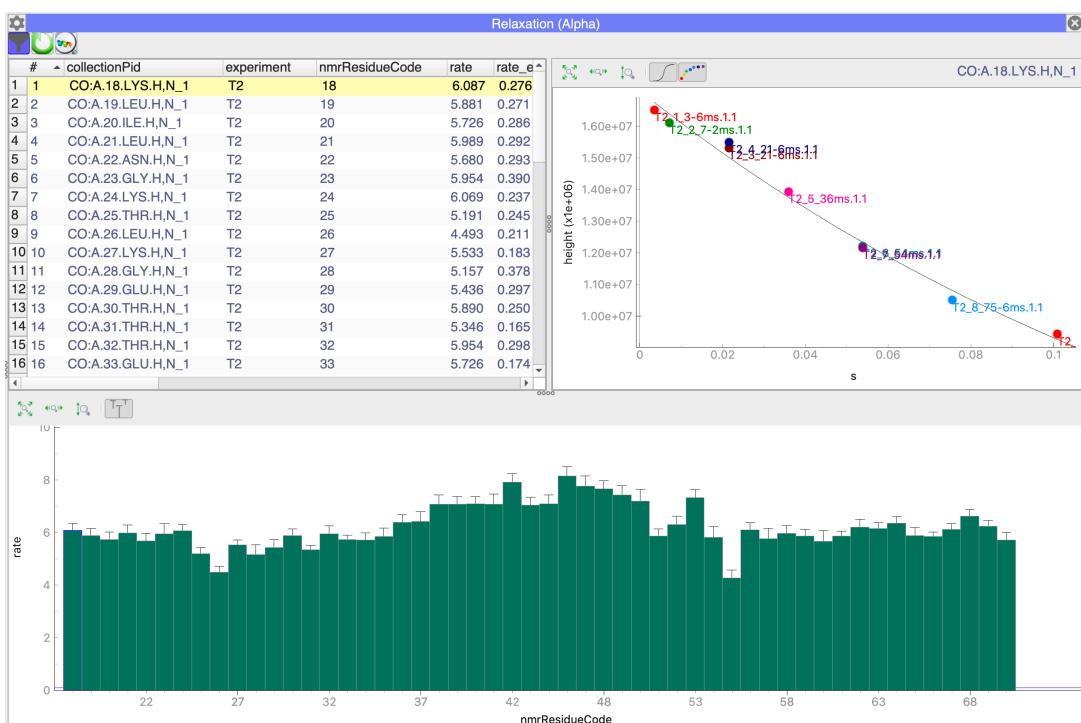


## Dynamics Tutorial (Alpha)



# Introduction

This tutorial will take you through the analysis of some dynamics data in CcpNmr Analysis Version 3.1 using the alpha-version of the Relaxation Data Analysis Module. We assume that you are already familiar with the basics of how the program works, e.g. by doing our Beginner Tutorial.

You can download the example data to go with this tutorial from the tutorials page of our website (<https://ccpn.ac.uk/support/tutorials/>). We are grateful to Dr Fred Muskett for making the spectra of GB1 available to us for use in this tutorial. You will be analysing T1 and T2 relaxation and heteronuclear NOE data, and then going on to do reduced spectral density mapping and Hsqc ETA( $\eta$ ) analysis. We have not included any theoretical background to these experiments.

Please see other publications for this information.

The tutorial is divided into sections, each of them has a set of simple actions: you will see a descriptive image on top and a full description below. (Note that images are representative, and that there may be small differences between your setup and that shown in the tutorial.)

## Contents:

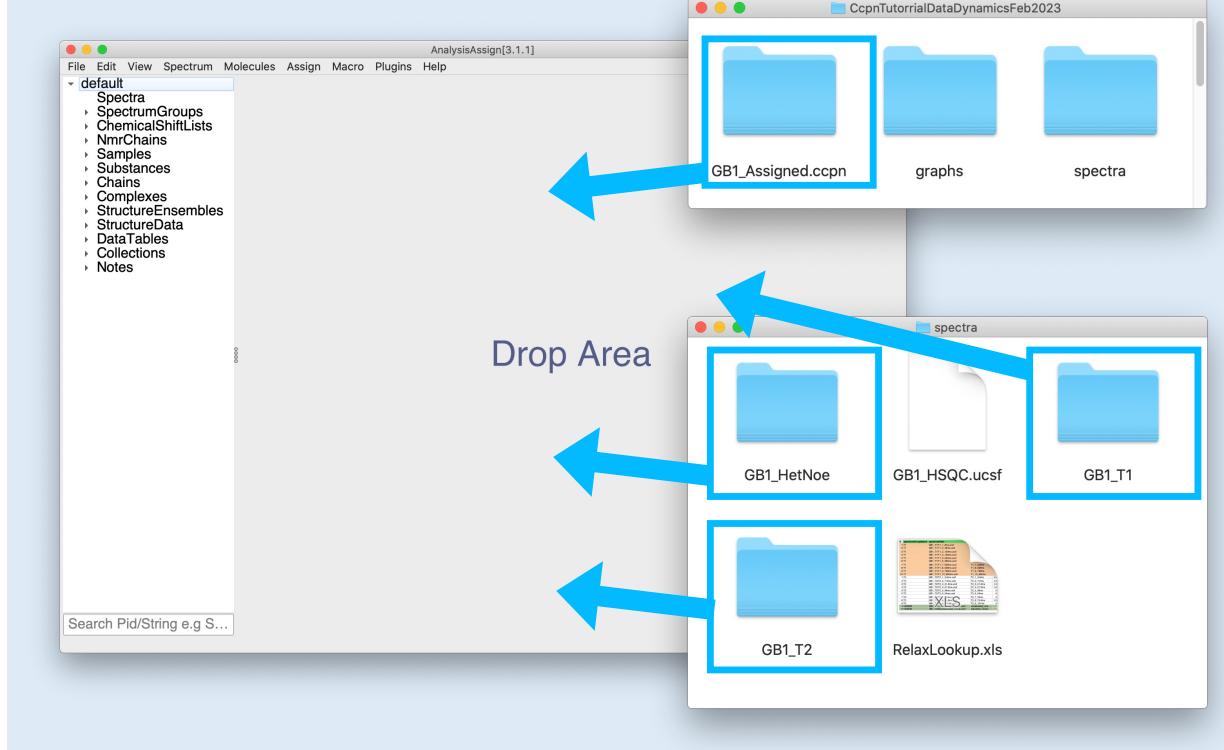
1. Loading Data
2. T1 and T2 Data
3. Heteronuclear NOE Data
4. Combined Analyses
5. Reduced Spectral Density Mapping
6. Hsqc- $\eta$  analysis
6. Exporting Graphs
7. Examining the Graphs

## Start CcpNmr Analysis V3

Apple/Linux users by using the terminal command *bin/assign* in the *ccpnmr* directory

Windows users by double-clicking on the *assign.bat* file in the bin directory of the *ccpnmr* directory

# Loading data



## 1A Open project and load spectra

- Find the **GB1\_Assigned.ccpn** project folder in the Dynamics Tutorial data directory. This project contains an assigned HSQC spectrum of GB1.
- Select the folder in your file browser and drag it onto the **Sidebar or Drop Area**.

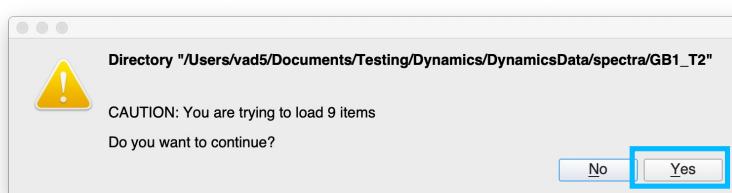
- Find the **spectra** directory in the Dynamics Tutorial data directory
- Select and drag the following three folders into the Sidebar or Drop Area:

**GB1\_T1**

**GB1\_T2**

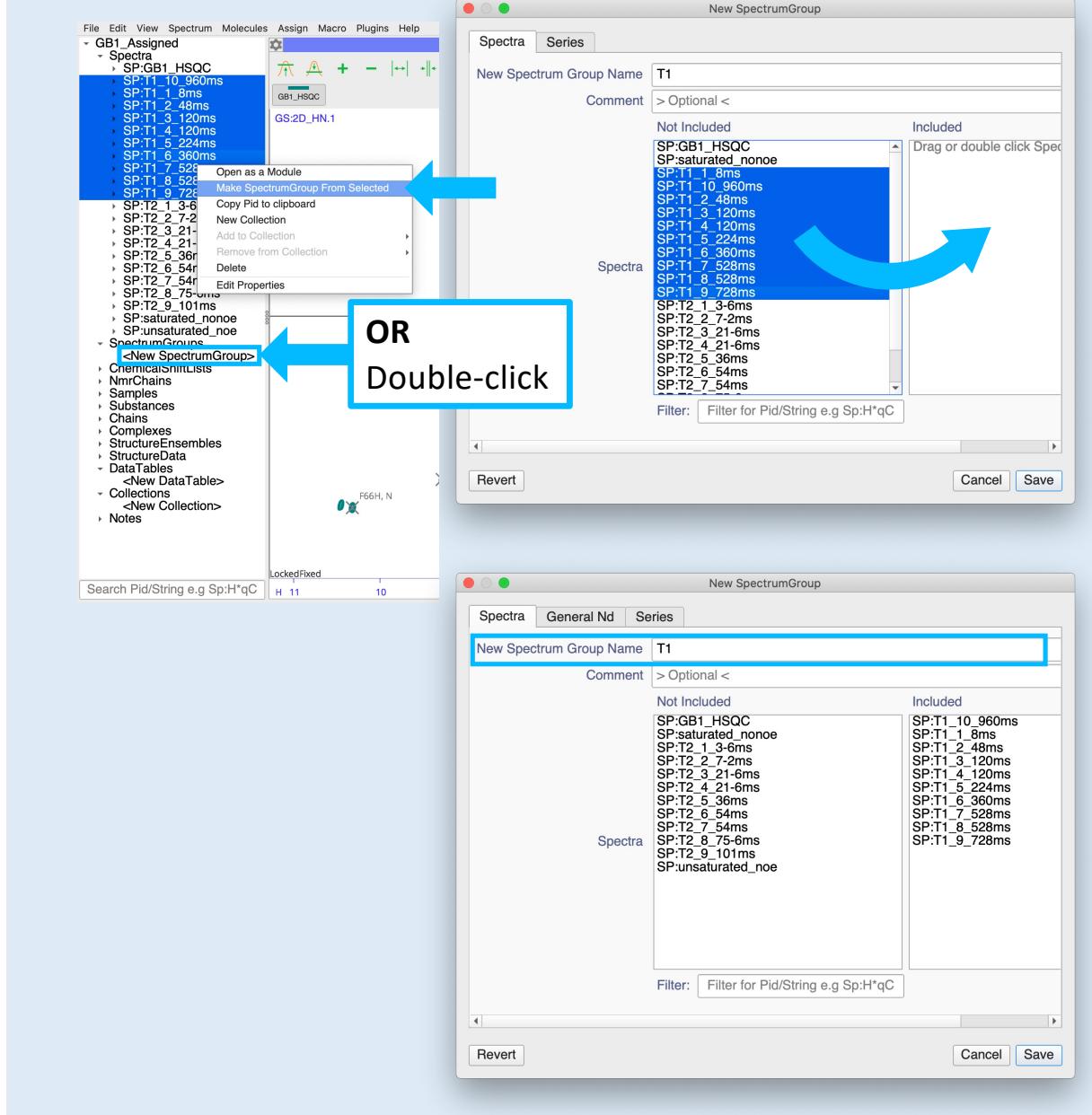
**GB1\_HetNOE**

If asked whether you want to continue loading multiple items, click **Yes**.



If you drop the folders into the Drop Area they will open directly. If you drop them on the Sidebar they will simply be visible in the **Spectra** section of the sidebar and can be opened in a SpectrumDisplay module at a later stage.

# Loading data



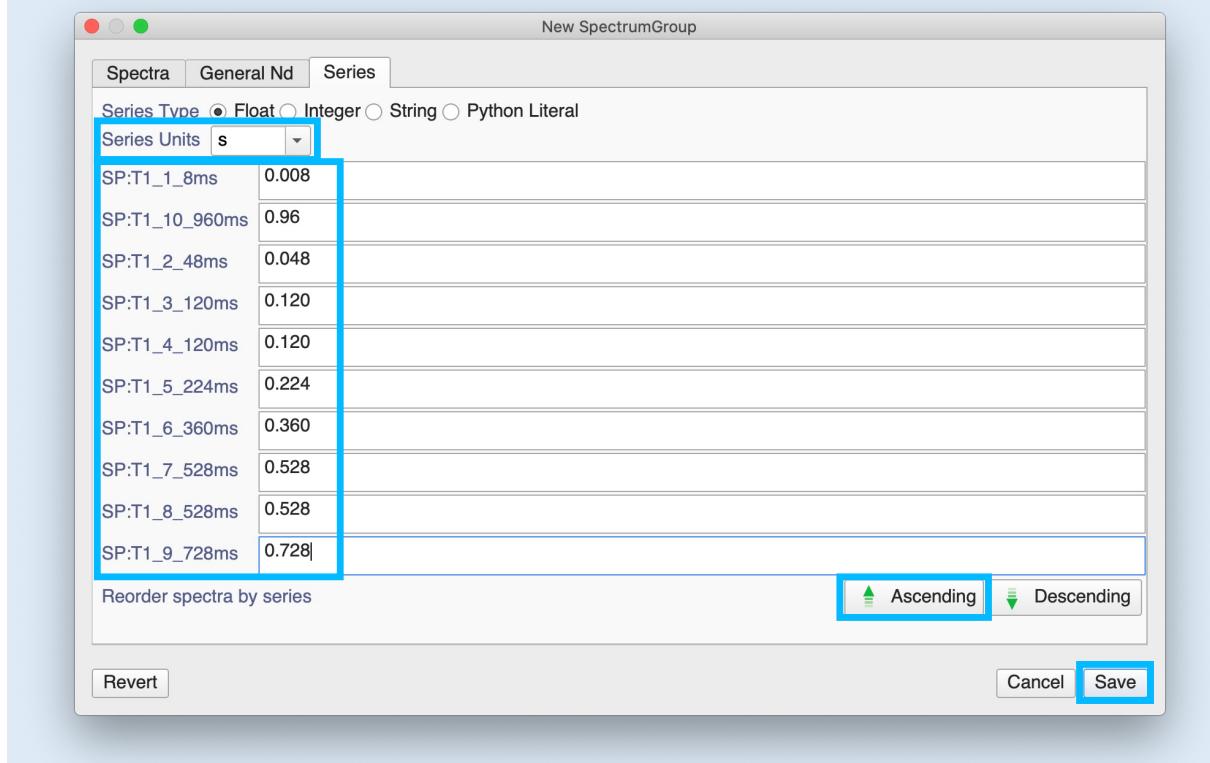
## 1B Create the T1 SpectrumGroup and Series

- Select all the T1 spectra in the sidebar, right-click and select **Make SpectrumGroup from Selected**

**OR**

- Expand **SpectrumGroups** in the sidebar and **double-click** on **<New SpectrumGroup>**
- In the **Edit SpectrumGroup** pop-up, **drag** all the T1 spectra from the left hand side the right hand side of the pop-up

- Give your SpectrumGroup a new Name, e.g. **T1**



### 1C Create the T1 Series

- Go to the **Series** tab of the Edit SpectrumGroup pop-up
- Enter **s** (seconds) as your unit (either type it or select from the drop-down menu).
- Enter the relaxation delay (in seconds) for each spectrum. You can derive these from the spectrum names (note that these are given in ms, not s).  
Note that some delay times are repeated in order to give an indication of the measurement error.
- If your spectra are not ordered in ascending order, then click the **Ascending** button to do so.
- Finally click on **Save**.

# Loading data

## T2Data

The screenshot shows the T2Data interface. On the left, a sidebar lists various spectra: SP:T1\_9\_728ms, SP:T2\_1\_3-6ms, SP:T2\_2\_7-2ms, SP:T2\_3\_21-6ms, SP:T2\_4\_21-6ms, SP:T2\_5\_36ms, SP:T2\_6\_54ms, SP:T2\_7\_54ms, SP:T2\_8\_75-6ms, SP:T2\_9\_101ms, and SP:saturated. A context menu is open over the SP:T2\_1\_3-6ms spectrum, with the 'Make SpectrumGroup From Selected' option highlighted. To the right, a 'New SpectrumGroup' dialog is open, showing a table of series. The 'Series' tab is selected. The 'Series Type' is set to 'Float'. The 'Series Units' dropdown is set to 's'. The table contains the following data:

| Spectrum       | Value  |
|----------------|--------|
| SP:T2_1_3-6ms  | 0.0036 |
| SP:T2_2_7-2ms  | 0.0072 |
| SP:T2_3_21-6ms | 0.0216 |
| SP:T2_4_21-6ms | 0.0216 |
| SP:T2_5_36ms   | 0.036  |
| SP:T2_6_54ms   | 0.054  |
| SP:T2_7_54ms   | 0.054  |
| SP:T2_8_75-6ms | 0.756  |
| SP:T2_9_101ms  | 0.101  |

## HetNOE

The screenshot shows the HetNOE interface. On the left, a sidebar lists spectra: SP:T2\_9\_101ms, SP:saturated\_nono, SP:unsaturated\_noe, and a SpectrumGroup named <New Spec>. A context menu is open over the SpectrumGroup, with the 'Make SpectrumGroup From Selected' option highlighted. To the right, a 'New SpectrumGroup' dialog is open, showing a table of series. The 'Series' tab is selected. The 'Series Type' is set to 'Float'. The 'Series Units' dropdown is set to 'AU'. The table contains the following data:

| Spectrum           | Value |
|--------------------|-------|
| SP:saturated_nono  | 1.0   |
| SP:unsaturated_noe | 0.0   |

## 1D Create T2 and Heteronuclear NOE SpectrumGroups and Series

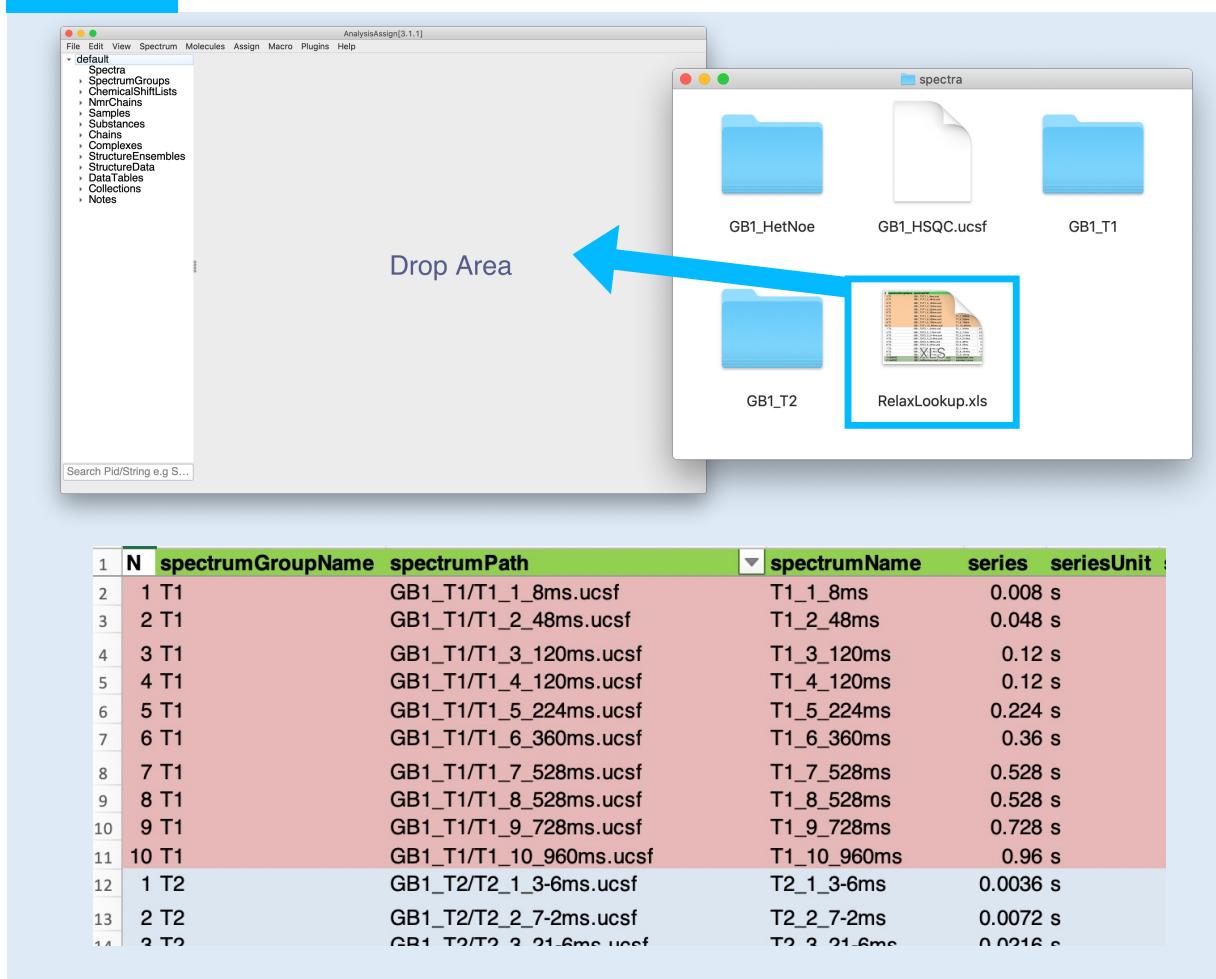
- Repeat the procedure for creating a SpectrumGroup and setting up the Series for the T2 data

Create a SpectrumGroup and Series for the Heteronuclear NOE data:

- Select the **saturated\_nono** and **unsaturated\_noe** spectra in the sidebar, right-click and select **Make SpectrumGroup from Selected**.
- Give the SpectrumGroup a **Name** (e.g. **HetNOE**)
- In the Series tab, set your units to **AU** (arbitrary units) and enter the following values:

|                        |            |
|------------------------|------------|
| <b>saturated_nono</b>  | <b>1.0</b> |
| <b>unsaturated_noe</b> | <b>0.0</b> |

# Loading data

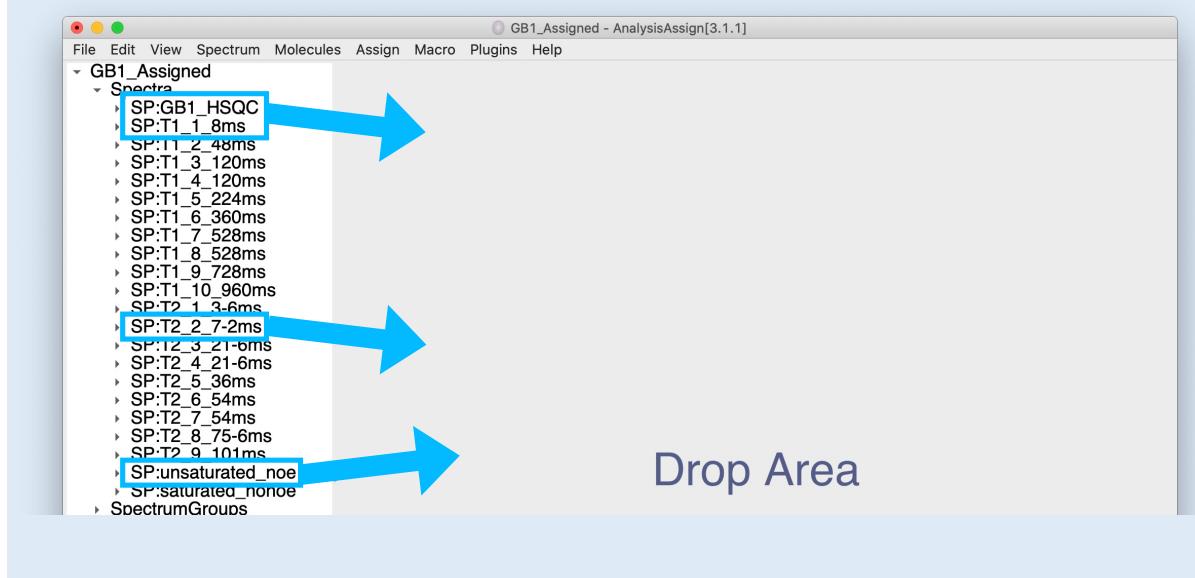


## 1E Import from Excel Lookup File (optional)

As an alternative to loading the spectra and setting up the SpectrumGroups and Series manually, you can also enter all the information into an Excel file and drag this into the program. This will automatically load the spectra and create the SpectrumGroups and Series for you.

The figure above shows the column headings required for the Excel file to load correctly. SpectrumPaths are relative to the location of the Excel file.

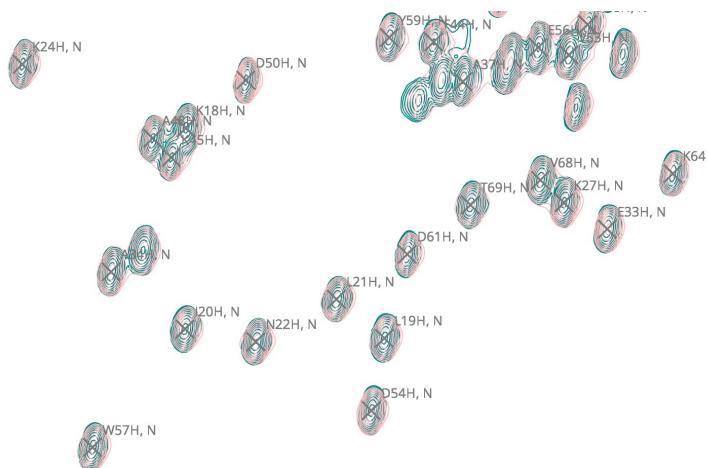
- Find the **GB1\_Assigned.ccpn** project folder in the Dynamics Tutorial data directory and drag it onto the **Sidebar** or **Drop Area**.
- Select **Yes**, if asked whether you want to open a new project or not
- Find the **RelaxLookup.xls** Excel file in the tutorial data **spectra** folder and drag it into the Sidebar or Drop Area.
- Expand the **Spectra** and **SpectrumGroups** sections of the sidebar to see that the data has been imported.



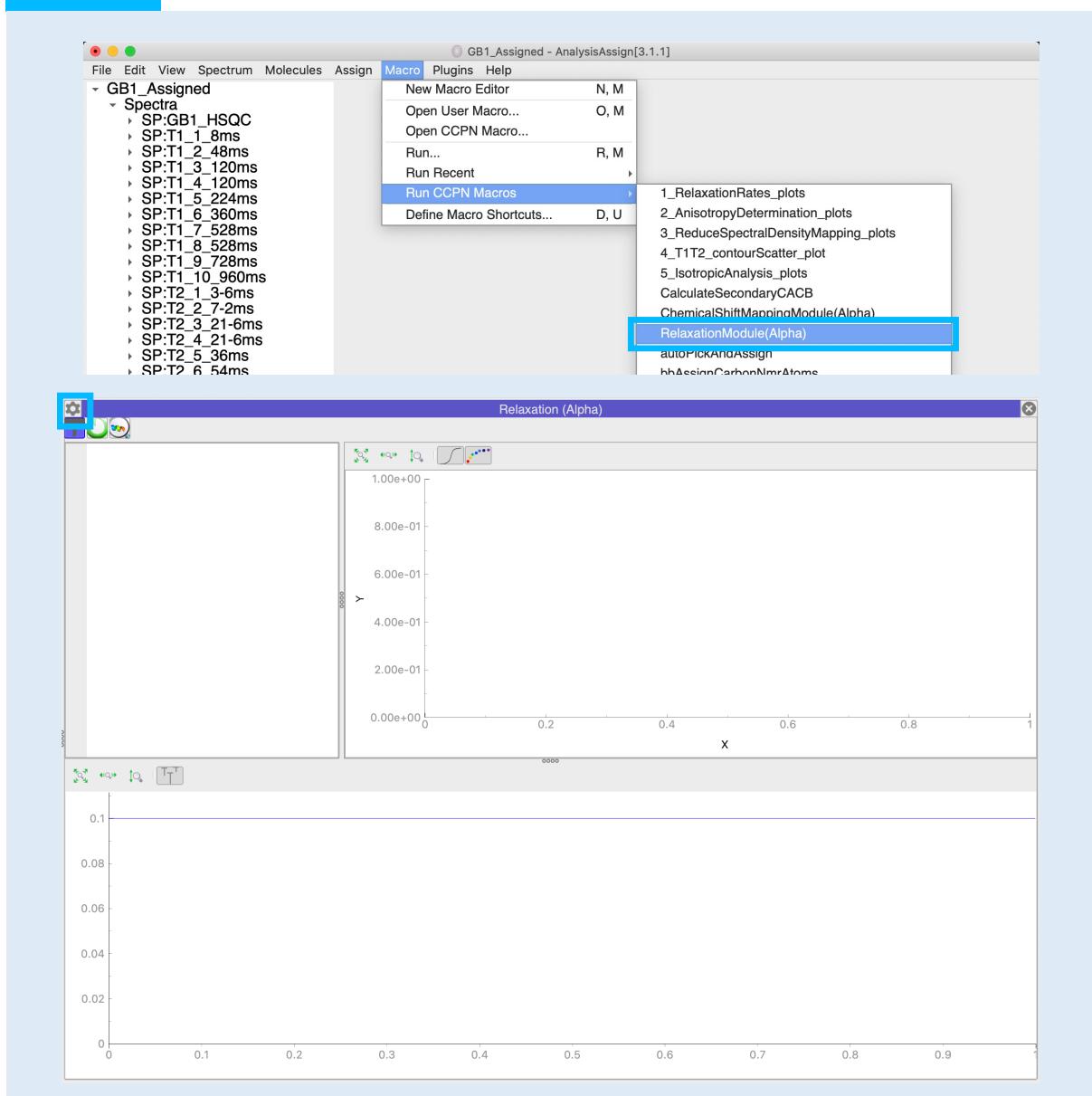
### 1F Check alignment to HSQC

- Close any open **SpectrumDisplays** (click on the in the top right corner).
- **Drag** the **GB1\_HSQC** spectrum from the sidebar into the DropArea.
- **Drag** the **T1\_1\_8ms** spectrum from the sidebar on top of the other spectrum.

These should overlay well, meaning that you will be able copy the peaks from the **GB1\_HSQC** spectrum to the T1 spectra without having to change their positions.



- **Drag** the **T2\_1\_3-6ms** and **unsaturated\_noe** spectra onto the **GB1\_HSQC** spectrum and check that these align well, too.



## 2A Open Relaxation Module

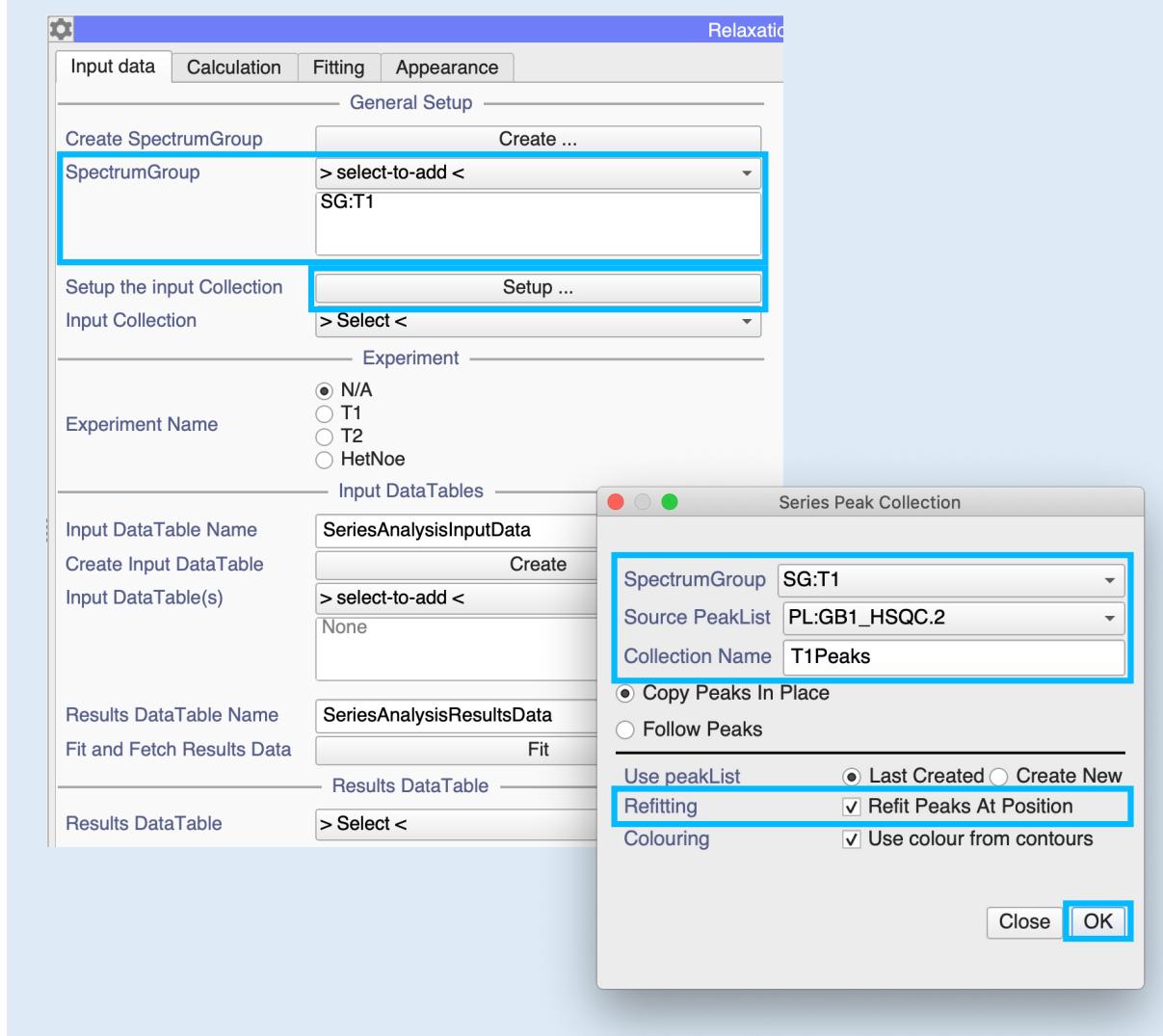
At this point you can either continue from Section 1 or start using our [Section1\\_completed ccpn project](#).

- Go to Main Menu → Macro → Run CCPN Macros → **RelaxationModule(Alpha)**.

This will open the alpha-version Relaxation Module.

- Open the Settings Panel by clicking the gear icon  in the top left of the module window.

This is where you will set up your data and run all the calculations required before inspecting it in the main module.



## 2B Copy Peaks

In the **General Setup** section you will need to select a **SpectrumGroup** (which specifies which spectra you want to use in your analysis) and a **Collection** (which is a collection of peak groups across the spectra).

We have already created our SpectrumGroups:

- Select the **T1** SpectrumGroup from the drop-down menu.

You will need to set up the Collection, as we don't have this yet:

- Click on the **Setup...** button to set up your Collection
- In the Series Peak Collection pop-up set:

Select SpectrumGroup: **SG:T1**

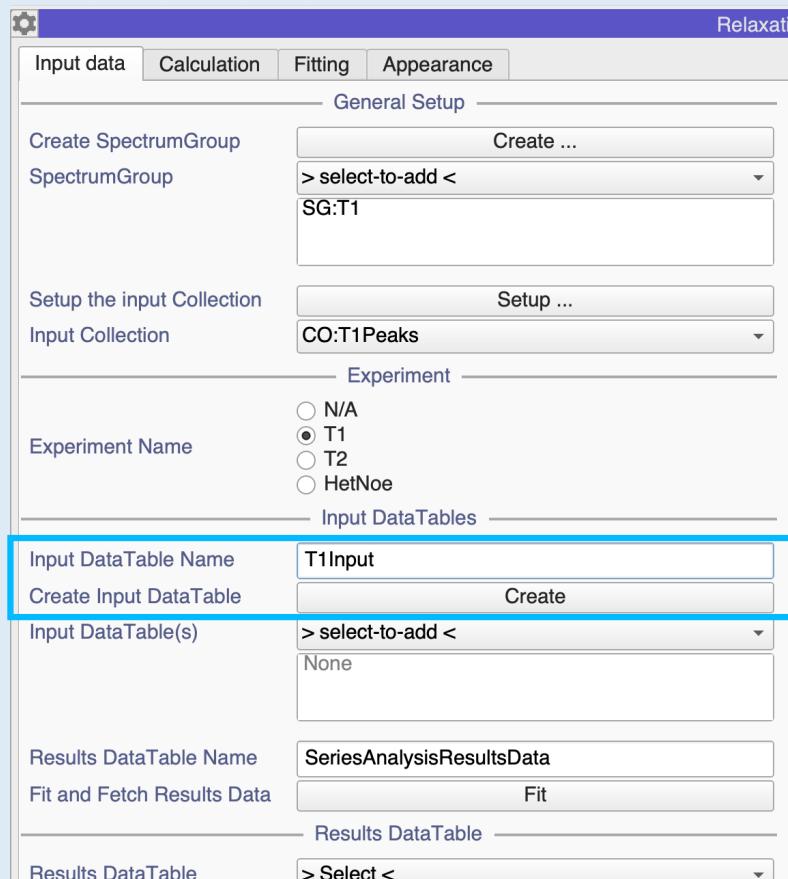
Source PeakList: **PL:GB1\_HSQC.2**

CollectionName: **T1Peaks**

Select **Refit Peaks At Position**

And keep the remaining default options, as shown above.

- Click **Okay** which will start the creation of the Peak Collections. This will probably take a minute or so.



## 2C Create Input DataTable

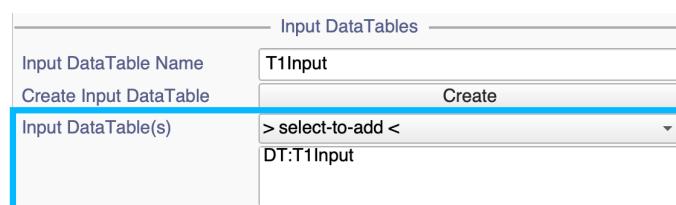
You will now create your Input DataTable, a table containing all the information needed to fit your data.

In the **Experiment** Section:

- Select **T1**

In the **Input DataTables** Section:

- Enter a **Input DataTable Name**, e.g. **T1Input**
- Click on the **Create** button to create your Input DataTable
- Check that this new Input Data Table is the only one shown in the **Input Data Table(s)** box.



# T1 and T2 Data

**Calculation Options**

- Blank
- HetNoe
- R2/R1
- Reduced\_Spectral\_Density\_Mapping

**Optimiser Options**

Optimiser Method: leastsq

Fitting Error Method: Default

**Fitting Options**

**Fitting Model**

- Blank
- OnePhaseDecay
- ExponentialDecay
- InversionRecovery

**Input DataTables**

Input DataTable Name: T1Input

Create Input DataTable: Create

Input DataTable(s): > select-to-add <

DT:T1Input

Results DataTable Name: T1Results

Fit and Fetch Results Data: Fit

## 2D Fitting

Move to the **Calculation** tab:

- Check that **Calculation Options** is set to **Blank**

Now move to the **Fitting** tab:

- Make sure the **Fitting Model** is set to **OnePhaseDecay**. Hover over this option to see information on the equation used).

A model to describe the rate of a decay.  
Model:  
$$Y = \text{amplitude} \cdot \exp(-\text{rate} \cdot X)$$
  
X: the various time values  
amplitude: the Y value when X (time) is zero. Same units as Y  
rate: the rate constant, expressed in reciprocal of the X axis time units, e.g.: Second-1.

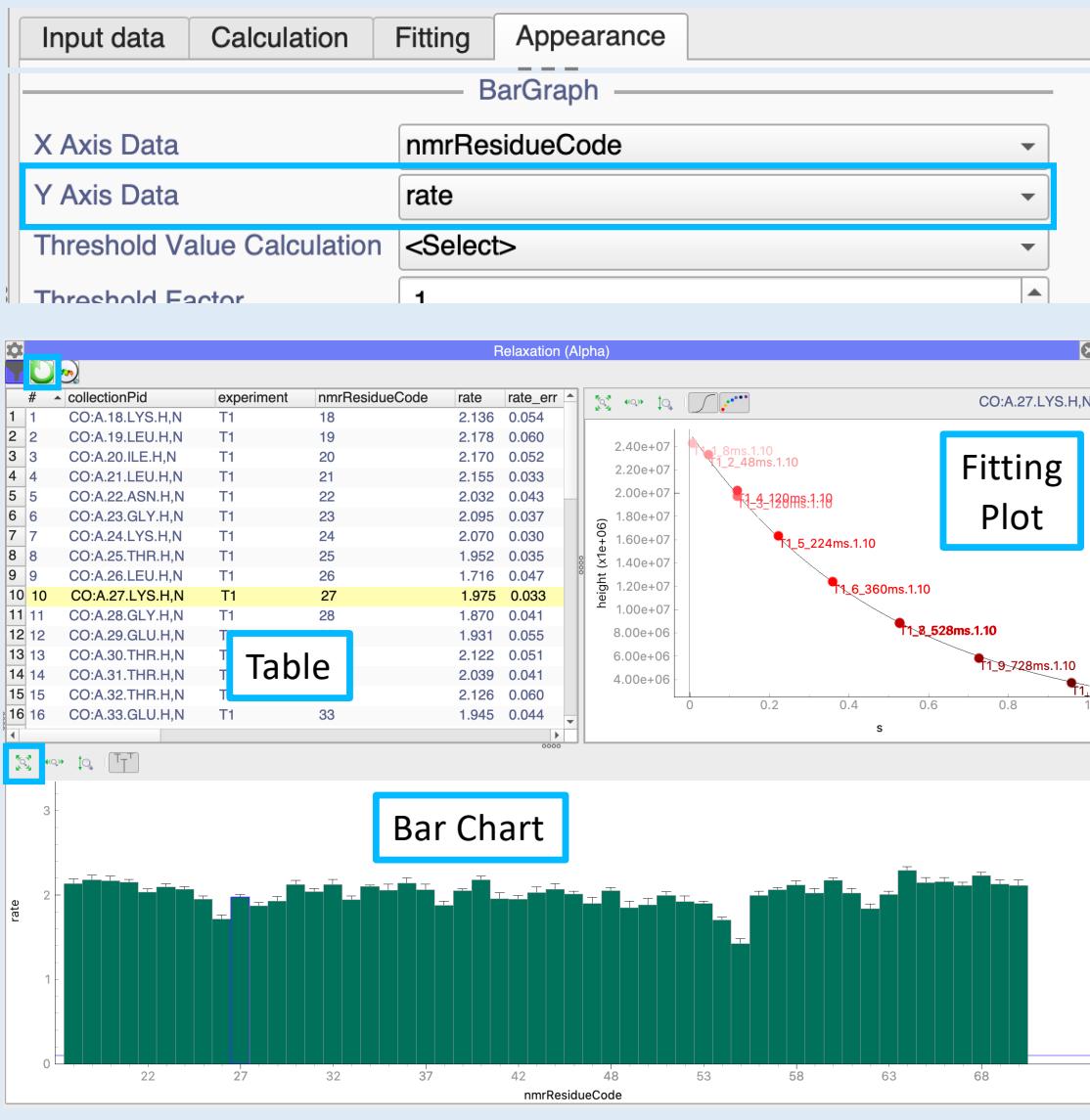
Move back to the **Input data** tab:

- Enter a **Results DataTable Name**, e.g. **T1Results**
- Click on the **Fit** button to run the fitting routine.

Your **Results DataTable** will then be automatically set to your new **T1Results** table. The table and graphs in the main module will be filled with this data.

Results DataTable

Results DataTable: DT:T1Results



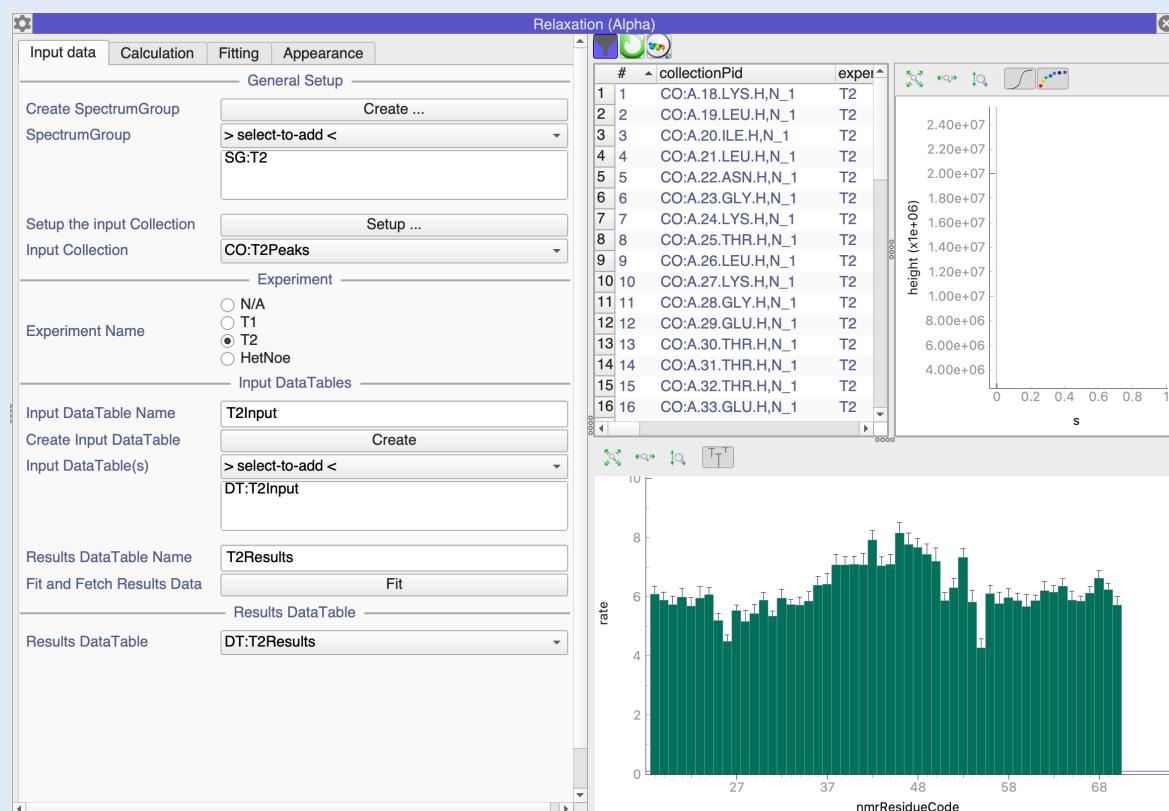
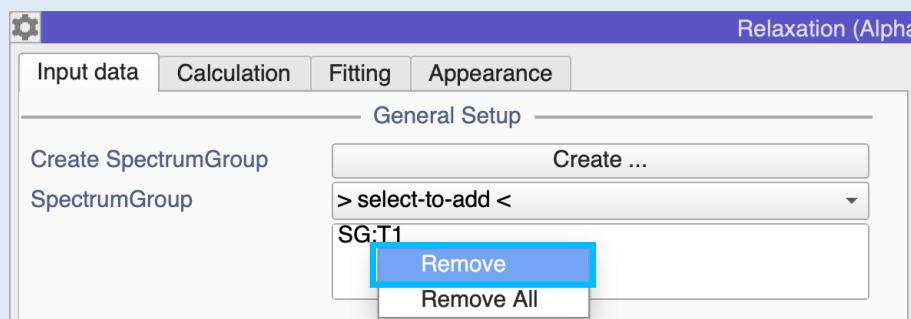
## 2E Inspect Results

Now move to the Appearance tab:

- Make sure the Y Axis Data is set to rate from the drop-down menu.
- Close the Settings tab by clicking on the gear icon in the top left again.
- If the Refresh button has gone orange , then press this to refresh the graphs and table.
- If the data aren't shown in full, then press the auto-zoom icon above the bar chart to auto-scale it.
- If you click on a row in the Table or on a bar in the Bar Chart, then the matching bar/row will be selected and in the Fitting Plot you will see a graph showing your data points (in spectrum colours) and the fit.

The table contains both the data points and fitting parameters.

If you have a SpectrumDisplay open this will navigate to the peaks corresponding to the residue selected.



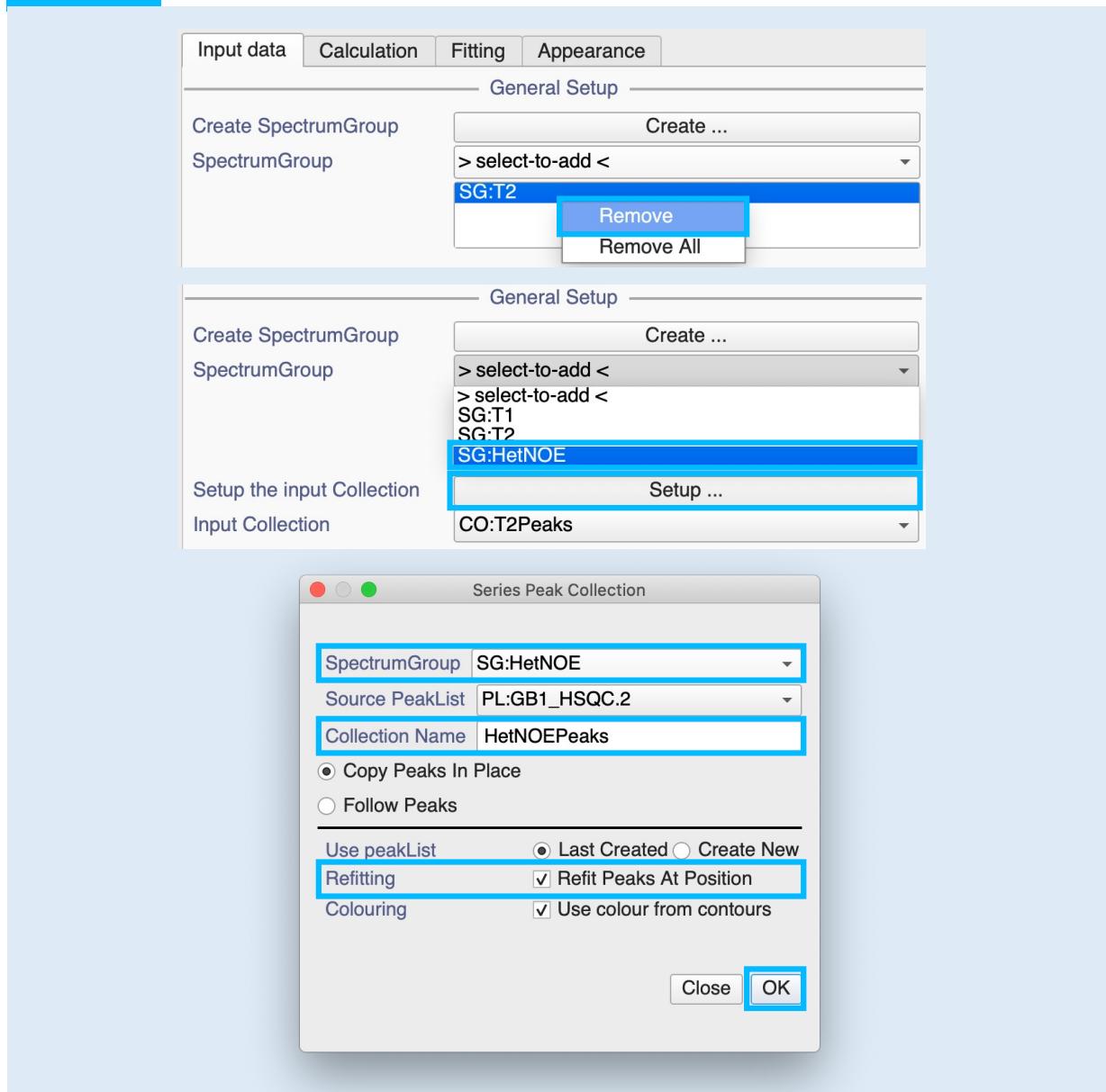
## 2F T2 Data

- Open the **Settings** panel with the gear icon.

In the **Input data** tab:

- In the **General Setup** section, right-click on your **SG:T1** SpectrumGroup and select **Remove** or **Remove all**.
- Repeat sections 2B–2E for the T2 data. Use the same options adjusting T1 to T2 in each instance and selecting **T2** as your **Experiment Name**.

# Heteronuclear NOE



## 3A Heteronuclear NOE Calculation Setup

- Open the **Settings** panel with the gear icon.

In the **Input data** tab:

- In the **General Setup** section, right-click on your **SG:T1** SpectrumGroup and select **Remove** or **Remove all**.
- Select **SG:HetNOE** as your **SpectrumGroup** from the drop-down menu
- Click on **Setup ...** to set up your Input Collection

In the Series Peak Collection pop-up:

- Select the **SG:HetNOE** SpectrumGroup
- Give your Collection a Name, e.g. **HetNOEPeaks**
- Select to **Refit Peaks At Position**
- Click **OK**

# Heteronuclear NOE

The screenshot shows the 'Experiment' settings for a Heteronuclear NOE calculation. The 'Experiment Name' is set to 'HetNoe'. The 'Input DataTable Name' is 'HetNOEInput'. Under 'Calculation Options', 'HetNoe' is selected. In the 'Fitting' tab, 'Blank' is selected as the 'Fitting Model'. The 'Results DataTable Name' is 'HetNOEResults'. The 'Fit' button is highlighted.

| Experiment  |  |
|---|--|
| Experiment Name   | <input type="radio"/> N/A<br><input type="radio"/> T1<br><input type="radio"/> T2<br><input checked="" type="radio"/> HetNoe                                       |
| Input DataTables  |  |
| Input DataTable Name  | HetNOEInput  |
| Create Input DataTable  | <b>Create</b>  |
| <input type="radio"/> Input data <input type="radio"/> Calculation <input type="radio"/> Fitting <input type="radio"/> Appearance |  |
| Peak Property   | height   |
| Calculation Options   |  |
| Calculation Options   | <input type="radio"/> Blank<br><input checked="" type="radio"/> HetNoe<br><input type="radio"/> R2/R1<br><input type="radio"/> Reduced_Spectral_Density_Mapping    |
| <input type="radio"/> Input data <input type="radio"/> Calculation <input type="radio"/> Fitting <input type="radio"/> Appearance |  |
| Optimiser Options   |  |
| Optimiser Method  | leastsq  |
| Fitting Error Method  | Default  |
| Fitting Options   |  |
| Fitting Model   | <input checked="" type="radio"/> Blank<br><input type="radio"/> OnePhaseDecay<br><input type="radio"/> ExponentialDecay<br><input type="radio"/> InversionRecovery |
| Results DataTable   |  |
| Results DataTable Name  | HetNOEResults  |
| Fit and Fetch Results Data  | <b>Fit</b>   |
| Results DataTable   |  |
| Results DataTable   | DT:HetNOEResults   |

## 3B Heteronuclear NOE Calculation

In the Settings **Input data** tab:

- Set the **Experiment Name** to **HetNoe**
- Give your Input DataTable a name, e.g. **HetNOEInput**
- Click on **Create**

In the Settings **Calculation** tab:

- Select **HetNoe**

In the Settings **Fitting** tab:

- Select **Blank**

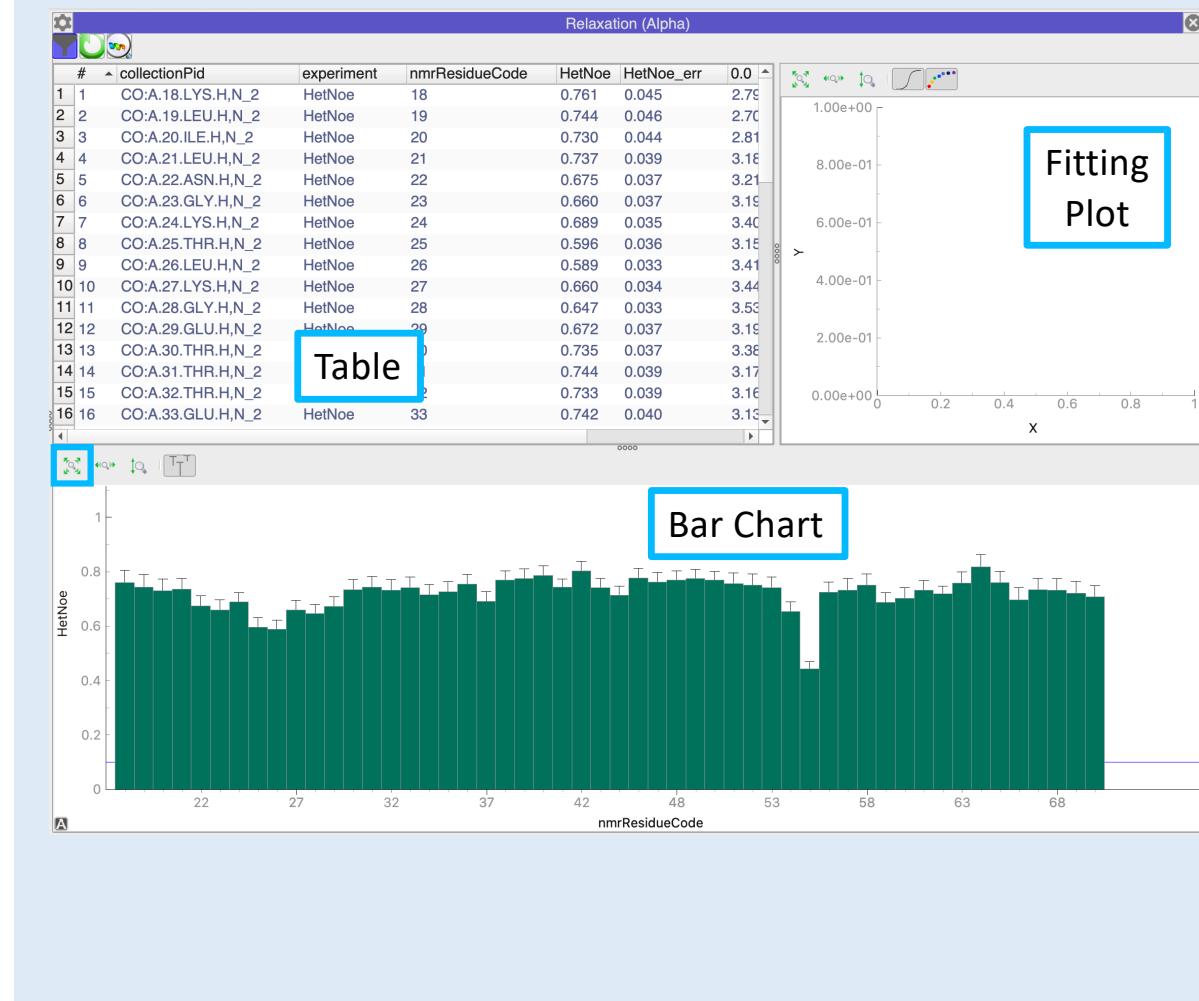
In the **Input data** tab:

- Give your Results DataTable a name, e.g. **HetNOEResults**
- Click on the **Fit** button to run the calculation.

Your **Results DataTable** will then be automatically set to your new

**HetNOEResults** table. The table and graphs in the main module will be filled with this data.

# Heteronuclear NOE



## 3B Inspecting the Heteronuclear NOE data

The bar chart should automatically show the Heteronuclear NOE on the Y-axis.

- Close the **Settings** tab by clicking on the gear icon.
- If necessary, press the auto-zoom icon above the bar chart to auto-scale it.
- If you click on a row in the Table or on a bar in the Bar Chart, then the matching bar/row will be selected.  
If you have a SpectrumDisplay open this will navigate to the peaks corresponding to the residue selected.  
The Fitting Plot area in the top right hand corner of the Relaxation module, will remain empty, as no fitting is required when analysing the Heteronuclear NOE data.

# Combined Data Analyses

The screenshot shows the CCPN Relaxation Module Settings panel. It has three main tabs: Input data, Calculation, and Fitting.

- Input DataTables Tab:**
  - Input DataTable Name: <default>
  - Create Input DataTable: Create
  - Input DataTable(s): > select-to-add < (highlighted with a blue box)
    - DT:T1Results
    - DT:T2Results
  - Results DataTable Name: R2R1Results
  - Fit and Fetch Results Data: Fit
- Calculation Tab:**
  - Peak Property: height
  - Calculation Options:
    - Blank
    - HetNoe
    - R2/R1** (radio button selected)
    - Reduced\_Spectral\_Density\_Mapping
- Fitting Tab:**
  - Optimiser Options:
    - Optimiser Method: leastsq
    - Fitting Error Method: Default
  - Fitting Options:
    - Fitting Model:
      - Blank** (radio button selected)
      - OnePhaseDecay
      - ExponentialDecay
      - InversionRecovery

## 4A R2/R1 Calculation Setup

At this point you can either continue from Section 3 or start using our **Section3\_completed ccpn** project.

- Open the **Relaxation Module Settings** panel with the gear icon.
- In the **Input data** tab, select the **Input DataTables** to be
  - DT:T1Results**
  - DT:T2Results**
- If need be, remove the **DT:HetNOEResults** DataTable by right-clicking on it and selecting **Remove**.
- Provide a **Results DataTable Name**, e.g. **R2R1Results**
- In the **Calculation** tab:
  - Set your **Calculation Options** to be **R2/R1**.
- In the **Fitting** tab:
  - Make sure the **Fitting Model** is set to **Blank**.

The screenshot shows the software interface for combined data analyses. At the top, the 'Input DataTables' section is visible, with 'Create Input DataTable' and 'Create' buttons, and a dropdown menu showing 'DT:T1Results' and 'DT:T2Results'. Below this, the 'Results DataTable Name' is set to 'R2R1Results' and the 'Fit and Fetch Results Data' button is highlighted with a blue border. The 'Results DataTable' dropdown shows 'DT:R2R1Results'. In the main area, the 'Relaxation (Alpha)' module is open. It contains a 'Table' view showing a list of residues with their R2/R1 values, and a 'Bar Chart' view showing the R2/R1 ratios for each residue. A 'Fitting Plot' area is shown in the top right corner of the Relaxation module window.

| #  | collectionPid   | nmrResidueCode | R2/R1 | R2/R1_err | Model | $\epsilon$ |
|----|-----------------|----------------|-------|-----------|-------|------------|
| 1  | CO:A.18.LYS.H,N | 18             | 2.850 | 0.201     | None  | ↑          |
| 2  | CO:A.19.LEU.H,N | 19             | 2.701 | 0.199     | None  | ↑          |
| 3  | CO:A.20.ILE.H,N | 20             | 2.638 | 0.195     | None  | ↑          |
| 4  | CO:A.21.LEU.H,N | 21             | 2.779 | 0.179     | None  | ↑          |
| 5  | CO:A.22.ASN.H,N | 22             | 2.795 | 0.204     | None  | ↑          |
| 6  | CO:A.23.GLY.H,N | 23             | 2.842 | 0.237     | None  | ↑          |
| 7  | CO:A.24.LYS.H,N | 24             | 2.931 | 0.157     | None  | ↑          |
| 8  | CO:A.25.THR.H,N | 25             | 2.659 | 0.173     | None  | ↑          |
| 9  | CO:A.26.LEU.H,N | 26             | 2.618 | 0.195     | None  | ↑          |
| 10 | CO:A.27.LYS.H,N | 27             | 2.801 | 0.140     | None  | ↑          |
| 11 | CO:A.28.GLY.H,N | 28             | 2.758 | 0.263     | None  | ↑          |
| 12 | CO:A.29.GLU.H,N | 29             | 2.815 | 0.234     | None  | ↑          |
| 13 | CO:A.30.THR.H,N | 30             | 2.775 | 0.185     | None  | ↑          |
| 14 | CO:A.31.THR.H,N | 31             | 2.621 | 0.134     | None  | ↑          |
| 15 | CO:A.32.THR.H,N | 32             | 2.800 | 0.219     | None  | ↑          |
| 16 | CO:A.33.GLU.H,N | 33             | 2.944 | 0.157     | None  | ↑          |

**Table**

**Bar Chart**

**Fitting Plot**

## 4B R2/R1 Calculation

In the **Settings Input data** tab:

- Click on the Fit button.
- Close the Settings tab with the gear icon and inspect your results in the main part of the module.
- If necessary, press the auto-zoom icon above the bar chart to auto-scale it.
- If you click on a row in the Table or on a bar in the Bar Chart, then the matching bar/row will be selected.

If you have a SpectrumDisplay open this will navigate to the peaks corresponding to the residue selected.

The Fitting Plot area in the top right hand corner of the Relaxation module, will remain empty, as no fitting was required for this calculation.

The screenshot shows the CCPN Relaxation Module Settings panel with three main tabs: Input data, Calculation, and Fitting.

- Input DataTables Tab:**
  - Input DataTable Name: <default>
  - Create Input DataTable: Create
  - Input DataTable(s): > select-to-add <
    - DT:T1Results
    - DT:T2Results
    - DT:HetNOEResults
- Calculation Tab:**
  - Peak Property: height
  - Calculation Options:
    - Blank
    - HetNoe
    - R2/R1
    - Reduced\_Spectral\_Density\_Mapping
- Fitting Tab:**
  - Optimiser Options:
    - Optimiser Method: leastsq
    - Fitting Error Method: Default
  - Fitting Options:
    - Fitting Model:
      - Blank
      - OnePhaseDecay
      - ExponentialDecay
      - InversionRecovery

## 5A Reduced Spectral Density Mapping Setup

At this point you can either continue from Section 4 or start using our **Section4\_completed ccpn** project.

- Open the **Relaxation Module Settings** panel with the gear icon.
- In the **Input data** tab, select the **Input DataTables** to be

**DT:T1Results**

**DT:T2Results**

**DT:HetNOEResults**

- Provide a **Results DataTable Name**, e.g. **RSDMResults**

In the **Calculation** tab:

- Set your **Calculation Options** to be **Reduced\_Spectral\_Density\_Mapping**

In the **Fitting** tab:

- Make sure the **Fitting Model** is set to **Blank**.

**Input DataTables**

|                            |   |
|----------------------------|---|
| Input DataTable Name       | <default>   |
| Create Input DataTable     | Create  |
| Input DataTable(s)         | > select-to-add <<br>DT:T1Results<br>DT:T2Results<br>DT:HetNOEResults |
| Results DataTable Name     | RDSMResults   |
| Fit and Fetch Results Data | Fit   |

**SpectrumDisplay**

|                         |                                   |
|-------------------------|-----------------------------------|
| Select SpectrumDisplays | > select-to-add <<br><Use active> |
|-------------------------|-----------------------------------|

**BarGraph**

|                             |                |
|-----------------------------|----------------|
| X Axis Data                 | nmrResidueCode |
| Y Axis Data                 | J0             |
| Threshold Value Calculation | JwX            |
| Threshold Factor            | JwH            |
| Threshold Value             | argA           |
| Above Threshold Colour      | argB           |
| Below Threshold Colour      | Rsqr           |
|                             | chisqr         |
|                             | redchi         |
|                             | aic            |
|                             | bic            |
| Untraceable Observation Col | CCPNpurple     |

## 5B Reduced Spectral Density Mapping Calculation

In the **Settings** **Input data** tab:

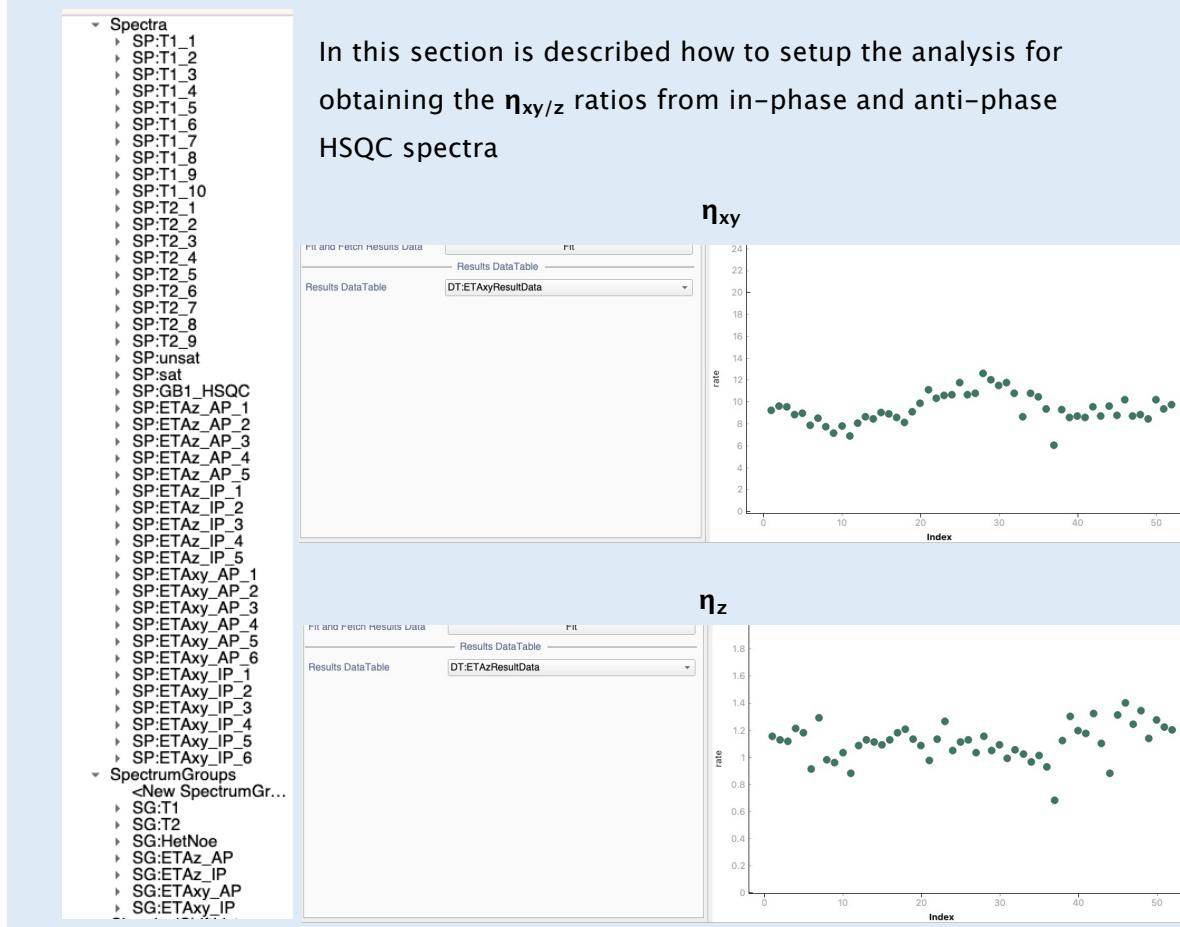
- Click on the **Fit** button.

In the **Appearance** tab:

- From the **Y Axis Data** drop-down menu select **J0**, **JwX** and **JwH** in turn to view the spectral densities at 0,  $\omega_N$  and  $\omega_H$ , respectively.
- If necessary, press the orange **Update** button  or auto-zoom button  to view the data on the bar chart.

The Table, Bar Chart and Spectrum Display are dynamically linked as usual and no fits are present.

## Relaxation Exchange rates determination via $\delta_{NH}$ and $\eta_{xy/z}$ analysis

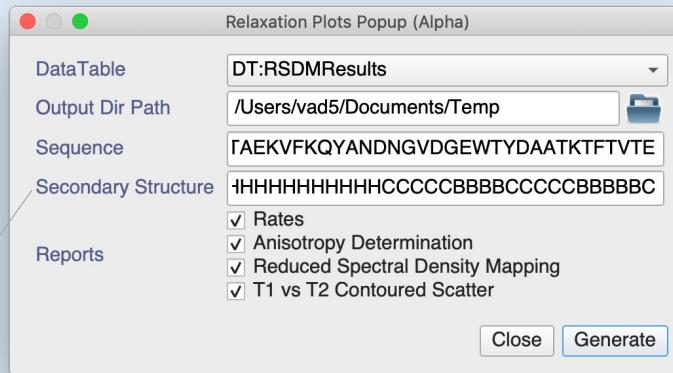


### 6A $\eta_{xy}$ and $\eta_z$ analysis setup

- If not continuing from step 5 of this tutorial, open the **Section5\_completed ccpn** project.
- Load the excel file **ETAs\_Lookup.xls** from spectra/GB1\_ETAs directory.
- Two new spectrumGroups and relative spectra will appear on the sidebar
- Run the macro **SetupETAsInputData**.  
main Menu > Macro > Run Ccpn Macros > SetupETAsInputData.  
Allow a couple of minutes to perform the macro.
- This macro will produce 2 new output DataTables containing the ETAx and ETAz values.  
More details about the performed actions are within the macro, open it with the macroEditor from the main menu.
- Open the RelaxationAnalysis module and select the the new result datatables to inspect the data.

On the following step, you will create the **Relaxation Exchange rates**

# Exporting Graphs



\* DSSP secondary structure coding:

*H*: *a*-helix

*G*:  $\beta_{10}$  helix

*I*:  $\pi$ -helix

*E*: extended strand

*B*: residue in isolated  $\beta$ -bridge

*S*: bend

*T*: *H*-bonded turn

*C*: no secondary structure

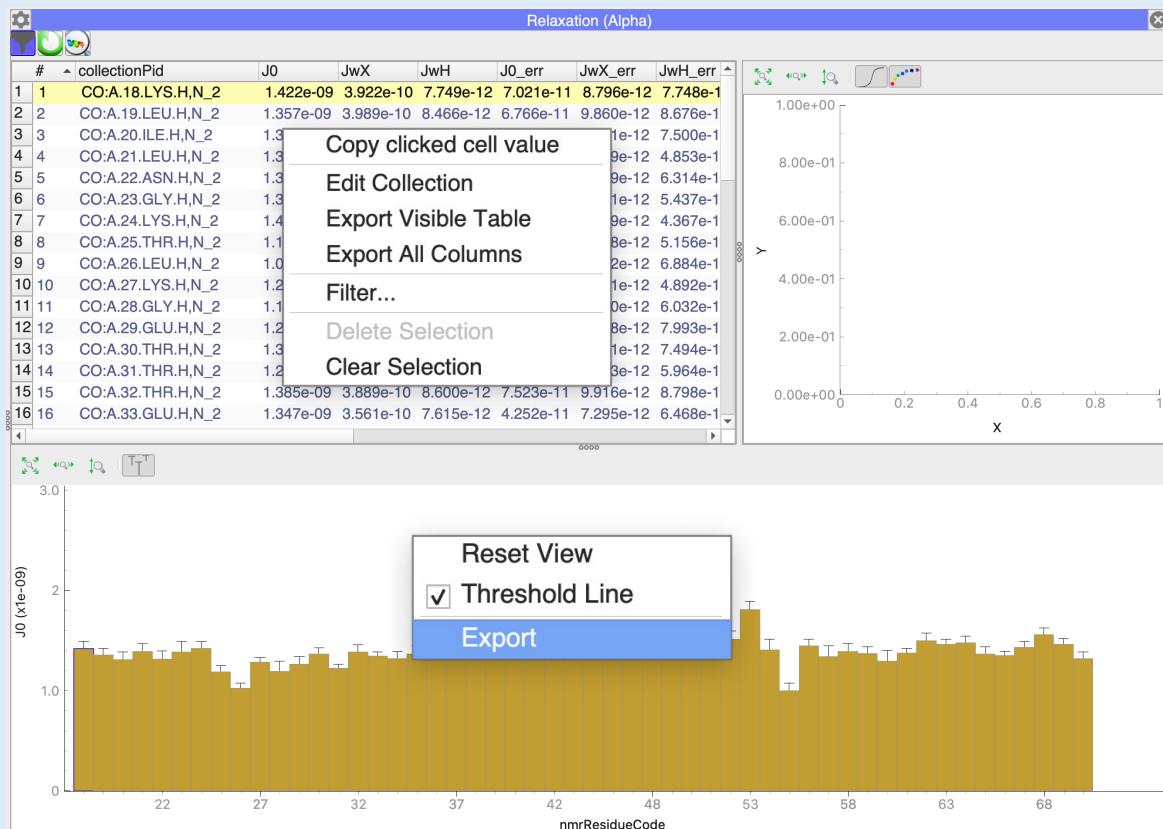
## 7A Export predefined plots in pdf format

At this point you can either continue from Section 6 or start using our **Section6\_completed ccpn** project.

- Go to Main Menu → Macro → Run CCPN Macros → Relaxation Plots Popup
  - As your DataTable, select your Reduced Spectral Density Mapping Results table (DT:RSDMResults)
  - Select a Directory where you want to save your plots
- The Sequence and Secondary Structure (in DSSP code\*) for GB1 are already provided in the pop-up.
- Keep all Reports selected
  - Click on Generate

## 7B Calculate and Export the Relaxation Exchange rates

- Go to Main Menu → Macro → Run CCPN Macros → Calculate\_RelaxationExchange\_via\_ETAs



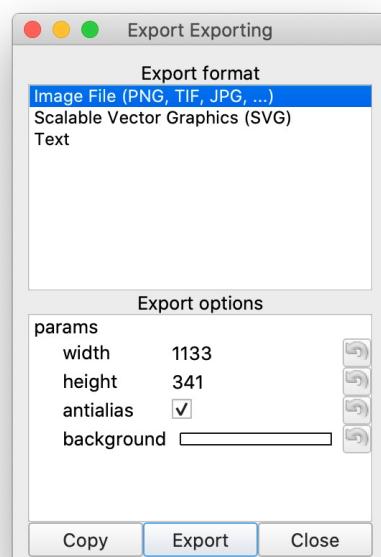
## 7C Exporting data for use in external graphing programs

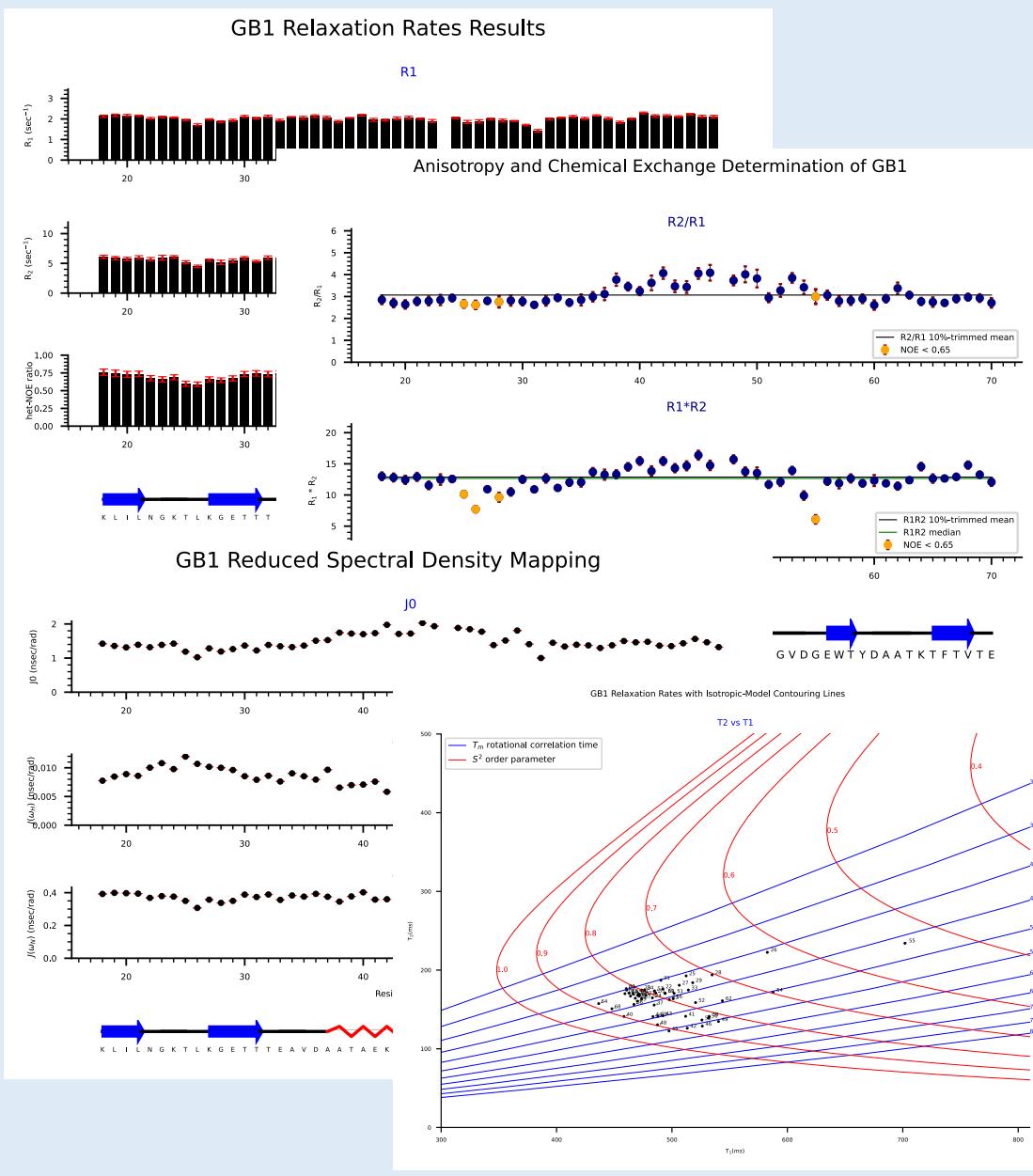
- Right-click on the table and select either **Export Visible Table** or **Export All Columns**. The former is sensitive to any filtering you might have done on the table while the latter is not.

## 7D Exporting individual charts

- Right-click on the bar chart or fitting graph and select **Export**.

You will be presented with a small pop-up offering you several options, including the ability to export in an image or a scalable vector graphics format.





## 8 Examine the graphs

The graphs are also available in the **graphs** folder of the tutorial data directory.

- Examine the various graph that you have produced
- For each graph, summarise what kind of data they display and what you can learn from them.
- What is your overall assessment of the dynamics of GB1? Is it adequately described by a small sphere tumbling in solution?

## Contact Us

**Website:**

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**Issues and bug report:**

<https://forum.ccpn.ac.uk/>

## Cite Us

Skinner, S. P. et al. CcpNmr AnalysisAssign: a flexible platform for integrated NMR analysis. *J. Biomol. NMR* (2016). doi:10.1007/s10858-016-0060-y