

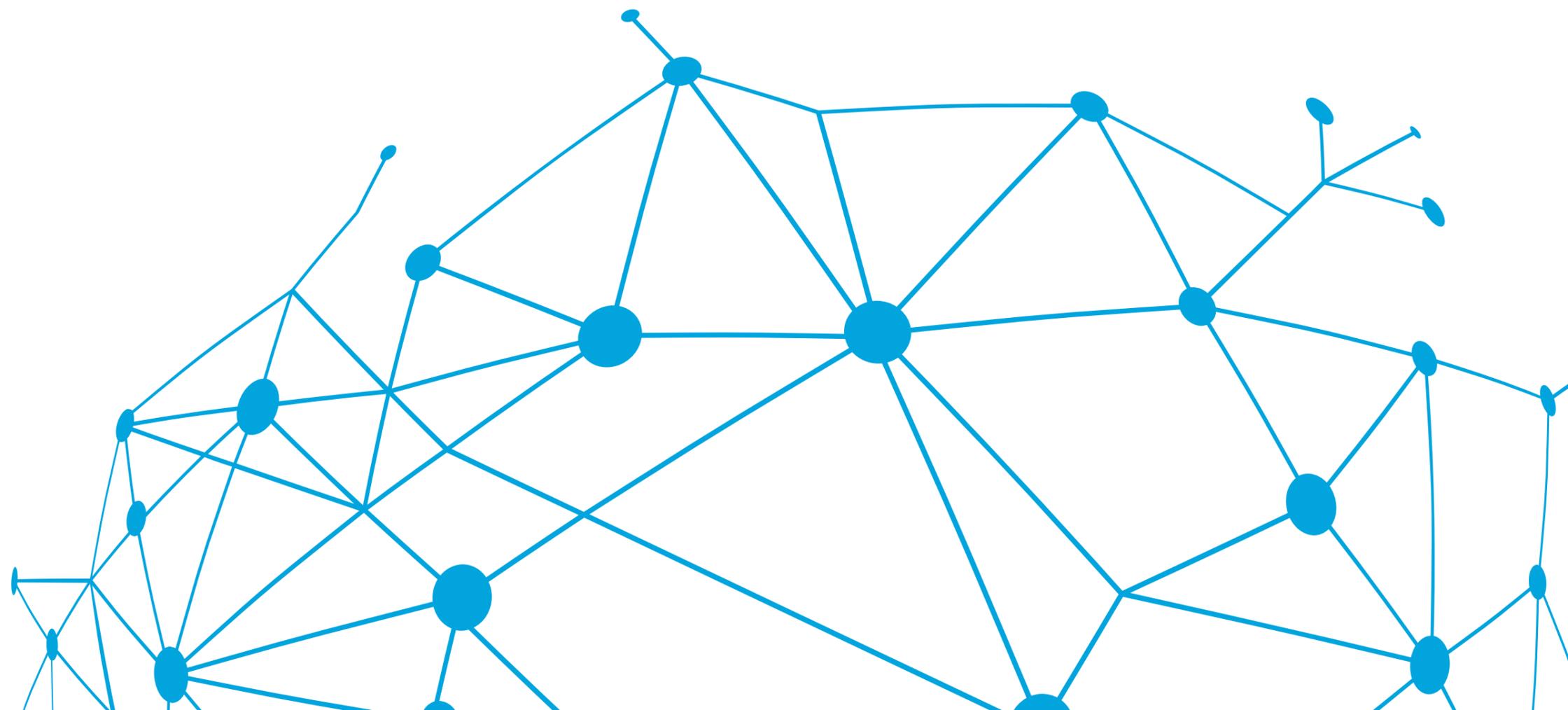


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LIFE SCIENCES CONSULTING

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Companies to Watch:
AI in Drug Discovery





Spun out of Google DeepMind in 2021, Isomorphic Labs is backed by Alphabet and a recent **\$600M funding round**

“AlphaFold broke new ground. Iso has built on it.”
Isomorphic

AI Strategy:

- Collaborative development with Google DeepMind of AlphaFold3 to create AI systems that **predict protein structures, molecular interactions and drug behaviors** with industry-leading accuracy
- Develop a **disease-agnostic unified drug design engine** that transforms the drug discovery process, to generate an **“ecosystem of proprietary predictive and generative models”**
- Operate a dual-track approach, **expanding pharma partnerships** while also advancing internal therapeutic programs in oncology and immunology, with plans to **advance a drug candidate into clinical trials in 2025**

Key Partnerships:



Focus Areas:

**Oncology
and
immunology**

API Commentary:

- Builds upon the already successful and **Nobel-winning AlphaFold technology**
- Major pharma partnerships confirm platform's credibility and expertise
- **AI-designed candidates are entering FIH clinical trials for pivotal testing**
- AI-driven drug design engine has the potential to open new therapeutic frontiers by targeting multiple therapeutic areas and modalities, including previously undruggable diseases with unprecedented speed and scope



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ATAVISTIK



Founded in 2021, Atavistik has **raised \$100M** to accelerate the discovery & development of precision allosteric therapeutics

“In a short period of time, Atavistik Bio has quickly identified novel allosteric binding pockets in a broad range of targets and built a deep discovery pipeline.”

- Dr. John Josey, Atavistik Board Chairman

AI Strategy:

- The **Atavistik Metabolite-Proprietary Screening (AMPS™)** technology utilizes the function of metabolites to identify novel cryptic (allosteric) binding pockets for a broad range of targets
- **Integration with an AI-enabled, structure-based drug discovery engine** enables the design of small molecule therapeutics
- Leverages the interaction between natural regulators in the body with proteins to **identify unique protein binding sites for potential drug development**

Key Partnership:



Focus Areas:

**Oncology
and
rare diseases**

API Commentary:

- Utilizing allosterism is a unique approach to **engage previously intractable targets**
- A clinical trial utilizing an oncology drug designed with AI assistance is underway, positioning Atavistik ahead of some competitors
- A partnership with Pfizer enables Atavistik's platform to **impact a broad range of oncology indications**



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Founded in 2018 by Daphne Koller, Insitro has **raised more than \$700M**, including more than \$400M in a single funding round alone

“Insitro is part of a growing field of AI companies promising to accelerate drug discovery by using machine learning to analyze huge datasets of chemical and biological markers.”

- Associated Press

AI Strategy:

Key Partnerships:



- The Insitro Human Platform combines multi-modal phenotypic cellular data with aggregate clinical data from human cohorts to internally generate **large-scale multi-modal databases** that appropriately model human disease states across an **array of genotypes and phenotypes**
- Self-supervised **deep machine learning and generative AI platforms** analyze these models of human disease
- **Novel drug targets** are identified for challenging diseases across multiple therapeutic areas

Focus Areas:

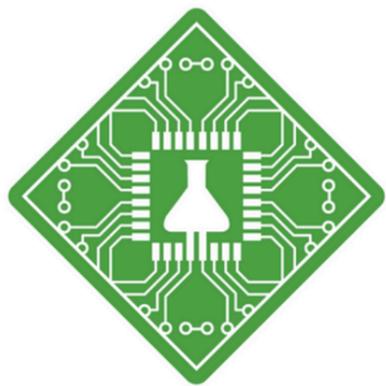
**Neurodegeneration
and
metabolic diseases**

API Commentary:

- Insitro is noted for its strong, experienced leadership
- **Multiple successful Pharma partnerships highlight the potential of the Insitro Human Platform**
- Despite these positives, Insitro laid off 22% of its workforce in May 2025, stressing the competitive nature of the AI/ML drug discovery space



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Insilico Medicine

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Since its inception in 2014, Insilico has **raised \$400M+** in funding and is **one of the few companies to have advanced AI-discovered drug candidates into human trials**, such as its lead anti-fibrotic drug, rentosertib

“With computational approaches like this, we have the potential to shorten the preclinical phase of drug discovery by years”

Dr. Igor Stagljär

AI Strategy:

- Leverages commercially available **proprietary Pharma.AI platform** that contains works across disciplines to use generative AI to **accelerate target identification, molecule design, and clinical trial prediction**
- **Deploys robotic labs** and AI-powered "Supervisor" humanoid robots to **automate synthesis, screening, and data analysis**
- The Company is also collaborating on advancing **Large Language of Life Models (LLLMs) to enable digital-omics experimentation**

Key Partnerships:

sanofi

FOSUN PHARMA
复星医药成员企业

MENARINI
group

EXELIXIS

Focus Areas:

**Oncology and
age-related
diseases**

API Commentary:

- Strength of pipeline and success in advancing programs, **with 7 clinical stage assets**, has attracted industry interest and partnerships
- AI-discovered anti-fibrotic therapy shows meaningful benefits in clinical trials
- The combination of technology and clinical validation positions Insilico **to deliver some of the first truly AI-discovered medicines, particularly for complex conditions** where traditional discovery methods have struggled



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Atomwise

Founded in 2012, Atomwise has **raised more than \$200M** to fund the AtomNet platform

“Results of the AIMS study show that AtomNet has a high success rate in finding hits for traditionally challenging biology, like allosteric or protein-protein interactions.”

- Dr. Gregory Bowman, UPenn

AI Strategy:

Key Partnerships:



翰森制药
HANSOH PHARMA



Focus Areas:

**Immunology
and
undisclosed
targets**

- The AtomNet platform is the **first application** of AI/ML based on a **deep convolutional neural network** (often used in image classification, speech recognition, etc.) for molecular recognition
- This platform **does not require a crystal structure or local ligand training**, a mainstay of earlier AI/ML drug discovery efforts where a novel model was required for each target
- Beyond Proof Of Concept: **predicted molecules have already become lead candidates and generated positive results in animal models**

API Commentary:

- Despite being part of the first generation of AI drug discovery companies, Atomwise has struggled thus far to translate candidates into clinical assets
- AtomNet is potentially differentiated in **not requiring novel models for each target as well as identification of "novel" compounds**
- Atomwise is seeking to advance its first candidate, a TYK2 inhibitor, into the clinic in 2025



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