APPLICATION NOTE

ACD/Labs

ADVANCED CHEMISTRY DEVELOPMENT, INC.

Eliminating the Logistical Challenges of NMR Data Processing with Browser-Based Software

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Introduction

NMR data acquisition and processing often occur separately in the modern laboratory. Scientists acquire data from instrument-vendor software run on a computer (workstation) physically connected to the instrument. To free up time on shared instruments, they then transfer the data to a different, unconnected computer for processing.

What software should be used for the processing step? The vendor software from the workstation seems like the obvious answer. But these programs are designed primarily for acquisition, not processing. Their processing tools are often difficult to use or don't allow you to get the information you need from your NMR data. Also, vendor software often can't process data acquired on other vendor's instruments. This creates problems for institutions with instruments from multiple vendors.

Third-party data processing software solves many of these problems. It provides advanced NMR processing tools in a vendor-neutral application. So users have all the necessary tools to process files from any instrument, without being tied to the instrument itself.

Still, one remaining factor has limited both third-party and vendor NMR data processing software: both must be locally installed. These individual installations require considerable equipment and time, including:

1. Significant amounts of computer memory
2. Substantial computing power
3. Discrete maintenance and updates of each installation

Also, for institutions with bring-your-own-device policies, locally installed software must be compatible with all operating systems for full accessibility. Finally, locally installed software can only be used on the computer where it is installed, recreating the problem of being tied to (and needing to share) equipment.

As part of the Spectrus JS family of vendor-neutral browser-based analytical data handling software, Spectrus Processor JS enables unparalleled flexibility for NMR and *x*C/UV/MS data analysis. The application is hosted from a central server or computer within the institution. Then, data that is uploaded to the Spectrus Processor JS server is stored with full chemical context and is accessible by users from any browser.

This application note describes the implementation of Spectrus Processor JS in a natural products researcher's NMR data handling workflow. The program was used at the University of North Carolina at Greensboro for isolating and characterizing bioactive compounds from fungi, plants, and bacteria. The discovered compounds may lead to new treatments for diseases such as malaria and cancer.

Switching to Browser-Based NMR Data Processing Software

The lab already used NMR data processing software and an established workflow to extract information from their spectra. It was therefore important for Spectrus Processor JS to fit into their workflow without requiring disruptive time and effort to set up.

Fortunately, Spectrus Processor JS needs no software download. The researcher accessed the software quickly and easily by opening a browser tab, navigating to the right page, and signing in with his username and password (Figure 1).

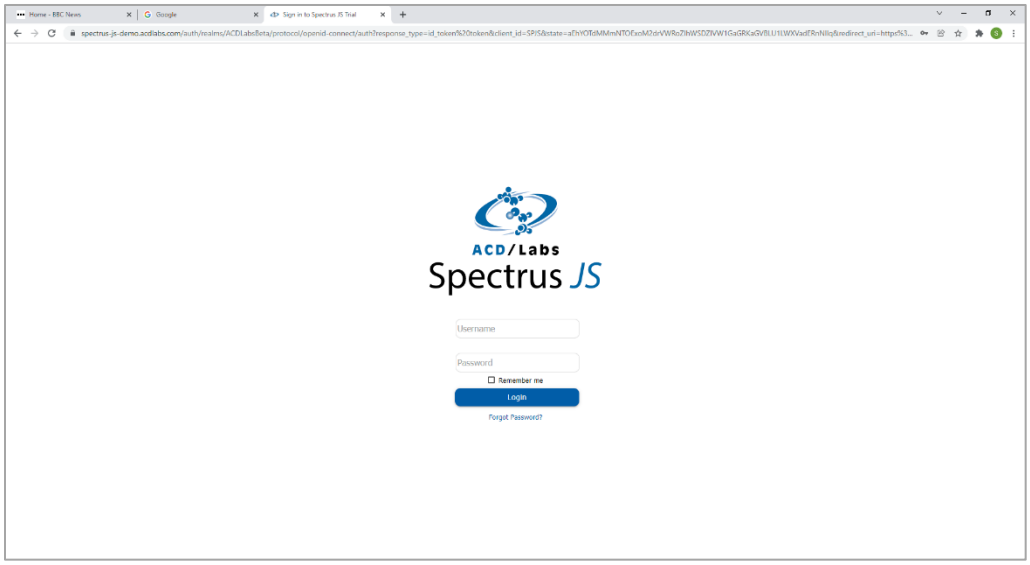

Figure 1: Spectrus Processor JS is accessed from a browser using a username and password to log in.

Both the researcher and his trainee, who had differing amounts of experience processing NMR data, found Spectrus Processor JS extremely easy to learn. The NMR data processing tools are clearly labelled and intuitive to use (Figure 2).

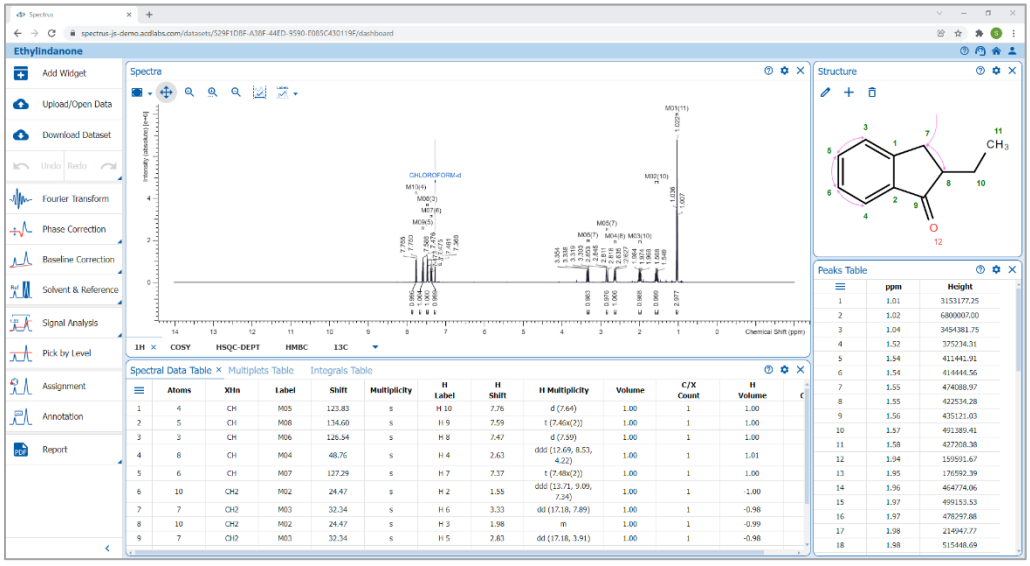

Figure 2: The Spectrus Processor JS interface and clearly labelled tools and widgets make it easy to learn to use.

They found the same keyboard shortcuts and spectra-stacking features that they were already familiar with, so they moved seamlessly through their previously established data processing routine. Though they received a tutorial video, they did not need it to get started. They reviewed it later but found nothing that they had not easily discovered on their own.

Processing Data from Multiple Shared Instruments

The researcher used shared 400 and 500 MHz JEOL instruments located on campus and a 700 MHz Agilent instrument shared between multiple organizations and located a 5–10 minute drive away. The campus workstation computers can process NMR data; however, since these instruments are shared, the researcher can spend only limited time on this computer. He does not perform the bulk of his processing there. For the off-campus instrument, alongside the same time restraints for a shared instrument, the workstation computer uses different NMR data processing software from the research lab. Though the researcher could quickly check the data quickly with the software, he had to transfer the raw data to his own software for more in-depth analysis.

The researcher's institution has a bring-your-own-device policy. Users download licensed NMR data processing software to their personally owned computers. Each person is allowed one license, so they are restricted to installing and using the software on one computer. Also, the researcher shared that computer with his trainee, further restricting data processing time and locations.

Though this previous NMR data processing setup allowed the researcher to obtain the necessary results, it required significant time and mental energy. With Spectrus Processor JS, most of these NMR data processing problems disappeared.

Since Spectrus Processor JS is cloud-enabled and browser-based, NMR data can be processed and uploaded from a browser on any workstation computers (Figure 3). The researcher can then return to his laptop (or any other convenient computer), bring up the data from his browser, and access it in the state it was last left in. His trainee could perform the same actions from his own computer, freeing up the researcher's computer time for himself.

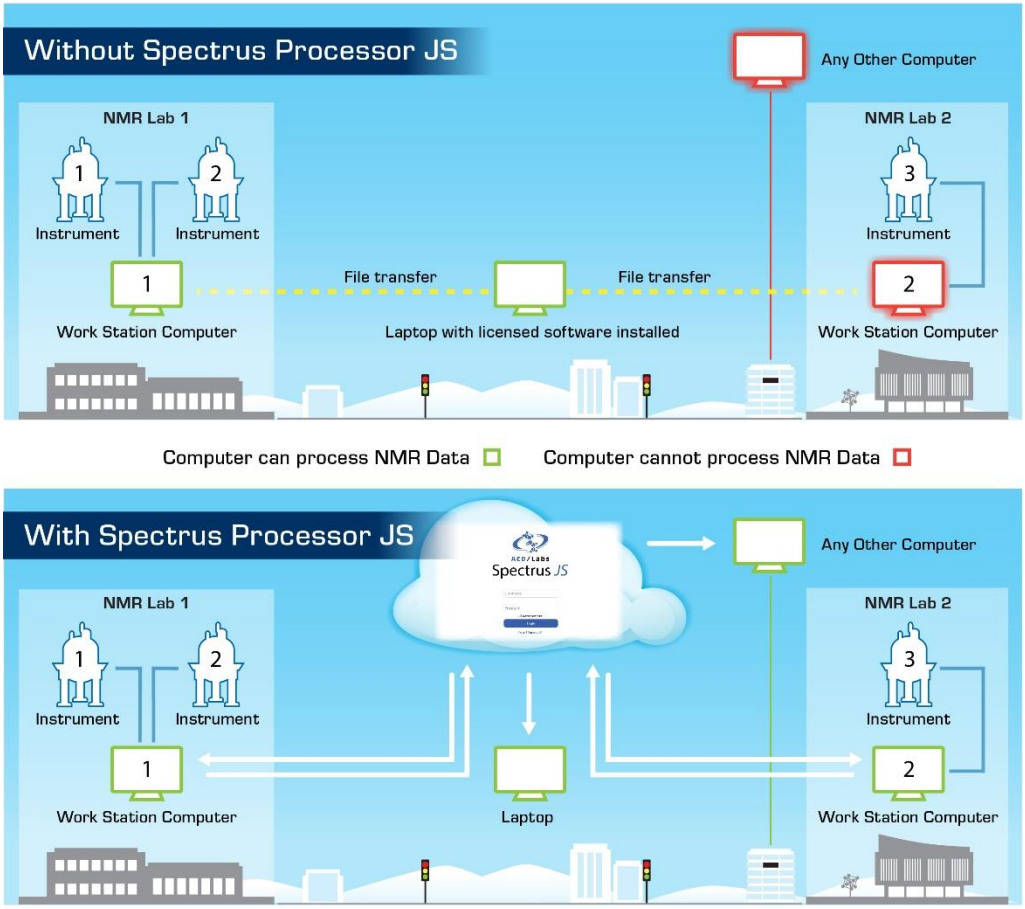

Figure 3: NMR data acquisition and processing architecture before and after implementing Spectrus Processor JS.

Improved Workflow and Records

Spectrus Processor JS also integrated well with existing laboratory-wide analytical data processing and storage systems.

For example, the researcher's lab keeps a library of NMR, MS, and chromatography data. The library contains more than 600 isolated and characterized fungal secondary metabolites. Before Spectrus Processor JS, the lab kept NMR data analysis records as images of processed spectra, and as peak assignment tables in word-processing software or on pieces of paper. This method was time-consuming and error prone.

With Spectrus Processor JS, the researcher generated consistent reports in a single click (Figure 4a). These contained processed spectra and his choice of tables displaying spectral data and experiment parameters (Figure 4b). The reports are helpful for the researcher's own reference and use in publications, but they also give everyone in the lab, now or in the future, access to the spectrum and details about the data and acquisition parameters.

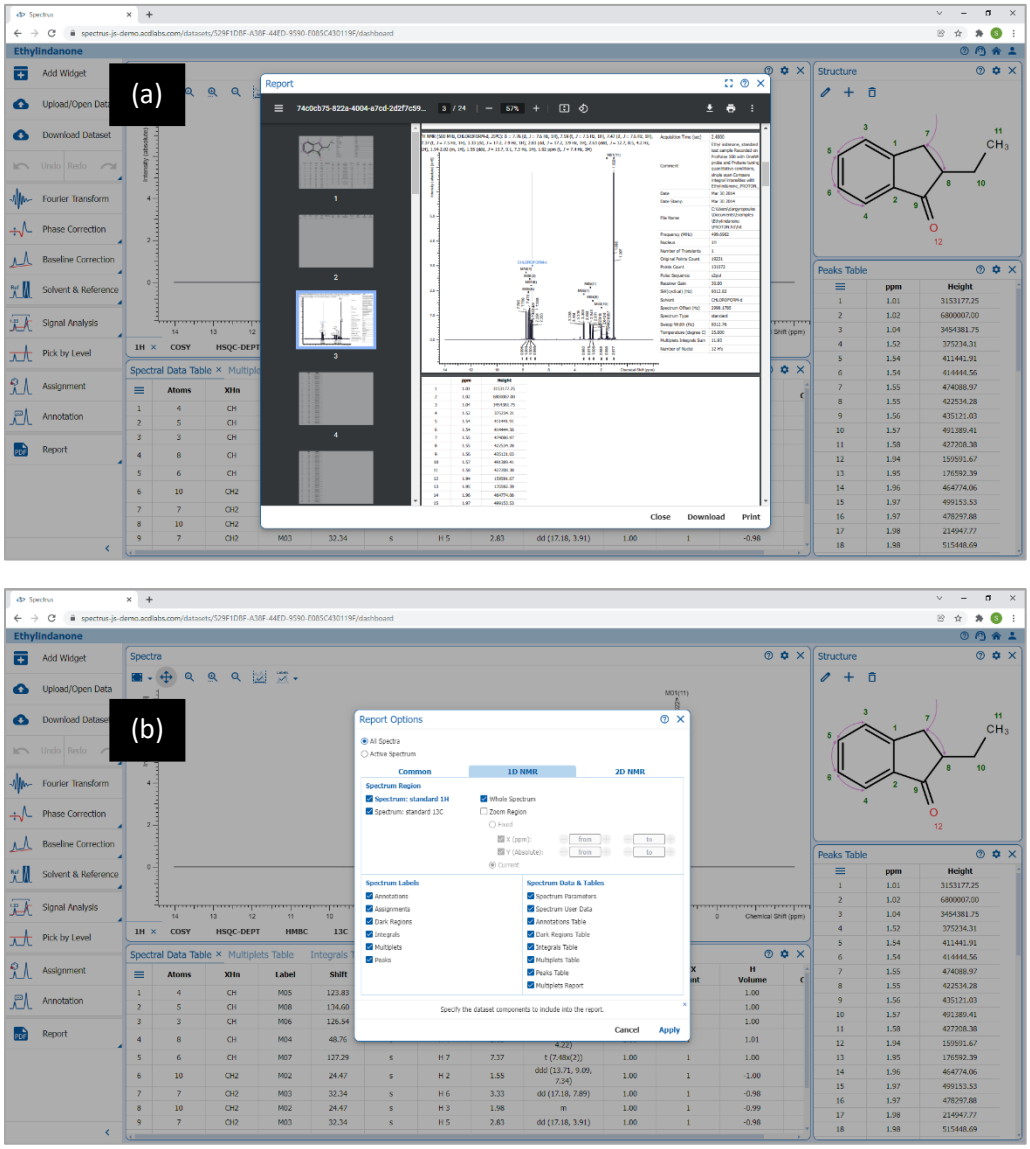

Figure 4: (a) Spectrus Processor JS reports are automatically generated with a single click (b) Spectrus Processor JS reports can be configured to display a variety of spectral data and experiment parameters.

"[Spectrus Processor JS] knows everything needed for natural product structure elucidation," said the researcher. It also paired well with software for other techniques, such as the MS fragment-prediction tool, ACD/MS Fragmenter.

Conclusions

Spectrus Processor JS made processing NMR data from shared and remote instruments significantly more convenient for natural products research. The scientist found it easy to switch from his previous software to Spectrus Processor JS. He could perform all the processing functions he required.

Without the logistical problems caused by local installations, the researcher had unlimited flexibility in when and where he processed his NMR data. Spectrus Processor JS also introduced features such as the multiplet table and one-click reports to his workflow. These accelerated his NMR data processing and allowed him to produce more accurate and meaningful results and records.