Getting Started with Spectrus Processor

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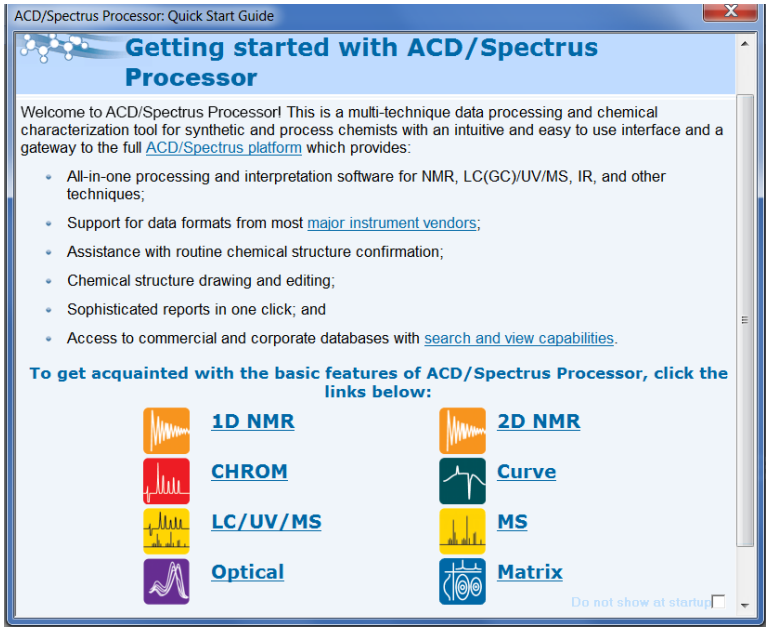
This document is an overview for the most popular functionality in Spectrus Processor and is a supplement to detailed Quick Start Guides offered by default in the software when you launch the program. Click on the links to launch detailed quick start guides for different data types (1D NMR, MS, etc.).



Detailed Quick Start guides are available when you launch the software.

Import Data

Import your data by simple 'drag-and-drop' from the left-hand navigation pane into the Processor interface (automatically populated with your computer and network directory structure), or 'double-click' on the data file.

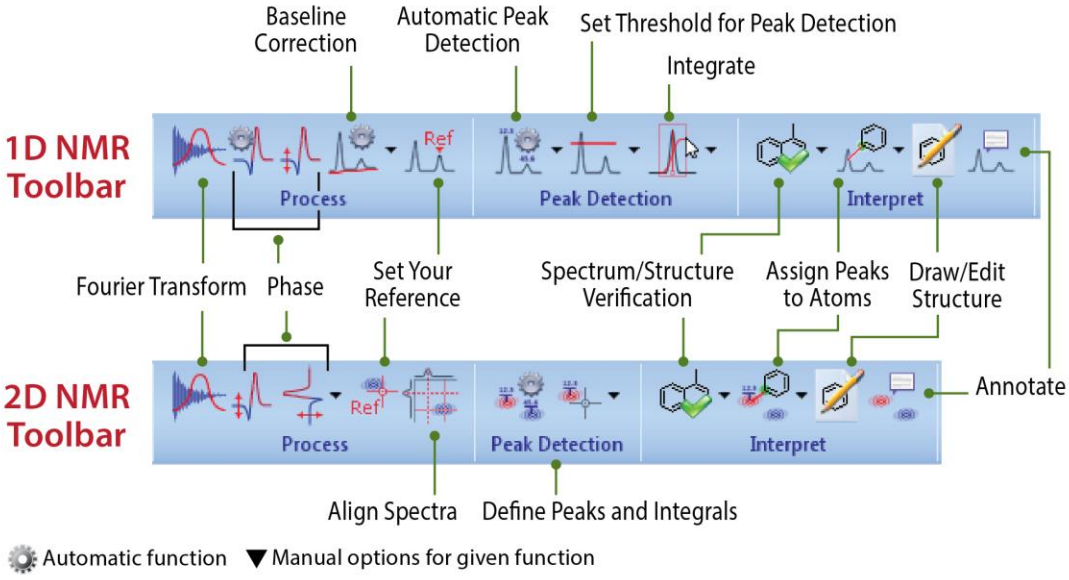
Processing and Interpreting Data

Toolbars automatically change, based on imported data, to provide technique-specific functionality for processing and interpretation.

Manual and automatic processing functionality is available in the software for 1D and 2D NMR, LC-MS, IR, Raman, and other analytical techniques. You will be able to import chemical structures relevant to your data, assign peaks to your structure, and annotate spectra and chromatograms.

NMR

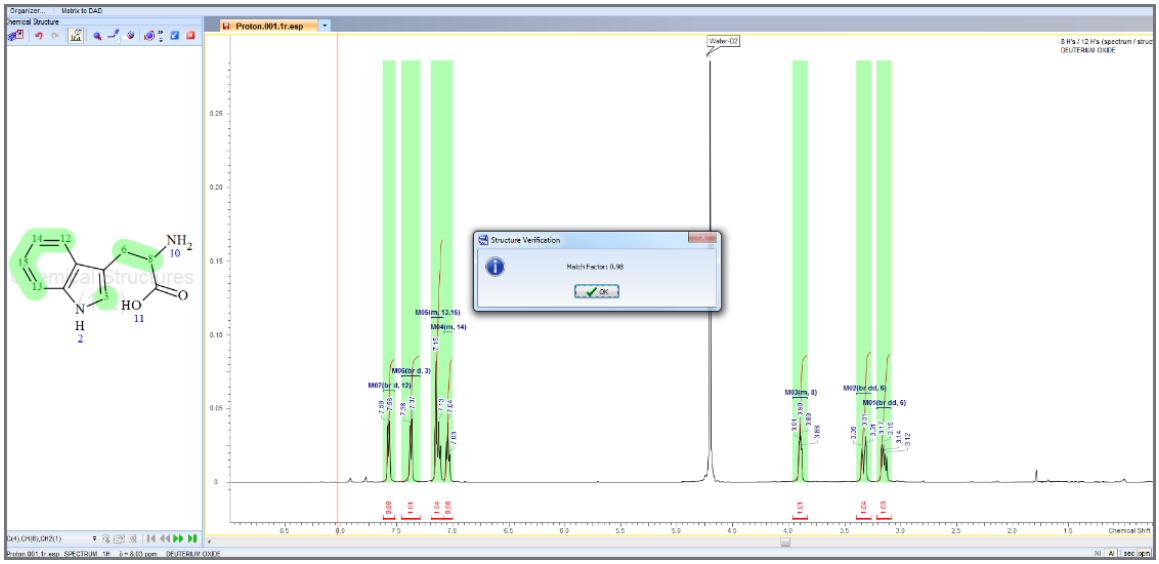
Simply drag-and-drop your NMR data (1D or 2D) into the Spectrus Processor interface and use the toolbar functions to process and analyze it. Note: pre-processed NMR spectra may also be imported with simple drag and drop for further manipulation/review.



Verify Structure/Spectrum Consistency

Draw a structure by launching the ChemSketch window (click **Draw/Edit Structure**).

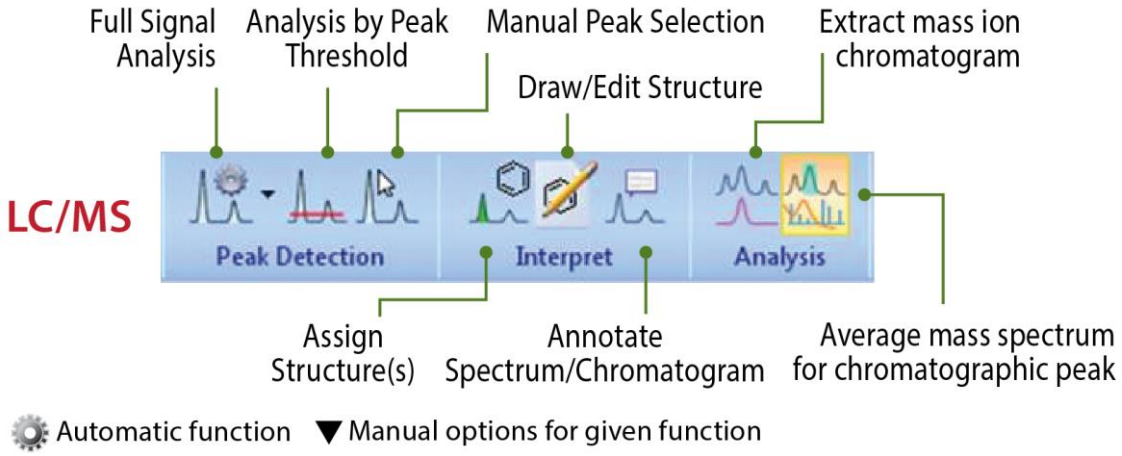
If verification does not occur automatically, simply click **Spectrum/Structure Verification** to find out if the suggested structure fits the spectral data.



Structure/Spectrum verification for NMR in Spectrus Processor maps spectral peaks to atoms on the structure and provides a Match Factor for how well a structure fits the data.

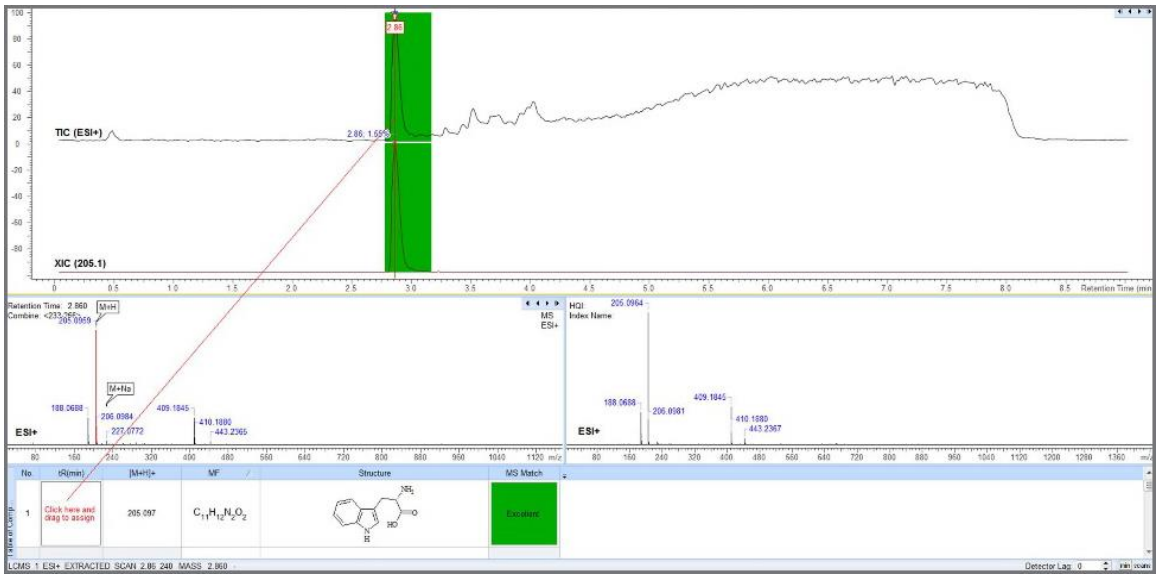
LC/MS & GC/MS

Functions on the toolbar allow you to manually detect peaks, extract the mass ion chromatogram, and assign structures to chromatographic peaks for hyphenated MS techniques.



To confirm that your LC/MS dataset is consistent with a given structure, draw the structure (click **Draw/Edit Structure**).

The software automatically extracts the mass ion chromatogram. Click and drag from the retention time column in the table to associate a chromatographic peak (green coloring on a chromatographic peak indicates consistency between the structure and the expected molecular ion and isotope pattern).

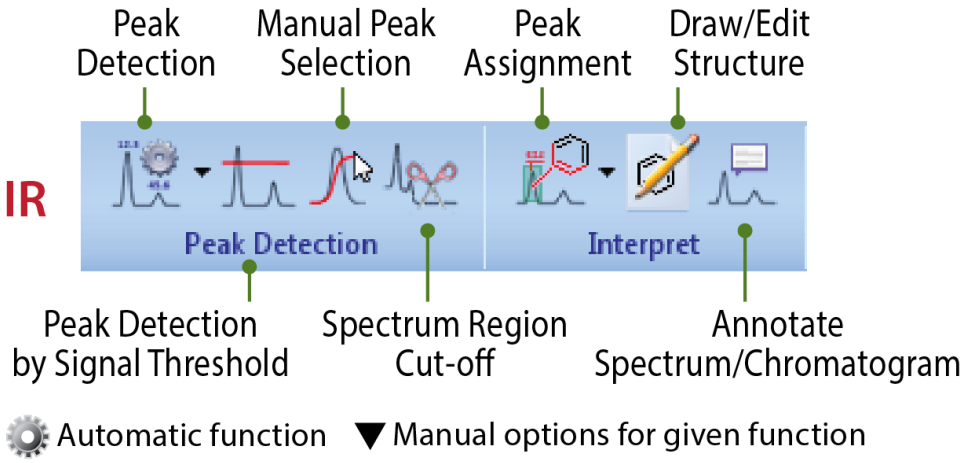


Adding a structure to an LC/MS data set in Spectrus Processor allows the user to quickly decide if the desired mass is present and assign the chromatogram. The software provides a binary (good or not) 'MS Match' factor to aid data interpretation (see the green box to the left of the structure indicating 'Excellent'.

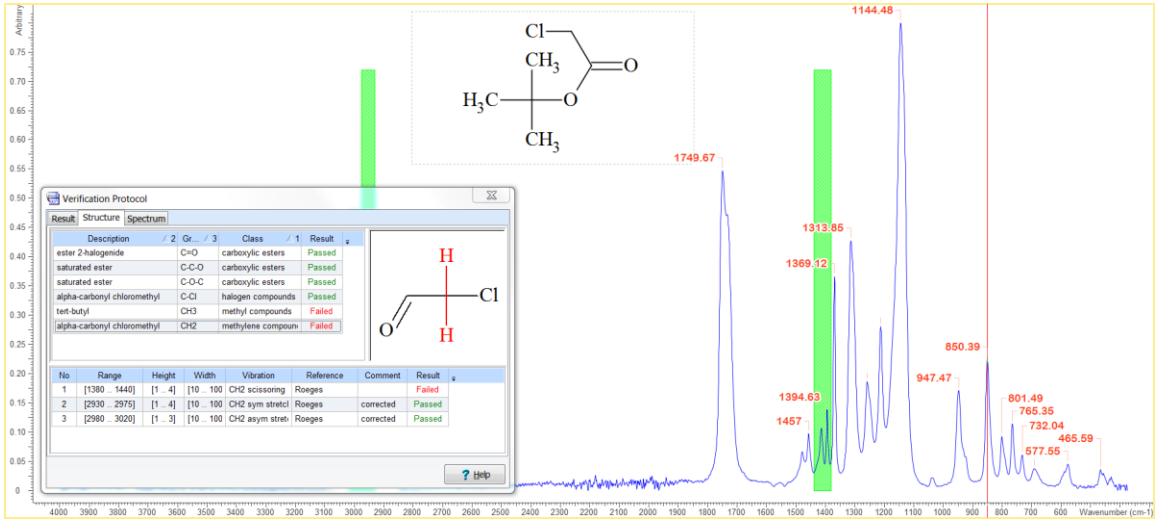
IR

To confirm the presence of particular functional groups/molecular fragments in your spectrum simply drag and drop your dataset into the interface and pick peaks by clicking **Peak Detection**.

Drag-and-drop (or draw) the proposed structure/structural fragment, and choose **Peak Assignment** from the options under interpretation.



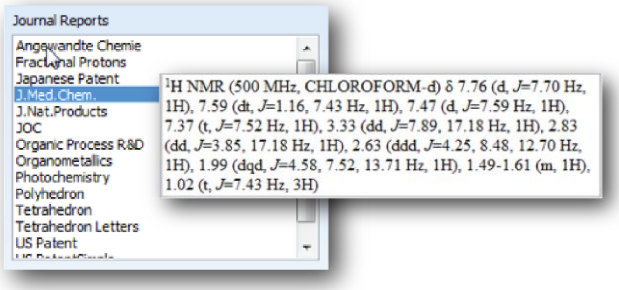
The software searches for component fragments in the spectrum and provides pass/fail results with an explanation of the expected peaks, their range, and a reference. 'Fail' results may be due to the absence of an expected peak/band, overlapping signals, or peaks shifted out of range.



Verification of a structure by IR provides visual highlighting of structural fragments and associated spectral peaks. The absence of expected peaks is indicated with a 'Fail' result.

Reporting

Generate standard individual reports for your analytical data by clicking **Report**.



You may be interested in creating multiplet reports for NMR in the Journal format of your choice. From the **Options** menu, choose **Multiplet Report**.

Copy/Paste spectra, table data, and multiplet reports for NMR from the ChemSketch interface where reports are generated, into Microsoft Office or documents of your choice.

Other Techniques

Spectrus Processor can be used to process and analyze data from other hyphenated MS techniques, other optical techniques (Raman, UV/Vis), thermal analyses, x-ray methods, calorimetry, and other analytical techniques. Similar technique-specific functionality is provided for each dataset as it is imported into the software.

General Information

Spectrus Processor is built with the capability for you to undock tables and windows in the interface to make the best use of screen space.

Alter your view of your data in the interface to suit your needs. Toggle between horizontal/vertical tile view (right top and bottom); or view individual techniques full screen with related data presented in different tabs (left below).