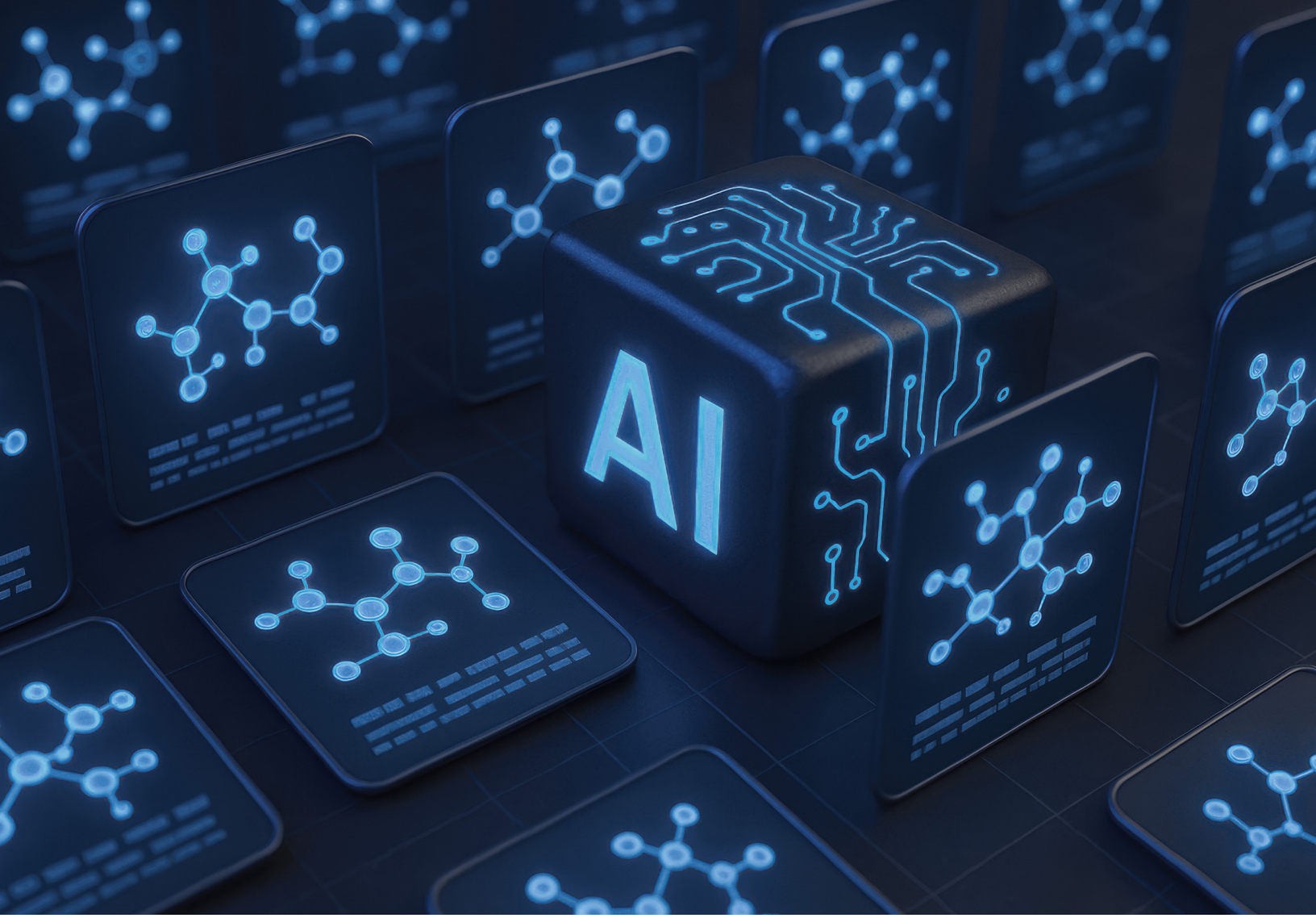

Accelerating Drug Discovery with AI: A Technetium Case Study

Technetium
THERAPEUTICS

Technetium Therapeutics, a pioneering drug discovery company, is at the forefront of leveraging artificial intelligence to transform the traditional drug development pipeline. In an industry where innovation is often stymied by long development cycles and the high cost of traditional research, Technetium Therapeutics has carved a unique path by focusing on de novo drug design from the ground up. This case study explores how Technetium Therapeutics leveraged SandboxAQ's SAIR (Structurally Augmented IC50 Repository) dataset, to significantly accelerate the discovery process and achieve remarkable hit rates in its drug development program.

From Patent Busting to De Novo Design

Traditional drug discovery often involves minor modifications to existing, patented drug structures to create a new, similar compound. While this can avoid legal issues, it rarely leads to novel treatments and can even result in less effective drugs. Technetium Therapeutics was founded on the principle of innovation over imitation. The company's mission is to design entirely new small molecules that are not only effective but also possess unique properties tailored to specific biological targets.

This approach, however, presents a significant challenge: the chemical search space for potential drug molecules is astronomically large. Traditional methods, which rely on synthesizing and screening thousands of compounds, are slow and expensive. Technetium Therapeutics' solution is a multi-agent AI platform that can virtually screen millions of molecules per day.

A Multi-Agent Approach to Molecular Design

Technetium Therapeutics' AI platform is built on a sophisticated, web-based system of multiple agents that communicate and collaborate. It includes the following:

- A **Generative Agent** that creates novel molecular structures. Using physics-based docking, a **Distillation Agent** filters the generated molecules, assessing their potential to bind to a specific protein target.
- The **Interaction Review Agent** is the core of Technetium's approach. Instead of just relying on docking scores, this agent analyzes the interaction profiles between the molecule and the protein, examining factors like the location and stability of hydrogen bonds.This level of detail ensures that the selected molecules have a high likelihood of being effective binders.

This stepwise, iterative process allows Technetium to refine a massive pool of potential molecules down to a few hundred promising candidates, which can then be further optimized.

Filling the Data Gap with SandboxAQ's SAIR Dataset

For its Interaction Review Agent to be effective, Technetium Therapeutics needed a robust dataset of real-world molecular interaction data. Initially, they trained their agent using the PDBBind dataset, which contains over 10,000 data points of small molecules bound to proteins. While valuable, this dataset was limited in size, a common problem in the drug discovery field where generating training data is expensive and time-consuming.

The introduction of SandboxAQ's SAIR dataset in June 2025 was a game-changer. The SAIR dataset, a synthetic, yet highly structured and organized collection of 5 million data points, provided the rich training data Technetium needed. By training their AI agent with SAIR data, Technetium was able to significantly enhance its predictive capabilities.

> We saw a fundamental flaw in the industry's approach, where everyone was chasing the same targets and just busting patents," said Cheng Hu, Co-founder and CEO of Technetium Therapeutics. "Our vision was to start from a clean slate with de novo design, but we were limited by the lack of rich, high-quality training data. The SAIR dataset from SandboxAQ was exactly what we needed to bridge that gap. It was the key to unlocking the true potential of our platform and achieving an outstanding success rate.
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> **Cheng Hu**, Co-founder & CEO of Technetium Therapeutics

The Results: A New Benchmark for Success

The impact of the SAIR dataset was immediate and measurable. After retraining their model, Technetium selected 18 compounds for laboratory testing in a program targeting ALS (amyotrophic lateral sclerosis). The results were a massive leap forward for the industry. Four of the 18 compounds tested showed significant activity, with potency under one micromolar. This translates to a 23% hit rate, a monumental improvement over the industry average of less than 1% for traditional methods and a typical 0.1 - 1% for AI-driven platforms.

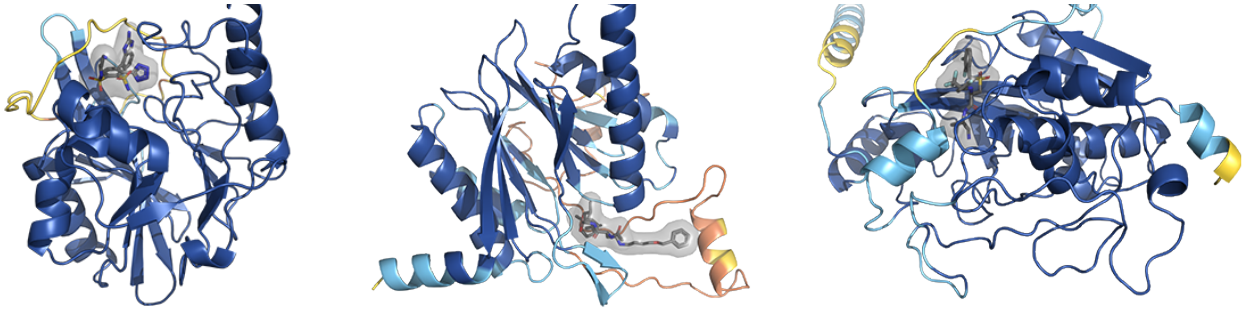
Technetium credits this success to two key factors: the sheer volume of high-quality data from SAIR and their innovative approach to feature selection. Instead of feeding the AI with random data, Technetium's team, with its deep domain expertise, extracts specific, meaningful features, e.g. whether a molecule is a hydrogen bond donor or acceptor, to ensure the AI learns the most critical information. This method avoids the pitfalls of simply relying on docking scores, which can often be misleading.

Technetium's team learned from the data itself, identifying instances where a high docking score didn't correspond to high potency and, conversely, where a low score concealed a potent molecule. By focusing on these specific, physics-based features, Technetium Therapeutics has created a system that goes beyond brute-force screening, delivering a new level of precision and success in drug discovery.

As the industry grapples with the limitations of existing data and the challenges of traditional drug development, Technetium Therapeutics is demonstrating a new path forward. By combining cutting-edge AI with a large, high-quality dataset, Large Quantitative Models (LQMs) are not only accelerating the discovery of new drugs but also paving the way for a more innovative, cost-effective, and more successful future for the entire pharmaceutical industry.

> AI models in drug discovery often feel like a black box. You feed them data and get a result, but you don't know why. Our system is different; it's built on a foundation of explainable, physics-based interactions. The SAIR dataset allowed us to train our models with a level of precision that other data simply couldn't provide. This is what gives us the confidence to go from millions of molecules to just a handful of promising candidates in a matter of weeks.

Chunlin Wang, Co-founder & CTO of Technetium Therapeutics



From Years to Weeks with Large Quantitative Models

Technetium Therapeutics is currently optimizing these four lead compounds to create preclinical and clinical candidates. Today they screen around 1 million molecules per day using their own hardware. To accelerate their development they joined the Nvidia Inception Program that provides them with access to GPUs on the DGX Cloud. While a significant part of the journey, including animal and human trials, still lies ahead, their AI platform has compressed the initial discovery phase from years to weeks.

Adam Lewis, SandboxAQ's Head of AI & Quantum Solutions said: "Technetium Therapeutics is a perfect example of what's possible when you combine advanced AI with rich, quantitative data. The SAIR dataset was designed to fill a critical void in scientific research, and Technetium Therapeutics' ability to leverage it so effectively demonstrates the power of our approach. With SAIR, we're enabling a new paradigm of discovery that moves beyond traditional methods and even existing AI models."

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To learn more about Technetium Therapeutics, please visit our website at https://technetiumtx.com. To download the SAIR dataset please visit: https://sandboxAQ.com/sair.