



AI FOR DRUG DISCOVERY, BIOMARKER DEVELOPMENT AND ADVANCED R&D LANDSCAPE OVERVIEW 2018 / Q2

Companies - 100
Investors - 220
Corporations - 30
R&D Centers - 20
Conferences - 20

AI for Drug Discovery, Biomarker Development and Advanced R&D Landscape Overview 2018 / Q2

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AI for Drug Discovery, Biomarker Development and Advanced R&D Landscape Overview 2018 / Q2

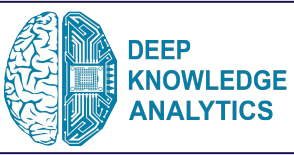
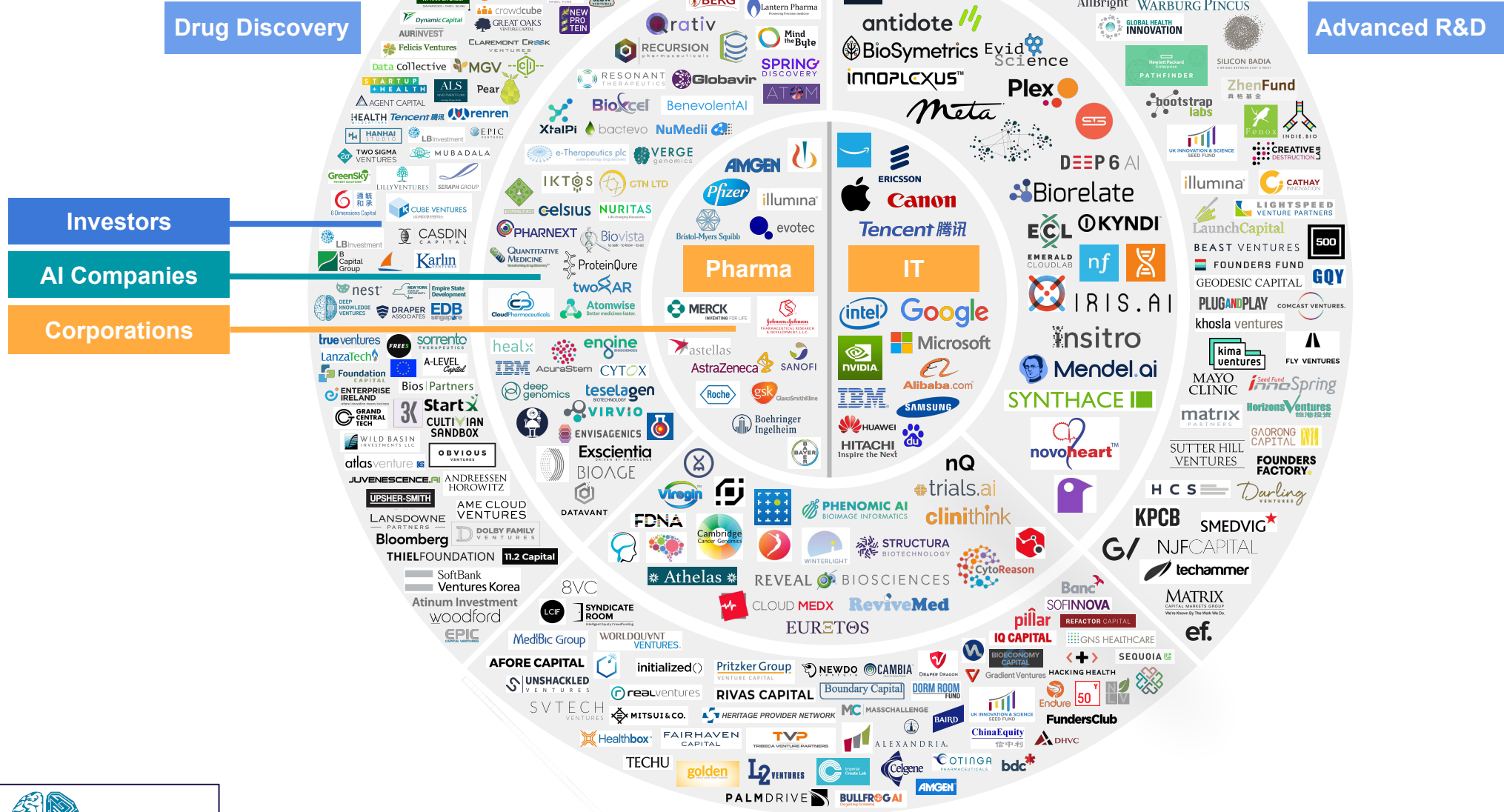
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AI for Drug Discovery, Biomarker Development and Advanced R&D Landscape / 2018 Q2

Companies - 100
Investors - 220
Corporations - 30



Biomarker Development

Diversification of AI for R&D and Drug Discovery process

Companies - 100
Investors - 220

Companies

Investors

Drug Design

Data Aggregation & Analysis

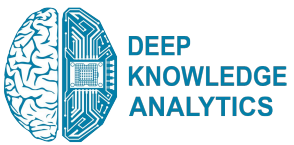
Clinical Trial Design, Optimization, Recruitment

Repurposing Existing Drugs

Researching Mechanisms of Disease

Design Preclinical Experiments

Preclinical Experiment Execution



AI for Drug Discovery, Biomarker Development and Advanced R&D Landscape / 2018 Q2

Companies - 100
Investors - 220
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Regional Position

Investors
AI Companies
Corporations

UK

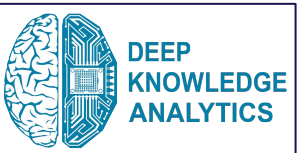
Canada

Other Regions

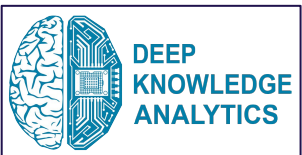
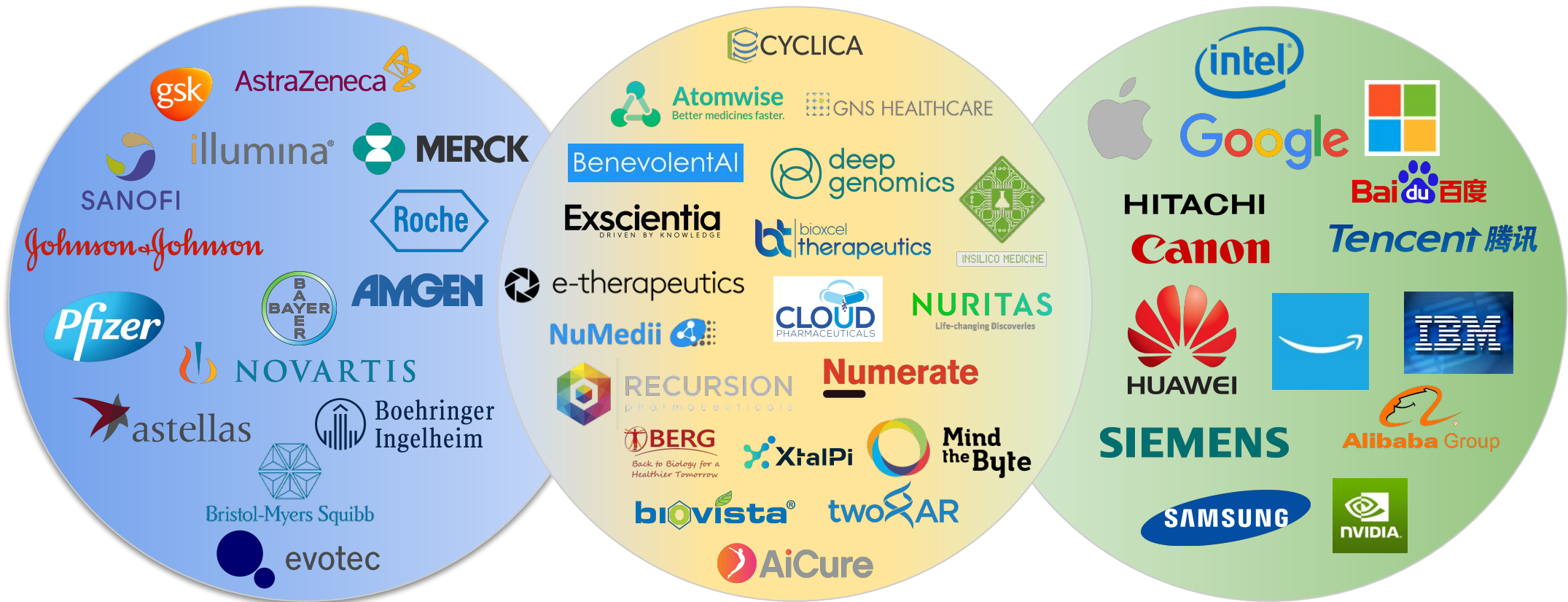
EU

Asia

USA



Leading IT and Tech Corporations / AI Companies / Pharma Corporations Advanced AI in Healthcare and Drug Discovery



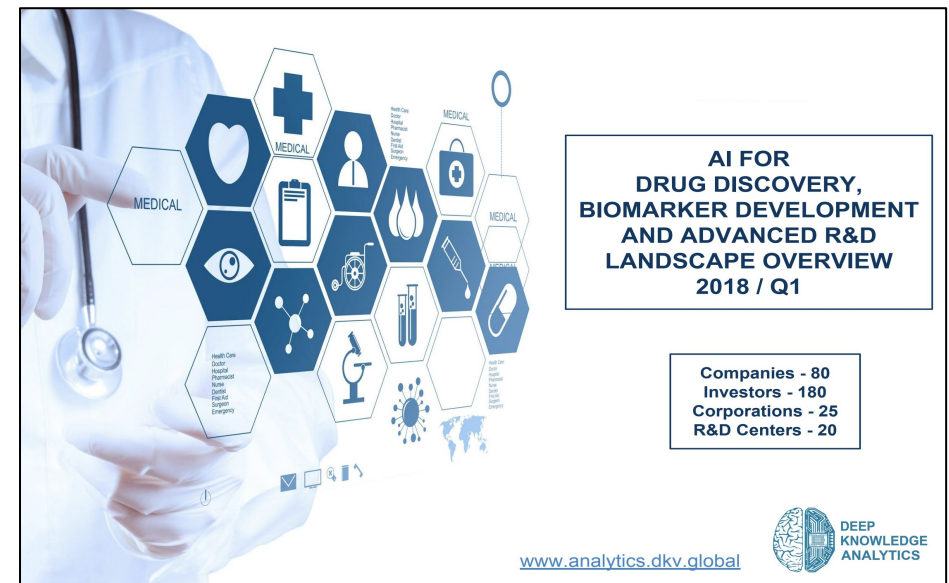
AI for Advanced R&D and Drug Discovery 2018 / Q2

In the end of 2017 our analytical department released its inaugural report on the state of AI for Drug Discovery industry, entitled "[AI for Drug Discovery Landscape Overview 2017](#)".

In April 2018 we released a subsequent report entitled "[AI for Drug Discovery & Advanced R&D Q1 2018](#)".

The present report is a significantly extended edition with more in-depth coverage of specific topics, and which has aggregated all important industry developments occurring in the second financial quarter of 2018.

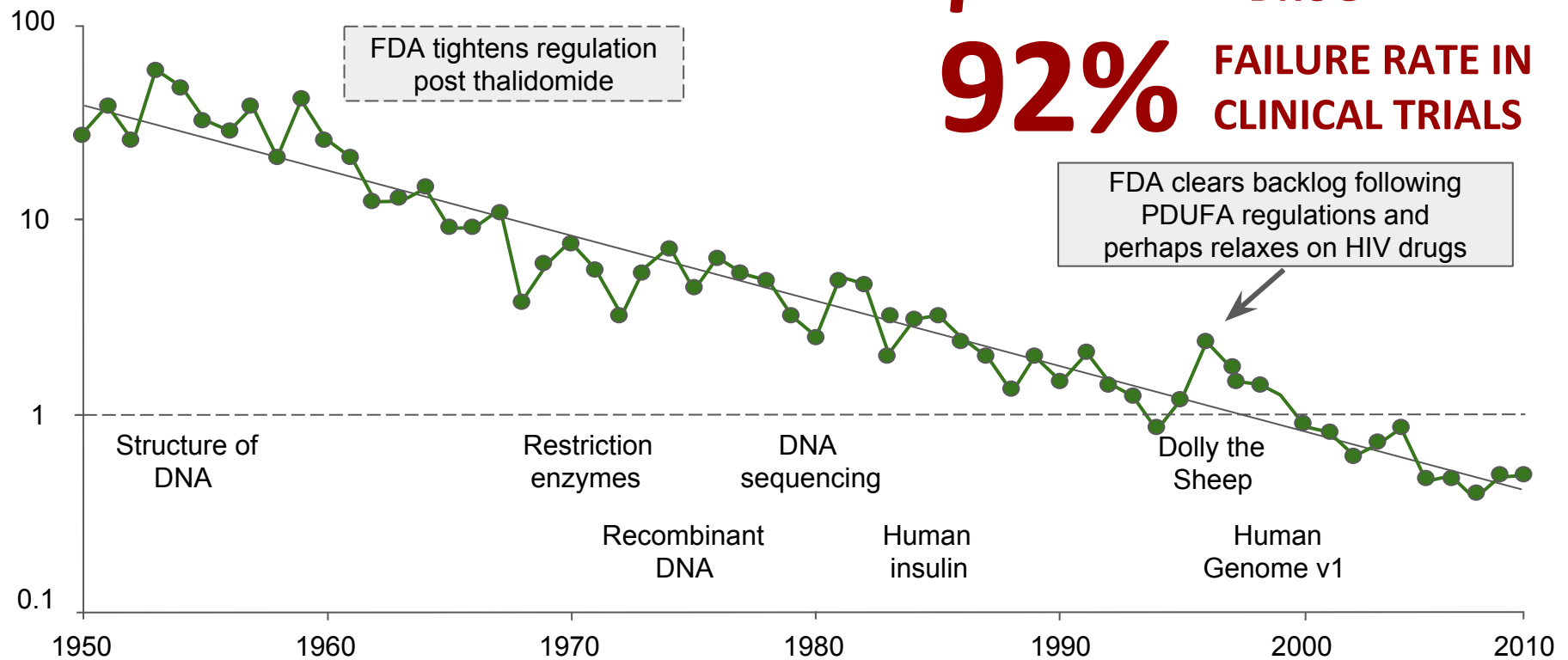
The second quarter of 2018 saw major changes, significant investments, acquisitions, and the establishment of substantial joint ventures. This serves as a stark reminder of how fast the AI for Drug Discovery, Biomarker Development and Advanced R&D sector is advancing. Many trends noted in our last report have continued and intensified, while other new trends have emerged as well.



Pharma Efficiency is Declining Steadily

>\$2.6B TO DEVELOP ONE DRUG
92% FAILURE RATE IN CLINICAL TRIALS

NMEs per \$B R&D spent (inflation adjusted)



Bernstein Research: The Long View - R&D Productivity, 2010

46 NEW DRUGS launched in 2014

Source: adapted from Insilico Medicine investor presentations, www.insilico.com

GLOBAL SALES:

>\$1 Trillion

GLOBAL R&D:

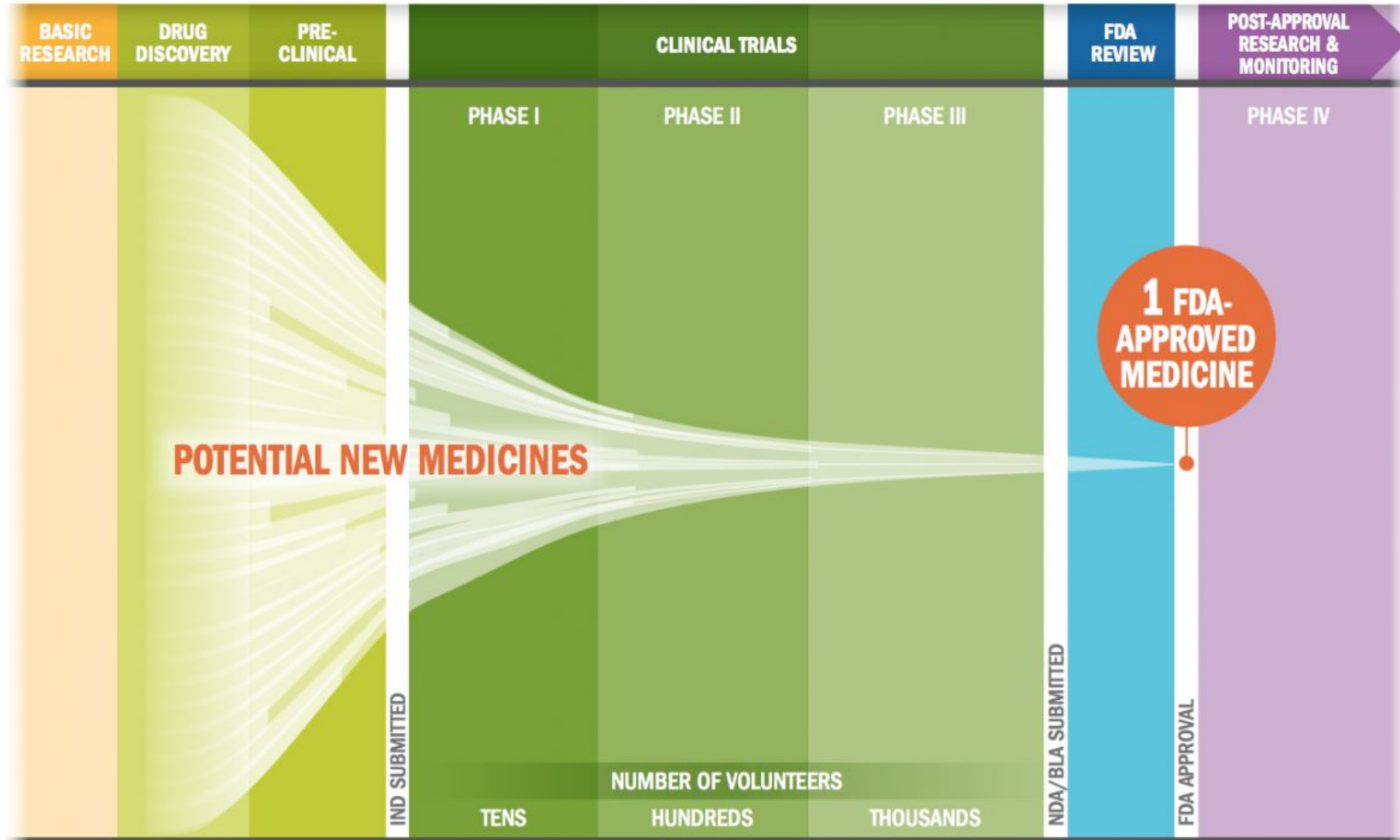
>\$150 Billion

>\$2.6B TO DEVELOP ONE DRUG

92% FAILURE RATE IN CLINICAL TRIALS

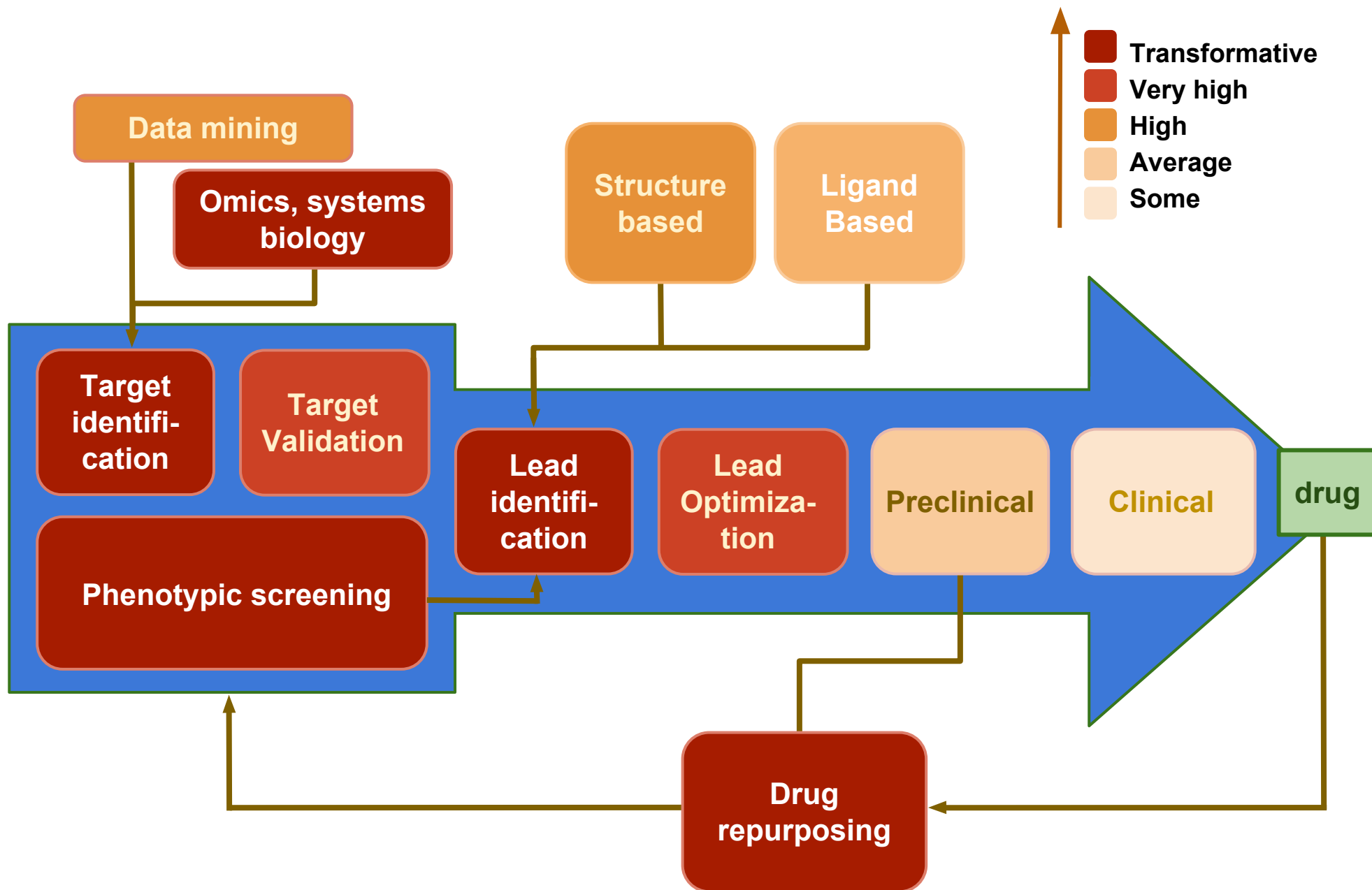


THE BIOPHARMACEUTICAL RESEARCH AND DEVELOPMENT PROCESS



Source: Biopharmaceutical Research & Development, PRMA http://phrma-docs.phrma.org/sites/default/files/pdf/rd_brochure_022307.pdf

The "heat map" of AI potential value for various R&D areas



The Application of AI for Advanced R&D

Generate Novel Drug Candidates

- 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

Aggregate and Synthesize Information

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

Repurpose 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

Design and Run 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

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

Computation-based Drug Discovery



Millions of
Compounds



1000s of
Compounds



Clinical Trials
FDA Approval
Process

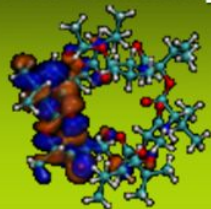
Synthesize new
Chemical Compounds

Robot-assisted screening
High Throughput Screening

Testing for Efficacy,
Side Effects, Safety

Computational Chemistry

- Synthesize compounds based on similarity



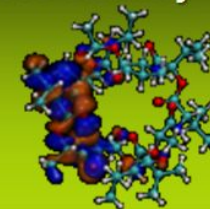
Virtual Screening

- Check if compounds bind to target proteins



Lead Optimization

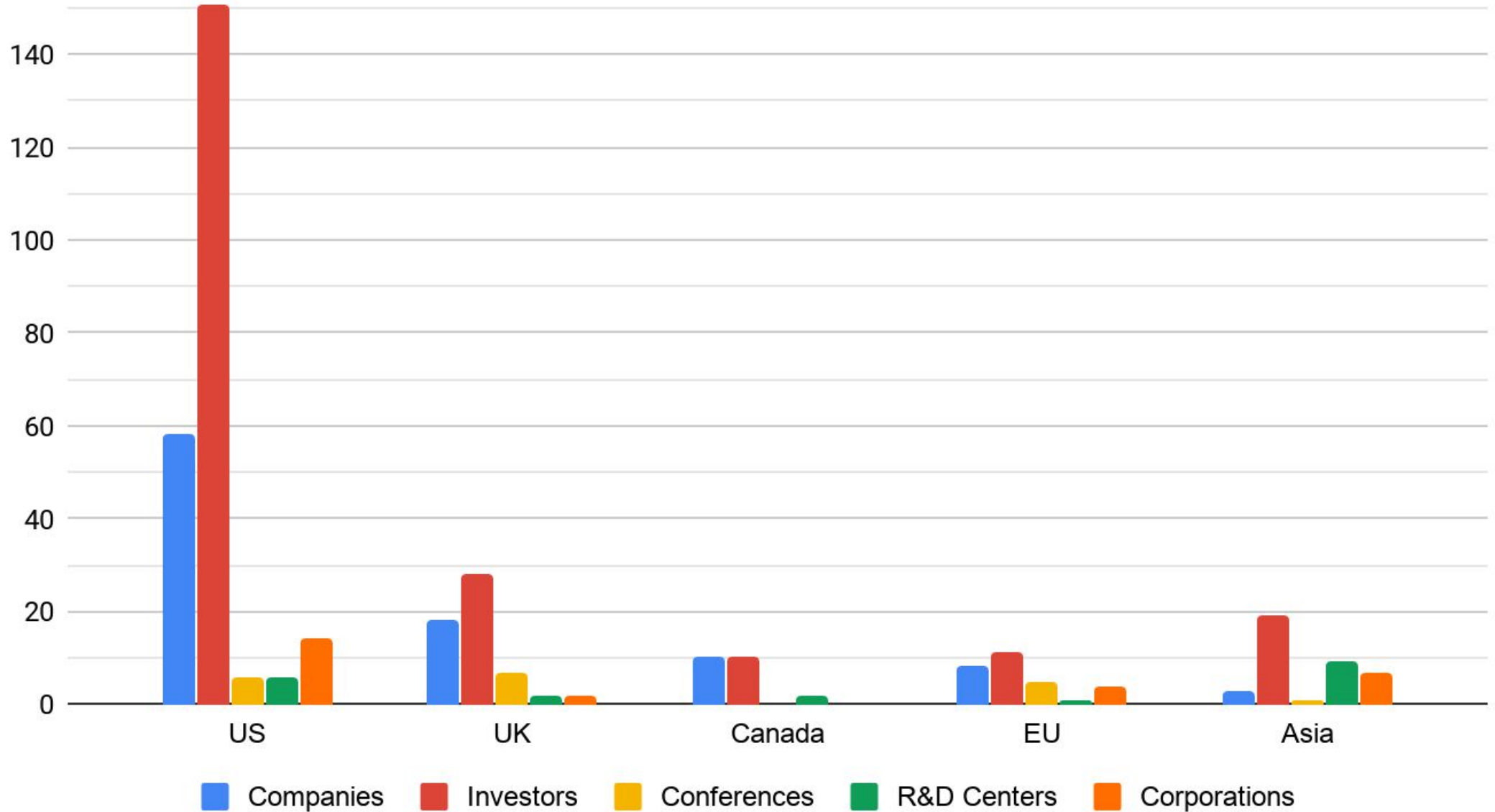
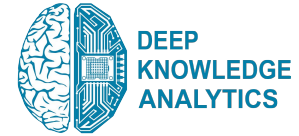
- Modify chemicals to improve efficacy



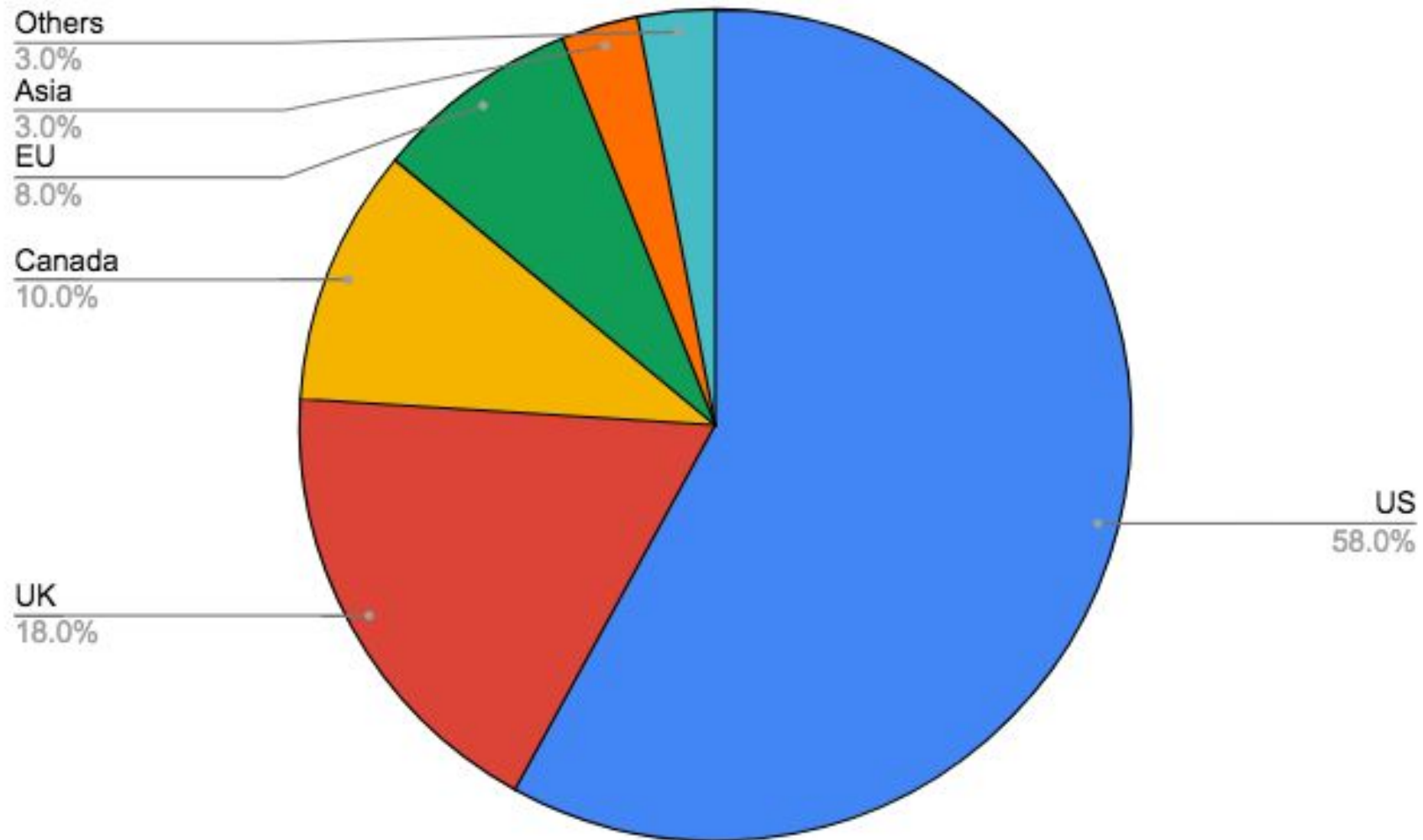
1

Source: <https://blogs.nvidia.com/blog/2010/01/22/accelerating-the-pace-of-drug-discovery-using-gpus/>

Regional Comparison of AI for Drug Discovery Companies/Investors/R&D Centers

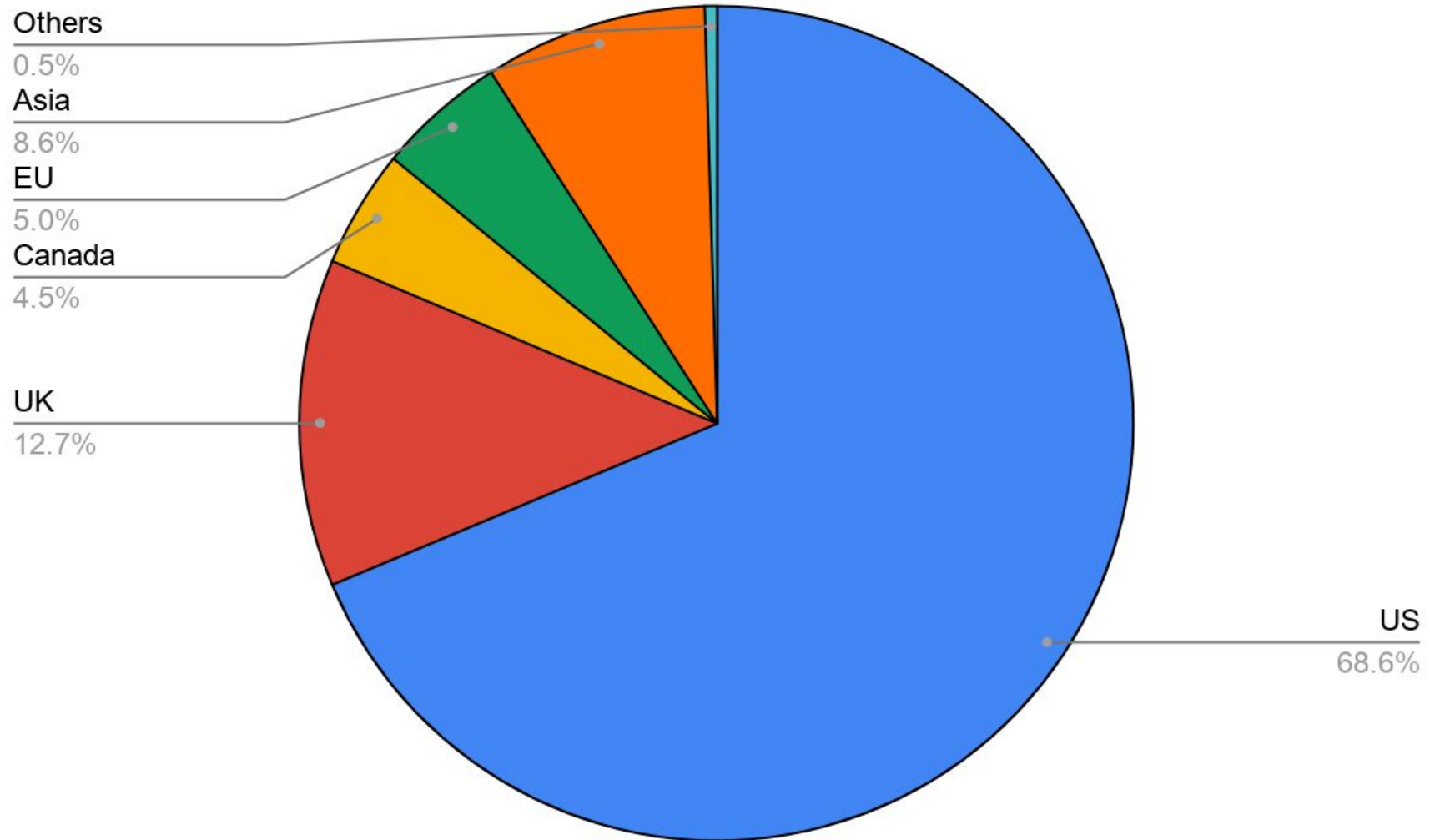


100 AI Companies: Regional Proportion



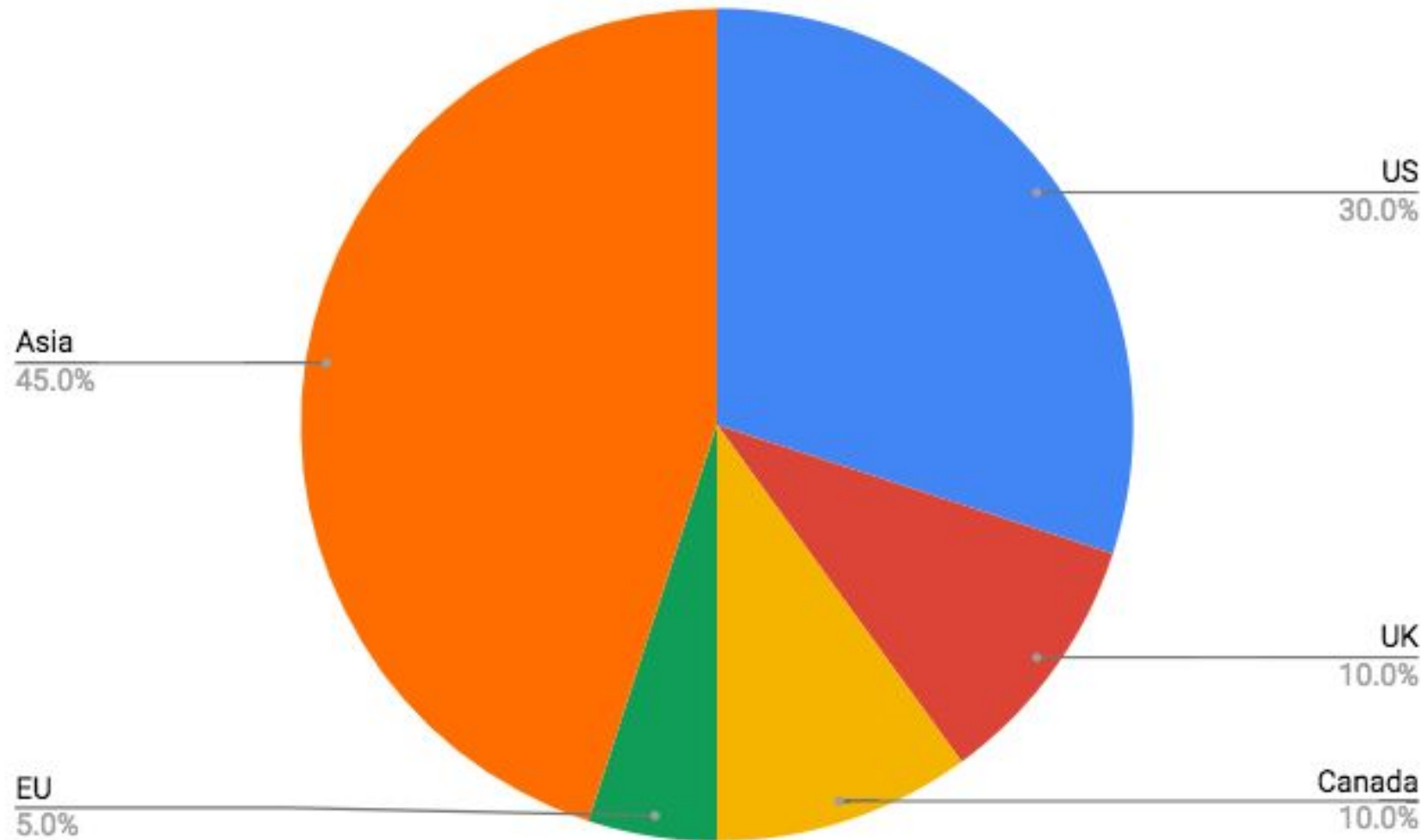
The US is still firmly in the lead in terms of its proportion of AI for Drug Discovery companies. Interestingly, Asia currently has the fifth-lowest proportion of AI for Drug Discovery companies. The Asia-Pacific region has, however, begin to aggressively increase their activity in the space in terms of investments into foreign companies (largely US-based companies), and we can 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.

220 Investors: Regional Proportion



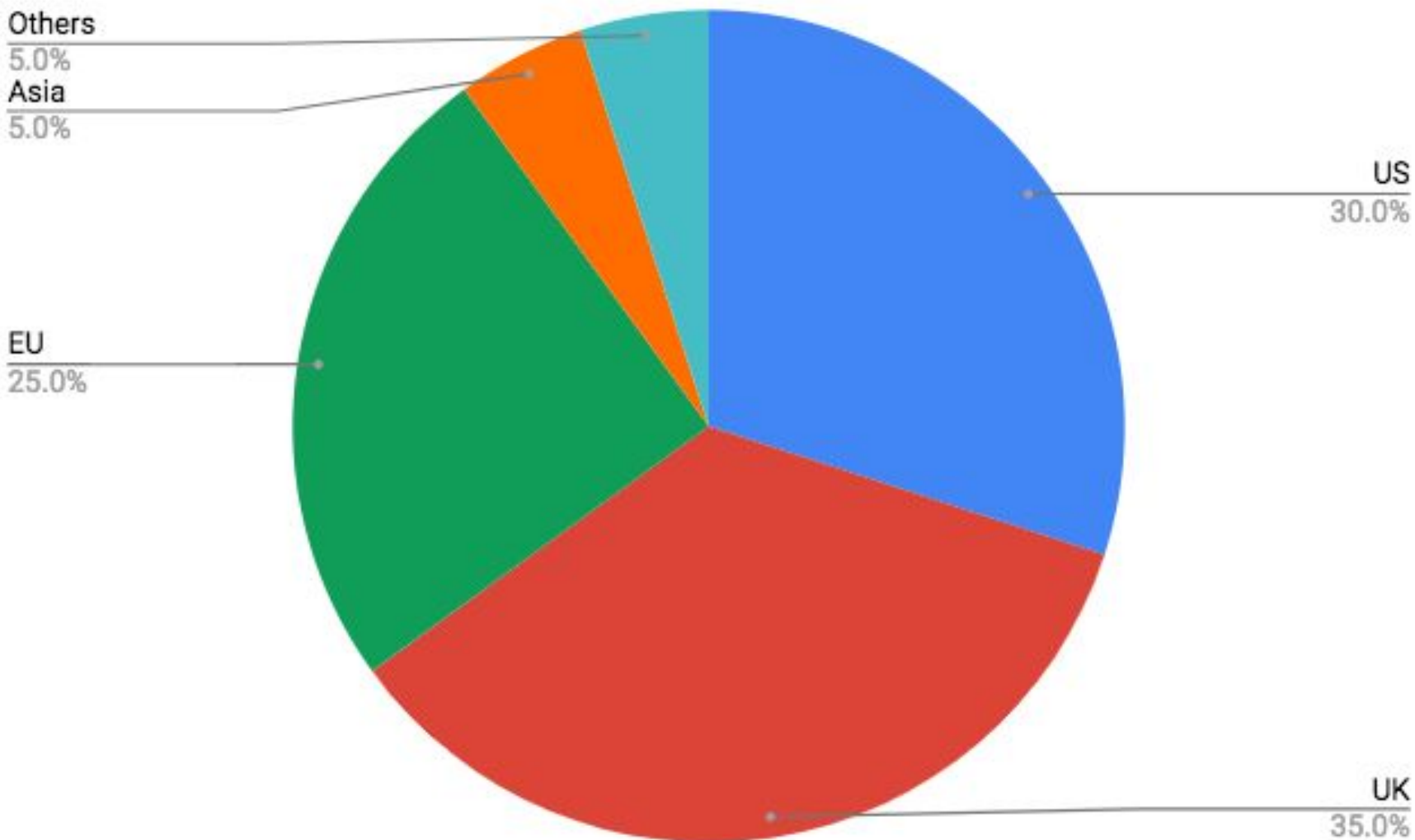
The US still leads the rest of the world in the proportion of AI for Drug Discovery Investors. This is sensible given that they also have the largest proportion of AI for Drug Discovery companies. However, it is interesting to note that, while the UK is home to the second-largest proportion of investors in this space, Asia has now overtaken the EU is rapidly advancing to acquire the #2 position. This past year has seen a substantial increase in the number of Asian investors, as well as Asian Tech & IT corporations, entering the AI for drug discovery industry.

20 Leading R&D Centers: Regional Proportion



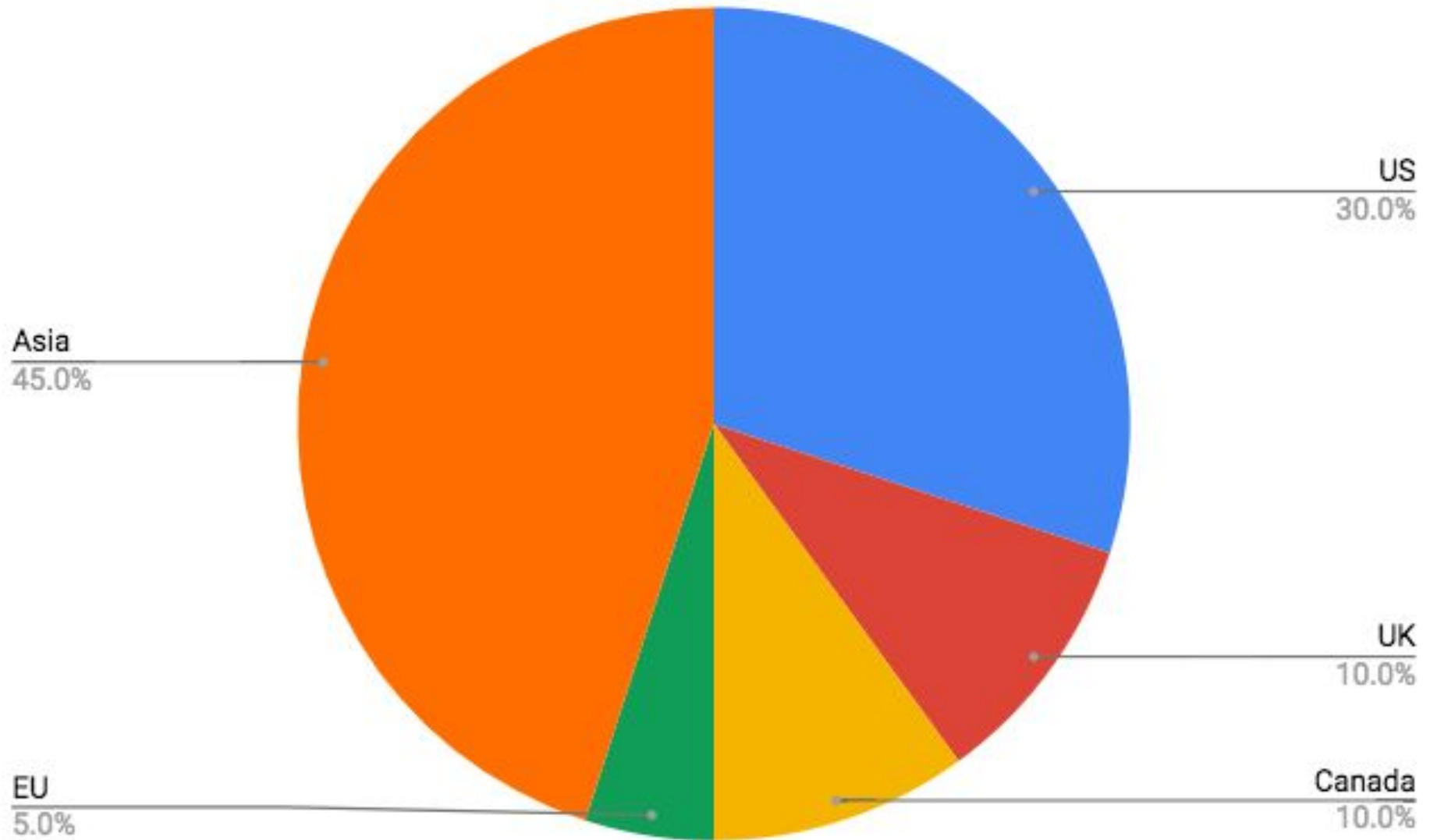
The figure above shows that while the US leads the world in terms of the number of R&D Centers focused on AI for Drug Discovery, China is rapidly catching up. This makes sense within the context of the recent increase in the number of Chinese investors entering the AI for Drug Discovery space, and the Chinese government's recent commitment to lead the world in AI by the year 2030.

Top-20 Conferences on AI for R&D and Drug Discovery 2018-2019: Regional Proportion

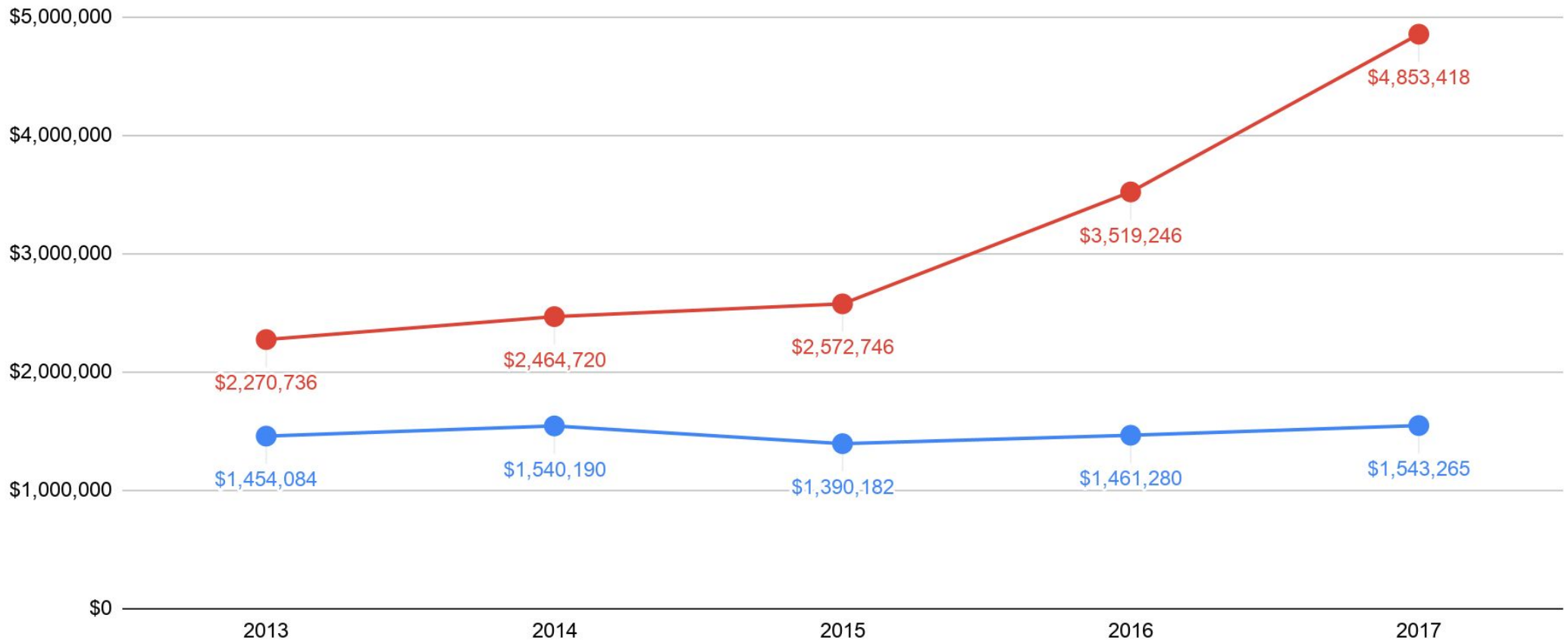


As can be seen in the figure above, whereas previously the US has dominated the AI for Drug Discovery conference landscape (which follows naturally from the fact that it also leads in terms of the total number of AI for Drug Discovery conferences and investors), we have seen a significant increase in the number of AI for Drug Discovery conferences located in the UK and EU.

30 Corporations Applying Advanced AI in Healthcare and Drug Discovery



Combined Capitalization of 15 IT & Tech Corporations vs 15 BioPharma Corporations In Millions of USD



As can be seen in the figure to the left, the combined capitalization of the 15 BioPharma corporations profiled in this report have remained on the same level for the past 5 years while the capitalization of the 15 IT & Tech corporations profiled in this report is growing significantly.

This can be considered as evidence that the BioPharma industry is stagnating in general, while the IT & Tech industry is progressing.

This is why it is so notable that the number of IT corporations has already matched the number of BioPharma corporations active in this subsector.

15 IT&Tech Corporations
15 BioPharma Corporations

Source: Deep Knowledge Analytics


Top 20 Global AI for Drug Discovery Conferences



AI Pharma
 10-11 Sep 2018 (remind.me)
 Tokyo, Japan

Interested Going

Cambridge Healthtech Institute's Inaugural
Artificial Intelligence & Machine Learning for Drug Discovery
 27 NOVEMBER 2018
 SHERATON LISBOA HOTEL & SPA | LISBON, PORTUGAL



12th June 2018
 De Vere Canary Wharf, London

AI IN PHARMA: OPPORTUNITIES & CHALLENGES

Get ahead of the curve in this AI strategy masterclass for executives in Pharma.
 Pre-Conference Think-Tank

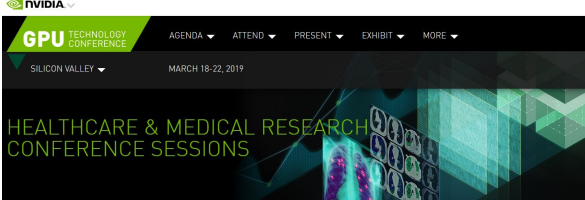


ADVANCED MACHINE LEARNING AND ARTIFICIAL INTELLIGENCE FOR DRUG DISCOVERY AND DEVELOPMENT
 Berlin, Germany 19-20th June



GPU TECHNOLOGY CONFERENCE
 SILICON VALLEY | MARCH 18-22, 2019

HEALTHCARE & MEDICAL RESEARCH CONFERENCE SESSIONS



ASDEvents
 conference, seminars & trainings

Artificial Intelligence in Pharma Industry Summit
 19 February, 2018 - 20 February, 2018,
 Berlin, Germany



The AI Health & Pharma Summit®
 Co-located with
The AI Summit LONDON
 14 JUNE 2018
 ExCeL EXHIBITION CENTRE, LONDON



Smi
 LINKING BUSINESS with INFORMATION



DRUG DISCOVERY
 21ST MARCH TO 22ND MARCH 2018,
 LONDON, UNITED KINGDOM



Cambridge Consultants

EVENT
AI in Pharma Summit 2018
 9th October 2018
 Boston, MA
 Venue: The State Room



Global Pharma R&D Informatics and AI Congress

WHEN
 29th-30th Oct 2018
 Registration from 8am

WHERE
 London, United Kingdom
 Radisson Blu Edwardian Heathrow

Home / Conferences / ARTIFICIAL INTELLIGENCE TO SPEED UP DRUG DISCOVERY: THE REVOLUTIONARY ROAD TO ADVANCING INNOVATION

ARTIFICIAL INTELLIGENCE TO SPEED UP DRUG DISCOVERY: THE REVOLUTIONARY ROAD TO ADVANCING INNOVATION

Top 20 Global AI for Drug Discovery Conferences



May 23, 2018
DoubleTree Suites Boston-Cambridge
Cambridge, MA



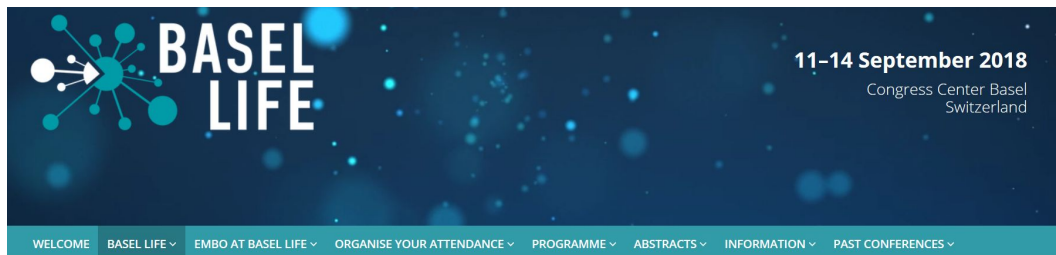
**2ND GLOBAL PHARMA R&D
INFORMATICS & AI CONGRESS**

29-30 OCTOBER 2018 – LONDON, UK



**Artificial Intelligence in Drug Development
Congress**

27-28 September 2017, London, UK



Artificial intelligence and blockchain in healthcare



**OXFORD
GLOBAL**

**2nd Annual Artificial Intelligence in Drug
Development Congress**

20-21 September 2018, London, UK

**AI PHARMA
INNOVATION
DRUG DISCOVERY**



**ARTIFICIAL INTELLIGENCE
TRANSFORMING PHARMA R&D**

11-14 September 2018

Congress Center Basel
Switzerland



11th & 12th July 2018,
Canary Riverside Plaza Hotel,
London UK

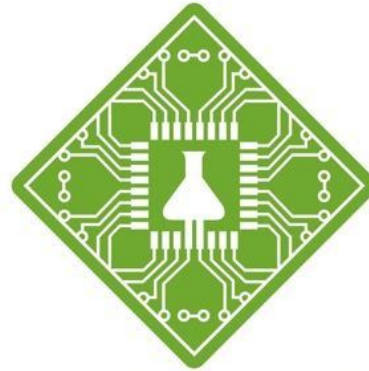


MAX PLANCK ALUMNI ASSOCIATION
Artificial Intelligence and Big Data in Pharma

Impact on drug development on the role of the industry

March 21, 2018
Max Planck Institute of Biochemistry, Munich

AI Companies in Longevity



INSILICO MEDICINE



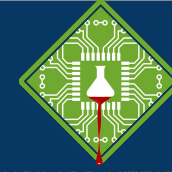
Atomwise
Better medicines faster.

Atomwise



BioAge

Insilico Medicine Aging.AI 2.0



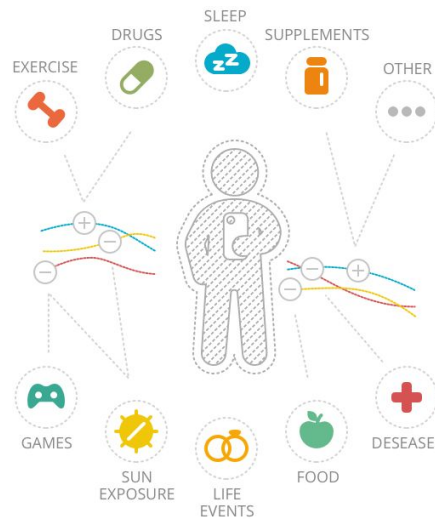
INSILICO MEDICINE

One of the most promising projects developed by Insilico Medicine is called Aging.AI 2.0, which is an AI-empowered platform integrating multiple predictors of clints age and used to track changes of health over time and optimize clints lifestyle.

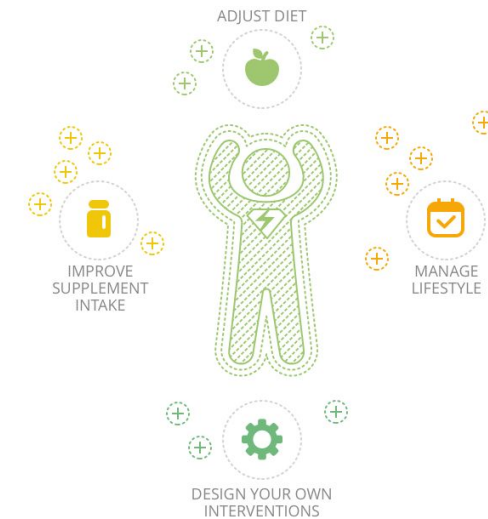
<http://young.ai/>



Track your age
at every level!



See what makes you
younger or older!



Stay young!

Insilico Medicine Earns Accolades from Frost & Sullivan

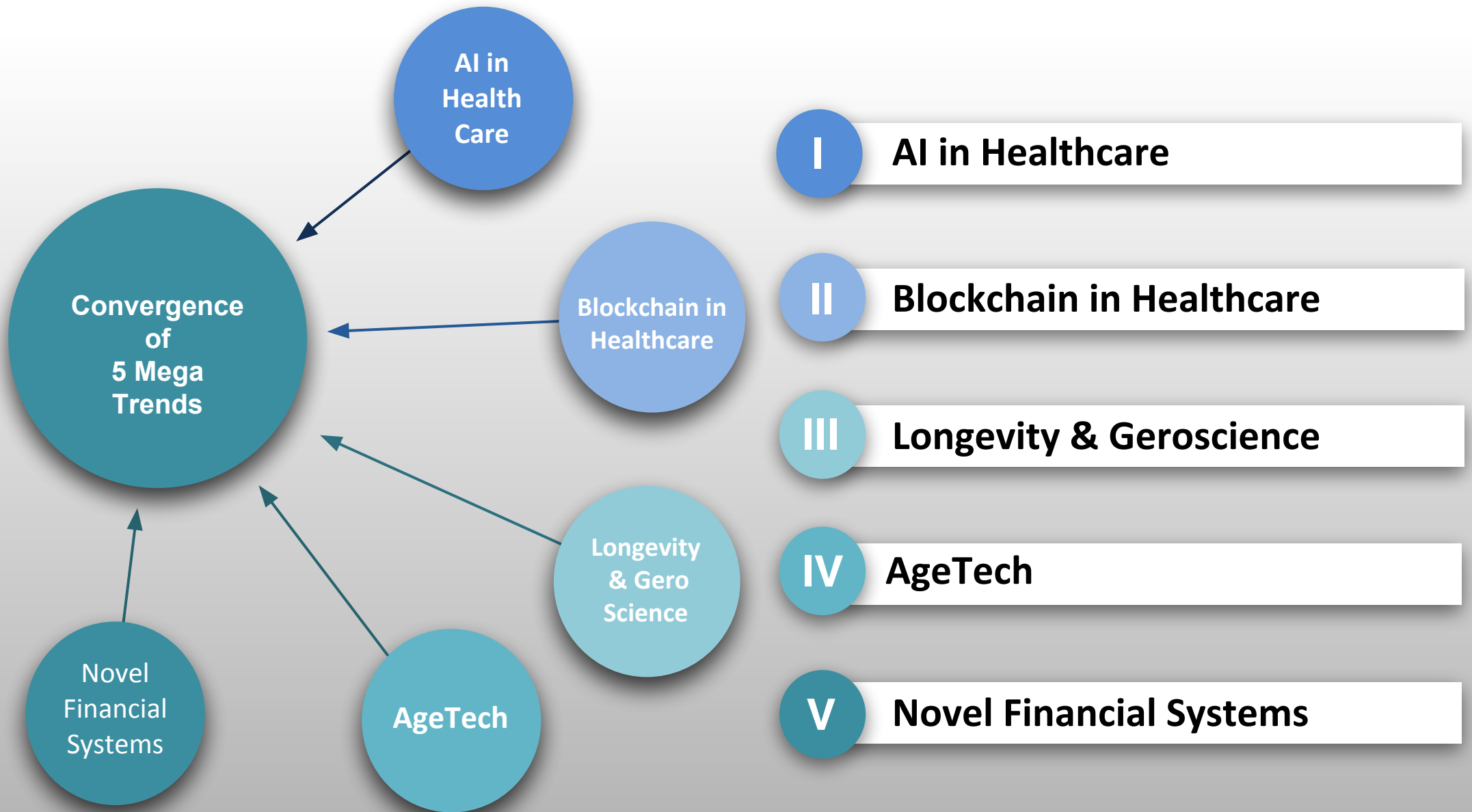
F R O S T & S U L L I V A N



INSILICO MEDICINE

2018 North American Artificial Intelligence for Aging Research
and Drug Development Technology Innovation Award

5 Mega Trends to Disrupt the BioTech & BioMedicine Industries in the next 5 Years

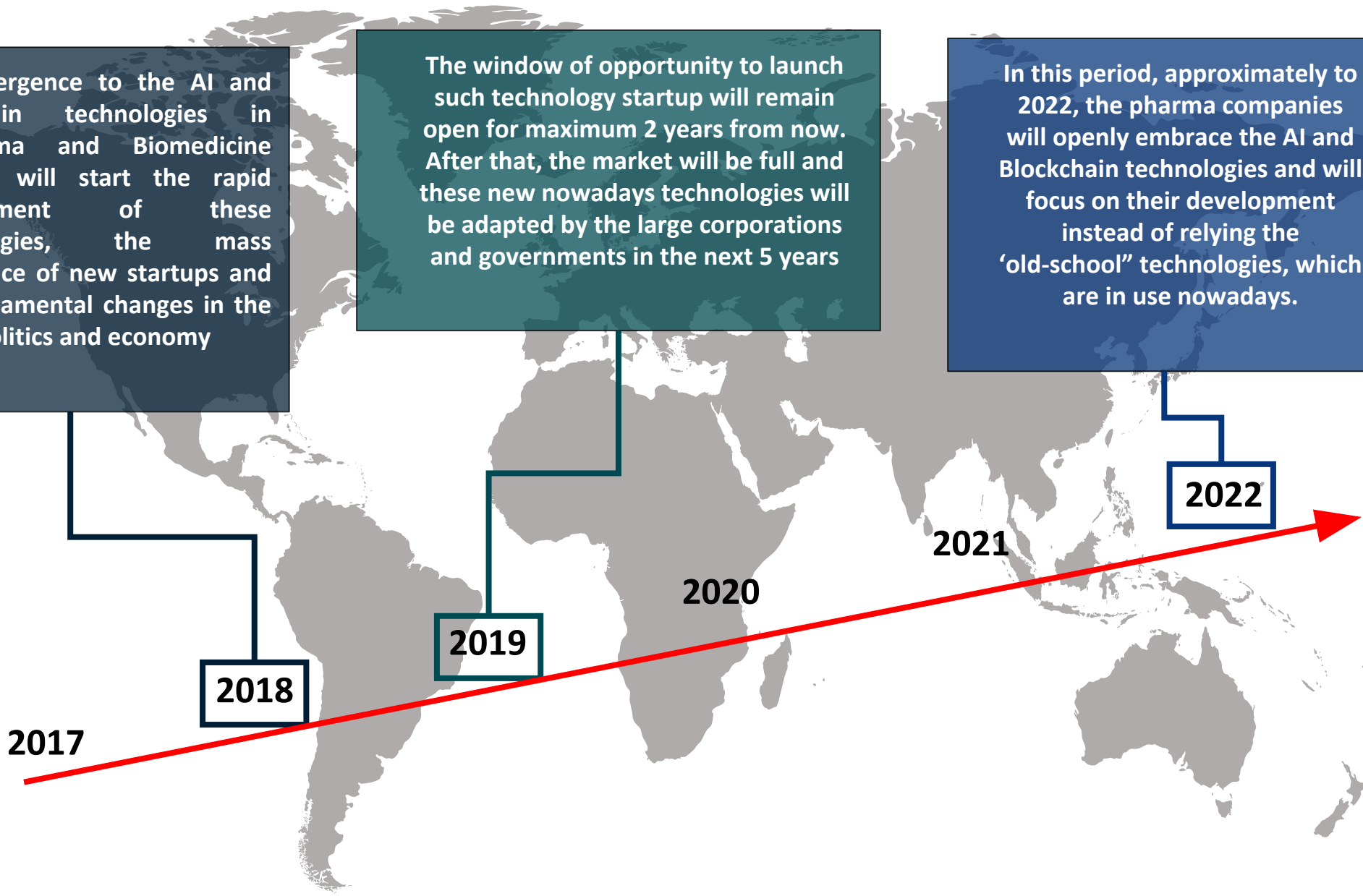


Consequence: The Major Shift in the BioMedicine Industry

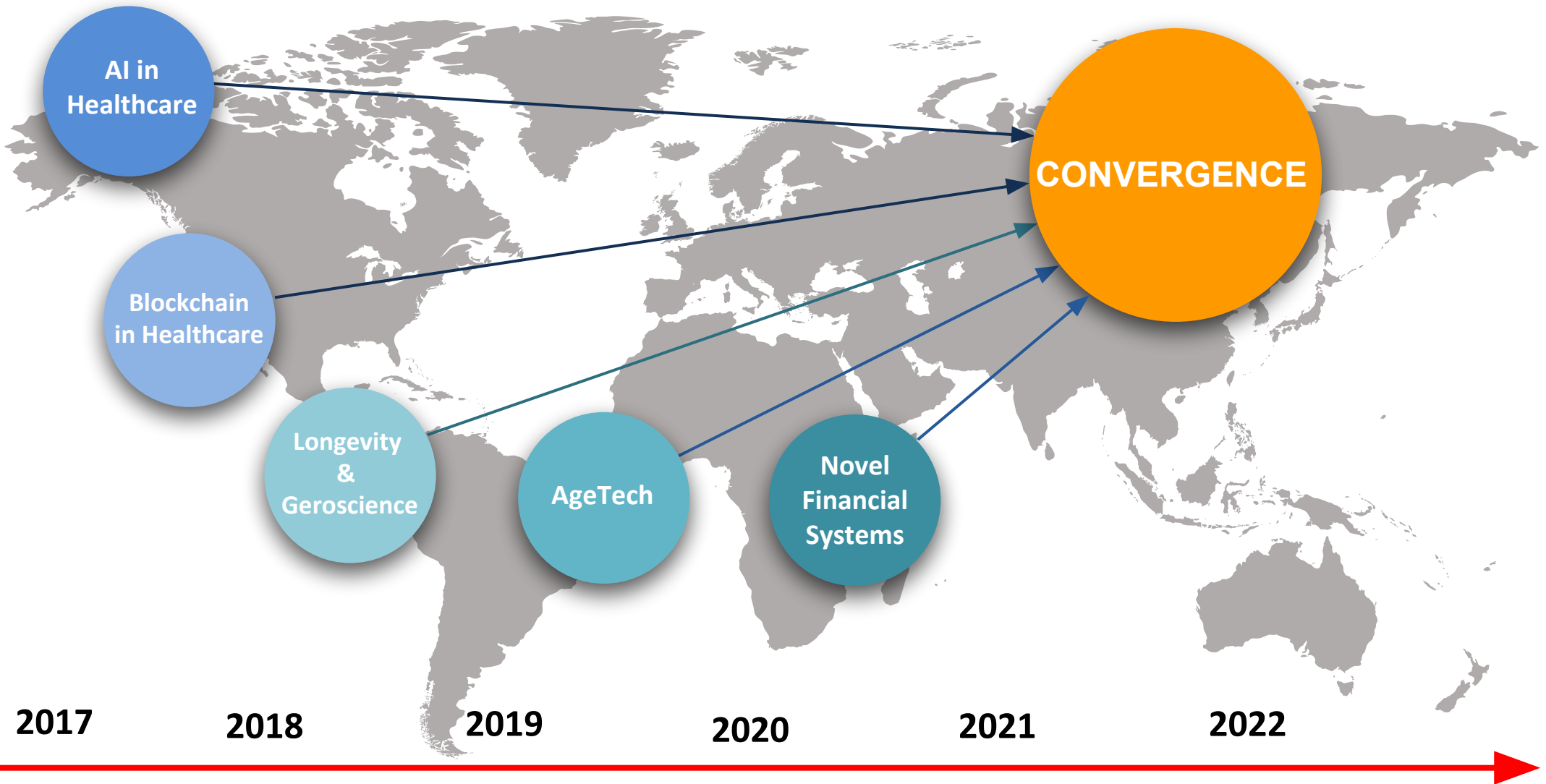
The emergence to the AI and Blockchain technologies in Biopharma and Biomedicine industry will start the rapid development of these technologies, the mass emergence of new startups and the fundamental changes in the world politics and economy

The window of opportunity to launch such technology startup will remain open for maximum 2 years from now. After that, the market will be full and these new nowadays technologies will be adapted by the large corporations and governments in the next 5 years

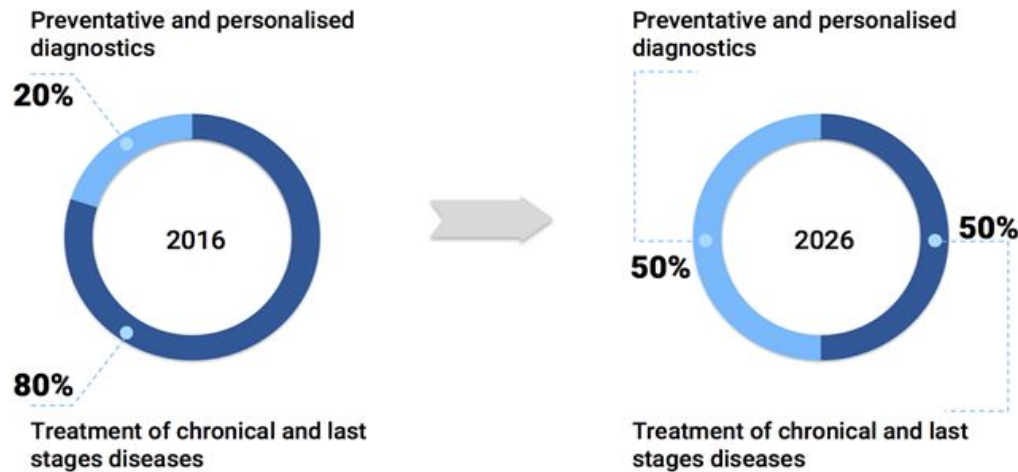
In this period, approximately to 2022, the pharma companies will openly embrace the AI and Blockchain technologies and will focus on their development instead of relying the 'old-school' technologies, which are in use nowadays.



Convergence of 5 Mega Trends

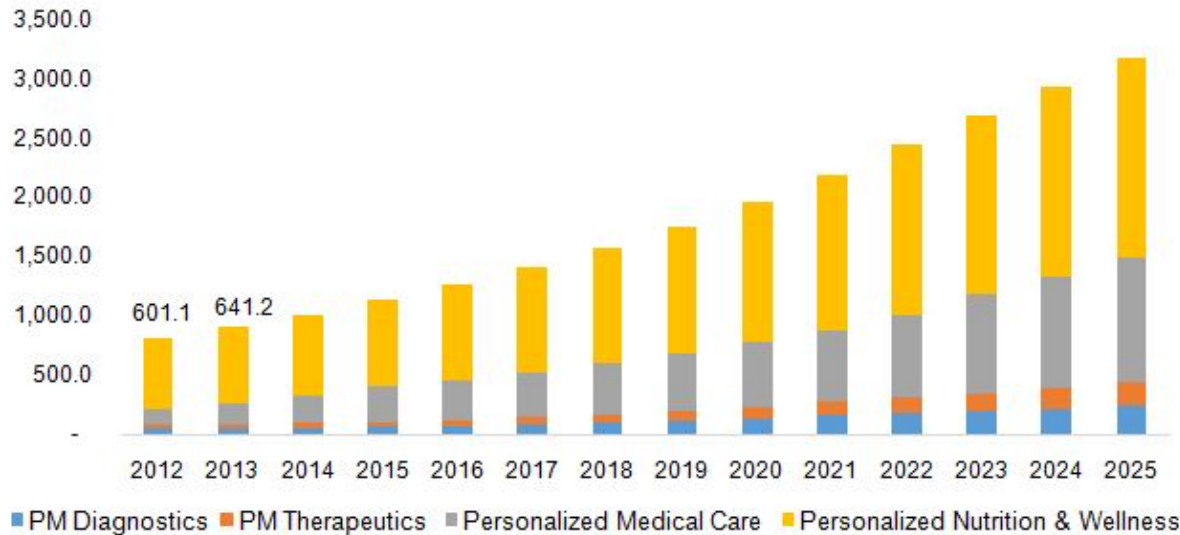


P3 medicine



It is expected that personalized and preventive approaches in the treatment of chronic diseases will become the prevalent one by 2026.

The changes in healthcare systems together with emerging technologies will double the P3 medicine market by 2022.



Source:
<https://www.grandviewresearch.com/industry-analysis/personalized-medicine-market>

**AI FOR
DRUG DISCOVERY,
BIOMARKER DEVELOPMENT
AND ADVANCED R&D
LANDSCAPE OVERVIEW
2018 / Q2**

Section III

Comparative Industry Analysis Classification Framework (Investor and M&A Guide)

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**Comparative Industry Analysis
Classification Framework
(Investor and M&A Guide)**

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Section III: Comparative Industry Analysis & Classification Framework (Investor and M&A Guide) is devoted to an in-depth comparative and quantitative analysis of the entire AI for Drug Discovery landscape, specifically tuned for investors and business analysts who wish to gain a deeper understanding of the industry in Q2 of 2018.

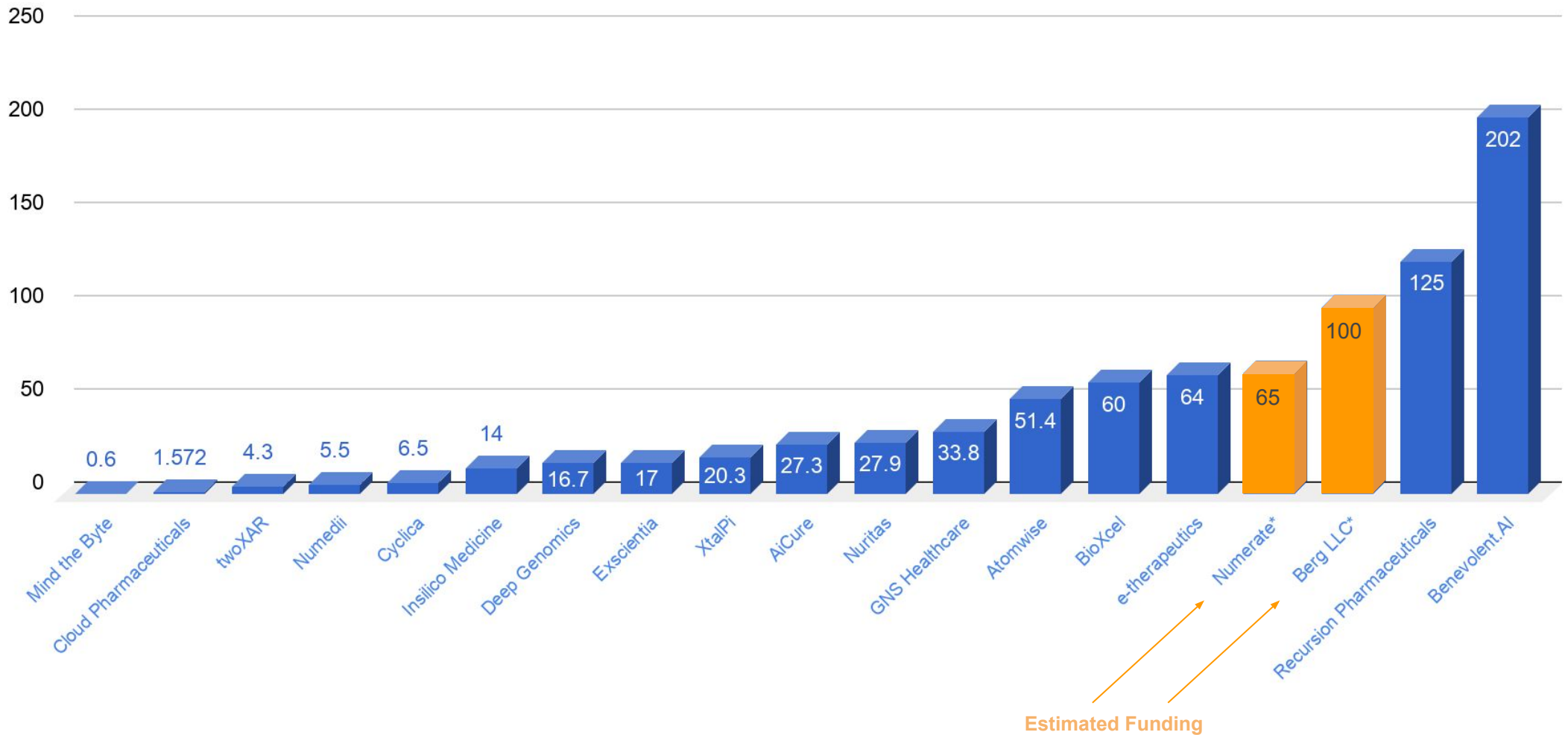
- **Chapter XI: Classification/Ratings of AI for Advanced R&D and Drug Discovery Companies** performs a quantitative analysis of many of the AI for Drug Discovery companies covered and profiled in this report using a variety of tangible metrics that can be used to acquire an understanding of their level of scientific validation and industry activity, including the proportion of AI specialists among their total staff, number of publications, number of patents, etc. It then uses these metrics to rank AI for Drug Discovery companies side by side, and to build a classification framework by which these companies can be better categorized according to their specific focus, application and industry segmentation.
- **Chapter XII: 2010 - 2016 - Investment Rounds, M&A Deals and Notable Events** summarizes some of the most notable investment rounds, M&As and other notable events from 2010-2016, including but not limited to Benevolent AI's \$87M raise, ThoughtSpot's \$100M raise and Meta's \$23M raise.
- **Chapter XIII: 2017 - Investment Rounds, M&A Deals and Notable Events** summarizes some of the most notable investment rounds, M&As and other notable events in 2017, including but not limited to Exscientia's €250M raise, AICure's \$15M raise and Insilico Medicine's \$10M raise.
- **Chapter XIV: Q1 2018 - Investment Rounds, M&A Deals and Notable Events** summarizes some of the most notable investment rounds, M&As and other notable events in Q1 of 2018, including but not limited to AtomWise's \$45M raise, XtalPi's \$15M raise, and twoXAR's \$10M raise.
- **Chapter XV: Q2 2018 - Investment Rounds, M&A Deals and Notable Events** summarizes the major investments, M&As and other notable events (e.g. joint ventures, public announcements, etc.) that have occurred within the AI for Drug Discovery space specifically in Q2 of 2018, including but not limited to ThoughtSpot's \$145M raise, Benevolent.AI's \$115M raise, Celsius Therapeutics' \$65M raise, and Datavant's \$40.5M raise

Chapter XI

Comparison of Leading AI Companies

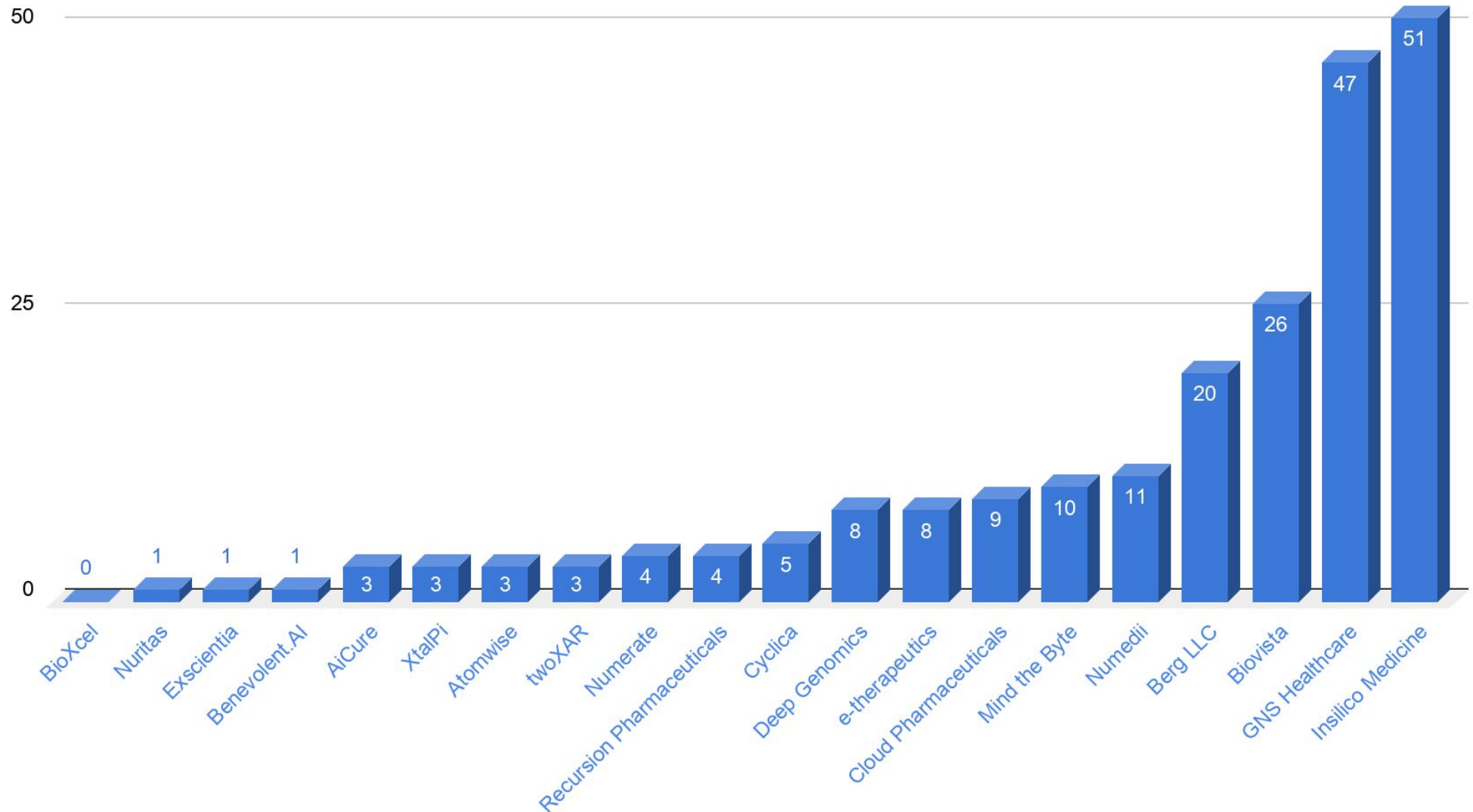
Comparison of Top-20 AI for Drug Discovery Companies

Funding, \$m *(as of 1 July 2018)*



Comparison of Top-20 AI for Drug Discovery Companies

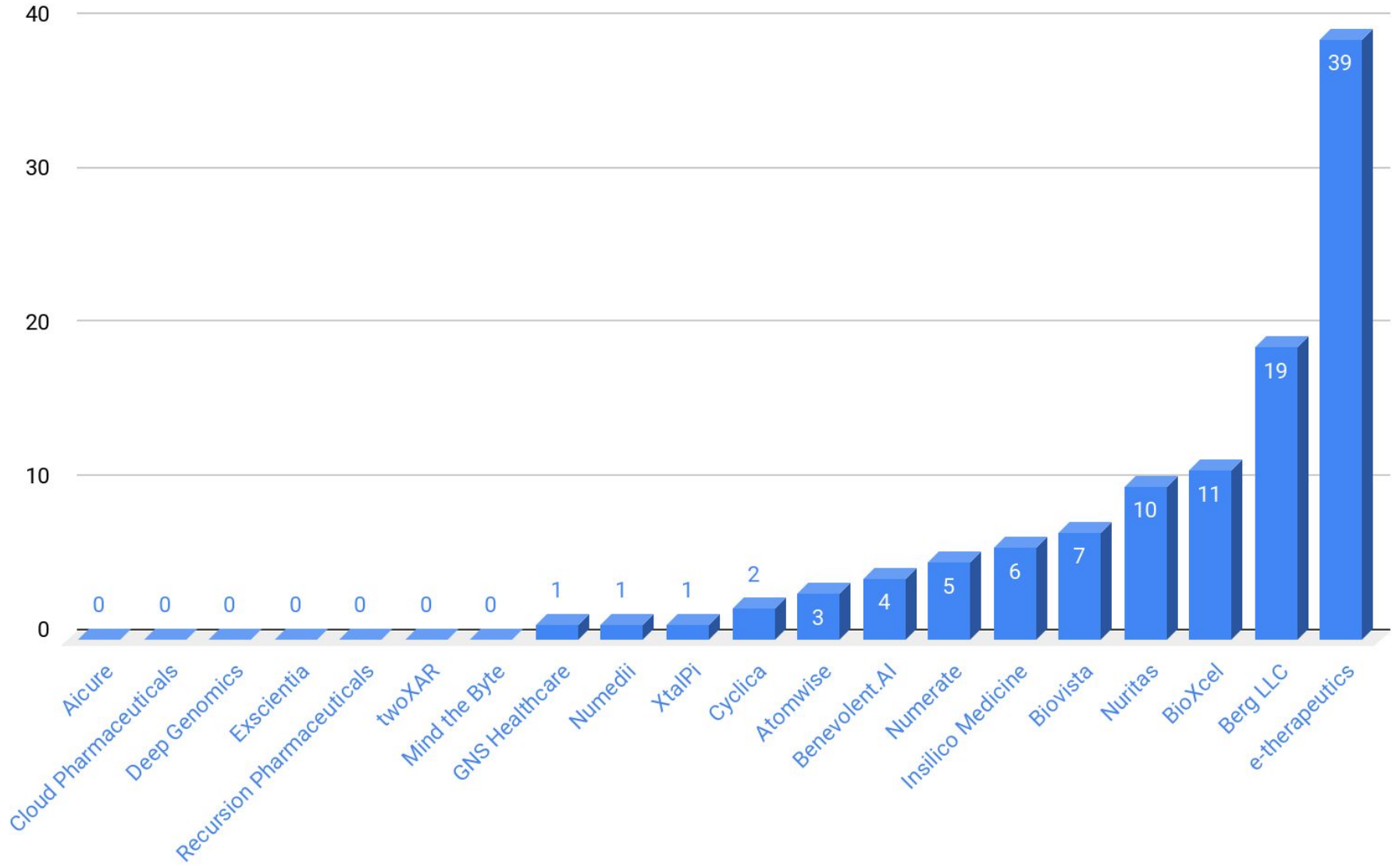
Number of Scientific Publications



Source: Company Website and PubMed

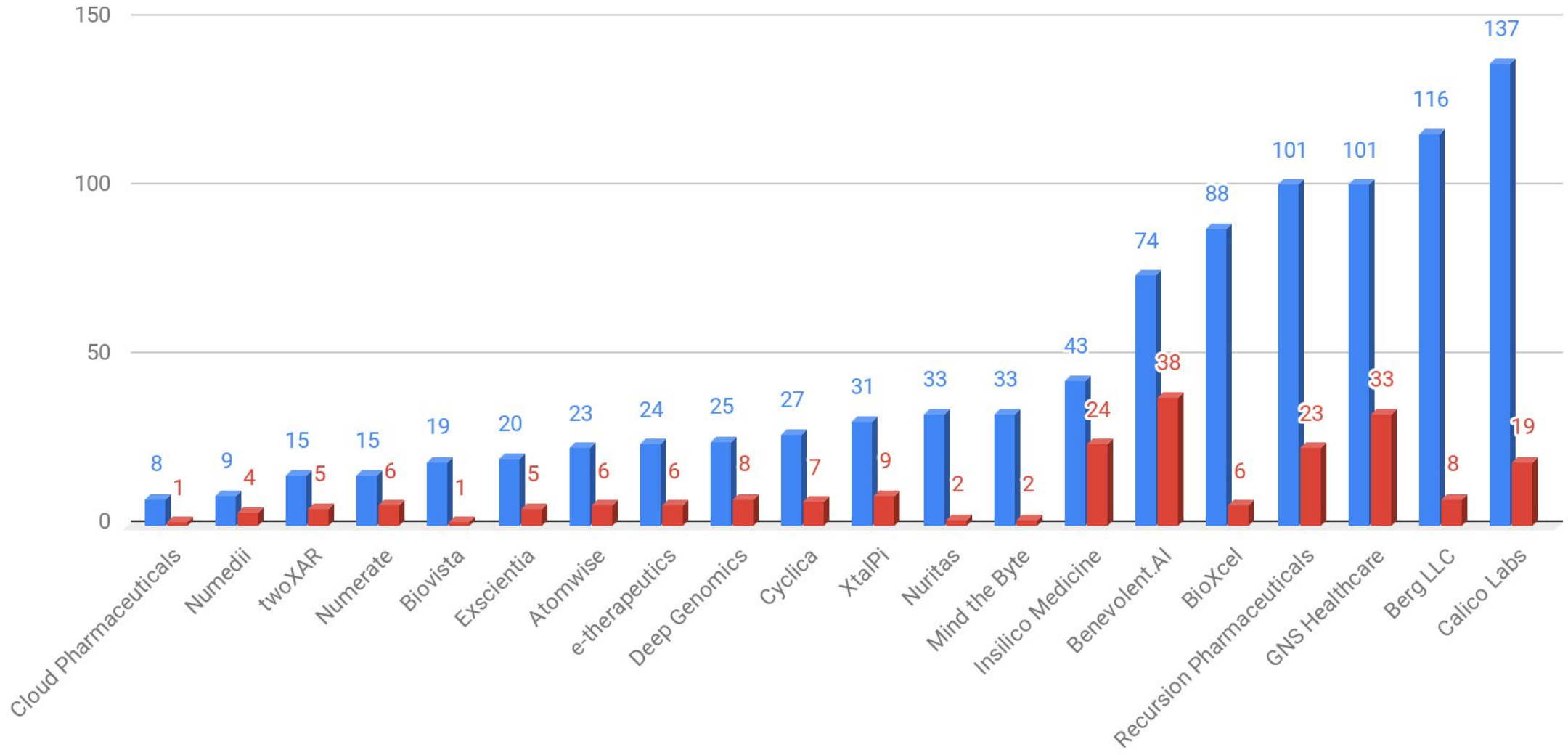
Comparison of Top-20 AI for Drug Discovery Companies

Number of Patents

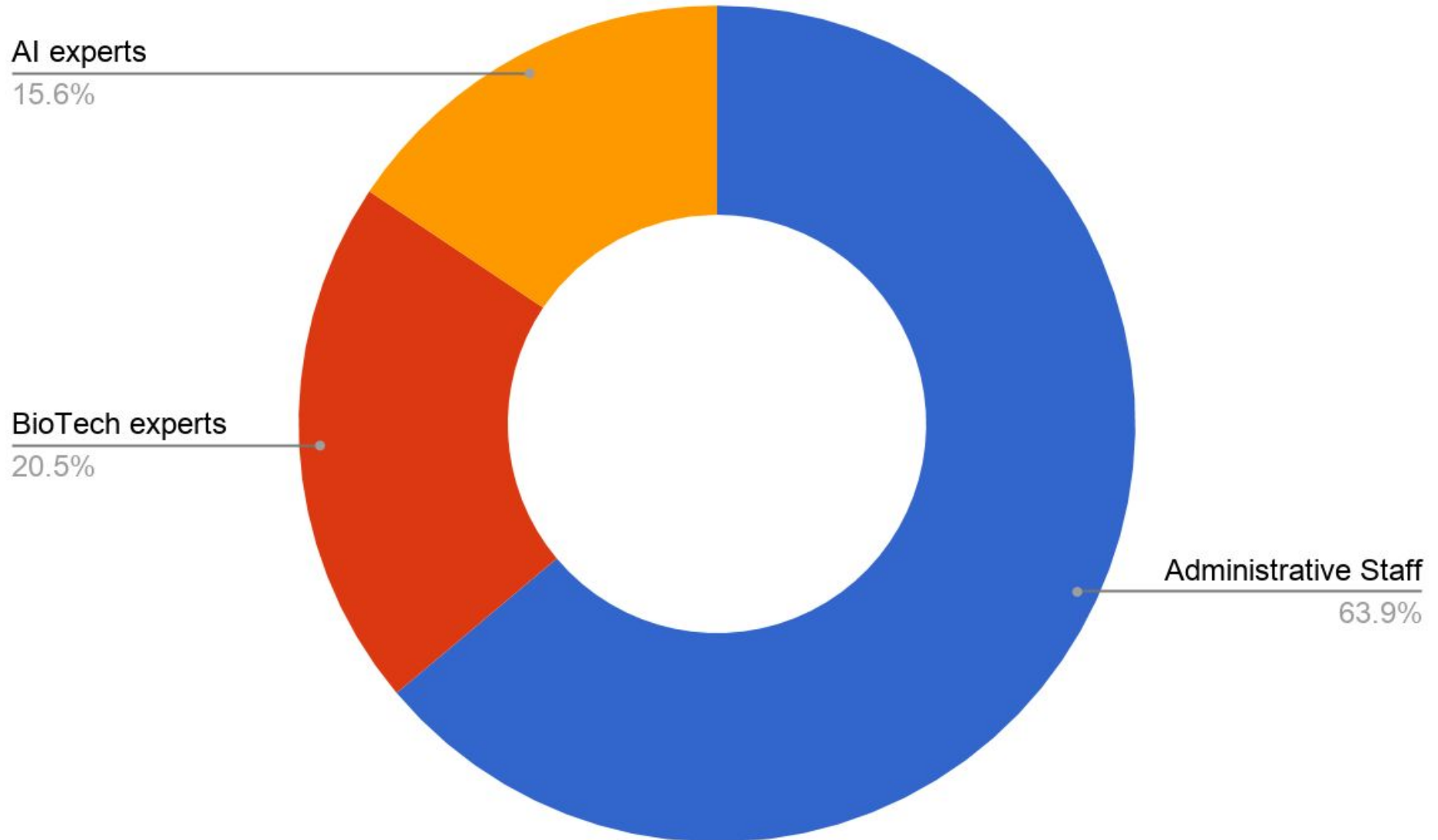


Comparison of Top-20 AI for Drug Discovery Companies

Total Number of Employees / AI experts

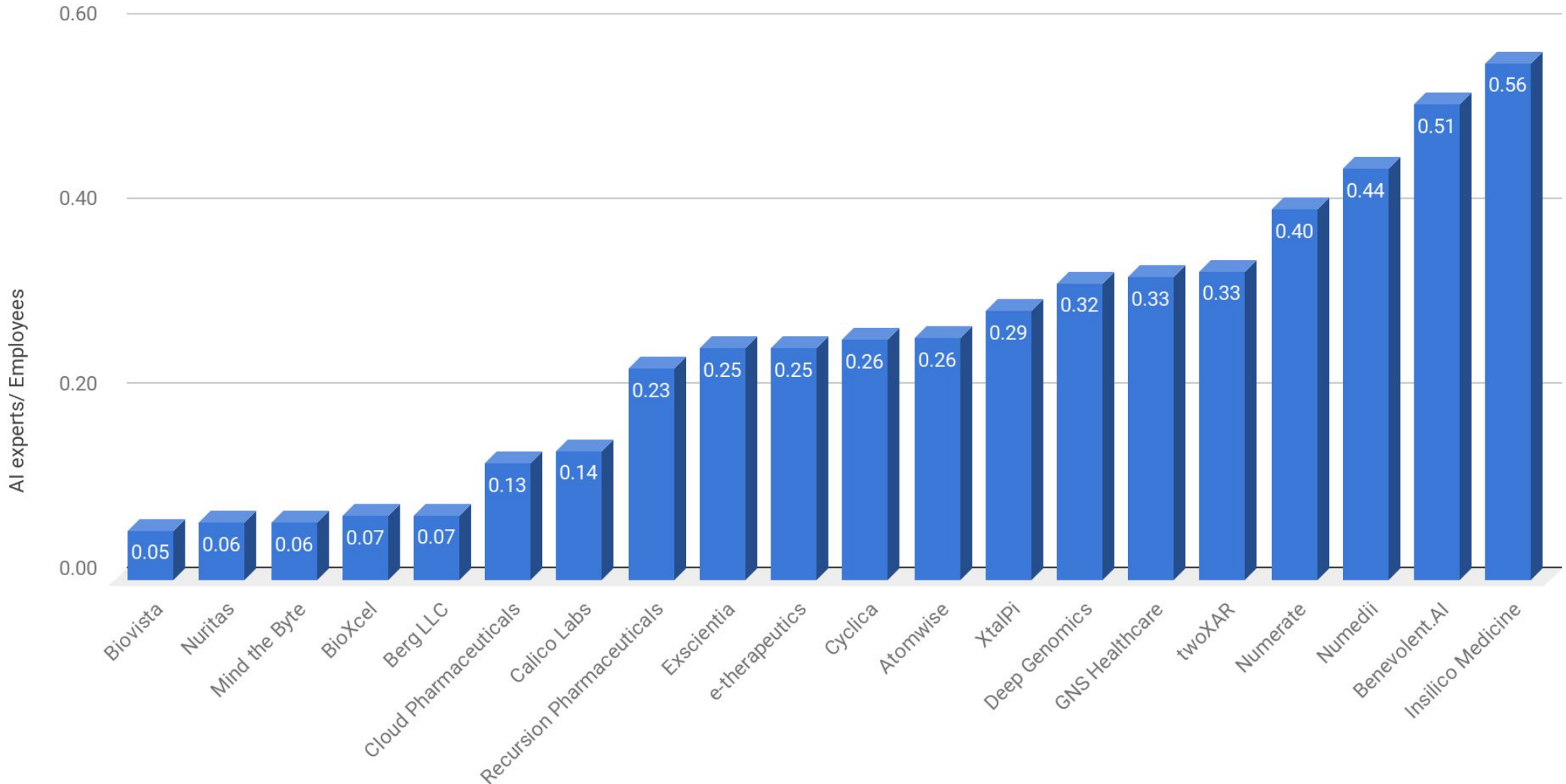


AI experts vs BioTech experts vs Administrative Staff



Comparison of Top-20 AI for Drug Discovery Companies

True AI companies
The ratio: **AI experts** vs
Total Number of Employees



Source: According to LinkedIn

Comparison of Top-20 AI for Drug Discovery Companies

Company	Scientific publications covering AI for Drug Discovery	Number of AI experts in the team / total number of employees	Public talks on AI for Drug Discovery	Validation
Atomwise	+	11/13	+	n/a
Benevolent.AI	+	18/74	+	n/a
Deep Genomics	+	10/26	-	n/a
Exscientia	+	2/12	+	+
GNS Healthcare	+	21/98	-	n/a
Insilico Medicine	+	24/43	+	+
NuMedii	+	4/9	+	+
Numerate	-	4/15	+	+
Recursion Pharmaceuticals	+	85/12	+	+
twoXAR	+	1/15	+	+

Comparison of Top-20 AI for Drug Discovery Companies

Company	Scientific publications covering AI for Drug Discovery	Number of AI experts in the team / total number of employees	Public talks on AI for Drug Discovery	Validation
Berg LLC	-	3/11	+	n/a
Mind the Byte	-	2/33	+	n/a
Biovista	+	1/19	+	+
AiCure	-	9/43	+	+
Cloud Pharmaceuticals	+	1/8	+	n/a
e-therapeutics	+	4/25	+	n/a
Nuritas	-	2/33	+	+
XtalPi	-	1/25	+	n/a
Cyclica	-	7/27	+	+
BioXcel	-	4/88	+	+

Comparison of Top-20 AI for Drug Discovery Companies

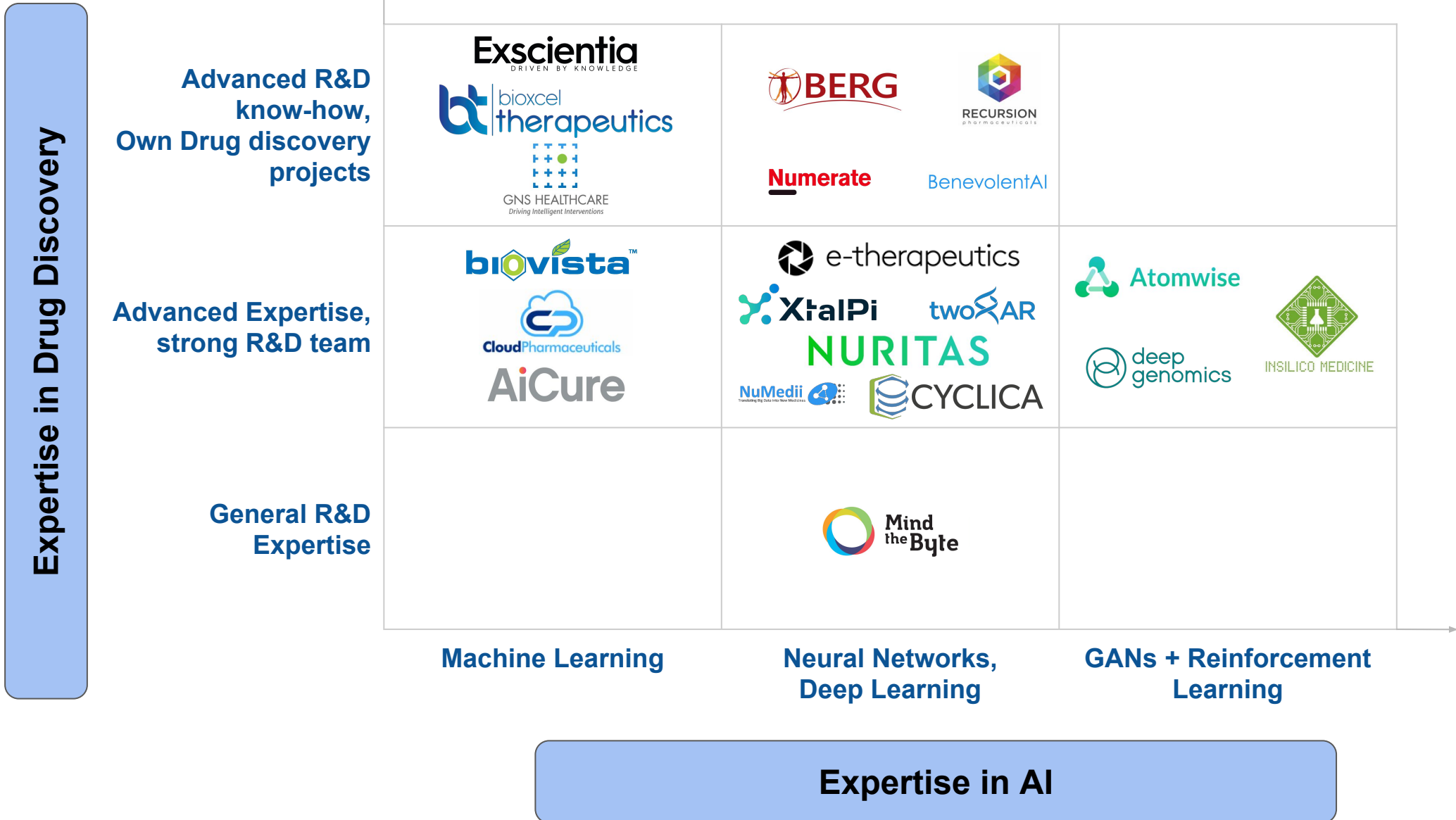
Companies	Computation method	Data Type
Atomwise	DL	Chemical notations; QSAR
Benevolent.AI	ML, DL, symbolic AI	Text; images; EHRs; omics
Deep Genomics	n/a	n/a
Exscientia	ML	Chemical notations; high-content screening; SAR
GNS Healthcare	ML	n/a
Insilico Medicine	DL, GANs, GANs + RL, symbolic AI	Omics; EHR
NuMedii	Big data analysis, DL, ML	Raw human, biological, pharmacological and clinical data, normalized and annotated.
Numerate	AI, cloud computing	Chemical notations; screening; high-content screening;
Recursion Pharmaceuticals	n/a	Images, high content screening data
twoXAR	n/a	Omics data, high content screening

Comparison of Top-20 AI for Drug Discovery Companies

Companies	Computation method	Data Type
Berg LLC	DL	Human Data
Mind the Byte	Big Data	protein ligand interactions
Biovista	ML	correlations between drugs, molecular targets, pathways, adverse events and diseases
AiCure	ML	n/a
Cloud Pharmaceuticals	legacy ML, cheminformatics	Chemical notations
e-therapeutics	Big Data	Chemical notations
Nuritas	DL	n/a
XtalPi	Quantum physics; machine learning; cloud computing	n/a
Cyclica	AI	Chemical notations
BioXcel	ML	n/a

Comparison of Top-20 AI for Drug Discovery Companies

Expertise in AI for Drug Discovery R&D / AI

























Comparison of Top-20 AI for Drug Discovery Companies

Expertise in AI for Drug Discovery Chemistry / Biology



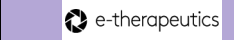












Expertise in Biology
































Classification of AI applications for R&D and Drug Discovery process

Data Mining	Biology Research	Drug Discovery			Drug Development	Biomarker Discovery
		Compound Generation	Compound Binding	ADME/Tox Predictions		
		 Atomwise Better medicines faster.	 Atomwise Better medicines faster.			
 benevolent.ai				 benevolent.ai		
 deep genomics						 deep genomics
		 e ^x scientia	 e ^x scientia	 e ^x scientia		
					 GNS HEALTHCARE Driving Intelligent Innovation	
	 INSILICO MEDICINE	 INSILICO MEDICINE	 INSILICO MEDICINE	 INSILICO MEDICINE	 INSILICO MEDICINE	 INSILICO MEDICINE
						 NuMedii
		 Numerate		 Numerate		
		 RECURSION pharmaceuticals				
	 twoXAR	 twoXAR				

Classification of AI applications for R&D and Drug Discovery process

Data Mining	Biology Research	Drug Discovery			Drug Development	Biomarker Discovery
		Compound Generation	Compound Binding	ADME/Tox Predictions		
						
						
						
						
						
						
						
						
						
						

Competitive Landscape

Hypothesis Knowledge Discovery	Target ID Biology	Compound Generation	Compound Binding	ADME Tox	Clinical Trials	Personalized Medicine	Real World Insights
 INSILICO MEDICINE BenevolentAI  IBM Watson  SPARKBEYOND nference	 INSILICO MEDICINE  IBM Watson twoAR NuMedii BIOAGE Standigm BERG deep genomics  RECURSION PHARMACEUTICALS WuXiNextCODE healx  iCarbonX 碳云智能	 INSILICO MEDICINE BenevolentAI inSili.com	 INSILICO MEDICINE Exscientia DRIVEN BY KNOWLEDGE  Atomwise  CYCLICA SCHRÖDINGER  XtalPi	 INSILICO MEDICINE Exscientia DRIVEN BY KNOWLEDGE Numerate	 INSILICO MEDICINE BenevolentAI  IBM Watson  SPARKBEYOND WuXiNextCODE  DEEP 6  Mendel.ai  trials.ai  OWKIN	 INSILICO MEDICINE  IBM Watson  FOUNDATION MEDICINE  flatiron  freenome GRAIL verily  iCarbonX 碳云智能 Over 1000 companies worldwide	 INSILICO MEDICINE  IBM Watson nference  Qrative  iCarbonX 碳云智能  SPARKBEYOND

Most Promising Players

Corporations

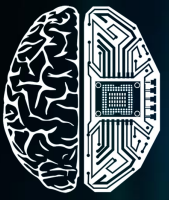


AI companies



BenevolentAI





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