillie Gifford**, and others. Recursion has also entered in drug discovery collaboration with Bayer to develop new treatments against fibrotic diseases of different organs. Recursion will receive $30M of upfront payment and could potentially receive $100M milestones for each discovery program and royalties on future sales.

— The **MELODY (Machine Learning Ledger Orchestration for Drug Discovery) project** initiated by 10 major pharmaceutical companies achieved its first goal — the deploying of a drug discovery platform. Together with **Nvidia** and **Owkin**, these companies are building the federated learning solution where AI can be trained on desperate datasets from different sites without the need to collect data together.

Industry Developments Q4 2019 — 2020

SEP

— **Exscientia** teams up with **Huadong Medicine** for the small molecules oncology program. The project is focused on DNA damage repair and specifically investigates the transcription control of DNA damage response genes, which disruption leads to the mutation accumulations. Both companies will share the responsibilities for the project. To design new molecules, Exscientia will apply the Centaur Chemist AI platform, which allows to design new molecules and prioritize them for synthesis. Meanwhile, Huadong Medicine will apply its expertise to generate data and improve Exscientia's AI design in a closed-loop cycle.

— **Insilico Medicine** is launching a new target and drug discovery platform Pandomics, that is the part of the **Pharma.ai**. The platform enables to analyse and interpret OMICS data without having an experience in bioinformatics and computational biology. The technology has been developing for 6 years, and proved itself in several collaborations and Insilico's own drug development programs.

OCT

— **Taisho Pharmaceutical** and **Insilico** have entered into a research collaboration to identify novel therapeutics against aging. Insilico Medicine will utilize both the target discovery and generative chemistry parts of its Pharma.AI platform in this collaboration. It will use its proprietary Pandomics Discovery Platform to identify novel targets for senolytic drugs and Chemistry42 platform for a molecular generation.

Appendix:
List of Entities

240 Companies Applying AI for Drug Discovery and Advanced R&D

1. A2A Pharmaceuticals
2. Accutar Biotech
3. Acellera
4. Acorn AI
5. AcuraStem
6. Aetion
7. AI Therapeutics
8. Ai-biopharma
9. AiCure
10. Aigenpulse
11. Alector
12. Alphanosos
13. Anima Biotech
14. Antidote
15. Antiverse
16. ApexQubit
17. Aqemia
18. Arbor Biotechnologies
19. Arctoris
20. Ardigen

21. Ariana Pharma
22. Arrakis Therapeutics
23. Arzeda
24. Athelas
25. Atomwise
26. Auransa Inc.
27. BenchSci
28. BenevolentAI
29. Berg LLC
30. Berkeley Lights
31. BioAge Labs
32. Biodesix
33. Biorelate
34. BioSymetrics
35. Biotx.ai
36. Biovista
37. BioXcel
38. Bioz
39. BlackThorn Therapeutics
40. BullFrog AI

41. C4X discovery
42. Cambridge Cancer Genomics
43. CaroCures
44. Causaly
45. Cellarity
46. Celsius Therapeutics
47. Chempass
48. Clinithink
49. Cloud Pharmaceuticals
50. CloudMedX
51. Collective Scientific
52. Concerto HealthAI
53. Cotinga Pharmaceuticals
54. Cyclica
55. CytoReason
56. Cytox
57. Data2Discovery
58. Data4Cure
59. Datavant
60. Deep 6 AI

240 Companies Applying AI for Drug Discovery and Advanced R&D

61. Deep Genomics
62. Deep Intelligent Pharma
63. DeepLens
64. DeepMatter
65. DeepMind Health
66. DeepPhenome
67. Delta4 AI
68. Denovicon Therapeutics
69. Desktop Genetics
70. DEXSTR
71. Dristi.ai
72. E-therapeutics
73. Eigengene
74. Elucidata
75. Emerald Cloud Lab
76. Empiric Logic
77. Engine Biosciences
78. EntheogeniX Biosciences
79. Entropica Labs
80. Envisagenics

81. Erasca
82. Euretos
83. Evaxion Biotech
84. Evid Science
85. Evoke Neuroscience
86. Evolutionary Genomics
87. Exscientia
88. FAR Biotech
89. FDNA
90. Fetch Biosciences
91. Flatiron Health
92. Foundation Medicine
93. Frontier Medicines
94. GenFit
95. Genialis
96. Globavir
97. GNS Healthcare
98. Gritstone Oncology
99. GTN Limited
100. Haystack Sciences

101. Healx
102. HelixAI
103. iCarbonX
104. Ideaya Biosciences
105. Iktos
106. Imagia
107. Inato
108. Indegene
109. Ingentium
110. Innophore
111. Innoplexus
112. Inside DNA
113. Insilico Medicine
114. Insitro
115. Intellegens
116. Intelligencia
117. Interprotein
118. Intomics
119. InveniAI
120. InVivo AI

240 Companies Applying AI for Drug Discovery and Advanced R&D

121.	Iris.ai	141.	Micar Innovation	161.	Olaris
122.	iTeos Therapeutics	142.	Micrographia Bio	162.	omicX
123.	Just Biotherapeutics	143.	Mind the Byte	163.	OneThree Biotech
124.	Juvenescence AI	144.	Molomics	164.	Optibrium
125.	Keen Eye	145.	Molplex	165.	Owkin
126.	Kite Pharma	146.	Mozi AI health	166.	Paradigm4
127.	KYAN Therapeutics	147.	Nanna Therapeutics	167.	PathAI
128.	Kyndi	148.	Neon Therapeutics	168.	PatSnap
129.	LabGenius	149.	NetraMark	169.	Pending AI
130.	LabTwin	150.	Nference	170.	Pepticom
131.	Lantern Pharma	151.	Nimbus Therapeutics	171.	Peptone
132.	Linguamatics	152.	Notable	172.	Percayai
133.	Longenesis	153.	Novoheart	173.	Perceiv Research
134.	MAbSilico	154.	nQ Medical	174.	Pharma.AI
135.	Massive Bio	155.	Nucleai	175.	Pharmacelera
136.	MediBIC Group	156.	NuMedii	176.	PharmCADD
137.	MedView Technologies	157.	Numerate	177.	Pharnext
138.	Mendel.ai	158.	Nuritas	178.	Pharos iBT
139.	Menten Biotechnology Labs	159.	OccamzRazor	179.	Phenomic AI
140.	Meta	160.	OKRA Technologies	180.	Plex Research

240 Companies Applying AI for Drug Discovery and Advanced R&D

181. PostEra
182. Precisionlife
183. Prognica Labs
184. Proscia
185. ProteinQure
186. Qrativ
187. Quantitative Medicine
188. Quertle
189. Qulab
190. Recursion Pharmaceuticals
191. Relay Therapeutics
192. Remedium AI
193. Repurpose.AI
194. Researchably
195. Resonant Therapeutics
196. Reveal Biosciences
197. Reverie Labs
198. ReviveMed
199. Roivant Sciences
200. Saama

201. Sangamo BioSciences
202. Satalia
203. Schrodinger
204. SEngine Precision Medicine
205. Sensyne Health
206. Sigma Technologies
207. Silexon
208. Silicon Therapeutics
209. Sirenas
210. Sophia Genetics
211. Sparrho
212. Spring Discovery
213. Standigm
214. StoneWise
215. Strateos
216. Structura Biotechnology
217. Synergy Pharmaceuticals
218. Syntekabio
219. Synthace
220. Systems Oncology

221. TARA Biosystems
222. Tempus
223. TeselaGen
224. ThoughtSpot
225. TrialJectory
226. Turbine AI
227. TwoXAR
228. uBiome
229. Unnatural Products
230. Verge Genomics
231. VERISIM Life
232. Virogin
233. Virvio
234. Vyasa Analytics
235. WinterLight Labs
236. WuXi NextCODE
237. Xbiome
238. XtalPi
239. ZappRx
240. ZebiAI

600 Investors - AI for Drug Discovery and Advanced R&D

1. 415
2. 10x Group
3. 11.2 Capital
4. 180 Degree Capital
5. 1984 Ventures
6. 360 Capital Partners
7. 3W Partners Capital
8. 500 Startups
9. 5AM Ventures
10. 6 Dimensions Capital
11. 7BC Venture Capital
12. 8VC
13. A-Level Capital
14. Abstract Ventures
15. Accel X
16. Accelmed Growth Partners
17. Access Industries
18. AcuraStem
19. Advantage Capital
20. Advent Life Sciences
21. Afore Capital

22. Agent Capital
23. AGORANOV
24. AJS Investments
25. Alan Cohen
26. Alchemist Accelerator
27. Alector
28. ALevel Capital
29. Alexa Accelerator, Powered by Techstars
30. Alexa Fund
31. Alexandria Real Estate Equities
32. Alexandria Venture
33. AllBright
34. Alpha Edison
35. Alphabet
36. ALS Investment Fund
37. Alta Partners
38. Altitude Life Science Ventures
39. Altos Ventures
40. Amadeus Capital Partners
41. Amazon

42. AME Cloud Ventures
43. Amgen Ventures
44. Amplify Partners
45. Amplitude Venture Capital
46. Andreessen Horowitz
47. Angels in MedCity
48. Anges Quebec
49. Angivest Ventures
50. Apeiron Investment Group
51. Aquarius Equity Partners
52. Arab Angel Fund
53. Arboretum Ventures
54. ARCH Venture Partners
55. Arkitekt Ventures
56. ArrowMark Partners
57. Artis Ventures (AV)
58. Arzeda
59. Asahi Kasei
60. Asset Management Ventures (AMV)
61. Astellas Pharma
62. Astia Angels

600 Investors - AI for Drug Discovery and Advanced R&D

63. AstraZeneca
64. Atinum Investment
65. Atlas Venture
66. Atomico
67. Aurinvest
68. B Capital Group
69. Babel Ventures
70. Baidu
71. Baidu Ventures
72. Baillie Gifford
73. Baird Capital
74. Bakken & Baeck
75. Balderton Capital
76. Bangarang Group
77. Baron Capital Management
78. Basis Set Ventures (BSV)
79. BCF Ventures
80. BDC Venture Capital
81. Beast Ventures
82. Big Pi Ventures
83. Bill & Melinda Gates Foundation

84. Bill Tai
85. Bioeconomy Capital
86. Biomatics Capital Partners
87. Bios Partners
88. Biotechnology Value Fund
89. Bioverge
90. Black Diamond Ventures
91. BlackRock
92. Bloomberg Beta
93. Blue Bear Ventures
94. Bold Capital Partners
95. BootstrapLabs
96. Boundary Capital Partners LLP
97. Boxer Capital
98. Bpifrance
99. BR Ventures
100. Brightspark Ventures
101. BristolMyers Squibb
102. btov Partners
103. Builders VC
104. Caffeinated Capital

105. Cambia Health Solutions
106. Canaan Partners
107. Canada Pension Plan Investment Board
108. Cantos
109. Capital One Growth Ventures
110. Carrick Capital Partners
111. Cascade Investment
112. Casdin Capital
113. Catalyst Health Ventures
114. Catapult Ventures
115. Cathay Innovation
116. CedarsSinai Accelerator
117. Celgene
118. Chiesi Pharmaceuticals
119. China Bridge Capital
120. China Canada Angel Alliance
121. China Equity
122. China Life Healthcare Fund
123. Cigna Ventures
124. Cisco
125. Citrix Startup Accelerator

600 Investors - AI for Drug Discovery and Advanced R&D

126. Citrix Systems
127. City Hill Ventures
128. Civilization Ventures
129. Clal Biotechnology Industries
130. Claremont Creek Ventures
131. Clarus Ventures
132. CLI Ventures
133. CM-CIC Capital Finance
134. Colt Ventures
135. Conversion Ventures LLC
136. Cormorant Asset Management
137. Cosine
138. Cota Capital
139. Creative Destruction Lab
140. CRG L.P.
141. Crowdcube
142. CRV
143. CTI Life Sciences Fund
144. Cultivian Sandbox Ventures
145. curative ventures
146. D. E. Shaw Research

147. D.A. Wallach Founding Partner
148. Daniel Curran
149. Darling Ventures
150. Darrin Disley
151. Data Collective DCVC
152. DCM Ventures
153. Debiopharm Innovation Fund
154. Deep Knowledge Ventures
155. Deerfield
156. Deerfield Capital Management
157. Density Ventures
158. Dentsu
159. Development Bank of Wales
160. Dexcel Pharma
161. DFJ
162. DFJ Growth
163. DHVC
164. Digital Science
165. DNA Capital
166. Dolby Family Ventures
167. Dorm Room Fund

168. Draper Associates
169. Draper Dragon
170. Driehaus Capital Management
171. Drive Capital
172. DROIA
173. Dynamk Capital
174. EASME EU Executive Agency for SMEs
175. Echo Health Ventures
176. EcoR1 Capital
177. EDBI
178. Eight Roads Ventures
179. Elad Gil Cofounder @ Color
180. Emerald Development Managers
181. Emerge Education
182. Endeavour Vision
183. Endure Capital
184. ENISA
185. Enterprise Ireland
186. Entrepreneur First
187. EPIC Capital
188. EPIC Ventures

600 Investors - AI for Drug Discovery and Advanced R&D

189. Esperante Ventures
190. Euclidean Capital
191. European Investment Bank (EIB)
192. European Union
193. Evotec
194. F-Prime Capital
195. Fairhaven Capital Partners
196. Farzad (Zod) Nazem
197. Federated Kaufmann Fund
198. Felicis Ventures
199. Fenox Venture Capital
200. Fidelity
201. Fifty Years
202. Finance Wales
203. Financiere Boscary
204. Finorpa
205. First Round
206. First Round Capital
207. First Star Ventures
208. Flare Capital Partners
209. Fly Ventures

210. Flybridge
211. Flybridge Capital Partners
212. Fond Vives II
213. Foresite Capital
214. Formic Ventures
215. Foundation Capital
216. Foundation for Technological Innovation
217. Founders Factory
218. Founders Fund
219. FPrime Capital
220. Frazier Healthcare Partners
221. FREES FUND
222. Fund+
223. FundersClub
224. Fusion Fund
225. Future Fund
226. Future Ventures
227. GEIF Ventures
228. General Atlantic
229. General Catalyst
230. Generation Investment Management

231. Geodesic Capital
232. Gi Global Health Fund LP
233. GlaxoSmithKline
234. Global Brain Corporation
235. Global Founders Capital
236. GM&C Life Sciences Fund
237. GNI Group
238. GNS Healthcare
239. Golden Ventures
240. Goldman Sachs
241. Goodman Capital
242. Google
243. Government of Canada
244. Government Of Quebec
245. GPG Ventures
246. Gradient Ventures
247. Great Oaks Venture Capital
248. Green Park & Golf Ventures
249. GreenSky Capital
250. Greenspring Associates
251. Greylock

600 Investors - AI for Drug Discovery and Advanced R&D

252. Grok Ventures
253. Groupe Roski
254. Grove Ventures
255. GV
256. Gyan Kapur
257. Hack VC
258. Hacking Health Accelerator
259. Hanhai Studio
260. HBM Partners
261. Health Velocity Capital
262. Health Wildcatters
263. Healthbox
264. HealthInc
265. Heritage Provider Network
266. Hewlett Packard Pathfinder
267. HIGHLINEvc
268. Hike Ventures
269. Hillhouse Capital Group
270. Hitachi
271. Hiventures Investment Fund

272. HOF Capital
273. Holtzbrinck Digital
274. Horizon Healthcare Services
275. Horizons Ventures
276. Human Capital
277. Hyperplane Venture Capital
278. IA Ventures
279. IBM
280. IDG Capital
281. Idinvest Partners
282. iGan Partners
283. Illumina Ventures
284. Inbio Ventures
285. INDEX: Design to Improve Life
286. IndieBio
287. Industry Ventures
288. Initialized Capital
289. Innospark Ventures
290. Innovate UK
291. Inovia Capital
292. Institut Català de Finances (ICF)

293. Intel Capital
294. Intermountain Ventures
295. International Private Bank (IPB)
296. Invoke Capital Partners
297. Invus
298. IPGL
299. IQ Capital
300. Ireland Strategic Investment Fund
301. IT-Farm
302. J. Hunt Holdings
303. James Hong
304. Jiantou Huawen Investment
305. JMI Equity
306. Johnson & Johnson Innovation
307. Juvenescence
308. Kakao Ventures
309. Kapor Capital
310. Karlin Ventures
311. KdT Ventures
312. Khosla Ventures
313. Kima Ventures

600 Investors - AI for Drug Discovery and Advanced R&D

314. Kingsley Advani
315. Kleiner Perkins
316. Konstantin von Unger
317. Korea Tech Incubator Program
318. KTB Network
319. La Famiglia
320. LabCorp
321. Lakestar
322. Lane Bess
323. Lansdowne Partners
324. Lanza Tech Ventures
325. LaunchCapital
326. Laurion Capital Management
327. LB Investment
328. LeFrak
329. Life Sciences Angel Network
330. Lifeforce Capital
331. LifeSci Venture Partners
332. Lightspeed Venture Partners
333. Lightstone Ventures

334. Lilly Asia Ventures
335. Lilly Ventures
336. Lim Teck Lee
337. Linden Mobile Ventures
338. Liquid 2 Ventures
339. London CoInvestment Fund
340. Lucas Venture Group
341. Lundbeck
342. Lux Capital
343. LVL1 Group
344. M12
345. MACSF
346. Madrona Venture Group
347. Magnetic Ventures
348. Manchester Tech Trust Angels
349. Marathon Venture Capital
350. Marketplace Funds
351. Masa Life Science Fund
352. MassChallenge
353. Matrix Capital Management

354. Matrix Partners
355. Maverick Ventures
356. Mayo Clinic
357. Mayo Clinic Ventures
358. MedTech Innovator
359. Menlo Ventures
360. Merck
361. Merck Global Health Innovation Fund
362. Mercury Fund
363. Michael Antonov
364. Michael J. Fox Foundation
365. Microsoft
366. Midven
367. Minneapolis Heart Institute Ventures
368. Mission and Market
369. Mission Bay Capital
370. MIT delta v
371. MITS Fund
372. Mitsui & Co
373. Monsanto Growth Ventures (MGV)

600 Investors - AI for Drug Discovery and Advanced R&D

374. Morgan Noble
375. MPM Capital
376. MRL Ventures Fund
377. Mubadala Capital Ventures US
378. Mubadala Investment Company
379. National Institutes of Health
380. NDRC
381. Neoteny
382. Nest.Bio Ventures
383. Nesta Ventures
384. New Enterprise Associates
385. New Leaf Venture Partners
386. New Wave Ventures
387. New York Presbyterian Ventures
388. New York State
389. New York State of Opportunity
390. NewDo Venture
391. Nex Cubed
392. Nextech Invest
393. Nikon

394. Nir Kalkstein
395. NJF Capital
396. Nordic Impact
397. Normandie Participations
398. Northleaf Capital Partners
399. Northpond Ventures
400. Northstar Ventures
401. Novaquest Capital Management
402. Novartis
403. Novartis Venture Fund
404. NPIF Maven Equity Finance
405. NVIDIA
406. Oak HC/FT
407. Obvious Ventures
408. OrbiMed
409. Origin Capital
410. OS Fund
411. Oseo
412. OUP (Osage University Partners)
413. Overkill Ventures

414. Palisades Growth Capital
415. Panache Ventures
416. Parinvest
417. Partner Fund Management
418. Pavilion Capital
419. Paxion Capital Partners
420. Pear VC
421. Pentech Ventures
422. Perceptive Advisors
423. Perivoli Innovations
424. Pfizer
425. Pfizer Venture Investments
426. Pi Campus
427. Pillar Companies
428. Pinnacle Ventures
429. Pioneer Fund
430. PivotNorth Capital
431. Plug and Play
432. Polaris Partners
433. PP Capital

600 Investors - AI for Drug Discovery and Advanced R&D

434. Prefix Capital	454. Revolution	474. Sapphire Ventures
435. Premier Partners	455. Rho Canada Ventures	475. Scale Asia Ventures
436. Primary Venture Partners	456. Right Side Capital Management	476. Schooner Capital
437. Pritzker Group Venture Capital	457. Rising Tide	477. Schrodinger
438. Qiming Venture Partners	458. Riva Capital	478. SciFi VC
439. QTV Financial	459. Rivas Capital	479. Sea Lane Ventures
440. Qualgro VC	460. Riverbank Capital Securities	480. Section 32
441. QVT Financial	461. Robin Hood Ventures	481. Seedcamp
442. RA Capital Management	462. Roche	482. Seneca Partners
443. Radical Ventures	463. Roche Venture Fund	483. Sequoia Capital
444. Ramen Ventures	464. Rock Health	484. Sequoia Capital China
445. Razor's Edge Ventures	465. Roivant Sciences	485. Seraph Group
446. Real Ventures	466. Romulus Capital	486. Serena
447. Redalpine	467. RTW Investments LLC	487. Service Provider Capital
448. Redmile Group	468. S.R.I.W.	488. ServiceNow
449. Redpoint	469. SAIF Partners	489. Seventure Partners
450. Refactor Capital	470. Salesforce	490. SFPIFPIM
451. Reneo Capital Management	471. Samsung Electronics	491. SGInnovate
452. Renren Inc.	472. Sanabil	492. Shangbay Capital
453. Rev1 Ventures	473. Sanofi	493. Shasta Ventures

600 Investors - AI for Drug Discovery and Advanced R&D

494. Shengding Equity Investment Fund	514. Sound Ventures	534. Synetro Group
495. Shunwei Capital	515. SPARK Impact	535. T. Rowe Price
496. Siemens	516. SpringRock Ventures	536. Tamarind Hill
497. Sierra Ventures	517. Square 1 Bank	537. Tavistock Group
498. Silicon Badia	518. SR One	538. TCP Venture Capital
499. Silicon Valley Bank	519. Stage Venture Partners	539. Team Builder Ventures
500. Singularity University Ventures	520. Stanford University Venture Fund	540. Techammer
501. Sinopharm Capital	521. Starlight Ventures	541. Techstars
502. Sinovation Ventures	522. Start Capital	542. TECHU
503. Sixty Degree Capital	523. StartUp Health	543. Temasek Holdings
504. Sky Ventures Group	524. Startupbootcamp	544. Tencent Holdings
505. Slow Ventures	525. StartX (StanfordStartX Fund)	545. TenOneTen Ventures
506. Smedvig Capital	526. Stripes	546. Terra Magnum Capital Partners
507. Sofinnova Partners	527. Summit Partners	547. The Cedars-Sinai Accelerator
508. SoftBank	528. Susa Ventures	548. The Column Group
509. Softbank Ventures Asia	529. Susquehanna International Group (SIG)	549. The Family
510. SoftBank Vision Fund	530. Sustainable Conversion Ventures	550. The Index Project
511. Soma Capital	531. SV Angel	551. The Longevity Fund
512. Sorrento Therapeutics	532. SV Tech Ventures	552. The Thiel Foundation
513. SOSV	533. Swisscom Ventures	553. Third Kind Venture Capital

600 Investors - AI for Drug Discovery and Advanced R&D

554. Third Rock Ventures	574. Universal Materials Incubator	593. Walking Ventures
555. TiE Angels	575. University of Birmingham	594. Washington Research Foundation
556. TIS Japan	576. Unshackled Ventures	595. Wavemaker Partners
557. Trancos Ventures	577. UpHonest Capital	596. Wellington Management
558. Travis May	578. Upsher Smith Laboratories	597. Western Technology Investment
559. Tribeca Venture Partners	579. Vanguard Atlantic	598. White Cloud Capital
560. Trinitas Capital	580. Varian	599. WI Harper Group
561. True Ventures	581. Velocity.Partners	600. Wild Basin Investments
562. Truffle Capital	582. VenBio Partners	601. Woodford Investment Management
563. TSVC	583. Versant Ventures	602. WorldQuant Ventures LLC
564. Tuesday	584. Vertex Ventures	603. Wren Capital
565. Two River	585. Vertex Ventures Israel	604. WuXi AppTec
566. Two Sigma Ventures	586. Vertex Ventures Southeast Asia & India	605. WuXi Healthcare Ventures
567. uBiome	587. VI Partners	606. Y Combinator
568. UCB Pharma	588. Viking Global Investors	607. Yael Capital Management Limited
569. UK Innovation & Science Seed Fund	589. Village Global	608. YF Capital (Yunfeng Capital)
570. UL Ventures	590. VisVires New Protein	609. Yitu Technology
571. Uncommon Denominator	591. Vives Fund	610. ZebiAI
572. Uni-Innovate Group	592. Walden Riverwood Ventures	611. ZhenFund
573. UnitedHealthcare Accelerator Powered by Techstars		612. Zhongyuan Union Cell & Gene Eng

30 Pharma Corporations Applying AI for Drug Discovery

COMPANY NAME	BASED IN	WEBSITE
1. AbbVie	United States	abbvie.com
2. Agios Pharmaceuticals	United States	agios.com
3. Amgen	United States	amgen.com
4. Astellas Pharma	Japan	astellas.com
5. Astrazeneca	United Kingdom	astrazeneca.com
6. Bayer	Germany	bayer.com
7. Biogen	United States	biogen.com
8. Boehringer Ingelheim	Germany	boehringer-ingelheim.com
9. Bristol-Myers Squibb	United States	bms.com
10. Celgene	United States	celgene.com
11. Ilumina	United States	illumina.com
12. Ipsen	France	ipsen.com
13. Janssen Pharmaceuticals	Belgium	janssen.com
14. Johnson & Johnson	United States	jnj.com
15. Merck	United States	merck.com

30 Pharma Corporations Applying AI for Drug Discovery

COMPANY NAME	BASED IN	WEBSITE
16. Mitsubishi Tanabe Pharma	Japan	https://www.mt-pharma.co.jp/
17. Novartis	Switzerland	novartis.com
18. Novo Nordisk	Denmark	novonordisk.com
19. Daewoong Pharmaceutical	South Korea	daewoong.com
20. Evotec	Germany	evotec.com
21. Genentech	United States	gene.com
22. Gilead Sciences	United States	gilead.com
23. GSK	United Kingdom	gsk.com
24. Pfizer	United States	pfizer.com
25. Roche	Switzerland	roche.com
26. Sanofi	France	m-en.sanofi.com
27. Santen	Japan	santen.com
28. Sumitomo Dainippon Pharma	Japan	ds-pharma.com
29. Takeda	Japan	takeda.com
30. Teva Pharmaceutical	Israel	tevapharm.com

15 Chemical Corporations Applying AI in Healthcare

COMPANY NAME	BASED IN	WEBSITE
1. Asahi Kasei	Japan	asahi-kasei.co.jp
2. BASF	Germany	basf.com
3. COVESTRO	Germany	covestro.com
4. DIC	Japan	dic-global.com
5. The Dow Chemical Company	United States	dow.com
6. DSM	The Netherlands	dsm.com
7. DUPONT	United States	dupont.com
8. ECOLAB	United States	de-at.ecolab.com
9. EVONIK INDUSTRIES	Germany	corporate.evonik.de
10. Henkel	Germany	henkel.com
11. Lonza	Switzerland	lonza.com
12. MITSUI CHEMICALS	Japan	mitsuichem.com
13. Solvay	Belgium	solvay.de
14. SUMITOMO CHEMICAL	Japan	sumitomo-chem.co.jp
15. SYNGENTA	Switzerland	syngenta.com

25 Tech Corporations Applying Advanced AI in Healthcare

COMPANY NAME	BASED IN	WEBSITE
1. Adobe	United States	adobe.com
2. Alibaba	China	alibaba.com
3. Amazon	United States	amazon.com
4. Apple	United States	apple.com
5. Baidu	China	baidu.com
6. Canon	United States	usa.canon.com
7. Cisco	United States	cisco.com
8. Dell Technologies	United States	delltechnologies.com
9. Foxconn Technology	Taiwan	foxconn.com
10. Fujitsu	Japan	fujitsu.com
11. Google	United States	google.com
12. Hitachi	Japan	hitachi.com
13. Huawei	China	huawei.com
14. IBM	United States	ibm.com
15. Intel	United States	intel.com

25 Tech Corporations Applying Advanced AI in Healthcare

COMPANY NAME	BASED IN	WEBSITE
16. Microsoft	United States	microsoft.com
17. Nvidia	United States	nvidia.com
18. Oracle	United States	oracle.com
19. Salesforce	United States	salesforce.com
20. SAP	Germany	sap.com
21. Samsung Electronics	South Korea	samsung.com
22. Siemens	Germany	siemens.com
23. Tencent	China	tencent.com
24. Unisys	United States	unisys.com
25. Workday	United States	workday.com

20 CROs AI in Healthcare

COMPANY NAME	BASED IN	WEBSITE
1. Aptuit	Italy	aptuit.com
2. BioClinica	United States	bioclinica.com
3. Charles River Laboratories	United States	criver.com
4. CMIC	United States	en.cmicgroup.com
5. Covance	China	covance.com
6. Galapagos NV	Belgium	glpg.com
7. ICON	United States	iconplc.com
8. IonsGate	Canada	ionsgate.com
9. IQVIA	United States	iqvia.com
10. Iris Pharma	France	iris-pharma.com
11. J-STAR Research, Inc. / Porton	United States	jstar-research.com
12. Open Orphan plc	Ireland	openorphan.com
13. PAREXEL	United States	parexel.com
14. Phastar	Great Britain	phastar.com
15. Phlexglobal	Great Britain	phlexglobal.com
16. PPD	United States	ppd.com
17. PRA International	United States	prahs.com
18. SGS	Switzerland	sgs.com
19. Synsight	France	synsight.net
20. WuXi AppTec	China	wuxiapptec.com

Overview of Proprietary Analytics by Deep Pharma Intelligence

About Deep Pharma Intelligence

Deep Pharma Intelligence is producing regular analytical reports on major areas of high-potential in the pharmaceutical and healthcare industries, maintaining ratings of companies and governments based on their innovation potential and business activity in the BioTech space, and providing strategic consulting and investment intelligence services to top-tier clients, including major investment funds and banks, family offices, insurance companies, government organizations, and big pharma companies among others. The company is a joint venture between the two highly specialized UK-based market intelligence hubs in Pharma / BioTech space:
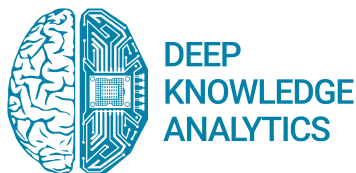
Pharma Division of Deep Knowledge Analytics (PD-DKA), a specialized subsidiary of Deep Knowledge Analytics (DKA), the leading analytical entity specifically focused on deep intelligence of the high-potential areas in the pharma industry, including artificial intelligence (AI) for drug discovery sector.

Deep Knowledge Analytics Pharma Division serves as the main source of investment intelligence and analytics for AI-Pharma, a specialized index hedge fund for the AI in the drug discovery sector. PD-DKA's insights are frequently covered by top media such as Forbes and the Financial Times, and are acknowledged by top pharma executives.

Recently, MIT named this division a top technology think-tank, acknowledging the AI ranking framework it developed.

BPT Analytics (BiopharmaTrend) - a rapidly growing analytical portal and media resource, dedicated to tracking emerging companies (startups/scaleups), innovations, investments, and trends in the pharma and biotech space.

BiopharmaTrend's reports and articles were referenced by Deloitte, Forbes, and other high profile media and consulting companies.

BiopharmaTrend is a media partner to a number of top-tier conferences and symposia in preclinical and clinical research, and healthcare research.

Overview of Proprietary Analytics by Pharma Division of Deep Pharma Analytics

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

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

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

Services:

- Investment landscape profiling, identifying investment ideas in the biotech/healthcare tech space.

- Preliminary due-diligence (business, science and technology, intellectual property (IP) profiling, freedom of operation assessment, legal assessment etc).

- Comprehensive due-diligence (deep business, science and technology assessment, IP and legal assessment, growth potential assessment etc).

- Infringement analysis of technology (i.g. If you plan to partner or invest in a data-analytics biotechs, or AI-development vendors, it is essential to understand their technological assets, both in terms of innovation potential and in terms of legal protection and non-infringement risk management).

- SWOT analysis of companies and technological sectors, competitive profiling.

- Industry profiling and growth strategy development for top-tier companies and governments.

Overview of Proprietary Analytics by Pharma Division of Deep Pharma Analytics

Proprietary Reports

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

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

The value our reports can deliver:

- Deep analysis of the deal-making prospects in the biotech and healthcare tech space, identification of top mini-trends and larger tendencies in innovations and technology adoption (e.g. AI, blockchain, eHealth tech, longevity biomarkers, new therapeutics and therapies etc.);

- Tangible forecasts on the 3-5 years horizon, providing an overview of future scenarios of the development of various technologies in the pharma industry;

- Practical guides for adopting various technological solutions and best practises, vendor profiling and contract research strategy building;

- Analysis of key market players in the emerging and high-growth areas of the pharmaceutical and biotech industries.

The parties who gain early access to these reports will have deep expertise on how their strategic agendas can be optimized in order to leverage novel research, new technologies, and emerging market opportunities, and stay competitive in a rapidly-changing technological environment, and taking into account shifting global priorities and trends.
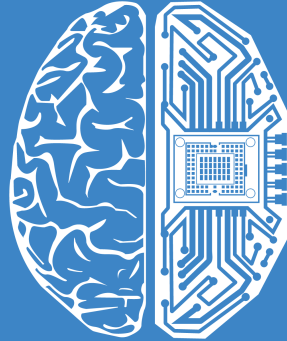
Deep Pharma Intelligence:
Upcoming Projects and Analytical Tools
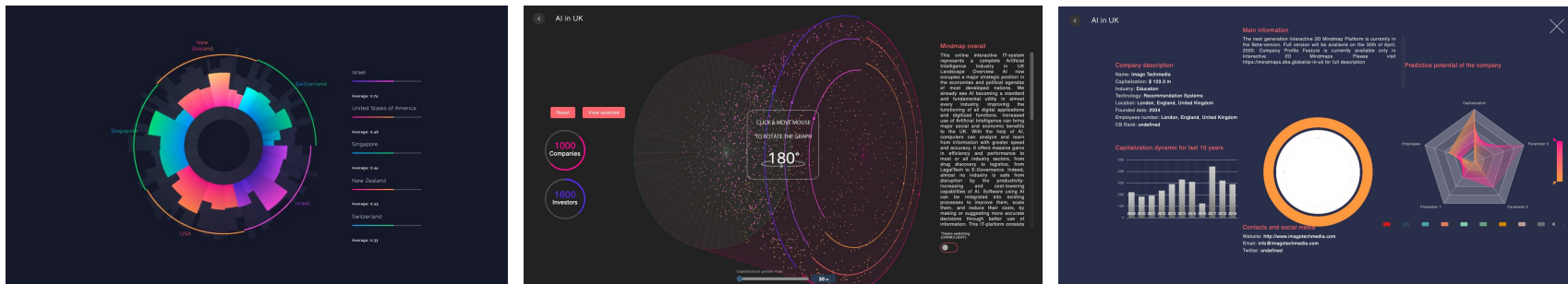
3D Visualisation Prototypes
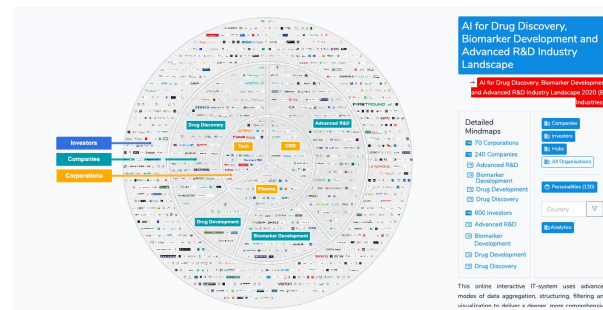
Deep Pharma Intelligence Big Data Analytics Dashboard

DEEP PHARMA INTELLIGENCE

Link to the Report: deep-pharma.tech/landscape-overview

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