Knowledge Management of Spectral Data

Authors: Marie Scandone and Gregory M. Banik, Ph.D.
Bio-Rad Laboratories, Informatics Division
3316 Spring Garden Street, Philadelphia, Pa 19104, USA
www.sadtler.com

Introduction

In a knowledge management system of spectral data, the ability to build, analyze and access analytical databases with the ability to create, manage, and communicate knowledge from those databases is essential. It is also vital that the management system has the ability to archive, share, compare, and search instrument data files to improve productivity in the laboratory. Putting all this data into one place, with a single, integrated user interface can aid product development and provide new ways of analyzing samples as well as make use of predictive models. By making real data and predictive data readily available and easy to use, a user can exploit new scientific developments and advance ahead of their competitors. The KnowItAll™ Analytical System can provide a complete knowledge management system.

One Interface

The KnowItAll Analytical System is modular and customizable so you can easily transfer information from plug-in to plug-in without having to leave the main interface and without having to open another software program. It allows movement from technique to technique, database to database and procedure to procedure. It handles spectra, structures, property information, peak tables, assignments, and any information pertinent to the spectroscopist or chemist.

Expandable Product with a Flexible Progressive Environment

With its state of the art design, additional software functionality can quickly and easily be plugged into the powerful KnowItAll architecture.

Solutions to Fit your Needs

- DrawIt
- IUPAC NameIt
- IUPAC DrawIt
- ReportIt
- MineIt IR, HNMR, CNMR, MS, UV/VIS, GC
- AnalyzeIt IR
- RefineIt IR, NMR
- SearchIt IR, HNMR, CNMR, MS
- PredictIt HNMR, CNMR
- AssignIt CNMR
- Database Building Option

Multiple Analytical Techniques

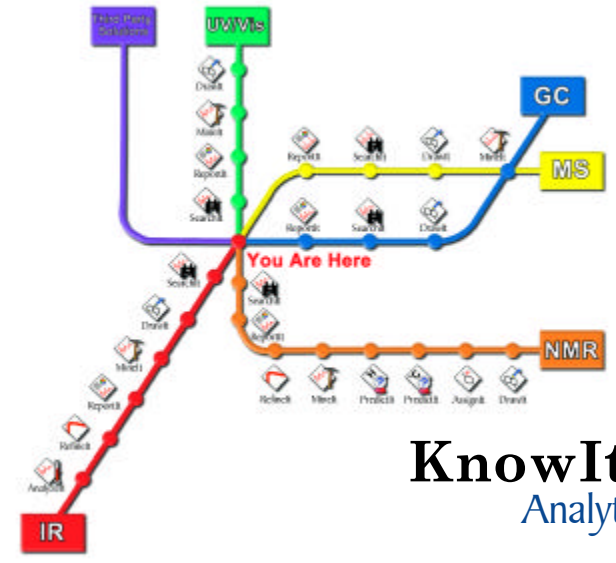
The system can support a number of analytical techniques such as:

IR	VP IR	RAMAN	GC	NEAR IR
HNMR	CNMR	UV/VIS	MS	

Unlimited Access to the High Quality Reference Databases

HaveItAll IR puts the world's largest infrared spectral collection of over 220,000 spectra of pure and commercial compounds all on one CD for secure searching from your desktop. HaveItAll NMR offers 12,000 HNMR spectra and over 140,000 CNMR spectra and growing that can be searched or used in prediction. HaveItAll MS allows searching of over 100,000 NIST mass spectra. All have been through comprehensive evaluations in order to provide the best possible data at the users finger tips.

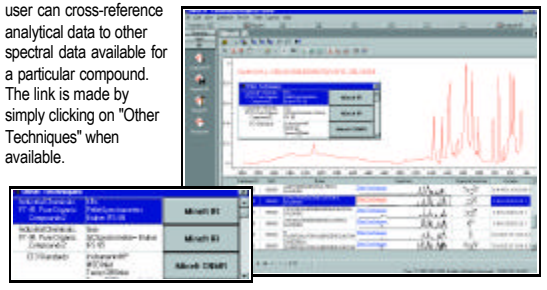
BIO-RAD
Informatics Division
Sadtler Software & Databases



KnowItAll™
Analytical System

Cross-Referencing to Other Techniques

With this feature, the user can cross-reference analytical data to other spectral data available for a particular compound. The link is made by simply clicking on "Other Techniques" when available.



Powerful Search Algorithms

The system allows the user to search reference spectra to identify or classify unknown spectra. Searches can be performed by spectrum, peak, name, structure, substructure and property fields. The analysis tools can identify new compounds, classify compounds, validate chemical compounds, deduce chemical, and physical properties, etc.

Communicate Knowledge

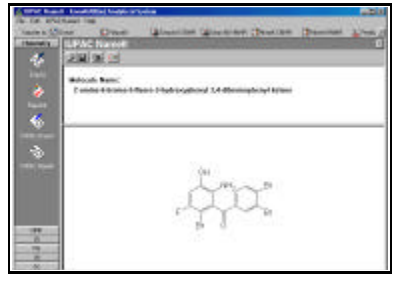
With DrawIt and ReportIt, a user can communicate knowledge according to his needs. In addition to a sophisticated chemical structure drawing tool, a user can create standard reports, design papers, presentations, and web publications that fits the user's specific needs and can include annotations, tables of data, spectra, structures, and much more.

Simplify Functional Group Analysis

AnalyzeIt can be used to help interpret the bands in an IR spectrum. Simply load a spectrum and click on a peak of interest to generate a list of all functional groups possible at that position. AnalyzeIt features over 200 functional groups and over 700 interpretation frequencies and helps to determine whether a structure matches a spectrum. You can draw a structure and break down the structure into its component functional groups to overlay with your spectrum.

Easy-to-Use Structure Naming Tool

IUPAC NameIt gives the user the ability to automatically assign systematic names to organic structures according to IUPAC nomenclature rules. IUPAC DrawIt understands IUPAC nomenclature rules and creates high-quality structures. These tools aid in the communication of information to and from the laboratory.

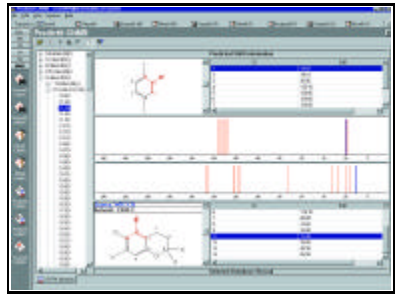


Process IR Spectra to Improve the Quality of the Data

RefineIt IR offers a variety of tools to process spectra. Spectra can be truncated, smoothed, baseline corrected and you can perform an ATR correction as well as spectral substraction.

Reliable Prediction for NMR

With HaveItAll NMR, you can view assigned data used for prediction and because prediction is not the only piece of information that you need, you can not only retrieve the real spectral data used to build your prediction, but you can also access all of the available information related to the reference spectrum, such as source of sample, solvent, methods of analysis, etc.



Database Building Option

If you are involved in research and spend a substantial portion of your overall R&D budget on costs directly associated with collecting instrument data, you now have a means to capture and manage this valuable resource. Get the most out of your data with KnowItAll. You can build your own searchable, cross-referenced databases for all analytical techniques including IR, Raman, Near IR, NMR, MS, UV/VIS, and GC.

Customizable Databases

Choose from over 100 pre-defined property fields to include spectral or chromatographical data, peak information, structures, and properties, such as melting point, CAS Registry Number, source of sample, or create your own user-defined fields such as lot number or instrument operator. Set your own parameters such as x- y-resolution.

Provides Tools to Handle CNMR Information

The AssignIt option provides access to tools to assign peak shifts, intensities, coupling constants, and multiplicities to the structures in a CNMR database. This information can be added to improve the information obtained in the laboratory.

Conclusion

By the management of data generated in a laboratory and by making reference data, processing tools and derived conclusions readily available to those who need it, you can give a user the ability to exploit new scientific developments and improve their productivity