

Atlas AI | The AI-Powered Drug Discovery Workbench



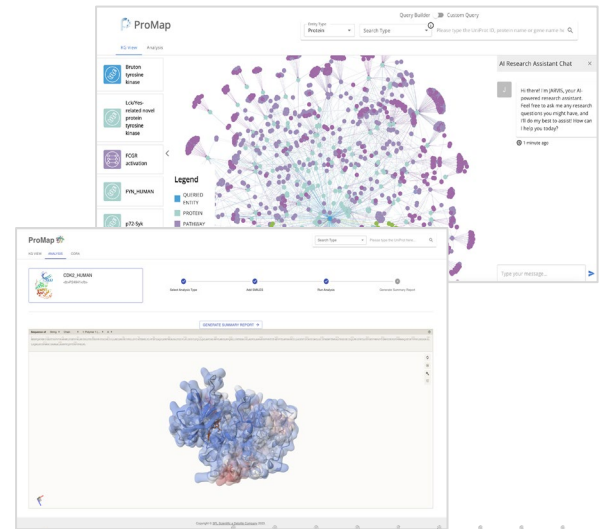
The Modern Lab's Dilemma

Pharmaceutical research and development (R&D) costs and timelines have skyrocketed in recent years due to increased therapeutic complexity and a corresponding influx of data to store and analyze. Overwhelmed research teams waste time on manual analyses and endless searching for hard-to-find data across disparate groups within their organization. Atlas AI leverages the power of knowledge graphs and generative AI to turn the huge growth of data into a strength, enabling truly innovative and modern approaches to pharmaceutical R&D.

Introducing Atlas AI: Research at the speed of AI

Atlas AI is an innovative, artificial intelligence (AI)-powered cloud native application that empowers scientists to generate and validate high-quality hypotheses quickly through three key pillars:

- 1 **Accelerate Insight Discovery:** The semantic knowledge graph captures connections between dozens of different data sources, from clinical data and diseases all the way down to the underlying biochemistry accelerating target identification, compound screening, and more.
- 2 **Generate Novel Hypotheses:** GenAI and Large Language Models (LLMs) assist scientists in synthesizing data and suggesting new hypotheses, including rapidly identifying candidates for drug repurposing or predicting the behavior of newly identified molecules.
- 3 **Simulate Experiments Quickly:** Customizable AI model pipelines allow scientists to simulate full experimental workflows & quickly validate ideas, such as efficient lead identification & optimization.



Atlas AI Semantic Knowledge Graph by the numbers

Summary statistics on current version of Knowledge Graph (* data current as of November 2023)
 11,229,138 total nodes and 96,355,621 relationships from 13 distinct high-quality scientific databases, including PubMed, UniProt, and PubChem, comprised of :

794,847

proteins including 102,402 variants, 89,754 mutations, and 885 antibodies

8,151

functional protein domains

431,029

detailed descriptions of protein function

7,630,236

chemicals/drug compounds

17,372

diseases and ailments

89,767

biological reactions across 22,020 biological pathways

1,386,431

drug-target pairs with experimental binding data

338,376

total PubMed citations across 121,267 unique PubMed references

2,356,105

distinct patents connected to compounds in the Knowledge Graph

142,469

links to experimentally-determined protein structures

Making it real: accelerating science through AI

CURRENT CHALLENGES

Clinical trials constitute a vital component of drug development; however, a significant number of these trials fail to gain approval, resulting in immense financial losses.

In order to avoid these costly mistakes, Atlas AI allows for faster and higher quality experiments in the pre-clinical stages of R&D, identifying potential issues earlier in the cycle.

ONCOLOGY TARGETS: AN EXAMPLE

A recent research paper meticulously evaluated 183 clinical trials, encompassing over 12,000 patients, focusing on 16 distinct drugs aimed at targeting the insulin-like growth factor-1 receptor (IGF-1R) for oncology treatment.

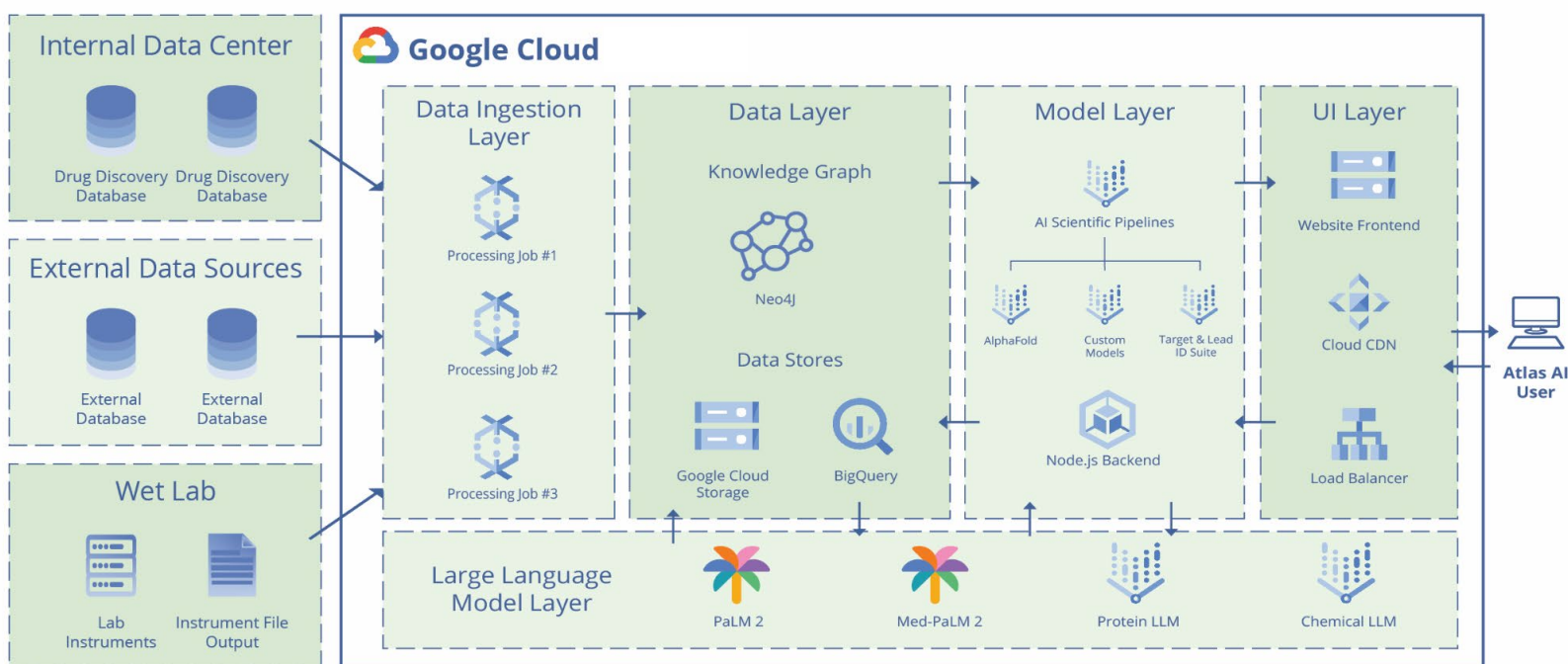
None of the aforementioned agents received approval for clinical use, incurring expenses of \$1.6-\$2.3 billion.

WHAT NEEDS TO BE PRIORITIZED

This scenario demonstrates that the industry requires enhanced preclinical models, rigorous target validation, and improved decision-making before embarking on clinical trials.

Atlas AI addresses these crucial areas by leveraging its Semantic Knowledge Graph to help researchers arrive at key insights more quickly and its AI scientific pipelines to validate these insights in hours instead of years.

Reference architecture on Google Cloud integrates Deloitte assets with scalable Google Cloud services



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