tetrascience

Simplifying ADME studies through data automation

CUSTOMER STORY

Rapid equilibrium dialysis followed by mass spectrometry (RED-MS) is a technique used in absorption, distribution, metabolism, and excretion (ADME) studies. It measures how small-molecule drugs interact with blood plasma proteins, which is crucial for understanding their bioavailability and efficacy in the body.

In RED-MS assays, a drug solution is added to a chamber separated by a semipermeable membrane with plasma proteins on one side. Drug molecules move between the two sides until an equilibrium is reached. Then, samples from both sides are analyzed by mass spectrometry (MS) to calculate the drug's bound/unbound ratio.

Challenge:

Scientists were spending significant time on manual file preparation and statistical calculations for RED-MS, which slowed down ADME screening.

Solution:

The Tetra Scientific Data and AI Cloud automatically prepares and processes data for RED-MS assays.

Result:

- Cut data preparation and processing time from hours to minutes
- Centralized and contextualized data for rapid search and retrieval
- Eliminated manual steps for improved scalability and data integrity

The Challenge

Scientists in the ADME group at a top 25 pharmaceutical company were spending a significant amount of time preparing files for MS analysis. They had to manually compile sample IDs, molecular weights, tandem MS transitions to be monitored, and more. After collecting the MS data, scientists performed time-consuming statistical calculations by hand. Previous attempts to automate these processes relied on a custom-built solution maintained by one scientist, creating a single point of failure. As a result, it was not widely adopted, and most scientists continued to use manual methods.

The Solution

A series of automated pipelines were created in the Tetra Scientific Data and AI Cloud™ to overcome the challenges of the existing workflow:

1. **Data replatforming.** Sample data is automatically ingested into the cloud.
2. **Data engineering.** The Scientific Data and AI Cloud contextualizes the data with relevant metadata, such as assay type, and transforms it into an open, vendor-agnostic format. The input data required for MS analysis is then converted into a format compatible with the mass spectrometer. The scientist uploads this file to the instrument before the run.
3. **Data normalization and analysis.** Once sample analysis is complete, the Scientific Data and AI Cloud automatically collects the results. Automated pipelines then normalize the data against internal standards and calculate necessary ADME statistics for reporting.

The Result

With the Tetra-enabled workflow, scientists spend minutes instead of hours on data preparation and processing, enabling them to focus on more valuable activities. Raw and processed datasets from RED-MS assays are centralized and contextualized in the cloud, facilitating fast search and retrieval. Moreover, data workflows are now highly automated (with robust pipelines) and standardized across the group, improving scalability and data quality.

AI Readiness

The Tetra Scientific Data and AI Cloud transforms raw data into AI-native Tetra Data. These large-scale, compliant, liquid, and purpose-engineered datasets ensure the ADME group can extract maximum value from their RED-MS data using advanced analytics and AI tools.