Analytical Data Management at CMLD-BU

The Center for Chemical Methodology and Library Development at Boston University (CMLD-BU) focuses on the discovery of new methodologies to produce novel chemical libraries of unprecedented complexity for biological screening. Dr. Aaron Beeler is the Associate Director of CMLD-BU, and is responsible for the open-access analytical laboratory at the university, where every day hundreds of samples are submitted for testing by a variety of analytical techniques.

With the high volume of samples processed by the laboratory, CMLD-BU needed a sample management system that could help coordinate the movement of samples through the analytical process, and that would centralize the collection and reporting of the results. Beeler and his staff worked closely with Professional Services staff and developers at ACD/Labs to implement a system that meets the needs of CMLD-BU and more.

The ACD/Labs Analytical Data Management Solution (ADMS) for CMLD-BU combines an analytical workflow component that controls sample submission, routing, and reporting, with vendor-neutral processing and data collection for NMR, MS, UV-IR and chromatography. In addition, an automated 2D NMR structure verification scheme automatic collection of structures, spectra, chromatograms, and metadata into a single centralized database; and the capability to automatically generate selected physicochemical properties was added.

Now, ADMS at CMLD-BU is able to smoothly flow samples through a variety of analytical techniques, collecting the disparate forms of data from the wide variety of instrument types employed in the lab; storing the data in a fully searchable database that can be accessed by staff and customers through workstations within the lab. Automated structure verification is used to validate entries in the database, then, validated structures are used to predict $\log P$, $\log D$, pK_a, solubility, and other parameters. Finally, customized reports are generated for the customer.

This system helps to improve efficiency and turnaround time in the laboratory by establishing a consistent treatment of data, and avoiding redundancy in testing. Adding automated structure verification and physicochemical property prediction contributes directly to CMLD-BU's goal of exploring and expanding the diversity of small-molecule chemical libraries.

To learn more about how ACD/Labs' ADMS can work in your organization, visit
www.acdlabs.com/adms/ or email info@acdlabs.com

Advanced Chemistry Development

ACD/Labs

Visionary Software   Advancing Research