WHAT IT TAKES TO **LEVERAGE AI IN PHARMA AND BIOTECH R&D**

Novasecta

Pharmaceutical R&D leaders must understand the potential of AI

Artificial Intelligence (AI) is a blanket term for a range of software applications that can be applied to achieve a diverse range of desired outcomes. By contrast Pharmaceutical Research and Development (R&D) is a complex and long-established multi-disciplinary activity that has a very clear desired outcome: a medicine that addresses an unmet need for a set of specific patients at a reasonable price.

The challenge for pharmaceutical R&D leaders is to first identify where AI can most make a difference, preferably through demonstrated results, or “use cases”, then find ways to leverage AI by addressing the challenges of practically applying it.

AI at its simplest comprises the application of computing power to identify patterns, predict outcomes, or validate hypotheses from datasets. Generative AI adds the ability to produce new content from the datasets.

The potential Pharmaceutical R&D applications for AI include drug discovery (e.g. target discovery and validation, drug design, in-vitro and in-vivo pharmacology, DMPK), clinical and translational science (e.g. trial protocol design, patient population identification and stratification), clinical operations (recruitment, site monitoring, processing clinical data), non-clinical development (e.g. safety, toxicology, pharmaceutical development, CMC), and pharmacovigilance.

Most AI R&D use cases so far have been for operational or process improvement

Most examples of successful AI use cases in pharmaceutical R&D have been either to improve operational efficiency or to improve the process of designing molecules in drug discovery. For example operational efficiencies can be made in clinical operations, creating first drafts of regulatory submissions, and pharmacovigilance and adverse event reporting.

For molecular design in drug discovery, AI can support discovery scientists, though owing to the limitations of public domain data, an estimated 80% of applications to date represent predicting docking for existing biological targets. While this may not yet be transformative, it is certainly an evolution from the early days of computational chemistry.

It is notable that in these “low hanging fruit” operational efficiency and drug discovery domains there are limited or no regulatory implications, so fewer constraints, to be considered in how AI is used. And it is the sponsor that bears the risk of the AI technology not working, rather than regulators, payers, patients, or governments.

Still early days for transformative AI R&D use cases

All the disciplines of pharmaceutical R&D can be influenced and informed using real world data concerning patients as well as health economic data for payers. The thoughtful use of patient and payer data represent a more transformative opportunity for AI. This is particularly the case for embedding such data in the activities of R&D to discover and develop new medicines that make a difference to patients in a way that is consistent with payer realities.

In the clinical/translational science domain, particularly where the use case involves the use of patient data, there has been less progress to date in applying AI. This is partly caused by data heterogeneity, and partly because regulatory implications become more important, which take time to be agreed on.

Future AI applications involving patient data are therefore still mostly work-in-progress. Such applications include identifying patient populations and cohorts that have high risk of disease progression. This can enable precision medicine approaches, methods to increase diversity and inclusion in clinical trials, and ensuring co-morbidities are comprehended. A more progressive approach can involve using Large Language Models (LLMs) to write protocols, though these are subject to the risk of hallucinations. Social listening is also a new work-in-progress application that seeks to assess the impact of medications on patients' lives, which could lend itself to future LLMs.

Multiple challenges in data and people

The biggest challenges of implementing AI in pharmaceutical R&D lie in data quality, particularly its heterogeneity and incompleteness, data availability, for example regulatory, payer and governmental concerns regarding the use of patient data, and people, for example misunderstandings between technologists, scientists, and physicians.

The data challenge is most pertinent for patient data, as it needs to cover diverse patient populations that may not uniformly engage with the healthcare system, and multiple complexities in connecting the effect of medication on disease progression. On top of these issues comes concerns about how such data can be anonymised and/or used in domains that the patient is not aware of or involved in. In clinical trials, there are also limitations about how many samples can be taken from patient populations to provide the datasets required for AI algorithms to produce insight.

For the people challenge, siloes between professionals in different disciplines, for example business development, R&D, and within R&D, create confusion and misunderstanding. There is a particular lack of common understanding between the basic skills required to get the most for AI: scientists, AI technologists, and physicians. Functional experts also tend to seek applications in their own areas rather than the more cross-functional applications that can be the most transformative for their company and the patients they serve.

For applying patient data to pharmaceutical R&D there is the further complication in many pharma companies of a lack of clear accountability for such applications, for example Chief Patient Officers, Medical Affairs heads, and Public Affairs all have interests in the collection of patient data. While clinical development professionals have interests in the use of this data.

How to best leverage AI for pharmaceutical R&D

AI is nothing without data and people. The reality is that software development has been taking place more quickly than quality data has been assembled, curated, and made available to the algorithms that can drive powerful AI applications. And to get the most from AI requires people that have a multi-disciplinary mindset and cross-functional awareness that is sadly not common in the highly specialised functions that are required for successful pharmaceutical R&D.

So the first step in leveraging AI for pharmaceutical R&D is acknowledging the limitations of current datasets, particularly those related to patients which are by their nature sensitive and subject to ethical considerations in their use. If the data are not good enough, pharmaceutical R&D professionals must engage with the physician, regulatory, payer, healthcare system, patient group, and government communities to find creative ways to make it available.

The second step is to address the people side of applying technology to create desirable outcomes. Deep generalists are required to bridge the misunderstandings between functional experts. And AI understanding and expertise must be embedded in the cross-functional project teams that drive progress of assets through drug discovery and development. This embedding and federating of AI expertise represents a core role for the emerging digital teams and leaders that are being added to corporate pharma executive teams and Information Technology functions.

CONCLUSION

With transparency, realism, and a truly multi-disciplinary and cross-functional mindset, AI has great potential in pharmaceutical R&D. The best is yet to come.