CASE STUDY

ACD/LABS [ADVANCED CHEMISTRY DEVELOPMENT, INC.]

Improving HTE Efficiency in Process Chemistry

Challenges in Traditional High Throughput Experimentation

Experimental set up of procedures for high throughput experimentation (HTE) traditionally involves electronic notebooks (paper lab notebooks) and Excel templates. Scientists at a top global pharmaceutical company also had reagent libraries integrated into their lab notebooks to ease the workflow. Post experiment execution, data was stored and visualized in a variety of software—their content management system, Spotfire, Tableau, Excel, or PowerPoint (Figure 1).

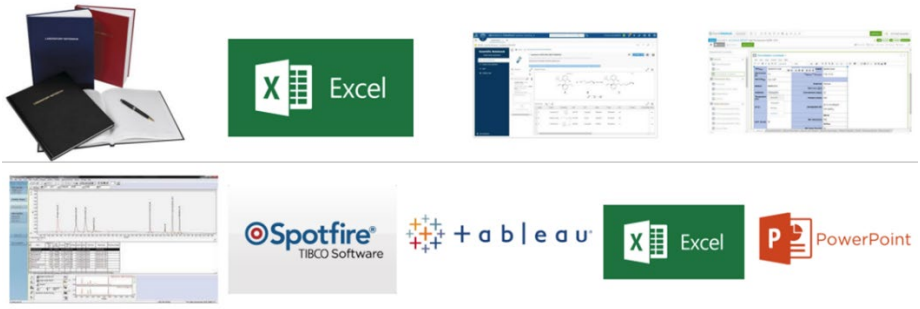

Figure 1. An array of software tools is used in the design, execution, and analysis of traditional HTE.

This ecosystem of disparate software tools is typical of pharmaceutical development organizations. It proliferates the risk of data transcription, makes collaboration and data sharing a challenge, and created inefficiencies.

> "These tools are not optimized for HTE. They lack workflow logic, and it's time-consuming to jump between different software, transcribe information between them and have no way to capture and visualize data automatically."

Streamlining HT Experimentation with Katalyst D2D

In 2018 the process chemistry team at a Fortune 500 corporation adopted Katalyst D2D to help realize their goals:

1. Accelerate reaction screening and decision-making timelines
2. Deal with the more complex molecules entering their pipeline more efficiently
3. Democratize high throughput experimentation for process chemistry and engineering

Katalyst fulfilled the requirements of intuitive end-to-end software that leads scientists through the design, execution, and analysis of experiments.

> "Katalyst is like an ELN for our high throughput experiments. It integrates with our experiment execution hardware and analytical instrument allowing us to visualize results in one place to make decisions and is a central place for us to document and manage HTE information and data."

Templated plate designs enabled the chemistry organization to easily see what experiments were being run and made HTE accessible to the broader chemistry team.

> "Colleagues not skilled in HTE were able to design a 96-well experiment in less than 5 minutes and get into the lab to run it the same day."

Flexible & Automated LC/MS Data Analysis for HTE

Katalyst also offers scientists flexibility in how they interact with experimental results. LC/MS instrument integration means that analysis plates are set up in Katalyst for execution. The results of these analyses may be assessed through:

Fully Automated LC/MS Data Processing

LC/MS data is pulled directly into Katalyst and processed automatically—peaks are labelled and area percent values calculated based on the specified internal standard. Scientists assess these results in tables, plot parameters graphically within the Katalyst interface, or export the data in JSON format for review in third-party tools, if desired.

Tailored Re-Processing of HTE Results

LC/MS results for individual wells or groups of wells can be re-processed quickly and conveniently within the software environment. Single wells can be manually reprocessed through web-based spectral processing software (Spectrus Processor JS) integrated with Katalyst—enabling tailored processing for non-standard data sets.

Offline LC/MS Data Analysis

The ability to import results for historical experiments or for experimental data inaccessible to automated routines adds the additional advantage of being able to leverage what was long thought to be dead data. Analytical data are processed and evaluated offline. A template is used to upload results into Katalyst as the centralized location for HTE Data.

> "Automated data processing is the biggest benefit of the software. Also, batch data processing [in the Spectrus environment] is a lot faster than by other means."

Accelerating HTE Success with Katalyst D2D

Katalyst is entrenched in the HTE process chemistry workflow, and used by dozens of chemists running hundreds of experiments a week. A summer co-op student with minimal training and no prior exposure to ACD/Labs software ran 4000 experiments in one month.

Buy-in from management and automated processing helped anchor Katalyst D2D in high throughput experimentation.

> "Analysis and processing of data that used to take days is now accomplished in a matter of minutes or within an hour. Peaks that may have been missed in the past are identified through a non-targeted screening algorithm."

More Resources

Webinar: Enabling AI and Dataset Production across the Chemistry Enterprise at BMS

Webinar: Practical Considerations for Improving High Throughput Synthesis