

Improving Analytical Data Management Across Multiple Experiments, Instruments, and Vendors

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Introduction

One key challenge confronted by analytical scientists is the growing need for contemporary informatics approaches that match advances in experimental methodologies. If this requirement remains unmet, the sheer amount of data generated by modern laboratories can lead to inadvertent sequestration and isolation of valuable information into discrete “data siloes”, causing important results to potentially be underutilized and/or inaccessible for future analyses. Moreover, widely used scientific informatics platforms, such as laboratory information management system (LIMS), electronic laboratory notebook (ELN), or chromatography data system (CDS) options, are not designed to manage diverse analytical data (raw values, spectra, chemical structures, etc.) and generally abstract this information into text, numbers, and images (Figure 1).

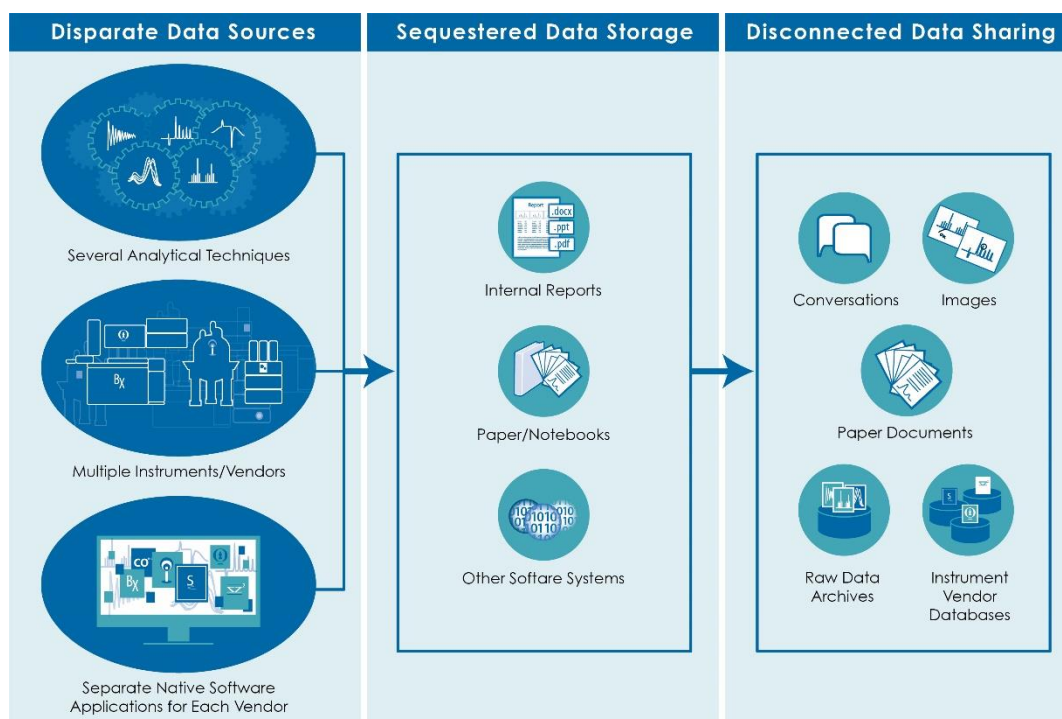


Figure 1. Outlining the modern challenges of analytical data management.

The ACD/Spectrus Platform, an analytical data management system (ADMS), addresses this challenge through a portfolio of interoperable products that link chemical and analytical data in a homogenous software environment. Regardless of technique and data format, varied analytical information can be assembled alongside its corresponding chemical context, while automation options help streamline analytical workflows. This brief application note presents a use-case for nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry (MS) data management on the Spectrus Platform, with a view to unify analytical processing and interpretation, as well as consolidate and simplify laboratory data management for a large and diverse group of research staff.

Challenges of Data Management in the Modern Analytical Lab

At the Friedrich-Schiller-Universität Jena (FSUJ), Drs. Peter Bellstedt and Nico Ueberschaar oversee the Faculty of Chemistry and Earth Sciences' NMR and MS programs, respectively. Relative to other institutions in the area, the FSUJ Faculty of Chemistry and Earth Science manages a complex analytical array that includes twelve MS instruments (orbitrap, ion trap, quadrupole, and Q-TOF variants) purchased from multiple vendors including Thermo Fisher Scientific, Bruker, Shimadzu, and Agilent. Their ten NMR instruments consist of nine conventional spectrometers from Bruker and one benchtop machine from Magritek. Attempts to reduce the experimental costs, time, and effort for these devices through consolidated data management were further complicated by their distribution in different locations within the department, with the MS instruments further divided among three distinct working groups.

Recognizing the value of better integrating NMR and MS analyses throughout FSUJ—for example, by designating singular technique managers—Drs. Bellstedt and Ueberschaar further determined that adoption of a chemically intelligent ADMS could improve efficiency. Between their responsibilities to guarantee all instruments are running smoothly, train students in various analytical techniques, answer specific questions from the different departmental working groups, and teach various courses, Bellstedt and Ueberschaar were left with little time to devote to ensuring all NMR and MS data were accessible and transferrable across working groups. Thus, the value of processing and storing data in ACD/Labs' vendor-independent analytical scheme was seen immediately, particularly for MS analyses.

Streamlining Collaboration and Data Sharing

An immediate benefit of adopting ACD/Spectrus at FSUJ was storage of experimental methods, data, and analyses in a centralized database environment, eliminating a major data distribution bottleneck. Whereas prior to software implementation key analytical technique knowledge was isolated in different working groups, and required self-directed training between incoming/outgoing PhD, MSc, and BSc students, now all methodologies and data are housed in a centralized server environment for easy sharing between individuals and laboratories. Moreover, the ACD/Spectrus feature of connected, live data (including spectra, structures, and metadata) means that research can also be easily stored in a consolidated database, and ongoing projects are immediately responsive to added knowledge and/or altered parameters. Critically, data from the multiple different vendor instruments can be imported, analyzed, integrated, and stored together, further increasing efficiency.

Standardizing Data Processing

The ambitions of Drs. Bellstedt and Ueberschaar did not cease at incorporating ACD/Labs solutions simply for research purposes. The value of efficient analytical data import, processing, storage, and sharing was also applied in various teaching contexts, where all undergraduate and graduate chemistry students at FSUJ are being trained in the use of ACD/Labs software. A key advantage to unifying the software environment for teaching purposes is removing the need to train students on multiple different vendor software platforms. Thus, the singular ACD/Spectrus Platform is able to help simplify the process of designing key courses in NMR and MS data processing and interpretation.

Though the above example focused on academia, the benefits of ACD/Spectrus for analytical data management are applicable across R&D in all industries. To learn more visit www.acdlabs.com/spectrus.