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Claude Science vs GPT-Rosalind vs Isomorphic Labs Compared

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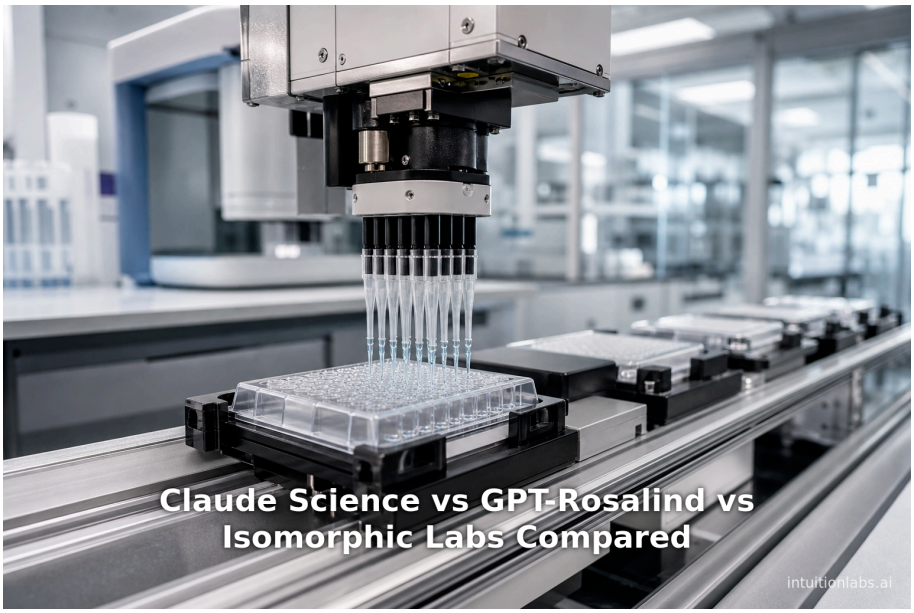

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Claude Science vs GPT-Rosalind vs Isomorphic Labs Compared

Executive Summary

As of November 2026, three organizations dominate discussion of AI-driven drug discovery, but they are not, strictly speaking, three competing products. **Claude Science**, released in beta by Anthropic on June 30, 2026, is a scientific workbench application built on the company's existing Claude models, bundled into the Claude subscription tiers that most buyers already pay for, which list Pro at **$17** per month on annual billing (**$20** if billed monthly) and Max at **$100** per month (claude.com) (www.anthropic.com). **GPT-Rosalind**, introduced by OpenAI on April 16, 2026, is a fine-tuned life sciences reasoning model gated behind a "trusted access"

enterprise review process, with pricing undisclosed during its research preview (openai.com). On September 8, 2026, OpenAI made the API model generally available to approved trusted-access customers at $5 per million input tokens and $25 per million output tokens (developers.openai.com). OpenAI later said GPT-Rosalind was coming out of research preview and is now available globally to eligible organizations through its trusted-access program (update of September 11, 2026), and on October 30, 2026 it released GPT-6 Rosalind (`gpt-6-rosalind`), again limited to organizations approved through trusted access. The benchmark figures discussed below come from OpenAI's April 2026 GPT-Rosalind launch and predate GPT-6 Rosalind.
Isomorphic Labs, the Alphabet-owned, Demis Hassabis-led spinout of Google DeepMind, is not a software product at all: it is a private drug-design engine, the Isomorphic Labs Drug Design Engine (IsoDDE), that the company uses internally and licenses through pharma partnerships (such as its January 2024 deals with upfront payments of $37.5 million to $45 million and milestone payments above $1 billion) rather than selling as a subscription (www.isomorphiclabs.com).

The three occupy different points in the drug discovery value chain and different business models, which makes "best" a function of what a buyer actually needs. Claude Science is a general-purpose research workbench, pre-configured for genomics, single-cell analysis, structural biology and cheminformatics, running on a lab's own laptop, HPC cluster or Modal account rather than sending raw data to Anthropic's servers by default. GPT-Rosalind is a specialized reasoning model that OpenAI reports achieved leading performance among models with published scores on a real-world bioinformatics benchmark, and it powers named deployments at Amgen, Novo Nordisk, Moderna, the Allen Institute and Thermo Fisher Scientific, described by trade press as a model used by organizations "to apply the technology across the discovery process" (www.fiercebiotech.com). Isomorphic Labs, by contrast, is a molecular-design system: as of February 2026 its IsoDDE release "doubled the performance of AlphaFold 3 on a protein-ligand structure prediction generalization benchmark," per an independent summary of the release (en.wikipedia.org). Isomorphic reaches the market not through seats but through deals: nearly $3 billion in combined biobucks with Eli Lilly and Novartis signed in January 2024, plus a strategic relationship with Johnson & Johnson, and a $2.1 billion Series B closed on May 12, 2026, led by Thrive Capital with Alphabet, GV, MGX, Temasek, CapitalG and the UK's sovereign AI fund (www.fiercebiotech.com) (www.prnewswire.com).

The broader market context tempers the hype attached to all three. A January 2026 PitchBook report found that more than $17 billion has been invested in AI-driven drug discovery since 2019, yet no AI-discovered drug has yet reached large-scale clinical trials (www.fiercebiotech.com). Grand View Research sizes the global AI-in-drug-discovery market at $2.3 billion in 2025, growing to $2.9 billion in 2026 and $13.8 billion by 2033 at a 24.8% compound annual growth rate (CAGR), though Fortune Business Insights puts the 2025 figure nearly twice as high at $4.46 billion, underscoring how much these estimates still vary by scope and methodology (www.grandviewresearch.com) (www.fortunebusinessinsights.com). Regulators have also drawn a boundary that matters to buyers: the FDA's January 2025 draft guidance on AI in drug development, a non-binding draft, is scoped to AI used to produce information or data intended to support regulatory decision-making about a drug's safety, effectiveness, or quality (www.fda.gov).

For buyers evaluating a platform, the practical distinction is access model, not raw capability. Claude Science and GPT-Rosalind are both usable, in some form, by an individual lab or enterprise research team today; Isomorphic Labs has no public product offering and is relevant chiefly to pharmaceutical companies capable of striking large partnership deals, or to industry observers benchmarking where the AlphaFold lineage has gone

since its 2024 Nobel Prize-winning breakthrough. This report examines each platform's capabilities, adoption, and strengths and limitations in turn, compares them on a common feature matrix, reviews the benchmark and market data underpinning vendor claims, and profiles named deployments including Xaira Therapeutics, Manifold Bio, Novo Nordisk, Amgen, Eli Lilly and Novartis before drawing conclusions relevant to life-sciences organizations deciding how, and whether, to adopt any of these systems.

Introduction and Background

The question of "Claude Science vs. GPT-Rosalind vs. Isomorphic Labs" has become common in life-sciences technology circles in 2026 because all three reached major milestones within a few months of each other. GPT-Rosalind launched April 16, 2026, as OpenAI's first purpose-built life sciences model. Trade press explained the underlying motivation: the model "is designed to reduce the time between target discovery and drug approval, a process that typically takes 10-15 years, according to industry group PhRMA" (www.fiercebiotech.com). Isomorphic Labs had moved first, on February 10, 2026, with its Drug Design Engine (IsoDDE), the first major technical update since AlphaFold 3, describing it in its own release as "excited to share an update on our progress towards a new frontier of drug design" and the clearest signal yet that the company, spun out of DeepMind in November 2021 to "build a computational platform to understand biological systems from first principles to discover new ways to treat disease," is moving from structure prediction toward an end-to-end, in-silico drug design system (www.isomorphiclabs.com) (techcrunch.com). Anthropic completed the trio on June 30, 2026, elevating Claude Science to the same product tier as Claude Code and Claude Cowork at an event for pharmaceutical executives, biotech founders and researchers in San Francisco (www.technologyreview.com).

These launches sit inside a much larger, and still largely unproven, industry bet. AI in drug discovery has attracted more than $17 billion in venture and corporate investment since 2019, a figure discussed further below. Although no AI-discovered drug had reached a large-scale clinical trial as of early 2026, Insilico Medicine announced on July 7, 2026 that it had initiated a Phase III trial of rentosertib, a program it says was discovered and designed through its Pharma.AI platform. (Insilico Medicine) Traditional drug development still takes more than a decade and typically costs upward of $2 billion per approved drug, the economic pressure that every AI drug-discovery pitch is built to address; one commonly cited industry estimate places the figure at 14.6 years and roughly $2.6 billion on average, per a 2019 Tufts Center analysis, with Cushman & Wakefield separately reporting that drug discovery and biotechnology accounted for 72% of 2022 U.S. venture funding in the life sciences (www.fortunebusinessinsights.com). AI's proposed role in closing that gap spans predicting patient outcomes, improving understanding of disease-progression predictors, and processing large real-world and digital-health datasets, per the FDA's own description of how sponsors are already using these tools (www.fda.gov). Some industry analyses suggest that AI-enhanced drug discovery and development can, in principle, shorten timelines and improve commercial-operations efficiency in adjacent functions, and McKinsey has separately estimated that AI could generate substantial annual value for the pharmaceutical industry, though these remain modeled projections rather than demonstrated outcomes at scale..

It is worth being precise about what each of the three organizations actually is, because the category label "AI drug discovery platform" obscures real differences. Anthropic and OpenAI are foundation-model companies extending general-purpose large language models (LLMs) into scientific workflows; their life-sciences offerings

are applications and specialized model variants layered on top of Claude and GPT model families respectively. Isomorphic Labs is a biotechnology company in its own right, majority-owned by Alphabet (the parent of Google and, separately, Google DeepMind), whose product is not software sold to end users but molecular designs and predictive models it applies to its own and partners' drug programs (en.wikipedia.org). This distinction, between accessible software and privately held scientific infrastructure, shapes every comparison in the sections that follow, including pricing, benchmarking methodology, and the kinds of organizations that can realistically become customers of each.

Regulatory context also frames the comparison. The FDA issued its first draft guidance on AI in drug development on January 6, 2025 (docket FDA-2024-D-4689), with Commissioner Robert Califf stating the agency is "committed to supporting innovative approaches for the development of medical products by providing an agile, risk-based framework that promotes innovation and ensures the agency's robust scientific and regulatory standards are met" (www.fda.gov). The FDA noted that "since 2016, the use of AI in drug development and in regulatory submissions has exponentially increased," and it published a companion draft guidance the same day specific to AI-enabled medical devices (www.fda.gov). The draft guidance provides recommendations on the use of AI to produce information or data intended to support regulatory decision-making about a drug's safety, effectiveness, or quality (www.fda.gov). Because the draft guidance is scoped to AI used to support regulatory decision-making, it does not by itself address discovery-only use of tools such as Claude Science, GPT-Rosalind, or Isomorphic Labs' IsoDDE, and it does not determine whether other FDA requirements apply; it remains a non-binding draft.

Claude Science

Capabilities

Claude Science is not a new model; it is an application that wraps Anthropic's existing Claude model family (Fable 5, Opus 4.8, Sonnet 5 and Haiku 4.5 at launch, depending on plan) in a research-specific environment. Anthropic has since moved to a newer generation, starting with Claude Opus 5.5 on September 22, 2026, and its pricing page now lists Fable 5.1, Opus 5.5, Sonnet 5.5 and Haiku 5.5 (www.anthropic.com) (claude.com). Anthropic describes the core product simply: "The Claude Science app runs analyses, searches databases, and traces every step from data wrangling to publication," using the same Claude models already included in a subscriber's plan rather than a separate, dedicated model (claude.com). It ships pre-configured for genomics, single-cell RNA sequencing, proteomics, structural biology and cheminformatics, and it reads literature and can query more than 60 curated scientific databases, including PubMed, UniProt, PDB, Ensembl, Reactome, ClinVar, ChEMBL and GEO, so users do not have to learn each database's schema individually (claude.com). It natively renders 3D protein structures, genome browser tracks, and chemical structures, and it connects to NVIDIA's BioNeMo Agent Toolkit for access to specialized open models including Evo 2, Boltz-2, and OpenFold3 (claude.com). Anthropic's broader claims about model capability in scientific contexts are also informed by outside researchers: Harvard physicist Matthew Schwartz has estimated, based on his own use of Anthropic's coding tools, that the underlying Opus 4.5 model series is "about as capable of executing scientific projects as a second-year graduate student," a data point cited by independent press covering the Claude Science launch (www.technologyreview.com).

A defining architectural choice is where computation happens. Claude Science installs on a lab's own laptop, a Linux box, or an HPC login node, and it writes and submits batch jobs over SSH to a lab's own compute cluster or through a Modal account, scaling from a single GPU to hundreds, so that large or sensitive datasets never have to leave the systems they are already on (www.anthropic.com). A background "reviewer" agent inspects outputs as a pipeline runs, flagging incorrect citations, untraceable numbers, and figures that do not match their underlying code, and every artifact carries the exact code, environment, and conversation that produced it, so results can be reproduced months later (www.anthropic.com).

Adoption

Claude Science was announced as available "in beta for Claude Pro, Max, Team, and Enterprise users," with Team and Enterprise admins needing to enable it for their organization (www.anthropic.com). Pricing runs through Anthropic's existing Claude plan structure rather than a standalone fee: the Pro plan is **$17** per month with annual billing ($200 billed up front) or $20 per month billed monthly (claude.com); Team Standard seats are $20 per seat per month annually ($25 monthly), and Team Premium seats, with 5x the usage of Standard, are $100 per seat per month annually ($125 monthly) (claude.com); Enterprise is priced at $20 per seat plus usage at API rates (claude.com). Anthropic is also funding up to 50 "AI for Science" projects with up to $30,000 in Claude credits each, alongside a discounted Team plan for research labs at academic institutions and nonprofit research organizations (www.anthropic.com).

Named early adopters cited by Anthropic and independent press include **Manifold Bio**; the **Allen Institute**, where researcher Jérôme Lecoq built a roughly 20-skill multi-agent pipeline that cut the time to write long-form literature reviews from as much as two years to a fraction of that; the nonprofit **Every Cure**; the AI-native biotech **Xaira Therapeutics**; and genomics data companies **LatchBio** and **Helix** (claude.com). MIT Technology Review reported that during the launch event, Anthropic staff member Alexander Tarashansky demonstrated the system autonomously identifying drug candidates for phenylketonuria, a rare genetic disease (www.technologyreview.com). Anthropic also announced it will use Claude Science to pursue its own internal drug-discovery research into "neglected" diseases that traditional biopharmaceutical companies do not consider commercially attractive, framing the effort around its status as a public benefit company that can "choose programs on patient benefit, including work the commercial market overlooks" (www.cnbc.com).

Strengths and Limitations

Claude Science's strength is breadth and accessibility: any Pro subscriber, individual academic or otherwise, can use it for **$17** to **$20** a month, with no enterprise gatekeeping, which stands in sharp contrast to GPT-Rosalind's approval process. Anthropic CEO Dario Amodei has compared the ambition directly to Claude Code, saying the technology is "going to be a general purpose technology that helps us to make sense of that complexity, in its full complexity, better," while cautioning "we don't know for sure if that's going to work out" (www.statnews.com). Its main limitation is that it is a workflow layer, not a specialized biological reasoning model: it uses the same general-purpose Claude models available elsewhere, and reception on Reddit reflects this trade-off directly, with one r/singularity poster summarizing that "openai shipped gpt-rosalind, an actual fine-tuned bio model, gated behind enterprise review. anthropic is betting on that the workflow layer matters more than a specialized model, same play as claude code" (www.reddit.com). Other early users flagged

practical friction, including the lack of native Windows support at launch, with one commenter asking bluntly, "Nor available for Windows?", and rate limits some found restrictive, while the discussion also covered point-solution wrappers around similar workflows (www.reddit.com). Windows support has since been added: Anthropic's documentation now describes Claude Science as "available in beta on macOS, Windows, and Linux" (claude.com). Academics on r/bioinformatics discussed Claude Science's role in bioinformatics workflows (www.reddit.com).

GPT-Rosalind

Capabilities

GPT-Rosalind is OpenAI's first entry in a dedicated life sciences model series, described as "a purpose-built model for life sciences research, designed to reason across biology, scientific evidence, data, and tools" (openai.com) that is meant to "work with scientific tools," connecting model reasoning to "approved tools, datasets, and repeatable workflows," and to "evaluate evidence" by comparing findings across papers, datasets, and scientific context (openai.com). Unlike Claude Science, it is a fine-tuned model variant, not merely a workflow wrapper around a general-purpose model, though it does share the "Codex" agentic coding backbone from OpenAI's mainline models; the June 3, 2026 update explicitly "combines GPT-5.5's agentic coding and tool-use capabilities with stronger model intelligence in core drug-discovery domains such as medicinal chemistry and genomics" (openai.com). The model is named after Rosalind Franklin, whose X-ray crystallography work was essential to understanding the structure of DNA (www.fiercebiotech.com). It is accompanied by two free "Life Sciences" plugins for OpenAI's Codex agentic coding environment, one for general research (literature review, sequence lookup, dataset discovery across more than 50 public multi-omics databases) and one for next-generation sequencing (NGS) analysis, that any user can access, not only trusted-access enterprise customers (openai.com).

A separate, adjacent initiative, Rosalind Biodefense, launched May 29, 2026 to sponsor trusted developers building pandemic-preparedness tools on top of GPT-Rosalind. OpenAI framed the effort around a broader belief "that frontier AI should meaningfully advantage those defenders," building on the fact that its ChatGPT agent, released in July 2025, was "the first model we treated as High Capability in biology under our Preparedness Framework" (openai.com). Early Rosalind Biodefense participants include Fourth Eon Biosecurity, which is testing the model in "AI-native biosecurity screening systems that analyze sequences and generate detailed threat assessments," and Lawrence Livermore National Laboratory, whose Bioresilience Incubator director said the collaboration is "examining how advanced AI tools can help scientists interpret complex data and existing knowledge, identify stronger candidates, and more efficiently connect design, simulation and experimental results" (openai.com). OpenAI also extended trusted access to Johns Hopkins Applied Physics Laboratory, which intends to integrate GPT-Rosalind into a protein-engineering platform, and to the Coalition for Epidemic Preparedness Innovations, "which is focused on its 100 Days Mission to accelerate the development of vaccines against epidemic and pandemic threats, including the current Ebola outbreak" (openai.com).

Adoption

GPT-Rosalind is not openly available. It is "launching through a trusted-access deployment structure for qualified Enterprise customers in the U.S. to start, with controls around eligibility, access management, and organizational governance," and organizations must apply and pass a safety and qualification review; for enterprises specifically, OpenAI's own access page frames the process as a way to "bring GPT-Rosalind into approved research workflows with governance review and enterprise-grade deployment controls" (openai.com). During the research preview period, "use of this model will not consume existing credits or tokens, subject to abuse guardrails," and OpenAI states it will share more details on pricing and availability as the program expands, meaning no public price list was available at the time of writing (openai.com). That changed on September 8, 2026, when OpenAI's API changelog announced that GPT-Rosalind (gpt-rosalind-research) "is now generally available through the trusted-access program for approved internal life sciences research," at $5 per million input tokens, $0.50 per million cached input tokens and $25 per million output tokens, with billing starting October 5, 2026 (developers.openai.com). OpenAI has also introduced Rosalind Workbench, a research-preview environment in the ChatGPT app that builds on GPT-Rosalind and offers guided scientific tasks; researchers who are eligible can request GPT-Rosalind access through it (developers.openai.com).

Named customers and partners include **Amgen**, **Moderna**, the **Allen Institute**, and **Thermo Fisher Scientific**, alongside **Novo Nordisk**, which is "partnering with OpenAI to deploy artificial intelligence across its business, from drug discovery to manufacturing and commercial operations" (www.reuters.com). Amgen's Sean Bruich, Senior Vice President of Artificial Intelligence and Data, framed the relationship as strategic: "Our unique collaboration with OpenAI enables us to apply their most advanced capabilities and tools in new and innovative ways with the potential to accelerate how we deliver medicines to patients" (openai.com). OpenAI's roster of pharma relationships extends beyond GPT-Rosalind's named launch partners: Sanofi and Formation Bio run a separate OpenAI-powered clinical-trial-recruitment tool, Moderna has "a wide-ranging initiative running with the AI stalwart," and Thermo Fisher "has also tapped OpenAI to help accelerate drug development," illustrating that OpenAI's life-sciences push is broader than any single model release (www.fiercepharma.com). Novo's own AI leader, Mishal Patel, framed the strategic rationale: "Life sciences research is complex, data-rich, and interdisciplinary. To deliver meaningful value for researchers, advanced AI models must be grounded in trusted scientific data" (openai.com). Eli Lilly has a separate, earlier OpenAI collaboration from 2024 focused on antibiotic-resistant bacteria, alongside its own Nvidia-built supercomputer (www.fiercebiotech.com).

Strengths and Limitations

GPT-Rosalind's strength is demonstrated, model-level performance on specialized scientific benchmarks, detailed in *Table 2* below. OpenAI reports the model out-performing GPT-5.5 at 27.5% versus 25.1% on MedChemBench while using 7.2% fewer output tokens, and achieving 21.6% versus 20.4% accuracy on GeneBench with 31% fewer tokens (openai.com). It also scores 63.2% versus 55.8% on LabWorkBench, a benchmark built from proprietary, uncontaminated wet-lab protocol data, using 5.3% fewer tokens (openai.com). In a joint evaluation with Dyno Therapeutics on an RNA sequence-to-function task, using

unpublished, uncontaminated sequences, best-of-ten model submissions ranked above the 95th percentile of 57 historical human expert scores on the prediction task, and around the 84th percentile on the sequence generation task (openai.com).

Its principal limitation is access: the trusted-access model, designed explicitly to guard against biological misuse, means most academic labs, small biotechs, and individual researchers cannot use GPT-Rosalind at all, regardless of budget, unless their organization clears OpenAI's governance and eligibility review, and it means Novo's own commitment that AI is "not replacing our scientists" is, for now, a promise most of the field cannot test firsthand (www.reuters.com). A further limitation was pricing opacity: GPT-Rosalind had no list price until OpenAI published per-token API rates in September 2026, and those rates apply only to organizations that clear trusted-access review, so most prospective buyers still cannot budget against it the way they can Claude Science's published per-seat rates.

Isomorphic Labs

Capabilities

Isomorphic Labs is structurally different from the other two: it sells no software product, publishes no price list, and offers no self-service signup. The company was announced publicly on November 4, 2021, established under Alphabet as a spin-off of Google DeepMind and led by DeepMind's own CEO, Demis Hassabis, who described biology at the time as "an information processing system, albeit an extraordinarily complex and dynamic one," while cautioning that it "is likely far too complex and messy to ever be encapsulated as a simple set of neat mathematical equations"; the company's own name reflects "the idea that information systems and biological systems may have a common structure," borrowing the mathematical sense of "isomorphic" as alike in shape though of different origin (techcrunch.com). Reporting at the time noted that Isomorphic was "essentially starting from scratch," building on DeepMind's research and drawing on the observation that "DeepMind's learning systems have shown a particular affinity for generality or knowledge transfer," while similarly ambitious AI-drug-discovery startups had, by that point, raised hundreds of millions of dollars without producing "any visible revolution or famous AI-discovered wonder drug" (techcrunch.com). The company, incorporated on February 24, 2021, was formally established under Alphabet as a DeepMind spin-off (en.wikipedia.org). By its own account, "Isomorphic Labs was launched from DeepMind, and many of our team contributed to the creation of the groundbreaking AlphaFold system" (www.isomorphiclabs.com). Its core technology, released in May 2024 alongside Google DeepMind, was AlphaFold 3, an AI system trained on nearly 100,000 known protein structures that predicts how proteins fold and interact with ligands and antibodies (en.wikipedia.org).

On February 10, 2026, Isomorphic went beyond structure prediction with the Isomorphic Labs Drug Design Engine (IsoDDE), a unified computational drug-design system the company describes as progressing "beyond AlphaFold 3 (AF3) in its predictive accuracy and introducing new capabilities which bridge the gap between structure prediction and real-world drug discovery" (www.isomorphiclabs.com). On antibody-antigen interface prediction, a proxy for biologics design, IsoDDE outperforms AlphaFold 3 by 2.3x and the competing open-source model Boltz-2 by 19.8x in the high-fidelity DockQ greater than 0.8 regime (www.isomorphiclabs.com).

Adoption

Because Isomorphic Labs sells no product, "adoption" here means partnership and internal use. In January 2024, Isomorphic signed two research collaborations worth nearly $3 billion combined: Eli Lilly agreed to pay $45 million upfront against more than $1.7 billion in milestone payments for small-molecule discovery on undisclosed targets, and Novartis agreed to $37.5 million upfront against $1.2 billion in milestones for three additional undisclosed targets, with "both Big Pharma firms" tasking Isomorphic "with using AlphaFold to discover small molecules for undisclosed targets" (www.fiercebiotech.com). Isomorphic said at the time that newer iterations of its underlying AlphaFold-derived technology were "expanding beyond protein predictions to include small molecules and nucleic acids," foreshadowing IsoDDE's broader scope two years later (www.fiercebiotech.com). Isomorphic later added Johnson & Johnson to its roster of strategic pharmaceutical partners, alongside continuing work with Novartis and Lilly (www.prnewswire.com), designing drug candidates with "AI models such as AlphaFold 3, a Google DeepMind-partnered model that can predict the structures and interactions of molecules," with new capital earmarked to "develop and deploy" IsoDDE and "accelerate its in-house drug pipeline into the clinic" (www.fiercebiotech.com). Beyond partnered programs, Isomorphic also runs an internal drug-candidate pipeline "focused in oncology and immunology," using IsoDDE on wholly owned assets rather than licensed-out capacity, from offices in London, Lausanne, and Cambridge, Massachusetts (www.isomorphiclabs.com).

Isomorphic's capital base has scaled to match its ambitions: after a first external funding round of $600 million in early 2025, the company closed a "ten-figure" $2.1 billion Series B on May 12, 2026, led by Thrive Capital, joined by Alphabet and Google's GV, with new backers including MGX, Temasek, CapitalG and the UK government's AI fund (www.fiercebiotech.com). Isomorphic president Max Jaderberg framed the raise around results already achieved: "this milestone is built on the strength of our AI drug design engine, which has already proven its worth across our internal programs by hitting key milestones and identifying viable candidates with unprecedented speed" (www.prnewswire.com), while Thrive Capital founder Joshua Kushner said his firm's "conviction in the team has only deepened as they've made significant progress in building a unified AI drug design engine to define a new age of drug discovery and design" (www.prnewswire.com). Its scientific advisory board includes four Nobel laureates, among them CRISPR pioneer Jennifer Doudna, reflecting the company's positioning as a scientific research organization first and a technology vendor a distant second, if at all (www.fiercebiotech.com).

Strengths and Limitations

Isomorphic Labs' strength is depth: IsoDDE's benchmark improvements over both AlphaFold 3 and the competing open model Boltz-2, summarized in *Table 2* below, are large by the standards of the field, and the company has published a technical report and citable manuscript alongside the February 2026 release. Isomorphic's own president, Max Jaderberg, is candid about how far the underlying science still has to go: "AlphaFold 3 was a major leap forward in understanding biological structures. But we know we're never going to solve drug design with AlphaFold alone. We'll need half a dozen more breakthroughs of that magnitude to reach our ambitious goal" (www.isomorphiclabs.com). The company's core limitation, for the purposes of this comparison, is inaccessibility: there is no plan, tier, seat, or price at which an outside organization can simply buy access to IsoDDE the way it can subscribe to Claude Science or apply for GPT-Rosalind trusted access.

Isomorphic is best understood not as a competing "platform" in the software sense but as a barometer of how far AI-based molecular design has advanced since AlphaFold, and as a potential partner only for organizations able to negotiate deals of the kind Isomorphic signed in January 2024, with upfront payments of tens of millions of dollars and larger contingent milestone payments.

Feature Comparison

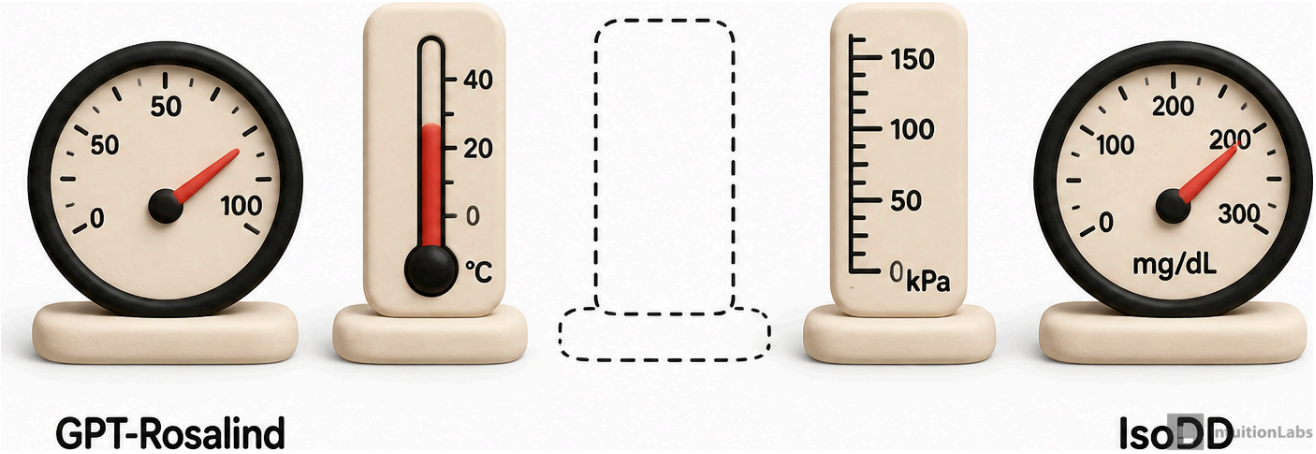
Table 1 below summarizes the three offerings across the dimensions most relevant to a prospective buyer: what each one is, how it is accessed, what it costs, and what kind of organization can realistically use it. Citations for each row's underlying facts appear in the sections above and below; the table itself restates them for side-by-side comparison.

Dimension	Claude Science (Anthropic)	GPT-Rosalind (OpenAI)	Isomorphic Labs / IsoDDE
What it is	Application layer on top of existing Claude models (Fable 5, Opus 4.8, Sonnet 5, Haiku 4.5 at launch; Claude 5.5 generation since September 2026)	Fine-tuned life sciences reasoning model built on GPT-5.5's agentic backbone	Private computational drug-design engine (IsoDDE), not sold as software
Launch date	Beta, June 30, 2026	Research preview, April 16, 2026; updated June 3, 2026; API generally available to trusted-access customers September 8, 2026	AlphaFold 3, May 2024; IsoDDE, February 10, 2026
Access model	Self-service signup, included in existing subscription tiers	Trusted-access review; enterprise application required	No public access; partnership/licensing deals only
Published price	$17-$20/mo (Pro); $20-$100/seat/mo (Team); $20/seat + usage (Enterprise)	Undisclosed at launch; since September 2026, API at $5 per 1M input and $25 per 1M output tokens (trusted access only)	None; $37.5M-$45M upfront plus $1.2B-$1.7B in milestones per deal
Compute/data location	Runs on the lab's own laptop, cluster, or Modal account by default	Hosted via ChatGPT Enterprise, Codex, or API	Runs on Isomorphic's own GPU fleet and proprietary "dataverse," a curated life-science data collection that "powers a cutting-edge research environment" (www.isomorphiclabs.com)
Primary published benchmark	None published as a standalone score (relies on underlying Claude model benchmarks)	BixBench: OpenAI-reported leading performance among models with published scores (no numeric score published)	2.3x-19.8x accuracy gain over AlphaFold 3/Boltz-2 on antibody-antigen prediction
Named enterprise users	Xaira, Manifold Bio, Allen Institute, Every Cure, LatchBio, Helix	Amgen, Novo Nordisk, Moderna, Allen Institute, Thermo Fisher	Eli Lilly, Novartis, Johnson & Johnson (deal partners); internal oncology/immunology pipeline

The table underscores that a head-to-head "which is best" verdict depends entirely on who is asking. For an individual academic lab or a well-funded biotech that wants an off-the-shelf research assistant today, Claude Science is the only one of the three that can be purchased outright, in minutes, at a published price. For an enterprise research organization that already has a formal AI governance function and can clear a vendor security review, GPT-Rosalind's specialized benchmarks make it a credible option, provided it can obtain trusted access. For a large pharmaceutical company with a balance sheet that supports nine-figure milestone payments, Isomorphic Labs offers what is arguably the deepest molecular-design technology of the three, but only through bespoke partnership, not procurement.

Performance and Benchmarks

Direct, apples-to-apples benchmarking across all three systems does not exist publicly, because they are evaluated on different tasks with different methodologies, a limitation this report treats as a finding rather than papering over. GPT-Rosalind's most consistently cited public benchmark is BixBench, a real-world bioinformatics and data-analysis benchmark, where OpenAI reports that GPT-Rosalind achieved leading performance among models with published scores (openai.com). OpenAI both defines and reports the benchmark results it publishes for GPT-Rosalind, a limitation common to nearly all proprietary AI benchmarks in this space.



Isomorphic Labs' benchmarks are structural and biophysical rather than agentic or workflow-based, and they are measured against a different reference point: prior model generations, not competing vendors. On the "Runs N' Poses" benchmark, designed to test generalization to novel binding pockets and ligands, "IsoDDE more than doubles the accuracy of AlphaFold 3 on the most difficult systems" (www.isomorphiclabs.com). On binding-affinity prediction, "IsoDDE surpasses all deep-learning methods by a considerable margin on three public benchmarks: FEP+4, OpenFE, and the recent CASP16" blind binding-affinity task, and in some cases exceeds physics-based free-energy perturbation methods that require experimental crystal structures IsoDDE does not need (www.isomorphiclabs.com).

Table 2 below consolidates the published benchmark figures for GPT-Rosalind and IsoDDE side by side, though, as the surrounding prose stresses, they are not measuring the same thing and should not be read as a single ranked leaderboard.

Platform	Benchmark	Reported Result	Comparison Point
GPT-Rosalind	BixBench	Leading performance among models with published scores (OpenAI-reported; no numeric scores published)	Other models with published scores (not itemized by OpenAI)
GPT-Rosalind	MedChemBench	27.5%	GPT-5.5 25.1% (7.2% fewer tokens)
GPT-Rosalind	GeneBench	21.6%	GPT-5.5 20.4% (31% fewer tokens)
GPT-Rosalind	LabWorkBench	63.2%	GPT-5.5 55.8% (5.3% fewer tokens)
GPT-Rosalind	Dyno RNA task (best-of-10)	>95th / ~84th percentile	57 historical human expert scores
Isomorphic IsoDDE	Runs N' Poses (hardest bin)	More than 2x accuracy	AlphaFold 3
Isomorphic IsoDDE	Antibody-antigen (DockQ > 0.8)	2.3x / 19.8x	AlphaFold 3 / Boltz-2
Isomorphic IsoDDE	FEP+4, OpenFE, CASP16 binding affinity	Surpasses deep-learning baselines	Published deep-learning methods

None of the figures in *Table 2* are directly comparable across the "Platform" column, because IsoDDE performs structural and biophysical prediction tasks, while GPT-Rosalind performs natural-language reasoning, literature synthesis, and workflow orchestration; Claude Science does not appear in the table at all because it publishes no standalone benchmark of its own, relying instead on the underlying Claude model a user selects (Opus 4.8, Sonnet 5, Fable 5, or Haiku 4.5 at launch, and the Claude 5.5 generation since September 2026). Anthropic instead points to qualitative case evidence, such as the Allen Institute literature-review pipeline discussed above, as its proof point. Independent, third-party, peer-reviewed benchmarking that places Claude Science, GPT-Rosalind, and IsoDDE on a single leaderboard does not exist at the time of writing, and buyers should treat every percentage figure in this report as a vendor-reported claim, evaluated on the vendor's own benchmark design, rather than as an independently audited result.

Data Analysis and Evidence

The market-sizing data around AI in drug discovery is itself a useful case study in how much estimates diverge depending on scope. Grand View Research values the global AI-in-drug-discovery market at $2.3 billion in 2025, rising to an estimated $2.9 billion in 2026 and $13.8 billion by 2033 at a 24.8% CAGR, with North America holding 52.85% of 2025 revenue (www.grandviewresearch.com). The drug optimization and repurposing application segment led the market with 52.46% of 2025 revenue, reflecting how much of today's spending goes toward extending existing molecules rather than discovering wholly novel ones (www.grandviewresearch.com). Fortune Business Insights, using different segmentation, estimates the 2025 market at $4.46 billion, nearly double Grand View Research's figure, rising to $5.00 billion in 2026 and $12.56

billion by 2034 at a 12.2% CAGR (www.fortunebusinessinsights.com). Comparable deal-level data illustrate the same dynamic at the transaction level: Fortune Business Insights notes that in November 2022, Insilico Medicine separately signed a $1.2 billion deal with Sanofi to discover up to six new targets, underscoring that large biobucks partnerships in this sector predate the current AI model wave by several years (www.fortunebusinessinsights.com). This report presents both top-line market figures rather than resolving the discrepancy, since the two firms appear to scope "AI in drug discovery" differently (application segments versus a broader technology and offering taxonomy), and readers evaluating market-sizing claims elsewhere should expect similar variance among research firms.

Investment data is more consistent across sources. PitchBook's January 2026 analysis, as reported by trade press, found more than $17 billion invested in AI-driven drug discovery since 2019 and, at that point, no AI-developed drug had reached a large-scale clinical trial. The finding was overtaken on July 7, 2026, when Insilico Medicine announced the initiation of a Phase III trial of rentosertib, which it says was discovered and designed through its Pharma.AI platform. (Insilico Medicine) Individual company-level figures corroborate the scale of capital involved: Isomorphic Labs alone has raised $600 million (2025) plus $2.1 billion (2026) and signed nearly $3 billion in partnership deal value with Eli Lilly and Novartis, while Xaira Therapeutics, an unrelated AI-native drug discovery biotech, launched in April 2024 with $1 billion in committed funding incubated by Arch Venture Partners and Foresite Labs (www.fiercebiotech.com).

On the regulatory side, the FDA reports an "exponential" increase in AI-related submissions since 2016, informed by an FDA-sponsored expert workshop convened by the Duke Margolis Institute for Health Policy and more than 800 public comments on two 2023 discussion papers, with the FDA's experience spanning more than 500 drug and biological product submissions with AI components since 2016 (www.fda.gov). Yet the agency's January 2025 document is non-binding draft guidance that provides a risk-based credibility-assessment framework for AI used to produce information or data intended to support regulatory decision-making about a drug's safety, effectiveness, or quality. Its stated scope does not determine whether other FDA requirements or oversight may apply to discovery-stage tools or their outputs. Taken together, these figures describe an industry with rapidly rising capital commitment and regulatory attention, but with as-yet-unproven clinical translation: billions of dollars, dozens of named partnerships, and improving benchmark scores have not yet, as of late 2026, produced an FDA-approved medicine whose discovery pathway ran primarily through one of these three platforms.

Case Studies and Real-World Examples

Xaira Therapeutics: Multi-Vendor AI Adoption in Practice

Xaira Therapeutics illustrates that leading AI-native biotechs do not necessarily commit to a single AI vendor. The company launched in April 2024 with more than $1 billion in committed funding, described at the time as the largest initial funding commitment in the history of its lead incubator, Arch Venture Partners, with financing that also included F-Prime, NEA, Sequoia Capital, Lux Capital, and Lightspeed Venture Partners, and was led by former Genentech chief scientific officer Marc Tessier-Lavigne, whose board recruits included former FDA Commissioner Scott Gottlieb and Nobel laureate Carolyn Bertozzi (www.fiercebiotech.com). By mid-2026, Xaira was a named Claude Science and Claude Code customer, with the company stating that the tools are

"accelerating that work, compressing the path from hypothesis to validation and advancing our therapeutic pipeline, enabling our scientists to focus on the discoveries that matter most" (claude.com). This demonstrates that even a company built around its own proprietary protein-design models (RFdiffusion and RFantibody, developed in David Baker's University of Washington lab) sees value in layering a general-purpose AI research workbench on top of its internal tooling, rather than treating AI drug discovery as a single-platform decision.

Anthropic's Internal Neglected-Disease Program

Rather than only selling Claude Science, Anthropic is using it to run its own drug-discovery program targeting "neglected" diseases that commercial biopharmaceutical companies typically decline to pursue because they lack a viable market. Anthropic said, in a statement to CNBC, that "as a public benefit company, we can choose programs on patient benefit, including work the commercial market overlooks" (www.cnbc.com). Life sciences head Eric Kauderer-Abrams explained the strategic logic: "We believe in the power of tight feedback loops, and there's no substitute for having our own experiences alongside you all in the trenches trying to develop drugs" (www.cnbc.com). As of the June 2026 launch, Anthropic had not disclosed what it would do with any promising drug candidates it discovers, including whether it would run clinical trials itself or seek a pharmaceutical partner (www.cnbc.com).

Isomorphic Labs and Eli Lilly / Novartis: The Milestone-Payment Model

The January 2024 Eli Lilly and Novartis deals remain the clearest illustration of how Isomorphic Labs actually monetizes its technology. Rather than a license fee or subscription, Isomorphic receives modest upfront cash, $45 million from Lilly and $37.5 million from Novartis, in exchange for large downstream "biobucks": payments contingent on the drug candidates it designs successfully clearing preclinical and clinical milestones, worth up to $1.7 billion and $1.2 billion respectively. This structure means Isomorphic's revenue is directly tied to clinical success, an incentive structure fundamentally different from Claude Science's flat per-seat subscription or GPT-Rosalind's usage-based enterprise licensing, and one that will not pay off, if it pays off at all, for years, given typical drug-development timelines of a decade or more. Alphabet's own president and chief investment officer, Ruth Porat, has described the opportunity in sweeping terms, calling AI in healthcare "a profound opportunity" and noting Isomorphic has "already made extraordinary progress in harnessing AI to accelerate drug discovery," adding that fresh funding "will be used to accelerate the work and bring important interventions to market with greater speed" (www.prnewswire.com) (www.fiercebiotech.com).

Novo Nordisk and GPT-Rosalind: An Enterprise-Wide AI Deployment

Novo Nordisk's April 14, 2026 partnership with OpenAI is the most extensively documented enterprise deployment of GPT-Rosalind. Reuters reported that the deal spans "drug discovery to manufacturing and commercial operations," with pilot programs beginning across research and development, manufacturing, and commercial functions, and full integration targeted by the end of 2026 (www.reuters.com). Trade press reported Novo says the collaboration will feature "strict data protection" and human oversight to "ensure ethical

and compliant use" (www.fiercepharma.com), and Novo CEO Mike Doustdar separately said the partnership gives Novo "the ability to analyze datasets at a scale that was previously impossible, identify patterns we could not see, and test hypotheses faster than ever" (www.fiercepharma.com). Reuters noted that "analysts expect annual revenue from weight-loss drugs to exceed $100 billion in the next decade," a market context for the partnership (www.reuters.com). OpenAI CEO Sam Altman characterized the partnership's ambitions broadly, stating it "will help them accelerate scientific discovery, run smarter global operations, and redefine the future of patient care" (www.reuters.com).

Implications and Future Directions

None of these three platforms is likely to remain static through the rest of 2026 and beyond. Anthropic has framed Claude Science as an early-stage beta that will keep evolving, and the recruitment of AlphaFold co-creator John Jumper away from DeepMind to Anthropic in mid-2026 suggests the company intends to deepen its scientific model capabilities rather than rely solely on general-purpose Claude models wrapped in a workflow layer (www.technologyreview.com). MIT Technology Review noted the timing is significant given that Anthropic "says it's set to see its first profitable quarter" as an IPO approaches later in 2026, meaning new pharmaceutical contracts around Claude Science could matter to the company's broader financial trajectory, not only its scientific ambitions (www.technologyreview.com). OpenAI has described GPT-Rosalind as the beginning of a broader life sciences model series and plans to keep expanding both trusted-access enterprise deployment and its freely available Codex research plugins, alongside the Rosalind Biodefense initiative for public-health and preparedness applications discussed above. Isomorphic Labs, which closed a $2.1 billion Series B in May 2026, has stated its intent to "scale its business globally and progress its drug candidate pipeline," suggesting the company may pursue additional pharma partnerships, deepen its internal oncology and immunology programs, or both (www.isomorphiclabs.com). In October 2026, Bloomberg reported that Isomorphic was in early talks to raise new funding at a valuation of $40 billion to $50 billion (siliconangle.com).

The broader digital-transformation context in pharma helps explain why buyers are receptive to all three platforms at once: cloud adoption and digital-platform spending in pharma have been growing broadly, independent of AI-specific spending. AI drug-discovery adoption is, in that sense, one strand within a much larger and already well-funded digitization wave, not a standalone trend.

The regulatory boundary between "AI used for drug discovery" and "AI used to support a regulatory decision" is likely to come under more scrutiny as these tools mature. Today, the draft guidance's credibility framework is scoped to AI used to support regulatory decision-making, so it does not by itself address discovery-stage use of a discovery engine like IsoDDE, a workbench like Claude Science, or a reasoning model like GPT-Rosalind; the guidance is a non-binding draft, and other FDA requirements may apply once a candidate's supporting data is formally submitted in an investigational new drug (IND) application or similar filing. As more AI-originated candidates move into human trials over the next several years, expect regulators in the U.S. and at the European Medicines Agency, which published its own AI reflection paper covering the full product lifecycle including discovery, to revisit whether that boundary still makes sense.

For life-sciences organizations evaluating this space, the practical implication is that "which AI drug discovery platform should we choose" is really several separate decisions layered together: whether the organization needs a general research productivity tool (pointing toward Claude Science), a specialized reasoning model

for target prioritization and evidence synthesis at enterprise scale (pointing toward GPT-Rosalind, subject to gaining trusted access), or a molecular-design partner willing to co-invest against milestone payments (pointing toward a relationship with Isomorphic Labs or a comparable AI-native biotech such as Insilico Medicine, Recursion (which completed its combination with Exscientia in November 2024), or Xaira) (ir.recursion.com). A useful evaluation checklist for organizations weighing these and other AI drug-discovery options includes: **data residency and compute location** (does the tool process data on the organization's own infrastructure or a vendor's cloud); **access model and lead time** (self-service versus multi-week enterprise review); **pricing transparency** (published per-seat rates versus negotiated, often multi-year, deal terms); **benchmark provenance** (whether performance claims come from independent, peer-reviewed evaluation or vendor-designed and vendor-reported benchmarks); and **regulatory posture** (whether outputs are intended only for internal hypothesis generation or are expected eventually to support a formal regulatory submission). Consultancies advising pharmaceutical and life-sciences organizations on AI adoption, including those focused on regulatory-compliant deployment architecture rather than on selling a competing discovery platform, generally recommend piloting against a narrowly scoped, measurable use case, such as a single target class or a defined literature-synthesis workflow, before committing to an enterprise-wide rollout of any of these systems, precisely because independent, cross-vendor benchmarking remains immature as of mid-2026.

Frequently Asked Questions (FAQs)

What is the best AI drug discovery platform in 2026? There is no single answer, because Claude Science, GPT-Rosalind, and Isomorphic Labs are not fully substitutable products. For accessible, affordable, general-purpose scientific research assistance today, Claude Science is the most readily available at $17 to $20 per month. For enterprise teams that can clear trusted-access review and need a specialized reasoning model, GPT-Rosalind is the purpose-built life sciences reasoning model of the three, having been adopted by major pharmaceutical players such as Amgen and Novo Nordisk. For deep, structural molecular design backed by a decade of AlphaFold-lineage research, Isomorphic Labs is the strongest technically, but is reachable only through partnership.

How does Isomorphic Labs compare to DeepMind? Isomorphic Labs is not DeepMind; it is a separate company, also owned by Alphabet, that spun out of DeepMind in 2021 and builds directly on DeepMind's AlphaFold research, including the jointly released AlphaFold 3 in May 2024, as discussed in the Isomorphic Labs section above. Demis Hassabis leads both organizations simultaneously as CEO. DeepMind remains a broad AI research lab within Alphabet, while Isomorphic Labs is a distinct, separately funded drug-discovery company with its own investors, board, and commercial deals.

What does Claude Science AI pricing and features actually include? Claude Science is bundled into Anthropic's existing consumer and business plans rather than sold separately: Free users do not get it, but Pro ($17 to $20/month), Max (from $100/month), Team ($20 to $100 per seat/month), and Enterprise ($20 per seat plus usage) subscribers all get access, with Team and Enterprise admins needing to enable it (claude.com).

Is GPT-Rosalind any good for drug discovery, based on independent review? OpenAI's own benchmark disclosures show consistent, if modest, gains over its general-purpose GPT-5.5 model on specialized tasks, for example 63.2% versus 55.8% on LabWorkBench, using fewer output tokens. Because the model is not

publicly available for independent testing outside the trusted-access program, no fully independent, third-party peer review of GPT-Rosalind's drug-discovery performance exists at the time of writing, and observers on Reddit have flagged that OpenAI shipped "an actual fine-tuned bio model, gated behind enterprise review," in contrast to Anthropic's broader workflow-layer approach, a framing that itself has not been independently validated.

How do I choose an AI drug discovery platform for my organization? Start from the use case, not the vendor: general research productivity favors an accessible tool like Claude Science; specialized target prioritization and evidence synthesis at enterprise scale favors a reasoning model like GPT-Rosalind, if trusted access is attainable; and molecular design for an actual drug candidate, where a pharmaceutical company can offer meaningful co-investment, may favor a partnership model like Isomorphic Labs. Evaluate data residency, access lead time, pricing structure, and benchmark provenance before committing, as outlined in the Implications section above.

What are the main alternatives to Isomorphic Labs? Because Isomorphic Labs is not purchasable, organizations seeking a comparable AI-native drug-discovery partner have looked to Xaira Therapeutics ($1 billion in committed funding, incubated by Arch Venture Partners and Foresite Labs), and to Insilico Medicine, which signed its own research and licensing collaboration with Eli Lilly in November 2025 using its Pharma.AI platform (www.grandviewresearch.com). Other names commonly cited in the same competitive set include Recursion (now combined with Exscientia) and BenevolentAI, though a full comparative analysis of those platforms is outside the scope of this report.

Is there published pricing to compare across all three platforms? Claude Science publishes per-seat list pricing. GPT-Rosalind had no public price during its research preview; since September 2026, OpenAI lists the gpt-rosalind-research API model at $5 per million input tokens and $25 per million output tokens, available only to approved trusted-access customers (developers.openai.com), and Isomorphic Labs has no list price at all, operating instead through negotiated upfront-plus-milestone deal structures disclosed only when a partnership is announced.

Conclusion

Comparing Claude Science, GPT-Rosalind, and Isomorphic Labs as though they were three checkboxes on the same shopping list misstates the market as it actually exists in late 2026. They are three different kinds of organizations solving overlapping but distinct problems: Claude Science is an accessible, low-cost research productivity layer for individual scientists and small teams; GPT-Rosalind is a gated, specialized reasoning model for enterprises able to clear a formal access review; and Isomorphic Labs is a private, capital-intensive molecular-design partner reachable only through negotiated deals that pair upfront payments in the tens of millions of dollars with contingent milestone payments that can exceed $1 billion. All three sit within an industry that has absorbed more than $17 billion in investment since 2019. The field reached a late-stage milestone on July 7, 2026, when Insilico Medicine announced the initiation of a Phase III trial of rentosertib, a program it says was discovered and designed through its Pharma.AI platform; the drug remains investigational and has not been approved by a regulator. (Insilico Medicine)

For most life-sciences organizations, the practical path forward is not to pick a single winner but to match tool to task: evaluate Claude Science or GPT-Rosalind for near-term research productivity and hypothesis generation, where pricing and access terms are relatively concrete, and treat a relationship with Isomorphic Labs, or a comparable AI-native biotech, as a longer-horizon, higher-stakes partnership decision governed by different economics entirely. Although AlphaFold 3 launched in May 2024 and the Lilly and Novartis collaborations were announced in January 2024, IsoDDE, GPT-Rosalind, and Claude Science all launched in 2026. Organizations that adopt any of these tools should plan for continued, rapid change in capability, pricing, and access policy rather than treating today's feature set as fixed (blog.google; Isomorphic Labs). The most durable advice, echoed across the FDA's own regulatory posture, is to keep the discovery-stage use of any of these systems clearly separated from the evidentiary standards that will eventually apply once a candidate moves toward an actual regulatory submission.

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