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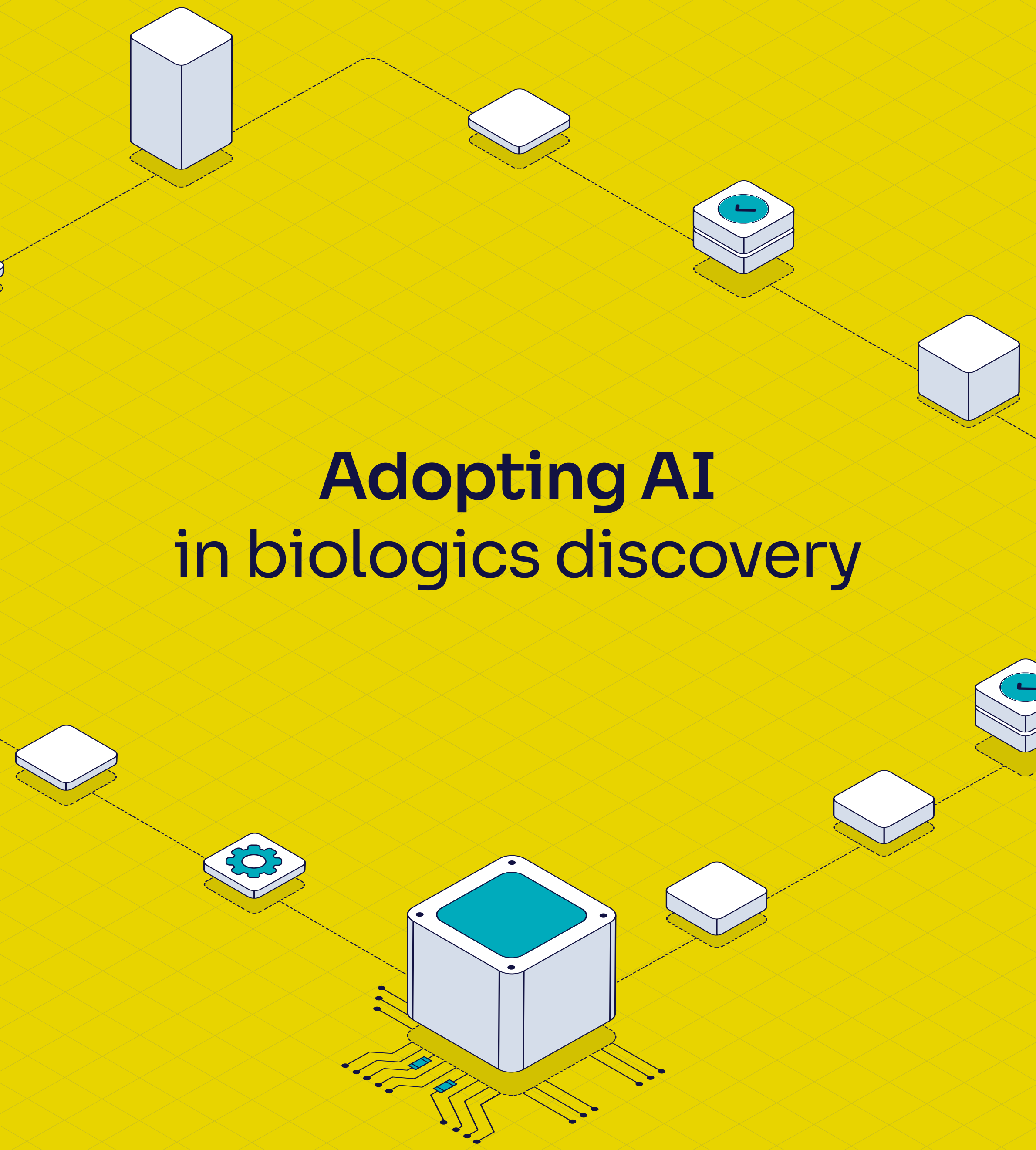

Adopting AI
in biologics discovery

In partnership with ENPICOM

Adopting AI in biologics discovery

AI-driven drug discovery is now a reality, shaping market expectations on development timelines, cost and efficiency, and candidate quality and viability. Nonetheless, AI-discovered drugs that have progressed beyond IND constitute only around 0.1% of the global biopharma pipeline.

Challenges connected with infrastructure adaptation for AI, access to usable data, and the transparency of an AI's output are part of the reason AI is not used more widely in drug discovery already. Addressing these challenges necessitates closer collaboration between life scientists and AI experts than was previously the case. To this end, dedicated bioinformatics platforms can help make data accessible to wet lab scientists and AI experts and encourage a multidisciplinary team dialogue.

Here, we discuss how these challenges connected with AI adoption relate to biologics discovery in particular.

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Introduction

Drug discovery and development have never been easy. R&D costs can amount to anywhere from over $800 million to nearly $3 billion over the course of 12 to 15 years, and the attrition rate of new drugs is high, as only up to 10% of candidates ever enter the market. While the majority of medicines have traditionally been small molecule drugs, the market share of biologics has been growing rapidly in recent years. By some estimates, biologics are expected to outpace small molecules in the market by 2027, even though they take longer to develop on average at up to twice the cost.

Biologics are a class of medicines derived from living cells used to treat a wide range of diseases, including cancer, autoimmune disease, and Alzheimer's. Biologics' three-dimensional structure contributes to their high target specificity, as well as desirable effectiveness and safety profiles.

As the biologics market grows, AI is increasingly becoming a valued computational tool for mitigating risk and increasing efficiency in biologics discovery due to its ability to rapidly analyze and interpret large amounts of data and identify patterns therein. For example, AI can facilitate accurate predictions on antibody structure, binding, and other properties, as well as generate de novo antibody sequences. AI can also assist scientists in target identification and screening for best candidate compounds.

"AI can uncover disease mechanisms, identify biomarkers for precision medicine, and leverage single-cell and spatial biology to pinpoint cell-specific or tissue-specific targets," says Lykke Hinsch Gylvin, Chief Medical Officer and Head of Global Medicine at Boehringer Ingelheim.

Moreover, workflows that used to be performed manually by human scientists are being automated by AI. Automation is vital to keeping abreast with growing volumes of data; by reducing the need for human intervention, errors are reduced and data quality and consistency is improved. Taken together, these applications of AI promise to reduce the time and cost of biologics discovery and dramatically increase its success rate.

We haven't seen the potential of AI adoption fully translated into actual successes when it comes to new medicines. But it has huge potential – AI is influencing drug candidates in development, increasing our probabilities of success, making us faster in a very different way.

Markus Kosch

Head of Oncology Europe and Canada at Daiichi Sankyo Europe GmbH

However, the life science industry is still in the early days of AI adoption in drug discovery overall.

“We haven't seen the potential of AI adoption fully translated into actual successes when it comes to new medicines,” says Markus Kosch, Head of Oncology Europe and Canada at Daiichi Sankyo Europe GmbH. “But it has huge potential - AI is influencing drug candidates in development, increasing our probabilities of success, making us faster in a very different way.”

AI’s potential is leading entrepreneurs to start companies specifically dedicated to using AI in drug discovery.

“There are probably now hundreds to thousands of companies using AI for drug discovery,” says Emmanuelle Martiano Rolland, COO and co-founder of the AI drug discovery startup AQEMIA.

As AI-driven drug discovery continues to gain traction, successful adoption of AI in biologics discovery will depend on a robust understanding of how the technology can address pertinent scientific and business needs. With this in mind, AI can help guide developers towards the best biologic candidates.

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Emmanuelle Martiano Rolland
COO and co-founder of AQEMIA

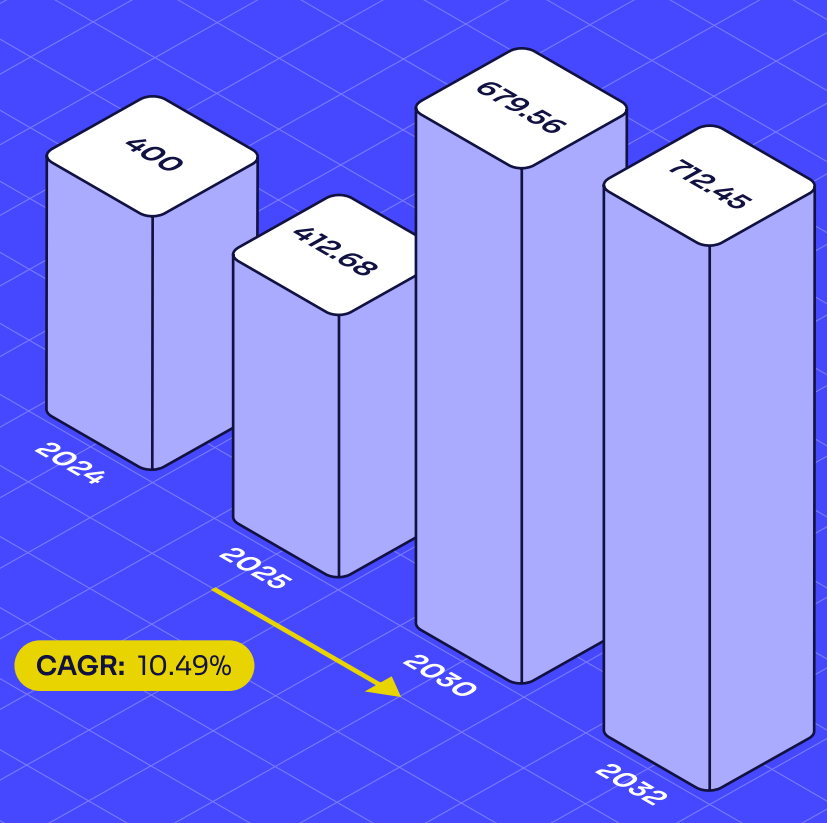


Figure: Evolution of Biologics market size

Challenges to AI adoption in biologics discovery

According to a recent MIT NANDA report, the majority of businesses across industries that have adopted AI see no return on their investment, even though most companies are interested in successfully adopting AI.

When it comes to following through, however, the MIT NANDA report identifies a growing divide between the companies that are successful and those that struggle in adopting AI. Companies that focus on AI systems capable of learning and adapting to the organization's need fare better than those who invest in static tools that do not integrate well into existing workflows.

"Heavy investment in models without matching investment in data, integration, and change management is why so many pilots never scale," explains Adnan Masood, Chief AI Architect at UST, a global digital transformation solutions provider.

So, as companies are being pitched by dozens of AI-tool developers each day, they must carefully consider how well an AI platform can adapt to their evolving needs.

In drug discovery, the adoption of AI requires an infrastructure consisting of the hardware, software and the data a model needs in order to generate an output.

Ofer Sharon is the CEO of OncoHost, a precision-oncology company. Prior to founding OncoHost, he held senior management positions at Merck and AstraZeneca and was part of the development and clinical launch team for Keytruda, a biologic cancer immunotherapy. Sharon explains, "AI's success in biologics discovery relies on a triad of robust data infrastructure, advanced computational capabilities, and multidisciplinary human capital."

Bringing the different factors needed for AI adoption together is not simple, as they each present distinct challenges.

Heavy investment in models without matching investment in data, integration, and change management is why so many pilots never scale.

Adnan Masood

Chief AI Architect at UST

Adapting infrastructures for AI integration

Infrastructure in the life science industry is still in the early stages of adopting AI in biologics discovery. To realize AI's full value, biologics developers must develop an infrastructure - including specialized hardware and cloud scale computing abilities - that enable seamless integration of AI into discovery workflows.

"Interoperable platforms and APIs ensure seamless integration between AI tools, databases, and research workflows, while secure storage and compliance systems protect sensitive data and adhere to regulations like GDPR and HIPAA," says Hinsch Gylvin.

However, infrastructure often has a long way to go before living up to the promise of seamless integration.

"AI's potential remains constrained by the immaturity of the ecosystem required to operate it at scale," Sharon states. "Data remain fragmented and siloed - between preclinical, translational, and commercial teams; between internal and external partners; and across incompatible platforms."

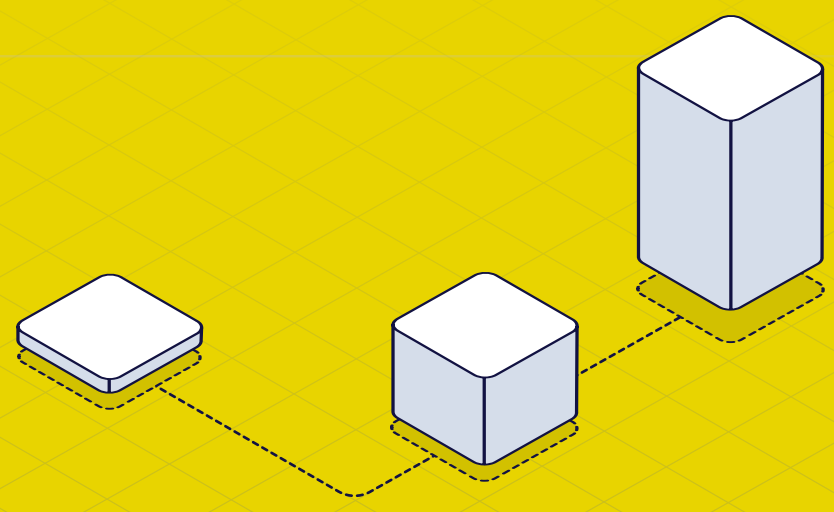
"An apt analogy here may be the industrial adoption of electricity at the turn of the 20th century," explains Nicola Bonzanni, CEO and founder of ENPICOM, a software company with a platform approach to unifying and integrating discovery workflows and data management. "It actually took some time for electricity to be adopted in factories, because the factories were built around steam engines and required a specific layout. Today, we must similarly redesign our infrastructure in order to fully integrate AI in biologics discovery."

For this reason, AI integration is oftentimes speedier with a specialized implementation partner rather than through internal IT or vendor-led approaches.

AI's potential remains constrained by the immaturity of the ecosystem required to operate it at scale. Data remain fragmented and siloed - between preclinical, translational, and commercial teams; between internal and external partners; and across incompatible platforms.

Ofer Sharon

CEO of OncoHost



The black box problem

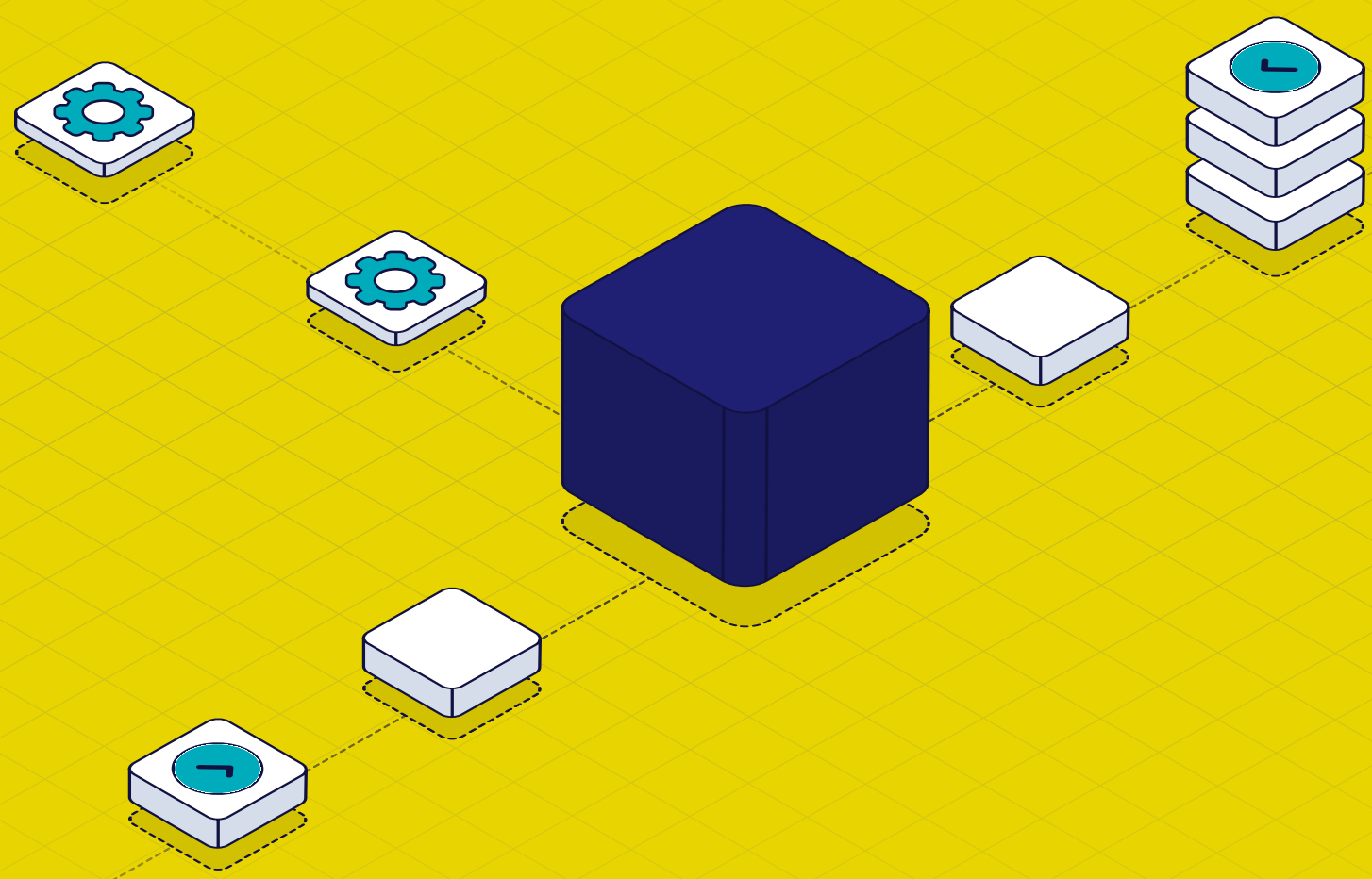
Furthermore, the perceived ‘black box’ around AI, or the lack of transparency relating to its analysis and decision-making process, can make it difficult for lab scientists to place their trust and funding in the technology. The black box phenomenon can detract from AI’s perceived utility, as it makes it difficult to understand how an AI’s predictions are made.

AI tools can become black boxes either because the developers intentionally withhold the source code, or as a result of how the AI is trained on data. Operating as a black box can also make it difficult to adapt an AI’s output in response to errors.

“AI tools must be intuitive, interpretable, and actionable,” says Sharon. “Results cannot remain “black box” abstractions; they must provide biological rationale and context for decision-making.”

However, making a black box more transparent is not easy. While sharing the source code of an algorithm can make its decision-making process clearer, more complex AI models are continuously adapting to incoming data. This learning process is not easily clarified to outside observers, even if the algorithm’s architecture is viewable. To place their trust in AI, researchers must retain control over the technology and be able to understand an AI’s output within a broader, critical context.

In protein engineering, for example, AI models are often used to optimize protein sequences by suggesting certain amino acid substitutions that human scientists could not think of on their own. In the best of cases, life scientists can understand the rationale behind these changes by inferring how they affect the protein’s structure and function. As a result, the issue of the ‘black box’ is resolved, as the transparency of the results speaks for itself.



The need for a standardized data foundation

Moreover, access to deep, broad, and standardized data on which to train AI often remains limited, which can compromise the technology's ability to make accurate predictions and integrate into existing drug discovery workflows. AI platforms necessitate a formalized agreement between life scientists and AI experts regarding data standardization. This is a key technical prerequisite for automating workflows in drug discovery.

Without this level of agreement, AI models are at a higher risk of being trained on noise, rather than meaningful data. In biologics discovery, datasets must also include molecular-level data like sequences, biophysical parameters, and functional assay results. Interestingly, standardized data is easier to come by for certain types of biologics than others.

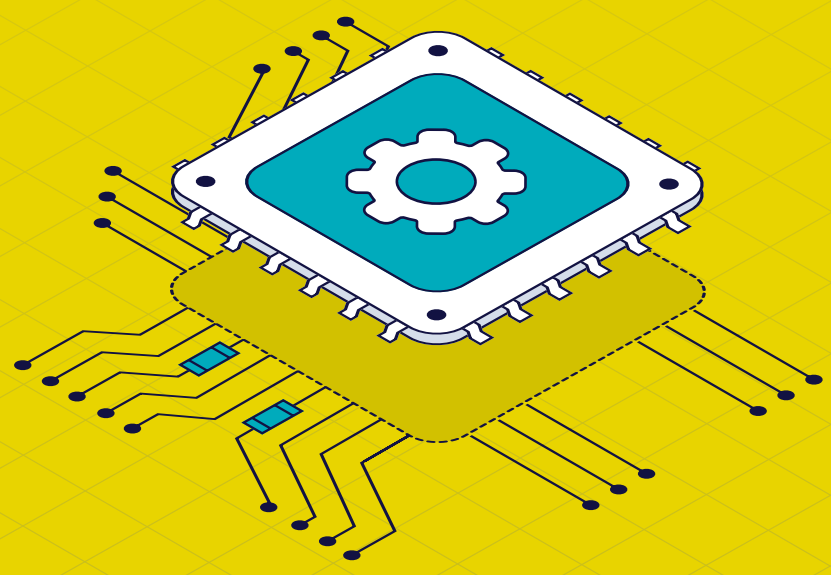
"Antibodies and other well-established protein therapeutics are comparatively 'AI-friendly' because they more readily come with large, standardized datasets and mature processes," says Masood. "Cell and gene therapies are harder due to their small and heterogeneous datasets, complex and evolving manufacturing, and strict privacy constraints that slow down data aggregation and model generalization."

Vaccines, mRNA therapeutics and antibody-drug conjugates (ADCs) form a middle ground, as the data available on the therapeutics is often still incomplete, and their biology highly complex. As a result, the impact of AI is likely to be more evident in antibody discovery first, before coming to the fore in other therapeutic modalities later on.

Antibodies and other well-established protein therapeutics are comparatively 'AI-friendly'.

Adnan Masood

Chief AI Architect at UST



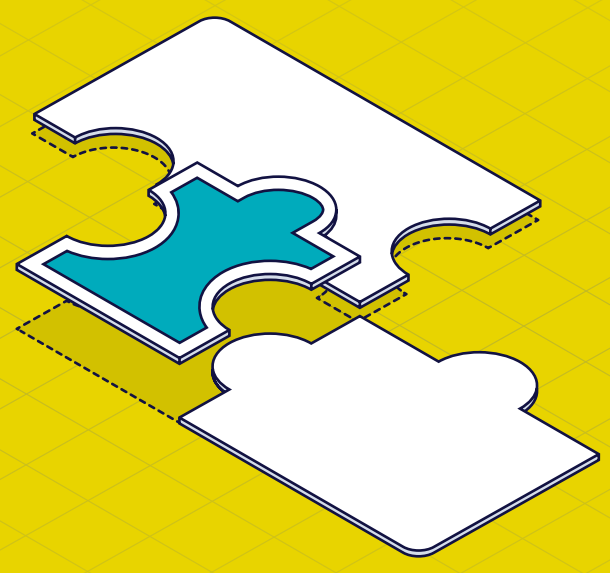
Interdisciplinary collaboration and coordination

The problem of silos does not pertain to data alone. Life scientists and AI experts are still compartmentalized within organizations and often work in isolation from one another. Connecting interdisciplinary teams of life scientists and AI specialists with one another is essential to integrating AI into biologics discovery.

“Beyond technology, organizational culture remains a barrier. The gap between R&D and market-access mindsets, between hypothesis-driven and data-driven thinking, often prevents meaningful integration,” Sharon elaborates. “Until companies address both the technical and cultural fragmentation, AI will remain a promising but under-leveraged asset.”

Successful AI adoption requires interdisciplinary expertise and coordination between molecular biologists, chemists, and pharmacologists with mathematicians, physicists and data scientists. This kind of collaborative, coordinated environment is needed for teams to make use of AI in a concerted way to drive drug discovery forward.

The challenge of bringing multidisciplinary teams together could become even more pronounced as more large organizations implement widespread AI adoption. This increases the importance of ongoing education, training and skill building.



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Ofer Sharon

CEO of OncoHost

Challenges to AI adoption in biologics discovery

Infrastructure	▪ Infrastructure – including specialized hardware and cloud scale computing abilities – is still in early stage of adapting to the needs of AI adoption and ensuring seamless integration between AI tools, databases, and research workflows. ▪ Current infrastructure limitations can be overcome by adopting AI with the help of a specialized implementation partner.
The black box	▪ The 'black box', or the lack of transparency connected with AI, can make it difficult for lab scientists to place their trust and funding in the technology. The black box can make it difficult to understand how an AI arrives at its output and adapt it in response to errors. ▪ The black box can arise as a result of how an AI is trained on data, or because the algorithms source code is withheld by its developer. Making AI more transparent is not easy. Ideally, scientists can infer an AI's 'rationale' if the output is clear and relatable.
Standardized data	▪ Access to deep, broad, and standardized data on which to train AI often remains limited. This can limit AI's ability to make accurate predictions and integrate into existing drug discovery workflows. ▪ Data standardization is necessary for workflow automation, and without it, AI models risk being trained on noise. ▪ In biologics discovery, the quality and quantity of data can vary depending on the therapy area in question. For example, antibodies and protein therapeutics are more likely to come with large, standardized datasets. Cell and gene therapies, on the other hand, have smaller, more heterogeneous datasets. ▪ Vaccines, mRNA therapeutics and antibody-drug conjugates (ADCs) form a middle ground, due to their complex biology and since available data is often incomplete.
Interdisciplinary collaboration	▪ Life scientists and AI experts are still compartmentalized within organizations and often work in isolation from one another. ▪ Successful AI adoption in biologics discovery requires interdisciplinary expertise and coordination between molecular biologists, chemists, and pharmacologists with mathematicians, physicists and data scientists. ▪ Furthermore, the gap between R&D and market-access mindsets, between hypothesis-driven and data-driven thinking needs to be bridged. ▪ Ongoing education, training and skill-building can help overcome these organizational challenges.

The Future of AI in biologics discovery

Ongoing education, training and skill building

To achieve closer interdisciplinary collaboration, researchers and AI experts will require ongoing education to enable fuller, more efficient use of AI in biologics discovery.

“Researchers need foundational knowledge of AI concepts, tools, and their applications, while AI experts must develop an understanding of biological systems, experimental workflows, and the challenges specific to biologics discovery,” explains Hinsch Gylvin. “This mutual education can be achieved through interdisciplinary training programs, hands-on workshops, and shared learning platforms that encourage both groups to engage with each other's expertise.”

“The fastest win is to put everyone on shared platforms where experimental data flows in automatically and models are exposed as easy-to-run components inside the scientist’s usual analysis environment, hiding the technical plumbing,” says Masood.

Collaborative approaches, even between organizations, will likely continue to be invaluable in bringing life scientists and AI experts together in biologics discovery.

“AI will not replace scientists; it will redefine what scientific intuition means. The true transformation lies not in replacing human reasoning but in augmenting it - amplifying the ability to see biological patterns invisible to the naked mind,” Sharon emphasizes.

As wet lab and in silico approaches become increasingly integrated with one another, the most successful organizations will likely be those that use AI as a tool that accelerates discovery and fosters scientific curiosity.

Researchers need foundational knowledge of AI concepts, tools, and their applications, while AI experts must develop an understanding of biological systems, experimental workflows, and the challenges specific to biologics discovery.

Lykke Hinsch Gylvin

Chief Medical Officer and Head of Global Medicine at Boehringer Ingelheim

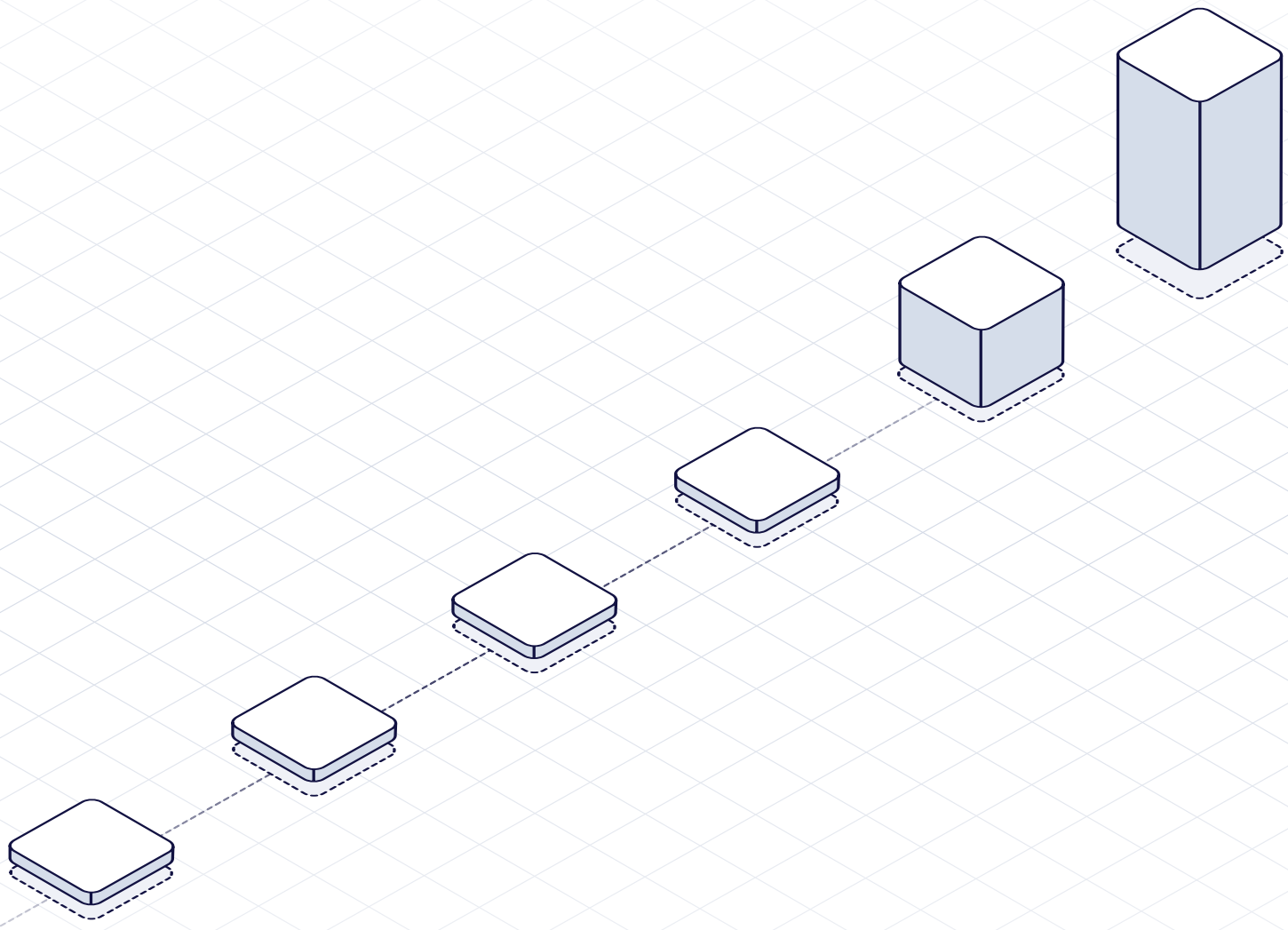
Adopting AI regulatory standards

AI is still in its early days of adoption in biologics discovery, and as a result, regulatory frameworks for the use of AI in drug discovery are still being developed. Here, a risk-based framework for assessing the use of AI could be helpful in differentiating the risk profile of using AI in different stages of development, from early discovery to later clinical stages with tangible patient outcomes.

Regulatory bodies must also address the degree to which AI output requires validation in order to be classified as reproducible and reliable, as this is essential in determining whether biologics made with AI meet general regulatory standards.

"We must first establish global AI development standards - the equivalent of GLP or GCP for model training and validation - to ensure reproducibility, reliability, and regulatory oversight," states Sharon.

A standardized data foundation is essential to achieving a high level of reproducibility and regulatory compliance.



Democratizing AI in biologics discovery

Attaining fuller integration of AI into existing workflows in biologics discovery will require the technology to become more accessible to and usable for all parties involved - not just AI experts, but wet lab scientists as well.

“No single organization can realistically build the required technology and data infrastructure alone,” explains Sharon. “The future likely lies in shared, standardized data ecosystems - a federated model of biological discovery akin to Asimov’s “Multivac” vision: a global, open-access supercomputer for drug discovery, where participants pay per access or contribution.”

To this end, the FAIR data principles could go a long way towards making it easier to share and reuse data. The FAIR principles state that, to facilitate the exchange and use of data, the data must be findable, accessible and readable by both humans and machines, and have a common structure. Furthermore, the data must be clearly sourced and have clear usage licenses.

Designated software platforms can help make data more accessible to and facilitate the use of AI models for multidisciplinary teams, in a trend the industry has termed ‘democratization’.

“Democratizing AI in this way means giving both life scientists and AI specialists access to the technology and data,” says Bonzanni.

In the future, the push towards more openly accessible data and models could drive up competition for big tech companies. For example, the release of Boltz-2 by MIT and Recursion introduced an open-source model for rapidly and accurately predicting molecular binding affinity, with potential applications in drug discovery. Boltz-2 was released in response to the limited accessibility of Google’s AlphaFold 3.

Democratizing AI means giving both life scientists and AI specialists access to the technology and data.

Nicola Bonzanni

CEO and founder of ENPICOM

Novel technologies and emerging business models

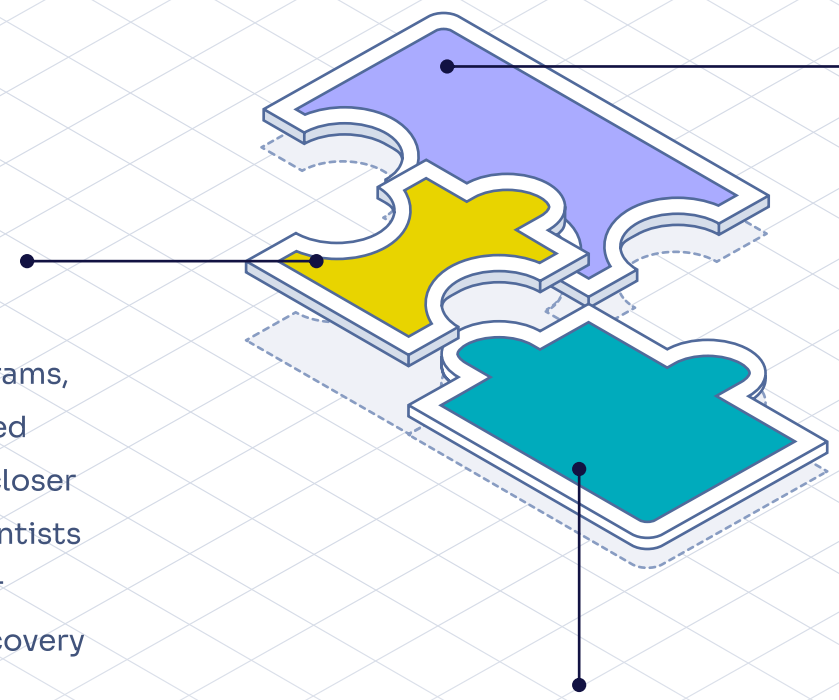
New approaches to AI-driven drug discovery that use quantum-physics algorithms to generate data may provide alternatives to models that rely on vast sets of standardized experimental data. These methods are encouraging scientists and entrepreneurs to tackle the business side of drug discovery in novel, creative ways as well.

“Our approach is different to most companies: It's not that we reproduce the science by MIT and Harvard and make a company out of it,” explains Maximilien Levesque, PhD, CEO and co-founder of AQEMIA. “Instead, we aim to literally invent the therapeutic molecules internally and build a company around one asset or a pool of coherent assets together, by using quantum inspired physics and machine learning approaches.”

“Pharmas come to us because they have a target they are struggling with, and we collaborate - for instance with Sanofi - to enhance their discovery approach. Alternatively, we have our own portfolio of assets in different stages of development,” Levesque elaborates. “Typically, the most advanced ones right now are in late-click optimization. And we discuss with our customers whether they want to partner or to in-license the programs.”

In time, such novel approaches to partnering or in-licensing AI-designed candidate programs could become a new norm in AI-driven drug discovery.

Figure: AI becomes a decision-guiding tool in biologics discovery



Democratization

Dedicated AI platforms and FAIR data principles are making AI models accessible to life scientists and facilitate integration into discovery workflows

Open source models make AI tools accessible to wider research community

Ongoing education, training and skill building

Interdisciplinary training programs, hands-on workshops, and shared learning platforms encourage closer collaboration between life scientists and AI experts, leading to fuller adoption of AI in biologics discovery

Data generation

Generating data using quantum physics algorithms to augment experimental data could alleviate reliance on vast standardized datasets

Concluding remarks

When it comes to the impact AI adoption can have on biologics discovery, perspectives in the life science industry vary. It is important for biologics developers to have realistic expectations of what the technology can offer.

“Just to manage expectations, I think AI supported or developed medicines will likely take a similar amount of time as other medicines to reach the markets, considering the need for clinical proof benefits, and looking at regulatory schedules and timelines,” says Kosch.

“In the next couple of years, fully AI designed therapies could reach patients following a similar clinical and regulatory approach to conventionally designed drugs,” Kosch elaborates. “The difference is AI designed therapies may come with a higher probability that their targets will actually be successful, with fewer negative trials.”

In the next couple of years, fully AI designed therapies could reach patients following a similar clinical and regulatory approach to conventionally designed drugs.

Markus Kosch

Head of Oncology Europe and Canada at Daiichi Sankyo Europe GmbH

AI adoption in biologics discovery can take years to fully implement and brings significant costs. Nonetheless, AI cost-saving benefits and applications in molecular design and candidate selection already appear to have a strong foothold in drug discovery, and the market for AI in drug discovery is expected to grow substantially over the next decade.

“AI can most effectively be used to avoid unnecessary investments in molecules and helps researchers decide for and focus efforts on the data-favored, higher likelihood molecules,” Hinsch Gylvin explains.

“AI-driven R&D adds data points that are critical for informed decision-making and should be a “routine” element of drug and target assessment,” says Hinsch Gylvin. “Integrating AI with biology-driven target discovery and chemistry-focused molecule design empowers scientists to make faster, data-driven decisions.”

AI-driven R&D adds data points that are critical for informed decision-making and should be a “routine” element of drug and target assessment.

Hinsch Gylvin

Chief Medical Officer and Head of Global Medicine at Boehringer Ingelheim

“If companies treat digital and cultural change as integral to AI adoption—and iterate on what works rather than chasing hype—the payoff will be faster, more reliable discovery across biologic modalities,” says Masood. Still, there are a number of steps AI has to take before it becomes a common decision-guiding tool.

“Once AI can be re-engineering for scale, handle messy real-world data, integrate into existing tools, and add governance around data lineage, model versions, and decisions influenced by the model,” says Masood, “it will become a trusted, everyday decision-aid.”

When it comes to AI adoption in drug discovery, there is no “one-size-fits-all” approach that will work for the life science industry as a whole. Instead, drug developers need to tailor AI adoption to the demands of their pipeline and candidates, and consider the time and cost needed to fully implement the technology in their organization. However, by focusing AI integration on specific tasks, AI can help inform research perspectives and guide decision-making in drug discovery.

Find out how ENPICOM accelerates AI adoption in biologics discovery here.

If companies treat digital and cultural change as integral to AI adoption, the payoff will be faster, more reliable discovery across biologic modalities.

Adnan Masood

Chief AI Architect at UST

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