APPLICATION NOTE

ACD/LABS [ADVANCED CHEMISTRY DEVELOPMENT, INC.]

Multi-Technique, Vendor Neutral Analytical Data Handling for Chemists

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Introduction

Scientists use diverse analytical techniques to confirm, identify, and characterize chemical structures. Instruments used to collect data are rarely from a single vendor, and each comes with its own software to process that data. The primary goal of this data is to help answer questions such as:

“Did I make what I think I made?” and

“How much is there…or…how clean/pure is it?”

This plethora of software is not only a training burden; valuable instrument time is often ‘tied up’ by scientists processing their data, and frustratingly, all the analytical information gathered to support a stop/go decision cannot easily be brought together and reviewed in one place. Furthermore, today more than ever, the primary responsibility for data interpretation often falls to non-specialists in analytical chemistry.

Wouldn’t it be great if you could use a single piece of software to answer these questions, no matter the analytical technique or instrument vendor?

Support of All Techniques and Instrument Formats in One Application

Whether you use NMR, chromatography, mass spectrometry, FT/IR, Raman, or other analytical techniques, Spectrus Processor allows you to view, process, interpret, and report data from all major vendor formats.

This application note will highlight the benefits of having a single software tool for analytical data handling. The software can be accessed from any computer meaning you no longer need be tied to the instrument, lab, or even a particular computer for data processing. In addition, this paper will address how simple, yet sophisticated, software tools can aid in the interpretation of analytical data, thus accelerating the decision-making process.

Convenient Comprehensive Analysis

Depending on the environment, accessing raw data can range from simplistic to cumbersome. When raw data processing and spectral analysis must be done at the instrument computer, it causes bottlenecks and is inefficient for more than a handful of chemists. In some cases, automated processing routines on instruments may be set up to reduce the amount of time spent using instrument software and reports are generated to communicate the results of experiments back to the chemist. While these reports provide a simple way to check if the desired compound is present on a routine basis, the reality is that not all reactions proceed as planned. Reports like those illustrated in Figure 1 are static and don't always lend themselves to closer inspection, and certainly not for deeper analysis of 'live' data. The need for reprocessing cannot be completely precluded.

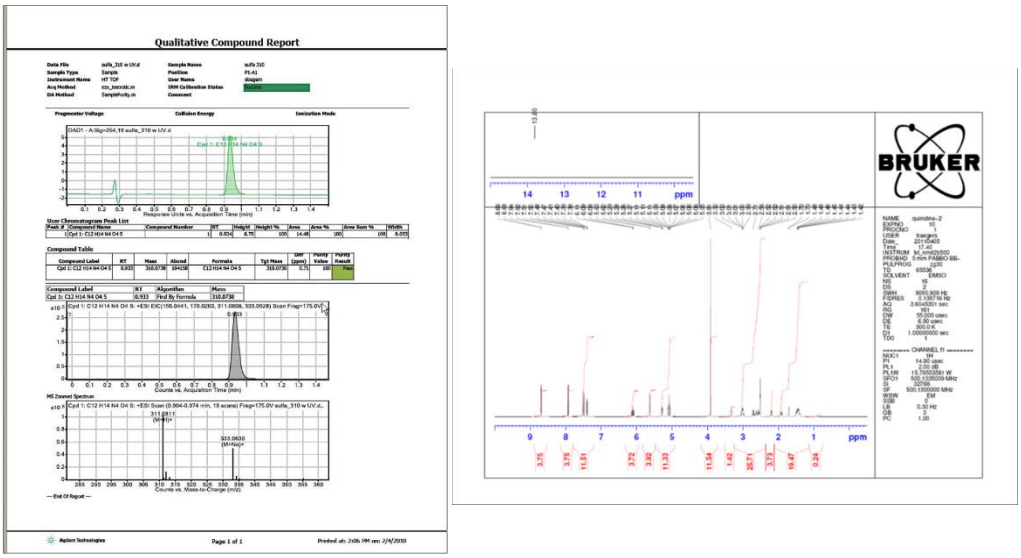

Figure 1.Examples of analytical data reports generated from walk-up NMR and LC/UV/MS systems.

Spectrus Processor provides an economical and easy way to provide chemists access to all analytical data in their own lab or office. Queues in the instrument room can be avoided while chemists are enabled to focus on their data in their own time, when they need it. With improved accessibility, synthetic chemists can inspect live data easily using a variety of beneficial features.

Fast and Efficient Manual or Automated Processing

Spectrus Processor can provide manual, partially automated, or fully automated data processing workflows. Figure 2a illustrates the result of various processing steps using Spectrus Processor—raw data from the instrument may be processed manually (in this case Bruker 1r and 2rr files), alternatively automated data processing and analysis will deliver a structure/spectrum verified result to help chemists make decisions as quickly as possible.

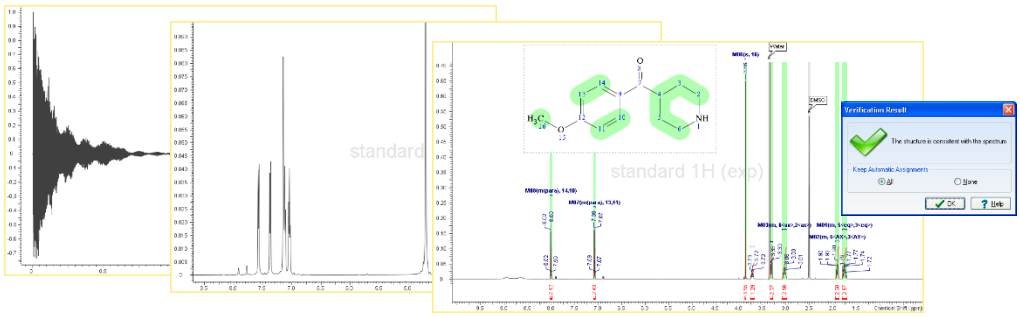

*Figure 2a: How do you like your data? From left to right: raw NMR data (Bruker FID), processed data (Bruker 1r), fully verified data (ACD/Labs *.spectrus and *.esp).*

Raw LC/UV/MS data, including associated analog channels, can be imported into Spectrus Processor. Manual or automated peak detection and processing (extraction of ion chromatogram, generation of average mass spectra across peak, spectral subtraction, etc.) is possible. Adding a structure automatically triggers a verification routine that indicates whether the expected molecular ion was observed in the dataset. See Figure 2b.

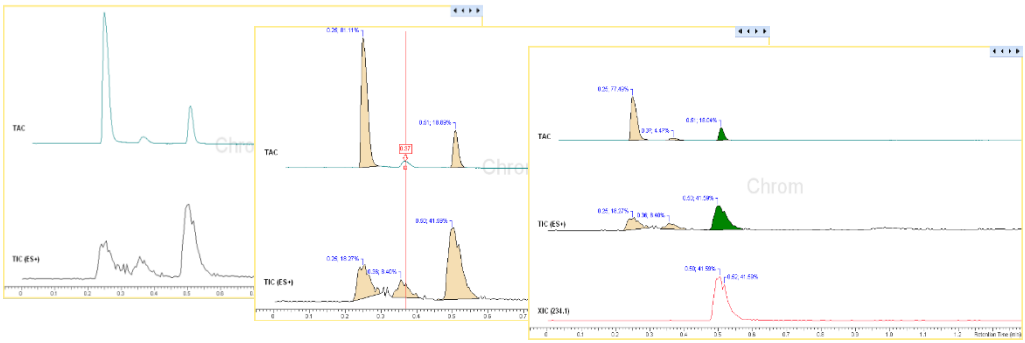

Figure 2b: How do you like your data? Left to right: LC/UV/MS data (Waters SQD raw data), post-import processed data, and assigned data.

Quick and Easy Formatted Multiplet Reports

Spectrus Processor automatically measures coupling constants (J-values) and prepares a formatted multiplet report in the specified journal format on-the-fly during processing, saving a significant amount of time in reporting NMR data.

^{1}H NMR (DMSO-d_6, 400 MHz) δ 9.17 (s, 1H), 8.93 (s, 1H), 8.86 (s, 1H), 8.81 (s, 1H), 6.70 (d, 1H, *J*=2.1 Hz), 6.6-6.7 (m, 1H), 6.57 (dd, 1H, *J*=2.1, 8.2 Hz), 5.87 (d, 1H, *J*=2.1 Hz), 5.66 (d, 1H, *J*=2.3 Hz), 4.86 (d, 1H, *J*=5.3 Hz), 4.46 (d, 1H, *J*=7.6 Hz), 3.79 (tt, 1H, *J*=5.4, 7.7 Hz), 2.63 (dd, 1H, *J*=5.3, 16.1 Hz), 2.33 (dd, 1H, *J*=8.1, 16.0 Hz)

Figure 3: Using Spectrus Processor, a chemist can quickly prepare a formatted multiplet report for their patents and publications like this one in real time.

Add Chemical Structures and Assign/Annotate Spectra

The capability to assign chemical structures/atoms/functional groups to peaks/multiplets/bands in spectra and chromatograms is a unique feature of Spectrus Processor. Simple click-and-drag motions in the processing window create electronic assignments that can be stored within the data file; providing more meaningful data for future review.

Digitally Assign NMR Data

Users may assign multiplets to atoms in a chemical structure or vice versa. In addition, the software suggests likely assignments (green/yellow) for interpretation assistance.

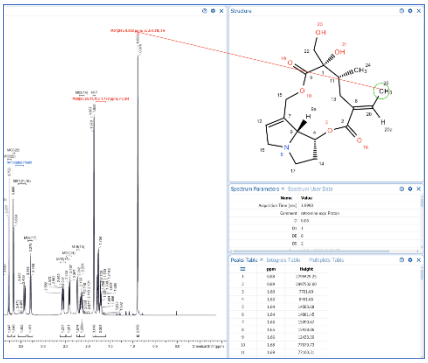

Figure 4: Using Spectrus Processor to assign a multiplet in a ^{1}H NMR spectrum.

Digitally Assign LC/UV/MS Data

Add a structure, formula, or mass to the Table of Components to automatically extract a relevant mass chromatogram, or assign a peak to generate a mass spectrum.

Color-coded MS match indicates consistency of monoisotopic mass and expected isotopic pattern.

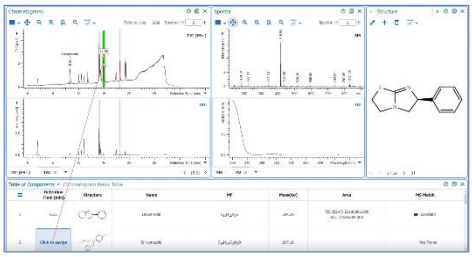

Figure 5: Using Spectrus Processor to assign a component structure to a peak in an LC/UV/MS dataset. Green in the MS Match column indicates structure/spectrum consistency.

Digitally Assign IR and Raman Data

Verify that expected bands for each fragment in your structure are present in the IR spectrum using the verification protocol in Spectrus Processor.

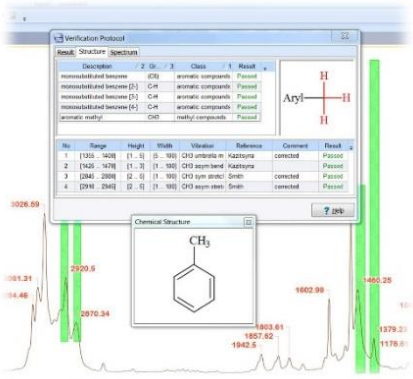

Figure 6: Spectrus Processor provides the capability to confirm if expected bands are present for proposed structure fragments with interactive highlighting of bands.

Accelerating the Chemist's Decision-Making Process

At the beginning of this document, we discussed two common questions asked of routinely collected ^{1}H NMR and MS or LC/UV/MS data by synthetic chemists—did I make what I think I made, and is it pure?

Spectrus Processor provides immediate feedback on the level of correspondence between a proposed structure and experimental mass spectrum, NMR spectrum, or IR spectrum. The chemist is able to confirm the expected structure or question the outcome of a reaction quickly, allowing them to make faster, more informed decisions about the relationship between a chemical structure and analytical data.

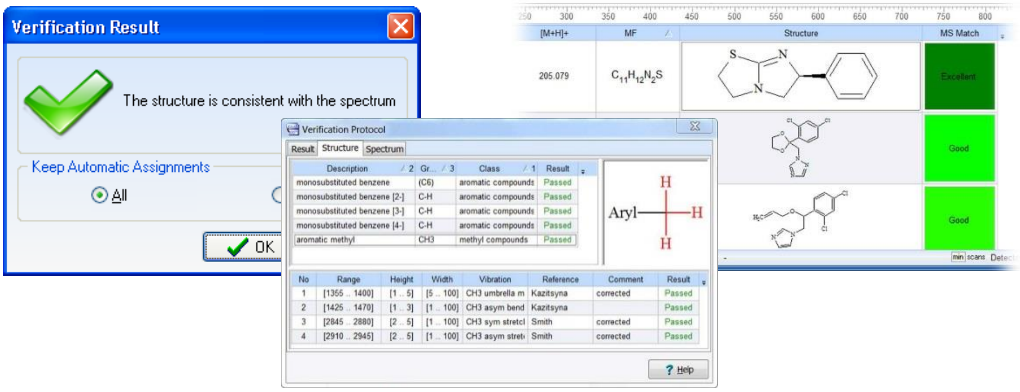

Figure 7: Verification output supports faster, more confident decision-making. Left to right: 1H NMR—a simple statement that the structure is (or is not) consistent with the spectrum; IR verification—pass/fail for correlation of fragments with bands in the spectrum; MS Match provides a binary result based on the presence of a monoisotopic mass and expected isotopic pattern.

When there is an inconsistency between the spectrum and structure for NMR, the user is informed of the specific reason for the inconsistency, as shown in Figure 8. The software provides an invaluable resource to help chemists confirm structure/spectrum consistency or investigate inconsistency.

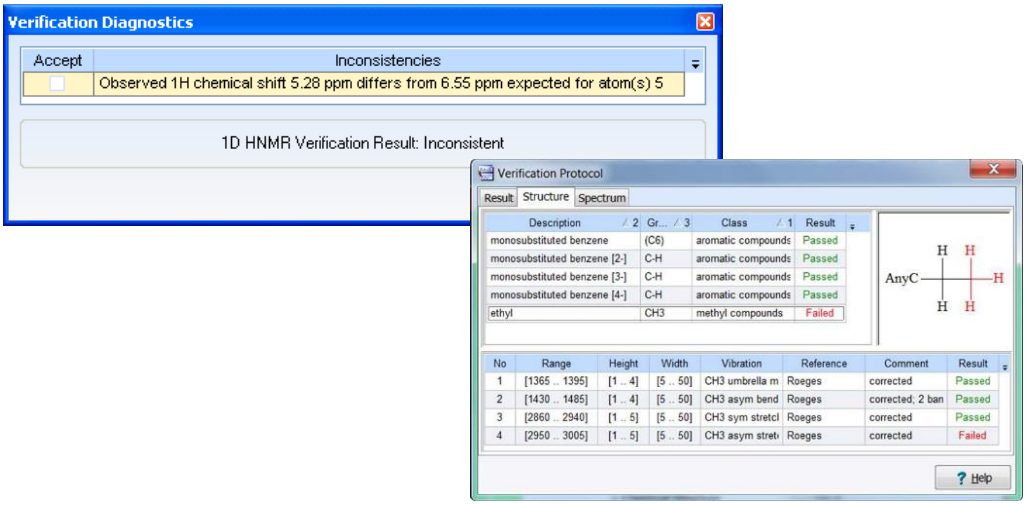

Figure 8: Verification output—(top) for NMR, Spectrus Processor provides information about the experimental chemical shift that significantly differs from the predicted for atom 5 in the chemical structure; (bottom) in the IR protocol inconsistencies between expected spectral bands and structural fragments are flagged for closer inspection.

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Create Comprehensive Multi-Technique Reports

Spectrus Processor helps organizations support the many options used to record results from spectral analysis. If you affix a copy of the spectrum into a paper lab notebook that is still possible. For organizations using systems such as electronic lab notebooks (ELNs), Spectrus Processor provides the capability to link to the electronic data files; export multi-technique analytical reports as PDFs; or paste images of spectra into the specific notebook record, in addition to providing a wealth of information about the spectrum in electronic form (i.e., experimental parameters, chemical structures, data tables, etc.).

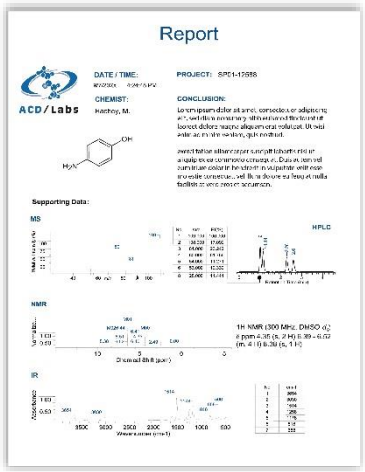

Figure 9: Example reports created by Spectrus Processor.

Choose the Deployment Option That's Right for You

Every lab and organization has their own unique needs, wants, and use patterns. This is why Spectrus Processor is designed to allow organizations to choose the deployment option that works for them.

The original multi-technique Spectrus Processor application is a windows-based desktop application that can be installed on individual computers or made available from an on-premises cloud installation, making it suitable for any number of users.

Meanwhile, browser-based Spectrus Processor JS provides ultimate user accessibility for NMR and *x*C/UV/MS data processing. The application is made available from a central computer or server in your IT environment. Users log in from their favorite web browser on any computer with network access. This means compatibility with Mac or PC devices and low IT overhead, making it ideal for groups of 5 or more users.

Conclusion

Spectrus Processor provides chemists with multi-technique, vendor neutral, easy-to-use, offline desktop processing, interpretation, and reporting. Once spectra are

processed and analyzed, software tools can be used to help the chemist make faster, smarter, and more independent decisions about the results of their reactions. Finally, this data can be used to quickly generate electronic reports complete with spectral expansions, instrument parameters, data tables, and more. Information can be archived as a PDF or elements copied and pasted into a word processing application. Furthermore, database search capabilities of Spectrus Processor enable searches of third-party and corporate analytical databases to aid comparisons from previous batches, material verification, or to help identify known compounds.

With the help of Spectrus Processor, routine analytical data analysis no longer needs to be a painful exercise of hopping between different software packages or spreading out spectra on your desk to direct next steps.