Processing and Managing Analytical Data to Extract and Share Knowledge–How Far We've Come and Why It's So Hard

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Introduction

Processing and managing analytical data is part of our everyday tasks. For many scientists, including those working in material analysis or material characterization, this work typically requires a multi-discipline approach involving a number of analytical techniques. Mastering all of these techniques is impossible for a single individual, so often a team approach is used.

Access to "historical" data is a desire not often achieved either because the data sits in discrete silos, or due to lack of access to the correct software to view the data.

In this paper we discuss ACD/Spectrus Processor–a new all-in-one analytical data processing and chemical characterization software, with powerful database search capabilities;s available for both the desktop and enterprise environments.

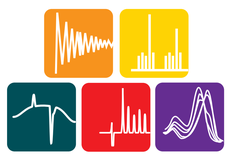
ACD/Spectrus Processor

For anyone looking to work with analytical chemistry data there are a number of basic workflow steps that need to be addressed:

- Import analytical data and meta data
- Process and interpret data to enhance knowledge extraction, and for reporting
- Associate structures and correlate with analytical data
- Create customized databases containing structures, band assignments, spectra, and text data
- Share a database and the knowledge it contains with associates in the next building, in another country, or somewhere in the future

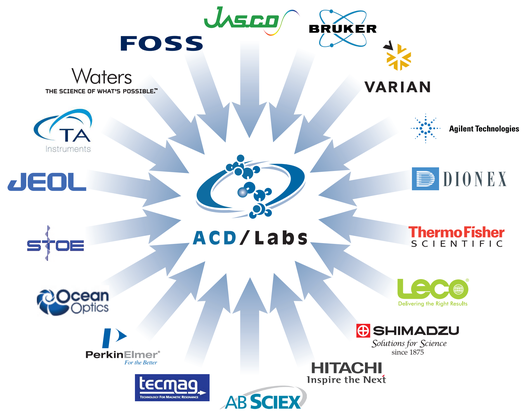
Analytical methods supported by Spectrus Processor include:

- **Optical**–IR, Raman, NIR, FAR IR, UV/Vis
- **Curves**–Thermal (DSC & TGA), XRPD, EELs, and general X-Y data
- **MS**–MS/MS, LC/MS, GC/MS
- **NMR**–1D, 2D, and hetero atom



Import, Access, & Process All Analytical Data in a Unified Software Environment

ACD/Labs' continuing collaborations with instrument vendors and standards committees allow us to provide an impressive array of import filters for analytical data.



In addition our professional services staff can assist with acquiring legacy data and linking to internal corporate databases.

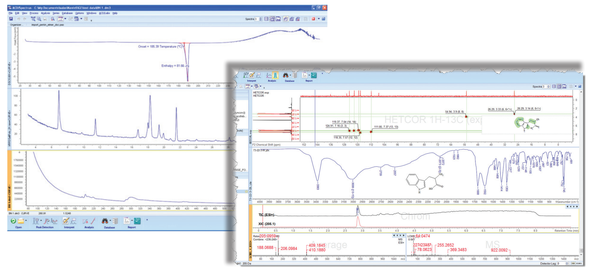


Figure 1: Import and access multiple data types in a unified interface with Spectrus Processor.

Integrate Structures with Data & Extract Answers

There is often a need to process or re-process data to gain greater insight into the problem under investigation, and an image of a spectrum is not sufficient. With Spectrus Processor you can view and access raw data from the instrument, pre-processed and interpreted data from corporate databases, or open access software. Simply drag-and-drop or copy-and-paste a chemical structure to receive immediate feedback on the consistency between structure and data.

Our unique ability to integrate structures with analytical data means you can interpret data to get answers and extract knowledge. Spectrus Processor provides assignments in NMR, spectra-structure correlations in IR and Raman, and more.

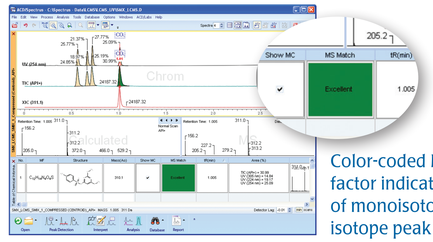


Figure 2: LC/MS–add a structure, formula, or mass data to the Table of Components to automatically extract a relevant mass chromatogram, or assign a peak to generate a mass spectrum.

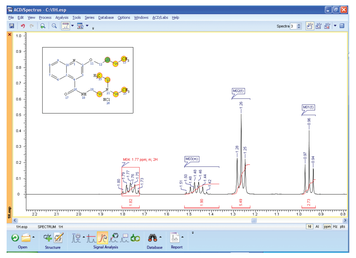


Figure 3: NMR Spectrum showing proposed assignment when selecting a multiplet.

The knowledge you extract can be kept with your data–our unique capabilities allow you to save analytical data, in its chemical context.

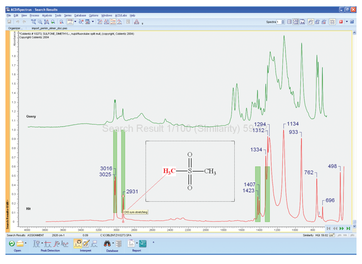


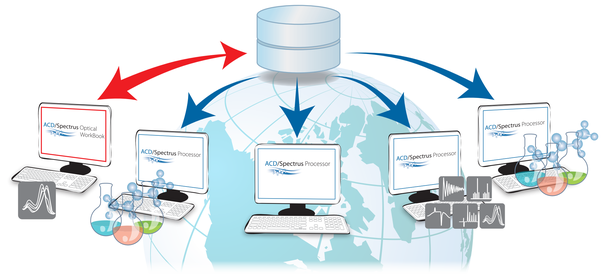
Figure 4: Spectral search results with the assignment feature being used to help identify the spectra-structure correlations of matching peaks. Spectrus Processor includes the ability for searching both corporate and commercial databases.

Sharing knowledge

Spectrus Processor allows you to share processed, and interpreted data through simple file-sharing. Colleagues can review assignments and your interpretation of the data, to learn more about a project, or perhaps use your data through re-processing and interpretation to address their own challenges.

Share your results through customized multi-technique reports.

Database creation tools such as ACD/Spectrus Optical Workbook are also available to create local desktop or enterprise wide databases for sharing across a global network of colleagues. Interpretations and knowledge generated can be saved as part of your corporate database, giving you the ability to share this hard earned knowledge with colleagues today and into the future.



Spectrus Processor provides access to databases to allow expert corporate knowledge to be re-used and applied in your organization. It is available as both a desktop application and enterprise package. Web-based access is also available for scientists that only need to search and access data.

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