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Intelligent drug discovery

Powered by AI

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Life sciences companies continue to respond to a changing global landscape, and strive to pursue innovative solutions to address today's challenges. Deloitte understands the complexity of these challenges, and works with clients worldwide to drive progress and bring discoveries to life.

Contents

Accelerating drug discovery

The Deloitte *Intelligent biopharma* series explores how artificial intelligence (AI) technologies will affect each step of the biopharma value chain.[1] This report, the second in our series, examines how AI is helping to accelerate the efficiency and cost-effectiveness of drug discovery.

DRUG DISCOVERY IS the first step of the value chain that identifies new candidate therapeutics for treating or curing human diseases.[2] It is the initial stage of biopharma research and development (R&D) and involves the identification and optimisation of potential new drugs and a preclinical *in vivo* validation through cell assays and animal models. Successful candidates that meet the regulatory requirements applied to drug discovery move into the clinical trial phase, where they are tested for efficacy and safety in humans.[3] Our next report in the series examines the impact AI is having on clinical trials *(Intelligent clinical trials: Transforming through engagement)*.

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. Progress was generally slow, frustrating and labour intensive. In some cases, discoveries occurred due to unexpected events and observations (such as penicillin). 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.[4] The advantages of small molecules include simple

manufacturing and administration routes, low specificity and a stable shelf life, meaning they are safe and effective for large groups of people. However, low specificity can also lead to side effects, reducing the chances of success in clinical trials.
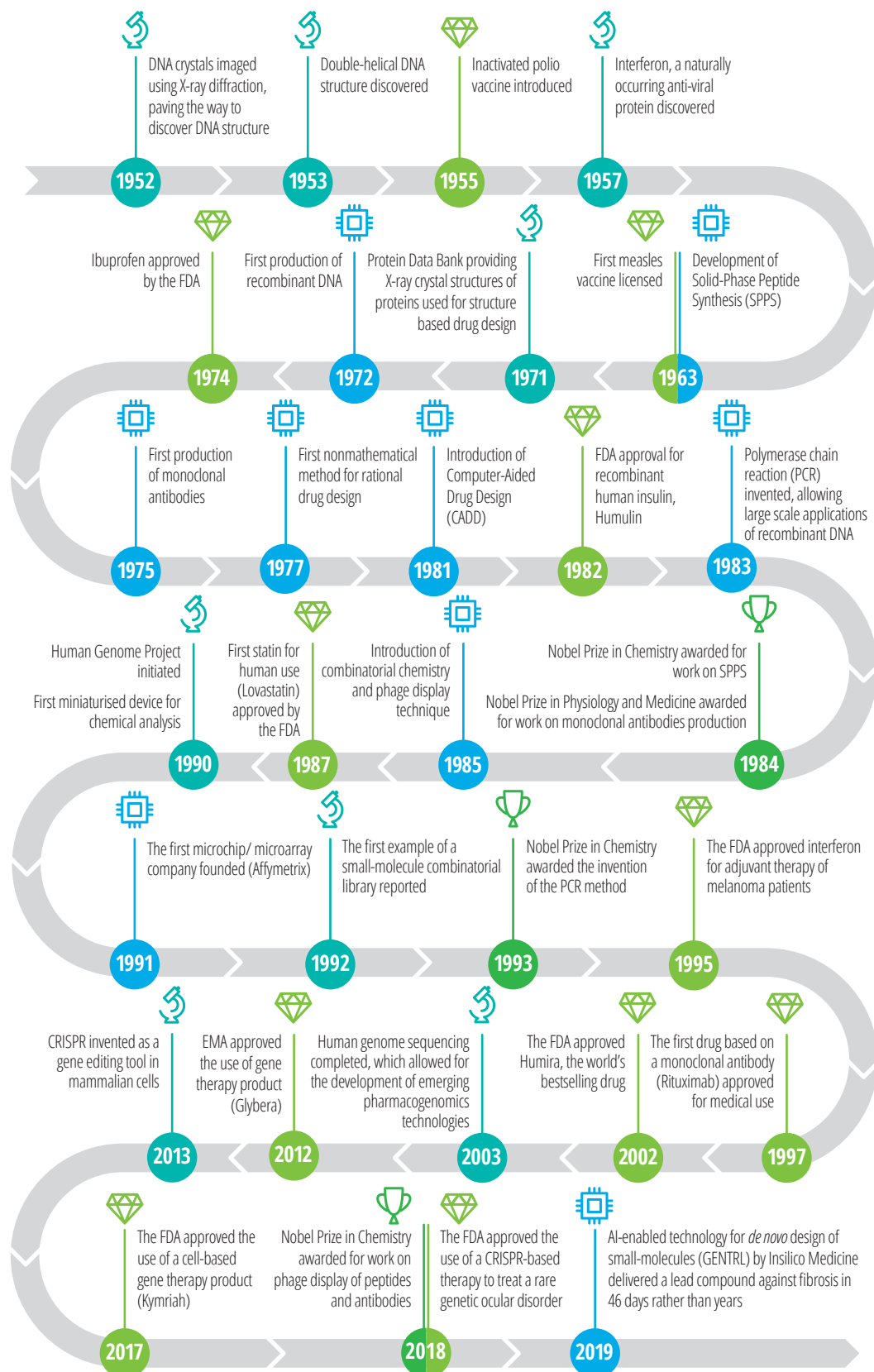
Since the 1990s, scientific and technological advances have led to the discovery of larger, more complex, biological therapeutics known as biologics. In contrast to chemically synthesised small molecules, biologics are produced or isolated from living organisms and include a wide range of products such as allergenics, antisense drugs, blood and blood components, recombinant therapeutic DNA and proteins, and vaccines.

Biologics are highly specific to their target and have invoked high levels of media and investor interest due to their innovative techniques and potential to cure previously untreatable diseases. Only 17 of the 59 drugs approved by Food and Drug Administration (FDA) in 2018 were biologics, largely due to the complex manufacturing and administration routes.[5] As most pharma companies have integrated biologics into their pipelines, for the purpose of this report we refer to all pharma companies as biopharma companies. Figure 1 provides a timeline on the history and progression of drug discovery paradigms.

FIGURE 1

The history and progression of drug discovery paradigms

🔬 Main research discoveries   💎 Drug approvals   🔲 Main technological advances   🏆 Main awards and prizes

1952 — DNA crystals imaged using X-ray diffraction, paving the way to discover DNA structure

1953 — Double-helical DNA structure discovered

1955 — Inactivated polio vaccine introduced

1957 — Interferon, a naturally occurring anti-viral protein discovered

1974 — Ibuprofen approved by the FDA

1972 — First production of recombinant DNA

1971 — Protein Data Bank providing X-ray crystal structures of proteins used for structure based drug design

1963 — First measles vaccine licensed; Development of Solid-Phase Peptide Synthesis (SPPS)

1975 — First production of monoclonal antibodies

1977 — First nonmathematical method for rational drug design

1981 — Introduction of Computer-Aided Drug Design (CADD)

1982 — FDA approval for recombinant human insulin, Humulin

1983 — Polymerase chain reaction (PCR) invented, allowing large scale applications of recombinant DNA

1990 — Human Genome Project initiated; First miniaturised device for chemical analysis

1987 — First statin for human use (Lovastatin) approved by the FDA

1985 — Introduction of combinatorial chemistry and phage display technique

1984 — Nobel Prize in Chemistry awarded for work on SPPS; Nobel Prize in Physiology and Medicine awarded for work on monoclonal antibodies production

1991 — The first microchip/ microarray company founded (Affymetrix)

1992 — The first example of a small-molecule combinatorial library reported

1993 — Nobel Prize in Chemistry awarded the invention of the PCR method

1995 — The FDA approved interferon for adjuvant therapy of melanoma patients

2013 — CRISPR invented as a gene editing tool in mammalian cells

2012 — EMA approved the use of gene therapy product (Glybera)

2003 — Human genome sequencing completed, which allowed for the development of emerging pharmacogenomics technologies

2002 — The FDA approved Humira, the world's bestselling drug

1997 — The first drug based on a monoclonal antibody (Rituximab) approved for medical use

2017 — The FDA approved the use of a cell-based gene therapy product (Kymriah)

2018 — Nobel Prize in Chemistry awarded for work on phage display of peptides and antibodies; The FDA approved the use of a CRISPR-based therapy to treat a rare genetic ocular disorder

2019 — AI-enabled technology for *de novo* design of small-molecules (GENTRL) by Insilico Medicine delivered a lead compound against fibrosis in 46 days rather than years

Source: Deloitte research supported by Deep Knowledge Analytics.

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.[6 7] Moreover, research published in 2017 found that the FDA had approved 1,578 drugs in total, targeting only 819 disease related molecular targets out of 20,000-25,000 genes composing the human genome.[8,9]

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

For the past 50 years, drug discovery has focussed largely on high-throughput screening for known disease-associated targets with progress driven by

massive improvements in computing power, advances in robotics and biological techniques, and improved methodologies in synthetic chemistry.[10]

The four main stages of drug discovery generally take five to six years to complete.

Drug discovery generally comprises four main stages (see figure 2). These stages take five to six years to complete, excluding the initial drug target identification and assay development steps, which are largely driven by academic and other research centres.[11]

FIGURE 2

The biopharma value chain for drug discovery

STAGE 1

First screening and hit identification
High-throughput screening of large libraries of chemicals to test their ability to modify the target positive hits are selected for further validation

STAGE 2

Hit to lead selection
Hits are confirmed and analogue clusters are synthetized three to six molecule clusters with better affinity and drug properties are selected

STAGE 3

Lead optimisation (drug candidate selection)
Lead molecules are further modified and improved a number of drug candidates are selected (1 in 5000 from initial screening)

STAGE 4

Preclinical testing
In vivo assays are performed to test pharmacodynamics, pharmacokinetics and toxicity of novel candidates 1 in 25 drug candidates that enter preclinical phase are selected for clinical trial studies

The drug discovery process usually takes five to six years from the start of stage I to the end of preclinical testing. Of 10,000 small molecules initially screened, 10 are selected for clinical trials.[12]

Source: Deloitte analysis.

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.[13] Our report, *Measuring the return from pharmaceutical innovation 2018*, examines the pipelines of the top 12 biopharma companies (both internally and externally sourced assets) and calculates the average cost of the R&D process as US$2.168 billion per drug – almost double the US$1.188 billion calculated in 2010.[14] At the same time, the average forecast peak sales per late-stage asset in the drug pipeline declined to US$407 million in 2018, less than half the 2010 value of $816 million. As a result, the expected return on investment from drug development has declined steadily from 10.1 per cent in 2010 to 1.9 per cent in 2018.[15] Finding ways of improving the efficiency and cost-effectiveness of bringing new drugs to the market is an imperative for the industry.

Around one-third of the above cost is spent on the drug discovery phase.[16] As shown in figure 2, of the 10,000 molecules initially screened, only 10 ever make it to clinical trials. Moreover, the chance of success for a compound entering phase I trials is slightly under 10 per cent and has not increased in a decade.[17] 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 (see figure 3), together with efficient drug delivery.[18] This is where the market for drug discovery is focussing its attention on using AI to improve the accuracy, predictability and speed of drug discovery. Other factors that lead to the drug failing in clinical trials include preclinical testing and animal models which often fail to mimic human physiology accurately.[19]

FIGURE 3

Drug and target binding

TARGET   SMALL MOLECULES   STRONG AND SECURE BINDING
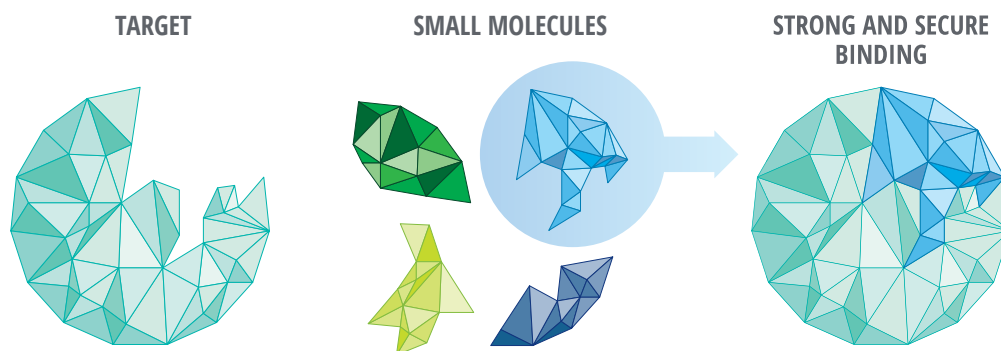
Source: Deloitte analysis.

AI DEFINITION

AI refers to any computer programme or system that does something we would 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. These technologies include computer vision, deep learning, machine learning, natural language processing, robotics, speech, supervised learning and unsupervised learning:

- **Machine learning (ML):** computer algorithms that learn from structured and unstructured data, identify hidden patterns, make classifications and predict future outcomes.

- **Deep learning (DL):** a machine learning-based approach that utilises a logic structure similar to the brain called neural 'networks' to recognise and discriminate patterns such as speech, image and video.

- **Natural language processing (NLP):** the application of computational techniques to the analyses and synthesis of natural language and speech.

Machine learning

Deep learning

Natural language processing
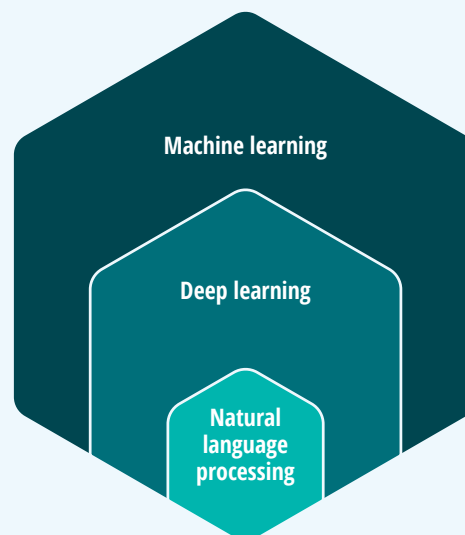
Why AI? Why now?

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. AI can also help cross-reference published scientific literature with alternative information sources, including clinical trials information, conference abstracts, public databanks and unpublished datasets. As described in the next chapters, AI applications in drug discovery have already delivered new candidate therapeutics, in some cases in months rather than years. 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.[20]

- **Increase the accuracy of predictions on the efficacy and safety of drugs** – currently, only one out of ten drugs are approved after clinical trials.[21] Most fail 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. Failure to demonstrate value compared to available therapies is a key factor undermining clinical trial progression. Finding new niches of competitive advantage could reduce withdrawals and improve asset sales.

While AI will have a role to play in the development of biologics, so far its use is largely focussed on chemical, small molecule research applications. Our research shows that this is due to the potential of AI to improve the understanding of structures and specificity of the target molecules as a result of the increasing amounts of structured and unstructured scientific data now available. The use of AI technologies to improve drug discovery is still at early stages and the applications available today are precursors to wider scopes such as biologics AI.

AI can also help cross-reference published scientific literature with alternative information sources.

The rise of AI drug discovery disruptors

In the past few years, the number of AI companies focussed on discovering new drugs using innovative approaches to discovery and preclinical testing has increased rapidly.

SINCE 2017, DEEP KNOWLEDGE ANALYTICS (DKA) has produced a series of quarterly reports providing in-depth, comparative and quantitative analysis of the AI for drug discovery landscape.[22] DKA's *Landscape of AI for Drug Discovery and Advanced R&D Q2 2019* report identifies significant growth across all areas. 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.[23] The AI R&D market increased from US$200 million in 2016 to more than US$700 million in 2018. Researchers expect it to reach US$20 billion in the next five years.[24] Some 120 (of the 170) companies are actively tackling different areas of drug discovery. Moreover, most major biopharma companies are now exploring AI-driven solutions for drug discovery, making a variety of deals to access this capability (see figure 4). These deals include acquiring the intellectual property rights to the assets, option exercise fees, royalties, technology access fees and income based on sublicensing or sale of drugs created under the collaboration.

FIGURE 4

AI-driven big biopharma deals disclosed in the market
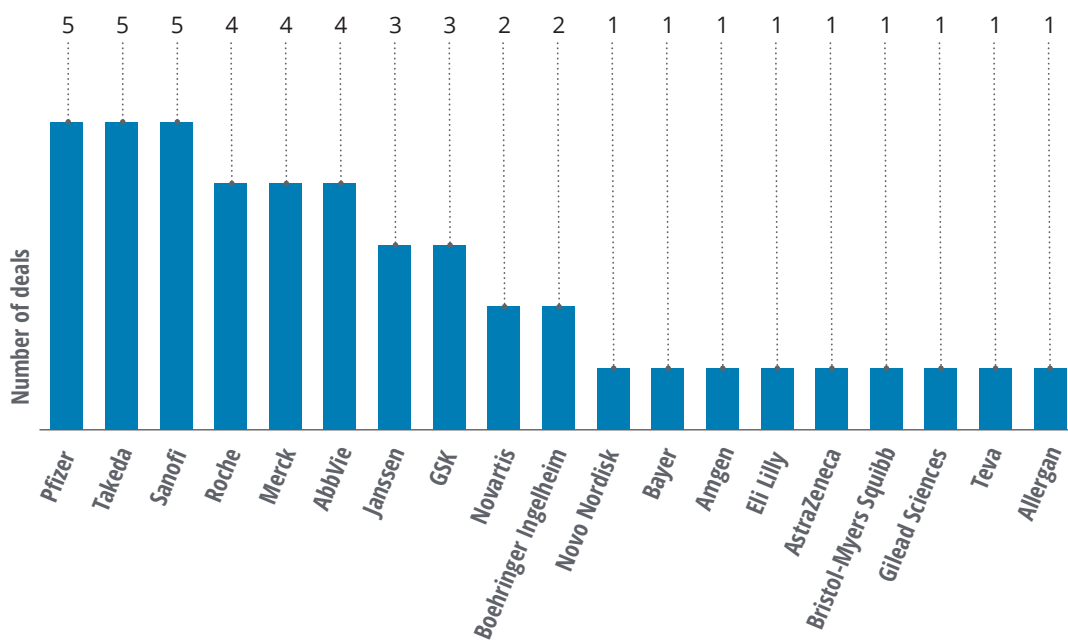
Source: Deloitte analysis (March 2019).

In the past three years, most biopharma companies have been adopting a variety of strategies to actively integrate AI into the discovery process, such as establishing their own dedicated teams by hiring AI experts and data analysts, investing in start-ups, and creating collaborations with tech giants and/or research centres.[25] While it is too early to evaluate which strategy will be more successful, the trend that is becoming consistent is the adoption of more than one AI solution at different stages of the drug discovery process and the diversification of deals and collaborations.

Biopharma companies are also increasingly outsourcing research activities to contract research organisations (CROs) to stay competitive and flexible in a world of exponentially growing knowledge, increasingly sophisticated technologies and an unstable economic environment.[26]

AI algorithms: Mining the data

In drug discovery, AI algorithms mostly use research data or available information on the 3D structure and binding properties of small molecules to 'recognise' the target specificity with greater accuracy than has been possible previously, using the same deep learning (DL) processes used for face recognition. This same concept is used to identify unwanted interactions causing toxicity. [27,28]

There are an increasing number of relevant sources of data for AI-enabled discovery and drug candidate selection. Having real-time access to as many datasets as possible will lead to new, promising and unbiased insights on rare diseases mecha-

nisms and help optimise drug efficacy and safety. Relevant data sources include or could include:

- The completed international human genome project in 2003 and the subsequent 'omics' (genomics, metabolomics, proteomics and structural genomics) revolutions, including the completion of the UK's 100,000 Genomes Project in 2018.[29,30]

- Proprietary and public research findings. About 80 per cent of scientific data is available only in intellectual property files. Grant applications and conference presentations are also rich in information that could be relevant to identifying new drug targets.[31]

- Small molecule libraries and protein structure information from research and clinical data. Each small molecule database is on average composed of 10 million compounds. By the mid-2000s, the available academic, commercial and proprietary databases of small molecules worldwide contained information related to 100 million different compounds. More recently, computer-aided *de novo* drug design has identified a list of 200 billion compounds with potential therapeutic activity.[32]

- Data related to the 90 per cent of drugs that do not make it is a valuable source of information for AI applications, including identifying unwanted interactions, and can be used to develop improved safety strategies and effective drug repurposing. Every year only ten per cent of all drugs evaluated in clinical trials reach the market.
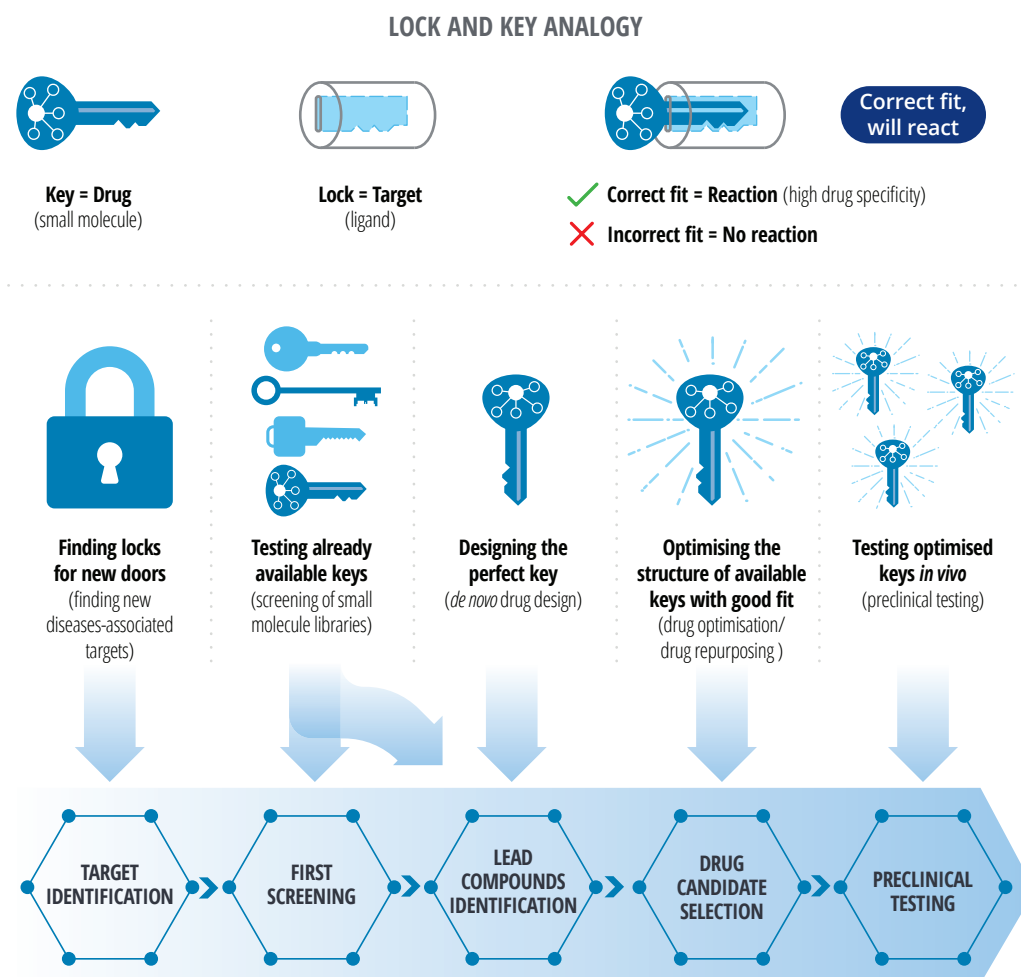
Five main AI challenges for drug discovery: Finding the ideal key for a complex lock

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 (see figure 5). AI solutions can visualise the 3D structure of the lock better than previously possible, for example, by screening small molecule libraries. They can also find new 'locks' to cure diseases by analysing research data more efficiently. 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 (see figure 6).

FIGURE 5

Lock and key analogy showing the five main challenges for AI in drug discovery

LOCK AND KEY ANALOGY

Key = Drug (small molecule)

Lock = Target (ligand)

Correct fit, will react

✓ **Correct fit = Reaction** (high drug specificity)

✗ **Incorrect fit = No reaction**

Finding locks for new doors (finding new diseases-associated targets)

Testing already available keys (screening of small molecule libraries)

Designing the perfect key (*de novo* drug design)

Optimising the structure of available keys with good fit (drug optimisation/ drug repurposing)

Testing optimised keys *in vivo* (preclinical testing)

TARGET IDENTIFICATION ›› **FIRST SCREENING** ›› **LEAD COMPOUNDS IDENTIFICATION** ›› **DRUG CANDIDATE SELECTION** ›› **PRECLINICAL TESTING**

Source: Deloitte analysis.

FIGURE 6

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
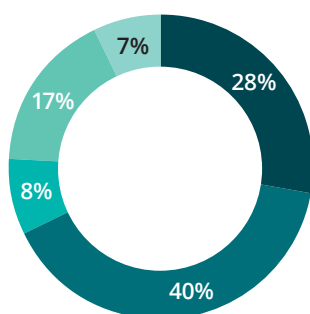
Source: Deloitte analysis.

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. This can lead to an easier identification of new diseases-associated pathways and new targets for drugs.

Start-ups that have secured collaborations with biopharma companies in these areas have developed competitive strategies for large data access.[33,34] Innoplexus for example, is pairing blockchain technology with AI to mine data 'trapped in silos' without compromising security and/or breaching ownership rights. With several large biopharma companies as clients, they are aiming to add the proprietary data of these companies to their own database and provide better predictions for their client portfolio.[35]

AI can tailor approaches for a more accurate understanding of pathological cellular and molecular mechanisms.

AI algorithms perform their analyses in the similar way as a systematic literature review, but in seconds rather than months. AI can tailor approaches for a more accurate understanding of pathological cellular and molecular mechanisms. The 'omics' real-time databases, whether disease agnostic or focussed on specific areas, are key assets for this type of approach, including single-cell genomics.[36] An increasing number of start-ups are targeting diseases with unmet medical needs, such as cardiovascular and neurodegenerative diseases.[37, 38] Case study 1 demonstrates how BenevolentAI has identified targets for ALS (amyotrophic lateral sclerosis, a rare motor neuron disease), and other diseases.

CASE STUDY 1. BENEVOLENTAI: USING MACHINE LEARNING TO IMPROVE TARGET PREDICTIONS

The Company

BenevolentAI, a UK company founded in 2013, creates and applies AI technologies to transform the way medicines are discovered, developed, tested and brought to market. The company has over 200 biologists, chemists, engineers, informaticians and data scientists working in cross-functional squads and is headquartered in London with a research facility in Cambridge (UK) and further offices in New York. BenevolentAI has active R&D drug programmes in disease areas such as ALS, Parkinson's, ulcerative colitis and sarcopenia. It has established partnerships with a number of major biopharma companies.[39]

The AI solution for drug discovery

BenevolentAI has the capability from early discovery right through to late-stage clinical development. The company has developed the Benevolent Platform® - a leading computational and experimental discovery platform that allows their scientists to find new ways to treat disease and personalise medicines to patients. The Benevolent Platform® focuses on three key areas, Target Identification, Molecular Design and Precision Medicine.

Main projects and diseases areas

- BenevolentAI's platform produced a ranked list of potential ALS, treatments, together with biological evidence. The BenevolentAI team was able to rapidly triage these predictions using strategies focussed on pathways implicated in multiple ALS processes. The five most promising compounds were taken to the Sheffield Institute for Translational Neuroscience (SITraN), a world authority on ALS. An ALS lead molecule emerged from a breast cancer drug, which showed delay of symptom onset when tested in the gold standard disease model.[40]

- In April 2019, the company began a long-term collaboration with AstraZeneca, aimed at using AI and machine learning to develop new treatments for chronic kidney disease (CKD) and idiopathic pulmonary fibrosis (IPF).[41]

- In September 2019, BenevolentAI signed a Framework Collaboration Agreement with Novartis Pharma AG ("Novartis"). This initial project with Novartis in oncology will see the application of AI and ML technology to stratify patients and gain a better understanding of patient and disease heterogeneity to more precisely target medicines for patients who need them.[42]

Achievements

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. BenevolentAI has published several pieces of research in distinguished scientific journals and world-renowned conferences.[43]

Screening of small molecule libraries to identify new drug candidates

Data from libraries of small molecules are driving new compound selection. Extremely accurate predictions of binding profiles can be created for targets, by using DL technologies, such as convolutional networks as demonstrated by Atomwise (see case study 2).

CASE STUDY 2. ATOMWISE USES DL TO SPEED UP DISCOVERY AND FIND MOLECULES FOR THE HARDEST TARGETS

The Company

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 company has 46 employees. It has set up over 300 partnerships with major biopharma companies and academic research centres around the world. In 2018, it secured US$45 million in venture capital funds for further development of the AI technology, with a total of US$51.3 million in funding to date.[44]

The AI solution for drug discovery

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.

Main Projects

They are working with partners across the globe on drug discovery projects for a variety of diseases, including Ebola, multiple sclerosis and leukaemia.

Achievements

The company used AI technology and algorithms in partnership with the University of Toronto for the rapid identification of treatments against the Ebola virus. The results of the research have been submitted to a peer-reviewed publication. Atomwise also found a new molecule targeting multiple sclerosis that inhibits a protein-protein interaction in the central nervous system and has been shown to be orally active in mouse models at very low dose. The drug has been licensed to an undisclosed biopharma company. More recent achievements include successes on Chagas disease, hand-foot-and-mouth disease, ischemic stroke and Parkinson's disease.[45,46]

In September 2019, Atomwise and Jiangsu Hansoh Pharmaceutical Group, a Chinese company behind this year's largest biopharma initial public offering, launched an up-to-US$1.5 billion collaboration to design and discover potential drug candidates for up to 11 undisclosed target proteins in cancer and other therapeutic areas.[47] In 2019, Atomwise also gained Eli Lilly and Charles River Laboratories as partners, along with a number of other strategic partners.[48]

A different approach, called network-driven drug discovery, tests a potential drug's ability to influence disease networks, rather than specific targets, using large-scale, proprietary databases and tailored computational tools. These have shown efficacy in at least 12 biological pathways.[49] This approach is part of an ongoing partnership with Novo Nordisk to find novel therapies for Type 2 diabetes.[50]

DL technology is not only transforming the small molecule research field, but it is also showing potential in the identification of new biologics such as therapeutic antibodies against cancer, fibrosis and other diseases. This approach has reduced the time required for antibody therapeutics discovery by three to 18 months.[51,52] Researchers seeking new antibiotics and novel antisense drugs for a subset of genetic diseases are using machine learning (ML) algorithms to help in the search.[53,54]

DL technology is not only transforming the small molecule research field, but it is also showing potential in the identification of new biologics.

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. In this case, only the information related to the structure of the target is necessary, avoiding the bias of small molecule screening. DL solutions are again at the core of this groundbreaking precision approach. The advantage is that drugs can be designed quickly, avoiding unwanted offset interactions,[55] with preliminary hit-to-lead results delivered in months.

In the past two years, at least nine AI tech providers have started offering tailored *de novo* drug design services, securing collaborations with major biopharma companies in different areas, including cardiovascular diseases and fibrosis.[56,57] *De novo* design of biologicals such as antibodies, DNA and peptides, is also an emerging trend that most AI for drug discovery companies are pursuing. [58,59,60] One AI drug discovery company, Insilico Medicine, has succeeded in using *de novo* AI to design a new molecule in 21 days and validate it in 25 days, 15 times faster than traditional biopharma process (see case study 3).[61]

CASE STUDY 3. INSILICO MEDICINE AND AI IMAGINATION FOR DRUG DESIGN

The Company

Initially established in the United States, Insilico Medicine moved its headquarters to Hong Kong in 2019,[62] Insilico is an AI drug discovery company employing over 85 AI experts and scientists in six countries (Belgium, South Korea, Russia, Taiwan, the UK and the US), sourced through hackathons and competitions. Founded in 2014, it is dedicated to extending human productive longevity and transforming every step of the drug discovery and drug development process. It uses DL approaches to identify protein targets and design novel lead molecules with specified properties. With revenues of US$4.5 million a year, it collaborates with over 150 academic and industry partners worldwide. By 2019, Insilico had raised US$51.3 million in funding.[63]

The AI solutions

Insilico 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 for the first time combines two distinct DL models. One example is AI Imagination, which 'imagines' molecules with specific properties using two competing networks: a generator, producing images with selected characteristics, and a discriminator, testing if the output is true or false. Once a target is identified, scientists use these DL algorithms to design molecular structures with desired physical and chemical properties.

Main Projects

In addition to working collaborations with large pharmaceutical companies, the company is pursuing internal drug discovery programs in a range of cancers, CNS diseases, dermatological diseases, fibrosis, metabolic diseases, sarcopenia and aging.[64]

Achievements

The GENTRL platform has generated new drug hits against fibrosis in 21 days and validated them, selecting one lead in another 25 days. The process from beginning of the design process took 46 days, 15 times less than traditional biopharma timings. The results were published in the journal *Nature Biotechnology* in September 2019.[65] The company believes the platforms built on its technology may save millions to tens of millions in R&D costs, and years in small molecule discovery time with better chances of passing through clinical trials.

In the past five years, Insilico has published 120 peer-reviewed scientific papers with over 3,300 citations. In 2017, it was named one of the top five AI companies by NVIDIA for its potential for social impact. In 2018, the company was named one of the global top 100 AI companies by CB Insights and received the Frost & Sullivan 2018 North American Artificial Intelligence for Aging Research and Drug Development award.

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. A drug interacts not only with a specific biological target but with a number of proteins, with as many as 300 causing adverse side effects. Cyclica, the first AI company to focus its technology development on the concept of polypharmacology, developed a drug-centric, proteome-wide approach to identify all the proteins that a small molecule can potentially interact with and provide information on unwanted targets or lead prioritization for other diseases (see case study 4). A number

of big biopharma companies, biotech start-ups and research institutions are currently collaborating with Cyclica to design novel multitargeted drug-like molecules with preferred properties, and ascertain the mechanism of action and safety profiles of their small molecule repositories, including drugs in discovery and early development, as well as exploring new applications for others.[66,67]

CASE STUDY 4. CYCLICA: WHERE AI MEETS BIOPHYSICS FOR DRUG DISCOVERY

The Company

Cyclica was founded in Toronto in 2013 and 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. Since it was founded, the company has raised US$12.5 million in venture capital and nondilutive funding and entered into research collaborations with Bayer, Eurofarma, Merck, and the Chinese biopharmaceutical giant WuXi AppTec. It has also formed multiple partnerships and joint ventures with start-up biotech companies and research institutions.[68,69] Cyclica currently has 31 employees, comprising computational scientists, experimentalists and software developers, operating across Asia, Europe, and North and South America.

The AI solution

Cyclica has two main patented AI solutions:

- Ligand Express, launched in 2018, is a cloud-based platform on which small molecule drugs are screened against repositories of proteomes to determine polypharmacological profiles. It identifies protein targets based on the structure, whilst also determining the drug's effects on these targets. The approach is based on a DL framework and can be used to identify unwanted drug interactions, reduce toxic effects, identify repurposing opportunities and generate new knowledge on disease mechanisms in a shorter period. They recently integrated the ML engine POEM, which provides a better understanding of pharmacokinetics and toxicology to predict the behaviour of potential drug candidates.

- Ligand Design, is used to produce novel lead-like compounds, optimised against multiple targets (both desirable targets and undesirable anti-targets) and multiobjective parameters. The platform *de novo* designs molecules by exploring chemical space in a generative or semigenerative manner while ensuring desired physicochemical, pharmacokinetic and polypharmacological characteristics. It can also screen large chemical catalogues of preexisting molecules against multiple targets for rapid purchase. It was launched in May 2019.

Main Projects

The Ligand Express platform is contributing to a number of projects to find drugs against Ebola, epilepsy and idiopathic pulmonary fibrosis. Several biopharma companies have selected Ligand Express to screen their proprietary small molecule repositories and investigate the possibility of repurposing or increasing the therapeutic index. Cyclica's proprietary drug discovery platform, featuring Ligand Design and Ligand Express, are being used to identify novel multitarget solutions for complex neurodegenerative diseases, such as Parkinson's, through a collaboration with the University of Toronto and Rosetta Therapeutics.[70]

Achievements

The company contributed to the understanding of a repurposed drug for the treatment of Ebola, identifying two main molecular pathways as possible mechanisms of action via the Ligand Express AI technology. Using the same 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. In August 2018, Bayer included Cyclica in its Grants4Apps programme, and in December 2018, Cyclica announced a collaboration with Merck KGaA aimed at providing important insights on target identification to support phenotypic screening and off-target profiling in general.[71,72]

Cyclica has also partnered with Tieös Pharmaceuticals to design anti-cancer molecules with a multitargeted approach via Ligand Design with the synthesised molecules showing good solubility and multitargeted biophysical interaction and evidence of good safety, efficacy and pharmacokinetics in its *in vivo* models.[73]

Preclinical testing

Animal models often fail in predicting accurately the human physiology response. A lack of good preclinical modelling is a key reason for low R&D returns. While there is a body of research focussed on finding better predictive preclinical technologies, such as organs-on-a-chip or 3D cell cultures, AI algorithms can help identify which animal models could be more accurate for certain diseases. A new statistical method called 'Found in Translation' uses ML algorithms to identify matches in gene expression profiles between mice and humans and better predict cross-species differences. The model can, with no experimental cost, identify information that, if missed, could cause false leads.[74]

Key considerations for biopharma's adoption of AI

Only a few of the 7,000 known rare diseases have seen any progress in the development of treatments. AI solutions have the potential to accelerate scientific research using quick and accurate *in silico* testing by using DL algorithms to identify new potential drugs faster and cheaper.

BIOPHARMA COMPANIES ARE increasingly adopting AI solutions to improve the discovery process. Like all innovation, 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 (see figure 7).

FIGURE 7

Five key considerations for the adoption of AI solutions

IMPROVING ACCESS TO ROBUST RELIABLE DATA
Collaborations, consortiums and partnerships

RECOGNISING THE DISRUPTIVE POTENTIAL OF TECH GIANTS
Tech companies have access to big datasets and are already investing in AI for healthcare

INCREASING DIVERSIFICATION OF DRUG DISCOVERY PIPELINE
AI can provide better predictive models and more agile research to understand rare disease mechanisms

ACQUIRING NEW AI SKILLS AND TALENT
AI experts are needed to implement solutions and evaluate collaboration with third parties

ESTABLISHING NEW KEY PERFORMANCE INDICATORS AND DESIGN THINKING
There is a need for new standardisation to evaluate milestone discoveries

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 the drug discovery process they need access to large datasets. While this can be achieved through industry collaborations, this is a challenge for a highly competitive traditional biopharma culture. That said, 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 three-year project, which began in 2019, has an estimated budget of €18.4 million euros. It has also received funding from the Innovative Medicines Initiative (IMI) as part of a public-private partnership.[75]

- 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.[76]

- 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.[77,78]

In the UK, a government-led initiative, Medicines Discovery Catapult, was created to help accelerate drug discovery, with informatics as a key theme (see case study 5).[79]

The benefits of achieving a better drug discovery process outweigh the risks of sharing knowledge.

CASE STUDY 5. MEDICINES DISCOVERY CATAPULT TO ACCELERATE AI FOR DRUG DISCOVERY

The AI in drug discovery mission

Medicines Discovery Catapult (MDC) is a national facility, funded by Innovate UK (the UK government's innovation agency). MDC accelerates innovative drug discovery by providing access to scientific resources and data, expertise, laboratory facilities and networks. It supports UK small and medium-sized enterprises (SMEs) to develop and industrialise new approaches to drug discovery. MDC also helps biotechs and academia to reduce discovery time and costs.

MDC collaborates to validate new ways of discovering therapeutics and driving key talent and expertise across the sector. For example, creating a drug discovery platform that can accurately predict the absorption, metabolism, toxicity, etc., of new drug candidates.[80]

Using AI to analyse drug data more efficiently and effectively reduces overall costs for companies that may be interested in data. These methods help to facilitate effective decision-making for assets to be optimised further and to create the best data assets. MDC uses its informatics skills, extensive proprietary databases and algorithms, and market understanding to help validate and drive adoption of data-driven approaches for data analysis and information extraction. For example, helping to derive more focussed compound subsets and supporting SMEs to undergo faster and more efficient drug screening.

They work with different types of companies and provide various services to each, contributing to an overall increase in the efficiency of the value chain (see figure 8).[81]

FIGURE 8

Medicines Discovery Catapult works with different companies to accelerate drug discovery

■ Unique biology model ■ Advanced technologies ■ Drug discovery expertise ■ Collaborative relationships
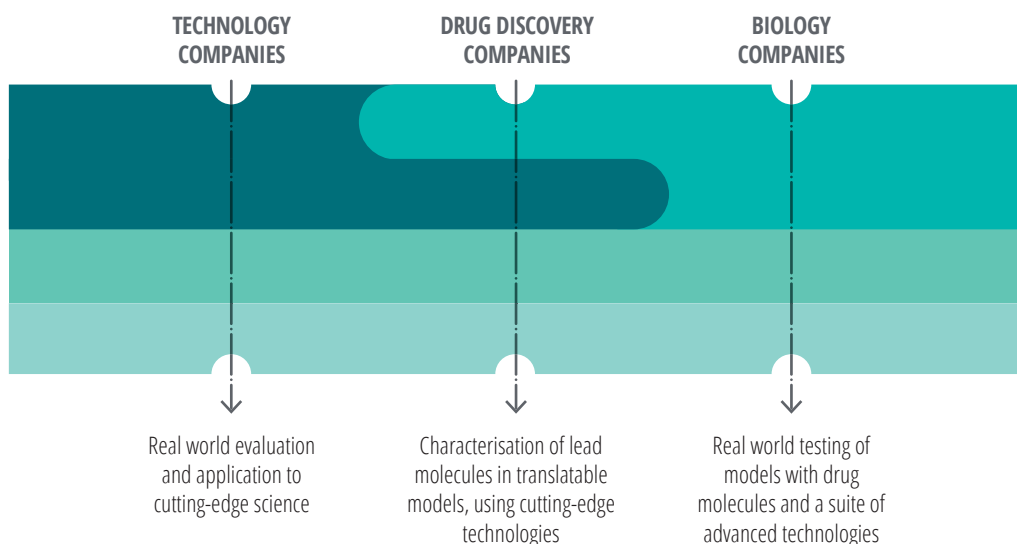
Source: Deloitte analysis.

Partnerships between biopharma and AI tech start-ups:

Most of the AI for drug discovery start-ups compete for access to large databases, especially when providing algorithms for specific types of data, such as 'omics' or certain disease areas. Some start-ups have set up contractual partnerships with academia and research centres, enabling them to benefit from access to proprietary data, as well as skills and talent. Some examples are included in the second part of the report and demonstrate how this arrangement can provide biopharma companies with access to a wider set of skills and data to help identify potential drug candidates more effectively.

Establishing partnerships requires biopharma companies to be able to evaluate AI start-ups and understand the solutions they provide. This is not a straightforward process, as most of these small companies are recent and the information available on the effectiveness of their solutions on delivering drug candidates are still limited.

One metric is the number of scientific publications and presentations at relevant scientific conferences. However, peer-review procedures often take time, thereby limiting the value of this metric in such an innovative field. The number of collaborations that AI start-ups have with leading research centres may provide an alternative metric. Another measure is the number of new drugs in the pipeline discovered or optimised using the technology and the number of deals and partnership that the start-up has with big biopharma companies.[82]

Recognising the disruptive potential of tech giants in drug discovery

Tech giants are increasingly disrupting the healthcare industry. What differentiates them is that these companies are already investing in AI for drug discovery, including several tech companies announcing partnerships with academic institutions, AI start-ups and biopharma companies:

- Google DeepMind's AI technology has developed a groundbreaking DL algorithm that predicts the 3D structure of proteins from primary sequences more accurately than earlier techniques, outperforming experienced computational biologists. The company is planning to develop the technology further, with the aim of using it to find new therapies.[83] Google has also started an Innovation Lab project with Sanofi in September 2019 to improve drug discovery and health services by using emerging technologies.[84] Google is also actively investing in other start-ups for drug discovery.[85]

- Tencent is expanding into the drug discovery space and participated to two multimillion-dollar deals just this year involving US-based companies Atomwise and XtalPi, both working on small molecule AI platforms.[86]

- In the UK, Vodafone Foundation (a registered charity) supported the Imperial College project DRUGS (Drug Repositioning Using Grids of Smartphones) to facilitate AI-enabled research against cancer through crowdsourcing.[87] An app called DreamLab diverts the unused processing power of thousands of phones, while charging at night, to support the work of a supercomputer in analysing billions of existing anti-cancer small molecules and improving their action against tumour targets. By plugging in 100,000 phones for six hours, the processing timings were reduced from 300 years for a single computer to only three months. The project led to the identification and validation of 110 anti-cancer molecules (this is discussed in a July 2019 *Nature* article).[88]

AI provides an opportunity to diversify pipelines

Exscientia, one of the first companies to use AI for the identification of new drug candidates, has secured relevant partnerships with a number of big biopharma companies over the past four years,

contributing to the understanding of key disease mechanisms to help diversify drug pipelines (see case study 6).

One of the most promising approaches for diversifying drug portfolios are 'omics' data, which are increasingly being used in areas such as research for

CASE STUDY 6. EXSCIENTIA: AT THE FOREFRONT OF THE AI-DRIVEN DRUG DISCOVERY PROCESS

The Company

Exscientia is a UK company founded in 2012, which has raised a total of US$43.7 million in funding. The most recent round took place in December 2018, where the company secured US$26 million.[89] They have also acquired a biophysics specialist company called Kinetic Discovery, to enable flexibility between genes and clinical candidates to identify targets.[90] It currently has 48 employees and ongoing partnerships with Celgene, GlaxoSmithKline plc (GSK), Roche, Sanofi and Shanghai biotech company GT Apeiron.[91]

The AI solution

The company has three main proprietary AI approaches:

- Single-target drug discovery projects: Identify targets most likely to be chemically tractable by investigating the drugability of each opportunity (i.e., the likelihood of a target to selectively bind to a well-balanced small molecule).

- Bispecifics: The design process for a bispecific molecule is like the approach for single targets, but the key difference is that potency must simultaneously satisfy two different targets.

- Phenotypic drug design: The system that automatically extracts key performance markers from high-dimensional phenotypic readouts and uses these to generate and optimise new iterations of compounds, to rapidly evolve compounds that satisfy key performance criteria.

Their model capitalises on 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 Centaur Chemist discovery process platform to generate phase I ready assets.

Achievements

To date, Exscientia has set up collaborations with several big biopharma companies. Below are some of the announced achievements from these collaborations:

- A two-year collaboration with Sanofi has resulted in a novel, bispecific small molecule that can target two pathways related to inflammation and the progression of fibrosis that is being advanced to clinical trials. As part of the collaboration, incentives have been agreed for certain development and sales milestones.[92]

- In April 2019, as a part of a £33 million collaboration with GSK that began in 2017, Exscientia delivered a lead molecule aimed at the treatment of chronic obstructive pulmonary disease.[93]

The company currently has a growing pipeline of approximately 20 drug compounds from collaborations and their own projects. These include one candidate ready to enter phase I. Five new assets have been delivered in under 14 months (compared to the five-year industry benchmark), with drug discovery cost savings of more than 80 per cent (30 per cent achieved for the entire drug development process). The company plans to double the pipeline yearly and with a number of projects reaching the commercialisation stage in 2020-2021. In its first year, Exscientia published a paper in *Nature*, which led to the development of a system that looks at the likelihood of binding between small molecules and targets to aid in drug candidate discovery.[94]

longevity therapeutics, including using AI technologies to help segment populations to identify novel pathways and associated pathologies involved in age progression.[95] For example, Aging Analytics Agency and its parent company Deep Knowledge Ventures, is establishing an AI Centre for Longevity in London that will focus on AI applications for drug discovery. A specific focus of the Centre will be the use of AI for the development of an optimal, actionable panel of biomarkers of aging, and devoting AI-driven R&D to some of the more neglected areas of research in longevity and personalised medicine.[96]

Need for new skills to optimise AI-enabled discovery

According to a 2018 survey by the Pistoia Alliance, a global, not-for-profit alliance that works to lower barriers to innovation in life sciences R&D, 72 per cent of life science professionals in Europe and the United States think that the industry is running behind in AI development. Forty-four per cent of respondents cite the lack of appropriate skills and talent as one of the main barriers, and 52 per cent state a lack of access to data. The report notes that to make AI technology work for the industry, companies require highly trained, specialist data experts and experts in AI and computational biology. The report also suggests that biopharma companies need to work closely with academic organisations and educators to attract the next generation of data scientists.[97]

A number of major companies are reorganising their internal structures and changing the skills and talent pool to align it with investments in AI technology.[98] GSK, which is one of the most active biopharma companies in the area of implementing emerging technologies, has recently hired 50 AI experts and created a specialised team.[99]

Establishing new metrics and key performance indicators

The lack of internal digitally skilled staff and the fact that digital solutions are often provided by third parties are limiting factors to establishing an objective evaluation of results.

In drug discovery, AI implementation requires a design thinking approach to modulate and resolve complex problems constructively. The creation of effective key performance indicators (KPIs) by dedicated internal teams with appropriate skills are needed to support and evaluate the progress of drug discovery projects and ultimately evaluate their integration into R&D pipelines.[100] Case study 7 illustrates one approach that is attempting to address this lack of objective measures.

CASE STUDY 7. DEVELOPING THE IMAGENET OF GENERATIVE DRUG DISCOVERY

Ongoing research in ML in general, and DL in particular, highlights the issues of reproducibility and fair comparison between different approaches. A major advance in AI was made in 2014 with the development of Generative Adversarial Networks (GANs), which allow the creation of novel molecular structures with a desired set of characteristics. Much of the core intellectual property related to the application of GANs and other generative models was invented in 2016, and was initially met with scepticism.[101,102] In 2018, however, the technique was widely adopted by the industry.[103] While there are multiple methods for generating novel molecular structures with ML models, there is no conventional way to run and evaluate the performance of generative models.

In September 2018, several AI companies formed the Alliance for Artificial Intelligence in Healthcare (AAIH).[104] In November 2018, AI researchers, led by the AAIH co-founders at Insilico Medicine, joined forces to develop the 'ImageNet' of generative drug discovery, to establish a set of standards for generative models in healthcare. AAIH launched a benchmarking platform that encompasses various ML techniques to compare them on a standard dataset. The MOSES (Molecular Sets) platform implements several popular molecular generation models and ranks them according to a predefined set of metrics.

MOSES aims to increase the pace of drug discovery, ease the sharing and comparison of new models and boost AI powered drug discovery, just as ImageNet boosted DL for imaging data. The MOSES platform provides a standardised benchmarking dataset, a set of open-sourced models with unified implementation and metrics to evaluate and assess the results of generation.[105] In 2019, the first experimental validation of generative models, utilising generative and reinforcement learning models, was demonstrated in cells and animals in 46 days.[106]

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.

Drug discovery and its role in the future of health

In 2018, the FDA's approval of 59 new drugs was 20 per cent more than in 2017 and 2016 and the highest number since 1996. The approvals included 19 first-in-class agents, 34 novel drugs for rare diseases and a record seven biosimilars.[107] The use of big data and AI is already accelerating the identification of more precise drugs and, although regulators have yet to approve any AI-derived drugs (nor have any been validated in clinical trials yet), the first milestone is expected to be reached by the end of 2020.[108] Indeed, it seems likely that

integrating more sophisticated bioinformatics, computational, engineering, nanotechnology and/or pharmacogenomics methods into the drug discovery process will lead to the next stage of advances in drug discovery.

Until now, AI for drug discovery companies have focussed on analysing large datasets, largely because DL requires big data. In future, disruption will come from big datasets combined with insights from small datasets, collected in real time from patients and individuals within the target population.[109] These small datasets will be added to algorithms trained on large datasets to drive the design of new precision drugs (see figure 9).

FIGURE 9

Intelligent drug discovery to deliver '4P' medicine

RADICALLY REFORMED
DATA ARCHITECTURE AND
DATA SHARING

AI HAS IMPROVED ACCURACY,
PREDICTABILITY AND SPEED OF
DRUG DISCOVERY

REGULATORY RELATIONSHIPS
BASED ON WIN-WIN
APPROACH

DRUG DISCOVERY BASED ON
NEW SKILLS AND TALENT

NEW GEOGRAPHIC
DISTRIBUTION OF AI FOR
DRUG DISCOVERY

PREDICTIVE
PREVENTIVE
PERSONALISED
PARTICIPATORY
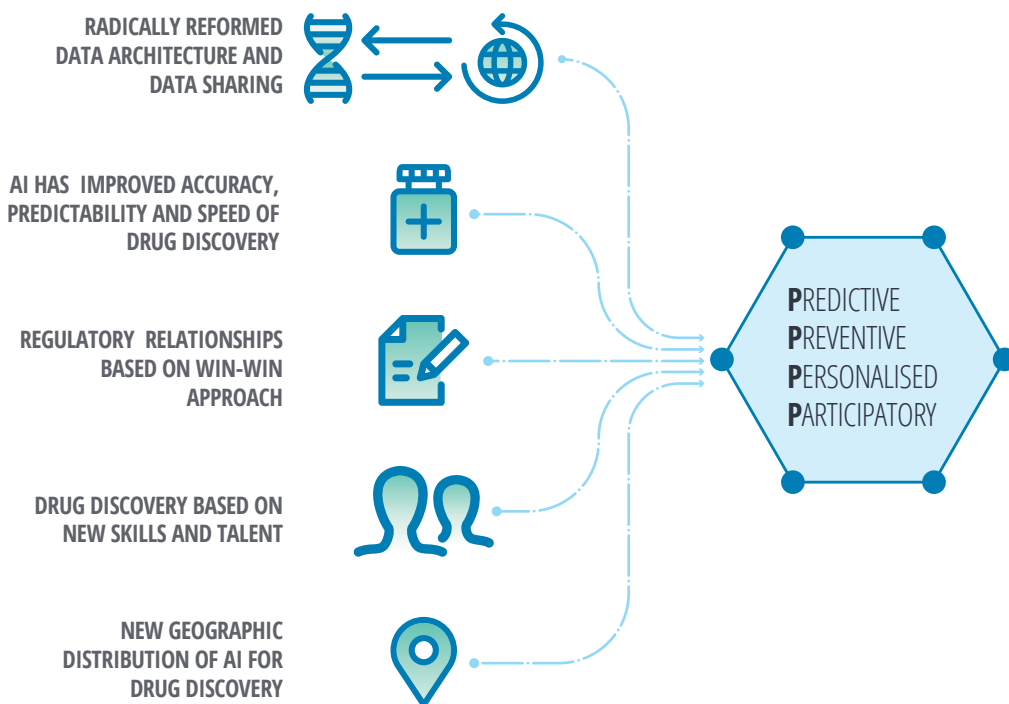
Source: Deloitte analysis.

As the number of compounds identified using AI increases, new drugs capable of treating very precise pathologies will become available, with personalised drugs designed *de novo* in a few weeks. These treatments will be highly specific to targets, linked to personal genetic backgrounds and avoid complications such as side effects. This transition will open up a new future for the health industry, as a higher level of knowledge on disease mechanisms both increases the number of treatments available and, in many cases, cures diseases that have not previously had effective treatments. This also suggests that IP will not only protect chemical formulas, but also products and services as part of the approval process.

While individual drug prices could rise as therapies become more efficacious and treat more targeted populations, overall drug spending could decrease as the total number of patients treated by individual drugs falls. Advanced early intervention and better adherence could also help improve the cost-effectiveness of these new therapies.[110]

Drug discovery and the future of work

The future skills of top-tier AI for drug discovery companies will include high levels of expertise in biopharmaceutical science, advanced proficiency in AI, specialist teams and constantly evolving internal knowledge. Some of these companies are developing advanced AI techniques to enable them to become the new unicorns of the biopharma industry.

AI start-ups are likely to be the main providers of drug discovery solutions, collaborating with big biopharma in the drug discovery process.[111] However, their relationships and terms of agreements are

already changing, as AI drug discovery companies no longer seek to be acquired, preferring to develop their own drugs and maintain autonomy. Some already have their own proprietary advanced drug pipelines. The increase in availability of venture capital (VC) funds in this sector (VC funding reached US$1.08 billion last year, from US$237 million in 2016) is helping drive this development.[112] Nevertheless, some form of partnership with big biopharma companies is required, if only to get access to clinical data. Indeed, compared to 2018, most large biopharma companies have increased their involvement in AI-related investment and research collaborations during 2019.[113]

Leaders with digital knowledge will need to integrate new strategies into their research units.

These investments in AI are helping biopharma improve their performance. DKA analysed the net income of the 15 top biopharma companies and found almost every company faced a negative trend before using AI, but this improved after implementing AI. The researchers identified that success for big pharma companies using AI for drug discovery depends on having highly skilled interdisciplinary leadership and skilled interdisciplinary AI experts who can innovate, organise and guide others, as well as AI-friendly CEOs and board members to drive the adoption of AI.[114] Characteristics of these biopharma leaders include being digitally sound and 'tech savvy', ready to support agile changes and new business and operating models.

For biopharma companies to thrive, they will need strong AI divisions and a strategy for acquiring or collaborating with the best AI start-ups. Leaders with digital knowledge will need to integrate new strategies into their research units. 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.

Another driver of change in drug discovery is likely to come from big tech companies who specialise in the use of big data and in developing new AI solutions. Both big tech and biopharma companies will be competing to hire and retain sufficient numbers of AI experts and biochemical specialists.[115] However, these and other key talents, such as bioinformatics and computational biologists, are in short supply. For biopharma companies, tech giants can be an opportunity as potential partners; a threat as competitors; or both an opportunity and a threat, for which they need to have a clear strategy for how to respond to this changing landscape.[116]

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. In recognition of the shortage of skills and talent, university science courses are beginning to include programmes on AI algorithms, big data and digital technologies and their application in life sciences. 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

To date, the United States 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 United Kingdom is the leading country after the United States in terms of investment and number of AI tech companies, and it is maintaining the same pace of growth. In the past year, the level of activity in the United Kingdom

and EU has increased by 10.8 per cent and 10.3 per cent respectively, due largely to government initiatives. 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.[117]

Trend analysis shows that geographical patterns are changing, with Asia and Europe becoming more competitive.[118] The past quarter has seen a sharp increase

The UK is the leading country after the US in terms of investment and numbers of AI tech companies.

in the number of Chinese investors encouraged by the country's government's ambition to lead the world in AI by the year 2030 (see case study 8).[119]

CASE STUDY 8. FOCUS ON CHINA

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.[120] 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.

The China Food and Drug Administration (CFDA) has introduced a number of important R&D reforms, one of which is that orphan drugs can apply for clinical trial waivers, drastically reducing the time it would take for the drug to reach the market. This, coupled with China's 2030 vision of becoming a global leader in AI, means China has set its sights on being at the forefront of innovative, digital approaches to drug design.

Over the past few years, China has been a major investor in biotech companies in the US.[121] Investments increased significantly in 2019, with US$1.4 billion of investments into US-based biotech and drug firms, compared to just US$125.5 million in 2018. However, an act called the Foreign Investment Risk Review Modernization Act of 2018, introduced by the Committee on Foreign Investment in the United States, has changed the way companies will be looking to invest. These changes will affect 27 industries, including the biotech research and development sector.

These developments, together with the fact that China has the largest number of AI R&D centres in drug discovery, will likely divert the investment into national products and drive the increase in the number of local AI companies providing solutions for drug discovery. As a result, the landscape of AI drug discovery companies is likely to be vastly different in ten years' time. The 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.[122]

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. For example, before any drug candidate can move into the clinical trial phase, all the information gathered about the molecule in the lead optimisation stage must be collated to prepare a target candidate profile. This, together with toxicological and chemical manufacture and control considerations, forms the basis of a regulatory submission to allow human administration to begin.[123]

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* (via computer modelling or simulation) 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, a transition that has already begun today.[124]

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. Significant advances in the techniques used will evolve to produce next generation AI methods and provide the framework for precision medicine to become mainstream.

Major disruption will come from biopharma companies that apply these next generation techniques (DL, generative adversarial networks and reinforcement learning) 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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