



Searching Spectral Databases With LabSpec 6

A typical Raman spectrum is rich in information about the analyzed material. Individual peaks within the spectrum provide information about the molecule's functional groups and their surrounding environment, whilst the full spectral profile provides a highly specific chemical fingerprint.

Using the Raman spectrum as a unique chemical identifier for a material is one of the great strengths of the technique, and offers a way to quickly identify an unknown material. To do this it is necessary to match the unknown spectrum to that of a known material – this requires a robust searching platform coupled with comprehensive spectral databases. With this in mind, HORIBA Scientific now offers the KnowItAll® HORIBA Edition (from the Informatics Division of Bio-Rad Laboratories, Inc.) for use with their LabSpec 6 Raman data acquisition and processing software – KnowItAll® provides users with a complete database searching and spectral database package.

Bio-Rad's HORIBA Edition of the KnowItAll® Informatics system offers an integrated environment for complete spectral searching, analysis and data mining. A seamless link is provided between LabSpec 6 and KnowItAll® - once a spectrum has been acquired, one click will export the data into KnowItAll®. From this point on, the full functionality of KnowItAll® is available for complete data mining.

KnowItAll® HORIBA Edition has a modular architecture, allowing a configuration to be built from a basic starter package through to a fully configured platform.

The basic package includes SearchIt™ for database spectral searching, Minelt™ for database visualization and mining (including Bio-Rad's patented Overlap Density Heatmap Analysis for visual data mining) and Mixture Analysis (which identifies individual components in a mixture spectrum, through database searching).

Beyond this, additional functionality can be added, to further enhance the package. Such functions include Database Building (allowing customized databases to be created, and searched upon), and the Analyzelt™ spectrum/structure correlation tool. This latter function will certainly be welcomed by Raman spectroscopists, for it allows them to quickly interrogate individual peaks within a spectrum, and see candidate functional groups contributing to it. Working through the spectrum in this way will lead to candidate

molecular structures being identified, and a detailed understanding of the spectrum composition.

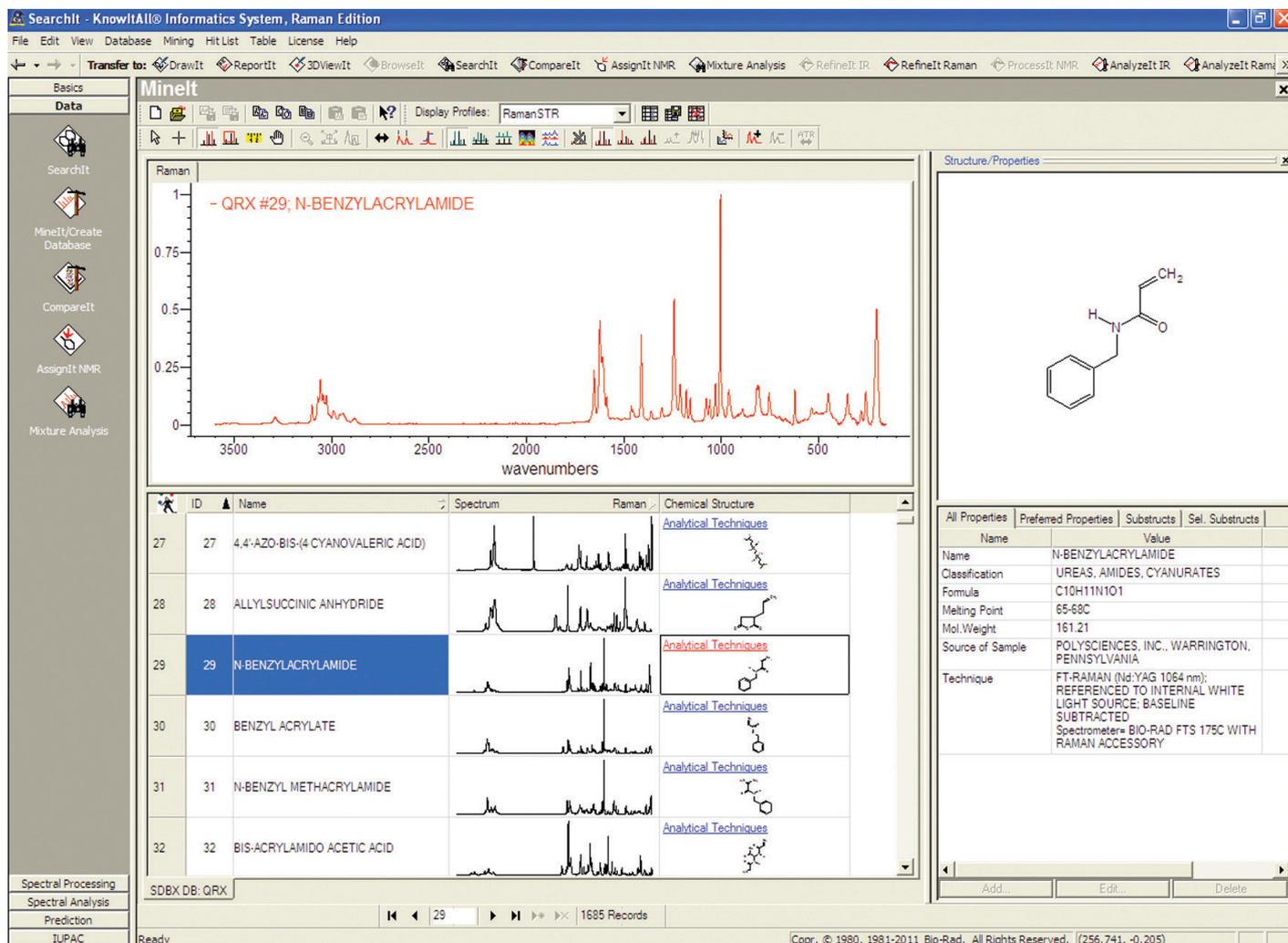
The SearchIt™ spectral searching module is reliant on good quality spectral databases. The HORIBA Edition of KnowItAll® includes the HORIBA Raman Database, comprising over 1500 spectra covering application areas such as forensics (including polymers, dyes/inks/pigments, and narcotics), semiconductors, bio-inorganics, and minerals.

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HORIBA Scientific and the Informatics Division of Bio-Rad Laboratories, Inc. offer a complete spectral searching and data mining tool for LabSpec 6 Raman software users.



In addition, users can optionally use Bio-Rad's own databases, either through the HavelAll® annual license with local PC or web searching, or through purchase of individual databases, such as Basic Monomers and Polymers (1680 spectra) or Inorganics (1630 spectra).

Spectral database searching is the accepted method to answer the ultimate analytical question: what is it? With the HORIBA Scientific Raman instruments a good quality Raman spectrum can be recorded in just a few seconds; KnowItAll® can translate that spectrum into a clear material identification, and advanced features such as AnalyzeIt™ provide invaluable links between spectrum and molecule.



HORIBA
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info.sci@horiba.com

USA: +1 732 494 8660
UK: +44 (0)20 8204 8142
China: +86 (0)21 6289 6060

France: +33 (0)1 69 74 72 00
Italy: +39 2 5760 3050
Brazil: +55 (0)11 5545 1500

www.horiba.com/scientific

Germany: +49 (0)89 4623 17-0
Japan: +81 (0)3 6206 4721
Other: +33 (0)1 69 74 72 00