EXECUTIVE INSIGHTS

Preparing for Innovation: A Maturity Framework for Artificial Intelligence in Life Sciences

Key takeaways

1. L.E.K. Consulting has developed an artificial intelligence (AI) maturity framework that can be deployed across use cases to assess the fit of AI, data availability, the strength of existing capabilities, the market environment and the extent of impact demonstrated
2. L.E.K. applies this framework to use cases within drug discovery — namely drug repurposing, drug target identification, small molecule drug design and antibody drug design — to assess the level of AI maturity
3. While some use cases (e.g. repurposing drug candidates) are more mature and have started demonstrating impact, barriers such as data availability are still being overcome in other use cases.
4. Advancements in technology, such as generative AI, are expected to lower barriers and accelerate the adoption of AI in life sciences.

Artificial intelligence has emerged as a transformative force in the life sciences industry, with a remarkable capacity to process extensive datasets, identify patterns and make predictions. AI is increasingly being used to accelerate drug discovery, optimise clinical trials and enhance patient care. These advancements hold promises from reshaping innovation and designing of life-saving therapies to shaping life sciences companies' strategic decision-making.

In this *Executive Insights*, we describe a framework for assessing the maturity of AI capabilities and utilisation across different use cases within drug discovery.

Framework to measure AI maturity

L.E.K. has devised a comprehensive framework to gauge the development and deployment stages of AI solutions, enabling organisations to gain precise insights into the readiness and potential of AI initiatives. Our framework considers five critical dimensions (see Figure 1) used to evaluate AI maturity (see Figure 2).

Right problem

Determines the suitability and advantages of AI solutions over traditional approaches

Right data

Evaluates current data availability, accessibility and quality

Right capabilities

Examines the available tools, platforms and expertise required for effective execution

Right market configuration

Considers the number of active players and the extent of collaboration interest from pharmacuetical companies

Demonstrated impact

Evaluates AI's ability to generate novel insights and identifies tangible successes achieved thus far

Figure 1

The AI use case framework

Dimensions	Key Questions
Right problem	• Are issues **suitable** for the deployment of AI? • Does AI provide a **clear advantage** compared with other methods (e.g., Datasets too large for human processing)?
Right data	• Is the data **available and suitable** for tackling the defined problems? • Is the data of **high quality and reliable**? • Are there widely accepted standards for **data sharing and utilisation**?
Right capability	• Are there **available tools** that are suitable and correctly deployed to solve issues? • Are there **specialists** with technical and commercial understanding to leverage the tools? • Is the solution well equipped to **adapt to the latest frontier developments in AI**?
Right market configuration	• Are there many **companies** that are leveraging AI to address issues? • Are there many **collaborations** between companies to cultivate a positive ecosystem? • Is adequate **funding/investment** available to deploy AI to solve issues?
Demonstrated impact	• Has the solution already demonstrated **significant efficiency, time and cost savings** through the deployment of AI? • Does the solution **expand current understanding** of the field and generate **novel insights**?

Note: the AI (artificial intelligence) maturity framework presented in other L.E.K. publications was adapted to Life Sciences use cases.
Source: L.E.K. research and analysis

Figure 2

Different levels of AI maturity and ranges

AI maturity	Low	Medium	High
Right problem	Problem-solving is left to humans		AI is well suited to provide additional value to problem-solving
Right data	No structured data capture		Data quality and access ubiquitous
Right capability	No suitable capabilities available		Wide availability of tools and specialists
Right market configuration	Market not configured to support AI implementation		Bustling ecosystem with multiple companies and collaborations
Demonstrated impact	Theoretical value/conceptual only		Proven and accepted to demonstrate value (i.e.cost savings and new insights)

Note: AI=artificial intelligence
Source: L.E.K. research and analysis

Assessment of AI in drug discovery use cases

Four AI use cases in drug discovery have been considered to illustrate the use of the framework in assessing AI maturity (see Figure 3).

Figure 3

Four use cases for AI in drug discovery in the life sciences

	Repurposing existing drug candidates	Drug target identification	Small molecule drug design	Antibody drug design
Description	Identification of existing molecules that can bind a given target to be used in other indications	Identification of druggable targets and biomarkers	Identification and optimisation of new **small molecule** candidate medicines	Identification and optimisation of new **antibody** candidate medicines
Example companies	• Atomwise • BenevolentAI • HealX • BioXcel Therapeutics	• Insitro • Insilico Medicine • Exscientia • BPGbio • e-therapeutics	• Recursion • Valo • Nuritas • Iktos • Deepcure	• BigHat Biosciences • MAbSilico • iBio • Antiverse

Note: AI=artificial intelligence
Source: L.E.K. research and analysis

1. Repurposing existing drug candidates

The use of AI in drug discovery so far is perhaps best demonstrated in drug repurposing, where AI can rapidly identify alternative indications for existing molecules. Over 250 companies are currently working on repurposing drugs through AI, with COVID-19 having provided a unique opportunity to apply this quick and flexible approach to drug discovery.

Baricitinib, a Janus kinase inhibitor for rheumatoid arthritis, was identified as a potential treatment for COVID-19 by BenevolentAI using their knowledge graph platform. It received emergency use authorization from the U.S. FDA in 2020 for treatment of COVID-19 in hospitalised patients followed by full approval in 2022, based on the results of four randomised clinical trials.

Most compounds identified by AI repurposing approaches are still under evaluation in clinical trials. The outlook is positive: data availability and quality are expected to improve as data becomes more diverse and accessible. That should fuel efforts in this space.

2. Drug target identification

AI techniques can rapidly build molecular disease models and much more efficiently identify druggable targets and biomarkers than traditional methods. An enormous volume of biomedical data is available, although the integration of multiple unstructured datasets is challenging. AI can be employed to extract and analyse findings from unstructured datasets, such as journal articles and omics databases as well as imaging and real-world patient data. Knowledge graphs are used to identify novel connections between entities, although the capabilities of these approaches are limited by the quality of standardisation and labelling of underlying datasets.

Initial programs using AI in drug target identification have moved through discovery and preclinical development, and at least 20 drugs with novel disease-target associations identified by AI are progressing through phase 1 and 2 studies. As companies expand datasets and feed findings back into AI algorithms, increasing numbers of drugs with novel disease-target associations — or entirely novel targets — are expected to emerge.

3. Small molecule drug design

Using available chemical structure data, AI can simulate complex chemical properties or enable the design of drug structures significantly faster and more accurately than traditional methods. Within this use case, companies can use AI to screen existing chemical libraries or to generate novel chemical designs. The availability and usability of underlying datasets remain key challenges in this use case, with training sets being comparatively small compared with the full chemical space of billions of compounds. In addition, data availability varies across different target classes, with kinases and G protein-coupled receptors being the most well characterised, which limits generalisable models and the novelty of resulting drug candidates.

Individual AI-driven tools are already an integral part of the drug design process for small molecules, with larger predictive solutions undergoing iterative development. Small molecules designed using AI are significantly more common than antibodies designed using AI at this point. Clinical programs from companies such as Exscientia and Insilico Medicine are part of the first wave of AI-designed small molecule drugs undergoing phase 2 trials, the results of which are likely to begin to illustrate the maturity and future potential of this use case.

4. Antibody drug design

Antibody design is a growing use case for AI through both optimisation of existing structures and de novo candidate design. To date, few AI-designed antibodies have reached the clinic, and the more complex nature of these molecules poses distinct challenges compared with small molecule drug design — such as with the computational capabilities required to run larger models. AI models for antibody design are also limited by the availability of datasets for antibody sequences and antibody-antigen pairs. In addition, with a large proportion of training data being derived from the same libraries used for traditional antibody design approaches, many of the traditional challenges, such as balancing specificity and affinity, persist.

The ecosystem of researchers and companies focused on AI for antibody drug design is growing, with a flurry of announcements from large pharma companies over the past year disclosing innovative internal capabilities or collaborations with start-ups or big tech. Most recently, more than US$1 billion was secured by Xaira Therapeutics, which plans to initially focus on de novo antibodies, having employed researchers with experience designing leading diffusion models for protein and antibody design alongside genomics and proteomics groups. Continued collaborations between AI platforms and pharma companies, as well as an increase in standardised and open source data, are expected to grow the maturity of this use case.

Outlook: Maturity of AI across use cases

AI maturity in life sciences is a diverse landscape and varies across use cases (see Figure 4). While applications like repurposing existing drug candidates and target identification have made significant strides, others like antibody drug design are still in the relatively early stages.

Figure 4

AI maturity across highlighted drug discovery use cases

	Repurposing existing drug candidates	Drug target identification	Small molecule drug design	Antibody drug design
Right problem	High	High	High	High
Right data	Medium	Medium	Medium	Low
Right capability	High	Medium	Medium	Low
Right market configuration	High	High	High	Medium
Demonstrated impact	High	Medium	Medium	Low

Note: AI=artificial intelligence
Source: L.E.K. research and analysis

Generative AI is one of the most significant developments in recent years for AI in life sciences. The ability to autonomously generate novel molecular structures and other complex data could accelerate innovation and cost savings above traditional predictive AI systems. In June 2023, Insilico's small molecule drug (INS018_055) for idiopathic pulmonary fibrosis became the first drug discovered and designed completely by generative AI to enter a phase 2 clinical trial. Insilico completed preclinical development at only c.10% of the typical cost and in less than half the time required for traditional method

Despite challenges in data availability and algorithm optimisation, innovation and collaborative efforts will continue to drive further enhancement. As these advancements take root and AI integrates further into the life sciences ecosystem, we anticipate a substantial shift in AI maturity, unlocking new possibilities in problem-solving capabilities and deliverable impact across a wide range of use cases.

How L.E.K. Consulting can help

With AI increasingly being used to accelerate drug discovery, optimise clinical trials and enhance patient care, L.E.K.'s AI maturity framework helps to gauge the development and deployment stages of AI solutions, enabling organisations to gain insights into the readiness and potential of their AI initiatives. More broadly, L.E.K. can support AI companies with business model choices, BD/M&A, valuation, organisation design and scale-up and key strategic choices.

To find out more and for a further discussion, please contact the partners below.

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About L.E.K. Consulting

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