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Insights

Intelligent biopharma: Forging the links across the value chain and

October 2019

Deloitte Centre *for*
Health Solutions

The pace and scale of medical and scientific innovation is transforming biopharma

Digital transformation is a strategic imperative for biopharma companies facing a complex and challenging environment

The biopharma value chain

According to a Deloitte/MIT Sloan Management Review survey:

- 20% of biopharma companies are **digitally mature** – a lack of clear vision, leadership and funding are holding companies back
- 58% of respondents said digital transformation is a **top management priority**
- 79% expect to **realise the value of digital initiatives** within the next five years

What is digital transformation?

Digital transformation is the use of innovative technologies to reimagine an organisation and drive change management. Digitally mature organisations are committed to transformative strategies that encourage collaboration and new ways of working, are open to taking risks and allow their leaders and employees access to the resources they need to develop digital skills and know-how.

Artificial intelligence technologies (blockchain, cloud, and virtual reality) are drivers of digital transformation -

Fundamental role of these technologies is to improve the quality of data and information flow and robustness of insights derived from data.

What is artificial intelligence?

AI refers to any computer programme or system that does something we would normally think of as intelligent in humans. AI technologies extract concepts and relationships from data and learn independently from data patterns, augmenting what humans can do and interacting with humans in a natural way.

Given biopharma's access to large data sets and the resources to access the required computing power and top technical talent, those companies who are willing to invest early are poised to capitalise on AI.

Machine learning
- Deep learning
- Supervised learning
- Unsupervised learning

Natural language processing

Speech

Computer vision

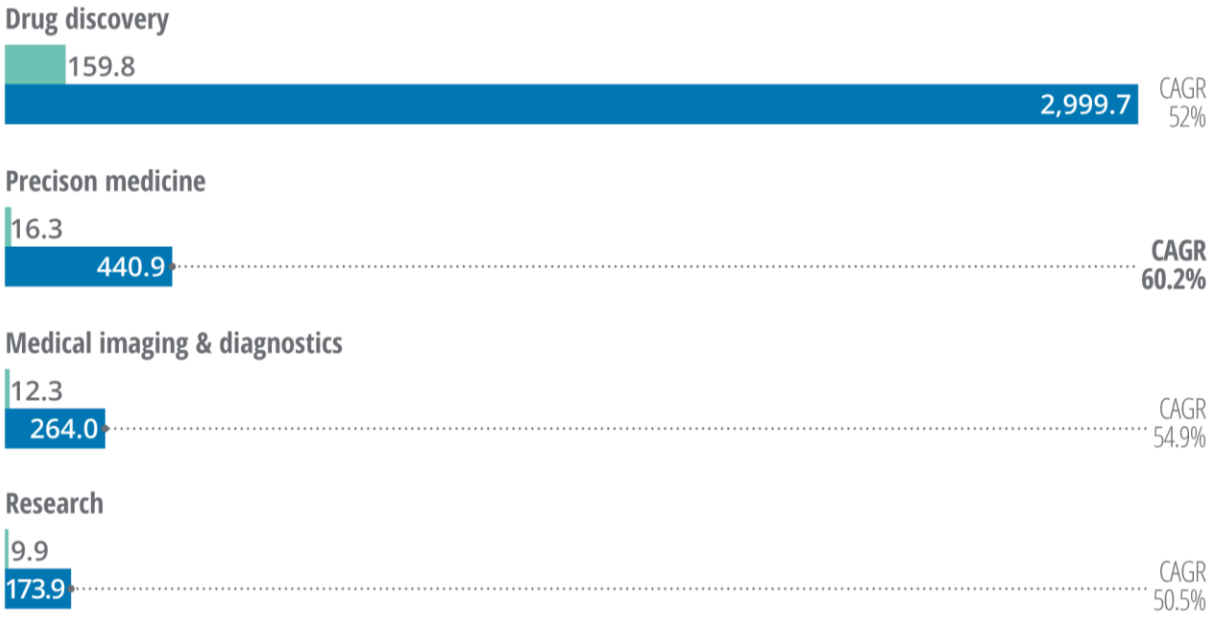
Planning

Expert systems

Robotics

The AI market in biopharma

Expected growth by application and geographical region, 2018-2025



NORTH AMERICA
2018 market share:
37.4%
2018-2025 CAGR:
53.9%
$74.1m to **$1.52b**

EUROPE
2018 market share:
30.1%
Expected 2018-2025 CAGR:
52.5%
$59.6m to **$1.14b**

APAC
2018 market share:
25.9%
Expected 2018-2025 CAGR:
53.8%
$51.4m to **$1.05b**

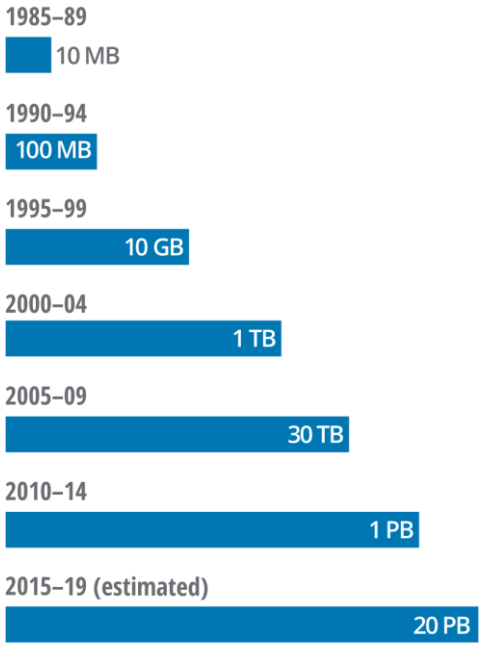
REST OF WORLD
2018 market share:
6.7%
Expected 2018-2025 CAGR:
43.7%
$13.2m to **$167.5m**

Factors driving the growth of AI across the value chain

Data volumes, computing power and computing costs

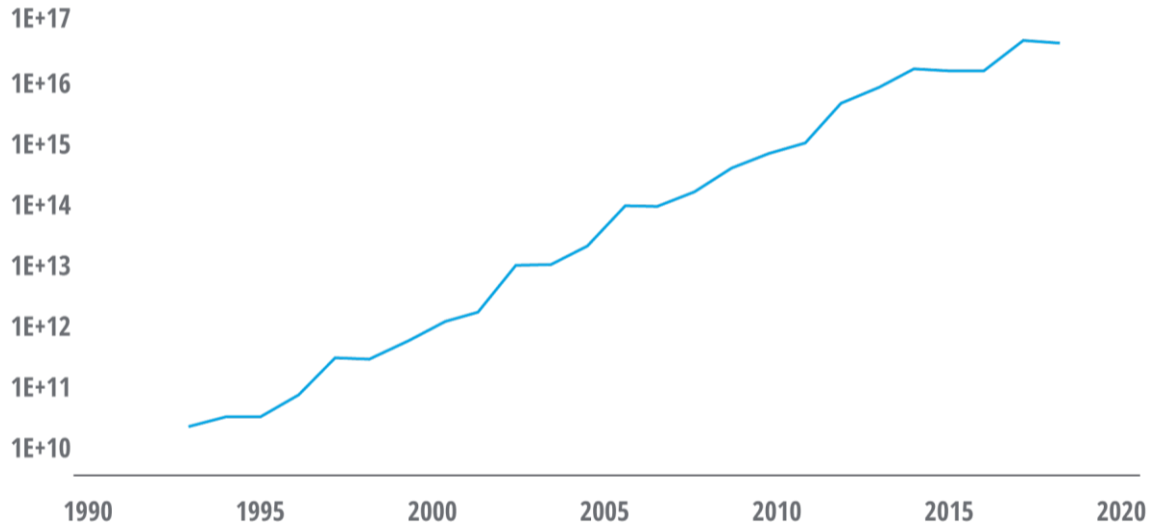
Increase in genomics data over time

Increase in volume of genomics data (base pairs/year)

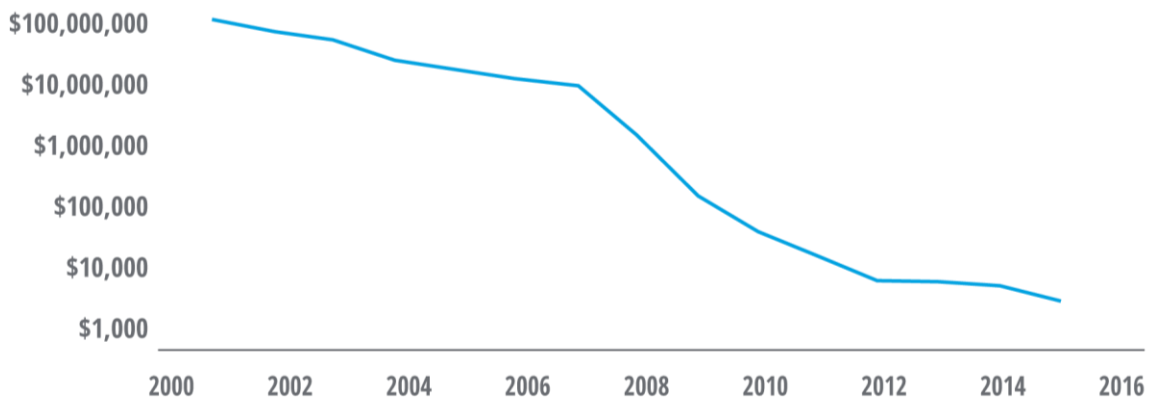


Supercomputer processing power

Floating-Point Operations per Second (FLOPS)

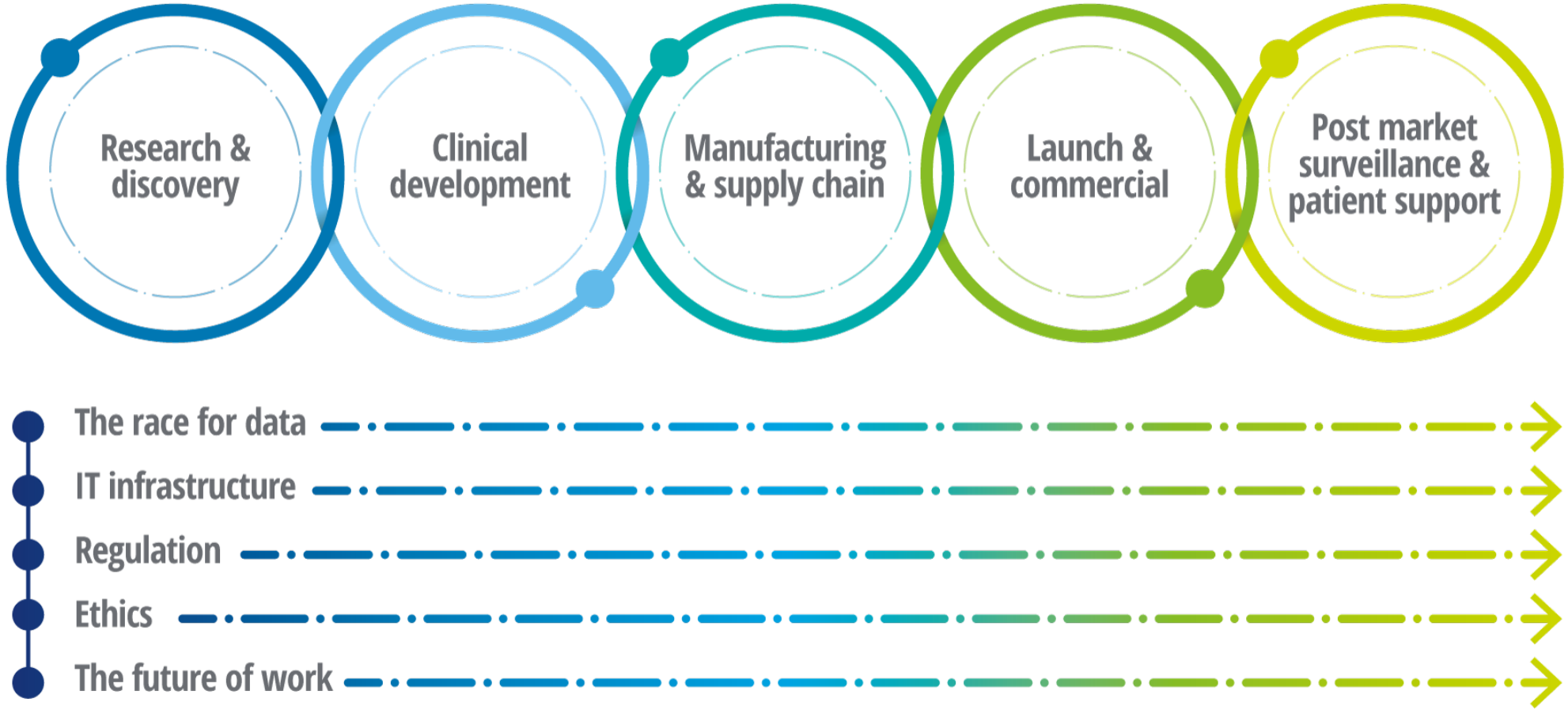


Cost of sequencing a full human genome



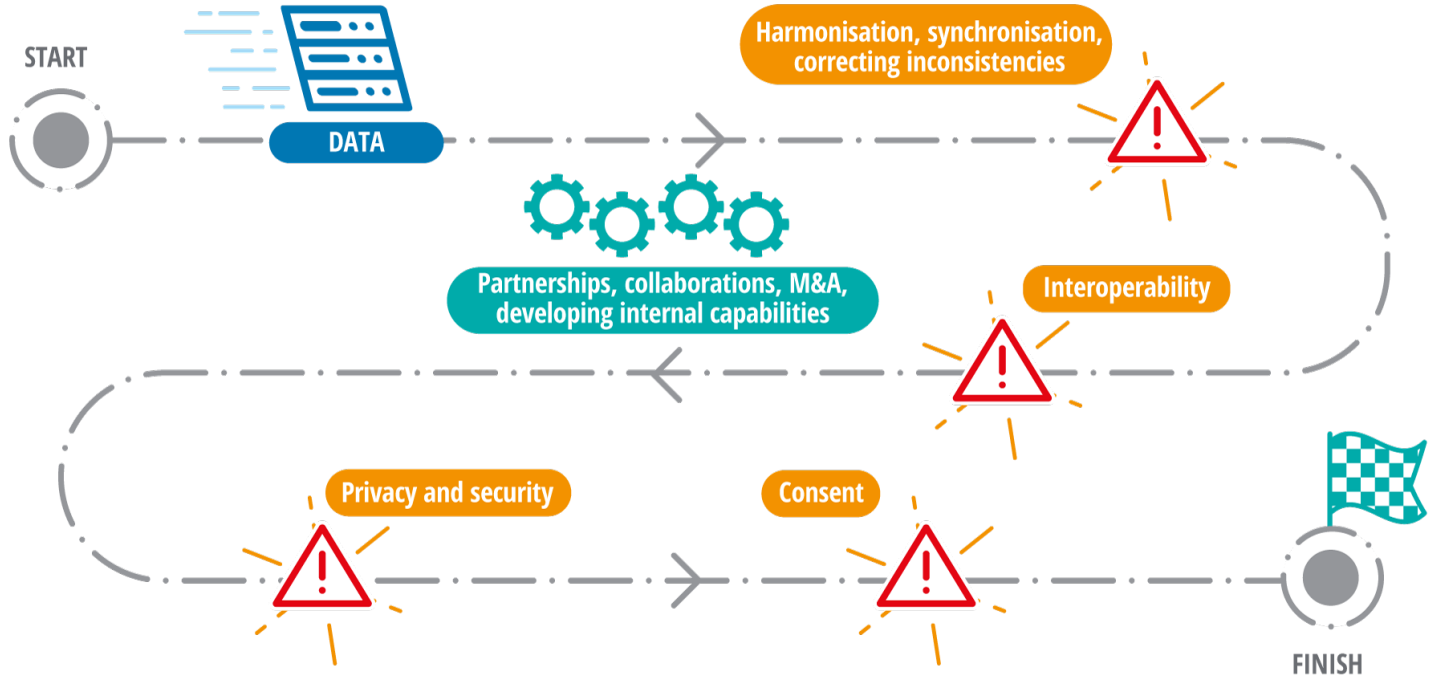
The challenges and opportunities in AI adoption

Critical themes that cut across the value chain are influencing AI implementation



The race for data

Winning the race for the highest quality data will be the deciding factor in determining which biopharma companies survive and thrive in a digitally transformed world



How to win

Biopharma companies need to ensure that any patient data they use has specific consent to be used for the specified purpose, and that it is private and secure. Improving information exchange between all stakeholders on threats, incidents, vulnerabilities, best practices and mitigation strategies is an imperative. Biopharma companies also need to commit to cybersecurity education across all tiers of the organisation and supply chain, and ultimately with customers. Tackling the interoperability challenge can be accelerated through the adoption of open platforms, based on open data standards.

Updating IT infrastructure

Improvements in the computer systems and infrastructure that perform the algorithms, including the hardware, software and services, are key factors enabling the rise of AI

Cloud computing and data storage offer potential advantages compared to on-premises if security, privacy and regulatory requirements are met

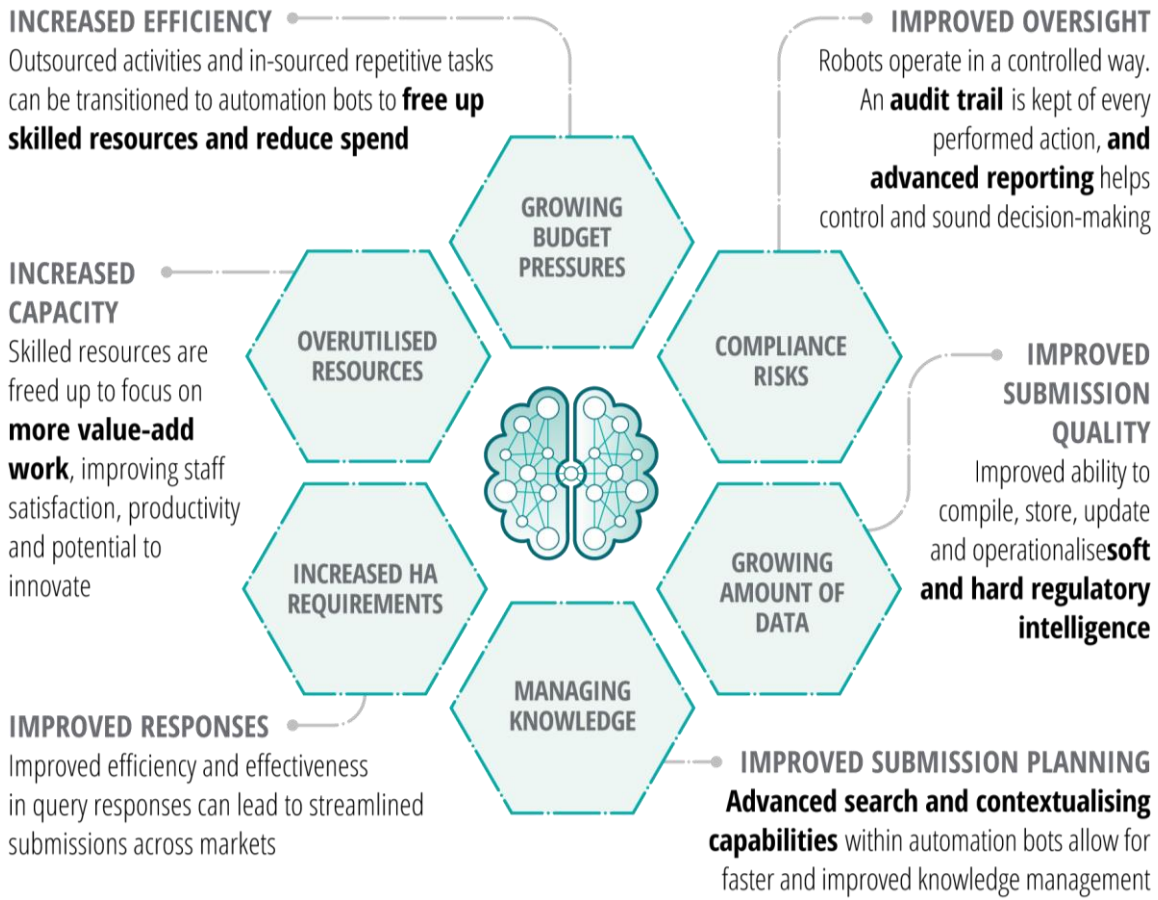
Deloitte Global predicts that in 2019:

- all industries will accelerate their use of cloud-based AI software and services
- among companies that adopt AI technology, 70% will obtain AI capabilities through **cloud-based enterprise software**
- 65% will create AI applications using **cloud-based development services**.

A **hybrid cloud** can be advantageous, which allows biopharma companies to store their core confidential data and applications on a private cloud while selectively utilising the public cloud when appropriate.

Navigating regulation

Biopharma companies can use AI to optimise the effectiveness of their response to the increasingly complex regulatory environment



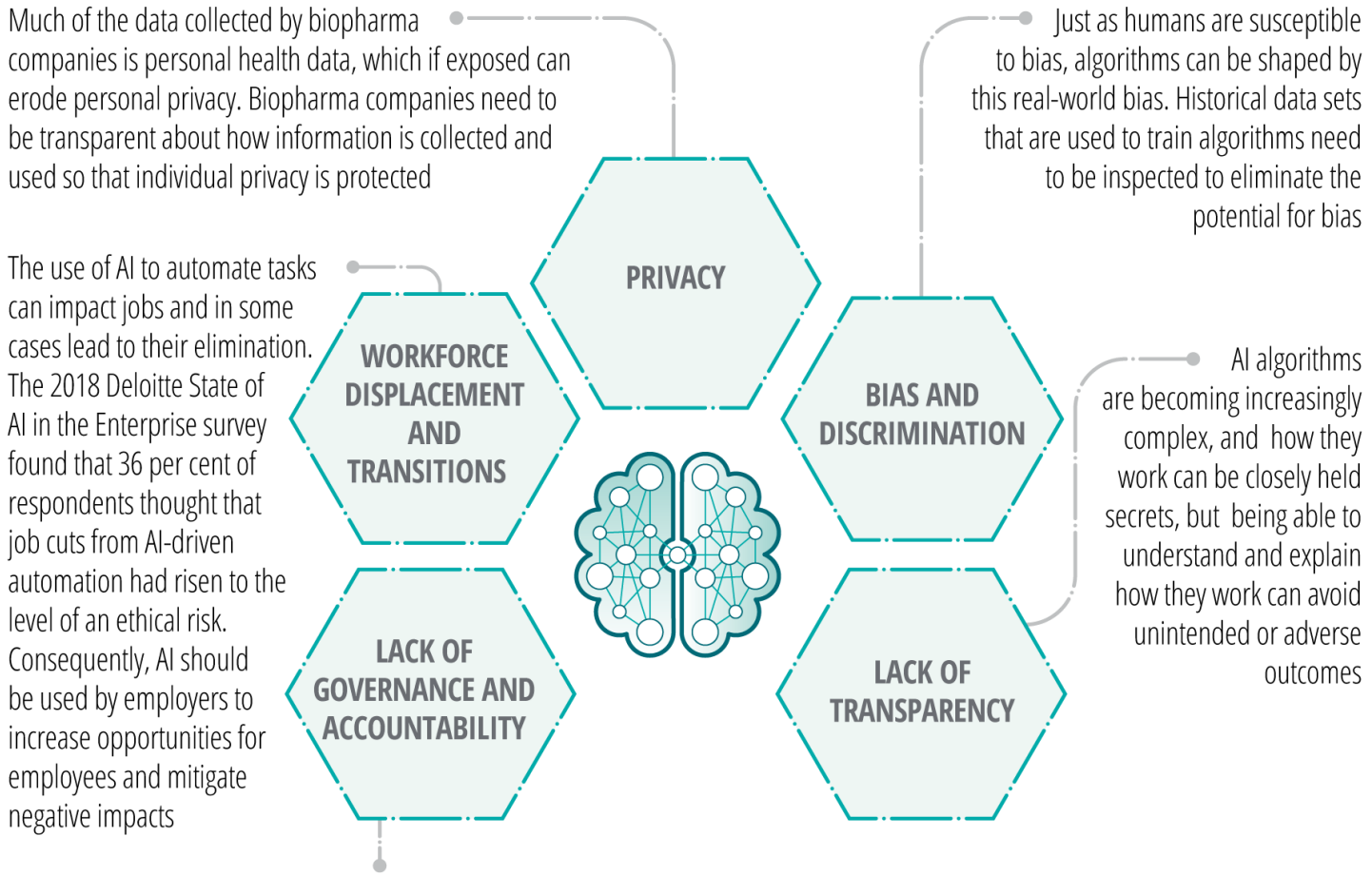
Biopharma companies should consider:

- taking steps to **standardise global operations** to facilitate regulatory convergence
- increasing the **transparency of operations and data** to highlight to regulators the benefits of partnerships, as well as improve public trust in the organisation
- transforming **culture, processes and operating models** to embrace the newfound interconnectivity of the regulation.

Ethical AI implementation

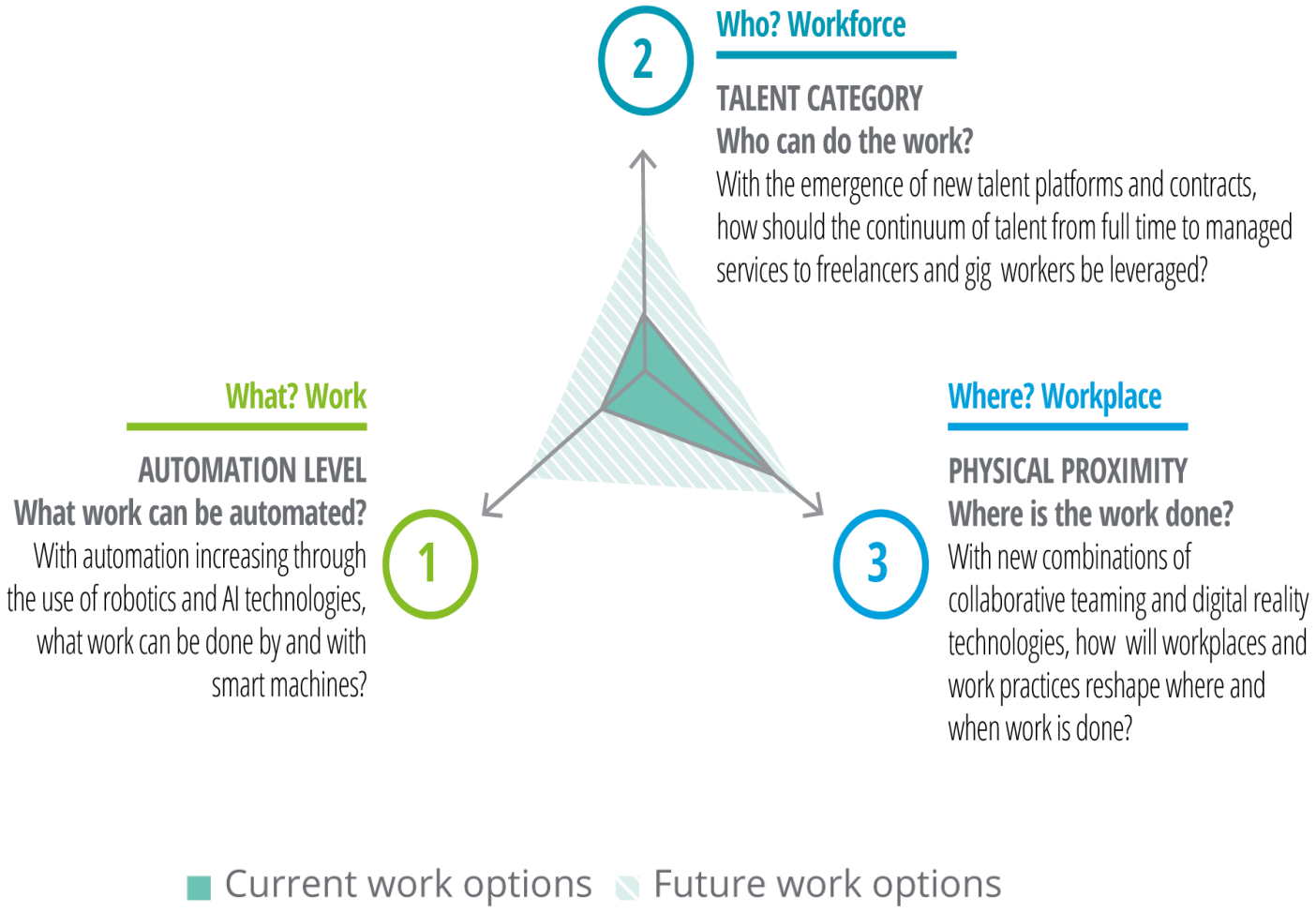
The five biggest issues around the ethics of data and AI technologies

As AI technologies become more powerful, so do the potential for unintended or adverse outcomes. The questions that surround AI ethics can be difficult, and the operational aspects of addressing AI ethics are complex, resulting in five main issues around the ethics of data and AI technologies.

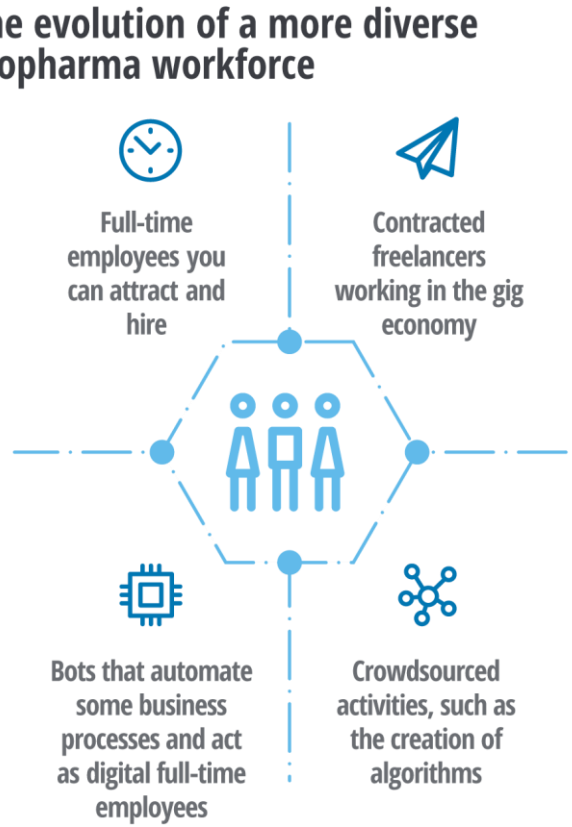


The future of work encompasses changes in who, what and where of work

AI technologies and digital transformation will result in major changes to roles and responsibilities within biopharma companies



The next generation of biopharma talent will need to be **agile, digitally literate and open to continuous learning** as part of their career development



Source: Deloitte analysis.

Biopharma's AI-fuelled future

AI will impact the entire biopharma value chain

FIGURE 15

Some of the main applications of AI across the biopharma value chain

- Aggregating and synthesising information
- Mining data to identify drug targets and molecule interactions
- Understanding disease mechanisms
- Drug candidate generation and selection

- Trial design
- Site selection
- Recruitment optimisation
- Process optimisation
- Predictive toxicity and risk monitoring
- Monitoring drug adherence

- Supply chain planning
- Predictive maintenance
- Inventory management
- Demand forecasting
- Logistics optimisation
- Workforce planning
- Procurement
- Medication tracking, safety and security
- End-to-end visibility

- Launch coordination
- Patient engagement
- Physician decision support
- Marketing operations
- Predictive pricing

- Medication adherence
- Adverse event recognition
- Patient monitoring
- Compliance monitoring
- Patient support programmes/ platforms

Source: Deloitte analysis.

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Intelligent drug discovery: Powered by AI

November 2019

Deloitte Centre *for*
Health Solutions

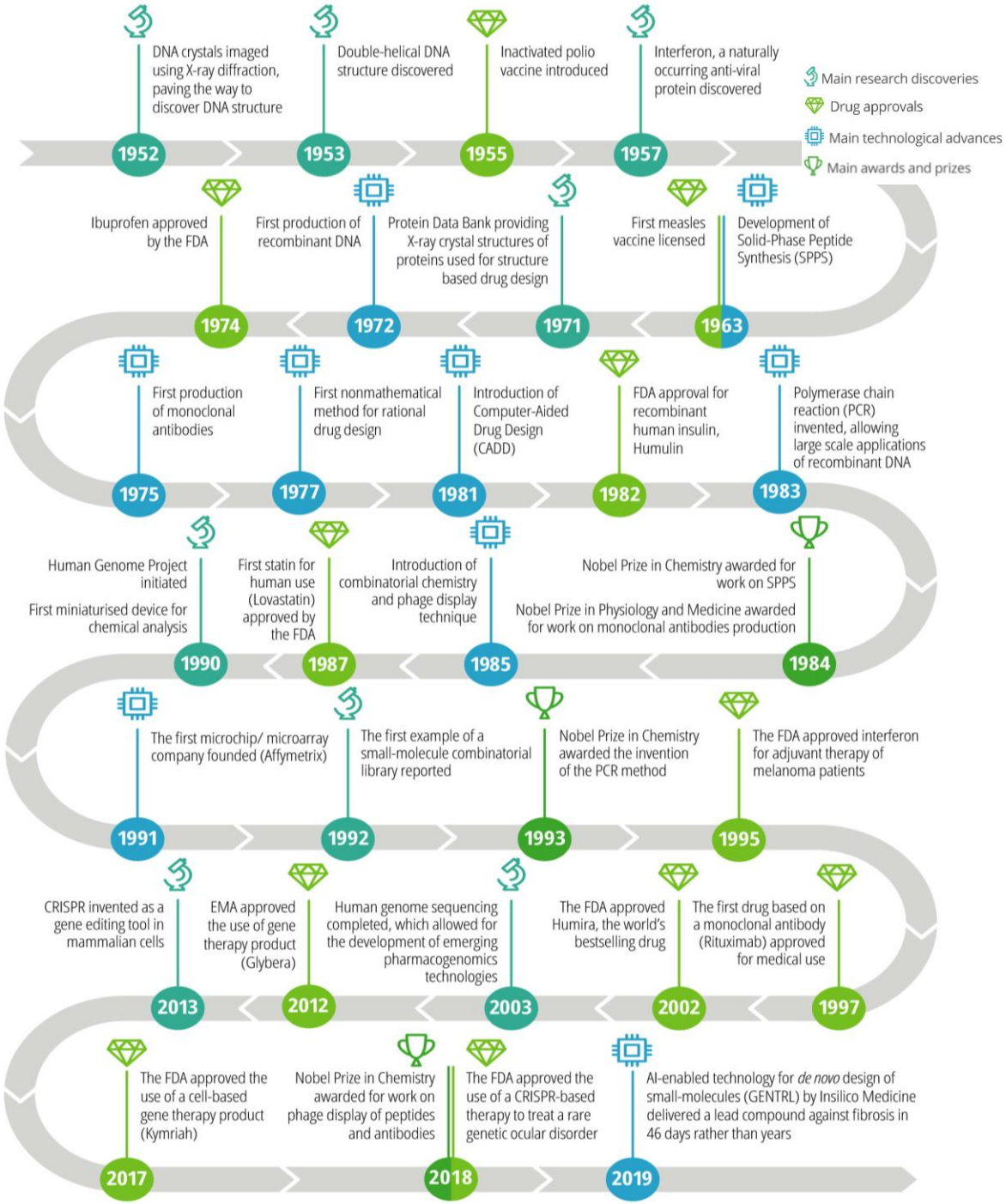
The evolution of drug discovery

Historically, the discovery of new therapeutics involved the extraction of ingredients from natural products and basic research to find potential treatments.

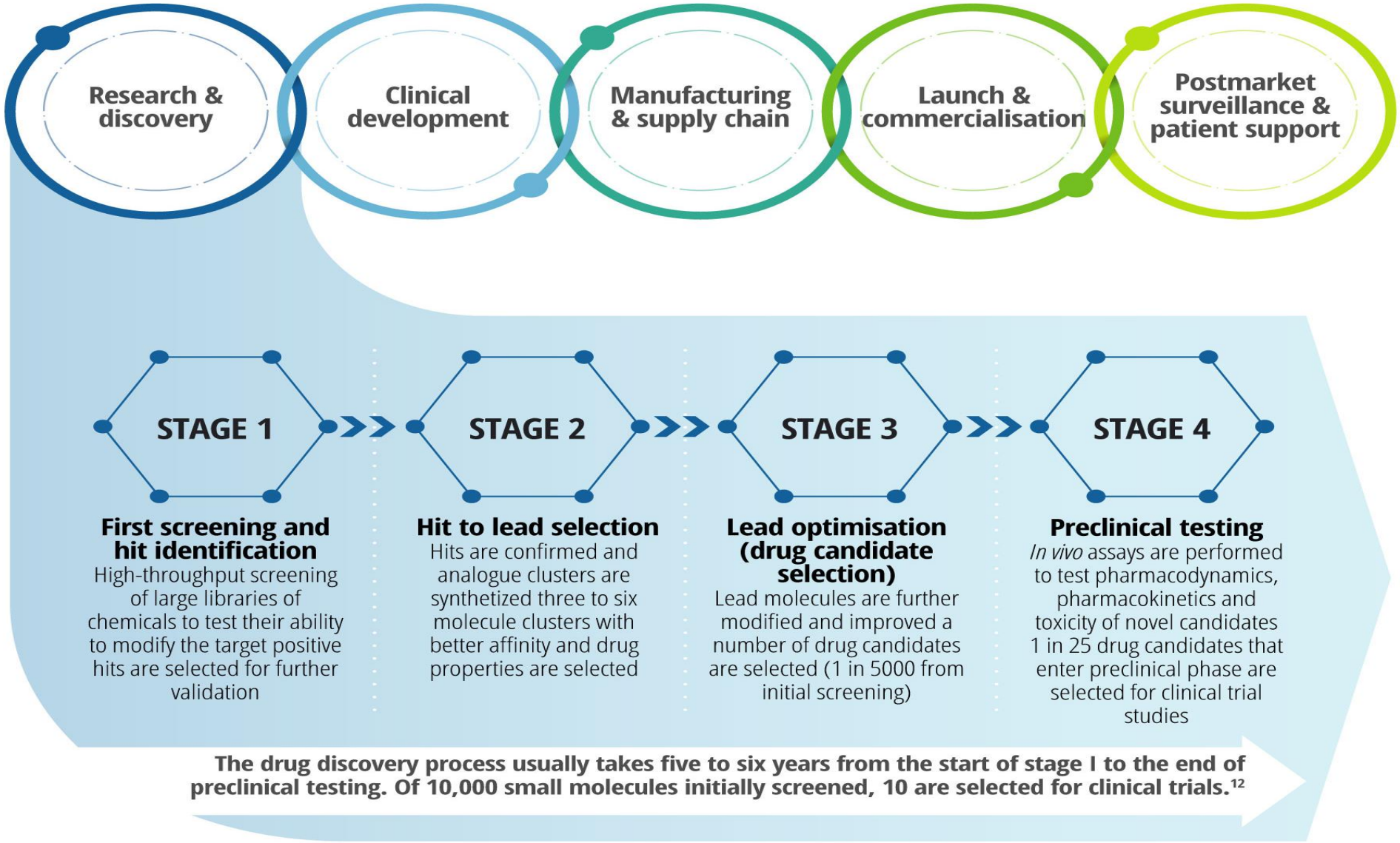
The majority of drugs discovered during the 20th century were chemically synthesised **small molecules**, which still make up 90 per cent of drugs on the market today.

Since the 1990s, scientific and technological advances have led to the discovery of larger, more complex, biological therapeutics known as **biologics**, which include a wide range of products such as antibodies, antisense drugs, blood and blood components, recombinant therapeutic DNA and proteins, and vaccines.

Despite advances in genomics, chemical synthesis and other molecular biology techniques, only around one-third of the estimated 20,000-30,000 known diseases have an adequate treatment.



Discovering drugs is a crucial first step in the biopharma value chain



Drug discovery is a long, expensive and often unsuccessful process

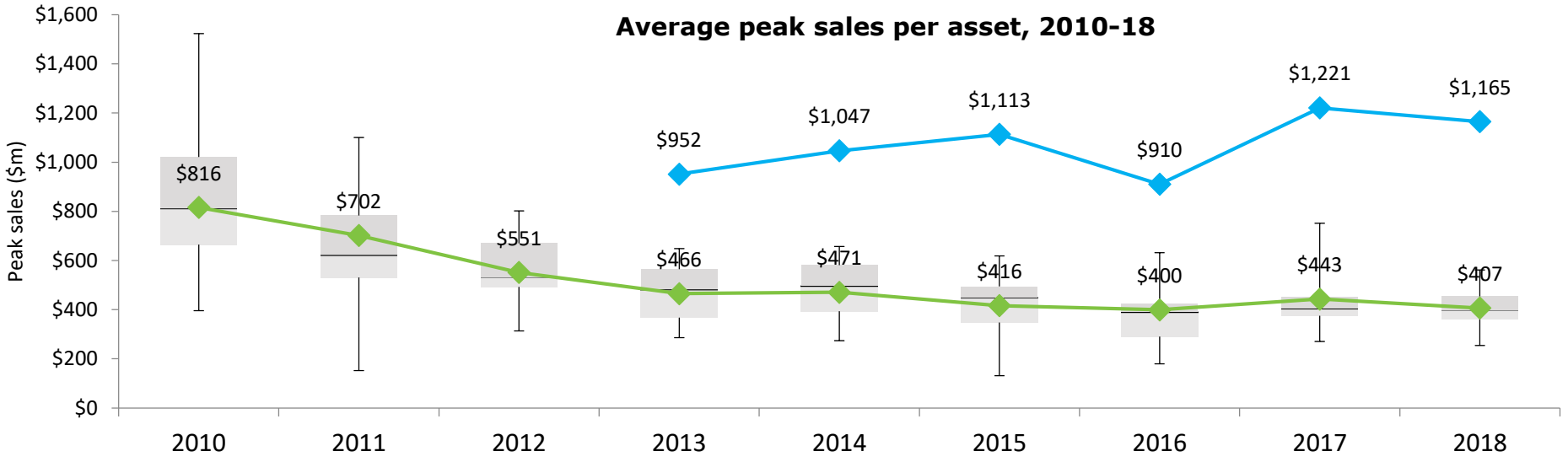
The average time to bring a molecule from discovery through to launch is 10-12 years.

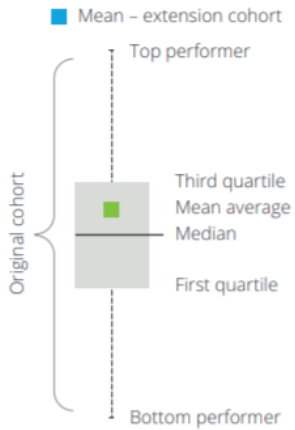
According to our report *Measuring the return from pharmaceutical innovation 2018*:

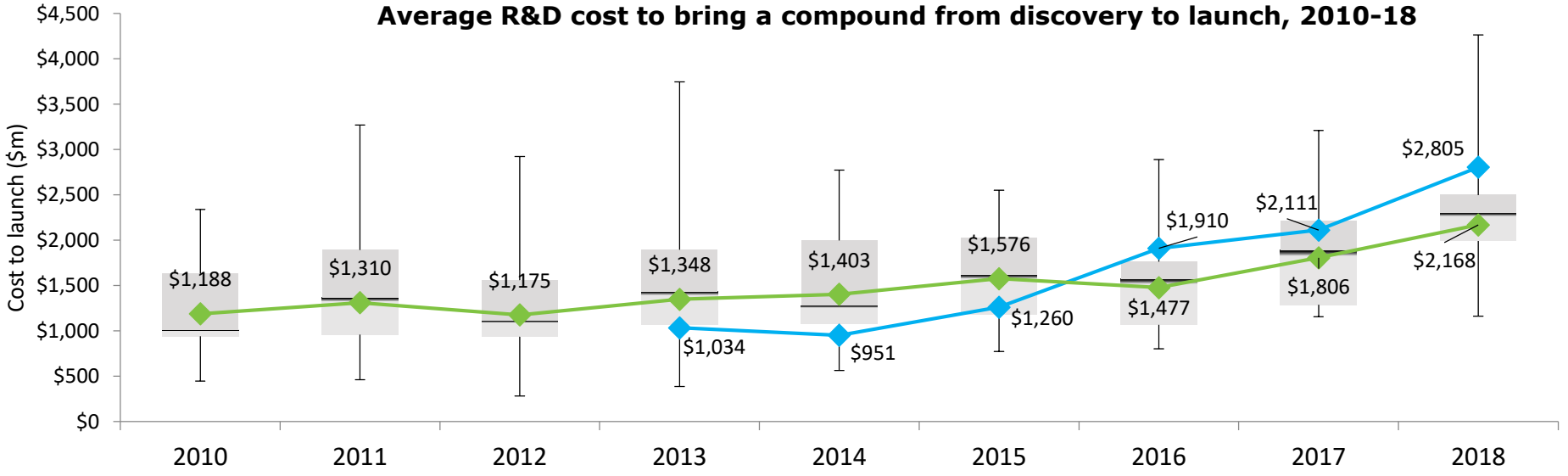
- The average cost of the cost of the R&D process calculated in 2018 was $2,168 billion, almost double the $1,188 billion value in 2010.
- The average forecast peak sales per late-stage asset in the drug pipeline in 2018 was $407 billion a significant decline of over 50% from the $816 billion in 2010
- The expected return on investment from drug development has declined steadily since 2010 from 10.1 to 1.9 % in 2019.

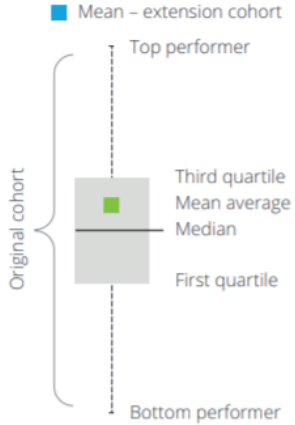
Finding ways of improving the efficiency and cost-effectiveness of bringing new drugs to the market is an imperative for the industry.

Peak sales per asset have stabilised but cost per asset has increased to a new high, partly driven by a decline in late-stage asset numbers









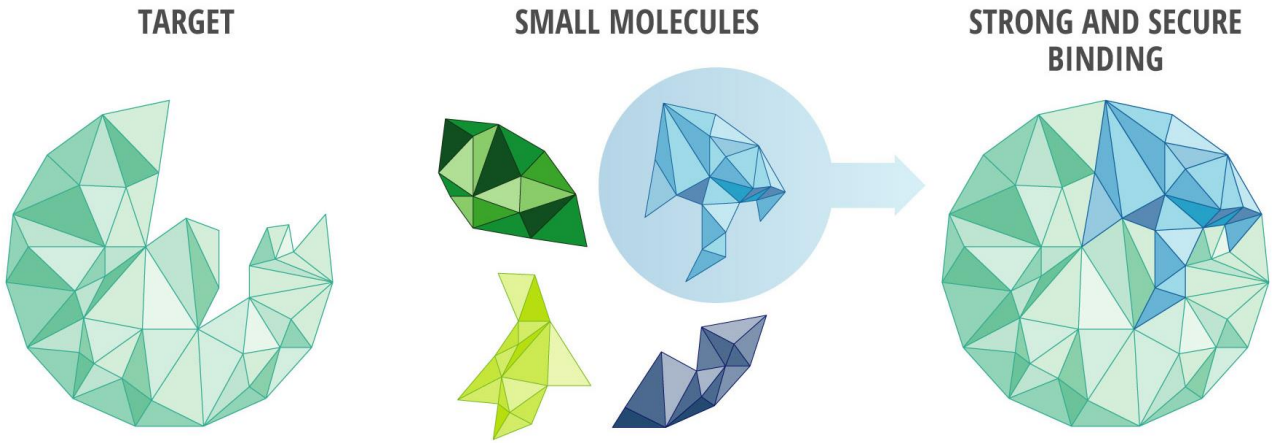
Source: Deloitte proprietary research

Around one-third of the R&D process cost is spent on the drug discovery phase

- Of the 10,000 molecules initially screened, only 10 ever make it to clinical trials
- The chance of success for a compound entering phase I trials is slightly under 10 per cent and has not increased in a decade

Improving discovery and clinical trial success rates is critical for the future of drug development

One of the factors that reduces the accuracy of the discovery process is the **lack of precise knowledge on the three-dimensional structure of drug compounds and targets**. Their binding affinity (specificity) and kinetics are ultimately what determine the efficacy of action together with efficient drug delivery



Intelligent drug discovery: Why AI? Why now?

AI-enabled solutions are emerging as a crucial tool for transforming the process of researching disease mechanisms of action and revolutionising the understanding of how drugs bind to targets, improving specificity. If adopted at the drug discovery stage, AI solutions have the potential to kick-start the productivity of the entire R&D process.

AI has the potential to:

Reduce timelines for drug discovery and improve the agility of the research process

The successful application of innovative technologies could speed up the discovery and preclinical stages by a factor of 15.

Increase the accuracy of predictions on the efficacy and safety of drugs

Currently, most drugs fail clinical trials due to efficacy and safety issues. Given the growing cost of bringing a drug to market, a ten per cent improvement in the accuracy of predictions could save billions of dollars spent on drug development.

Improve the opportunity to diversify drug pipelines

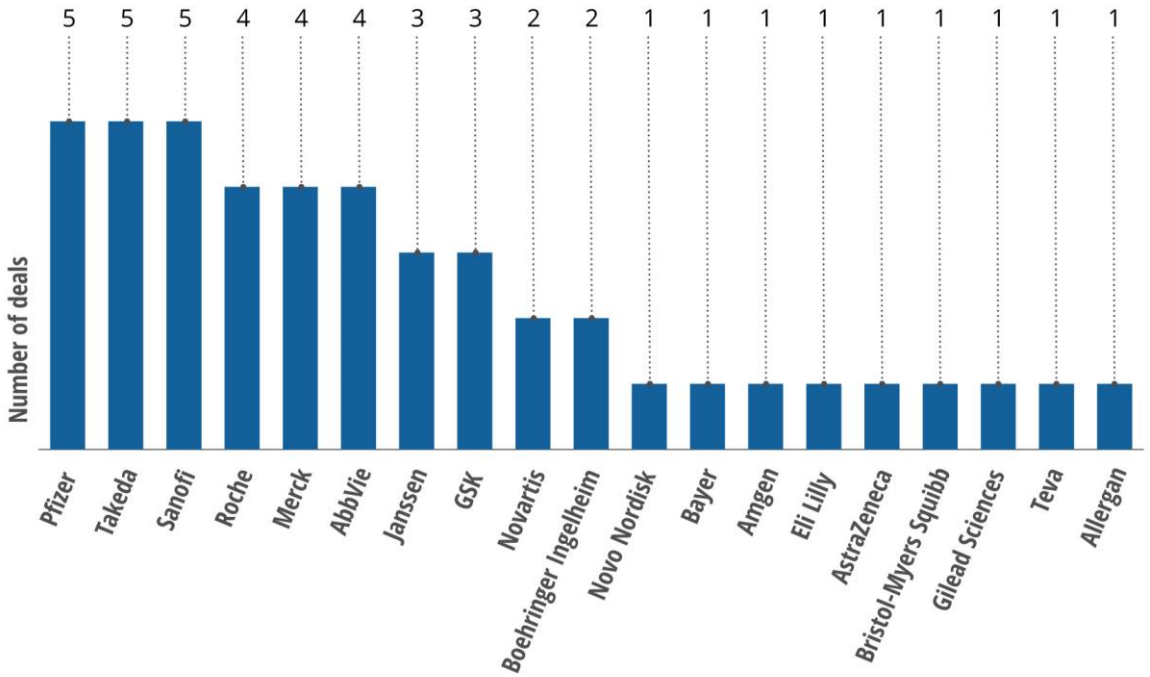
AI-enabled prediction tools could improve the speed and precision of discovery and preclinical testing, opening up new research lines and enabling more competitive R&D strategies. Finding new niches of competitive advantage could reduce withdrawals and improve asset sales.

The rise of AI drug discovery disruptors

According to our report DKA's report *Landscape of AI for Drug Discovery and Advanced R&D Q2 2019*:

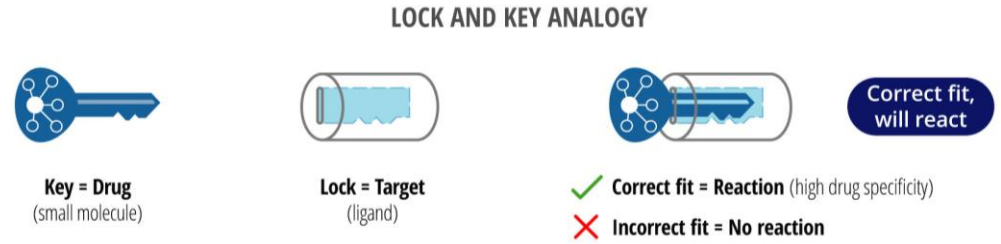
- As of July 2019, there are 170 AI companies, 50 corporations, 400 investors and 35 major R&D centres.
- In the second quarter of 2019, the number of R&D centres increased by five, start-up companies increased by 20, collaborations increased by 30 and investors increased by 50 compared to the first quarter
- 120 out of the 170 companies are actively tackling different areas of drug discovery.

Most major biopharma companies are now exploring AI-driven solutions for drug discovery, making a variety of deals to access this capability

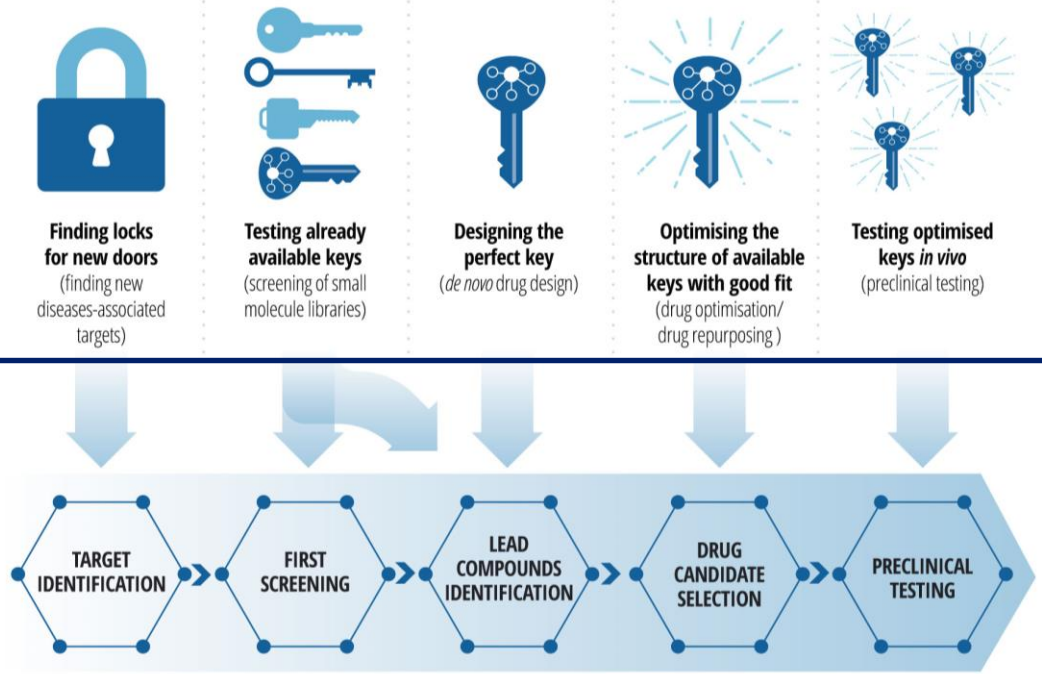


Five main AI challenges for drug discovery: Finding the ideal key for a complex lock

The approach to finding new drug candidates for disease targets is like trying to find the perfect key for a specific lock.



The majority of AI solutions for drug discovery available today are focussed mainly on **five different approaches to this challenge**

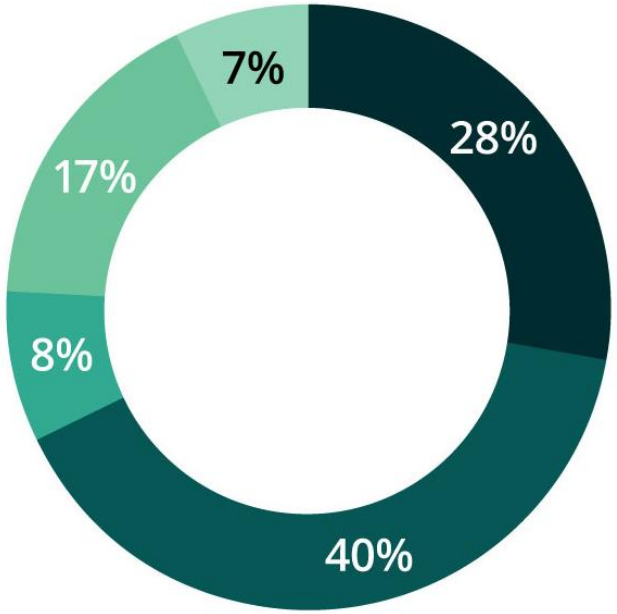


Five main AI challenges for drug discovery

AI for drug discovery companies frequently provide algorithms and platforms to address more than one of these challenges of biopharma research and discovery, although currently **40 per cent of their focus is on screening**

Number of AI for drug discovery start-ups by area

- Finding new targets
- Screening of small molecule libraries to find new candidates
- *De novo* drug design
- Drug optimisation and repurposing
- Preclinical testing



Finding new diseases-associated targets

- AI algorithms leverage large amounts of basic research data from public and private sources to enable a better understanding of diseases mechanisms.
- AI can tailor approaches for a more accurate understanding of pathological cellular and molecular mechanisms.

Case Study 1

BenevolentAI, a UK company founded in 2013, is creating and applying AI technologies to to transform the way medicines are discovered, developed, tested and brought to market. The company has the capability from early discovery right through to late-stage clinical development.

The company aims to use the power of AI to put patients first, and tangibly transform their lives by creating a way to lower drug discovery and development costs, decrease failure rates and increase the speed at which medicines are delivered to patients.

Screening of small molecule libraries to identify new drug candidates

Extremely accurate predictions of binding profiles can be created for targets, by using DL technologies, such as convolutional networks.

Case Study 2

Atomwise, a US company founded in 2012, uses AI technology to predict small molecule-protein binding affinities and focusses on identifying potential therapeutics for any disease target.

The AI platform AtomNet is a patented structure made of DL Convolutional Neural Networks for hit discovery and lead compound identification and optimisation. It learns the three-dimensional features of drug-to-target molecular binding and identifies discriminators. The platform can select hits that have key features such as the ability to cross the blood-brain barrier in a short amount of time with new lead compounds obtained in days, bypassing the need for costly and long high-throughput screening experiments.

De novo design of new drug candidates

A step forward from AI-enabled screening of small molecule libraries is *de novo* design of new compounds that fit, with precision, the structural criteria required to bind specific targets.

Only the information related to the structure of the target is necessary, avoiding the bias of small molecule screening. DL solutions are at the core of this groundbreaking precision approach.

Case Study 3

Insilico Medicine, a Hong Kong-headquartered company initially founded in 2014 in the US, uses deep generative models, which are ML techniques based on neural networks that produce new data objects.

They recently developed a platform called Generative Tensorial Reinforcement Learning (GENTRL), which combines two distinct DL models and has generated new drug hits against fibrosis in 21 days and validated them, selecting one lead in another 25 days.

Drug optimisation and repurposing

Better insights on the polypharmacology of drugs could be used to improve drug development success rates by identifying offset targets and unwanted toxic effects and also providing opportunities for drug repurposing.

Case Study 4

Cyclica, a company founded in Toronto, Canada, in 2013, provides an integrated cloud-based and groundbreaking AI-augmented platform for drug design, off-target profiling, system biology linkages, structural pharmacogenomics insights and drug repurposing based on polypharmacology.

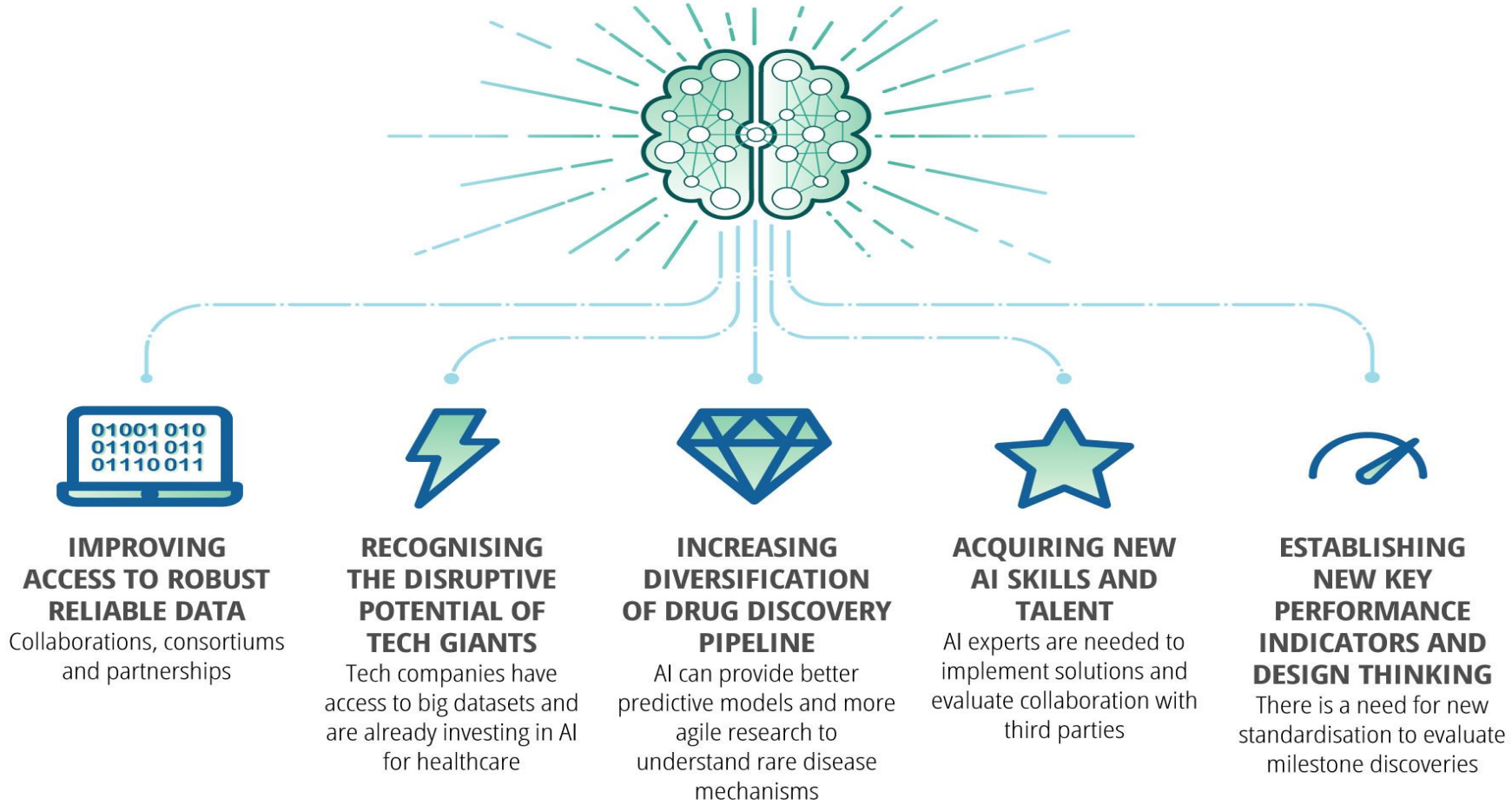
They have developed two proprietary drug discovery platforms that are now being used to identify novel multi-target solutions for complex neurodegenerative diseases, through a collaborative environment.

Importantly, by using their platform, Cyclica discovered the molecular reason leading to the fatal side effects exhibited by a chronic pain treatment drug candidate in clinical trials in 2016, identifying a plausible toxic protein target.

Five key considerations for biopharma's adoption of AI

The integration of AI into traditional processes needs to be underpinned by a robust strategy

Developing successful strategies requires biopharma companies to consider five key actions

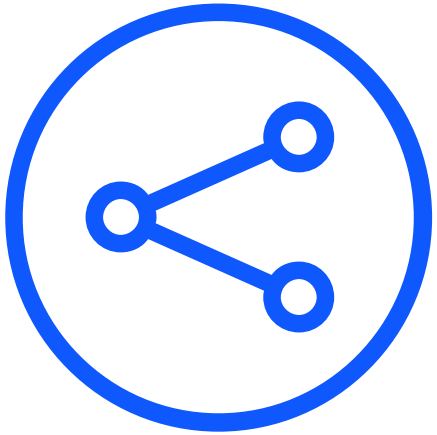


Source: Deloitte analysis.

Improving access to robust and reliable data: Data sharing is the new competitive advantage

Collaborations and consortiums:

For biopharma companies to use AI to improve drug discovery they need access to large datasets. While this can be achieved through industry collaborations, this is challenging in the highly competitive traditional biopharma culture. **The benefits of achieving a better drug discovery process outweigh the risks of sharing knowledge** and lead to more successful R&D pipelines, saving billions of dollars. Examples include:



- **The Machine Learning Ledger Orchestration for Drug Discovery MELLODDY** project is a consortium of 17 partners created to enable effective sharing of the chemical libraries of ten biopharma companies, specifically for AI drug discovery applications. The collaboration is underpinned by the use of blockchain technologies aimed at improving the accuracy of predictions for identifying better drug candidates.
- The **Machine Learning for Pharmaceutical Discovery and Synthesis Consortium** is a collaboration started in 2018 by the Massachusetts Institute of Technology involving 13 major biopharma companies. It aims to facilitate the design of useful algorithms for the automation of small molecule discovery.
- The **Accelerating Therapeutics for Opportunities in Medicine (ATOM) consortium** is another US-based collaborative initiative for the development of state-of-the-art, AI-enabled drug discovery processes. Established in 2017 by GSK, Lawrence Livermore National Laboratory, University of California San Francisco and Frederick National Laboratory for Cancer Research, it aims to significantly reduce the preclinical drug discovery timeframe for the patients' benefit

AI provides an opportunity to diversify pipelines

Case Study 6

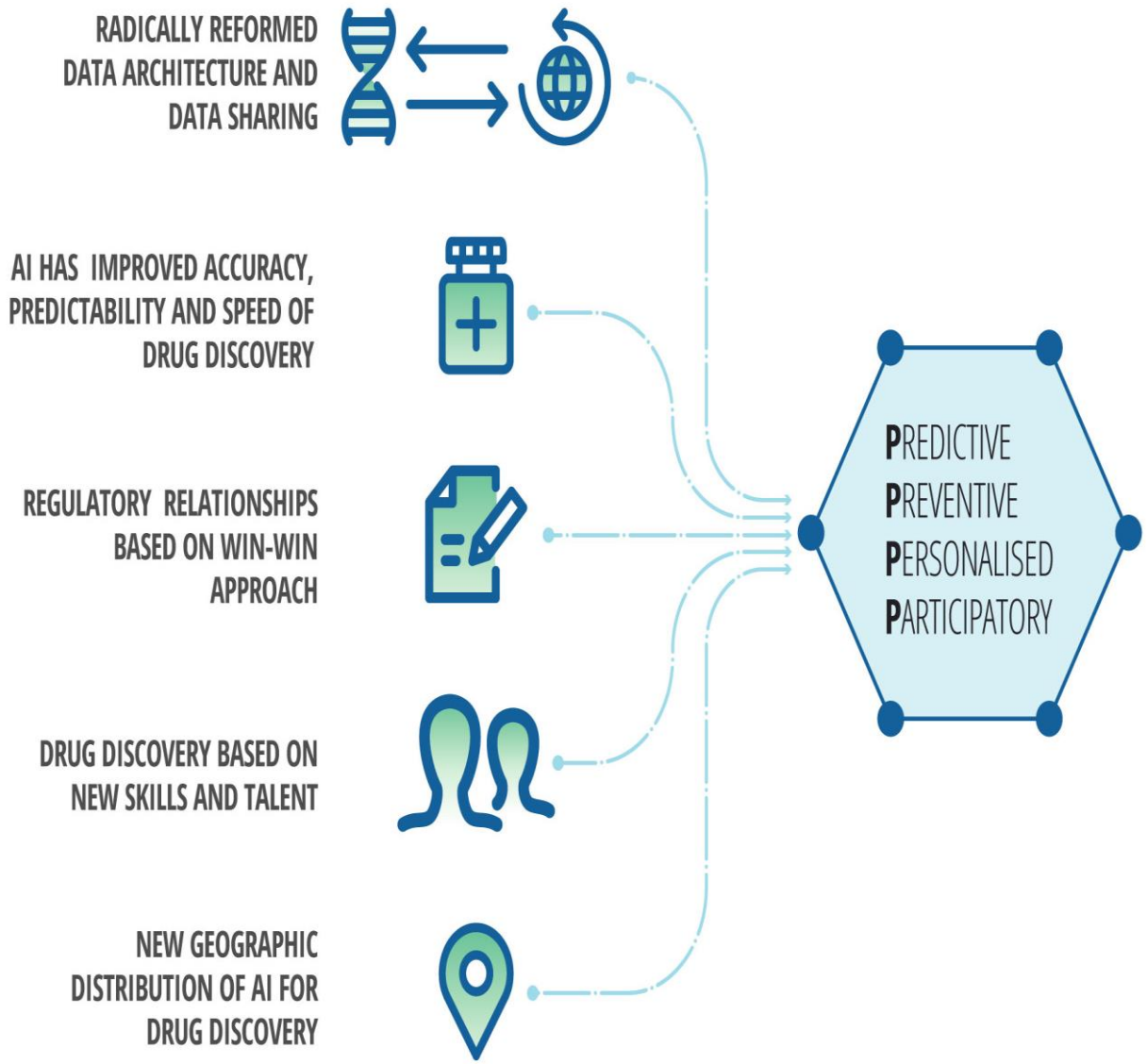
Exscientia, a UK company founded in 2012, has developed a model that three main proprietary AI approaches, which capitalises on accessing data from academic collaborations and the use of crowdsourcing and translational disease models. This data is fed into predictive models from big data, and active learning from small data, and then input to a bespoke discovery process platform to generate phase I ready assets.

The company has secured relevant partnerships with a number of big biopharma companies over the past four years, and is contributing to the understanding of key disease mechanisms to help diversify drug pipelines

The future of drug discovery: Delivering '4P' medicine

The adoption of AI and other innovative technologies, and the use of big data from multiple sources is enabling **more precise targeted treatments** and shifting the health ecosystem toward a future where medicine is personalised, predictive, preventative and participatory (the '4Ps'), leading to **new, more efficient and effective models of care**.

Over the next decade, these shifts will have a significant impact on treatments and on patient outcomes, particularly in those areas of medicine with unmet need.



Source: Deloitte analysis.

Drug discovery and the future of work

- Success for companies using AI for drug discovery depends on having **highly skilled interdisciplinary leadership**, as well as **AI-friendly CEOs** and board members to drive the adoption of AI
- For biopharma companies to thrive, they will need **strong AI divisions** and a strategy for acquiring or collaborating with the best AI start-ups.
- **Agility and effective communication between departments with interdisciplinary skills** in both business and technology, including deep experience in AI, computer science, data science, engineering, life sciences, mathematics and statistics, will be a strategic asset.
- Both big tech and biopharma companies will be competing to **hire and retain sufficient numbers of AI experts and biochemical specialists**. However, these and other key talents, such as bioinformatics and computational biologists, are in short supply.
- This **changing drug discovery landscape will transform biopharma R&D laboratories and research facilities**. While they will continue to employ biologists and chemists, they will also employ AI experts and data scientists. Academia should consider partnering with biopharma, tech companies and CROs to develop education exchange programmes to enhance the required technology capabilities across the ecosystem.

The changing geography and rise of emerging markets in the future of drug discovery

The US currently leads the AI drug discovery sector in both investment (63.5 per cent) and number of AI for drug discovery companies (60 per cent of start-ups).

The UK is the leading country after the US in terms of investment and number of AI tech companies, and it is maintaining the same pace of growth.

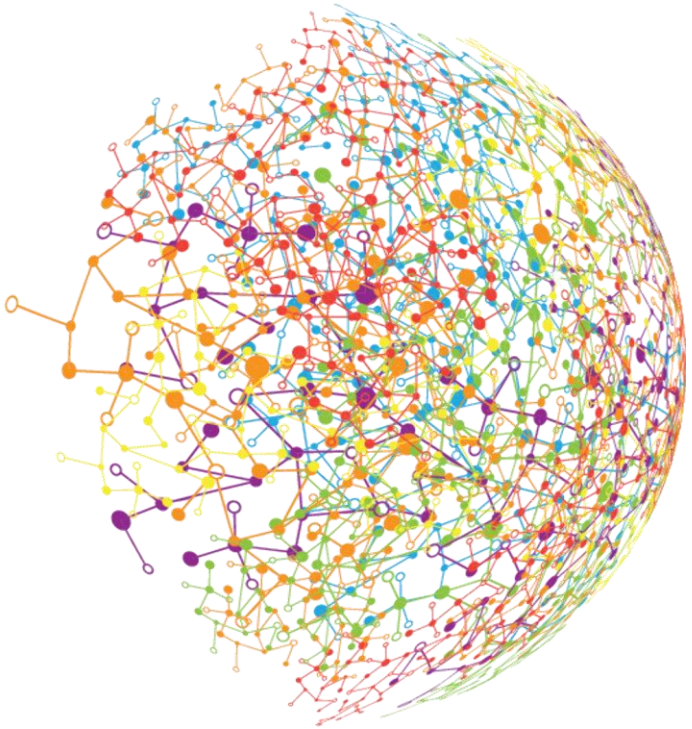
Although Asia has the fifth-lowest proportion of AI for drug discovery companies, Asia's activity in this space is increasing, especially in investments in foreign companies, mostly US-based

Case Study 7

China has swiftly become one of the largest biopharma and medical product markets in the world, projected to reach US$145-175 billion in sales by 2022.Quicker regulatory approval and widening market access are among the changes that have made China a target market for biopharma companies to launch innovative medical products.

China aims to become a global leader in AI and to be at the forefront of innovative, digital approaches to drug design. The Chinese government is creating programmes to increase AI skills and talent. Considering the rise of personalised and precision medicine in the next decade, China has a significant competitive advantage because there is the potential to collect data from more than 1 billion citizens.

Regulating the new AI drug discovery landscape



- **Regulations and laws are changing rapidly** in response to the use of new technologies across industries, requiring biopharma companies to develop legal and ethical expertise in AI drug discovery.
- AI start-ups and biopharma companies are increasingly promoting open collaboration and data sharing through the cloud; in order to avoid data ownership, safety and privacy breaches, they are increasingly **adopting blockchain technologies to be able to demonstrate compliance with regulations**.
- A key challenge will be how to address **health inequalities related to genetic differences**. Organisations need to create **ethical boards and develop an improved regulatory system that covers the use of AI solutions for drug discovery, including the use of personalised data**.
- As drug discovery begins to use the wider sources of data discussed in this report, a set of new **regulations protecting data safety, privacy and access to electronic health records will also be required**.

What next?

- By 2030, drug discovery processes are likely to be mostly outsourced to external AI companies, where research will be done mostly *in silico* and in collaboration with academia.
- The timings from screening to preclinical testing will be reduced to a few months rather than five/six years, and new potential drug candidates will be identified at increasingly lower costs.
- In the next five to ten years, the number of companies using AI for drug discovery will increase exponentially and new drugs capable of treating very precise pathologies will become the norm.
- Major disruption will come from biopharma companies that apply these next generation techniques to biomarker development, drug discovery and drug repurposing.
- Over the next decade, patients can expect these developments to have a significant impact on the effectiveness of their treatment options and on disease outcomes, particularly in areas with no treatments available currently.

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