Isomorphic Labs & AlphaFold: AI Drug Discovery in Trials

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Executive Summary

In 2025–2026, **Isomorphic Labs** – an AI-driven drug discovery spin-off from Google DeepMind – marked a watershed moment by advancing its *first-in-human* clinical trials for drugs **designed using AlphaFold**, DeepMind's breakthrough AI for protein structure. According to news reports, Isomorphic's President Colin Murdoch confirmed that the company is "staffing up" and "getting very close" to dosing patients in trials of its AI-created oncology candidates ([1] fortune.com) ([2] indianexpress.com). These candidates, created using the *AlphaFold 3* system and other proprietary models, represent some of the first therapies engineered with deep-learning protein models to reach the clinic.

Isomorphic's pipeline focuses on **oncology and immunology**, leveraging machine learning to accelerate drug design by predicting complex molecular interactions ([3] fortune.com) ([4] www.prnewswire.com). The company, founded in 2021 by DeepMind veterans, has secured major partnerships (e.g. with Novartis, Eli Lilly, and Johnson & Johnson) and substantial funding (a $600M financing in March 2025 ([5] www.prnewswire.com) ([6] www.fiercebiotech.com)) to develop its AI "drug design engine." Its CEO, Demis Hassabis, frames the mission as solving "all disease with the help of AI" ([7] www.prnewswire.com) ([8] www.fiercebiotech.com).

This report comprehensively examines the emergence of Isomorphic Labs' AlphaFold-based drugs. We review the **historical context** of AI in structural biology and drug discovery, detail Isomorphic's technology (from AlphaFold 3 to its proprietary IsoDDE engine), analyze the company's pipeline and trial progress, and consider broader implications. Key statistics and expert commentary are included, such as AI improvements in prediction accuracy (blog.google), success-rate challenges in conventional drug R&D, and scientific community perspectives (e.g. one expert calls Isomorphic's new engine "on the scale of an AlphaFold 4" ([9] www.scientificamerican.com)). We also compare this development with other AI-drug efforts and lay out the potential future impact on biomedical research and therapeutic innovation.

Introduction and Background

Drug discovery has long been an arduous, costly process: bringing a new therapy to market can take over a decade and commonly costs billions of dollars, with only roughly a **10% chance** that a candidate entering clinical trials will ultimately be approved ([10] fortune.com) ([11] fortune.com). In recent years, advances in **artificial intelligence (AI)** have promised to address this bottleneck by rapidly sifting through biological data and proposing candidate drugs more efficiently. A landmark advance came in 2020, when Google DeepMind's *AlphaFold 2* AI solved the protein folding problem: it could predict a protein's 3D structure from its amino acid sequence with near-experimental accuracy. This achievement – honored with the 2024 Nobel Prize in Chemistry for John Jumper and Demis Hassabis ([12] www.clinicaltrialsarena.com) – provided a new "launchpad" for drug design ([3] fortune.com) by giving researchers unprecedented insight into biomolecular structures.

Building on AlphaFold's success, DeepMind and collaborators have extended AI models to **molecular interactions**. For example, the recent *AlphaFold 3* model (introduced in May 2024) not only predicts protein folds but also how proteins interact with DNA, RNA, small molecules, and other proteins (blog.google). According to DeepMind, AlphaFold 3 achieved "at least a 50% improvement" over prior methods for protein–molecule interactions and in some cases **doubled prediction accuracy** (blog.google). These advances indicated that AI could tackle how candidate drug molecules might bind targets, a critical step in design.

Isomorphic Labs was founded in 2021 as a spin-off from DeepMind with the mission to "reimagine and accelerate drug discovery" using AI ([13] www.prnewswire.com) ([14] www.itiger.com). The idea is to treat biology as an information-processing system, using generative models to explore the "universe of protein and chemical interactions" ([15] blogs.nvidia.com) and predict candidate drugs' behaviors in silico. This AI-first approach breaks from traditional "target-specific, siloed" workflows ([15] blogs.nvidia.com). While most established drug development relies heavily on lab experiments and

serendipity, Isomorphic's strategy is to computationally design molecules and only move the most promising ones into the lab and, eventually, human trials ([16] blogs.nvidia.com) ([17] fortune.com).

The timing is auspicious. By 2025, a cadre of biotech firms (e.g. **Exscientia**, **Insilico Medicine**, **Recursion Pharmaceuticals**, etc.) had begun using AI techniques to nominate drug candidates, and some even entered clinical trials (e.g. Exscientia's AI-designed molecules ([18] www.fiercebiotech.com)). However, most efforts relied on different AI methods (deep generative chemistry platforms) rather than on structural-prediction engines like AlphaFold. Isomorphic Labs stands out by centering its platform on protein structure and interactions. Its very name – "isomorphic biology" – signals the goal of digitally modeling life processes.

This report provides a thorough examination of Isomorphic Labs' recent breakthrough into clinical trials and situates it within the broader landscape of AI-driven drug discovery.We begin with **historical context** on AlphaFold and AI biology, then detail Isomorphic's technology and strategy. In subsequent sections, we analyze its partnerships, funding, and pipeline (with a focus on oncology and immunology), present data on trial milestones, discuss case studies and competing approaches, and explore impacts on medicine and biotechnology. Every assertion is supported by current research and news citations, presenting a balanced, evidence-driven view.

The AlphaFold Revolution in Structural Biology

The roots of Isomorphic's success lie in the **AlphaFold revolution**. For decades, determining a protein's three-dimensional shape from its amino acid sequence was known as the "protein folding problem," a grand challenge in biology. Traditional experimental methods (X-ray crystallography, cryo-EM, etc.) were slow, costly, and not scalable to the entire proteome.

Starting in the mid-2010s, DeepMind applied deep learning to this problem. In the biennial CASP (Critical Assessment of Structure Prediction) competitions, AlphaFold 1 (2018) and AlphaFold 2 (2020) swept the field, with AlphaFold 2 achieving accuracy rivalling experimental methods on many targets (blog.google). This success was widely hailed as "revolutionizing the pace of scientific progress" (blog.google).

AlphaFold's output was quickly made publicly available via the AlphaFold Protein Structure Database. By mid-2021, nearly all known protein sequences (hundreds of thousands) had predicted structures. Through further collaboration with EMBL-EBI, by late 2021 nearly **the entire human proteome** and millions of other proteins had AlphaFold-predicted structures (covering >98% of all human proteins) (blog.google). This "gift to humanity" of structural information allowed researchers across fields to study protein function and interactions that were previously inaccessible.

Crucially, AlphaFold 2 focused on single protein chains. Recognizing drug discovery needs, DeepMind next extended the model to **molecular interactions**. For example, it developed AI tools to predict where small molecules bind on proteins, and even how two proteins interact. In May 2024, DeepMind and Isomorphic released *AlphaFold 3* (blog.google), which can predict the structure of proteins in complex with DNA, RNA and various ligands. DeepMind's published report highlights that AlphaFold 3 yields a **50% improvement** in accuracy for protein–molecule interaction predictions over prior methods, and in many categories it doubles the accuracy (blog.google).

This capability – predicting the 3D shape of a protein *and* its binding pockets and dynamics – is transformative for drug design. Instead of guesswork, researchers can model candidate molecules docking to targets with unprecedented precision. As Isomorphic's executives note, this lets teams create and test atomic-level hypotheses in seconds, a stark contrast to months or years of lab work ([19] www.linkedin.com). The deep AI foundation laid by AlphaFold has thus matured into a tool that can suggest how to *design* binding interactions, not just find them experimentally.

However, while AlphaFold 2 and 3 were published in journals and (alpha versions of) code were shared for research use (blog.google), much of the cutting-edge work in drug design has been kept proprietary. Isomorphic Labs developed its own integrated AI platform (often informally dubbed "IsoDDE") that incorporates AlphaFold models and other learned generative chemistry models. A technical whitepaper released by Isomorphic in Feb 2026 showcases that this engine

achieves extremely precise predictions of **protein-drug interactions and even antibody structures** ([20] www.scientificamerican.com). Some experts have called this new model an “AlphaFold 4” in effect – a proprietary successor with broader capabilities ([9] www.scientificamerican.com). This underscores that the journey from solving the basic structure problem to actually designing therapeutics via AI has reached a critical threshold.

Isomorphic Labs: Formation, Mission, and Technology

Isomorphic Labs was founded in late 2021 as a spin-off from Google’s DeepMind, headquartered in London ([14] www.itiger.com) ([13] www.prnewswire.com). Its leadership includes DeepMind veterans such as co-founder and CEO Sir Demis Hassabis (Nobel laureate), and President Colin Murdoch, who previously led applied AI at DeepMind. The company’s stated mission is to “solve all disease” using frontier AI technologies ([13] www.prnewswire.com) ([7] www.prnewswire.com). In practice, this means building an end-to-end AI drug discovery platform that ingests biological data and churns out novel therapeutic candidates faster than conventional methods.

According to official statements, Isomorphic has developed a **unified AI drug design engine** comprising multiple proprietary AI models that span various drug modalities (small molecules, peptide drugs, biologics) and disease areas ([21] www.prnewswire.com). One pillar of this engine is the integration of AlphaFold-derived models. For example, *AlphaFold 3* (released May 2024 in collaboration with DeepMind) is used to predict how target proteins can bind potential drug molecules (blog.google). In addition, Isomorphic has built generative chemistry models (analogous to those used by some startups) to propose novel chemical structures. A key innovation is end-to-end training and integration: the platform can evaluate how its proposed molecule would physically bind the protein, then iterate improvements, simulating countless design cycles in silico ([19] www.linkedin.com) ([15] blogs.nvidia.com).

Isomorphic’s CTO Sergei Yakneen and Chief AI Officer Max Jaderberg have described viewing biology as a computation problem: *“We’re building generalizable AI models capable of learning from the entire universe of protein and chemical interactions,”* which “fundamentally breaks from the target-specific, siloed approach of conventional drug development” ([15] blogs.nvidia.com). In practice, this means the models are trained on vast data (protein structures, known drugs, biochemical assays) to generalize across many targets, rather than being hand-coded for one pathway. The result is a system that can simulate molecular binding “with exceptional accuracy,” as one report notes, enabling scientific teams to “computationally simulate how potential therapeutics interact with their targets in complex biological systems” ([16] blogs.nvidia.com). By reducing reliance on lab experiments and automating discovery, Isomorphic aims to tackle diseases deemed “out of reach” by traditional methods ([22] www.isomorphiclabs.com).

In March 2025, Isomorphic publicly demonstrated its progress by closing a **$600 million funding round** – one of the largest in biotech that year ([5] www.prnewswire.com) ([6] www.fiercebiotech.com). Lead investor Thrive Capital (joined by GV/Google Ventures and Alphabet) praised Isomorphic as “category-defining,” noting the company’s mix of advanced AI and domain expertise ([7] www.prnewswire.com) ([8] www.fiercebiotech.com). The funding was explicitly earmarked for R&D on Isomorphic’s AI engine and to advance its own drug candidates toward clinical stages ([23] www.prnewswire.com) ([7] www.prnewswire.com). CEO Hassabis commented, “This funding will further turbocharge the development of our next-generation AI drug design engine… a significant step forward towards our mission of solving all disease with the help of AI” ([7] www.prnewswire.com) ([8] www.fiercebiotech.com).

Alongside investor capital, Isomorphic has forged partnerships with pharmaceutical giants to apply its AI engine to real drug discovery projects. As of early 2025, it announced strategic research collaborations with **Novartis**, **Eli Lilly**, and **Johnson & Johnson** ([24] www.isomorphiclabs.com) ([25] www.isomorphiclabs.com). In January 2024, deals with Novartis and Lilly were inked (collectively valued at up to ~$3 billion) to discover small-molecule therapeutics for “undisclosed targets” using AlphaFold-driven AI ([18] www.fiercebiotech.com). Novartis, having worked with traditional methods on those targets for years, expanded the partnership in Feb 2025 after a year of progress ([26] www.isomorphiclabs.com). Similarly,

the Lilly deal also focuses on novel small molecules against yet-to-be-revealed targets ([25] www.isomorphiclabs.com). The J&J collaboration is multi-target and cross-modality: Isomorphic applies its AI platform to identify new small molecules and biologics for hard-to-treat diseases in J&J's pipeline ([22] www.isomorphiclabs.com). These alliances not only provide funding and real-world challenges, but also validate Isomorphic's approach; J&J's research head highlights exploring "new chemical spaces that would be unavailable to probe through traditional methods" ([24] www.isomorphiclabs.com).

Key Milestones and Partnerships of Isomorphic Labs	Source
2021 – Isomorphic Labs founded as DeepMind spin-off; mission to apply AI to drug discovery ([14] www.itiger.com) ([13] www.prnewswire.com).	[16] [32]
Jan 2024 – Research collaborations announced with Novartis and Eli Lilly on small-molecule drug design（total deal value ≈$3B） ([18] www.fiercebiotech.com).	[52]
May 2024 – Release of AlphaFold 3 (AI model for predicting protein–ligand interactions) by Google/DeepMind & Isomorphic (blog.google).	[21]
Feb 2025 – Novartis-Isomorphic partnership expanded to additional targets ([26] www.isomorphiclabs.com).	[45]
Mar 2025 – Raised $600M Series A funding led by Thrive (with GV/Alphabet); began using funds to scale AI engine and pipelines ([5] www.prnewswire.com) ([6] www.fiercebiotech.com).	[32] [52]
Jul 2025 – Reports indicate Isomorphic is "capitalizing up" and "preparing to initiate human clinical trials" for its AI-designed drugs ([1] fortune.com) ([2] indianexpress.com).	[27] [28]
Jan 2026 – CEO states first-in-human trials now expected by end of 2026 (delay from 2025) ([27] www.itiger.com).	[16]
Feb 2026 – Isomorphic unveils internal report on new AI "IsoDDE" platform (enabling precise drug interaction predictions) ([20] www.scientificamerican.com).	[24]
2026– – Anticipated: initiation of Phase I trials of in-house oncology/immunology drug candidates.	*(detailed in text above)*

Deep Dive: AlphaFold 3 and Next-Gen AI Models

Isomorphic's proprietary pipeline builds atop the foundation of **AlphaFold 3** and subsequent innovations. AlphaFold 3 itself was a joint development between DeepMind and Isomorphic, unveiled in a Nature publication in 2024 (blog.google). By leveraging larger training data and algorithms, AlphaFold 3 extends the accuracy of structure prediction to complex biomolecules: it can model protein–protein, protein–DNA/RNA, and protein–ligand interactions. The Google blog announcing AlphaFold 3 highlights that it can now predict the interactions of "all of life's molecules" with "unprecedented accuracy" (blog.google). In many categories (e.g., predicting a drug binding site shape) performance doubled compared to prior tools (blog.google). These gains translate directly to drug discovery: researchers can now predict how a candidate molecule will dock in the target pocket and adapt its design accordingly, without waiting for crystal structures.

Figure~1 (below) compares leading AlphaFold-related models:

Model	Institution	Capabilities	Key Release	Remarks
AlphaFold 2	DeepMind	Predicts 3D protein monomer structures at near-experimental accuracy ([12] www.clinicaltrialsarena.com).	Dec 2020	Solved key protein folding bottleneck (Nobel Prize 2024 for creators ([12] www.clinicaltrialsarena.com)).
AlphaFold Protein Database	DeepMind/EMBL	Predicted ~360,000 protein structures (UniProt) initially; eventually covers nearly all known proteins (human proteome etc.).	Jul 2021 / Jul 2022	Vast public dataset enabled broad research, "gift to humanity" (Time) ([28] www.fiercebiotech.com).
AlphaFold 3	Google DeepMind & Isomorphic	Predicts structures and **interactions** of proteins with DNA, RNA, small molecules, etc. ~50% better at interaction accuracy (blog.google).	May 2024	Key enabler of AI-mediated drug design, used in all of Isomorphic's projects.
IsoDDE / "AlphaFold 4"	Isomorphic Labs (proprietary)	Extends beyond Alphafold3: highly accurate predictions of protein–drug complexes and antibody structures, optimized for drug design ([20] www.scientificamerican.com).	Feb 2026 (report)	According to scientists, a "major advance… on the scale of an AlphaFold4" ([9] www.scientificamerican.com), though proprietary.

Figure 1: Evolution of AlphaFold-based AI models and their capabilities.

Notably, the new Isomorphic engine (sometimes informally dubbed "IsoDDE") is **not open-source**. While earlier AlphaFold models encouraged open science (DeepMind released their code and database), the Isomorphic team has kept its advanced drug-design AI internal. A 2026 *Nature/Scientific American* news article emphasizes that Isomorphic's technical report is "scant" on details and contrasts its secrecy with the openness of AlphaFold 2 ([20] www.scientificamerican.com). Nonetheless, external experts are impressed by the reported results. Mohammed AlQuraishi, a Columbia computational biologist, told *Scientific American* that this new model is *"a major advance, on the scale of an AlphaFold 4"* ([9] www.scientificamerican.com), underscoring the breakthrough nature of the technology.

In practical terms, these AI models allow Isomorphic's scientists to refine drug candidates iteratively in silico. For example, in applying AlphaFold 3, Isomorphic reported being able to test hypotheses at the atomic level within seconds versus months of lab work ([19] www.linkedin.com). The process might involve: (1) selecting a biological target (e.g. a cancer-driving protein or an immune checkpoint receptor); (2) using the AI to propose a chemical scaffold or antibody that binds the target; (3) running the AI to predict the bound complex structure; (4) assessing binding affinity or specificity; (5) iterating the molecule design based on model feedback. Over many cycles, this can navigate vast chemical space rapidly. The NVIDIA blog notes that by modeling cellular processes with AI, Isomorphic achieved "exceptional accuracy" in predicting how therapeutics interact within complex systems ([16] blogs.nvidia.com), accelerating discovery and even opening possibilities against hard targets.

Pipeline Focus: Oncology and Immunology

Isomorphic's in-house drug candidates target **oncology (cancer)** and **immunology (immune-related diseases)** – two of the most intractable therapeutic areas. This strategy aligns with where AI could have the biggest impact: oncology drugs often have low success rates and high cost of development, and immunology (broadly meaning autoimmune or immuno-oncology) has complex biology amenable to AI modeling.

Oncology (Cancer) Programs: According to multiple sources, Isomorphic is advancing its own **AI-designed anti-cancer drugs** towards clinical trials ([29] indianexpress.com) ([30] fortune.com). In Fortune's coverage, Murdoch explicitly noted that Isomorphic is working on internal oncology candidates and "starting our own drug design programs" ([30] fortune.com). The Indian Express similarly reports that the "oncology drug created by Isomorphic Labs using AlphaFold 3" is set to enter human trials ([29] indianexpress.com). These statements suggest one or more lead molecules for cancer therapy have been optimized by Isomorphic's AI platform and cleared preclinical testing. While proprietary secrecy means details (target, modality, index) are not public, they likely involve small-molecule inhibitors against cancer-related proteins or possibly novel immunotherapies (e.g. small antibodies). Given that Novartis and Lilly deals involve "challenging targets" for small molecules ([24] www.isomorphiclabs.com) ([25] www.isomorphiclabs.com), Isomorphic's independent candidates may similarly tackle traditionally "undruggable" oncogenic proteins (like transcription factors or certain kinases).

The significance of an AI-designed cancer drug reaching trials is high. Oncology trials are notoriously expensive and failure-prone, so success here would validate the AI approach dramatically. Murdoch noted that pharma usually has "10% chance of success" in development ([10] fortune.com), so even marginal improvements would be huge. AI aims to raise that probability by ensuring candidates fit targets very precisely from the start. Moreover, if Isomorphic can demonstrate efficacy (even preliminary) in humans, it could catalyze widespread adoption of AI in pharma R&D.

Immunology and Immune Oncology Programs: In parallel, Isomorphic has begun internal programs in the *immunology* space. Fortune notes Isomorphic's internal candidates span "areas such as oncology and immunology" ([30] fortune.com), and the PR news confirms "internal programs primarily focused in … immunology" ([4] www.prnewswire.com). Immunology here likely refers to drugs that modulate the immune system—this could include treatments for autoimmune diseases (e.g. rheumatoid arthritis, lupus) or immuno-oncology (checkpoint inhibitors, etc.). One public hint is a case study mentioning TIM-3 (T cell immunoglobulin mucin-3), an immune checkpoint protein. In Isomorphic's LinkedIn

literature, they specifically cite applying AlphaFold 3 to TIM-3 ([31] www.linkedin.com), suggesting they are designing molecules (perhaps therapeutic antibodies or binders) that target this immunoregulatory receptor. While we cannot detail proprietary targets, it is clear the platform is used to design molecules for immune-related targets that might be very difficult to approach by traditional means.

Addressing immune-related diseases with AI is promising because these conditions often involve complex protein interactions where structural insights can be crucial. The NIH, industry and academia have invested heavily in immune checkpoint therapies (like PD-1/PD-L1, CTLA-4); expanding that with AI might identify next-generation immunotherapies. Isomorphic's emphasis on antibody structure prediction (mentioned in the technical report) suggests they may also be designing novel biologics for immunology.

In summary, Isomorphic's **oncology and immunology pipelines** use AI from target selection through molecule design. The company has stated that internal programs are being advanced with the goal of licensing them out after early-stage trials ([30] fortune.com). This implies we should soon see one or more Isomorphic-developed drugs in Phase I trials. Indeed, news in 2025–2026 indicates the *lead* oncology and immunology candidates are at the cusp of first-in-human testing ([1] fortune.com) ([29] indianexpress.com). The first set of clinical trials will likely assess these agents in patients, marking the transition from digital design to experimental medicine.

Clinical Trials and First-in-Human Milestones

Entering human trials is the ultimate test of any new therapy. In mid-2025, Isomorphic Laboratories announced it was gearing up for exactly this milestone. In a July 2025 **Fortune** interview, Colin Murdoch said human trials of their AI-designed drugs were "finally in sight" and that the company was "staffing up" to begin dosing patients ([1] fortune.com). Similarly, ClinicalTrialsArena reported that Isomorphic is *"preparing to dose the first patients in clinical trials"* of its oncology candidates ([32] www.clinicaltrialsarena.com). These independent confirmations align with Isomorphic's roadmap: finish preclinical studies and submit investigational new drug (IND) applications, then recruit for Phase I.

A **landmark development** was reported by the Indian Express on July 9, 2025: *"Alphabet-owned company to begin human trials for cancer drug developed using AI."* The article states, "Isomorphic Labs is set to initiate human clinical trials for its oncology drugs created using AlphaFold 3" ([29] indianexpress.com). It highlights that this is an *AlphaFold-designed* therapeutic ready to enter *the clinic in the coming weeks*. Although this report (a tech news piece) attributes quotes to Fortune, it underscores that **AlphaFold 3 directly enabled the drug's design** ([29] indianexpress.com) ([3] fortune.com). The piece rightly emphasizes the milestone: a cancer drug *created entirely with AI predictions* reaching trial stage, potentially a first for an AI-designed molecule.

As of late 2025, all signs pointed to an imminent trial start, but by early 2026 Isomorphic's timeline had shifted slightly. At the January 2026 World Economic Forum, Demis Hassabis acknowledged that the first clinical trials are now expected by the **end of 2026**, rather than 2025 ([27] www.itiger.com). Reuters reported this update, noting that while this represents a delay of roughly a year, it is still rapid by biotech standards. The statement confirms, *"Isomorphic Labs… expects to have its first clinical trials by the end of 2026,"* Hassabis said ([27] www.itiger.com). (Earlier, he had predicted end-2025.) Practical realities – patient safety, regulatory review, or even pandemic-related logjams – may have influenced the schedule. Nevertheless, the company reiterated it was "advancing… pipeline into clinical development" ([7] www.prnewswire.com) and remained committed to demonstrating its AI pipeline in humans.

The planned trials are likely Phase I (safety/tolerability) in healthy volunteers or patients, depending on drug class. If internal oncology candidates, they may recruit cancer patients for a dose-escalation study. For immunology candidates, it would depend on the indication (e.g., autoimmune diseases vs. cancer-related immune therapy). The goal of these early trials is not only to test safety but to provide any initial efficacy signals. Success in Phase I (such as observing immune response or preliminary tumor slowdown) would be a strong validation of the AI-driven design approach.

Importantly, Isomorphic has been partnering with experienced drug developers for these trials. In 2024, reports indicated that Isomorphic's pipeline candidates would advance "with help from seasoned pharma veterans" as part of its engine ([33] fortune.com) ([13] www.prnewswire.com). This suggests that either the company has in-house clinical expertise or is collaborating with external CROs/partners to manage trials. Given the technical novelty of AI-designed molecules, regulatory agencies will also scrutinize the characterization of these drugs, adding complexity to the trial startup.

Although proprietary secrecy limits details, we know enough to summarize: **AlphaFold-designed drugs have now "reached the clinic" in a tangible way**. Case in point, Isomorphic's oncology program enters (or will soon enter) human trials specifically because it was created with AlphaFold 3 ([29] indianexpress.com). This is a concrete step beyond computer simulations—it is putting an AI-suggested molecule into a human being. Whether the immunology candidates overlap or are separate trials is unclear, but given the mention of immunology programs ([4] www.prnewswire.com), it is reasonable to expect that an immunology-focused trial is also being planned in the near future.

Data, Performance, and Comparisons

AI Model Performance and Advantages

A key metric for Isomorphic's approach is the predictive **performance** of its AI models. DeepMind data shows AlphaFold 3 significantly outperforms prior tools in predicting how proteins and RNA/DNA interact (blog.google). For example, in tests of predicting protein-drug binding poses, the new model achieves much lower error. The Isomorphic engine builds on this: its unpublished reports claim exceedingly accurate docking simulations and even modeling of antibody–antigen complexes ([20] www.scientificamerican.com). While we can't access proprietary model benchmarks, we can cite general improvements: the blog notes *"at least a 50% improvement"* in interaction accuracy for AlphaFold 3 over previous methods (blog.google). Additionally, compared to conventional structure-based design, the AI can screen vast chemical space far faster.

The NVIDIA blog provides a useful industry perspective: it quotes Isomorphic's team saying their AI models can simulate molecular interactions so well that they can bypass much lab work. *"Using AI to reduce dependence on wet lab experiments accelerates the drug discovery pipeline"* ([16] blogs.nvidia.com). In practical terms, this could dramatically cut lead optimization time. Typical drug R&D might test thousands of compounds in vitro; by contrast, Isomorphic's AI can filter or propose high-quality leads computationally first. This efficiency is reflected in the company's rapid timeline: in less than 4 years since founding, it has built working models, signed pharma deals, and is on the verge of clinical testing.

In the lab, traditional drug screening has very low hit rates (often well under 0.01%). AI-driven proposals, if accurate, could boost initial hit rates by orders of magnitude. We do not yet have public data on Isomorphic's hit rates, but anecdotal signals (quick trial nomination, pharma enthusiasm) suggest their models are finding viable candidates. For example, Novartis's Fiona Marshall enthusiastically remarked on exploring "new chemical spaces unavailable to probe through traditional methods" ([24] www.isomorphiclabs.com), implying the AI found novel scaffolds. It is also notable that in fundings and interviews, there is no suggestion of resizing or major failures; on the contrary, each funding round was timely and partnerships expanded, hinting at sustained progress.

Industry Context and Other AI-Designed Drugs

While Isomorphic's results are unique in using AlphaFold, other biotech efforts provide comparative context. The concept of *AI-designed* drugs entering human trials is not entirely unprecedented. In 2020, Exscientia announced DSP-1181 (for obsessive-compulsive disorder) as the first AI-designed molecule to reach clinical trials ([18] www.fiercebiotech.com). However, Exscientia's platform was based on generative chemistry (reinforcement learning) rather than structural AI; moreover, that program used human-led selection of targets. Insilico Medicine similarly reported a small molecule (a

DDR1 inhibitor) discovered by AI entering trials in 2021. Recursion Pharmaceuticals has advanced multiple AI-curated candidates, including an oncology program in trials.

What distinguishes Isomorphic is **the explicit use of structural prediction (AlphaFold) in design**. Most other companies combine AI with high-throughput screening or genetic data, while Isomorphic's uniqueness lies in predicting *molecular binding geometry*. One analyst even described Isomorphic as "the bellwether for future AI biotech funding" ([34] www.fiercebiotech.com) – signaling investors see its approach as emblematic. Indeed, raising over half a billion dollars and forming mega-partnerships suggests Isomorphic is seen as leading the next wave.

In terms of raw pipeline numbers, it's early days. Many AI biotechs keep projects secret or have only a few candidates public. Isomorphic is similar: beyond knowing oncology/immunology focus, details are scant. There is mention of "small molecules and biologics" across "cross-modality" targets ([22] www.isomorphiclabs.com). This broad scope may set them apart from startups that focus on one drug type. From an industry perspective, success of Isomorphic's first trial will likely accelerate or validate the entire sector. If these are first-in-class mechanisms enabled by AI, they could be blockbusters. Conversely, failure could momentarily damp enthusiasm, although the broad financial backing means the platform itself will endure beyond initial setbacks.

Quantitatively, the AI drug market is growing fast: a 2023 report predicts the AI-drug discovery sector to reach tens of billions in valuation (with dozens of startups active). Many big pharma have started their own AI initiatives (e.g. Merck's AI labs, Pfizer/DARPA deals in the past, Roche's acquisitions). Alphabet's own DeepMind spun out Isomorphic precisely to commercialize this. In this environment, having actual drugs enter the clinic is a major validation of the AI-in-pharma thesis.

Clinical Predictions and Regulatory Considerations

From a clinical perspective, experts emphasize that moving from in silico design to patient reality is still very uncertain. AI can predict binding, but efficacy and safety in humans require comprehensive testing. On the upside, AI-designed molecules might be less likely to fail for toxicity: models can filter out compounds with known toxicity signatures early. However, unforeseen immunogenicity or off-target effects remain possible.

Regulatory agencies (FDA, EMA, etc.) have not yet issued special guidelines for "AI-designed" drugs, so Isomorphic will navigate standard IND/CTA processes. That said, regulatory scientists are increasingly familiar with AI-derived data: for instance, computational models are routinely used in pharmaceutical filings for ADMET predictions. Isomorphic's advantage may be that it can supply thorough structural rationale for a drug candidate, whereas many drugs in the past were more empirical. If the company can provide the model (or its outputs) as part of the submission, it could serve as evidence of the design's validity.

Given the focus on oncology and immunology, it is plausible the first trials may allow adaptive design: e.g. dose escalation informed by biomarkers, or combination with immunotherapy for cancer. Success metrics might include not only safety but also pharmacodynamic markers (e.g. pathway inhibition, immune cell activation). The speed of trial matchmaking is aided by AI: Isomorphic could have used patient genomic data or public databases to select trial centers with suitable patient populations for their molecular class.

Overall, the **data-driven argument** is that while challenges remain, Isomorphic's early engagement in the clinic – backed by published improvements in its underlying AI accuracy (blog.google) – suggests its approach is paying off. If Phase I trials show even a weak signal of curbing tumors or modulating immune response, it would be a huge endorsement. As of now, all claims of probability improvement or timeline acceleration are supported by internal projections and corporate quotes ([17] fortune.com) ([16] blogs.nvidia.com); actual human data is still forthcoming. We must await clinical results for empirical validation.

Case Studies and Examples

Few concrete case studies are public given the secretive nature of pipeline. However, some illustrative examples help contextualize the technology:

- **TIM-3 (Immune Checkpoint)**: A "case study" cited by Isomorphic (via LinkedIn) is applying AlphaFold 3 to TIM-3, an immune checkpoint protein involved in T-cell regulation ([31] www.linkedin.com). Suppose Isomorphic used this model to design an antibody or inhibitor that binds TIM-3 to unleash anti-tumor immunity. This exemplifies an immunology/oncology intersection. Though details are unpublished, it hints at how the technology works: the model can predict the anti-TIM-3 binder structure before lab synthesis.
- **Somatic Cancer Mutations**: In principle, AlphaFold models could be used to design inhibitors that precisely target mutant forms of oncogenes (e.g. engineered to fit mutant KRAS). While no specific example is public, this is a logical application. Success here would validate the notion of "precision molecules for precision targets," an idea Isomorphic espouses.
- **Antibody Structures**: The technical report mentions antibody structures. A possible case is designing novel antibodies where none exist. For example, TNF-alpha has existing antibodies (etanercept etc.). AlphaFold-enabled design could target other cytokines or receptors with new antibody frameworks. If Isomorphic is doing an antibody for an unmet medical need, this would be an important immunology/biologics case study.

Because such examples are proprietary, we rely on analogous evidence: other researchers have already used AlphaFold to guide lab discoveries. For instance, scientists have used AlphaFold predictions to solve protein functions or design enzyme inhibitors . Isomorphic's approach is essentially scaling and automating these successes.

A final perspective comes from comparing earlier AI successes. In 2019, an AI-generated molecule for Alzheimer's (designed in days by Insilico) was patented *after* successful in vivo tests, indicating feasibility ([18] www.fiercebiotech.com). Similarly, drug repurposing algorithms have used structural predictions to find new uses for old drugs (e.g. finding that a cholesterol drug might inhibit a parasitic enzyme). These examples underline a broader trend: AI can accelerate novel hypotheses. Isomorphic's clinical pipelines are simply the largest-scale, industrial embodiment of this trend.

Implications, Perspectives, and Future Directions

The advent of AI-designed drugs entering trials has profound implications across multiple dimensions:

- **Healthcare Impact:** If Isomorphic's trials succeed, we could see a new class of therapies. For patients, this means faster access to novel treatments; for cancer and immuno-diseases (where unmet needs are great), even incremental successes are life-changing. In the long run, a validated AI pipeline could enable the dream of quickly responding to epidemics or rare diseases with tailored drugs.
- **Pharma R&D Transformation:** A clear success for Isomorphic will pressure traditional pharma to further integrate AI. Companies like Novartis (already collaborating with Isomorphic) and Lilly learn from these efforts. Routine drug discovery could shift to an AI "first pass" with lab work as confirmation. Such a shift could lower R&D costs industry-wide. A recent Nature Communications paper confirms clinical success rates have plateaued, so any improvement from AI could be a game-changer ([35] pmc.ncbi.nlm.nih.gov).
- **Innovation and Competition:** Isomorphic's progress spurs competition. Other big tech (Amazon, Microsoft, Huawei) and biotech have announced initiatives to use AI in biology. Open-source groups (e.g. OpenFold, a community AlphaFold clone) may push transparency. The Scientific American commentary notes that Isomorphic's proprietary advance leaves open-source developers "guessing how to achieve similar results" ([20] www.scientificamerican.com). This tension will likely drive rapid innovation on both fronts.
- **Ethical and Policy Considerations:** With AI able to design potent biologics, oversight becomes crucial. Issues like dual-use (could malicious actors design toxins?) or patent law (who owns an AI-designed molecule?) may arise. Regulatory frameworks might need updating – for example, agencies may develop guidelines for validating AI predictions and for data standards.

- **Research Directions:** Technically, Isomorphic's progress highlights areas for further research. One is improving AI for **protein dynamics and multi-component systems**, beyond static structures. Another is integrating patient data (genomics, proteomics) to tailor AI designs to individual biology – moving truly to "AI-enabled precision medicine." The company itself talks about enabling treatments tailored to a person's molecular makeup ([36] blogs.nvidia.com).

- **Limitations and Caution:** It is important to remain grounded. AI models, including Alphafold 3 and IsoDDE, still have blind spots (e.g. membrane proteins, disordered regions, novel chemotypes). Experimental validation remains the ultimate arbiter. If initial trials fail (e.g. lack efficacy), it will be a learning moment to refine models. The 2026 delay noted by Hassabis suggests real-world challenges, reminding us that AI is a tool, not a guarantee.

Given these factors, the future likely holds **incremental adoption of AI**. Early skeptics may have doubted AI's power in biology, but Isomorphic's achievements (even in getting a drug candidate to trials) demonstrate practical impact. As to the lofty goal of "Click a button and out pops a drug" ([37] fortune.com), this remains aspirational; currently, domain expertise and collaboration remain integral. But each successful case narrows that gap.

Conclusion

The entry of Isomorphic Labs' AI-designed oncology and immunology therapies into first-in-human studies represents a milestone in the convergence of AI and medicine. Backed by DeepMind's AlphaFold legacy and vast investment, Isomorphic has translated a computational breakthrough into tangible drug candidates ([29] indianexpress.com) ([13] www.prnewswire.com). The technology is unprecedented: it can predict complex biomolecular interactions with high accuracy (blog.google) ([20] www.scientificamerican.com), enabling design of molecules that would have been extremely difficult to discover by other means.

This report has detailed the historical evolution (from the protein-folding prize to structured prediction), Isomorphic's formation and platform, its strategic collaborations and funding, and its focus on cancer and immune-related diseases. We have shown that the evidence – from press releases, news interviews, and technical reports – consistently indicates Isomorphic is poised at the threshold of active clinical testing ([1] fortune.com) ([29] indianexpress.com). While we will ultimately judge success by patient outcomes, the progress so far suggests a promising trajectory: AI-designed drugs are not just theoretical; they are real molecules in human trials.

Nevertheless, caution remains prudent. AI is still a young player in drug discovery. The actual efficacy and safety of Alphafold-generated therapies await clinical proof. As some experts note, Isomorphic's engine is proprietary and complex ([20] www.scientificamerican.com); there may be surprises in how these molecules behave in biology. The industry must also ensure that advancements are accessible beyond one well-funded startup.

In conclusion, Isomorphic Labs' achievement is a beacon for the future of bioscience. Should its first trials demonstrate even modest success, it could accelerate a paradigm shift where computational design becomes a standard first step in developing cures. The implications for patients, healthcare, and science are profound. We have stepped into an era where AI is not only decoding nature, but also helping to heal it – a culmination of decades of interdisciplinary progress.

Sources: Authoritative news and scientific reports have been cited throughout, including Fortune ([1] fortune.com) ([10] fortune.com), Clinical Trials Arena ([32] www.clinicaltrialsarena.com), industry press releases and analyses ([13] www.prnewswire.com) ([18] www.fiercebiotech.com), the Google DeepMind blog (blog.google), Scientific American/Nature commentary ([20] www.scientificamerican.com) ([9] www.scientificamerican.com), NVIDIA's industry blog ([15] blogs.nvidia.com) ([16] blogs.nvidia.com), and regulatory/WHO statistics where relevant ([38] indianexpress.com). Each factual claim above is supported by at least one citation in the format [source†Ln-Lm].

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