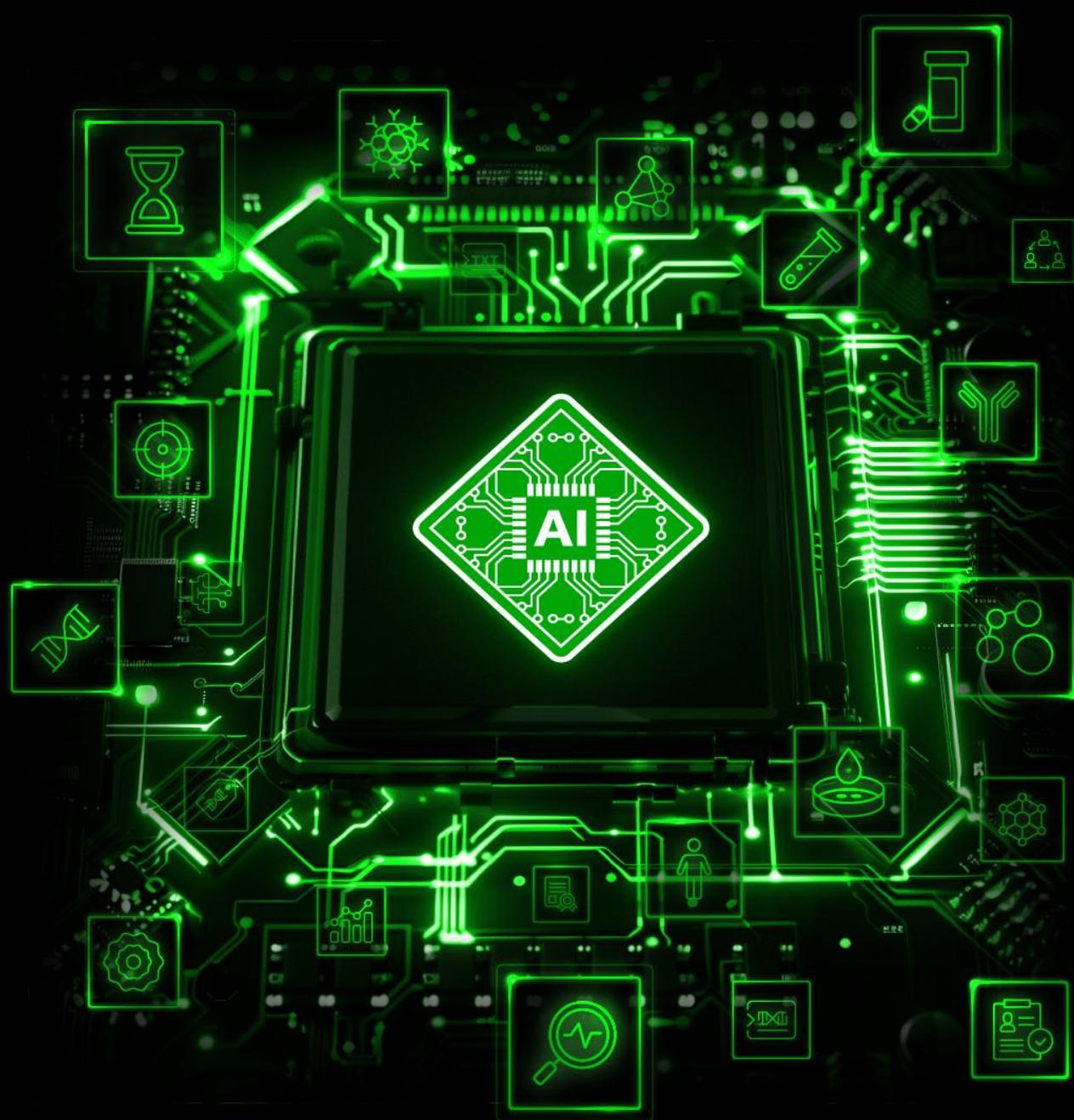


**Insilico
Medicine**

Company Presentation

February 2026



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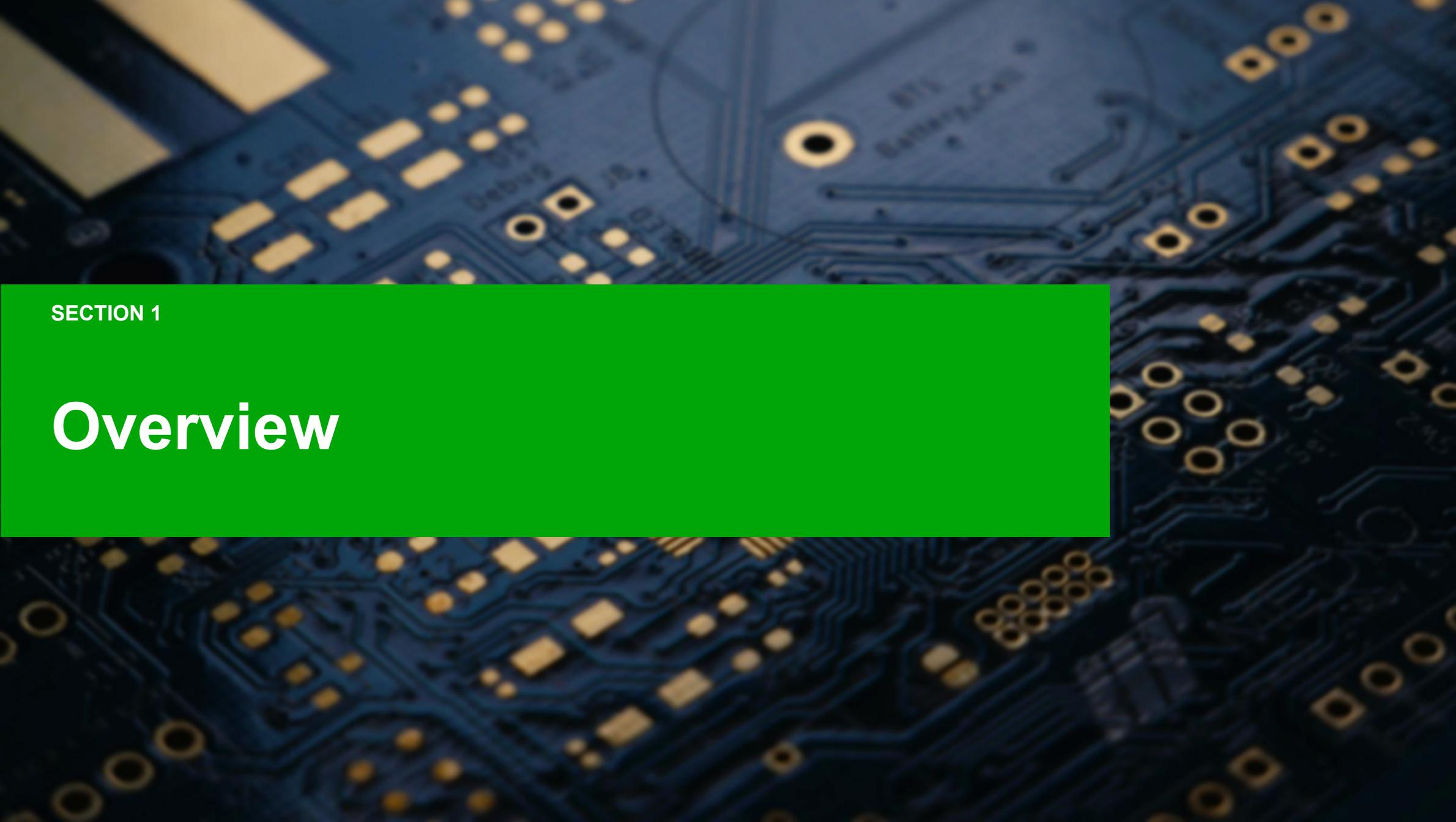
1 Overview

2 AI Platform

3 Asset Pipeline

4 Business Model

5 Financials



SECTION 1

Overview

A Leading and Global AI-driven Biotech Company Established in 2014

To accelerate drug discovery and development by leveraging our rapidly evolving, proprietary Pharma.AI platform



VALUES



PATIENT FIRST



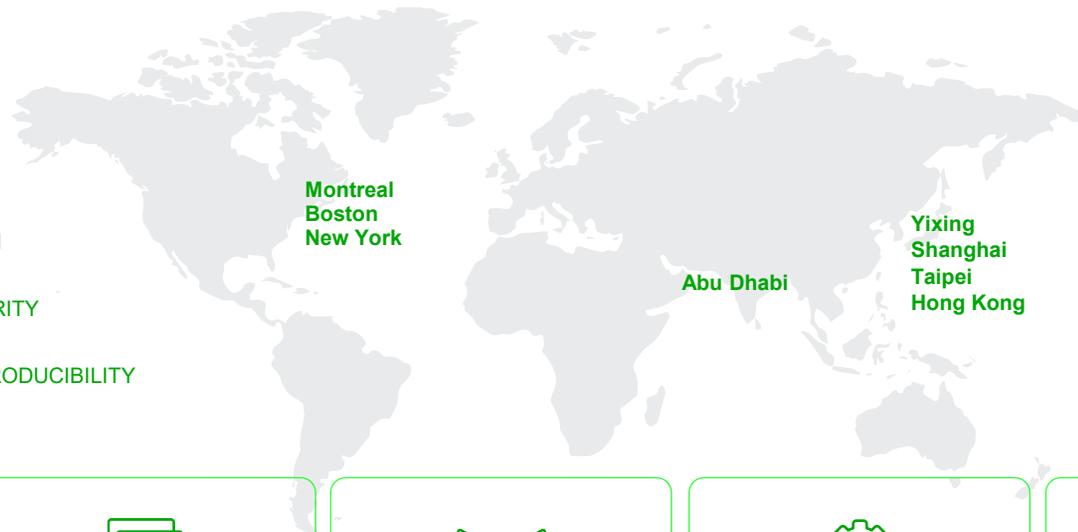
RELENTLESS INNOVATION



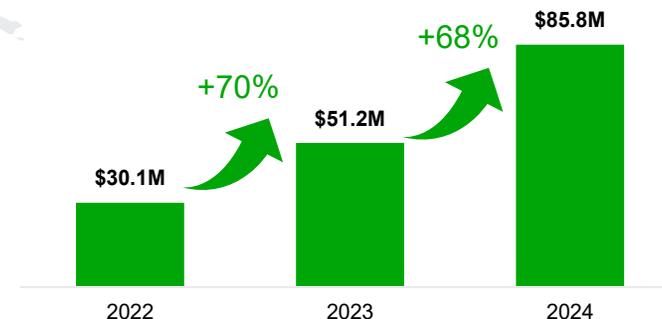
TRANSPARENCY & INTEGRITY



HIGHEST QUALITY & REPRODUCIBILITY



Revenue



>\$4B

Total Contract Value



9

Since 2021

Out-licensing / Collaboration Deals



>50

AI Platform Revenue Generating Customers



2

Large Collaborations in Non-pharma Sectors

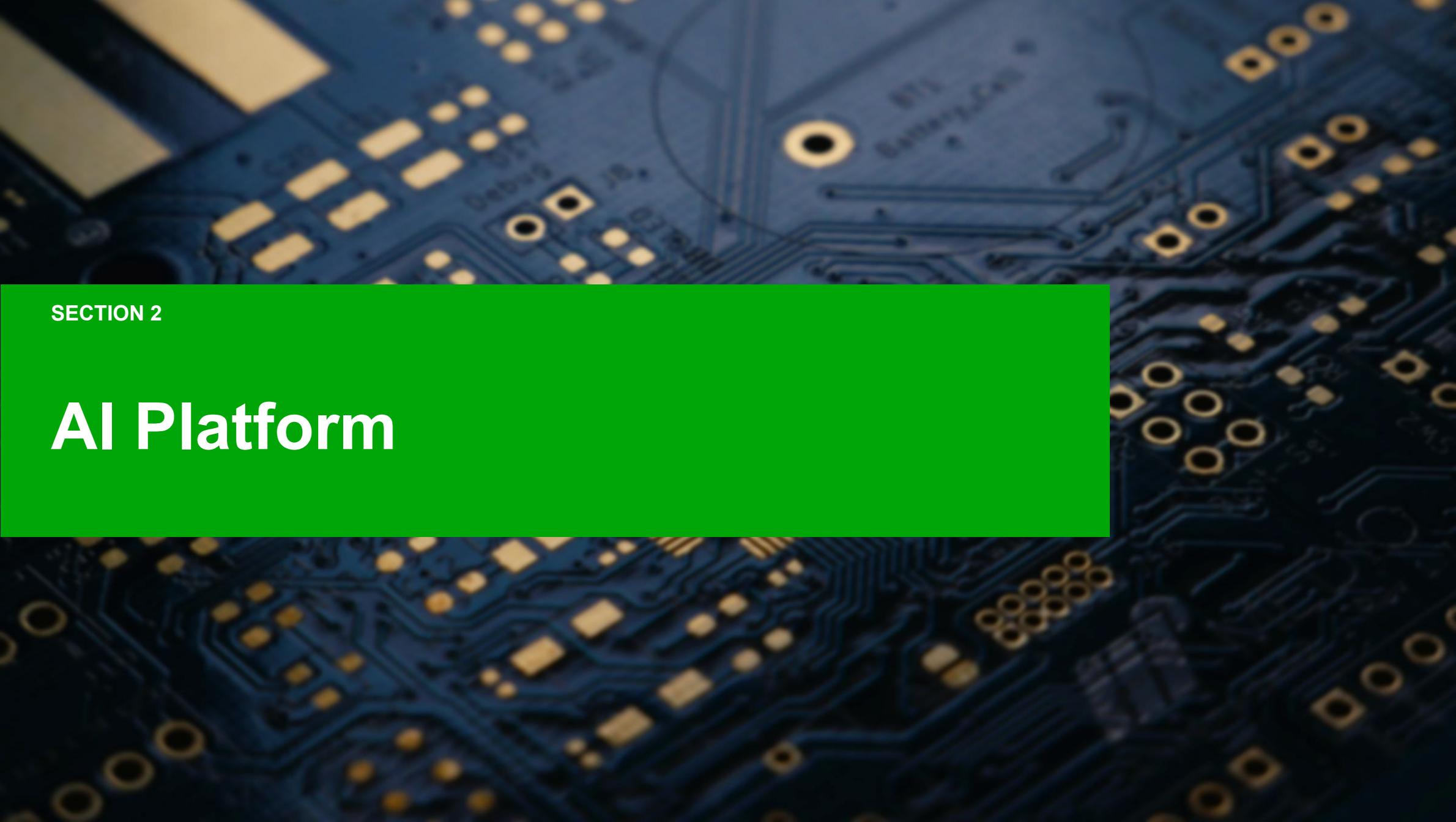


> 20 clinical / IND-enabling stage assets

Lead Asset: Potentially Most Clinically Advanced AI-Discovered Drug Candidate Globally



Strong Cash Position



SECTION 2

AI Platform

World's Leading Generative AI-powered Drug Discovery and Development Platform with End-to-end Capabilities



Biology42



PandaOmics

Discover and Prioritize Novel Targets



Generative Biologics

Discover and Optimize Novel Biomolecules



Life Star 2

Automated Lab Operating Environment

Large Language of Life Models (LLMs)



Precious1GPT

Multimomics Age Prediction & Target ID



Precious2GPT

Multimodal Multimomics Biological Data Synthesis



Precious3GPT

Multi Tissue Multispecies Multimomics Multimodal Life Model

Chemistry42



Generative Chemistry

Generate Novel Molecules



Alchemy

Physics-based Relative Binding Free Energy Engine



ADMET & Off-target

On-the-fly Optimization



MDFlow

End-to-end simulation workflows



Retrosynthesis

Predict Synthetic Routes for Molecular Structures



Model Training

Train a State-of-the-art Model on the Data



MolSpace

Visualize the result of generations using GTM and compare it with the entirety of public data



Nach01

Multimodal Natural & Chemical Languages Foundation Model

Medicine42



inClinico

Design and Predict Clinical Trials

Science42



DORA

Multi-agent Generative Research Assistant

LLM Assistant



Copilot

Generative Conversational Agent



Environmental Sustainability

Generative AI Technologies for Environmental Sustainability



Data Warehouse

Seamless Cross-application Data Flow via Efficient Integration & Standardization



MMAI Science Gym

Boost the LLM's intelligence in drug discovery and development

Experienced

Advisory Board of experts in field of AI



Bud Mishra, PhD

Professor at the Courant Institute, Mathematical Sciences, New York University
Computer Scientist, ISI highly cited researcher in Computer Science



Alán Aspuru-Guzik, PhD

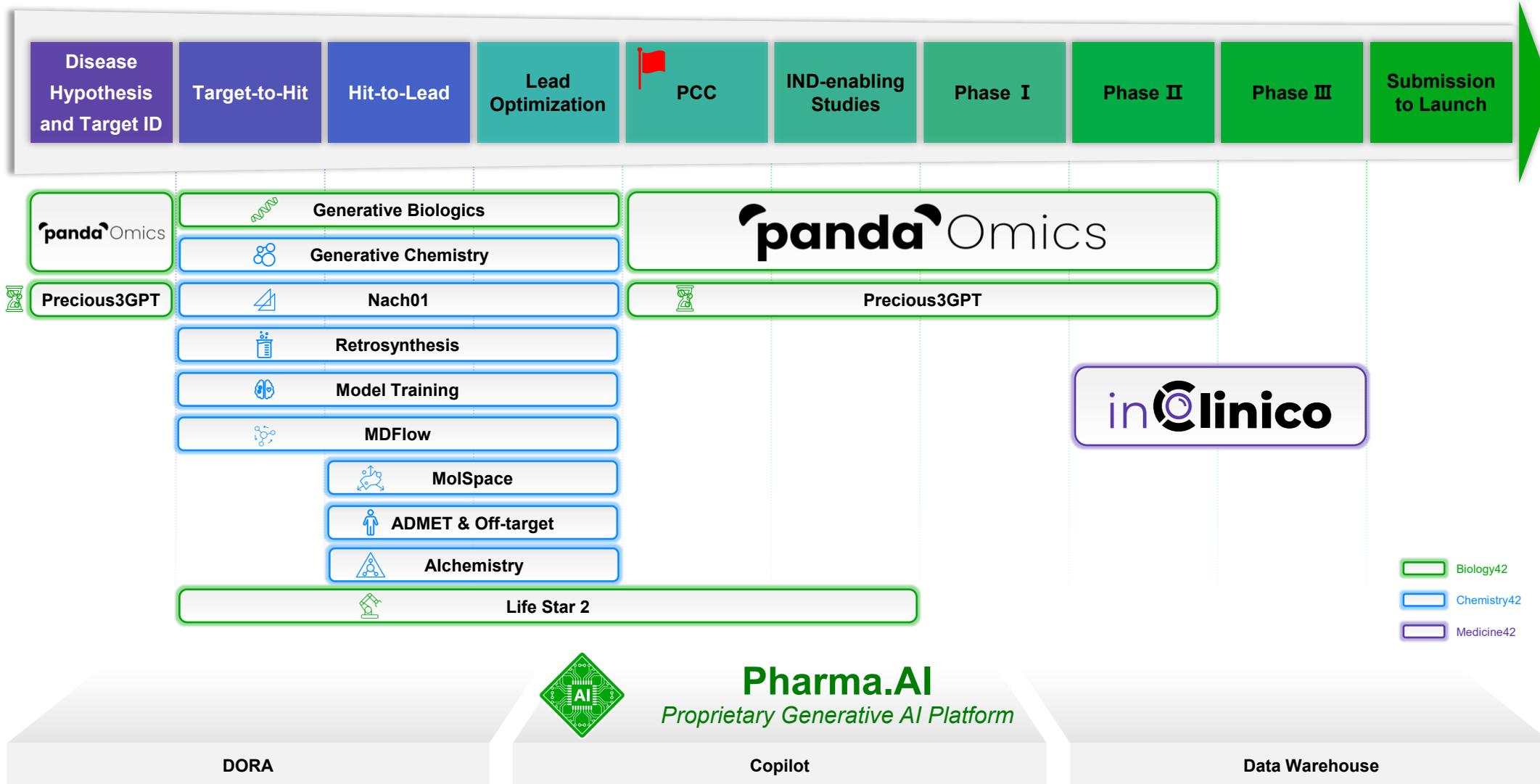
Professor and Director, Vector Institute, University of Toronto,
Former Professor, Harvard University
Expert in Generative Chemistry and Quantum Computing



Michael Levitt, PhD

Professor, Stanford University
Professor, Weizmann University
Expert in Computational Biology and Structural Biology,
2013 Nobel Laureate in Chemistry

Insilico Generative AI for Drug Discovery Process: Code to Cure



Differentiated Generative AI Platform Empowered by AI + Scientists

Full Integration of Pharma.AI and Our Biology Teams Allowing for Real-time Feedback to Enhance Platform's Capability



AI-powered Drug Discovery

- ✓ Customized generation of millions of hit molecules for a given target
- ✓ Can handle very large datasets to screen and optimize drug properties
- ✗ Inability to adapt to the complexity of the real world
- ✗ Experimental results cannot be effectively translated into model optimization
- ✗ Required massive training sets



AI + Scientists

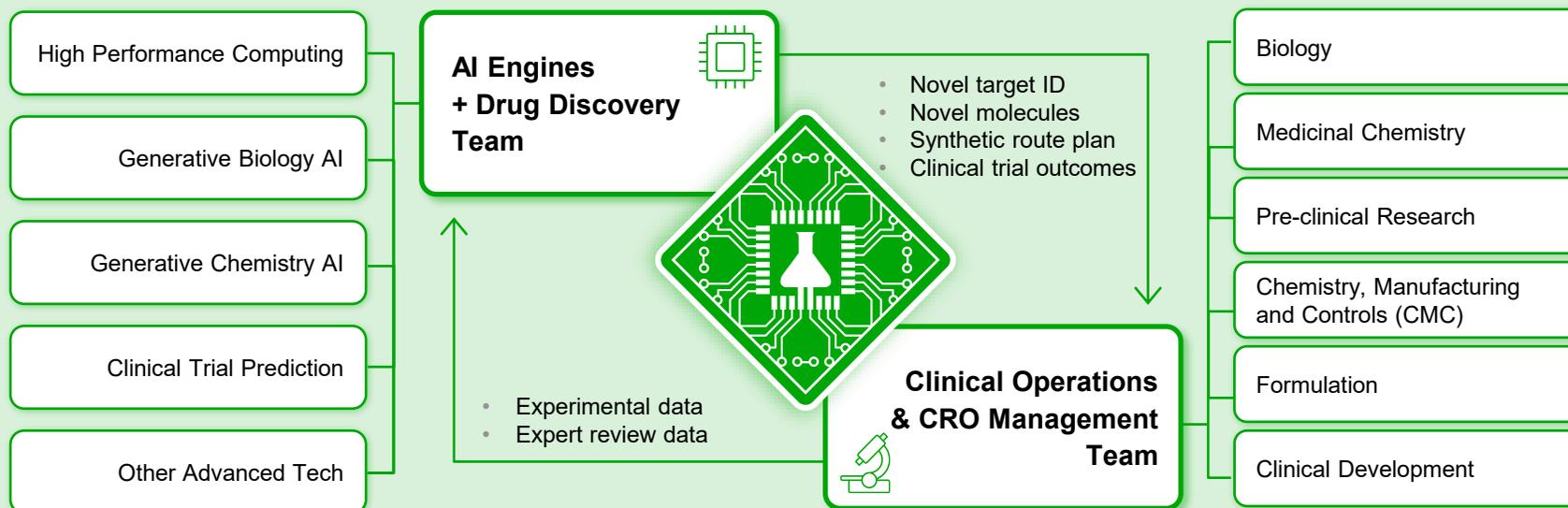
- ✓ Discover novel target and design novel molecules
- ✓ Accuracy enhanced by real-time feedback loops
- ✓ Multi-dimensional screening and optimization by handling large datasets
- ✓ Highly efficient
- ✓ Labor-saving and cost-effective



Traditional Drug Discovery

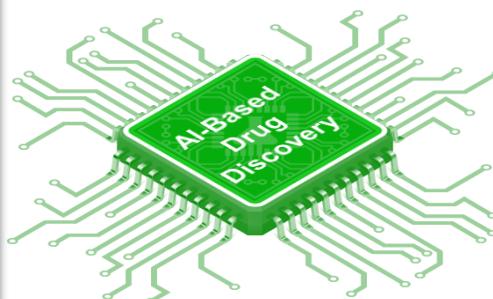
- ✓ No model training set required
- ✓ Optimization based on real world feedback
- ✓ Easier to develop mechanism-driven theories and avoid data bias
- ✗ Begins at experimental screening of existing limited libraries of molecules
- ✗ Manual testing and optimization through trial and error
- ✗ Slow and Costly

Unique Dual CEO Structure Combining Technological Innovation and R&D Execution



Alex Zhavoronkov,
Ph.D.
CEO, Artificial Intelligence

- Leading expert in the field of generative AI
- Oversees innovation of generative AI platform and implementation of business and strategic initiatives
- 300+ peer-reviewed research papers, 3 books



Feng Ren,
Ph.D.
CEO, Drug Discovery

- Pharmaceutical industry veteran
- Guides R&D strategy and operational oversight and execution of our growing R&D organization
- 80+ peer-reviewed papers and 120+ patents





SECTION 3

Asset Pipeline

>20 Asset Pipeline Discovered from Our Generative AI Platform with Leading Asset Most Advanced Globally among Peer Companies



Development Strategy

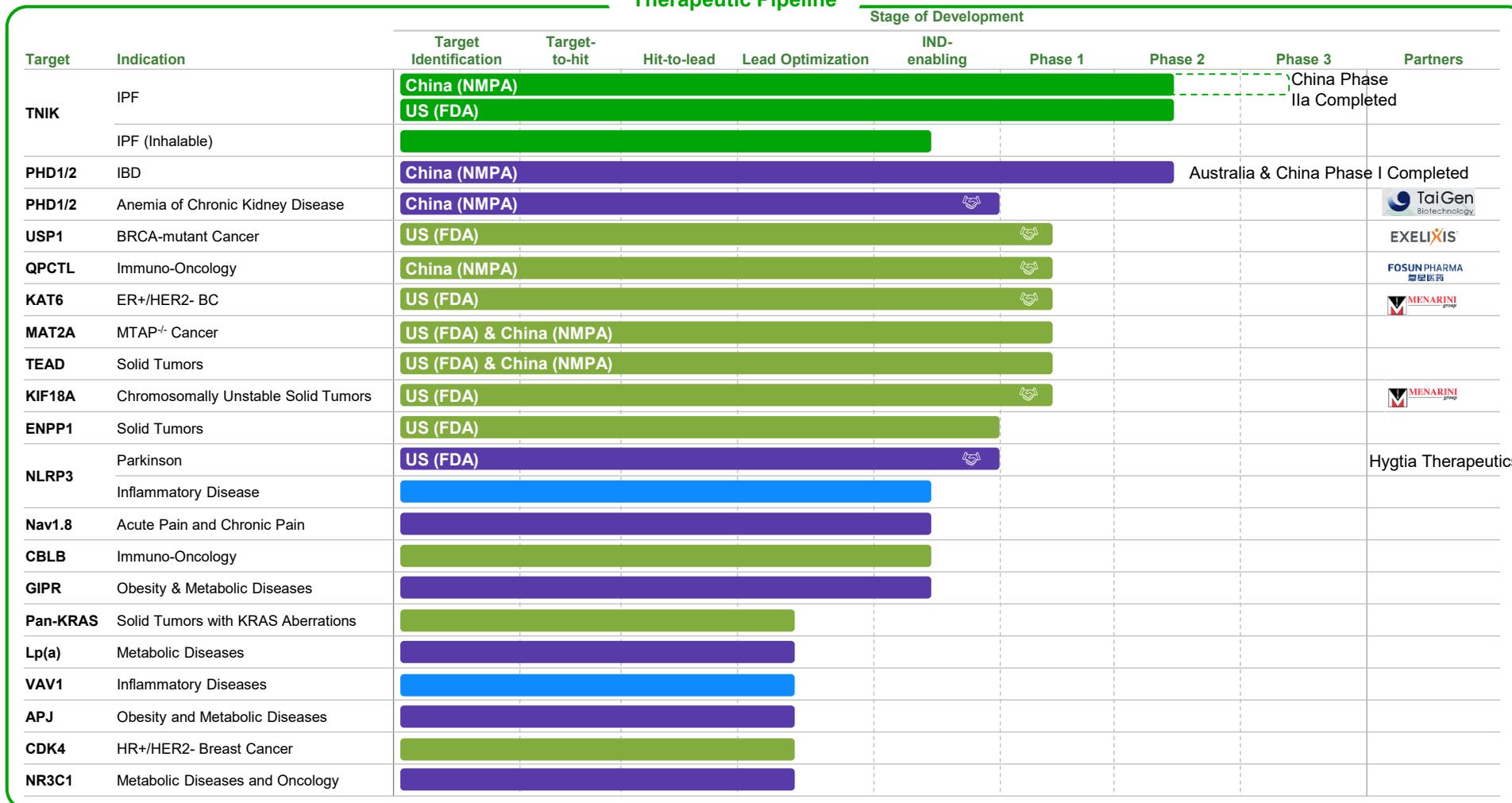


To Discover Novel Targets



Optimization on Existing Targets/Drugs

Therapeutic Pipeline



Notes:

- All programs are designed for oral administration unless otherwise indicated
- FDA granted ISM001-055 the orphan drug designation for its IPF indication
- All pipeline is entirely the product of internal generation, with global rights and no targets or compounds in-licensed from pharmaceutical companies

200+ Peer-reviewed Publications & 600+ Patents

nature medicine



Article | [Open access](#) | Published: 03 June 2025

A generative AI-discovered TNIK inhibitor for idiopathic pulmonary fibrosis: a randomized phase 2a trial

Zuojun Xu ¹, Feng Ren, Ping Wang, Jie Cao, Chunting Tan, Deqiong Ma, Li Zhao, Jinghong Dai, Yipeng Ding, Haohui Fang, Huiping Li, Hong Liu, Fengming Luo, Ying Meng, Pinhua Pan, Pingchao Xiang, Zuke Xiao, Sujata Rao, Carol Satler, Sang Liu, Yuan Lv, Heng Zhao, Shan Chen, Hui Cui, ... Alex Zhavoronkov ¹

[+ Show authors](#)

Nature Medicine (2025) | [Cite this article](#)

[Metrics](#)

Abstract

Despite substantial progress in artificial intelligence (AI) for generative chemistry, few novel AI-discovered or AI-designed drugs have reached human clinical trials. Here we present the results of the first phase 2a multicenter, double-blind, randomized, placebo-controlled trial testing the safety and efficacy of rentosertib (formerly ISM001-055), a first-in-class AI-generated small-molecule inhibitor of TNIK, a first-in-class target in idiopathic pulmonary fibrosis (IPF) discovered using generative AI. IPF is an age-related progressive lung condition with no current therapies available that reverse the degenerative course of disease. Patients were randomized to 12 weeks of treatment with 30 mg rentosertib once daily (QD, $n = 18$), 30 mg rentosertib twice daily (BID, $n = 18$), 60 mg rentosertib QD ($n = 18$) or placebo ($n = 17$). The primary endpoint was the percentage of patients who have at least one treatment-emergent adverse event, which was similar across all treatment arms (72.2% in patients receiving 30 mg rentosertib QD ($n = 13/18$), 83.3% for 30 mg rentosertib BID ($n = 15/18$), 83.3% for 60 mg rentosertib QD ($n = 15/18$) and 70.6% for placebo ($n = 12/17$). Treatment-related serious adverse event rates were low and comparable across treatment groups, with the most common events leading to treatment discontinuation related to liver toxicity or diarrhea.

nature biotechnology



Brief Communication | [Open access](#) | Published: 11 December 2024

Intestinal mucosal barrier repair and immune regulation with an AI-developed gut-restricted PHD inhibitor

Yanyun Fu, Xiao Ding, Man Zhang, Chunlei Feng, Ziqi Yan, Feng Wang, Jianyu Xu, Xiaoxia Lin, Xiaoyu Ding, Ling Wang, Yaya Fan, Taotao Li, Yushu Yin, Xing Liang, Chenxi Xu, Shan Chen, Fadi E. Poulos, David Gennert, Frank W. Puri, Petrina Kanya, Feng Ren, Alex Aliper & Alex Zhavoronkov ¹

Nature Biotechnology (2024) | [Cite this article](#)

6789 Accesses | 134 Altmetric | [Metrics](#)

Abstract

Hypoxia-inducible factor prolyl hydroxylase (PHD) inhibitors have been approved for treating renal anemia yet have failed clinical testing for inflammatory bowel disease because of a lack of efficacy. Here we used a multimodal multimodal generative artificial intelligence platform to design an orally gut-restricted selective PHD1 and PHD2 inhibitor that exhibits favorable safety and pharmacokinetic profiles in preclinical studies. ISM012-042 restores intestinal barrier function and alleviates gut inflammation in multiple experimental colitis models.

nature medicine



Review Article | Published: 14 February 2024

Validation of biomarkers of aging

Mahdi Moari, Chiara Herzog, Jesse R. Poganik, Kejun Yin, Jamie N. Justice, Daniel W. Belsky, Albert T. Higgins, Chen Brian H. Chen, Alan A. Cohen, Georg Fuetten, Sara Hågg, Riccardo E. Marioni, Martin Wildschwendter, Kristen Fortney, Peter O. Fedichev, Alex Zhavoronkov, Nir Barzilai, Jessica Lasky-Su, Douglas P. Kiel, Brian K. Kennedy, Steven Cummings, P. Elaine Slagboom, Eric Verdin, Andrea B. Maier, ... Luigi Ferrucci ¹ [+ Show authors](#)

Nature Medicine 30, 360–372 (2024) | [Cite this article](#)

27k Accesses | 84 Citations | 175 Altmetric | [Metrics](#)

nature biotechnology



Brief Communication | [Open access](#) | Published: 22 January 2025

Quantum-computing-enhanced algorithm unveils potential KRAS inhibitors

Mohammad Ghazi Vakil, Christoph Gorpella ¹, Jamie Snider, Akshat Kumar Nigam ², Dmitry Bezukov, Daniel Varoli, Alex Aliper, Danil Polykovskiy, Krishna M. Padmanabha Das, Huel Cox III, Anna Lyakisheva, Ardalan Hosseini Mansob, Zhong Yao, Lela Bitar, Danielle Tahoulas, Dora Cerina, Eugene Radchenko, Xiao Ding, Jimin Liu, Faraz Meng, Feng Ren, Yudong Cao, Igor Stojiljar ³, Alan Assouar-Guzik ⁴ & Alex Zhavoronkov ¹

nature biotechnology



Article | [Open access](#) | Published: 08 March 2024

A small-molecule TNIK inhibitor targets fibrosis in preclinical and clinical models

Feng Ren, Alex Aliper, Jian Chen, Heng Zhao, Suata Rao, Christoph Kusube, Ivan V. Gostov, Man Zhanna, Klaus Witte, Chris Kusan, Vladimir Aleksovski, Tami Isakovski, Danil Polykovskiy, Jianyu Xu, Eugene Babkin, Junsen Qiao, Xing Liang, Zhenzhen Mou, Hui Wang, Frank W. Puri, Pedro Torres, Ayuso, Alexander Veviorskiy, Dandan Song, Sang Liu, ... Alex Zhavoronkov ¹ [+ Show authors](#)

Nature Biotechnology (2024) | [Cite this article](#)

100k Accesses | 41 Citations | 891 Altmetric | [Metrics](#)

ADVANCED SCIENCE



Research Article | [Open Access](#) | [Cite this article](#)

Utilizing AI for the Identification and Validation of Novel Therapeutic Targets and Repurposed Drugs for Endometriosis

Bonnie Hai Man Liu, Yuezheng Lin, Xi Long, Sze Wan Hung, Anna Gaponova, Feng Ren, Alex Zhavoronkov, Frank W. Puri, ... Ch. Chao Wang ¹

First published: 12 December 2024 | <https://doi.org/10.1002/advb.202406565> | Citations: 1

nature medicine



WORLD VIEW | 07 February 2023

Caution with AI-generated content in biomedicine

Generative artificial intelligence tools such as chatGPT have many uses in medicine, but a lack of accuracy poses problems.

nature biotechnology



> *Nat Biotechnol.* 2020 Oct;38(10):1127–1131. doi: 10.1038/s41587-020-0686-x.

Artificial intelligence, drug repurposing and peer review

Jeremy M Levin ^{1, 2}, Tudor I Oprea ^{3, 4, 5, 6}, Sagie Davidovich ⁷, Thomas Ciozel ⁸, John P Overington ⁹, Quentin Vanhaelen ¹⁰, Charles R Cantor ¹¹, Evelyn Bischof ^{12, 13, 14}, Alex Zhavoronkov ¹⁵

nature biotechnology



Brief Communication | Published: 02 September 2019

Deep learning enables rapid identification of potent DDR1 kinase inhibitors

Alex Zhavoronkov ¹, Yan A. Ivanovskiy, Alex Aliper, Mark S. Veselov, Vladimir A. Aladinovskiy, Anastasia V. Aladinovskaya, Victor A. Seredev, Danil A. Polykovskiy, Maksim D. Kuznetsov, Aris Asakubayev, Yury Volkov, Artem Zhulov, Rim S. Shavakhmetov, Alexander Zhetokas, Lidya I. Mirnaya, Boudien A. Zeyherbosch, Lemert H. Lee, Richard Seli, David Madge, Li Xing, Tao Guo & Alan Assouar-Guzik ¹

Nature Biotechnology 37, 1038–1040 (2019) | [Cite this article](#)

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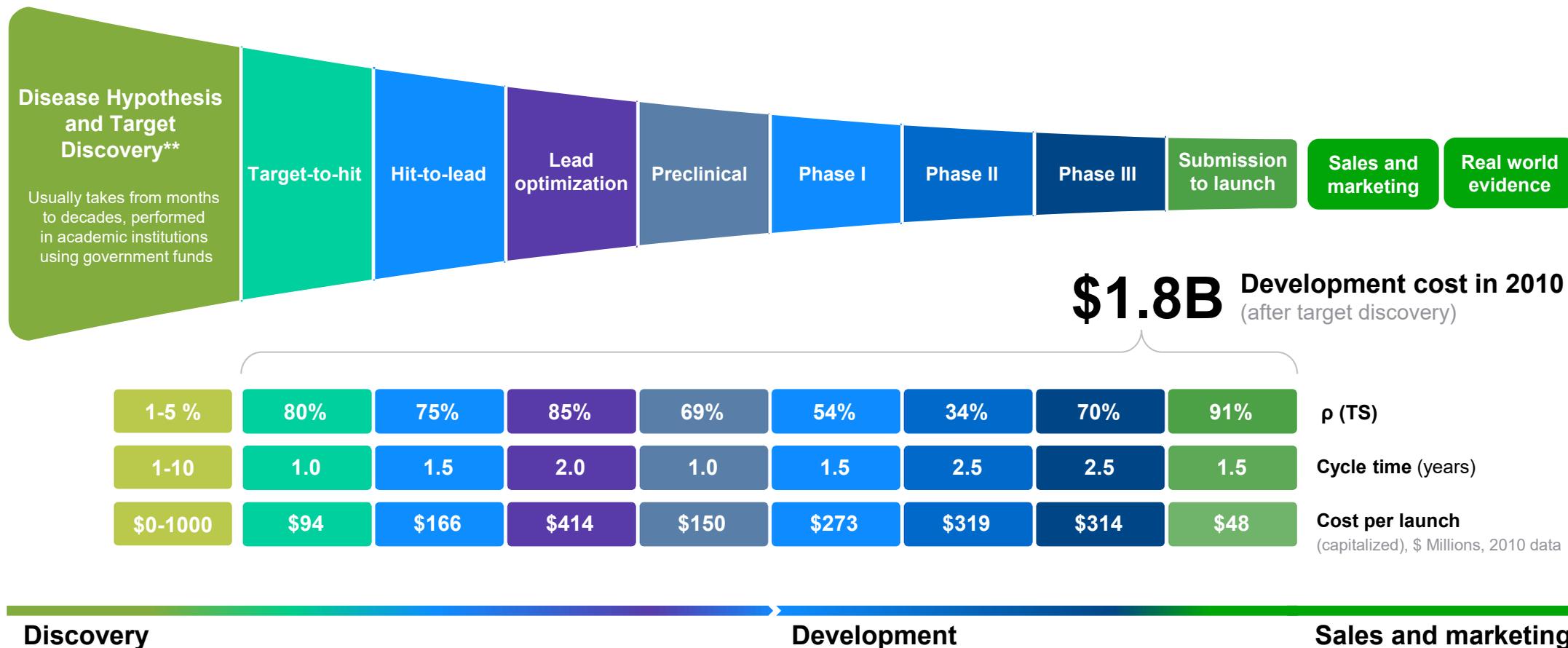
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Donald Small, MD, PhD
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Oncology and Professor,
Johns Hopkins Medical Institute (JHMI)
Expert in Pharmaceutical Research
in Target Discovery

Traditional Drug R&D Takes >10 Years and >\$2B*

From the discovery to the launch of a new drug

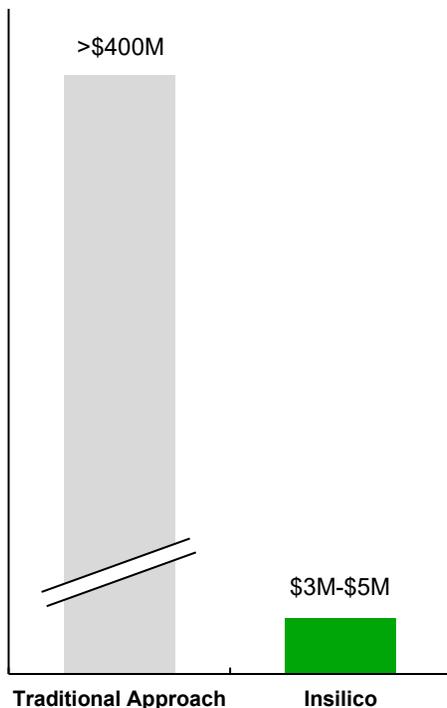


* Modified from Paul et al, How to improve R&D productivity: the pharmaceutical industry's grand challenge. Nature Reviews Drug Discovery, 2010
 ** Based on interviews with the pharmaceutical industry executives

AI-based Drug R&D is Cheaper, Faster, and has Higher Success Rate than Traditional R&D

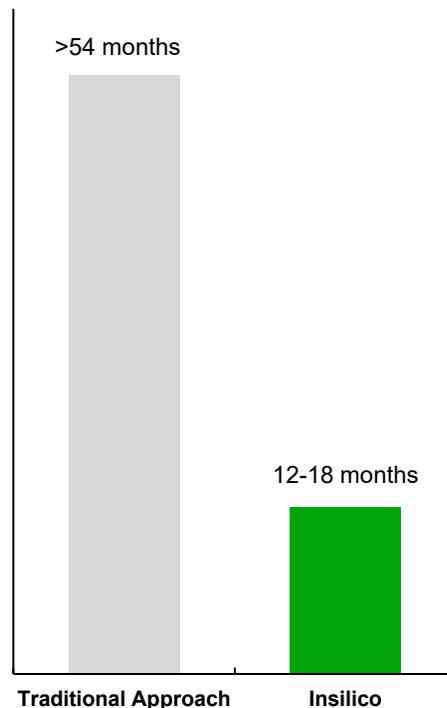
Cheaper

Cost in Preclinical Candidate Selected



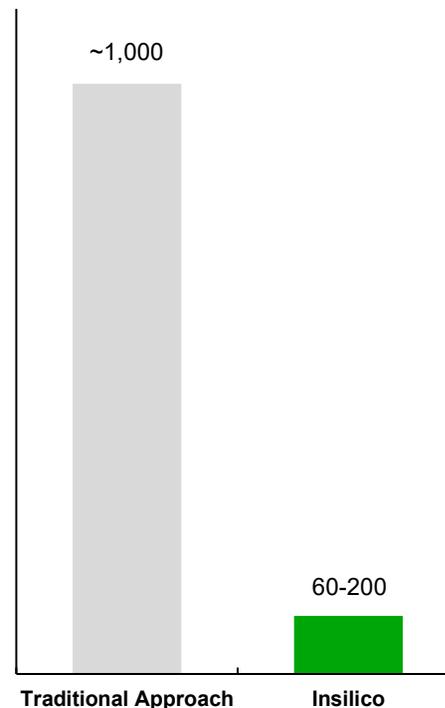
Faster

Months from Target Discovery to Preclinical Candidate Nomination



Higher Success Rate

Molecule Synthesized to Identify Preclinical Candidates



AI Application in Drug R&D

84%
AI upgraded the prediction precision of protein folding to

20%
AI can improve the precision of compound screening by

75%
Accuracy of AI-based drug toxicity prediction reached to

92%
AI models categorize compounds with a precision of

Pharma.AI Catalyzed Drug Discovery Breakthroughs from 2021-2024

27 Total Developmental Candidates (DC)

2021:
2 DC

2022:
9 DC

2023:
6 DC

2024:
5 DC

2025:
5 DC

12 Molecules Received IND Clearance

Completed **Phase IIa** in IPF

Completed Two **Phase I** in IBD

Shortest Time To DC:

8 Months

Average Time To DC:

12-15 Months

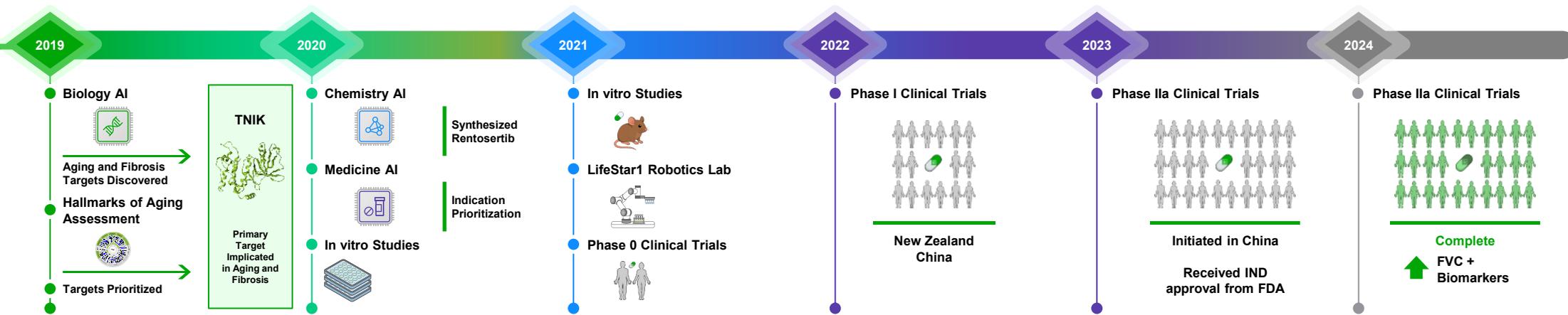
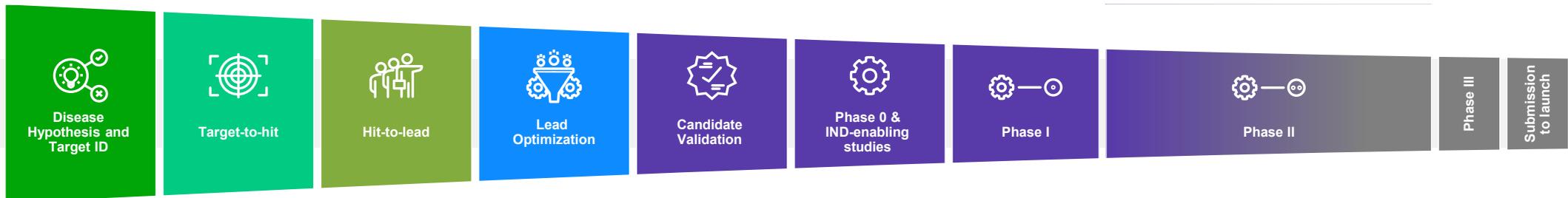
Longest Time To DC:

18 Months

60~200 Molecules Synthesized Per Program

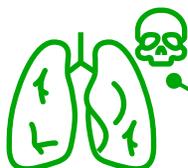
4 Nature Biotechnology Publications

Case Study: ISM001_055 (TNIK Inhibitor) is the Most Clinically Advanced AIDD Candidate Globally



High Unmet Medical Needs in IPF with Limited Treatment Options

Market Opportunity



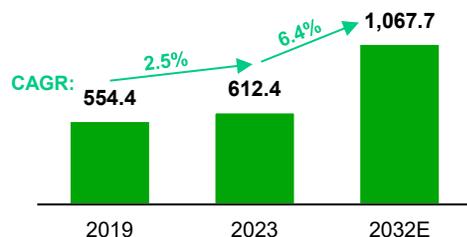
Fibrosis is a pathological feature of many chronic inflammatory diseases that refers to the scarring and hardening of tissues and organs

Among these, idiopathic pulmonary fibrosis (IPF) stands out as a particularly severe and complex form of the disease

Due to its progressive nature, limited treatment options, and poor prognosis, IPF has become a major focus of current research and drug development

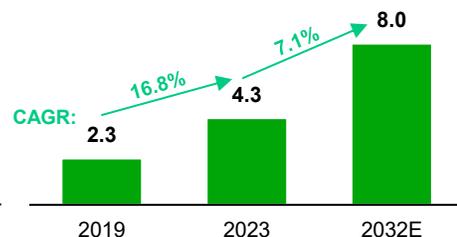
Global Incidence of IPF

Thousand



Size of the IPF Drug Market

US\$ Billions



Growth Drivers of the Global IPF Drug Market



Increasing incidence and prevalence of IPF patients



Growing awareness of IPF



Improvement in IPF diagnosis



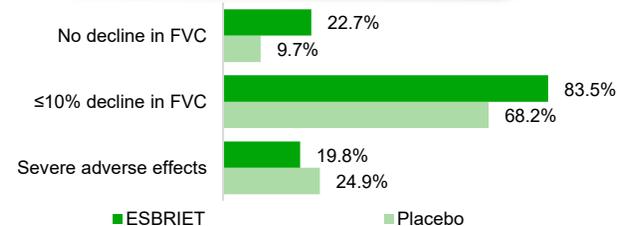
Government support for drugs targeting orphan disease

Competitive Landscape

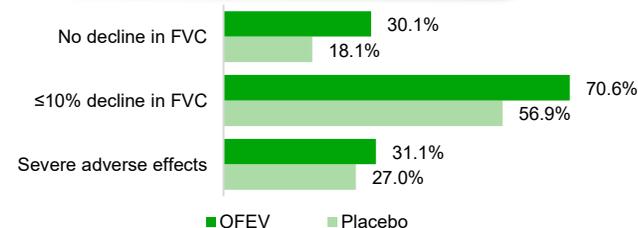
Approved Drugs

Generic name	Brand Name	Original Drug Manufacturer	FDA Approved Date	Drug Target	Original Drug Approved Region
Pirfenidone	Esbriet®	Roche/ Genentech	2014-10-15	TGF-β, TNF-α and interleukin 6	FDA, EMA, PMDA
Nintedanib	OFEV®	Boehringer Ingelheim	2014-10-15	Tyrosine kinases	FDA, EMA, NMPA, PMDA
Nerandomilast	Jascayd®	Boehringer Ingelheim	2025 -10-08	PDE4B	FDA, NMPA

ESBRIET vs placebo for IPF

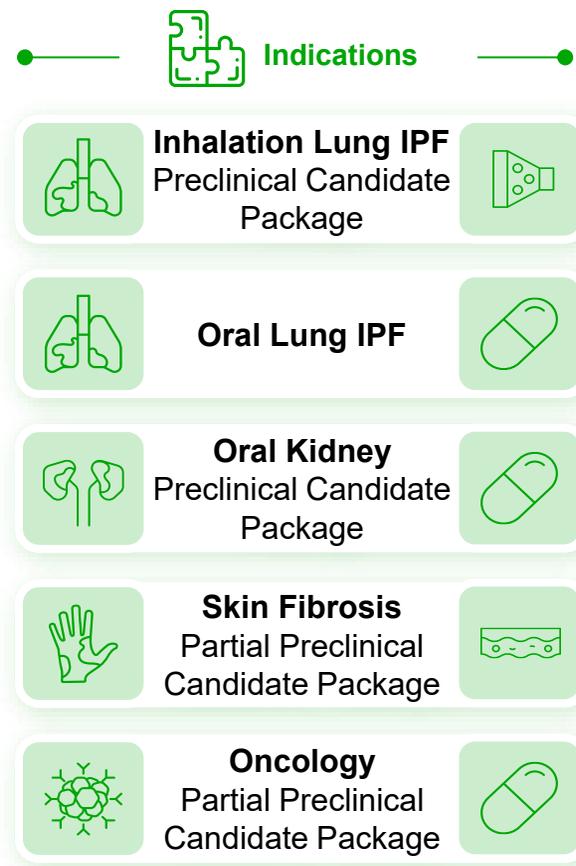
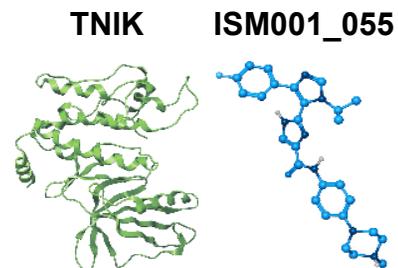
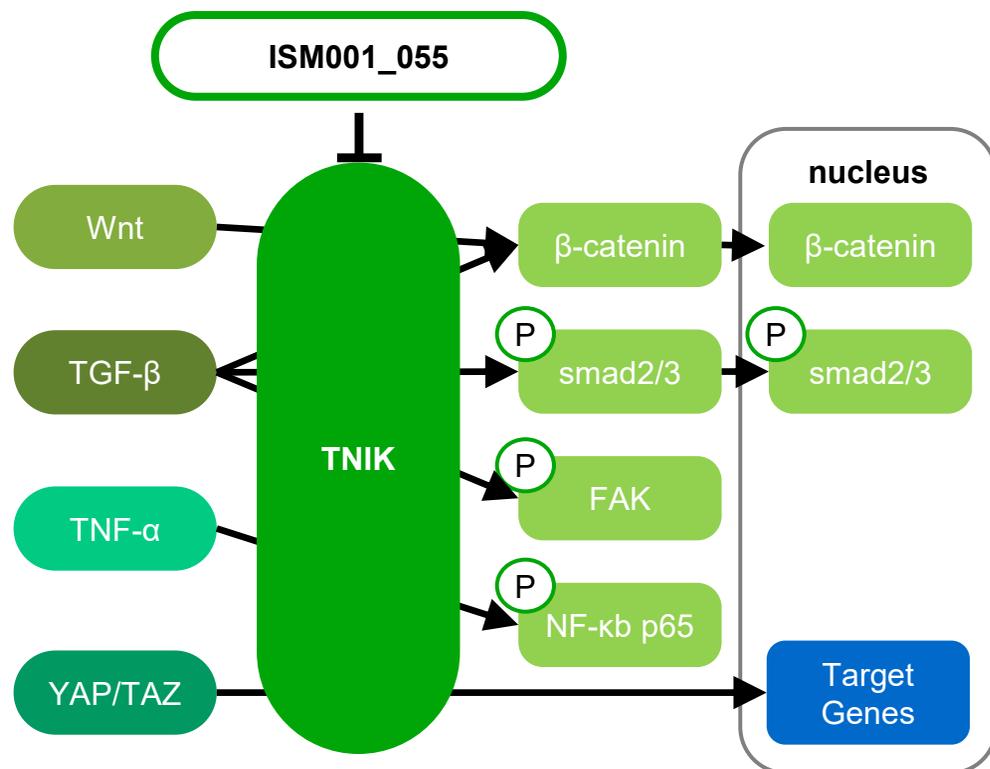


OFEV vs placebo for IPF

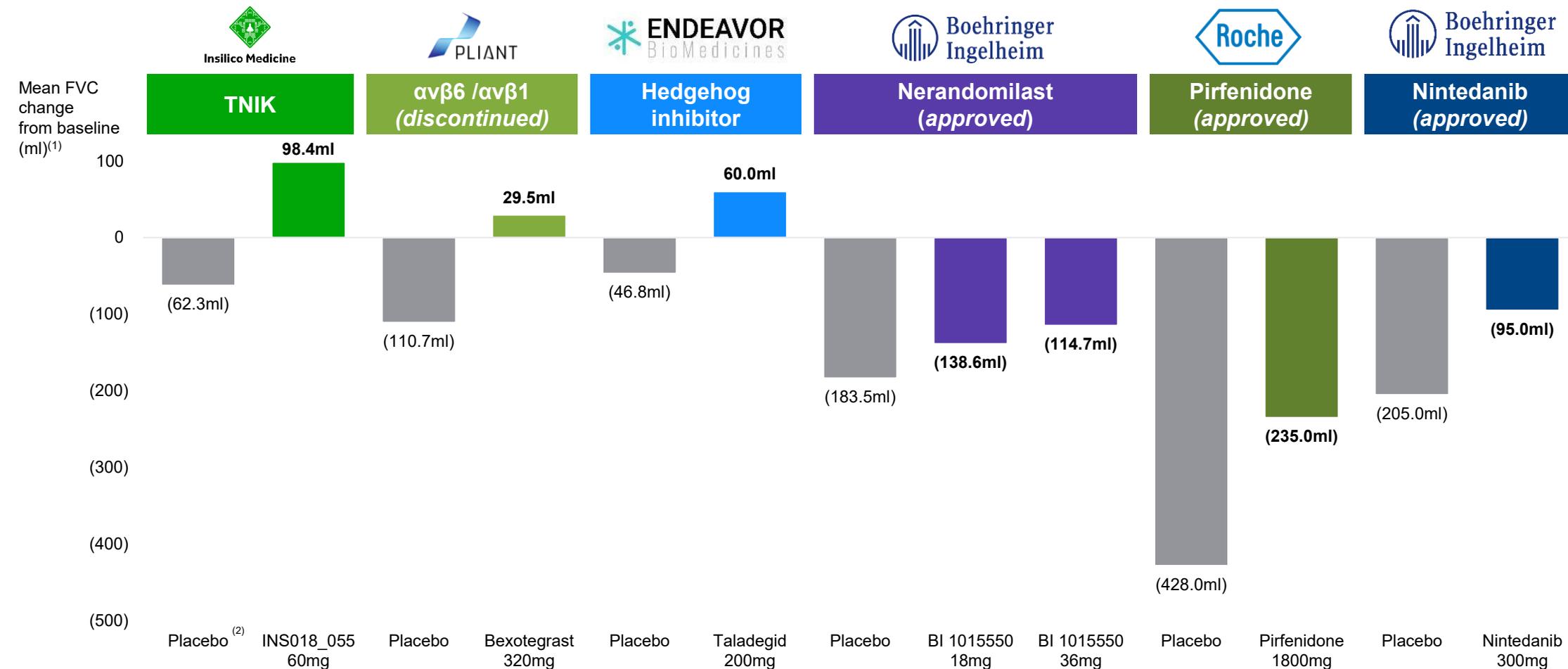


ISM001-055: Target Identified and Molecule Created by our Generative AI Platform

INS018_055 (ISM001-055): Small-molecule drug candidate designed by our generative AI platform to treat fibrosis-related indications by inhibiting the TRAF2- and NCK-interacting kinase (TNIK)



ISM001-055 Out-performs Other Investigational Agents in Cross Trial Data Comparison



Source: Pliant Therapeutics poster; ICLAF 2024 presentation; Richeldi, L., Azuma, A., Cottin, V., Hesslinger, C., Stowasser, S., Valenzuela, C., Wijsenbeek, M. S., Zoz, D. F., Voss, F., & Maher, T. M. (2022). Trial of a preferential phosphodiesterase 4B inhibitor for idiopathic pulmonary fibrosis. *New England Journal of Medicine*, 386(23), 2178–2187. <https://doi.org/10.1056/nejmoa2201737>; FDA approved drug label; Boehringer Ingelheim website

Note:
 1. For investigational agents, data are compiled from published phase 2 results at week 12; For NDA and approved drugs, data are compiled from published phase 3 results at week 52
 2. One outlier was noted: One outlier was randomized to the placebo treatment group and excluded from the analysis

Life Star 2: AI-Driven Automated Laboratory Accelerates Drug Discovery and Development

Target discovery and target verification

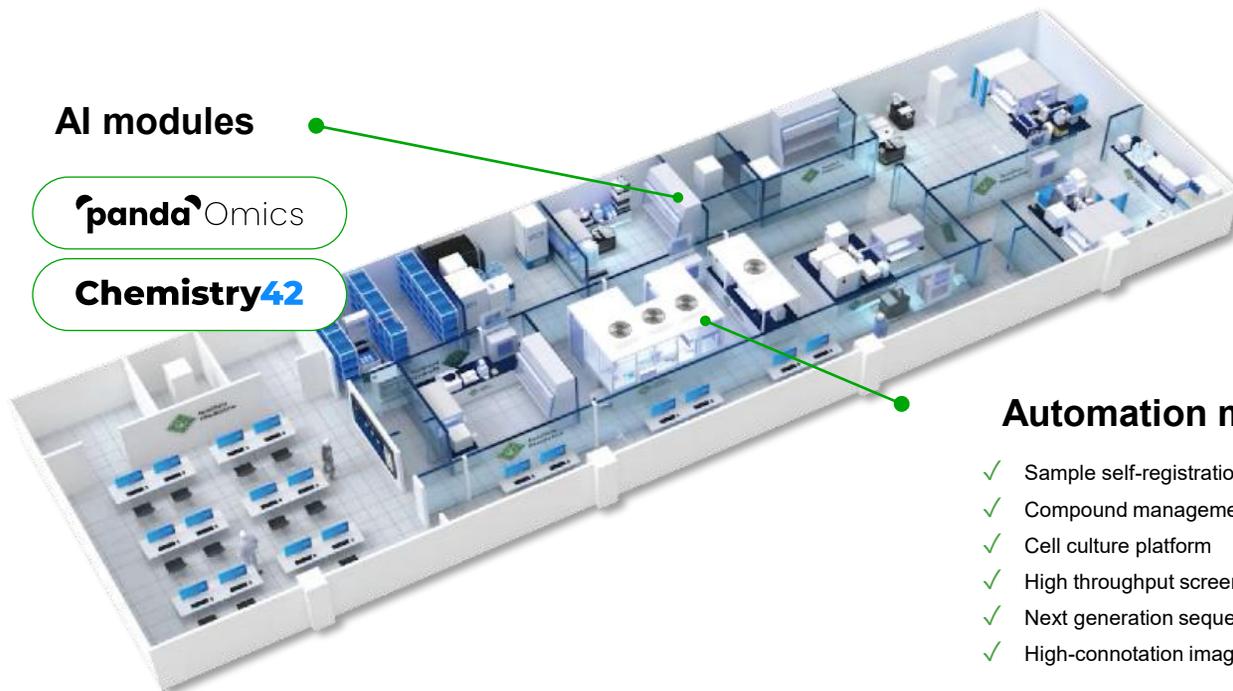
Drug development and translational medicine

Algorithm verification

AI modules

pandaOmics

Chemistry42



Automation module

- ✓ Sample self-registration
- ✓ Compound management platform
- ✓ Cell culture platform
- ✓ High throughput screening platform
- ✓ Next generation sequencing platform
- ✓ High-connotation imaging platform



Towards Chemical and Biological Superintelligence: Insilico Medicine's MMAI Gym for Science

After MMAI Gym training, LLMs can achieve up to 10-fold performance gains on key drug discovery benchmarks, compared to their baseline performance where they fail on approximately 75–95% of tasks.

LLMs trained at the Gym demonstrated substantial gains on target search benchmarks

- ✓ Qwen3-4B outperformed all frontier LLMs in the retrieval of clinical targets after one training session at the MMAI Gym

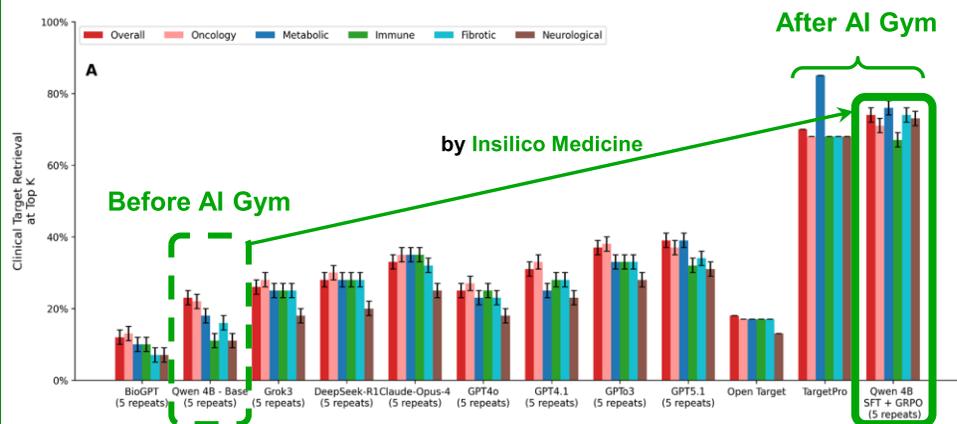


Figure 1 . Metrics on the TargetBench benchmark¹

LLMs trained at the Gym demonstrated substantial gains on clinical trial prediction benchmarks

- ✓ Prediction of clinical trials outcomes based on trial description and time split. Qwen3-4B base model's F1 increased from 0.82 to 0.94 after an MMAI Gym session, outperforming GPT5 (0.87)

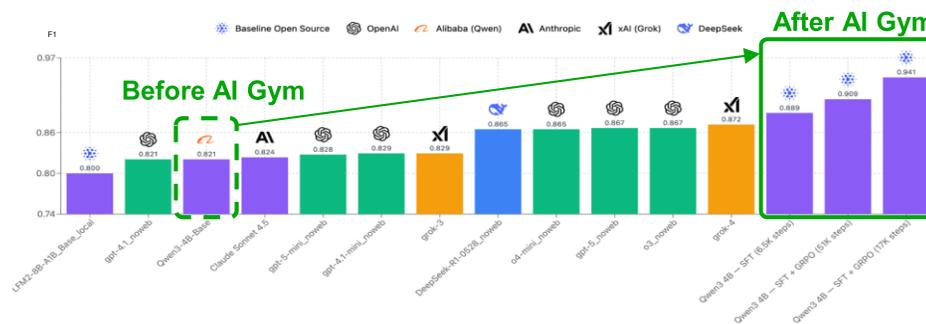
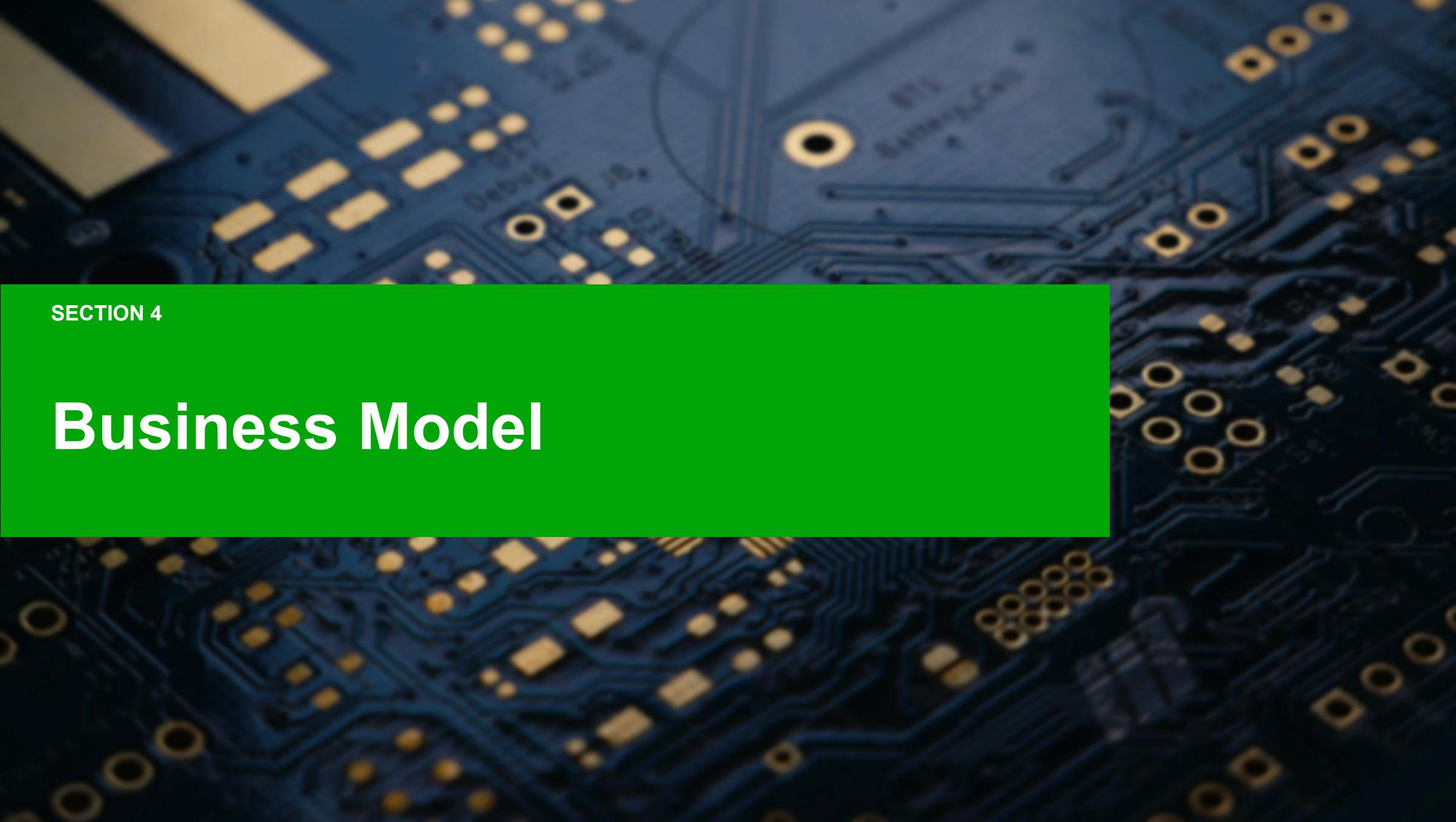


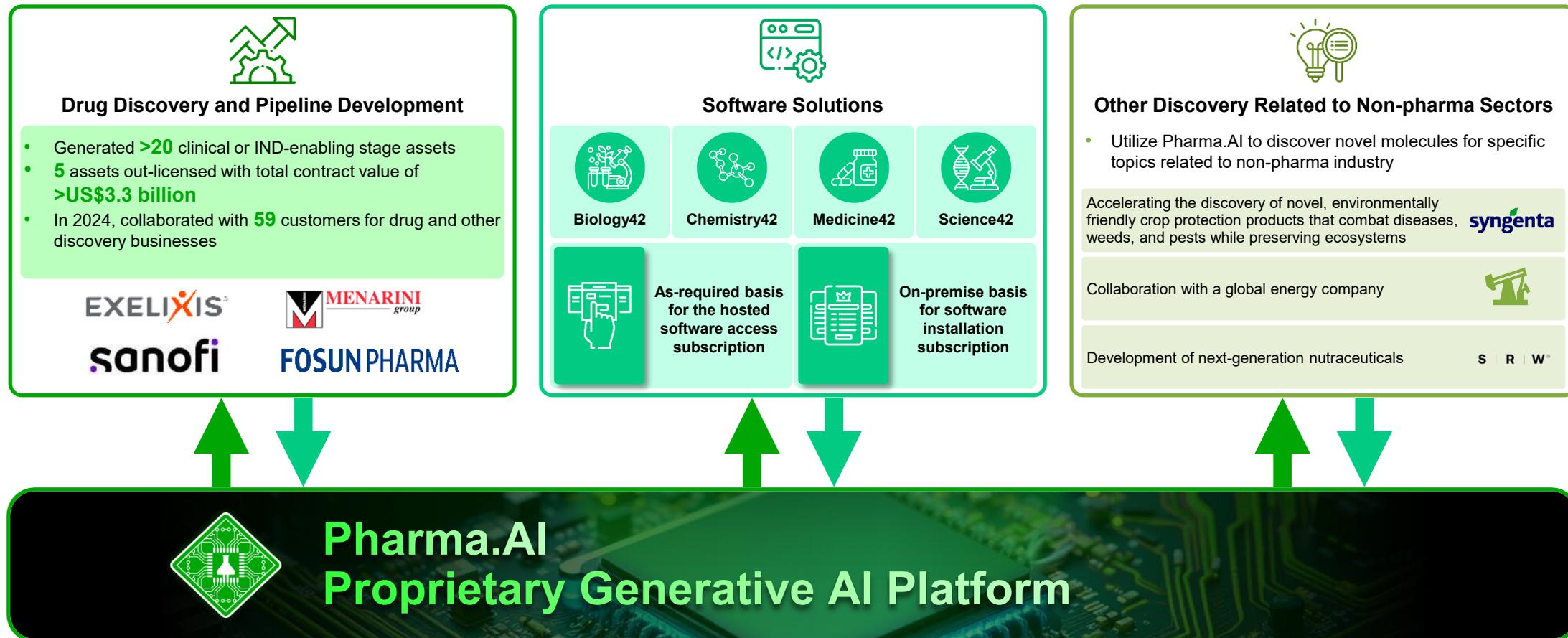
Figure 2. Metrics on the TrialBenchX benchmark



SECTION 4

Business Model

Multi-Pronged Revenue Generating Business Model for Long-term Growth



Multiple Collaboration and Out-Licensing Agreements with Leading Pharmaceutical and Biotech Companies since 2021



FOSUN PHARMA

2021

QPCTL Co-development & 4 Collaboration Targets

Upfront of **\$13 million** + **\$15 million** equity investment

Total deal value up to **\$82 million**

sanofi

2022

Up to 2 + 4 Collaboration Targets

Upfront plus target nomination fees of **\$21.5 million**

Total deal value up to **\$1.2 billion**, plus royalties

EXELIXIS

2023

USP1 Out-licensing

Upfront payment **\$80 million** plus milestones

Total deal value close to **\$1 billion** plus royalties

MENARINI group

2023

KAT6 Out-licensing

Upfront payment **\$12 million** plus milestones

Total deal value over **\$500 million**, plus royalties

MENARINI group

2024

KIF18A Out-licensing

Upfront payment **\$20 million** plus milestones

Total deal value over **\$550 million**, plus royalties

Lilly

2025

Research Collaboration

Total deal value over **\$100 million**, plus royalties

SERVIER

2026

Research Collaboration

Upfront and near-term R&D payments **\$32 million** plus milestones

Total deal value over **\$888 million**, plus royalties

Hygtia Therapeutics

2026

NLRP3 Co-development

Upfront payment **\$10 million** plus milestones

Total deal value **\$66 million**

齐鲁制药 QILU PHARMACEUTICAL

2026

Research Collaboration

Total deal value near **\$120 million**, plus royalties

Note: Notable agreements by total deal value

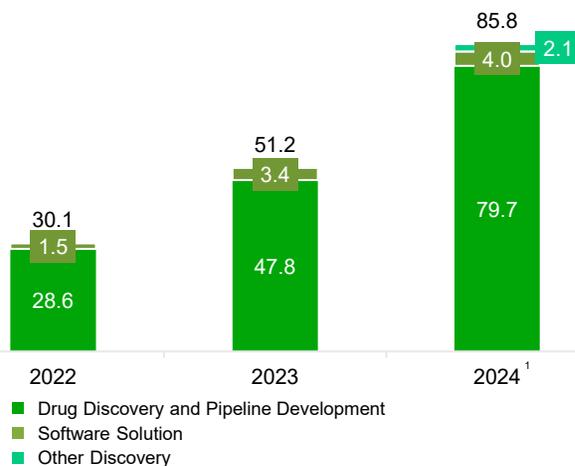


SECTION 5

Financials

Financial Highlights

Revenue (USD MM)



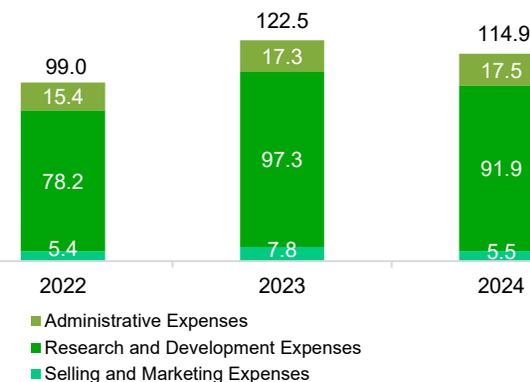
- Revenue generated from drug discovery and pipeline development increased from 2022 to 2024 due to an increase in revenue from out-licensing arrangements
- Revenue generated from software solution increased from 2022 to 2024 due to increased subscription from customers of existing software solutions and introduction of new software solutions in 2024

Gross Profit (USD MM)



- Gross profit margin increased from 2022 to 2024 due to the higher gross profit margin associated with out-licensing transactions from drug discovery and pipeline development business. Gross profit margin from software solution remains 100% during the same period
- Plan to strengthen collaborations with third-party contractors, enabling us to negotiate more favorable agreements and achieve greater cost efficiency

Expenses (USD MM)



- Research and development expenses increased from US\$78.2 million for 2022 to US\$97.3 million for 2023. The increase was primarily attributable to the increase in third-party contracting costs paid to CROs and CDMOs and the increase in labor costs, which is in line with the expansion of our pipeline
- Research and development expenses slightly decreased from US\$97.3 million in 2023 to US\$91.9 million in 2024. The decrease was primarily attributable to decreases in share-based compensation expenses and third-party contracting costs

Notes:

1. Revenues from non-pharmaceuticals segments, which were not material in prior years and therefore disclosed in combination with drug discovery, are now disclosed separately for 2024

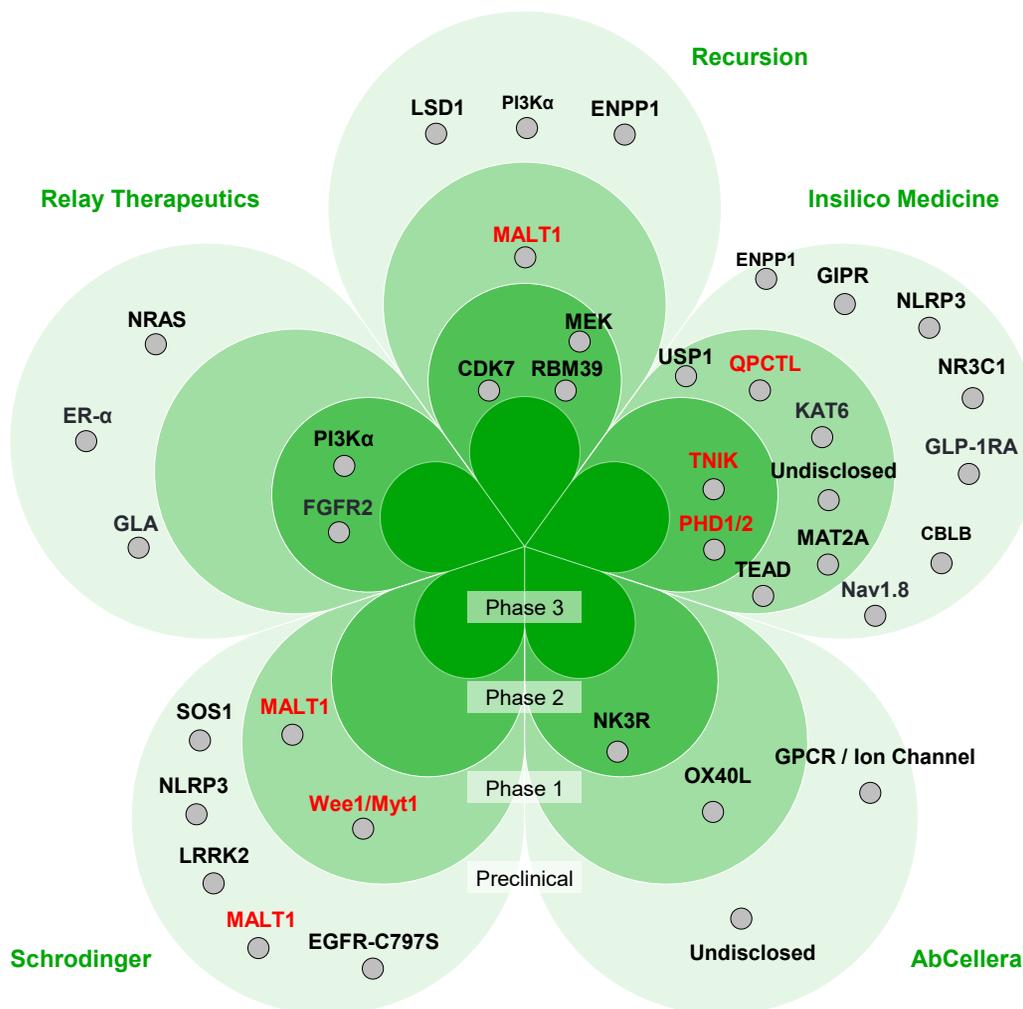
AI-Based Drug Discovery and Development Market Financial Landscape

Financial Performance Comparison

Company	Revenue			Trend	2024A P/S	2025E P/S ²	Market Cap as of Jan 15, 2026
	2022	2023	2024				
 Insilico Medicine	\$30.1 M	\$51.2 M	\$85.8 M		45.8x ¹	NA	\$3,932.9 M ³
 XtalPi 晶泰科技	\$19.3 M	\$24.6 M	\$36.5 M		190.4x	74.9x	\$6,951.3 M
 Schrödinger	\$181.0 M	\$216.7 M	\$207.5 M		6.5x	5.4x	\$1,349.8 M
 RECURSION	\$39.8 M	\$44.6 M	\$58.8 M		42.9x	41.0x	\$2,523.3 M
 RELAY THERAPEUTICS	\$1.4 M	\$25.5 M	\$10.0 M		139.8x	109.6x	\$1,398.2 M
 AbCellera	\$485.4 M	\$38.0 M	\$28.8 M		44.6x	35.6x	\$1,283.7 M

Note: 1. Calculated by Post-money valuation of E-series financing dividing by revenue in 2024; 2. based on Capital IQ market consensus; 3. Post-money valuation of E-series financing, as of May 2025; NA refers to Not Applicable

Largest Pipeline and is the Most Innovative among AIDD Companies



Company	Number of AI Discovered Target in Proprietary Pipeline	Novel : Non-novel Target
Insilico Medicine	27	3:24
Relay Therapeutics	5	0:5
Schrödinger	7	3:7
Recursion	7	1:6
AbCellera	4	0:4



Source: Frost & Sullivan Analysis

Note:1. A "high novelty target" is defined as a target that has been identified through AI discovery and has not previously been subject to clinical development