

OMNIC Spectra: Next Generation Spectroscopy

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Key Words

- Identification
- OMNIC
- Spectra

Forensics and analytical laboratories require tools to analyze many kinds of unknown samples. There is no typical sample – fibers (loose or embedded in a product), fisheye distortions in polymer films, trace quantities of unknown materials or samples containing low levels of contaminants are among the possibilities. The newest infrared spectroscopy instruments from Thermo Scientific, the Nicolet™ iS™ 10 FT-IR spectrometer and Nicolet iN™ 10 infrared microscope, coupled with the OMNIC™ and OMNIC Picta™ software packages, have elevated data collection and routine analyses for the above purposes to new levels of simplicity and confidence. The next link in the laboratory productivity chain involves extracting information from the data, through processing and analysis.

The analysis of spectral information has evolved substantially from the days when consulting a reference book was sufficient. Excellent tools – like spectral subtraction and searching algorithms – have long been available, but multi-step processing may be inefficient, inconsistent from worker to worker or time consuming. The OMNIC Spectra™ spectroscopy software presents a revolutionary approach to laboratory data analysis. Placing all of the tools at your fingertips, eliminating the need for creating spectral libraries, making interactive processing visible and, most spectacularly of all, bringing spectral identification tools into a new era of productivity are just some of the features of OMNIC Spectra. Using a workflow that moves the analyst from original spectrum to final report, OMNIC Spectra will rapidly become the standard for laboratory data analysis operations.

Traditionally, spectral analysis of a multi-component system begins with processing of the spectrum, through ATR or baseline corrections. A search against a spectral library is then carried out to identify best matches. One match from the list is moved to the active window and a subtraction is carried out. The difference spectrum is searched against the same or different libraries, and a second best choice is drawn out. Ideally, this can be subtracted from the first difference spectrum, and another round of searches can be carried out.

These processes are difficult to bring under control. Litigation or production line shut-downs can hinge upon proper choice of subtraction factor, and reproducibility from operator to operator is low. OMNIC Spectra was designed around two core considerations: improvement of analysis workflows and the obtaining of consistent results between operators of varying skill levels. The traditional processing tools are available in a completely new interface which provides immediate and interactive control over the results. New tools supply remarkable, automated ways to extract information about your spectra, providing consistency and elevated confidence in your results.

Features Follow Function

The OMNIC Spectra interface emphasizes function rather than the tools, moving the user from spectral processing to interpreting to reporting in a smooth progression, using a simple toolbar structure as seen in Figure 1. This environment keeps the tools primed for action. The workspace lets you see the affect of actions taken, as it happens. Reports can be built with just a few moves of the mouse. The operations take place in a circular fashion about the workspace, flowing from data to action to result, then back to action or on to a report.

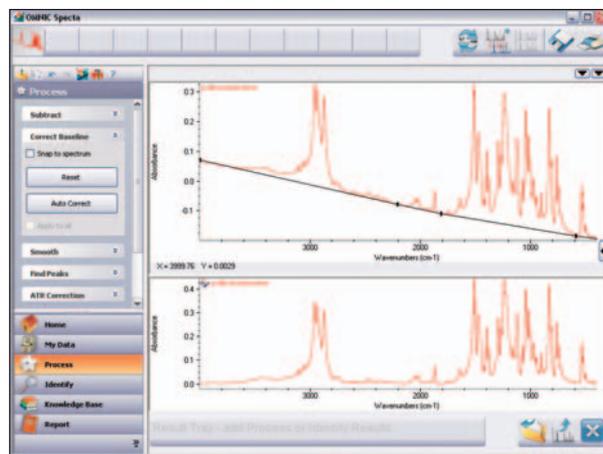


Figure 1: The OMNIC Spectra working environment. The data tray at the top contains spectra being worked on, while the tools are ready at the left.

My Data

OMNIC Spectra treats your hard disk as a database, starting with the construction of an index of all readable files. The index “opens” spectral groups (.spg files) and libraries, so that you see all spectra as separate listings. This permits the use of advanced file-finding tools to be used, as shown by the example in Figure 2. This capability coupled with the preview screen provides great vision into your data. A simple double click readies your data for processing and analysis by moving it into the Data Tray, where your data resides ready for action.



Figure 2: Finding spectra on the hard disk with OMNIC Spectra is easier than ever, with searching tools and access to libraries and spectral groups.

Processing

Basic processing functions, like ATR correction, baseline correction and subtraction are accessible from the Process menu. The selected spectrum and the processed spectrum are seen simultaneously, as shown in Figure 3, so the affect of the process can be seen interactively. A single click moves the processed result into the workspace, but

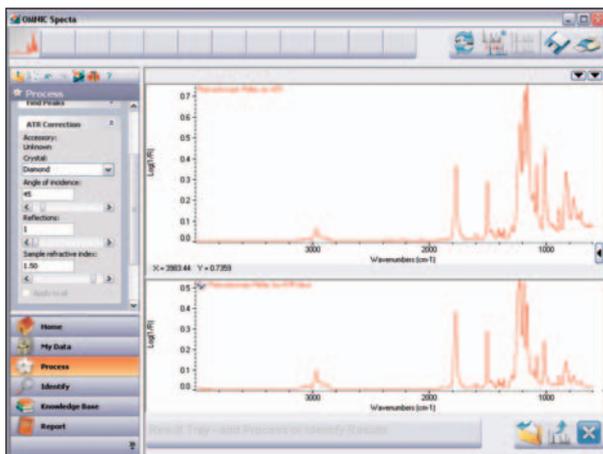


Figure 3: Processing occurs in a specific window, with the action on the left, the spectrum on the upper right and the working result below it. The buttons at the lower right either store an intermediate result in the Results tray, perform the action and close the process, or skip the action and close the process.

leaves the original data (still in the data tray) untouched. Further, each process attaches a “bread crumb” to the spectrum, so you can reprocess a spectrum from the source file, undoing each processing step, even after storing the result of a complete analysis. The new “Optimize” tool performs a sequence of automated procedures on spectra, which can assist in rapidly improving the appearance of spectra for further analysis.

Identify

The real horsepower of OMNIC Spectra lies in the identifier tools. Besides traditional searches, peak search and an interpretation function provide tools for extraction of information. Even more novel, the searches may use directories on your hard drive, or the contents of the entire hard drive, in tandem with commercial or OMNIC libraries. There is no need to build new libraries – spectra with different resolutions or spectra ranges can be placed into a common directory, and then used as a database for the search. The software automatically accounts for different formats (transmission versus absorption), and has enormous power to handle spectra collected using different experimental conditions.

Figure 4 shows the result from a traditional processing procedure. A spectrum has been searched against a collection of commercial libraries. Not all of the spectral features are accounted for, so a subtraction is needed. Right clicking on the best match automatically moves the search result to the workspace, defines this as the subtraction reference, and takes the user into the subtraction processing menu (Figure 4). Even the problem with totally absorbing peaks (huge residuals) is averted. The display in Figure 4 shows none of the residuals – they have been cleared. One click, multiple activities: simplicity exemplified.

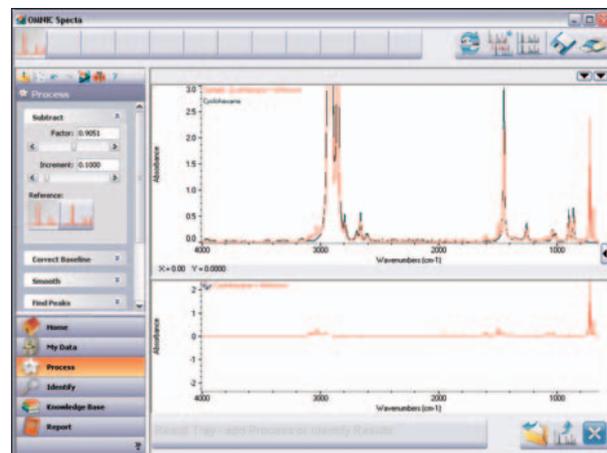


Figure 4: After a search, you can come straight to processing results with a right-click. The two spectra are shown at the top, and the result (with totally absorbing peaks not shown) is below. The sliders in the Subtract menu to the left can be used to adjust the results.

The extra power of this is clear when considering a typical analysis. A sample exhibiting contaminant peaks is searched against a library of production materials. The best match spectrum – representing the main component – is subtracted (one click away) and the residual spectrum is ready for searching against a database of known contaminants. An ideal library of contaminants would include materials known to be present in the factory, like lab coats, ceiling tile dust, hair or plaster. This would identify the source of the contamination in a useful manner with a very small number of clicks.

Figure 5 shows an identification result based on peak searching. This is an excellent tool for identifying possible origins for smaller peaks not accounted for in the initial search. Focusing between 1400 and 1180 cm^{-1} in this case draws out a flame retardant match. This does not appear on the basic search result match list, which is dominated by the bulk polymer.

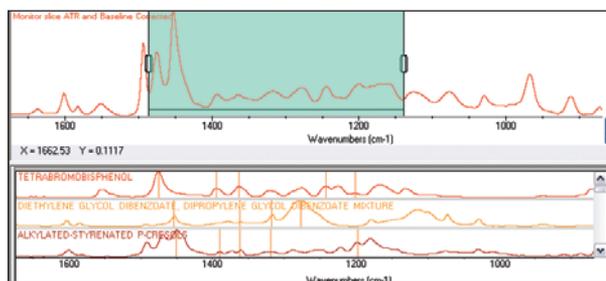


Figure 5: Narrow range peak search performed on an ABS plastic containing a flame retardant

Many samples coming into the analytical laboratory contain multiple components, either intentionally or through contamination. This is why chromatography like GC-MS is common in these settings – separate and identify. Infrared spectra of these materials are complex, and require sequential subtractions to deconvolute. Now, this process of spectral searching takes a huge leap with the unique Multi-component search embedded in OMNIC Spectra. The user chooses the number of components expected (two to four) and selects the databases for the search. The algorithm then does a series of concerted comparisons, combining spectra within the databases to perform a composite search. The resulting set of composite matches is assembled, and the user can visually scan the results. An example three-component pharmaceutical mixture is analyzed in this way in Figure 6. The result clearly identifies the three components, and provides a stunning visual through the spectral comparison showing how effective the algorithm is.



Figure 6: A multi-component search done on a pharmaceutical mixture. All three of the main components are correctly identified.

The productivity leap provided by this tool relative to the traditional search and subtract method is profound. Any user selecting the same database and number of components will arrive at the same result. The composite versus original comparison in the top window gives visual confirmation. Simplicity, confidence and consistency: a powerful combination adding up to productivity for the laboratory analyst.

In the absence of satisfactory database spectra, the spectral interpreter function can identify chemical moieties associated with spectral features. There are 145 entries in the interpreter database, covering all of the basic organic building blocks, and the user can add more. The interpreter also includes HTML files for the 145 entries, giving additional reference materials – almost like an organic chemistry book at the click of a button.

Report

Most workflows must result in a report. Once again, OMNIC Spectra supplies simplified tools, using the industry standard PDF format for document portability. Any workspace action – a process result, an identify result, or a simple spectrum – can be moved to the Results tray. Additionally, any information in a PDF knowledge base, such as the Thermo Scientific “IR Spectroscopy of Polymers” book or locally produced SOP documents, can be viewed and pages extracted to the Reports tray. Report preparation then involves moving these items through a PDF generator, seen at the lower left of Figure 7, to generate the report.

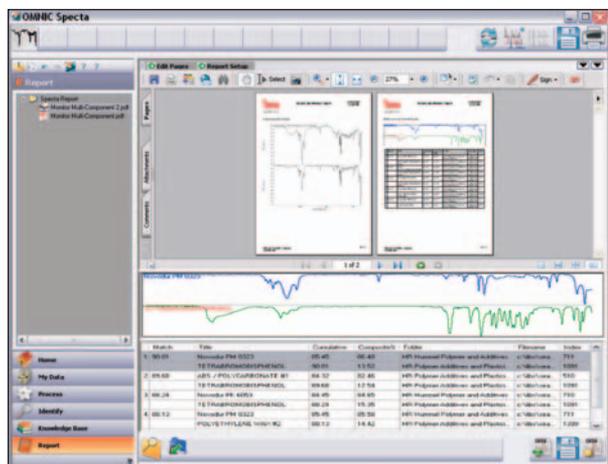


Figure 7: Report generation in OMNIC Spectra. All materials are converted to a PDF format. The report is shown in the upper pane, while the working material is shown below. The two buttons at the lower right create the PDF and clear the space for the next report.

Summary

OMNIC Spectra combines the familiar with the revolutionary to simplify your spectroscopy needs. The workflow is smooth and driven by function rather than the tools themselves. High levels of built-in intelligence give consistent, reliable results for any user. Building on our tremendous experience with the OMNIC spectroscopy platform, OMNIC Spectra will increase productivity by applying our cumulative experience in spectral analysis to your laboratory needs.

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