AI FOR DRUG DISCOVERY, BIOMARKER DEVELOPMENT AND ADVANCED R&D LANDSCAPE OVERVIEW 2018 / Q3

Companies - 125
Corporations - 30
R&D Centers - 20
Investors - 260

DEEP KNOWLEDGE ANALYTICS

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AI for Drug Discovery, Biomarker Development and Advanced R&D Landscape Overview 2018 / Q3

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Companies - 125
Investors - 260
Corporations - 30

Drug Discovery

Advanced R&D

Investors

AI Companies

Corporations

Pharma

IT

Biomarker Development

DEEP KNOWLEDGE ANALYTICS

Diversification of AI for R&D and Drug Discovery Process

Companies - 125
Investors - 260

Companies

Investors

Design Preclinical Experiments

Preclinical Experiment Execution

Data Aggregation & Analysis

Drug Design

Clinical Trial Design, Optimization, Recruitment

Repurposing Existing Drugs
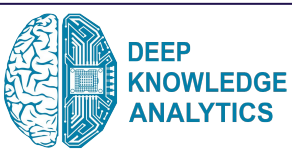
Researching Mechanisms of Disease
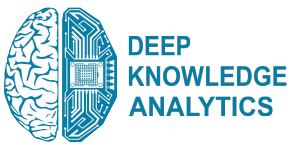
DEEP KNOWLEDGE ANALYTICS

AI for Drug Discovery, Biomarker Development and Advanced R&D Landscape / 2018 Q3

Companies - 125
Investors - 260
Corporations - 30

Regional Position

Investors
AI Companies
Corporations

USA
Canada
Other Regions
Asia
EU
UK

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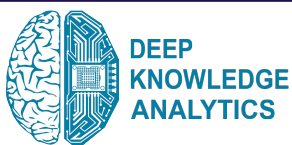
Leading
IT and Tech Corporations / AI Companies / Pharma Corporations
Advanced AI in Healthcare and Drug Discovery
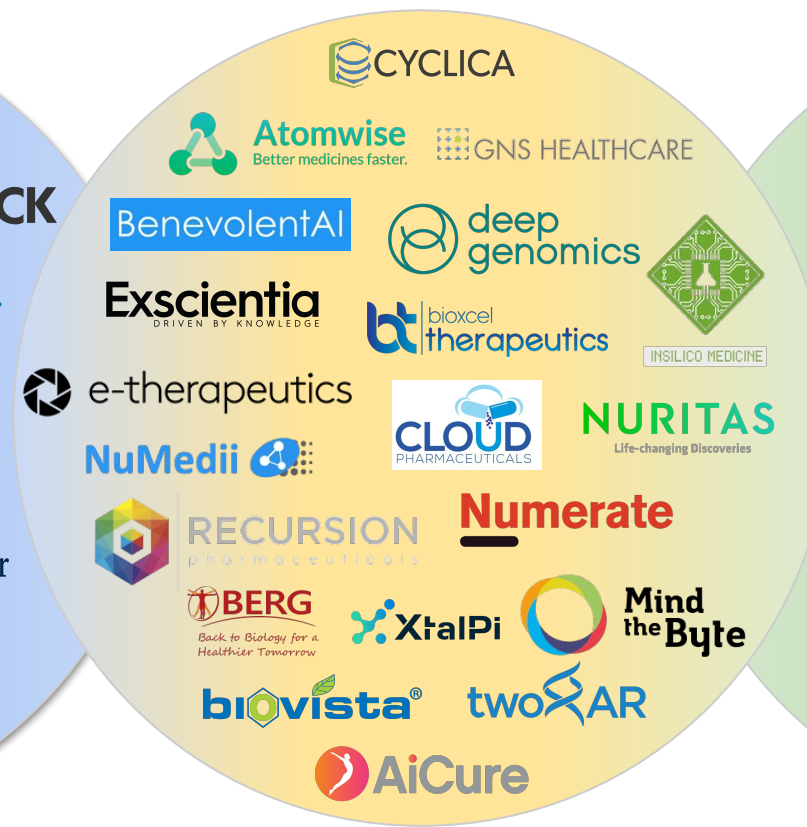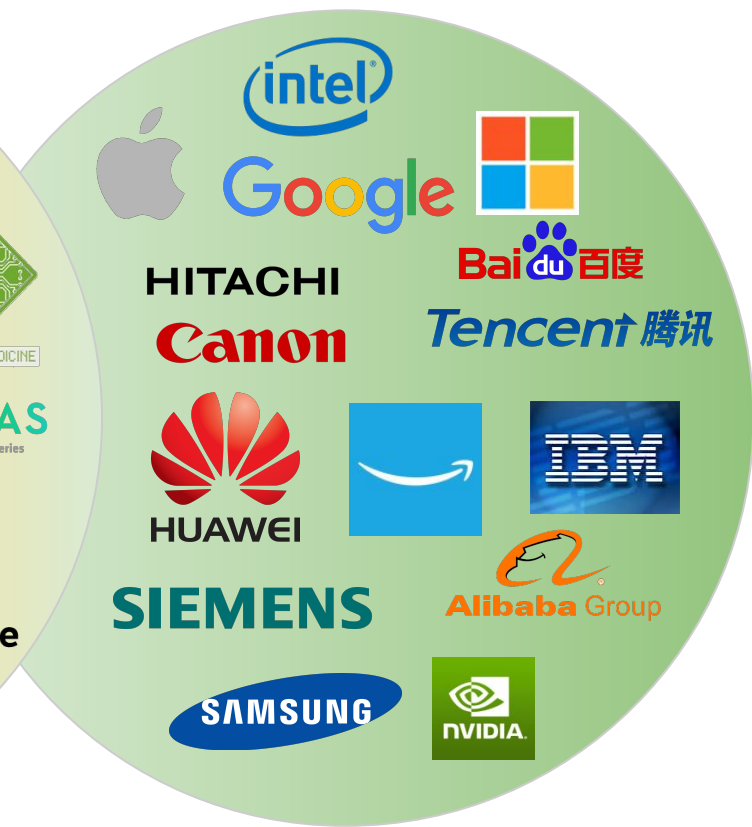
GLOBAL SALES:
>$1 Trillion

GLOBAL R&D:
>$150 Billion

>$2.6B TO DEVELOP ONE DRUG

92% FAILURE RATE IN CLINICAL TRIALS

AI in Healthcare by 2024:
>$10 Billion

AI for DD by 2024:
>$4 Billion

AstraZeneca
$ 23.641 M

GILEAD
$ 32.693 M

Johnson&Johnson
1 $ 70.074

SANOFI
$ 34.542 M
9   9

Roche
2 $ 50.111 M

gsk GlaxoSmithKline
$ 36.566 M
8   8

Sales per annum

7   7

Pfizer
3 $ 48.851 M

MERCK
$ 39.498 M
6   6

BAYER
$ 51.407 M
5   5

4 $ 49.414 M

NOVARTIS
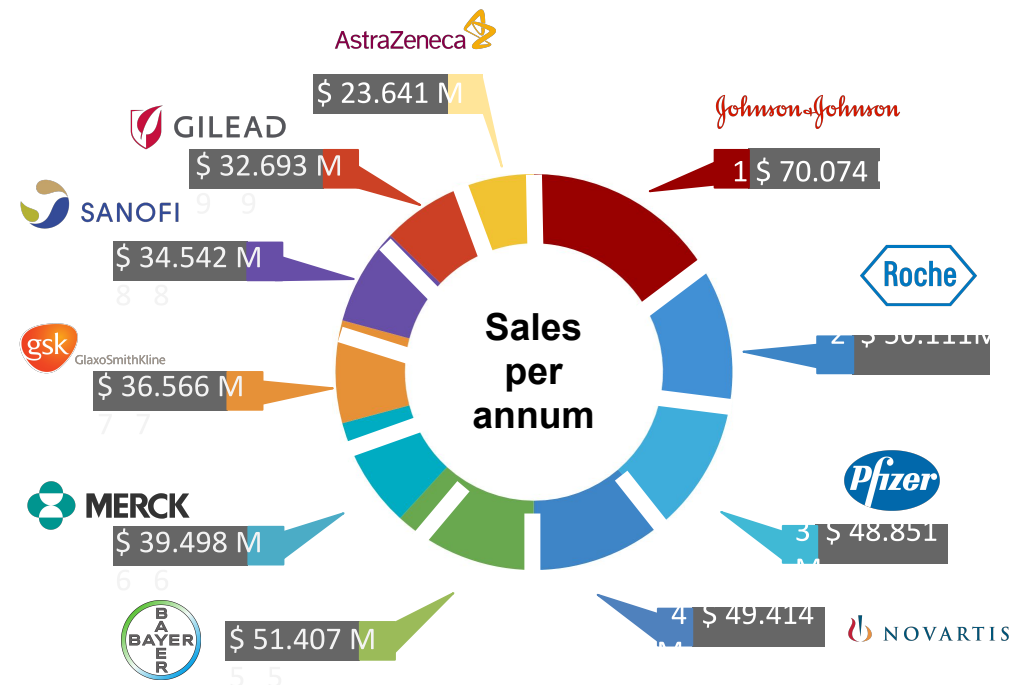
Pharma Efficiency is Declining Steadily

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

>$2.6B TO DEVELOP ONE DRUG

92% FAILURE RATE IN CLINICAL TRIALS

FDA tightens regulation post thalidomide

FDA clears backlog following PDUFA regulations and perhaps relaxes on HIV drugs

Structure of DNA

Restriction enzymes

DNA sequencing

Dolly the Sheep

Recombinant DNA

Human insulin

Human Genome v1

1950   1960   1970   1980   1990   2000   2010
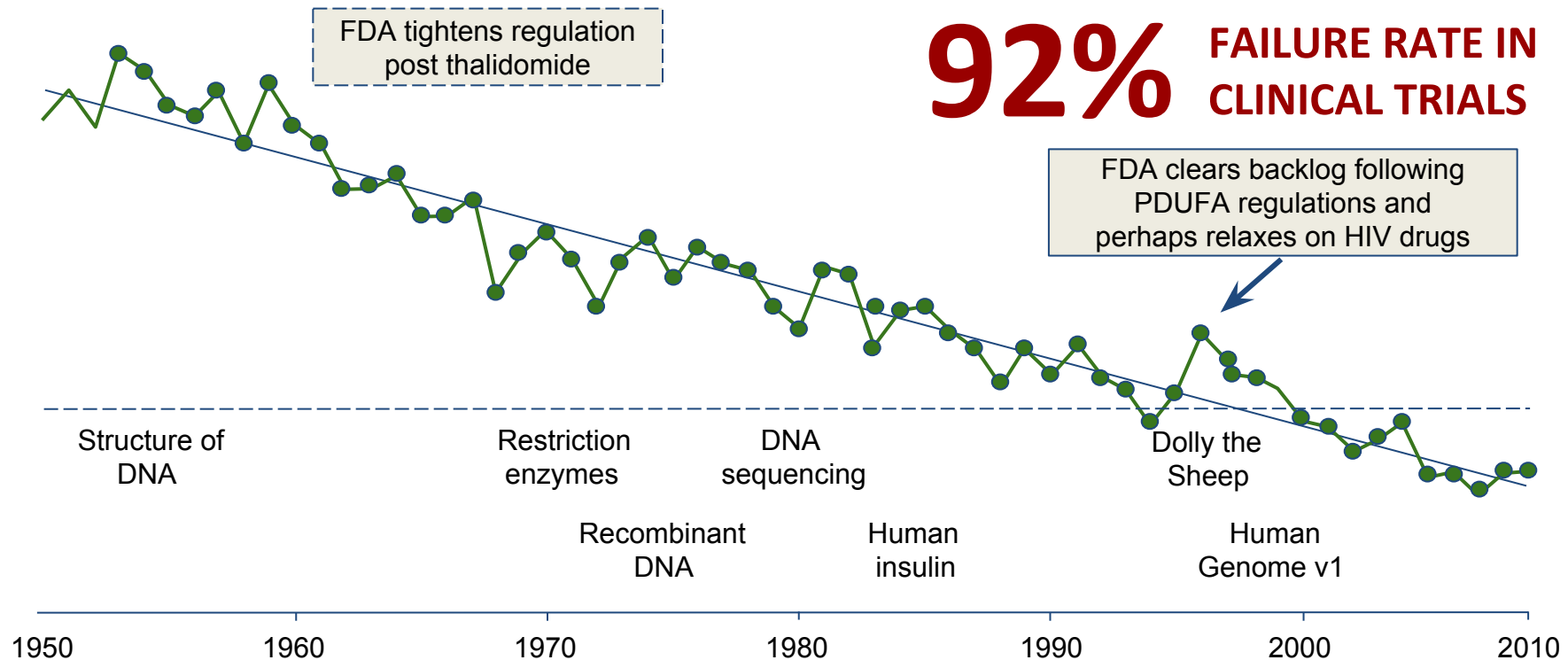
Bernstein Research: The Long View - R&D Productivity, 2010

46 NEW DRUGS launched in 2014

Biopharmaceutical R&D Process / Low efficiency
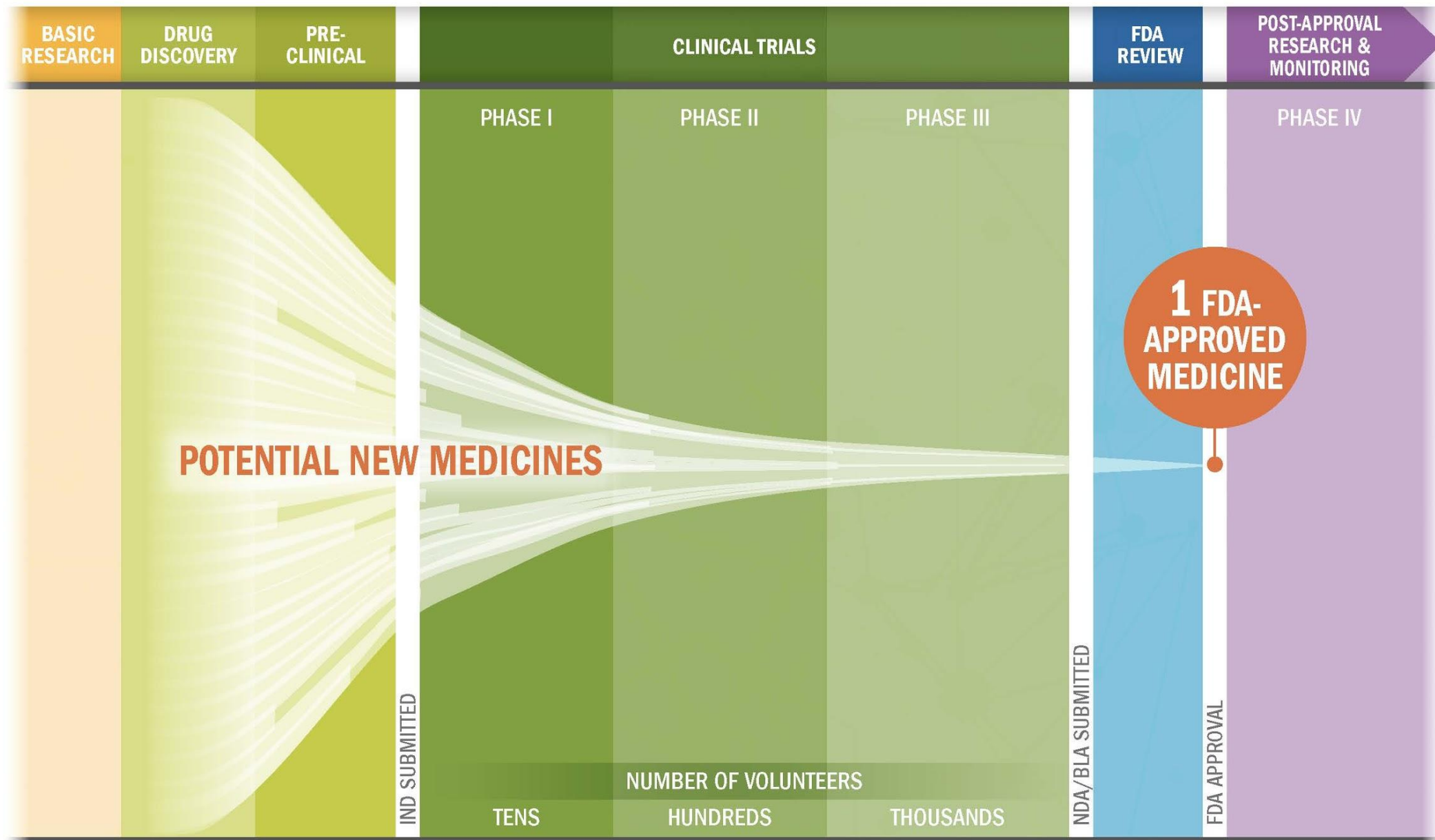
Key: IND: Investigational New Drug Application, NDA: New Drug Application, BLA: Biologics License Application

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

Combined Capitalization of 15 IT & Tech Corporations vs 15 BioPharma Corporations In Millions of USD
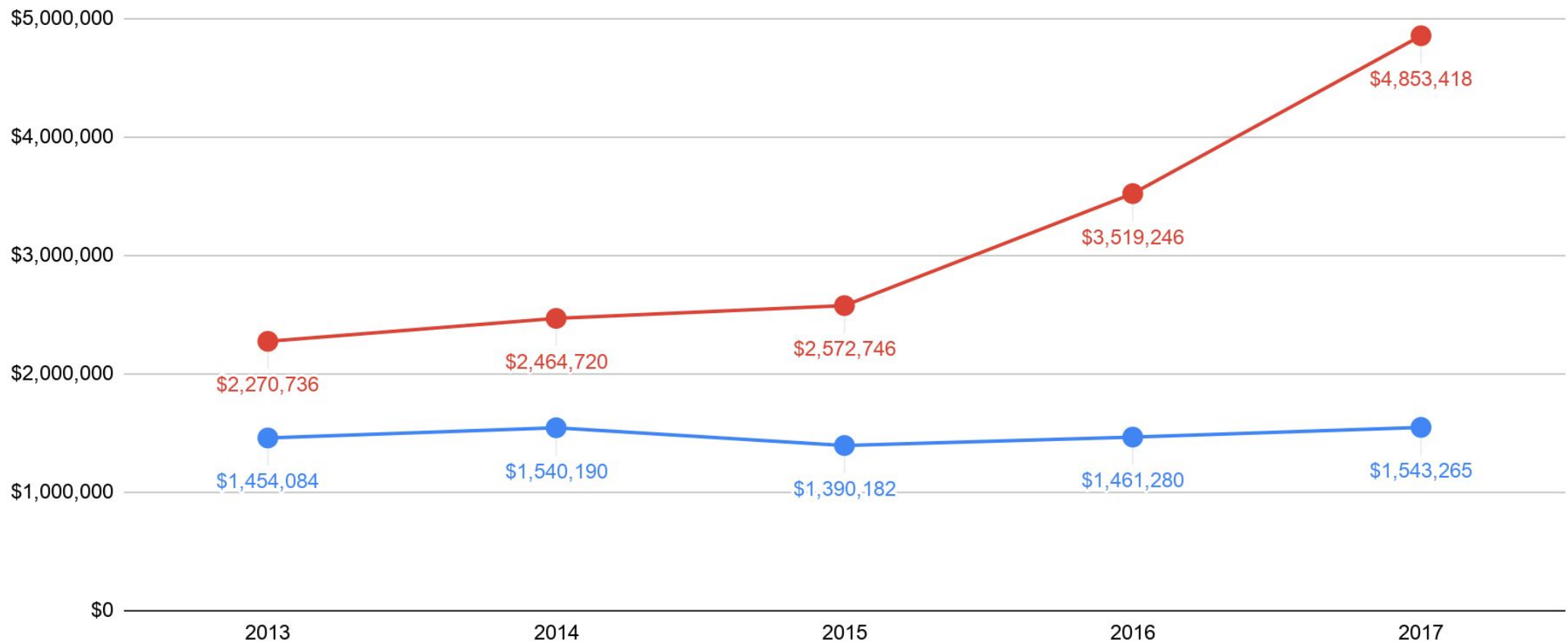
As can be seen in the figure to the above, the combined capitalization of the 15 BioPharma corporations profiled in this report have remained on the same level for the past 5 years while the capitalization of the 15 IT & Tech corporations profiled in this report is growing significantly.

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

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

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

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

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

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

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

Legend:
- Transformative
- Very high
- High
- Average
- Some

Data mining

Omics, systems biology

Structure based

Ligand Based

Target identification

Target Validation

Phenotypic screening

Lead identification

Lead Optimization

Preclinical

Clinical

drug

Drug repurposing
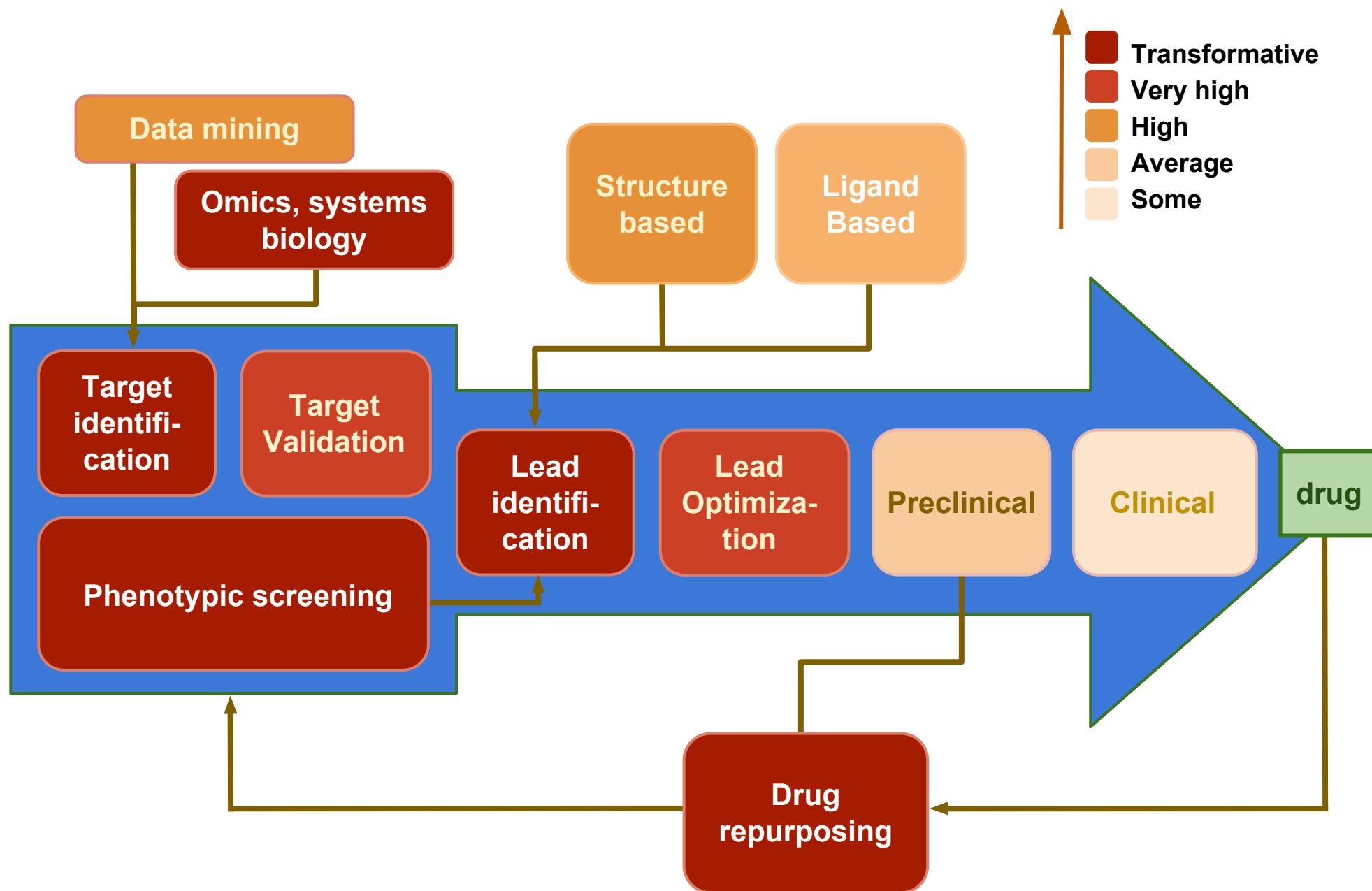
Top 30 Conferences - AI for Drug Discovery and Advanced R&D
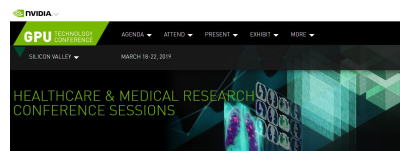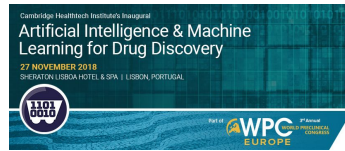
Executive Summary

This 110-page report marks the fourth installment in a series of reports on the topic of the Artificial Intelligence in Drug Discovery Industry that Deep Knowledge Analytics have been producing for more than 1 year now. We released the first edition of these reports, entitled "AI for Drug Discovery Landscape Overview 2017", in the end of 2017, followed by "AI for Drug Discovery & Advanced R&D Q1 2018" in the first quarter of 2018, and by "AI for Drug Discovery & Advanced R&D Q2 2018" in the second quarter of 2018.

The present edition consists of a shortened version of our previous 600-page report on the state of the industry in Q2 of 2018, updated with major developments having occurring in Q3 of 2018, and can be considered as a summary of the major insights, data analysis, conclusions and forecasts of our previous report.

The report is organized as follows:

- **Infographic Summary** - provides comprehensive mind maps and diagrams.

- **Executive Summary** - provides a major summary of the report.

- **AI for Drug Discovery Landscape Overview** aggregates, lists and categorizes 125 AI-companies, 260 investors, 15 BioPharma corporations, 15 IT & Tech corporations, 30 industry-specific conferences and 20 journalists writing on the topic of AI for Drug Discovery.

- **BioPharma and Tech Corporations Onboarding AI for Advanced R&D and Drug Discovery** charts how the BioPharma industry is now actively participating in the AI for Drug Discovery and biomarker development space via internal R&D, partnerships, investments and acquisitions, in contrast to 2017, during which time they remained largely skeptical of the disruptive impact of AI.

- **Industry Developments - Q3 2018** gives an overview of major industry developments in Q3 of 2018 from the side of new company initiatives, new investment deals, new mergers and new acquisitions. Through specific examples, it shows how the industry continues to grow, how China continues to aggressively enter the AI for Drug Discovery sphere, and how new countries in Asia (like South Korea) are also beginning to participate in the industry.

- **Major Government Initiatives in the US, UK, EU and Asia Pacific** - provides and overview of major government initiatives, and how certain progressive countries like the UK continue to launch pivotal initiatives to strengthen their national position in the global AI in Healthcare race.

Executive Summary

- **Investment Trends, Tech Corporation Affairs & Government Initiatives** offers a detailed overview of 2018 industry developments on the side of investments, M&As, Tech Corporations and Government Initiatives. This section details how IT & Tech Corporations are continuing to enter the space; this was already a major trend in 2017, and it is continuing apace into 2018, remaining one of the strongest hallmarks of the subsector's exponential dynamic of development. This section also offers a broad overview of trends in investments and M&A deals specifically tuned to industry progress in Q3 of 2018, detailing an overall increase in investments, the increasing activity of IT and Tech corporations, and the surge of activity from Chinese investors and Tech corporations.

- **Novel Technologies & Trends (Industry Forecast 2019-2020)** is devoted to in-depth coverage of the science and technology behind the industry, and to analysis of emerging subsectors, charting the near future of the industry from 2019 to 2020. It first gives an overview of topics, trends and advancements occuring in deep learning for drug discovery, one of the specific forms of AI which has now emerged as the leading technology delivering practical and tangible results in the industry, and pays particular attention to the emergence of Generative Adversarial Networks (GANs) as a highly disruptive sub-class of deep learning that may come to dominate industry progress in the years to come. It then turns its attention to to the use of AI in Drug Discovery for Longevity research, which can be considered to have started in mid-2017 with an event held at the Buck Institute for Research on Aging, at which Atomwise, BioAge and Insilico Medicine held a workshop, and which has just recently been formally solidified through Insilico Medicine being awarded the 2018 North American Artificial Intelligence for Aging Research and Drug Development Technology Innovation Award by leading business consulting firm Frost & Sullivan. Finally, it concludes by analyzing the ongoing convergence of AI for Drug Discovery with other advanced technologies including blockchain, personalised medicine and digital medicine, illustrating how these technologies and industries are being synergistically integrated so as to expedite the dynamic of progress in the AI for Drug Discovery sphere.

- **Appendix**

  - Overview of extended 600-page version of "AI for Drug Discovery and Advanced R&D Q2 2018".

  - Overview of the specialized chapter "Comparison of 20 Leading AI Companies" from our extended report "AI for Drug Discovery and Advanced R&D Q2 2018".

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Executive Summary

Our previous report noted a reversal of what we referred to in our first three reports on the subject of AI in Drug Discovery as the "**Big Gap**", i.e., the fact that throughout 2016 and 2017 IT and Tech corporations recognized and supported AI for healthcare startups, in terms of both investment and acquisitions, while BioPharma corporations lagged behind, still skeptical of the impact that AI could make upon drug discovery, biomarker development and other BioPharma niches.

Our most recent analysis indicates that this **"Big Gap" is now to a large extent neutralized**, and the BioPharma industry now has significant interest in AI, and belief in its ability to facilitate fundamental paradigm shifts in their traditional modes of operation. Some BioPharma companies have now become actively involved in the AI for Drug Discovery sector, while others still lag behind, skeptical of the sector's potential for impact and disruption, or finding themselves unable to acquire or implement these novel technologies in any relevant capacity. All indications still point to the conclusion that 2019 will mark the year that will test the strength, resolve and foresight of BioPharma as a whole.

Those BioPharma companies that commit significant will and resources to acquiring strong AI specialists, technologies and acquisitions will flourish, and those that do not will stagnate, and by the time their profit margins force them to realize the disruptive potential of AI for Drug Discovery and other biomedical niches, they will have missed the boat, with the majority of talent, technology and companies having already been acquired by their competitors.

Meanwhile, Chinese IT and Tech corporations, such as Alibaba, Baidu and TenCent, have made significant investments and acquisitions in the AI in Healthcare and Drug Discovery sector in particular, showing that the number of IT-corporations committing to the sector is growing not just nationally but also globally. This trend was noted in our last report Q2 2018, and continued to gain momentum, with even more investors in the Asia-Pacific region entering the space in Q3 2018.

At the same time, the lack of AI specialists that was alluded in our previous reports is still present. The majority of talented AI specialists in general have been acquired by traditional IT-corporations and have been applied for purposes other than AI in healthcare, creating a lack of enough specialists to support the activities of AI for Drug Discovery companies in particular.

Executive Summary

And it is not just traditional BioPharma companies that are suffering from this lack of specialists; indeed, even companies specializing specifically in AI for Drug Discovery are feeling the effects of this lack, **with AI specialists still comprising only 15.6% of such companies staff.** One of the central aims of this report is to summarize this gap, and chart the possible ways forward in order to neutralize it.

Deep Learning in general, and Generative Adversarial Networks (GANs) in particular, have started to be applied intensively by the leading AI for Drug Discovery companies, and this specific niche is now recognized by some progressive stakeholders as the most promising subsector for the entire AI for Drug Discovery industry.

Overall, the AI in healthcare and BioPharma subsector is growing at a steady rate, both in terms of new companies, investments and acquisitions, and in terms of the extent with which it is disrupting the traditional modes of operation of BioPharma as a whole. What is now a subsector and niche is poised to grow into perhaps the leading sector in BioPharma in the next 2-3 years, one that will have the greatest transformational impact on the industry, and one that will distinguish the leaders of the industry from the stagnators. We can predict that in 2019-2020 there will be intensive competition between the largest BioPharma companies and the largest IT and Tech corporations for the acquisition of new AI specialists, technologies and startups, in much the same way that 2014 – 2016 saw intense competition between IT-corporations to acquire the best AI assets and resources.

The total valuation of the AI for Drug Discovery subsector grew approximately 1.5 - 2x during the first half of 2018. Notably, this appears to be a result of the general growth of the industry itself, and the entry of several new large players, companies and investors, rather than due to breakthrough practical applications in any particular AI for Drug Discovery company itself. While companies are achieving steady progress, with indications that a few such companies could progress to the point of achieving practical applications in the clinic by 2020, no one company has yet brought a new blockbuster drug to market. Given the current dynamic of industry and technology progress, we can reasonably project that such a moment could occur as soon as 2020. Meanwhile the fact that the industry is witnessing steady growth despite any one company yet bringing a blockbuster drug to the market shows that AI for Drug Discovery is still an undervalued space. Therefore we can expect to see the total capitalization of this subsector grow significantly (e.g. on the order of 5-10x). At the same time, there is a possibility that a global financial crisis could occur within the next few years according to the opinions of several notable financial market players, which could temporarily decrease the dynamic of progress that we have seen in this space in the first half of 2018.

Executive Summary

Another significant trend developing in Q2-Q3 of 2018 is the emergence of new geographic locations, such as the EU, Asia and China, which are beginning to participate much more actively in the industry. The US was the main epicenter of activities in this space throughout the past several years, but we are now seeing industry involvement and a profusion of AI for Drug Discovery-themed events and conferences in the UK, Germany and Switzerland. Meanwhile, the number of investors based in the Asia-Pacific region, including China and Singapore, are also beginning to increase significantly, with a slew of large investment rounds occuring in the first half of 2018 alone.

2018 has also seen an increase in the number of Chinese investors entering the space. The Chinese IT-corporation Tencent, for instance, led a $155 million round of funding held by AI in healthcare company iCarbonX. Tencent also recently co-invested in a $15 million round held by AI for Drug Discovery company XtalPi with Google and Sequoia China. Chinese IT-corporation Alibaba has also entered the AI for healthcare space with the launch of what they refer to as the "ET Medical Brain", a platform that leverages Alibaba's formidable computational resources in order to generate new AI medical applications. Similarly, in Q3 2018, Sequoia Capital China led a $115 Series B investment round into Chinese AI for Drug Discovery company Deep Intelligent Pharma (DIP). And in Q3 2018 Ping An Good Doctor (backed by Softbank), the biggest online health care services provider in China, announced their plans to build 'hundreds of thousands' of its telephone booth-sized, unstaffed AI-assisted clinics and roll these out across the country over the course of the next three years.

In June 2018 prominent Chinese pharma company Wuxi AppTec invested in AI for Drug Discovery company Insilico Medicine alongside Pavilion Capital (a VC firm owned by the Singaporean government), as well as several Western VC firms including BOLD Capital Partners and Juvenescence Limited. In a recent Forbes article on the subject of Wuxi AppTec's recent investment Insilico's CEO Alex Zhavoronkov noted: *"I think this really shows that China is becoming a bigger player in AI. The emergence of China in AI, in research in particular, shows they are no longer a follower. So the US needs to invest in AI and biotech more than in military or trade wars that only make geopolitical tensions worse. Investing in biotech benefits everyone on the planet. It's a pretty good trend."*

In terms of whether it is the USA, EU, UK or Asia-Pacific region that comes out on top will remain to be seen. There are however, some factors that could be used to the advantage of the Asia-Pacific region generally, and China in particular, in the coming years. China currently is low on the list of the top countries competing in the Pharma industry. It falls significantly behind its Western competitors, due chiefly to the fact that it has focused on selling drugs that were innovated elsewhere, and lags behind in terms of actual pharma innovation. But that may be about to change.

Executive Summary

We have seen an influx of Chinese investors into life sciences industries over the past several years. For instance, the entry of Chinese investors into the broader biotech and drug industry landscape also mounted significantly in 2018, rising to $1.4 billion of investments into US-based biotech and drug firms compared to just $125.5 million during the same period the previous year. Furthermore, the Chinese government has recently shown significant interests in building up their AI industry, and in prioritizing AI in healthcare in particular. In an AI Strategic Plan released in July 2017, they outlined their intentions to catch up in the AI race by 2020, make major breakthroughs by 2025 and become the world leader in AI by 2030. But, in order to excel within the BioPharma industry they will need to reformulate their IP regulations, which are currently not tight enough to retain proprietary control over novel pharma innovations that they might develop in the coming years.

There are two additional advantages that China could possibly use in the coming AI for Drug Discovery race. Firstly, they have shown success in generating a massive amount of real-time medical data from their enormous population of citizens, as well as their current flexible privacy laws. Since AI in general (and machine learning and deep learning in particular) feed on data, this could potentially be used to the nation's benefit. Secondly, they have the raw materials needed for the most scarce resource in the industry: namely, a large quantity of Data scientists and AI specialists. If the Chinese government were to commit substantial resources to the training of additional AI and data scientists, they could potentially grow to surpass their Western competitors over the next 3-5 years. In the West, players in the AI for Drug Discovery race will suffer a severe scarcity of AI specialists in the coming years because the majority of them have been acquired by the IT and Tech industry for other purposes. China has the potential to leapfrog this issue.

Furthermore, while we can expect to see IT & Tech Corporations battle it out for supremacy in the AI for Drug Discovery race over the next several years. There are several factors that put IT & Tech corporations at an implicit advantage over BioPharma corporations. Firstly, IT & Tech corporations work from a solid foundation of AI and IT specialists, IP, resources and expertise, which is the very area that is the most scarce in the race, and the factor that constitutes the primary bottleneck in the ongoing progress of the AI for Drug Discovery industry. There is a limited number of AI specialists and resources to go around, and IT & Tech corporations already have the large majority of them. Secondly, IT and Tech corporations are used to and familiar with change, and with reformulating their business models and internal operations from the ground up in order to keep pace with the increasing rate of change in their industry.

Executive Summary

- **IT & Tech corporations are now outcompeting BioPharma corporations in the AI for Drug Discovery race**.
It is notable that the combined capitalization of the 15 BioPharma corporations that we have profiled in this report has 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 and the gap is increasing. This can be considered as an evidence that the BioPharma industry is stagnating in general, while the IT & Tech industry is progressing. This is why it is so remarkable that the number of IT corporations has already matched the number of BioPharma corporations active in this sector.

- **The industry is growing at a steady pace**, with a substantial increase in investments and joint ventures in Q1-Q3 of 2018 compared to 2017. We are also seeing a significant increase in industry participation and activity from large corporations. As can be seen in the BioPharma Corporations Onboarding AI for Drug Discovery section of this report, whereas BioPharma corporations were previously resistant and skeptical towards the disruptive impact of AI for Drug Discovery, many BioPharma corporations are now actively participating through the investment of joint ventures and M&A deals. Meanwhile, as can be seen in the same section, the number of IT and Tech corporations active in this space is also steadily increasing, and still surpasses activity from BioPharma corporations.

- **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 companies, investments and industry conferences, we are seeing an increased level of activity from the UK, particularly in the form of government initiatives. We are also seeing a dramatic increase in activity from the Asia-Pacific region generally, and from China in particular. Chinese investors are now aggressively investing in AI for Drug Discovery startups, and Chinese IT & Tech corporations are entering the space with level of activity that at least equals US IT & Tech giants. Furthermore, China's massive population and governmental will to rapidly advance their global leadership position in AI means that if they prove committed to increasing the number of AI specialists and Data scientists, China could overtake their Western competitors in this subsector in the next 3-5 years, when USA, UK and EU companies begin to really suffer from the impact of the coming scarcity of AI-specialists and Data scientists in the coming years.

- **We could see the arrival of the AI-industry's first blockbuster drug by 2020**. While no AI for Drug Discovery company has brought a blockbuster drug to market yet, many now have drugs developed using AI in clinical trials. The first arrival of such a drug to market will signal the tangible scientific validation of the entire AI for Drug Discovery approach, and will cause a massive increase of investments and capitalization of this industry in general.

Emerging Trends in AI for Drug Discovery

- Today, drug discovery is a trial-and-error process that eats up enormous amounts of research time. AI can significantly narrow the focus of researchers by rapidly assimilating and analyzing the information in public and proprietary databases.

- Beyond scanning health records to help providers identify chronically ill individuals who may be at risk of an adverse episode, AI can help clinicians take a more comprehensive approach for disease management, better coordinate care plans and help patients to better manage and comply with their long-term treatment programmes.

- The use of AI is enabling review and translation of mammograms 30 times faster with 99% accuracy, reducing the need for unnecessary biopsies.

- Researcher Frost & Sullivan said artificial intelligence systems will generate $6.7 billion in global revenue from healthcare by 2021, compared with $811 million in 2015.

- In 2018, even more extreme challengers and disruptors will arrive with the convergence of next generation AI, blockchain and precision medicine.

- The global healthcare AI market is highly fragmented and is characterized by the presence of large number of industry players, while the AI for Drug Discovery segment has a comparatively lower level of competition because this market segment only accepts companies with very high levels of expertise. There are more than 1000 AI in Healthcare companies on global scale, but only 125 of them are capable of entering the AI in Drug Discovery and advanced R&D sector.

- The breakthroughs in AI for Drug Discovery will change the R&D process of Bio Pharma, and it will have a tremendous impact on whole BioPharma industry.

- That is why the players from the AI for Drug Discovery market can become new game changers and significantly influence the capitalization of BioPharma corporations.

Highlights of Major Events in Q3 2018

- **August 2018** - China's largest online healthcare platform, Ping An Good Doctor, has announced that it will launch 300,000 AI-assisted medical consultation booths across southeast Asia.

- **September 2018** - US consortium Alliance for Artificial Intelligence in Healthcare (AAIH) (a consortium founded to "educate and advocate for policies and regulations to promote rapid integration and utilization of AI in healthcare") meet at the Basel Life Congress to finalize their plans for the first 12 months of operation. Founding members of the consortium include Insilico Medicine, GE Healthcare, Benevolent AI, OWKIN, NuMedii, Numerate, Recursion, Cyclica, Envisagenics, BlackThorn Therapeutics, University of Pittsburgh and the Buck Institute for Research on Aging.

- **October 2018 -** Chinese AI and blockchain for drug development company Deep Intelligent Pharma (DIP) raises $15 million Series B funding from Sequoia Capital China, which will be used for "research and development of AI-powered drug development technology." This deal highlights the increasing aggressiveness of Chinese startups entering the AI for drug development sphere, a trend highlighted in our Q2 2018 report, which only continues to grow as we approach 2019.

- **October 2018** - Chinese company XtalPi raises an additional $46 million in Series B add-on led by China Life Healthcare Fund and with SIG and Yael Capital as co-investors, on top of its original $15 million Series B round from Sequoia China, Google and Tencent that closed in January 2018, bringing XtalPi's total funding to date to over $66 million.

- **October 2018** - Pfizer announces at the AI Applications Summit for BioPhama conference that it now has over 150 separate AI projects underway, though few of them are believed to be at the core of AI for drug discovery.

- **October 2018** - Berkeley Lights, Inc. (BLI), a leader in digital cell biology, announces the completion of a $95 million financing round led by Nikon and backed by existing investors Sequoia Capital, Walden-Riverwood Ventures, Black Diamond Ventures, and Paxion Capital, and joined by new investors Cota Capital, KTB Network, Atinum Investment, Shangbay Capital, AJS BioTree Healthcare Fund, and Varian.

Highlight of Major Events in November 2018

- **November 2018** - The UK announces that five new AI medical clinics will open across the UK in 2019 via £50 million in funding through the Department for Business, Energy and Industrial Strategy. These AI clinics will use software to digitise scans and biopsies, and use AI-enabled tools to perform early disease diagnostics.

- **November 2018** - German pharma company Bayer has announced that it will use AI to accelerate patient safety data analysis to detect drug-related side effects through its pharmacovigilance systems.

- **November 2018 -** UK company Exscientia acquires UK start-up Kinetic Discovery to enable a "full stack" of AI driven drug discovery, adding Kinetic's expertise in specialist protein engineering, biophysical screening and structural biology to their existing assets.

- **November 2018** - UK company Escientia expands its presence at Oxford University by establishing a lab at the new Schrödinger Building on The Oxford Science Park, uniting its computer scientists, drug specialists and biologists under one facility to accelerate its platform and portfolio development activities, and to expand its ecruitment activities at Oxford University.

- **November 2018** - Korean pharmaceutical company Daewoong Pharmaceutical makes a public commitment to adopt AI for drug discovery in partnership with Ulsan National Institute of Science and Technology (UNIST), signalling that South Korea is beginning to enter the AI for Drug Discovery market alongside other countries in the Asia-Pacific Region like China and Singapore.

In conclusion, the large majority of the trends, insights and forecasts made in our previous reports remain true today, at the end of Q3 2018. The number of new AI in Drug Discovery startups continue to grow, and the funding flowing into the industry continues to rise. IT and Tech corporations continue to enter the sphere of AI in Healthcare. BioPharma corporations continue to on-board AI for drug discovery, though nonetheless remain slow to move in the face of disruptive change, and remain susceptible to being overtaken by more progressive Tech Corporations and AI for Drug Discovery startups. And while the US remains the global leader of this sphere, it is very quickly losing ground to the UK and the Asia pacific region (and China in particular), who are rapidly enhancing their position in the global AI for Drug Discovery race through strategic financing, acquisitions, and government initiatives.

AI for Drug Discovery and Advanced R&D Landscape Q3 2018

AI for Drug Discovery and Advanced R&D Landscape Q3 2018

The present section aims to deliver an overview of the AI for Drug Discovery landscape, including lists of Companies, Investors, R&D Centers, Conferences & Media in one fell swoop.

It features detailed lists of:

- 125 companies applying AI for Drug Discovery & Advanced R&D
- 260 investors in AI for Drug Discovery companies
- 20 leading AI for Drug Discovery R&D centers
- 15 IT and Tech corporations embracing AI for Drug Discovery and advanced AI in Healthcare
- 15 Biopharma corporations applying AI for Drug Discovery
- 30 conferences focused on AI for Drug Discovery and advanced R&D
- 20 journalists regularly covering AI for Drug Discovery in media with a certain level of expertise and specialization in the topic

All of these entities are profiled in depth in this report's appendices. Here, our aim is simply to list them and, where applicable, to classify them according to application, industry segmentation, and regional location. Companies, for instance, are categorized according to industry segmentation (i.e. focusing on Drug Discovery, Biomarker Development, or Advanced R&D, respectively), while investors are classified according to their regional location and the companies in which they invested.

These lists have been extended in comparison to our previous report (AI for Drug Discovery, Biomarker Development and Advanced R&D Q2 2018) in order to include those companies, investors and entities that rose into prominence in Q3 of 2018. We have added, 25 AI companies, 40 investors, 10 conferences, and 10 conferences.

20 Leading R&D centers

R&D Centers	Location
Astellas Drug Discovery Research Centre	Japan
Babraham Research Campus	UK
Center for Computational Health - IBM Research	US
Centre for Drug Research and Development	Canada
China R&D Center (CRDC) - Pfizer	China
Chinese Thoracic Oncology Group (CTONG)	China
Drug Discovery Oxford	UK
Janssen Pharmaceutical Companies of Johnson & Johnson	US
Johnson & Johnson Pharmaceutical Research and Development	China
Korea Pharmaceutical and Bio-Pharma Manufacturers Association	South Korea
La Jolla Laboratories	US
Merck Exploratory Science Center (MESC)	US
Merck Serono Pharmaceutical R&D Co., Ltd	China
Pande Lab - Stanford University	US
Ritsumeikan Research Center for Drug Discovery and Development Science	Japan
Roche Innovation Center Copenhagen	Danmark
Sanofi Pasteur R&D Centre	Canada
The Development Center for Biotechnology	Taiwan
The R&D Centre China LTD (RRDCC)	China
Warren Family Research Center for Drug Discovery and Development	US

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

1. A2A Pharmaceuticals
2. AccutarBio
3. Acellera
4. Acurastem
5. AiCure
6. Antidote
7. Antiverse
8. Arbor Biotechnologies
9. Athelas
10. ATOM
11. Atomwise
12. Bactevo
13. BenchSci
14. BenevolentAI
15. Berg LLC
16. Berkeley Lights
17. BioAge Labs
18. Biorelate
19. BioSymetrics
20. Biovista
21. BioXcel
22. Brite Health
23. BullFrog AI
24. C4X discovery
25. Cambridge Cancer Genomics
26. Causaly
27. Celsius Therapeutics
28. Clinithink
29. Cloud Pharmaceuticals
30. CloudMedX
31. Cotinga Pharmaceuticals
32. Cyclica
33. CytoReason
34. Cytox
35. Datavant
36. Deep 6 AI
37. Deep Genomics
38. Deep Intelligent Pharma
39. Desktop Genetics
40. e-therapeutics
41. Emerald Cloud Lab
42. Engine Biosciences
43. Envisagenics
44. Euretos
45. Evaxion
46. Evid Science
47. exscientia
48. FDNA
49. Genialis
50. Globavir
51. GNS Healthcare
52. GTN
53. Healx
54. HelixAI
55. IBM Watson Health
56. Iktos
57. Imagia
58. Inato
59. Innoplexus
60. Insilico Medicine
61. Insitro
62. Intellegens
63. Intelligencia.AI
64. Interprotein
65. InveniAI
66. InVivo AI
67. Iris.ai
68. Juvenescence AI
69. Kyndi
70. LAM Therapeutics
71. Lantern Pharma
72. MediBIC Group
73. Mendel.ai
74. Meta
75. Micar21
76. Mind the Byte
77. Molomics
78. Mozi
79. nference
80. Novoheart
81. nQ Medical
82. NuMedii
83. Numerate
84. Nuritas
85. Owkin
86. PathAI
87. PatSnap
88. Pepticom
89. Peptone
90. Pharnext
91. Phenomic AI
92. Plex Research
93. ProteinQure
94. Qrativ
95. Quantitative Medicine
96. Recursion Pharmaceuticals
97. Remedium AI
98. Researchably
99. Resonant Therapeutics
100. Reveal Biosciences
101. Reverie Labs
102. ReviveMed
103. Scibite
104. sciNote
105. Sensyne Health
106. Sparrho
107. Spring Discovery
108. Standigm
109. Structura Biotechnology
110. Synthace
111. TeselaGen
112. ThoughtSpot
113. Transcriptic
114. Trials.ai
115. Turbine
116. TwoXAR
117. uBiome
118. Verge Genomics
119. VERISIMLife
120. Virogin
121. Virvio
122. Vyasa
123. WinterLight Labs
124. XtalPi
125. ZappRx

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

1. 10x Group
2. 11.2 Capital
3. 500 Startups
4. 6 Dimensions Capital
5. 8VC
6. A-Level Capital
7. Accelerate Long Island
8. Accelerate@Babraham
9. Advantage Capital
10. Afore Capital
11. Agent Capital
12. AGORANOV
13. Alexandria Real Estate Equities
14. AllBright
15. Alphabet
16. ALS Investment Fund
17. Amadeus Capital Partners
18. AME Cloud Ventures
19. Amgen Ventures
20. Amplify Partners
21. Andreessen Horowitz
22. ARCH Venture Partners
23. Atlas Venture
24. Aurinvest
25. B Capital Group
26. Baidu Ventures
27. Baird Capital
28. Bakken & Baeck
29. BDC Venture Capital
30. Beast Ventures
31. Bioeconomy Capital
32. Biomatics Capital Partners
33. Bios Partners
34. Bloomberg Beta
35. BOE Technology Group
36. Bold Capital Partners
37. BootstrapLabs
38. Boundary Capital Partners LLP
39. Caffeinated Capital
40. Cambia Health Solutions
41. Capital One Growth Ventures
42. Casdin Capital
43. Cathay Innovation
44. Celgene
45. China Equity
46. Citrix Systems
47. Claremont Creek Ventures
48. CLI Ventures
49. Comcast Ventures
50. Creative Destruction Lab
51. Crowdcube
52. CrunchFund
53. CRV
54. Cultivian Sandbox Ventures
55. Danhua Capital
56. Darling Ventures
57. Data Collective
58. DCM Ventures
59. Deep Knowledge Ventures
60. Dentsu
61. DFJ Growth
62. Digital Science
63. DNA Capital
64. Dolby Family Ventures
65. Dorm Room Fund
66. Draper Associates
67. Draper Dragon
68. Dynamk Capital
69. EASME - EU Executive Agency for SMEs
70. EDBI
71. Emerge Education
72. Empire State Development
73. Endure Capital
74. Eniac Ventures
75. Enterprise Ireland
76. Entrepreneur First
77. EPIC Capital
78. EPIC Ventures
79. European Union
80. Fairhaven Capital Partners
81. Faridan
82. Felicis Ventures
83. Fenox Venture Capital
84. Fifty Years
85. Finance Wales
86. First Star Ventures
87. Fly Ventures
88. Foundation Capital
89. FounderFuel
90. Founders Factory
91. Founders Fund
92. FREES FUND
93. Frontier IP Group plc
94. FundersClub
95. Gaorong Capital

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

96. General Catalyst
97. Geodesic Capital
98. GlaxoSmithKline
99. GM&C Life Sciences Fund
100. Golden Venture Partners
101. GQY
102. Gradient Ventures
103. Grand Central Tech
104. Grand Challenges Canada
105. Great Oaks Venture Capital
106. GreenSky Capital
107. GV
108. Hacking Health Accelerator
109. Hanhai Studio
110. Health Wildcatters
111. Healthbox
112. Heritage Provider Network
113. Hewlett Packard Pathfinder
114. Horizons Ventures
115. IA Ventures
116. Illumina
117. Indie Bio
118. Initialized Capital
119. InnoSpring Seed Fund
120. iNovia Capital
121. IQ Capital Partners LLP
122. J. Hunt Holdings
123. Jiantou Huawen Investment
124. Juvenescence
125. Kapor Capital
126. Karlin Ventures
127. KdT Ventures

128. Khosla Ventures
129. Kima Ventures
130. Kleiner Perkins Caufield & Byers
131. KTB Network
132. Lansdowne Partners
133. Lanza Tech Ventures
134. LaunchCapital
135. LB Investment
136. LeFrak
137. Lenovo
138. Life Sciences Angel Network
139. Lightspeed Venture Partners
140. Lilly Ventures
141. Linden Mobile Ventures
142. Liquid2 Ventures
143. London Co-Investment Fund
144. Lucas Venture Group
145. Lundbeck
146. Lux Capital
147. Marathon Venture Capital
148. Masa Life Science Fund
149. MassChallenge
150. MassDevelopment
151. Matrix Partners
152. Mayo Clinic
153. MedTech Innovator
154. Menlo Ventures
155. Merck Global Health Innovation Fund
156. Mission and Market
157. MIT delta
158. MITS Fund

159. Mitsui & Co
160. Monsanto Growth Ventures (MGV)
161. Mubadala Investment Company
162. National Institutes of Health
163. National Science Foundation
164. Nest.Bio Ventures
165. Nesta Ventures
166. New Leaf Venture Partners
167. New Protein Capital
168. New Wave Ventures
169. NewDo Venture
170. Nikon
171. NJF Capital
172. Obvious Ventures
173. Octopus Ventures
174. OS Fund
175. Otium Capital
176. Palm Drive Capital
177. Pavilion Capital
178. Pear Ventures
179. Pentech Ventures
180. Perivoli Innovations
181. Pillar Companies
182. Pitch@Palace
183. PivotNorth Capital
184. Plug and Play
185. Presence Capital
186. Pritzker Group Venture Capital
187. Qiming Venture Partners
188. Qualgro VC
189. Real Ventures
190. Redalpine Venture Partners

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

191. Refactor Capital
192. Renren Inc.
193. Rivas Capital
194. Rough Draft Ventures
195. Seneca Partners
196. Sequoia Capital
197. Sequoia Capital China
198. Seraph Group
199. Serena Capital
200. ServiceNow
201. Shunwei Capital
202. Silicon Badia
203. Silicon Valley Bank
204. Slow Ventures
205. Smedvig Capital
206. Sofinnova Partners
207. Softbank Ventures Korea
208. Sorrento Therapeutics
209. SOSV
210. Square 1 Bank
211. SR One
212. Stage Venture Partners
213. Starlight Ventures
214. StartUp Health
215. StartX
216. StartX (Stanford-StartX Fund)
217. Summit Partners
218. Sutter Hill Ventures
219. SV Angel
220. SV Tech Ventures
221. SyndicateRoom
222. Techammer

223. TechU Angels
224. Temasek Holdings
225. Tencent Holdings
226. TenOneTen Ventures
227. The Thiel Foundation
228. Third Kind Venture Capital
229. Third Rock Ventures
230. TIPS
231. Tribeca Venture Partners
232. True Ventures
233. Truffle Capital
234. TSVC (formerly TEEC Angel Fund)
235. Two Sigma Ventures
236. uBiome
237. UK Innovation & Science Seed Fund
238. Uni-Innovate Group
239. Unshackled Ventures
240. Upsher Smith Laboratories
241. Vanguard Atlantic
242. Varian
243. Vertex Ventures
244. Vertex Ventures Southeast Asia & India
245. VTF Capital
246. Walden Riverwood Ventures
247. Warburg Pincus
248. Westcott LLC
249. White Cloud Capital
250. WI Harper Group
251. Wild Basin Investments
252. Woodford Investment Management
253. WorldQuant Ventures LLC

254. Wren Capital
255. WuXi AppTec
256. Y Combinator
257. Yuansheng BioVenture
258. Zappos
259. ZhenFund
260. Zillionize Angel

15 Pharma Corporations applying AI for Drug Discovery

Company Name	Based in	Website
1. Amgen	United States	https://www.amgen.com/
2. Astellas Pharma	Japan	https://www.astellas.com/
3. Astrazeneca	United Kingdom	http://www.astrazeneca.com/
4. Bayer	Germany	http://bayer.com/
5. Boehringer Ingelheim	Germany	https://www.boehringer-ingelheim.com/
6. Bristol-Myers Squibb	United States	https://www.bms.com/
7. Evotec	Germany	https://evotec.com/
8. GSK	United Kingdom	http://www.gsk.com/
9. Ilumina	United States	https://www.illumina.com/
10. Johnson & Johnson	United States	http://www.jnj.com/
11. Merck	United States	http://www.merck.com/
12. Novartis	Switzerland	http://www.novartis.com/
13. Pfizer	United States	https://www.pfizer.com/
14 Roche	Switzerland	http://www.roche.com/
15. Sanofi	France	http://m-en.sanofi.com/

15 Tech Corporations Interested in Advanced AI Applications in Healthcare

Company Name	Based in	Website
1. Alibaba	China	http://www.alibaba.com/
2. Amazon	United States	http://amazon.com/
3. Apple	United States	http://www.apple.com/
4. Baidu	China	http://www.baidu.com/
5. Canon	United States	https://www.usa.canon.com/internet/portal/us/home
6. Google	United States	http://www.google.com/
7. Hitachi	Japan	http://www.hitachi.com/
8. Huawei	China	http://huawei.com/
9. IBM	United States	http://www.ibm.com/
10. Intel	United States	http://www.intel.com/
11. Microsoft	United States	http://www.microsoft.com/
12. Nvidia	United States	http://www.nvidia.com/
13. Samsung Electronics	South Korea	http://www.samsung.com/us
14. Siemens	Germany	https://www.siemens.com/global/en/home.html
15. Tencent	China	https://www.tencent.com/en-us/

Top-30 Conferences on AI for R&D and Drug Discovery 2018-2019

Name	Date	Location	Website
2nd Annual Artificial Intelligence in Drug Development Congress	20-21 September 2018,	UK	https://www.oxfordglobal.co.uk/artificialintelligence-congress/
2nd Global Pharma R&D Informatics and AI Congress	29th-30th October 2018	UK	http://www.global-engage.com/event/pharma-informatics-congress/
ADVANCED MACHINE LEARNING AND ARTIFICIAL INTELLIGENCE FOR DRUG DISCOVERY & DEVELOPMENT	19th - 20th June 2018	EU	https://www.bisgrp.com/portfolio/conferences/pharmaceutical/advanced-machine-learning-and-artificial-intelligence-for-drug-discovery-development
AI Health & Pharma Summit	14 June, 2018	UK	https://theaisummit.com/health/
AI in Pharma Summit 2018	9th October 2018	US	https://www.cambridgeconsultants.com/events/ai-pharma-summit-2018
AI IN PHARMA: OPPORTUNITIES & CHALLENGES	12th June 2018	UK	https://telecomstechacademy.knect365.com/ai-in-pharma-opportunities-challenges/
AI Pharma	10-11 September 2018	Japan	https://10times.com/ai-pharma-japan
AI Pharma Innovation: Drug Discovery Summit	26-28 February 2018,	US	http://ai-drugdiscovery.com/
Artificial Intelligence and Big Data in Pharma	March 21 2018	EU	http://www.mpg-alumni.de/conferences/aiworkshop/
Artificial Intelligence and Machine Learning for Drug Discovery	November 27, 2018	EU	http://www.worldpreclinicaleurope.com/AI-ML-Drug-Discovery

Top-30 Conferences on AI for R&D and Drug Discovery 2018-2019

| Name	Date	Location	Website
Artificial Intelligence for Drug Discovery	May 23, 2018	US	https://www.BioPharmatrend.com/post/57-artificial-intelligence-for-drug-discovery-may-23-2018-cambridge-ma-usa/
BioData World	28 - 29 November 2018	Switzerland	https://www.terrapinn.com/conference/biodata/index.stm
Artificial Intelligence in Pharma Industry Summit	19- 20 February 2018	EU	https://www.asdevents.com/event.asp?id=17278
Artificial intelligence to speed up drug discovery: the revolutionary road to advancing innovation	4th December 2018	EU	https://www.biofit-event.com/conference/artificial-intelligence-speed-drug-discovery-revolutionary-road-advance-innovation/
Artificial Intelligence Transforming Pharma R&D	Feb 21-22, 2018	US	https://benevolent.ai/events/previous/artificial-intelligence-transforming-pharma-r-d/
BASEL LIFE Artificial intelligence and blockchain in healthcare innovation forum	11–14 September 2018	Switzerland	https://www.basellife.org/basel-life-2018/basel-life/innovation-forums/scientific-programme/artificial-intelligence-and-blockchain-in-healthcare.html
HEALTHCARE & MEDICAL RESEARCH CONFERENCE SESSIONS	March 18-22, 2019	US	https://www.nvidia.com/en-us/gtc/topics/healthcare-and-life-sciences/
Pharma AI & IoT 2018	11th-12th July 2018	UK	http://www.virtueinsight.com/pharma/Pharma-AI--IoT-2018/
SMi's 2nd annual Drug Discovery conference	21-22 March 2018	UK	https://www.drugtargetreview.com/news/29432/new-2018-role-artificial-intelligence-drug-discovery/
THE Summit for ChangeMakers Using AI in Biopharma	25-26 October 2018	US	https://pharmaphorum.com/events/ai-applications-summit-BioPharma/

Top-30 Conferences on AI for R&D and Drug Discovery 2018-2019

| Name	Date	Location	Website
Machine Learning and Artificial Intelligence	11-13 March 2019	USA	https://www.bio-itworldexpowest.com/AI
2nd AI Pharma Innovation: Drug Discovery Summit 2019	27-28 February 2019	USA	http://ai-drugdiscovery.com/register/register/
The AI Application Summit Biopharma	25-26 October 2019	USA	https://www.aiapplicationssummit.com/register-your-interest/?eventID=2826
Advanced Machine Learning And Artificial Intelligence For Drug Discovery And Development	28-29 May 2019	UK	https://www.drugdiscoverydevelopmentforum.com/#faq-gallery
Intelligent Health AI	11-12 September 2019	Switzerland	https://intelligenthealth.ai/
BioData World West 2019	10-11 October 2019	USA	https://www.terrapinn.com/template/live/go/9939/20103
3rd Annual Artificial Intelligence in Drug Development Congress	September 2019	UK	https://www.oxfordglobal.co.uk/artificialintelligence-congress/
Precision Medicine World Conference 2019	20-23 January 2019	USA	https://www.pmwcintl.com/registration/?page_scroll=2019sv
Deep Learning in Healthcare Summit	23-24 May 2019	USA	https://www.re-work.co/events/deep-learning-in-healthcare-summit-boston-2019
Pharma AI & IoT 2018	11-12 July 2018	UK	https://pharmaphorum.com/events/pharma-ai-iot-2018/

20 Journalists Specializing in AI for R&D and Drug Discovery

Name	Based in	Associated Media Entity
1. Richard Staines	United Kingdom	Pharmaphorum
2. Nick Paul Taylor	United Kingdom	Freelance
3. Joy Persuad	United Kingdom	Freelance
4. Alaric DeArment	United States	MedCity News
5. Dave Muoio	United States	MobiHealthNews
6. Derek Lowe	United States	Science Translational Medicine
7. Amirah Al Idrus	United States	FierceBiotech
8. Bill Siwicki	United States	HIMSS Media
9. Heather Mack	United States	The Wall Street Journal
10. Jeff Lagasse	United States	HIMSS Media
11. Bernie Monegain	United States	HIMSS Media
12. Mike Miliard	United States	HIMSS Media
13. Conor Hale	United States	FierceMedTech, FierceBiotech
14. Andrew McConaghie	United Kingdom	Pharmaphorum
15. Joseph Keenan	United States	FierceBiotech, FiercePharma
16. Julian Upton	United Kingdom	Pharmaceutical Executive
17. Gemma Jones	United Kingdom	PMLiVE
18. Phil Taylor	United Kingdom	Freelance
19. Kumba Sennaar	United States	Kumba Sennaar
20. Daniel Faggella	United States	TechEmergence

# Regional Comparison of AI for R&D and Drug Discovery Companies / Investors / R&D Centers
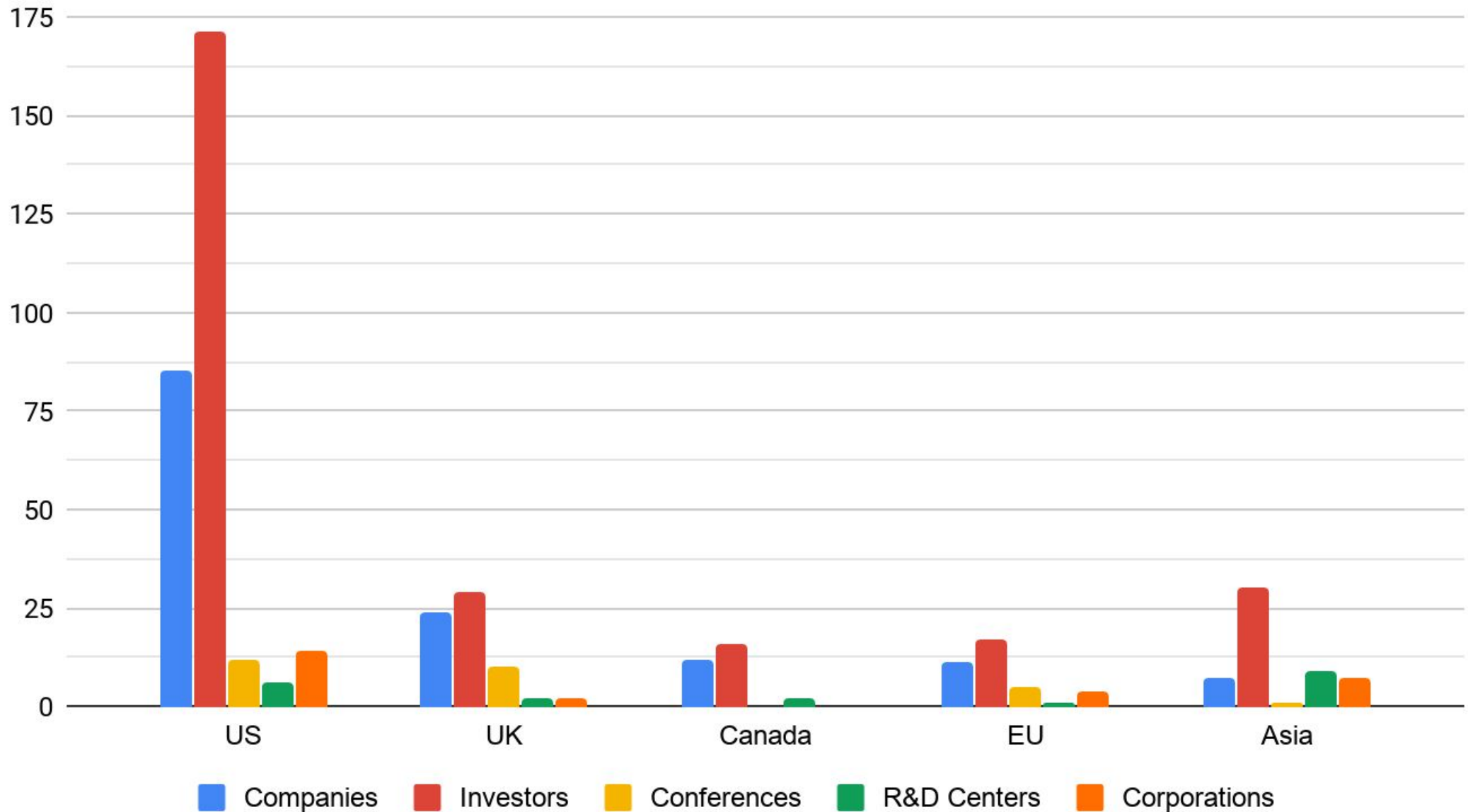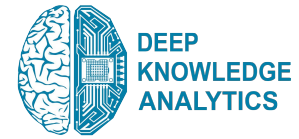
125 AI Companies: Regional Proportion

Others
3.5%

Asia
4.9%

EU
7.6%

Canada
8.3%

UK
16.7%

US
59.0%
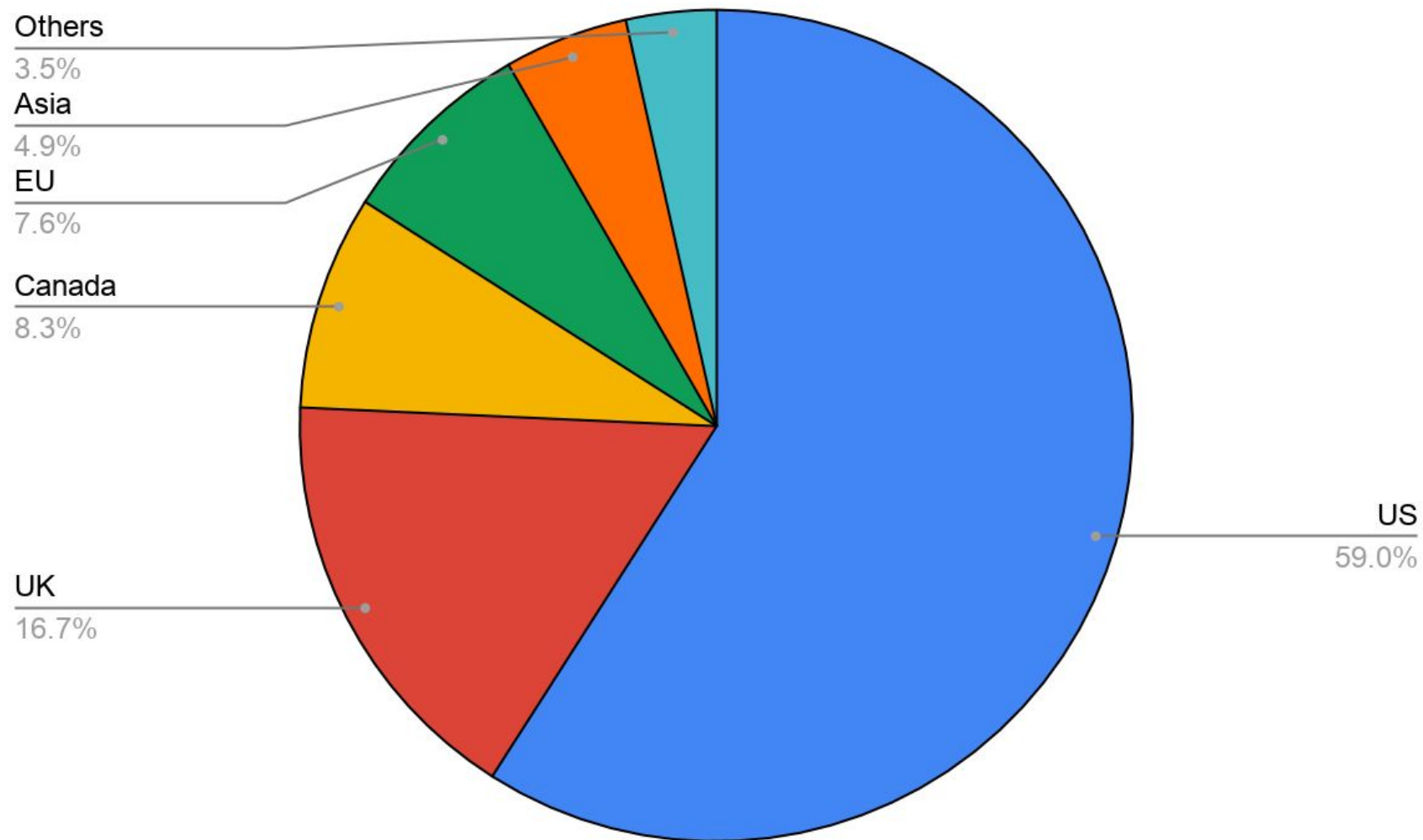
The US is still firmly in the lead in terms of its proportion of AI for Drug Discovery companies. Interestingly, Asia currently has the fifth-lowest proportion of AI for Drug Discovery companies. The Asia-Pacific region has, however, begin to aggressively increase their activity in the space in terms 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.

260 Investors: Regional Proportion

Others
0.8%
Asia
11.3%
EU
6.4%

Canada
6.0%

UK
10.9%

US
64.5%
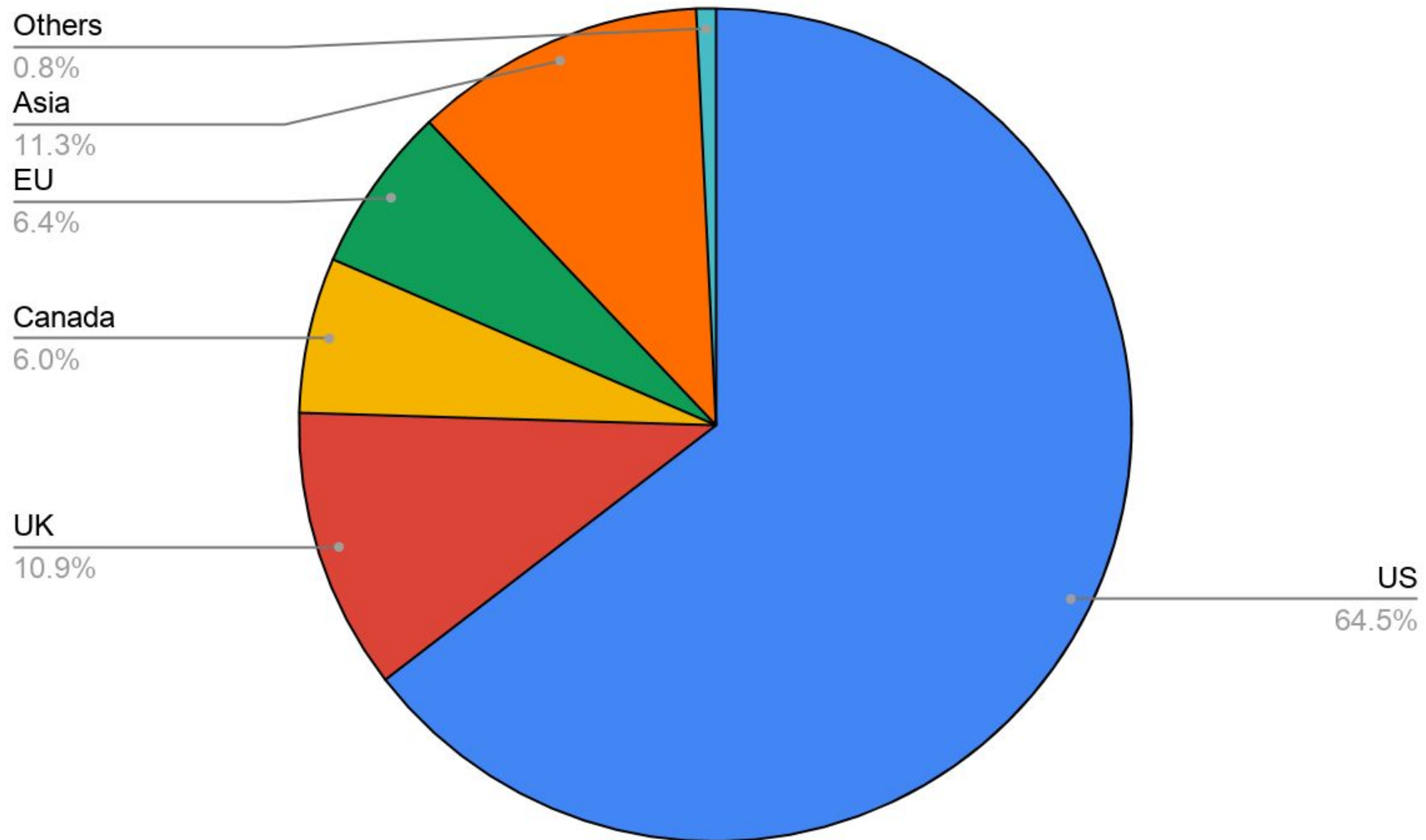
The US still leads the rest of the world in the proportion of AI for Drug Discovery Investors. This is sensible given that they also have the largest proportion of AI for Drug Discovery companies. However, it is interesting to note that, while the Asia Pacific Region is home to the second-largest proportion of investors in this space, now having surpassed the UK, which has dropped down to the #3 position, having previously occupied the #2 position in this regard in our previous reports.

20 Leading R&D Centers: Regional Proportion
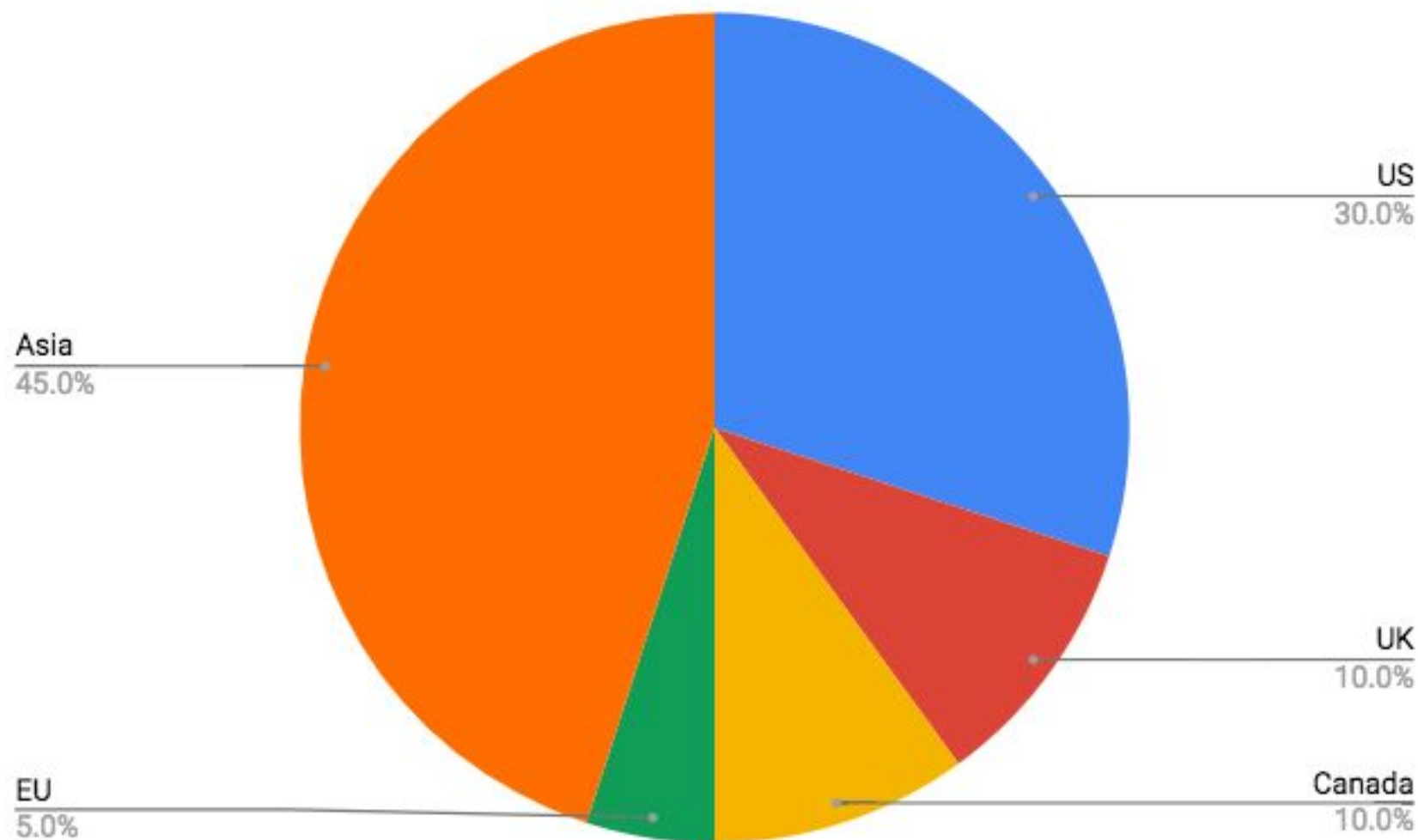
Whereas data in our previous reports indicated that the US leads the world in terms of the number of R&D Centers focused on AI for Drug Discovery, Asia has now surpassed them. This is sensible within the context of the recent increase in the number of Chinese investors entering the AI for Drug Discovery space, and the Chinese government's recent commitment to lead the world in AI by the year 2030.

Top-30 Conferences on AI for R&D and Drug Discovery 2018-2019:
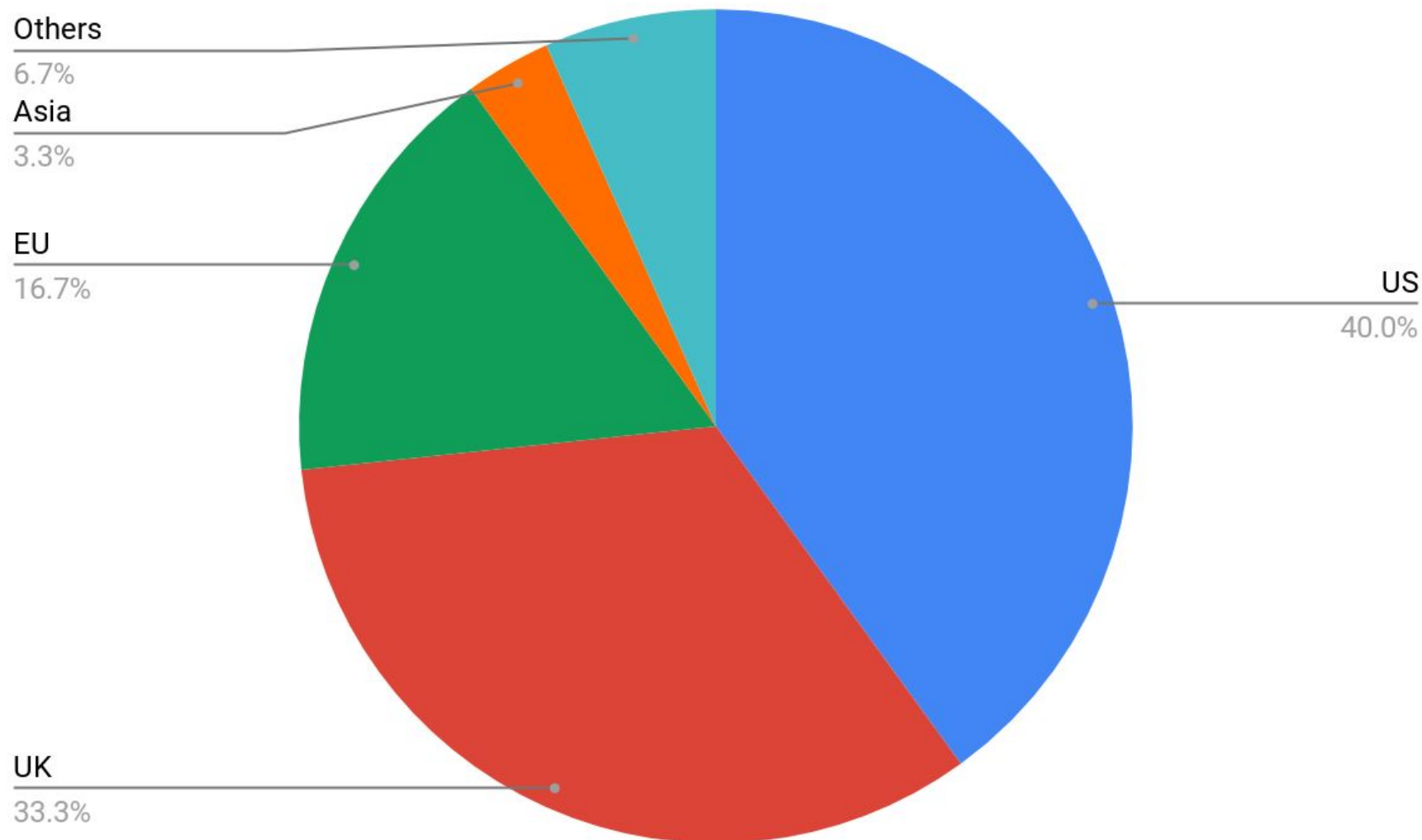
As can be seen in the figure above, whereas previously the US has dominated the AI for Drug Discovery conference landscape (which follows naturally from the fact that it also leads in terms of the total number of AI for Drug Discovery conferences and investors), we have seen a significant increase in the number of AI for Drug Discovery conferences located in the UK and EU.

30 Corporations Applying
Advanced AI in Healthcare and Drug Discovery
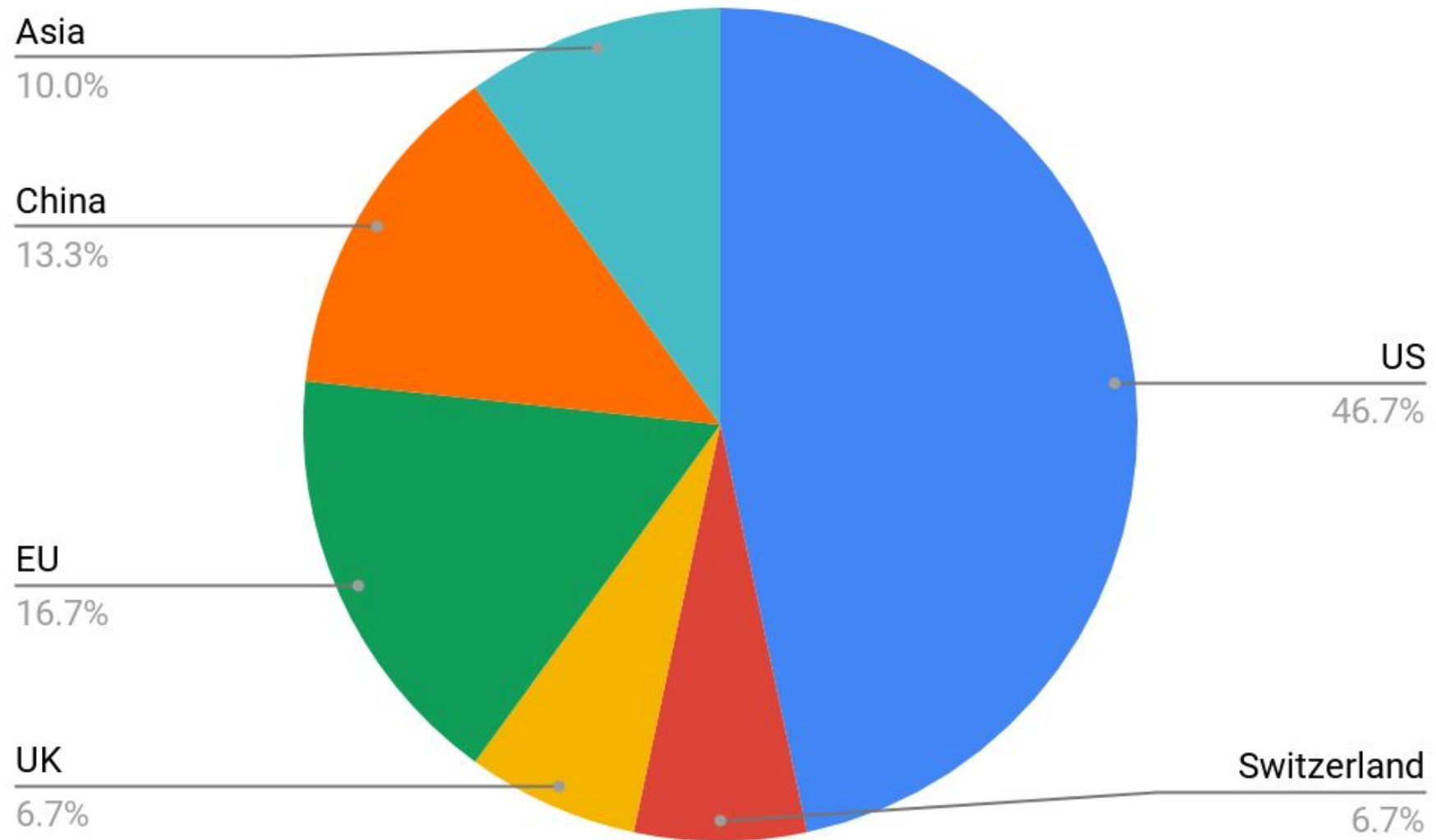
Region	Percentage
Asia	10.0%
China	13.3%
EU	16.7%
UK	6.7%
US	46.7%
Switzerland	6.7%

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 number of AI companies, volume of investments and number of industry specialized conferences, in 2018 we are seeing an increased level of activity from the UK, Switzerland and China.

AI experts vs BioTech experts vs Administrative Staff
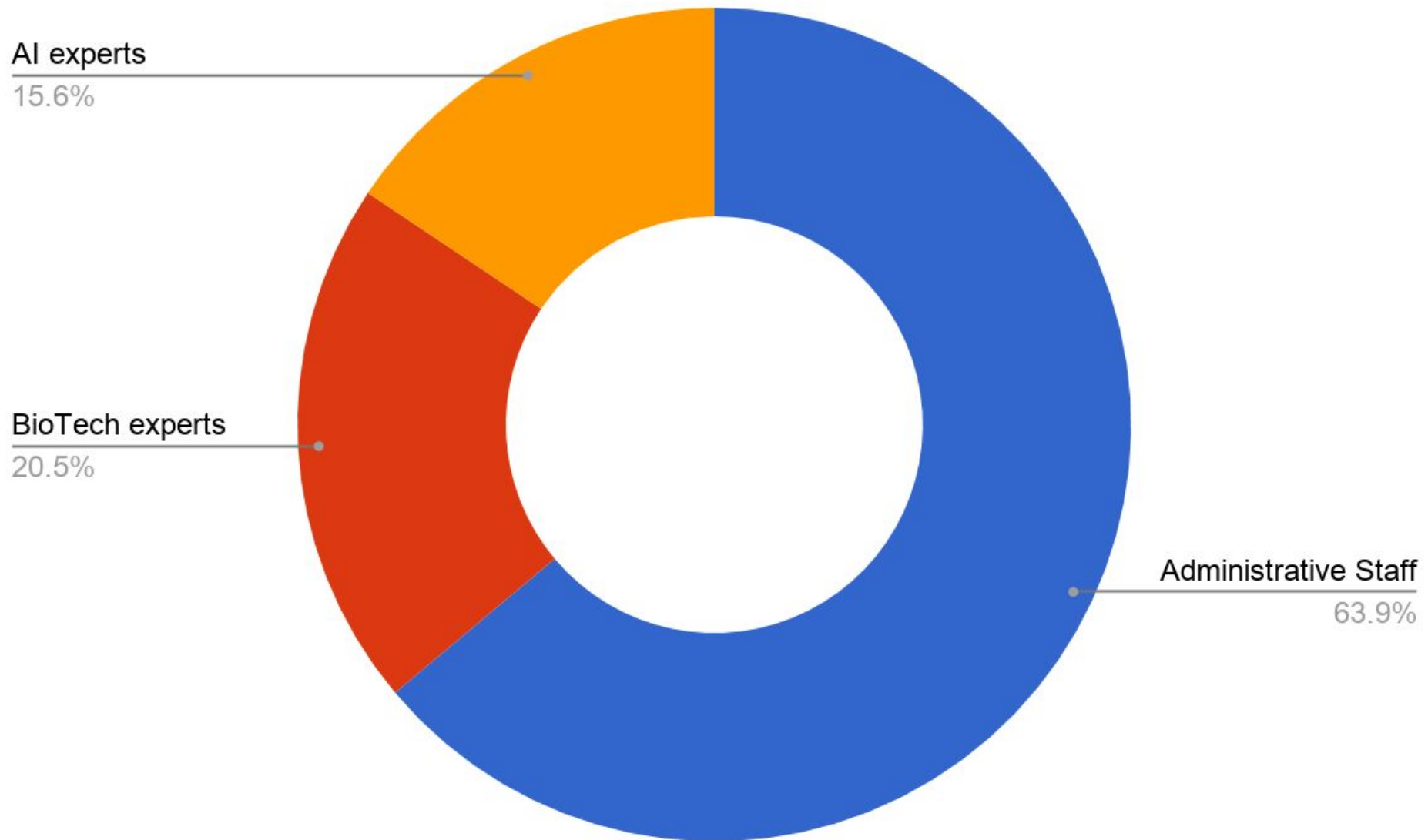
Despite the recent hype, there is an obvious lack of AI-specialists in the Drug Discovery space and therefore a lack of **"True AI"** companies in this sector. Administrative staff outnumber AI specialists at a 4:1 ratio. We are already beginning to see the effects of the coming AI talent winter.

Does 2018 Signal the Rise of China as a New Epicenter of AI for Drug Discovery Activity?

In terms of whether it is the USA, EU, UK or Asia region that comes out on top will remain to be seen. There are however, some factors that could play out to the advantage of the Asia region generally, and China in particular, in the coming years that may be worth noting.

China currently is low on the list of the top countries competing in the Pharma industry. It falls significantly behind its Western competitors, due chiefly to the fact that it has focused on selling drugs that were innovated elsewhere, and lags behind in terms of actual pharma innovation. But, we have seen an influx of Chinese investors into life sciences industries over the past several years. For instance, the entry of Chinese investors into the broader biotech and drug industry landscape also mounted significantly in 2018, rising to $1.4 billion into US-based biotech and drug firms compared to just $125.5 million during the same period the previous year.

Furthermore, the Chinese government has recently shown significant interests in building up their AI industry, and in prioritizing AI in healthcare in particular. In an AI Strategic Plan released in July 2017, they outlined their intentions to catch up in the AI race by 2020, and to make major breakthroughs by 2025 and become a world leader in AI by 2030. But, in order to excel within the BioPharma industry they will need to reformulate their IP regulations, which are currently not tight enough to retain proprietary control over novel pharma innovations that they might develop in the coming years.

There are two additional advantages that China could possibly use in the coming AI for Drug Discovery race. Firstly, they have shown success in generating a massive amount of real-time medical data from their enormous population of citizens, made possibly by their sheer population size, as well as their current flexible privacy laws. Since AI in general (and machine learning and deep learning in particular) feed on data, this could potentially be used to the nation's benefit. Secondly, they have the raw materials needed for the most scarce resource in the industry: namely, a large quantity of Data scientists and AI specialists.

If the Chinese government were to commit substantial resources to the training of additional AI and data scientists, they could potentially grow to surpass their Western competitors over the next 3-5 years. In the West, players in the AI for Drug Discovery race will suffer a severe scarcity of AI specialists in the coming years because the majority of them have been acquired by the IT and Tech industry for other purposes. China has the potential to leapfrog this issue.

Could UK, EU or Asia Government Initiatives be the Key to match with the US in the AI for Drug Discovery Race?

The US has led the AI for Drug Discovery race in terms of both total investments and the number of US-based companies focusing on AI for Drug Discovery. The USA is also home to the largest pharma corporations in the world, putting it in an excellent position to grow its AI for Drug Discovery industry if, as recent trends seem to indicate, the BioPharma industry continues to build up their internal AI for Drug Discovery resources and increase their number of AI for Drug Discovery startup acquisitions.

With that being said, there is also mounting interest in the AI for Drug Discovery sector from the EU, UK and Asia Pacific region as well. While the USA leads the pharma race generally, as we have discussed elsewhere in this and earlier reports, the AI for Drug Discovery sector is poised to become the central factor that will determine who is the winner of the drug discovery race more generally in the years to come.

If the EU, UK or China proves more willing to grow their AI for Drug Discovery industry, especially through something akin to a national development strategy, whereby a significant amount of government funds are earmarked for such a purpose, then it is possible that the US could be overtaken in terms of its current leadership position in the pharmaceutical industry. It all depends on the actions and commitments taken by the US government, as well as by the current US-based leaders of the BioPharma industry, and by US-based IT-corporations.

The Chinese government, for instance, does appear to be committed to prioritizing Artificial Intelligence industry. In an AI Strategic Plan released in July 2017, they outlined their intentions to catch up in the AI race by 2020, make major breakthroughs by 2025 and become the world leader in AI by 2030.

In a parliamentary meeting held around the same time as the report's release, China science and technology minister Wan Gang noted that government finance will lead the way in AI research, including the development of supercomputers, and high performance semiconductor chips, software and the hiring of key talent to lead the field. If they remain true to their commitment, they could succeed in building up the necessary resources in order to dominate the AI for Drug Discovery space.

Could UK, EU or Asia Government Initiatives be the Key to match with the US in the AI for Drug Discovery Race?

The UK has also had a recent increase in governmental support for AI generally, as well as for AI in healthcare in particular. In April 2018, the UK government confirmed its commitment to keep up with other countries in the AI race through a very large government initiative worth £1 billion titled the AI Sector Deal, a deal between government and industry (involving over 50 leading UK tech companies) announced by Business Secretary Greg Clark and Digital Secretary Matt Hancock, which will involve more than £300 million in new private sector investment, as well as 1000 new government-funded AI PhDs.

In a press release on the topic of the initiative, the UK government noted that "The deal will help establish the UK as a research hotspot, with measures to ensure the innovators and tech entrepreneurs of tomorrow are based in the UK, with investment in the high-level post-graduate skills needed to capitalise on technology's huge potential. It includes money for training for 8,000 specialist computer science teachers, 1,000 government-funded AI PhDs by 2025 and a commitment to develop a prestigious global Turing Fellowship programme to attract and retain the best research talent in AI to the UK."

This new initiative builds upon the commitment already made by the UK government in its Industrial Strategy and AI grand challenge, which put AI's use in healthcare at the forefront of their commitment. Coinciding with the recent £1 billion pact between industry and government to put the UK on the forefront of the global AI race, the government also commissioned an independent review to assess the need of NHS staff to be trained in AI in order to equip them with the skills required to keep abreast of the latest developments in healthcare. The review was announced in April 2018 by Jeremy Hunt, Secretary of State for Health and Social Care.

Furthermore, UK Business Secretary Greg Clark recently announced £103m in funding for a new institute that will aim to utilize AI for Drug Discovery. The Rosalind Franklin institute will utilize AI to create new drugs, diagnostics and treatments. Founded as part of the UK's AI and Data Grand Challenge, it will build upon the UK Government's modern Industrial Strategy and aim to keep the UK on the forefront of the pharma and life sciences industry. Remarkably and ambitiously, its stated aim is to "generate new drugs for clinical testing within a few weeks."

Major Trends

Generally speaking, our analysis has revealed the continuation and intensification of several trends identified in our previous reports, AI for Drug Discovery & Advanced R&D Q1 2018 and Q2 2018, as well as the emergence of several new trends:

- The US continues to lead investments in AI for Drug Discovery companies from a total-landscape perspective.

- The UK remains the home of the highest-valuated Drug Discovery company, Benevolent AI, which recently raised an additional $115 million at a $2 billion valuation.

- The industry is seeing an increasing influx of investors from the Asia-Pacific region, and most particularly from China and Singapore. The Chinese IT-corporation Tencent, for instance, led a $155 million round of funding was held by AI in healthcare company iCarbonX. Tencent also recently co-invested in a $15 million round held by AI for Drug Discovery company XtalPi with Google and Sequoia China. Chinese IT-corporation Alibaba has also entered the AI for healthcare space with the launch of what they refer to as "ET Medical Brain", a platform that leverages Alibana's formidable computational resources in order to generate new AI medical applications. In June 2018 prominent Chinese pharma company Wuxi AppTec invested in AI for Drug Discovery company Insilico Medicine alongside Pavilion Capital (a VC firm owned by the Singaporean government), as well as several Western VC firms including BOLD Capital Partners and Juvenescence Limited.

- 2018 has seen increased governmental support for AI in healthcare from both the UK and Chinese government. Large-scale government initiatives could prove to be the key for certain nations to overtake the US in the AI for Drug   Discovery   race.

- The general trend of IT & Tech corporations entering the AI for healthcare space continues to spread, previously applying most particularly to US-based entities, but now including prominent Chinese IT and Tech corporations, including Tencent and Alibaba.

Most Promising Players

Corporations

nVIDIA

gsk GlaxoSmithKline

AstraZeneca

Google

Baidu 百度

AI companies

INSILICO MEDICINE

BenevolentAI

Atomwise
Better medicines faster.

GNS HEALTHCARE

deep genomics

BioPharma and Tech Corporations in the AI for Drug Discovery and Advanced R&D sphere

BioPharma Corporations Onboarding AI for Drug Discovery.
AI in BioPharma R&D: Pharma Companies Started to Close "The Big GAP"

- Biopharma budgets are significantly related to spending on R&D and failures in clinical trials. Meanwhile, the breakthroughs in applying AI for Drug Discovery will have dramatic impact on not just BioPharma companies but all biotech startups and biotech VC funds. All of them will be disrupted by AI for Drug Discovery.
- The major progress in these technologies is coming not from biotech side but from IT and Data Science.
- Due to the lack of AI specialists and promising AI & Drug Discovery startups, only a select few BioPharma players will emerge as the leaders of this trend.
- Meanwhile others, even with substantial budgets and the will to succeed in this area, will fail if they are even one year late to the race because all of the top AI specialists and AI in healthcare startups will have been acquired by then.
- The number of experts in the field of AI for Drug Discovery is insufficient to meet the demand of all big pharma companies, so only those few pharma companies and investors who will partner with the best AI for Drug Discovery companies in time will benefit from these collaborations and increase their capitalization accordingly.
- In the past ninth months a large number of deals and acquisitions have been made between Big Pharma companies and AI startups.
- Those BioPharma companies that will create strong AI for Drug Discovery divisions and that will succeed to acquire the best AI startups will become the leaders of the field as little as 3 to 5 years from now. Consider the acquisition of DeepMind by Google for $0.5B in 2014. Those companies that will invest heavily in their AI for Drug Discovery departments will see their market capitalization skyrocket in coming years.
- Those BioPharma companies that do not accept AI will repeat the mistakes of Kodak, who were once the leader of their industry, but went to bankruptcy because they failed to embrace digital photography as the disruptive trend it was, even despite the fact that the digital camera was invented inside Kodak labs.
- If BioPharma would find the courage to spend 10% of their marketing budget on R&D in AI, they could blow IBM Watson out of the water by learning from their mistakes. We see now that our forecasts in the previous version of the report were true. Big Pharma companies are now actively investing in and collaborating with smaller companies and startups from the AI for Advanced R&D industry.

Pfizer: Involvement with $1.4 billion Government Initiative to Boost the UK's AI Industry (April 2018)

An April 2018 release also indicated that Pfizer was involved in a UK-based initiative that would increase government funding for UK AI initiatives.

The specific context in which Pfizer would be participating, however, remains unclear and undisclosed.

Nonetheless, when coupled with Pfizer's historical and recent partnerships with AI for Drug Discovery companies, and the recent launch of its own in-house AI analytics platform, this could signal that Pfizer is indeed gearing up to join a select few other Big Pharma corporations in committing its own internal resources to the AI for Drug Discovery race.

Q Search

Bloomberg

Technology

U.K. Unveils $1.4 Billion Drive Into Artificial Intelligence

By Jeremy Kahn and Alex Morales

April 25, 2018, 7:00 PM EDT *Updated on April 26, 2018, 1:29 PM EDT*

- ▶ Ministers announce 300 million pounds of new expenditure
- ▶ Sector deal is fourth under May's flagship industrial strategy

Source: https://www.bloomberg.com/news/articles/2018-04-25/u-k-announces-1-4-billion-drive-into-artificial-intelligence

AI in Drug Discovery Survey

AI for Drug Discovery company BenchSci recently conducted a survey among 330 scientists working in the area of drug discovery and drug development, to determine the extent with which their institutions currently use or plan to incorporate AI into their drug discovery efforts. Their results appear to show that:

- The use of AI for Drug Discovery may be on the horizon for more pharma companies than previously expected.
- Lack of education and understanding of AI is one of the foremost barriers for institutional adoption.
- Nearly half of respondents expected their institutions use of AI to stay the same, while 38% expected it to increase, and 16% expected it to increase substantially.

When asked about the specific activities that their companies and institutions utilize AI for, 40% said that they use AI for target identification and validation, 34% for safety tests, 29% for compound discovery, 25% for lead optimization, and 21% for preclinical studies. The survey also analyzed the perceived vs. real benefits of applying AI to drug discovery, finding the following use-cases had differences in the real vs. perceived level of benefits:

- increasing speed of drug discovery: 44% real benefits, 61% perceived benefits;
- increasing research comprehensiveness: 32% real benefits, 46% perceived benefits;
- increasing opportunities for existing compounds: 25% real benefits, 45% perceived benefits;
- increasing novelty of targets and compounds: 28% real benefits, 45% perceived benefits;
- decreasing cost of drug discovery: 22% real benefits, 41% perceived benefits;
- decreasing experimental failure: 18% real benefits, 29% perceived benefits.

When asked about the biggest barriers preventing the broader adoption of AI for Drug Discovery in the pharma industry, 62% selected lack of knowledge and expertise, 43% selected prohibitive cost,, 42% selected lack of knowledge regarding available companies and tools, and 28% selected lack of relevant case studies at their particular organization.

Source: https://blog.benchsci.com/6-things-we-learned-about-artificial-intelligence-in-drug-discovery-from-330-scientists

GSK: Partnership with Insilico Medicine

GSK also announced a August 2017 partnership with Insilico Medicine, starting with GSK evaluating Insilico's proprietary technology for identifying novel biological targets and pathways of interest. In an associated press release John Baldoni, Senior Vice President, Platform Technology Sciences at GSK, stated: "We are delighted to be working with the Insilico team, as they have exhibited curiosity, agility and AI expertise that we value. GSK recently established a drug discovery unit to explore how this rapidly developing field might drive drug discovery at a higher velocity, with greater precision and at a reduced cost. The collaboration with Insilico Medicine represents one of several approaches we are exploring to take advantage of emerging technology that might make us more effective and efficient, always keeping in mind the patients who need new medicines."
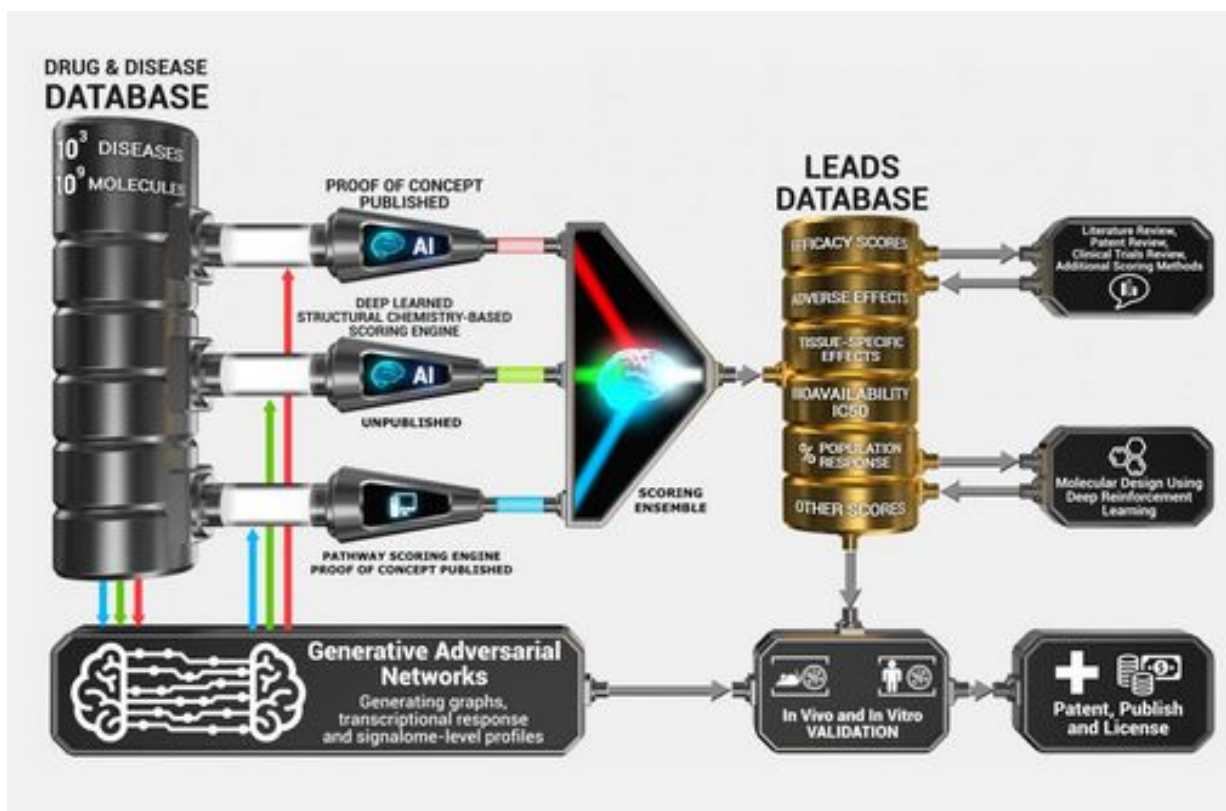
Source: https://www.eurekalert.org/pub_releases/2017-08/imi-iec081417.php

GSK: Partnership with Cloud Pharmaceuticals

And in May 2018, GSK announced a partnership with Cloud Pharmaceuticals to use AI to design novel small-molecule agents for GSK-specified targets.

In an associated press release, Ed Addison, CEO of CLoud Pharmaceuticals, stated: "Application of Cloud Pharmaceuticals technology has been proven to dramatically shorten the time from target validation to lead molecule. We believe this agreement validates the strength of this process and reinforces the value we can offer accelerate the discovery of novel, high-quality drug candidates." In the same release, Cloud Pharmaceuticals COO, Don Van Dyke, added: "It is estimated that the traditional discovery process to arrive at a clinical candidate molecule takes greater than 5 years. Cloud has consistently been able to reduce that to a matter of a few months."

In addition to both its in-house AI for Drug Discovery unit, and three partnerships with leading AI for Drug Discovery companies, GSK is also a part ot the Accelerating Therapeutics for Opportunities in Medicine (ATOM) Consortium, which has the ambitious aim to leverage AI for Drug Discovery so as to reduce the timeline from drug target identification to a clinic-ready drug to less than a year. Their involvement with ATOM involves providing ATOM with chemical and *in vitro* biological data for more than 2 million compounds that GSK has screened.

Pfizer: Partnership with XtalPi for Machine Learning and Quantum Mechanics for Drug Discovery (May 2018)

In May 2018, Pfizer announced a partnership with XtalPi to develop an "artificial intelligence-powered platform to model small-molecule drugs as part of its discovery and development efforts."

The partnership combines quantum mechanics and machine learning to predict pharmaceutical properties of candidate compounds. The two companies are currently collaborating on crystal structure prediction and screening to optimize the process of drug design and solid-form selection.

In a press release associated with the announcement Shuhao Wen, XtalPi's co-founder and chairman of the board, stated:

"The collaboration allows us to apply our expertise in molecular modeling, AI, and cloud computing towards improving existing computational methods while exploring new algorithms to address a wide range of drug design challenges.

Source:
https://www.prnewswire.com/news-releases/xtalpi-inc-announces-strategic-research-collaboration-with-pfizer-inc-to-develop-artificial-intelligence-powered-molecular-modeling-technology-for-drug-discovery-300644351.html

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Pfizer: Launch of In-House AI Analytics Platform (May 2018)

Pfizer also appears to be developing its own AI analytics platform, which may signal that it is gearing up to, like a select few other Pharma corporations, begin commiting internal resources and in-house staff to the AI for Drug Discovery race.

A recent Wall Street Journal article, which appeared in May of 2018, stated: "Pfizer Inc.'s recently-built analytics platform is helping employees from different divisions within the company collaborate in an effort to identify patients with rare diseases that might previously have gone undiagnosed, company executives said. With the help of machine-learning algorithms, the analytics platform is now yielding new insights that were previously difficult to identify in a short amount of time because there too many disparate datasets to sift through. The cloud-based Virtual Analytics Workbench tool officially launched in 2017 and more than 350 employees are using it including mainly data analysts and research and development teams. The goal is to scale it more broadly across different departments."

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Seeking Insights into Rare Diseases, Pfizer Scales AI Analytics Platform

Data science shouldn't be confined to mathematicians, says CIO Jeff Keisling

Source: https://blogs.wsj.com/cio/2018/05/09/seeking-insights-into-rare-diseases-pfizer-scales-ai-analytics-platform/

Bristol-Myers Squibb: Partnership with Sirenas (February 2018)

2018 also saw pharma corporation Bristol-Myers Squibb ink a deal with Sirenas, a machine learning company utilizing ML to discovery microbiome-based therapeutics.

The deal involves utilizing Sirena's proprietary data mining technology (ATLANTIS) to identify drug candidates from among Sirena's microbiome-based chemical library.

In a press release associated with the announcement, Sirenas CEO Jake Beverage stated:

"We believe science-focused BioPharma companies can benefit from our innovative approaches to access breakthrough chemistry in delivering drug candidates for difficult biological targets. We look forward to a fruitful collaboration with Bristol-Myers Squibb, one of the finest drug discovery teams in the world, to identify potential new therapies to treat the world's highest unmet medical needs."

Phil Baran, Co-Founder of Sirenas added: "Sirenas has built a remarkably effective platform that combines powerful computational approaches, deep natural product expertise, and state of the art synthesis to rapidly deliver new drug candidates. We are committed to using computational approaches like ATLANTIS™ with our partners to uncover novel therapies from the profound chemistry hidden in the diversity of nature."

Source: https://www.prnewswire.com/news-releases/sirenas-enters-into-multi-target-collaboration-with-bristol-myers-squibb-300596468.html

Amgen: Partnership with Owkin & Involvement in MIT's Machine Learning for Pharmaceutical Discovery and Synthesis Consortium (May 2018)

Amgen was revealed in May 2018 to be a member of MIT's Machine Learning for Pharmaceutical Discovery and Synthesis Consortium.

As with many of the companies listed as members of the consortium, little is known about the specifics of their involvement, but it does signal that they have a vested interest in machine learning for drug discovery.

A later report the same month also announced a partnership between Amgen and medical machine learning company Owkin.

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MedTech

Amgen-partnered Owkin bags $11M to scale AI platform

by Nick Paul Taylor | Jan 17, 2018 7:45am

AMGEN

MIT MLPDS
Machine Learning for Pharmaceutical Discovery and Synthesis Consortium

OWKIN
Artificial Intelligence for Predictive Medicine

Source: https://www.fiercebiotech.com/medtech/amgen-partnered-owkin-bags-11m-to-scale-ai-platform

Awards & Grants

- **Johnson & Johnson Innovation** and **Janssen Research & Development** launched the Artificial Intelligence for Drug Discovery QuickFire Challenge. Johnson & Johnson Innovation will award up to $100,000 in grants, one year of JLABS residency & mentorship to the individuals or teams who submit the best ideas, technologies, or solutions that are using artificial intelligence to advance healthcare.

- **Novartis** provides funding opportunities for innovative, high-risk projects that have the potential to open up novel research directions beyond incremental innovation and discovery. In this year's call, proposals in the field of AI will be accepted, namely: AI in Drug Discovery, AI in clinical development and medical practice, AI and the patient. Grants are for a period of 18 months. A maximum of 15 projects will be funded, depending on the quality of the proposals as judged by the review committee.

- **Merck**, a leading science and technology company, announced in 2017 recipients of €1 Million Grant at the fifth annual Grant for Multiple Sclerosis Innovation (GMSI) during the 7th Joint ECTRIMS-ACTRIMS Meeting in Paris, France.

Acquisitions

- **Johnson & Johnson** Medical Devices Companies, through French affiliate Apsis S.A.S., announced in 2018 the acquisition of Orthotaxy, a privately-held developer of software-enabled surgery technologies, including a differentiated robotic-assisted surgery solution. This proprietary technology is currently in early-stage development for total and partial knee replacement, and the Johnson & Johnson Medical Devices Companies plan to broaden its application for a range of orthopaedic surgery procedures. Financial terms of the transaction were not disclosed.

- **Roche** in 2018 acquired Flatiron Health, developer of a cancer electronic health record software that collects and aggregates data from cancer patients, for $2.1B.

- **Roche** acquired in 2017 Viewics Inc., a laboratory business analytics platform. Under the terms of the agreement, Roche is acquiring all shares of the company. Financial details of the acquisition were not disclosed.

- **Astrazeneca** acquired in AlphaCore Pharma, an Ann Arbor-based biotech company working on a drug to treat atherosclerosis in 2013 through MedImmune (its the biologics division). The terms of the deal were not disclosed.

- **Astellas Pharma**, a Japanese pharmaceutical and biotechnology company, is acquiring in 2018 Seattle biotech Universal Cells. Astellas will pay up to $102.5 million for Universal Cells in up-front and milestone payments, assuming the company hits certain benchmarks in developing its universal stem cell technology.

- **QIAGEN** announced in 2018 that they entered into an agreement to acquire STAT-Dx, a privately-held company developing the next generation of multiplex diagnostics for one-step, fully integrated molecular analysis of common syndromes using a novel system based on real-time PCR technology and proven QIAGEN chemistries.

Collaborations

- **Genentech**, a member of the Roche Group, in the summer of 2017 announced their own collaboration with Cambridge, MA-based GNS Healthcare. GNS Healthcare's mission statement is to use the latest innovations in machine learning to turn biomedical data into solutions and treatments on cancer therapy.

- **Johnson & Johnson** and IBM announced in 2015 plans to collaborate around a new generation of intelligent virtual coaching solutions and applications designed to enhance the patient experience and deliver improved health   outcomes.

- **Janssen Research & Development**, LLC, another organization in the Johnson & Johnson family of companies, has been working with WinterLight Labs and their speech-based AI platform to analyze Janssen's growing collection   of   speech   data   acquired   from   ongoing   clinical   trials.

- **Johnson & Johnson's** medical device company, **Ethicon**, is collaborating with Google on an initiative aiming to integrate   big   data   analytics   capabilities   into   a   digital   surgery   platform.

- **Pfizer** in late 2016 announced a collaboration that will utilize IBM Watson for Drug Discovery. Pfizer is using IBM's AI technology for its immuno-oncology research, a strategy of using the body's immune system to help fight cancer.

- **GlaxoSmithKline** has invested $43 million into Scottish artificial intelligence (AI) company Exscientia, which aims to use deep learning to develop new drugs. It also partnered with Insilico Medicine "after completing over 18 months of pilots". The terms were not disclosed.

- **AstraZeneca** teamed up in 2017 with US biology and technology company Berg to search for new drugs to treat Parkinson's Disease and other neurological disorders using artificial intelligence.

- **Sanofi** has signed a 250 million euro ($273 million) research collaboration and licence option agreement in metabolic disease with Exscientia in 2017.

Sources: https://www.techemergence.com/machine-learning-drug-discovery-applications-pfizer-roche-gsk/

IT & Tech Corporations Involvement in BioPharma

- In April 2017 **Amazon Web Services** and Merck announced a developer competition that plans to harness artificial intelligence for diabetics. Dubbed the Alexa Diabetes Challenge, and powered by Luminary Labs, the contest aims to incentivize startups and individual developers to create apps that harness Amazon's Alexa, particularly for patients recently diagnosed with Type 2 diabetes.

- In 2014 **Google** bought DeepMind, a British AI startup for around $600 million. DeepMind's work is based on a solid grounding in neuroscience. Another DeepMind project involves a collaboration with London's Moorfields Eye Hospital. DeepMind has been given access to one million images from historical eye scans, along with associated patient data.

- In 2017 **IBM** developed machine learning models to analyze correlations between diseases and side effects commonly caused by the medications used to treat them. IBM also built an association engine to identify significant associations between predicted therapeutic indications and side effects, and a visual analytics system to support the interactive exploration of these associations.

- In September 2016 **Microsoft** announced a quartet of new initiatives focusing on using artificial intelligence in health care. One such initiative from Microsoft is to apply AI to radiology, using machine vision tools to analyze CT scans of tumors. Microsoft's Project Hanover is using ML technologies in multiple initiatives, including a collaboration with the Knight Cancer Institute to develop AI technology for cancer precision treatment, with a current focus on developing an approach to personalize drug combinations for Acute Myeloid Leukemia (AML).

- In March 2017 MedyMatch Technology, Ltd. and Samsung NeuroLogica Corporation, the healthcare subsidiary of **Samsung Electronics** Co., Ltd. announced a collaboration to integrate artificial intelligence clinical decision support applications with Samsung NeuroLogica's medical imaging hardware in the acute care marketplace. This collaboration aims to create support tools which provide a second read capability to help caregivers quickly and accurately assess patients in prehospital environments.

IT & Tech Corporations Involvement in BioPharma

- In April 2018 **NVIDIA** and **Canon Medical Systems** partnered to accelerate Deep Learning in healthcare. NVIDIA and Canon Medical Systems expect to make a significant contribution to promoting the use of data-intensive deep learning techniques in medical and related research, as well as to driving the uptake of AI in the healthcare sector. Canon Medical Systems will use NVIDIA DGX systems to process large volumes of medical data generated by Abierto VNA, the proprietary, in-house, medical data management system it launched in January.

- In July 2017 **Alibaba** announced that it is charting a way to push the application of artificial intelligence (AI) in diagnostics and healthcare to make medical treatment more accessible, timely, and affordable. Alibaba Cloud is actively working on AI-powered solutions to tackle health care problems in China and globally. In March 2017 Alibaba Cloud launched ET Medical Brain, a suite of AI solutions designed to ease the workload of medical personnel. Alibaba Health also unveiled its first AI service for medical diagnostics called 'Doctor You,' which can use imaging in the early diagnosis of cancer. Other projects include the partnership between Alibaba Cloud and Wuhan Landing Medical High-tech Co. on a system that leverages AI and visual computation technologies to detect early stage cervical cancer by using cell cytology. Alibaba Cloud is also working on a project to train machines to detect lung cancer using high-resolution CT scans.

- In February 2017 **Baidu** pushed further into the AI market with the acquisition of Raven Tech, a startup behind the 'Flow' digital assistant. Baidu is looking to use artificial intelligence algorithms for drug discovery technology so it can significantly shorten the duration of drug development.

- In February 2018 **Medopad** teamed up with Chinese tech giant **Tencent** to develop artificial intelligence-enabled clinical decision support software and medical chatbots. The partnership will combine Tencent's data assets and AI technology with Medopad's mobile apps. According to Forbes the collaboration gives Medopad access to the nearly 1 billion users of Tencent's WeChat messaging service.

- In March 2018 **Mitsubishi Tanabe Pharma** and **Hitachi** announced a partnership to use AI to more efficiently develop drugs. The aim of the collaboration is to use Hitachi's advanced digital technology, including AI, to shorten the development period for news drugs and reduce development costs, while reducing the possibility of expensive trial failures.

IT & Tech Corporations Entering the AI for Drug Discovery Space

Tech Corporations are more flexible with new technologies. Moreover, their revenue depends on cutting edge technologies, which they are using and implementing in their products. AI and machine learning technologies became a part of their technologies. These technologies are used in advanced R&D and drug discovery. In our opinion using advanced technologies by Tech Corporations give them a huge advantage over BioPharma companies on drug discovery.

The interest and application of AI is relatively faster in healthcare and life sciences, and many tech corporations like Google, Apple, IBM, Qualcomm, AT&T, GE, Amazon, and Microsoft have shown interest by investing in, acquiring and partnering with life sciences companies in this space. In the life sciences sector, an enormous amount of data has been generated and the big data is getting bigger and bigger by the minute from omics, biomarker research, drug discovery, clinical trials, smart pills and devices, manufacturing supply chain sensors, patient data and from commercial functions.

AI & Machine Learning are horizontal technologies that can be used in various industries, and drug discovery is not an exception. Tech Corporations are more flexible than BioPharma companies, and have much more capabilities to implement new technologies in advanced R&D and drug discovery sectors. The future of the BioTech sector may lie on their shoulders.

Additionally, companies like Facebook, Google and Amazon have other advantages; these companies have access to billions of customers worldwide, who can be monitored and researched. Based on this information and developed biomarkers, the industry of drug discovery will make a step forward and would be more precise than ever.

In this section 15 Tech Corporations and their involvement in advanced R&D and drug discovery were analysed. It's important to mention that every and each company has its own vision and the level of involvement differs from one company to another, however, overall, IT Corporations are interested in advanced R&D and drug discovery sector.

Will Tomorrow's BioPharma Corporations Be Today's IT & Tech Corporations?

While we can expect to see traditional BioPharma and IT & Tech Corporations battle it out for supremacy in the AI for Drug Discovery race over the next several years, they do not necessarily start from level playing fields. There are several factors that put IT & Tech corporations at an implicit advantage over BioPharma corporations.

Firstly, IT & Tech corporations work from a solid foundation of AI and IT specialists, IP, resources and expertise, which is the very area that is the most scarce in the race, and the very factor that constitutes the chief bottleneck in the ongoing progress of the AI for Drug Discovery industry.

There are only so many AI specialists and resources to go around, and IT & Tech corporations already have the large majority of them.

Meanwhile, there is no such scarcity among pharma and life sciences staff.

It will be much harder for BioPharma corporations to build up their internal AI and IT staff and resources than it will be for IT & Tech corporations to build up their internal pharma and life sciences departments.

It is not impossible for BioPharma to succeed in launching internal AI for Drug Discovery units, as we have seen with several pharma corporations including GSK, Pfizer and Merck, but they will need to pay top dollar in order to attract AI specialists away from their current positions at AI and Tech corporations.

Secondly, AI, IT and Tech corporations are used to change, and to reformulating their business models and internal operations from the ground up in order to keep pace with the increasing rate of change in their industry.

Will Tomorrow's BioPharma Corporations Be Today's IT & Tech Corporations?

They operate within a space that changes more rapidly than any other industry, and in order to have become an AI, IT or Tech corporation in the first place, they need to have been willing and able to absorb and embrace change in a fundamental and systemic manner.

This is not so with traditional BioPharma, which has operated with the same business model in mind for several decades.

The BioPharma industry is often thought of as an elitist and stagnant industry which is very resistant to change.

This is a state of affairs recognized both within and outside of the Pharma industry, with Job Landoni, Senior VP of Platform Science and Technology at GSK, and one of the most outspoken pharma executives on the disruptive impact of AI for Drug Discovery, admitting that "pharma is using a model that was becoming increasingly dated."

Another factor putting AI, It and Tech corporations at an advantage is the comparatively larger market cap of their industry, and the larger revenues they generate.

This means that they have more resources to play with, and can offer more monetary incentives to keep their AI specialists in place.

However, while the AI, IT and Tech corporations begin the race from a more advantageous starting line, their success is not set in stone.

If the BioPharma industry were to show enough will and commitment to embrace change, and allocate enough funding and resources to the acquisition of AI specialists and AI for Drug Discovery startups, it is not impossible for them to win the race.

Will Tomorrow's BioPharma Corporations Be Today's IT & Tech Corporations?

Furthermore, when it comes to will and commitment, they may even be at an advantage in comparison to AI, IT and Tech corporations, in the sense that they have more to lose.

For AI, IT and Tech corporations, entering into healthcare and drug discovery will be an additional revenue stream, auxiliary to their main focus.

Another factor to consider is the fact that the combined capitalization of the 15 BioPharma corporations that we have profiled in this report has 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 and the gap is increasing. This can be considered as an 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.

For BioPharma corporations, to lose the race is to lose everything, and amounts to either keeping or losing their main source of revenue. Whether this proves enough to overcome the stangantion and resistance to change typical of BioPharma will remain to be seen in the years to come.

Pharma Increases its Commitment to Adoption AI for Drug Discovery

In 2013, US start-up Berg was asked by the Department of Defense to help improve the detection of prostate cancer, a disease common among pilots. Less than five years later, an artificial intelligence-driven tool has been tested on more than 1,000 patients with promising results. Excitement about AI, machine learning and big data have prompted a boom in health-tech start-ups in a market traditionally dominated by big pharma.

Despite debate over the extent to which AI will revolutionise medical science, billions are being bet on something revolutionary emerging to drive the next big leaps in drug development This year has seen a jump in investment from big pharma and a range of joint ventures with health tech groups. In 2018, at least 15 companies have integrated AI into their drug discovery processes, according to Deep Knowledge Analytics, an analysis company.

"We've seen huge interest from many of the major pharma companies" in the past 18 months, says Andrew Hopkins, chief executive of Exscientia, an AI-driven drug discovery company working with GlaxoSmithKline.

Other partnerships include AstraZeneca's and Sanofi's projects with Berg, and Merck's work with Numerate, another drug design company. In-house developments include Pfizer using AI to mine patient data — stored anonymously in electronic medical records — for signs of a rare form of heart failure. Novartis hopes a drug part-developed with AI will be registered within the next 36 months.

 "We see ourselves shifting from the mindset of a traditional pharma company to [one] more inherently agile, typical of a tech company," says Badhri Srinivasan, Novartis's head of global development operations. About $5bn was invested in AI companies in 2016, according to consultancy IP Pragmatics, with healthcare one of the fastest growing sectors. By 2021, the value of the segment is expected to reach $6.6bn, with particular growth in China.

In the UK, five new government-funded technology centres will open in 2019, using AI to accelerate disease diagnosis with the aim of making the National Health Service more efficient. In early-stage drug discovery, start-ups such as BenevolentAI use algorithms to comb through enormous quantities of data for patterns humans alone might not find and generate new hypotheses to medical problems.

Source: https://www.ft.com/content/e450a688-ddfb-11e8-b173-ebef6ab1374a

Pharma Increases its Commitment to Adoption AI for Drug Discovery

With hypotheses come potential solutions: companies such as Insilico Medicine are using AI to design treatments not yet found in nature or chemical libraries; others use AI to simulate clinical trials, before selecting real-life candidates. The hunt for efficiencies is particularly important in an industry suffering from miserable statistics.

It takes an average of 12 years and costs of $2bn to bring a drug to market, and most clinical trials are unsuccessful. According to a report from Deloitte, projected returns on drug discovery R&D investment fell to their lowest level in eight years in 2017, while spending increased.

Inefficiencies and inaccuracies mean "all we're doing is magnifying the trial and error process," says Niven Narain, Berg's chief executive. High attrition rates are one of the reasons for expensive drug prices, as pharma companies look to offset the cost of failed projects against the few successful ones.

Improving productivity "hopefully will have downstream effects", says Julie Schiffman, vice-president of business analytics at Pfizer. Others are uncertain. "AI won't necessarily drive the cost of drugs down," says Eric Sandor, of consultancy company Genpact.

"What it will probably do is identify drugs that can be specifically formulated for small groups of patients . . . that are more specialised, which could therefore be more expensive." AI is not a silver bullet, says Simon Smith, chief growth officer at BenchSci, an AI-driven biomedical search engine. "The risk inherent in developing a drug isn't going to go away just because you used a machine to do it," he says.

Despite the recent hype, there is a lack of AI specialists and "promising" drug discovery start-ups, according to Deep Knowledge Analytics. Moving beyond the "low-hanging fruit" to discoveries that make drug development drastically faster or cheaper will be "much harder" than achievements to date, says Mr Smith. It may be that current algorithms are focusing on the wrong things, he says. "If the processes themselves aren't going to make the next big breakthrough, it doesn't matter if we expedite them by 100 times."

Source: https://www.ft.com/content/e450a688-ddfb-11e8-b173-ebef6ab1374a

Trends

Thus, we are seeing a vast increase in the number of pharma corporations who are entering the AI for Drug Discovery space, either through the development of in-house AI departments and resources (as in the case of GSK most prominently, as well as Pfizer), or through M&As.

Meanwhile, it is very possible that more activity is going on in this sphere among the boardrooms of large pharma companies without having publicly-available indication of such a situation. Pharma companies do not typically announce what new activities and plans the have on the horizon prior to the official launch of a new in-house unit or project, for example.

In a recent Forbes article Simon Smith, Chief Growth Officer at BenchSci, noted that "It's possible we'll see it in 2018. Most companies plan to expand the use of AI for Drug Discovery this year. Fifty-nine percent of scientists told us their organization will do so, and 94% told Pistoia they'll increase use of machine learning within two years." If this proves true, then it is likely that a larger number of pharma companies will be on-boarding AI into their operations over the next several years than we have concrete publicly-available indication of through the announcement of new projects, departments, investments and M&As.

The pharma industry is a typically-bureaucratic industry resistant to change, and one that is somewhat more conservative than other industries, and less willing to try what might seem like "untested" and "non-validated" technologies given the tremendous 99% failure rate that they experience even with methods that have been tried and true for decades, and which brought the worlds biggest blockbuster drugs to market.

Nonetheless, they seem to be taking note of the paradigm shift already visible on the horizon. They face an up-hill battle against the advantages held by IT and Tech corporations venturing into the AI for Drug Discovery space, what with their possession of the scarcity of resources in the industry - namely, AI specialists and IP - but with enough will and commitment, they could emerge to win the race in the years to come, and retain their positions as the leaders of the pharma industry.

Industry Developments Q3 2018

Industry Developments Q3 2018

- **August 2018** - China's largest online healthcare platform, Ping An Good Doctor, has announced that it will launch 300,000 AI-assisted medical consultation booths across southeast Asia.

- **September 2018** - US consortium Alliance for Artificial Intelligence in Healthcare (AAIH) (a consortium founded to "educate and advocate for policies and regulations to promote rapid integration and utilization of AI in healthcare") meet at the Basel Life Congress to finalize their plans for the first 12 months of operation. Founding members of the consortium include Insilico Medicine, GE Healthcare, Benevolent AI, OWKIN, NuMedii, Numerate, Recursion, Cyclica, Envisagenics, BlackThorn Therapeutics, University of Pittsburgh and the Buck Institute for Research on Aging.

- **October 2018 -** Chinese AI and blockchain for drug development company Deep Intelligent Pharma (DIP) raises $15 million Series B funding from Sequoia Capital China, which will be used for "research and development of AI-powered drug development technology." This deal highlights the increasing aggressiveness of Chinese startups entering the AI for drug development sphere, a trend highlighted in our Q2 2018 report, which only continues to grow as we approach 2019.

- **October 2018** - Chinese company XtalPi raises an additional $46 million in Series B add-on led by China Life Healthcare Fund and with SIG and Yael Capital as co-investors, on top of its original $15 million Series B round led by Sequoia China, Google and Tencent that closed in January 2018, bringing XtalPi's total funding to date to over $66 million.

- **October 2018** - Innovate UK invests £1 million in a project led by AI company Intelligens, software company Optibrium and drug discovery company Medicines Discovery Catapult to apply deep learning to drug design and testing and to create "a next generation platform that will better predict the absorption, distribution, metabolism, excretion and toxicity (ADMET) of new drug candidates."

Industry Developments Q3 2018

- **October 2018** - Pfizer announces at the AI Applications Summit for BioPhama conference that it now has over 150 separate AI projects underway, though few of them are believed to be at the core of AI for drug discovery.

- **November 2018** - The UK announces that five new AI medical clinics will open across the UK in 2019 via £50 million in funding through the Department for Business, Energy and Industrial Strategy. These AI clinics will use software to digitise scans and biopsies, and use AI-enabled tools to perform early disease diagnostics.

- **November 2018** - German pharma company Bayer has announced that it will use AI to accelerate patient safety data analysis to detect drug-related side effects through its pharmacovigilance systems.

- **November 2018 -** UK company Exscientia acquires UK start-up Kinetic Discovery to enable a "full stack" of AI driven drug discovery, adding Kinetic's expertise in specialist protein engineering, biophysical screening and structural biology to their existing assets.

- **November 2018** - UK company Escientia expands its presence at Oxford University by establishing a lab at the new Schrödinger Building on The Oxford Science Park, uniting its computer scientists, drug specialists and biologists under one facility to accelerate its platform and portfolio development activities, and to expand its recruitment activities at Oxford University

- **November 2018** - Korean pharmaceutical company Daewoong Pharmaceutical makes a public commitment to adopt AI for drug discovery in partnership with Ulsan National Institute of Science and Technology (UNIST), signalling that South Korea is beginning to enter the AI for DD market alongside other countries in the Asia-Pacific Region like China and Singapore.

XtalPi Raises Additional $46 million in Series B Add On (October 2018)

Chinese AI drug discovery startup XtalPi has raised another $46 million this year, in an extension of its venture capital round, to finance expansion of its computerized pharmaceutical research platform.

The new investment was led by China Life Healthcare Fund, with participation from SIG and Yael Capital, and adds to the original $15 million series B round that closed in January. That round, which included support from Sequoia China, Google and Tencent, brings XtalPi's total fundraising to over $66 million.

XtalPi was launched with the goal of integrating quantum physics and AI to create drug discovery and development applications that predict the properties of small molecules, and help researchers accelerate and de-risk new projects.

"For the next step, we want to open our base solution platform to support other developers of drug research and development algorithms," Shuhao Wen, XtalPi's co-founder and chairman, said in a statement.

"Through this, we will help global pharmaceutical companies connect with a wide range of the latest AI research tools in an easily accessible way, and thereby further improve the efficiency of drug discovery and development," he added. Founded in 2014 by a group of Massachusetts Institute of Technology physicists, the company has since grown to three locations, in Cambridge, Massachusetts, Beijing and Shenzhen, China.

The new financing will support XtalPi's AI applications in drug R&D that expand the searchable chemical space for discovery work, as well as optimize later stages of development. It also intends to upgrade the cloud-computing power and data security of its Intelligent Digital Drug Discovery and Development platform, known as ID4, to offer customized solutions to pharmaceutical companies.

In May, Pfizer announced an expansion of its collaboration with XtalPi to drug design and solid form selection; previously the two companies worked on crystal structure prediction and screening. As part of project, a portion of the molecular mechanics parameters generated using public-domain compounds will be made available to the public, XtalPi said at the time.

Sources: https://www.fiercebiotech.com/medtech/ai-drug-miner-xtalpi-raises-another-46m-series-b-add;

Exscientia acquires Kinetic Discovery (November 2018)

Exscientia announces that is has acquired the biophysics specialists, Kinetic Discovery, a private UK company. The acquisition builds up Exscientia's capabilities for tackling novel drug targets to create first-in-class drug candidates by seeding its algorithms with data generated through the use of fragment screening and structural biology.

The addition of Kinetic's complementary expertise enables Exscientia to create a 'full stack' AI-driven drug discovery company to go rapidly from gene to clinical candidate for any druggable target of choice. The acquisition of Kinetic is part of Exscientia's growth strategy to develop a proprietary drug pipeline and to enhance its support of existing and future partnerships.

Kinetic Discovery brings specialist protein engineering, biophysical screening and structural biology expertise that is highly synergistic to Exscientia's current drug design, pharmacology and computational science platform. The integration of these capabilities will scale Exscientia's ability to discover new drug molecules for its ambitious portfolio plans.

Dr Andy Bell, Chief Research Officer of Exscientia, said: "Our aim is to revolutionise the drug discovery process through the application of a systematic, AI-driven approach. We see huge synergy in combining Kinetic Discovery's biophysics capabilities with Exscientia's AI drug design platform. We have been working extensively with Kinetic for over two years and our scientists have been incredibly impressed with their ability to rapidly generate high-quality data on a wide range of projects. The evidence we are seeing is that our offering has the potential to radically improve the current drug discovery paradigm."

Kinetic Discovery's operations and employees will relocate from their current facilities at Harwell, Oxfordshire to Exscientia's new state-of-the-art facilities in The Schrödinger Building on the Oxford Science Park. Kinetic's founder and Chief Scientific Officer, Dr Iva Navratilova, will join Exscientia as its Chief Biophysicist. The merging of Kinetic will increase Exscientia's head count to 35 employees, representing 16 different nationalities. Dr Navratilova added: "We are very excited to join forces with Exscientia and become an integral part of its unique platform. Over the last couple of years working with Exscientia's outstanding team, we have seen the value of an integrated service to the drug discovery process, and we look forward to building on this to create better drugs faster and more cost-effectively."

Sources: https://www.prnewswire.com/news-releases/exscientia-builds-full-stack-ai-driven-drug-discovery-capabilities-through-acquisition-of-kinetic-discovery-870079484.html

Korean Daewoong Pharmaceutical Adopts AI to Boost Drug Discovery (November 2018)

Daewoong Pharmaceutical said it would adopt artificial intelligence (AI) to boost drug discoveries. The drugmaker and Ulsan National Institute of Science and Technology (UNIST) signed an agreement to apply big data and AI technologies to the existing system of the new drug development at the university's main building in Ulsan, Friday.

Under the agreement, Daewoong will engage in data processing for new drug development and experimental analysis of new drug candidates, and UNIST will develop data analysis algorithms and AI technologies.

Pharmaceutical firms have searched for drug candidates one by one. Now, however, they can hunt for drug candidates using AI, which will learn itself from existing data. To find candidates using AI, the "Data Science" technology was essential, the company said. The technology helps the company extract knowledge and insight from diverse and vast amounts of data.

Experts in the area are working at the UNIST's School of Management Engineering, which was established in March 2016. Out of the eight faculty members, seven are experts in data science. The school specializes in research and education of data science. Lee Jung-hye, a professor at the UNIST's School of Management Engineering, said multinational pharmaceutical firms were increasingly using big data and AI to discover a drug candidate or verify therapeutic efficacy. "AI that learns various kinds of data including medicine, drugs, and genomes will drastically reduce the time for new drug development," she said.

UNIST President Jung Moo-young said, "The biomedical industry is one of the fastest growing industries in the Fourth Industrial Revolution era." He went on to say, "Working with Daewoong, which has various experiences in drug development and know-how, will lead to influential research and creation of new industries."

Daewoong Pharmaceutical CEO Jeon Seung-ho said the joint research with UNIST was part of the company's healthcare business aimed at the public interest. "Developing a platform technology using big data will help Daewoong build new pipelines," Jeon added.

Source: http://www.koreabiomed.com/news/articleView.html?idxno=4572

Chinese AI for Drug Discovery Company Secures $15m in Funding (October 2018)

Deep Intelligent Pharma (DIP), a Chinese startup that offers artificial intelligence (AI) and blockchain technology for drug development, has raised US$15 million in Series B funding from Sequoia Capital China, according to reports.

Leveraging the AI technology, Beijing-based DIP provides new drug research and development services for pharmaceutical companies, offering services to help its clients accelerate drug discovery and development.

Its end-to-end, AI-driven platform enables pharmaceutical companies to move compounds from the lab to the marketing stage with great quality, according to information posted on the firm's website.

One of its main products is "Medical Translations," a multi-language medical machine translation engine equipped with Natural Language Processing (NLP) technology. It also offers the medical content generation and publication service, "A.I.M medical", which helps to create multilingual educational materials and publications.

DIP was founded in 2017 by Li Xing, who has 11 years of experience in new drug development, including with pharmaceutical companies Pfizer, Sanofi, and Johnson & Johnson.

In an interview, Li told Chinese tech media site 36Kr that the fresh capital will be mainly used for research and development of AI-powered drug development technology.

Li said the company currently has over 50 corporate clients, including multinational pharmaceutical companies and top domestic pharmaceutical firms. It runs with a team of about 100, with AI talents and new drug R&D professionals each accounting for half.

According to Crunchbase data, DIP raised US$6.6 million in its Series A funding round from Chinese venture capital Zhen Fund, which also participated in an undisclosed Seed round in the company in 2017.

Source:
ttp://www.ejinsight.com/20181010-china-ai-drug-startup-secures-us15-mln-new-funding-from-sequoia/?fbclid=IwAR3PidnmirTt9So1H9XM4xsMZaMY9AAbmBAj7vR-s-ail8i5v6vcBIOffpg

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Berkeley Lights Raises $95m in New Financing Round (October 2018)

Berkeley Lights, Inc. (BLI), a leader in digital cell biology, announces the completion of a $95 million financing led by Nikon and backed by existing investors Sequoia Capital, Walden-Riverwood Ventures, Black Diamond Ventures, and Paxion Capital; and joined by new investors Cota Capital, KTB Network, Atinum Investment, Shangbay Capital, AJS BioTree Healthcare Fund, and Varian. BLI has developed a unique nanoscale technology that accelerates drug discovery and development processes through the combination of bioscience, technology, and information. Funds from the newest investment will be used to expedite solutions for cell therapy development and manufacturing, including CAR T and endogenous T-cells, as well as increase research and development and expansion of commercial activities.

"This investment from new and past investors is a testament to the significant strides that BLI has already made in transforming the future of drug discovery and development with our digital cell biology platform. In the past 12 months, we have more than doubled the adoption rate of our Beacon platform; and we've only just begun," said Eric Hobbs, Ph.D., CEO, Berkeley Lights. "As we continue to strengthen our technology's global presence, we will be focusing on adding platform capabilities that will, ultimately, make personalized cell therapeutics accessible to all."

"Our continued support of Berkeley Lights speaks to growing evidence that the company's technology is poised to revolutionize drug discovery and development," said Yasuyuki Okamoto, Senior Vice President and Director, Healthcare Business Unit, Nikon Corporation. "We look forward to seeing continued adoption of their digital cell biology platform by the biotechnology and pharmaceutical industry throughout the globe, as well as development of additional capabilities that will speed discovery and development for life-saving therapeutics."

The Beacon platform has been adopted by more than half of the top 25 global pharma companies. With BLI technology, these customers are seeing improvements in their workflows and the potential of digital cell biology to transform the industry. The Beacon platform delivers extraordinary efficiencies to current cell biology processing and speeds discovery and development by using optofluidic light technology to individually isolate, culture, perform assays and export thousands of live cells in conjunction with visual and digital monitoring. The rich digital and analytical insights provided allows scientists to make more informed decisions, so they can select and retrieve the best cells, leading to more consistent and potent production of therapeutics in a dramatically reduced timeframe.

Source:
https://www.prnewswire.com/news-releases/berkeley-lights-closes-95-million-funding-round-to-expedite-commercial-expansion-and-platform-development-for-cell-therapy-300730472.html?fbclid=IwAR23WOTpcjpdL5W9ZlbHf3vQSI7f3q40O4hIrF-ZeESzbhJeqT7VV-AUwMk

Trends of Investment and M&A Deals

- **2013-2015.** During these years 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.

- **2016-2017.** 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. Therefore, there were significant concerns regarding the scalability of such an approach, and whether they could deliver truly disruptive results, above and beyond traditional R&D departments in BioPharma. By the beginning of 2017 the first tangible results were achieved by a number of AI companies and new benchmark methods for the application of AI were established, and new collaborations between Pharma and AI startups yielded much better results. Since then the race for the acquisition of the best AI startups began.

- **2018.** Now the capitalization of the industry is continuously growing. If there will be major breakthroughs, the growth leading up to 2020 could approach 20x or more. 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 so as to bet on the entire subsector, in such a way as to tie the performance of the fund to the performance of the entire sector rather than any individual company.

- **Diversification:** In 2015 and 2016, 26 and 22 investment rounds were conducted, and this number increased to 30 in 2017.

- **Increased amount of investments:** 2017 and 2018 showed significant growth of investments. Comparing to 2015 and 2016, when AI R&D startups raised $231M and $230M accordingly, 2017 showed significant growth to $469M. The industry saw a total of $455M in Q2 of 2018, compared to $159M in Q1 2018. This is almost as much as was raised in all of 2017 combined ($468M).

- **Consistency:** During 2013-2016 there was some growth in the amount of capital raised by the industry players, however the trend was not steady. In 2017-2018 we observed stable growth of the investments in the industry, an increase in the number of IT and Tech corporations entering the field, and active participation from traditional BioPharma corporations, largely in the form of joint ventures.

Major Government Initiatives in the US, UK, EU and Asia Pacific

AI for Drug Discovery Major Government Initiatives in the US, UK, EU and Asia Pacific

Just as the past several years has seen astark rise in the number of AI for Drug Discovery companies, investments, M&As, collaborative ventures, public recognition, conferences and media coverage, the past few years have also brought an increased interest in and commitment to AI for Drug Discovery by several governmental bodies in the USA, UK, EU and Asia Pacific region.

This is sensible given the increasingly widespread consensus that AI will disrupt the BioPharma industry, and that existing drug companies, as well as entire health care systems, will need to begin investing time, funds and other resources into AI for Drug Discovery in order to stay competitive.

Some countries, for instance, seem to see it as one of the means by which they can increase their global leadership position in AI generally, such as China. Others simply recognize the need to begin investing public funds and resources into it in order to keep their healthcare systems in step with the ongoing pace of technological change.

The increased commitment and interest of governmental bodies will bode well for the broader AI for Drug Discovery industry. Aside from increasing the total amount of funding available for AI for Drug Discovery and Advanced R&D generally, it also helps to keep governments aware of the secondary effects of the industry, once companies begin to bring practical results into the clinic.

Foremost among these is the likelihood that the time and cost it takes to go from concept to trial to clinic will be substantially reduced, which will necessitate changes to existing pharmaceutical regulatory frameworks. By keeping abreast of industry and R&D developments, governmental bodies can gain a deeper understanding of what to expect and how to reformulate existing operating procedures in order to account for them.

The present chapter aims to provide readers with an overview of the largest and most important government initiatives relating to AI in Drug Discovery and Advanced R&D that have occurred both within the past few years generally, and in 2018 in particular.

USA

The US has led the AI for Drug Discovery race in terms of both total investments and the number of US-based companies focusing on AI for Drug Discovery.

The USA is also home to the largest pharma corporations in the world, putting it in an excellent position to grow its AI for Drug Discovery industry if, as recent trends seem to indicate, the BioPharma industry continues to build up their internal AI for Drug Discovery resources and increase their number of AI for Drug Discovery startup acquisitions.

With that being said, there is also mounting interest in the AI for Drug Discovery sector from the EU, UK and Asia-Pacific region as well.

While the USA leads the pharma race generally, as we have discussed elsewhere in this and earlier reports, the AI for Drug Discovery sector is poised to become the central factor that will determine who is the winner of the drug discovery race in the years to come.

If the EU, UK or Asia Pacific region proves more willing to grow their AI for Drug Discovery industry, especially through something akin to a national development strategy, whereby a significant amount of government funds are earmarked for such a purpose, then it is possible that the US could be overtaken in terms of its current leadership position in the pharmaceutical industry.

It all depends on the actions and commitments taken by the US government, as well as by the current US-based leaders of the BioPharma Industry, and by US-based IT corporations.

China

In an article in South China Morning Post, Andy Chun notes that "AI relies greatly on data for machine learning and predictive analytics, and China has no shortage, with its population generating massive amounts of real-time medical data. The Chinese population is eager to use technology and adopt AI."

According to recent data from the UN, China is aging more rapidly than any other country in the world, largely as a result of its previous one-child policy, and will have roughly 330 million citizens over the age of 65 by the year 2050.

Thus, the Chinese government have perhaps more incentive than any other developed nation to prioritize innovations in healthcare that could help them avoid economic turmoil due to the healthcare costs associated with an aging population. The Chinese government does seem to be setting their sights on prioritizing AI in healthcare as well. In an AI Strategic Plan released in July 2017, they outlined their intentions to catch up in the AI race by 2020, make major breakthroughs by 2025 and become the world leader in AI by 2030.

In a parliamentary meeting held around the same time as the report's release, China science and technology minister Wan Gang noted that government finance will lead the way in AI research, including the development of supercomputers, and high performance semiconductor chips, software and the hiring of key talent to lead the field. If they remain true to their commitment, they could succeed in building up the necessary resources in order to dominate the AI for Drug Discovery space.

Indeed, as we have noted elsewhere, the current bottleneck that limits progress in AI for Drug Discovery, and the most crucial factor that will determine who emerges as the leader of this space in the years to come, is the limited pool of AI specialists available to be acquired. Given China's formidable population, they have the raw materials to generate, via education, incentives and prioritization, the most valuable resource in the entire AI for Drug Discovery landscape: AI specialists.

Source: https://www.scmp.com/tech/article/2077845/future-here-china-sounds-clarion-call-ai-funding-policies-surpass-us;
https://www.scmp.com/tech/enterprises/article/2103568/world-dominance-three-steps-china-sets-out-road-map-lead-artificial;
https://www.scmp.com/comment/insight-opinion/article/2152087/artificial-intelligences-greatest-contribution-may-be-health

In April 2018, the UK government confirmed its commitment to keep up with other countries in the AI race through a very large government initiative worth £1 billion Titled the AI Sector Deal. The deal between government and industry (involving over 50 leading UK tech companies) was announced by Business Secretary Greg Clark and Digital Secretary Matt Hancock, and will involve more than £300 million in new private sector investment, as well as 1000 new government-funded AI PhDs.

Commenting on the initiative, UK Digital Secretary Matt Hancock noted that "Artificial Intelligence is at the centre of our plans to make the UK the best place in the world to start and grow a digital business. We have a great track record and are home to some of the world's biggest names in AI like Deepmind, Swiftkey and Babylon, but there is so much more we can do. By boosting AI skills and data driven technologies we will make sure that we continue to build a Britain that is shaping the future."

In a press release on the topic of the initiative, the UK government noted that "The deal will help establish the UK as a research hotspot, with measures to ensure the innovators and tech entrepreneurs of tomorrow are based in the UK, with investment in the high-level post-graduate skills needed to capitalise on technology's huge potential. It includes money for training for 8,000 specialist computer science teachers, 1,000 government-funded AI PhDs by 2025 and a commitment to develop a prestigious global Turing Fellowship programme to attract and retain the best research talent in AI to the UK."

Source: https://www.gov.uk/government/news/tech-sector-backs-british-ai-industry-with-multi-million-pound-investment--2;
https://www.gov.uk/government/publications/artificial-intelligence-sector-deal;
https://www.gov.uk/government/publications/industrial-strategy-the-grand-challenges/industrial-strategy-the-grand-challenges#artificial-intelligence;
https://www.gov.uk/government/topical-events/the-uks-industrial-strategy
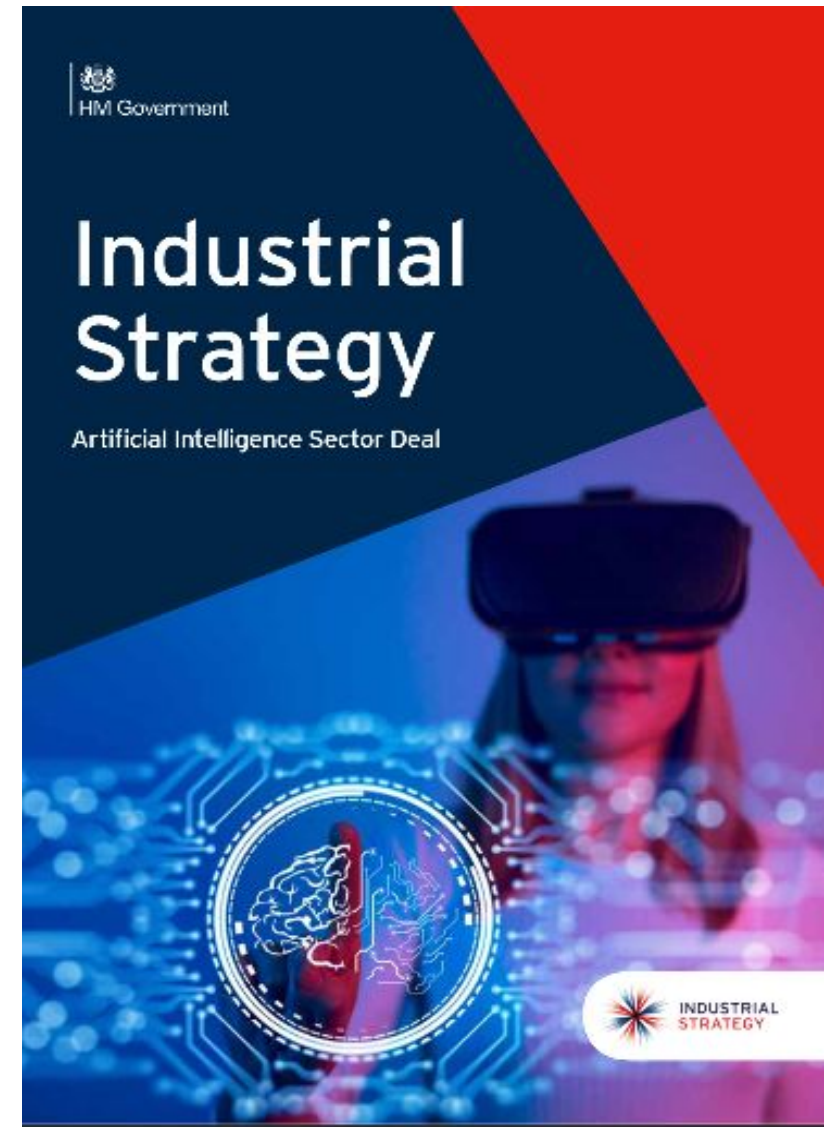
United Kingdom

"The new Rosalind Franklin Institute will lead a revolution in drug development and diagnosis to improve the lives of millions of patients. And with over 10 million people in Britain alive today expected to live to 100, now more than ever it is vital that the Government invests in the development of new technologies and techniques which will support people to have healthier lives. The RFI will pioneer disruptive technologies and new ways of working to revolutionise our understanding of biology, leading to new diagnostics, new drugs, and new treatments for millions of patients Worldwide. It will bring university researchers together with industry experts in one facility and embrace high-risk, adventurous research, that will transform the way we develop new medicines."

- **Greg Clark, Secretary of State for Business, Energy & Industrial Strategy**

UK & NHS To Launch 5 AI Medical Clinics in 2019

Five new medical technology centres are set to open in the UK next year which will use artificial intelligence to speed up disease diagnosis. The clinics will be built in Leeds, Oxford, Coventry, Glasgow and London with funding from the Department for Business, Energy and Industrial Strategy. It is part of the Government's drive to use AI to improve healthcare and treatments.

The centres will have software that will digitise scans and biopsies as well as tools that should help speed up the process of conducting early diagnosis. The new clinics are planned to open in 2019 and will be based at universities and NHS facilities. In total the centres will cost £50m. One of the centres, the London Medical Imaging and Artificial Intelligence Centre for Value-Based Healthcare, will use AI pattern recognition software to detect anomalies in scans with the aim of helping to carry out earlier diagnosis. Business Secretary Greg Clark said the new centres should free up more time for NHS staff to spend on direct patient care. Health Secretary Matt Hancock said: "Artificial intelligence will play a crucial role in the future of the NHS and we need to embrace it by introducing systems which can speed up diagnoses, improve patient outcomes, make every pound go further and give clinicians more time with their patients.

"As part of our long-term plan, we will transform the NHS into an ecosystem of enterprise and innovation that allows technology to flourish and evolve." AI has become increasingly common in all parts of medicine and healthcare. Moorfields Eye Hospital and Google's DeepMind are implementing an algorithm that will enable computers to analyse high-resolution 3D scans of the back of the eye to detect more than 50 eye conditions. Great Ormond Street Hospital (GOSH) has also paired up with Cambridge-based technology giant Arm to develop smart "person recognition" cameras that can spot intruders and monitor staff on its premises, in a move that could speed up operations and improve security.

The technology will be used by the children's hospital in London to track doctors and nurses on site, while also keeping track of visitors as they pass from the reception area to wards.

Source: https://www.telegraph.co.uk/technology/2018/11/06/five-new-ai-medical-centres-open-across-uk-next-year/

Novel Technologies and Trends 2019-2020

Deep Learning in Drug Discovery

Deep learning is a subset of machine learning consisting of artificial neural networks, famous for its capacity to learn in an unsupervised manner by being "trained on" unstructured and/or unlabelled data.

Its distinction with respect to traditional machine learning can be best thought of as its depth - i.e., deep learning uses "deeper" layers of artificial neural networks with are layered on top of each other.

Machine learning has been in use for almost two decades in the process of in drug discovery.

Since an early flush of optimism in the 1950's, smaller subsets of artificial intelligence - first machine learning, then deep learning, a subset of machine learning - have created ever larger disruptions.
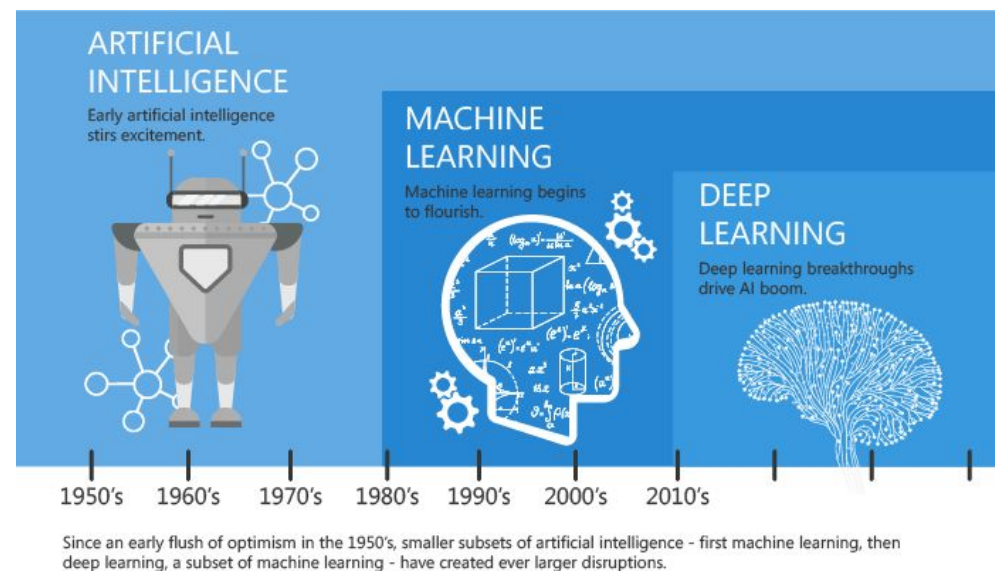
Since the inception of deep learning as a field, it has progressed by leaps and bounds, and has become famous in the public eye for replicating many functions which previously were once thought of as the exclusive domain of humans.

For instance, over the past few years deep learning algorithms have allowed computers to see, read, and write, in ways that are less error-prone than older, more traditional methods of AI, such as decision trees.

For instance, the use of deep learning algorithms trained to analyze and interpret medical images with an error rate of just 6%, which some experts claim to be less error-prone than human doctors. Deep learning has a place in a wide variety of healthcare niches, including medical image analysis, medical device data evaluation, sequencing data analysis, virtual drug screening, drug adherence analysis, drug efficacy analysis, metabolomic profiling, sequencing, molecule profiling, biomarker identification, and drug lead identification, virtual testing and optimization.

Source: https://www.rootsanalysis.com/reports/view_document/deep-learning-in-drug-discovery-and-diagnostics-2017-2035/156.htm

Deep Learning in Drug Discovery

Importantly, deep learning algorithms have show substantial capacities in significantly reducing the time and cost required to bring a drug to market.

Bringing the average drug to market has been known to cost as much as $2.5B over a period of 12 years, and deep learning algorithms have in some cases been shown to reduce the cost of bringing a drug to market by as much as 50%.

Some experts predict that the annual cost savings associated with the development and deployment of deep learning-based solutions to drug discovery could result in cost savings nearing $100B, with nearly $35B projected savings in the diagnostics niche alone.

One of the most ripe commercial opportunities for the picking with regards to deep learning for healthcare is the AI-supported diagnostic imaging subsector, due to the abundance of data available, as well as the consistency of how such data is organized across different databases.

One of the starkest examples of the power of deep learning is in AlphaGo, popularly known to have bet the world champion in the game Go in a remarkably short amount of time. By emulating the computational patterns of human thought in a much more naturalistic manner than, for example, traditional, brute-force decision trees, it required less computational steps in order to arrive at the decisions it needed go make, and managed to win 100 out of 100 games after training on Go data for just three days.

Remarkably, more than 55% of deep learning companies focusing on the image recognition sector are applying their efforts to diagnostic imaging. Of these 55%, a remarkable 78% focus on medical imaging. Meanwhile, out of all deep learning companies, 35% are focusing their efforts on drug discovery, and 57% of those 35% aim to provide deep learning based drug discovery platforms.

Source: http://www.gbm.hsbc.com/solutions/global-research

Deep Learning in Drug Discovery

Deep learning has been proven capable of achieving lower error rates in image and voice recognition and natural language processing compared to traditional machine learning algorithms. Famous in the eyes of the public for things like self-driving cars, natural language processing and image/voice recognition, its impacts on the drug discovery process have only recently begun to accumulate. So, if deep learning is supposed to be a closer approximation to the kinds of information processing occurring in the human brain, then how does it differ? One of the starkest differences is that, whereas humans require relatively little data in order to extrapolate trends and patterns, deep learning algorithms are famous for their dependence on very little data. Consider the example of a human seeing a pattern one time, and extrapolating it to other instances.

This, in deep learning, is referred to as one-shot learning. Research has shown that deep learning algorithms perform better when the datasets they are trained on are large. While work on specific architectures that allow for deep learning-based classifiers and predictors to be built that operate according to one-shot and even zero-shot learning, for now, the performance deep learning algorithms are somewhat limited to the available size of the datasets used to train them. Deep learning algorithms have proven highly effective in modeling the chemical reactions between candidate drugs and their molecular targets, through which they exert their mechanisms of action. This has allowed researchers to hone in on a much more precise suite of candidate molecules in silico, prior to in vitro validation.

While much work in the real of deep learning for drug discovery is happening in the US, such as through the work of Insilico Medicine, a Baltimore-based AI for age-related drug discovery and biomarker development company, important work in this arena is also occurring abroad as well.In the UK for example, researchers from Warwick's School of Engineering have developed a deep learning algorithm capable of predicting whether or not a candidate drug molecule will bind to its target protein with 99% accuracy. Take, for instance, the case of Chuna, which recently launched a next-generation AI development plan which includes such AI platforms as Baidu's self-driving car algorithms, AliCloud's "city brain", Tencent's medical imaging algorithms and iFlytek's natural language processing algorithms. The Chinese healthcare system is ripe for the development of deep learning algorithms, because China's network of hospitals and healthcare institutions generated vast swatches of data regularly, so much so that the digitisation, classification and processing of such data was baluated at RMB30b in 2016

Source:https://www.sciencedirect.com/science/article/pii/S1359644617303598; https://www.sciencedaily.com/releases/2017/12/171214144442.htm

Generative Adversarial Text to Image Synthesis

Scott Reed, Zeynep Akata, Xinchen Yan, Lajanugen Logeswaran, Bernt Schiele, Honglak Lee

(Submitted on 17 May 2016 (v1), last revised 5 Jun 2016 (this version, v2))

Automatic synthesis of realistic images from text would be interesting and useful, but current AI systems are still far from this goal. However, in recent years generic and powerful recurrent neural network architectures have been developed to learn discriminative text feature representations. Meanwhile, deep convolutional generative adversarial networks (GANs) have begun to generate highly compelling images of specific categories, such as faces, album covers, and room interiors. In this work, we develop a novel deep architecture and GAN formulation to effectively bridge these advances in text and image model– ing, translating visual concepts from characters to pixels. We demonstrate the capability of our model to generate plausible images of birds and flowers from detailed text descriptions.
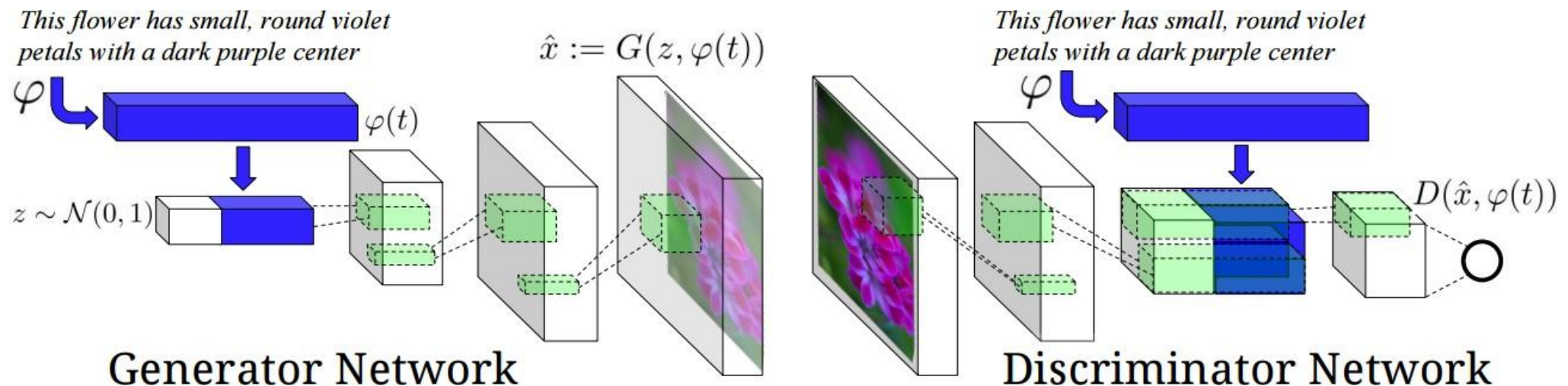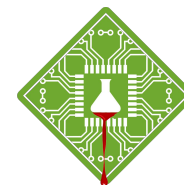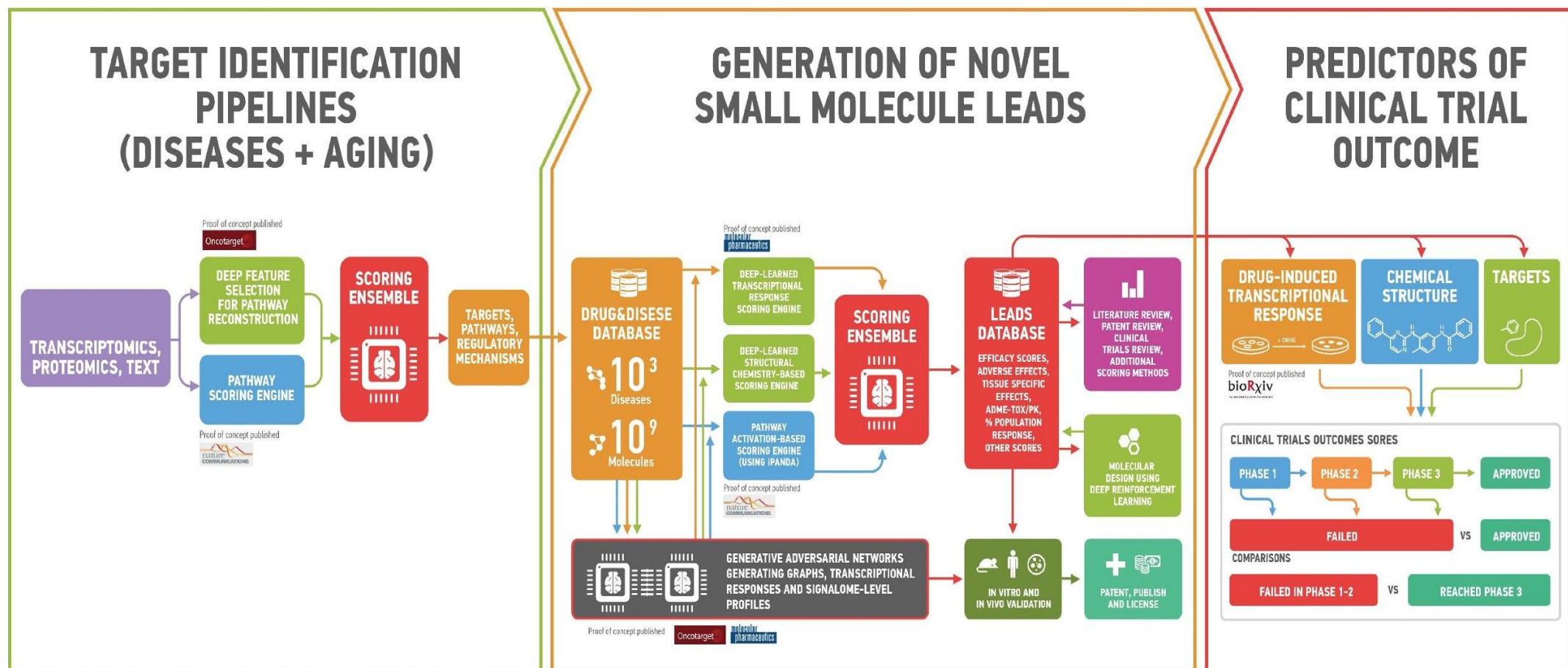
AI for Advanced R&D in Longevity Research
Insilico Medicine

INSILICO MEDICINE

Insilico Medicine's mission is to extend healthy longevity through innovative AI solutions for drug discovery and aging research. Insilico Medicine is committed to transforming the pharmaceutical industry with next-generation artificial intelligence. They are developing new tools for drug discovery and repurposing, biomarker development and pursuing novel strategies for rapid validation. Their projects combine advances in genomics, big-data analysis, deep learning and reinforcement learning.

Insilico Medicine and Biotime announced in 2016 the launch of a beta version of Embryonic.AI, an artificially intelligent system for analyzing the embryonic state of human cell samples using gene expression data. Insilico established in 2017 a collaboration with GSK to discover novel biological targets and molecules. As a first stage of the collaboration, GSK will evaluate Insilico's technology in the identification of novel biological targets and pathways of interest to GSK.

In 2018 a collaboration occurred between Insilico Medicine and Juvenescence AI Limited, which is a drug development and artificial intelligence company focused on ageing and age-related diseases. Juvenescence AI combines advances in artificial intelligence with classical development expertise in order to prioritize and develop compounds from Insilico Medicine, Inc.'s end-to-end automated drug discovery pipeline through to clinical proof of concept.

By using AI and deep learning, the company can analyze how different compounds will affect certain cells, determine what drugs can be used to treat the symptoms, and any possible side effects that may occur. Even though it's only been around a few years, Insilico has already been named by NVIDIA as one of the 5 top AI companies. With R & D resources spread out across the globe in the UK, Russia, and Belgium and a backing of $14 million behind it.

Source: https://www.eurekalert.org/pub_releases/2017-08/imi-iec081417.php
https://www.businesswire.com/news/home/20180205005024/en/Insilico-Medicine-Juvenescence-Announce-Drug-Candidate-Joint

Atomwise is the creator of AtomNet, the first Deep Learning technology for novel small molecule discovery, characterized by its unprecedented speed, accuracy, and diversity.

Today, drug-resistant bacteria and pandemic viruses threaten to send us back to the time of plague and smallpox. Persistent, neglected diseases remain a dark spot on our collective conscience. And while we're all living longer, diseases of aging like Alzheimer's still have no cure. Atomwise has the unique ability to research hundreds of millions of potential medicines rapidly, making it fundamentally easier to tackle these big problems.

Atomwise's AtomNet platform uses structural information to predict binding between molecular targets and small molecules by processing millions of data points regarding successful and unsuccessful ligand-binding interactions. The company has more than 50 molecular discovery programs, including confidential projects with AbbVie Inc. and Merck & Co. Inc.

In April 2017, Atomwise started a program to motivate academic scientists to explore the drug-hunting potential of its technology. Researchers can apply to the company's Artificial Intelligence Molecular Screen (AIMS) awards program by identifying the disorder they hope to treat, and the disease-causing biomolecules they want to defeat with a drug. Successful applicants will receive 72 compounds that Atomwise predicts are most likely to work as that drug.

Atomwise has been partnering up with big pharmaceutical firms, biotechnology companies, and university research labs in an effort to speed up the discovery of new drug candidates for neurodegenerative diseases, cancer, and other disorders. In June, the startup also announced a collaboration with Monsanto to find compounds that might protect crops against pest infestations and diseases.

Source: http://www.chematria.com/
http://www.4-traders.com/ABBVIE-12136589/news/AbbVie-AI-drug-discovery-company-Atomwise-raises-51M-series-A-26122374/
https://www.xconomy.com/san-francisco/2018/03/07/atomwise-raises-45m-to-grow-ai-driven-drug-discovery-business/

BioAge is committed to contribute to and support the evidence-based medical approach to a healthy lifestyle, accomplished through diet, exercise, supplementation and the use of integrative medicine.

The overall aim of the proposed staff exchange programme is to build, extend and strengthen sustainable international collaborations between the partners so as to create a knowledge base for biomarker based research related to aging, sampling techniques in the elderly and biomonitoring studies.

BioAge develop biomarkers and drugs that impact human aging by coupling genomic data with machine learning. BioAge is building a platform that doesn't require waiting for its subjects to actually age. Instead, it wants to measure biological age using signals floating in a drop of blood.

BioAge Labs raised $10.9M in Series A financing to accelerate drug discovery for aging in 2017. BioAge is betting on the power of high-throughput human data, coupled with innovative machine learning, to substantially accelerate drug discovery for aging. The company take a hybrid experimental and computational approach to identifying the molecular signatures that drive aging, working with multiple partners in academia and industry. The funding will enable BioAge to build their team, refine and test their signatures of aging, and begin in vivo evaluation of drug candidates. Their initial targets for drug development will be specific diseases where aging is causal; however, their ultimate goal is more ambitious — to combat the suffering and disability caused by all aging-related diseases, and to restore both the quality and quantity of life that is so often lacking in old age.

"Cure a disease in a year" program

In November 2018 was announced that Insilico Medicine, a Rockville-based company developing the end-to-end drug discovery and real world evidence pipeline utilizing the next generation artificial intelligence, will present its research and introduce the "Cure a disease in a year" program at the World's leading congress for big data in precision medicine - Biodata World Congress 2018 on 28-29 November 2018 at Congress Center Basel.

Alex Zhavoronkov, PhD, Founder, and CEO of Insilico Medicine, Inc. said:

"Our company published the many proofs of concept for the applications of modern AI in drug discovery and completed many pilots. However, the pharmaceutical industry is not moving fast enough. Several pharmaceutical companies are claiming to have hundreds of data scientists and the many petabytes of legacy data that will help them turn into the data companies. But so far with no tangible results coming out of these efforts. It is time to unveil our end-to-end drug discovery pipeline and offer rare disease foundations a chance to collect the data required for this pipeline and get the targets and molecules for testing. For the first time we will present our "Cure a disease in a year" program at Biodata World Congress 2018, which gathers the key opinion leaders from the academia and industry."
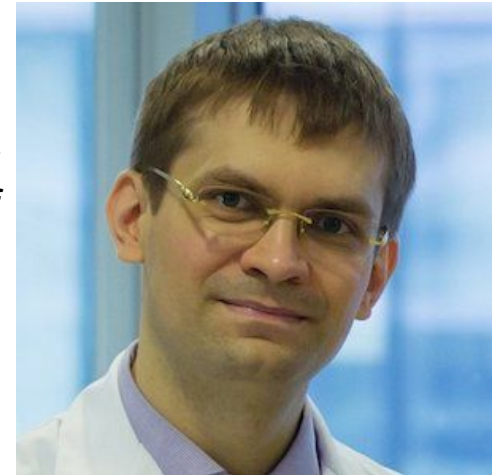
Alex Zhavoronkov

"Artificial Intelligence (AI) techniques, such as deep learning (DL), reinforcement learning (RL), and generative adversarial networks (GANs) play a pivotal role in studying the biology of aging on many levels. We are excited to share our vision and latest results at the industry's leading event for Data and AI in healthcare"

According to the Chair of "AI in Ageing Research and Longevity" Round Table, **Tina Woods**, Founder of Collider Health:

"This is an exciting time in health and longevity. Insights can be gathered from DNA and other health, behavioral and environmental information with astonishing efficiency using AI- and all this can drive 'smarter' research and more personalized strategies to increase our 'healthspan'. I hope one day we can each have our own 'Life Dashboard' giving us the power to leverage our genetic, health, wealth and life data, and nudging us in the right ways to live a longer, healthier life while helping billions of others too".

Buck Institute Brings Insilico Medicine CEO on as Adjunct Professor to Spearhead their AI for Longevity Research Activities

Following this mini-conference, the Buck Institute also acquired Insilico Medicine's CEO Alex Zhavoronkov as an Adjunct Professor, in order to spearhead the Buck's activities in utilizing the latest advanced in AI and deep learning for longevity research.

The fact that the leading aging research foundation in the United States is devoting their time and resources towards the use of AI and deep learning for geroscience research is yet another indication that AI, machine learning and deep learning is now recognized as a legitimate niche within the broader geroscience community.

In a press release associated with the announcement, Buck Institute CEO Eric Verdin stated:

"We are incredibly excited about the potential of AI to accelerate aging research. The Buck has been at the forefront of asking the most important questions in the field. Now, with the latest in bioinformatics and artificial intelligence, and with the involvement of world-class experts like Dr. Zhavoronkov, we will finally have the tools to answer them. Fully utilizing these powerful technologies, we will dramatically increase our understanding of how aging works, and what we can do about it."

Artificial Intelligence for Aging and Longevity Research: Recent Advances and Perspectives

Pharmaceutical Artificial Intelligence Department, Insilico Medicine, Inc., Baltimore, MD, United States
Biogerontology Research Foundation, London, United Kingdom
Buck Institute for Research on Aging, Novato, CA, United States
Department of Computer Science, University of Oxford, Oxford, United Kingdom
Center for Healthy Aging, Department of Cellular and Molecular Medicine, University of Copenhagen, Denmark
George Mason University, Fairfax, VA, United States

Highlights:
Presentation of the most recent advances for the design of deep learned aging clocks.
Description of achievements in the development AI de novo molecular generators.
Strategies for developing AI-based of cross species aging studies.
Algorithms are combined within a pipeline to optimize the drug discovery process.
Strategies to select and extract features relevant to aging research.

Abstract
The applications of modern artificial intelligence (AI) algorithms within the field of aging research offer tremendous opportunities. Aging is an almost universal unifying feature possessed by all living organisms, tissues, and cells. Modern deep learning techniques used to develop age predictors offer new possibilities for formerly incompatible dynamic and static data types. AI biomarkers of aging enable a holistic view of biological processes and allow for novel methods for building causal models—extracting the most important features and identifying biological targets and mechanisms. Recent developments in generative adversarial networks (GANs) and reinforcement learning (RL) permit the generation of diverse synthetic molecular and patient data, identification of novel biological targets, and generation of novel molecular compounds with desired properties and geroprotectors. These novel techniques can be combined into a unified, seamless end-to-end biomarker development, target identification, drug discovery and real world evidence pipeline that may help accelerate and improve pharmaceutical research and development practices. Modern AI is therefore expected to contribute to the credibility and prominence of longevity biotechnology in the healthcare and pharmaceutical industry, and to the convergence of countless areas of research.

Source: https://www.sciencedirect.com/science/article/pii/S156816371830240X?fbclid=IwAR1Ej-snAXI-cSc0vJmoZRNeCrqp0xMPg-lwgi-vLRn_xcAGjAKRmdxvTyY

Meanwhile, in 2018, AI for Drug Discovery was cemented as a legitimate and official subsector within the broader longevity research landscape, and longevity research as a legitimate niche within the broader drug discovery landscape, with both subsets having attained a new degree of recognition.

This occurred when leading business consulting firm Frost & Sullivan awarded Insilico Medicine the North American Artificial Intelligence for Aging Research & Drug Development Technology Innovation Award, as part of their 2018 Best Practices Awards.

More than this, the fact that a highly respected business consulting firm like Frost & Sullivan created a specific category of award for this specific area of research and development is highly indicative of the increasing level of repute that AI in Drug Discovery for aging research is garnering from both the broader geroscience community as well as the wider drug development communities.

This new development may also serve to highlight the high degree of synergy that is possible through the convergent integration of two cutting-edge and highly innovative classes of R&D.

Appendix

This 100-page report marks the fourth installment in a series of reports on the topic of the Artificial Intelligence in Drug Discovery Industry that we have been producing for more than 1 year now.

We released the first edition of these reports, entitled "AI for Drug Discovery Landscape Overview 2017" in the end of 2017, followed by "AI for Drug Discovery & Advanced R&D Q1 2018" in the first quarter of 2018, and by "AI for Drug Discovery & Advanced R&D Q2 2018" in the second quarter of 2018.
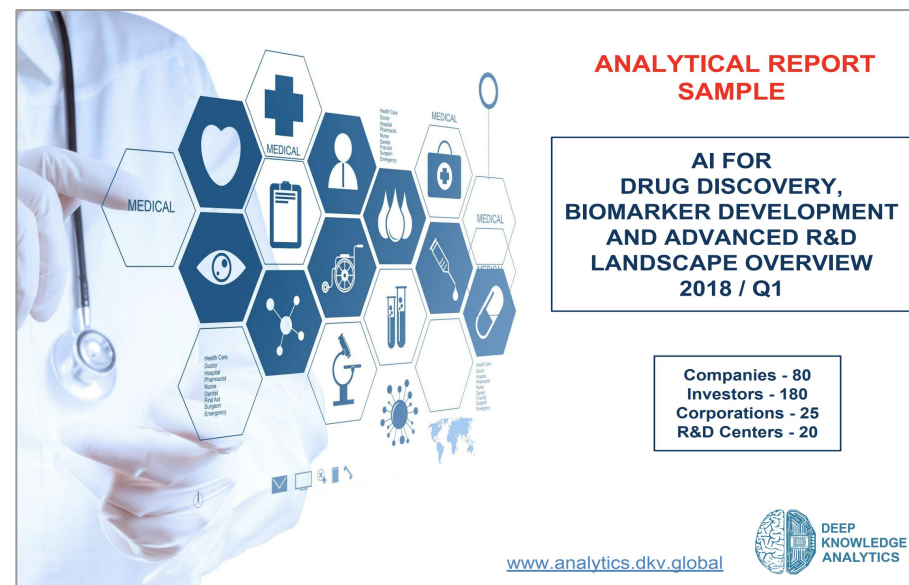
The present edition consists of a shortened version of our previous 600-page report on the state of the industry in Q2 of 2018, updated with major developments having occuring in Q3 of 2018, and can be considered as a summary of the major insights, data analysis, conclusions and forecasts of our previous report. The following two slides show a detailed table of contents from our previous report.

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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Appendix / Profiles

Comparison
of 20 Leading
AI Companies

Comparison of Top-20 AI for Drug Discovery Companies
True AI companies
The ratio: AI experts vs
Total Number of Employees
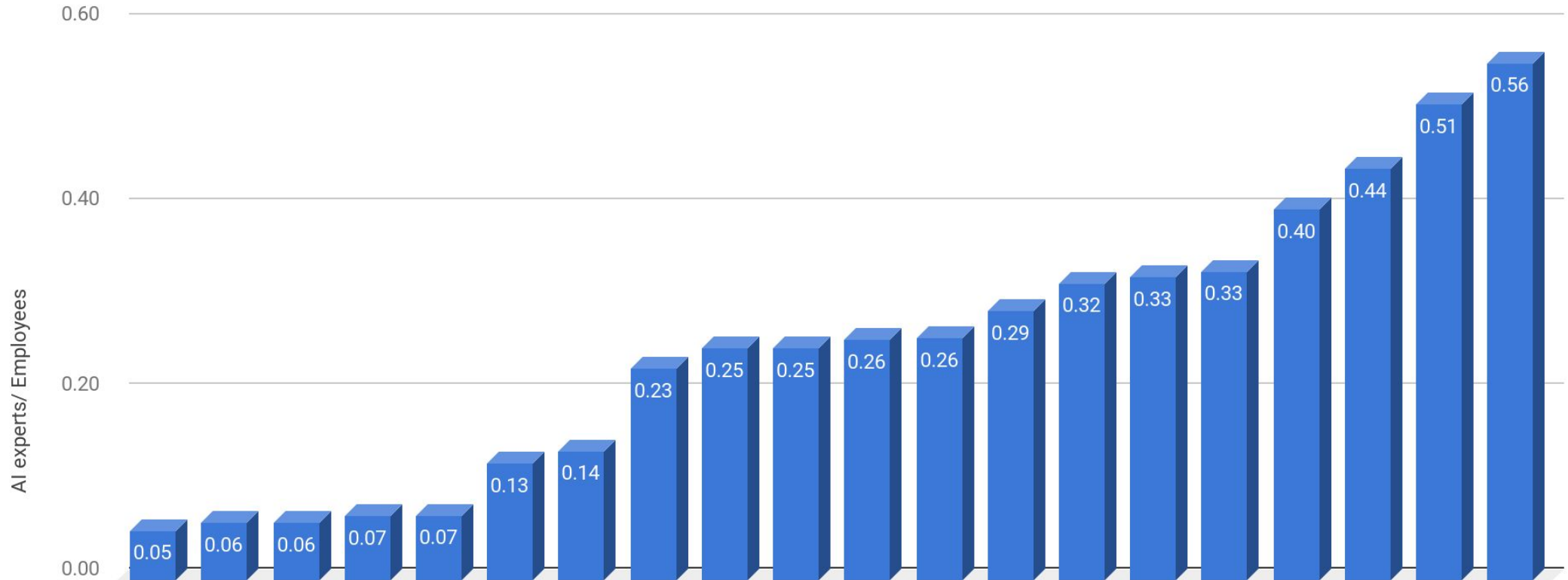
Source: According to LinkedIn

Comparison of Top-20 AI for Drug Discovery Companies

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

Source: Crunchbase, Google
Securities and Exchange Commission

228
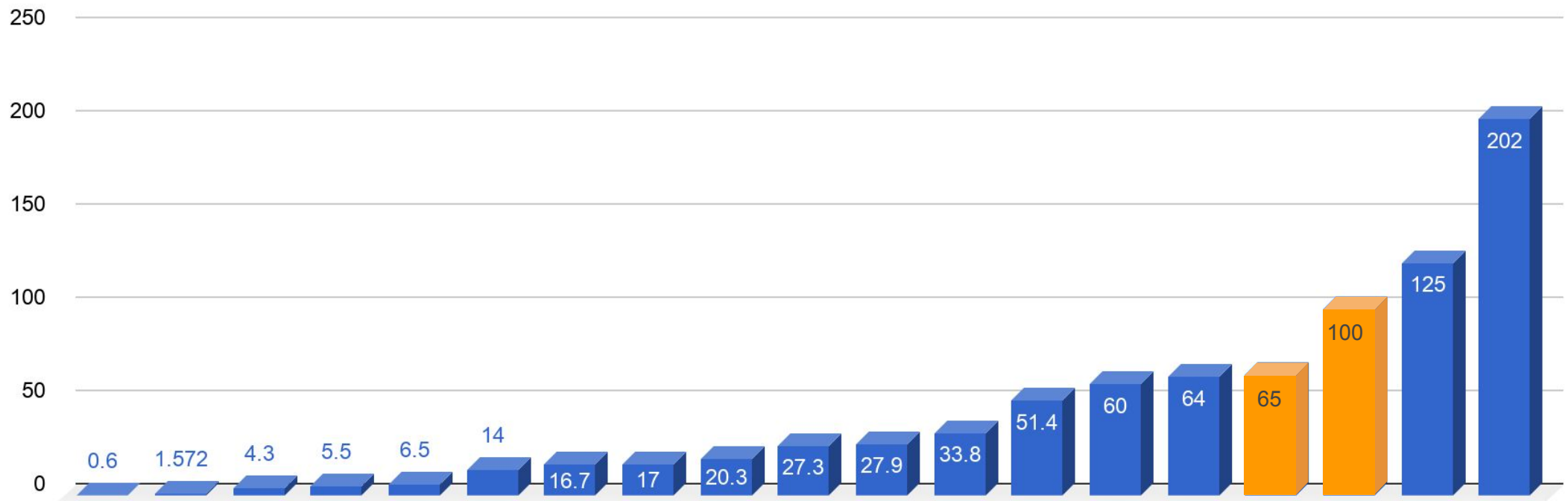
Comparison of Top-20 AI for Drug Discovery Companies

Number of Scientific Publications
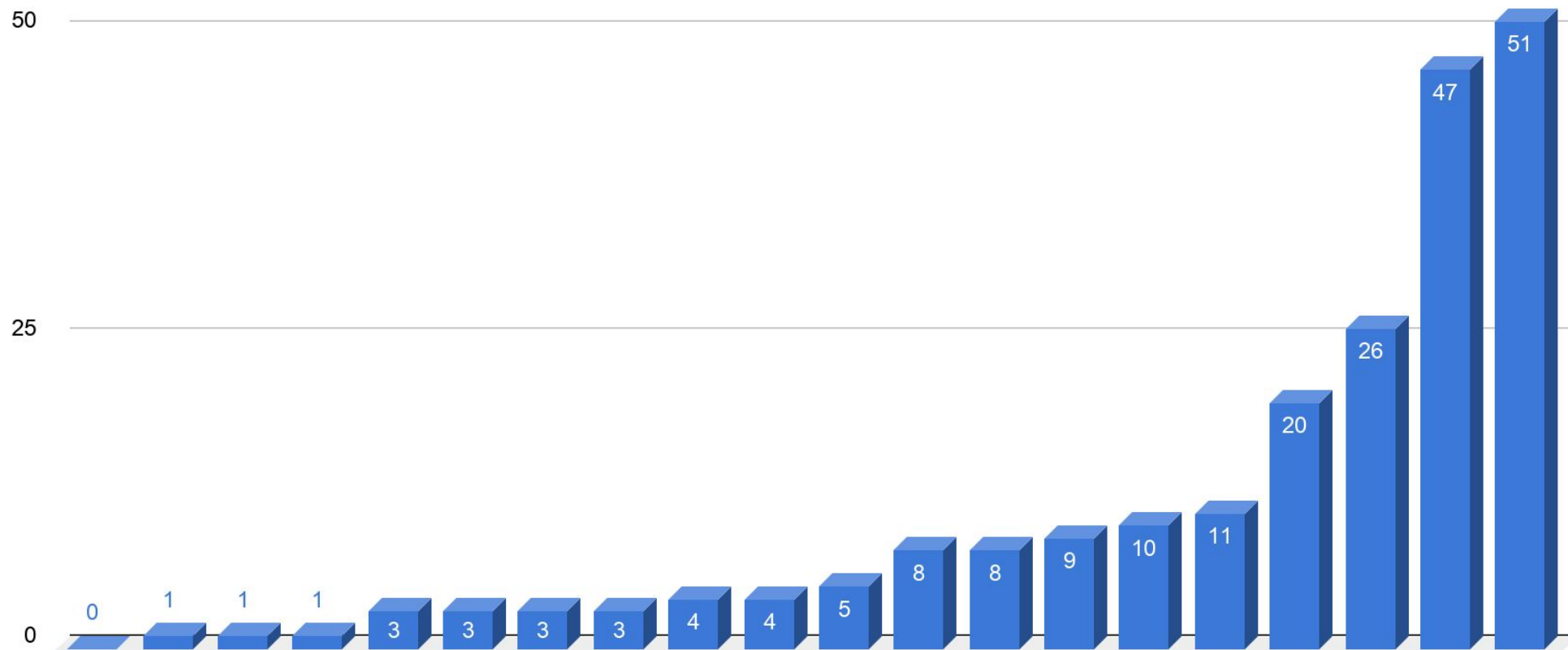
Comparison of Top-20 AI for Drug Discovery Companies

Number of Patents

Source: patents.google.com
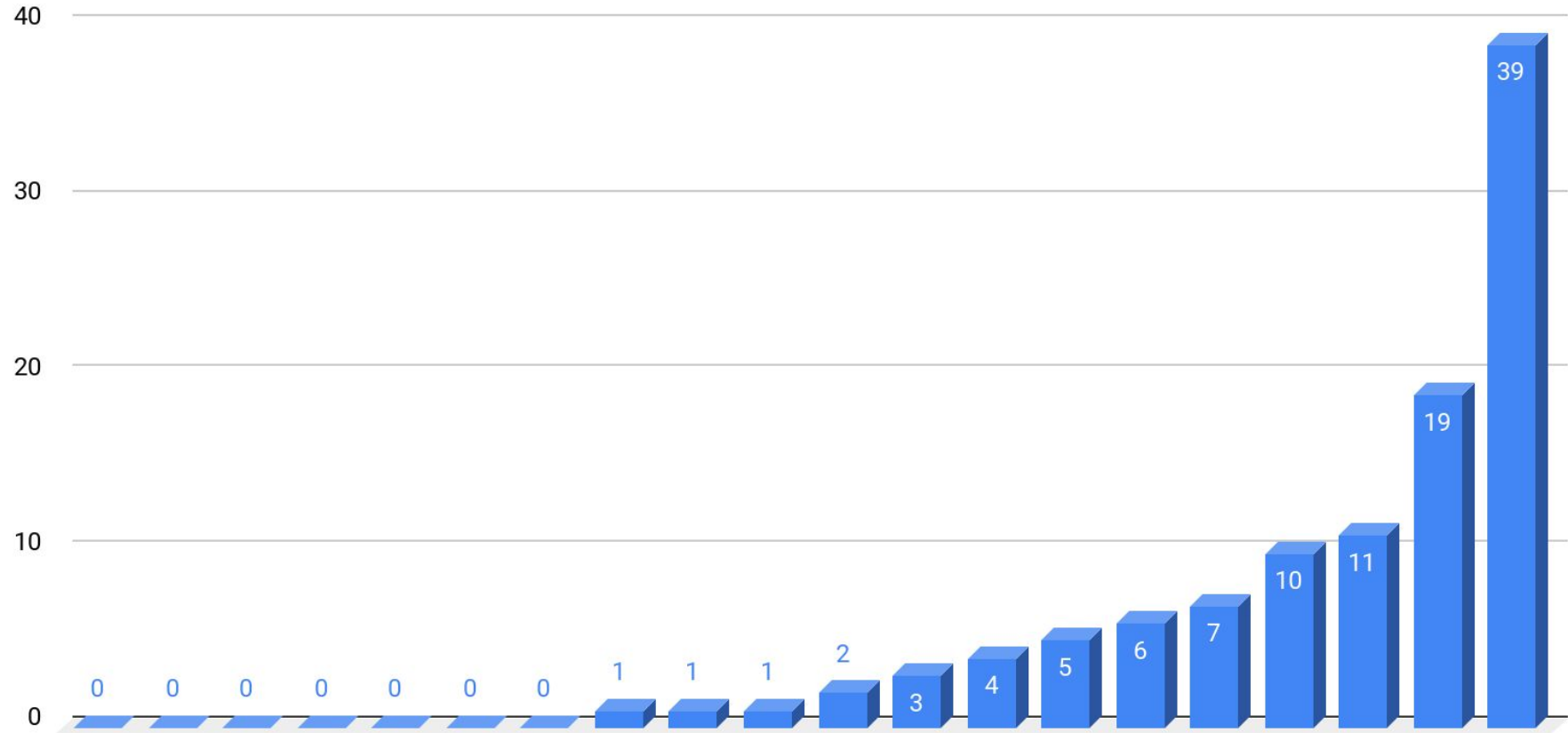
Comparison of Top-20 AI for Drug Discovery Companies

Total Number of Employees / AI experts

Source: According to LinkedIn

Deep Knowledge Analytics (DKA) Disclaimer