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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 – worked toward its first *first-in-human* clinical trials for drug candidates **designed using AlphaFold-based AI**, DeepMind's breakthrough AI for protein structure. In a July 2025 Fortune interview, President Colin Murdoch said the company was "staffing up" and "getting very close" to clinical trials of its AI-designed candidates; the company's stated target is now the end of 2026, and no first-in-human dosing had been publicly announced when this article was last checked in November 2026 (fortune.com) (indianexpress.com). These candidates, created using the *AlphaFold 3* system and other proprietary models, are intended to become among the first therapies engineered with deep-learning protein models to enter the clinic.

Isomorphic's pipeline focuses on **oncology and immunology**, leveraging machine learning to accelerate drug design by predicting complex molecular interactions (fortune.com) (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 (www.prnewswire.com) (www.fiercebiotech.com) and a $2.1B Series B in May 2026 (www.isomorphiclabs.com)) to develop its AI "drug design engine." Its CEO, Demis Hassabis, frames the mission as solving "all disease with the help of AI" (www.prnewswire.com) (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" (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 (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, shared by John Jumper and Demis Hassabis with David Baker (nobelprize.org) (www.clinicaltrialsarena.com) – provided a new "launchpad" for drug design (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 (www.prnewswire.com) (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" (blogs.nvidia.com) and predict candidate drugs' behaviors in silico. This AI-first approach breaks from traditional "target-specific, siloed" workflows (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 (blogs.nvidia.com) (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 (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 progress toward 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.

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 (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), Isomorphic Labs applies proprietary models to drug design. 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 (www.scientificamerican.com). Some experts have called this new model an "AlphaFold 4" in effect – a proprietary successor with broader capabilities (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 (www.itiger.com) (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 (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 (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 (www.linkedin.com) (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" (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" (blogs.nvidia.com). By reducing reliance on lab experiments and automating discovery, Isomorphic aims to tackle diseases deemed "out of reach" by traditional methods (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 (www.prnewswire.com) (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 (www.prnewswire.com) (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 (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” (www.prnewswire.com) (www.fiercebiotech.com).

Alongside investor capital, Isomorphic has forged partnerships with pharmaceutical giants to apply its AI engine to real drug discovery projects. It has announced strategic research collaborations with **Novartis** and **Eli Lilly** (both in January 2024) and, in January 2026, **Johnson & Johnson** (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 (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 (www.isomorphiclabs.com). Similarly, the Lilly deal also focuses on novel small molecules against yet-to-be-revealed targets (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 (www.isomorphiclabs.com). These alliances not only provide funding and real-world challenges, but also validate Isomorphic’s approach; Novartis’s Fiona Marshall, President of Biomedical Research, says the collaboration has seen “the exploration of new chemical spaces that would be unavailable to probe through traditional methods” (www.isomorphiclabs.com).

Key Milestones and Partnerships of Isomorphic Labs
2021 – Isomorphic Labs founded as DeepMind spin-off; mission to apply AI to drug discovery (www.itiger.com) (www.prnewswire.com).
Jan 2024 – Research collaborations announced with Novartis and Eli Lilly on small-molecule drug design（total deal value ≈$3B） (www.fiercebiotech.com).
May 2024 – Release of AlphaFold 3 (AI model for predicting protein–ligand interactions) by Google/DeepMind & Isomorphic (blog.google).
Feb 2025 – Novartis-Isomorphic partnership expanded to additional targets (www.isomorphiclabs.com).
Mar 2025 – Raised $600M Series A funding led by Thrive (with GV/Alphabet); began using funds to scale AI engine and pipelines (www.prnewswire.com) (www.fiercebiotech.com).
Jul 2025 – Reports indicate Isomorphic is “staffing up” and “preparing to initiate human clinical trials” for its AI-designed drugs (fortune.com) (indianexpress.com).
Jan 2026 – Johnson & Johnson and Isomorphic announce a cross-modality, multi-target research collaboration (www.isomorphiclabs.com).
Jan 2026 – Hassabis says at Davos that first clinical trials are expected by the end of 2026; he had previously said AI-designed drugs would be in trials by the end of 2025 (investing.com).
Feb 2026 – Isomorphic unveils internal report on new AI “IsoDDE” platform (enabling precise drug interaction predictions) (www.scientificamerican.com).
May 2026 – Isomorphic announces a $2.1B Series B round led by Thrive Capital, with Alphabet and GV participating (www.isomorphiclabs.com).
2026– – Anticipated: initiation of Phase I trials of in-house oncology/immunology drug candidates.

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 (www.clinicaltrialsarena.com).	Dec 2020	Solved key protein folding bottleneck (Nobel Prize 2024 for creators (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) (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.
IsoDDE / "AlphaFold 4"	Isomorphic Labs (proprietary)	Extends beyond Alphafold3: highly accurate predictions of protein–drug complexes and antibody structures, optimized for drug design (www.scientificamerican.com).	Feb 2026 (report)	According to scientists, a "major advance… on the scale of an AlphaFold4" (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 **proprietary**. DeepMind released code and a database for earlier AlphaFold models. A 2026 *Scientific American* news article discusses Isomorphic's technical report in comparison with AlphaFold 2 (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"* (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 (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 (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 Fortune, Isomorphic designs its own internal drug candidates, including in oncology, and is moving them towards clinical trials (fortune.com). In Fortune's coverage, Murdoch explicitly noted that Isomorphic is working on internal oncology candidates and "starting our own drug design programs" (fortune.com). Isomorphic has not disclosed the target, modality, or identity of these candidates, whether an investigational new drug (IND) application or equivalent has been filed, or what its first indication will be. The Novartis and Lilly deals involve "challenging targets" for small molecules (www.isomorphiclabs.com); the targets of Isomorphic's own candidates have not been disclosed.

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 (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" (fortune.com), and the PR news confirms "internal programs primarily focused in ... immunology" (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 (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 (fortune.com). This implies we should soon see one or more Isomorphic-developed drugs in Phase I trials. Indeed, in July 2025 Fortune and the Indian Express reported that Isomorphic was preparing for first-in-human testing (fortune.com) (indianexpress.com). The company has since said its first clinical trials are expected by the end of 2026, and it has not disclosed an IND filing or a first indication. Whenever the first trials begin, they 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 Labs said it was gearing up for exactly this milestone. In a July 2025 **Fortune** interview, Colin Murdoch said, "We're staffing up now. We're getting very close." (fortune.com). Similarly, ClinicalTrialsArena reported that Isomorphic is *"preparing to dose the first patients in clinical trials"* of its oncology candidates (www.clinicaltrialsarena.com). These reports are consistent with Isomorphic's stated aim of starting clinical trials; the company has not publicly disclosed an investigational new drug (IND) filing or the first indication it will pursue.

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" (indianexpress.com). It described the drugs as set to enter the clinic in the coming weeks, a July 2025 expectation that was later overtaken by the delay of Isomorphic's first clinical trials to the end of 2026. Although this report (a tech news piece) attributes quotes to Fortune, it says the drugs were created using AlphaFold 3 (indianexpress.com) (fortune.com). The piece frames this as a potential milestone for AI-designed molecules, but no human dosing had been announced as of this article's last check.

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 (investing.com). Reuters reported on 20 January 2026 that Hassabis said, at an event at the World Economic Forum in Davos, that Isomorphic expects to have its first clinical trials by the end of 2026 (investing.com).. (Earlier, he had predicted end-2025.) Reuters gave no reason for the shift, and this article has found no public announcement of a first dosing as of November 2026.

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.

Fortune's July 2025 report describes Isomorphic's planned drug design engine as "a system that combines machine learning researchers with pharma veterans to design new medicines faster" (fortune.com). Isomorphic has not publicly disclosed who will run its first clinical trials, whether in-house clinical teams or external partners. Given the technical novelty of AI-designed molecules, regulatory agencies will also scrutinize the characterization of these drugs, adding complexity to the trial startup.

Based on public reporting, we can summarize: **Isomorphic's candidates have not yet been publicly reported to be in human trials**; the company's stated target for its first clinical trials is the end of 2026. Reaching that stage would be a concrete step beyond computer simulations. Whether the immunology candidates overlap or are separate trials is unclear; Isomorphic has described immunology programs (www.prnewswire.com), but it has not disclosed a first indication or a trial timetable for them.

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 (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"* (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 says it expects to begin clinical trials by the end of 2026.

In the lab, traditional drug screening has very low hit rates. 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" (www.isomorphiclabs.com), implying the AI found novel scaffolds.

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 (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.

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" (www.fiercebiotech.com) – signaling investors see its approach as emblematic. Indeed, raising a $2.1B Series B in May 2026 and forming mega-partnerships suggests Isomorphic is seen as leading the next wave.

In terms of raw pipeline numbers, it's early days. Public information about Isomorphic's pipeline identifies an oncology and immunology focus without candidate-level details. There is mention of "small molecules and biologics" across "cross-modality" targets (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.

Alphabet's own DeepMind spun out Isomorphic precisely to commercialize this. In this environment, if its drugs do enter the clinic, that would be 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.

FDA states that it recognizes the increased use of AI throughout the drug product life cycle and across a range of therapeutic areas (fda.gov). 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.

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).

Overall, the **data-driven argument** is that while challenges remain, Isomorphic's progress toward the clinic – backed by published improvements in its underlying AI accuracy (blog.google) – suggests its approach is promising, though it remains unproven in humans. 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 (fortune.com) (blogs.nvidia.com); actual human data is still forthcoming. We must await clinical results for empirical validation.

Case Studies and Examples

Few concrete pipeline case studies are publicly available. 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 (www.linkedin.com). The following is a hypothetical illustration only, not an Isomorphic disclosure: a team could use an AlphaFold 3-type model to design an antibody or inhibitor that binds TIM-3 and predict the binder structure before lab synthesis. The LinkedIn case study describes a general application of AlphaFold 3 and is not evidence of a pipeline program; Isomorphic has not published details of any TIM-3 program.
- **Somatic Cancer Mutations**: In principle, AlphaFold models could be used to design inhibitors that precisely target mutant forms of oncogenes (a generic illustration, not an Isomorphic disclosure). Isomorphic has not disclosed a program against any specific oncogene. 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. This is a generic illustration, not an Isomorphic disclosure: no antibody program has been announced.

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, Insilico Medicine researchers reported in *Nature Biotechnology* that their GENTRL generative model had been used to discover potent inhibitors of DDR1, a kinase target implicated in fibrosis, in 21 days, a preclinical result (www.nature.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 planned clinical pipeline would be simply the largest-scale, industrial embodiment of this trend.

Implications, Perspectives, and Future Directions

The prospect 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 (pmc.ncbi.nlm.nih.gov).
- **Innovation and Competition:** Isomorphic's progress spurs competition. Open-source groups (e.g. OpenFold, a community AlphaFold clone) may push transparency. The *Scientific American* commentary discusses ongoing open-source efforts to develop similar capabilities (www.scientificamerican.com).
- **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 (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 reported slip of the trial target to the end of 2026 is a reminder that timelines can move; no reason was publicly given, and 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 progress toward the clinic points to practical impact. As to the lofty goal of "Click a button and out pops a drug" (fortune.com), this remains aspirational; currently, domain expertise and collaboration remain integral. But each successful case narrows that gap.

Conclusion

Isomorphic Labs' planned first-in-human studies of its AI-designed oncology and immunology candidates, if they begin as targeted by the end of 2026, would represent a milestone in the convergence of AI and medicine. Backed by DeepMind's AlphaFold legacy and substantial investment, Isomorphic is working to translate a computational breakthrough into clinical drug candidates (indianexpress.com) (www.prnewswire.com). The technology is unprecedented: it can predict complex biomolecular interactions with high accuracy (blog.google) (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 (fortune.com) (indianexpress.com). While we will ultimately judge success by patient outcomes, the progress so far suggests a promising trajectory: AI-designed drug candidates still await their first human trials, which Isomorphic has said it expects by the end of 2026.

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. Isomorphic's engine is proprietary (www.scientificamerican.com), and its drug candidates still require clinical evaluation.

In conclusion, Isomorphic Labs' progress 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 (fortune.com), Clinical Trials Arena (www.clinicaltrialsarena.com), industry press releases and analyses (www.prnewswire.com) (www.fiercebiotech.com), the Google DeepMind blog (blog.google), Scientific American/Nature commentary (www.scientificamerican.com), NVIDIA's industry blog (blogs.nvidia.com), and news coverage (indianexpress.com).

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