

Application Note:

Simple and powerful software for spectroscopy

Increasingly complex instrument and software landscapes in the spectroscopic laboratory create the need for standardization and simplification in routine tasks and in spectra identification.

Today, modern optical spectrometers are unthinkable without software. Software controls spectra acquisition, handles and processes spectra, and provides numerous tools for analyzing measured data.

This includes the identification of unknown samples by searching reference libraries. Such spectra databases are commercially available; in addition, laboratories can build their own spectra collections over time.

Each spectrometer manufacturer offers their own software tools for this purpose, to control their own spectrometers, sometimes offering powerful and specialized functionality for processing the data. The latter often represents a unique selling point and may offer competitive advantages on the market, because special applications are made possible for the user in the first place. For simple routine tasks, on the other hand, especially if equipment and software from different manufacturers are available in a laboratory, the large number of software programs can become an obstacle. The users have to master the handling of the processing tools in different software, algorithms differ from manufacturer to manufacturer, and often advanced functionality is not needed at all in everyday life and can even overtax the users.

"Smaller" spectrometer manufacturers who develop their own software are often not able to offer some functionalities at all, so that a search function, for example, may not be available at all.

Moreover, since database and file formats are not standardized, libraries and spectra are not always interchangeable between different software packages. A comparison of spectra from different instruments is thus made difficult, if not impossible. There have been several attempts to create comprehensive data formats (such as JCAMP, AnIML or Allotrope, to name just a few), but unfortunately these have not yet been able to gain widespread acceptance.

The machete in the software jungle

For routine sample identification tasks, especially in laboratories with diverse instrument inventories, it is therefore desirable to have uniform software that allows fast and easy processing and comparison of spectra from different file formats and supports powerful spectra searches in commercial spectra databases as well as in one's own spectra collection.

Addressing these needs was the guiding principle behind S.T.Japan-Europe's design of SpectraGenius. For more than 20 years, S.T.Japan-Europe GmbH has been offering high-quality spectral databases for ATR-FTIR, transmission IR, NIR and Raman in various formats worldwide. Users looking for easy-

to-use, straightforward software for routine processing and identification of spectra in a wide variety of formats need a solution that works with S.T.Japan's spectral databases and delivers results quickly.

Katja Holland-Moritz, CEO of S.T.Japan-Europe GmbH, explains, "We don't want to compete with spectrometer manufacturers' software, but rather offer a complement that is affordable and attractive, especially for smaller laboratories and educational institutions."

Over 60 spectra formats

SpectraGenius software can read spectra in more than 60 file formats from different vendors such as Thermo, Bruker, Perkin-Elmer, Shimadzu and many more. The preview mode allows a quick preview of the data to be loaded, so that only those spectra actually to be processed end up in the workspace.

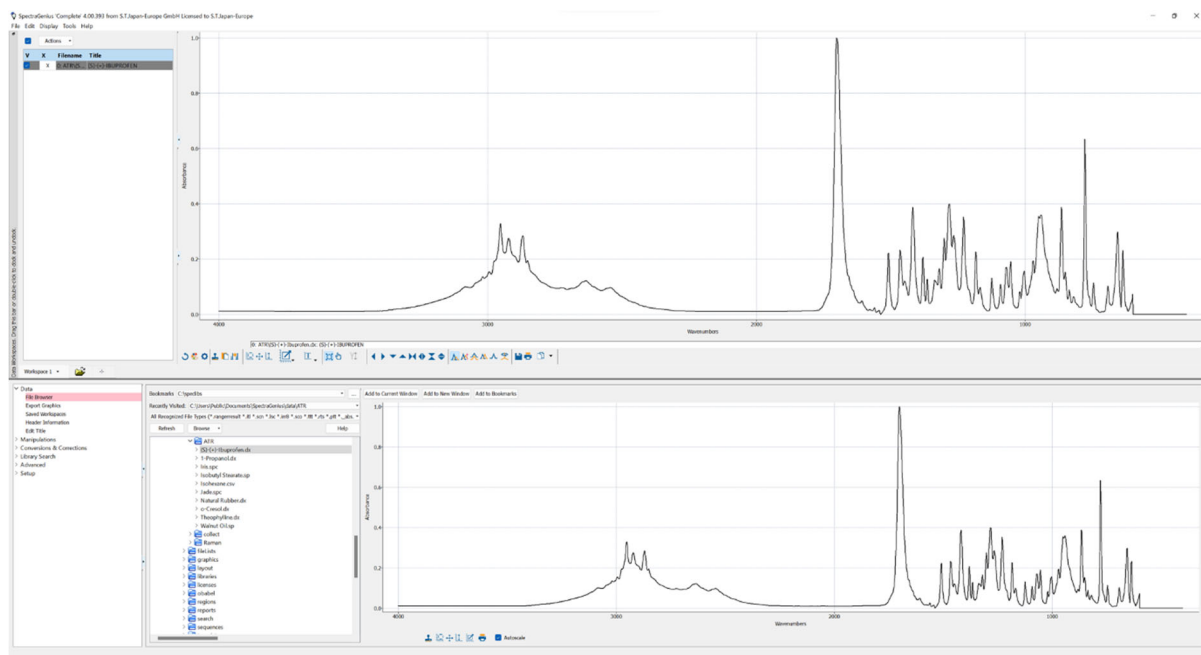


Figure 1: The intuitive user interface of SpectraGenius with Preview Mode

Once loaded, single or multiple spectra can be processed simultaneously. In addition to various axis conversions, spectral range and resolution adjustments, SpectraGenius offers automatic and manual baseline corrections, smoothing, offset correction, normalization and more. All operations can be completely undone at any time. Thus, spectra can be processed quickly, transparently, efficiently and, above all, uniformly, preparing them for a spectrum search regardless of the spectrometer on which they were previously recorded.

For routine tasks, all operations can also be automated very easily and without any programming knowledge in the Batch Processing tool. Processing sequences are then applied to multiple spectra simultaneously with just a few clicks. Only a few spectra - if any - have to be processed manually, which saves the user a lot of time and effort.

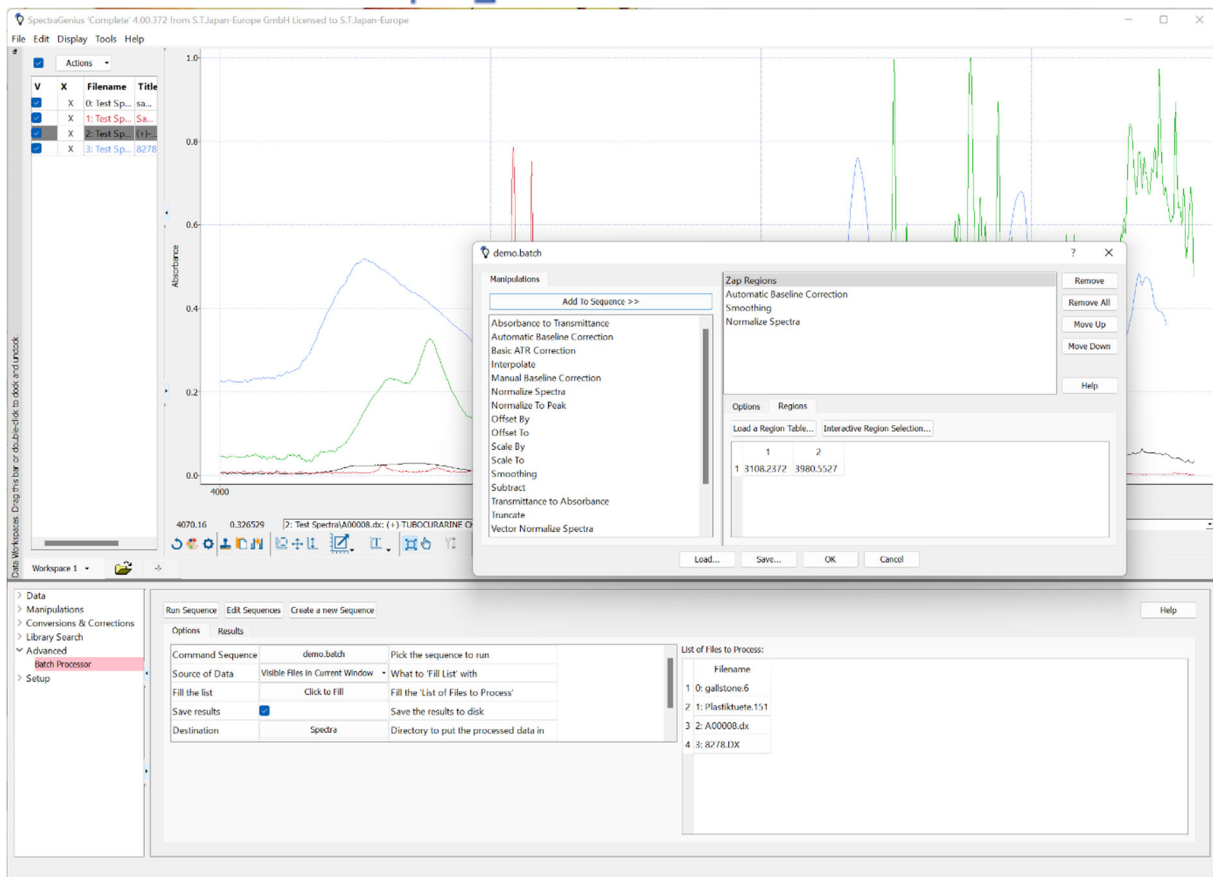


Figure 2: The Batch Processing Mode allows simple automation of routine processes without any programming knowledge.

The ability to create several different workspaces in the software and even save them for later use ensures a clear overview when working on different projects. This prevents data from being mixed up.

Fast search in spectral databases

For easy identification of unknown samples or incoming goods inspection, the measured spectrum can be compared with a reference spectrum. The identity and purity of the sample can thus be quickly checked. In the age of digitization, automated spectrum searches in reference databases have taken the place of manual comparisons with printed spectra from thick spectral atlases. Using powerful comparison algorithms, spectra are compared with each other and the degree of agreement is indicated by a numerical value. The results, sorted by this numerical value, are then displayed on the screen and can be subsequently checked by the user.

SpectraGenius offers a particularly fast search, which compares tens of thousands of spectra within a few seconds and displays the results. The list of hits can not only be viewed, but also exported for further processing, e.g. to Microsoft Excel or Word, or output as a printed report or PDF.

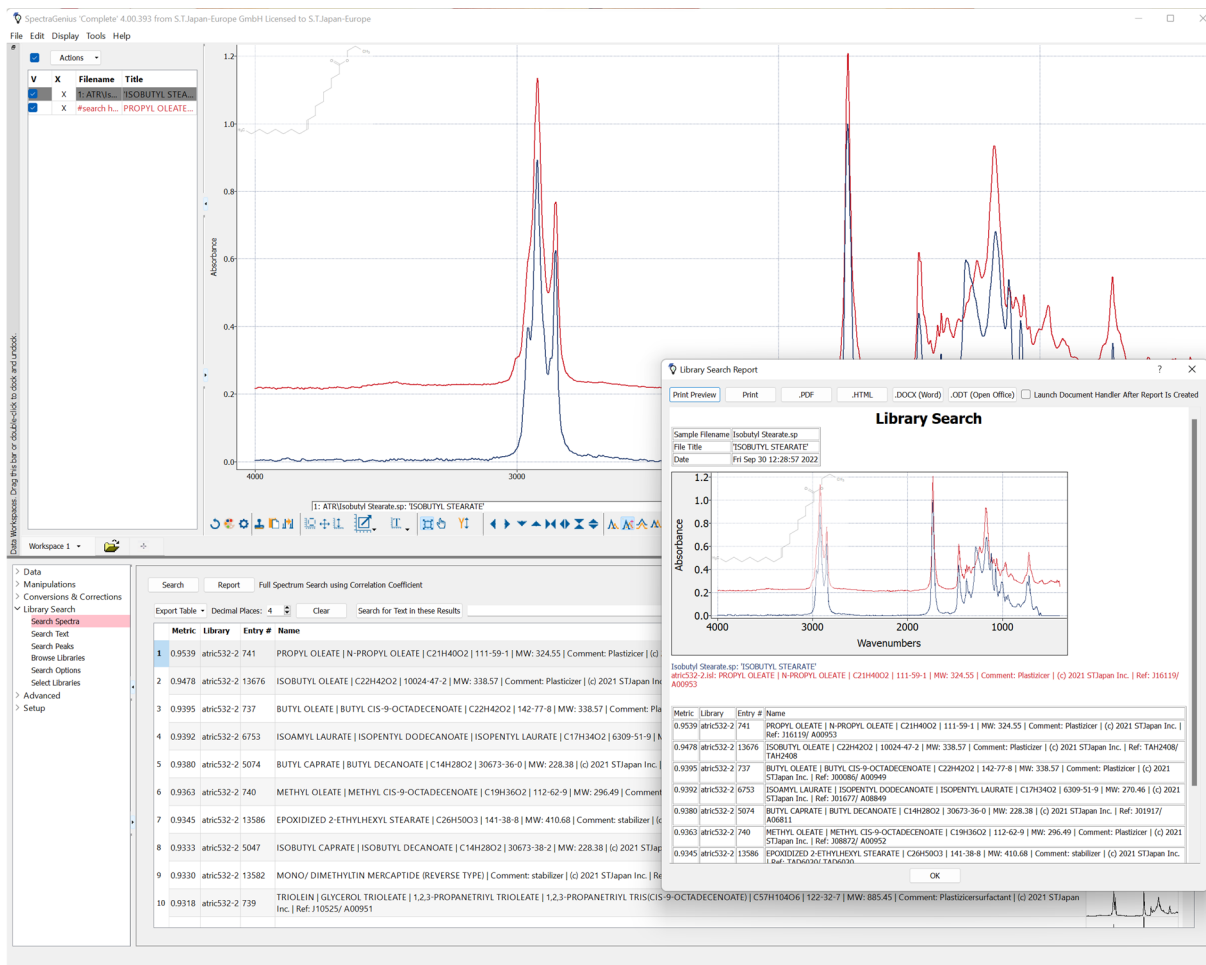


Figure 3: Spectra search in SpectraGenius is fast and allows easy output of result reports.

Spectrum databases in some common formats (Thermo Galactic, Thermo Nicolet, Perkin-Elmer SPL) can be used for this purpose; either already self-created ones from the respective manufacturer software or commercially acquired ones like for example the dozens of libraries with tens of thousands of spectra from S.T.Japan-Europe. Furthermore, it is possible to specify a directory on the file system as a basis for the search, so that also the search in own spectra collections is made possible.

Spectra searches in SpectraGenius can be performed on the full spectral range or on selected spectral regions. Furthermore, it is possible to search for specific peaks or to search for text in the description of the spectra. A result of a spectrum search can thus be further narrowed down by a subsequent text search.

Simple further processing of the results

As already mentioned, result lists of searches can be easily output to the printer and exported to e.g. PDF or Microsoft Office. It is also possible to save data in selected formats as a spectrum or as an image for further processing in other software, e.g. for report generation.

For simple printed reports, SpectraGenius also offers a layout editor so that the output layout can be customized according to your own wishes.

A wide range of options

SpectraGenius is available as a 30-day demo version as well as in various packages with specially selected ATR and/or Raman databases, optionally with English or Japanese user interface and corresponding databases. All S.T.Japan spectral databases are also available for SpectraGenius.

Dr. Maren Fiege

CTO

S.T.Japan-Europe GmbH

www.stjapan.de