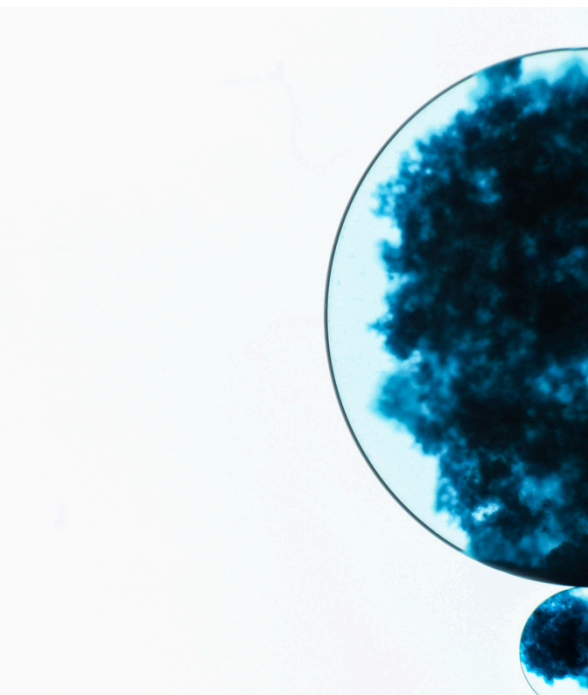
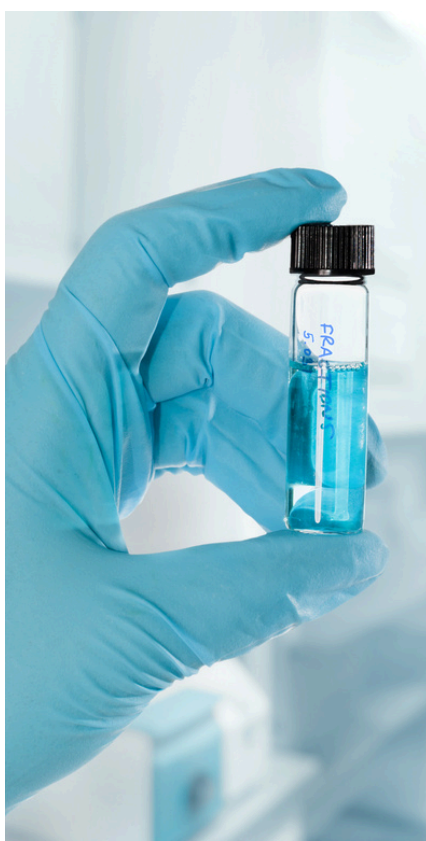




AI BASED DRUG DISCOVERY



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AI-Powered Drug Discovery: Reshaping the Pharmaceutical Frontier

An in-depth analysis of artificial intelligence applications transforming the drug discovery pipeline from target identification to clinical development.

Artificial intelligence is no longer a peripheral tool in drug discovery. It is rapidly becoming the central engine of pharmaceutical R&D, compressing timelines from over a decade to as few as three years, while dramatically reducing attrition and capital burn.

Traditional drug development costs upwards of \$2.6 billion per approved molecule, with failure rates exceeding 90% in clinical trials. AI-native approaches encompassing generative molecular design, protein structure prediction, multi-omics integration, and adaptive trial design are dismantling each of these constraints simultaneously. The result: a market in structural transformation, with legacy pharma partnering aggressively with AI-first biotechs and technology firms.

\$1.9 T	45B	70%	45+
GLOBAL PHARMA MARKET (2025)	AI DRUG DISCOVERY MARKET BY 2030	REDUCTION IN TARGET ID TIME	AI DISCOVERED DRUGS IN TRIALS

Four AI Capabilities Driving Disruption

Generative Molecular Design

LLMs and diffusion models generate novel molecules with targeted properties, expanding chemical-space exploration beyond traditional HTS. Examples include MolGPT, REINVENT 4.0 and DiffSBDD.

Protein Structure Prediction

AlphaFold 3 and RoseTTAFold predict protein–ligand, protein–DNA and protein–RNA interactions, accelerating structure-based drug design at unprecedented scale.

Target Validation

Graph neural networks and transformers integrate genomics, proteomics, metabolomics and clinical data to uncover disease mechanisms and patient-stratification biomarkers.

Adaptive Clinical AI

AI enables patient matching, synthetic control arms, dropout prediction and dose optimization, potentially shortening trials while reducing development costs.

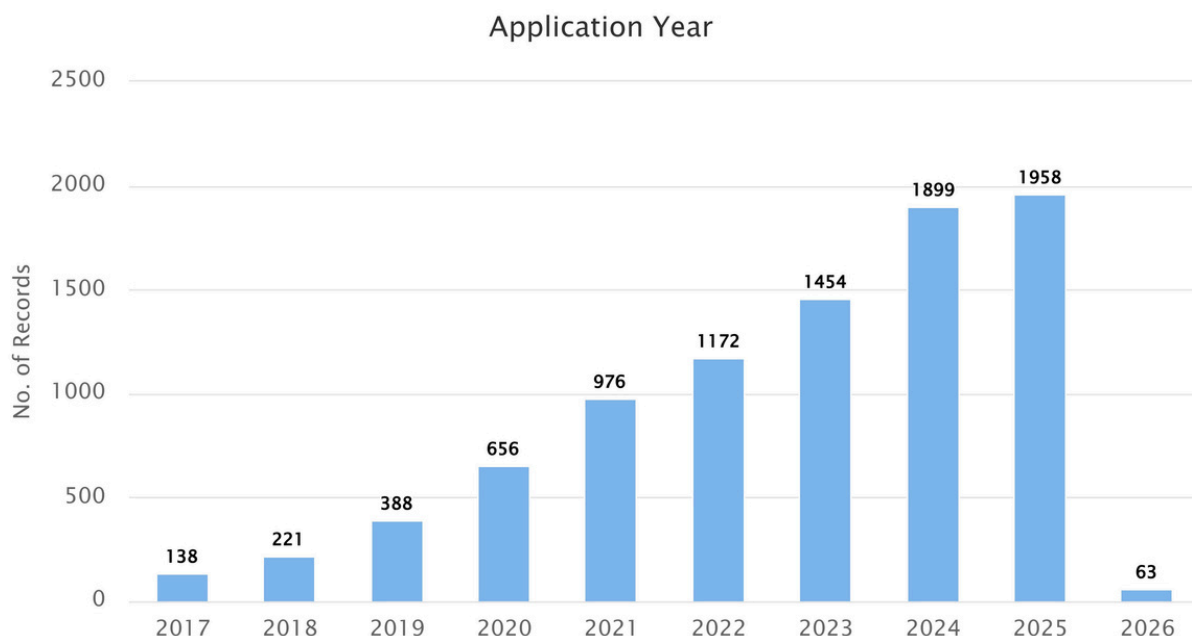
Executive Summary

AI-based drug discovery represents a structural transformation in how pharmaceutical innovation is generated, protected, and commercialised. This report analyses the global patent landscape for AI-driven therapeutic platforms across five disease verticals and five core AI technology types, surfacing trends in IP strategy, competitive positioning, and commercial readiness.

- IP activity is highly concentrated: neural networks and machine learning account for the majority of filings, with oncology representing the dominant therapeutic focus across all AI categories.
- Foundational AI platforms are gaining strategic ground: filings using foundational model architectures have grown at 34% CAGR since 2020, reflecting a shift toward general-purpose molecular intelligence platforms.
- Language models show strongest emergence at the clinical stage: LLM-based applications dominate trial design, biomarker identification, and regulatory submission automation.
- Reinforcement learning commands a distinct niche: RL filings are concentrated at hit identification and lead optimisation stages, reflecting their strength in iterative molecular design.
- Geographic IP competition is intensifying: China has overtaken Europe in annual AI drug discovery patent volumes since 2022, with India emerging as a strategically positioned filer.
- Post-peak filing trends signal consolidation: a cumulative 44% decline from peak volumes indicates dominant players are building density rather than exploring breadth.
- Royalty and licensing potential is material: the Glenmark-AbbVie transaction demonstrates India-origin AI-enabled biologics IP can command billion-dollar licensing valuations.
- Royalty and licensing potential is material: the Glenmark-AbbVie transaction demonstrates India-origin AI-enabled biologics IP can command billion-dollar licensing valuations.

9500+ AI Drug Discovery patents Analysed	34% CAGR Foundational AI filings 2020–24	70% Decline from filing peak 2018–2024	45+ Landmark AI-pharma Licence value
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Overall Filing Trend



Post-2020 is a structural inflection, not growth: AI shifted from experimental tooling to core R&D infrastructure.

Momentum indicates permanent integration into drug discovery, not a crisis-driven spike.

From platforms to products: Filing focus is moving toward AI-generated molecules and targets, signaling ownership of therapeutic outcomes.

New entrants reshaping IP landscape: AI-native biotechs and tech players are now central patent drivers, not just pharma incumbents.

Data advantage is compounding filings: Proprietary datasets + feedback loops are accelerating innovation velocity for early movers.

Emerging patent thickets: Dense filings in core areas (target ID, molecular design) will increase freedom-to-operate risks.

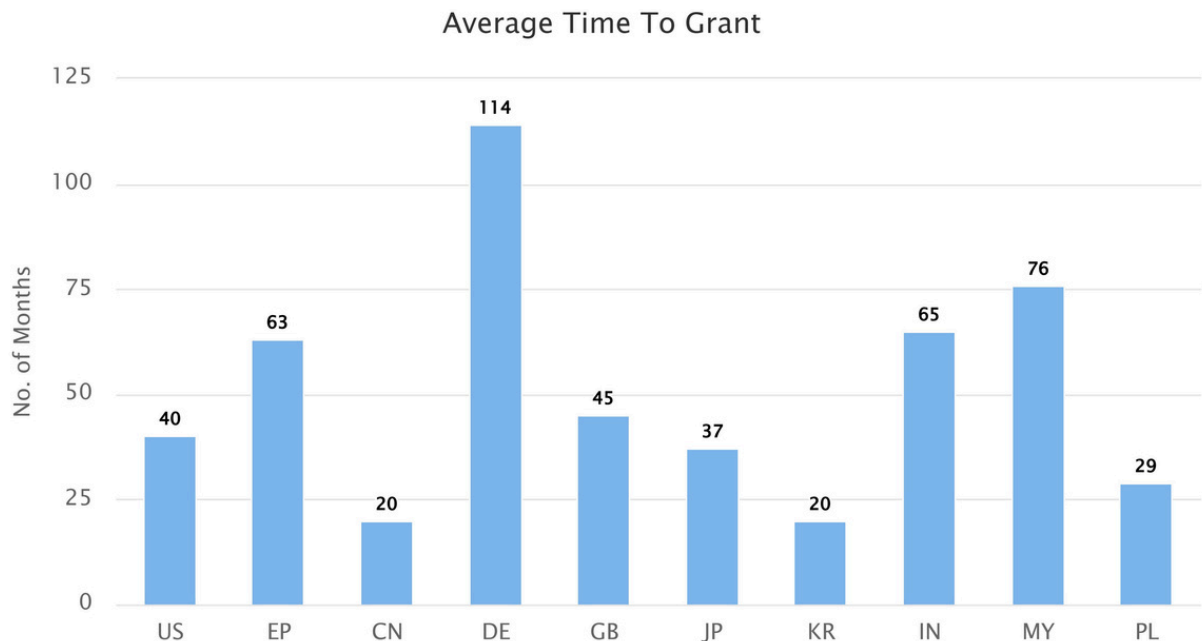
Land-grab phase underway (2022–2025): Volume surge suggests quantity over quality, expect future tightening and litigation.

Early signs of consolidation (2025): Slowing growth hints at a shift toward portfolio strength and commercialization.

2026 dip is artificial: Likely due to publication lag, not a real decline in innovation.

Strategic shift ahead: Advantage moving from filings to data control, model performance, and clinical validation.

Average Time to Grant (Jurisdictional Impact)



Grant speed is now a strategic lever, not admin detail: Jurisdictions like China and Korea enable faster IP crystallization, accelerating commercialization timelines.

Europe reflects rigor over speed: Germany's long timelines signal deep examination intensity, often translating into stronger but slower-moving rights.

US sits in a strategic middle ground: Balanced timelines allow both speed and claim robustness, making it a preferred anchor jurisdiction.

Shorter grant cycles enable companies to assert rights sooner in competitive races, especially in fast-moving AI domains.

Longer timelines often correlate with more defensible patents, critical for high-value therapeutics.

Portfolio sequencing matters: Companies are likely prioritizing early grants in fast jurisdictions, while using slower ones for long-term strength.

Asia is optimizing for speed: China and Korea timelines reflect a policy-driven push to accelerate innovation protection cycles.

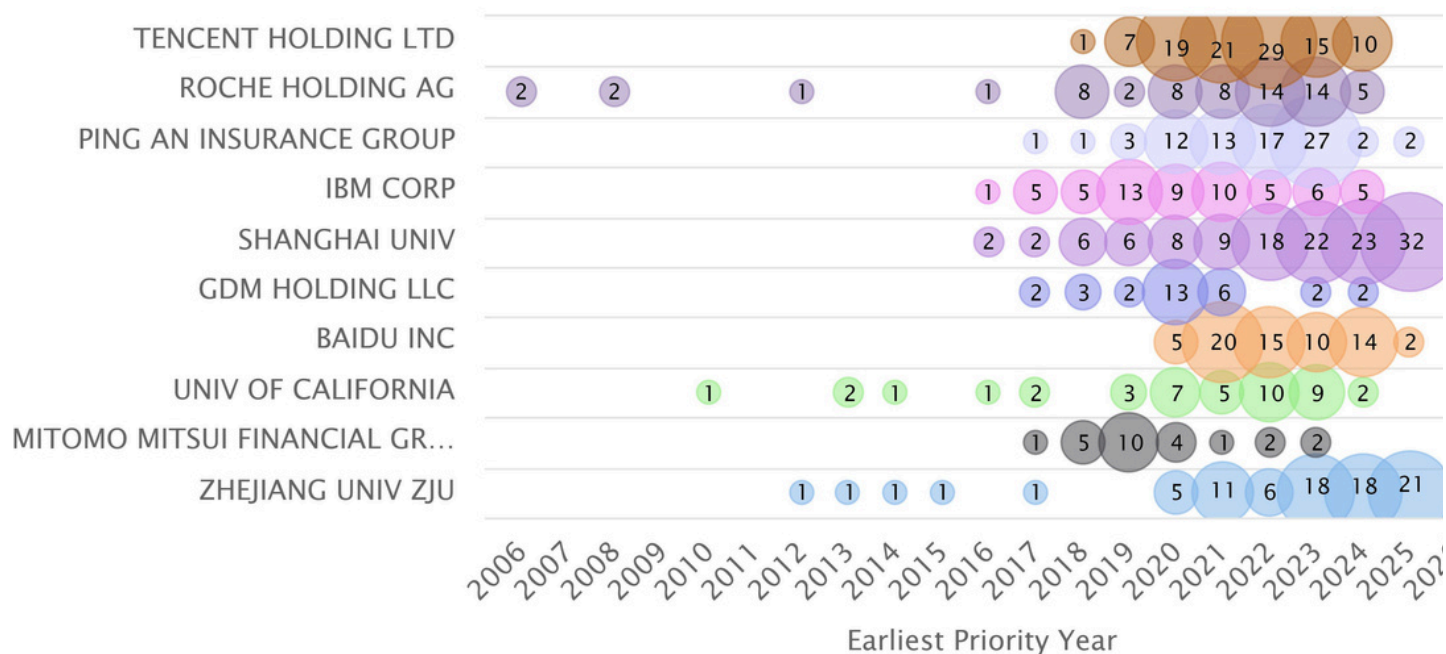
Hidden cost of delay: Longer grant times can compress effective patent life, especially in fast-evolving AI-driven pipelines.

Divergence creates arbitrage opportunities: Smart filers can stagger filings to balance early protection and long-term enforceability across regions.

Implication: IP strategy is no longer global-first, it's jurisdiction-optimized, aligning speed, strength, and market entry timing.

Top Assignees Filing Trend

Assignee Innovation Timeline



Late-stage clustering (post-2018): Most assignees show sharp activity only in recent years, indicating synchronized market entry rather than long-term incumbency.

Minimal early presence, followed by rapid expansion by Tencent suggests a fast-follow, scale-first IP strategy.

Roche shows continuity: Early filings + steady recent activity reflect sustained, research-led positioning rather than reactive entry.

Shanghai & Zhejiang Univ = volume engines: Consistent, high-density filings indicate institutionalized IP generation pipelines, not sporadic innovation.

Ping An & IBM signal cross-industry convergence: Their timelines show non-pharma players entering and scaling in parallel with core biotech actors.

Concentrated recent filings by Baidu suggests AI capability redeployment into drug discovery, not organic pharma evolution.

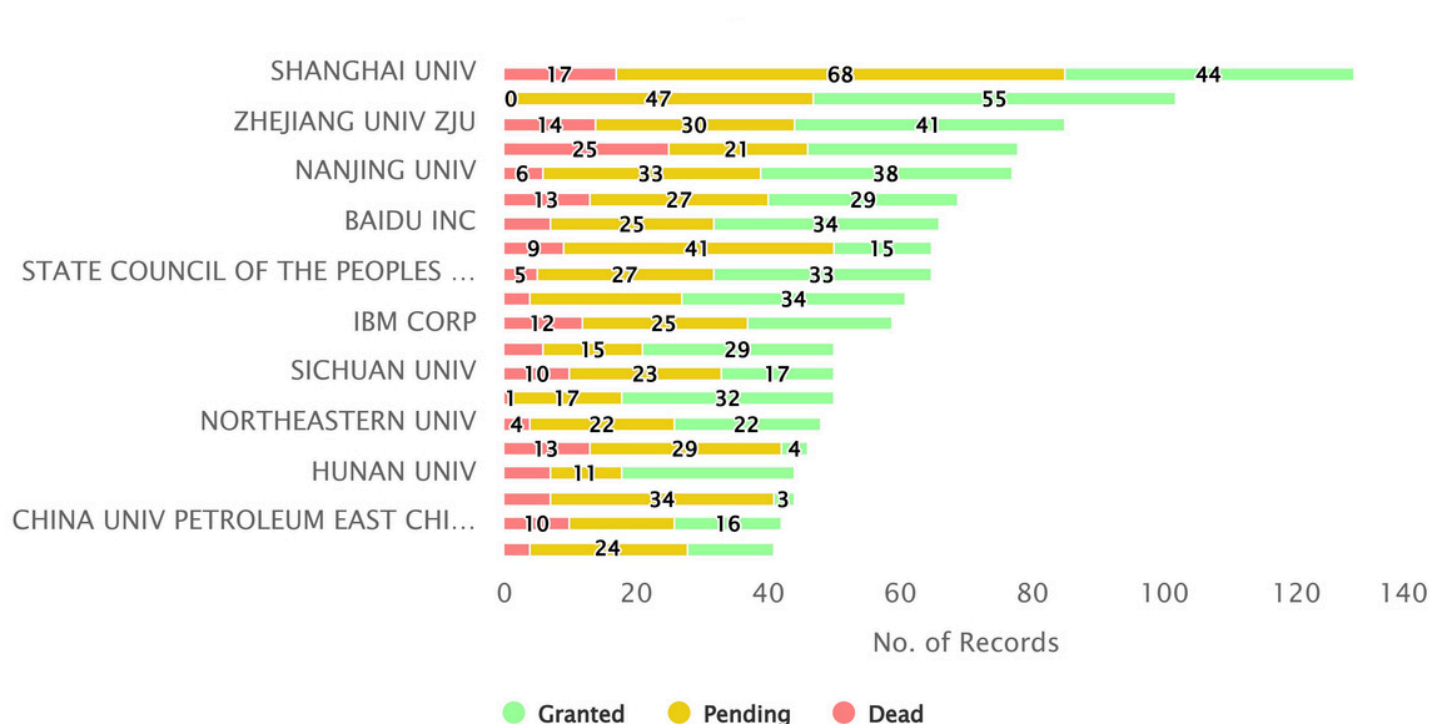
US academia is early but selective: Sparse but earlier entries indicate high-value, research-driven contributions rather than volume play.

Japanese players are steady but contained: Gradual timelines imply measured participation, likely in niche or precision domains.

Post-2020 synchronization effect: Multiple assignees ramp simultaneously, pointing to a global inflection where AI drug discovery became mainstream.

With most players entering late and scaling fast, differentiation will depend less on timing and more on depth

Portfolio Legal Status



High pending ratios signal pipeline-heavy portfolios: Most assignees hold a large share of pending cases, indicating future IP strength is still under construction, not yet enforceable.

Corporate portfolios skew more pending-heavy: Players like IBM and Baidu show forward-loaded pipelines, suggesting recent entry or ongoing expansion.

Shanghai Univ leads in conversion efficiency: Strong granted base alongside high filings suggests mature IP management, not just volume generation.

State-linked entities show mixed efficiency: Higher pending and moderate granted counts reflect scale-first filing with slower conversion cycles.

Zhejiang Univ shows balanced maturity: A relatively even split across granted and pending reflects steady progression from filing to enforceable rights.

Portfolio depth > portfolio size: Leaders are distinguished not by filings alone, but by granted-to-pending balance and lifecycle management.

Dead portfolio share remains controlled: Low abandonment rates across players indicate disciplined filing strategies with selective pruning.

Execution capability is the differentiator: Variation in grant ratios highlights that IP strategy (prosecution, claim design) is as critical as innovation itself.

Academic institutions are not just filing more they are successfully converting into granted IP at scale as compared to corporates.

Implication: Competitive advantage will hinge on who converts fastest to enforceable rights, not who files the most.

Technology Taxonomy

APPLICATION

APPLICATION



CLINICAL &
REGULATORY
(1411)



DISCOVERY &
TARGET BIOLOGY
(7756)



HIT IDENTIFICATION
& DESIGN
(578)



LEAD
OPTIMIZATION
(745)



PRECLINICAL &
SAFETY
(473)

ARTIFICIAL INTELLIGENCE

ARTIFICIAL
INTELLIGENCE



FOUNDATIONAL
AI
(2029)



LANGUAGE
MODEL
(214)



MACHINE
LEARNING
(2057)



NEURAL
NETWORK
(4755)



REINFORCEMENT
LEARNING
(425)

DATA TYPE

DATA TYPE



BIOLOGICS/
GENOMICS
(5204)



CLINICAL AND REAL-
WORLD DATA
(1835)



EXPERIMENTAL &
PHARMACOLOGICAL DATA
(3969)



IMAGING AND
SPATIAL DATA
(1942)



MOLECULAR &
CHEMICAL DATA
(4053)

DISEASE TYPE

DISEASE TYPE



AUTOIMMUNE
(157)



CARDIAC
(183)



INFECTIOUS
(405)



NEUROLOGICAL
(408)



ONCOLOGY
(1230)

Market Overview



AI-based drug discovery is undergoing a structural shift from experimental augmentation to becoming a core layer of pharmaceutical R&D infrastructure. What was once limited to discrete applications such as target identification or virtual screening is now evolving into integrated, end-to-end platforms that span discovery through early clinical development. This transition is being driven by persistent industry pressures escalating R&D costs, high attrition rates in clinical trials, and the need to compress development timelines positioning AI not as a peripheral tool, but as a strategic enabler of productivity and decision-making.

The competitive landscape reflects this maturation. Early-stage point solutions are giving way to platform-centric models that combine machine learning, generative chemistry, and physics-based simulations into unified workflows. At the same time, large pharmaceutical companies are increasingly internalizing AI capabilities, while continuing to engage in high-value partnerships and acquisitions to access specialized technologies and data assets. This has led to a market dynamic where capability aggregation and platform depth are becoming more important than standalone innovation.

A defining feature of the market is the centrality of data. Competitive advantage is shifting decisively toward companies that control high-quality, proprietary datasets and the infrastructure required to curate, standardize, and continuously refine them. Multimodal data integration spanning genomics, chemical structures, imaging, and real-world clinical data is emerging as a key differentiator, enabling more robust and generalizable models. In parallel, closed-loop systems that integrate computational predictions with experimental validation are proving critical in improving translational success.

Investment trends further underscore this evolution. Capital is increasingly directed toward scalable platforms with demonstrated validation rather than single-asset pipelines, while deal activity reflects a move toward larger, milestone-driven collaborations.

Despite this progress, the path to scale remains constrained by structural challenges. The translation of *in silico* predictions into clinical success continues to be a key bottleneck, compounded by regulatory uncertainty and the inherent complexity of biological systems.

In this context, AI-based drug discovery is best understood not as a standalone market segment, but as an evolving operating model for life sciences.

Key Players



Recursion Pharmaceuticals

Jurisdiction: North America

Technology: Recursion OS

AI Type: ML, DL, Generative AI, LLMs, Computer Vision

Primary Stage: Drug Discovery

Secondary Stage: Preclinical Research

Sub-stage Focus: Target ID to Preclinical Testing

Core Use Case: AI-driven automated drug discovery platform (design–test–learn loop)

- ✓ AI-driven drug discovery platform with automated lab integration
- Uses biological data for target ID and molecule design
- Robotic systems enable high-throughput testing
- Continuous design–test–learn loop
- Applied in discovery and preclinical stages



In Silico Medicine

Jurisdiction: North America

Technology: Rentosertib

AI Type: Generative AI, NLP, Causality Inference

Primary Stage: Drug Discovery

Secondary Stage: Preclinical

Sub-stage Focus: Target Discovery, Molecule Design, Preclinical Testing

Core Use Case: AI-designed fibrosis drug

- ✓ AI identified novel fibrosis target using omics + literature mining
- Generative AI designed and optimized candidate molecules
- Multi-parameter evaluation (binding, stability, permeability)
- Preclinical validation in fibrosis mouse models
- Optimized ADME, solubility, and safety profile
- Advanced to Phase II clinical trials

Mergers & Acquisitions

Siemens → Dotmatics

Year 2025

Deal \$5.1 Billion

Indication AI-powered scientific R&D data management

Technology AI lab data management linking research to manufacturing

- Purchased Dotmatics, leading AI scientific software used by 1,400+ pharma companies.
- Enables Siemens to connect laboratory data management directly to manufacturing workflows.
- Accelerates drug research timelines through integrated AI data analysis.

GE HealthCare → Intelera

Year 2025

Deal \$2.3 Billion

Indication Outpatient imaging AI & SaaS diagnostics

Technology Cloud AI, SaaS radiology platform

- Expands GE HealthCare's AI presence in high-growth outpatient imaging markets.
- Intelera contributes ~\$270M in annual revenue with ~90% recurring and 30% EBITDA margins.
- Accelerates GE HealthCare's shift toward SaaS and recurring digital revenue.

BioNTech → InstaDeep

Year 2023

Deal ~\$549M (£362M upfront + £200M milestones)

Indication AI-powered immunotherapy & vaccine design

Technology DeepChain biological sequence design platform

- Fully acquired InstaDeep, operator of the DeepChain biological sequence design ML platform.
- Embeds machine learning across drug discovery, immunotherapy design, and vaccine pipelines.
- Strengthens BioNTech's pioneering position in AI-powered drug discovery and design.

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