

Omega Position Paper: Artificial Intelligence and its Role in Drug Discovery

CURB YOUR COMMERCIAL ENTHUSIASM

A breakthrough in engineering is not necessarily a breakthrough in medicine

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How should investors assess AI's role in drug discovery amid all the hype? It is a fair question, as AI continues to dominate nearly every financial news cycle. In addition, tech entrepreneurs and leaders with strong track records of delivering value to their investors are increasingly trying to apply their skills to biology. Last but not least, lest one gets too comfortable dismissing them as having gotten over their skis: last year, both the Physics and the Chemistry Nobel prizes were awarded for work in machine learning – the latter specifically for applications to life sciences¹ (the chemistry prize was awarded for the development by Google's DeepMind division of AlphaFold and its “decoding” of protein structure).

And yet, we at Omega have not joined the rush to fund these companies – are we being overly cautious?

In the pages below, we highlight the latest developments, and what we believe the potential impacts and limitations of AI at each step of drug discovery are so that you can develop your own understanding of the right timing and the right problems. Think of this as a guide to what we believe are the most important pivot points in the field – the areas with the greatest potential returns on innovation – and their cousins, the pitfalls – where we expect value to be destroyed.

We will also give you our bottom line up front: Machine learning models identify patterns within and between datasets, enabling them to make informed predictions – about what comes next, what fits best, or what belongs together – when given something new. Models are therefore only as good as the quality and quantity of the data on which they are trained. And – this is even more important – as with *any* solution (machine learning or not) they are only as valuable as the significance of the problems to which they are applied. If there is a limit on the size of the prize to be won, there is a limit to how much it makes sense to spend on the innovation required to win it – at least if you are looking for returns.

And therein lies the rub. We believe there are two reasons to be skeptical of the current impact of machine learning on the business of drug development:

- **First, you have a data problem.** The human body is an extremely complex system of overlapping and often redundant positive and negative feedback loops across multiple cellular pathways. We do not currently understand (even remotely) the role of each protein or metabolite operating across our organism and/or how they interact with each other in healthy individuals (let alone in disease states). And that is before taking into account the myriad genetic and environmental factors that affect these pathways, proteins, and metabolites. And the data that could help make sense of this variability? Much of it is yet to be generated – and the remainder is locked up within large pharmaceutical companies – and not publicly available.
- **Second, you have an application problem.** In our experience, the machine learning approaches currently being deployed in drug discovery and development are not geared toward the rate-limiting steps of the process. We believe that capacity added at these steps will not materially increase the pace of drugs reaching approval – which is the endpoint for which one is ultimately – and economically – rewarded.

To be clear, we are in the business of developing successful therapeutics – work that not only benefits human health – but also leads to sustained and uncorrelated returns for our investors².

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As investors in healthcare, we have been active since 2004 (and many of our team members have been investing in the space even longer), and we are extremely proud of the fact that our portfolio companies have so far launched 52 drugs on the market³. We would therefore be supportive of *anything* that we believe makes drug development cheaper, easier, faster, or more reliably successful.

But we do not get excited unless and until we are on a path to that point. We named our firm after the last letter of the Greek alphabet because everything we do needs to end with a clear path to a drug that makes a difference for patients, physicians, and ultimately the pharmaceutical companies that often acquire or partner with our portfolio companies to advance their products. We will wait for the right technology to be applied to the right problems. And for this, we expect our prudence to be rewarded as this cycle unfolds⁴.

Finally, we should state that our scope here is a narrow one – AI and drug development. There are, and will continue to be, many promising AI applications in healthcare more broadly: we are thinking specifically of business processes such as clinical trial enrollment and recruiting (a key and expensive bottleneck in drug development), filing regulatory applications for drugs (these filings can be millions of pages), but also in diagnostics and imaging, healthcare IT, mental healthcare, and many other applications. They are beyond the scope of this paper.

It is true that there is enormous opportunity in biotech...

“There is no question that digital biology is going to be... one of the biggest revolutions ever... [F]or the very first time in our history, biology has the opportunity to be engineering, not science...”

Jensen Huang, Nvidia (Dean’s Speaker Series, Apr 2024)

“The next big game-changing revolution is in biology.”

Eric Schmidt, Google (Time, Apr 2024)

“AI could 10x the rate of [discovery], giving us the next 50-100 years of biological progress in 5-10 years.”

Dario Amodei, Anthropic (Dario Amodei Essay, Oct 2024)

....but we will also see value get destroyed, where approaches are ill-informed.

“[T]here is one problem. AI needs masses of high-quality data to be useful for science, and databases containing that sort of data are rare.”

David Baker, 2024 Nobel Laureate (MIT Tech Review, Oct 2024)

“AI has been startlingly effective... where lots of high-quality data are available; [but] in [most] areas, no such database exists – and biotech companies are still making aggressive AI investments. I would...bet that we are going to have some whopping failures.”

Derek Lowe (Science, Sep 2024)

THE EARLY BIRD DOES NOT ALWAYS GET THE WORM

Before diving into the specifics of drug discovery, let us consider a broader pattern: Markets have historically rewarded prudence in the long run, but have very often been driven by FOMO and groupthink in the short run.

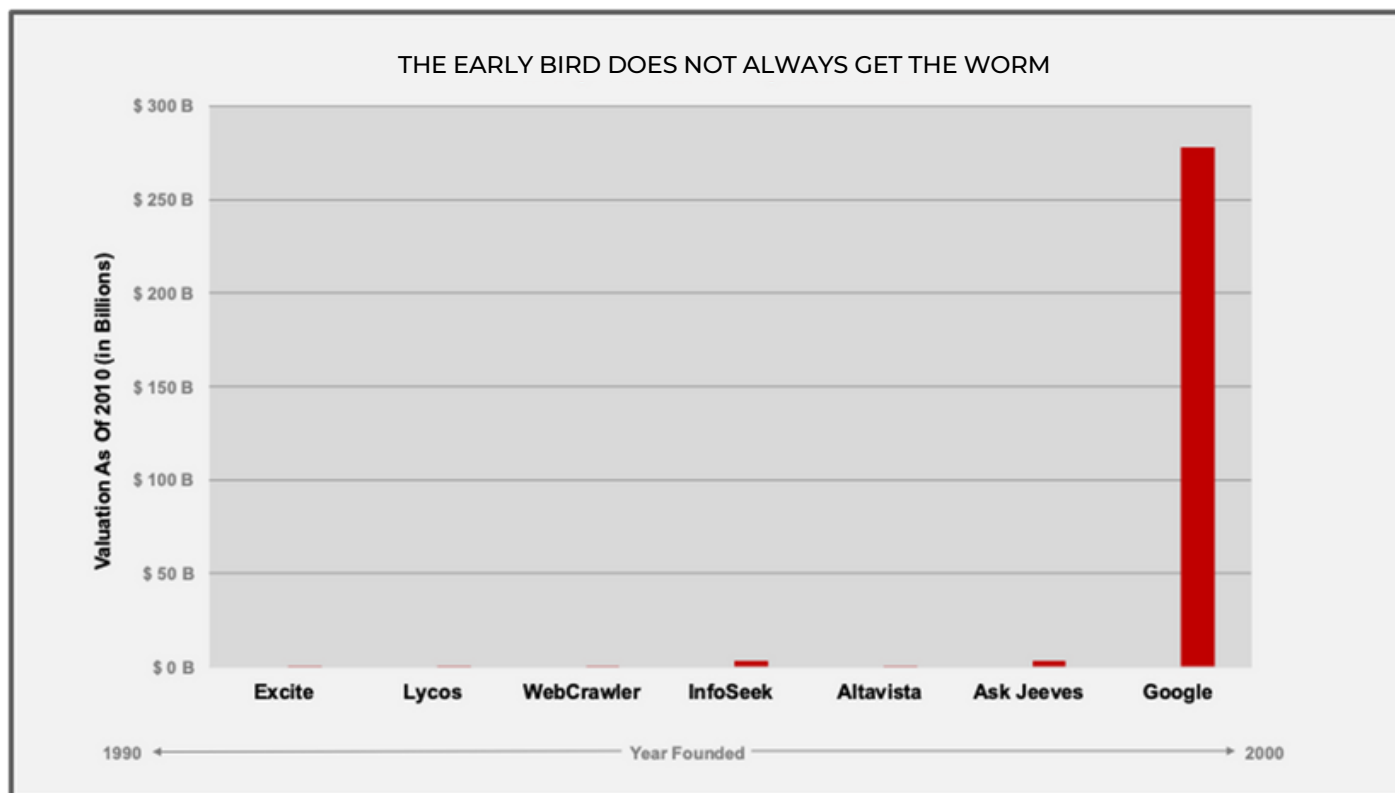
You have all seen the scale of investment in AI: according to PitchBook, AI companies received more than 60% of all U.S. VC dollars last quarter – plus another ~\$150B in investments made by public companies last year. That is equivalent to ~7% of U.S. GDP⁵. For context, when personal computers took the world by storm in the 80's and 90's, spending peaked at only ~2% of GDP. *Is anyone who was not invested in AI five years ago too late to be rewarded?*

If you are selling microprocessors, you probably are too late, as NVIDIA has seemingly captured the market (at least for the time being). Can it continue to grow at this torrid pace when people stop buying a colossal amount of their chips for training models? Perhaps, but that is not our investment focus.

If, on the other hand, you are in the business of applying AI tools to solve problems in other domains, it is just as likely that you are still *too early*. Take the historical example of the internet, and the business of search: by the early 1990s, following on the heels of the telecom infrastructure boom (and subsequent bust), there was an “application” boom: most knew search, for example, was going to be huge in the internet age. Investors piled on (Lycos, Excite, WebCrawler, and Yahoo – all founded in 1994; AltaVista – 1995; Infoseek and Ask Jeeves – 1996) at eye-watering prices. And all these companies went to zero. *But you need not have invested a dollar in search until Google – founded in 1998 – to have captured 99% of the eventual value in the space. Or think about it this way: Facebook (founded in 2004) was not the first social network, and the iPhone (first released in 2007) was not the first smartphone.*

It is not the first mover who wins, but the one who fits new capabilities into the right form factor for the right problem.

FIGURE 1: THE RIGHT APPLICATIONS ARE ULTIMATELY VALUED MORE THAN THE EARLY APPLICATIONS



Source: Bloomberg data, Omega Funds Analysis as of 30 September 2025 | Companies shown founded 1990-2000, valuations shown as of 2010. For illustrative purposes only.

Now apply this to biotech: Everyone is excited to use AI in life sciences – but we have seen this movie before, and we know how it ends. The first applications are not necessarily the right applications – and markets reward those with vision to see this and the discipline to wait⁶. In this case, we believe that investors should wait for biotech applications that specifically target the steps in drug development where innovation is most likely to yield returns of massive scale – exactly what is required to justify these investments⁷.

WHERE IS THE OPPORTUNITY IN BIOTECH?

Economists use the concept of "marginal returns" to highlight a crucial truth: Not all steps in a production process are equally valuable. The limiting factor – the slowest step, or the input in the shortest supply – sets the pace of progress. For an air force, both planes and pilots are essential, but when you are out of planes, adding more pilots will not help. *And what we think is that, for the time being at least, AlphaFold (the subject of last year's Nobel) and its cousins are, at the moment, excess pilots for planes not yet built.*

THE RIGHT PROBLEM VS. THE ACCESSIBLE PROBLEMS

To understand why this is the case, let us talk about the "inputs" to, or steps of, the process by which a drug product is brought to market. It can be (roughly) divided into three stages:

- 1. Target Selection:** Identifying a biological target (a molecule – usually, not always, a protein) that plays a critical role in a disease, or, more commonly, a set of diseases.
- 2. Drug Discovery and Development:** Designing and optimizing molecules (drugs) that can interact with the biological target and modulate its activity (either enabling or disabling it) – while also being easy to manufacture, easy to administer, and have minimal unintended effects (do not modulate the activity of molecules beyond their intended target).
- 3. Clinical Trial Testing:** Demonstrating that the drug has its intended effect and has no deleterious side effects in human subjects.

In our experience, **Steps 1 and 3 are – by far – the most capacity-constrained and the least susceptible to AI disruption.** If you locked the world's top drug developers in a room and asked them to write down every target where they are 100% sure that *if* they could manipulate it, the disease would be "solved," the list would be short – less than a page, depending on the font they use. Nothing that comes even remotely close to covering the full spectrum of human disease. (According to the WHO, there are roughly 30,000 diseases known.)⁸

Now, consider how hard it is to *add* to this list: Identifying and then validating a novel drug target is a high-stakes scientific gamble. It takes a massive investment to prove a molecule is involved in a disease – and not essential to any healthy function – and many of these experiments fail. They fail because biology is enormously complex, and – relatively speaking – still poorly mapped: By analogy, if biology were the planet, we would have explored many of the major cities, but vast continents remain uncharted. Because the costs are so high and failure so frequent, few organizations are willing to make these investments. As a result, most drug development concentrates on the existing small set of well-understood proteins as targets – those "major cities" we have already mapped – the targets that are on the single page. This has produced many valuable drugs, but it also creates bottlenecks: when everyone works on the same targets, competition increases, margins are eroded, and opportunity costs rise – other diseases and untapped mechanisms with enormous potential are left waiting.

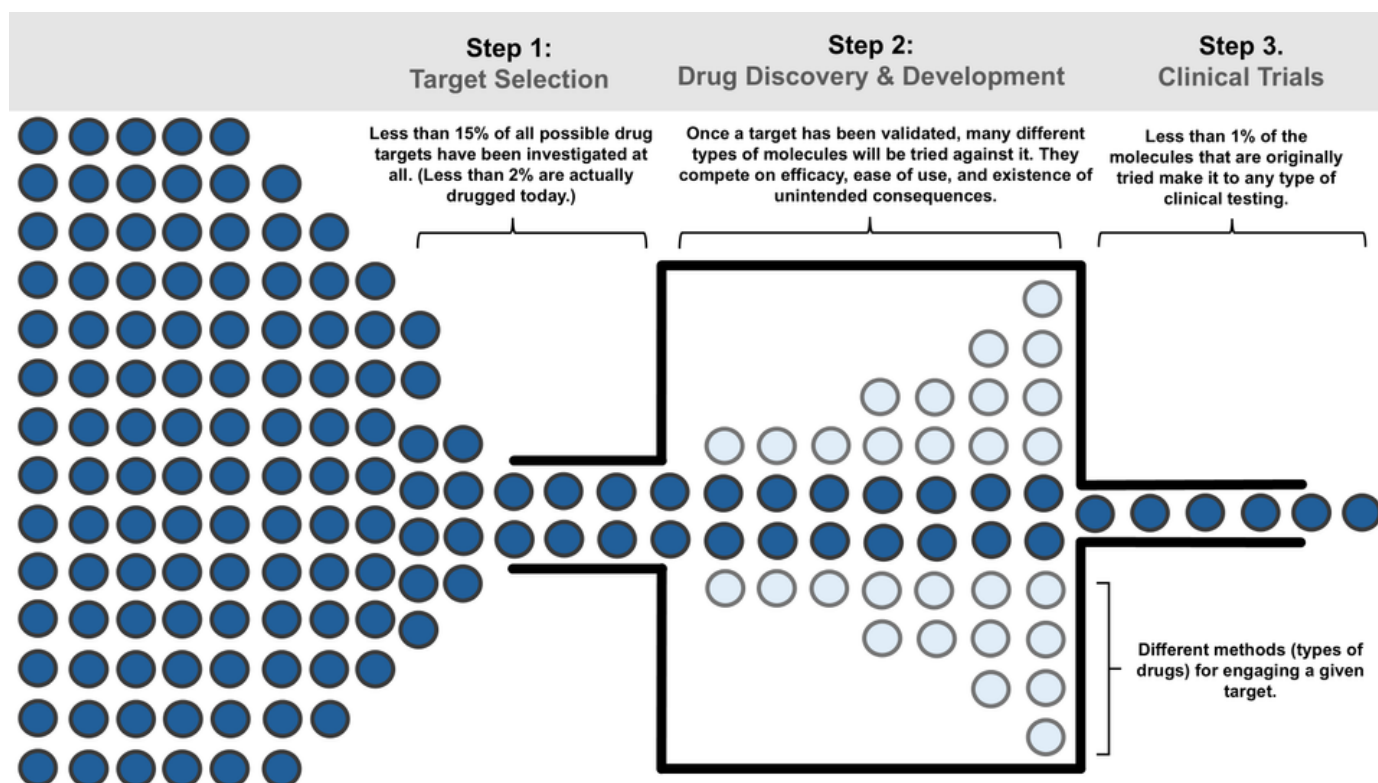
Clinical trials, on the other hand, are capacity-constrained because they are *logistical* gauntlets and almost inefficient by design: first, you identify patients with the disease, which means developing relationships with hospitals, accessing medical records, and relying on already busy doctors to flag potential participants. Then you screen them to make sure the drug is tested on the specific sub-population for which it was designed – right

disease stage, treatment history, and labs – which means tests and manual review. Next, you need to enroll this sub-population. These are sick people who – in addition to the burden of their disease – need to travel, take time off work, and accept the risk of side effects. And once enrolled, you must keep them engaged. Even small gestures – like checking in personally by phone – can make the difference between someone staying in or dropping out, but these are manual, time-consuming tasks.

As the most capacity-constrained steps in the drug development process, we believe that target selection, clinical trials, and indication selection are the areas in which there is the greatest return on innovation.

Step 2, however – the stage where you produce a molecule that can interact with your drug target and alter its activity – is where most AI applications in biology live today. If you read about “AI-enabled drug design” in the popular press, it is almost certainly a story about a company designing new molecules for an existing target. But this step is not the choke point; it is not (generally speaking) capacity-constrained. Today, we have many methods for making molecules of many types to suit a variety of circumstances. These methods can always be better and cheaper – but they are already rather good, relatively cheap, and the return on their being *faster* is minimal primarily because we already are producing drug candidates at a faster rate than we can test in the clinic⁹.

FIGURE 2: TARGET SELECTION AND CLINICAL TRIALS ARE THE PRIMARY BOTTLENECKS TO DRUG DISCOVERY

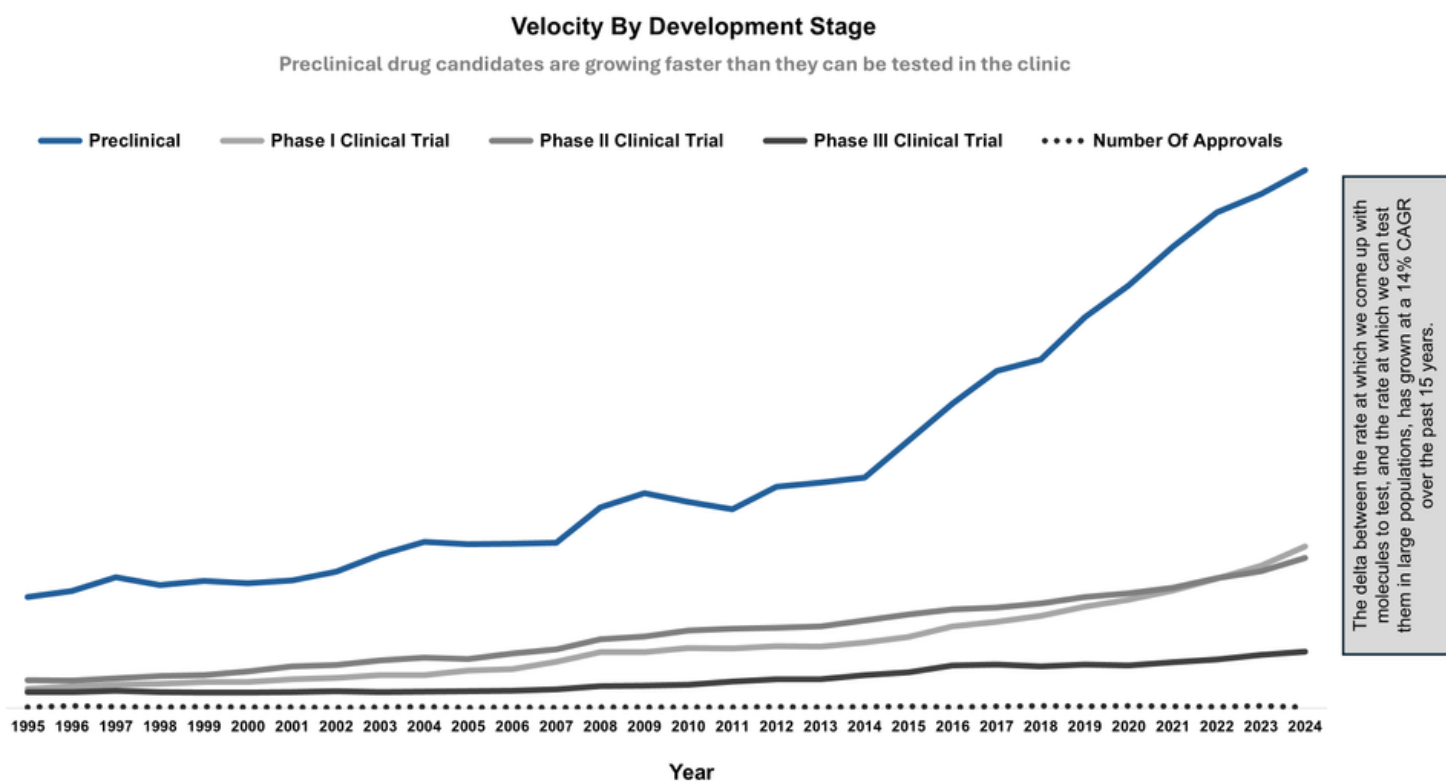


You do not have to take our word for this; you can see it in the data. The rate at which the industry is generating “drug candidates” (new molecules to interact with a target and modulate its activity) has far outstripped the rate at which we are able to test them (which has grown only very modestly, due to the constraints described above). And this rate of generation has far outstripped the rate at which new drugs are approved (which has increased, but relatively anemically).

Ironically, one reason there is already so much ‘drug candidate’ capacity is because there existed *earlier generations* of computational tools: the 1990s were as exciting a time for computational chemistry as they were for

internet search. In *The Billion Dollar Molecule*, for example, Vertex, founded in 1989, is summarized as “smart ex-Merck guys making drugs with computers.” History does not always repeat itself, but it certainly tends to rhyme.

FIGURE 3: GROWTH OF DRUG CANDIDATES BY DEVELOPMENT STAGE



Source: Citeline data, Omega Funds analysis | As of October 2024

So why the Nobel Prize? Modeling the shape of proteins is incredibly interesting *mathematically* and is an incredible feat of *engineering*. We also believe that accelerating the understanding of unknown protein structures (via AlphaFold and its brethren) is a very useful tool and will help design better biologic drugs.

But, as we stated up front, a breakthrough in engineering is not the same as a breakthrough in medicine. To beget a breakthrough in medicine – to bring more drugs to more patients that result in more years of life – and to change biotech economics and get a return on your investment, you have to solve the rate-limiting problems above.

THE RATE-LIMITING PROBLEMS ARE NOT SOLELY LIMITED BY INTELLIGENCE

As we close, you might be wondering: Why not simply apply these new methods – with all their raw horsepower – to the *rate-limiting* problems (target identification; clinical trial execution)? And the short answer is that, for these problems, intelligence is not the key – or the only – missing ingredient.

Target discovery, for example, as mentioned in our preamble, is throttled by the quantity and quality of basic biological data available. Google (DeepMind, which developed AlphaFold) started with protein folding not because it was the most important problem in medicine, but because it was the rare problem that was both hard and had copious high quality extant data on which to train – it was the only place they *could* start. AI models are only as good as their input data. Drug discovery involves vast, heterogeneous data – “omics” data (genomics, transcriptomics, proteomics, metabolomics, etc.), chemical libraries, pre-clinical experimental data in animals, clinical records – much of which is absent, and/or noisy and/or locked up in proprietary databases. (For example, there exist valuable proprietary data on the efficacy/toxicity of all the drug candidates that pharmaceutical companies have tested over the last few decades.) Wider adoption and deeper impact will require not only substantial new data generation, but also the establishment of industry norms for data sharing and better curation.

There are some initiatives trying to address this, which we are following with interest (Eli Lilly's recent TuneLab initiative, for one; with others highlighted below), but we are not there yet¹⁰.

Indeed, there are multiple groups trying to tackle these constraints: Companies like BenevolentAI use natural language processing to mine the extant literature and link genes, pathways, and diseases in ways that others may have overlooked in the past. Others, like Insilico and Retro Biosciences (an OpenAI partner) are combining these methods with in-house data generation of their own to complement and extend the publicly available data. And still others – like Xaira (which raised a \$1B Series A last year), New Limit (founded by Coinbase's Brian Armstrong), Lila ("the world's first scientific superintelligence platform"), Recursion (\$RXRX; currently valued at \$2.6B)¹¹ and the Arc Institute (backed by a team led by Stripe's Patrick Collison) are taking those data generation efforts to the next level of scale – with large-scale lab automation. They pick a small number of cells to use as model systems, systematically manipulate each gene, one at a time, and measure the effects on the cell, thousands of times over – feeding all this information into a model of a "virtual cell." The hope is that this will allow us to identify new drug targets, in the future, in silico – and then design the right drugs for these targets using the AI tools already on the scene.

But these efforts remain patchy, likely sub-scale, and early: *As of today, no drug backed by an AI-native company has yet to reach FDA approval*, after nearly a decade of effort. Indeed, none of these companies have completed the first step – identifying a novel and valuable target, inherently and *causally* linked to a human disease. Why? The models that exist today rely on literature and publicly available datasets that are smaller, more skewed, and more biased than commonly recognized. And it is quite difficult, it turns out, to infer the full universe of biological diversity from a small number of cells from a small number of donors (especially diseased cells, which are unusual by definition). As promising as they seem, these are still first attempts to create the kind of broad, high-quality data infrastructure and biological sampling that truly transformative models will require. We are not betting against progress – but we are betting it will not come from these efforts alone (*and not yet*).

And when it comes to clinical trials: we believe the linchpin for success in clinical trials is execution leadership and experience, not necessarily incremental intelligence, or processing power. Technology can be an enabler, but legacy infrastructure and human bottlenecks still dictate the pace: think of it like boarding a plane. Yes, maybe someone produces a new technology to scan your ticket faster, but you are still waiting while your fellow travelers block the aisle rearranging their carry-ons. In clinical trials, sometimes you need to work really hard to convince the pilot (the physician who has access to patients) to fly the plane to your destination (to try your drug in those patients).

In our experience, what really drives success is sharp judgment, strategic foresight, the right network, and experience. In short: content and connectivity.

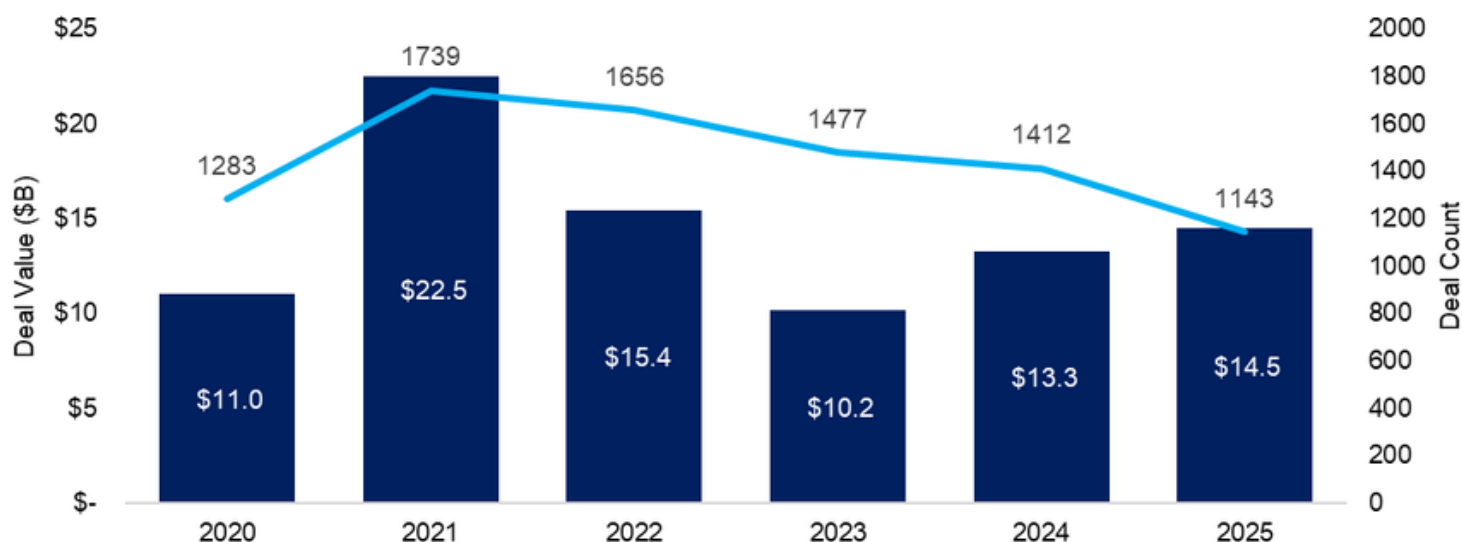
The right people to run your trial – the ones who know how to do this – are a limited resource, and one that we cultivate assiduously (and expensively, we might add). Patient recruitment underscores the point. Precision medicine fragments eligible populations, making it harder – not easier – to reach the required N of patients in your trial. AI may pinpoint and contact candidates more efficiently, but it cannot create additional patients or relocate them closer to trial sites. As with executive talent, patients are a finite asset; securing their participation still depends on leaders who know how to engage both them and their physicians on a human level.

CONCLUSION

Allow us to leave you with three additional parting observations: First, the market is converging (for some time now, it seems) on our initial perspective that we have held now for several years; second – the opportunity within drug discovery remains vast and it is fundamentally uncorrelated to the current AI investment boom (which, if that bubble bursts, means our companies should escape the worst of the fallout); and finally, you cannot "pattern match" your way to capturing this opportunity because the economics differ fundamentally from consumer technology. First principles thinking (often cited; rarely practiced) is important here.

1. The market is converging on our perspective: As in previous FOMO waves – from the dot.com book, to early fintech to cleantech 1.0 – capital has poured in faster than viable business models have formed, leaving investors at risk of substantial losses. Now, a few years in, others in the market are starting to share the perspective we have held from the start: AI healthcare VC deal activity peaked in 2021, before contracting in 2022 and 2023, and leveling off in 2024. We believe this trend not only reflects macroeconomic pressures, but also the relatively poor results so far (see appendix), and a broader shift toward a more rational approach to investing in the AI drug development space. At the same time, companies themselves are correcting course. The nimblest are redirecting their models toward the most tractable bits of the most high-value problems we’ve described here – such as using their ‘virtual cell’ platforms to identify patients most likely to respond in a clinical trial, a bounded sorting problem, rather than trying to solve the open-ended challenge of all biology at once. This is the sweet spot for innovation we describe above – technically feasible and economically valuable.

FIGURE 4: AI HEALTHCARE VC FUNDING



Source: PitchBook, Global AI Healthcare VC funding | As of 30 September 2025

2. Drug discovery remains one of the largest and most exciting markets imaginable: Progress in this field is never linear, but it is inevitable – and its potential impact is staggering. Every person on Earth is already, or will certainly one day be, a “customer” of medicine, which makes the opportunity as large as any market can be. Far from being a niche or speculative pursuit, biology remains one of the most consequential frontiers of innovation.

3. Success in this market will demand first-principles thinking, rather than pattern-matching to consumer tech: the path forward in capturing the opportunity in drug discovery will not mirror that of consumer technology. In software, scale comes from abundant data, problems with transferable patterns, and general-purpose models. Once you have trained on enough text, the next language comes quickly; once you have built one app, the next reuses its infrastructure. The economics of artificial general intelligence, which assume exponential returns to scaled output, rely on this. But in biology, we face a paradox in terms of transferability. Life is deeply interconnected – organisms share profound similarities, from their genes to their metabolic pathways – yet our ability to act on disease only improves when we slice problems ever more finely, down to specific mechanisms, patient subgroups, and molecular contexts. And unlike consumer AI, the data to power this cannot be scraped, commoditized, or outsourced to some emerging country with vast reserves of cheap labor; it must be generated purposefully, in the lab, often at scale (and that is expensive). This tells us that while the opportunity is just as vast, the route to scale must look different. To succeed, you cannot pattern-match against consumer tech; you must think from first principles.

— ABOUT OMEGA FUNDS

Omega Funds is a leading international investment firm that creates and invests in life sciences companies that target our world's most urgent medical needs. Omega Funds has raised approximately \$2.5B since the firm's inception in 2004.

The last letter of the Greek alphabet “Ω” encompasses Omega’s brand and its investment strategy. Omega specializes in identifying and powering companies through value inflection points across the full arc of innovation, from company formation through clinical milestones and commercial adoption. These impactful, value-creating inflection points are achieved by targeting severe, unmet medical needs with novel therapeutics, devices, or platform technologies. Omega Funds’ portfolio companies have brought 52 products to patients in multiple therapeutic areas, including oncology, rare diseases, precision medicine, and others, resulting in 50 M&A exits and 48 public listings¹².

— APPENDIX

For those interested in continued learning on the topic of AI in drug discovery, we have provided additional reading options along with a link to our previous webinar on the topic for viewing at your leisure. Please note the Financial Times article requires a subscription to view.

- [Omega Funds Webinar – AI in Drug Discovery & Development: Hype or Revolution?](#)
- [Financial Times Article – Why is AI Struggling to discover new drugs?](#)

FIGURE 5: TOP AI HEALTHCARE VC EXITS BY VALUE SINCE 2020¹

Company	Close date	Exit Value (\$M)	Location	Exit Type	Post Exit Performance ²
Caris Life Sciences	6/17/2025	\$5,911	US	IPO	54.0%
Yidu Technology	1/15/2021	\$3,059	China	IPO	-74.9%
Recursion Pharmaceuticals	4/16/2021	\$2,312	US	IPO	-72.9%
Exscientia	10/1/2021	\$2,298	UK	IPO	-75.8% ³
Brii Biosciences	7/13/2021	\$1,704	China	IPO	-91.0%
Absci	7/22/2021	\$1,446	US	IPO	-81.0%
Relay Therapeutics	7/16/2020	\$1,338	US	IPO	-73.9%

Source: PitchBook as of 30 September 2025 | ¹Only funding rounds for companies focused on drug discovery and therapeutics shown. ²Post exit performance is measured as price change from IPO issue price to closing price as of 30 September 2025. ³Exscientia was acquired in November 2024. Performance is measured as change in market cap from IPO to acquisition price. The companies reflected above are provided for illustrative purposes and educational purposes only and are not Omega investments and may not be representative of the performance of any Omega investments. Such investments are also not representative of all relevant AI healthcare exits since 2020.

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Footnotes:

1. [Press Release for The Nobel Prize in Chemistry 2024](#)

2. For illustrative purposes only. There can be no assurance Omega vehicles will achieve its investment strategy or that any such returns will ultimately be achieved.

3. Past performance is not indicative of future results or success.

4. There can be no assurance any such results will ultimately be achieved.

5. Source: PitchBook | As of 30 September 2024

6. This dynamic of the early bird often being too early and missing the worm should be even more pronounced within biotech. Many of the consumer-technology tools referenced captured value through network effects and true economies of scale. They iterated to find the right application, but once that was established, network effects created competitive advantages and a winner takes all dynamic. Biopharma products lack “network effect” mechanics. Thus, we believe investors may face even less penalty for waiting until the technology and market matures.

7. For illustrative purposes only. There can be no assurances any such returns will ultimately be achieved.

8. Source: The Washington Post | As of 2016

9. To be clear, this is not to say that there is no value in making a better molecule for a given target – there are indeed existing targets (on that short list of targets in whose role in disease we’re already pretty confident) that are poorly engaged, and targets no one’s yet cracked (often referred to as “undruggable targets”). These are waiting for better drugs to be designed, so that they can be harnessed. But relative to the opportunities described above, the value unlocked here is limited – especially when considering the capital investment required to develop the tools that will result in these better drugs.

10. [Lilly launches TuneLab platform to give biotechnology companies access to AI-enabled drug discovery models](#)

11. As of 8 October 2025

12. Past performance is not indicative of future results and there can be no assurance any historical trends will continue in the future.