JASON Overview: Where to Find What You Need

Contents

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. *(note we will add comments for Mac users once the Mac versions is up and running)*
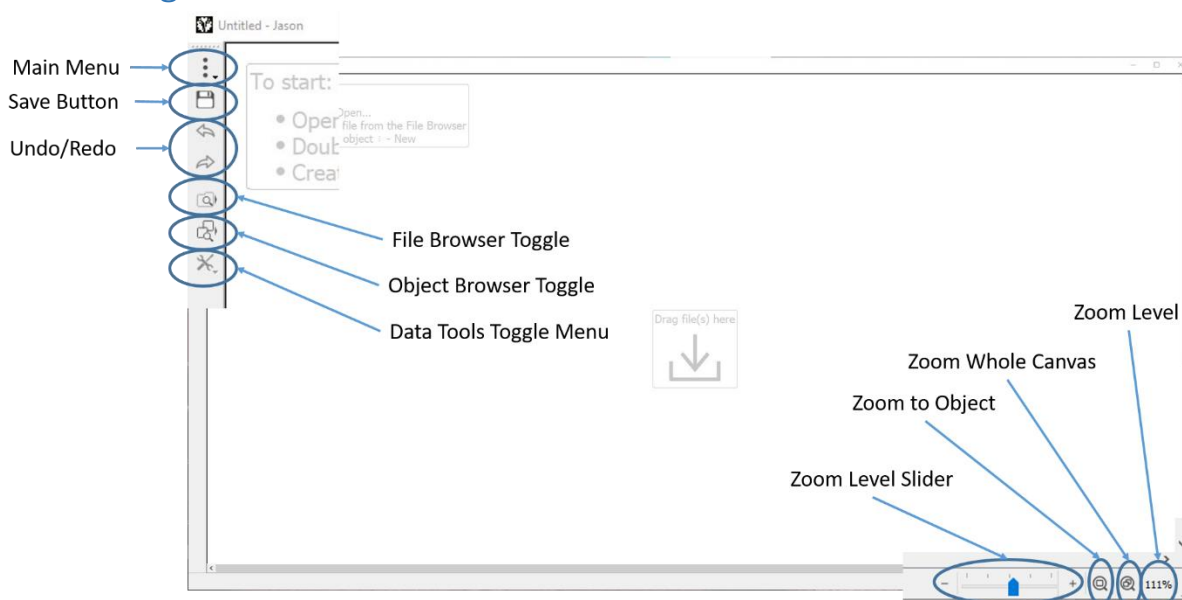
1   Getting Started

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 new molecular structure drawing and spectral simulations and the general settings interface.
2. **Quick save button,** which once the file has been saved initially allows the user to quickly save their current progress
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. **Data tools toggle menu**, which provides a menu of option 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.

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 figure 2).
2. Use the open option on the main menu to navigate to the file of choice, then open

3. Use the file browser toggle button to make the file browser visible the use it to navigate to the relevant files.
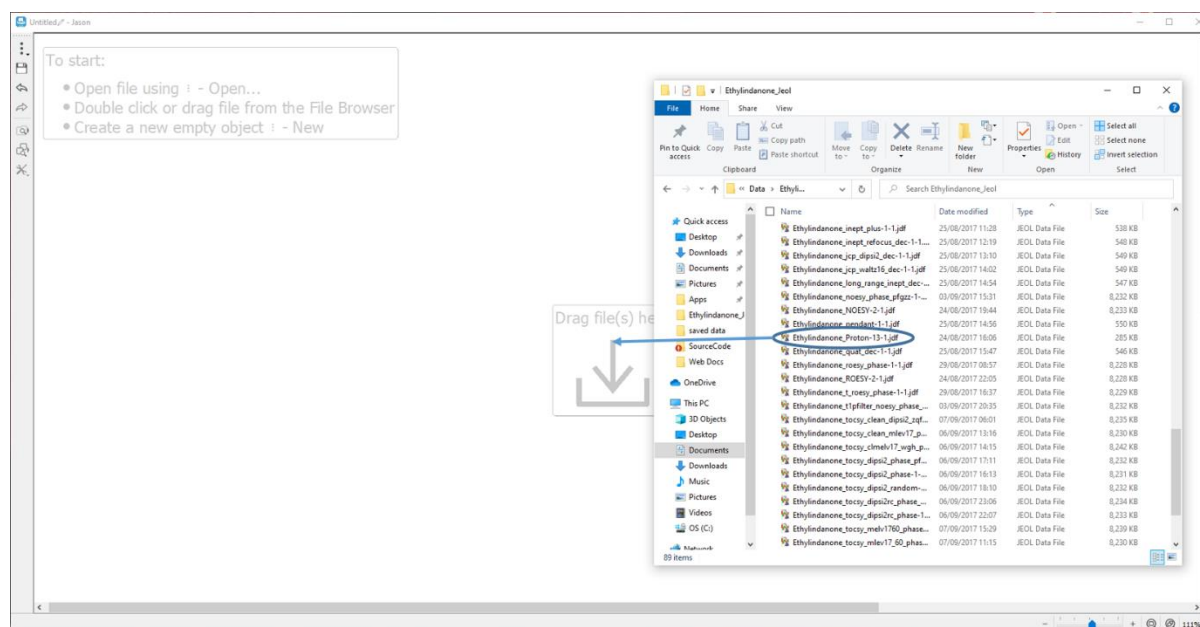
2.1 Loading from Windows Explorer

Figure 2: Loading a file from Windows Explorer

A suitable data file can simple 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 explore 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 where a file can be loaded by either double-clicking on the file or dragging it onto the canvas. Multiple files can be loaded using the usual methods for selecting multiple files in Windows Explorer.

2.3 Loading from the File Browser

The file browser toggle button can be used to make the file browser visible on JASON. By default it will appear by the left hand edge of the canvas, see figure 3. 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.
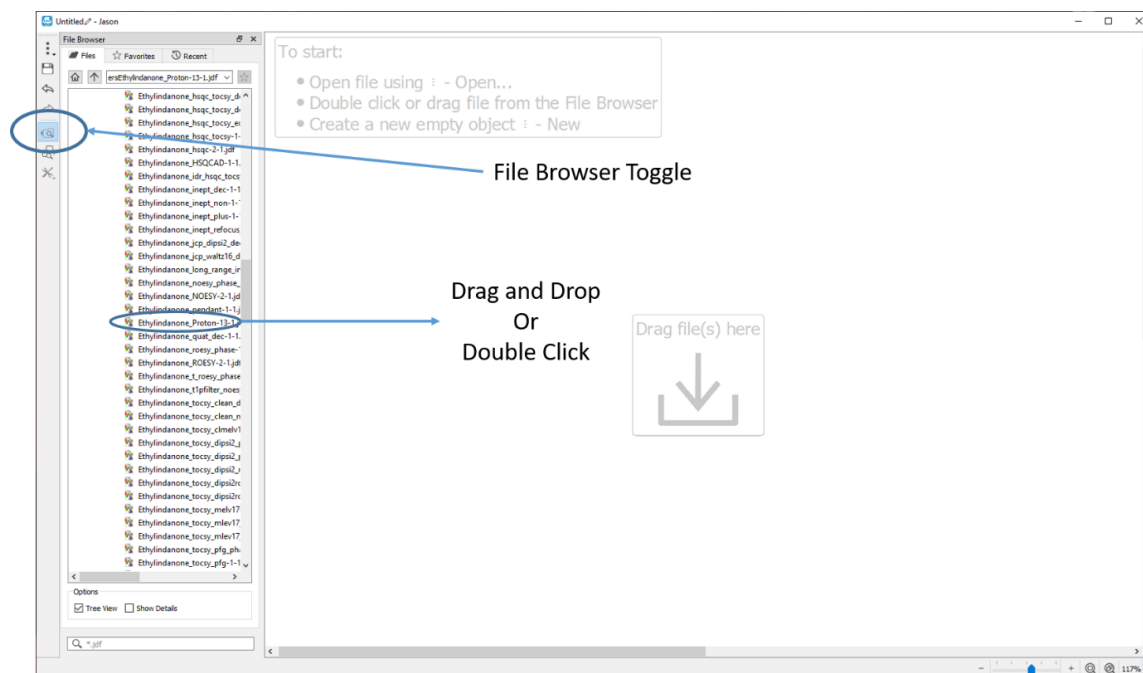
Figure 3: Loading data from the JASON file browser

The file browser itself comprises three panels (see figure 4)

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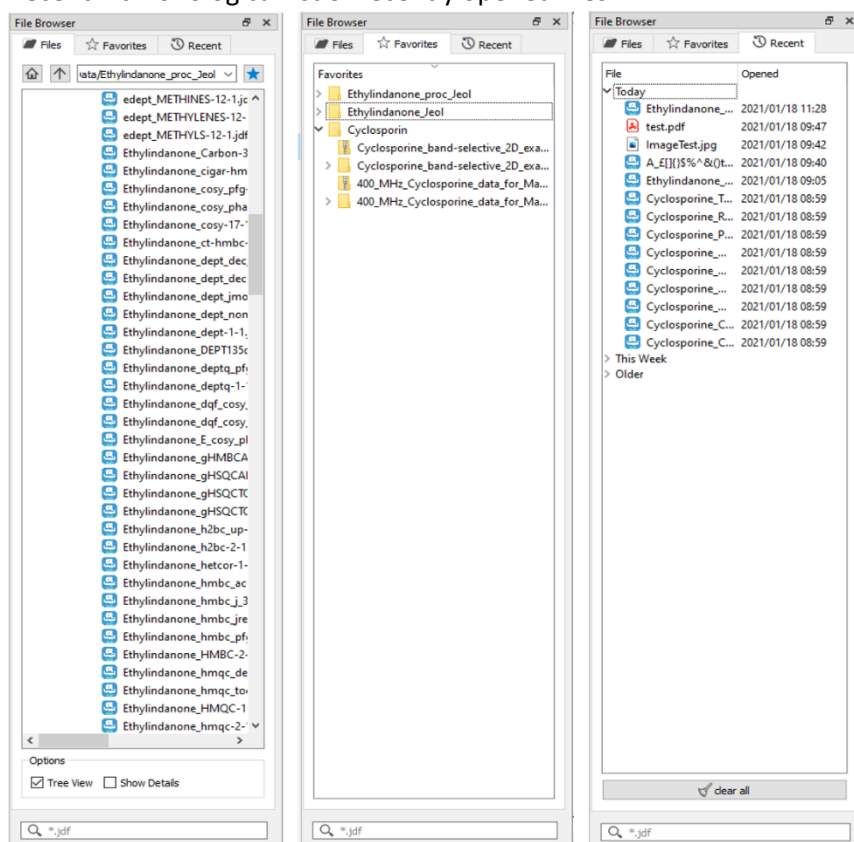3. Recent – chronological list of recently opened files.

Figure 4: The file browser tabs

A file can be loaded from the file browser by simply navigating to the directory of choice and selecting the desired file. Files are selected with a left mouse button click and 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 figure 5.
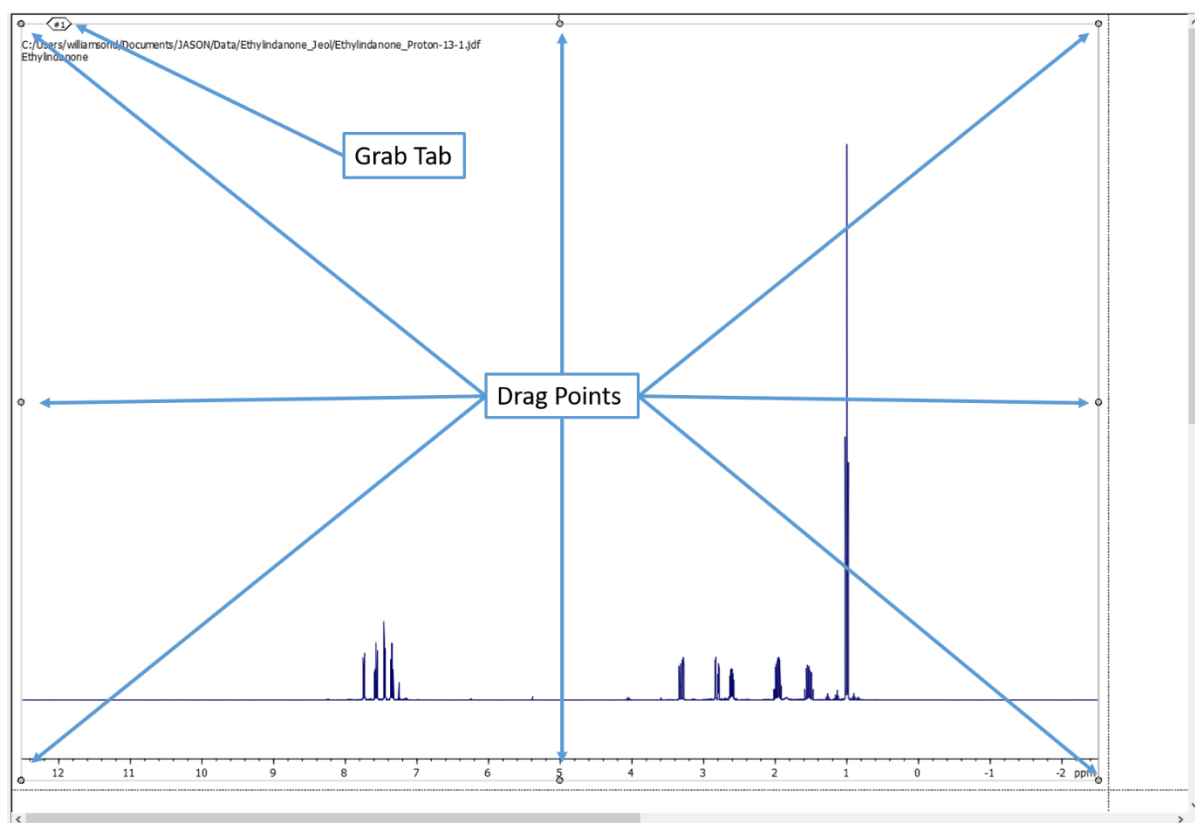
2.4   Arranging data on the Canvas

Figure 5: Grab tab and drag points for moving and rescaling canvas objects

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 the object is selected and currently the active focus. These circles can be used to rescale the object by 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.

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. 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 following section.

Figure 6: 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, see figure 7. In this case these are the panels for NMR spectra.

3.1 Context Tool Bar

Figure 7: Context Tool Bar

When an object is selected in JASON the **context tool bar,** shown in figure 7, becomes available in the top left hand corner of the spectrum. This is a set of tools for manipulating and analysing the current object. A tool is selected by left clicking the icon of choice or clicking the appropriate short cut key. In addition, a particular functionality can be temporarily activated by holding down the short cut. 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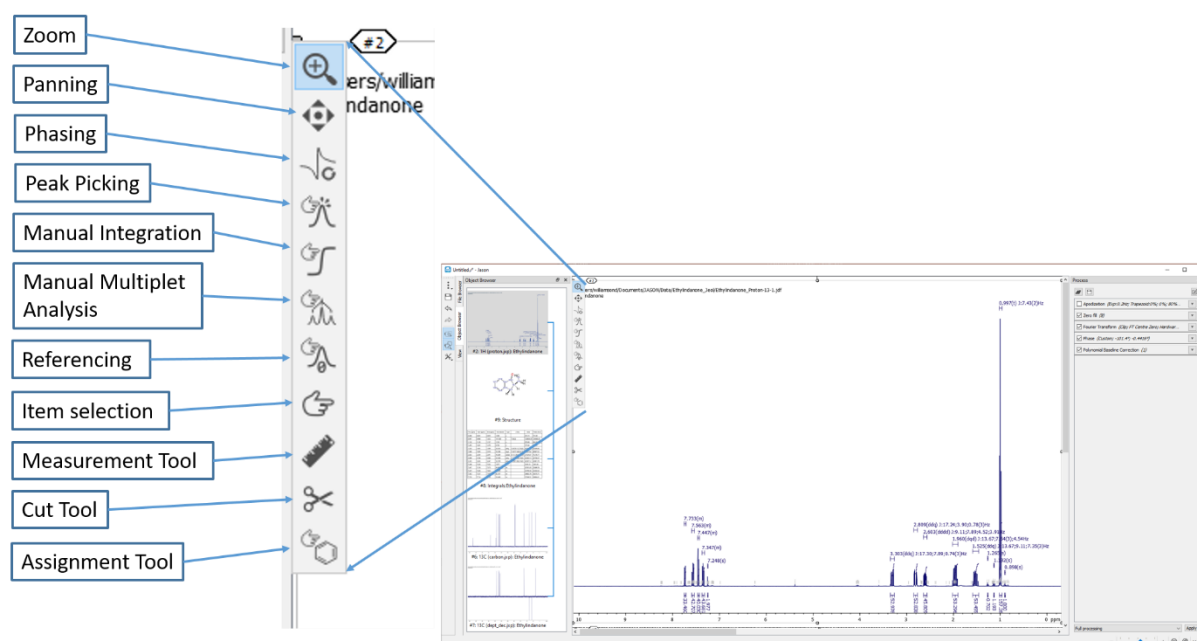 release of the "z" key control will return to the phasing functionality. In the following description the shortcut key is given in parenthesis after the mode name. The short cut is not case sensitive. There are some generic functions, double clicking the left mouse button resets the zoom level to full view and scrolling the mouse where 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. On release of the mouse button the view will zoom to the newly selected region.

Panning (P): In panning 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 8.

Figure 8: Interactive Phasing Mode
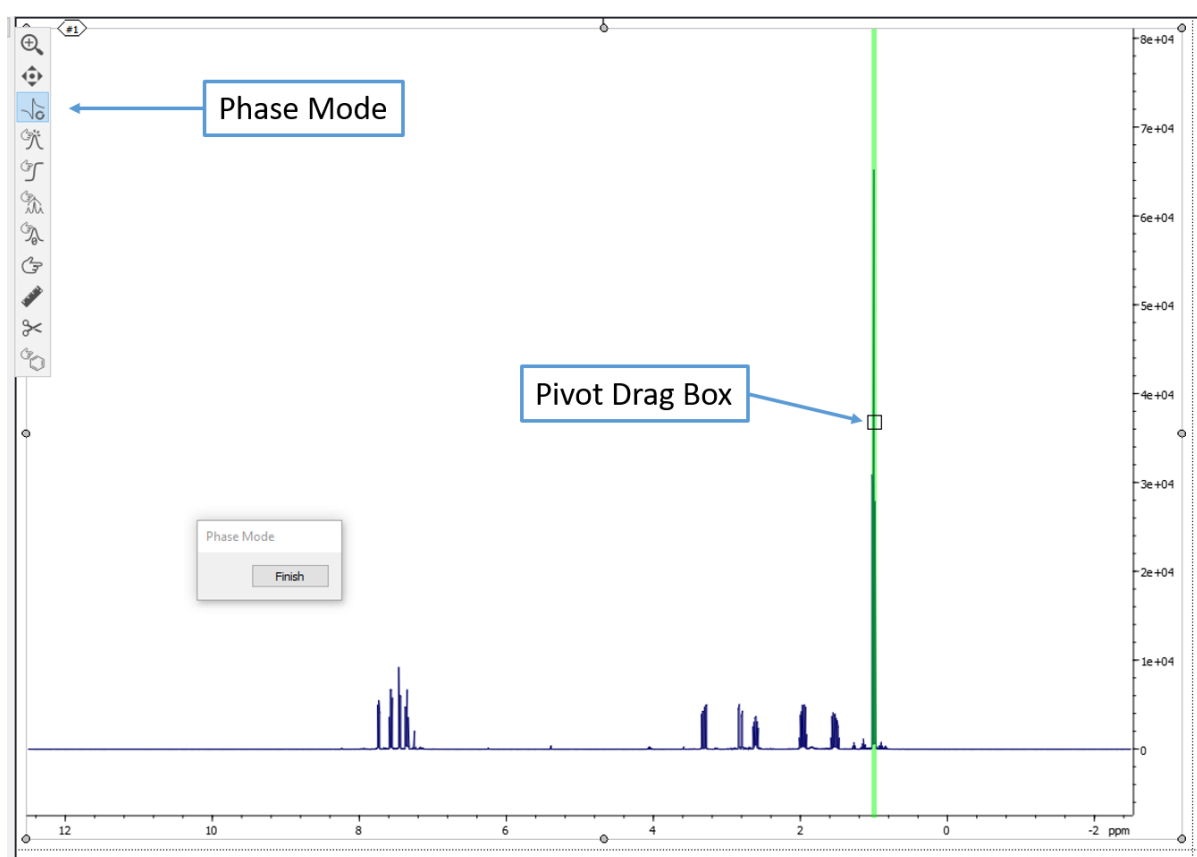
The pivot point can be moved by left clicking and dragging the grab box on the green pivot line. Zero order phasing is performed by holding down the left mouse button and moving the mouse. The mouse can be moved in any direction, allowing users to move the mouse in the manner they are most accustomed to. First order phasing is carried out in a similar manner holding down the right

mouse button. Once the spectrum has been satisfactorily phase, the user can exit phase mode by clicking the finish button on the phase mode dialogue box.

2D NMR data is phased in a similar manner, see figure 9. When the phase mode is selected, the largest positive peak in the spectrum is selected as the pivot point. If "Show Traces" box has been checked in the phase mode dialogue 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 9: Interactive Phasing 2D

If the "show 2nd 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 changes 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.

Once the phasing has been completed successfully, the user can exit the phase mode by clicking the **Finish** button on the phase mode dialogue.

Peak Picking (K): In peak picking mode, a user can manually place a label to mark a peak. This is done my moving the mouse to the desired position and left clicking, see figure 10. 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.
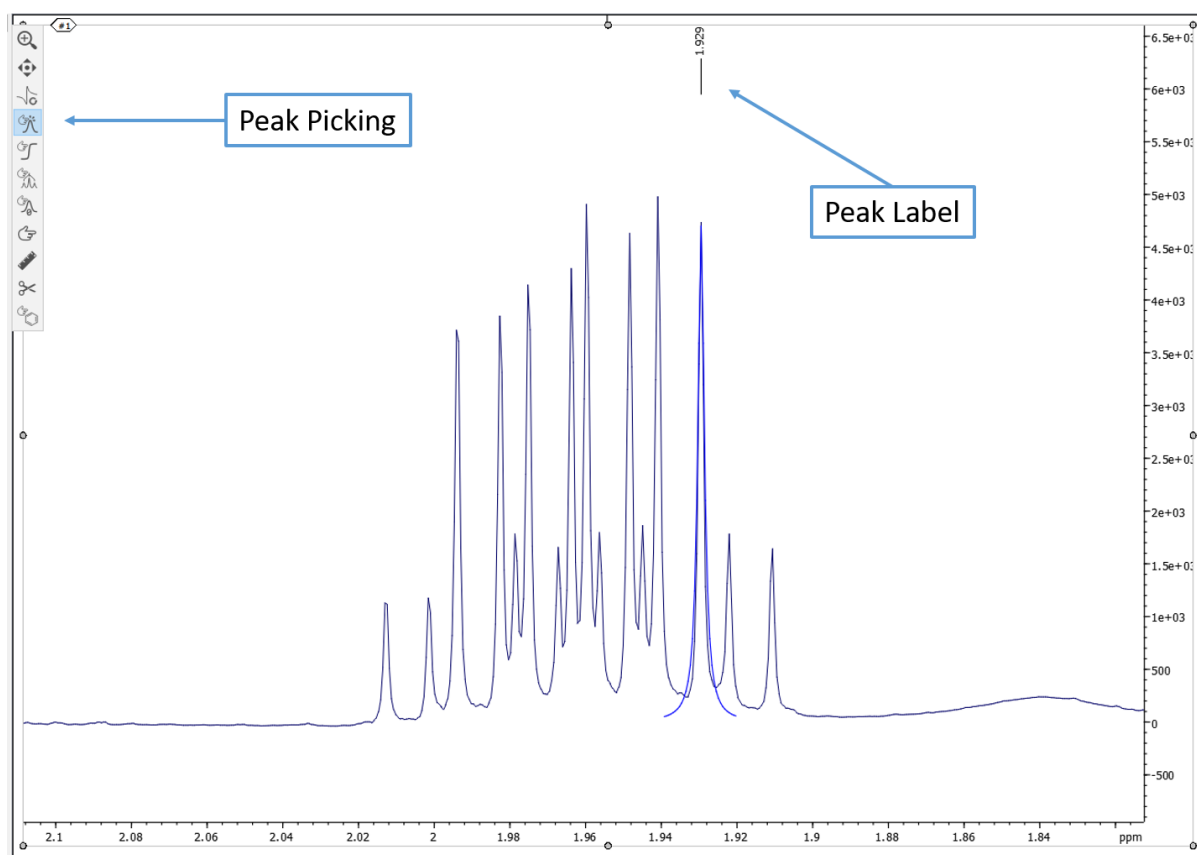

Figure 10: Peak Picking Mode

A table of peaks can be created by right clicking on the spectrum and selected the Create -> Peak Table option from the menu. Tables will be discussed in more detail in a following section. A peak can be delete 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 11. 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 dialogue. 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, the arrows at the top of the dialogue box can be used to navigate between them. The normalized values are relative to all integrals in the spectrum and changing one value will change the value for all other integrals.

Figure 11: 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 12.

Figure 12: 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 and additionally

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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 dialogue box.

Referencing (R): The referencing mode allows a user to select a peak or a position on a spectrum and set the frequency 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 dialogue. 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.
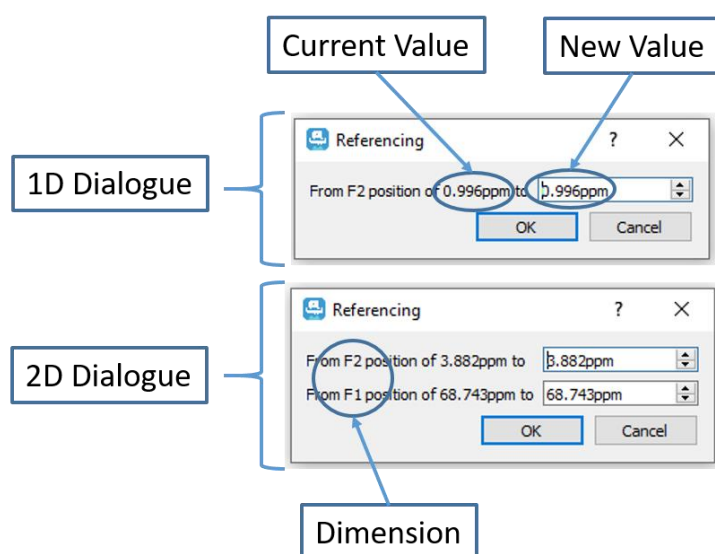

Figure 13: Referencing Dialogue

The referencing dialogue is shown in figure 13 with the current frequency value of the dimensions shown as part of the description and the new value as a text box. In the case of multi-dimensional spectra the dialogue 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 positions.

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.

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 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 coordinated, and a second label is created at the end of the measurement. The end point label contained the coordinated of the end point and the differences between the coordinates of the end point and start point, see figure 14. 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 option to make only a single measurement, as a new measurement is made the previous is deleted. The multiple measurement mode maintains each measurement as the user makes them.
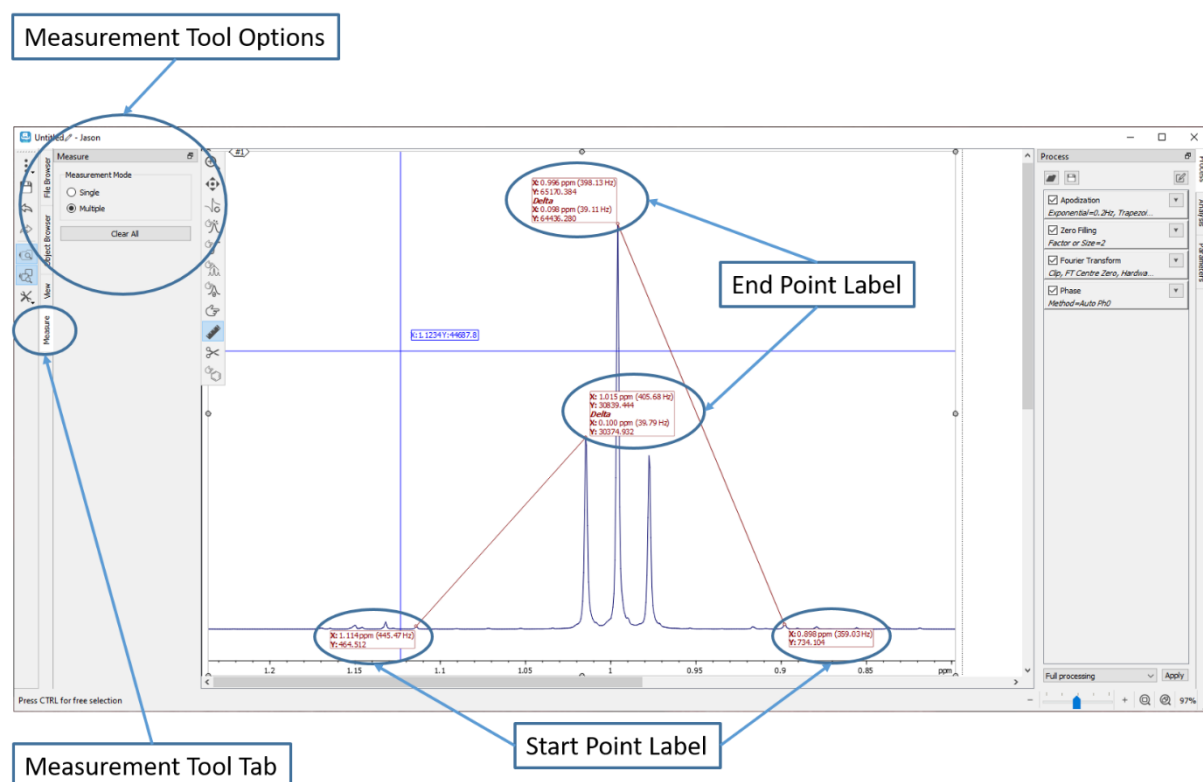
Figure 14: Measurement tool

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.
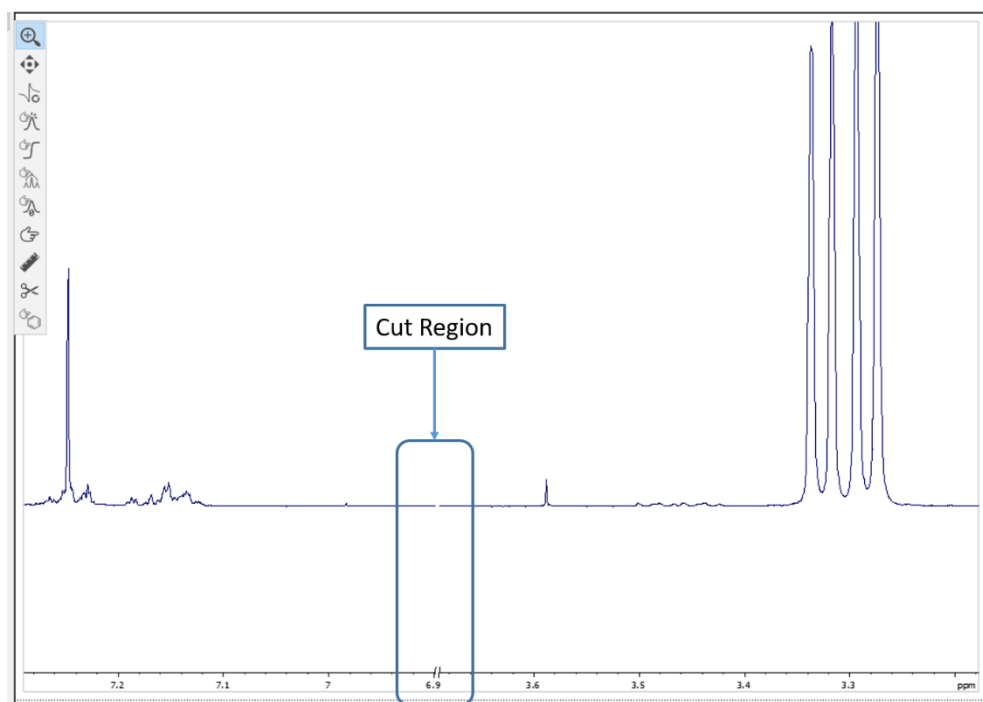
Cut Tool (T):

Figure 15: 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 bottom 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 15. For a 2D data set the cut region is selected by holding down the left mouse button and dragging in both dimensions to select a rectangular cut region. The cut region is shown as discontinuities in the axes, see figure 16.

Figure 16: Cut regions in a 2D spectrum

It is worth noting that if a 1D spectrum is used as the projection, as in figure 16, then the cut region in the appropriate dimension will be shown as a discontinuity in the base line of the spectrum.

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. 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 data tools toggle menu described in an earlier section. The panels available for an NMR spectrum are shown in figure 17. 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 17, or stacked vertically as in figure 18.

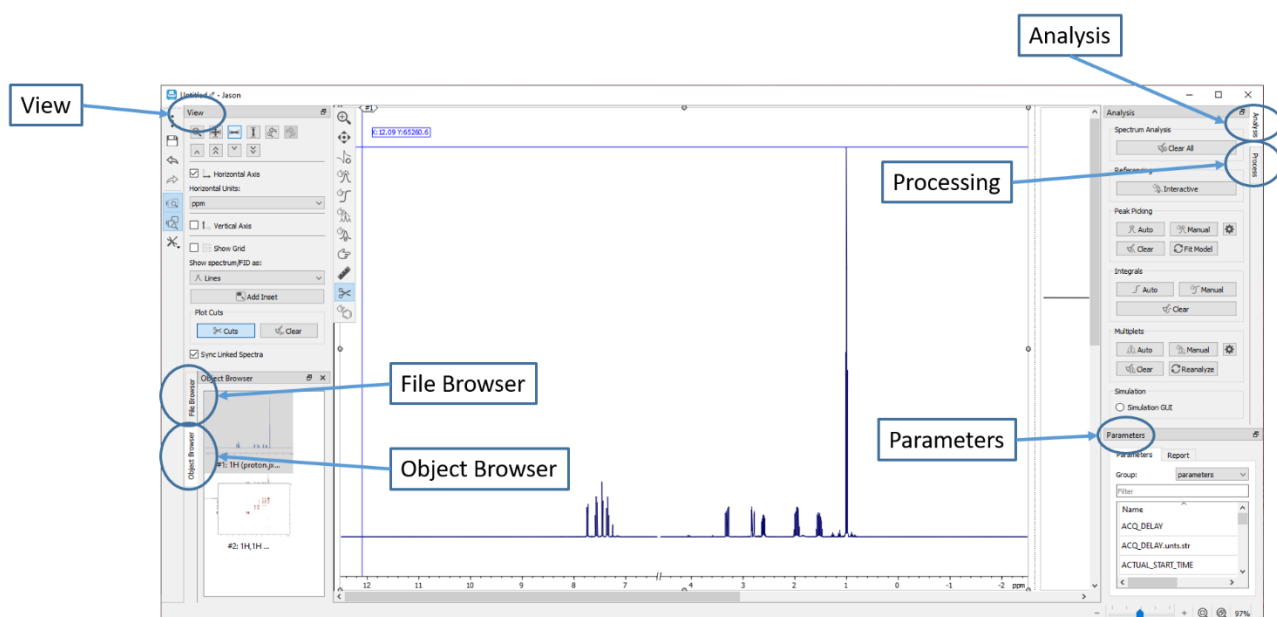*Figure 17: Data Context Tools panels for NMR spectra*

Figure 18: 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
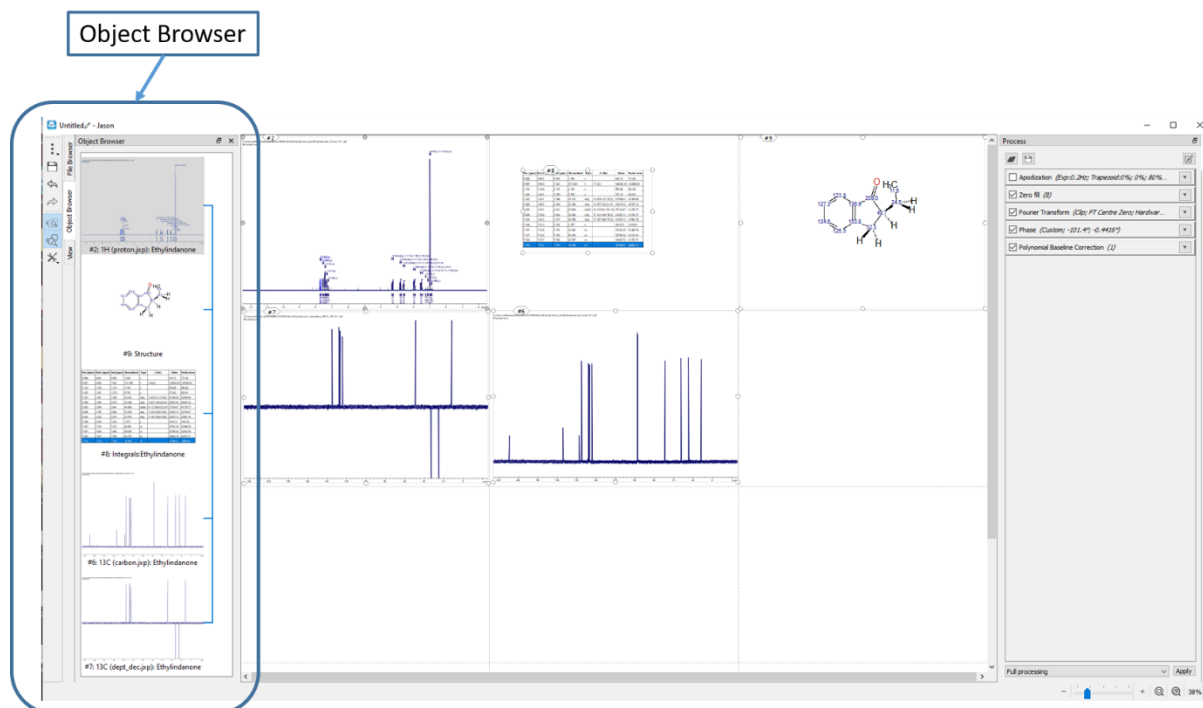

Figure 19: The Object Browser

The object browser is a visual list of all objects on the canvas, see figure 19. 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 19 the proton spectrum 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 dialogue, see figure 20. This dialogue 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 synchronised.

There is also a checkbox option to interlink all the selected spectra. If this option is selected then all the selected items in the link target panel will be mutually linked when the ok button is pressed. To avoid confusion it is important to note that having this box checked will create mutual linking between all selected items, however, unchecking the box, does not reverse the process. Objects on the canvas must be explicitly unlinked pair by pair.

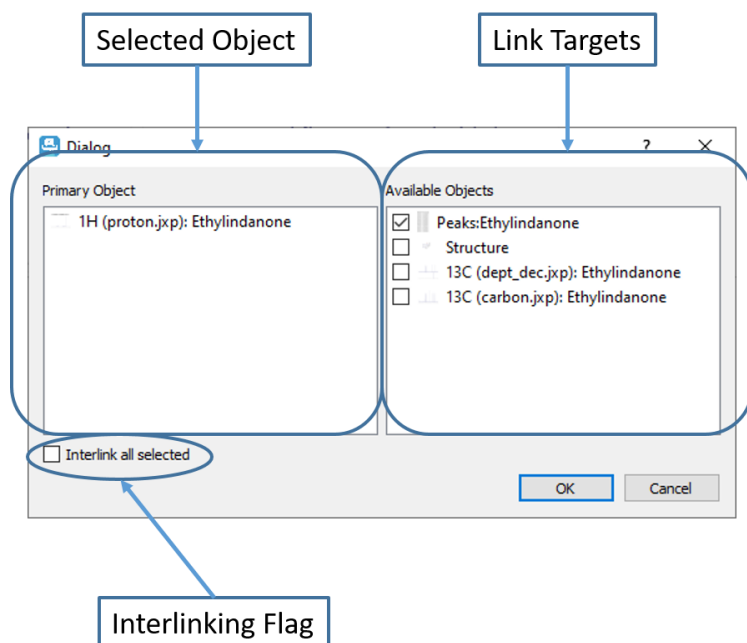The links between objects are shown as the blue connecting line to the right of object browser display area.

Figure 20: The object linking dialogue

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.
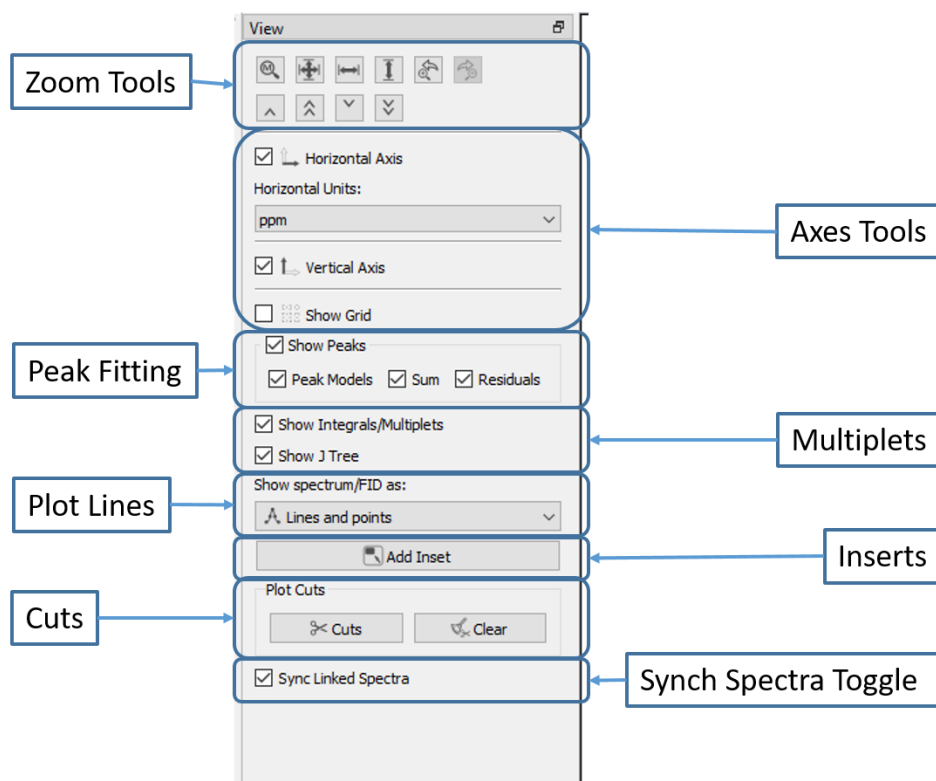

Figure 21: The View Panel

The view options for a 1D spectrum are shown in figure 21.

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

Axes 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 (residual).

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 lined 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 22. 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.
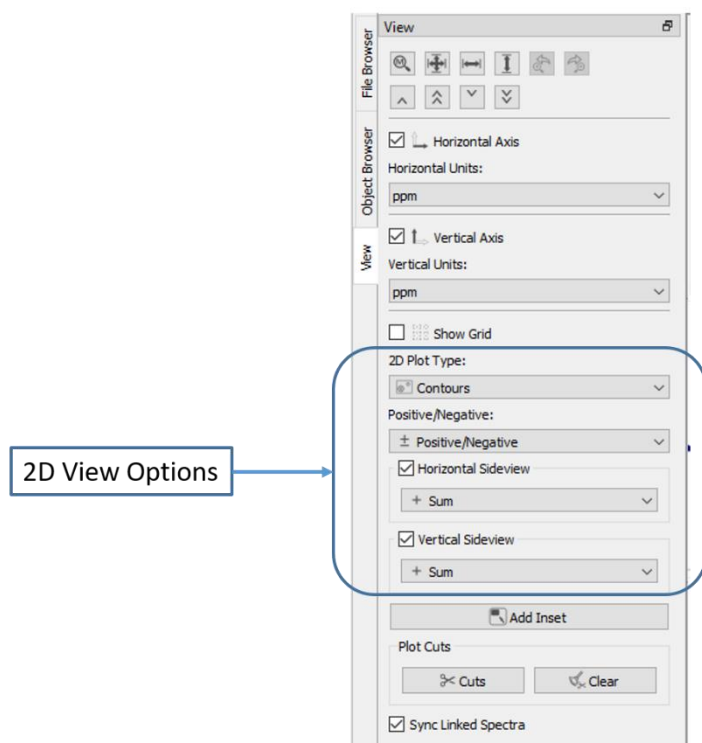
Figure 22: 2D Options in the view panel

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 23 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.
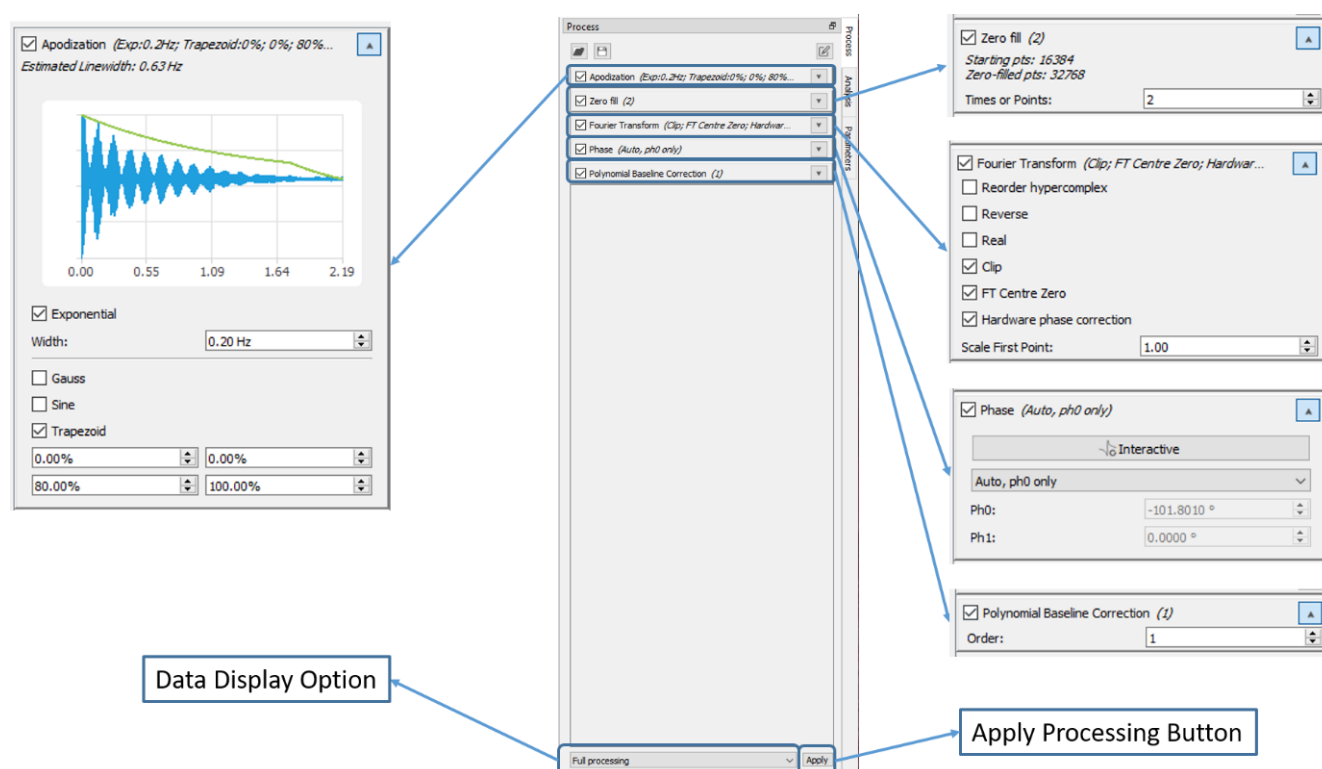

Figure 23: The Processing Panel

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 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 a later section (8).

Apodization: this panel displays the options and parameters for signal apodization. In addition to the 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 multipler, for values less than 10 or as a number of points.

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 phase is determined automatically
2) Custom: in this mode the phase can be changed manually by typing values into the dialogue boxes below.
3) Absolute: the spectrum is displayed in magnitude mode.
4) Auto Ph0: the first order phase is determined from the acquisition parameters and the zero order phase is corrected automatically.

The Ph0 and Ph1 fields display the current zero and first order phase correction and in custom mode they can be used to manually change the phase.

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

Data Display Options: The data display options allows the user to view the data at different points in the processing chains, the options are:

1) Show raw data, which displays the original time domain data
2) F2 time domain processing, which displays the time domain signal after processing 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.
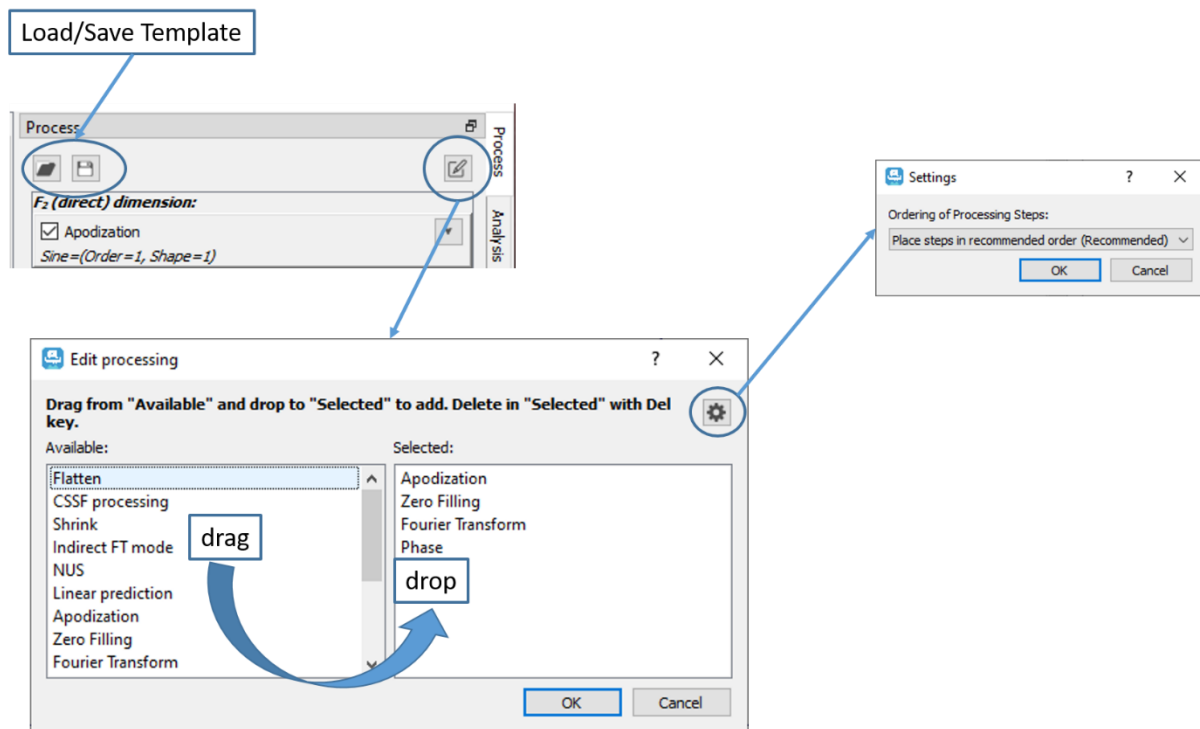
Figure 24: Processing List options

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 24. The edit processing dialogue 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 selection have been made, the processing list is updated when the ok button is pressed.

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.

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 dialogue, see figure 24. 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.

3.6 The Analysis Panel

The analysis panel contains a list of analysis tools that might be used to examine an NMR a spectrum. The list of functionality shown is figure 24 is typical for a 1D NMR spectrum.
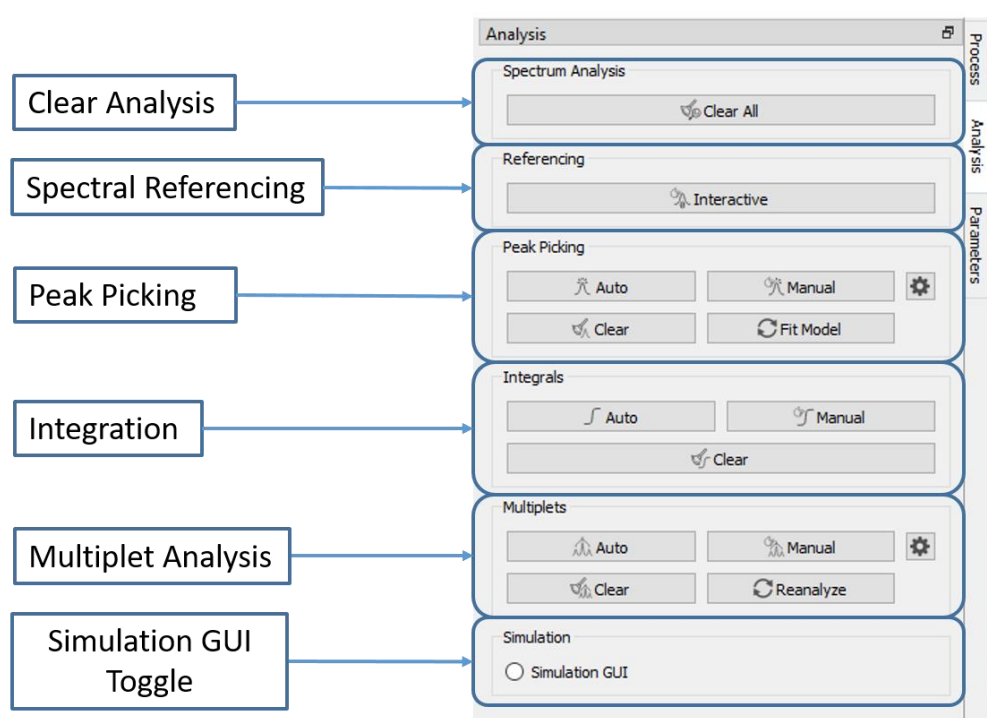

Figure 25: The Analysis Panel

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.

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 mode to the data.

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 a subsequent 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 a regional analysis as carried out in the peak picking and integration analysis steps, assuming these have not already been performed, 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 reanalyse button can be pressed to redo the multiplet analysis.

The clear button clears all multiplets.

Simulation GUI Toggle: If a user has created a simulation and no longer needs to see the simulation GUI it can be hidden using the simulation GUI radio button.

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 26 shows the two tabs for the parameter panel of a 1D NMR spectrum.
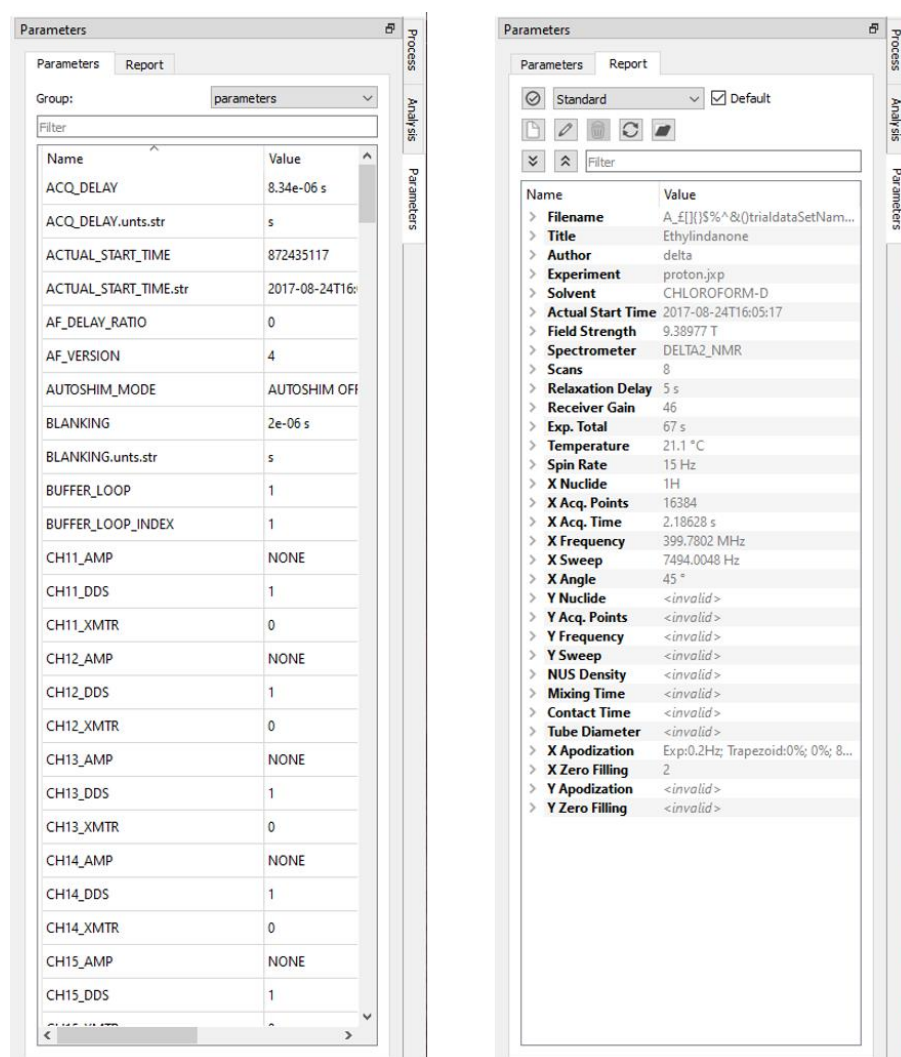

Figure 26: The Parameters Panel

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 4 options:

4.1.1   Parameters Table

The **parameter table** option from the **create** menu places a parameter table next to the spectrum, see figure 27. 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 26) into the displayed table.
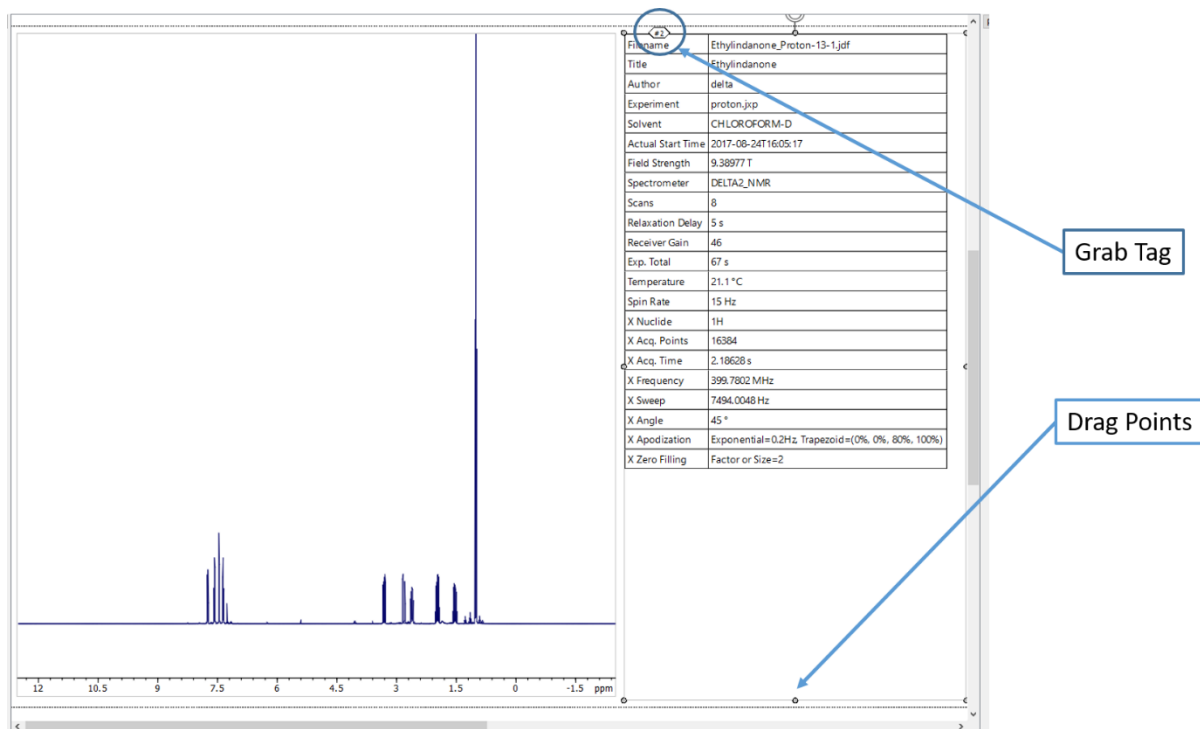

Figure 27: Parameter Table
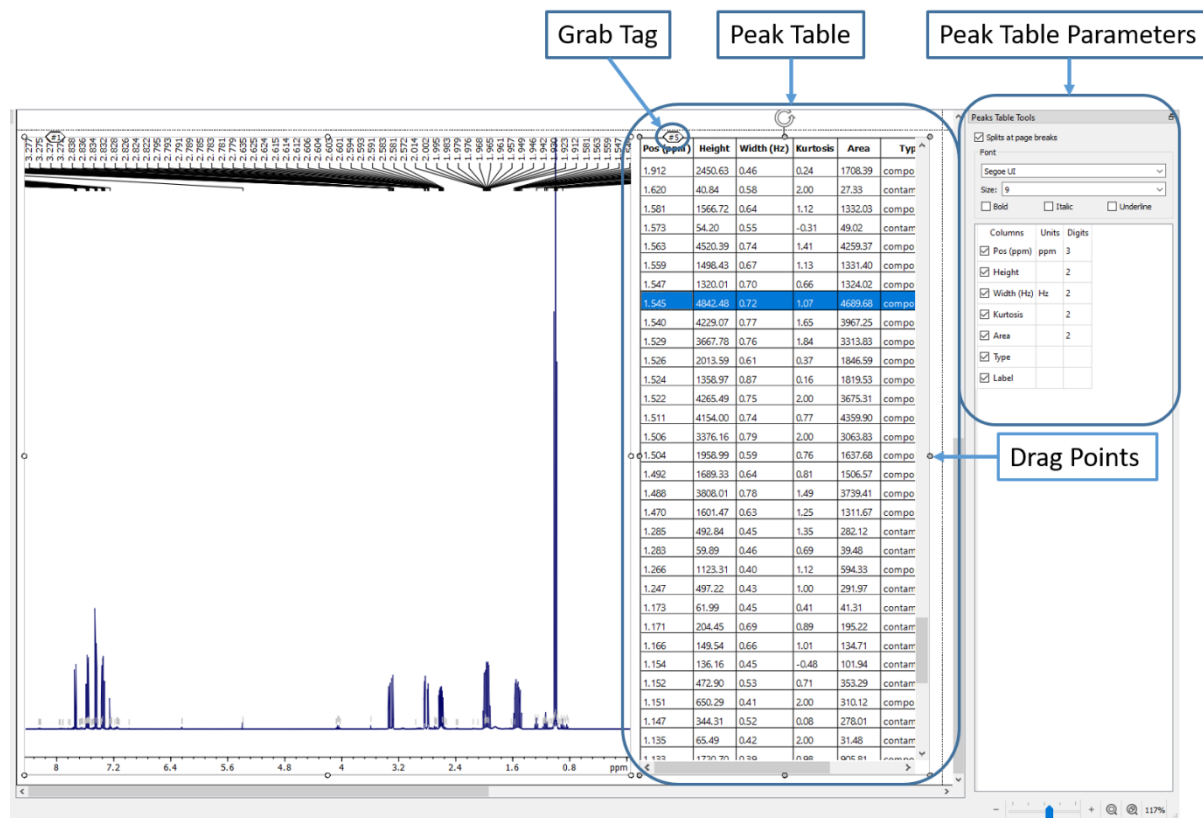
4.1.2   Peak Table

Figure 28: Peak Table

Once a peak picking has been carried out the **create** menu in the right mouse button context menu will have an option for **peak table**, see figure 28. Clicking on is 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 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
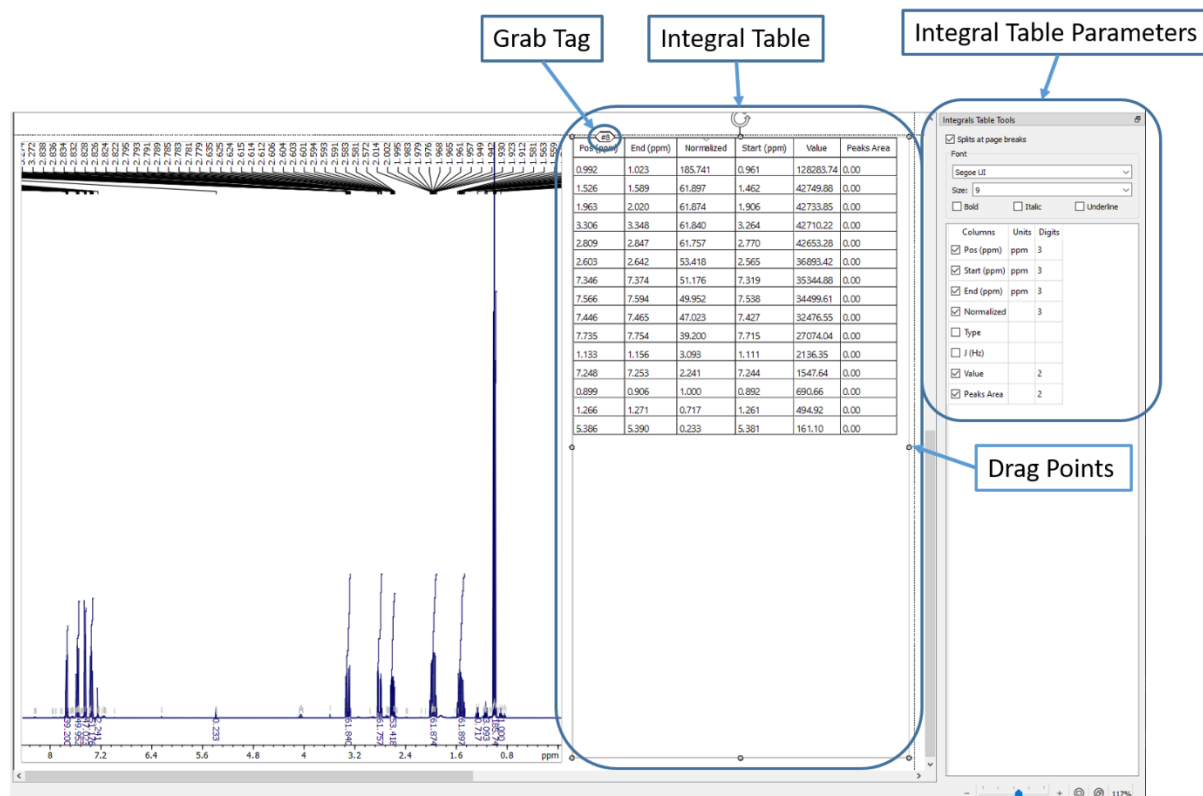
4.1.3   Integral/Multiplet Table

Figure 29: Integral Table

Once integrals has been created the **create** menu in the right mouse button context menu will have an option for **Integral/Multiplet table**, see figure 30. Clicking on is 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, see figure 30.

4.1.4   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 30. 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 journal formats .
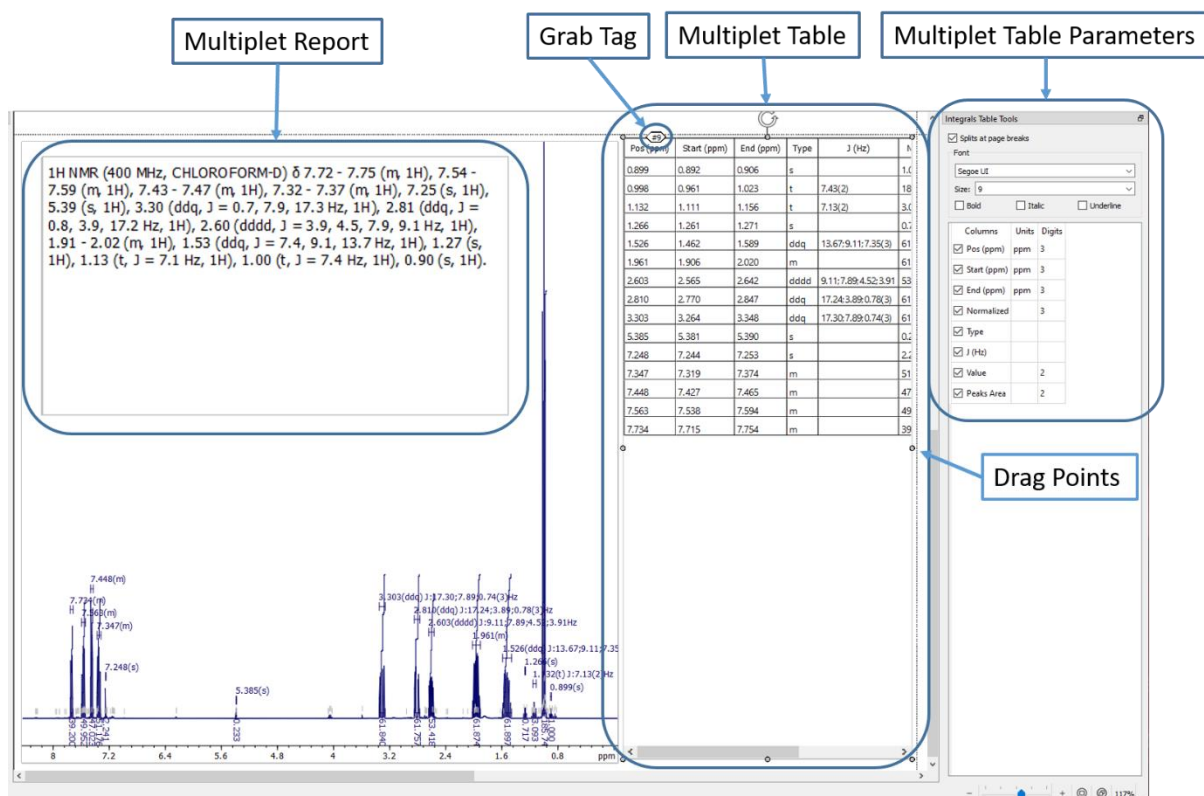
Figure 30: Multiplet Table and Report

5 The Settings Menu

There is a large array of option 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 31.
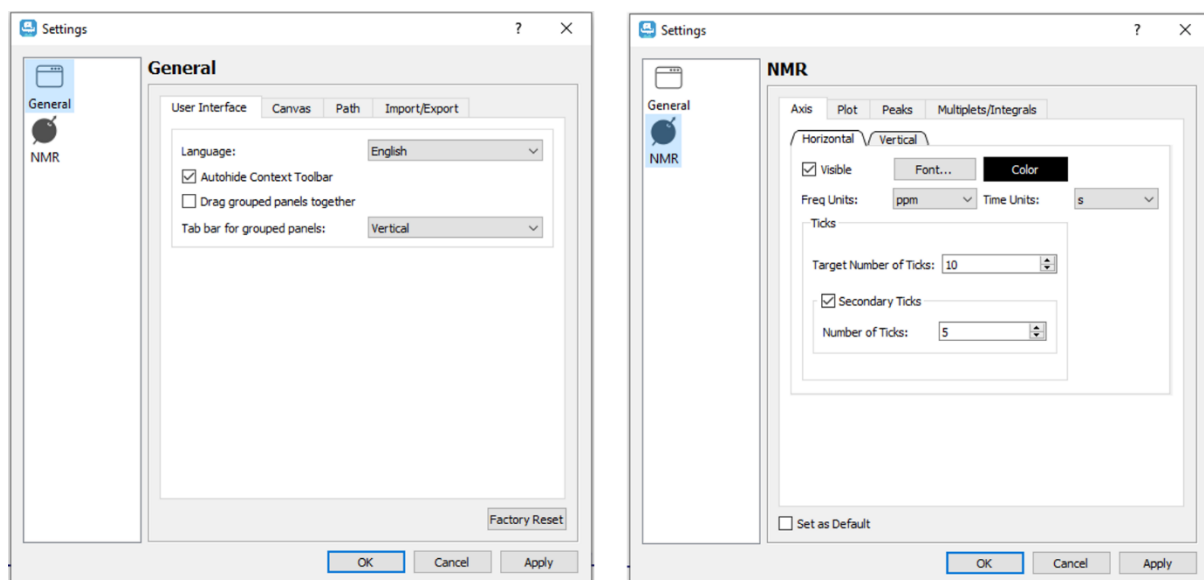

Figure 31: The Settings Menu, the general setting (left) and NMR settings (right)

The settings menu can be accessed from the main menu in the top left hand corner of JASON or from the menu opened on a right mouse button click anywhere in the canvas. When the menu is first opened the user will see the general settings section. If the NMR icon is selected, the menu will

display the NMR settings. The settings menu comprises two section, the general settings and the NMR settings. Each of these sections has its own set of tabs which are described below.

5.1   The General Settings

Figure 32: The General Settings
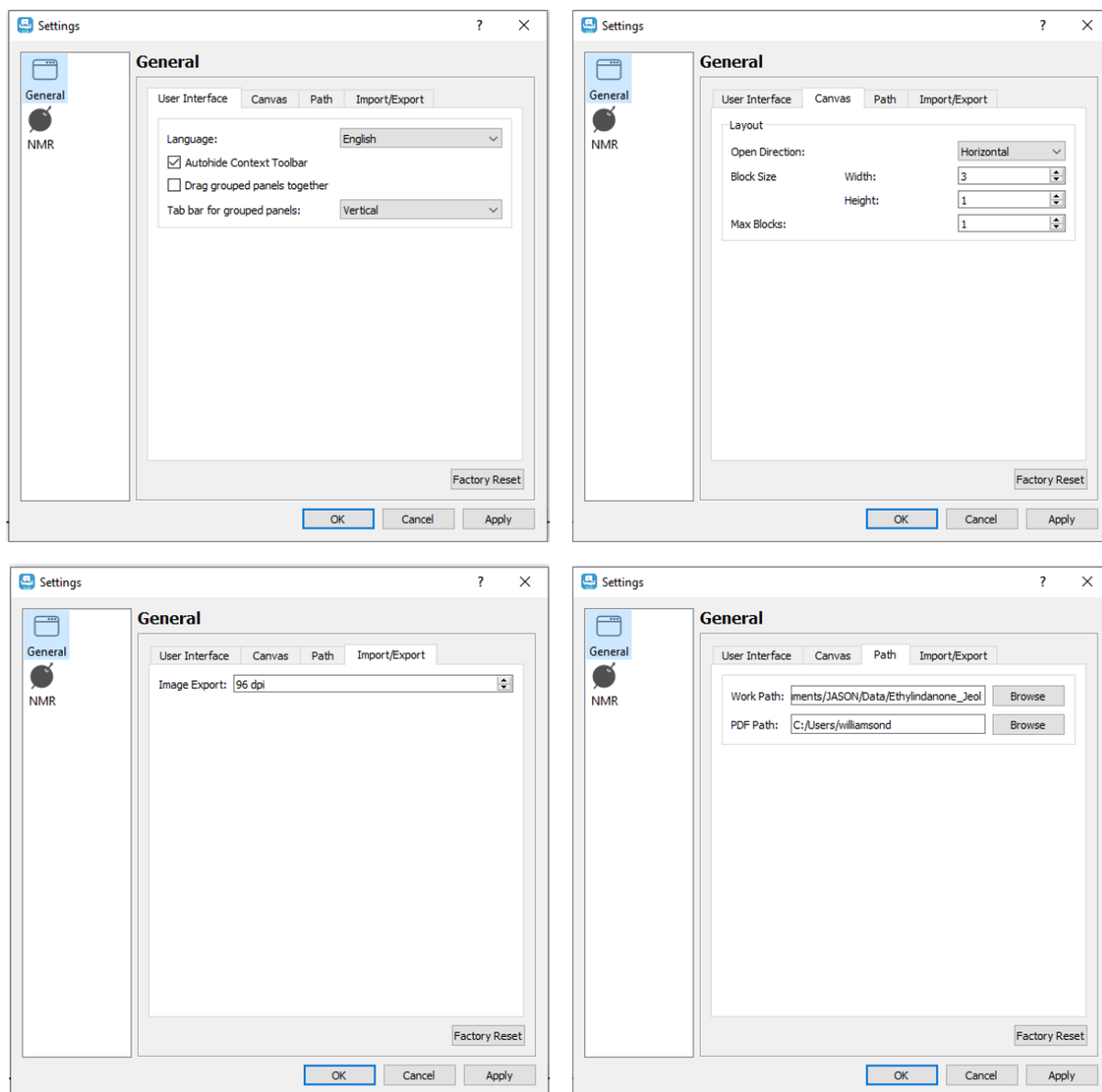
The general settings panel has 4 tabs:

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.

Autohide Context Tool Bar: when this box is checked, the context tool bar discussed in section 3.1 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 and subsequent sections that are stacked on top of each other can be moved as a single object, see figures 17, 18 and 33.

Tab Bar for Group Panels: When the context sensitive panels are grouped together by stacking then one on top of another, the tabs can be displayed either horizontally or vertically as shown in figure 33.
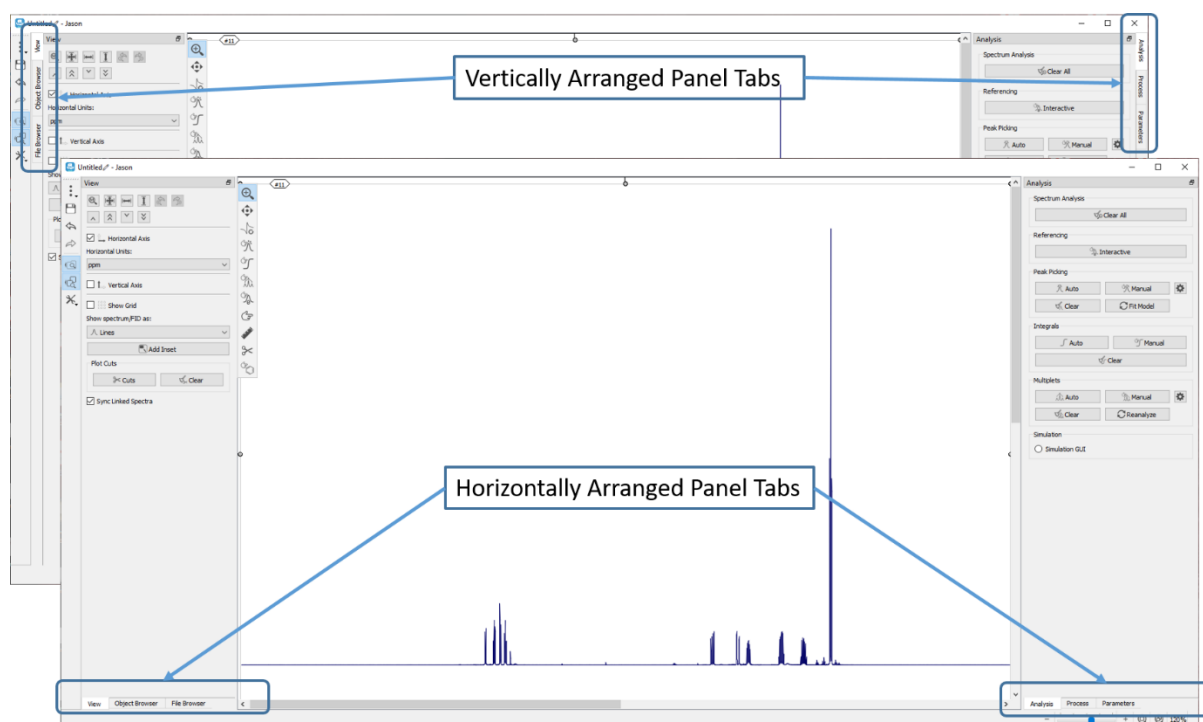

Figure 33: Alternative arrangements of grouped panels.

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 make in the **Open Direction** option.

If the user wishes the objects can be added in blocks, the size of these blocks are defined by the **Block Size Width** option and the **Block Size Height** option. As an example, if the open direction is horizontal and the block width and height are set to 2, then the first object will be placed in the top left hand corner (column A, row 1). The next object will be placed one step horizontally (column B, row 1). The third object will be placed one row below the first object (Column A, row 2), because the width of the block was set to 2. The fourth object will now be placed one column along from the third object and below the second object (Column B row 2). This completes a block.

If the **Max Blocks** option is set to 1, all subsequent objects will be added horizontally or vertically in in 2 x 2 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 x 2 blocks up to a grid of a x 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 typing the

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 typing the

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 34. Each panel is describe in the section below. Any settings can be set as default using the **Set as Default** checkbox at the bottom.
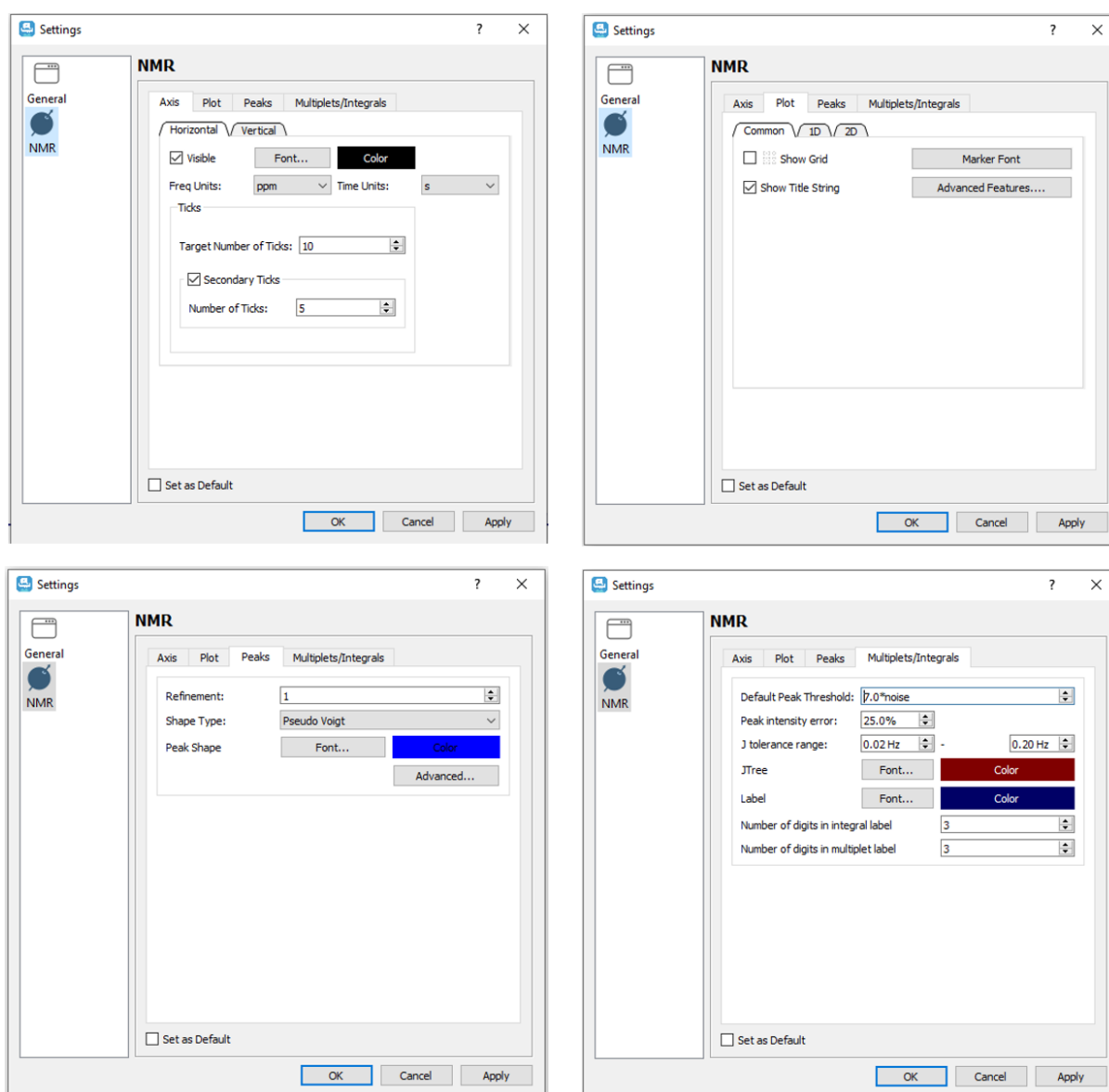

Figure 34: The NMR Settings main tabs

Any changes can be applied using the **Apply** button or when all the changes have been completed the user can quit the settings dialogue by pressing **ok**, which will apply the setting and quit or by pressing the **cancel** button which will quit without applying the settings.

5.2.1   Axis

The axis settings contains the options for modifying the axis in an NMR spectrum and it comprises two panels, settings for the horizontal axis and settings for the vertical axis, see figure 35.
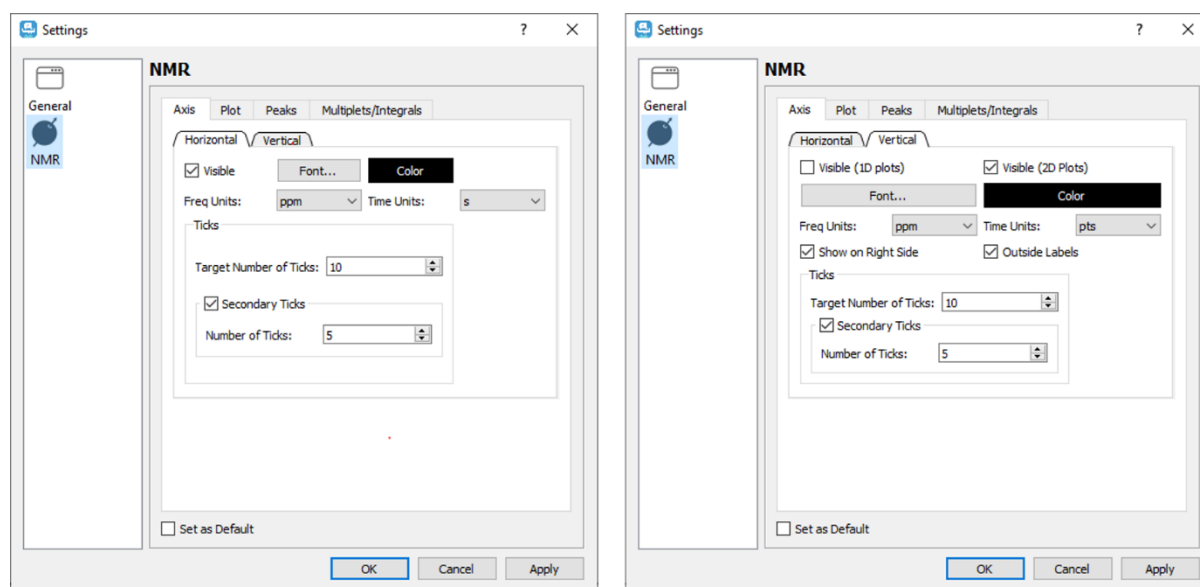

Figure 35: NMR setting axis tabs

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

Visible checkbox to toggle the visibility of the axis.

Font and **Color** buttons open dialogues that allow the user to change the font and style of the axis and the colour.

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 dialogue 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 minimising 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** dialogue 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.
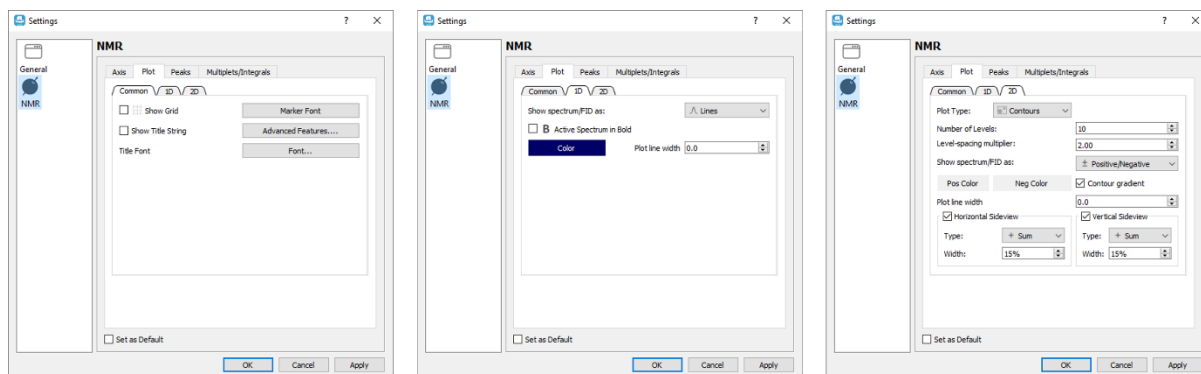

Figure 36: NMR settings plot tabs

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 dialogue. The **Marker Font** button allows the user to change the font, style and colour 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 dialogue shown in figure 37. The options determine the joint zoom behaviour of a parent spectrum and an insert.
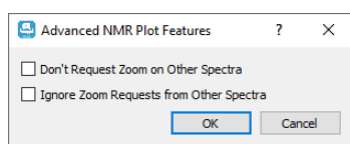

Figure 37: The NMR settings plot advanced options

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 38:

Refinement, which controls the number of iterations or cycles 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 Generalised 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 colour of the peak labels and the peak lines.

The **Advanced** button opens up a dialogue box that contains all the options used in peak picking and peak fitting, see figure 38. These values should only be changed by an expert user who fully understands the peak picking process.
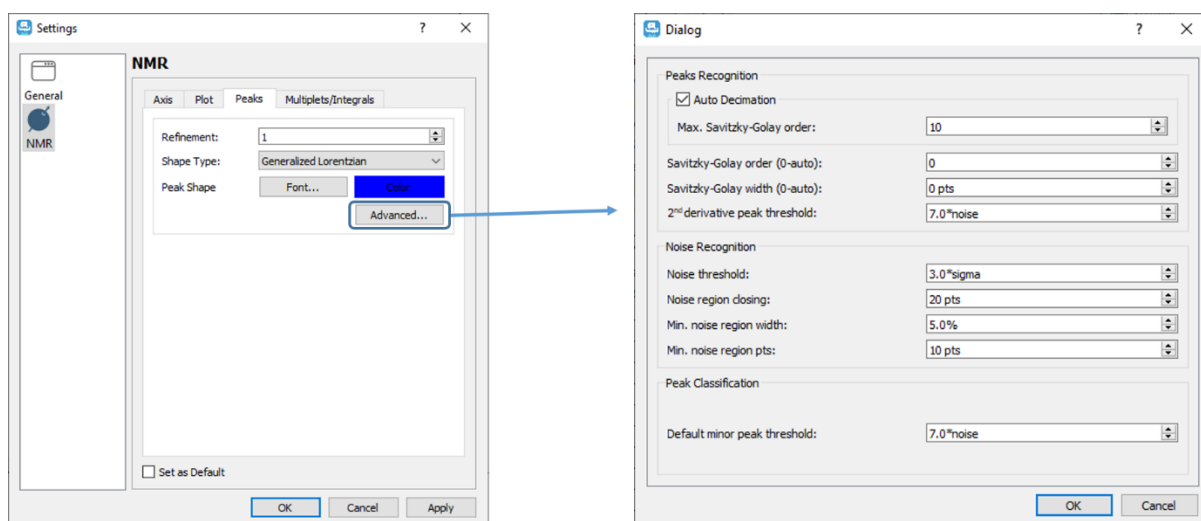
Figure 38: NMR Peak Setting

5.2.4   Multiplets/Integrals

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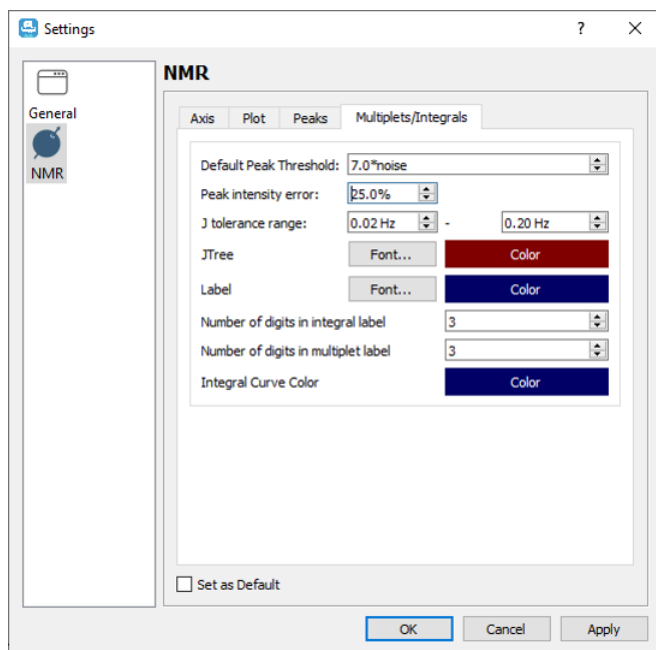

Figure 39: Multiplets and Integral Settings

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 varying degrees of second order effect. 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.

JTree: These options allow the user to define the font and colour of the J-coupling tree displayed on a spectrum

Label: These options allow the user to define the font and colour 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 Colour: this option allows the user to pick the colour 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.
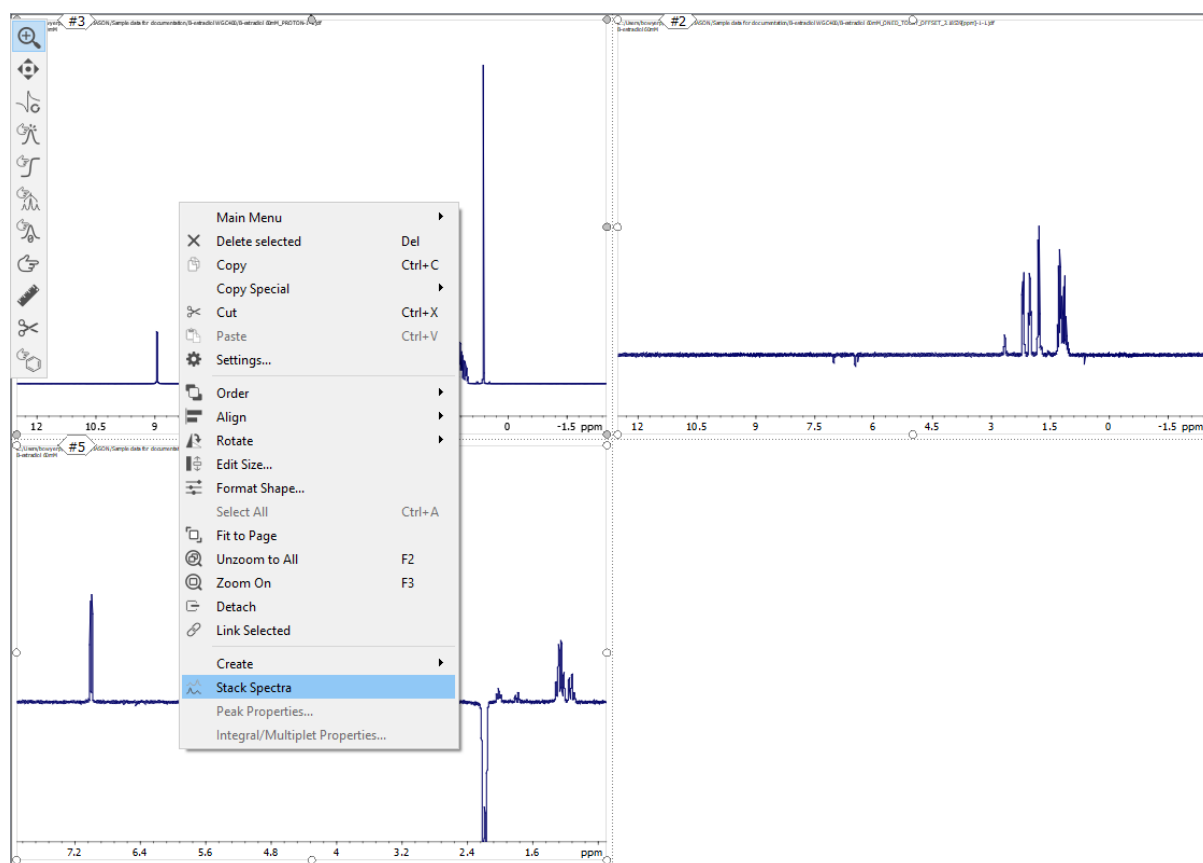

Figure 40: Selecting and stacking individual spectra

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

Figure 41: 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 42: 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.
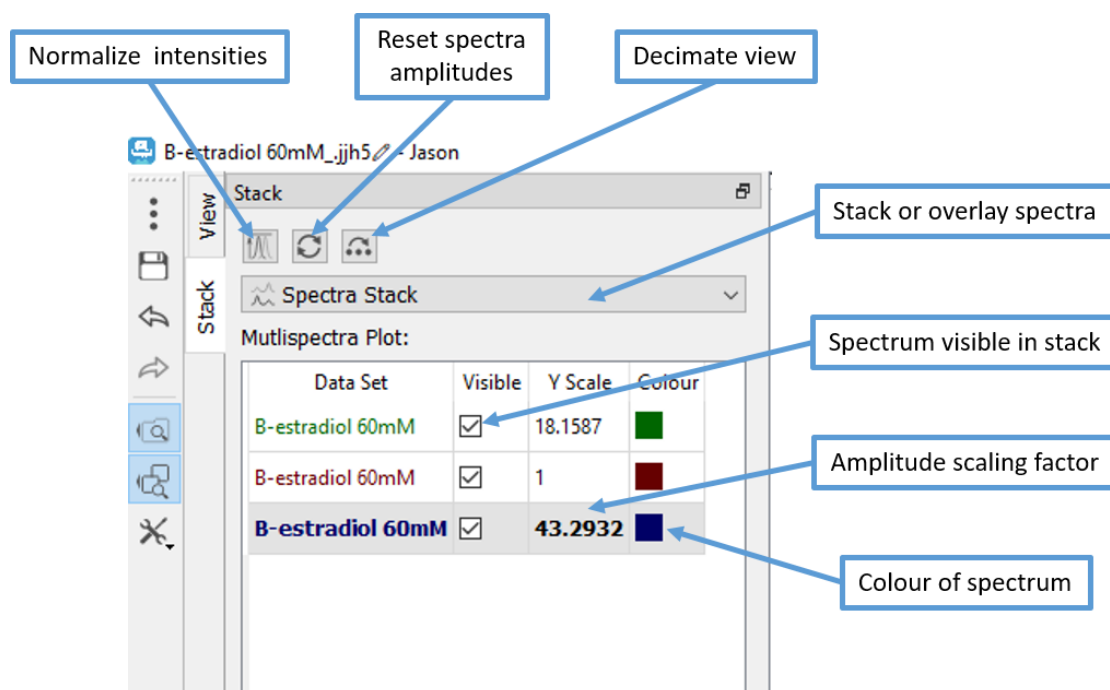
The currently active spectrum in the stacked plot is also indicated by bold font for the row. To make another spectrum in the stack active, double-click on the appropriate row in the table. To adjust the order of the spectra, click on a row and drag it to the desired location, above or below other rows in the table.
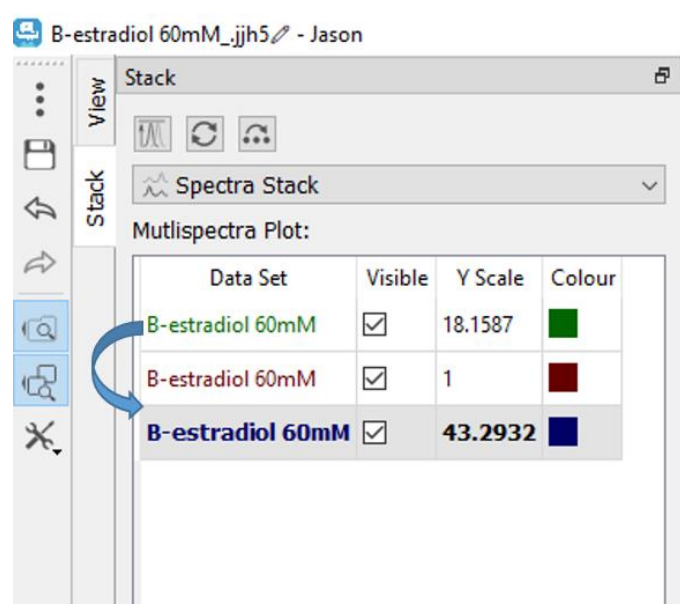

Figure 43: Reordering spectra in the stacked plot by dragging rows in the table

To change the colour of a spectrum in the stacked plot, double-click on the coloured square at the right-hand side of the row and select or configure the desired colour on the "Select Colour" 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^{th} spectrum in the stack (e.g. every 10th spectrum). To do this, use the "Decimate view" button and enter the decimation factor.

To overlay spectra instead of stacking them, select "Spectra Overlap" from the dropdown menu.
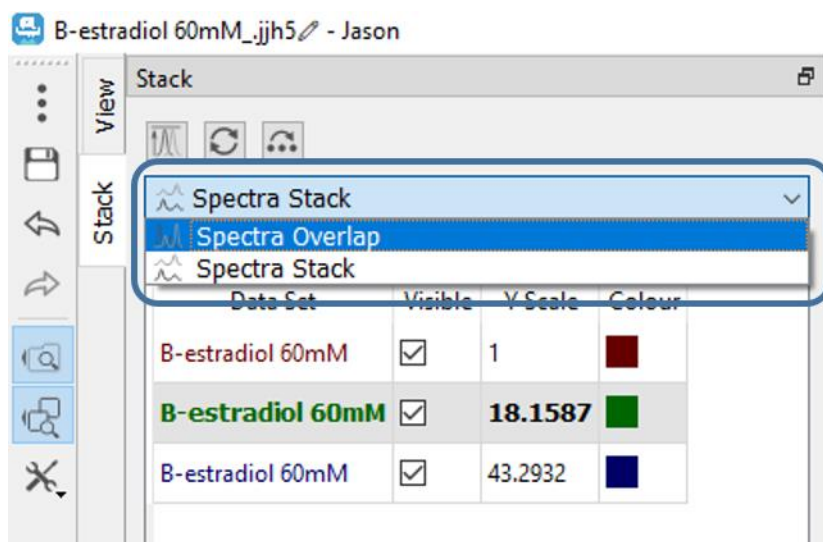

Figure 44: Overlaying spectra using the Stack panel

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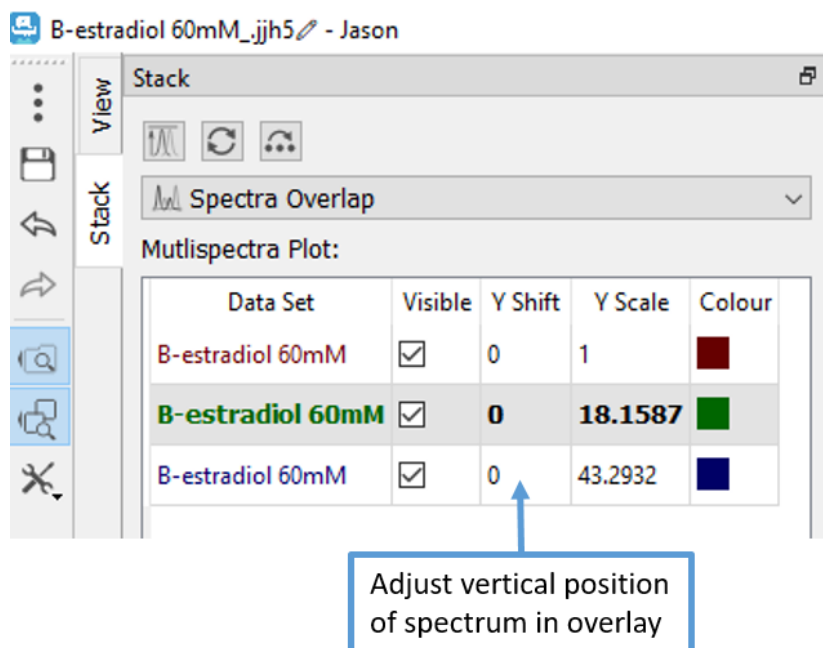

Figure 45: Adjusting the vertical positions of overlaid spectra

7   Spin Simulations

Spin simulations of 1D spectra can be performed in JASON but selecting the simulation option from the **main menu.** When a simulations has been selected it opens the simulation dialogue panel, see figure 40. This allows the user to enter the chemical shifts and coupling constants for the spins along with other relevant parameters. As the data is entered the simulated spectrum will appear in a new panel on the canvas.
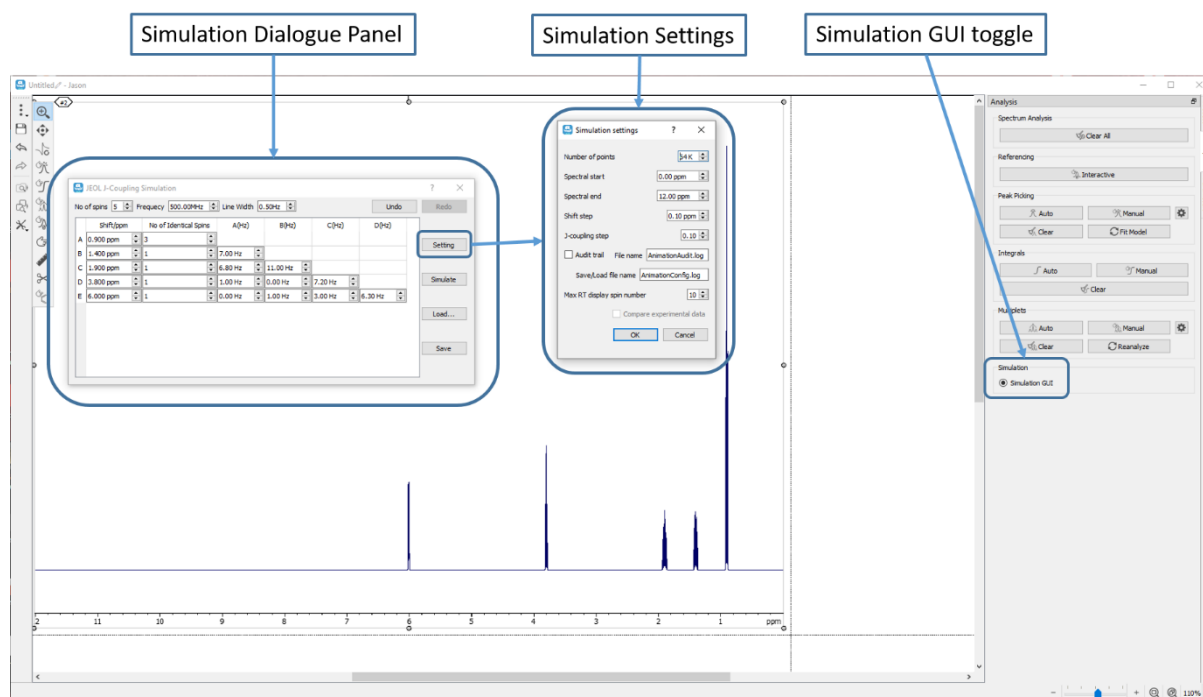

Figure 46: Spin Simulation interface

7.1   Simulation Dialogue 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 dialogue.

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 spins

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 chemicals 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 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 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: As 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   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. 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 41. 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.
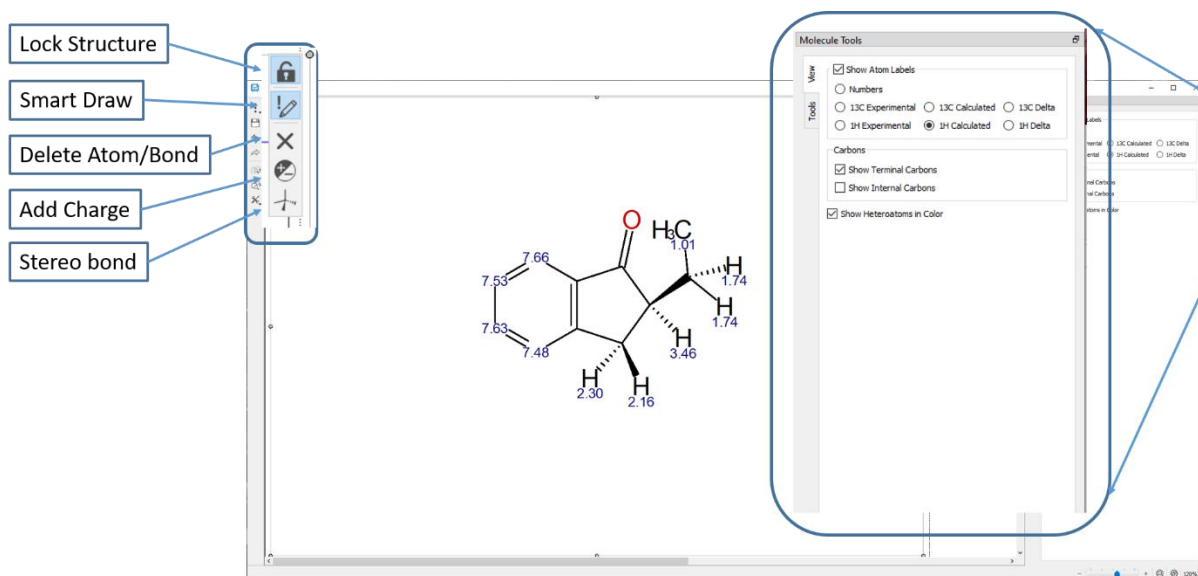
Figure 47: Molecular drawing interface

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 togged 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.

13C Experimental/Calculated/Delta: These options show the chemical shift value of the carbonsatoms 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).

1H 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 Colour: This toggles the option to show heteroatoms in colour.

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 42.
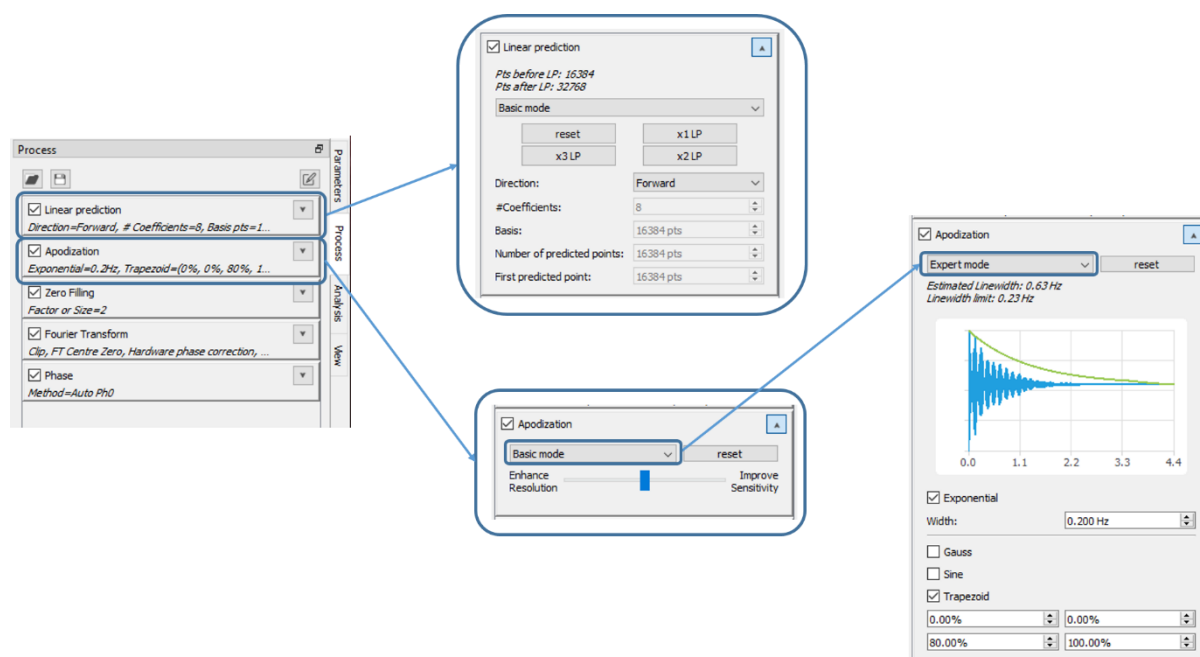

Figure 48: Extended Processing Options

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. At this point in time that is no additional points.

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 option 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.