

Artificial Intelligence
In Drug Discovery

MARKET SURVEY 2020

Insights from
industry experts on:

- AI Applications
- Partnerships & Collaboration
- AI Implementation



Artificial Intelligence (AI) is attracting a huge amount of attention in almost every sector, and one often-cited potential application of this technology is in drug discovery. AI as an umbrella term can cover a range of tools and technologies such as machine learning, deep learning, neural networks, voice recognition, and image recognition. The potential for AI to allow powerful analysis of huge data sets and see or predict patterns better than human scientists means that many consider it inevitable that AI will have a transformative impact on every aspect of the drug development continuum and beyond. Thus, we decided to survey those working in this space on their thoughts on the current state of the market.

It takes billions of dollars and more than a decade to develop a new drug, and AI has been seen as the enabling technology that could reduce both the cost and time to market. With total investment exceeding \$7.20 billion across 300+ deals between 2013 and 2018, the pharmaceutical industry continues to lead the healthcare sector in terms of attracting AI-related venture funding, and major pharmaceutical companies have embraced AI as part of their digitisation efforts. As such, research has found that artificial intelligence in drug discovery will be worth \$1,434 million by the end of 2024, increasing from \$259 million in 2019. These tools have many potential applications in pharma and healthcare; they can carry out or augment tasks that have until now been completed by humans, or have not been possible previously.

AI presents significant opportunities for saving money, improving care, and saving lives.

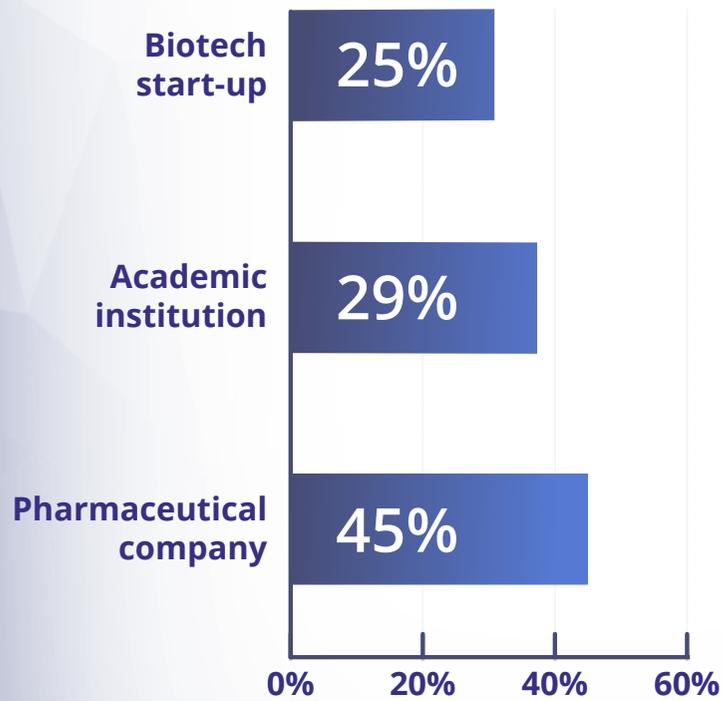
However, it is important to not overstate the current impact of AI, and instead focus on its usefulness now and its likely near-term future impacts. This survey aims to focus on the use and implementation of AI across drug development. It also investigates and identifies the current challenges and where AI is likely to see successful uptake, garners insight from respondents from pharma, biotech, and research organisations who are applying these tools and technologies, and assesses how those in this field see the market developing.

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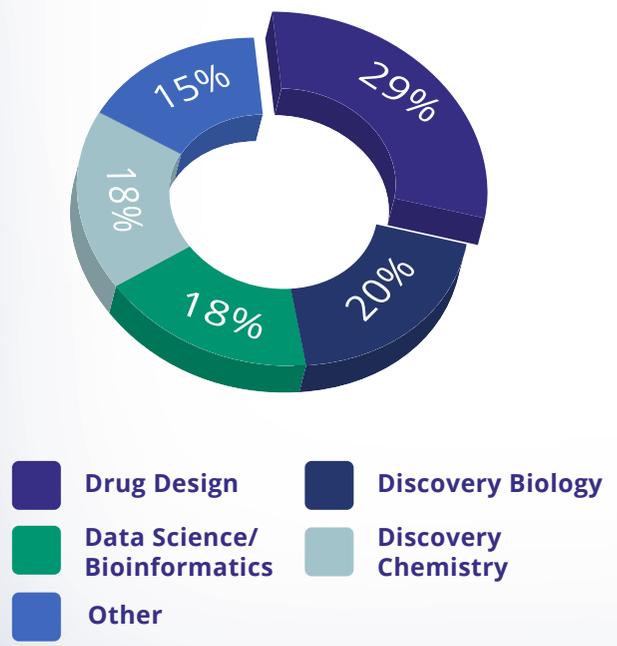


1 What type of organisation do you belong to?

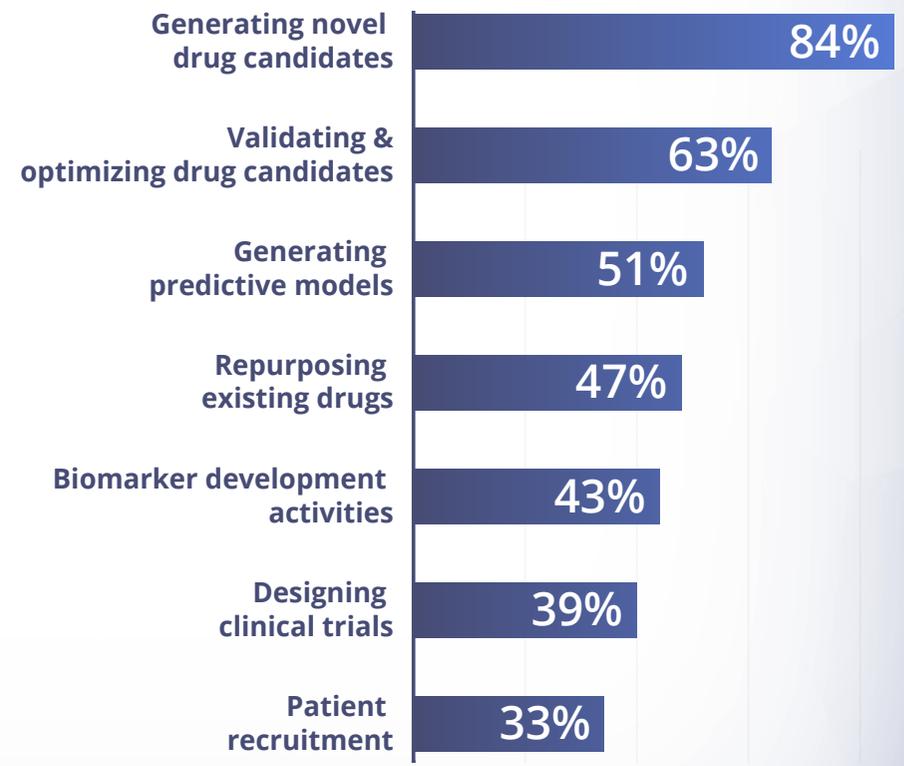


2 What kind of research do you engage in?

Organisations utilising AI for drug discovery engage in a variety of activities. These include generating novel drug candidates, repurposing existing drugs, generating predictive models, validating and optimising drug candidates, biomarker development activities, designing clinical trials, and patient recruitment



3 What activities do your organisation engage in?





AI is described as having the potential to revolutionise the pharmaceutical industry in the future, but what about the present?

Many companies have now been seriously exploring the applications of AI and are already putting it to work in a variety of ways.

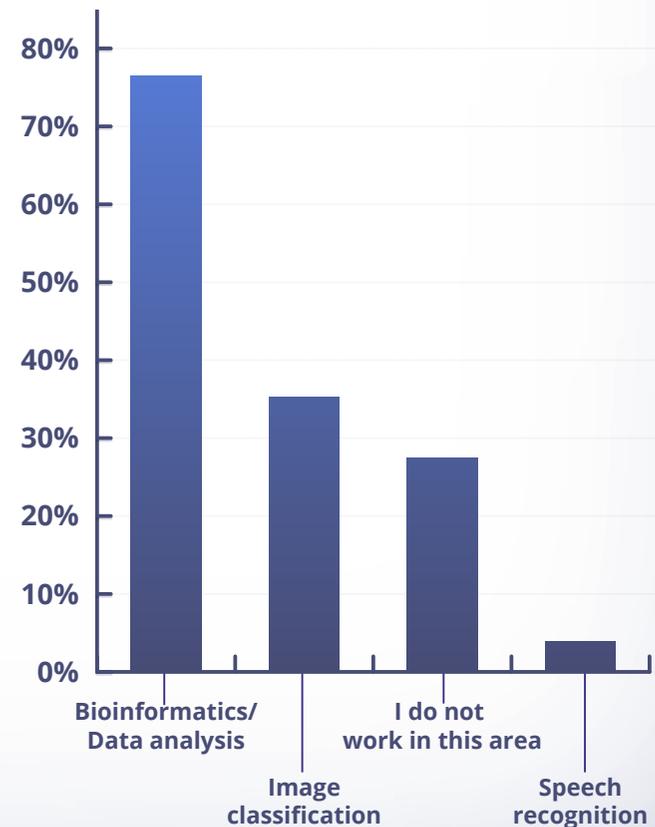
“Machine learning has the potential to play a significant role in the future of drug discovery. This is because drug discovery is a data-intensive endeavour, and the volumes and types of data are now reaching levels of size and complexity where only computers and algorithms are going to be able to identify novel patterns and hypotheses.”

Jim Weatherall,
Vice President of Advanced Analytics and Head of the
Advanced Analytics Centre, AstraZeneca

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Which deep learning techniques do you apply in Drug Discovery?

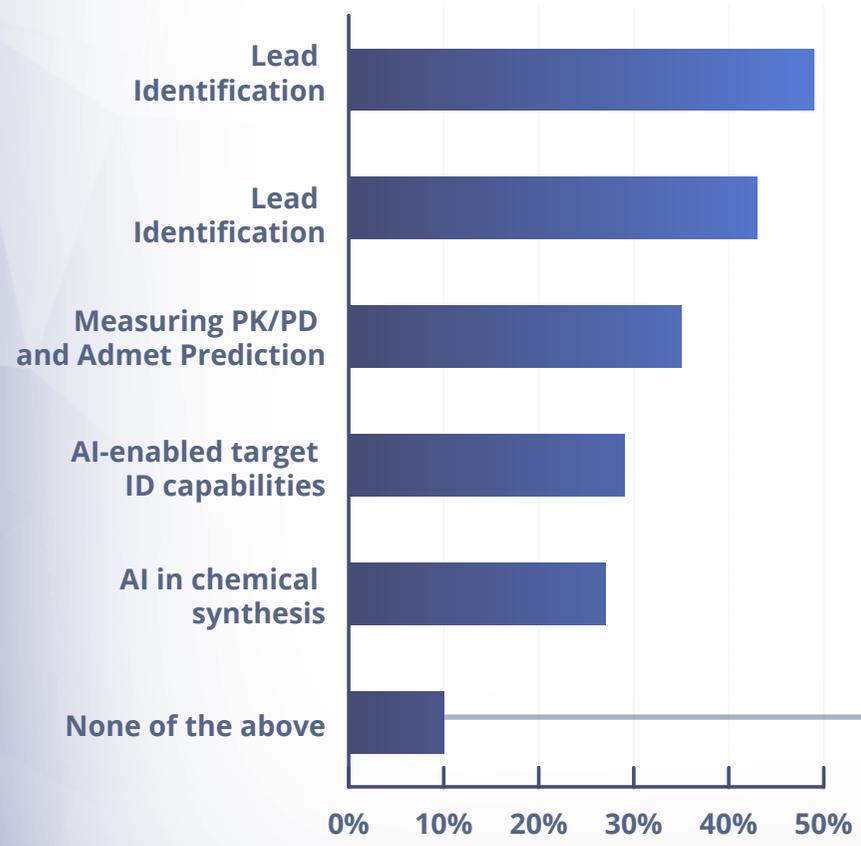
While deep learning has been investigated as a tool for speech recognition and image classification, bioinformatics or data analysis remains by far the most common use.





THE CURRENT APPLICATIONS IN AI

5 In which areas do you apply AI in Drug Discovery?



6 If none of the above, which areas do you use AI in?





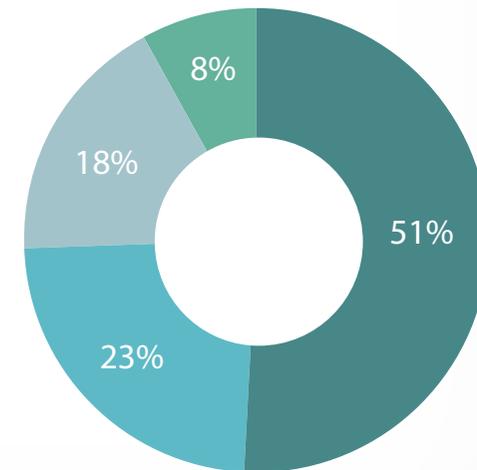
The disruptive potential of AI technologies means that organisations are changing the ways in which they work. The rise of start-ups and small biotechs that are specialist AI companies, and the lack of the necessary specific skillsets within the workforce of large pharma companies, means that partnerships and collaborations have become prevalent in the implementation of AI-driven drug discovery and development programmes. However, some pharma companies do now have their own AI teams, although the model of adoption and implementation of these technologies varies.



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Who in your organisation is responsible for AI implementation?

There are differences in the ways in which AI implementation is co-ordinated. This responsibility being under the jurisdiction of R&D is the most common model, but it is interesting to note that almost 25% of respondents indicated that AI implementation is not co-ordinated centrally, suggesting a fragmented or more ad-hoc pattern of uptake.



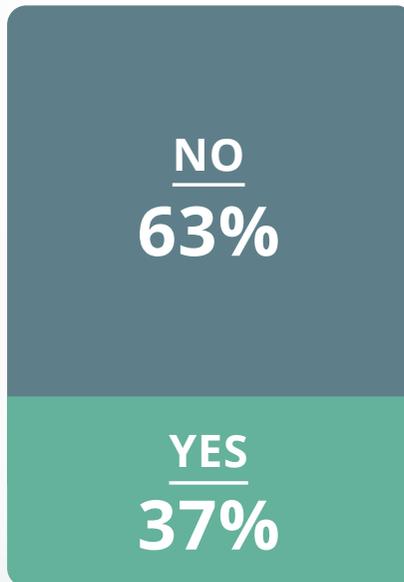
- R&D
- Chief Technology Officer
- Not centrally co-ordinated
- Chief Information Officer



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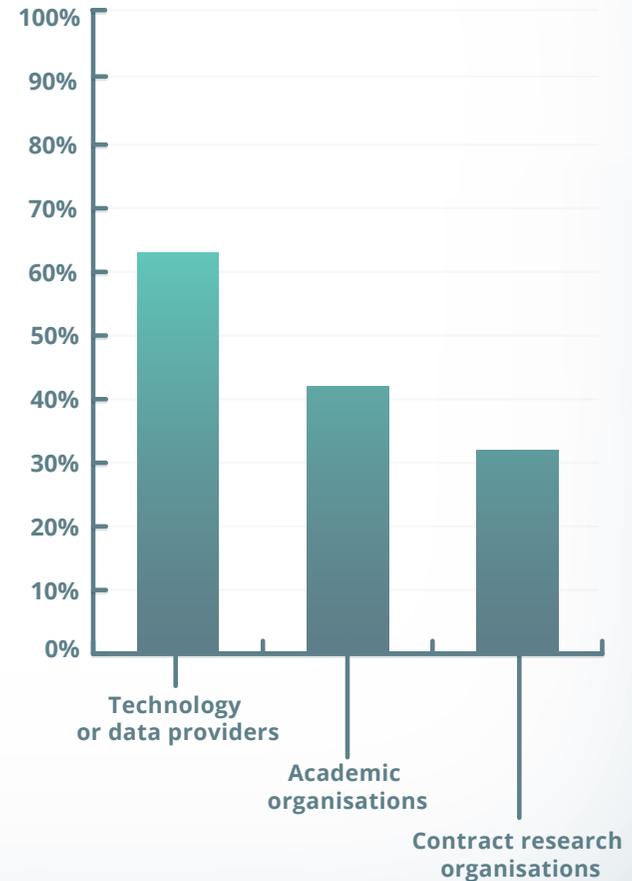
Do you partner with any other organisation to implement AI?

Similarly, while numerous companies do not partner with others with regards to AI, there are many that do. For those in partnerships, these collaborations are a mix of technology or data providers, academic organisations, and contract research organisations (CROs) and most commonly relate to drug discovery, drug design, and data analysis.



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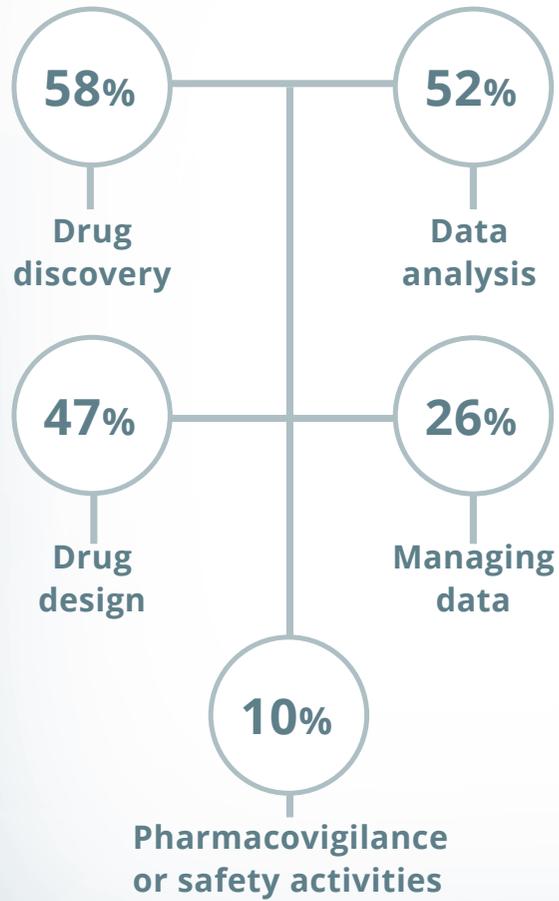
If yes, what type of organisation do you partner with?





10

Which areas do your partnerships relate to?





ORGANISATIONAL CHANGE

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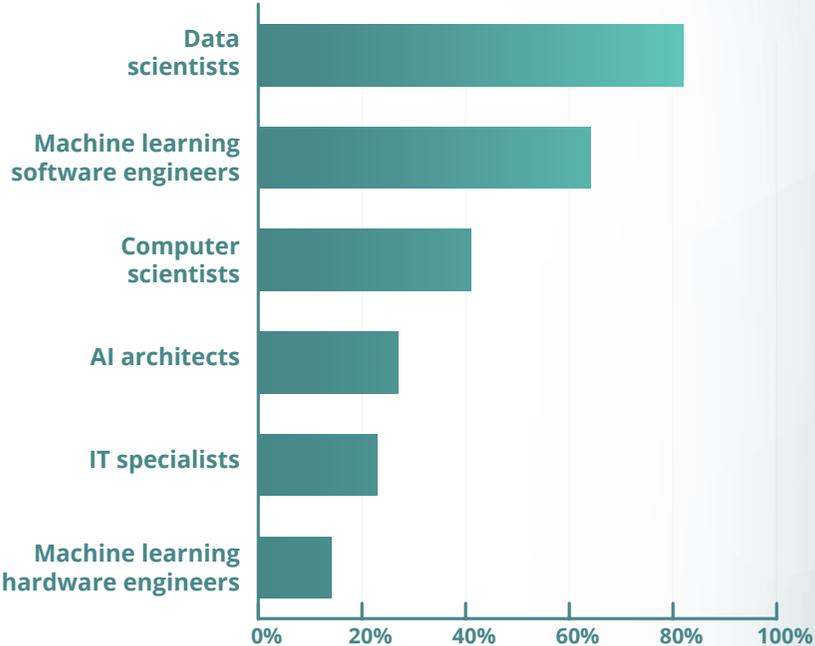
Do you plan to expand AI staff through next year?



"We've seen more organisations embrace the AI branding and create job roles and departments that reflect this, moving past the hype and replacing scepticism with action."
 Jim Weatherall, Vice President of Advanced Analytics and Head of the Advanced Analytics Centre, AstraZeneca

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What type?



"There are too few people that understand machine learning and the drug discovery and development process. You need some of these experts. The problem is we don't have them yet, and we can't train them fast enough."
 Brandon Allgood, CTO and Cofounder, Numerate



One widely-cited criticism of AI is that the term has become a catch-all and poorly defined buzzword, and that the term has been overhyped by big tech companies. Indeed, some point to the fact that some of what is described as 'AI' are just machine learning methods that are actually several decades old. As such, it is important to consider what the hype surrounding AI really is, how much is justified, and what this means for the usefulness of its associated tools.

"Thanks in no small part to the marketing and commercially driven interests of Google, Facebook, Amazon, Apple, Microsoft, and the startup ecosystem, the term Artificial Intelligence has lost all meaning."

Brian Martin, Head of AI in R&D Information Research, Senior Principal Data Scientist

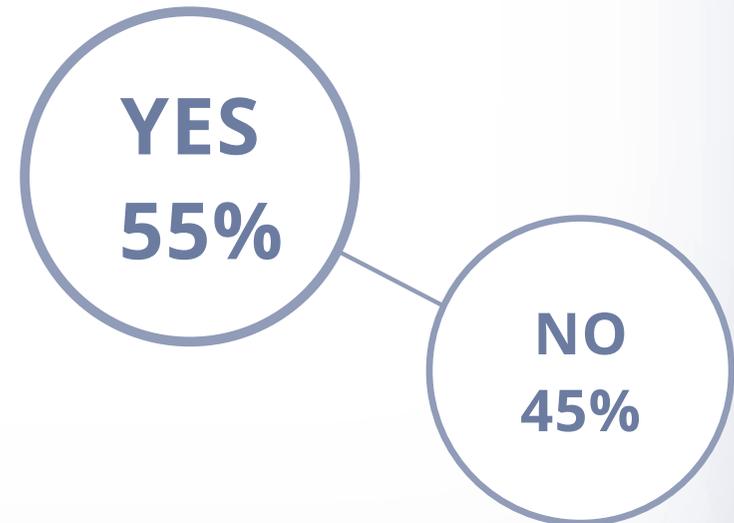
"The machine learning and AI effect is real, it's not just hype... We're making big strides in machine learning and applying it here, but there's still a long way to go. This is far from being a magic bullet."

Brandon Allgood, CTO and Cofounder, Numerate

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Do you agree that there is a lot of hype surrounding AI in drug development?

There is a clearly a need to consider whether the hype surrounding AI is justified, or whether it is becoming somewhat of an empty buzzword. It is pertinent to think about how much of this excitement is justified in regard to AI's novelty, universality usefulness, and transformational ability.





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If yes, what is the hype?

Novelty



Universality

New promise of AI to solve every problem

Is it just a branch/rebranding of machine learning?

A buzz-word

It has been around for some time in computational chemistry

Promises to solve every problem

Every prediction technique is marketed as AI

Magic bullet to solve all problems

Can be used in everything without validation and tuning



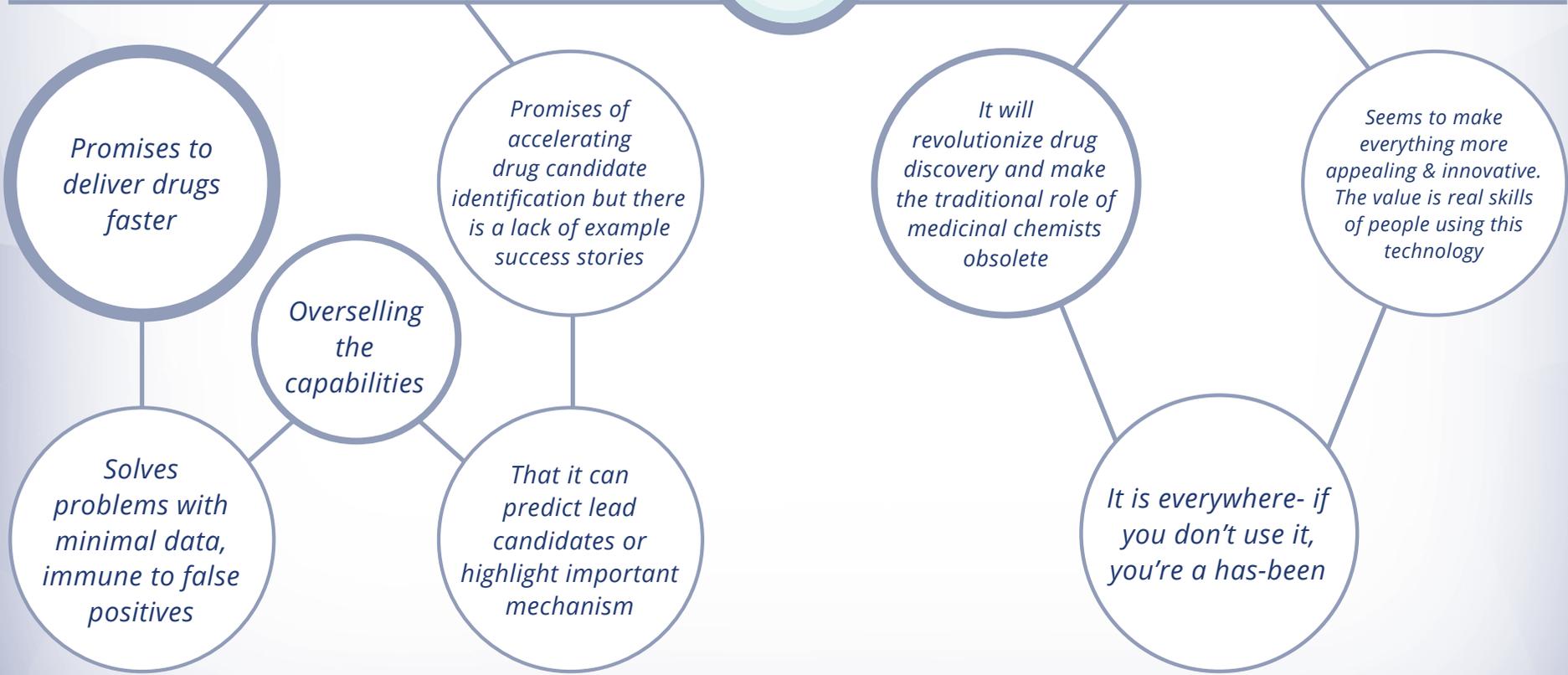
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If yes, what is the hype?

Usefulness



Transformational

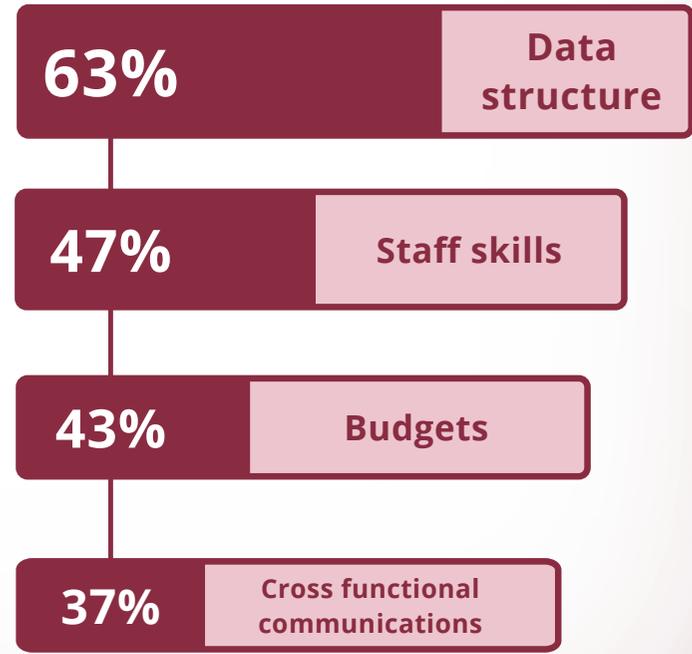


Ambiguous nomenclature and driverless-car-driven hype are not the only issues facing the adoption and implementation of AI. Companies will have to make considerable effort to change organisational and individual mindsets on what it is to be a scientist in drug discovery, and also invest in ensuring that they have the people with the required skills and data literacy. If the full potential of these technologies is to be realised, these challenges must be acknowledged and addressed.

15

What are the challenges of AI implementation in Drug Discovery?

There are challenges with regards to the implementation of AI in the drug discovery process, with respondents all concurring that staff skills, data structure, budgets, cross functional communications are four significant hurdles to overcome.



"We have to treat AI as much as a 'human problem' as a 'machine problem'. That is, we are trying to understand how best people can interact with AI, what will lead them to trust the outputs, and how to effectively blend their own soft subjective judgement with the outputs of a hard mathematical engine."

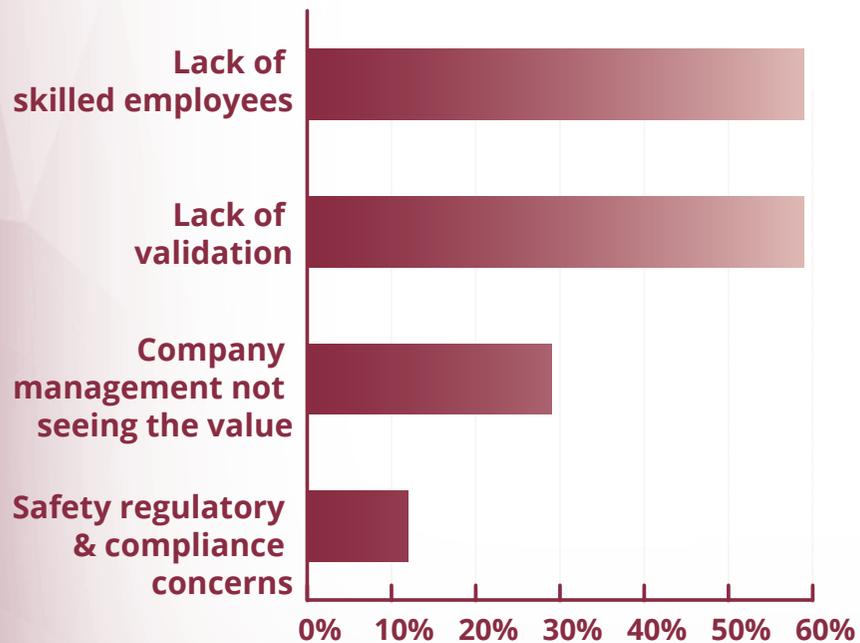
Jim Weatherall, Vice President of Advanced Analytics and Head of the Advanced Analytics Centre, AstraZeneca



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Which of the following would you identify as hurdles to the broad adoption of AI?

In particular, lack of skilled employees and lack of validation are the two most important obstacles in the way of broad adoption.



Despite the caveats of the AI revolution, it is clear that these technologies have the potential to be an incredibly transformative and effective force on every stage of the drug development process. For the most efficient implementation of AI, it is essential to consider where exactly the current technologies can have the biggest impact and produce the greatest benefits.

"Imagine if you were able – with a certain degree of accuracy and uncertainty – to confidently predict the clinical efficacy and safety of your medicine, before it ever makes it in to clinical trials."

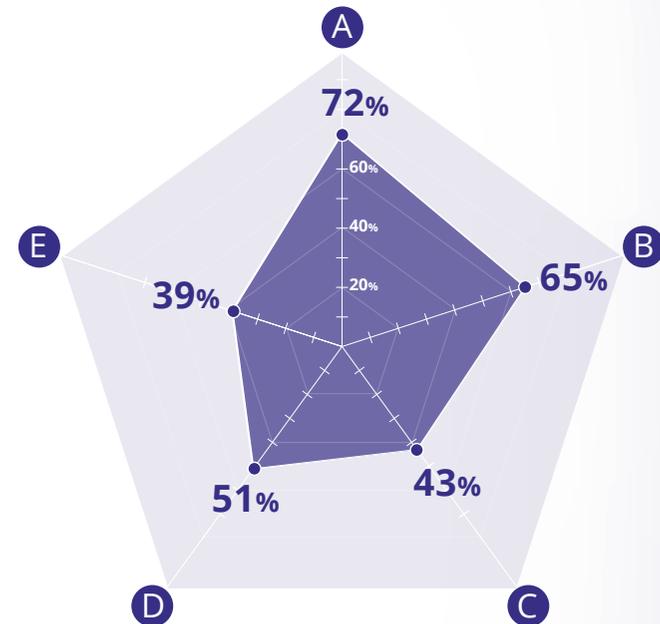
Jim Weatherall, Vice President of Advanced Analytics and Head of the Advanced Analytics Centre, AstraZeneca



"In pharmaceutical research and development, this means the concept of drug R&D as a pipeline with a start and an end is history"

Brian Martin, Head of AI in R&D Information Research, Senior Principal Data Scientist, AbbVie

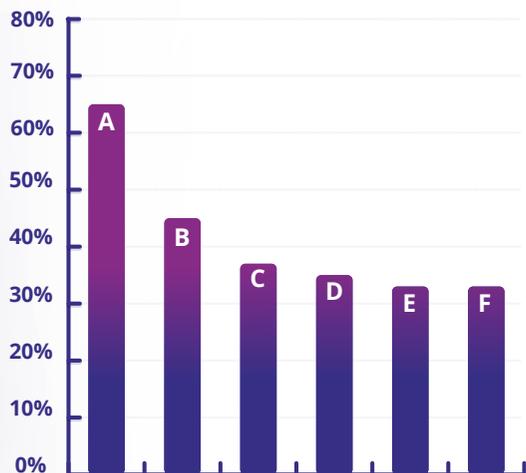
17 Where can AI and machine learning be most helpful in drug development?



- A. Data analysis
- B. Drug design
- C. Improving in basic biological understanding
- D. Model management & managing big data
- E. Synthesis design

18 **What do you think is going to drive AI forward in Drug Development?**

Discovery and design of novel/biological targets was emphasised as the most significant area for driving forward AI for drug development.



- A. Discovery and design of novel/biological target
- B. Genomic Driven Research
- C. Phenotyping
- D. Genetic Driven Research
- E. Understanding of Biology
- F. Digital Biomarkers

“Learning new underlying disease driving mechanisms from data, however, which could significantly support pharma R&D strategies, can hardly be done with today’s AI technologies, but it is one of the main areas of AI research today.”

Andreas Schuppert, Key expert, Bayer AG and Professor, Aachen University

“Artificial intelligence – or more specifically, narrow or specialized artificial intelligence techniques – play key roles in enabling value delivery in all steps of the cycle”

Brian Martin, Head of AI in R&D Information Research, Senior Principal Data Scientist, AbbVie

As the survey has demonstrated, AI has many applications in many areas of drug discovery and companies are already using it in a variety of ways. Having addressed the hype surrounding AI and with the recognition that there will be no magic silver bullet, it can nevertheless be concluded that specific AI tools and technologies hold significant promise for transforming the R&D process, developing new drugs more quickly and cheaply and ultimately delivering benefits to the lives of patients.



ADDITIONAL CONTENT

Oxford Global sat down with industry leaders to discuss further areas on AI in Drug Discovery. We reflect on topics such as machine learning, advanced analytics with AI, development pipeline with AI and more.

Visit our **Content HUB** for more expert insight into AI in Drug Discovery



BREAKING THE DISCOVERY AND DEVELOPMENT PIPELINE WITH AI

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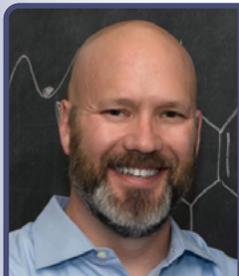


UNLOCKING THE FULL POTENTIAL OF DATA THROUGH ADVANCED ANALYTICS

"[...] AI could have an impact on the wider healthcare industry. We have already seen chat bots and virtual assistants, with whom you can have a 'conversation', in order to discuss your health or medical issues."

Jim Weatherall, Vice President of Advanced Analytics & Head of the Advanced Analytics Centre, AstraZeneca

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THE FUTURE OF MACHINE LEARNING AND AI WITHIN DRUG DISCOVERY

"With machine learning one can get to a drug faster/cheaper, having made fewer compounds and having spent less money and less time, which is great. But that's just taking an existing process and making it more efficient."

Brandon Allgood, CTO and Cofounder, Numerate Inc.

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HIGH PERFORMANCE ACTIVITIES IN ARTIFICIAL INTELLIGENCE

"Recent results indicate that AI methods, such as reinforcement learning, may provide new options to monitor or even improve the impact of therapeutic strategies on patient outcome."

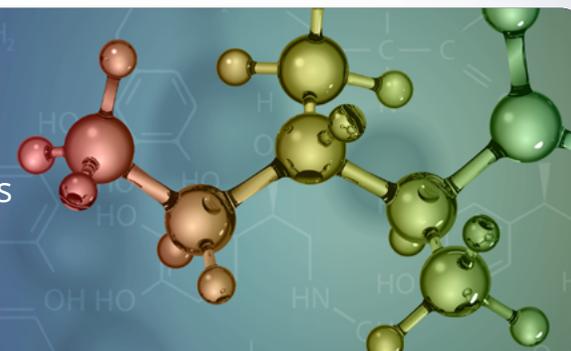
Andreas Schuppert, Key Expert, Bayer AG and Professor, Aachen University

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Drug Discovery Summit | Drug Design and Medicinal Chemistry Congress
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The **R&D Series** features 3 outstanding programmes bringing together Europe's most successful pharmaceutical organisations, top biotech companies and internationally renowned academic institutions specialising in therapeutic areas. The event includes over 100 cutting-edge presentations and workshops, over 8 hours of valuable networking sessions, and an exhibition hall showcasing 40 vendor companies.

Join us in Berlin this May to gain valuable insights on the most critical updates on empowering drug discovery with chemical biology as well as overcoming challenges with handling discovery data. Enabling technologies that facilitate quicker drug development timelines such as protein degradation tools, target-based discovery techniques including RNA as novel targets, cutting edge computational chemistry and drug design methods as well as AI are also addressed.

> Download the Agenda 



Featured Presentations from the R&D Series Include

Computational Design Of Target-Focused Chemical Libraries To Address RNA-Binding Proteins

John Karanicolas, Professor



A Perspective On AI In Drug Discovery - A Case Study From Bayer

Rolf Jautelat, Vice President Medicinal Chemistry



AI In Lead Optimisation

John Griffin, Vice President and Head, Translational Sciences

