

Kebotix Case Study: Autonomous Optimization

Summary Highlights

- 5x reduction in costs for lab supplies and HTE run-time achieved thanks to Kebotix's artificial intelligence-driven adaptive optimization.
- Fully autonomous assay optimization (extendable to >10 free parameter).
- Easy plug-in of Kebotix smart experimentation software into existing HTE platforms.

Speed Saves Lives

For the National Center for Advancing Translational Sciences (NCATS), it's all about delivering new treatments and cures for diseases faster.

If you ask a patient when they want their cure, they'll say yesterday. Generating a new therapeutic takes 10 to 15 years and billions of dollars. We need to find better drug development methods that are efficient.

Looking toward a better tomorrow for patients, NCATS reached out to Kebotix, a technology platform company for new chemicals and materials, to enhance productivity of NCATS' high-throughput experimentation (HTE) via

artificial intelligence-driven optimization of assay conditions for biosynthesis inhibitors.

NCATS had been running systems in a very open loop fashion. They have their assay and fixed chemical libraries, they run the experiment, get results, and then iterate. What they weren't taking advantage of were some of the technologies out there, especially when it came to machine learning.

Kebotix provides NCATS with the ability to organize its operation and automate at a level where it has all the data in a very structured format ideally suited for machine learning and ready for running experiments autonomously.

Kebotix Smart Algorithm

1. Use each experimental result to update a surrogate AI model.
2. Kebotix (KBX) algorithm selects the next experiment to run.
3. Gain more information with fewer experiments.

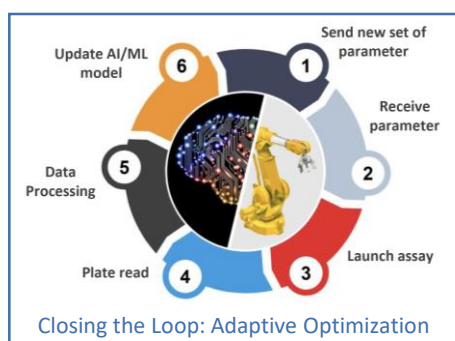


Leveraging Kebotix AI-driven optimization, 54 experiments were sufficient to replace a 294-experiment factorial DOE.

Finding a Better Way

Kebotix partnered with NCATS to demonstrate fully autonomous optimization of assays performance for biosynthesis inhibition. Kebotix software processed and learned from previous experimental results leading to submission of new AI-generated assay conditions via remote access to the HTE facility at NCATS for experimental testing.

The goal of the multi-objective optimization was to reduce lab consumables (enzyme and substrate)



while maintaining a sufficiently high signal-to-noise ratio defined in terms of statistical effect size.

Prior to partnering with Kebotix, NCATS had been using a high-throughput approach and factorial design of experiment (DOE) that required the team to run a full set of 294 experiments in a brute force fashion. Despite the moderate complexity of the optimization task, executing the factorial DOE kept an expensive HTE facility occupied for two days. This approach often wastes testing materials and time. For an agency focused on finding treatments for rare diseases, of which there are over 7,000, a better way was needed.

Optimizing Experiments Quickly

Instead of testing a set of predefined parameters as in the traditional DOE approach, Kebotix uses adaptive optimization to gain more information using fewer experiments.

By employing an advanced proprietary AI-driven optimization algorithm, Kebotix found suitable conditions and optimal assay performance with only 55 measurements with up to 20 running simultaneously. This output was sufficient for the Kebotix algorithm to identify and test the global optimum of the full 294 DOE experiments with a high probability (>95%). NCATS achieved a five-fold reduction in costs for lab supplies and HTE run-time, reduced from 49 hours to a mere 9.

Who We Are

Kebotix (www.kebotix.com) is a platform company for chemicals and materials ushering in a new age of high-speed innovation using artificial intelligence and robotic automation. Kebotix has built the world's first self-driving lab for materials discovery powered by AI and robotics. Kebotix, founded in 2017, is accelerating the exploration, discovery, use and production of new molecules and materials that can solve some of the world's most urgent problems.

How can you benefit from adaptive optimization?

Kebotix's adaptive optimization works for a wide variety of applications of optimization problems, going beyond the demonstrated bio-application. Opportunities include:

- Industrial process optimization
- Chemical or biological reaction optimization
- Cost reduction through substitution testing
- Formulation testing and optimization
- Any process with a variety of choices and the opportunity to iterate and evaluate

Our adaptive optimization approach allows you to save the cost of expensive experiments, find optimal settings in a shorter time, and experiment in richer and more complicated parameter spaces.

Kebotix AI suggests new experimental parameters that are remotely submitted to NCATS' HTE facility that runs experiments every 10 minutes.

