



# 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 operating system.*

# 1 Getting Started

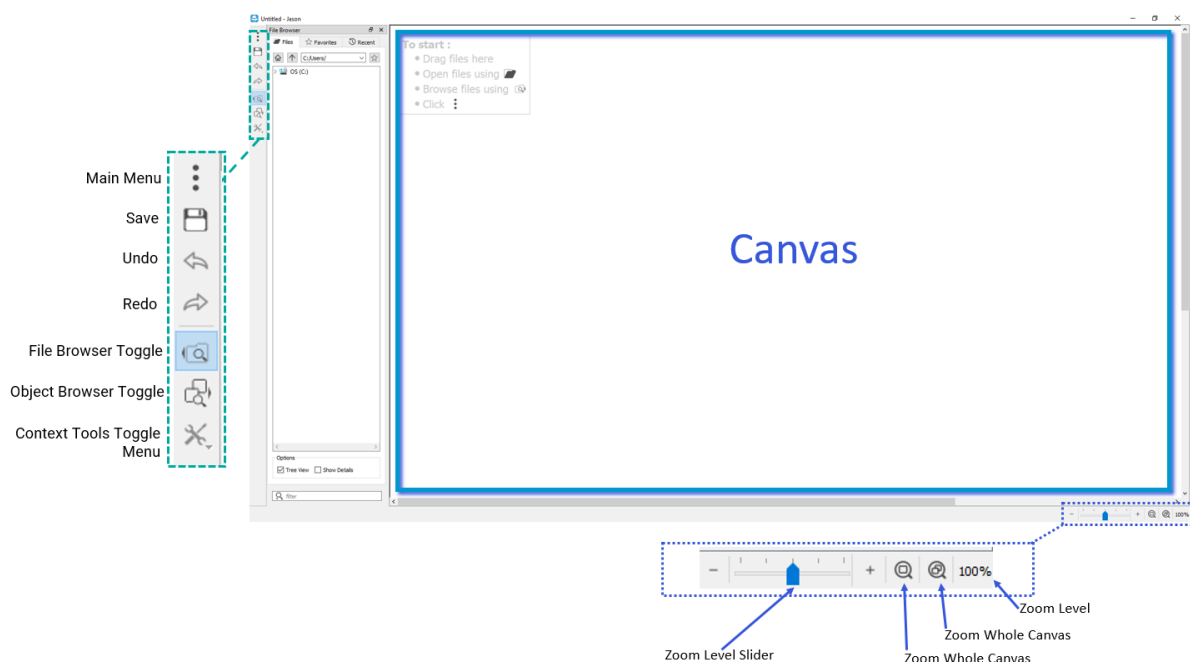


Figure 1: JASON canvas when the software is first opened.

When a new instance of JASON is opened, by double clicking the desktop icon, the user is presented with an empty workspace are 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 dialogue allowing the user to choose where to save the file and what to name it. A previously saved file will automatically be save 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. **Context tools toggle menu**, which provides a menu of options for toggling the visibility of various data manipulation tools.

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

## 2 Loading Data into JASON

There are three primary methods for loading data into JASON:

1. Drag and drop a file from Windows Explorer onto the canvas (see **Error! Reference source not found.**).
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

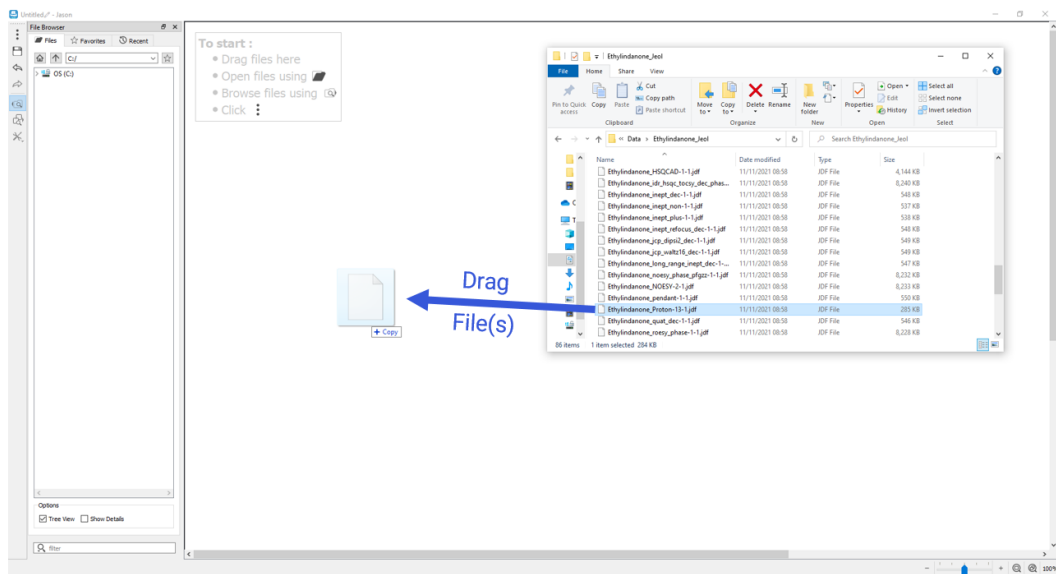


Figure 2: Loading a file from Windows Explorer

A suitable data file 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.

### 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.

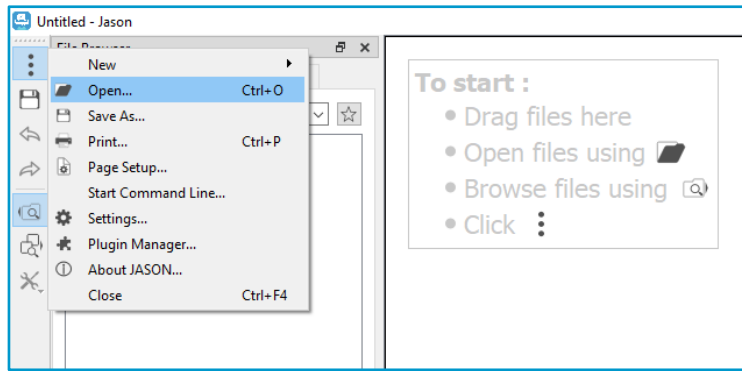


Figure 3: Loading a file from the Main Menu

### 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 **Error! Reference source not found.**. Note that the layout of JASON is configurable and the file browser can be detached and reattached at any edge of canvas simply by dragging the whole browser using the name bar at the top of the file browser frame.

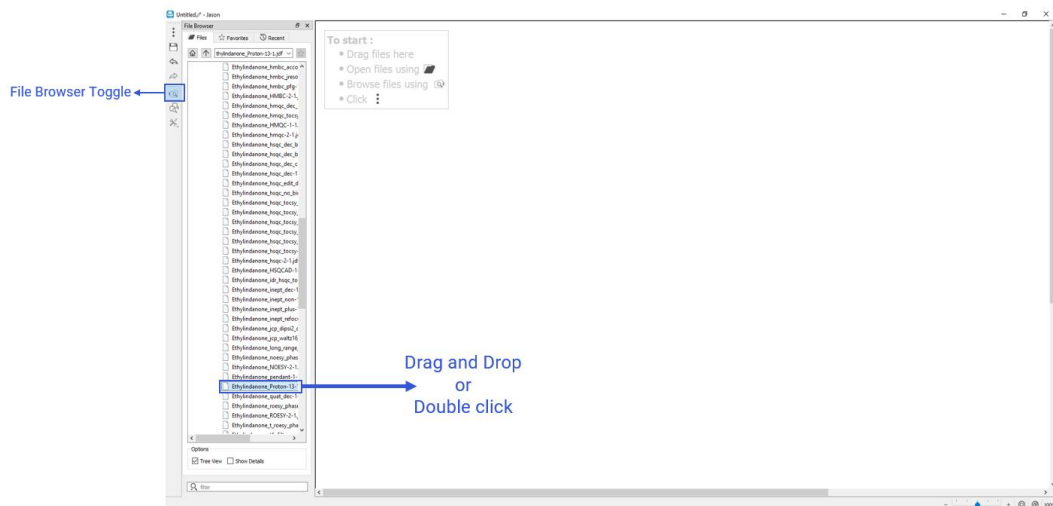


Figure 4: Loading data from the JASON file browser

The file browser itself comprises three panels (see **Error! Reference source not found.**)

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

A file can be loaded from the file browser by simply navigating to the directory of choice and double clicking on the desired file. 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 control and selecting individual files, see **Error! Reference source not found.**. The selection is then dragged to the canvas to load the files.

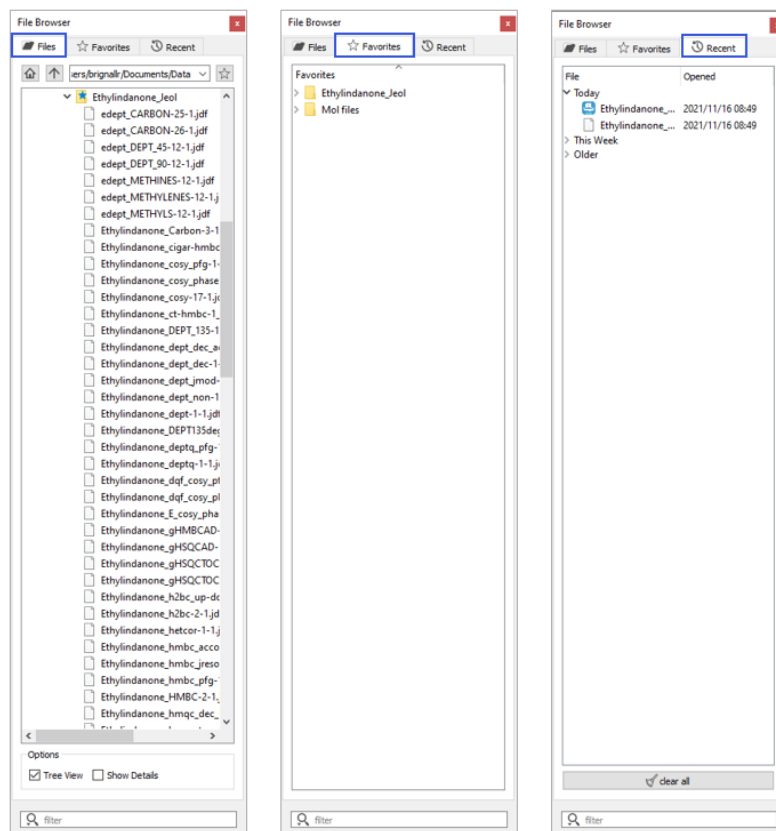


Figure 5: The file browser tabs

## 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. More details of how to manipulate canvas objects are given in the following section.

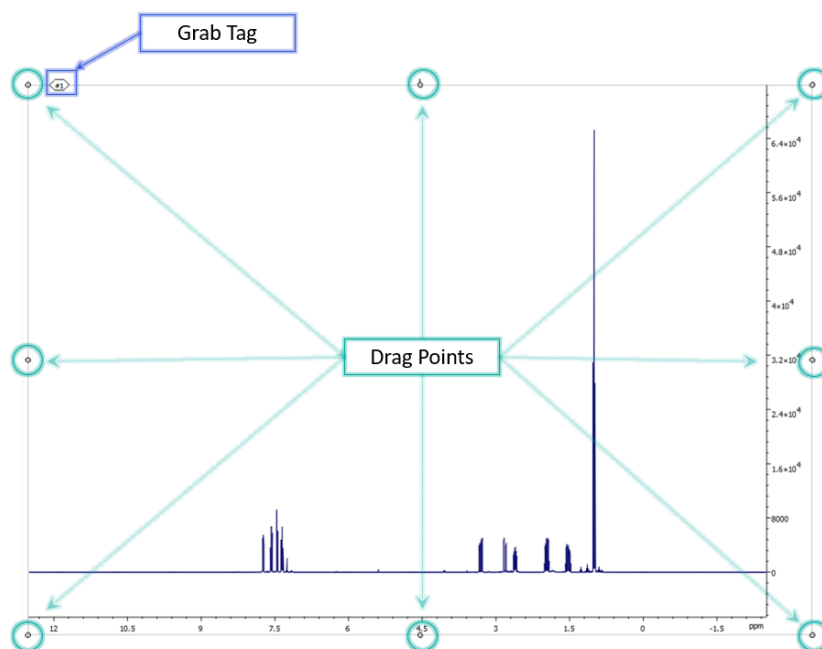


Figure 6: Grab tab and drag points for moving and rescaling canvas objects

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 create 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 7). The settings menu is accessed from the main menu in the top left-hand corner of JASON and will be described in more detail in a Section 5.

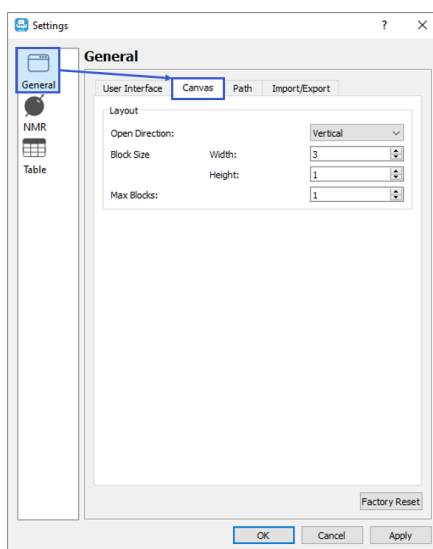


Figure 7: Canvas Settings



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

An overview of the tools a 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 8 shows those typical for a 1D NMR spectrum.

### 3.1 Context Tool Bar

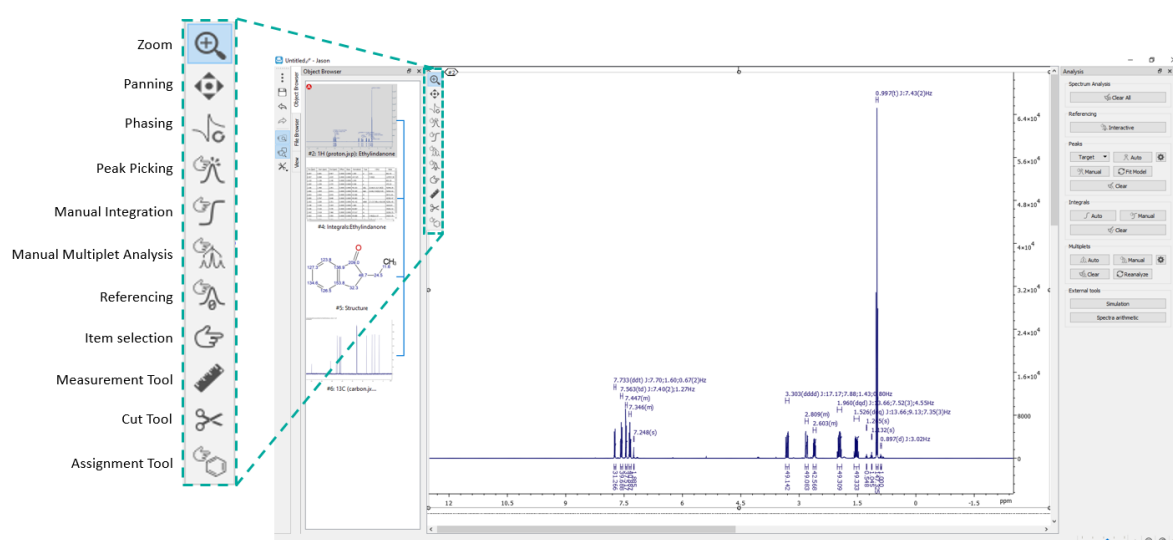


Figure 8: Context Tool Bar

When an object is selected in JASON the **context tool bar**, shown in Figure 8, 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 the icon of choice or pressing the appropriate short cut key on the keyboard. In addition, a particular functionality can be temporarily activated by holding down the short cut key. For example if a user is phasing a spectrum but need to zoom into a region of the spectrum, they can simply hold down the “z” key (the short cut for zoom), zoom into the desired region and on release of the “z” key control will return to the phasing functionality. In the following description, the shortcut key is given in parenthesis after the mode name. The short cut is not case sensitive. There are some generic functions, double clicking the left mouse button resets the zoom level to full view and scrolling the mouse wheel increases or decrease the intensity of a spectrum.

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

**Phasing (F):** In 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 9.

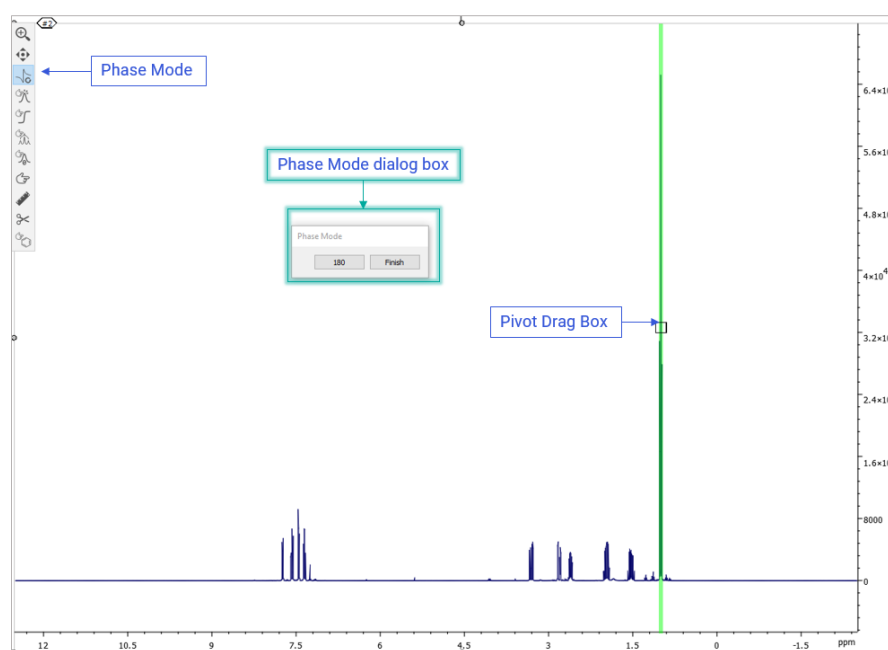


Figure 9: Interactive Phasing Mode

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 users 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 phase mode by clicking the finish button on the phase mode dialog box.

The Phase 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.

2D NMR data is phased in a similar manner, see Figure 10. 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.

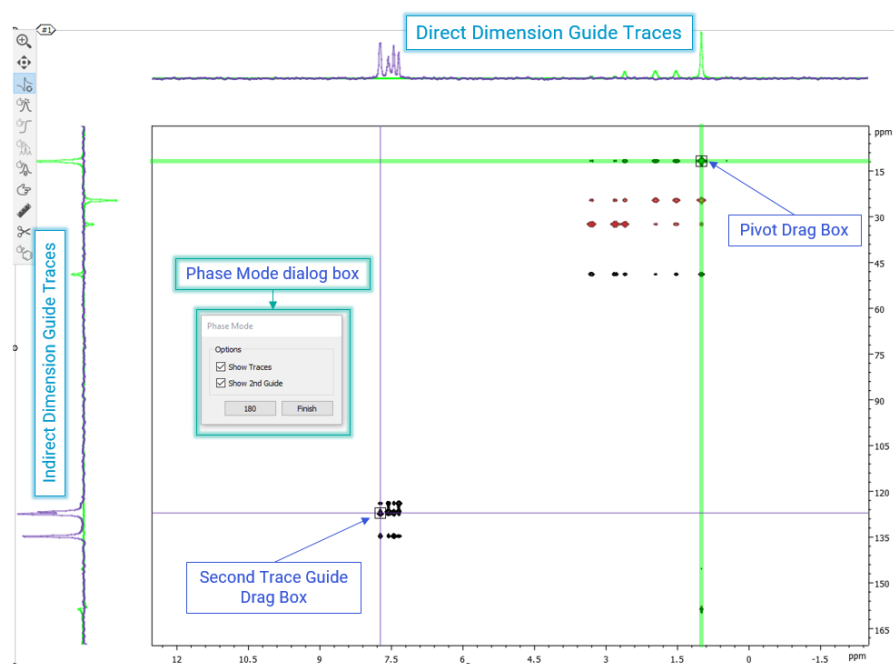


Figure 10: Interactive Phasing 2D

The Phase 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** 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.

**Peak Picking (K):** In peak picking mode, a 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 **Error!**

**Reference source not found.** By default, the cursor will attempt to “snap to” potential peaks, but if the **Ctrl** button is held down the user can place the peak flag freely.

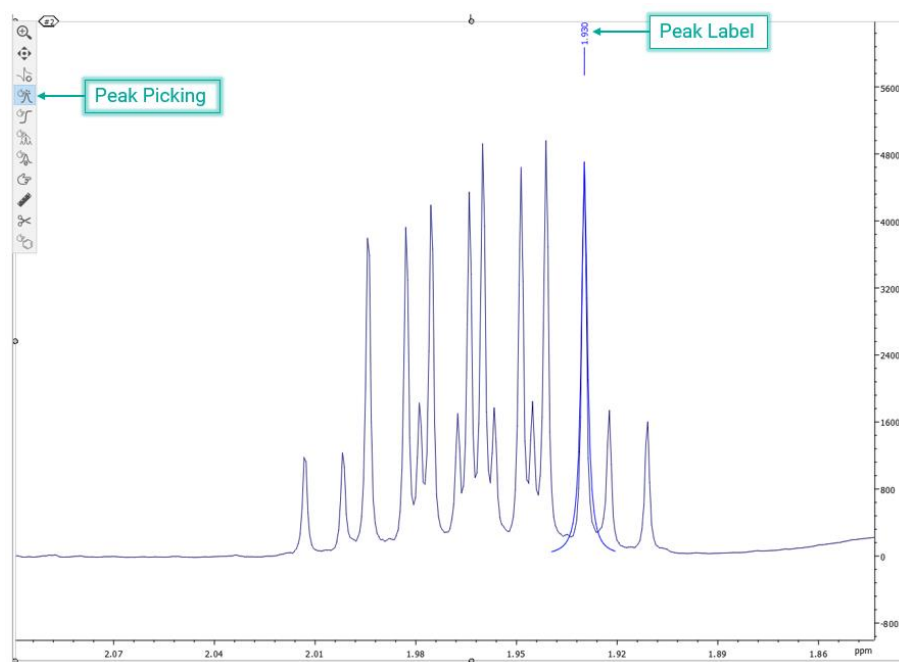


Figure 11: Peak Picking Mode

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. 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 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 12. 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**.

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.

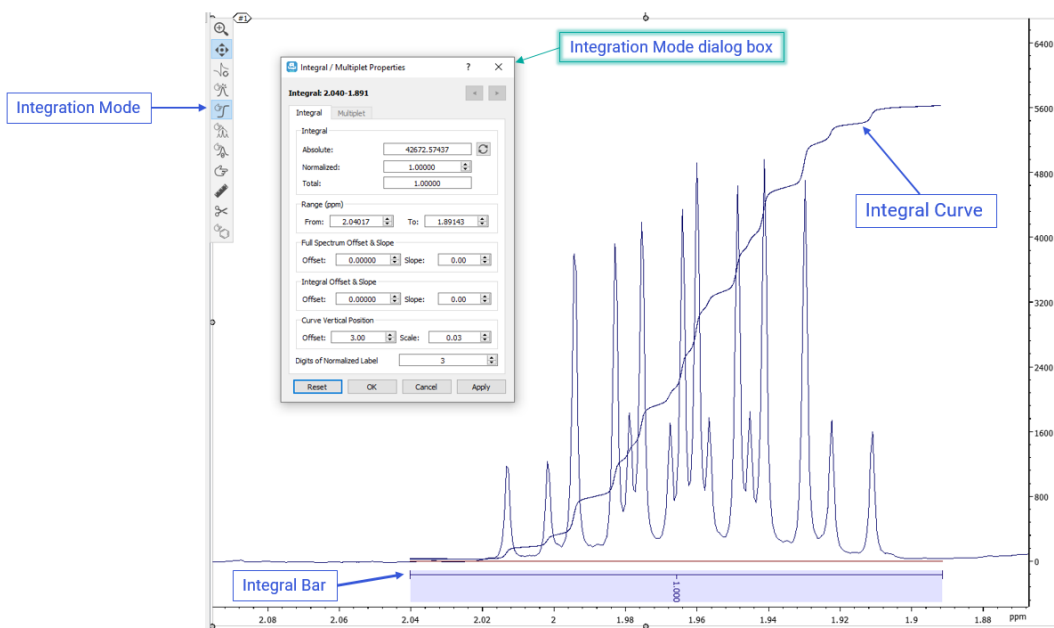


Figure 12: Manual Integration Mode

**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 13.

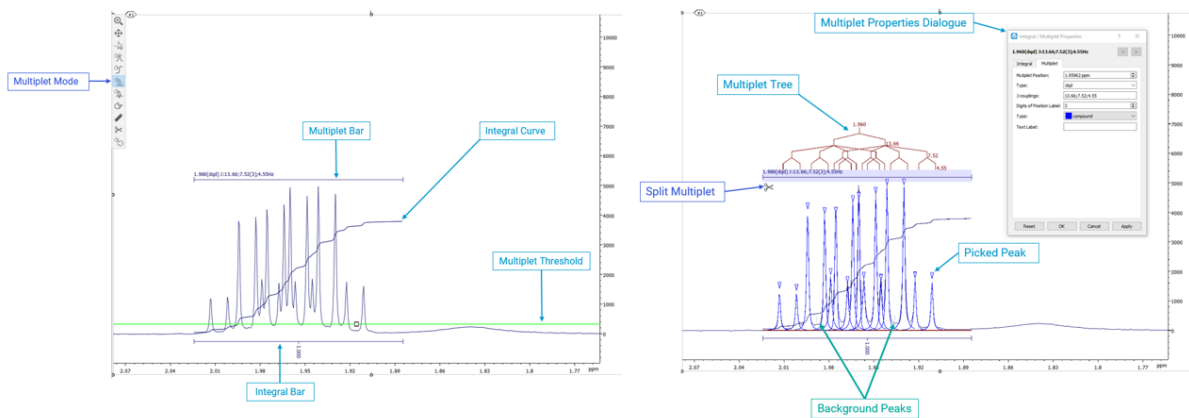


Figure 13: Manual Multiplet Analysis Mode

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 appears. Peaks above the threshold will be used in multiplet analysis, while peaks below 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 as shown. When the

multiplet bar is highlighted, peaks belonging to the multiplet are marked with a blue triangle label while background peaks, i.e., those that were smaller than the threshold are marked with small grey ticks. 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.

**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** key should be held down.

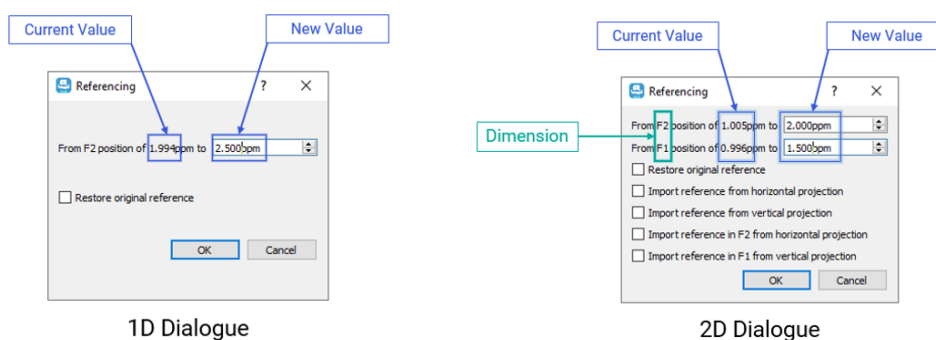


Figure 14: Referencing Dialog

The referencing dialog is shown in Figure 14, 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).

**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.

**Measurement Tool (D):** When the measurement tool mode is selected, a user can make accurate measurements between two points on a spectrum. The first point is selected by moving the mouse to a point on the spectrum and holding down the left mouse button. The measurement is then performed by dragging from the first point to the end point, which is defined by releasing the mouse button. In default mode on a 1D spectrum, the cursor will snap to the top of the nearest peak but a free selection can be made by holding down the **Ctrl** key. 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 15. When the measurement mode is selected, an extra tab, labelled "measure" opens to the left-hand side of the canvas (in this configuration). This tab contains the measurement tool options. These are the options that allow the user to make a single measurement, in this mode if a new measurement is made then the

previous is deleted. The multiple measurement mode maintains each measurement as the user creates them.

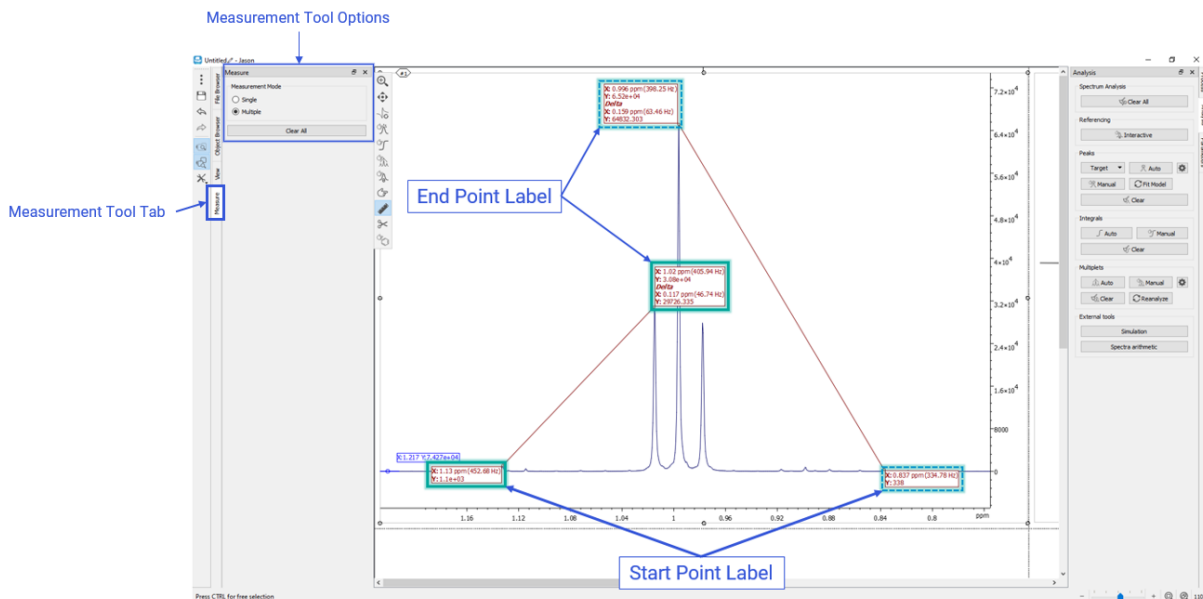


Figure 15: Measurement tool

The **Clear All** button deletes all current measurements. If a user wishes to delete a particular measurement, this can be done by moving the cursor close to one of the measurement lines. A red cross will appear and the line can be deleted using the red cross.

**Cut Tool (T):**

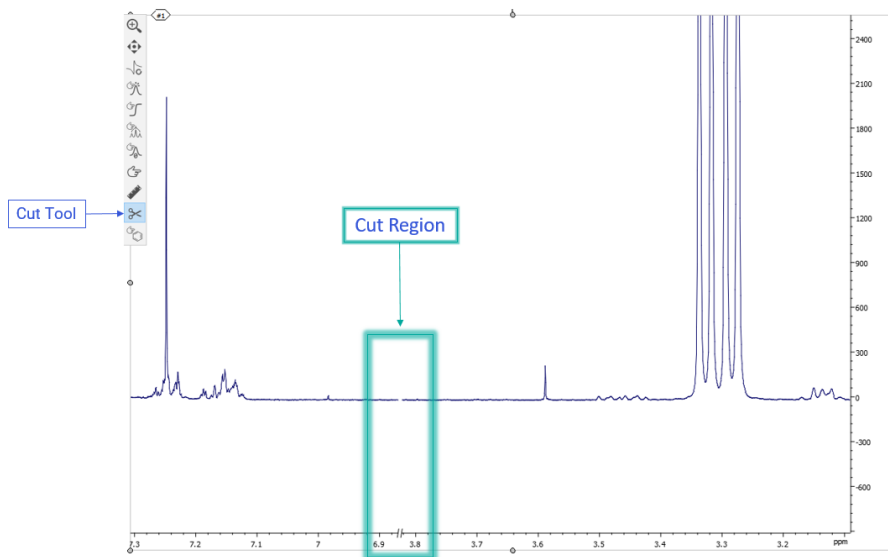


Figure 16: Cut region in a 1D spectrum

Selecting the 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 16. 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 17.

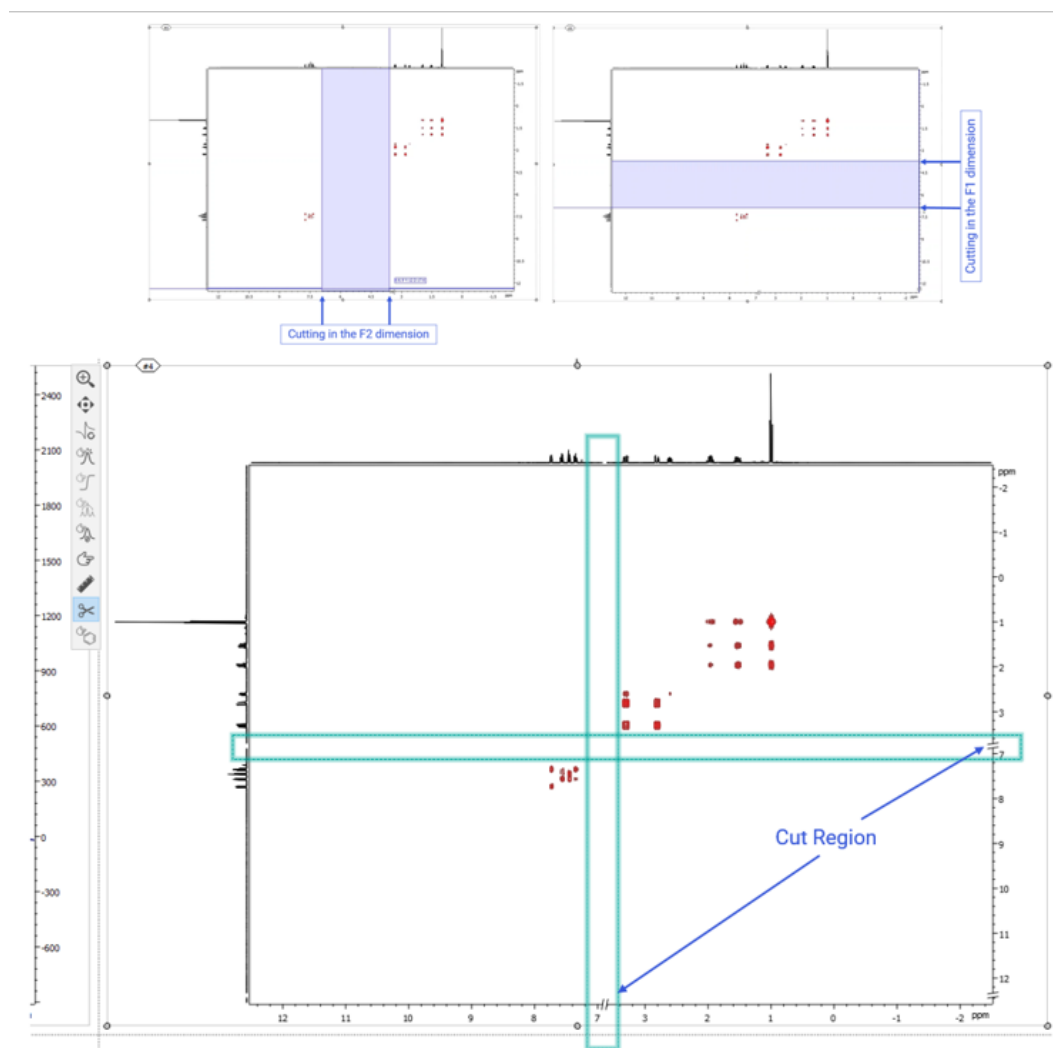


Figure 17: Cut regions in a 2D spectrum

It is worth noting that if a 1D spectrum is used as the projection, as in Figure 17, then the cut region in the appropriate dimension will be shown as a discontinuity in the base line of the spectrum.

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

**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 a molecular structure (see Section 8). 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

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 18. 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 18, or stacked vertically as in Figure 19.

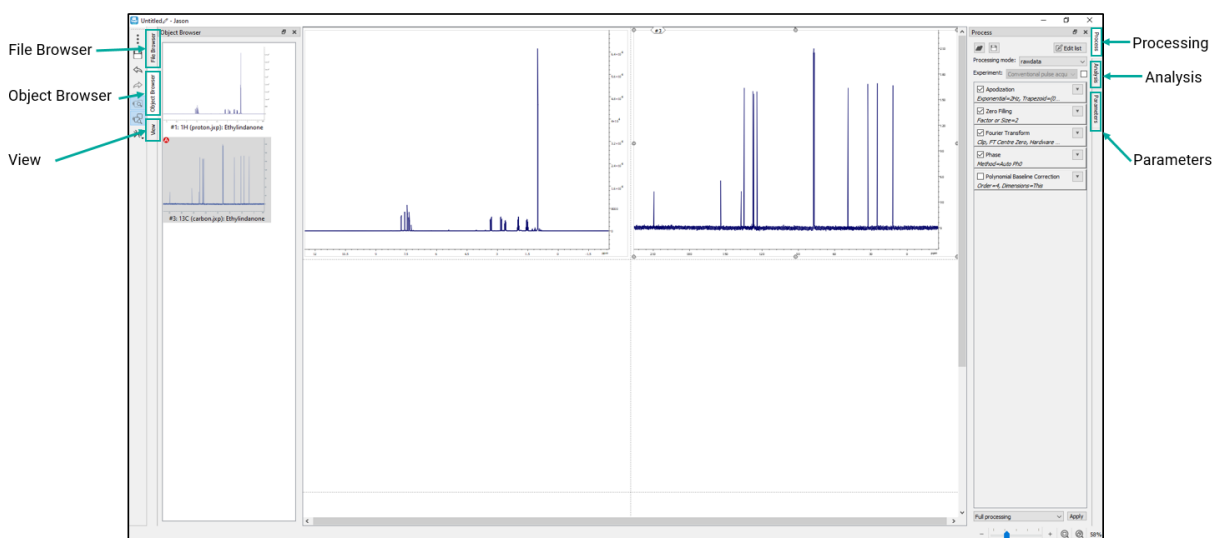


Figure 18: Data Context Tools panels for NMR spectra

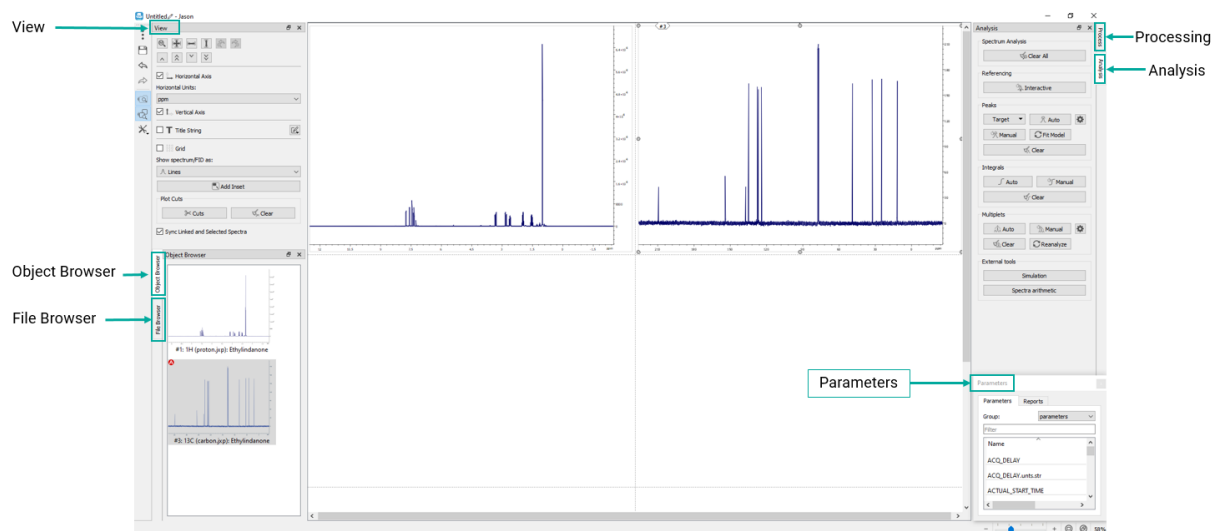


Figure 19: Alternate Configuration of Panels

There are six principal panels for an NMR spectrum, the file browser was described in an earlier section. The other panels are described below.

### 3.3 The Object Browser

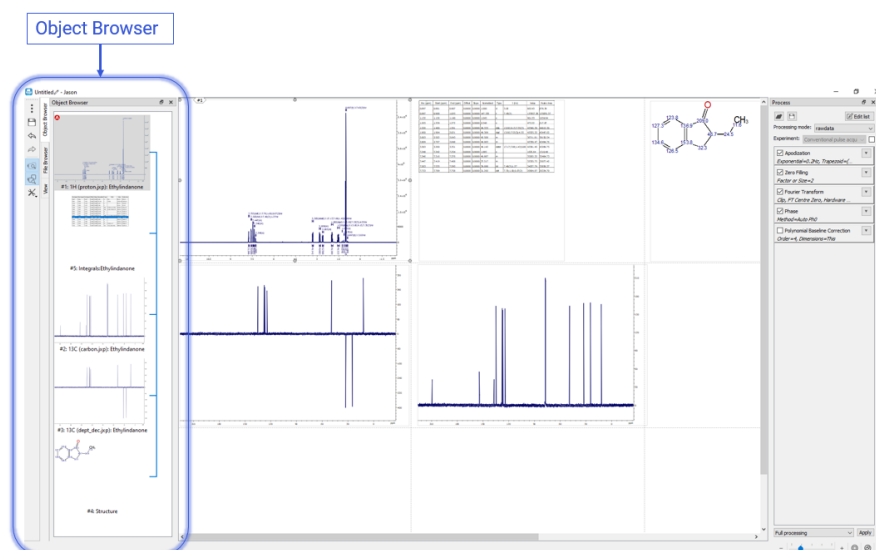


Figure 20: The Object Browser

The object browser is a visual list of all objects on the canvas, see Figure 20. 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 grey and on the canvas because the rescaling drag points around the object on the canvas are filled. In Figure 20 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 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 pressing the delete key. The second option opens the object linking dialog, see Figure 21. 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 peaks, integral or multiplet table is created, a link from the corresponding spectrum to the table will automatically be created

The links between objects are shown as the blue connecting line to the right of object browser display area.

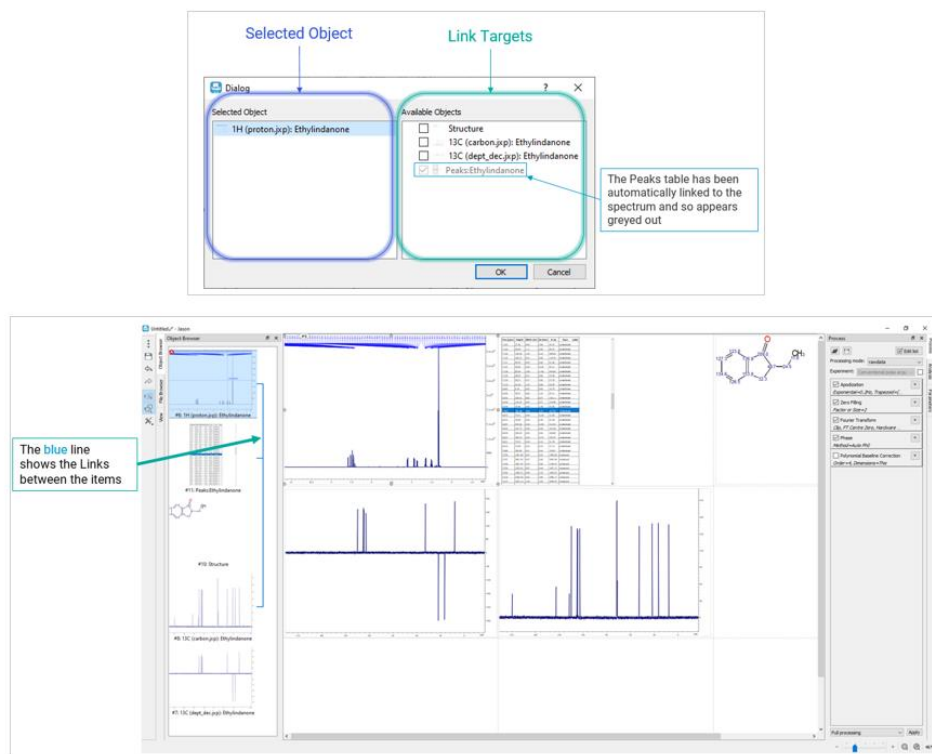


Figure 21: The object linking dialog

### 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 22.

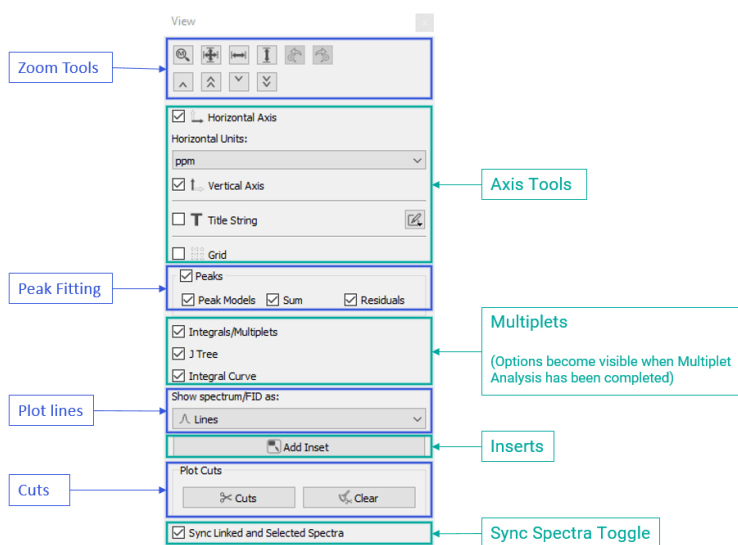


Figure 22: The View Panel

**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 a previous and next zoom buttons to undo or redo zoom steps

**Axis Tools:** The axes tools allow the user to toggle the visibility of the axes and to change the units the axes display.

**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 allows 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.

**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 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.

**Cuts:** The cuts button works identically to the cut tool in the context tool bar. Pressing the cuts button starts the cuts tool mode and the clear button removes all cuts.

**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 23. In addition to the options described for a 1D spectrum, a 2D spectrum has the following additional options.

**2D View Options:** Within the 2D options the user can choose how the data should be plotted. For a 2D spectrum (Fourier transformed in both dimensions) this can be a contour plot or a raster plot. For pseudo-2D data (Fourier transformed in the direct dimension F2) this could be as an overlay plot or a stacked plot. The positive/negative option allows the user to plot only positive or negative values or both.

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, often referred to as the projection. 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.

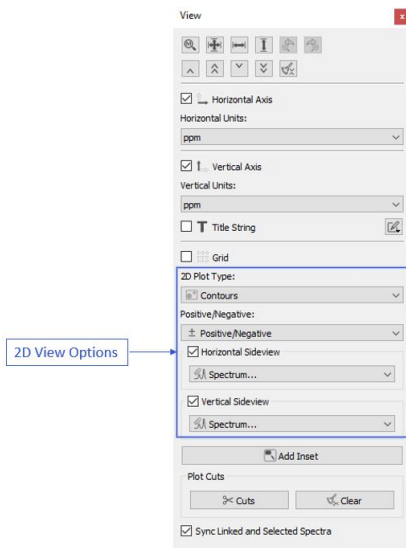


Figure 23: 2D Options in the view panel

### 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 24 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.

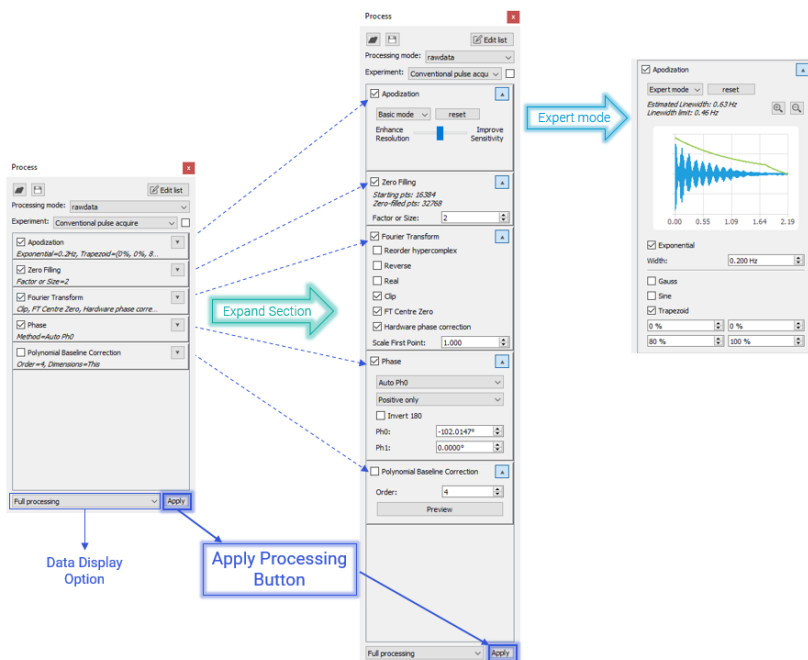


Figure 24: The Processing Panel

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 option related to the processing step. A number of the processing steps have extended modes of use, a basic mode and an expert mode. These are discussed in the Extended Processing Options section.

**Apodization:** this panel displays the options and parameters for signal apodization. In addition to the available apodization functions, the panel also displays the FID and the apodization envelope.

**Zero Fill:** this panel displays 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:** this panel 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.

**Phase:** this panel 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.

**Polynomial Baseline Correction:** This option displays the parameters for a simple polynomial baseline correction. The order of the polynomial used can be changed in this panel.

**Data Display Options:** The data display options allows 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, 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 **Error! Reference source not found.** 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.

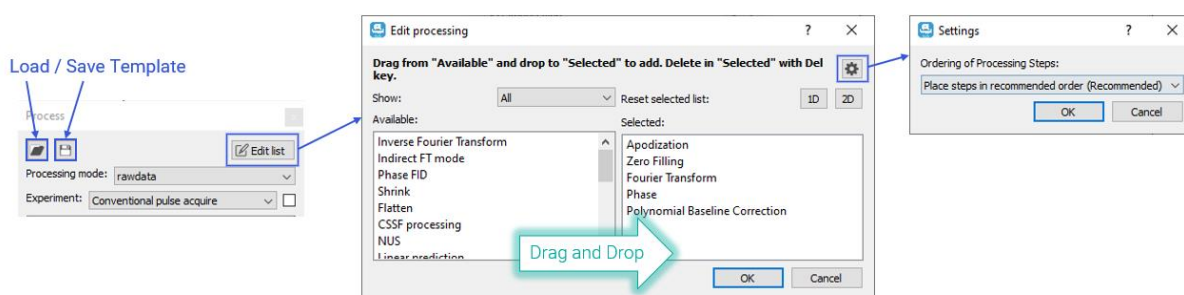


Figure 25: Processing List options

**Settings:** In default mode, JASON will arrange the processing steps in the most appropriate order automatically. If a situation arises where a user wishes to change the order of the processing steps this can be done by selecting the settings button in the top right-hand corner of the edit processing dialog, see **Error! Reference source not found.** 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:** 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 26 is typical for a 1D NMR spectrum.

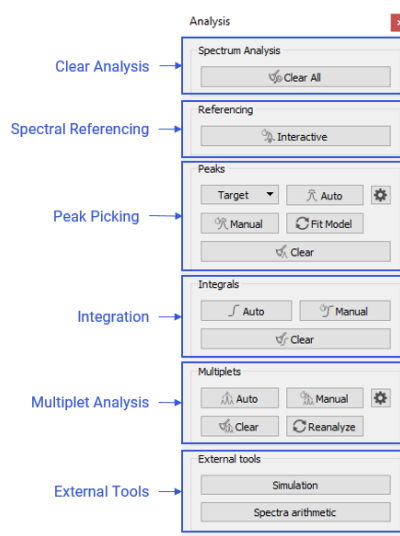


Figure 26: The Analysis Panel

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

**Spectral Referencing:** This button is identical to the referencing mode on the context tool bar.

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

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

Automatic peak picking 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.

The fit model button allows the user to refine the fitting, either by changing the fitting model (deleting/adding peaks, changing parameters in the peak table) or simply by 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 in to regions containing groups of peaks likely to belong to a single multiplet.

Manipulation of the integral regions and labels is identical to the description of the integration mode in the context tool bar section.



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 a 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 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.

**External Tools:** Advanced analysis tools

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 spectra together.

### 3.7 The Parameters Panel

The parameter panel comprises two tabs; the parameter 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 27 shows the two tabs for the parameter panel of a typical 1D NMR spectrum.

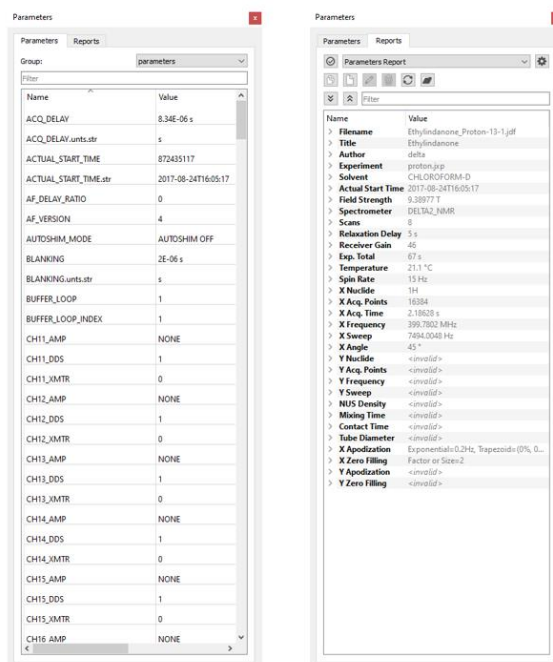


Figure 27: The Parameters Panel

## 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:

#### 4.1.1 Parameters Report

The **parameter report** option from the **create** menu places a parameter table next to the spectrum, see Figure 28. The contents of the parameter table are defined in the parameter report tab. 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 users preferred location while the drag points allow the user to resize the table. 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 29) into the displayed table.

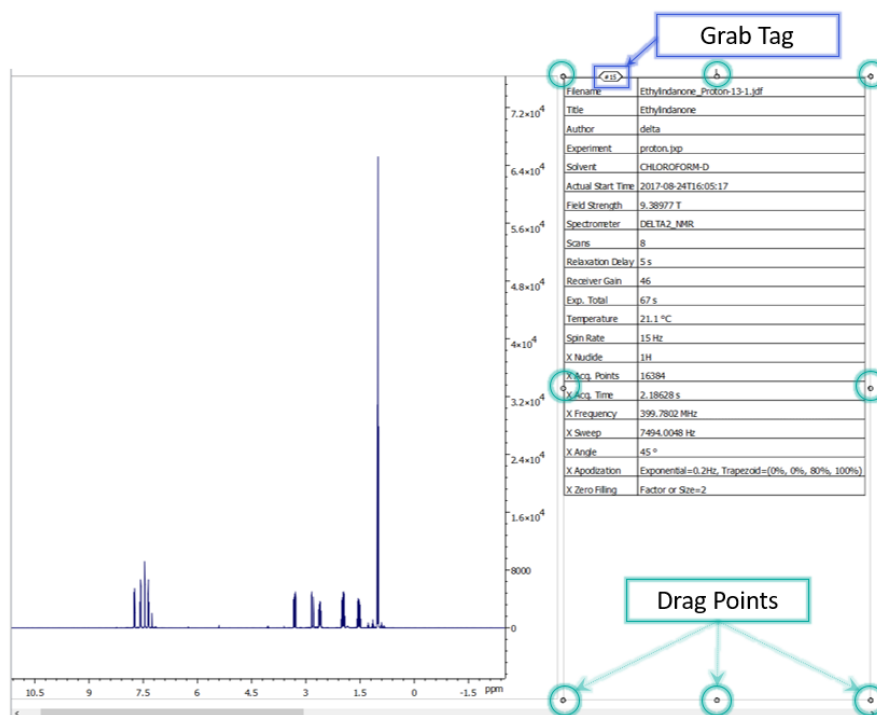


Figure 28: Parameter Table

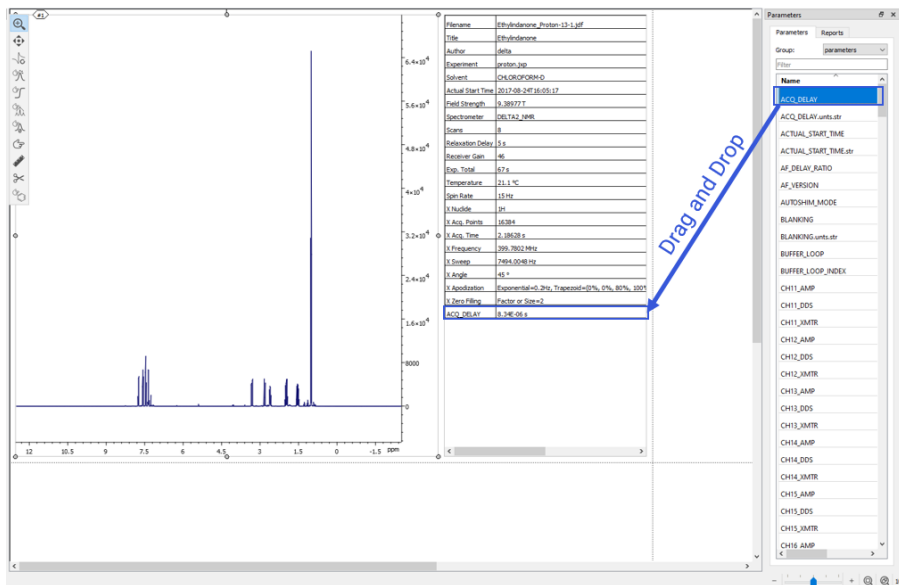


Figure 29 Adding Parameters to the Parameter Table

### 4.1.2 Processing Report

The **processing report** option from the **create** menu places a processing table next to the spectrum, see Figure 30 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 users 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

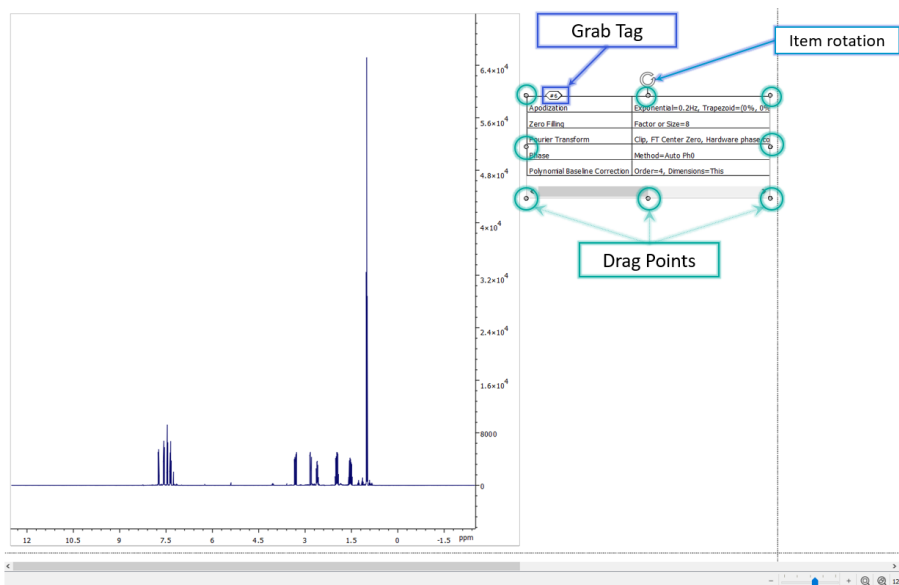


Figure 30 Processing Report

### 4.1.3 Peak Table

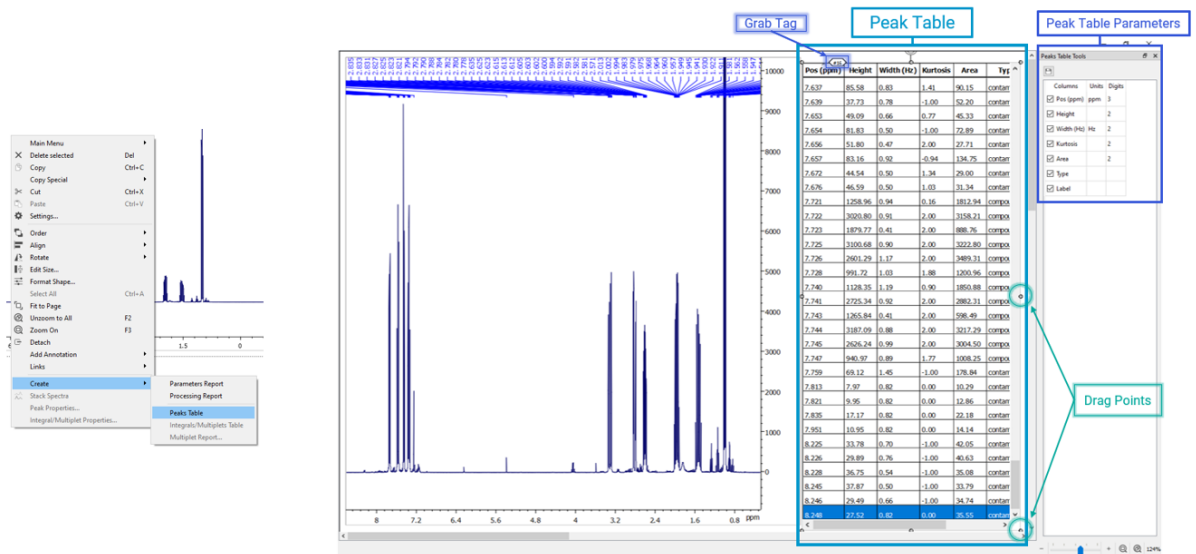


Figure 31: Peaks Table

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 31. Clicking on this option creates a table of peaks next to the spectrum. 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 change 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 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

### 4.1.4 Integrals/Multiplets Table

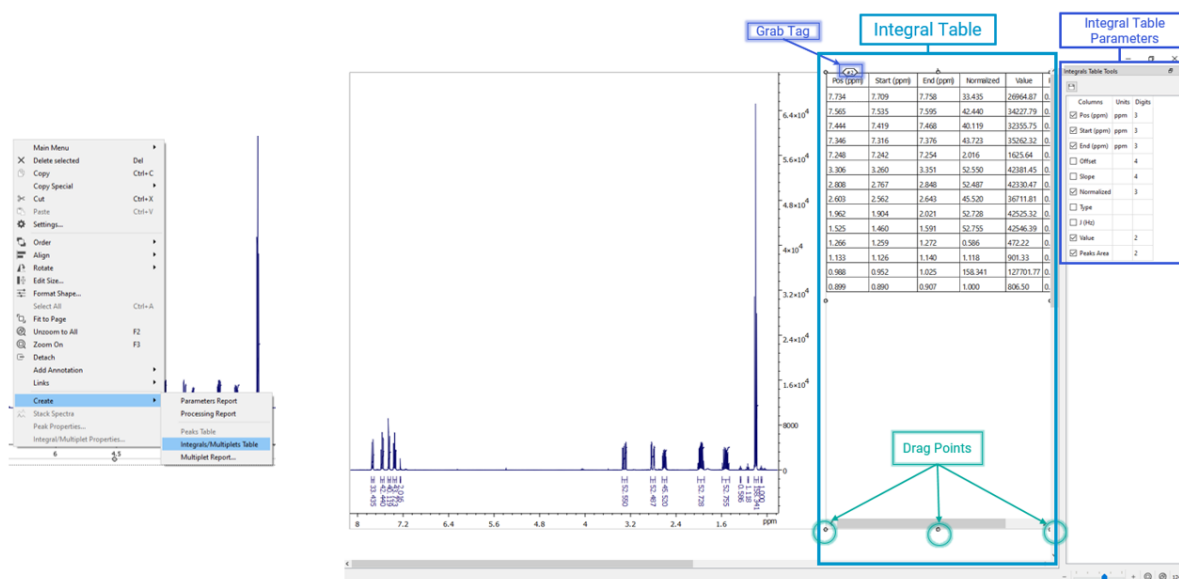


Figure 32: Integral Table

Once integrals has been created the **create** menu in the right mouse button context menu will have an option for **Integrals/Multiplets table**, see Figure 32. Clicking on this option creates a table of integrals next to the spectrum. 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 change 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 Multiplet Report

In addition to the multiplet table, the multiplet information can also be displayed as a **multiplet report** using the option in the **create** menu, see Figure 33. 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.

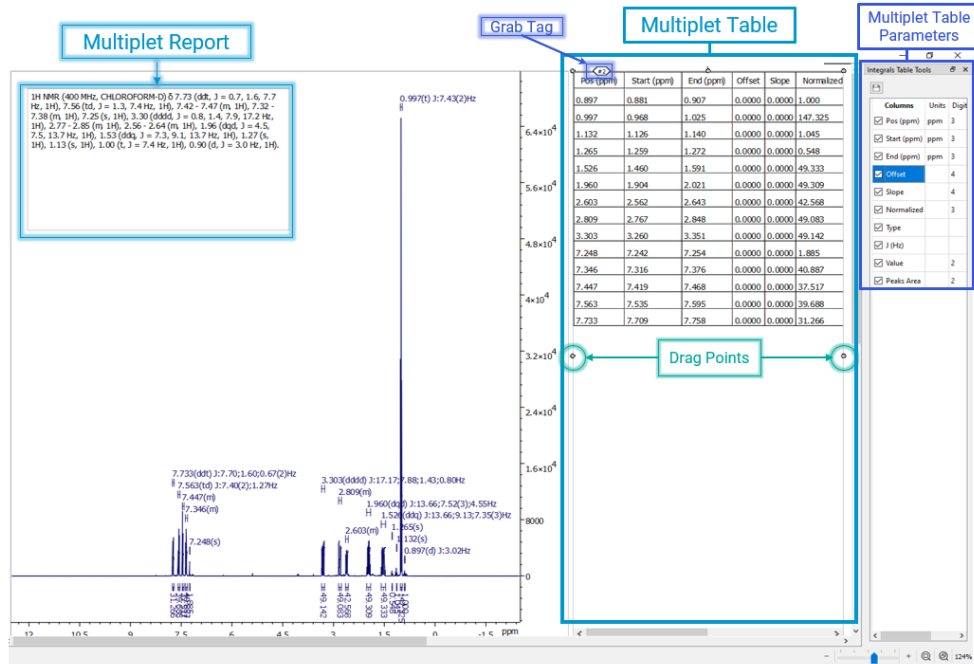


Figure 33: Multiplet Table and Report

## 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 34.

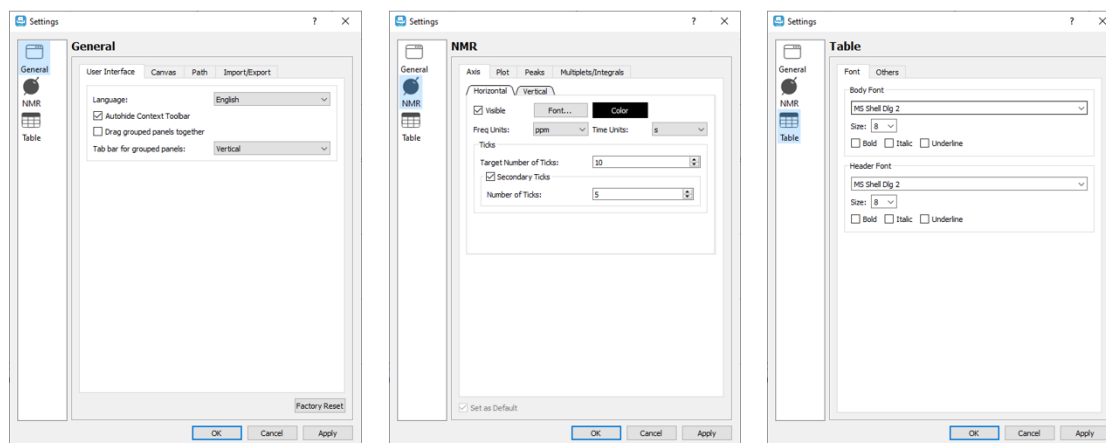


Figure 34: The Settings Menu, the general setting (left), NMR settings (middle) and Table settings (right)

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 setting 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 setting and quit. Pressing the **cancel** button will quit without applying the settings.

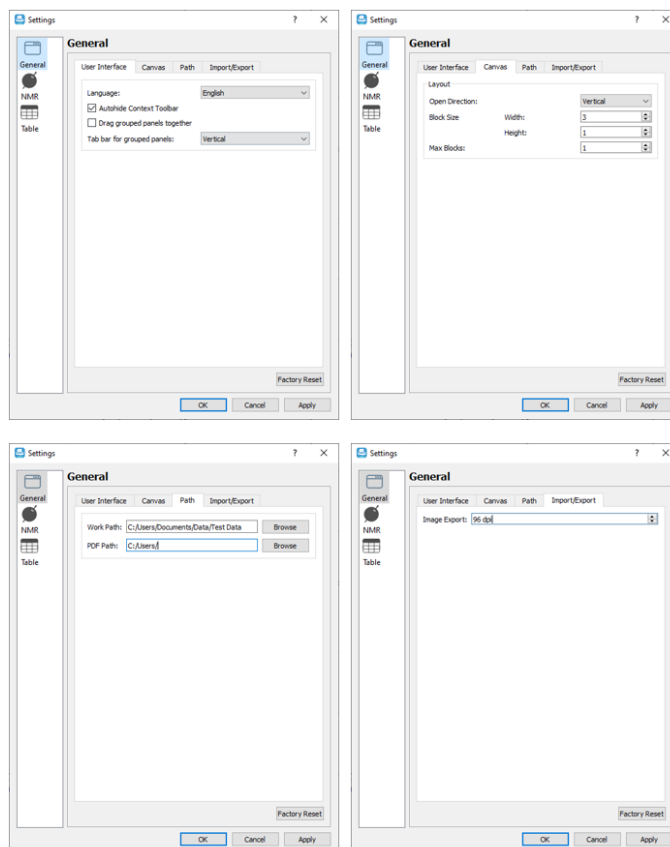


Figure 35: The General Settings

The general settings panel has 4 tabs:

### 5.1.1 User Interface

There are four options in the user interface tab.

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

**Autohide Context Tool Bar:** when this box is checked, the context tool bar discussed in section 3.1 Context Tool Bar will become invisible unless the cursor is moved into the top left-hand corner of a spectrum.



**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 18, Figure 19 and Figure 36.

**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 36.

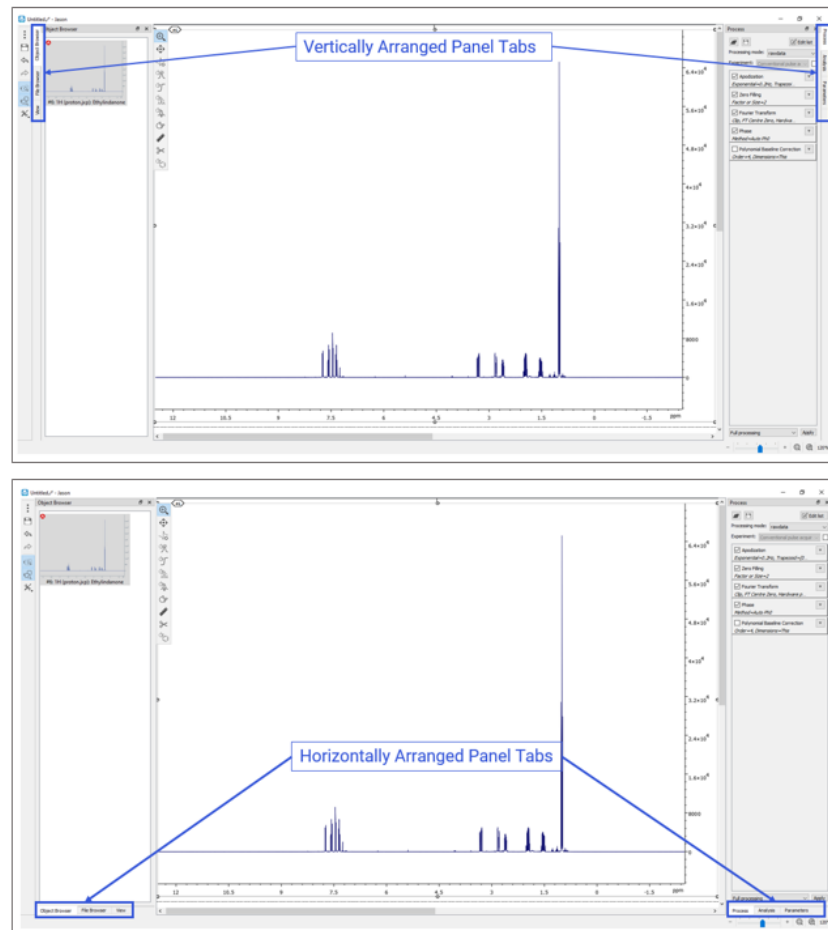


Figure 36: Alternative arrangements of grouped panels.

### 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.

Layout is based on a “block” structure. A block consist of several pages/objects and specified by its height and width (as numbers of pages). The layout procedure places objects within the blocks first, and then places blocks within the canvas itself. The

smallest and simplest block has a height and width of 1 and contains only a single page/object.

“Open direction” specifies the open-end direction along which more and more objects can be placed without restrictions. For example, “vertical” open direction means that if significant number of new objects are opened, then only a restricted number will be allowed horizontally but any number of objects are allowed vertically. The alternative to the open direction will be referred below as a “restricted” direction. So, if “open” direction is “vertical”, the “restricted” direction is “horizontal” and vice versa.

The placement of new object follows the following layout rules:

- 1) The top-left page is used for the first placement on an empty canvas
- 2) All newly opened objects fill the block first. The restricted direction is the faster changing direction: objects are placed in this direction till the max height or width is reached.
- 3) When the block is complete, the new block is started. The new block will be positioned in the restricted direction till the user-defined “Max. blocks” is reached.
- 4) If the “Max. blocks” number is reached, the new block will be started along the open direction.

If the **Max Blocks** option is set to 1, all subsequent objects will be added horizontally or vertically in in width x height blocks depending on what option was selected for the **Open Direction** option.

If the **Max Blocks** option is set to 2, the canvas will be filled in blocks of 2 x 2 objects and in a 2 x 2 grid of blocks after which the canvas will continue to fill horizontally or vertically as before.

By extension if the **Max Blocks** option is set to a value  $a$ , the canvas will be filled in  $2 \times 2$  blocks up to a grid of  $a \times a$  blocks.

### 5.1.3 Path

**Work Path:** This is the default path when a JASON document is saved. The directory can be changed by browsing the file system using the **browse** button or by typing in the path.

**PDF Path:** When the JASON document is saved as a PDF this is the default directory. The directory can be changed by browsing the file system using the **browse** button or by typing in the path.

### 5.1.4 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 four associated tabs, see Figure 37. Each panel is describe in the section below. Any settings can be set as default using the **Set as Default** checkbox at the bottom.

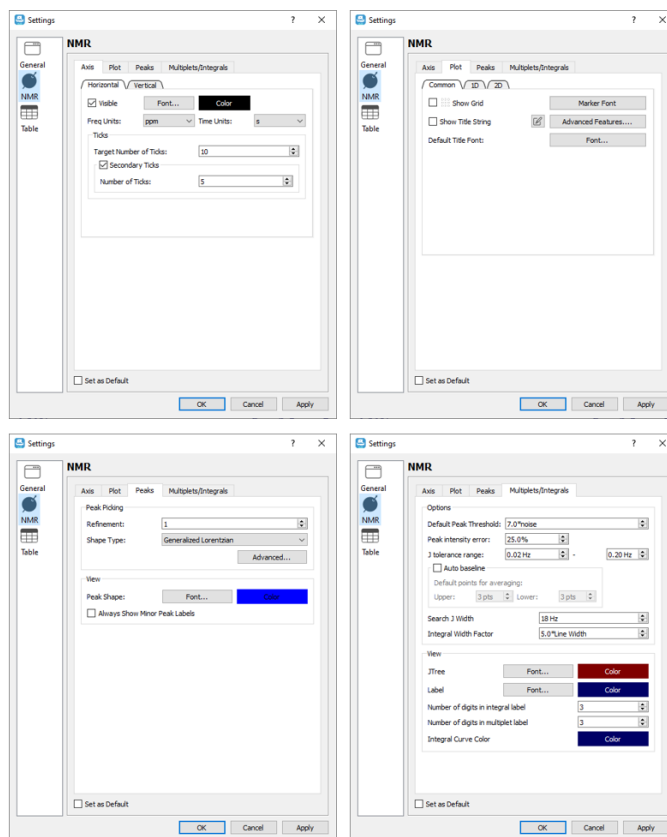


Figure 37: The NMR Settings main tabs

### 5.2.1 Axis

The axis settings contains the options for modifying the axes in an NMR spectrum and it comprises two panels, settings for the horizontal axis and settings for the vertical axis, see Figure 38.

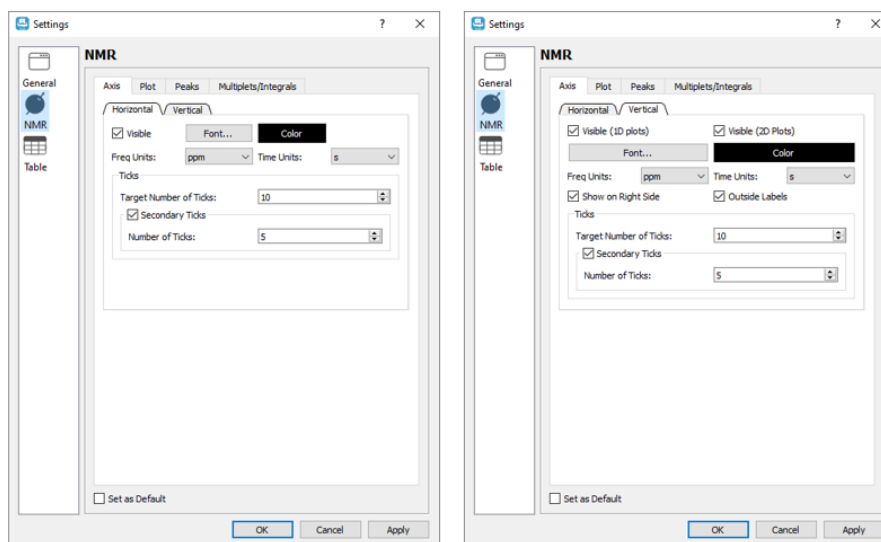


Figure 38: NMR setting axis tabs

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

**Visible checkbox** 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 the color.

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

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 insure 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.

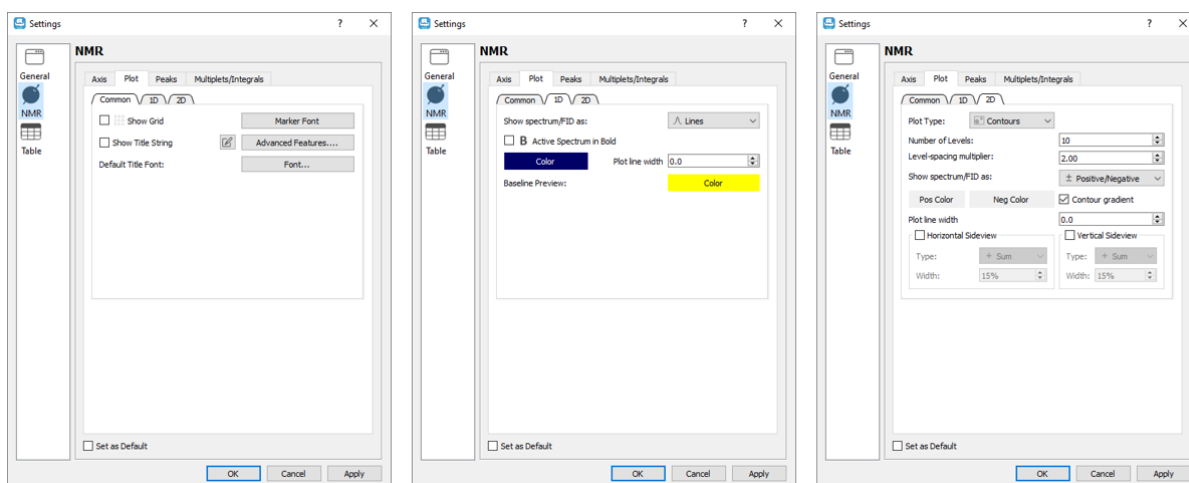


Figure 39: NMR settings plot tabs

The **Show Grid** checkbox toggles the visibility of the grid on a spectrum. The **Show Title String** checkbox toggles the visibility of the title on a spectrum.

The **Common** tab has two buttons that open the standard font dialog. The **Marker Font** button allows the user to change the font, style and color of the crosshair marker. The **Title Font** button allows the user to change the font of the spectrum title. The **Advanced Features** buttons opens the dialog shown in Figure 40. The options determine the joint zoom behaviour of a parent spectrum and an insert.

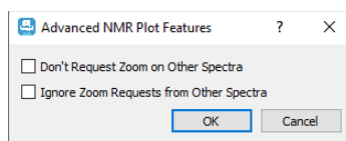


Figure 40: The NMR settings plot advanced options

The first checkbox, toggles whether the current active spectrum should send a request to update the zoom of linked spectra. The second checkbox toggles whether a linked spectrum acts on the request from the currently selected spectrum.

### 5.2.3 Peaks

The peaks tab has three main options, see Figure 41:

**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 **Advanced** button opens up a dialog box that contains all the options used in peak picking and peak fitting, see Figure 41. These values should only be changed by an expert user who fully understands the peak picking process.

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

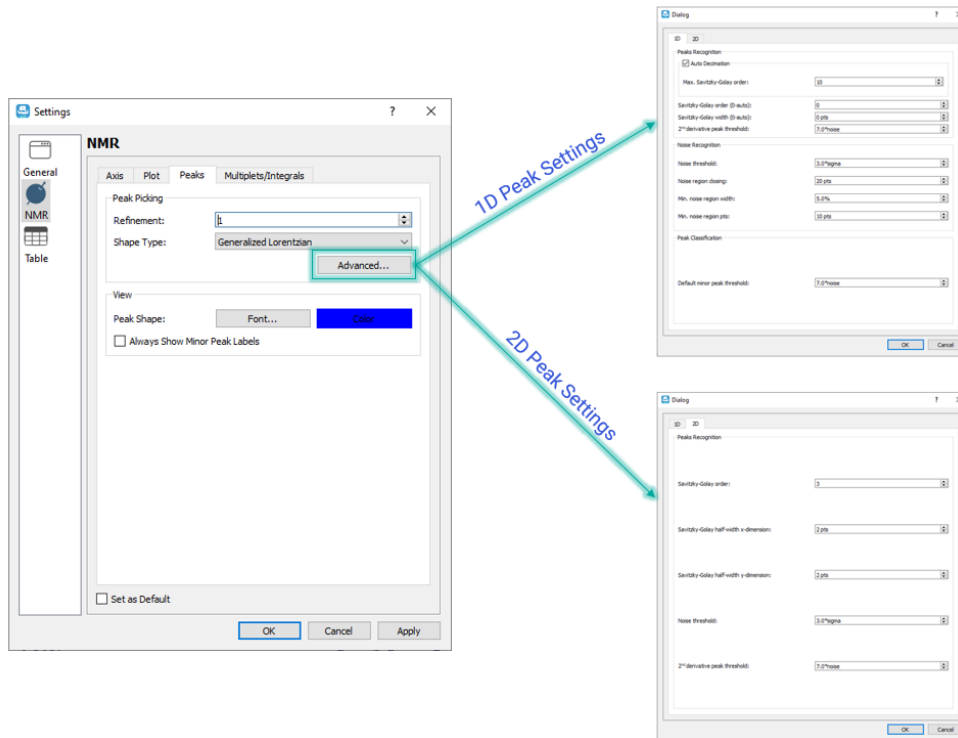


Figure 41: NMR Peak Setting

### 5.2.4 Multiplets/Integrals

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

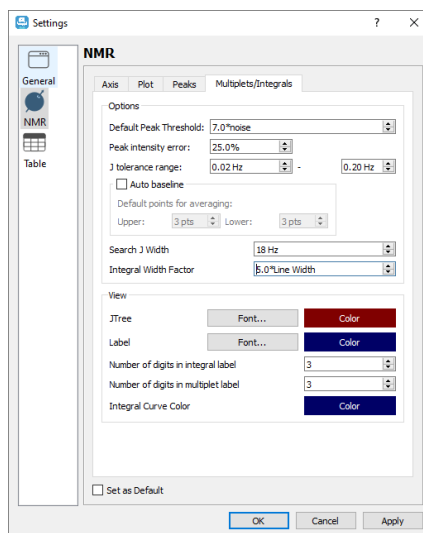


Figure 42: Multiplets and Integral Settings

The options available are:

**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

**JTree:** 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.

## 6 Stacking and Overlaying Spectra

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 “Stack Spectra” from the context menu.

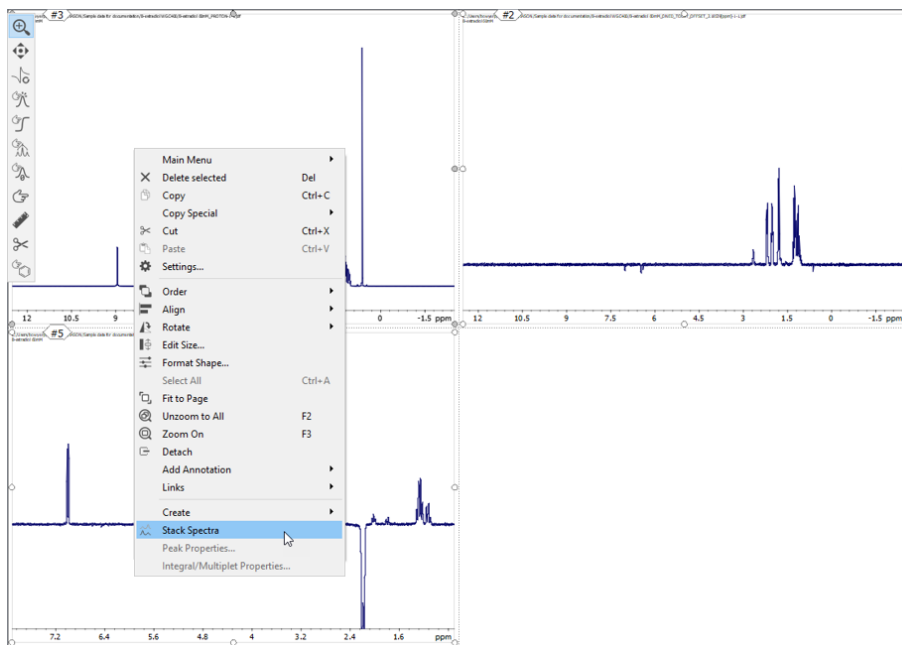


Figure 43: Selecting and stacking individual spectra

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

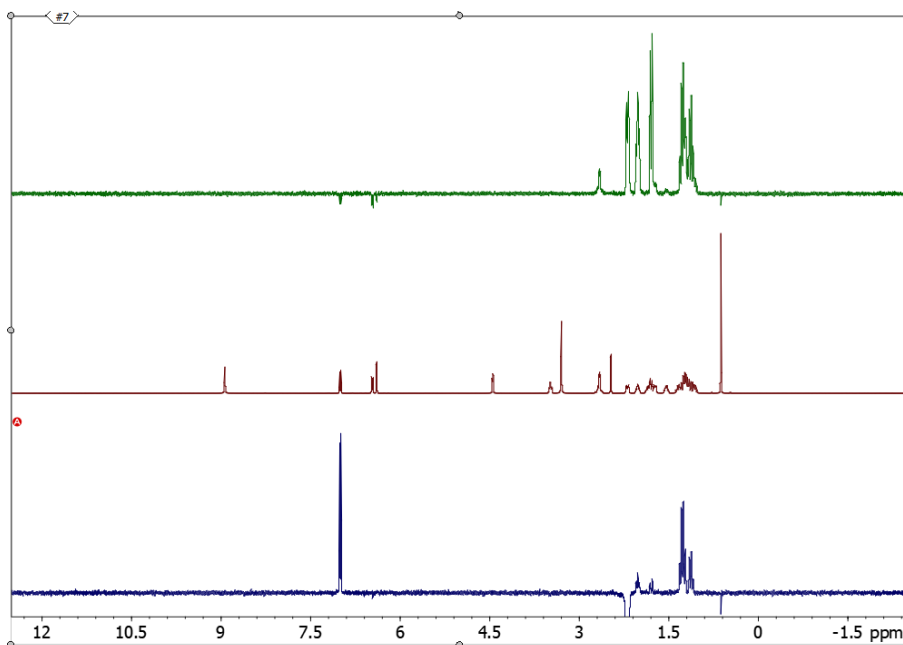


Figure 44: Stacked spectra



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.

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.

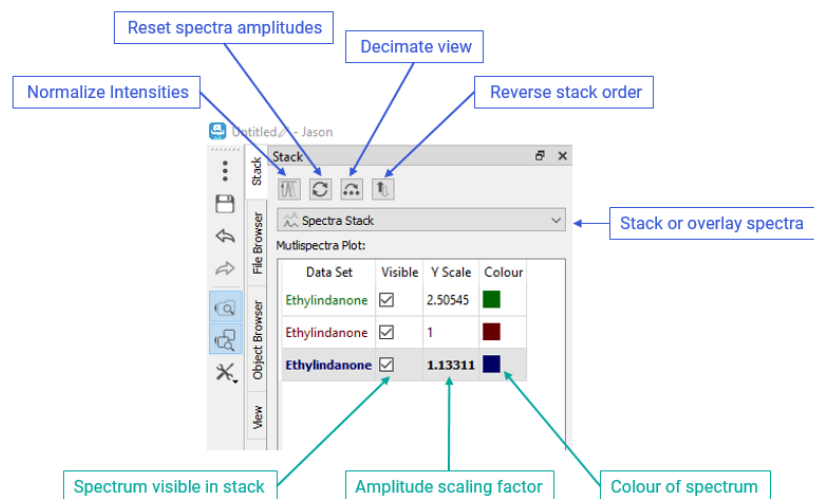


Figure 45: Stack panel

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.

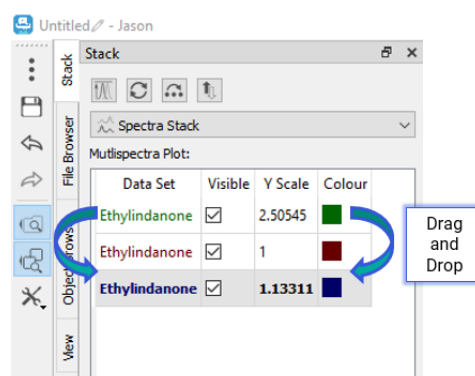


Figure 46: Reordering spectra in the stacked plot by dragging rows in the table

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 on 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  $n^{\text{th}}$  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.

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

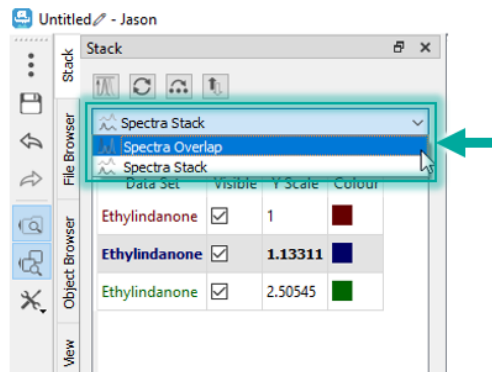


Figure 47: Overlaying spectra using the Stack panel

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

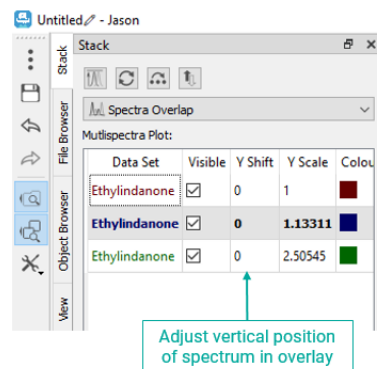


Figure 48: Adjusting the vertical positions of overlaid spectra

## 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 49. This allows the user to enter the chemical shifts and J-coupling constants for up to 10 spins along with other relevant parameters. As the data is entered the simulated spectrum will appear in a new panel on the canvas.

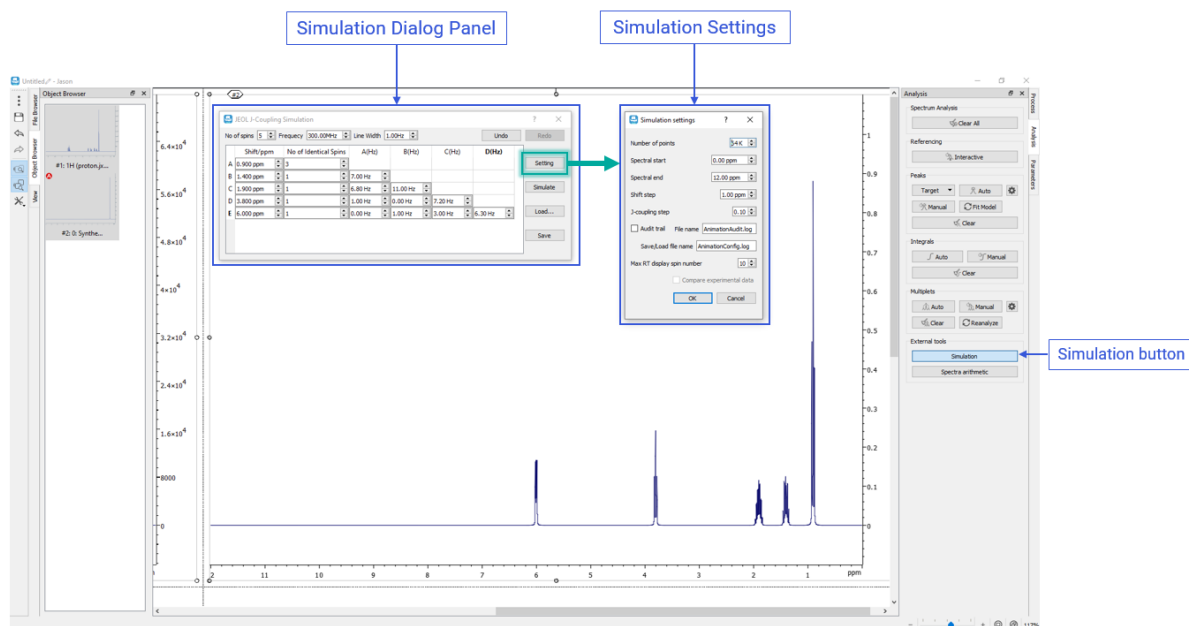


Figure 49: Spin Simulation interface

### 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:** Perform the simulation with the current simulation parameters.

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

**Save:** Save 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 simulation settings contain some general parameters for the simulations

**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 simulation 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 simulation 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:** As the simulation 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 option.

## 8 Molecular Structures

Molecular structures can be drawn or loaded from files. A file can be loaded by simply using the **Open** options in the **File Menu** or dragging and dropping a file onto the canvas. Supported formats are .mol and .sdf. A new structure can be drawn by selecting the **New->Structure** options from the **File Menu**. When the structure is selected the user will see the options displayed in Figure 50. The structure interface comprises a **context menu** 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.

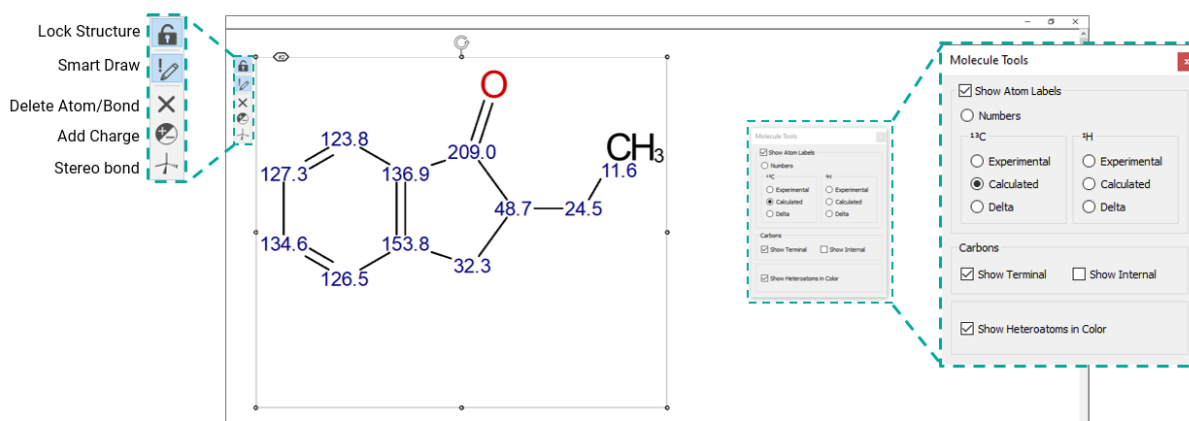


Figure 50: Molecular drawing interface

### 8.1 Context Menu

**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:** Smart draw 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.

**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.

## 8.2 Molecular Tools View

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

**Numbers:** This options label 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).

**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.

## 9 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 51.

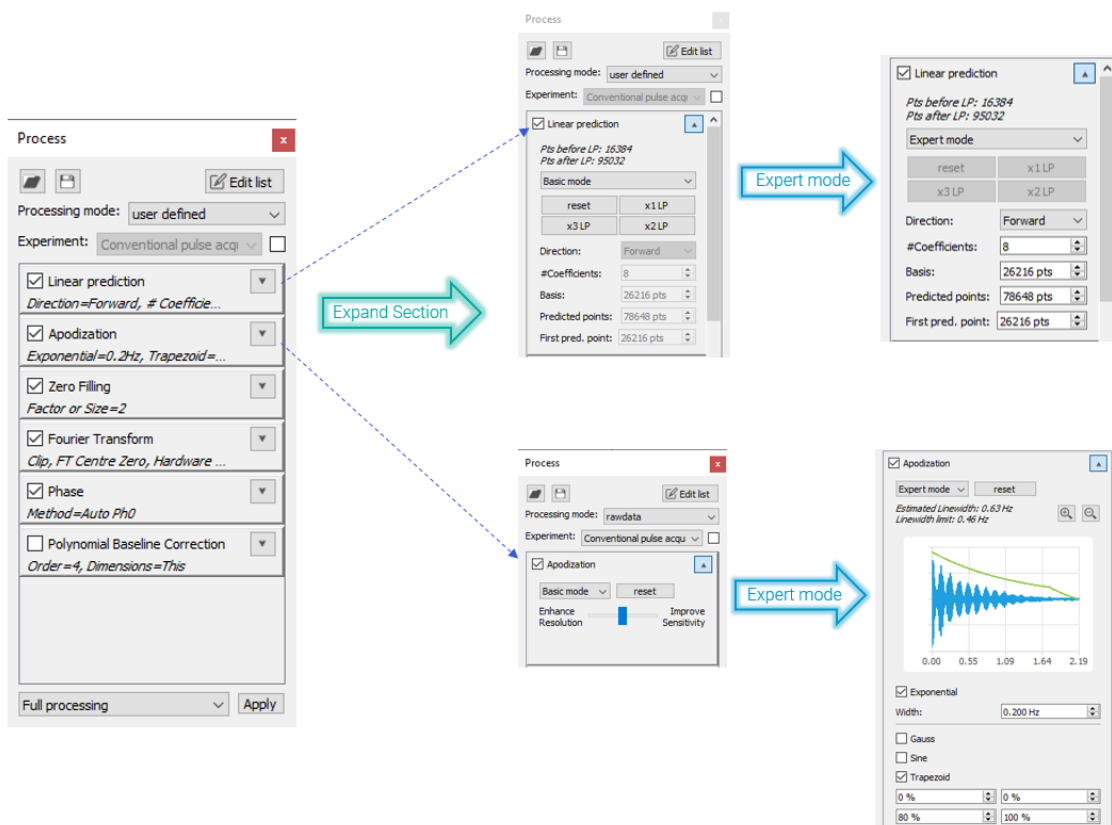


Figure 51: Extended Processing Options

### 9.1 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**.

In basic mode, the user is able to select the direction of the linear predictions, **forward** or **backward** from the dropdown menu, **direction**.

If **basic mode** and **forward** linear prediction are selected then the four boxes directly below the mode options are available, these are:

**Reset:** reset the linear prediction to the default..

**x1 LP:** increase the FID length to double the original number of points, FID plus the fid length in linear predicted points.

**x2 LP:** increase the FID length to triple the original number of points, FID plus twice the fid length in linear predicted points.

**x3 LP:** increase the FID length to quadruple the original number of points, FID plus three times the fid length in linear predicted points.

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

When **basic mode** is selected, the advanced linear prediction parameters, below the **direction** dropdown box are not accessible.

If **backward** linear prediction or **expert mode** are selected then the **x1 LP**, **x2 LP** and **x3 LP** buttons will no longer be available to the user.

If expert mode is selected, the advanced options are available to the user.

## 9.2 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 (the signal to 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.

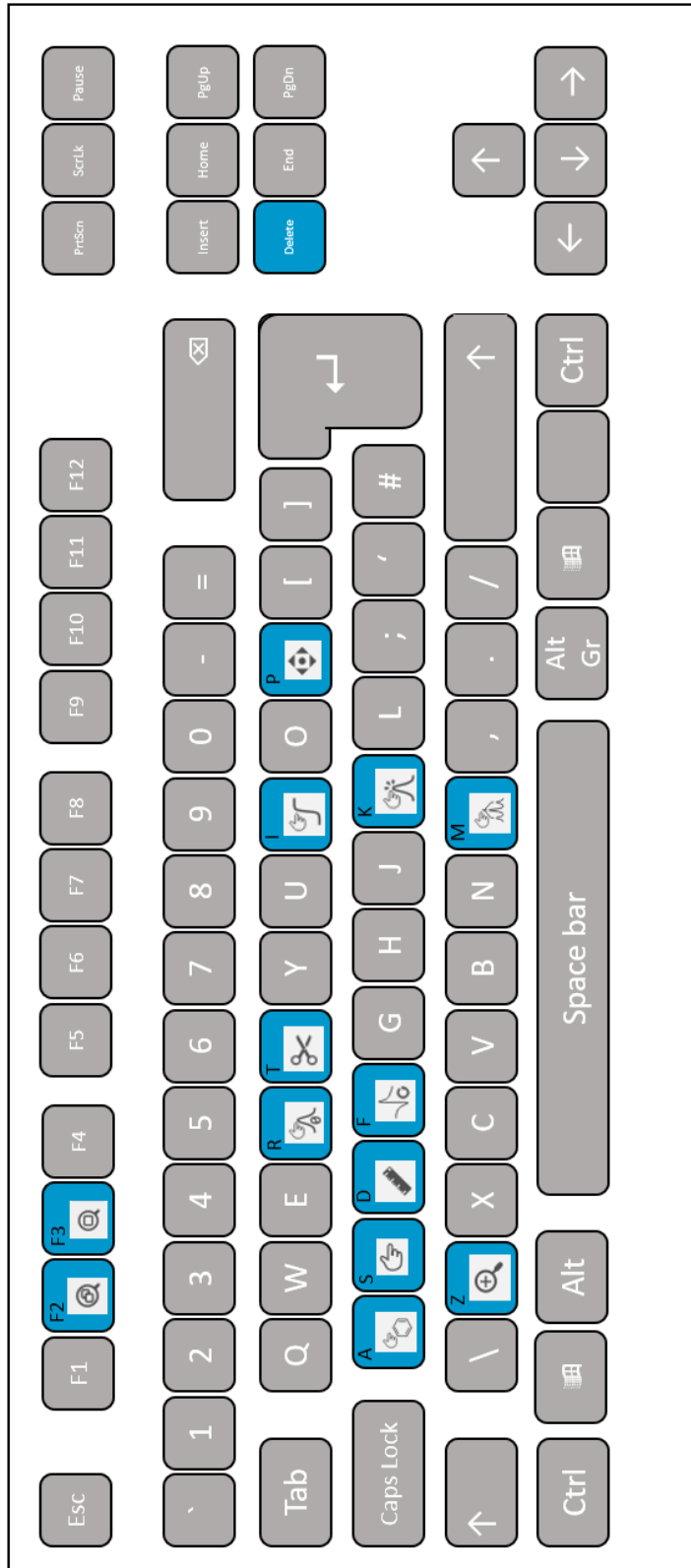
Full control over the apodization functions and their parameters is offered in **expert mode**. The expert mode uses parameters from the processing list associated with the data as its default and a preview of the apodization envelope is also shown in this mode.



## 10 Appendix

### 10.1 Windows Keyboard Shortcuts

Windows (UK keyboard, TKL)



Other useful Windows keyboard shortcuts and keyboard combinations are listed below

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

Where **Ctrl** and one other key are indicated, press and hold the **Ctrl** key then press the second key