



# JASON

# User Guide

# JASON Overview:

## Where to Find What You Need

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*This document is intended to give the user an overview of JASON and to allow them to orient themselves within the software. It is assumed that the user has a working knowledge of NMR processing and that JASON is running under the Windows or macOS operating systems.*

# 1 Getting Started

- Click here for a video tutorial on [Getting started with JASON](#).

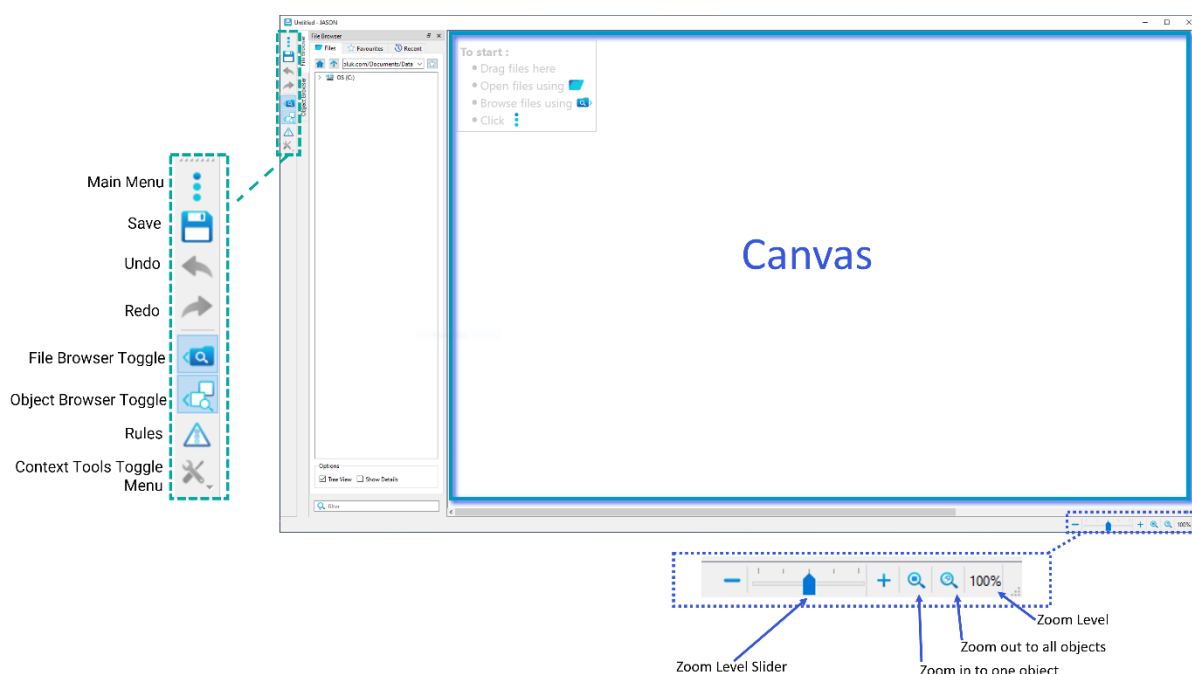


Figure 1: JASON canvas when the software is first opened.

When a new instance of JASON is opened, by double clicking the desktop icon, the user is presented with an empty workspace called the **Canvas** (see Figure 1). With no data loaded, the Canvas has the following functions in the menu in the top left-hand corner:

1. **Main Menu**, which contains options for loading, saving and printing data, starting a new molecular structure drawing, spectral simulations and the general settings interface.
2. **Quick Save button**, if the current instance of JASON is untitled, clicking this button will open the 'Save' dialog allowing the user to choose where to save the file and what to name it. A previously saved file will automatically be saved under its current name to its current location.
3. **The Undo/Redo arrows**, which allow the user to undo or redo the most recent action.
4. **File Browser toggle button**, which toggles the visibility of the File Browser.
5. **Object Browser toggle button**, which toggles the visibility of the Object Browser.
6. **Rules button**, which opens the Rules panel to allow the user to create or select rules.
7. **Context Tools toggle menu**, which provides a menu of options for toggling the visibility of various data manipulation tools.

It is possible to add text to the Canvas by using the right mouse click and selecting **Main Menu -> New -> Text**.

**Images** can be pasted from the clipboard onto the Canvas using the usual 'Paste' command or opened from the File Browser. Open images can be copied and pasted onto the JASON canvas from an image viewer.

**Annotations** can be added to items on the Canvas which are active by right clicking on the item and selecting 'Annotation' from the menu list and following the instructions on the appearing pop-up; the currently available options are: Rectangle, Arrow, Text, Ellipse, Triangle, and Curve. For drawing curved polyline annotations, select [Annotation] → [Curved Polyline] from the context menu. Click on the Canvas to set the starting point of the curve; click to add each point where you want the curve to bend. Double-click to complete the drawing.

The bottom right-hand corner has **Zoom controls**, which will be discussed in the context of data viewing and manipulation (see Section 3).

## 1.1 Plugin Manager

The Plugin Manager is accessed via the three dots Main Menu button and displays all the available plugins for the opened instance of JASON (see Figure 2 as an example: please note that the list of available plugins constantly grows and not all of them are presented in Figure 2).

From the Plugin Manager, users can enable or disable a plugin and set properties such as enabling auto-update.

The 'Plugin Details' section displays information about the selected plugin, such as the version number. If an update is available for the selected plugin, this will be highlighted in the 'Version' section.

For the current version (6.1), the following plugins are available:

**Affinity Screen** - provides an interface for manual and automatic analysis of 1D NMR fragment-based ligand screening data.

**Binning** – provides Binning analysis tools ('Bins' section in the 'Analysis' panel)

**MAGRES** File Filter

**SIMPSON** File Filter

**SMILEQ** - quantitative analysis of NMR data

**Solid Spin** - provides solid-state NMR simulation in JASON using SIMPSON, which is a general simulation program for solid-state NMR.

**TECMAG** File Filter

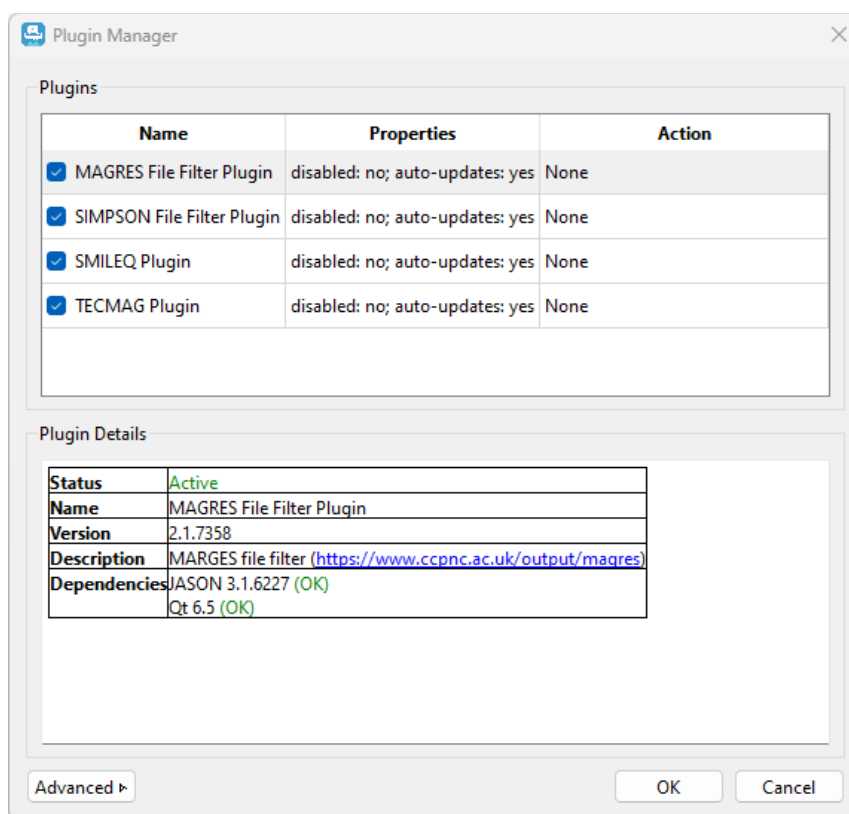


Figure 2: Plugin Manager

## 2 Loading Data into JASON

There are three primary methods for loading data into JASON:

1. Drag and drop a file, folder or zip archive from Windows Explorer onto the Canvas (see Figure 3).
2. Use the 'Open' option on the Main Menu to navigate to the file of choice, then click 'Open'.
3. Use the 'File Browser' toggle button to make the File Browser visible and then use it to navigate to the relevant files.

## 2.1 Loading from Windows Explorer or Finder

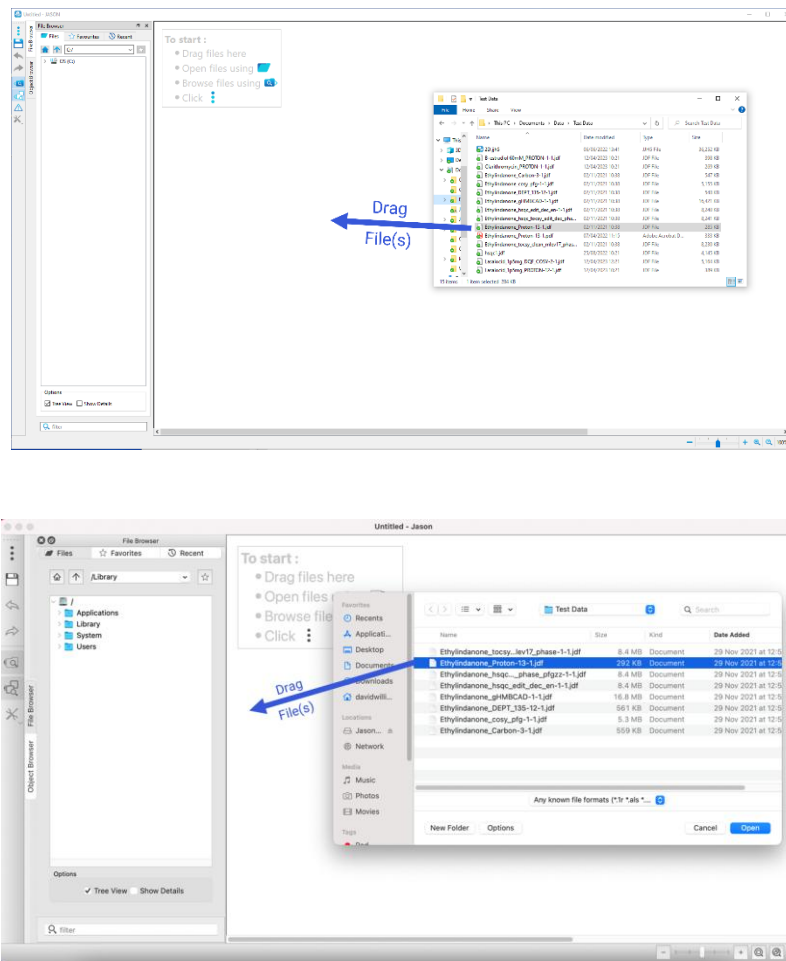


Figure 3: Loading a file from Windows Explorer or Mac Finder

A suitable data file or folder can simply be dragged and dropped from a standard Windows File Explorer window onto the Canvas. It is also possible to use the 'Open with' option in Windows explorer and select JASON as the chosen software, however it is worth noting that this will start a new instance of JASON rather than loading the data into an existing one.

A ZIP archive can also be simply dragged and dropped to JASON. JASON will automatically extract all files that it can open.

Files or images can also be copied from the File Browser or Desktop onto the Canvas.

## 2.2 Loading from the Main Menu

Left clicking on the Main Menu and selecting the 'Open' option, opens a Windows file browser which can be used to navigate to an appropriate directory. Here, a file can be loaded by either double-clicking on the file or dragging it onto the Canvas or clicking the

'Open' button on Windows explorer. Multiple files can be loaded using the usual methods for selecting multiple files in Windows Explorer.

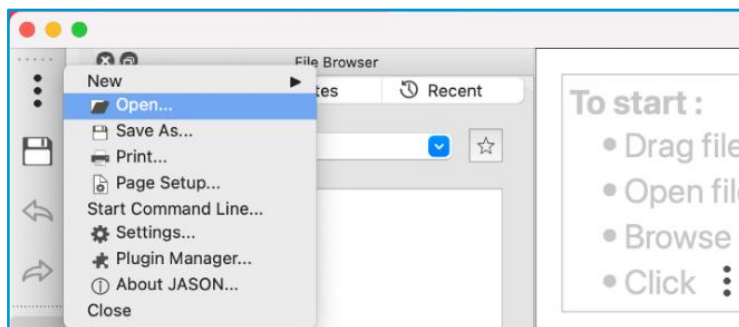


Figure 4: Loading a file from the Main Menu

## 2.3 Loading from the File Browser

The 'File Browser' toggle button can be used to make the File Browser visible in JASON. By default, it will appear by the left-hand edge of the Canvas, see Figure 5. Note that the layout of JASON is configurable, and the File Browser can be detached and reattached at any edge of the Canvas simply by dragging the whole browser using the name bar at the top of the File Browser frame.

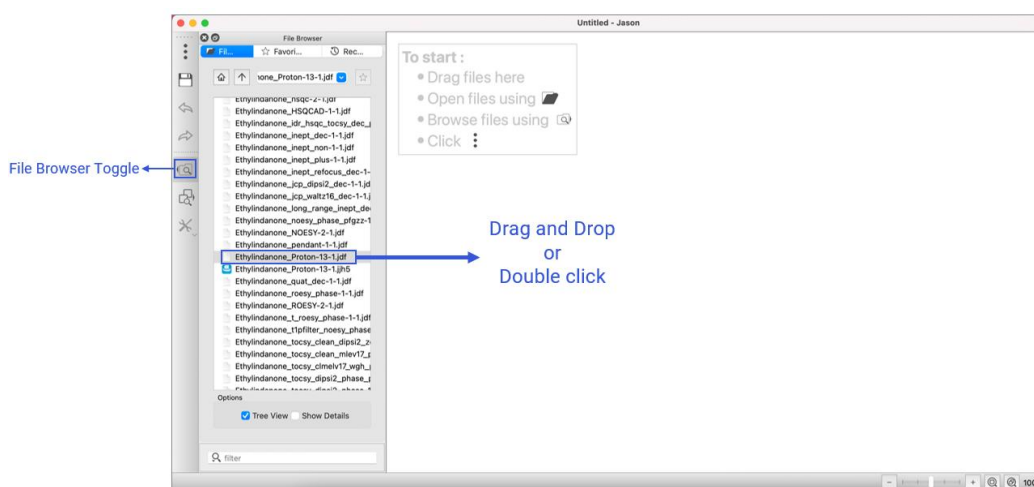


Figure 5: Loading data from the JASON file browser

The File Browser itself comprises of three panels (see Figure 6)

1. **Files** – a straightforward file navigator panel.
2. **Favorites** – a list of favorite directories.
3. **Recent** – a chronological list of recently opened files.

A folder can be loaded from the File Browser by simply navigating to the directory of choice and double clicking on the desired folder. Files can be selected with a left mouse button click. Multiple files can be selected by holding down **Shift** and selecting a second

file to select all the files in between or holding down **Ctrl** or **Cmd** and selecting individual files, see Figure 6. The selection is then dragged to the Canvas to load the files.

Folders can be added to the 'Favorites' tab by selecting them in the 'Files Browser' panel and clicking on the 'star' icon or by right-clicking on the folder and selecting 'Add to Favorites'. Folders in the 'Favorites' panel may be given an alias name by right-clicking on the folder and selecting 'Edit Alias' from the menu.

Right click on any entry in the 'Recent' tab to display menu options. From this menu, items in the 'Recent' list can be deleted, the list cleared, a file opened, or the file path copied as a text string.

Note that for the ease of navigation, for the data formats: JEOL Delta, TopSpin, VNMR, and JCAMP-DX, JASON parses the title file from Bruker data and display it in the File Browser.

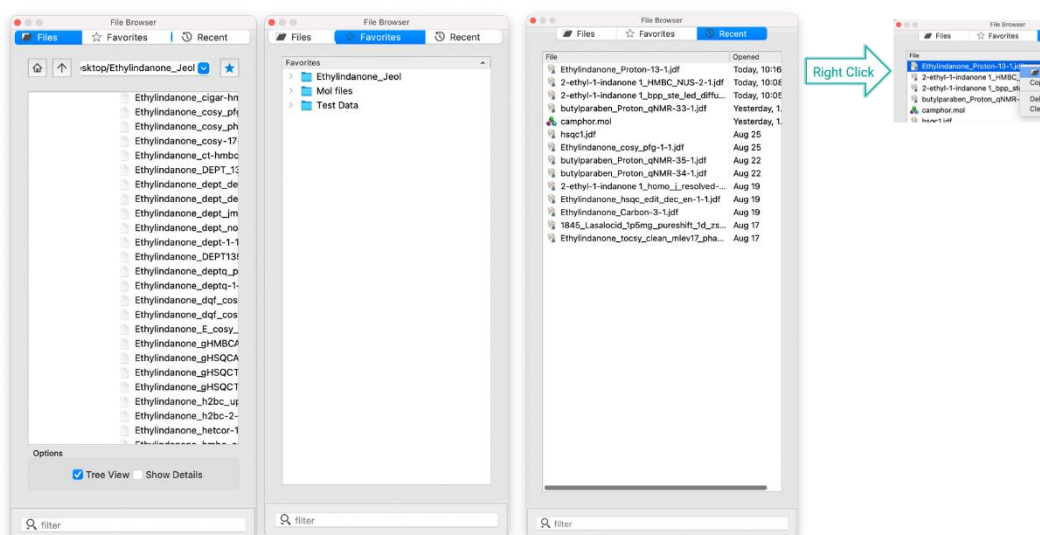


Figure 6: The file browser tabs

## 2.4 Arranging data on the Canvas

When an object on the Canvas is selected in JASON, you will see eight small circles around the edge of the object. If these circles are filled in, then the object is selected and currently the active focus. These circles can be used to rescale the object by clicking and dragging. In addition, when selected, each object has a small numbered tag in the top left hand corner. This is used to manually move the object around the Canvas. When resizing or moving an item on the Canvas, it “snaps” to the edges of the page or relatively to the edges of other items on the same page. Keep ‘Ctrl’ pressed for **free placement** and resizing; **‘mirror’ resize** is activated with the ‘Ctrl+Shift’ key combination; ‘Alt’ + left mouse button is used for **pan navigating** the Canvas. More details of how to manipulate Canvas objects are given in the following section.

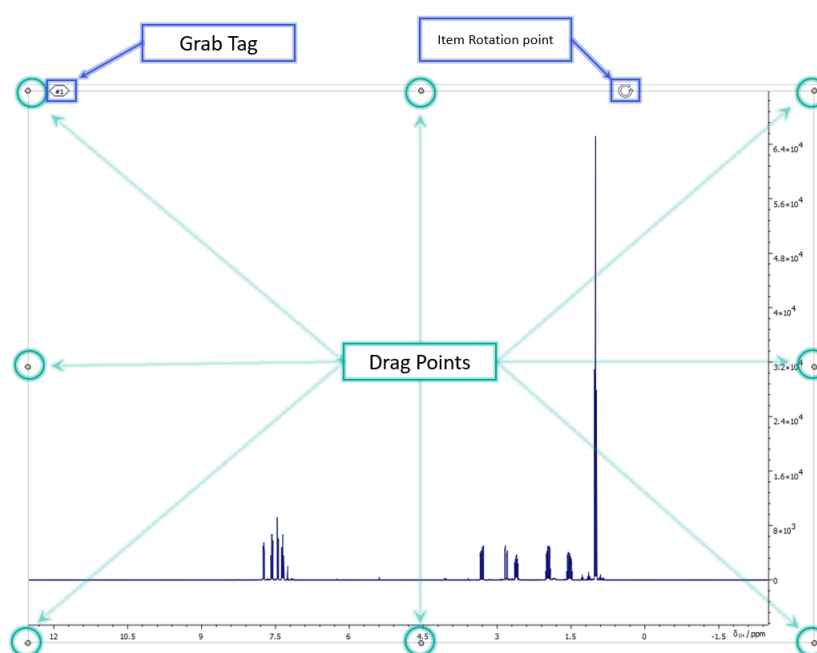


Figure 7: Grab tab and drag points for moving and rescaling canvas objects

The pattern in which items are placed on the Canvas as they are opened in JASON, is determined by the method of opening the object file. If the file is dragged and dropped on a blank part of the Canvas, the file will be opened at that position. If the file is opened by double clicking on it, then the object created will be placed automatically on the Canvas in a pattern that is defined in the ‘Settings’ menu, in the ‘General’ section under the ‘Canvas’ tab (see Figure 8). The ‘Settings’ menu is accessed from the Main Menu in the top left-hand corner of JASON frame and will be described in more detail in Section 5.

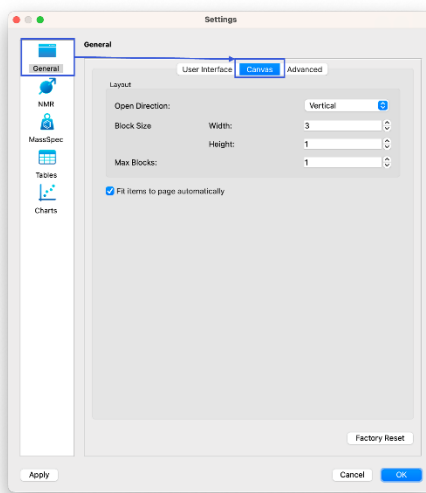


Figure 8: Canvas Settings

Objects on the Canvas are arranged in a kind of table, with vertical columns and horizontal rows. For the convenience of rearrangement, it is possible to insert empty 'columns' or 'rows' next to existing objects on the Canvas; the corresponding options ('Insert Row' and 'Insert column') are found in the right-click menu on the objects, section 'Appearance' (see Figure 9):

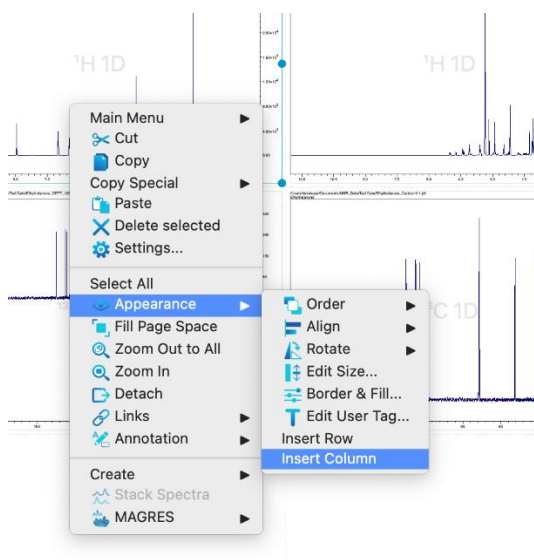


Figure 9: Inserting columns/rows while rearranging objects on Canvas

Right-clicking on an item on the Canvas or on the Canvas itself, displays a context menu, under the 'Canvas' submenu of which the options for adding more space on the Canvas are found. Selecting "Insert Column" will insert a column to the left of the selected item. Items in the same column as the selected item, as well as those in columns to its right, will be shifted one column to the right. The same logic applies to the 'Insert Row' option,

with the new row being placed above the row containing the selected object (Figure 10: 'Canvas' submenu in context menu).

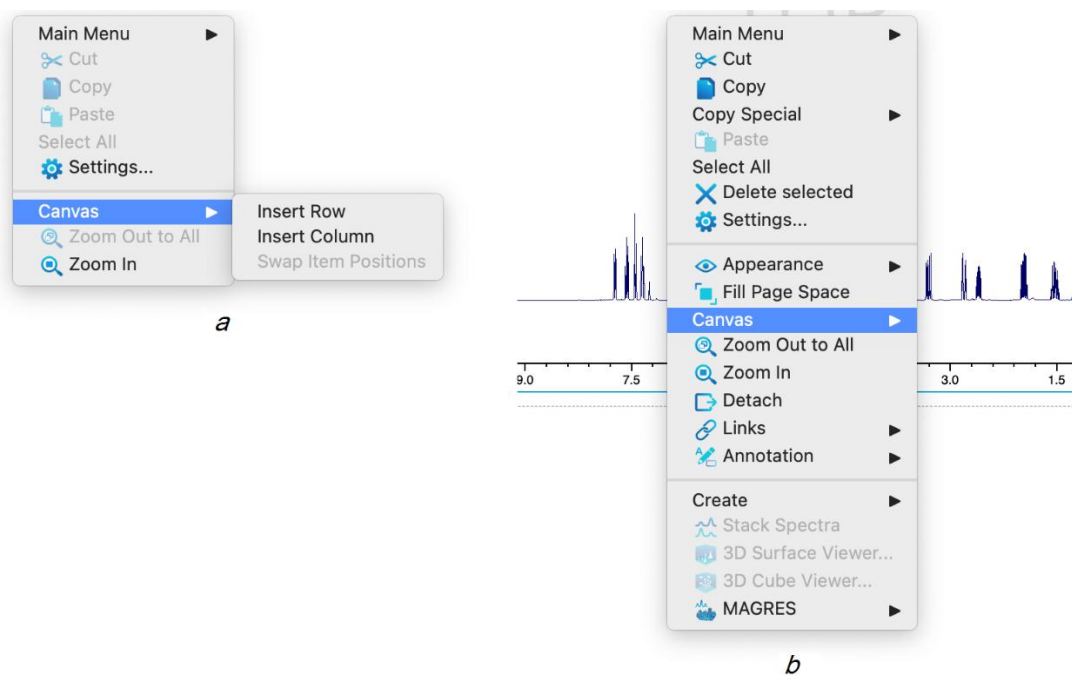


Figure 10: 'Canvas' submenu in context menu

It is possible to **switch the place of items on the Canvas** provided that:

- Only two items are selected.
- The selected items are on different pages.
- The selected items do not have a parent item.
- Each page contains only the selected items and their child items.

**To swap two items**, select them first (holding 'Ctrl' or 'Cmd'), then right-click on one of the selected items to get the context menu and choose the "Swap Item Positions" option in the Canvas' section. When this option is selected, the selected items – along with their child items – are swapped between their respective positions. Swapping positions is covered by undo/redo.

### 3 Data Manipulation Overview: Viewing, Processing and Analysis

An overview of the tools the user can use to manipulate data objects on the Canvas is provided in this section. A more detailed discussion of each of these tools will be given in a later section.

Once data has been loaded into JASON, the user will see that a number of context dependent panels have opened up. For example, Figure 11 shows those typical for a 1D NMR spectrum.

### 3.1 Context Tool Bar

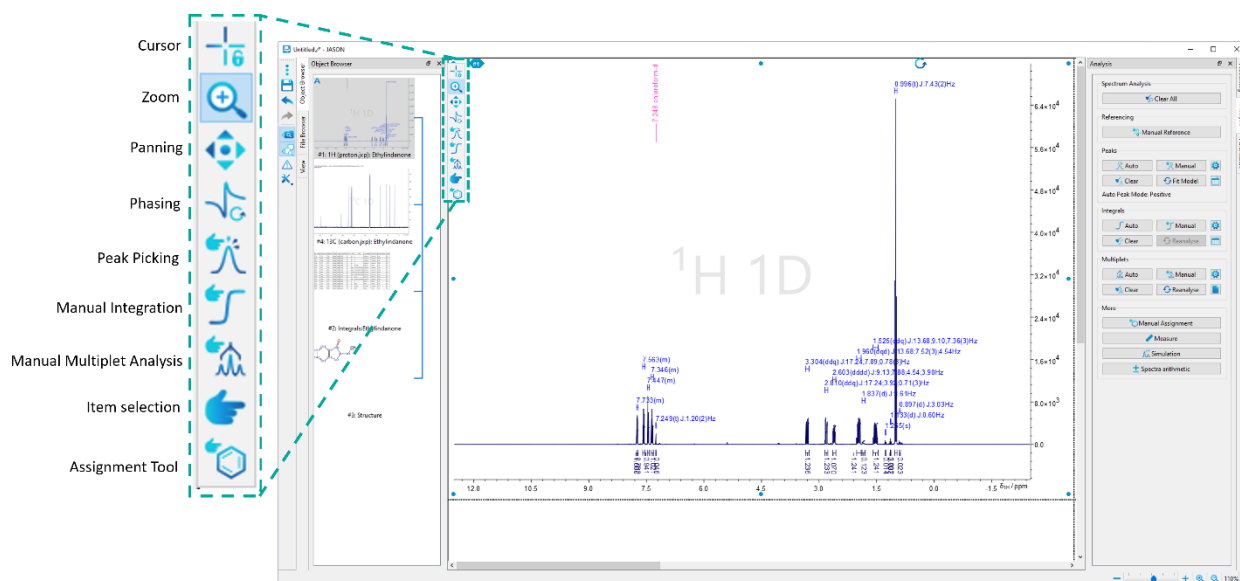


Figure 11: Context Tool Bar

When an object is selected in JASON, the **Context Toolbar**, shown in Figure 11, becomes available in the top left-hand corner of the spectrum. This is a set of tools for manipulating and analyzing the current object. A tool is selected by left clicking on the icon of choice or pressing the appropriate shortcut key on the keyboard. In addition, a particular functionality can be temporarily activated by holding down the shortcut key. For example, if a user is phasing a spectrum and needs to zoom into a region of the spectrum, they can simply hold down the **Z** key (the shortcut for zoom) on the keyboard and zoom into the desired region, and on release of the **Z** key the control will return to the Phasing functionality. In the following description, the shortcut key is given in parenthesis after the mode name; the shortcuts in JASON are not case sensitive. There are some generic functions for NMR spectra; double clicking the left mouse button resets the zoom level to full view and scrolling the mouse wheel increases or decreases the intensity of a spectrum.

**Cursor (C):** Cursor Mode locks all Zooming and Panning functionality. In addition, it can be used to examine homonuclear 2D spectra (COSY, TOCSY, NOESY, ROESY). Placing the cursor on the diagonal of this type of spectrum and moving horizontally or vertically opens a box allowing the user to identify the relevant cross peaks. In cursor mode, the double cursor also appears on INADEQUATE spectra (Figure 12). The second cursor points to the cross-peak on the other side of the INADEQUATE diagonal (the option to turn the diagonal on / off is found in the '2D Plot' section of the 'View' panel).

In some cases, JASON cannot recognize the double-quantum/single quantum (DQ-SQ) experiment type. For example, it could happen for some solid-state DQ-SQ experiments. Setting the diagonal slope to 2.0 (in Settings-Plot-2D) will force the experiment type "DQ-SQ" to be assigned to the unrecognized dataset. After that, the cursor, diagonal and other tools work on that DQ-SQ experiment as expected, taking the double frequency values at the indirect dimension into account."

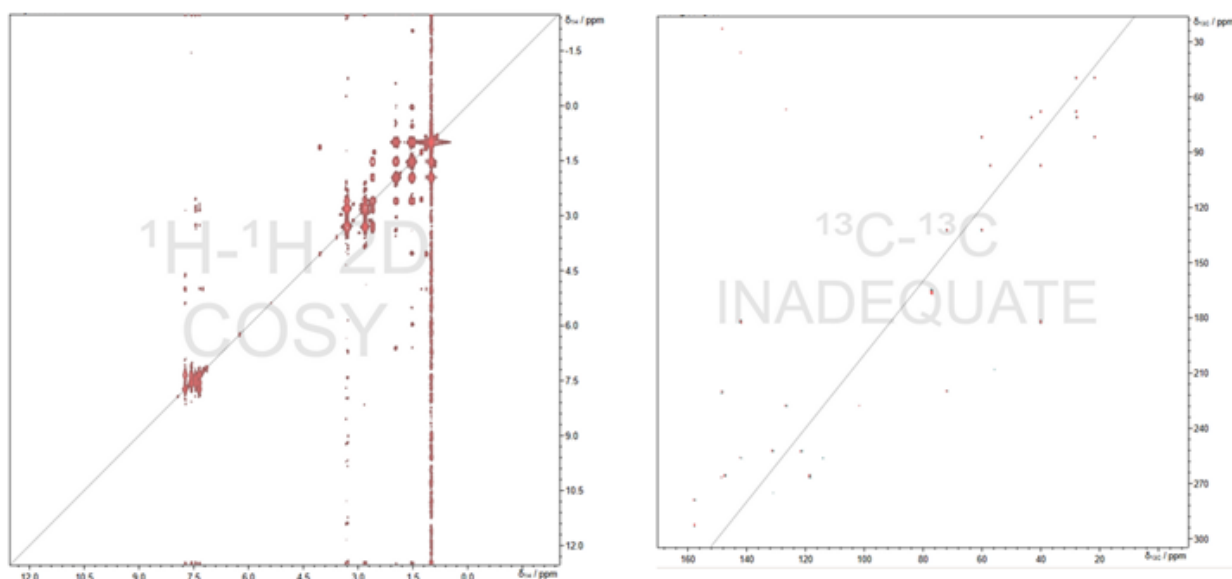


Figure 12: Diagonal on 2D homonuclear experiments and INADEQUATE spectra

**Zoom (Z):** In the Zoom mode, clicking the left mouse button and dragging the cursor selects the new zoom view region. On release of the mouse button, the view will zoom to the newly selected region.

**Move/Scale spectrum (P):** In the Move/Scale mode, a left click and drag moves the position of the spectrum

**Phasing (F):** In the Phasing mode, the user can interactively change the phase of the spectrum. On selecting the Phase mode, the pivot point is set on the largest peak in the spectrum by default (the green line in Figure 13).

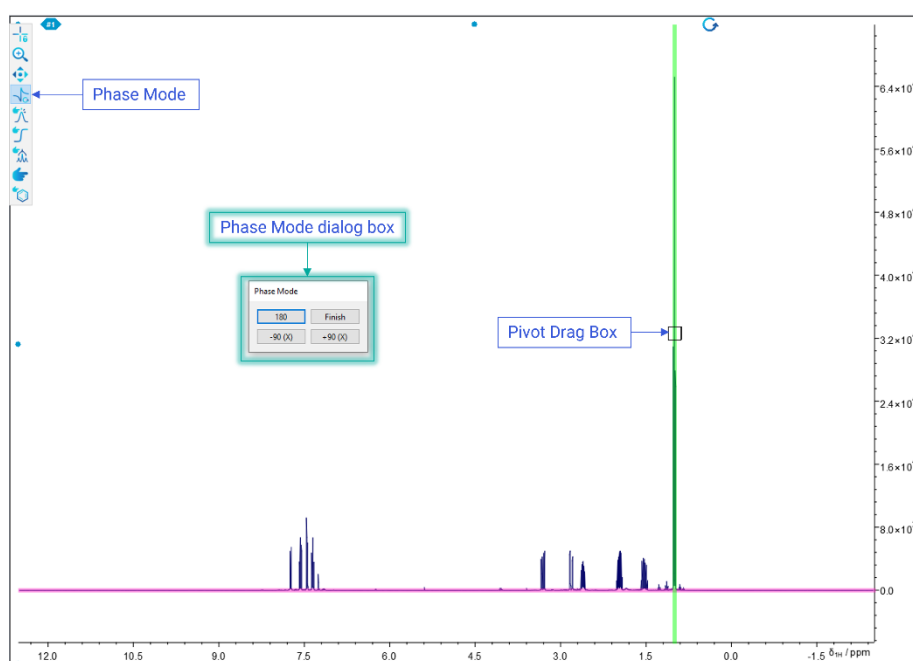


Figure 13: Interactive Phasing Mode

The pivot point can be moved by left clicking and dragging the grab box on the green pivot line. Zero order phasing is performed by holding down the left mouse button and moving the mouse. The mouse can be moved in any direction, allowing the user to move the mouse in the manner they are most accustomed to. First order phasing is carried out in a similar manner, holding down the right mouse button. Once the spectrum has been satisfactorily phased, the user can exit the Phase mode by clicking the 'Finish' button on the 'Phase mode' dialog box.

The 'Phase mode' dialog box contains several buttons. Clicking the '180' button will flip the phase of the spectrum by 180°. The 'OK' button applies all changes and closes the dialog, 'Cancel' button cancels changes and closes the dialog, exiting the Phasing mode, and the 'Reset' button resets values to those before changes were made, leaving the dialog open ()..

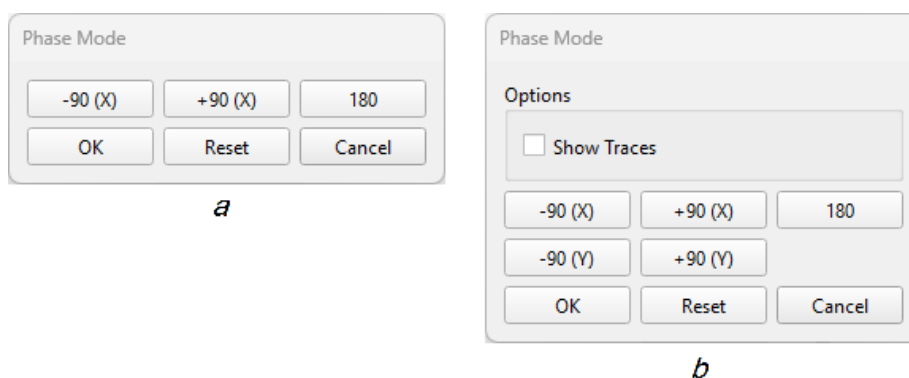


Figure 14: 'Phase' mode dialog for 1D and 2D NMR

2D NMR data is phased in a similar manner, see Figure 15. When the Phase mode is selected, the largest positive peak in the spectrum is selected as the pivot point. If the 'Show Traces' box has been checked in the 'Phase mode' dialog box, then the X and Y traces (green lines) that pass through the pivot point will be displayed at the appropriate edge of the spectrum to help guide the phasing. The pivot point can be moved by left clicking and dragging on the pivot grab box.

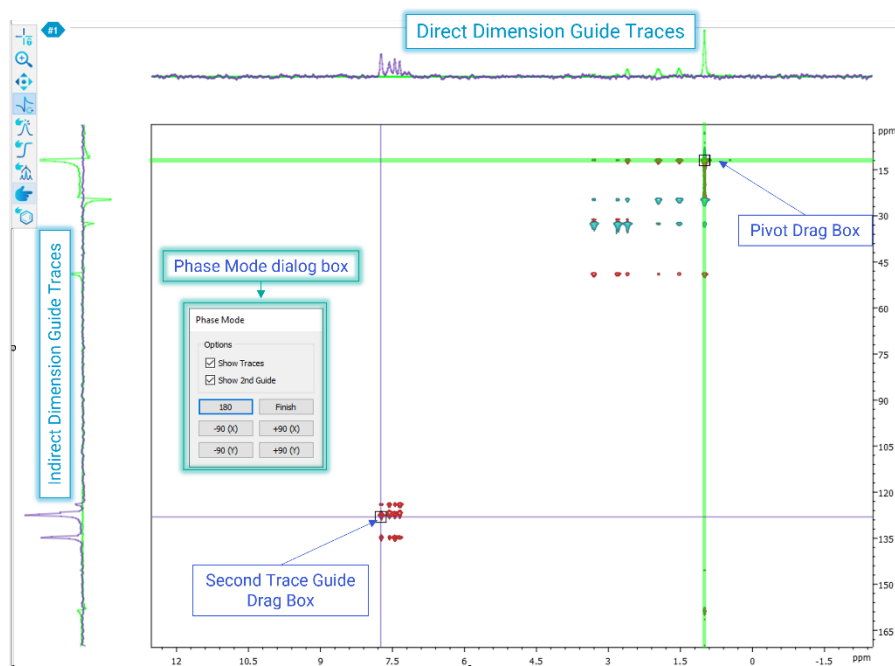


Figure 15: Interactive Phasing 2D

The 'Phase mode' dialog box contains two buttons, '180' and 'Finish'. Clicking the '180' button will flip the phase of the spectrum by 180°. Clicking on the 'Finish' button will exit the Phasing mode. If the 'Show Traces' checkbox is ticked, the 'Show 2<sup>nd</sup> Guide' checkbox becomes visible.

If the 'show 2<sup>nd</sup> guide' box is checked, a second set of traces can be selected; these are shown as the blue lines and can be moved using the second trace grab box. The guide traces are also displayed at the edges of the spectrum.

The zero order phasing of the 2D spectrum is carried out by holding down the left mouse button. The direction of movement now corresponds to the direction of the phasing. Moving the mouse vertically changes the phase of the indirect dimension, also referred to as F1 or the Y axis. Moving the mouse horizontally changes the phase of the direct dimension, also referred to as F2 or the X axis. Moving the mouse diagonally will change the phase of both axes simultaneously.

The first order phasing is carried out identically to the zero order phasing; however, the right mouse button is held down instead of the left mouse button. Holding down **Ctrl** or **Cmd** while phasing gives the user finer control over the phase changes.

Once the phasing has been completed successfully, the user can exit the Phase mode by clicking the 'Finish' button on the 'Phase Mode' dialog.

**Manual Peak Picking (K):** In the Manual Peak Picking mode, the user can manually place a label to mark a peak. This is done by moving the mouse to the desired position and left clicking, see Figure 16. By default, the cursor will attempt to "snap" to potential peaks, but if the **Ctrl** or **Cmd** button is held down, the user can place the peak flag freely.

For 2D, in a similar manner, peaks can be selected anywhere if no key pressed, but in the vicinity of a peak the cursor will snap to it. Press 'Ctrl' for a free selection of peaks

(ignoring gridlines); with the 'Shift' pressed, the cursor will snap to the nearest gridline. In HSQC, the cursor snaps to intersections or horizontal gridlines; in HMBC it snaps to intersections or horizontal or vertical gridlines.

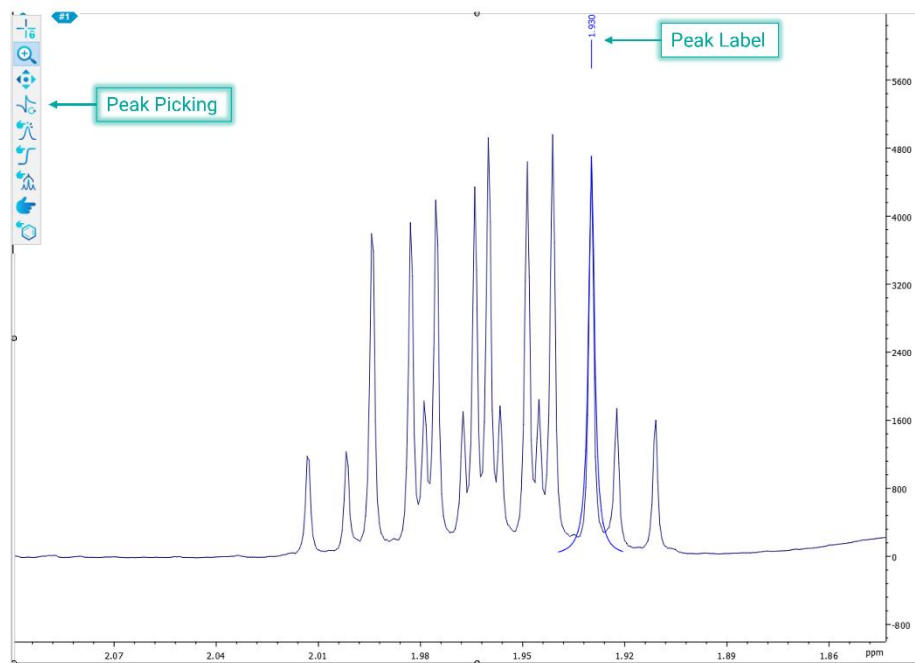


Figure 16: Peak Picking Mode

The **'Text Label'** option in the **'Peak Properties'** dialog allows for editing a peak label: right-click on the label and choose the **'Peak Properties'** option in the context menu to get the dialog.

A **table of peaks** can be created by right clicking on the spectrum and selecting the **'Create -> Peak Table'** option from the menu. Tables will be discussed in more detail in the **'Tables'** section. The data can also be represented as a chart by clicking on a table and selecting the **'Create chart'** option from the menu. Charts will be discussed in more detail in the **'Charts'** section. A peak can be deleted by using the Selection mode to select the peak, then pressing the **Delete** key. The selection tool is discussed below.

**Manual Integration (I):** In the Manual Integration mode, the user can integrate a region of the spectrum to calculate the peak area summing point by point. This is achieved by selecting the Integration mode, then holding the left mouse button and dragging the cursor horizontally to define the integration region. On releasing the left mouse button, the integration is performed, see Figure 17. The range of the integral is shown as the **integral bar** below the base line, and the cumulative sum is shown as the **integral curve**. The most recent integral is shown as selected with its control points available to drag the range. Similarly, if the user hovers the mouse over the integral label, the integral becomes highlighted, and if user use left click at this point, then that makes this integral to be the editable one, i.e. selected and its control points shown on the plot. The implementation considers all types of plots.

Clicking on an integral bar reveals a blue icon with 2 integral curves on its left side; click and drag the icon to the desired position to **split the integral** (Figure 17)

Double clicking on the integral bar opens the 'Integral Properties' dialog. This provides a set of options that allow the user to change the integral properties, from the appearance of the lines and labels to the actual range of the integral and the normalization of the peak area. If there are multiple integrals defined across the spectrum, the arrows at the top of the dialog box can be used to navigate between them. The normalized values are relative to all integrals on the spectrum and changing one value will change the corresponding value(s) for all other integrals.

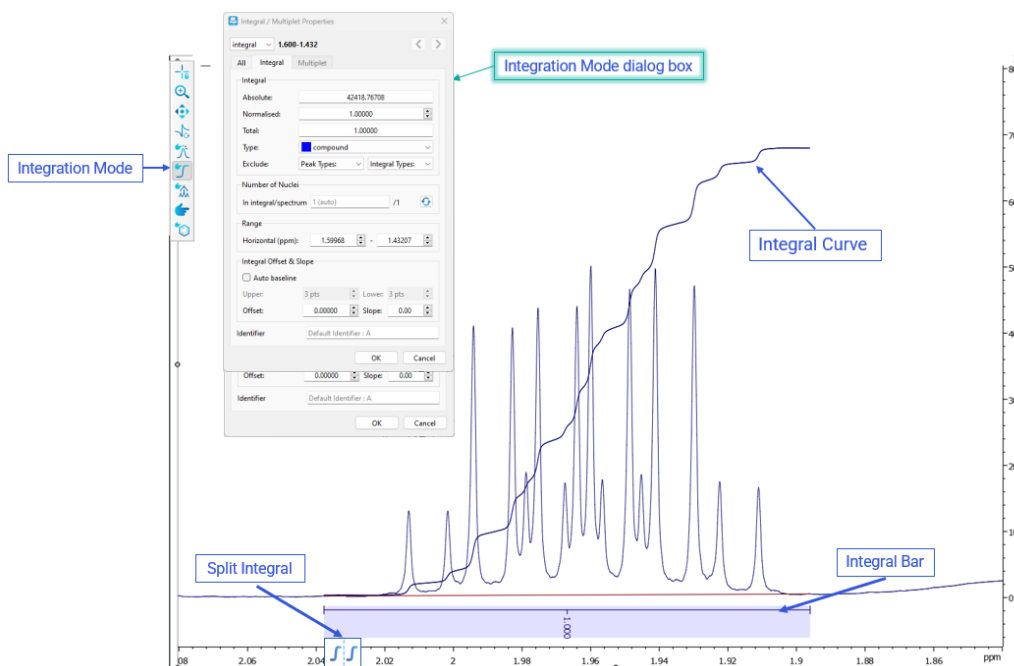


Figure 17: Manual Integration Mode

**Manual Multiplet Analysis (M):** When the Multiplet mode is selected, the user can perform first order multiplet analysis on a manually selected region of the spectrum, see Figure 18.

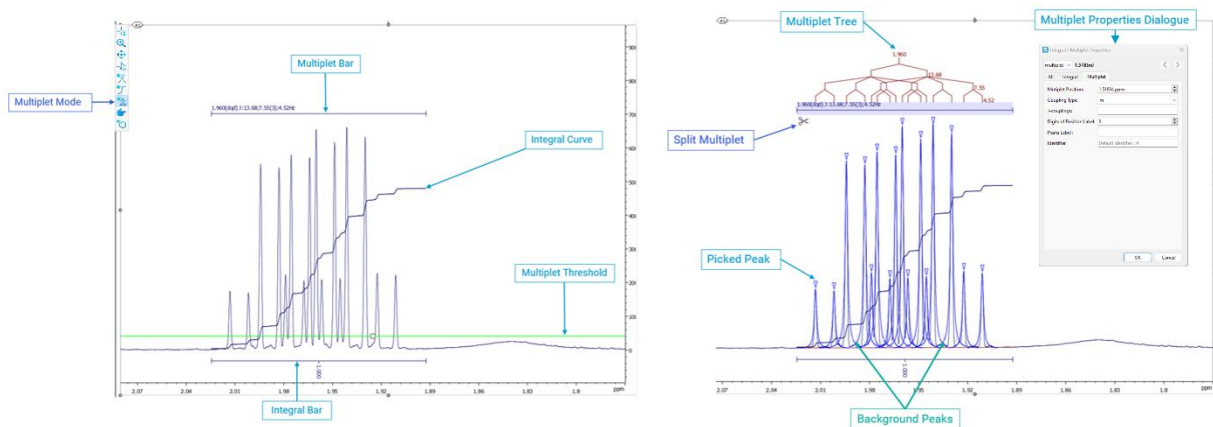


Figure 18: Manual Multiplet Analysis Mode

The region is selected in the same way that an integral region is selected, by holding down the left key and dragging. When the Multiplet mode is first selected, a **threshold line** appears. Peaks above the threshold will be used in multiplet analysis, while peaks below it will be ignored. If there are peaks that have already been picked in the region, then these will be used in the multiplet analysis. If no peaks have been picked, then JASON will perform an automatic peak picking before the multiplet analysis. Information about the multiplet is reported on the multiplet bar, above the peaks. Additionally, the integral of the region is also reported, and the **integral bar** and **integral curve** are shown. When the multiplet bar is highlighted, peaks belonging to the multiplet are marked with a blue triangle label. If the multiplet is resolved, the **J-coupling tree diagram** is also presented. As with the Integral mode, double clicking on the multiplet bar brings up the 'Multiplet Properties' dialog box.

**Item Selection (S):** The Selection mode is a general-purpose mode and is used to select individual items on a Canvas object. This might be anything from a single peak label to an entire multiplet. This tool can also be used to select annotations.

**Assignment Tool (A):** The Assignment tool is used in conjunction with a molecular structure to select a multiplet or peak on a spectrum and assign it to an atom in the structure. This is done by left clicking on the label of a peak or multiplet and dragging it to the atom on the molecular structure (see Section 9). The atom will then be assigned the central chemical shift of the multiplet or the position of an individual peak.

### 3.2 Context Sensitive Panels

- Click here for an [Introduction to the Panels](#).

There are six principal panels for an NMR spectrum. The File Browser was described in an earlier section; the other panels are described below.

When data is loaded into JASON, the user will notice that some additional panels become visible. The particular panels that become available are dependent on the current active object. The visibility of each panel can be toggled on and off using the Context Tools toggle menu described in an earlier section. The panels available for an NMR spectrum are shown in Figure 19. It is important to note that the arrangement of the panels is flexible, and they can be rearranged according to the user's preference simply by dragging a panel by its name bar to a preferred location. The panels can be stacked on top of each other as in Figure 19, or stacked vertically as in Figure 20.

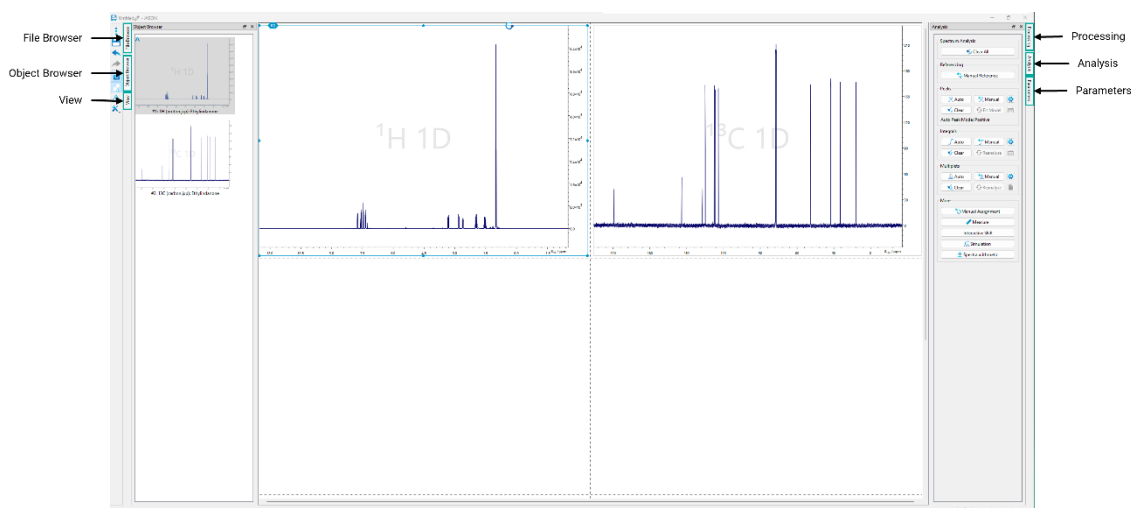


Figure 19: Data Context Tools panels for NMR spectra

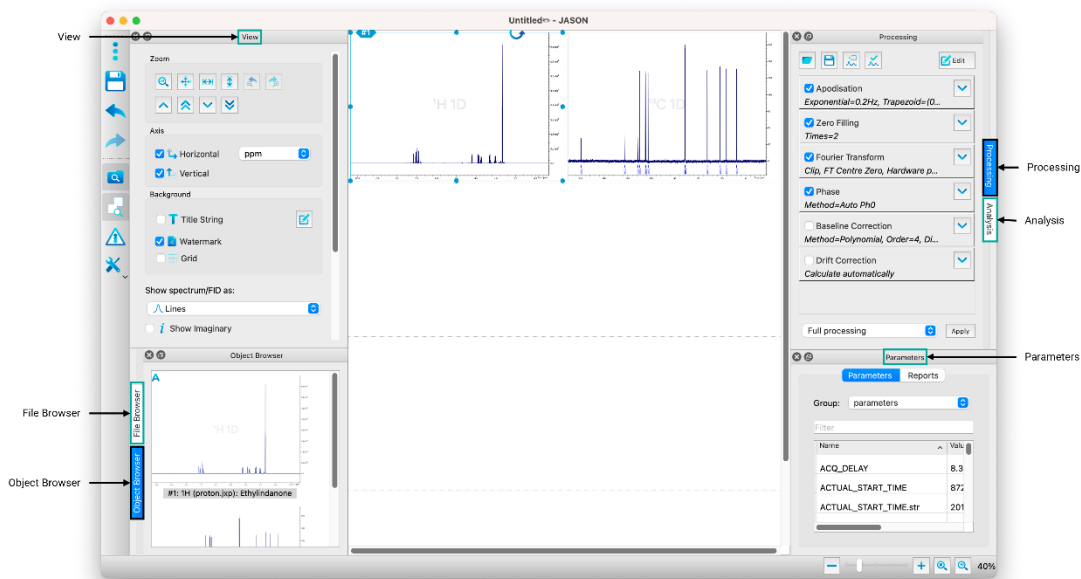


Figure 20: Alternate Configuration of Panels

### 3.3 The Object Browser

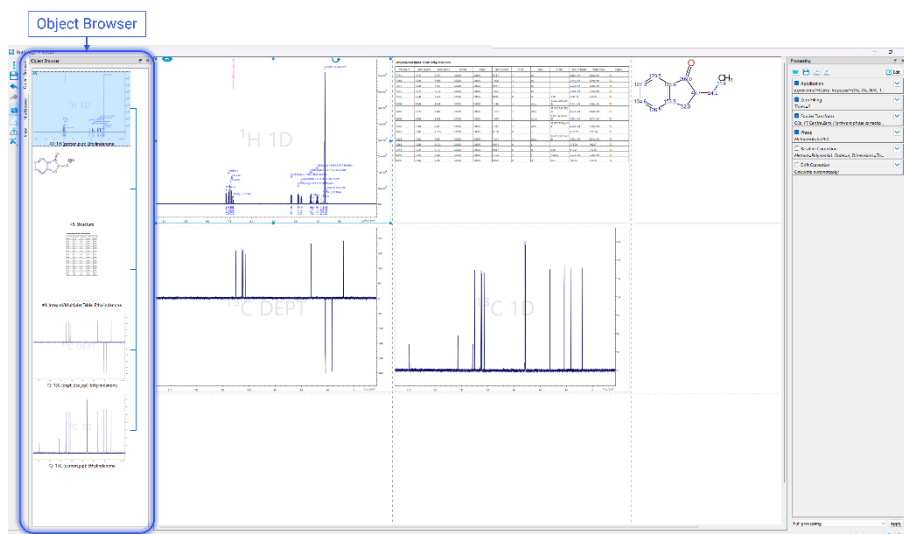


Figure 21: The Object Browser

The Object Browser is a visual list of all objects on the Canvas, see Figure 21. A single left click on an item in the Object Browser makes that item the active selection. The active selection can be identified in the Object Browser because it is shaded gray, and on the Canvas because the rescaling drag points around the object on the Canvas are filled. In Figure 21, the proton spectrum in the top left is the current active selection. Double left clicking on an object makes that object the active selection and zooms the canvas onto the object.

A single right click on an item in the Object Browser brings up two options; the first, Delete, allows the user to delete an object from the Canvas (and the Object Browser). It is worth noting that this can also be done by selecting an item and hitting the **Delete** key. The second option, Links, opens the 'Object Linking' dialog, see Figure 22. This dialog comprises two panels, the left-hand panel shows the current active selection, and the right-hand panel shows the possible targets to link to the active selections. The items in the 'Link Target' panel can be selected by checking the tick boxes next to their name. When the user presses 'Ok', a link is created between the items; and, where appropriate, the axes of the linked spectra and the zoom levels are synchronized.

If a Peak, Integral or Multiplet table is created, a link from the corresponding spectrum to the table will be created automatically.

The links between objects are shown as the blue connecting line to the right of the 'Object Browser' display area.

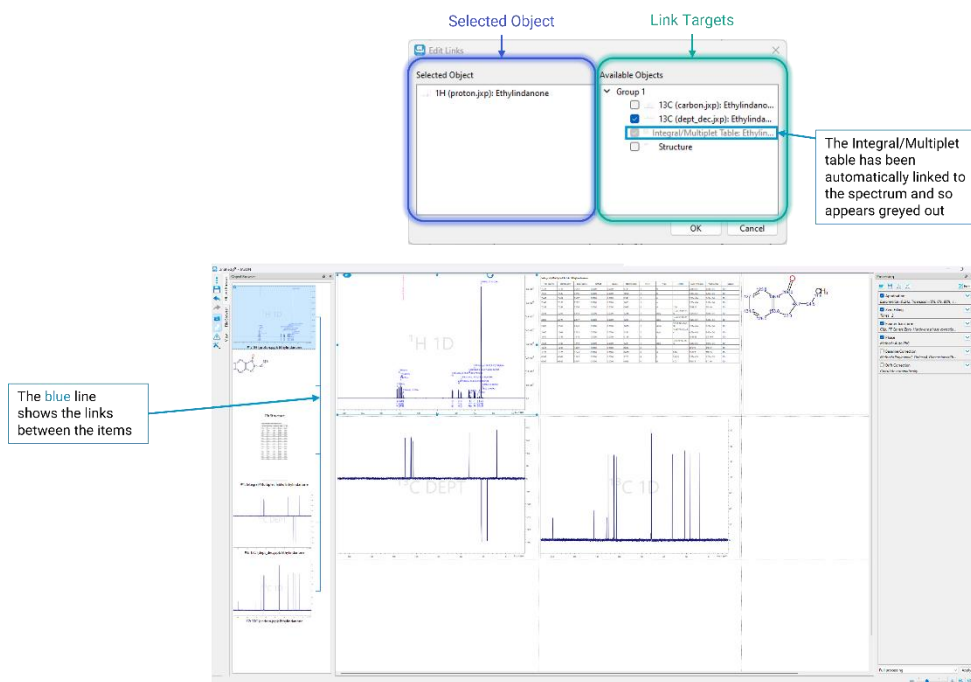


Figure 22: The object linking dialog

### 3.4 The View Panel

The 'View' panel contains the options for how an object is displayed on the Canvas. It is context sensitive and, in this section, the 'View' panel for a spectrum is described.

The view options for a 1D spectrum are shown in Figure 23.

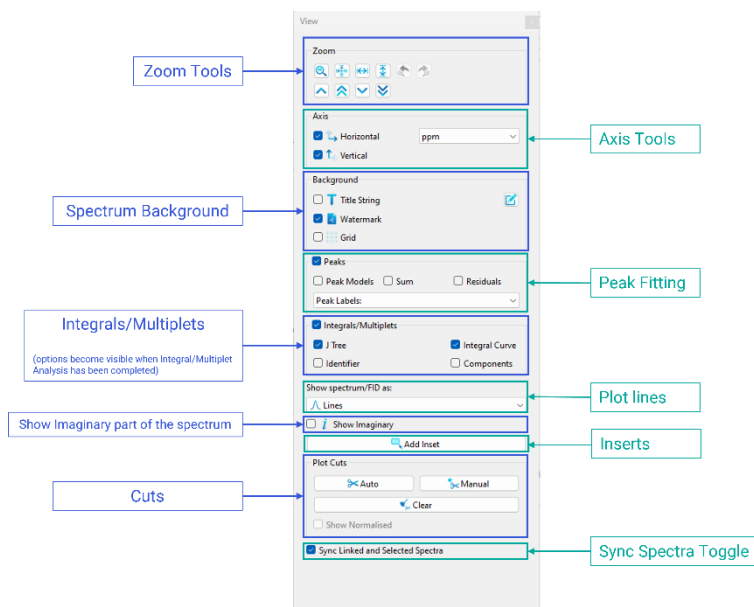


Figure 23: The 'View' panel

**Zoom Tools:** The zoom tools are a set of manual zooming controls that provide the user with more precise control of their zoom level in situations where the mouse zoom control does not provide sufficient sensitivity. This includes 'Previous' and 'Next' zoom buttons to undo or redo zoom steps. For 2D data, the manual zoom tool enables the user to set the Horizontal and Vertical zoom and enter level settings including 'Floor' and 'Ceiling'. The 'Reset Zoom' button resets the zoom to the default zoom level settings.

**Axis Tools:** The axes tools allow the user to toggle the visibility of the axes and to change the units the axes display and their direction ('Show Opposite').

**Peak Fitting Display:** Peak picking is a two-stage process; the first stage involves identifying potential peaks and the second stage involves fitting the parameters of those peaks to the data. The 'Peak Fitting' display option allows the user to toggle the visibility of the individual model peaks, the full model spectrum (sum) and the difference between the experimental data and the model (residuals).

**Multiplet Analysis Display:** Once a multiplet analysis has been carried out, the 'Multiplet' section of the 'View' panel allows the user to toggle the visibility of the J-coupling tree and the multiplet and integral labels.

**Plot Style:** The 'Plot Style' options allow the user to change the type of plot used to plot the experimental spectrum. The options are: 1) line where the spectrum is simply drawn as a continuous line joining the data point; 2) stick, where each point is drawn as a vertical line positioned at the frequency of the data point, running from the x axis to the amplitude of the data point; 3) lines and points, the data is shown as a continuous line as in option 1 but the data points are also shown if the zoom level is high enough.

**Add Insert:** The 'Add Insert' button allows the user to select a region of the spectrum and have it displayed as an insert on top of the parent spectrum. To use this functionality, the user presses the 'Add Insert' button and then the left mouse button drags on the main spectrum to select the region for the insert. The insert and parent spectra are linked but are independent with respect to zooming and panning.

**Plot Cuts (T):**

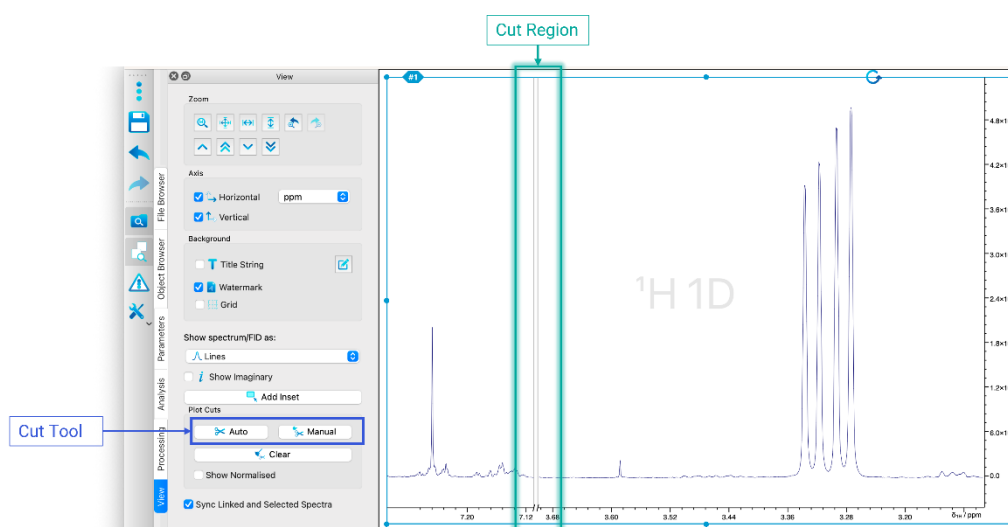


Figure 24: Cut region in a 1D spectrum

Selecting the Manual Cut tool mode allows a user to cut out a region of spectrum. In a 1D spectrum this is done by holding down the left mouse button and dragging horizontally to select the region to be cut out. The selected region is removed on release of the left mouse button. A cut region is shown as a discontinuity in the baseline of the spectrum and in the axis, as shown in Figure 24. For a 2D data set, the cut region is selected by holding down the left mouse button and dragging first in one dimension and then in the other dimension to select a rectangular cut region. The cut region is shown as discontinuities in the axes, see Figure 25.

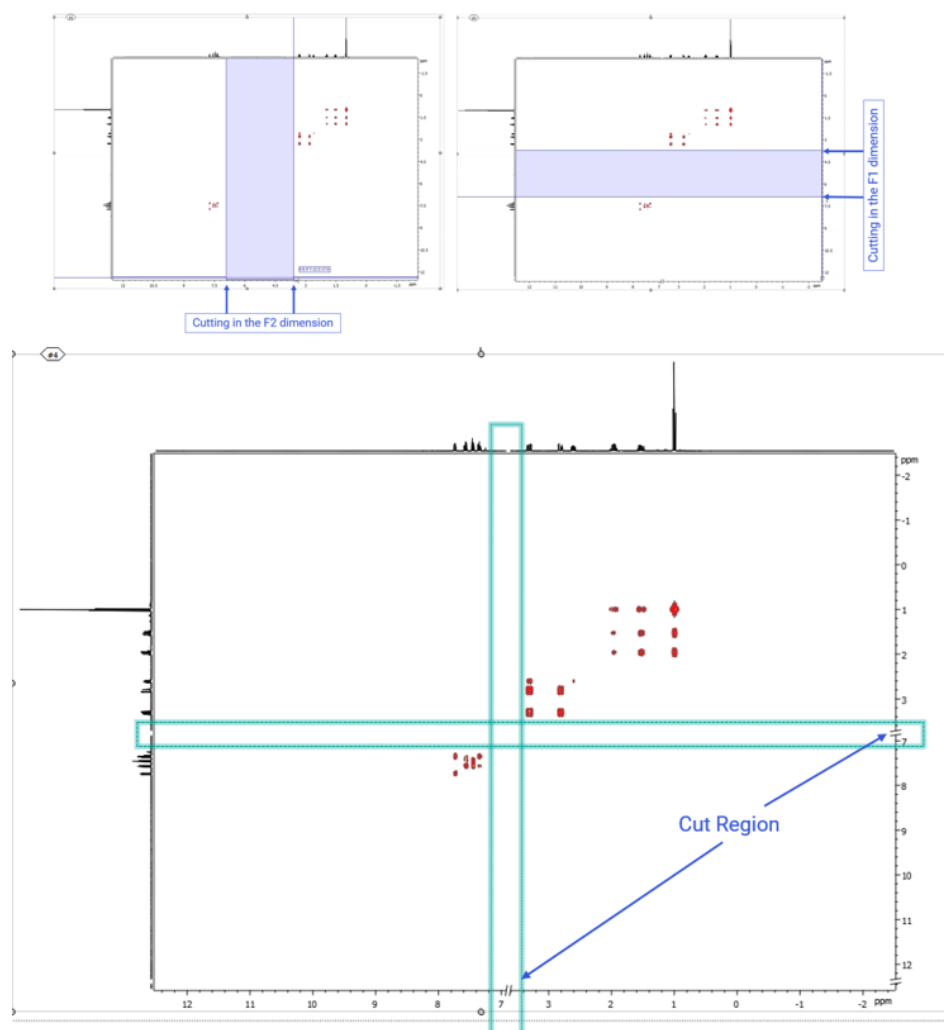


Figure 25: Cut regions in a 2D spectrum

It is worth noting that if a 1D spectrum is used as the projection, as in Figure 25, then the cut region in the appropriate dimension will be shown as a discontinuity in the base line of the spectrum.

The 'Auto cuts' button sets the plot cuts automatically. It is based on automatic recognition of the peak regions and cuts out the unnecessary plot regions, where no relevant peaks were found.

To clear a cut region, select the 'Clear' option in the 'Plot Cuts' section of the 'View' panel.

**Sync Spectra Toggle:** The 'Sync Spectra' toggle checkbox determines whether linked spectra on the Canvas should have their axes synchronized with respect to zooming and panning.

The view options for a 2D spectrum are shown in Figure 26. In addition to the options described for a 1D spectrum, a 2D spectrum has the following additional options.

**Show Normalized:** For **1D** spectra only, the 'Show Normalized' checkbox is displayed. When this box is checked, each visible section is normalized. The normalization coefficients are shown in the plot. 'Show Normalized' option works on both the main spectrum and on insets to the spectrum.

**2D View Options:** Within the 2D options the user can choose how the data should be plotted. For **2D** and **pseudo-2D** spectra, there are four view modes available: Contour plot, Raster plot, Overlay plot, and Stacked plot. The 'Positive/Negative' option allows the user to plot only positive or negative values or both.

2D NMR data is plotted with direct and indirect dimension data along horizontal and vertical axis. Users can swap it to plot for example the  $^{13}\text{C}$  axis horizontally and  $^1\text{H}$  axis vertically for an HMBC spectrum using the '**Transpose**' function found among processing items (please refer to 3.5 'The Processing Panel' section, 'Adding More Processing Steps' paragraph). For transposing nD processing, the user can select two dimensions out of the existing dimensions, and they will be transposed.

The axes control has an additional option in the form of a drop-down box. This option determines what is plotted at the edge of the 2D spectrum, referred to as the 'sideview' in JASON. The options are: 1) Sum, which is just the sum of all points across a row or column, depending on the axis; 2) Skyline, which is the maximum value across each row or column; 3) Spectrum, the user can select a 1D spectrum from the Canvas; 4) Trace, the user is able to plot a specific trace from the 2D spectrum using the cross hair cursor. More than one trace can be plotted on an axis projection.

**Sideviews** can be scaled using the mouse scroll wheel and moved up or down by holding down the **Shift** key whilst using the scroll wheel.

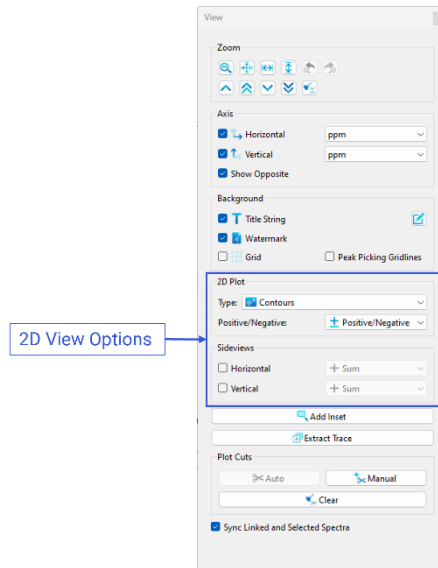


Figure 26: 2D Options in the 'View' panel

### 3.5 The Processing Panel

The 'Processing' panel contains all the steps in the processing chain used to convert the raw data into an NMR spectrum.

Figure 27 shows a typical processing list for a 1D NMR spectrum. In this section, it is assumed that the user is familiar with routine NMR processing.

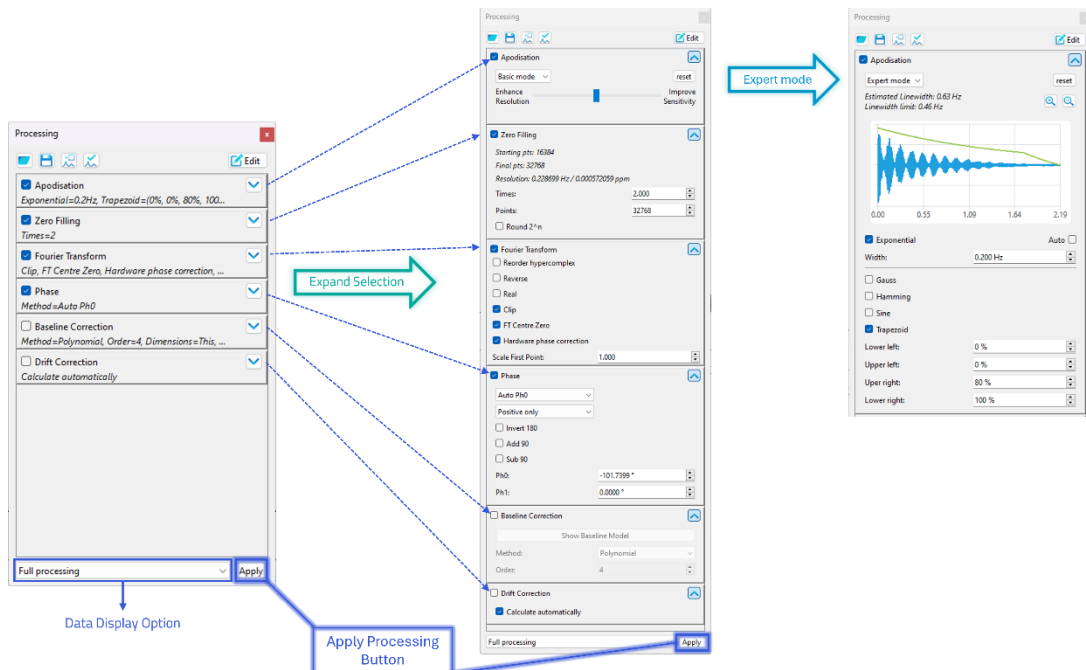


Figure 27: The Processing Panel

Any change that is made to the processing list has to be applied; this is done by pressing the 'Apply' button at the bottom of the processing list. All entries in the processing list have a checkbox to the left of the name and an 'Open/Close' toggle arrow to the right. The checkbox allows the user to turn on or off that processing step. To turn a step off, the user unticks the checkbox and then presses the 'Apply' button. By toggling the button to the right of the name, the user can see and modify parameters and options related to the processing step. A number of the processing steps have extended modes of use, a basic mode and an expert mode which are discussed below Extended Processing Options.

At the top of the 'Processing' panel, JASON reports the **experiment type** if it is determined by the experiment recognition system. To the left of it, there are buttons allowing the customer to **Load and Save processing lists**. The current processing list can be saved in the .jpp (JASON processing list) or the .cjp (compact format) and can be applied later using either the 'Open and apply processing list' button or by dragging and dropping in the file. The 'Edit Processing List' button opens up a dialog which is described in detail in the 'Adding More Processing Steps' section.

**Apodization** section displays the options and parameters for signal apodization; both 'Basic' and 'Expert' modes are available. In addition to the available apodization functions, 'Enhance Resolution' and 'Improve Selectivity', 'Open Interactive' button switches to the Interactive mode in which the FID and the apodization envelope are displayed.

**Zero Fill** section contains the options available for zero-filling. The zero fill can be defined as a multiplier, for values less than 10 or as a number of points in the final zero-filled data set.

**Fourier Transform** section displays all the options for the Fourier transform. There are a number of options available, a number of which are only applicable to the indirect dimension of a 2D spectrum. The 'Round' option allows for not adding zero to odd sized datasets.

**Phase** section shows the options for phasing. The 'Interactive' button is equivalent to the Phasing mode on the Context Tool bar. In addition to the interactive mode, there are:

- 1) Auto: in this mode the applied phase correction is determined automatically
- 2) Custom: in this mode the phase can be changed manually by typing values into the dialog boxes below.
- 3) Absolute: the spectrum is displayed in magnitude mode.
- 4) Auto Ph0: the zero order phase is corrected automatically, with the first order correction set to zero.

The Ph0 and Ph1 fields display the current zero and first order phase correction, and in Custom mode they can be used to manually set the phase of the spectrum.

The 'Invert 180' tick box will apply a zero order phase correction of 180 degrees to the current phase. For a phased spectrum this will essentially invert all the peaks.

**Normalize Intensity** section contains the controls for normalizing the spectra intensity:

- 1) 'Scale to' - scale highest intensity to specified value;
- 2) 'Add': a constant value added to all points after the multiplication;
- 3) 'Position': for maximum search as % of spectrum, where left edge is 0% and right edge is 100%; by default, it is middle of spectrum.

- 4) 'Range' – find maximum intensity in range specified (and at defined position) to normalize the spectral intensity.

The last two arguments by default means searching whole data for maximum, and it can be used to setup for a region around a peak which will be scaled.

**Baseline Correction** section has the following options: Polynomial, Cubic Spline, Linear Spline, Whittaker, Bernstein, Akima Spline; parameters of each of the options can be changed in the same section. 'Show Baseline Model' button allows the user to preview the result and opens access to interactive tools to manipulate manual baseline points. Hover the mouse cursor over the interactive buttons and controls to see tool tips for the short description of their functionality.

**Data Display Options** allow the user to view the data at different points along the processing chain; the options are:

- 1) Show raw data, which displays the original time domain data, if available
- 2) F2 time domain processing, which displays the time domain signal after the processing steps which apply only to time domain data have been applied, but prior to the Fourier transform
- 3) F2 after FT, which displays the frequency domain data immediately after the Fourier Transform
- 4) Full Processing (default option), which displays the data after the application of the full processing chain.

**Adding More Processing Steps:** When a new data set is opened, JASON will attempt to read and interpret any processing list that has been saved with the data and apply it automatically. There may be other processing steps that the user wishes to apply, and these can be added using the 'Edit processing' button at the top right-hand corner of the 'Processing' panel, see Figure 28. The 'Edit processing' dialog has a list of available processing functions in the left-hand panel. The right-hand panel has the list of processing steps in the current processing list. A new step is added to the list by simply dragging it from the left-hand panel and dropping it in the right-hand panel. In default mode, JASON will automatically place the processing step at the most appropriate position in the list. An item can be removed from the processing list by simply selecting it in the right-hand list and pressing the 'Delete' key. Once the selections have been made, the processing list is updated when the 'OK' button is pressed.

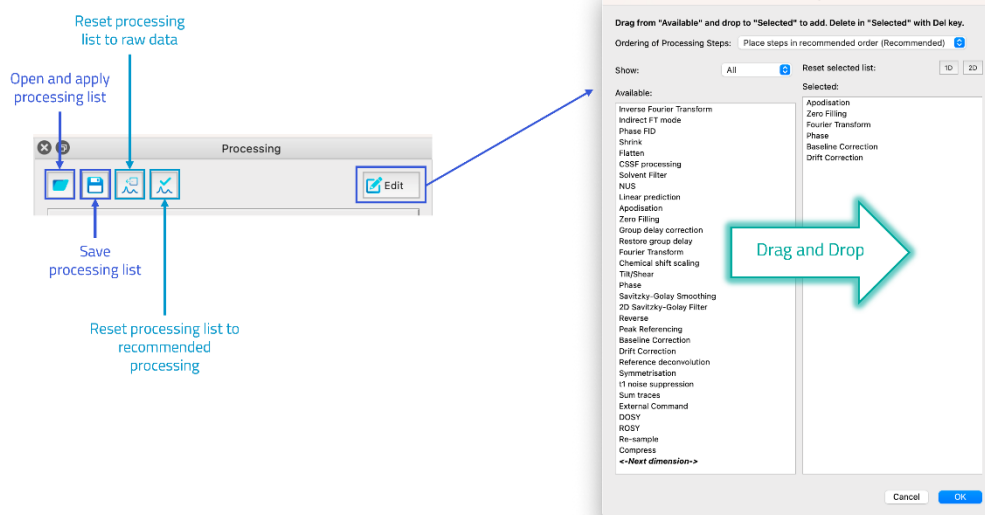


Figure 28: Processing List options

Settings of **Ordering of processing steps**: In default mode, JASON will arrange the processing steps in the most appropriate order automatically. To change the order of the processing steps, the user can select 'Settings' button in the top right-hand corner of the 'Edit processing' dialog, see Figure 28. This brings up a drop-down list of modes. The first is the default mode, the second and third modes allow the user to place a processing step where they like. The second mode will give a warning if JASON thinks the placement is inappropriate (i.e., placing zero-filling or apodization after the Fourier Transform). The third mode, expert mode, provides no warnings.

**Save and Load Template**: as a reminder, the processing list can be saved to a template file, or an existing template can be loaded using the two buttons on the top left-hand side of the 'Processing' panel.

### 3.6 The Analysis Panel

The 'Analysis' panel contains a list of analysis tools that might be used to examine an NMR spectrum. The list of functionality shown in Figure 29 is typical for a 1D NMR spectrum.

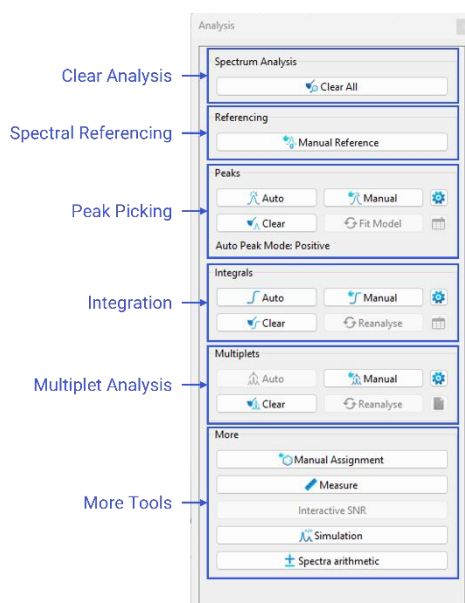


Figure 29: The 'Analysis' Panel

**Clear Analysis** button clears all levels of analysis.

**Referencing (R):** The Referencing mode allows a user to select a peak or a position on a spectrum and set the chemical shift to a value of choice. To make a selection, the user moves the cursor using the mouse to the desired position, then left clicks to open the 'Referencing' dialog. It is worth noting that in default mode the cursor will snap to the nearest peak. In order to have a free selection, the **Ctrl** or **Cmd** key should be held down.

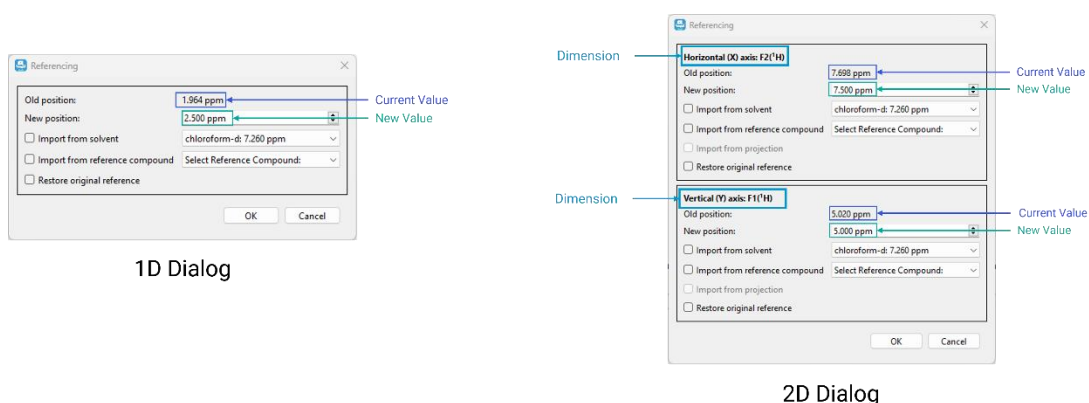


Figure 30: 'Referencing' Dialog

The 'Referencing' dialog is shown in Figure 30, with the current chemical shift value of the dimensions shown as part of the description and the new value as a text box. In the case of two-dimensional spectra, the dialog box contains a line for each dimension of the

spectrum. Once the user enters the new value and clicks 'OK', the spectrum will be reset using the new reference position(s).

**Peak Picking:** There are two modes for peak picking, automatic and manual. The Manual Peak Picking mode is identical to the Peak Picking mode in the Context Tool bar.

**Target button** allows the user to define whether the pick peaking algorithm should identify positive peaks only, negative peaks only, or both positive and negative peaks.

**Automatic Peak Picking** mode asks the user to set a threshold for the amplitude of peaks of interest, then automatically picks all peaks across the spectrum and fits the subsequent model to the data. The threshold itself does not change the peaks that are picked but simply labels the peaks as contaminants if the peak amplitude is below the threshold, or compound if the peak amplitude is above the threshold. Additional options for auto peak picking are described in more detail in the 'Peaks' paragraph of the 'The NMR Settings' section.

The '**Fit model**' button allows the user to apply fitting on the existing peaks. It is a convenient tool to get fitted peak models after deleting/adding peaks, changing parameters in the peak table, etc. It is equivalent to forcing more fitting iterations of the current model.

Manipulation of the individual peaks after peak picking is identical to the description in the 'Peak Picking' section of the Context Tool bar.

The 'Clear' button will clear all picked peaks.

The 'Settings' button to the right of this section opens the 'Peak' tab of the 'NMR settings', which is described in The NMR Settings section.

**Integration:** There are two integration modes; the Manual mode is identical to the Integration mode in the Context Tool bar. The Automatic mode will attempt to separate the spectrum into regions containing groups of peaks likely to belong to a single multiplet. The Integration mode is available for 1D, 2D and pseudo-2D spectra.

Manipulation of the integral regions and labels is identical to the description of the Integration mode in the Context Tool bar section.

The integral baseline can be adjusted using the control points highlighted in [x] below. Hovering the mouse over either control point displays a tooltip explaining what the control point does.

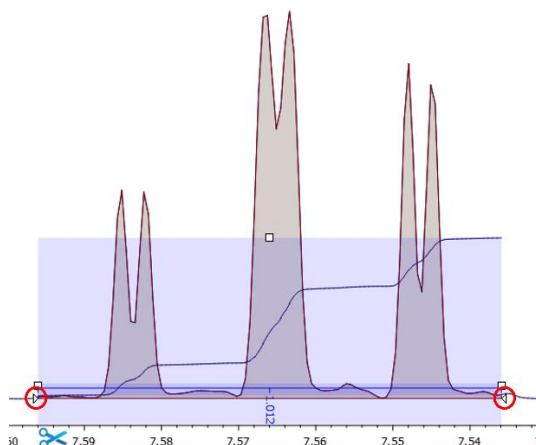


Figure 31: Integral baseline control points

The 'Clear' button will clear all integrals across the spectrum.

**Multiplet Analysis:** There are two modes for multiplet analysis. The manual mode is identical to the Multiplet mode described in the Context Tool bar section. Automatic mode will perform peak picking and cluster peaks into groups or regions that are likely to belong to a single multiplet as carried out in the peak picking and integration analysis steps. If peak picking was performed beforehand, it will use these results to perform multiplet analysis on the regions and the peaks within each region. The multiplet analysis mode is available for 1D and 2D spectra.

The individual multiplets can be manipulated with the range being extended, peaks being added or removed from the multiplet. Once the user is happy with the changes, the 'Reanalyze' button can be pressed to redo the multiplet analysis. The 'Clear' button clears all multiplets.

**More Tools:** Additional analysis tools

**Manual Assignment (A):** The 'Assignment' tool is used in conjunction with a molecular structure to select a multiplet or peak on a spectrum and assign it to an atom in the structure. This is done by left clicking on the label of a peak or multiplet and dragging it to the atom on a molecular structure (see Section 9). The atom will then be assigned the central chemical shift of the multiplet or the position of an individual peak.

**Measure Tool (D):** The 'Measure' tool allows the user to make accurate measurements between two points on a spectrum and is discussed in detail below.

**Interactive SNR Tool** allows the user to select signal and noise regions and is also discussed in detail below.

The **Simulation** button opens the JEOL J-Coupling Simulation panel allowing a user to create a simulated spectrum.

The **Spectra Arithmetic** button opens the Arithmetic panel which allows a user to add or subtract spectra.

**Measure Tool (D):** The 'Measure' mode allows the user to make accurate measurements between two points on a spectrum. Selecting the 'Measure' mode opens a dialog which contains two tabs. One of them has the 'Measure' tool options. The 'Single' option allows the user to make a single measurement; in this mode if a new measurement is made then

the previous is deleted. The 'Multiple' mode maintains each measurement as the user creates them. To make a measurement, the user needs to select the first point on the spectrum by the mouse and drag to the end point holding down the left mouse button. If the 'Snap to Peaks' option is selected, the cursor will snap to the top of the nearest peak; otherwise, a free selection of the starting and end point can be made. Once the measurement is made, a label is created at the starting point of the measurement, with the starting coordinates, and a second label is created at the end of the measurement. The end point label contained the coordinates of the end point and the differences between the coordinates of the end point and start point, see Figure 32.

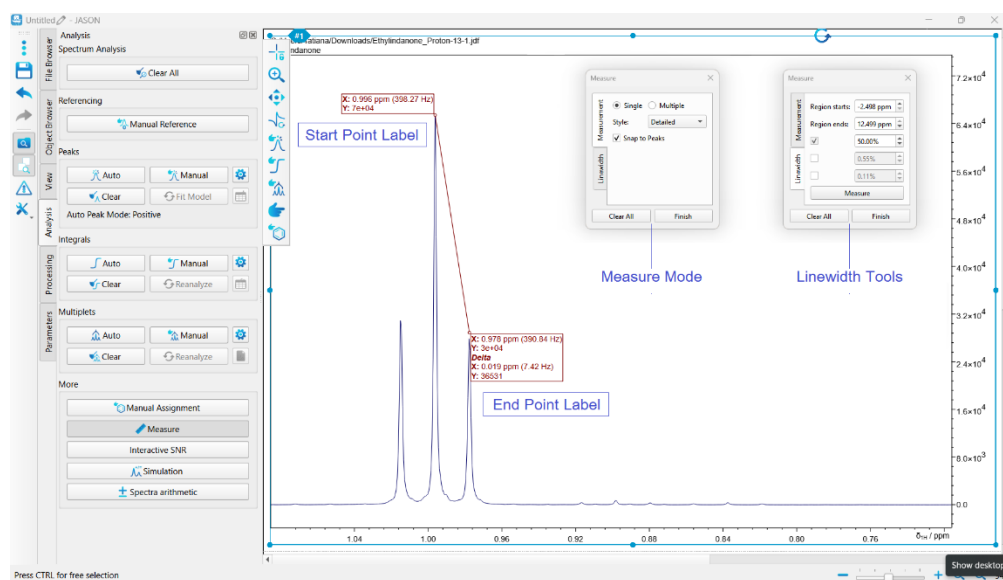


Figure 32: 'Measure' Mode and 'Linewidth' tools

The 'Clear All' button deletes all current measurements. A particular measurement can be deleted by a click on the red cross that appears if point the cursor at the measurement line.

Clicking on the 'Finish' button closes the 'Measure' dialog and exits the mode; the 'View' panel has a check box for measurements visibility outside the Measure mode.

**Linewidth tools** is the second tab of the 'Measure' dialog and is part of the "Measure" tools (in Figure 32, 'Measure' and 'Linewidth Tools' are shown next to each other for demonstration purposes only). On the NMR spectrum that should be measured, the peak range will be taken from the current zoom. The routine will search for the maximum intensity point within this range and then descend on both sides looking for intensities, at which the width should be measured. Between one and three measurements can be created at the same time. Toggle checkboxes for additional measurements and enter the intensity at the measured points (50%, 0.55% and 0.11% by default). Clicking "Measure" creates measurements on the plot; if any issues are detected, they will be reported in the 'Warning' pop-up. The measurements are standard JASON measurements in "Delta Hz" style. They can be reported in the Measurement table and so on. The 'Clear All' button deletes all present measurements; this action can be undone.

**Interactive SNR Tool** opens an 'Interactive SNR Calculator' dialog, in which signal and noise regions can be set by using the control points on the region indicators on the

spectrum (Figure 33: Interactive SNR Tool). Additional signal regions can be added using the '+' icon in the dialog. After a new signal region is added, it appears at the right edge of the spectrum and becomes editable by entering the digits in the 'From' and 'To' fields. Signal regions can be deleted using the 'Trash Bin' icon, The 'Delete' option will remove the currently edited signal region; this can't be used if only 1 region is left. The arrows let the user cycle through the multiple signal regions; the order of signal regions is not the one on the plot but the history of creating them. The visibility of the SNR labels is controlled in the 'View' panel by the 'Show SNR' checkbox.

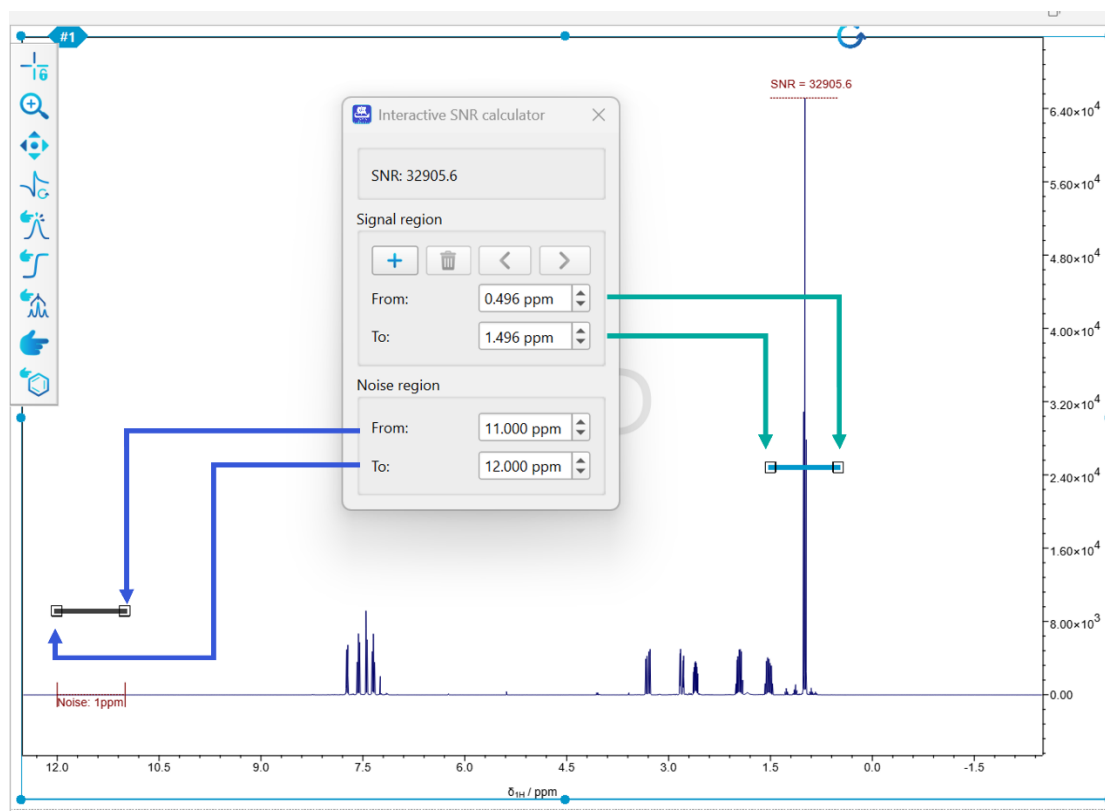


Figure 33: Interactive SNR Tool

### 3.7 The Parameters Panel

The 'Parameters' panel comprises two tabs; the 'Parameters' tab is a list of all parameters available for the selected data, and the 'Report' tab is a list of all parameters that will be displayed if a parameter table is created. Figure 34 shows the two tabs for the 'Parameters' panel of a typical 1D NMR spectrum.

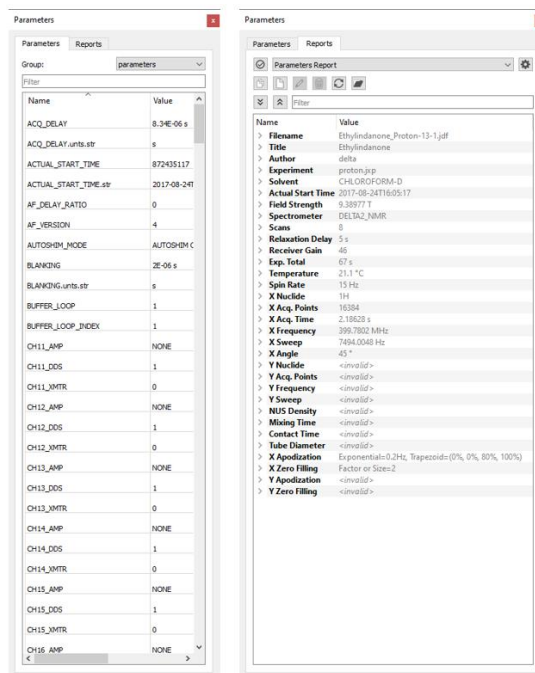


Figure 34: The 'Parameters' Panel

### 3.8 The Table Tools Panel

When a table is created and selected as the active item, the 'Table Tools' panel will appear. The 'Table Tools' panel allows users to customize how a table is displayed. Table settings can be restored to the factory default settings by clicking on the 'Restore Factory' button, or new settings saved as the default setting using the 'Set as Default' button.

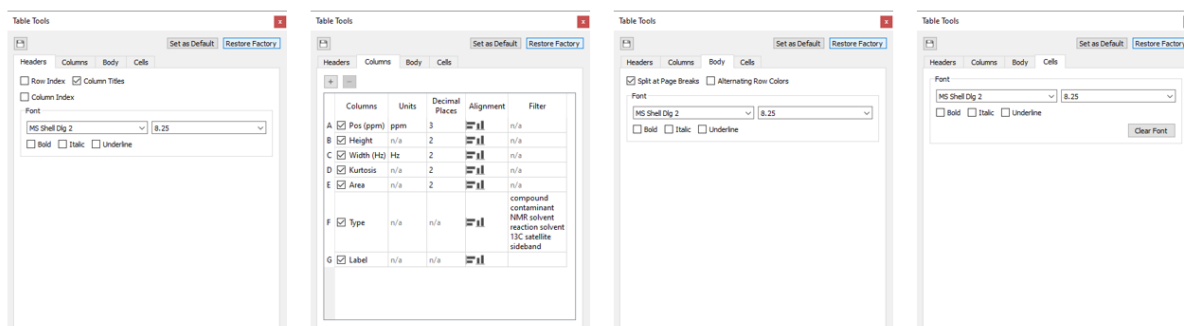


Figure 35: The 'Table Tools' Panel

The **Headers** tab contains the settings for the table header. The 'Row Index' and 'Column Index' checkboxes display the indexes of the rows and columns which can be especially useful when using equations in the custom columns in the table, Figure 35.

The **Columns** tab allows users to add or remove custom columns ('+', plus, or '-', minus, buttons), set units, adjust decimal places, customize font for the entire column, set the alignment of column entries and filter the values. Please note that the individual font cell settings have priority over the column settings. Adding custom columns is useful if more information should be added manually to the table. It is possible to add numbers, strings or Excel-like equations to the cells of custom columns.

The **Body** tab contains general settings for the font in the body of the table.

The **Cells** tab enables users to set font settings for a selected cell or cells.

### 3.9 The Chart Tools Panel

A chart can be created by selecting an item in a table and choosing the 'Create Chart' option from the menu available by a right click. Use the standard keyboard shortcuts: Ctrl + U (Cmd + U) to undo zoom, and Ctrl + I (Cmd + I) to redo zoom on charts.

When a chart is created and selected as the active item, the 'Chart Tools' panel will appear. The 'Chart Tools' panel allows users to customize how the chart is displayed.

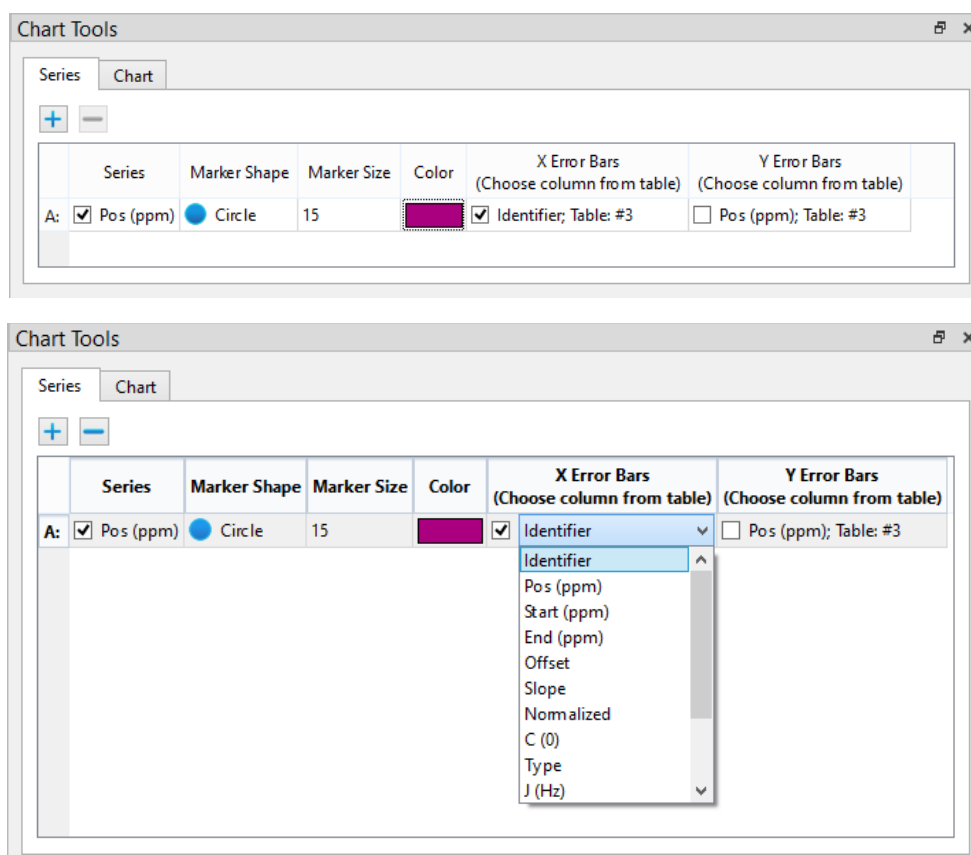


Figure 36: The 'Chart Tools' Panel, 'Series' tab

The **Series** tab contains the settings for the visual data representation across different series. The 'Series' checkbox allows the user to choose the data from what column of the table to display, and the 'Data unit marker' settings ('Marker Shape', 'Size', and 'Color') determine how this data will be presented on the chart visually, along with the data accuracy representation ('X' and 'Y Error Bars'), Figure 36.

The user can set the data accuracy visual representation (error bar) parameters by choosing which column from the table is to be used for drawing the error bars. This can be accomplished by selecting the column from the drop-down menu that shows up when editing the 'X Error Bars' or 'Y Error Bars' columns in the 'Chart Tools' panel under the 'Series' tab. When creating a series from a peaks table, the columns responsible for the drawing the error bars will be automatically selected as the corresponding error columns for both X and Y data points. All changes made to the error bar are supported by the Redo / Undo framework and can be saved.

**Note:** the error bars functionality is only available for data taken from the tables and not from 'Fit Data' (best fit line series).

The **Chart** tab allows users to adjust the parameters of the chart and contains settings regarding the Legend and Axes. It is worth mentioning that showing / hiding the axes as well as axis range modifications are supported by Undo / Redo; the corresponding buttons can be found in the 'Axes Ranges' section or the actions can be performed by the shortcut keys combinations: Ctrl + U (Cmd + U) for undoing, and Ctrl + I (Cmd + I) for redoing the changes.

The controls for setting the axis properties to default are found in the 'Axes Properties' section; these are integrated into the global JASON undo / redo stack, The horizontal and vertical axes properties on the chart tools panels GUI are dynamically updated in real-time to reflect any changes made.

Chart settings can be restored to the factory default settings by clicking on the 'Restore Factory' button; or new settings saved as the default setting using the 'Set as Default' button in the 'Chart' tab. The Cogwheel button opens up the 'Global Settings' dialog, Figure 37.

More settings to the chart display parameters may be found in the 'Chart' tab in the 'Global Settings' dialog, and like that for the 'Table' tab, those settings affect the default settings, but not the currently active chart.

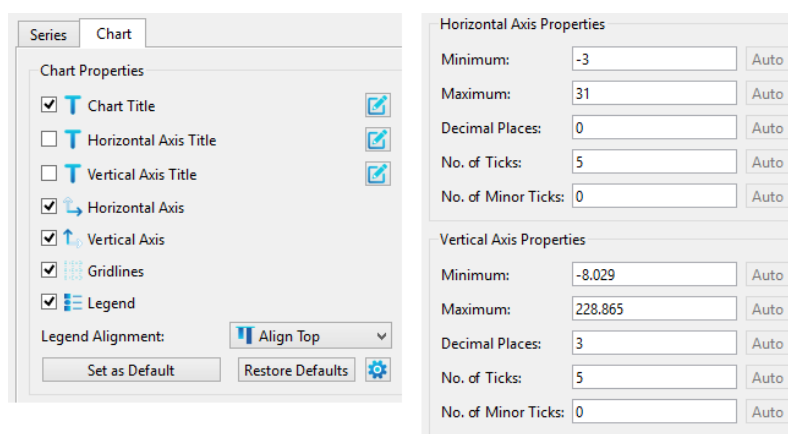


Figure 37: The 'Chart Tools' Panel, 'Chart' Tab

## 4 Reporting: Tables and Parameters

When a user has performed a peak picking, integration or created a series of multiplets it is often useful to display the data in the form of a table for reporting.

### 4.1 Tables

To **create a table** in JASON, the user right clicks on the object to bring up the right click context menu. At the bottom of the menu is the option 'Create' that contains a menu with 5 options; these options are only selectable if the corresponding analysis has been carried out.

Tables can be **copied and pasted** by selecting the table as the active item and then using 'Ctrl+C' or 'Cmd+C' to copy and 'Ctrl+V' or 'Cmd+V' to paste. If a row or cell is selected (this will be shown as highlighted blue), only these items will be copied. 'Ctrl+Click' in the column header to select the entire column. 'Cut' and 'Delete' operations are available via the context menu (available by a right-click) if the content of at least one of the selected cells is editable, with an exception to this logic for the 'Parameters' table, for which both 'Delete' and 'Cut' actions remain enabled regardless of whether the selected items are editable. The 'Cut' action is supported by the undo/redo functionality within JASON.

**Table titles** are set by default with a name which represents its origin, for example a Peak Table created from a spectrum which is item 3 on the canvas will have a title 'Peak Table from #3'. The table title is user editable by double clicking on the title as per spectrum titles. The table title editor dialog has tool buttons to insert placeholder text for table titles and parent tags in the format: <Table Title> from #X; see Figure 38.

Users can insert the following placeholders:

`${object_title}` – will be replaced with the table's title.

`${tag}` – will be replaced with the tag of the parent object the table was created from.

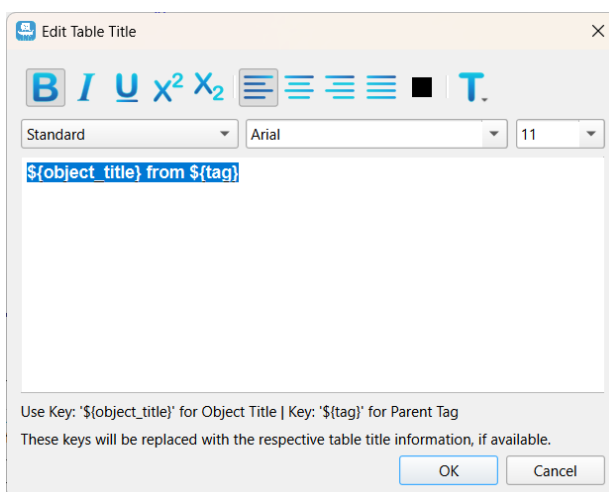


Figure 38: 'Edit Table Title' dialog

The **table border** and **grid** can be made visible or hidden using the checkbox on the 'Table Tools' panel. The default border and grid setting can be set from the 'Settings' menu.

Changing the **column width** manually is an action supported by Undo/Redo.

Right-clicking on a table brings in a context menu which also contains a lot of useful options. The **'Expand Vertically'** option found in the right-click context menu, will expand the table fully vertically, displaying all the rows.

#### 4.1.1 Parameters Report

The **Parameters Report** option from the 'Create' menu places a parameter table next to the spectrum, see Figure 39. The parameter table can be manipulated on the Canvas as any other object in JASON; the grab tag allows the user to drag and drop the table to the user's preferred location while the drag points allow the user to resize the table.

The contents of the parameter table are defined in the 'Parameters Report' tab. JASON shows the parameters in the Vendor sorted order; clicking on the name column header allows the parameters to be sorted alphabetically A to Z or Z to A. The order of the rows in the parameter table can be changed by left clicking on the row and dragging it up or down the table.

New items can also be dragged directly from the 'Parameters' tab in the 'Parameters' panel (see Figure 40) into the displayed table.

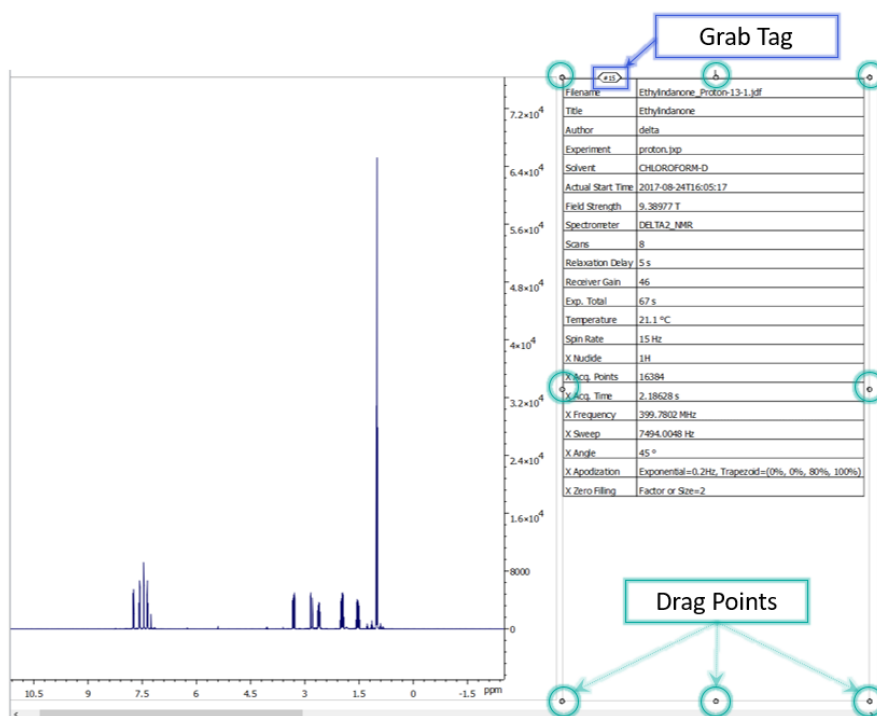


Figure 39: 'Parameter' Table

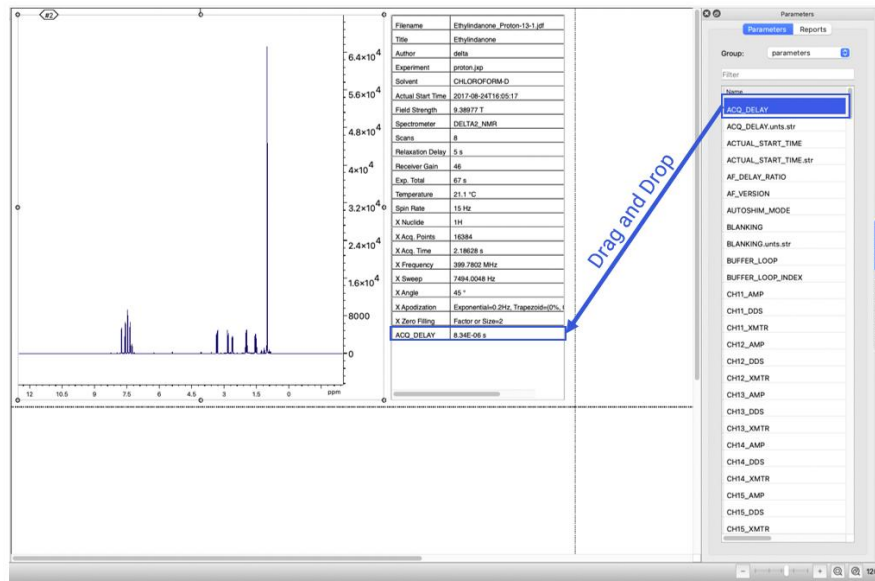


Figure 40 Adding Parameters to the 'Parameter' Table

#### 4.1.2 Processing Report

The **Processing Report** option from the 'Create' menu places a processing table next to the spectrum, see Figure 41 Processing Report. The contents of the processing table are defined by the processing steps applied to the spectrum. The processing table can be manipulated on the Canvas as any other object in JASON. The grab tag allows the user to drag and drop the table to the user's preferred location while the drag points allow the user to resize the table. The order of the rows in the processing table can be changed by left clicking on the row and dragging it up or down the table

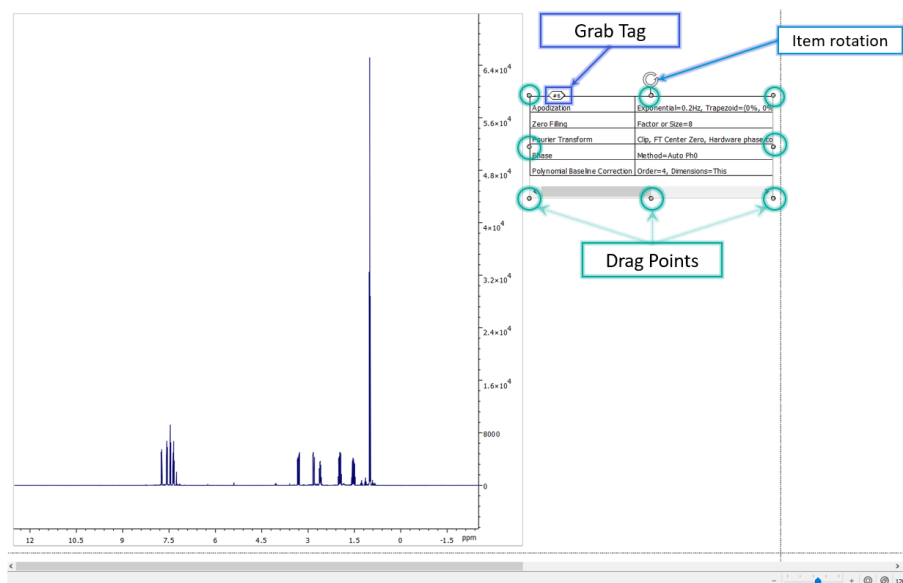


Figure 41 Processing Report

### 4.1.3 Peak Table

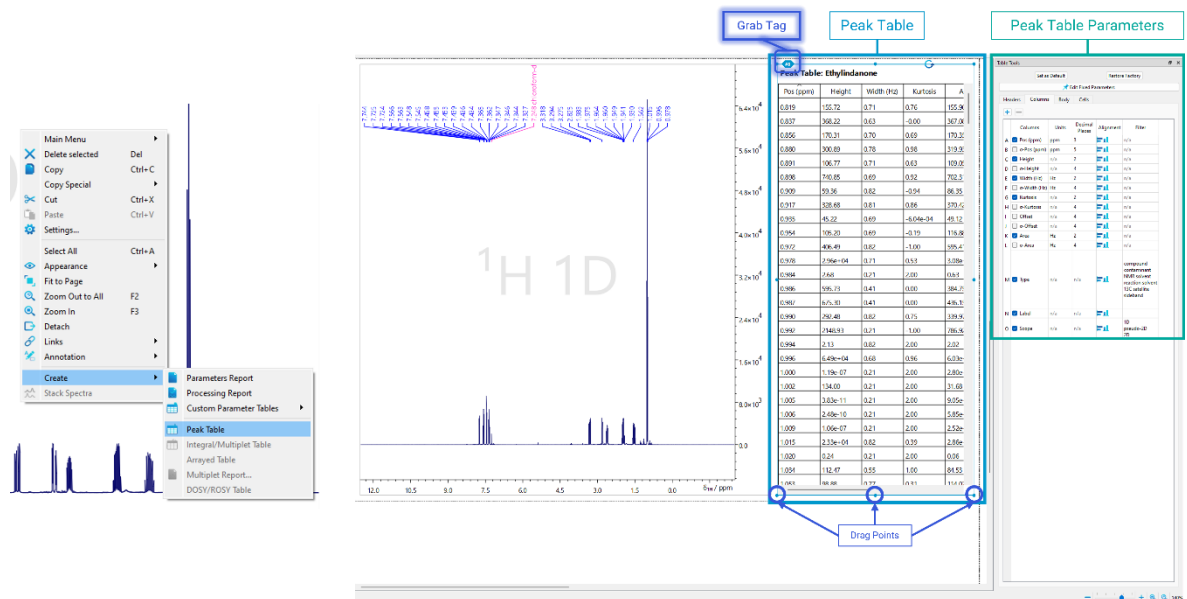


Figure 42: Peaks Table

Once a peak picking has been carried out, the 'Create' menu in the right mouse button context menu will have an option for **Peaks Table**, see Figure 42. Clicking on this option creates a table of peaks. The table can be manipulated using the grab tag to move the position of the table and drag points to resize the table. If the box containing the table is smaller than the size of the table, then the table will have scroll bars for both horizontal and vertical movement. In addition to the table, a 'Peak Table Parameters' panel is also created. The panel allows the user to choose which columns to display in the table. The font and size of the characters in the table can be changed as well as the number of decimal places to display for each value. The checkbox 'Splits at page breaks' will split the table if it is resized to cover multiple pages. The '**Expand Vertically**' option expands the table vertically downwards to show all the rows; it can be found in the context menu available by a right-click on the table body (cell).

The **order of the columns** in the table can be changed by dragging the first cell of a column to the preferred position.

### 4.1.4 Integrals/Multiplets Table

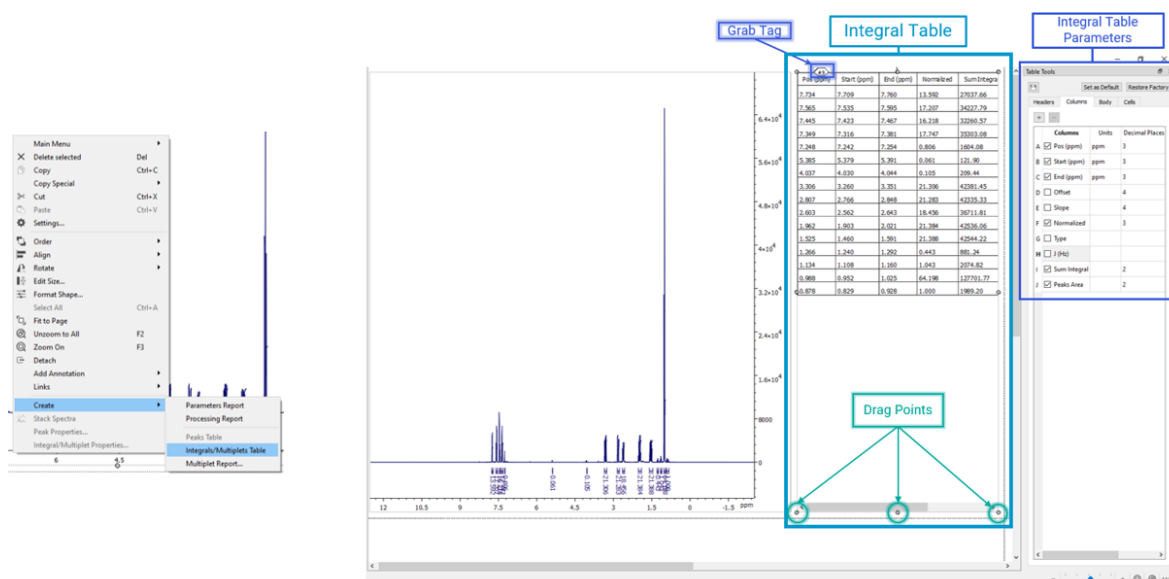


Figure 43: Integral Table

Once integrals have been created, the 'Create' menu in the right mouse button context menu will have an option for **Integrals/Multiplets table**, see Figure 43. Clicking on this option creates a table of integrals. The table can be manipulated using the grab tag to move the position of the table and drag points to resize the table. If the box containing the table is smaller than the size of the table, then the table will have scroll bars for both horizontal and vertical movement. In addition to the table, an 'Integral Table Parameters' panel is also created. The panel allows the user to choose which columns to display in the table. The font and size of the characters in the table can be changed as well as the number of decimal places of each value. The checkbox 'Splits at page breaks' will split the table if it is resized to cover multiple pages. The order of the columns in the table can be changed by simply left clicking on the first cell of a column and dragging it to the preferred position.

If multiplet analysis has been carried out, the **Integral/Multiplet table** option from the 'Create' menu will display the **Multiplet Table**. The multiplet table is identical to the integral table but will contain information about the type of multiplet identified and the J-couplings if the multiplet structure was successfully resolved.

### 4.1.5 Measurements table

Once the user is done with measurements and the 'Measurements' mode exited, a **Measurements table** can be created by a right-click on the spectrum and choosing the corresponding option in the 'Create' menu. In the table, the user can adjust the position of the starting and end points by clicking on and editing the corresponding cells. The type of information displayed on the label can be chosen between the 'Detailed' and 'Delta Hz'

options in the 'Select Value' dialog that appears upon clicking in a corresponding cell in the 'Display Style' column; the value will be changed for that cell only.

### 4.1.6 Multiplet Report

In addition to the multiplet table, the multiplet information can also be displayed as a **multiplet report** using the corresponding option in the 'Create' menu or by clicking on the 'Create Multiplet Report' button in the 'Multiplet' section of the 'Analysis' panel, see Figure 44. The report is in the style used in academic journals and can be cut and pasted from JASON into a manuscript. When the option is selected, the user will see a dropdown list of available journal formats.

It is also possible to add identifier labels to the multiplet report. For this, the %IDENTIFIER field is found in the multiplet report template options. Once added to a template, and that template is applied, the multiplet identifiers appear in the multiplet report, e.g.: "... F: 1.96 (dq, J = 4.5, 7.5, 13.7, 1H), ..." If an assignment is applied, the identifiers are changed to the numbers of the assigned atoms on both the spectrum plot and multiplet report. If the user modifies the identifier in the 'Multiplet Properties' dialog, it is modified in both the spectrum plot and multiplet report.

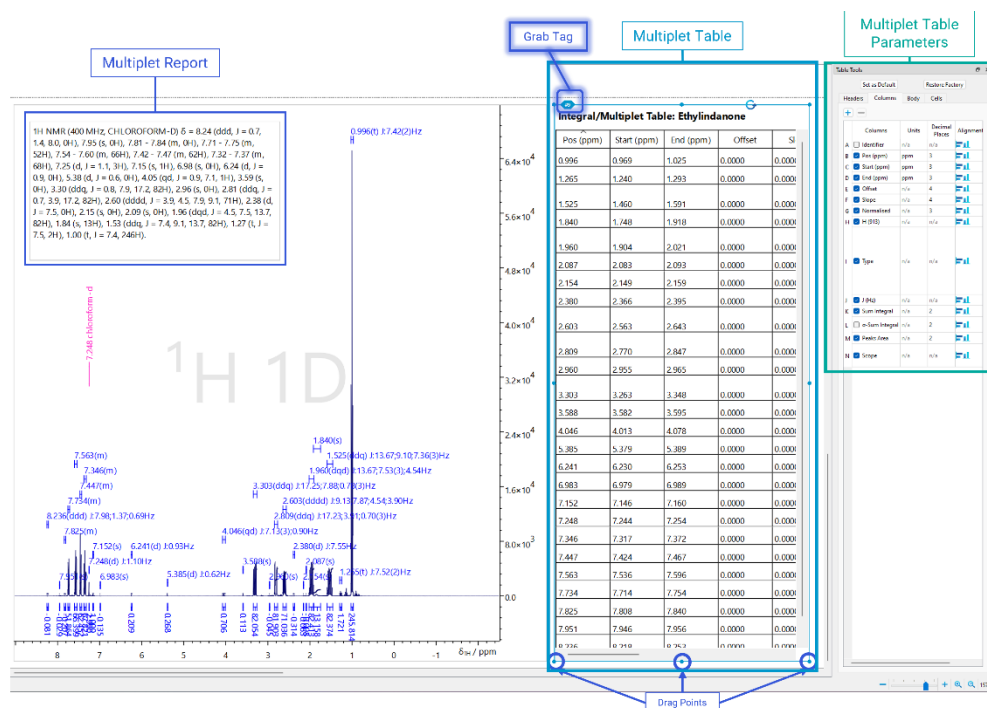


Figure 44: Multiplet Table and Report

### 4.1.7 Custom table

The option to create a custom table is found in the **Main Menu** → **New** → **Custom Table...** (also available by a right-click on the Canvas); it opens a dialog allowing the user to specify the number of rows and columns.

Newly created custom tables are initially empty except for the column titles which are A, B, C, etc. And can be edited later, allowing the user to fully customize header and cell data as needed.

**Rows can be added or removed** via the table's context menu:

'Add Row(s)...' opens a dialog to specify how many rows to add (supports undo/redo).

'Remove Selected Rows' deletes the currently selected rows and is only enabled when a selection is active (supports undo/redo).

'Delete Selected' provides the same functionality as 'Remove Selected Rows' (supports undo/redo).

**Columns can be added or removed** using the "+" and "-" buttons in the 'Table Tools' panel, 'Columns' tab.

**Table column titles** can be changed in the same 'Table Tools' panel, 'Columns' tab.

## 4.2 Printing objects

The option to print out objects from JASON can be found in the Main Menu and is also available from the menu appearing after right clicking on the currently active object.

By default, JASON sends all of the objects currently existing on the Canvas to print. To print out selected objects of interest, select them in the Canvas first and chose the 'Selected Objects' option in the 'Range' section of the 'Print' dialog (Figure 45):

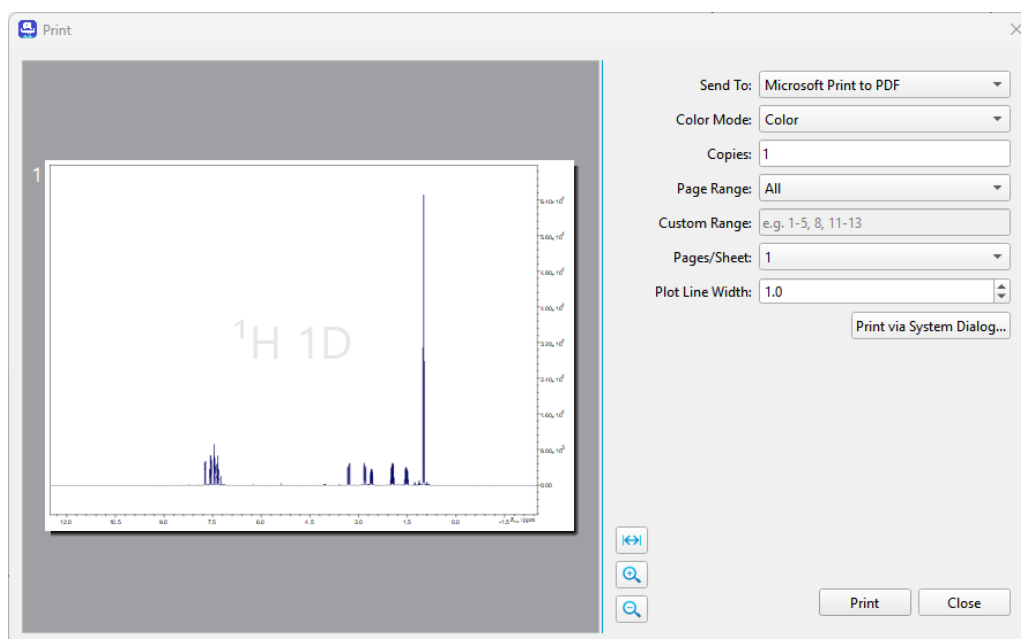


Figure 45: Printing selected objects

Please note that the 'Plot Line Width' affects the line width for printing of the object only, which can be seen in the printing preview, but not that displayed on the Canvas.

## 5 The Settings Menu

There is a large array of options for customizing the look and feel of JASON, as well as preferences for the analysis tools. These are controlled using the 'Settings' menu, shown in Figure 46.

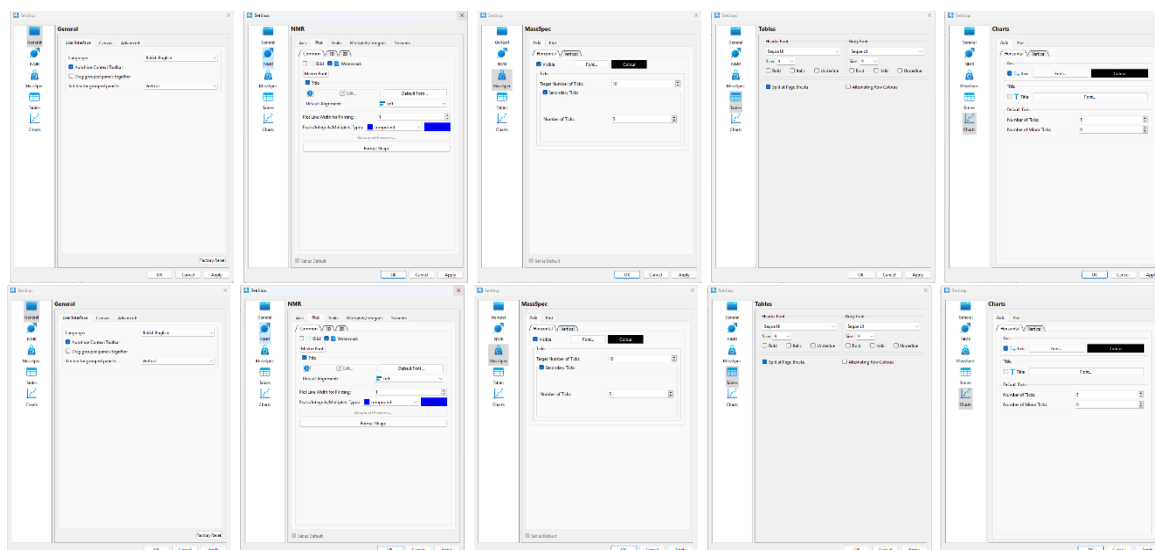


Figure 46: The 'Settings' Menu

The 'Settings' menu can be accessed from the Main Menu in the top left-hand corner of JASON or from the menu opened by a right mouse button click anywhere in the Canvas. When the menu is first opened, the user will see the 'General Settings' section. The 'Settings' menu comprises of three sections, the **General Settings**, the **NMR settings** and the **Table settings**. Each of these sections has its own set of tabs which are described below.

**Factory Reset button:** this button sets all options in settings to their original factory default values.

## 5.1 The General Settings

Any changes can be applied using the 'Apply' button, or when all the changes have been completed the user can quit the settings dialog by pressing 'OK', which will apply the current settings and quit. Pressing the 'Cancel' button will quit without applying the settings.

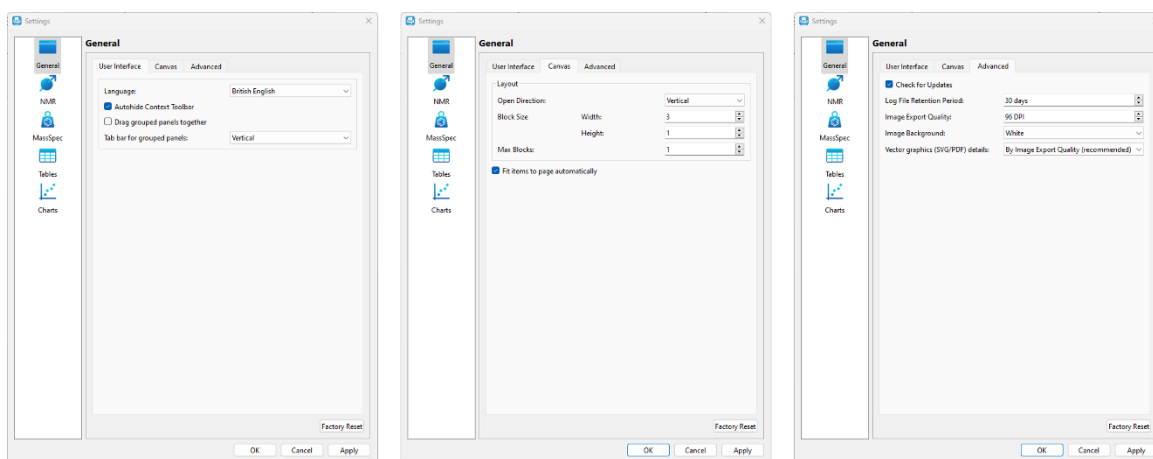


Figure 47: The General Settings

The 'General Settings' panel has 3 tabs:

### 5.1.1 User Interface

There are four options in the 'User Interface' tab.

**Color Scheme:** this option allows the user to choose between Light and Dark mode of the JASON interface. JASON color theme can be chosen independently of the OS theme, or follows the system theme if that is chosen.

**Language:** this option allows the user to select the language for the software. Currently, English and Japanese are supported.

**Context Tool bar** option refers the Context Tool Bar discussed in section 3.1 and contains three options:

'Always Visible' is self-explanatory;

'Auto-Hide' will make to the Context Tool bar invisible unless the cursor is moved into the top left-hand corner of a spectrum;

'Deactivate' will hide the Context Tool bar away unless the option is changed.

**Drag Grouped Panels Together:** when this box is checked, the context sensitive panels, described in section 3.2 Context Sensitive Panels and subsequent sections that are stacked on top of each other, can be moved as a single object, see Figure 19, and Figure 48.

**Tab Bar for Group Panels:** when the context sensitive panels are grouped together by stacking them one on top of another, the tabs can be displayed either horizontally or vertically as shown in Figure 48.

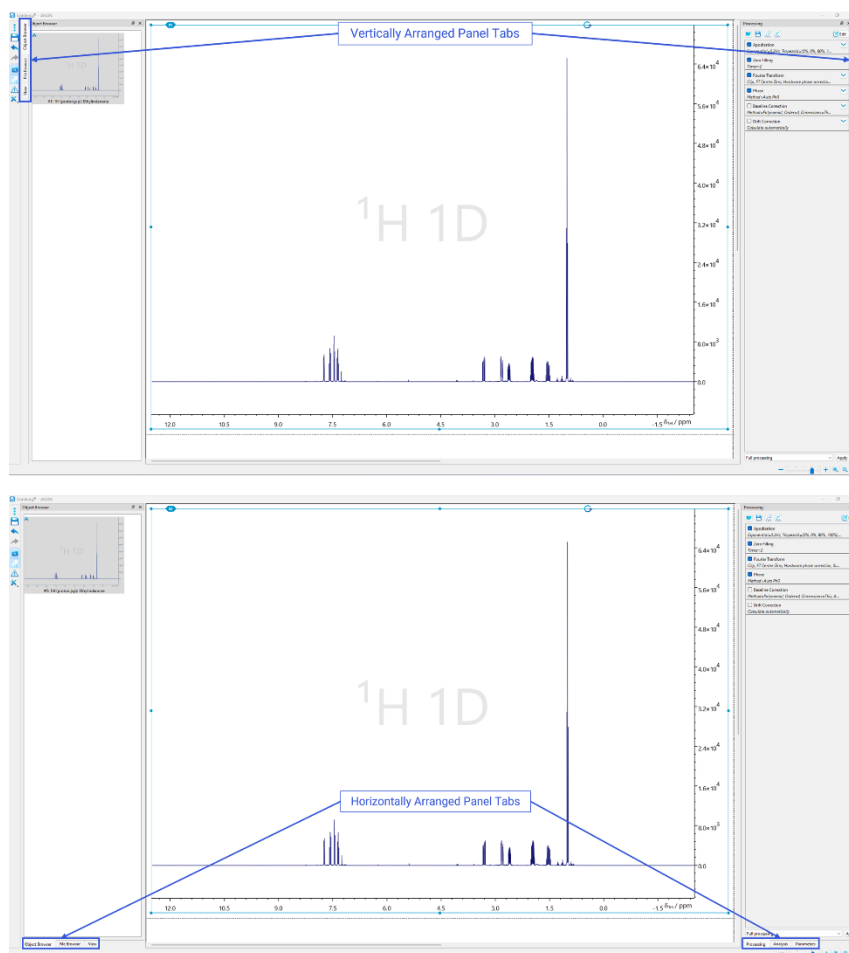


Figure 48: Alternative arrangements of grouped panels.

### 5.1.2 Canvas

This tab allows the user to **define how new objects are added to the Canvas**. By default, objects are added sequentially either horizontally or vertically on the Canvas depending on the choice made in the 'Open Direction' option.

New objects are placed on the Canvas using a layout which has two logic layers of placement. In the first logic layer, objects fill a block of width and height as specified in the settings. Once this block is full, then new blocks are created on the Canvas, following similar rules.

The second logic layer defines which direction the Canvas can grow in. When placing the blocks on the Canvas within the second layer, the user can choose in what direction (horizontal or vertical) the Canvas can grow without restriction while more and more blocks are added. This direction is called the 'Open Direction; in Settings. For clarity, we

will refer to the direction perpendicular to the open direction as the 'Restricted Direction'. The restricted dimension size is limited by the value of the 'Max Blocks' parameter.

Below we describe some details and examples of this layout system.

When a new object is placed on the Canvas, e.g. by double clicking in the file browser, the placement of this new object on the Canvas is determined by the following rules:

- 1) On an empty Canvas, the top-left page is used first.
- 2) Newly opened objects fill a block first. Objects are placed along the restricted dimension first (i.e. perpendicular to the open dimension) until the maximum height or width is reached (as appropriate).
- 3) When the block is complete, a new block is started. This new block will be positioned along the restricted direction until the number of blocks is equal to the user-defined 'Max Blocks' setting.
- 4) When the 'Max Blocks' number is reached, the new block will be started along the open direction. This new block is then populated using these rules.

If the 'Max Blocks' option is set to 1 and the block size is 1×1 (this means that a block corresponds to a single object), all subsequent objects will be added horizontally or vertically depending on what is selected for the 'Open Direction' option. I.e. all new objects will be added either vertically or horizontally in a single column or row.

If the 'Max Blocks' option is set to a number N and the block size is 1×1, then the object will be added in restricted dimension till it reaches N objects, after that a new row/column of the objects will be started according to the open direction setting.

If the block size is an arbitrary set of values A×B, then the 'Max Blocks' and 'Open Direction' settings are applicable for the blocks, not just the individual objects. A block of the size A×B will be filled first according to the rules above. Then the placement of the next block will be determined by the parameters 'Max Blocks' and 'Open Direction' using the same rules as for individual objects. This is shown in the figure below in the case of a 3×2 arrangement with max blocks set to 2 and the open direction being vertical.

To **create an addition row of items in the Canvas**, right-click on the object of interest and find the 'Insert Row' option in the context menu. A click on it will insert a row above the selected item and move the items in the row containing the selected item and the row below it down one row; Undo/Redo functionality is supported for this operation.

### 5.1.3 Import/Export

**Image Export:** this option controls the quality of images created from the JASON document.

## 5.2 The NMR Settings

The 'NMR Settings' panel has six associated tabs: Axis, Plot, Peaks, Multiplet/Integrals, Solvents, and Bins, see Figure 49. Each panel is described in the section below. Any settings can be set as default using the 'Set as Default' checkbox at the bottom.

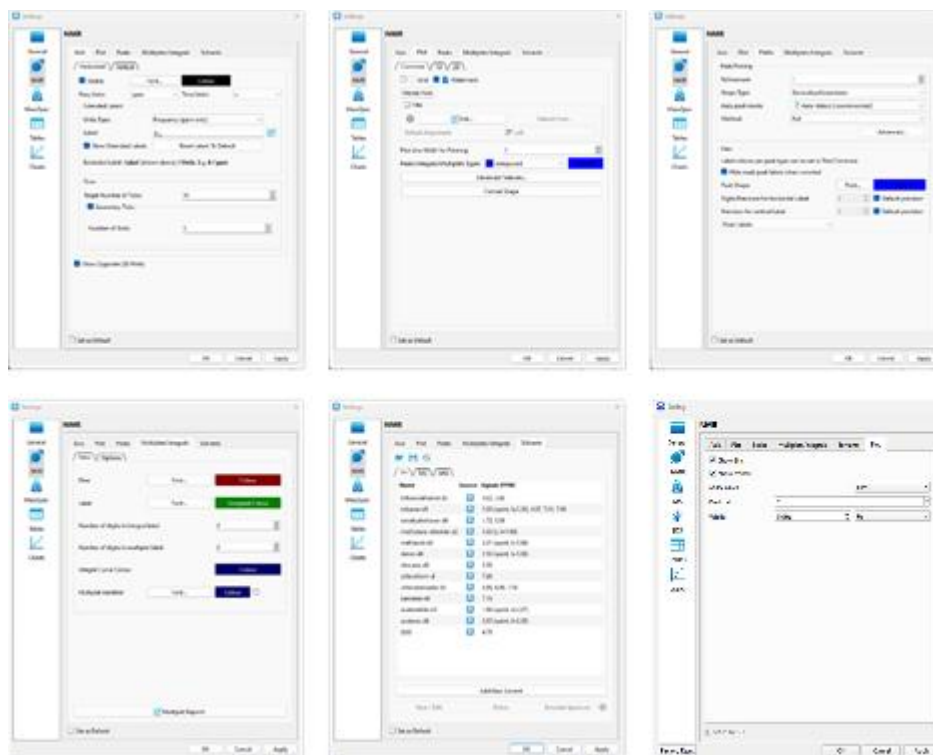


Figure 49: The 'NMR Settings' main tabs

### 5.2.1 Axis

The 'Axis' settings contain the options for modifying the axes in an NMR spectrum and it comprises three panels, settings for the horizontal axis and settings for the vertical axis, see Figure 50.

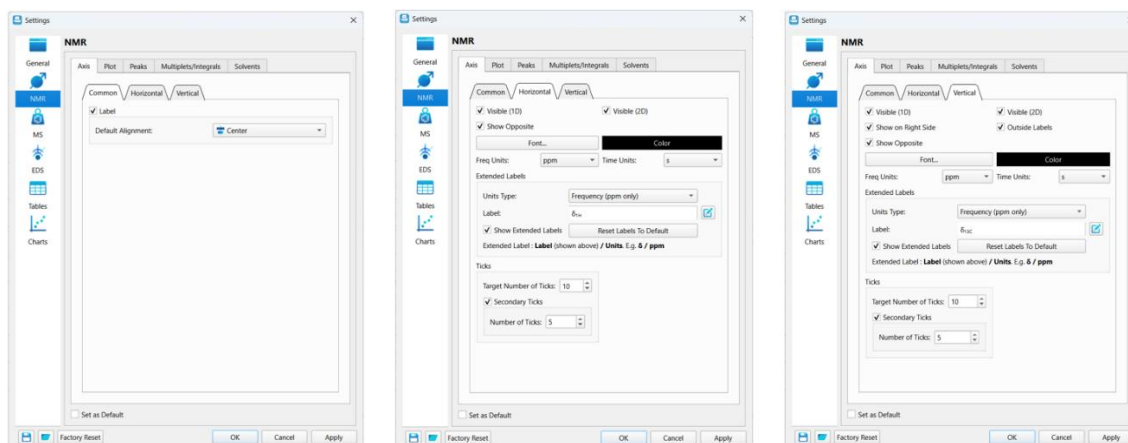


Figure 50: 'NMR setting', 'Axis' tabs

The 'Common' tab contains the settings for the **axis label**: the user can choose whether the axis title (label) should be visible and its default position (select between right/left side or middle). Clicking on the 'OK' button will apply the changes and close the dialog. Clicking on 'Apply' will apply the changes without closing the dialog.

Both 'Horizontal' and 'Vertical' tabs contain settings regarding the Axis.

The **Horizontal** tab has the following controls:

**Visible** checkbox is to toggle the visibility of the axis.

**Font** and **Color** buttons open dialogs that allow the user to change the font and style of the axis and their color.

The display units for frequency domain data and for the time domain data are chosen from the dropdown lists of **Freq Units** and **Time Units**.

In the **Extended Labels** section, users can customize the axis label displayed. Clicking on the 'Edit' button to the right of the 'Label' field opens the 'Edit Axis Label' dialog. From this dialog, the user can enter their required axis label information, including isotope number, element name, and enable superscript and subscript font.

In the 'Ticks' options, the user can set a **target number of ticks** using the dialog box. JASON will try and set the number of major ticks for the current display range as close to this target number as possible while minimizing the number of decimal places displayed on each tick. This is to ensure that the axis labels do not look overcrowded for display and printing purposes.

The secondary ticks are optional and can be toggled on and off using the **Secondary Tick** checkbox. The user can set the number of secondary ticks between each major tick in the **Number of Ticks** dialog box.

The **Vertical** tab has the same options as the 'Horizontal' tab with the following additions.

The axis visibility option for 1D and 2D spectra can be toggled separately using the **Visible (1D plots)** and **Visible (2D plots)** checkboxes.

The position of the vertical axis can be swapped between the left and right-hand side of a plot using the **Show on Right side** checkbox, and the axis labels can be displayed inside or outside the spectrum, with this option being toggled using the **Outside Labels** toggle box.

## 5.2.2 Plot

The Plot tab has three panels containing the options that are **common** to all spectra or specific to **1D** spectra and **2D** spectra.

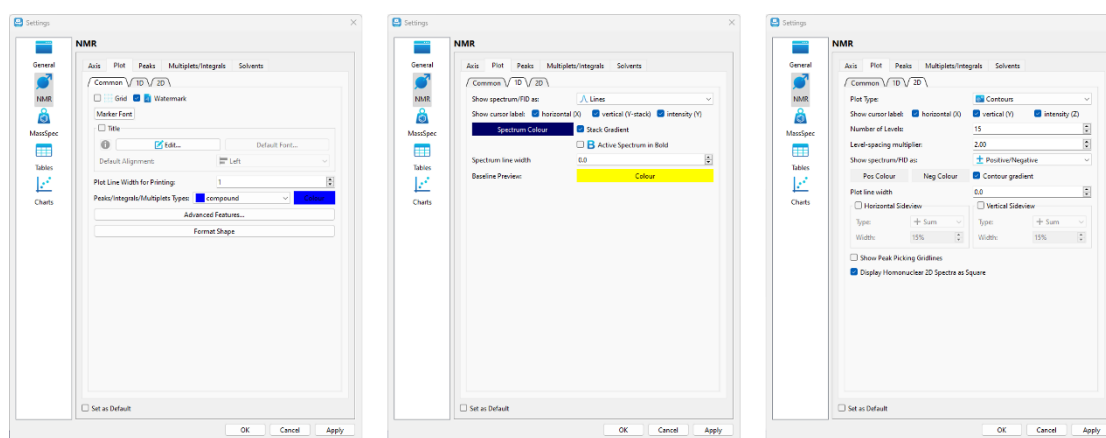


Figure 51: 'NMR settings', 'Plot' tabs

In the **Common** tab, the **Grid** checkbox toggles the visibility of the grid on a spectrum. The **Watermark** checkbox adds the experiment type to the spectrum background as a watermark.

- Click here to see how to [add a Watermark](#) and [here to see how to display gridlines](#).

The **Marker Font** button opens the standard font dialog and allows the user to change the font, style and color of the crosshair marker.

The **Title** checkbox toggles the visibility of the title on a spectrum. The **Title Font** button allows the user to change the font of the spectrum title. The **Advanced Features** button opens an advanced menu.

The **1D** and **2D** tabs contain controls for the appearance of the corresponding type of a spectrum and the cursor label.

In the 2D tab, there is also the option to **Show Pick Picking Gridlines**. In the 'Homomuclear 2D spectra' section, the **Display as Square** and **Show Diagonal** check boxes are self-explanatory, and the **Diagonal Slope** option allows the user to set the slope manually.

## 5.2.3 Peaks

The 'Peaks' tab has three main options, see Figure 52:

**Refinement**, which controls the number of iterations used when fitting the peak model to the spectral data.

**Shape Type** is a dropdown list of model shapes for the peak models; the current options are Generalized Lorentzian and Pseudo-Voigt.

**Peak Shape** has two buttons associated with it, the **Font** button allows the user to change the font of the peak labels on a spectrum and the **Color** button allows the user to change the color of the peak labels and the peak lines.

The **Method** of peak detection includes the following options: Full, Derivative Only, Local max only, and ML only. The Machine Learning algorithm is currently implemented for 1D and pseudo2D spectra only; this can be set as the default peak picking method if desired.

The **Advanced** button opens a dialog box that contains all the options for 2D and nD peak picking autotype settings and those used in peak picking and peak fitting, see Figure 52. These values should only be changed by an expert user who fully understands the peak picking process.

The 'View' section contains the '**Hide weak peak labels when crowded**' checkbox option. If checked, the hidden labels will be plotted as soon as user adjusts zoom close enough for all the labels to fit horizontally; the same settings option applies to both 1D and pseudo2D plots.

Once parameters have been changed, the user can save these as their new default value by checking the **Set as Default** tick box.

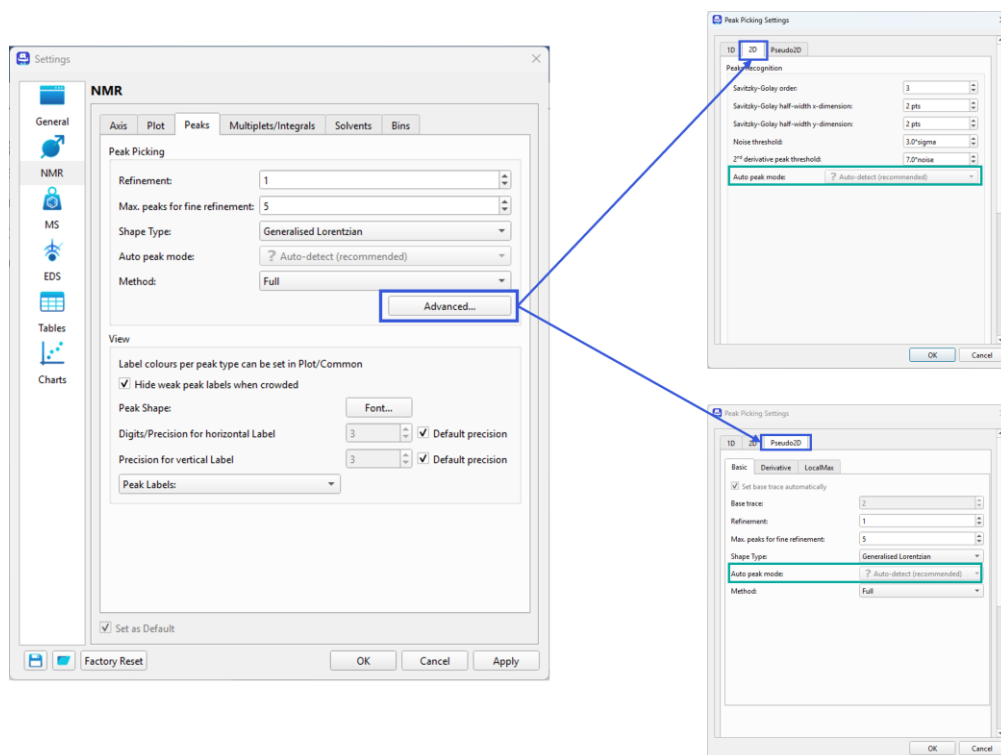


Figure 52: 'NMR Peak' Setting

## 5.2.4 Multiplets/Integrals

The **Multiplets/Integrals** tab combines the options for both analysis functionalities

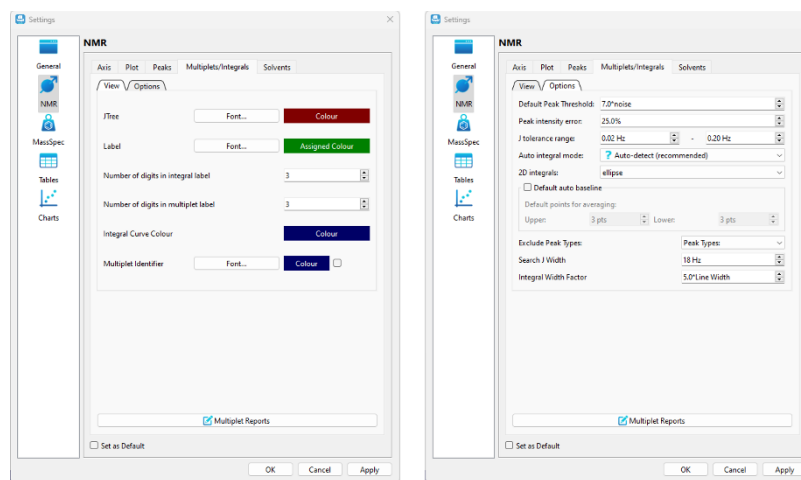


Figure 53: 'Multiplets' and 'Integrals' Settings

The 'View' sub-tab contains options for the display of multiplets and integrals:

**J-Tree:** these options allow the user to define the font and color of the J-coupling tree displayed on a spectrum

**Label:** these options allow the user to define the font and color of the multiplet and integral labels.

**Number of digits in integral label:** this option allows the user to define the number of decimal places displayed on the integral label.

**Number of digits in multiplet label:** this option allows the user to define the number of decimal places displayed on the multiplet label.

**Integral Curve Color:** this option allows the user to pick the color of the integral curve; the check box next to the it toggles the visibility of the integral curve.

**Multiplet marker** and **Integral marker** checkboxes toggle the visibility of corresponding markers; both checkboxes are checked by default.

The 'Options' sub-tab contains the available options:

**Default Peak Threshold:** in the automatic multiplet selection this is the first pass default threshold for including peaks as part of a multiplet.

**Peak Intensity Error:** the multiplet analysis assumes a perfect first order multiplet, however in real data there will be the effects of strong coupling present to a greater or

lesser extent. This parameter provides a tolerance to the peak intensity to accommodate the variation.

**J Tolerance range:** while a perfect multiplet should have peaks spaced at exact separations, overlap and uncertainties in the peak picking introduce small errors in the peak positions. During the multiplet analysis if at any step the analysis is unable to resolve the multiplet structure satisfactorily, the peak tolerance is allowed to increase, starting from a lower bound and terminating at the upper bound. The range of this tolerance is defined here.

**Autobaseline:** if this box is checked JASON will automatically detect whether the integral region is sitting on a flat base line with no bias. If not, it will calculate a correction and apply it to the integral.

**Search J Width:** this parameter defines the maximum separation between two adjacent peaks in the same multiplet or integral region.

**Integral Width:** this parameter defines how far an integral region should extend from the outer most peak in a multiplet or integral regions.

## 5.2.5 Solvents

The 'Solvents' settings panel has three sections, see Figure 54. Any changes can be applied by pressing the 'Apply' button or by pressing the 'OK' button which will also close the settings dialog. Changes can be rejected by clicking the 'Cancel' button which will close the settings dialogue without applying the changes.

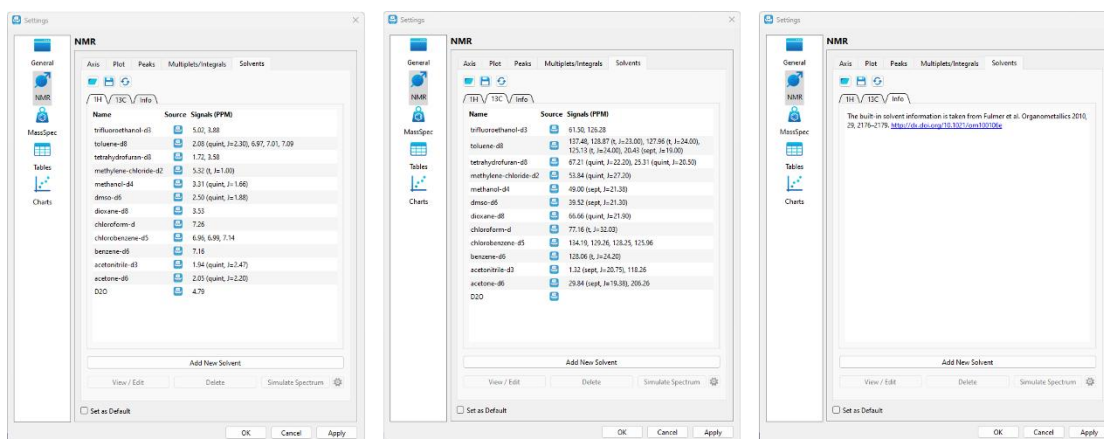


Figure 54 'Solvent' Settings

The user can add new solvents by clicking on the 'Add New Solvent' button near the bottom of the panel.

## 5.2.6 Bins

The 'Bins' tab contains settings for visualization and calculation of bins/buckets on 1D NMR plot, see Figure 55:

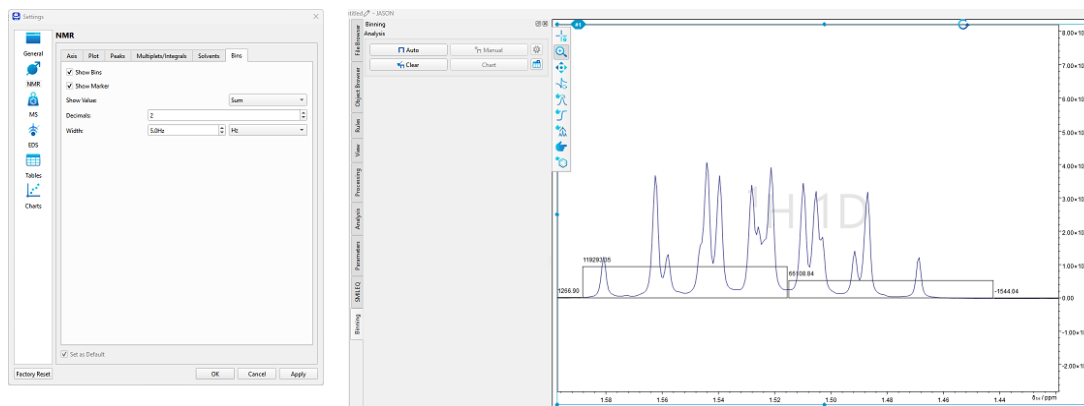


Figure 55: 'Bins' tab and bins visualization

The 'Show Bins' option works locally for selected spectrum and globally when no spectrum is selected; the user may need to zoom in to see the bin markers.

In the dialog, the user can specify the number of decimals and set the width of buckets/bins. Changing the width of the bins/buckets works for any new analysis conducted after the change, and the specified value will be used when automatic binning is requested.

If the user opens the 'Bin' settings without an NMR plot selected, then, as usual, the default options will be saved. If the settings are open from an NMR plot, then the default is only modified if 'Save as Default' checkbox is selected by the user.

## 5.3 MS

The 'MS Settings' panel has two associated tabs, 'Axis' and 'Plot'; see Figure 56. Each of the panels is described in the section below. Any of the settings can be set as default using the 'Set as Default' checkbox at the bottom.

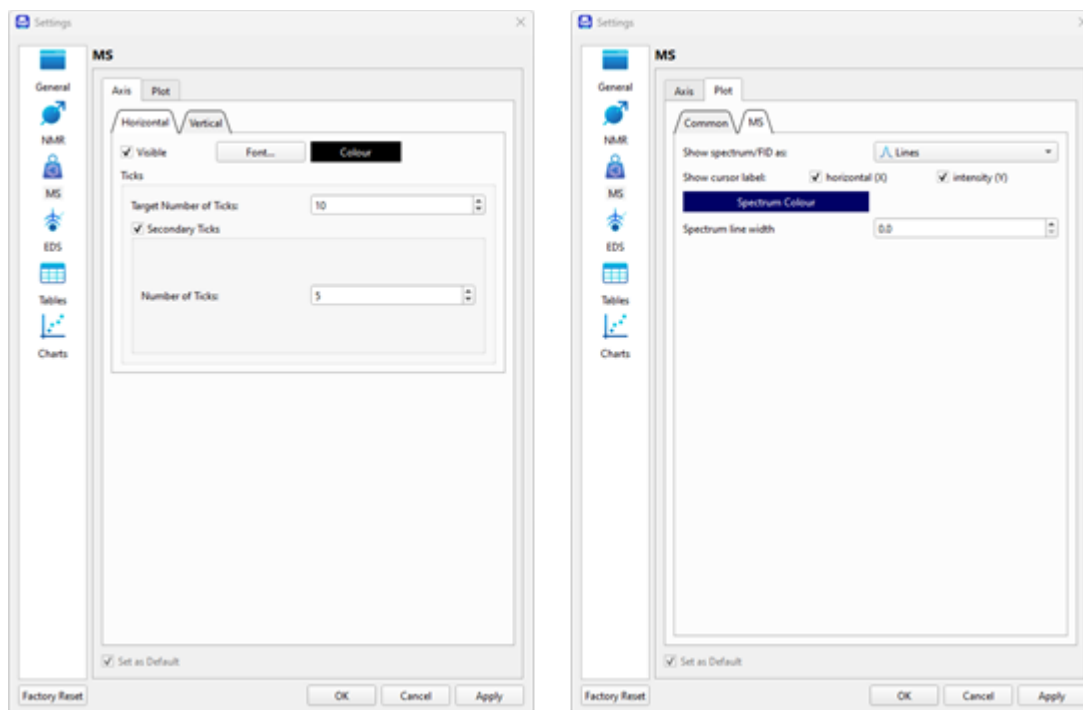


Figure 56 'MS' Settings

### 5.3.1 Axis

The 'Axis' settings contain the options for modifying the axes display in an MS spectrum and it comprises three panels, settings for the axis label, horizontal axis and settings for the vertical axis, see Figure 57.

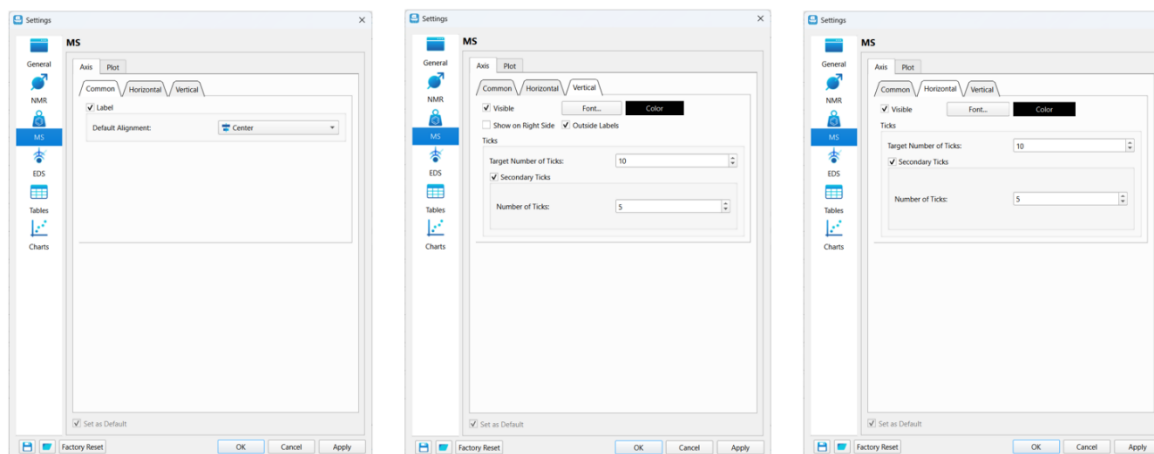


Figure 57 'MS Axis' Settings

### 5.3.2 Plot

The plot tab has two panels containing the options that are **common** to all spectra or specific to **MS** spectra as shown in Figure 58.

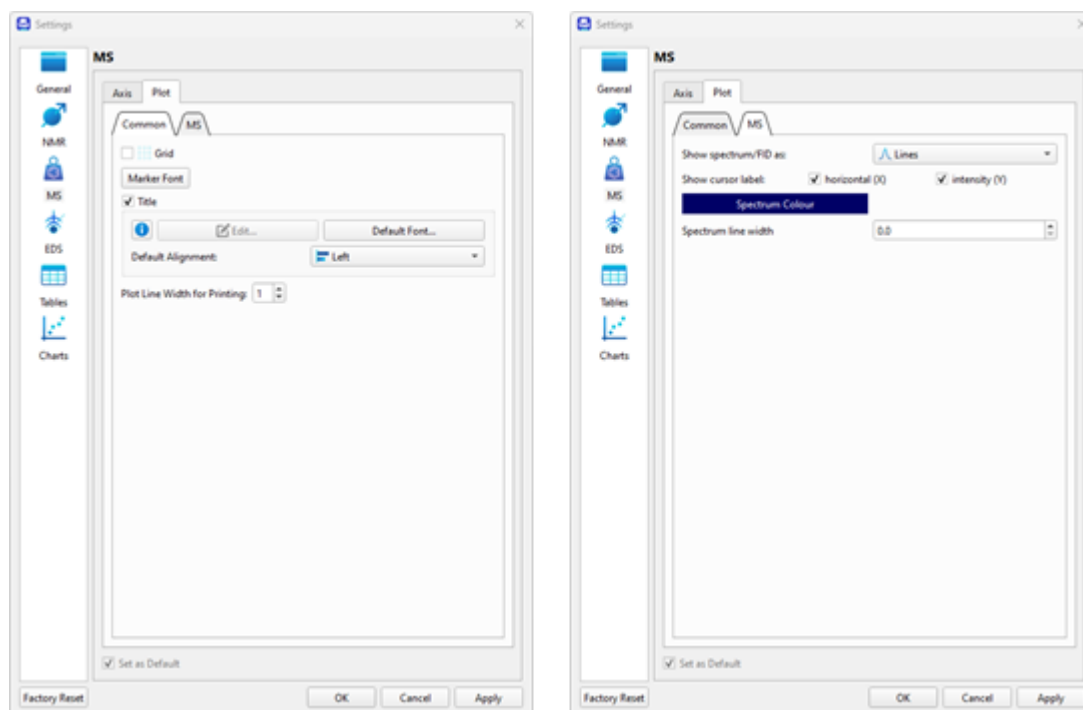


Figure 58 'MS Plot' Settings

## 5.4 Tables

The 'Tables' settings panel has two sections, see Figure 59. Any changes can be applied by pressing the 'Apply' button or by pressing the 'OK' button which will also close the settings dialog. Changes can be rejected by clicking the 'Cancel' button which will close the settings dialog without applying the changes.

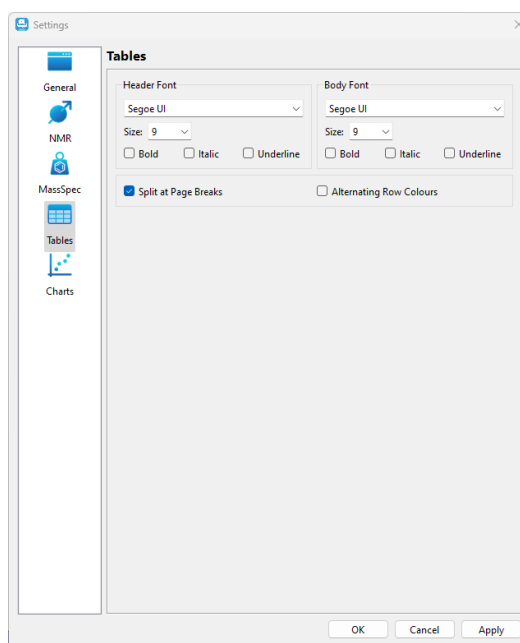


Figure 59 'MS Table' Settings

The user can change the fonts for the header or the body of a table in the 'Header Font' and 'Body Font' sections, respectively. The other two options allow the user to define the behaviour of a table if it extends beyond the boundaries of a single page on the Canvas and to display a table with alternating colors for each row.

## 5.5 Charts

The 'Charts' settings panel contains the settings of the chart display and has two sections, 'Axis' and 'Plot'; see Figure 60. Any changes can be applied by pressing the 'Apply' button or by pressing the 'OK' button which will also close the settings dialogue. Changes can be rejected by clicking the 'Cancel' button which will close the settings dialogue without applying the changes.

Please note that like that for the 'Tables' setting tab, changing the settings of the chart display parameters in the global 'Settings' dialog affects the default settings, but not the currently active chart.

In the **Plot** tab, the user can define the Legend placement on the chart; change the fonts for the header of the title of a chart, and turn on or off gridlines as well as chose their color.

2D **Gridlines** in JASON is a powerful tool aimed to help with manual assignment:

- during assignment of 2D spectra, gridlines related to different carbon CHn can be displayed in different colors when carbon CHn is known and the chemical shift is not assigned (CHn usually appear after HSQC peaks are defined)
- when a peak is assigned, the peak picking gridline changes its appearance to less prominent which allows the user to focus on unassigned signals.

The **Axis** tab consists of two tabs, containing separate settings for the **Horizontal** and **Vertical** axes of a chart display parameters. The user can adjust the font of horizontal and vertical axes labels and the axes color in the 'Axis' section, and the font of horizontal and vertical axes titles in the 'Title' section; as well as modify the default number of ticks and minor ticks for each axis of the chart.

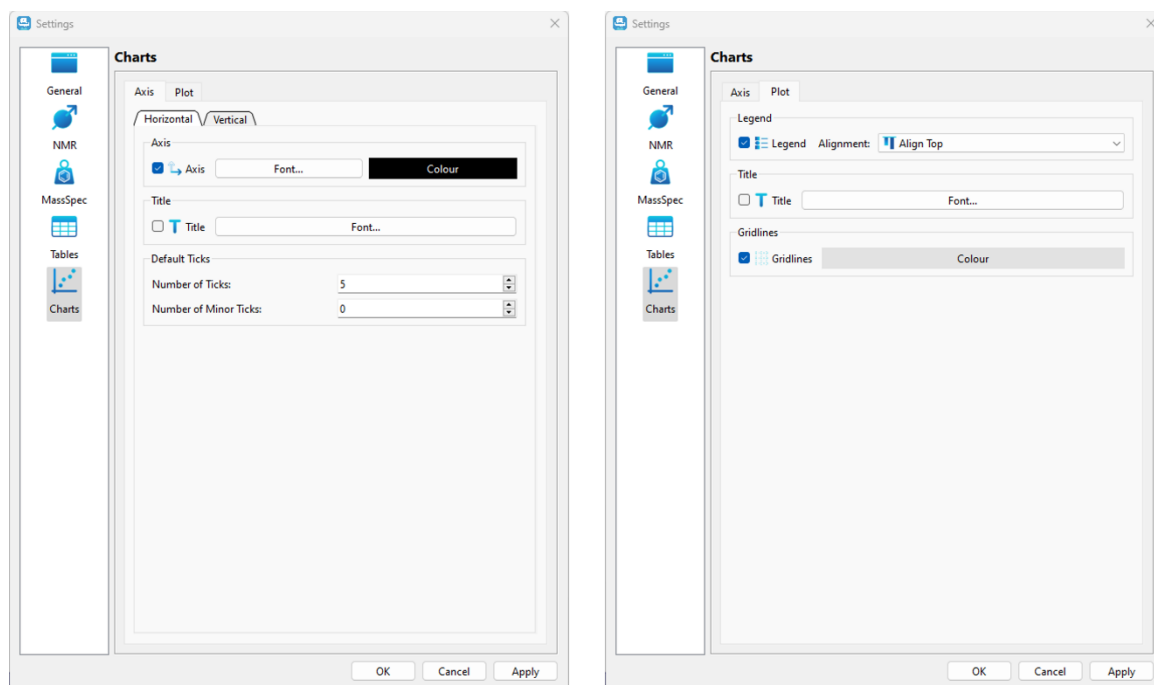


Figure 60: Chart Settings

## 6 Stacking and Overlaying Spectra

- Click here for a video on [Stacking or overlaying spectra](#). You can also create a stack using [Drag and Drop](#).

A stacked plot or overlay of spectra in the current JASON document can be created by first selecting the spectra to stack and then right-clicking on the Canvas and selecting the 'Stack Spectra' option from the context menu.

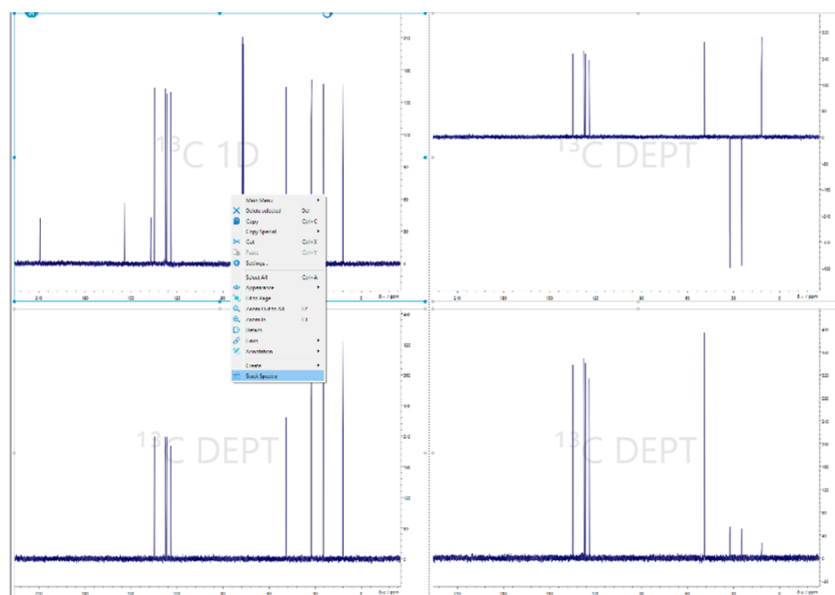


Figure 61: Selecting and stacking individual spectra

A new stacked plot of the spectra will be added to the Canvas.

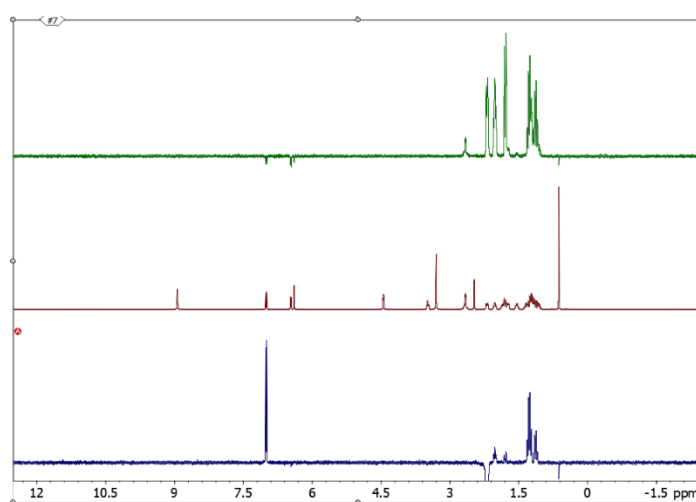


Figure 62: Stacked spectra

The currently active spectrum in the stacked plot is indicated by an “A” in a red circle to the left of the spectrum. Additional processing and manipulation of the active spectrum (e.g. phasing) can be performed as necessary in the usual manner.

The ‘Clip 1D Spectra in Stack’ option, found on the ‘Plot’ section of the 2D NMR tab in the global Settings dialog, controls clipping for drawing of 1D spectra and traces in stack, see Figure 63. ‘Off’ by default, it also works for pseudo-2D and multiplot spectra.

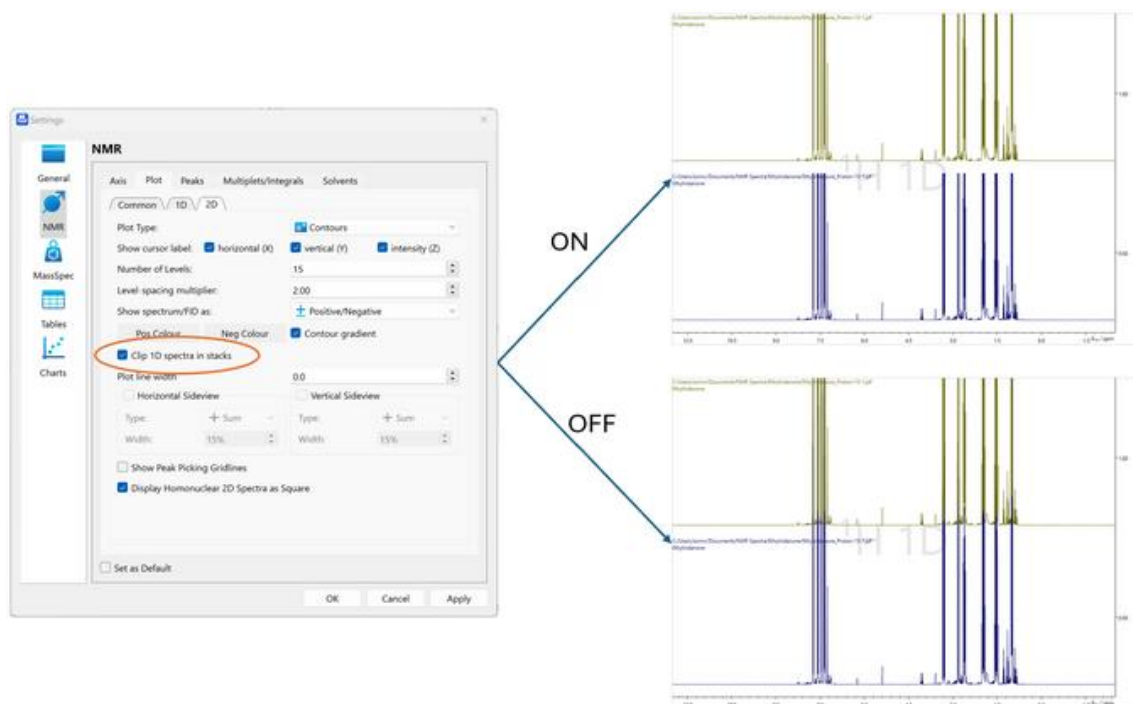


Figure 63: ‘Clip 1D Spectra in Stack’

## 6.1 The Stack Panel

When a stacked plot is selected, the ‘Stack’ panel from the ‘Context Tools’ becomes available. The ‘Stack’ panel allows easy manipulation of the order and amplitude scaling of each spectrum in the stacked plot.

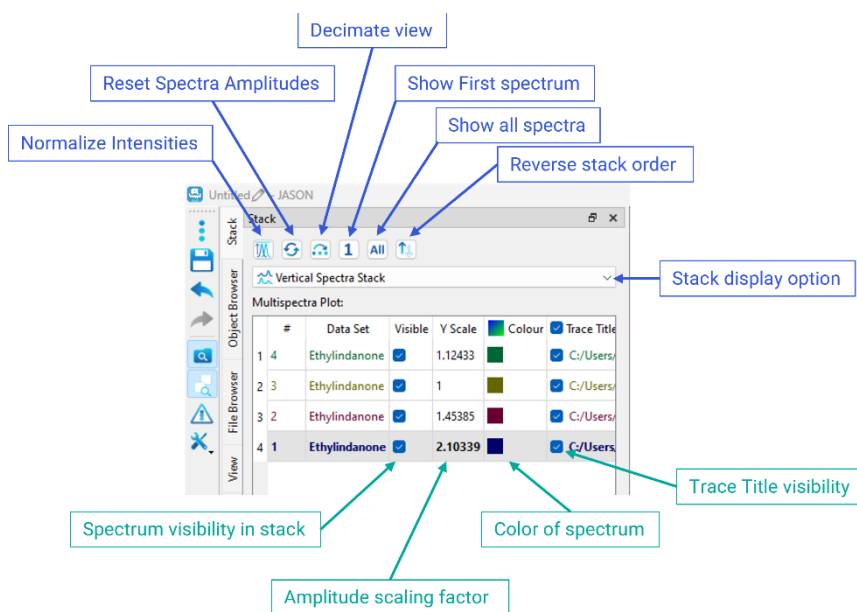


Figure 64: Stack panel

To **adjust the amplitude scaling** applied to a given spectrum, enter a value for the 'Y Scale' into the appropriate row of the table on the 'Stack' panel. To **normalize the intensities** of the spectra, click the 'Normalize intensities' button at the top-left-hand side of the 'Stack' panel. To **reset the amplitude scaling and shifts**, click the 'Reset 1D spectra scaling and shifts' button.

The **currently active spectrum in the stacked plot** is also indicated by bold font for the row. To make another spectrum in the stack active, double-click on the data set name of the appropriate row in the table. To **adjust the order of the spectra**, click on a row and drag it to the desired location, above or below other rows in the table.

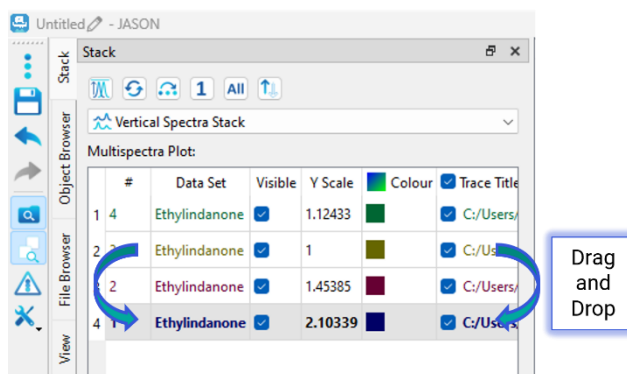


Figure 65: Reordering spectra in the stacked plot by dragging rows in the table

To **change the color of a spectrum** in the stacked plot, double-click on the colored square at the right-hand side of the row and select or configure the desired color in the 'Select Color' window.

To **hide a spectrum**, uncheck the 'Visible' box in the appropriate row. For large numbers of stacked spectra, it is sometimes desirable to display only every n<sup>th</sup> spectrum in the stack

(e.g. every 10<sup>th</sup> spectrum). To do this, use the 'Decimate view' button and enter the decimation factor.

The 'Show Tilt' check box toggles the visibility of the triangle slider which is used to **control the tilt of the stacked plot** (the horizontal shift of the spectra relative to each other); this works the same for pseudo2d and multispectrum stacks.

The 'Stack' panel also provides access to a text editing dialog so font, sub/superscript, Greek characters etc. can be included in the title string. To **edit titles of individual traces** in a stack plot:

- Right-click on a trace title in the 'Trace Title' column to see the context menu;
- Double-click in a title box also allows editing the title (Figure 66).

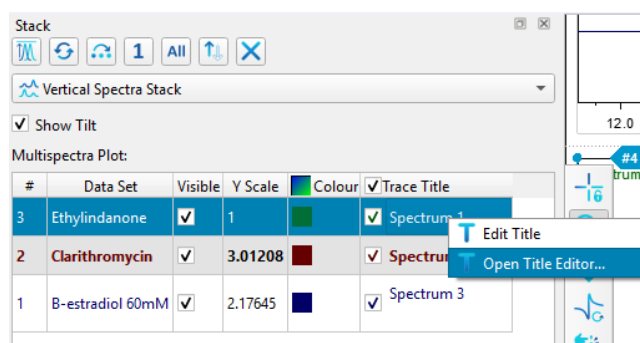


Figure 66: Editing titles of individual traces in a stack plot

To **overlay spectra** instead of stacking them, select 'Spectra Overlay' from the dropdown menu.

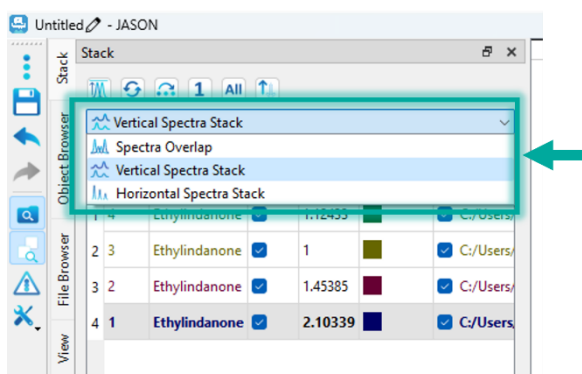


Figure 67: Overlaying spectra using the 'Stack' panel

In spectra overlay mode, the vertical position of each spectrum can be adjusted by entering a value for the 'Y shift'

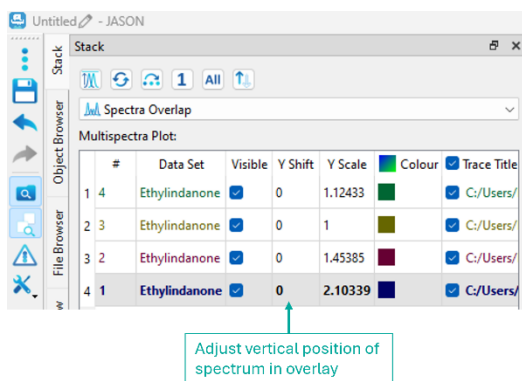


Figure 68: Adjusting the vertical positions of overlaid spectra

In a multispectral stack, rotating the mouse wheel over the stack will change the scaling of all spectra (Figure 69)..

Rotating the mouse wheel with **Shift** pressed will change the scaling of an individual (active) spectrum in both 1D and 2D multispectral overlaps. The scaling value in the 'Stack' panel table ("Y Scale" for 1D spectra and "Amp. Scale" for 2D) is updated dynamically.

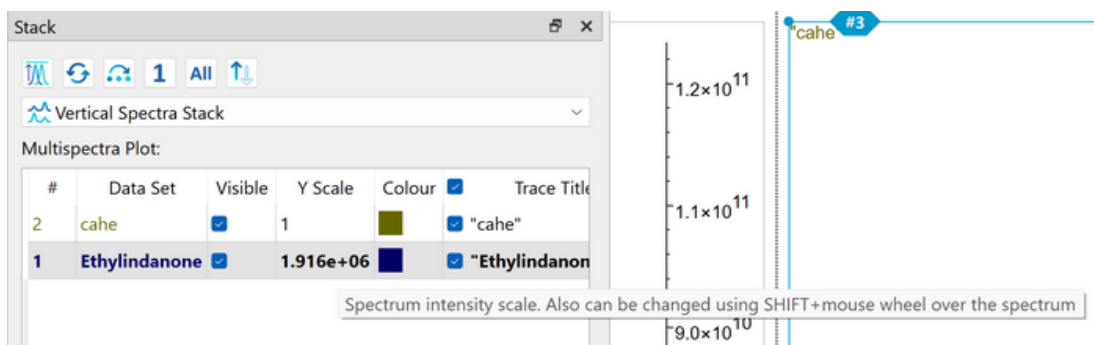


Figure 69: Changing the spectrum intensity scale in a multispectral stack

In a multispectral stack, **individual traces can be phase-corrected independently**. To do so, in the 'Phase' section of the 'Processing' panel, the user should select the 'Custom' mode (instead of the default 'Auto Ph0') and uncheck the 'Global' settings checkbox; this will bring in an active 'Edit' button (Figure 70: Phase-correction traces in a slack individually). A click on the 'Edit' button will open the 'Edit Phase Values per Trace' dialog; a double click on a cell in the dialog will allow for editing the value.

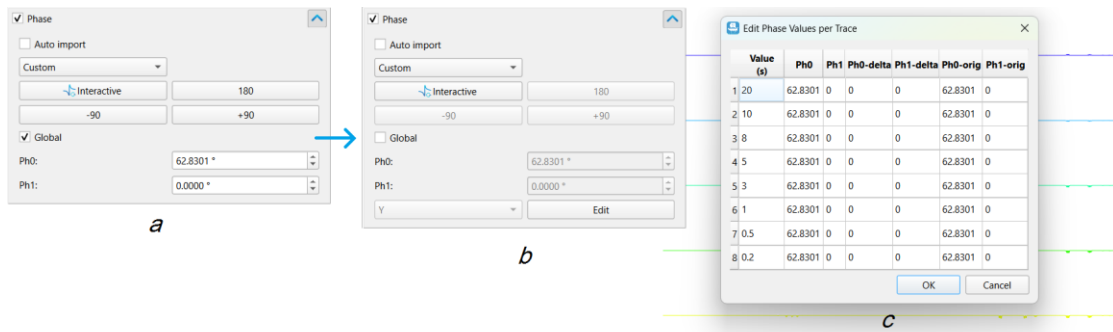


Figure 70: Phase-correction traces in a slack individually

It is possible to specify a new phase value by entering it in the 'Ph0' or 'Ph1' cell or by entering a change of phase from the current value in the 'Ph0-delta' or 'Ph1-delta' cells – for example '+180' will add 180° to the currently applied value. Once the values have been entered, press the 'OK' button on the dialog and then press the 'Apply' button on the 'Processing' panel to apply the phase changes.

For 2D data, the dimension is automatically selected, for 3D data, the user can specify the dimension to apply phase corrections to.

Like that for a regular 2D spectrum, it is possible to attach **1D projections along the axes of overlaid 2D spectra.**

The projection behavior with multi-spectra 2D plots is as following:

**Overlapped:** both projections are allowed

**Vertical stack:** a horizontal projection is allowed

**Horizontal stack:** a vertical projection is allowed

If the "Skyline" or "Sum" projection is activated on multiplot-2D, then projections for each spectrum are created. The projections are colored according to the Pos. color of the corresponding 2D spectrum. To subtract spectra, enter the coefficient as "-1".

If the "Spectrum" projection is set on multiplot-2D, then the projection is associated with the active spectrum (at the time the projection is created). The color of the spectrum is set as before but could be changed. In the current implementation, the trace colors follow just the same scheme as for a single 2D spectrum: cycling between a predefined set of colors, according to when the traces were created.

If "Trace" is set on multiplot-2D, then the trace(s) is taken from the active spectrum. The color of the trace is set as before. It's possible to take traces from different spectra by switching the active spectrum and using the "multiple" mode for trace selection. Visibility of the spectra also controls the visibility of the projections, associated with this spectrum.

Drag&drop from Object Browser is supported for the allowed projection types.

**Note:** it is possible to convert a stack of spectra to pseudo 2D. The corresponding 'Convert to Pseudo 2D' button found in the 'View' panel opens up a dialog where the user can specify all the essential parameters for a new dimension with many domain type options (not everything but several options), see Figure 71.

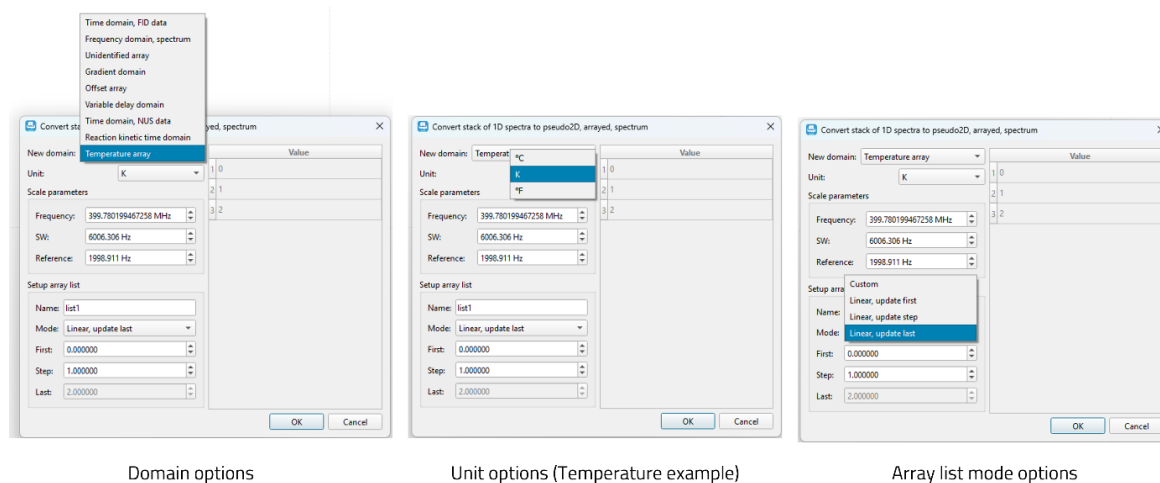


Figure 71: Convert to Pseudo 2D options

## 6.2 Pseudo 2D Data

When an arrayed (pseudo 2D) data set is opened in JASON, the stack of 1D traces is displayed in JASON; the visualization is via vertical lines at the peak positions in each plot rectangle of each visible trace, link connected by horizontal lines at the top and bottom of traces on the vertical stack plot of pseudo2D NMR data.

The context 'Stack' panel contains options relevant for the pseudo-2D display. The user can toggle the traces visibility in the corresponding table or set up a decimated visibility with the 'Decimate' button.

Pseudo 2D data can be converted to a 1D stack in the 'View' panel by selecting the 'Convert' button in the 2D plot section. Once this conversion has been performed, the 'Stack' panel contains usual controls for multiple 1D spectra in a stack.

**Note:** pseudo2D is effectively a single dataset with a single processing list, whereas a stack is individual datasets each with their own processing list.

## 7 Spin Simulations

Simulation of 1D spectra can be performed in JASON by selecting the 'Simulation' option from the Main Menu. When a simulation has been selected, it opens the 'Simulation' dialog panel, see Figure 72. This allows the user to enter the chemical shifts and J-coupling constants for up to 20 spins along with other relevant parameters. As the data is entered, the simulated spectrum will appear in a new panel on the Canvas.

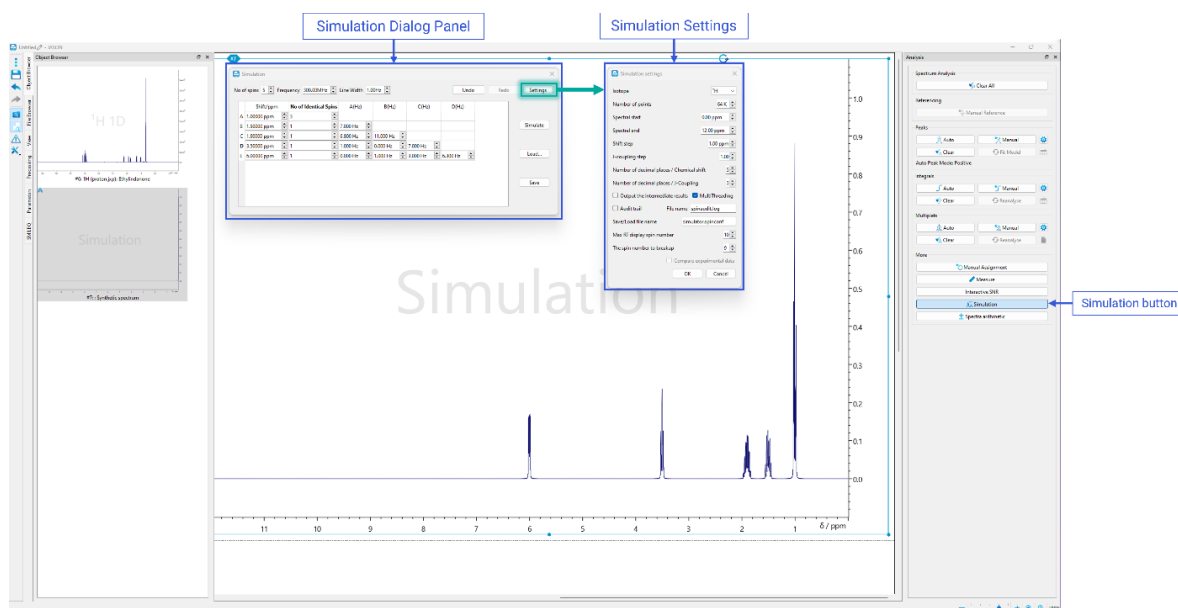


Figure 72: Spin Simulation interface

### 7.1 Simulation Dialog Panel

**No of Spins:** this is the total number of non-identical resonances in the simulations.

**Frequency:** this is the base frequency of the simulation in MHz.

**Line Width:** this is the line width (Hz) of the peak model for the simulation.

**Undo/Redo:** allows the user to undo the previous command or redo the last undo.

**Settings:** opens the simulations settings dialog.

**Simulate:** performs the simulation with the current simulation parameters.

**Load:** loads a previously saved set of simulations parameters.

**Save:** saves the current simulations parameters.

The following parameters are related to the spin system which will be simulated. The spin system is described using a spreadsheet-like table of cells. Depending on the number of spins in the simulations, the rows of the cells are labelled A, B, C, etc. These labels also

correspond to the labels for the spins and are used to label the third column and beyond. The column headings are explained below.

**Shift/ppm:** this is the chemical value in ppm of the spin(s).

**No of Identical Spins:** more than 1 spin can be associated with a given resonance frequency; for example, a methyl group will comprise 3 identical spins. This can be accommodated in this column. It is important to note that if two spins have the same chemical shift but are not magnetically equivalent, then it will be necessary to add each spin to the simulation explicitly.

**A(Hz), B(Hz), C(Hz), etc.:** these column headings are related to the spin labels assigned in the table rows. Each cell contains the J-coupling between two spins, for example column A; row B contains the coupling constant  $J_{AB}$  in Hz.

## 7.2 Simulation Settings

The 'Simulations settings' panel contains some general parameters for the spin simulation:

**Number of points:** the number of real data points used to create the spectrum.

**Spectral Start:** the starting chemical shift value for the x-axis, in ppm.

**Spectral End:** the last chemical shift value for the x-axis, in ppm.

**Shift Step:** the step size for changing the chemical shift values in the simulations table when using either the mouse wheel or the up and down arrows at the edge of the cell.

**J-coupling Step:** the step size for changing the J-coupling values in the simulations table when using either the mouse wheel or the up and down arrows at the edge of the cell.

**Audit Trail:** this toggles on/off an audit trail for the simulation with the audit information saved in the file **File Name**

**Save/Load File Name:** this is the file into which the simulation parameters are saved and loaded.

**Max RT display spin number:** when the simulations parameters are changed, the simulated spectrum will update in real time provided the total number of spins (sum of identical and non-identical) is less than the number set in this options.

## 8 3D Spectrum Viewer

This option is accessible from the right-click context menu on an NMR spectrum and selecting either **3D Surface Viewer** or **3D Cube Viewer** from the available options. Typically, a 2D NMR spectrum enables the 3D Surface Viewer, while a 3D NMR spectrum enables the 3D Cube Viewer.

The 3D Spectrum Viewer provides common GUI controls available for all plot types, as well as additional tools specific to surface and cube plots.

### 8.1 3D Surface Viewer

The 3D Surface Viewer creates a 3D surface representation of a 2D NMR spectrum, where spectral intensity is displayed as peaks rising from a flat baseline across two chemical shift dimensions (Figure 73: 3D Surface Viewer):

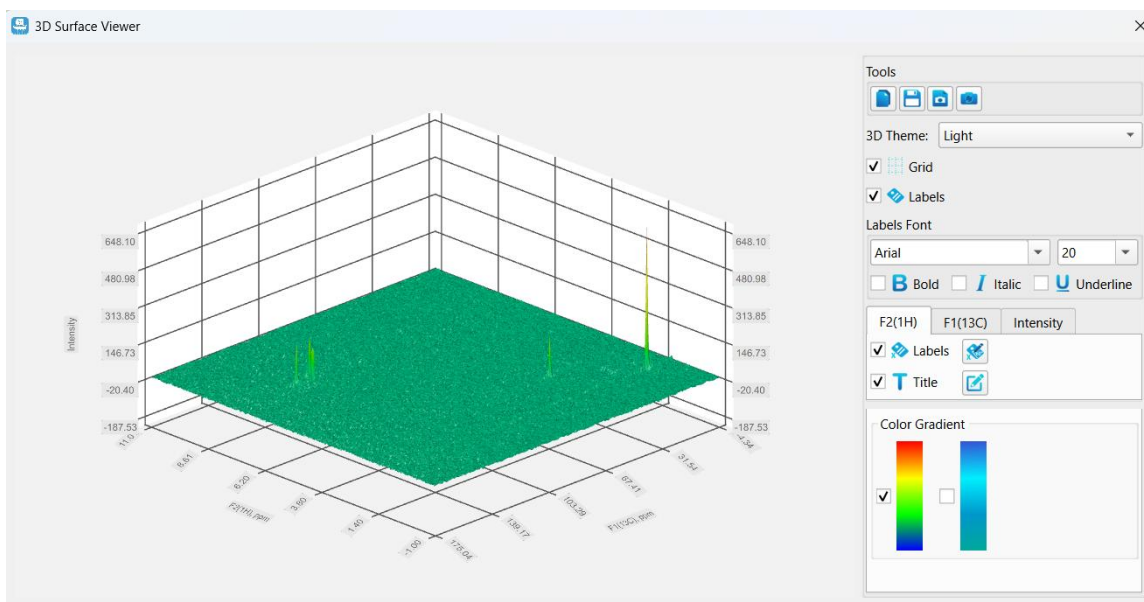


Figure 73: 3D Surface Viewer

## 8.2 3D Cube Viewer

The 3D Cube Viewer creates a 3D cube representation of an NMR spectrum, where detected resonances appear as isolated volumetric blobs (isosurfaces) within the spectral space (Figure 74: 3D Cube Viewer):

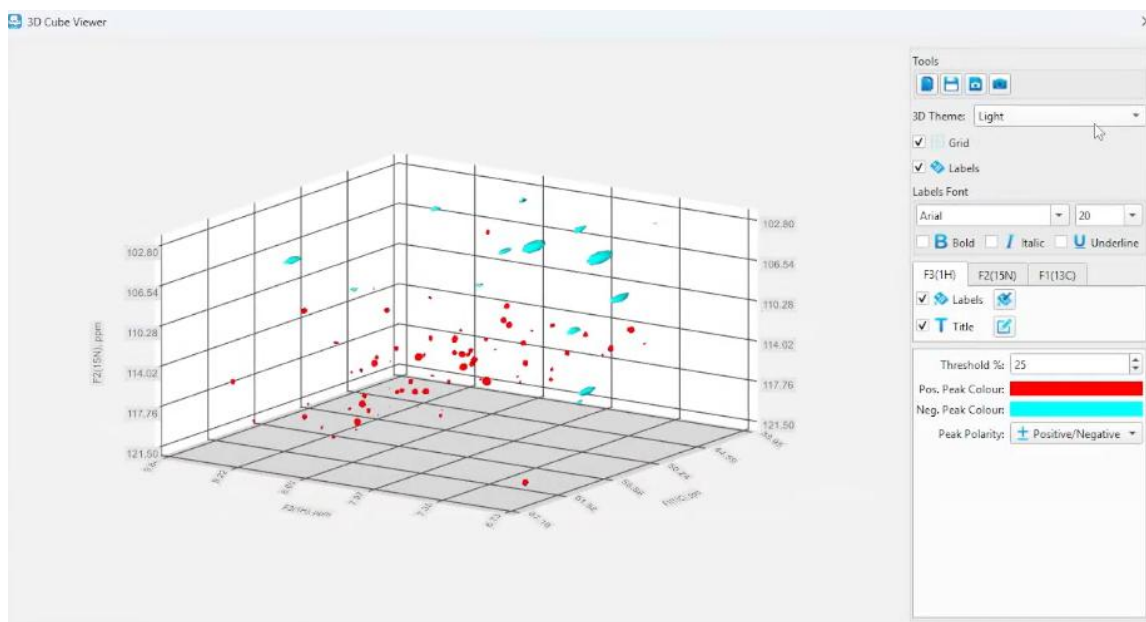


Figure 74: 3D Cube Viewer

## 8.3 3D Spectrum Viewer common GUI controls

The 2D Spectrum Viewer common GUI controls available for all plot types include:

**Copy Image:** Captures a screenshot of the current 3D spectrum and copies the image to the clipboard.

**Save Image:** Captures a screenshot of the current 3D spectrum and opens a save dialog allowing the user to save the image.

**Place Image:** Captures a screenshot of the current 3D spectrum and places the image onto the JASON canvas, then closes the 3D Viewer. Double-clicking the image on the canvas will reopen the 3D Viewer and restore it to match the captured view.

**Reset Camera:** Resets the camera position to its default view.

**Viewer Theme:** Allows the user to change the viewer theme. By default, the viewer uses JASON's current color theme. The theme can be changed using a drop-down menu with the following options: **System** (user system default), **Dark**, or **Light**.

**Grid** visibility checkbox: Shows or hides all grid lines in the spectrum viewer.

**Labels** visibility checkbox: Shows or hides the axis labels for the X, Y, and Z axes.

**Labels Font:** allows the user to specify the font used for all axis labels (X, Y, and Z axes).

Settings for **Axis-Specific Properties** allow the user to specify a configuration of properties for each individual axis, including:

Axis **Labels** visibility checkbox: Show or hide the axis label.

Axis **Labels Rotation/Angle**: Adjust the rotation angle of the axis label.

Axis **Title** visibility checkbox: Show or hide the axis title.

Axis **Title Text**: Edit the title displayed for the axis.

## 8.4 3D Spectrum Viewer specific GUI controls

**3D Surface Viewer specific GUI controls** include:

**Color Gradient**: Allows the user to modify the color gradient used to render the surface. Two gradient options are available:

**Blue to Red (default)**: A heat-map style gradient where warmer colors (red) represent higher signal intensity and cooler colors (blue) represent lower intensity.

**JASON Colors**: Uses the color gradient based on JASON's current color scheme.

**3D Cube Viewer specific GUI controls** include:

**Threshold**: Allows the user to adjust the iso-surface threshold level by changing the threshold percentage used to display peaks. The default value is 25%; after entering a new value, press 'Enter' to apply the change.

**Positive and Negative Peak Colors**: By default, peak colors are taken from JASON NMR settings, but they can be customized by the user. Clicking on the positive or negative peak color opens a color picker dialog, allowing the user to select a preferred color.

**Peak Polarity**: The peak polarity can be adjusted using a drop-down menu, which allows the user to display positive or negative peaks only or both. The default setting is taken from the JASON NMR settings.

## 9 Molecular Structures

- A video describing [Drawing a Structure in JASON](#) can be found here.

Molecular structures can be drawn, loaded from files or entered as a text.

A file can be loaded by simply using the 'Open' options in the Main Menu or dragging and dropping a file onto the Canvas. Supported formats are .mol, .sdf, and .cdxml.

A new structure can be drawn by selecting the **New ->Structure** options from the Main Menu. When the structure is selected, the user will see the options displayed in Figure 75. The structure interface comprises a **context toolbar** at the top left-hand corner of the panel and a 'View' tab, in this case displayed to the right of the canvas but as with the other panels, this is configurable. These are described in more detail below.

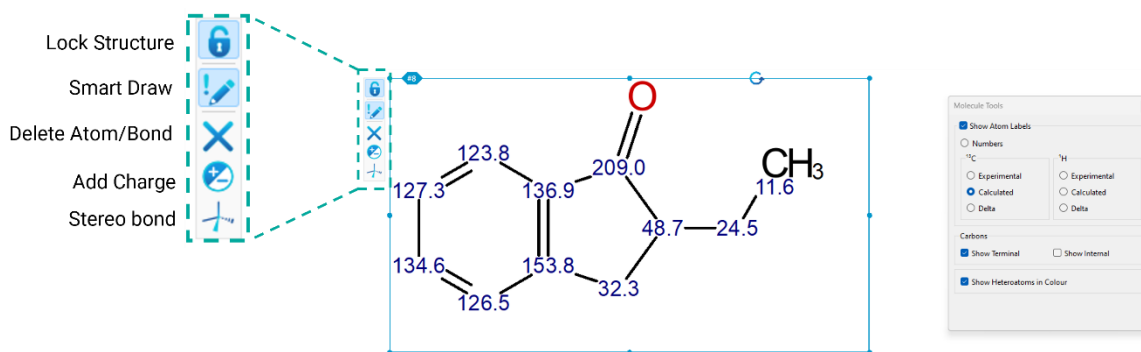


Figure 75: Molecular drawing interface

The functionality for creating a structure from text is found in the 'Molecule Tools' panel, under a 'Create Structure from Chemical Text Notation' button. JASON supports pasting text directly from clipboard and thus molecular packages; various formats, including .mol, .sdf, SMILES, InChI, SMARTS, plain text, and HTML are supported. The system automatically identifies the format and creates the corresponding items on the JASON canvas. If the format cannot be determined, a default text item will be created using the pasted clipboard content.

Note 1: For .sdf text formats, JASON processes them similarly to .sdf files, handling only the first molecule block.

### 9.1 Context Toolbar

**Lock Structure:** once a structure has been created to the satisfaction of the user, it can be locked to prevent accidental changes being made during spectral assignment. The lock is toggled on/off using this button.

**Smart Draw:** this is the primary tool for drawing or editing structures. It is a context sensitive mode.

- 1) In this mode if the user left clicks on a blank part of the panel, a carbon atom will be drawn.
- 2) If the user clicks on an atom and drags, a bond will be drawn terminating in a new carbon atom.
- 3) If the user clicks on a bond and drags, the structure will be extended creating a ring structure. The number of atoms in the ring is dependent on the length of the drag. As the drag is being performed, the proposed ring structure is shown to the user.
- 4) Clicking on an atom will cycle through a list of possible alternative nuclei, providing the user with a method to change a carbon atom to another atom, oxygen or nitrogen for example.
- 5) Clicking on a bond will cycle through a series of options for the bond, for example bond multiplicity or stereo representation of the bond. Note that when the bond multiplicity changes, the hydrogens attached are also adjusted to take this into account.
- 6) A nucleus can be set by clicking on an atom and then typing the appropriate nucleus letter on the keyboard.

**Delete Atoms/Bonds:** this mode is used to delete atoms or bonds in the structure.

**Add Charge:** this mode is used to add charges to atoms.

**Stereo Bonds:** this mode is used to specifically edit the stereo representation of bonds.

## 9.2 Molecular Tools View

**Show Atom Labels:** this toggles on/off the label chosen in the options below.

**Numbers:** this option labels the atoms numerically.

**<sup>13</sup>C Experimental/Calculated/Delta:** these options show the chemical shift value of the carbon atoms as labels. The chosen chemical shift value may be the value assigned from a spectral assignment ('Experimental'), a predicted value ('Calculated') or the difference between the experimental and calculated values ('Delta').

**<sup>1</sup>H Experimental/Calculated/Delta:** these options show the chemical shift value of the hydrogen atoms as labels. The chosen chemical shift value may be the value assigned from a spectral assignment ('Experimental'), a predicted value ('Calculated') or the difference between the experimental and calculated values ('Delta').

It is possible to choose the shifts for both <sup>13</sup>C and <sup>1</sup>H on a structure to be displayed simultaneously, the <sup>1</sup>H shifts in this case are displayed in parenthesis.

**Carbons, Show Terminal Carbons:** this option toggles on/off whether the terminal carbons in a chain are shown explicitly with their attached hydrogens.

**Carbons, Show Internal Carbons:** this options toggles on/off whether all carbons and their attached hydrogens are show explicitly.

**Show Heteroatoms in Color:** this toggles the option to show heteroatoms in color.

To change an atom label, hover the mouse over and enter the desired text ('Structure' widget should be active); to remove an atom label / display default number: press the space key once.

More options, related to assignment, can be found in the context menu available by a right-click on the structure. Apart already mentioned options of displaying assignment information (**Show on Structure** and **Show on Atom**), there is also an option to **Show Correlations** and the **Add / Remove explicit hydrogens** command. Along with the options for **Auto Assignment**, the **Clear Structure Assignment** option is available when the structure is selected; and the option to remove assignment from a particular atom (**Remove Assignment from Atom #x**) available when the molecule is selected and the mouse is positioned over a specific atom. For assigned structures, **Assignment Info (RMSD)** can be shown for C and H and updates automatically in background; the corresponding check box is found under the 'Show on Structure' option.

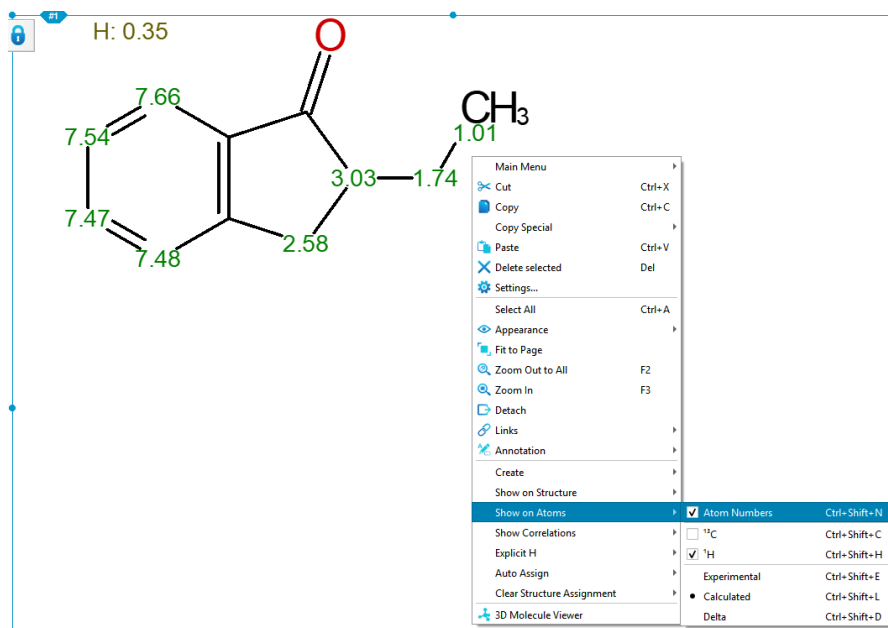


Figure 76: Assignment Tools in Structure Context menu

### 9.3 3D Molecule Viewer

The option for 3D viewing a molecule structure is found in the context menu available by a right click in the 'Molecule' window. It allows for rotating the molecule model by any angle using the mouse or touchpad.

The 'Tool' tab in the 3D Molecule viewer has the following functionality:

**Copy Image** – to capture and copy the 3D model image to the clipboard;

**Save Image** – opens the 'Save File' dialog to let the user save an image of the molecule;

**Place Image** – captures a screenshot of the 3D model and creates an image on the Canvas, automatically closing the 3D Viewer. Double-clicking on such an image reopens the 3D Viewer with the same properties it had when the image was created. The stored properties include Camera position, 3D Model representation, Measurements, and Show / Hide crystal unit cell.

**Reset Camera** – resets the Camera position to the default view;

**Reload Molecule** – resets to default all the settings in the 3D Molecule Viewer.

The user can choose between 3 styles of displaying the molecule (Ball and Stick; Ellipsoid; or Lines) under the '**Update 3D presentation**' control, as well as choose black or white for the **background**.

The 'Measurement' tab allows for measuring the **distance** between 2 atoms, the **angle** between 3 atoms, and the **torsion** between 4 atoms by the user's choice.

## 10 Extended Processing Options

Some of the processing options have two modes of operations; a basic mode for the inexperienced user and an expert mode for those users who have a deeper understanding of NMR processing. In the basic mode JASON will assist the user to make sensible choices of parameters but allowing the user to choose what effect they would like, for example, sharper lines or doubling the number of points. JASON will then attempt to select appropriate parameters. The extended options for linear prediction and apodization are shown in Figure 77.

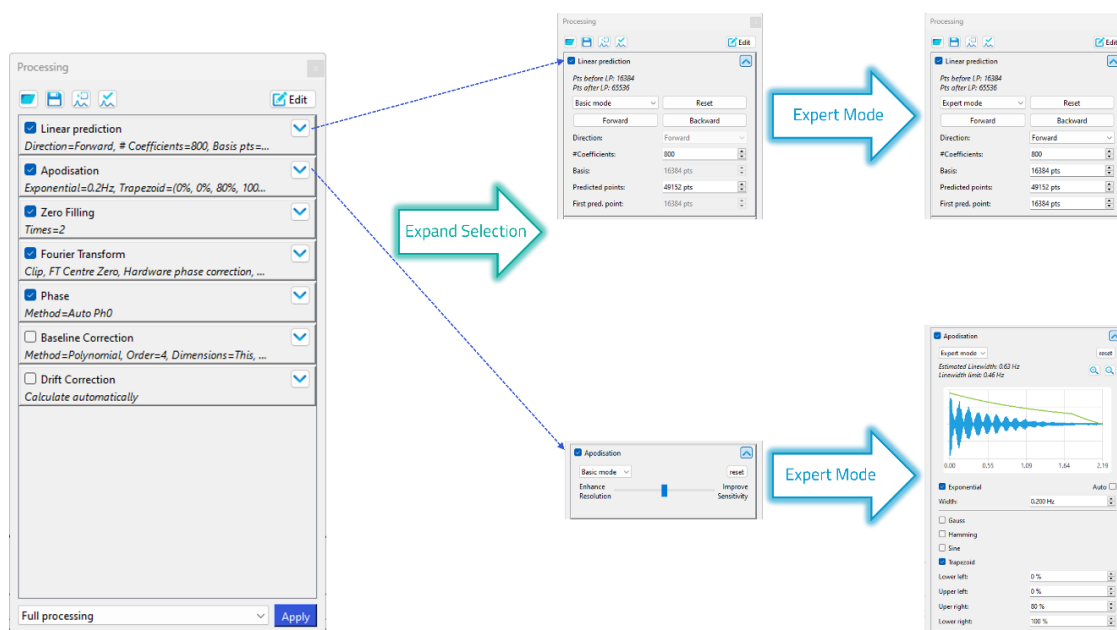


Figure 77: Extended Processing Options

### 10.1 Linear Prediction

On expanding the linear prediction options, using the arrow in the top right-hand corner of the 'Linear Prediction' option box, the user is presented with the full options for linear prediction. The first option is a drop down box from which the user may select **basic mode** or **expert mode**.

The default parameter values are imported from the data when specified in the original vendor format, similar to Apodization and other parameters. When linear prediction was not used for a 2D data, JASON inserts an inactive linear prediction element to the processing list with its parameters automatically set to provide four times improved resolution.

The **Reset** button resets the linear prediction to the default, including removing the LP processing if it was not applied at the time of data import into JASON.

The **Forward** or **Backward** buttons provide automatic setup of the linear prediction parameters for the appropriate direction of prediction.

In **basic mode** only a few options are editable by the user, these are:

**#Coefficients:** the number of linear prediction coefficients used.

**Predicted points:** the number of points which are predicted by the linear prediction

The user does not need to set any of the Linear Prediction parameters, JASON will automatically selected a suitable set of parameters.

In expert mode, the advanced options are available to the user including a group delay correction when backward LP is applied in the direct dimension on digitally filtered data.

## 10.2 Apodization

As with Linear Prediction, Apodization has two modes, **basic** and **expert**, selectable using a dropdown menu.

In the **basic mode** only a slider is presented to the user. The slider allows the user to adjust the quality of their spectrum between enhancing the resolution of the spectrum (the sharpness of the lines) and enhancing the sensitivity (Signal / Noise). As default, JASON will select a balance based on the average linewidth of the spectrum. Currently this mode is only available for 1D spectra.

Full control over the apodization functions and their parameters is offered in **expert mode**. The expert mode uses parameters from the processing list associated with the data as its default and a preview of the apodization envelope is also shown in this mode.

## 11 Rules

In JASON, **Rules** allow the user to determine a set of actions which occur when a spectrum or item of this type is opened and placed on the Canvas.

There are three types of Rules: **Processing**, **Analysis**, and **Layout**. Once a spectrum is opened on the Canvas, the first thing JASON looks for is a processing rule. If there is one, then the actions prescribed in it will be applied. Otherwise, standard processing will be applied. JASON will then apply the analysis and layout rules. If there are multiple matching rules of each type, the first one is applied.

All three types of rules have the same set of potential conditions. Typically, processing rules will have more conditions selected, whereas analysis and layout rules will use fewer conditions. This is shown in the condition checkboxes ticked by default in the corresponding dialog boxes (see Figure 78).

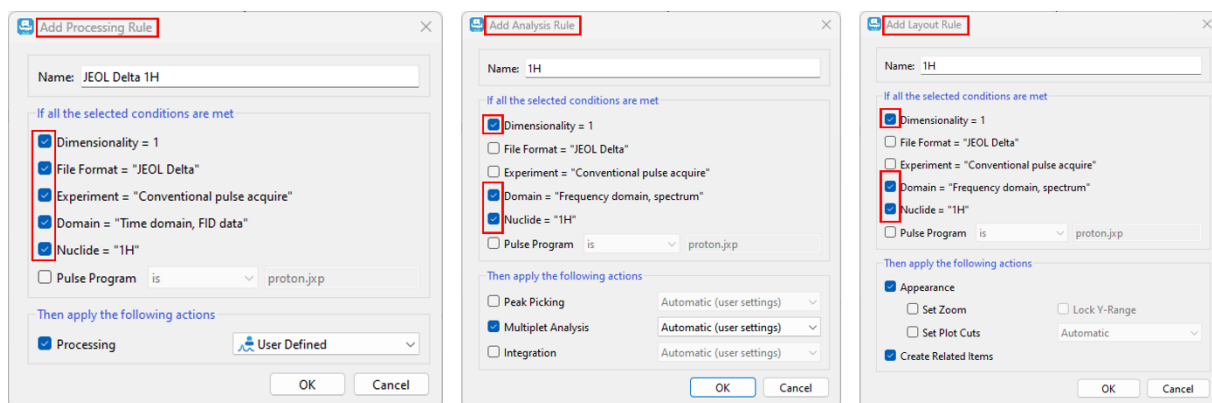


Figure 78: Rule Dialog Boxes

If the type of experiment is not known, then pulse program name will be suggested as an alternative condition. Also, in the case of the JCAMP-DX format data, an additional 'Origin' condition checkbox is added.

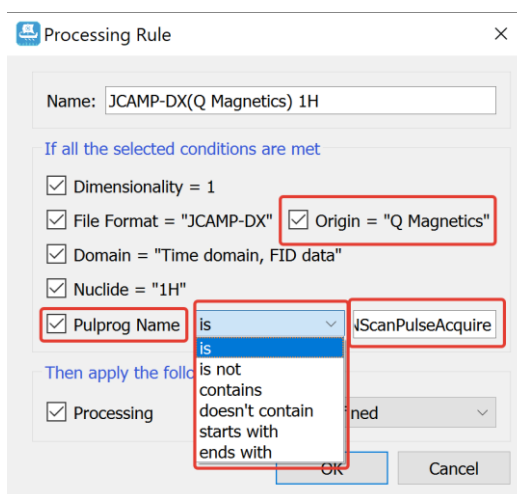


Figure 79: Processing Rule by Pulse Program

For 2D spectra, the conditions of the Y-dimension become available.

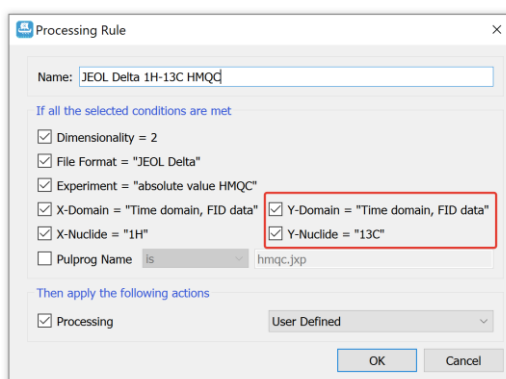


Figure 80: 2D Experiment Processing Rule Dialog

## 11.1 Managing Rules

Rules can be managed in the 'Rules' panel available by a click on the 'Rules' panel toggle button on the toolbar:

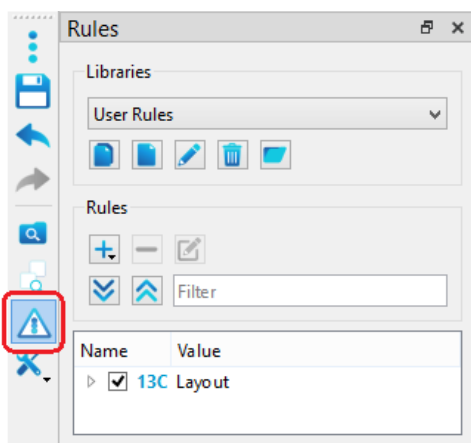


Figure 81: Managing the Rules Panel

## 11.2 Rule Libraries

Rules can be grouped into libraries, allowing users to organize different rule sets for different applications.

The ability to add new rules is available when there is an active spectrum on the Canvas.

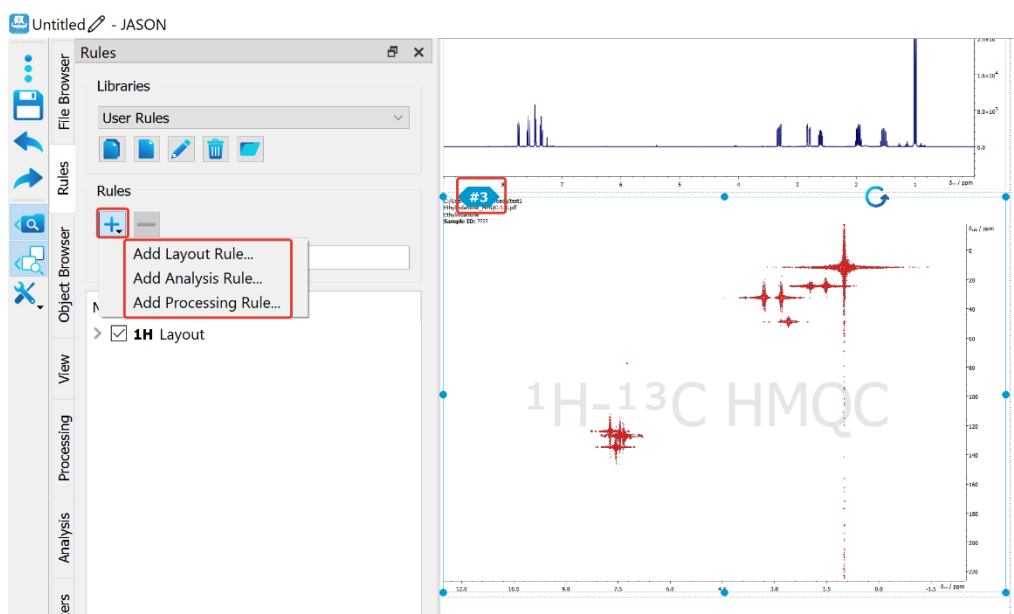


Figure 82: Adding a new Rule

### 11.3 Processing Rules

As with the 'Processing Rule' panel, the user is given the option to choose between 'User Defined', 'Recommended', and 'Rawdata' processing types.

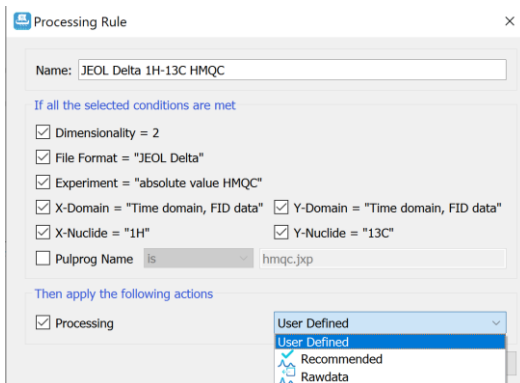


Figure 83: The Processing Rule Dialog

### 11.4 Analysis Rules

Analysis rules currently support Automatic Peak Picking, Integration, and Multiplet Analysis. The corresponding checkboxes are ticked automatically depending on what was set in the original spectrum.

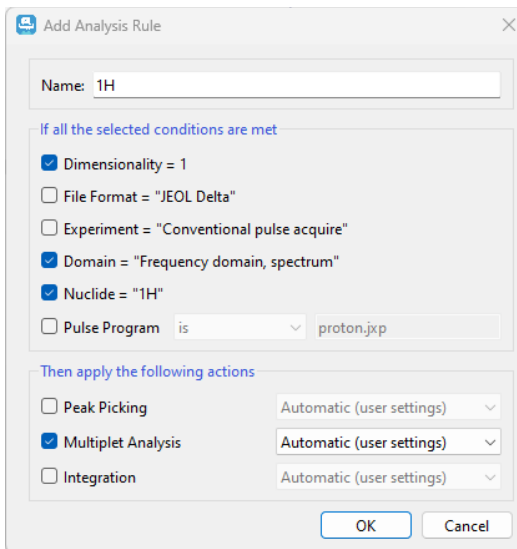


Figure 84: The Analysis Rule Dialog

## 11.5 Layout Rules

In the case of Layout rules, there are currently only two options available (Appearance and Related Items), but each of these is very powerful. **Appearance** refers to the geometry, styles, zoom, annotations, and any cuts applied to the spectrum. **Related Items** are all the linked tables, multiplet reports, insets, molecules, as well as the same items of the same type, such as insets, created from the original spectrum. In addition, Related Items include all images and text boxes located on the same page with the spectrum and any of the related items listed above. The spectrum layout rule therefore actually defines a whole cluster of items.

### 11.5.1 Important Features of the Layout Rules

1. Layout rules store information on the position of the spectrum and other items so that when a rule is applied, the spectrum and its associated items are all positioned correctly. The spectrum does not need to be in the same location on the Canvas as when the rule was created. This ensures that a spectrum can be placed anywhere on the Canvas, and the layout will be applied correctly.
2. Tables will remember their appearance. For example, the parameter table will remember the template from which it was created and so will appear the same.
3. When applying layout rules containing molecules, empty molecule items will be created, where the user can later either draw or drag and drop a .mol file. Even though the molecule object is empty, its properties are taken from the layout rule.
4. Text boxes and images are placed by layout rules as they originally were.
5. In the Appearance action, the ability to control the zoom is provided. There is a checkbox that controls whether zoom information is stored by the rules. Additionally, for 1D spectra there is a checkbox that controls whether the rules will store the vertical zoom range. The set plot cuts check box allows the user to include automatic or user defined plot cuts within the layout rules. If the spectral item used to create the layout rule includes cuts, the combo box will offer Custom Ranges or Automatic options. If the spectral item does not contain cuts, only the Automatic option will be displayed.

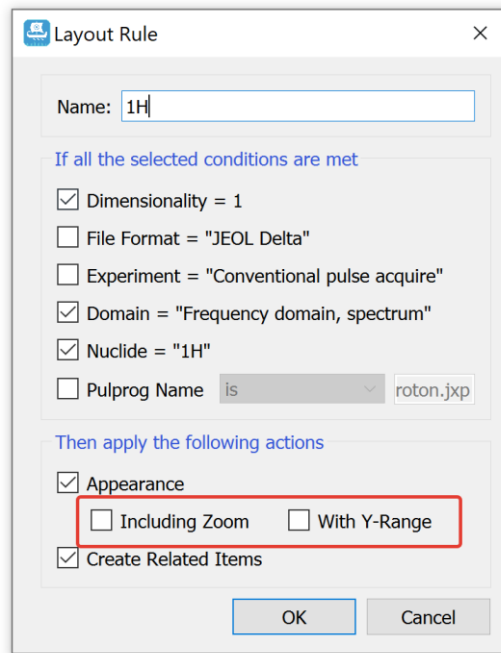


Figure 85: Layout Rules; Appearance options

## 11.6 Created Rules

The created rules appear in the list of rules in the 'Rules' panel. For the rules, the operations of deletion, disabling, renaming, editing (via the right mouse click), reordering (via drag and drop) are available.

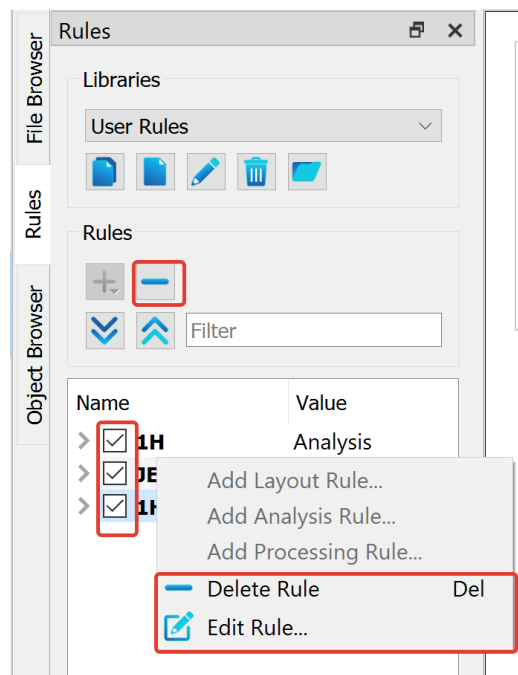


Figure 86: Editing Rules

The rules applicable to the active spectrum are highlighted in the list of rules with the active color. If multiple rules of the same type are applicable, the potentially applicable rules are highlighted with a dim active color.

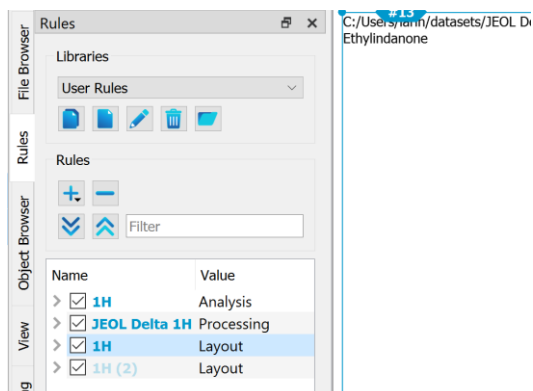


Figure 87: Applicable rules to the Active Spectrum are highlighted

The 'Apply Rule' button (as well as the context menu 'Apply Rule item') becomes enabled when both a spectrum and an applicable rule is selected in the Rule Browser. The 'Apply Rule' feature also works with multiple selected spectra. In that case, one of the spectra needs to be active:

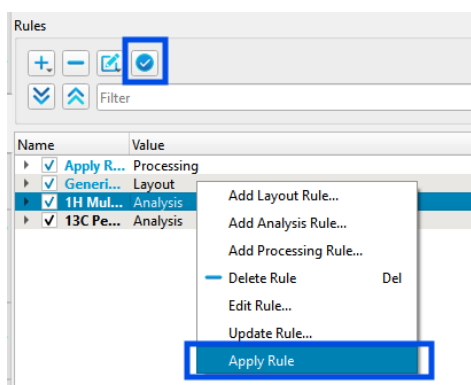


Figure 88: 'Apply Rule' option

Rules can be updated using the 'Update Rule' option. The 'Update Rule' option will only be enabled if the selected rule is applicable to the chosen spectrum.

## 11.7 Rule Names

Rule names are generated automatically, but are editable. The automatic name is generated based on the chosen conditions and so as to be meaningful. Names do not need to be unique and can be set by the user to aid their usage.

## 12 Mass Spectrometry

From JASON version 3.2, mass spectrometry data is supported for the JEOL JMS-S3000 SpiralTOF instrument.

The JASON canvas works in the same way for mass spectrometry data as for NMR data.

### 12.1 Opening MS data

To open data, use the JASON File Browser to locate the desired file(s) and then either double click on the file or drag and drop it onto the Canvas. Files can also be opened from the JASON main menu or by using 'Ctrl + O' ('Cmd' on Mac).

The final way to open files is to drag them from the Windows File Explorer or Mac finder window onto the Canvas. The file(s) will be opened on the Canvas wherever the mouse cursor dropped them and organized as per the settings in Settings -> General -> Canvas -> Layout.

### 12.2 Viewing and interacting with MS data

When MS data is opened on the JASON Canvas, the context menu for the spectrum is shown on the top left of the spectrum. The context menu contains the available tools for interacting with the spectrum as shown below:

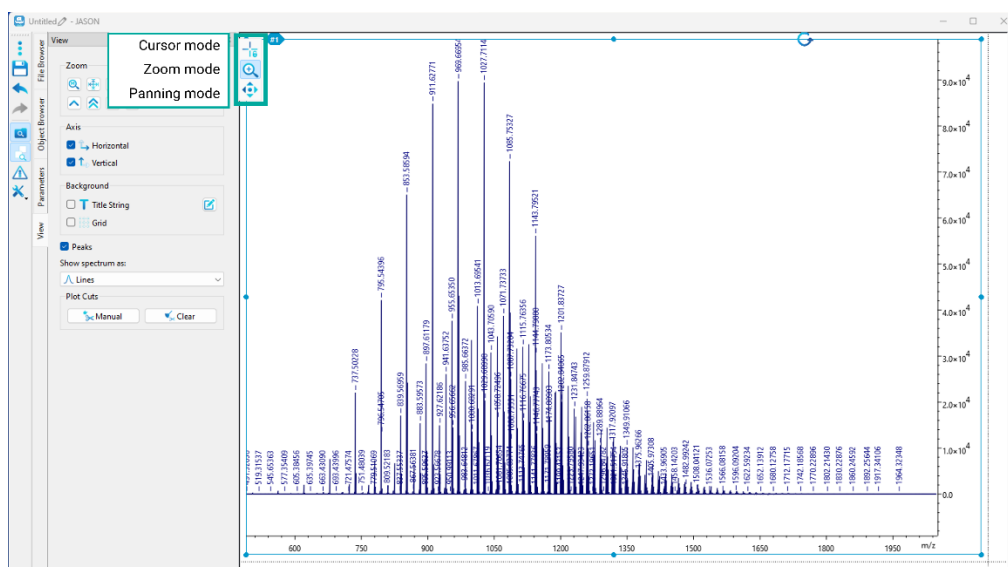


Figure 89: Mass Spectrometry context menu

## 12.2.1 The View Panel

The 'View' panel contains the available tools for viewing the MS data.

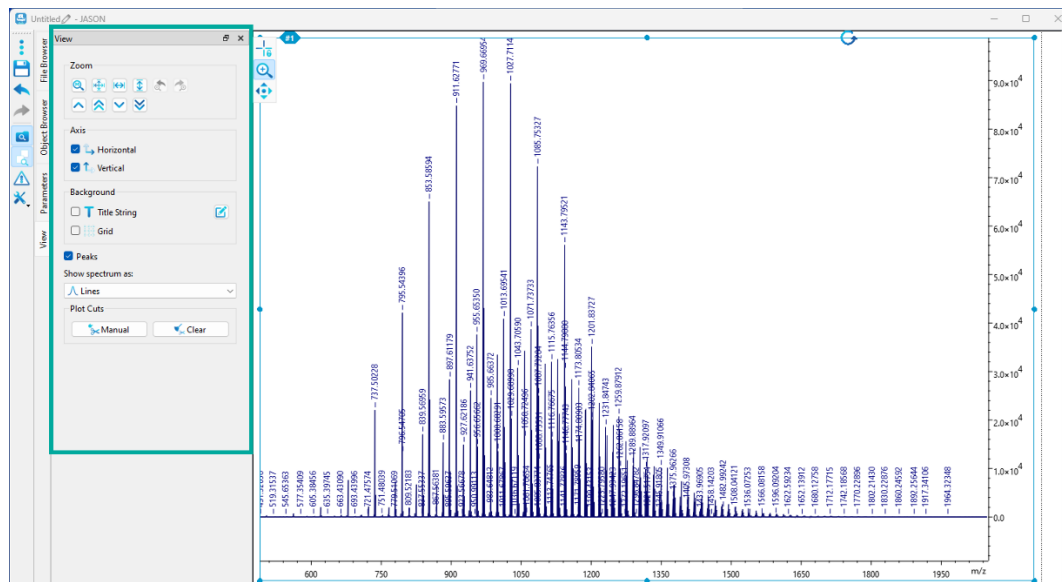


Figure 90: View Panel; Mass Spectrometry data

It is possible to use the **Zoom** tools to change the zoom of the displayed spectrum.

The **Axis** tools allow the user to turn on or off the respective axes.

The **Background** settings allow the users to show/hide and edit the spectrum title and to view a grid on the spectrum if desired.

The **Peaks** checkbox turns on or off the display of the peaks on the spectrum and it is possible to change the **display** of the plotted peak type (Lines, Sticks, Lines and points) using the drop down box.

The **Plot Cuts** section allows the cutting of areas of the spectrum using the manual tool. Cuts can be cleared using the clear button.

## 12.2.2 The Parameters Panel

The 'Parameters' panel displays the parameters associated to the spectrum, the 'Reports' tab enables the user to create a parameters report.

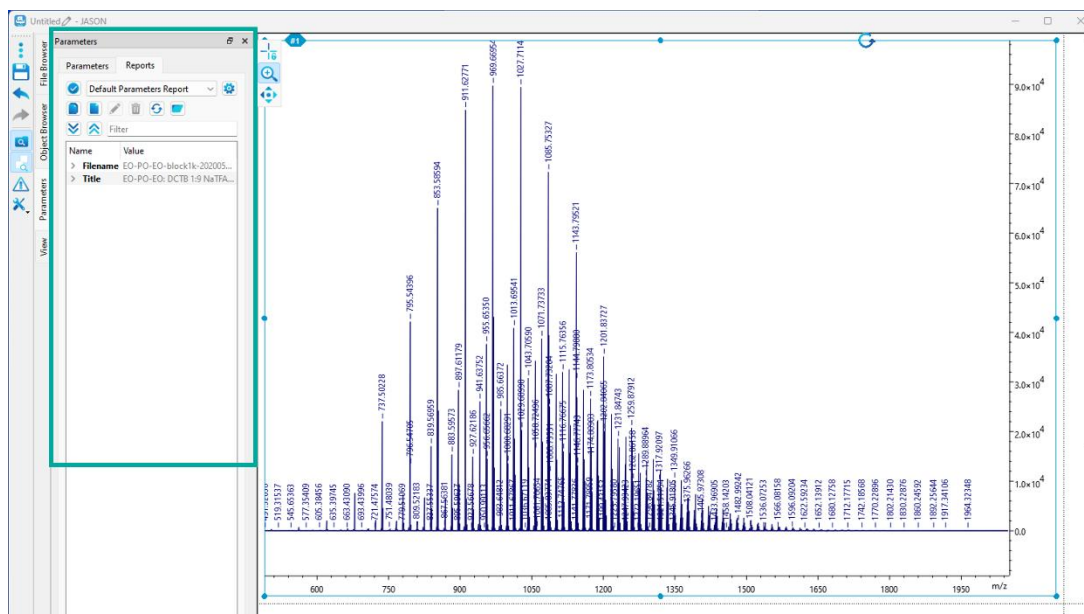


Figure 91: Parameters Panel; Mass Spectrometry data

### 12.3 Saving MS data

MS data from JASON can be saved in the JASON jjh5 and jjj formats and as JCAMP-DX files, as well as the standard JASON options including PDF, jpeg, png and svg.

To save data, navigate to the 'Save' button on the JASON menu bar, or by using 'Ctrl + S' ('Cmd' on Mac). The 'Save as' option can be found under the JASON three dots main menu button.

## 13 Appendix

### 13.1 Keyboard Shortcuts

Other useful: keyboard shortcuts and keyboard combinations are listed below:

Windows	MacOS	Functionality
Key	Key	Functionality
Del	Del	Delete selected item
<b>Ctrl+A</b>	<b>Cmd+A</b>	Select all
<b>Ctrl+Z</b>	<b>Cmd+Z</b>	Undo
<b>Ctrl+X</b>	<b>Cmd+X</b>	Cuts selected items to clipboard
<b>Ctrl+C</b>	<b>Cmd+C</b>	Copy selected item
<b>Ctrl+V</b>	<b>Cmd+V</b>	Paste item
<b>Ctrl+S</b>	<b>Cmd+S</b>	Save
<b>Ctrl+U</b>	<b>Cmd+U</b>	Undo Zoom
<b>Ctrl+I</b>	<b>Cmd+I</b>	Redo Zoom

Where **Ctrl** (Cmd) and one other key are indicated, press and hold the **Ctrl** (Cmd) key then press the second key.

## 13.2 Supported File Formats

- Bruker TopSpin:
  - raw (fid/ser): conventional 1D, 2D, and 3D; 2D NUS, DOSY, pure shift
  - processed (1r, 2rr, 3rr, 4rr,..8rr) data
- Bruker WinNMR:
  - raw and processed 1D and 2D data
- CCP-NC MAGRES (free plugin) compatible with output files created by:
  - CASTEP
  - Quantum ESPRESSO
- Chemagnetics/Varian Spinsight: 1D, 2D raw and processed data
- JCAMP-DX from any other software, including vendor-specific 1D and 2D data:
  - ACDLabs
  - Bruker TopSpin
  - JEOL Delta
  - Nanalysis
  - NUTS
  - Magritek
  - Mestrelab
  - Oxford Instruments
  - ThermoFisher picoSpin
  - Q\_Magnetics
  - Varian/Agilent
- JEOL Delta (JDF):
  - raw: conventional 1D, 2D, and 3D; 2D NUS, DOSY, pure shift
  - processed: 1D, 2D and 3D
  - JDA (JEOL Data Archive)
- JEOL Alice 2: 1D and 2D data
- Magritek:
  - SpinSolve: 1D, 2D, and 2D DOSY
  - SpinSolve Expert: 1D, 2D
- NMRPipe:
  - Processed 1D and 2D, (no support for DOSY)
- RS2D SPINit:
  - 1D and 2D including versions both before and after 2022.06

- QOne SpinStudioJ
- SIMPSON (free plugin): 1D
- TECMAG/TNMR (free plugin): 1D, 2D
- Varian/Agilent VnmrJ:
  - Raw (fid): conventional 1D, 2D; 2D NUS and DOSY