# Achieving Great Science: Bringing Together Physical Measurements and Chemical Analysis

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## Abstract

In today's laboratory it is common to be involved in many aspects of the physical or chemical analysis of materials. Having the ability to keep track of all this disparate data can be a major challenge—whether we are generating all of the data ourselves or whether it is coming from several departments. In addition, using a multitude of different data types increases the possibility of misplacing or misattributing results to the wrong samples more so than we would like to admit.

This poster will look at a tool that can be used to manage, analyze, annotate, and create reports from data sources as diverse as TGA, DSC, XRPD, optical spectroscopy, chromatography, Mass Spec, NMR, chemical structures, and metadata. Having all of the data available to review and share across an organization improves the decision-making process and allows great science to be achieved.

## Objectives

- Create a customized database containing curves, spectra, structures, and metadata
- Process data to add chemical information, structures, annotations, and peak information
- Provide local or enterprise access to stored data through desktop or Web-based client applications

## Data Types

**Solid State Characterization**

- TGA, DSC, and XRPD

**Spectra and Chromatograms**

- IR, Raman, SS-NMR, mass spec, and all chromatography techniques

**Chemical Structures**

- Searchable structures

**Metadata**

- Instrument parameters and sample properties

## Software

**Primary ACD/Labs Software**

- Curve Manager—thermal curves, XRPD, and others

**Additional ACD/Labs Software**

Including:

- UV-IR Manager—optical spectra
- ChromManager—chromatograms
- MS Manager—MS spectra
- 1D and 2D NMR Manager—NMR spectra

## Step One—Importing Data Into the System

The first step in any data management system is to get the measured data into the system. As anyone who has been involved in trying to do this can attest, this is not a trivial task. Although there are some public formats that can be used, they are not universally converted in a consistent manner due to either misinterpretations of the standard or to unauthorized additions implemented to meet custom needs. It is much better to directly import the native file format using official specifications provided by the instrument vendor or scientific body. However, because of the constant evolution due to new instruments, scientific advances, or new software versions, maintaining up-to-date data format converters is not always feasible. Any data management system will always rely heavily on the ability to import free-form or generic data formats, and will often resort to using ASCII imports to bring data into a system. Since some instrument companies are unable or unwilling to share their data file formats, this further reinforces our reliance on good support for generalized formats.


ACD/Labs has spent over 10 years as an independent third-party software company, building and maintaining relationships with instrument companies to allow them to access native file formats. The result of that effort is that today the software can import data from over 70 data file formats, and we continue to implement additional file converters.


*Figure 1*: Current list of file formats supported by ACD/Labs software and the instrument relationships that have been built.

## Step Two—Processing the Data

Once data is in the system, the next step is to have the ability to process or analyze it. The various ACD/Labs modules allow a wide range of processing steps from peak picking or smoothing, to operations on large groups of data and making structure spectra correlations for some spectroscopies.

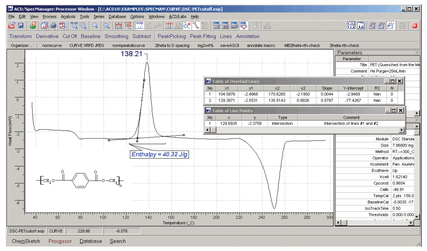


*Figure 2*: Table of Mass Chromatograms after IntelliXtract processing of 'Metabolized' sample dataset with Peak Tag filtering for monoisotopic parent ions.

## Step Three—Data Management

Having the ability to manage and keep track of many different data types can be an invaluable aid in achieving great science. This software tool allows one, or many, users to keep different data types together in a single record in a database of many records. With search tools to query the database on text data, structures or sub-structures, and several spectral data types, finding the data you need is no longer a nightmare experience that leaves you wondering if you looked in all the right places.

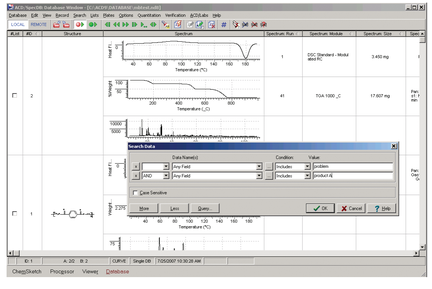

*Figure 3*: Database view showing records with three data types in each record—set to do a text query. (Note: The example data is for demonstration purpose only, and is not necessarily of the same material.)

## Step Four—Visualizing and Sharing the Data

Once the data has been saved, it then becomes useful only if the information is made available to the people who need it. A database can be added to, browsed, or searched by the creator of the database and anyone else who has the desktop client tools. In addition, there may be cases where access to browsing and searching is needed but not the ability to add or modify data in records. In that case, a Web client can be used to access an enterprise-wide database.

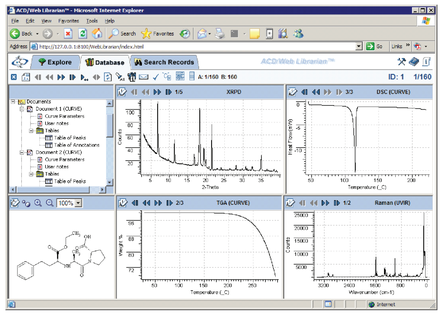


*Figure 4*: Web client view of database entry. Note the ability to combine physical, chemical, and structural information in one record and on one screen.

## Discussion & Conclusions

Solid state characterization of new material is a multi-disciplinary field using a variety of analytical techniques. It is practically impossible for any one technique to unambiguously answer all the questions for chemical and physical solid-state characteristics. Currently, different data types are often collected in different data system silos, making data coordination, reconciliation, and interpretation often very difficult.

In this poster, we show that it is possible to manage live analytical data of different types in the same data system.

- Extensive proprietary and generic file format support
- Centralized processing independent of the instrument
  - Instrument-independent analysis and processing
  - Consistent high-quality reports
- Centralized data management system
  - Multi-technique data coordination and access
  - Find appropriate data easily by text, structure, or spectrum searching

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