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AI-Discovered Drugs in Clinical Trials 2026: Full Pipeline

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AI-Discovered Drugs in Clinical Trials 2026: Full Pipeline

Executive Summary

As of July 2026 (with dated updates through October 2026), the field of artificial intelligence (AI) driven drug discovery has moved from a speculative narrative to a measurable clinical pipeline. FDA approval records do not classify products by whether AI was used in discovery, so claims about a field-wide first approval depend on the methodology of the tracker making them. A conference abstract presented at the American Society of Clinical Oncology (ASCO) in 2026 counted **117 AI-enabled therapeutic assets across 63 companies** that had entered interventional human trials, of which 60 (51.3 percent) had completed Phase 1 and only 8 (6.8 percent) had completed Phase 2 (doi.org). Two third-party publications estimate a broader universe of more than **173 AI-designed programs** in clinical development in early 2026 and roughly **$60 billion** invested in AI drug discovery since 2019, respectively (medspark.ai) (ai2.work). These estimates use their publishers' own classifications and are not reconciled to the ASCO/JCO asset-level analysis, so they should not be treated as authoritative pipeline totals.

Among the named late-stage candidates, Insilico Medicine's **rentosertib** (formerly ISM001-055/INS018-055) is a TNIK inhibitor for idiopathic pulmonary fibrosis (IPF) that reported Phase 2a results in Nature Medicine showing a mean forced vital capacity (FVC) improvement of +98.4 mL versus a -20.3 mL decline on placebo over 12 weeks (nature.com). Insilico announced and registered its 320-patient Phase III study (NCT07687459) on July 7, 2026. At registration in July 2026, the study was listed as not yet recruiting, with an estimated start date of August 30, 2026. Update (October 2026): Insilico dosed the first patient in the trial, named GENESIS-

IPF-3, on September 9, 2026, and the registry now lists it as recruiting (prnewswire.com) (clinicaltrials.gov). Generate:Biomedicines announced on December 1, 2025 that it planned to initiate two global Phase 3 trials, SOLAIRIA-1 and SOLAIRIA-2, of its AI-engineered antibody GB-0895 (prnewswire.com).

Behind Insilico, **Recursion Pharmaceuticals** (which absorbed Exscientia in a $688 million all-stock merger that closed November 20, 2024) (reuters.com) runs a pipeline including REC-4881 (Phase 2, a 43 to 53 percent reduction in polyp burden in familial adenomatous polyposis, detailed below), REC-617 (a confirmed partial response in platinum-resistant ovarian cancer) (ir.recursion.com), and other clinical-stage candidates. **Isomorphic Labs**, the Alphabet/DeepMind spinout built on AlphaFold and backed by a $2.1 billion Series B round in May 2026 (biospace.com), had **not yet disclosed a clinical candidate or dosed a patient** as of mid-2026.

Beyond these three, a wider field of AI-native biotechs has clinical-stage assets, including Schrödinger (SGR-1505, a 22 percent overall response rate in lymphoma) (ir.schrodinger.com), Absci (ABS-101, its first AI-designed biologic for inflammatory bowel disease to enter a Phase 1 trial) (investors.absci.com), Generate:Biomedicines (GB-0895, moving to Phase 3 for severe asthma) (prnewswire.com), and Iambic Therapeutics (IAM1363, a 28 percent response rate in heavily pretreated HER2 cancer) (iambic.ai). A frequently cited 2024 BCG analysis found AI-discovered molecules had an 80 to 90 percent Phase 1 success rate, but only roughly 40 percent in Phase 2, comparable to historic industry averages (pubmed.ncbi.nlm.nih.gov), and the 2025 Nature Medicine rentosertib paper explicitly cautioned that "AI-discovered drugs have experienced similar levels of phase 2 trial failure as non-AI-discovered drugs" and that none had yet progressed through Phase 3 at the time of writing (nature.com). The global AI-in-drug-discovery market itself is estimated at roughly $2.3 to $2.6 billion in 2025, rising to $2.9 to $3.3 billion in 2026, with several research firms projecting a compound annual growth rate (CAGR) near 25 percent through the early 2030s (grandviewresearch.com). This report examines selected companies across that pipeline and details the clinical events, positive and negative, that define where AI drug discovery stands in 2026.

Introduction and Background

Artificial intelligence has been promoted as a way to compress the traditionally slow, expensive process of drug discovery, which the Tufts Center for the Study of Drug Development estimated in a landmark 2014 analysis costs roughly $2,558 million per approved compound (the origin of the commonly cited "$2.6 billion" figure) (globenewswire.com). A 2025 Nature Medicine paper puts the current industry benchmark at roughly $2 to $3 billion spent over 10 to 15 years to bring a single new drug to market (nature.com). Against that backdrop, a wave of "AI-native" biotechs, spinouts, and pharma-AI partnerships emerged over the past decade promising to shrink target discovery, molecule design, and preclinical timelines using machine learning, generative chemistry, and structure-prediction models such as AlphaFold.

The symbolic starting point most often cited is January 2020, when Sumitomo Dainippon Pharma (now Sumitomo Pharma) and Exscientia announced that **DSP-1181**, a serotonin 5-HT1A receptor agonist for obsessive-compulsive disorder (OCD), had entered Phase I trials in Japan after "requiring less than 12 months to complete the exploratory research phase," versus an industry average closer to 4.5 years (sumitomo-pharma.com). The BBC covered the milestone as, "in a world first for machine learning in medicine" (bbc.co.uk). As of mid-2026, with later developments flagged as updates, the field has both matured and been

humbled. Insilico Medicine announced and registered a Phase III study of rentosertib, its first Phase III program, on July 7, 2026; the registry initially listed the study as not yet recruiting, with an estimated start date of August 30, 2026 (a later first-patient dosing is noted in the dated update above). At the same time, no AI-discovered drug has yet received full FDA marketing approval, per industry tracking sources (medspark.ai).

This report is a data-driven, selected survey of the AI-discovered drug clinical pipeline as of mid-2026, covering companies with named candidates in the clinic, their reported trial stages and data, funding evidence, and comparisons of sector success and failure rates with traditional drug development. Life-sciences organizations evaluating whether and how to adopt AI in research and development increasingly need this kind of grounded, source-verified picture rather than vendor narrative; industry commentary often repeats the claim that AI-enhanced drug discovery and development can accelerate timelines by up to 60%, attributed to Deloitte research, a claim this report tests against the actual, verifiable trial record rather than taking it at face value.

Defining the Field: What Counts as an "AI-Discovered" Drug

"AI-discovered" is not a regulatory term, and the industry uses it loosely to cover several distinct levels of AI involvement. At one end are candidates for which AI systems proposed the novel biological target and generated the specific molecular structure, such as Insilico Medicine's rentosertib, discovered using the company's Pharma.AI platform, which the company states discovered both a novel target and a novel molecule "in under 18 months," versus a typical multi-year, $430 million-plus preclinical program (insilico.com). At the other end are programs where AI accelerated an existing discovery process, for example structure prediction, virtual screening, or clinical trial design, without AI generating the core molecule from scratch. The distinction matters for interpreting success-rate statistics, since studies that aggregate all "AI-enabled" assets, such as the 2026 ASCO/JCO conference abstract that identified 117 such assets across 63 companies with a median founding-to-Phase-1 time of 6.5 years (doi.org), necessarily mix these categories.

Multiple trackers now attempt to quantify the field's size. Medspark, an industry tracking outlet, reported that the number of AI-designed drug programs in clinical development "surged to over 173 in early 2026, up from roughly two dozen in late 2023" (medspark.ai). A separate 2026 industry analysis estimates that approximately $60 billion has flowed into AI drug discovery since 2019, producing about 175 clinical-stage programs, explicitly framing the moment as a "Phase III reckoning" given the absence of approvals to date (ai2.work). A January 2026 review in Pharmacological Reviews lists the positive Phase IIa results for Insilico Medicine's TNIK inhibitor, then still designated ISM001-055, in idiopathic pulmonary fibrosis, alongside the Recursion-Exscientia merger, among the field's defining developments since 2024 (sciencedirect.com), underscoring that peer-reviewed literature has begun treating individual AI-discovered clinical results, rather than platform capabilities alone, as the field's primary evidence base. No single authoritative, government-maintained registry of "AI-discovered drugs" exists; ClinicalTrials.gov records individual trials but does not tag AI-driven discovery, meaning every figure in this space, including the ones cited above, ultimately depends on a private company's or research group's own classification criteria. This report treats a candidate as AI-discovered when the sponsoring company itself, in a Tier 1 disclosure (press release, SEC/regulatory filing, or peer-reviewed paper), attributes target identification or molecular design substantially to an AI or machine-learning platform, and notes where that framing is contested.

The AI-Native Leaders: Insilico Medicine, Recursion Pharmaceuticals and Exscientia

Insilico Medicine, a Hong Kong-listed biotech that completed the largest Hong Kong biotech initial public offering (IPO) of 2025, raising HKD 2.277 billion and reaching a market capitalization of roughly HKD 20.7 billion (about $2.7 billion USD) after its December 2025 listing (insilico.com) (pharmaphorum.com), is the clearest current leader by clinical-stage volume. As of an April 2026 company disclosure, Insilico had nominated 30 preclinical candidate compounds and initiated three Phase II clinical trials (insilico.com). CEO Alex Zhavoronkov stated in mid-2025 that the company had nominated 22 developmental candidates, 10 of which had reached the clinical stage (drugdiscoverytrends.com). Its lead program, **rentosertib**, targets TNIK to block TGF-beta-dependent fibrogenesis and inflammation in IPF (insilico.com), and announced and registered a Phase III study (NCT07687459) on July 7, 2026, led by Professor Zuojun Xu of Peking Union Medical College Hospital and designed to enroll approximately 320 patients over 52 weeks of dosing. The registry listed the study as not yet recruiting, with an estimated start date of August 30, 2026 (insilico.com) (clinicaltrials.gov). The first patient was dosed on September 9, 2026, at Peking Union Medical College Hospital; the trial plans to enroll 320 participants across 47 centers in China, with the annual rate of decline in FVC over 52 weeks as its primary endpoint (prnewswire.com). Beyond rentosertib, Insilico's **ISM6331**, a pan-TEAD inhibitor for advanced malignant mesothelioma nominated in June 2023 using the company's Chemistry42 structure-based design tool (prnewswire.com), with first-in-human Phase 1 data scheduled for a Rapid Oral presentation at the European Society for Medical Oncology (ESMO) Congress in October 2026 (the congress outcome is not independently verified here) (insilico.com). A separate NLRP3 inflammasome inhibitor, **ISM8969**, partnered with Hygtia Therapeutics for up to $66 million in upfront and milestone payments, completed first-in-human dosing in June 2026 (hkexnews.hk). Insilico projected H1 2026 revenue of approximately $102.5 million to $106.5 million, up roughly 273 to 287 percent year on year (insilico.com). Its interim results, released August 26, 2026, reported H1 2026 revenue of $106.3 million, up 287.2 percent, and a net profit of $35.54 million (prnewswire.com).

Recursion Pharmaceuticals (Nasdaq: RXRX) took a different route to scale: acquisition. On August 8, 2024, Recursion agreed to buy Exscientia, its closest AI-drug-discovery rival, for $688 million in an all-stock deal (reuters.com), a combination that closed November 20, 2024, delisting Exscientia's Nasdaq shares (Nasdaq: EXAI) and creating a combined pipeline the companies described as "more than 10 clinical and preclinical programs," with over $450 million in upfront and realized milestone payments received to date against more than $20 billion in potential deal value (ir.recursion.com). The combined company's active clinical pipeline includes **REC-4881**, a MEK1/2 inhibitor in Phase 2 for familial adenomatous polyposis (FAP) that reported "a median 43% reduction in polyp burden at Week 13, deepening to 53% at Week 25" in its Q1 2026 update (ir.recursion.com); **REC-617**, a CDK7 inhibitor for advanced solid tumors that produced a confirmed durable partial response in a platinum-resistant ovarian cancer patient in December 2024 interim data (ir.recursion.com); **REC-1245**, an RBM39 degrader in Phase 1/2 that advanced from biological discovery to development candidate in 18 months, "more than twice as fast as the industry average," per the company (ir.recursion.com); and **REC-3565**, a MALT1 inhibitor. Legacy Exscientia asset **EXS74539/REC-4539**, an LSD1 inhibitor, began a new Phase 1 dose-determining ENLYGHT trial (NCT07517198) on April 13, 2026, sponsored by Exscientia AI Ltd. as a wholly owned Recursion subsidiary (clinicaltrials.gov). In May 2025, Recursion announced a pipeline update that discontinued three clinical-stage programs, REC-2282 (NF2), REC-994

(cerebral cavernous malformation), and REC-3964 (C. difficile infection), and paused REC-4539 (fiercebiotech.com). Recursion's Q1 2026 results reported a net loss of $117.5 million (versus $202.5 million a year earlier) and $665.2 million in cash (ir.recursion.com), underpinned by partnerships including a 2021 Roche/Genentech collaboration ($150 million upfront, up to $12 billion in aggregate potential across 40 programs) (ir.recursion.com) and a 2023 Bayer oncology deal (up to $1.5 billion in milestones) (ir.recursion.com). Nvidia had earlier invested $50 million in Recursion in July 2023 via a private investment in public equity (PIPE), pairing capital with cloud-computing access for AI foundation-model development (fiercebiotech.com).

Exscientia, before the merger, earned its own place in the field's history. Its DSP-1181 partnership with Sumitomo Dainippon Pharma is generally credited as the first AI-designed drug into human trials, and the company later signed a Merck KGaA (Darmstadt) collaboration worth $20 million upfront and up to $674 million in milestones for three programs (ir.recursion.com), and a Bristol Myers Squibb (BMS) collaboration, a roughly $1.2 billion "biobucks" discovery deal through which BMS obtained the EXS4318 PKC-theta inhibitor in 2021, before BMS discontinued that asset in October 2025 as part of a $1.5 billion cost-cutting initiative (fiercebiotech.com).

Isomorphic Labs and the Platform-Partnership Model

Isomorphic Labs, launched out of Alphabet's DeepMind in 2021 to commercialize AlphaFold protein-structure-prediction technology (prnewswire.com), uses a platform-partnership model backed by external funding. In January 2024 Isomorphic Labs signed same-day collaborations with **Eli Lilly** ($45 million upfront, up to $1.7 billion in milestones) (prnewswire.com) and **Novartis** ($37.5 million upfront, up to $1.2 billion in milestones) (prnewswire.com), a combination the company itself described as worth "nearly $3 billion" excluding royalties (isomorphiclabs.com); the Novartis scope was expanded by up to three additional research programs in February 2025 on the same financial terms (isomorphiclabs.com). Isomorphic Labs then raised $600 million in its first external funding round in March 2025, led by Thrive Capital (isomorphiclabs.com), with Hassabis stating the capital would "help us advance our own programs into clinical development" (prnewswire.com), and then a **$2.1 billion Series B** in May 2026, characterized by BioSpace as "the second largest biotech round of all time," trailing only Altos Labs' $3 billion 2022 raise (biospace.com). Isomorphic Labs president Max Jaderberg said in the Series B announcement that "our drug design engine works, and it's giving us a repeatable way" to advance programs (storage.googleapis.com).

As of mid-2026, Isomorphic Labs had **not put a molecule into human trials**. BioSpace reported in May 2026 that the company "hasn't yet disclosed a molecule or reached the clinic" (biospace.com). The company describes its wholly owned internal pipeline as concentrated in oncology and immunology (biospace.com), but as of mid-2026, no Tier 1 or Tier 2 source confirms a named clinical candidate or an FDA IND clearance for the company. Isomorphic Labs is therefore included in this report as a platform-partnership company with an internal pipeline focused on oncology and immunology; as of the July 31, 2026 cutoff, the article's cited sources did not identify a named clinical candidate or FDA IND clearance.

The Broader Pipeline: Additional AI-Native Biotechs in the Clinic

Beyond the three leaders, a wider set of AI-native biotechs has reached the clinic with varying degrees of success. **Schrödinger** (Nasdaq: SDGR), which uses a physics-based computational chemistry platform, reported in June 2025 that its MALT1 inhibitor **SGR-1505** achieved a 22 percent overall response rate across dose levels in relapsed/refractory B-cell lymphoma, with dose escalation complete (ir.schrodinger.com).

XtalPi, whose platform combines quantum physics, AI, and robotics, has enabled several clinical-stage molecules through partnerships. Company announcements name PEP08 (with PharmaEngine), RTX-117 (from its incubated ReviR Therapeutics) and SIGX1094 (with Signet Therapeutics) among these molecules; this report does not independently verify their regulatory clearances or designations.

Absci Corporation became a clinical-stage company in May 2025 when it dosed the first patient in a Phase 1 trial of **ABS-101**, which it described as its "first AI-designed biologic" for inflammatory bowel disease, with attributes including "high affinity, low immunogenicity, and extended dosing interval" that were "intentional attributes achieved through AI" (investors.absci.com). By November 2025, interim Phase 1 data showed an extended half-life versus first-generation anti-TL1A competitors, but Absci decided not to fund further internal development itself, instead seeking an out-licensing partner (sec.gov).

Generate:Biomedicines is advancing **GB-0895**, a long-acting anti-TSLP antibody for severe asthma, into two global Phase 3 trials (SOLAIRIA-1 and SOLAIRIA-2) enrolling approximately 1,600 patients, announced in December 2025 (prnewswire.com), after Phase 1 data in 96 patients showed an approximately 89-day half-life (prnewswire.com); the company's CEO said reaching Phase 3 within four years demonstrated that "an antibody engineered with AI can achieve a potentially best-in-class profile" (prnewswire.com). An earlier Generate program, **GB-0669**, an AI-generated antibody against SARS-CoV-2, moved "from computer to clinic in just 17 months" (generatebiomedicines.com), though the company later paused prophylactic development given shifting market conditions.

Iambic Therapeutics' HER2 inhibitor **IAM1363** showed partial responses in 28 percent of evaluable patients with measurable disease, including patients previously treated with trastuzumab deruxtecan (T-DXd) and tucatinib, per October 2025 ESMO data (iambic.ai); the company's CEO called it "one of the first clear demonstrations of a drug candidate with compelling clinical activity and safety from a TechBio company" (iambic.ai), noting the program moved from start to clinical trial initiation in two years (iambic.ai). The Phase 1/1b trial (NCT06253871) remained active and recruiting as of early 2026 (centerwatch.com).

Relay Therapeutics' RLY-2608 (zovegalisib), designed with the company's Dynamo motion-based drug design platform, reported an 11.0-month median progression-free survival in PI3K-alpha-mutated breast cancer as of June 2025 updated data (ir.relaytx.com). A Phase 3 trial, ReDiscover-2, comparing zovegalisib plus fulvestrant with capivasertib plus fulvestrant, has been recruiting since August 2025 (clinicaltrials.gov).

Analysis of Key Segments

The pipeline that emerges from these company-level surveys is heavily weighted toward early-phase, oncology-focused, small-molecule programs, with several program discontinuations noted in the company profiles. *Table 1* below summarizes the clinical-stage status of the AI-discovered and AI-enabled drug

candidates covered in this report as of July 2026.

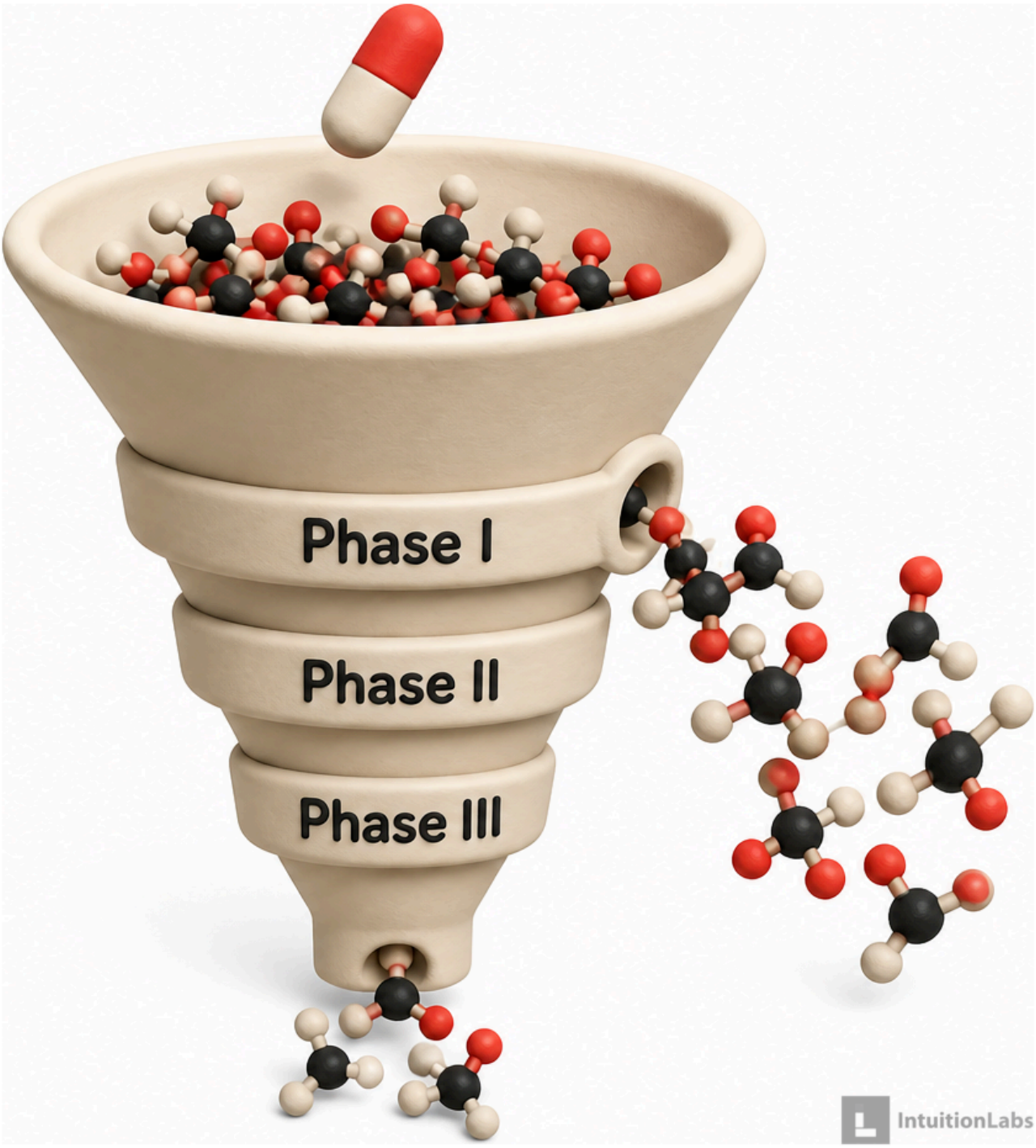

Table 1: Selected Clinical-Stage AI-Discovered and AI-Enabled Drug Candidates, 2026 Snapshot

Company	Lead Candidate	Indication	Phase (mid-2026)	Status Note
Insilico Medicine	Rentosertib (ISM001-055)	Idiopathic pulmonary fibrosis	Phase III	Initiated July 7, 2026 (insilico.com); first patient dosed September 9, 2026 (prnewswire.com)
Recursion Pharmaceuticals	REC-4881	Familial adenomatous polyposis	Phase 2	43 to 53% polyp reduction reported (ir.recursion.com)
Recursion Pharmaceuticals	REC-617	Advanced solid tumors	Phase 1/2	Confirmed partial response, ovarian cancer (ir.recursion.com)
Recursion (Exscientia legacy)	EXS74539/REC-4539	Select solid tumors, including SCLC	Phase 1	New trial started April 13, 2026 (clinicaltrials.gov)
Isomorphic Labs	Undisclosed	Oncology, immunology	Preclinical	No molecule disclosed as of May 2026 (biospace.com)
Schrödinger	SGR-1505	B-cell lymphoma	Phase 1	22% overall response rate (ir.schrodinger.com)
XtalPi / Signet Therapeutics	SIGX1094	Diffuse gastric cancer	Phase I	Company-reported clinical-stage program; regulatory designations not independently verified
Absci	ABS-101	Inflammatory bowel disease	Phase 1	Absci's first AI-designed biologic for IBD to enter a Phase 1 trial (investors.absci.com)
Generate:Biomedicines	GB-0895	Severe asthma	Phase 3	~1,600-patient SOLAIRIA-1/2 trials (prnewswire.com)
Iambic Therapeutics	IAM1363	HER2-altered cancers	Phase 1/1b	Preliminary sponsor-reported partial responses in 28% of 18 evaluable participants (iambic.ai)
Relay Therapeutics	RLY-2608 (zovegalisib)	PI3K-alpha-mutated breast cancer	Phase 3	11.0-month median PFS (ir.relaytx.com); Phase 3 ReDiscover-2 recruiting (clinicaltrials.gov)

The table shows a bifurcated pipeline: a small number of programs, principally rentosertib and GB-0895, are in or planned for late-stage Phase 3 development, while most remaining candidates cluster in Phase 1 or Phase 1/2. Oncology and immuno-oncology dominate by indication count, reflecting both the availability of well-characterized molecular targets for generative design and the field's origins in computational structural biology; fibrosis (rentosertib) and immunology (GB-0895, EXS4318 before discontinuation) are secondary clusters. Modality is also split: while small-molecule inhibitors dominate (rentosertib, REC-617, REC-4881, SGR-1505, ISM6331), a growing share are AI-designed biologics, notably Absci's ABS-101 and Generate:Biomedicines' antibody programs, indicating that generative AI design techniques originally proven on small molecules are extending into protein and antibody engineering.

Program-level pace also varies widely within the sector: the JCO conference abstract found a median of 6.5 years from company founding to Phase 1 entry across the 63 companies it tracked (doi.org), a timeline several multiples longer than the sub-30-month, target-to-Phase-1 pace Insilico reports for individual programs such as rentosertib (insilico.com), a reminder that company-level infrastructure buildout, not just per-molecule AI design speed, determines how quickly a young AI-native biotech reaches its first clinical trial. Insilico's own pipeline

also illustrates the field's therapeutic diversification beyond oncology and fibrosis: alongside rentosertib and ISM6331, the company lists a USP1 inhibitor for BRCA-mutant cancer (insilico.com), and its most recently nominated preclinical candidate, as of April 2026, originated from a research collaboration in the United Arab Emirates (insilico.com), pointing to an increasingly international discovery footprint rather than one confined to the United States, Western Europe, and China.

Data Analysis and Evidence

The clearest quantitative test of AI drug discovery's clinical performance comes from a peer-reviewed 2024 analysis, authored by Boston Consulting Group (BCG) researchers and published in Drug Discovery Today, which found that "AI-discovered molecules have an 80-90% success rate," substantially higher than historic industry averages, in Phase 1 trials, but that "in Phase II the success rate is approximately 40%, albeit on a limited sample size," comparable to historic industry averages (pubmed.ncbi.nlm.nih.gov). A subsequent 2025 Nature Medicine paper, reporting Insilico Medicine's own rentosertib Phase 2a results, offered a more cautious update: "AI-discovered drugs have experienced similar levels of phase 2 trial failure as non-AI-discovered drugs," and, as of that publication, "none has so far progressed through phase 3 trials" (nature.com). Rentosertib's Phase III study was announced and registered in July 2026 (HKEX announcement), but the registry initially listed it as not yet recruiting with an estimated August 30, 2026 start (the first patient was dosed later, on September 9, 2026); in any event, registration or initiation is not the same as progressing through or completing Phase III. The Nature Medicine statement therefore remains accurate for the status at the time of publication. *Table 2* summarizes the wider clinical-asset counts and market-size estimates behind these dynamics.

Table 2: AI Drug Discovery, Selected Quantitative Benchmarks (2024 to 2026)

Metric	Figure	Source and As-Of Date
AI-enabled clinical assets (interventional trials)	117 assets, 63 companies	JCO/ASCO 2026 conference abstract, data as of Dec. 1, 2025 (doi.org)
Share of those assets completing Phase 1	51.3% (60 of 117)	Same source (doi.org)
Share completing Phase 2	6.8% (8 of 117)	Same source (doi.org)
Median founding-to-Phase-1 time	6.5 years	Same source (doi.org)
AI-designed drug programs in clinical development	Over 173 (early 2026), up from ~24 in late 2023	Medspark, July 19, 2026 (medspark.ai)
AI-in-drug-discovery global market, 2025	$2.3 billion (est.)	Grand View Research (grandviewresearch.com)
Same market, 2026 to 2033 forecast	$2.9 billion to $13.8 billion, 24.8% CAGR	Grand View Research (grandviewresearch.com)
Alternate market estimate, 2026 to 2031	$3.25 billion to $10.29 billion, 25.94% CAGR	Mordor Intelligence (mordorintelligence.com)

Metric	Figure	Source and As-Of Date
VC funding for AI drug development, first 3 quarters 2025	$2.7 billion	PitchBook, Nov. 12, 2025 (pitchbook.com)
AI-ML drug discovery partnership deals, 2025	114 deals, $43.4 billion potential value	DealForma, Jan. 13, 2026 (dealforma.com)
AI-ML drug discovery M&A, 2025	99 deals, $12.3 billion	DealForma (dealforma.com)
Cumulative AI drug discovery investment since 2019	~$60 billion into ~175 clinical-stage programs, 0 approvals	ai2.work, July 24, 2026 (ai2.work)

These figures paint a market that is small in absolute revenue terms (a $2 to $3 billion software and platform market as of 2025-2026) relative to the tens of billions of dollars committed as venture capital and pharma-partnership deal value, and relative to the roughly $60 billion cumulative investment tracked since 2019. That gap is a structural feature of the industry: AI drug discovery companies mostly monetize through milestone-laden partnerships and platform licensing rather than product sales. FDA approval records do not classify products by whether AI was used in discovery, so they cannot independently establish a field-wide approved-product-revenue total. On timelines, Insilico's own claims are illustrative of the field's central efficiency argument: the company's target-discovery-to-Phase-I timeline for rentosertib was "under 30 months," versus a typical multi-year, $430-million-plus preclinical program (insilico.com), and in a July 2026 interview, Insilico's CEO told a wire-service reporter that traditional drug discovery "takes about 4.5 years to get to a drug developmental candidate," versus the company's typical 13-month and record 9-month AI-driven timelines in China (979weve.com). Insilico separately claimed its rentosertib preclinical program cost roughly one-tenth of, and took a fraction of the time of, a traditional program it estimated "would have taken years and cost over $400 million" (techstrong.ai). Recursion's REC-1245 program, discussed above, moved from biological discovery to development candidate more than twice as fast as the industry average by the company's own account. These vendor-reported acceleration figures should be read as company claims rather than independently audited benchmarks; no peer-reviewed, cross-company study in this report's fact base independently verified a specific multiple of time or cost savings, though the directional finding, materially faster preclinical timelines with clinical-stage attrition broadly similar to the traditional industry, is consistent across the BCG, Nature Medicine, and JCO sources cited above.

Funding concentration is a further, and underappreciated, feature of the data. One funding tracker estimated that Isomorphic Labs' $2.1 billion Series B alone accounted for approximately 87 percent of all disclosed AI-drug-discovery venture capital raised in the first half of 2026 (newmarketpitch.com). This concentration means sector-level funding totals reflect an uneven distribution of capital across companies. Recursion's own SEC filing on the Exscientia combination documents the transaction's structure as a UK court-sanctioned Scheme of Arrangement that took legal effect through "the delivery of such order to the Registrar of Companies in England and Wales" (sec.gov), an unusually cross-border legal structure for a Nasdaq-listed AI drug discovery merger, and upon closing, Exscientia's American Depositary Shares (ADSs) "ceased trading and will be delisted from Nasdaq" (nasdaq.com).

Case Studies and Real-World Examples

The case studies below examine the most advanced programs in the pipeline, beginning with rentosertib.

Rentosertib: From a Phase 2a Signal to a Registered Phase III Study

Insilico Medicine's rentosertib is the field's central proof-of-concept case. The GENESIS-IPF Phase 2a trial randomized 71 idiopathic pulmonary fibrosis patients across 22 sites in China to 12 weeks of 30 mg once daily, 30 mg twice daily, or 60 mg once daily rentosertib, or placebo (insilico.com). The primary endpoint was safety: the percentage of participants with at least one treatment-emergent adverse event. A secondary lung-function endpoint, change in forced vital capacity, favored the high-dose arm: a mean improvement of +98.4 mL (95 percent confidence interval, 10.9 to 185.9) versus a mean decline of -20.3 mL on placebo (nature.com), with an even larger 187.8 mL improvement in the subgroup not on standard background antifibrotic therapy (drugdiscoverytrends.com). The study's authors concluded that "these results suggest that targeting TNIK with rentosertib is safe and well tolerated" and merited larger, longer trials (nature.com). Insilico acted on that conclusion by announcing and registering a 320-patient Phase III study (NCT07687459) on July 7, 2026, its first Phase III program. The registry initially listed the study as not yet recruiting, with an estimated start date of August 30, 2026. The trial, GENESIS-IPF-3, subsequently dosed its first patient on September 9, 2026 (prnewswire.com).

Implications and Future Directions

Two trends should shape how life-sciences organizations interpret the AI drug discovery pipeline over the next several years. First, the sector is consolidating: Recursion's absorption of Exscientia for $688 million (reuters.com) suggests that stand-alone AI-native biotechs face pressure to either scale through acquisition or convert into platform-licensing businesses rather than independent drug developers. Second, funding concentration, with a single company's $2.1 billion raise accounting for an estimated 87 percent of first-half-2026 sector venture capital (newmarketpitch.com), means aggregate investment figures reflect how capital is distributed across companies; company-level trial data provides separate context from sector-level funding headlines.

For pharmaceutical and life-sciences organizations evaluating whether and how to build or buy AI drug discovery capability, the picture as of mid-2026 includes preliminary, sponsor-reported findings: REC-4881 produced a median 43% Week-13 reduction in polyp burden among 12 efficacy-evaluable participants in an ongoing open-label Phase 2 study, while IAM1363 showed partial responses in 28% of 18 evaluable participants in a Phase 1/1b study (ir.recursion.com) (iambic.ai), and multiple Phase III programs, set against industry trackers' reported zero-approval record, Phase 2 attrition that the Nature Medicine authors themselves describe as comparable to the traditional industry (nature.com), and several named program discontinuations across the companies surveyed in this report. This is the kind of source-verified evidence base needed to separate a vendor's platform narrative from its verified clinical track record before committing R&D budget or partnership capital to any single AI drug discovery approach.

Looking ahead, the next 12 to 18 months will help show whether recent Phase 3 announcements, registrations, and ongoing studies translate into successful pivotal-trial readouts and, eventually, regulatory approvals. Further clinical updates from rentosertib, GB-0895, REC-4881, REC-617, SGR-1505, and IAM1363 will help show whether Phase 1 efficiency gains translate into Phase 2 and Phase 3 approval rates that meaningfully beat, rather than merely match, the traditional industry baseline.

Frequently Asked Questions (FAQs)

How many AI-discovered drugs are in clinical trials as of 2026? Industry trackers put the number of AI-designed drug programs in clinical development at over 173 as of early 2026 (medspark.ai), while an ASCO/JCO conference abstract counted 117 AI-enabled therapeutic assets across 63 companies in interventional trials as of December 2025 (doi.org). The discrepancy reflects differing definitions of what counts as "AI-discovered" or "AI-enabled," discussed above.

What does "AI-enabled" versus "AI-discovered" mean in these pipeline counts? "AI-enabled" is the broader term, covering any use of machine learning in target identification, molecular design, or trial optimization, while "AI-discovered" more narrowly implies AI generated the specific molecular structure or target hypothesis, as with Insilico Medicine's rentosertib (insilico.com). The JCO analysis of 117 assets across 63 companies used the broader "AI-enabled" framing, which is one reason its count differs from narrower trackers (doi.org).

Has an AI-discovered drug been approved by the FDA yet? No. As of mid-2026, no AI-discovered drug has received full FDA marketing approval, per industry tracking sources (medspark.ai). Insilico Medicine announced and registered a Phase III study of rentosertib on July 7, 2026; the registry initially listed it as not yet recruiting, with an estimated start date of August 30, 2026 (insilico.com), and Generate:Biomedicines' GB-0895 is in Phase 3 for severe asthma (prnewswire.com), but neither has yet completed pivotal testing. Rentosertib's Phase III trial, GENESIS-IPF-3, dosed its first patient on September 9, 2026 (prnewswire.com). One late-stage drug whose design is described as AI-assisted is Takeda’s zasocitinib (TAK-279), a TYK2 inhibitor for plaque psoriasis designed by Nimbus Therapeutics in collaboration with Schrödinger (dermatologytimes.com). Whether it counts as AI-discovered depends on each tracker's definition.

What is the success rate of AI-discovered drugs compared with traditional drug discovery? A 2024 BCG-authored, peer-reviewed analysis found an 80 to 90 percent Phase 1 success rate for AI-discovered molecules, well above historic industry averages, but only about 40 percent in Phase 2, in line with historic industry averages (pubmed.ncbi.nlm.nih.gov). A 2025 Nature Medicine paper similarly found AI-discovered drugs experience Phase 2 failure rates "similar" to non-AI drugs (nature.com).

Which biotech companies currently have AI-discovered drugs in clinical trials? Companies with named clinical-stage AI-discovered or AI-enabled candidates as of mid-2026 include Insilico Medicine, Recursion Pharmaceuticals (including former Exscientia programs), Schrödinger, XtalPi (and its partners PharmaEngine, ReviR Therapeutics, and Signet Therapeutics), Absci, Generate:Biomedicines, Iambic Therapeutics, and Relay Therapeutics. Isomorphic Labs' disclosed work remained preclinical as of mid-2026 (biospace.com).

Is there a single, authoritative tracker of AI drug discovery pipelines? No government or single industry body maintains an authoritative AI-drug-discovery tracker. ClinicalTrials.gov records individual trials, but “AI-discovered” is not a standard registry classification, so counts depend on each research group’s definitions and inclusion criteria.

Conclusion

By July 2026, AI-discovered and AI-enabled drug candidates have moved decisively past the proof-of-concept stage that defined the field when DSP-1181 entered Phase I in January 2020. Industry trackers reported that the field had not yet delivered an FDA marketing approval, but that conclusion depends on their AI-discovery classifications because FDA approval records do not use such a category. Insilico Medicine announced and registered a Phase III rentosertib study following a Phase 2a study whose primary endpoint assessed treatment-emergent adverse events and whose secondary endpoints included FVC; the registry initially listed the Phase III study as not yet recruiting, with an estimated August 30, 2026 start; the first patient was subsequently dosed on September 9, 2026. Recursion Pharmaceuticals, having absorbed Exscientia, is generating Phase 2 efficacy data in familial adenomatous polyposis and Phase 1 responses in ovarian cancer, while simultaneously discontinuing multiple programs as part of ordinary portfolio management. A broader field of six additional AI-native biotechs profiled here, from Schrödinger and XtalPi to Absci, Generate:Biomedicines, Iambic Therapeutics, and Relay Therapeutics, has produced credible early clinical data alongside a number of program discontinuations. Isomorphic Labs had raised substantial capital and remained in preclinical development as of mid-2026.

The quantitative evidence assembled in this report supports a measured conclusion: published analyses report 80 to 90 percent Phase 1 success and roughly 40 percent Phase 2 success for the studied AI-discovered molecules, with the Phase 2 estimate based on a limited sample and broadly comparable to historical industry performance. Company reports describe faster preclinical timelines and several candidates have produced clinical signals, but the evidence does not yet show that AI materially changes the probability of surviving Phase 2 and Phase 3 testing. Whether that changes will be determined largely by the data rentosertib, GB-0895, and the next cohort of Phase 2 assets generate over the following one to two years, and life-sciences organizations tracking this space should weigh individual, verified clinical results over platform-level funding and timeline claims when assessing where the technology genuinely stands.

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