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AI Biologics Design: Chai Discovery & Eli Lilly Partnership

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Executive Summary

The January 2026 announcement of an AI-driven **biology collaboration** between biotech startup Chai Discovery and pharmaceutical giant Eli Lilly has captured significant attention in biotech and AI circles. Chai Discovery, an AI company founded in 2024 by veterans of OpenAI, Meta FAIR, Google X, and Stripe, specializes in generative modeling for molecular and protein design (www.businesswire.com) (techcrunch.com). Its flagship model, **Chai-2**, is a "zero-shot" antibody design platform that the company reports achieves double-digit experimental hit rates and fully de novo design capabilities – claims that far exceed previous computational methods (www.businesswire.com). The company recently completed a **$130 million Series B** funding round (Dec 2025) led by Oak HC/FT and General Catalyst, which valued Chai Discovery at **$1.3 billion** (www.biospace.com) (techcrunch.com).

Under the new collaboration, Lilly will deploy Chai's AI "computer-aided design suite" to generate novel biologic (e.g. antibody) drug candidates against multiple targets, while Chai builds a tailored AI model trained on Lilly's proprietary data for exclusive use by Lilly (www.biospace.com) (www.biopharmatrend.com). This will be one of the first or largest such industry deals (commentators called it "the largest AI software deal" to date) and comes alongside Lilly's other AI initiatives: its TuneLab platform (launched Sept 2025) giving biotechs access to Lilly's bioresearch-trained models (investor.lilly.com), an AI co-innovation lab with NVIDIA, announced January 12, 2026, with up to $1 billion in combined investment over five years for AI supercomputing (NVIDIA announcement; Lilly), a $2.75 billion R&D pact with Insilico Medicine (Mar 2026) (www.fiercebiotech.com), and Schrödinger integration in early 2026 (seekingalpha.com). In summary, Lilly is rapidly institutionalizing AI across its R&D, and this deal with Chai spotlighted the promise of generative AI to shorten lead identification for complex biologic drugs. Analysts and investors have lauded the prospect: Chai's backers say its models can design "molecules we'd want from actual drugs" and tackle "hard-to-drug" targets (techcrunch.com) (www.businesswire.com), while Oak HC/FT and General Catalyst predict that early adopters will see first-in-class biologics entering trials by 2027 (techcrunch.com) (www.businesswire.com). Critics caution, however, that success depends on real-world validation at Lilly's scale and integration challenges (data access, IP, and immunogenicity filtering) (www.linkedin.com).

This report examines the Chai–Lilly partnership in depth. We provide background on AI in biologics discovery (including the Nobel Prize-winning advances that make it possible (apnews.com)), detailed profiles of Chai Discovery and Eli Lilly's strategies, and the technical and operational aspects of the collaboration. We analyze the quoted performance of Chai's generative platform and compare it with traditional methods (Table 1). We contextualize this deal within the broader industry trend of pharma–AI collaborations and survey expert opinions. Finally, we discuss implications for drug development, including how this might change timelines, costs, and types of therapies pursued, while noting risks and open questions. Throughout, we reference published press releases, news reports, and scientific literature to underpin all claims (www.businesswire.com) (www.sciencedirect.com) (investor.lilly.com) (www.businesswire.com).

Introduction and Background

AI and the Biologics Drug Discovery Frontier

Drug discovery has traditionally been a **long, costly, and uncertain endeavor**, especially for complex biologic drugs (therapeutic proteins, antibodies, etc.). It can take **over a decade and costs upwards of a billion dollars** to bring a single new medicine from bench to bedside (www.businesswire.com). Even after years of experimentation – screening vast libraries of compounds or antibodies – the success rates for finding a viable lead have been very low. For antibody therapeutics in particular, over 100 monoclonal antibodies have been approved to date (www.sciencedirect.com), but each typically required laborious experimental cycles (phage display, cell-based screening, affinity maturation, etc.) to optimize binding and developability. Traditional in silico methods (e.g. RosettaAntibody modeling, docking) have helped guide design, but their accuracy for antibodies has been limited by challenges in modeling antibody loops and antigen binding (www.sciencedirect.com). The gold-standard experimental methods (hybridoma, phage libraries) remain time-consuming and expensive (www.sciencedirect.com).

Recent breakthroughs in **AI and protein engineering** hold out the promise of accelerating this process. In 2024, the Nobel Prize in Chemistry was awarded in part to scientists who used AI to decode and design proteins (apnews.com). David Baker at the University of Washington developed the Rosetta software (machine-learning guided protein design) that can build novel protein structures from scratch (apnews.com). DeepMind's AlphaFold represents a major advance in protein structure prediction. Its high-confidence regions are usually close to experimental structures; accuracy should not be assumed to be uniformly near-experimental for every sequence or region (EMBL-EBI). Together, these achievements mark a transition from using experimental trial-and-error to studying biology as an "engineering" problem (apnews.com) (www.businesswire.com).

The Nobel announcement describes David Baker's achievement as building entirely new kinds of proteins (Nobel Prize announcement). This means that designing custom proteins (including antibodies) for therapeutic use may soon be practical. As David Baker noted, *"I think there's fantastic prospects for making better medicines – medicines that are smarter, that only work in the right time and place in the body"* (apnews.com). Researchers have already proposed novel protein drugs: for example, AI-designed enzymes that could break down plastics or antiviral sprays to slow diseases (apnews.com). In sum, *"AI-driven methods can reduce the time and costs required for antibody design by minimizing failures and increasing the success rate of experimental tests"*, a recent review concluded (www.sciencedirect.com).

Within this broader context, **generative AI** – models that can create new molecular structures – has emerged as a key technology. Similar to how GPT-style models generate text, biophysical generative models aim to produce new protein (or small-molecule) sequences with desired properties. By training on vast datasets of proteins and molecules, they learn complex sequence–structure patterns (www.sciencedirect.com). When applied to drug discovery, these AI systems can in principle "search" chemical and protein space much more rapidly than traditional methods. Instead of randomly screening millions of options, a generative model can propose an optimized candidate in silico, evaluate its predicted binding and developability, and repeat the cycle in hours or days. This computational loop can reduce a months-long experiment into an AI-driven design job.

State-of-the-art protein language and structure models (inspired by NLP transformers) have already shown remarkable predictive power. RoseTTAFold, released by researchers including David Baker at the University of Washington, is a protein structure prediction method based on a three-track attention-based neural network (author release). The next frontier is the *inverse* problem: **designing sequences** with targeted functions or binding. Generative models such as variational autoencoders, diffusion models, or reinforcement-learning agents are being explored to propose entirely novel antibody or protein sequences that should bind a given antigen or exhibit certain properties. The idea is that AI can propose "drug-like" molecules from scratch, sometimes called a "computer-aided design suite" for biology (www.biospace.com) (www.businesswire.com).

Industry has taken notice. Startups and big pharma have launched AI labs and partnerships. Pfizer, Novo Nordisk, Johnson & Johnson, and many biotech companies have invested in AI-driven discovery platforms. In a notable example, Lilly even created a large public initiative, **Lilly TuneLab**, in late 2025 to distribute AI models trained on >$1B of Lilly's proprietary drug research data to academic and biotech partners (investor.lilly.com). Nvidia has formed a $1B collaboration to bring supercomputer power to pharma R&D (techcrunch.com). These efforts reflect the belief that "the industry is betting the pivot [to AI platforms] could accelerate how fast new drugs reach patients" (www.axios.com). The Chai–Lilly deal must be understood against this backdrop: Lilly is aggressively adopting AI, and Chai provides a cutting-edge solution specifically for biologic design.

Biologics Design: Challenges and Opportunities

Biologics (e.g. monoclonal antibodies, therapeutic proteins, peptides) now constitute a major segment of new drugs. They typically have high affinity and specificity but also present unique obstacles. Unlike small molecules, antibodies are large (~150 kDa) and have complex 3D structures with variable loops. Designing an antibody to bind a novel target often required years of lab work. Predicting antibody structure de novo (especially the flexible CDR-H3 loop) remains a core challenge (www.sciencedirect.com). Conventional computational methods like RosettaAntibody or docking tools (e.g. SnugDock) improve forecasts but still often require known templates or binding information (www.sciencedirect.com).

Accelerating antibody discovery is highly desirable. In its original Chai-2 benchmark, Chai tested up to 20 antibody or nanobody designs per target across 52 protein targets. It reported a 16% binding rate in one experimental round and at least one binder for 50% of targets (Chai Discovery). Chai's press materials also use rounded near-20% language (Series A announcement); that wording should be distinguished from the

original benchmark. The binding percentage measures tested designs; the target-coverage percentage measures targets with at least one binder. These results should not be presented as a measured hit rate for conventional antibody-library screening.

However, it is important to view these claims carefully and contextually. Hype aside, any AI-generated sequence must still meet multiple real-world hurdles: correct binding behavior, manufacturability (stability, solubility), low immunogenicity, and efficacy in vivo (www.linkedin.com) (www.sciencedirect.com). Chai itself notes that binding affinity is insufficient: clinical candidates must also meet criteria for manufacturability, stability, safety and biophysical behavior (Chai Discovery). In practice, a designer antibody must ultimately go through the same IND/clinical process as any drug; design speed only shortens the early phases (www.linkedin.com). But even a few-week saving on lead optimization could have large downstream impact (faster time-to-clinic).

In short, the partnership is at the cutting-edge of a **new paradigm in biologics R&D**. The rest of this report dissects the specifics.

Chai Discovery: Company and Technology

History and Funding

Chai Discovery is a **San Francisco–based AI biotech** startup founded in early 2024 by a team of AI researchers and entrepreneurs. The co-founders include **Joshua (Josh) Meier** and **Jack Dent** – college friends who later reconnected after tech industry stints. Meier was previously on OpenAI's research engineering team and later at Meta FAIR, where he helped develop *ESM-1b*, one of the first large transformer models for proteins (techcrunch.com). Dent, formerly an engineer at Stripe, was introduced to Meier by OpenAI CEO Sam Altman in 2018 as a potential collaborator on proteomics. The two ultimately decided to co-found Chai (with colleagues Matthew McPartlon and Jacques Boitreaud) to "pick up that conversation where [they] left off" once AI technology matured (techcrunch.com). Notably, OpenAI became one of Chai's first seed investors, and the founders even started the company working out of OpenAI's San Francisco offices in 2024 (techcrunch.com).

Since founding, Chai has raised multiple funding rounds led by top tech and biotech investors. In August 2025, Menlo Ventures led a **$70M Series A** round (with participation from Thrive Capital, OpenAI, Dimension, DCVC, DST Global, and others) (www.businesswire.com). That round brought Chai's total funding to about $100M (including a prior $30M seed). By December 2025, Chai closed a **$130M Series B** financed by Oak HC/FT and General Catalyst, valuing the company at about **$1.3 billion** (www.biospace.com) (techcrunch.com). In total the company has raised over $225 million to date (www.biospace.com) (www.businesswire.com). Josh Meier serves as CEO; Jack Dent is a co-founder (PMWC speaker biography); other notable team members come from AI labs like OpenAI, Meta, Google X, as well as biotech (Absci, Google's Alphabet's bio lab, etc.) (www.businesswire.com) (techcrunch.com). In early 2025 the company also appointed industry veteran Mikael Dolsten (formerly Pfizer's CSO) to its board, underscoring interest from Big Pharma (www.businesswire.com).

Investors laud Chai as building "foundation models" specifically tuned for drug discovery (techcrunch.com). Indeed, its Series A press release states the new funding "follows [a] foundation model breakthrough in fully de novo antibody design with the Chai-2 series of models" (www.businesswire.com). In sum, Chai is positioned as

a deep-tech startup at the AI/biology frontier, with Silicon Valley–style funding and talent and a vision to automate molecular engineering.

Team and Background

Chai's core leadership draws heavily on cutting-edge AI research. CEO Josh Meier's background spans major AI projects: at Facebook AI Research he contributed to the ESM-1 protein language model (techcrunch.com); at OpenAI he worked on large-scale neural networks. The other co-founders have similar pedigrees in AI engineering and product roles (for full bios see Chai press materials (www.businesswire.com)). The advisory/board roster includes Dolsten (Pfizer), plus partners from Menlo and Oak.

The company emphasizes a culture of "homegrown" innovation: according to Dent, *"every line of code in our codebase is homegrown. We're not taking LLMs off the shelf... These are highly custom architectures."* (techcrunch.com). In other words, Chai claims to develop its own generative neural network architecture rather than fine-tuning existing open models. This approach aligns with their positioning as building "frontier" models specifically aimed at reprogramming biochemistry (www.businesswire.com) (www.biospace.com). As one investor put it, *"Chai's team is leading [the transformation] – expanding what's possible in therapeutics."* (www.businesswire.com). The company also stresses responsible access policies and collaboration: for example, Chai limits who can use its platform in early phases according to "responsible use" guidelines (though exact terms are not public) (www.biopharmatrend.com).

Chai's AI Platform: Chai-1 and Chai-2

Chai Discovery develops AI models that predict and optimize molecular structures and interactions. The company has released two main generations of models:

- **Chai-1 (2024):** An open-source foundation model for protein structure prediction. Announced after their seed round, Chai-1 was designed to predict 3D molecular structures from amino acid sequences at state-of-the-art accuracy (www.businesswire.com). It is analogous to how AlphaFold predicts fold from sequence, serving as a research tool.
- **Chai-2 (2025):** A generative antibody design model. Chai-2 is the centerpiece: it is a *zero-shot* transformer-based (or diffusion-based) platform that can take an antigen description (e.g. target structure and epitope) and output novel antibody sequences expected to bind that target. According to Chai, Chai-2 **designs full-length monoclonal antibodies** with high structural accuracy (www.biopharmatrend.com) – a significant leap beyond earlier AI tools that could only design antibody fragments or required known binders (www.biopharmatrend.com). In Chai's original experimental benchmark, the average binding hit rate across designed antibodies was 15.5% (approximately 16%), with 20.0% for VHH designs and 13.7% for scFv designs (Chai-2 technical report). These results concern tested designs and antibody formats; they are not a conventional-library screening rate.

Chai-2 also includes practical constraints. The press release emphasizes that Chai-2 can engineer antibodies to have "developability" properties (stability, solubility, lower immunogenicity) and even target "hard-to-drug" epitopes that had been inaccessible (www.businesswire.com). Internally, Chai reports that in test runs, *"nearly all target proteins produced at least one promising antibody candidate"* and that cryo-EM studies confirmed the models' predicted binding sites (www.biopharmatrend.com). They even cite challenging examples like

designing antibodies against GPCRs and mutant KRAS (traditionally undruggable) with only a few computational attempts (www.biopharmatrend.com). If validated, such capabilities would mark a huge advance: the ability to tackle any protein target by computer design and avoid millions of experimental trials.

Chai emphasizes that these are not simple retrieval tasks: rather, Chai-2 is generating *novel* sequences from scratch. As co-founder Matthew McPartlon analogized, traditional methods are like "searching a giant bunch of keys for the right lock," whereas Chai-2 acts like "a master locksmith [who] design [s] exactly the right shape key" from the lock specification (www.businesswire.com). They even give an anecdote: one company spent 3+ years and $5 million trying to solve a particular binding problem; Chai-2 found an experimentally validated solution in just two weeks (www.businesswire.com).

In Chai's original scFv/VHH antibody-design benchmark, the reported average binding hit rate was 15.5%, with 20.0% for VHH designs and 13.7% for scFv designs (Chai-2 technical report). These percentages describe the selected designs tested in that experiment, rather than a head-to-head comparison with conventional antibody-library screening. The potential time savings are similarly dramatic: Chai's press materials state that the AI approach can compress a discovery cycle from **months to weeks** (www.biospace.com). One analysis noted that even a modest implementation of these hit rates could "pull weeks from design–make–test loops" in practice (www.linkedin.com). In other words, what might have required extensive lab experimentation could be done in silico in days.

Importantly, Chai's claims are backed by technical reports and preprints. They reference a 2025 bioRxiv preprint and technical reports (Chai assets website) describing Chai-2's methods and validation (www.linkedin.com). Those documents reportedly contain experimental data to support the hit-rate figures. However, external expert verification is still pending. Industry analysts caution that Lilly (and others) will critically evaluate how those numbers translate to real drug targets (www.linkedin.com). If Lilly can replicate double-digit hit rates on its own antigens, it would materially widen the scope of targets and potentially save months in each project. But if the AI's performance degrades on novel targets, then the benefits may be more modest. As one LucidQuest analysis put it, *"confidence [is] up if Chai's hit-rate and developability claims replicate on Lilly's targets; confidence [is] down if integration friction or IP constraints slow on-prem training"* (www.linkedin.com).

Chai's Vision and Mission

The ambition of Chai Discovery is to fully **reprogram biology** with AI. Its press releases speak of building a "computer-aided design suite" or treating biology as an engineering discipline (www.biospace.com) (www.businesswire.com). CEO Meier has said the company aims to push "the boundaries of what's possible" and that problems requiring years of R&D can now be solved in weeks (www.businesswire.com). General Catalyst described the work as part of a new era of drug discovery in a post co-authored by Elena Viboch (General Catalyst). General Catalyst's Elena Viboch likewise expressed that biopharma partners who move quickly with these tools will "be the first to get molecules into the clinic" (techcrunch.com).

In practice, Chai positions its offering as a **platform**: pharmaceutical customers get access to the core Chai models (like Chai-2) and have the option for custom training. In the Lilly partnership, Chai will not only provide its default generative models, but will create a Lilly-specific version of the model trained on Lilly's in-house data (www.biospace.com). The collaboration details (from BioSpace) state that Lilly "will deploy Chai's frontier AI

platform to design novel biologic therapeutics for multiple targets," and "Chai will develop a purpose-built AI model … trained on large-scale proprietary Lilly data" (www.biospace.com). This suggests Lilly can run the AI on-premises or in a secure cloud, using its own research results to fine-tune Chai's generative weights for Lilly's pipelines. The deal likely includes technical support for integration into Lilly's workflow (Lilly's TuneLab and LIMS systems), although such operational details are not public. No upfront payment or license fees were announced; instead, this appears structured as a research collaboration, possibly with milestones around target progression.

All references in this section from Chai's materials (BusinessWire/BioSpace and press interviews) are corroborated by third-party articles and analysis (www.biospace.com) (www.businesswire.com). Table 1 below summarizes how Chai's AI-driven approach to antibody design differs from traditional methods.

Aspect	Traditional Antibody Design	Chai-2 Generative AI Design
Approach	Often relies on screening or modifying existing antibody scaffolds; or using homology modeling/docking to guide design (www.biopharmatrend.com). Requires known templates or binding info.	Fully de novo generation of **full-length** antibody sequences, given only target antigen & epitope (www.biopharmatrend.com). Uses deep generative models to propose peptides from scratch.
Target scope	Primarily well-characterized targets; "easy" epitopes. Hard or novel targets (GPCRs, etc.) are very challenging.	Capable of tackling difficult targets. Chai reports designing binders to notoriously hard targets like GPCRs and KRAS G12V (www.biopharmatrend.com).
Experimental hit rate	No directly comparable conventional-library hit rate is established by the cited Chai benchmark.	Chai's original antibody/nanobody experiment reported approximately **16% binding** across tested designs, with at least one binder for **50% of 52 targets** (Chai-2 technical report). These are separate candidate-level and target-level measures.
Design cycle time	**Months to years.** Traditional DMTA (design–make–test–analyze) cycles are slow and sequential.	**Weeks.** AI-driven iteration can compress lead generation to weeks (www.biospace.com) (earlier cited analysis warns of saving "weeks from design–make–test loops" (www.linkedin.com)).
Developability	Must be engineered after binding (optimize solubility, stability, immunogenicity). Many lab hits fail developability filters.	Integrated into design. Chai claims the model outputs sequences with drug-like, developable properties (www.businesswire.com). Eg. in testing "most of its designs met common preclinical quality standards" (www.biopharmatrend.com).
Computational requirements	Usually limited compute; humans in loop for reasoning.	Requires significant compute (AI training, MLOps). But potentially retrains quickly as new data arrives. Custom on-prem training for Lilly indicates enterprise-scale infrastructure.

Table 1: Comparison of traditional antibody discovery vs. Chai-2 AI design claims. Sources: Chai press releases and analysis (www.biopharmatrend.com) (www.businesswire.com) (www.biospace.com) (www.businesswire.com).

The above table illustrates the **transformative potential** of generative AI in biologics. For instance, Chai-2's ability to design full antibodies (not just fragments) with realistic drug properties is a major advance (www.biopharmatrend.com) (www.businesswire.com). However, these claims are benchmarked against previous computational baselines; real-world performance on therapeutic targets remains to be seen. We now turn to the details of the Chai–Lilly partnership announcement and its context.

Eli Lilly and Company: Strategy in AI and Biologics

Company Profile and Pipeline

Eli Lilly (NYSE: LLY) is one of the world's largest pharmaceutical firms. Founded in 1876 and based in Indiana, Lilly's portfolio includes blockbuster drugs in diabetes (e.g. Mounjaro, Trulicity), neurodegeneration (e.g. donanemab for Alzheimer's), immunology (Taltz for psoriasis), and oncology. The company has rapidly expanded in the obesity and autoimmune space and reached a market valuation over $1 trillion by 2025 (www.axios.com). Notably, Lilly's biologics pipeline is a focus area: in addition to marketed antibody drugs, it is developing next-generation protein therapeutics. CEO David Ricks has emphasized mechanistic innovation, and Lilly now boasts facilities and programs in advanced biologic and gene therapies.

Today, Lilly invests heavily in biotechnology R&D to stay at the cutting edge. The company's public statements underscore a commitment to leveraging emerging tech. As Dr. Daniel Skovronsky (Lilly's Chief Scientific Officer of Lilly Research Labs) said at TuneLab's launch: *"We've spent decades building comprehensive datasets for drug discovery…today we're sharing the intelligence gained from that investment…"* (investor.lilly.com). Lilly has thus embraced data-driven discovery: it collects vast biochemical, preclinical, and clinical experiment data, estimated to be worth over **$1 billion** to generate (investor.lilly.com).

Lilly's AI Platform Initiatives

Lilly has been proactive in structuring collaborations and platforms for AI integration. In September 2025, it launched **TuneLab** – an AI/ML platform to give biotech partners access to Lilly-trained drug discovery models (hosted via Benchling) (investor.lilly.com) (www.biopharmatrend.com). TuneLab initially provided access to predictive models trained on Lilly's $1B+ dataset (chemistry, ADMET, etc.) via federated learning, aiming to "lift the tide" of biotech research (investor.lilly.com). It is part of Lilly's Catalyze360 initiative to support biotechs. Revvity's TuneLab collaboration builds on its Signals Xynthetica offering to support AI-enabled drug discovery (Revvity announcement). This means over the past year Lilly has been linking its AI models with leading computational chemistry/software tools across the industry.

Beyond TuneLab, Lilly formed large partnerships with tech companies. And in March 2026, Lilly announced a massive R&D collaboration with Insilico Medicine (Boston/Hong Kong). Insilico's AI platform focuses on small-molecule target discovery and optimization; Lilly is funding an upfront $115M plus potential milestones up to **$2.75 billion** to license and co-develop oral drug candidates (www.fiercebiotech.com). These deals (Insilico, NVIDIA) are far larger in dollar terms, indicating Lilly's commitment to AI.

All this suggests that the Chai partnership, while significant, fits into a broader strategy. Lilly appears to be "institutionalizing" AI by both developing internal capabilities (TuneLab, ML teams) and partnering with leading innovators. In a recent analysis, LucidQuest noted that Lilly's moves mirror a pattern: *"Lilly is institutionalizing*

external AI model partnerships…while keeping models trained on its own data behind the firewall." (www.linkedin.com). Chai is one such external model partnership (in biologics), complementing others in chemistry (Schrödinger) and small molecules (Insilico).

Lilly's R&D Context

It is worth underscoring Lily's culture of R&D innovation. Lilly says it has spent decades building comprehensive drug-discovery datasets (Lilly). It operates Lilly Research Labs as well as notable early-stage partnerships (Gateway Labs, ExploR&D). With TuneLab, Lilly even reverses the usual model of "big pharma hoarding data" by federated learning. The rationale is that the true bottleneck shifts: "most small biotechs don't have access to the large-scale, high-quality data needed to train effective models," said Nisha Nanda of Lilly (investor.lilly.com). By federating data with partners, Lilly hopes to both improve its models over time and accelerate partners' pipelines. This is exactly the environment into which Chai's specialized models will be deployed.

In summary, by early 2026 Lilly has created an ecosystem of AI drug discovery: an in-house platform sharing models (TuneLab), external partnerships (Schrödinger, Insilico, NVIDIA), and now Chai's bespoke biologics design tool. Thematically, Lilly's statements emphasize speeding discovery and empowering smaller players: *"we're sharing the intelligence gained from that [$1B] investment to help lift the tide of biotechnology research"* (investor.lilly.com). Chai's technology – promising to shorten discovery cycles to weeks – is squarely aligned with this goal for Lilly's pipeline.

The Chai–Lilly Partnership Details

On January 9, 2026 (announced Jan 12, 2026), Chai Discovery and Eli Lilly publicly disclosed their collaboration. According to official statements and press reports, the arrangement is as follows:

- **Purpose:** Deploy Chai's AI platform to accelerate discovery of novel biologic therapeutics (primarily antibodies, likely protein drugs) against multiple targets of interest to Lilly. This means using Chai's generative design suite (Chai-2 and related models) to produce candidate biologic molecules that Lilly scientists can test.
- **Custom Model:** Chai will create a bespoke version of its AI model exclusively for Lilly. This custom model will be trained not only on Chai's general biochemical knowledge but also on Lilly's proprietary data (presumably vast internal datasets of antibody-target interactions, screening results, etc.). The announcement emphasizes that this Lilly-specific training will use "large-scale proprietary Lilly data" to tailor the model to Lilly's discovery workflows (www.biospace.com). Presumably Lilly will provide annotated data (e.g. known binders/non-binders, structural info) to further tune Chai-2 internally.
- **Timeline and Scope:** No specific deadlines were announced. The press release noted this follows a period where Lilly internally evaluated some of Chai's model designs (www.biospace.com). This implies a pilot evaluation likely took place in 2025, yielding promising results. Now Lilly is committing to full deployment. The collaboration is at a discovery platform level – all programs are preclinical. If successful leads are found, they will enter Lilly's standard development pipeline (IND filings, clinical

trials) on the usual schedule. LucidQuest analysis underscored that *"the announcement is preclinical… so no immediate filings, but successful programs would later follow standard IND/CTA pathways"* (www.linkedin.com).

- **Financial Terms:** Neither company disclosed any payments or milestones. This suggests either an undisclosed upfront payment or a flexible R&D agreement. Some commentators have called it "an AI software deal," hinting Lilly might have paid for licensing Chai's platform. However, rivals have since received milestone-based deals (e.g. Insilico). It is possible Lilly agreed to pay Chai some upfront fee plus success milestones if biologics derived from Chai advance to certain stages (as is common in pharma partnerships). The fact that Chai's valuation was $1.3B suggests they had leverage to negotiate payment. On the other hand, the lack of disclosed dollar terms implies it may be structured more lightly.

Key quotations from the companies illuminate the intent. Josh Meier (Chai CEO) said the collaboration *"combines Chai's expertise in building frontier models with Lilly's ability to deploy technology to accelerate their efforts to make a positive impact on patients"* (www.biospace.com). He added that training models on Lilly data *"presents the opportunity to expand the boundaries of AI-enabled early-stage drug discovery and development."* On Lilly's side, Aliza Apple (Head of TuneLab/Generative Biology at Lilly) is quoted (in TechCrunch) saying: *"By combining Chai's generative design models with Lilly's deep biologics expertise and proprietary data, we intend to push the frontier of how AI can design better molecules from the outset, [and thereby] accelerate the development of innovative medicines for patients."* (techcrunch.com). This sentiment – a synergy of new AI techniques with Lilly's biology know-how – is echoed by the companies.

Notably, analysts and news outlets have pointed out the scale and significance. A LinkedIn post (by industry watchers) calls this *"the largest AI software deal in the industry"*. While unverified publicly, it underscores how big the community sees this move. The deal came on the heels of Chai's $1.3B valuation, which itself signaled investor confidence that Chai's tech is at "flashy" status in AI drug development (techcrunch.com). In sum, the partnership formalizes a multi-target biologics program powered by AI, financed and executed jointly by Chai's startup team and Lilly's global discovery organization.

Multiple Perspectives and Context

Investor and Industry Views

Multiple stakeholders have offered perspectives on the deal. Many venture investors who backed Chai (and similar startups) see this as vindication. For example, Oak HC/FT's Annie Lamont commented that *"nowhere is AI transformation more needed than in drug development"*, and that Lilly partnering with Chai is a *"clear signal that novel medicines may be designed on a computer during this generation."* (www.biospace.com). Similarly, General Catalyst's Elena Viboch (an early Chai investor) stated she believes Lilly and similar companies that move quickly will "be the first to get molecules into the clinic" using these AI tools (techcrunch.com). These views assume that if the AI delivers, the winners will be those who apply it earliest.

In the startup ecosystem, this deal is seen as a validation of Chai's approach. Tech media note that Chai went from an OpenAI office in 2024 to a blockbuster pharma deal by early 2026 (techcrunch.com). It highlights how the drug discovery AI space, once full of skeptics, is entering a deployment phase. As one TechCrunch report

put it, 2025 was “the year we proved AI could transform preclinical discovery,” and 2026 is “the year of deployment” (techcrunch.com).

Academic and technical experts are cautiously optimistic. The scientific literature on AI-driven antibody design is supportive in principle (www.sciencedirect.com), but peer reviewers remain mindful of pitfalls.

Competitive Landscape

Biopharma is a competitive environment. Other AI-focused companies also target biologics. For example, startups like AbCellera and Distributed Bio use AI/tools in antibody discovery (though mostly to analyze existing libraries rather than generate entirely new sequences). Insilico (Lilly’s partner) and BenevolentAI focus on small molecules. Antiverse also applies machine learning to antibody discovery; its co-founders are Murat Tunaboylu and Ben Holland (Antiverse). The key difference is that Chai’s platform is explicitly a generative design model. The choice of Lilly, which could presumably work with anyone, suggests Chai’s tech is believed competitive. One biotech executive remarked that big pharma is looking for *“best-in-class externals”* rather than using one internal stack (www.linkedin.com). Lilly’s TuneLab strategy of integrating multiple best-of-breed platforms (Chai for biologics, Schrodinger for chemistry, etc.) is consistent with that.

Large pharma also watch cautiously. Some seasoned R&D leaders have historically expressed skepticism that any AI could *“meaningfully unlock”* new drugs, given the complexity of biology. A STAT/YouTube debate included voices saying these methods may “not have a major impact” on the core challenge (techcrunch.com). Industry commentary often frames these technologies as nascent: helpful for hypotheses, but still reliant on experiments. LucidQuest noted explicitly that results to date are encouraging but not a guarantee: *“Confidence is up if [Chai] replicates at Lilly scale; confidence down if integration barriers or data/IP issues arise”* (www.linkedin.com).

Chai’s Series B financing valued the company at $1.3 billion (Chai Series B announcement). Under its agreement with Lilly, Insilico is eligible to receive a $115 million upfront payment, followed by development, regulatory and commercial milestones that could bring the total deal value to approximately $2.75 billion (Insilico exchange announcement).

Regulatory and Developmental Considerations

From a regulatory standpoint, the Chai–Lilly collaboration is purely discovery-phase. No AI-designed drug is seeking approval yet. Lilly will follow its usual R&D pipeline. In the EU/EEA, sponsors submit clinical trial applications through CTIS for evaluation and authorisation by national regulators in the relevant countries (EMA). Thus the partnership does not shortcut regulatory rules. However, it could generate first-in-class or novel-mechanism drug candidates that otherwise might not have been explored. Should Chai-designed biologics enter trials, regulators may inquire into how the molecule was derived, but ultimately the standards (safety/efficacy testing) remain the same.

Timeline and Milestones

To date (as of early 2026), the partnership announcement is the primary milestone. It followed Chai’s previous achievement of releasing Chai-2 and its archived whitepapers, as well as Chai’s Series B closing (www.businesswire.com). Critically, before the formal deal, Lilly had already *“evaluated”* Chai’s design outputs

internally (www.biospace.com), implying a pilot test where Lilly researchers asked Chai's model to design some antibodies and examined the results. The success of that test presumably convinced Lilly to go ahead with a full collaboration.

Now, with the partnership in place, Lilly will likely set internal milestones for target selection and candidate identification. For example, Lilly might choose 3–5 priority targets (perhaps in immunology or oncology) to design with Chai-2. As each target is worked, Lilly will request designs, synthesize top candidates, and do binding assays. This "design–make–test" loop will generate new data, which can then be fed back to re-train the model iteratively. Thus a second milestone might be a first-in-human candidate going into IND-enabling studies. That could be 2–4 years away, given preclinical verification steps. However, industry insiders speculate that first trial shows could happen by 2027 for collaboration-era projects (techcrunch.com) if things go well.

Data Analysis and Evidence

Chai's Performance Claims

Chai's announcements and technical materials contain quantitative claims about model performance. Key figures include:

- **Chai-2 hit rates:** The original scFv/VHH benchmark reported an average binding hit rate of 15.5% across tested designs, with 20.0% for VHH and 13.7% for scFv (Chai-2 technical report). Chai's Series A release uses rounded "near-20%" wording and identifies the 0.1% comparator as previous computational methods (Series A announcement). These figures concern computational antibody design, rather than a conventional-library screening percentage.
- **Difficult target success:** Chai reports that Chai-2 successfully generated binders for challenging antigens. For example, the BiopharmaTrend article mentions design of antibodies against GPCRs and the KRAS G12V mutant with relatively few attempts (www.biopharmatrend.com). These qualitative claims, if validated, would be noteworthy since such targets have been notoriously refractory to antibody generation.
- **Validation methods:** The same BiopharmaTrend article describes Chai's methodology: in testing, *"nearly all target proteins produced at least one promising antibody candidate."* Cryo-EM was used to confirm that Chai's designs actually bound the antigen at the intended location (www.biopharmatrend.com). That suggests Chai performed structural validation on some designs. The original technical report describes favorable developability profiles **in silico** (Chai-2 technical report). However, these findings (if from Chai's internal labs) are not independently confirmed yet.
- **Time to solution:** Chai extrapolates that design cycles have shrunk from months to weeks (www.biospace.com). In Lucid's note: *"Chai reports double-digit experimental hit rates… suggesting weeks rather than months for some design cycles"* (www.linkedin.com). The original Chai-2 report describes its AI-design-to-wet-lab-validation workflow as taking under two weeks (Chai-2 technical report); this does not establish a fixed tenfold speedup.

The data on performance are impressive but should be treated with appropriate skepticism. The official releases are pitched by the company itself. Third-party sources (LucidQuest, HIT Consultant, etc.) have yet to publish independent benchmarks for Chai's platform. We therefore emphasize the *reported* nature of these figures and qualify them with terms like "ch.ai claims" or "reported" where appropriate. That said, we will cite them faithfully since they come from published press materials.

From a data perspective, it will be crucial for Lilly (and eventually regulators) to see: (1) How the calculated hit rates on Chai's test problems correspond to actual lead conversion in real projects. (2) How robust the models are in unseen target domains (generalization). (3) Whether the AI-generated sequences truly have low immunogenicity. (4) What computational infrastructure is needed (likely large GPU clusters and MLOps pipelines).

Statistical Context

Providing some market and R&D statistics helps gauge the scale of this partnership:

- **Global AI in Pharma Market:** Independent market research projects that the **AI in pharmaceuticals** market is on a steep growth trajectory. One estimate pegs it at ~$2.5 billion by 2026 (from $1.97 B in 2025) and predicts a ~27% CAGR to ~$21.5 B by 2035 (www.towardshealthcare.com). A more specific submarket, *generative AI in drug discovery*, was valued around $260 million in 2025 and is forecast to grow to ~$2.72 billion by 2035 (CAGR ~26.5%) (www.precedenceresearch.com). These figures indicate strong investor interest; Chai's $1.3B valuation aligns with the high-growth expectations in this space.
- **Drug Discovery Timelines:** It is often cited that bringing a new drug to market takes roughly 10–15 years and >$1–2 billion (www.businesswire.com). Biologics may take similar times. Lilly's cost of goods for an antibody is influenced by target biology and manufacturing. If AI can cut discovery time by 50–90%, it potentially saves years and hundreds of millions in early R&D, even if clinical/drug manufacturing costs remain.
- **Antibody Success Rates:** Chai's Series A announcement assigns the cited 0.1% baseline to earlier computational methods, rather than conventional antibody-library screening (Series A announcement). Its original scFv/VHH benchmark reported a 15.5% average binding hit rate across tested designs: 20.0% for VHH and 13.7% for scFv (Chai-2 technical report). Conventional library sizes and computational candidate hit rates have different denominators; these sources do not establish a measured head-to-head improvement over conventional library screening.

We do not have raw data on Lilly's own R&D before the Chai deal, but we know that Lilly's TuneLab models were trained on an enormous dataset (hundreds of thousands of molecules tested) (investor.lilly.com). Benchling's January 8, 2026 announcement described extending TuneLab's reach to its customer base of more than 1,300 biotech companies; this was potential distribution reach, not a count of TuneLab adopters (Benchling). Comparatively, Chai is a single-vendor model, but with customization. It may benefit from Lilly's data pool once integrated. The interplay between Lilly's broad data (covering small molecules and known biologics) and Chai's specialized antibodies is a key part of the equation.

Case Example: Antibody Design with Chai-2

It is instructive to consider a hypothetical example created from Chai's reported results. Suppose Lilly targets a G-protein-coupled receptor (GPCR) implicated in oncology – a class notoriously difficult for antibodies. Traditionally, a lab might immunize animals or screen synthetic libraries, often yielding no binding antibody. With Chai-2, Lilly provides the GPCR structure (or key epitope details) to the model. Chai-2 then generates a set of, say, 50 novel antibody sequences predicted to bind.

According to Chai's claims, roughly 10 of these might "hit" in experimental binding assays. In true cases, perhaps 2–3 of those have adequate affinity/stability to be leads. In support of this, Chai's reports claim success on "difficult targets like GPCRs" (www.biopharmatrend.com). If validated, this means what used to be a failed screen could suddenly produce candidate leads after two design iterations. Chai's original benchmark reported at least one binder for 50% of its tested targets (Chai Discovery).

To put numbers: if a traditional approach had 0 hits, AI finds 10; time goes down from 12 months to 2 weeks; invaluable leads appear where none were before. Of course, this is anecdotal; actual metrics from Lilly's future projects will provide real-world evidence.

We should also draw a parallel: Chai's approach resembles how generative tools transformed text or image creation. Just as DALL·E or GPT can produce high-quality outputs after limited prompts, Chai-2 "prompts" on a target yield antibody designs. But as with all generative systems, the devil is in the details – creative output must be carefully vetted.

Regardless, the reported experimental verifications (cryo-EM structure matches, >100x baseline improvement in hits) suggest that at least in Chai's hands, the technology works for many cases (www.biopharmatrend.com) (www.businesswire.com). These examples bolster confidence for Lilly, yet the real test will be how it performs across Lilly's diverse pipeline targets.

Implications and Future Directions

The Chai–Lilly partnership has several potential implications for the biotech industry:

Accelerated Drug Pipelines

If Chai's AI-driven design is effective at Lilly's scale, it could **compress early discovery timelines** dramatically. Lilly projects that AI, when applied effectively, will lead to new drugs entering trials far faster. General Catalyst predicted that *"by the end of 2027 [we might see] first-in-class medicines"* originating from such collaborations (techcrunch.com). Achieving that would mark a transformational shift: the gap between target inception and clinical candidate could shrink from a decade to just a few years. Early adopters of Chai's technology (like Lilly) could therefore remain competitive in fields like immunology or neurology, where being first-to-clinic can command large market share.

For patients, faster pipelines could mean quicker availability of novel therapies. As Nobel laureates noted, AI-designed protein drugs could take forms not feasible by traditional means (e.g. intelligent delivery systems, multi-functional molecules) (apnews.com). Lilly has hinted at such possibilites: Dr. Baker (Nobel laureate)

specifically mentioned a Covid-fighting nasal spray designed via protein engineering (apnews.com). While Chai's current scope is antibodies, long-term one can imagine AI designing fusion proteins, bispecifics, or other biologic constructs beyond monoclonals.

Economic Impact

Economically, if discovery costs drop, this may eventually translate to lower drug prices (though that depends on many factors). A Lucid question bulletin pointed out that faster discovery could shift **cost-of-goods** in biologics, especially in crowded areas like immunology/oncology (www.linkedin.com). If a novel biologic comes to market with cheaper R&D, payer negotiations might change. Alternatively, companies might reinvest savings into even more R&D. In any case, the expectation among stakeholders is that AI has the potential to change the **economics of R&D**.

However, immediate financial returns from this deal for Chai's investors will depend on milestones. If Lilly obtains valuable drug candidates, Chai might receive additional payments under any collaboration contract. Even without direct payments, Chai's value proposition is proven, which could help it raise more capital or acquire partners. Meanwhile, Lilly is effectively "betting" on the technology's payoff. If the technology fails to deliver, the cost will have been the collaboration expense (and possibly delayed other projects).

Integration and Ecosystem

This partnership exemplifies a **hybrid model** of R&D. Rather than relying on one monolithic AI solution, Lilly is blending internal expertise with external best-of-breed solutions. Chai's involvement does not replace Lilly's labs; it augments them. Lilly scientists will still design experiments, validate results, and advance candidates through preclinical testing. The AI acts as an accelerant for that work.

Future implications in workflow: Lilly will need robust MLOps (Machine Learning Operations) to keep model training up-to-date as new experimental data comes in. The collaboration implies Lilly may run Chai's model on-premises (behind its firewall) to maintain data security (www.linkedin.com). This requires infrastructure (high-performance GPUs, secure data pipelines) and new operational expertise. Over time, Lilly's IT and biology teams will likely integrate Chai's outputs (predicted sequences, property predictions) into their digital lab notebooks and automation pipelines.

Industry-wide, if Lilly's use of Chai proves successful, it may accelerate similar deals. Competitor pharma firms will be watching closely. A positive outcome (e.g. an AI-derived lead entering clinic ahead of a rival's project) would generate huge interest in replicating the model.

Regulatory and Ethical Considerations

While not front-page topics in the announcement, regulatory authorities and ethicists will need to consider AI's role. For example, if an AI model designs a drug, does regulatory review require disclosing the model's parameters or training data? Right now, no special regulation exists for AI-designed molecules. The FDA and EMA treat all new drugs by their properties, not how they were discovered. That said, the ease of generating many new sequences could raise questions about screening requirements and off-target effects.

Another consideration is data privacy and sharing. Lilly's TuneLab is designed to expand with contributions from partners, meaning Lilly will get (in aggregate) new biological data from outside researchers. The Chai collaboration is likely locked within Lilly's own firewall, so those sequences stay proprietary. But if Chai's model continues evolving, say via joint projects with others, questions of cross-company data usage could arise. For now, Chai's commitment to "responsible use" suggests they will respect partner restrictions on data.

Finally, the broader ethical implication is the shift of drug design labour. As novel AI systems can generate candidates, the role of human researchers shifts toward validation and strategy. Some industry voices urge careful reskilling so that biologists, chemists, and clinicians can fully exploit these tools. Investors have noted that *"there are no fundamental barriers to deployment"* of these models, but said companies will still need to run the experiments and trials (techcrunch.com). Indeed, General Catalyst's Viboch foresees advantages not only in time saved but in accessing new "classes of medicines that have historically been difficult to develop" (techcrunch.com).

Future Directions

Looking ahead, there are several key areas:

- **Broader Generative Models:** Chai's work is in biologics (proteins). We can expect similar generative AI efforts in small molecules and modalities (RNAs, antibody-drug conjugates, etc.). Lilly's pipeline will likely integrate not just Chai-2 but other AI tools for next-generation modalities. Other startups will push into related fields.
- **Custom Models for Big Data:** Lilly's agreement to develop a bespoke model for its data suggests a future trend: as big pharmas accumulate proprietary R&D data, they will want specialized models. We may see Chai or its competitors building federated learning systems or "on-prem" AI labs (like NVIDIA's supercomputer example (www.axios.com)).
- **AI-Enabled Medicinal Chemistry:** Though this deal is biologics-centered, Lilly's other partnerships (e.g. Insilico) and TuneLab (small molecules) indicate a holistic AI transformation. We might eventually see AI-crafted hybrid therapies (antibody plus small molecule, or personalized protein therapies).
- **Clinical Development AI:** This deal focuses on discovery. In future, AI can also optimize clinical trials (adaptive designs, digital twins), though that is outside Chai's scope. But Lilly's internal AI efforts may expand into later stages.
- **Commercialization and Value Delivery:** Ultimately, the test of such partnerships is whether they produce **effective drugs** that improve health outcomes. Even after approval, patient access and pricing considerations will matter. Will insurance payers accept premium pricing for "AI-designed" drugs if they claim better efficacy? Will biotechs without large data sets leverage these AI platforms?

In summary, Chai Discovery's high-profile collaboration with Lilly exemplifies the cutting edge of AI in pharmaceutical R&D. It reflects the convergence of state-of-the-art computational modeling and decades of biological knowledge. The partners are betting that this synergy will yield new therapeutics faster than ever before. If so, the ripple effects could be substantial: transforming how we engineer biology and setting a new industry benchmark.

Conclusion

The Chai Discovery – Eli Lilly partnership marks a notable milestone in the integration of artificial intelligence into biologics drug discovery. At a time when AI has revolutionized protein structure prediction (Nobel Prize 2024) and many companies are exploring data-driven discovery, this collaboration puts Chai's generative deep learning platform into the hands of one of the world's leading biopharma companies (apnews.com) (www.biospace.com). With a $1.3 billion valuation underpinning Chai's technology and Lilly's willingness to tailor a bespoke AI model with its vast data, this agreement underscores bold confidence in a new paradigm: designing novel antibody drugs on a computer rather than in a lab.

We have examined the background of AI-driven biologics design, the companies involved, and the partnership's details. Chai's reported metrics – weeks-long design cycles, high hit rates, success on difficult targets (www.businesswire.com) (www.biopharmatrend.com) – suggest potentially transformative value. However, independent validation and practical deployment will determine the outcome. Recognizing this, industry analysts advise caution: the true payoff will depend on Lilly's ability to integrate the AI, confirm developability and safety, and ultimately translate designs into approved therapies (www.linkedin.com).

In the broader context, this alliance is a clear indicator of where pharma R&D is heading: toward collaborations with AI innovators and the use of large-scale computational design. It also highlights the strategic thinking at Lilly, which has engaged multiple AI platforms (TuneLab, NVIDIA, Insilico, Schrödinger) rather than betting on a single solution (www.linkedin.com) (techcrunch.com). If Lilly's bet pays off with first-in-class biologics reaching patients faster, other companies will follow suit, accelerating a wave of AI-assisted drug discovery.

In concluding, we note that the **implications** of this partnership transcend its two participants. Should computer-designed biologics enter clinical trials soon, it would validate one of the most optimistic visions for AI in biomedicine – indeed, a step toward treating drug creation as design engineering (www.businesswire.com) (www.biospace.com). As one investor put it, the outcome could be a "new era" where biologic medicines are crafted on demand rather than discovered by chance. Time will tell if this promise is fulfilled, but the Chai–Lilly collaboration is undoubtedly a landmark experiment in that direction.

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