M&A trends in AI for drug discovery

What pharma companies need to consider on their journey to optimise drug development

Content

Executive Summary

Artificial intelligence (AI) promises to make drug discovery and development faster and cheaper, or may even identify completely new drugs beyond the reach of traditional methods. While the technology is still young, a host of players such as pharma companies, biotechs, start-ups and established tech giants have started to use AI in the hope of revolutionising the biopharma industry.

For this paper, we analysed ten years of partnerships and deal-making to understand industry dynamics and show how the race to transform drug discovery and development with AI is reflected in biopharma M&A activity. Our aim is to offer insights to M&A and business development (BD) teams as they prepare to empower their organisations with AI capabilities developed by the businesses they acquire or partner with.

Key takeaways from 10 years of deal-making in AI for drug discovery…

1
Pharma is actively partnering but does not seem to go all-in on individual deals:

Pharma companies are very active in partnering with AI drug discovery start-ups and tech companies, but are de-risking their partnerships through low upfront payments. Overall, in five years, we expect data and AI to be an element of up to one-third of all partnership deals.

2
The AI-related M&A market is small, but heating up:

While the number of M&A transactions related to AI in drug discovery is still small, increasing momentum is reflected in growing deal volumes and larger deal sizes. We expect both the number and the size of deals to increase in the next five years.

3
While there are early signs of consolidation and capability build-up – pharma is not buying yet and AI-related deals pale in comparison to other pharma M&A activity:

Thus far, acquirers are predominantly AI-focused companies, indicating consolidation that reflects a maturing of the market and the need to hunt for capability and technology. Pharma companies are not yet acquiring companies in the space.

…and what it means for the biopharma business model

The potential of AI to transform drug discovery and development is not in question, but many pharma companies appear to take a careful external approach towards deals. While the traditional pharma business model will not change, companies need to establish AI across their value chain to reduce the cost, success rate and time to market of their programmes. Finding the right levers to accelerate internal efforts with external innovation through deals will be a key differentiator for biopharma companies. In our work we highlight **four recommendations for success:**

1
Build a valuation framework that includes technology: Assessing the technology of an AI model is a core challenge of every AI deal; M&A teams need to work with functional experts to build practical approaches, e.g. sandboxing to test the quality of the underlying models.

2
Understand the scalability and generalisation of AI use cases: Transformative deals need a vision for scaling AI modules across the organisation and potentially beyond. Too often, the data that fuels the AI engine is locked within data silos, models cannot be generalised or data ownership questions prevent scaling.

3
Build a computing and data strategy: Some companies are adapting their cloud vs on-premise decisions for certain AI models with sensitive data. Any potential target or partner needs to fit into this new operating strategy.

4
Have an integration plan that focuses on shifting people's mindset: An AI deal is not about acquiring a technology but the minds who make it run. The people in a potential target as well as in the buyer organisation need to re-think processes and be open to changing their mode of operating. Therefore, a collaboration model should be at the core of an integration plan.

The uptake in partnership and deals related to AI in drug discovery seen in recent years shows that many players are now seeking to scale AI in their organisations. If companies succeed in making drug development smarter, they can bring life-saving therapies to patients faster at lower cost.

Introduction

AI is vital to making drug development more sustainable

From original idea to launch, the process of developing a new drug can – based on different estimates[1,2] – take upwards of 12-15 years and cost between US$1-6 billion. While development costs have been estimated to double every nine years since the 1950s[3], returns for marketed therapies have decreased. Novel therapies that are often targeted at narrower patient groups will further increase the pressure to reduce costs. While these personalised treatments offer great hope to millions of patients, their development costs will ultimately be borne by healthcare systems that are already under stress. To sustain the future of pharma and biotech, therefore, companies need to find ways to make drug development faster and more efficient – a task that AI is increasingly being deployed to achieve.

The ability of AI methods such as machine learning (ML) or deep learning (DL) to analyse vast amounts of data and identify correlations and patterns has significant potential to improve many steps along the drug discovery and development process. The increase in patents and publications related to AI and drug discovery is one indicator of the intense research activity over the last 10 years (Figure 1). As the technology has matured and computing power has increased, investment activity has also intensified, leading to billions flowing into the sector[4]. The expectation is that, in combination with knowledge of biological and pharmacological diseases, AI methods will bring greater efficiency to today's cumbersome, trial-and-error, drug discovery and development approach.

The results of this are becoming increasingly evident, with the pipeline of AI drug discovery companies growing by more than 37% each year[5] and more and more companies showing how they were able to accelerate established processes.[6] In light of these developments regulators have also recognised the importance of this fast-developing field. Just this year, the US Food and Drug Administration and the European Medicines agencies have both published papers aiming to consolidate their perspectives on this topic[7,8].

Figure 1: Publications and patents related to AI in drug discovery and development from (*first five months in 2023), Sources: Espacenet, Pubmed.

Number of patent families and publications related to AI in drug discovery
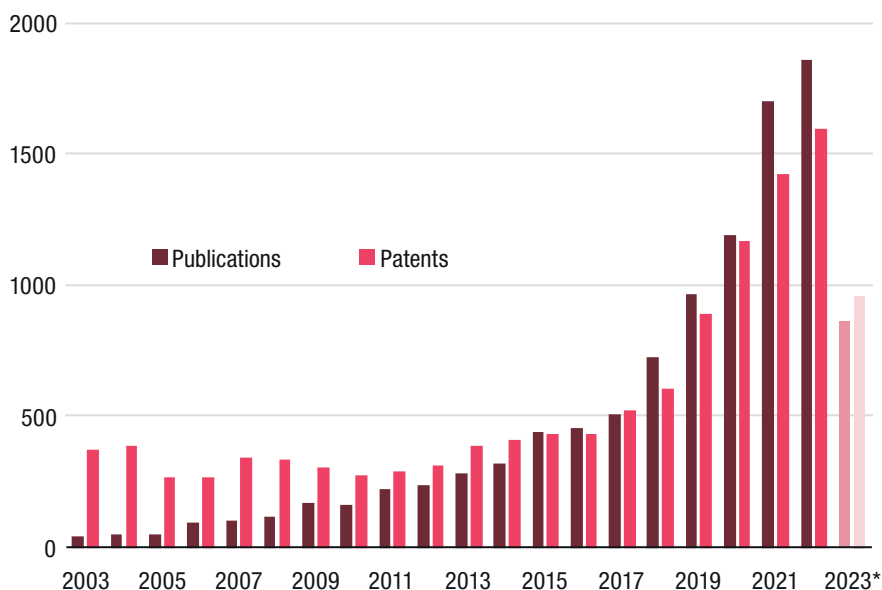
Partnering with AI drug discovery start-ups

Pharma companies have realised the potential of AI, but are seeking to de-risk the partnerships they enter into

Pharma companies have recognised the potential impact AI can have on their drug discovery efforts, and have started to drive numerous internal projects and initiatives to build up their capabilities and develop real applications[9]. In addition, pharma is building heavily on partnerships with smaller innovative start-ups, academic institutions and tech companies. An analysis of Biomedtracker data reveals more than 250 alliances related to AI in drug discovery (Figure 2), with 25% of these partnerships involving a large pharmaceutical company. Sanofi has recently been the most active in partnering, with approximately ten published partnerships, reflecting its "all-in" approach to AI and data science[10]. Most other big pharma companies have shown a similar commitment to using AI in drug discovery by announcing major alliances and data-driven projects for their R&D efforts.

Across the industry, AI technology has become an element in up to 10% of partnership deals in discovery. We predict that AI, along with data and analytics, will be a key element in more than one-third of all partnerships within the next five years. The value of these partnership deals has also risen steadily, reaching up to US$14 bn in total published deal value.

However, while these numbers illustrate the increasing importance of AI, a deeper analysis reveals that companies are taking a cautious approach to structuring these deals. In most cases, the allocation of the deal sum is heavily shifted towards milestone payments, i.e. the part of the deal sum that only gets paid if certain agreed goals (milestones) are achieved. In one of every two deals, milestone payments represent more than 90% of the total consideration, and in one in every four deals as much as 100%. This ratio is atypical compared to the industry average, and reflects a degree of uncertainty. From our discussions with industry professionals, we conclude that this uncertainty is not linked to the question of if AI will have a significant impact for drug discovery, but rather which player or model will be the one to bring it to life fastest.

Figure 2: Pharmaceutical partnerships with AI from 2013 to 2022, Source: Citeline Biomedtracker.

Partnership and published deal value related to AI drug discovery
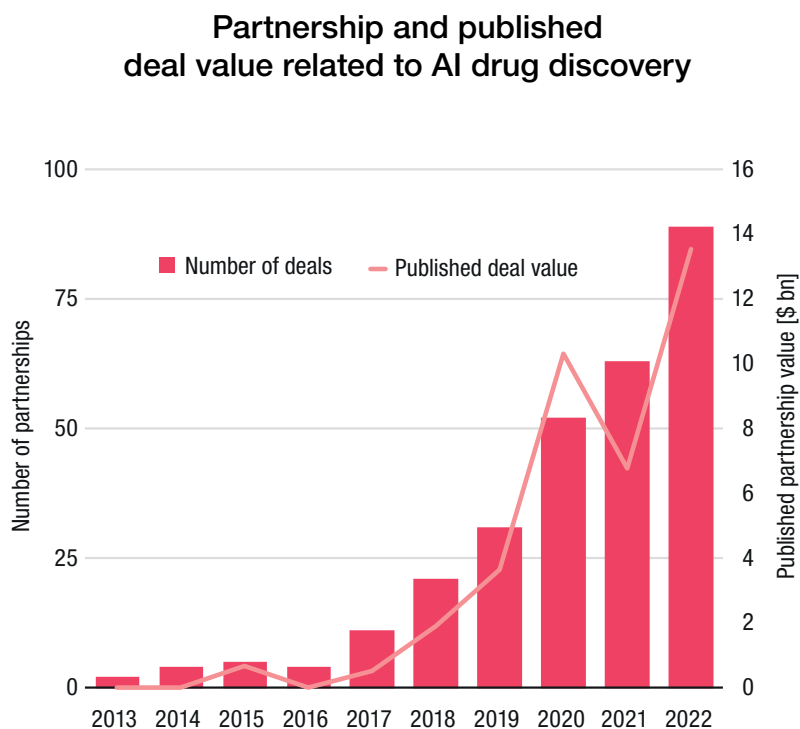
Key takeaway 1

Pharma is actively partnering but does not seem to go all-in on individual deals: Pharma companies are very active in partnering with AI drug discovery start-ups and tech companies, but are de-risking their partnerships through low upfront payments. Overall, in five years we expect data and AI to be an element in up to one-third of all partnerships deals.

AI deals' upward trajectory

M&A in AI for drug discovery is increasing, but pharma is not buying yet

In the biopharma industry, deal-making has always been a key tool to accelerate innovation. To analyse the extent of M&A in AI in drug discovery, we combined the Biomedtracker and CB Insights deal databases and screened for acquisitions in drug discovery that include AI-related key words. While this data may not capture very small deals, it still might serve as a proxy for M&A activity in the industry.

Excluding asset deals we found a total of 49 company acquisitions in the last ten years, a number that is small compared with the more than 1,000 biopharma deals in the same period. This probably (and accurately) reflects the relatively nascent state of applied AI in the field, and we see the same careful attitude towards M&A as we saw for partnerships. However, we can identify a clear momentum in deal activity, both in number and size over the last five years. Over 90% of deals have taken place since 2018 (see Figure 3). In this period, AI-related deals correspond to about 4.7%-6.6% of the total deal volume in biopharma as published in Biomedtracker. Moreover, in the first five months of 2023 we have already
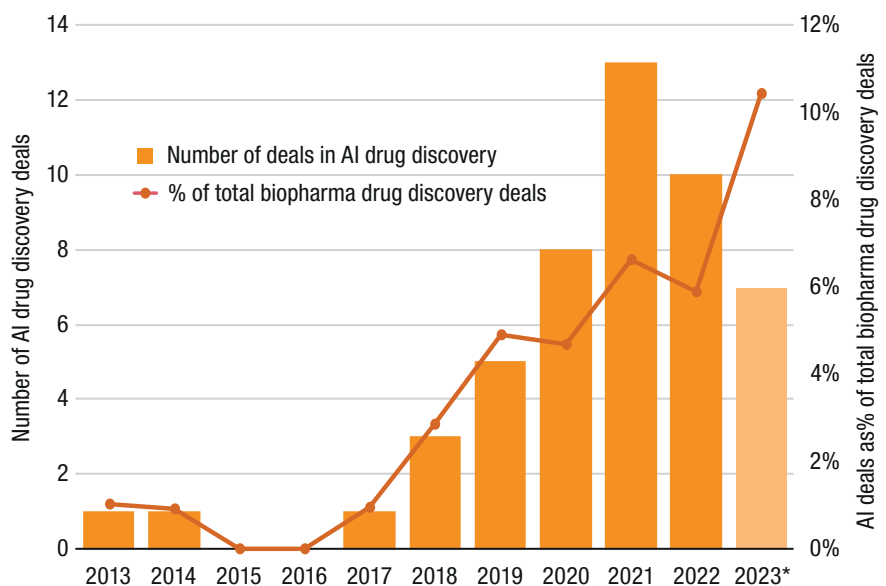
seen seven deals (about 10% of the total volume). The biggest deals also took place in 2023, with BioNTech's acquisition of InstaDeep for US$ 540m leading the field (see Table 1 for the biggest deals).

Examining the size of deals reveals a similar trend. While deal size is not published in most private transactions, we note that total deal value and the number of large acquisitions above US$ 100m have been increasing sharply since 2021 (see Figure 4 The comparative contraction in AI-related deal size seen in 2022 is much smaller than for the biopharma industry overall, which saw average deal size shrink by more than half[11]. Table 1 below lists the five largest deals in the last 10 years, which have all taken place within the last three years.

In summary, looking at the number and size of deals makes it clear that while overall M&A activity in AI for drug discovery is still small, there are obvious signs that momentum is picking up. We expect the trend of large M&A deals related to AI and drug discovery to significantly increase in the coming years.
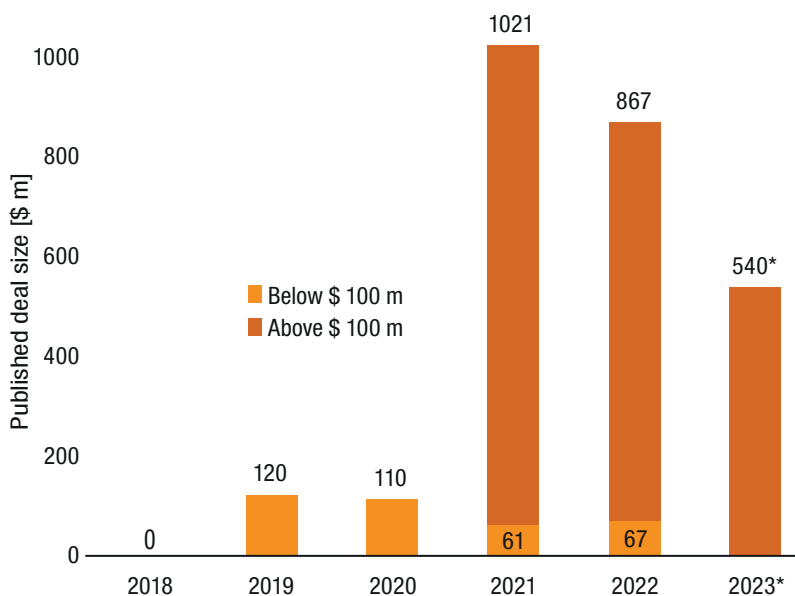
Figure 3: Number of AI discovery deals and percentage of deals compared to total biopharma deals from (*first five months of 2023), Source: Citeline Biomedtracker, CBInsights.

Number of AI drug discovery deals and % of total biopharma deals

Published deal size of AI drug discovery deals

Key takeaway 2

The M&A market is small, but heating up: While the number of M&A transactions related to AI in drug discovery is still small, increasing momentum is reflected in growing deal volumes and larger deal sizes. We expect both the number and size of deals to increase in the next five years.

Table 1: Top 5 AI deals in drug discovery in terms of deal volume.

Acquirer	Acquirer type	Target	Target type	Date	Deal volume [US$ m]	Comment
BionTech	Pharma	InstaDeep	AI Tech	10.01.2023	540	BionTech acquired InstaDeep, a company that provides decision-making systems, including analysis of protein sequences
Valo Health LLC	AI Drug Discovery	Courier Therapeutics Inc.	Biotech	28.05.2021	510	Valo Health acquired Courier Therapeutics, a biotech that developed a protein therapeutics platform
Cadence Design Systems, Inc.	AI Tech	OpenEye Scientific Software, Inc.	AI Tech	25.07.2022	500	Cadence Design Systems acquired the computational drug design company OpenEye Scientific Software, which produces molecular modelling and simulation software
Roivant	AI Biotech	Silicon Therapeutics	AI Tech	26.02.2021	450	Roivant acquired Silicon Therapeutics for US$ 450 m in equity. Silicon has built a proprietary computational physics platform for the in-silico design and optimisation of small molecule drugs
Ginkgo Bioworks	Other	Zymergen Inc.	AI Biotech	25.07.2022	300	Ginkgo Bioworks acquired Zymergen Inc, an AI biotech that applies machine learning to research and genetically-modified organism design

AI market dynamics and pharma's challenges

What do these deals tell us about the dynamics of the market? And is pharma using deals as an innovation accelerator? To better understand the rationale behind them, we grouped companies leveraging AI in drug discovery into the following three main categories:

1.

AI drug discovery companies aim to completely change the drug discovery and development process and make AI a core element across several process steps. These companies often own or co-own a pipeline of clinical drug candidates. According to our categorisation, companies like Exscientia and Insilico medicines that own drug assets, or Schroedinger and AbCellera that mostly work through partnerships, fall into this category*.

2.

AI tech companies use AI for one or a few specialised steps in drug discovery such as knowledge graphs or protein folding, or they may have more general AI models. Typically, these companies work in a service model. In our categorisation we put companies like InstaDeep (solves data and decision-making problems for pharma and other industries) or GinkoBioworks (offers several individual services across the discovery and development chain)*.

3.

AI biotechs are more traditional biotechs that leverage AI along with conventional methods and core capabilities. An example is Roivant Sciences, a biotech company with an innovative portfolio model, whereby subsidiaries are created to give a certain therapeutic area focus and a flexible financing structure. Roivant also emphasises AI as a key means to speed up drug discovery*.
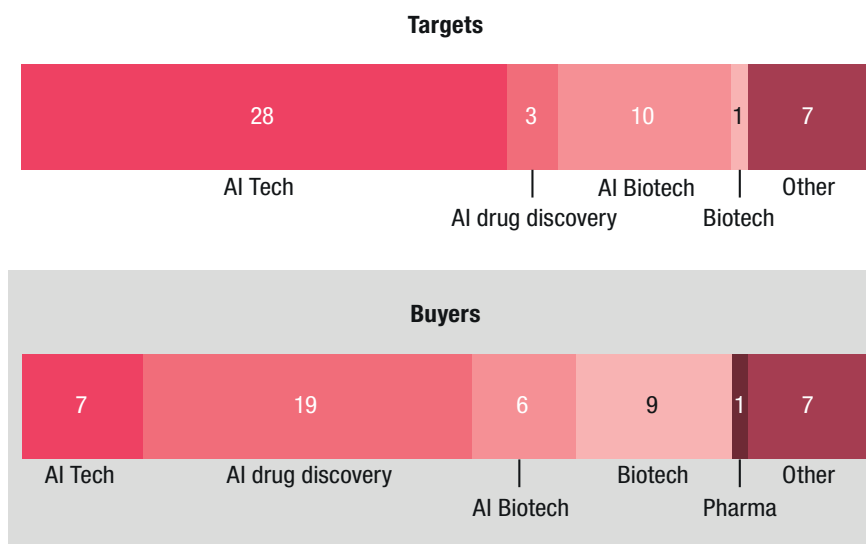
* Depending on the perspective, some companies may fall into several/other categories

Through this lens, we can see that in one-third of M&A deals AI drug discovery companies have been on the acquirer side (see Figure 5 for more details). These, mostly smaller deals indicate a degree of consolidation and capability building, especially since more than half of the targets are AI tech companies that have the potential to extend capability (see Figure 5 for more details). These signs of consolidation may point to the rise of larger AI drug discovery players that will establish themselves and set the pace in the field.

Figure 5: Number of AI M&A deals by the type of acquirer or buyer.

Number of deals by company type

Targets

AI Tech	AI drug discovery	AI Biotech	Biotech	Other
28	3	10	1	7

Buyers

AI Tech	AI drug discovery	AI Biotech	Biotech	Pharma	Other
7	19	6	9	1	7

Three fundamental challenges

What stands out is that until the beginning of this year, large pharma companies had not yet used bigger M&A deals as a tool to acquire capabilities at scale in AI drug discovery. This mirrors the careful spin on deal-making, where we found that deals are heavily shifted towards milestone payment. For an AI-related M&A deal there are limited options for de-risking, and these three fundamental challenges add additional complexity to a biopharma deal and explain pharma's limited commitment:

1.

The evaluation challenge

AI in drug discovery is a crowded space made up of start-ups, technology companies and other solution providers, and it's therefore difficult to identify which of them will bring the greatest value to a company. The ultimate test, to be faster or have a higher success rate in bringing drugs to market, takes several years to complete. Although there have been several accounts of AI-enhanced drug development passing faster through pre-clinical and clinical stages (e.g. Insilico Medicine's recent announcement that it is advancing its clinical candidate into phase 2 in an estimated one-third of the time compared to traditional methods[12]), it will take years before there is empirical evidence to help us understand which models provide better outcomes in the long run.

For companies that offer a specific service, it may be possible to assess the performance of a model based on validation datasets or case studies. However, pharma leaders we spoke to are often reluctant to provide their companies' data. Besides the data security risk, they also do not want to train a potential competitor's model during a test run. Interestingly, our analysis of six publicly traded AI drug discovery start-ups show that for these companies, investors still seem to focus on the asset pipeline (see 'Valuing AI drug development companies' on next page).

"It is a people business – much more than for other deals. In the end, you are buying an algorithm, but you also need these people in the organisation."

– Head of M&A of a large pharma company

2.

Scalability

In many cases it is not clear how to scale. In some cases, the full potential of the AI company cannot be exhausted by one company. A pharma company only has the capacity to bring a limited number of molecules through development and commercialisation. If the target AI company keeps its services available to third parties, that opens up a new set of data security and ownership risks (similar to the ones discussed above). In other cases, the data used for training a model might be too narrow to scale it across an organisation, for example to other therapeutic areas. An AI model is only as good as the data used to train it.

3.

Integration

People are a key asset of an AI drug discovery company. Many M&A executives we spoke to raised the concern that it would be difficult to retain the talent behind a potential target after an acquisition, given the inherently different cultures of an AI start-up and a pharmaceutical company. However, integrating technologists is critical to making any deal a long-term success.

Valuing AI drug development companies

In order to understand further how AI drug discovery companies are valued in the market, we studied publicly traded companies which develop assets along the entire pipeline. Analysis included the team experience, number of publications in peer-reviewed journals, public partnership as well as the clinical pipeline companies own or partner with. The six AI drug development companies had negative EBITDA in FY22, which is not untypical for preclinical and clinical biotechs with no or few drugs yet on the market. No clear correlation for factors like scientific publication, team experience and partnerships was found, which can be partly explained by the different strategies the companies take for example regarding partnerships. However, if we look at enterprise value as at 31 December 2022, we see that not unlike traditional biotech, investors value a strong clinical pipeline. Depending on the operating model of these companies, the assets in the pipeline are either owned solely by the company or developed in collaboration through co-ownership or partnership deals that often include milestone revenues. For comparison, we also included an AI biotech company (i.e. a company where AI is one of several core capabilities, see definition above). It has to be noted that this relationship reflects a general tendency. When zooming into the different companies, we see a more differentiated value perception that takes into account factors like the maturities of assets, therapy area focus or commercial prospects of the indications.

Enterprise value vs clinical pipeline of publicly traded AI drug discovery companies
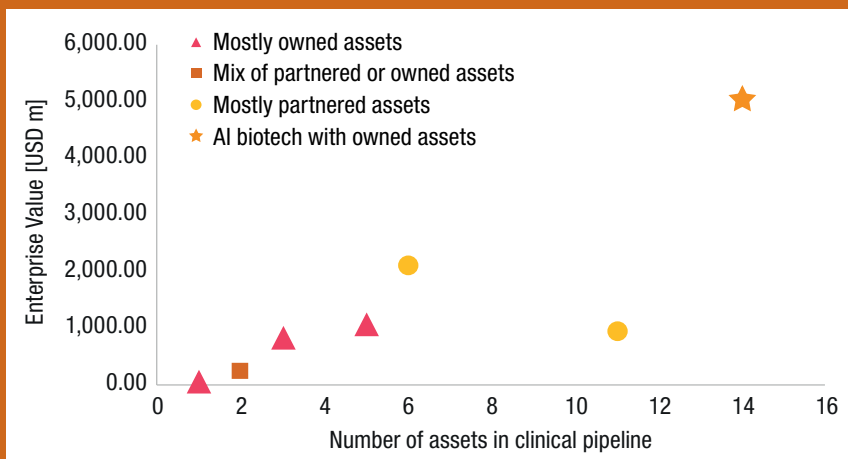
Figure 6/box: Correlation of enterprise value with assets in the clinical pipeline of publicly listed, pure play AI drug development companies (both as at 31.12.2022).

What this means for pharma companies

Will traditional business models be disrupted?

Given early successes and the advancing power of AI technologies such as deep learning models or generative AI, there is no question about the disruptive nature of AI for drug discovery. Our analysis has shown that although pharma companies are very active in the field, they also appear to be taking a cautious approach to bringing in external innovation. We also highlight the challenges of accelerating the deployment of AI though deals. Looking at the considerable change AI is bringing to other industries, it's natural to ask whether traditional pharma companies will be fast enough to redesign their R&D efforts around AI and data or whether they will be disrupted by a new breed of more digital players.

In the short to medium term large pharma companies will still be able to rely on their traditional business model, which bets, in part, on identifying the most promising drug candidates from smaller, potentially AI-augmented biotechs and bringing them to the market with their clinical, regulatory, manufacturing and commercial capabilities[2]. However, sooner or later companies need to have AI implemented across the discovery and development process to increase efficiency across the value chain. Without it, they risk rapidly losing competitiveness. Their drug programmes will be too expensive, too slow and, arguably, less relevant if they cannot focus on the right targets to get the right data to inform insights in a timely way. To succeed with AI, pharma companies need to find the right mix of internal and external capability building and scale AI across their often-siloed organisations. Making the right deals and partnerships with AI drug discovery and tech companies can be a critical accelerator for innovation. The recent BionTech InstaDeep acquisition signals that some companies have identified significant value in jump-starting their capabilities through an acquisition. It is likely that we will see more of this trend.

To make these deals a success, business development and M&A teams need to tailor their deal-making approach to incorporate a focus on AI and data.

"We are heavily building up our own capabilities. But as well as this, there will be more experimenting through partnerships, collaborations and potentially acquisitions in the next few years."

– Head of M&A of a large pharma company

Four key areas pharma M&A and partnering teams need to focus on

1

Build a valuation framework: AI drug discovery companies are inherently difficult to value. We consider five dimensions as critical for an outside-in valuation of these companies (See Figure 7 below). Assessing the technology requires a level of technical expertise in data and AI and working with functional experts to be able to assess the quality of the underlying models. Strategies to evaluate models require a set of benchmark measures that are universal (e.g. accuracy, sensitivity, specificity or, recall and computational cost) and specific to an AI problem (e.g. multilabel evaluation metrics for predicting side effects). In addition, companies may use the curation of real or synthetic datasets that can be used to run these evaluations or develop ways to sandbox an algorithm to avoid data leaking or to improve the model.

Figure 7: Suggested variables to assess the enterprise valuation of AI companies.

Expertise, team & culture	Is there a strong leadership and experienced team? • AI expertise • Clinical and TA expertise
Financials & business case	Is the financial and commercial assessment realistic (due diligence)? • Business plan and case, funding • Competitive landscape • USP, market potential
Pipeline & drug candidates	If applicable: how strong is the pipeline and success rate? • Clinical and pre-clinical data • History of approval
Technology	Is the AI effective, defendable, and scalable? • AI models • Data sources & analysis • IP
Track record & validation	What has the company achieved? • Quality of case studies • History of partnerships • Relevant publications

2

Understand the scalability of the data and generalisation of AI use cases: M&A teams need to be able to understand the opportunities from – and complexities of – integrating an existing AI model into a pharma organisation that has data and processes siloed within therapeutic areas and functions. In addition, teams need to understand if the data is available for scaling to additional use cases, if it can be used compliantly across different jurisdictions and if it is safe. This assessment also includes the understanding of legal and ethical barriers that may limit the use of AI with other patient groups[13].

3

Build a computing and data strategy for a target: In recent years, companies have benefited from shifting data and computational power to the cloud to benefit from high flexibility, scalability and predictable cost. However, concerns about compliance, data sovereignty, data security and cost have led companies in some cases to reconsider their cloud vs on-premise decisions for new models such as hybrid or private clouds, federated models or even fully on-premise solutions. Before a deal, companies need to have a clear strategy of how an AI platform of a potential acquisition fits into the evolving strategies to avoid costly surprises in the integration.

4

Have an integration plan that focuses on shifting people's mindsets: A deal is about the technology and the people who run it. It's essential to have a change strategy to shift employees' mindsets, both in the target or alliance partner and the acquirer. The full potential of an AI deal will only be realised if people across functions adopt new standards and think about processes differently. Succeeding in this requires significant education and change management. If, for example, an AI start-up remains isolated, it can end up just operating as an internal service provider instead of achieving its potential to fundamentally shift the acquirer company to achieve more efficient drug development. A successful deal should be a step towards a new operating model to achieve smarter drug discovery and data use across the company.

M&A and business development teams need to build new capabilities

Artificial intelligence and machine learning offer a tremendous potential to identify new therapies and bring them to patients more efficiently. Our partnership data shows how established pharma companies are ramping up collaborations with start-ups or tech companies like Microsoft, Google, Amazon or Nvidia. However, we also see signs of uncertainties. First, partnership deals are de-risked with low upfront and high milestone payments, and secondly, there are a limited number of acquisitions of AI players by pharma companies. Nevertheless, with the rapid maturing of the industry, the importance of AI-related drug discovery deals will continue to grow significantly in the next years. Considering this development, M&A and business development teams have to build new competencies to understand the strategic and practical impact of these deals. Only then can they successfully maximise the potential of external innovation and scale newly acquired capabilities across the organisation.

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