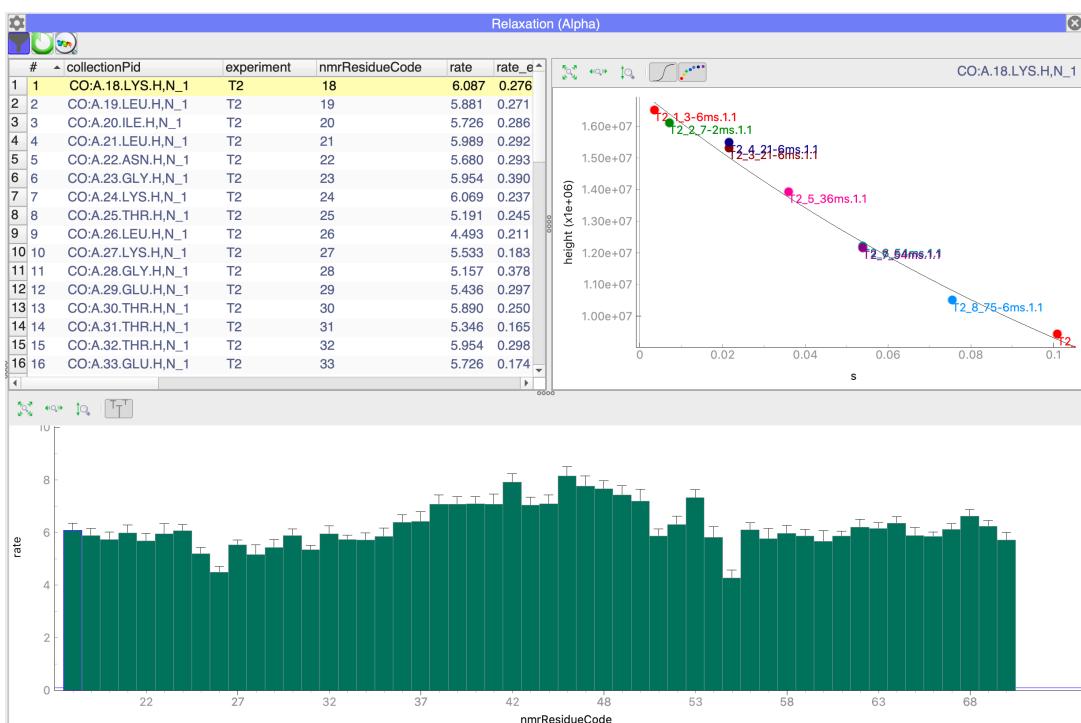


Dynamics Tutorial (Beta)



Introduction

This tutorial will take you through the analysis of some dynamics data in CcpNmr Analysis Version 3.2 using the beta 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. 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:

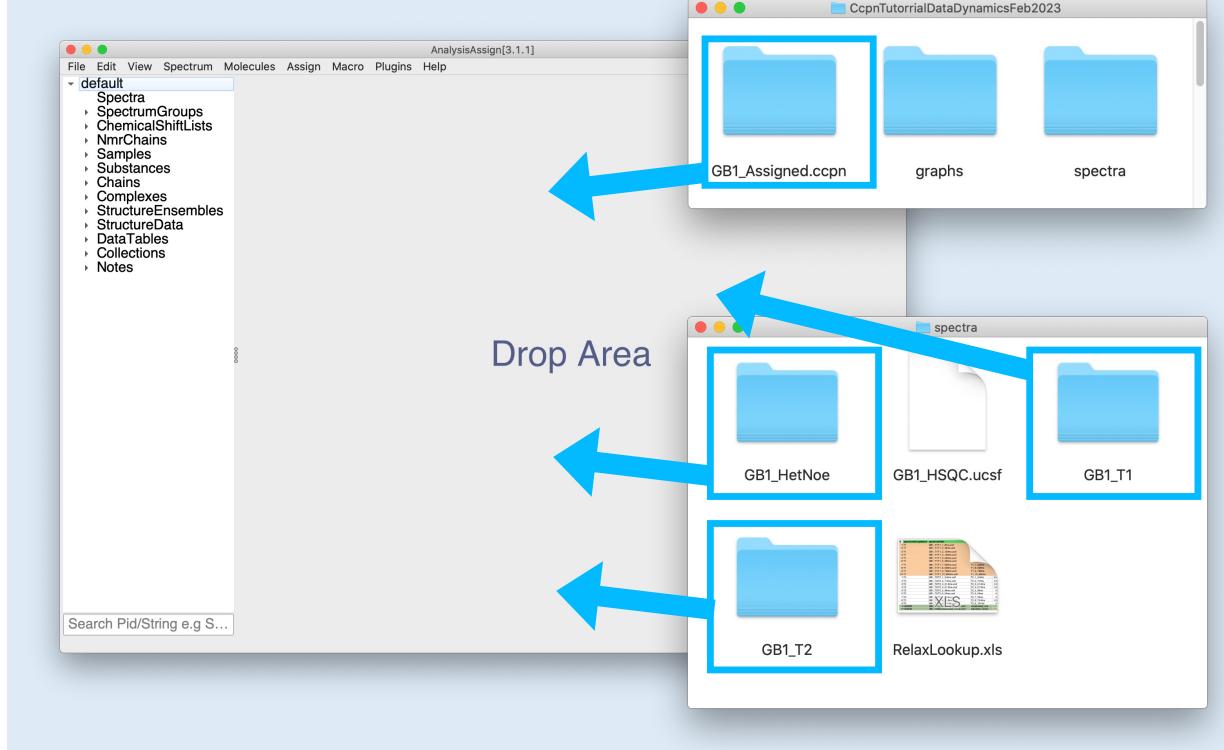
1. Loading Data
2. T1 and T2 Data
3. Heteronuclear NOE Data
4. Combined Analyses
5. Reduced Spectral Density Mapping
6. Exporting Graphs
7. Examining the Graphs

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**.

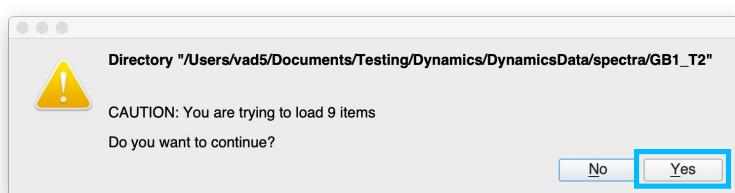
- Find the **spectra** directory in the Dynamics Tutorial data directory
- Select and drag the following three folders into the Sidebar or Drop Area:

GB1_T1

GB1_T2

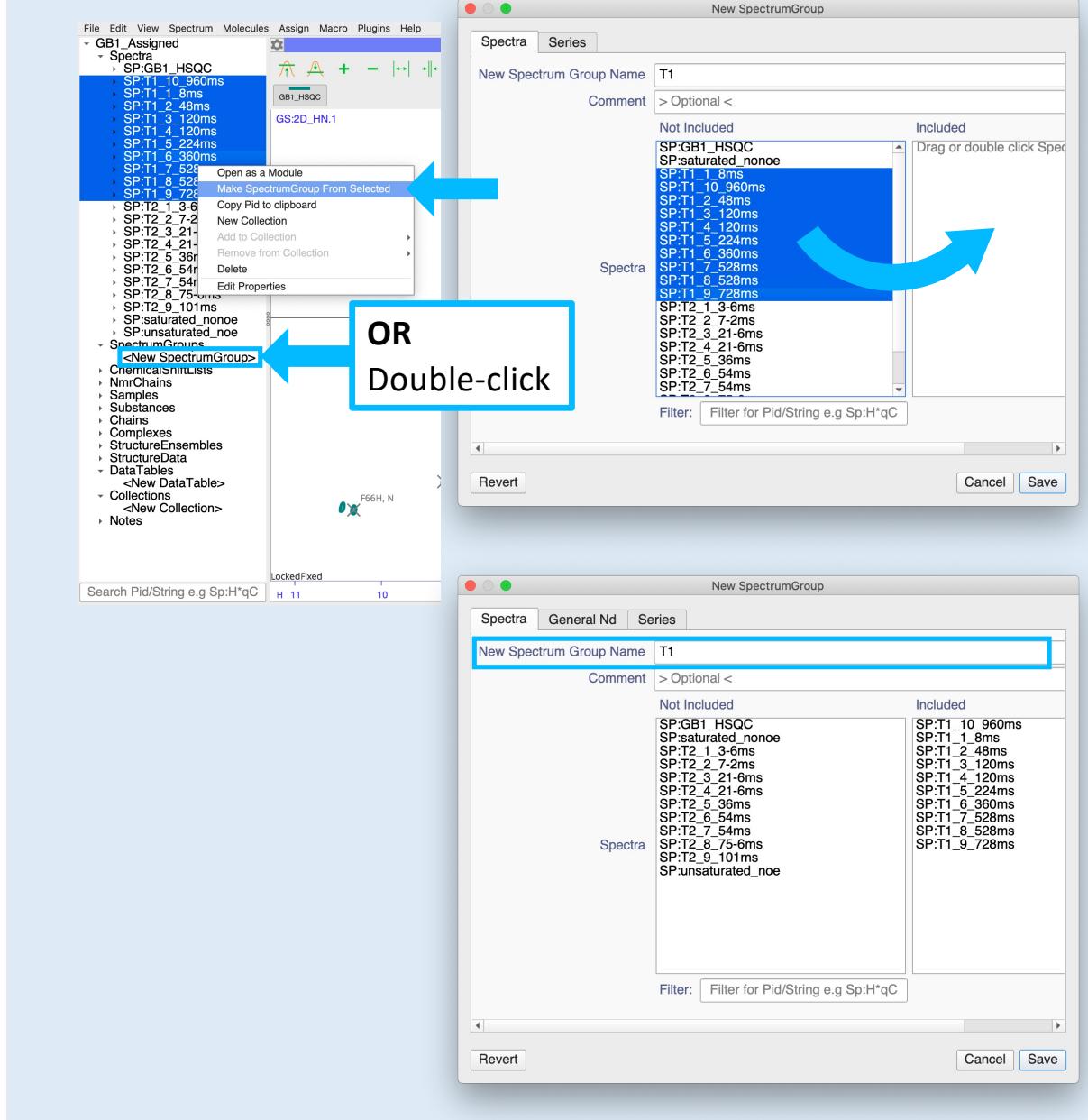
GB1_HetNOE

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



If you drop the folders into the Drop Area the spectra will open directly. If you drop the folders on the Sidebar the spectra 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

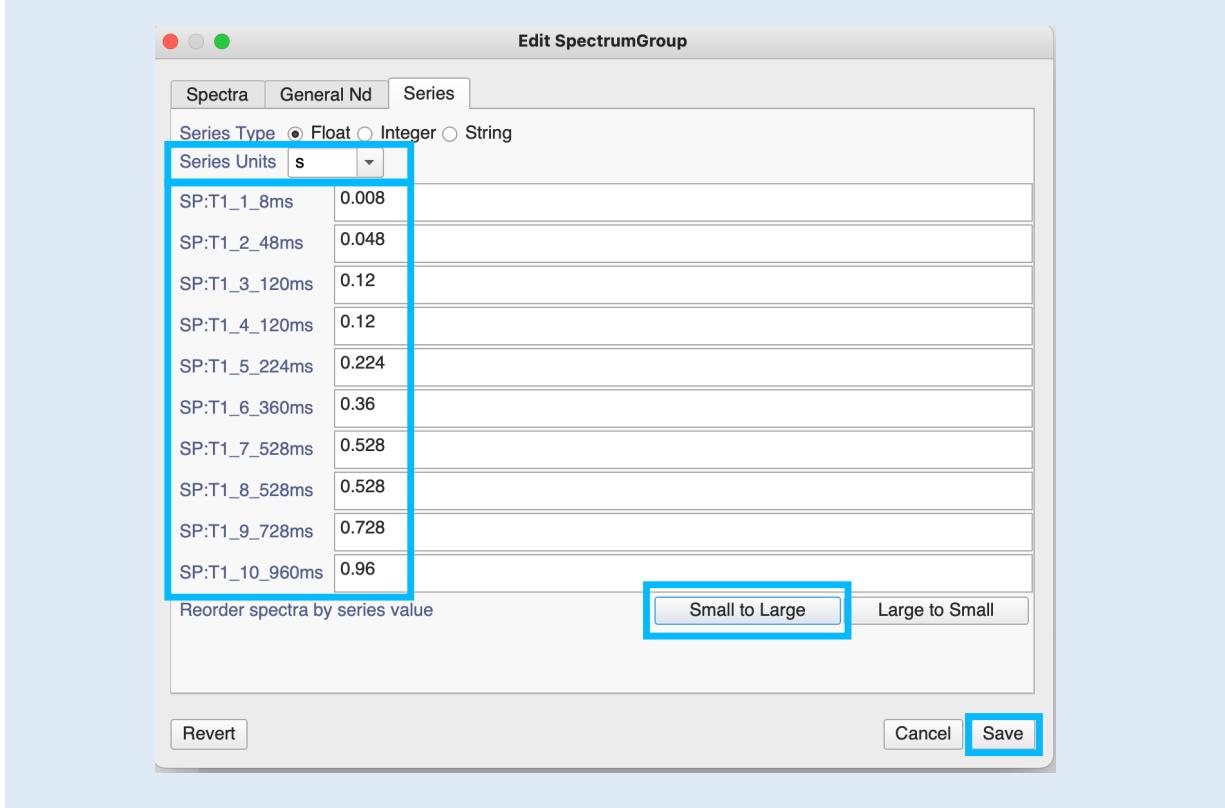
- Select all the T1 spectra in the sidebar, right-click and select **Make SpectrumGroup from Selected**

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**

Loading data



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 **Small to Large** button to do so.
- Finally click on **Save**.

Loading data

T2Data

The screenshot shows the T2Data sidebar with a context menu open over several spectra. The menu includes options like 'Open as a Module', 'Make SpectrumGroup From Selected', 'Copy Pid to clipboard', 'New Collection', 'Add to Collection', 'Remove from Collection', and 'Delete'. The 'Make SpectrumGroup From Selected' option is highlighted. To the right, a 'New SpectrumGroup' dialog is open, showing a table of T2 values. The 'Series' tab is selected, and the 'Series Type' is set to 'Float'. The 'Series Units' dropdown is set to 's'. The data table contains the following rows:

Spectrum	Value (s)
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 sidebar with a context menu open over several spectra. The menu includes options like 'Open as a Module', 'Make SpectrumGroup From Selected', 'Copy Pid to clipboard', 'New Collection', 'Add to Collection', and 'Delete'. The 'Make SpectrumGroup From Selected' option is highlighted. To the right, a 'New SpectrumGroup' dialog is open, showing a table of HetNOE values. The 'Series' tab is selected, and the 'Series Type' is set to 'Float'. The 'Series Units' dropdown is set to 'AU'. The data table contains the following rows:

Spectrum	Value (AU)
SP:saturated_nono	1.0
SP:unsaturated_noe	0.0

1D Create T2 and Heteronuclear NOE SpectrumGroups and Series

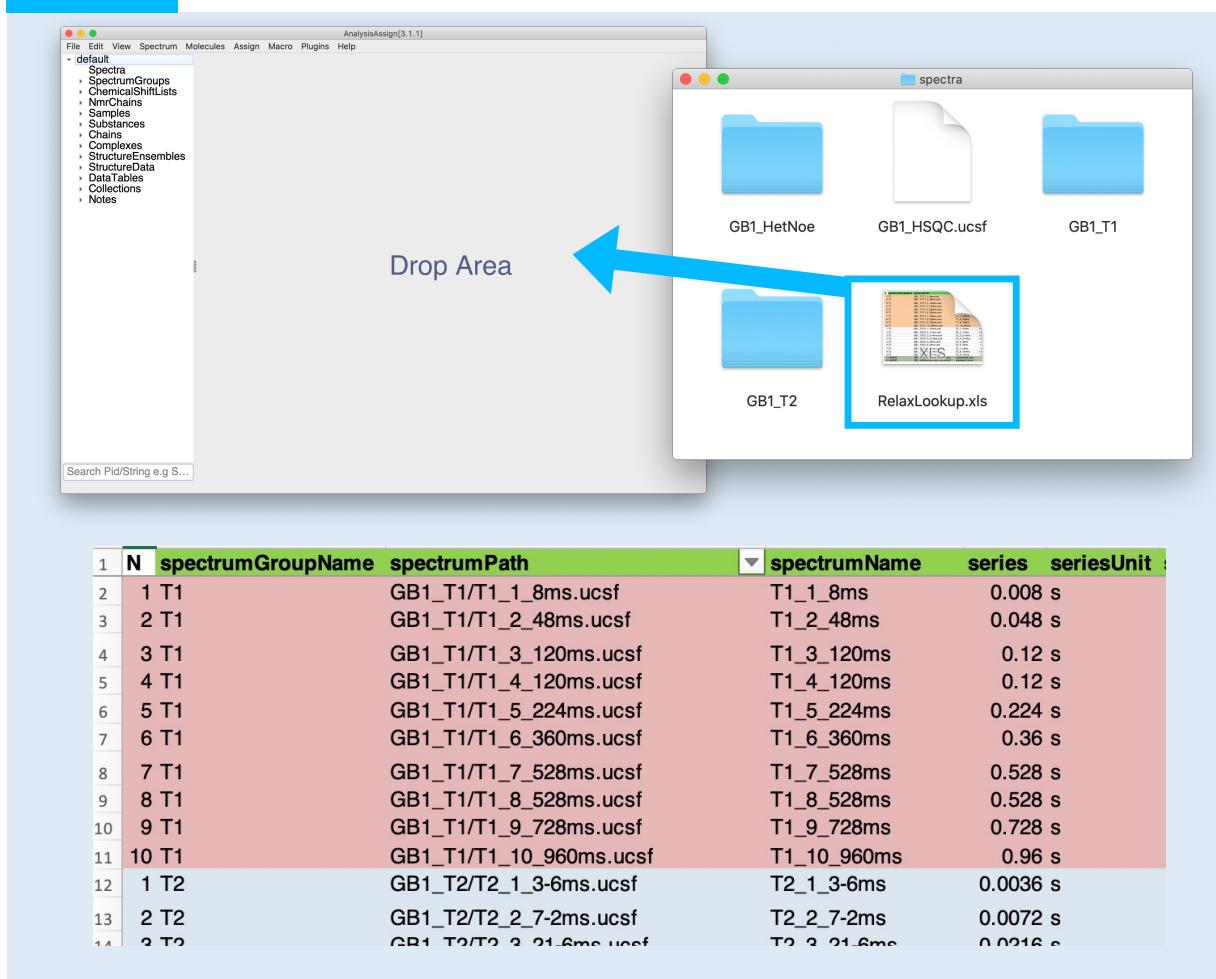
- Repeat the procedure for creating a SpectrumGroup and setting up the Series for the T2 data

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:

saturated_nono	1.0
unsaturated_noe	0.0

Loading data

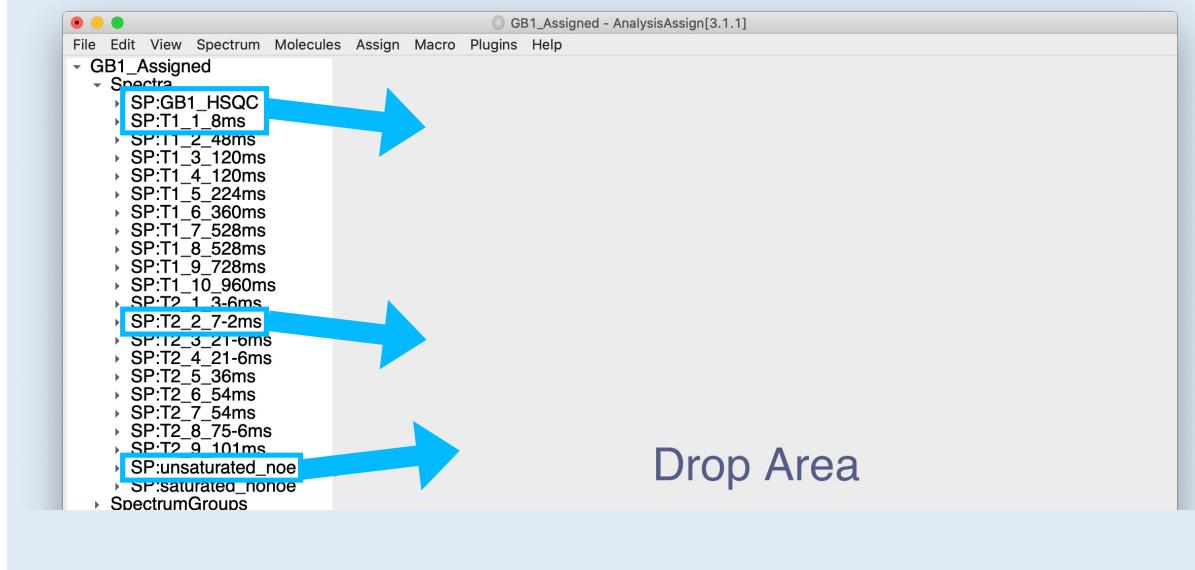


1E Import from Excel Lookup File (optional)

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.

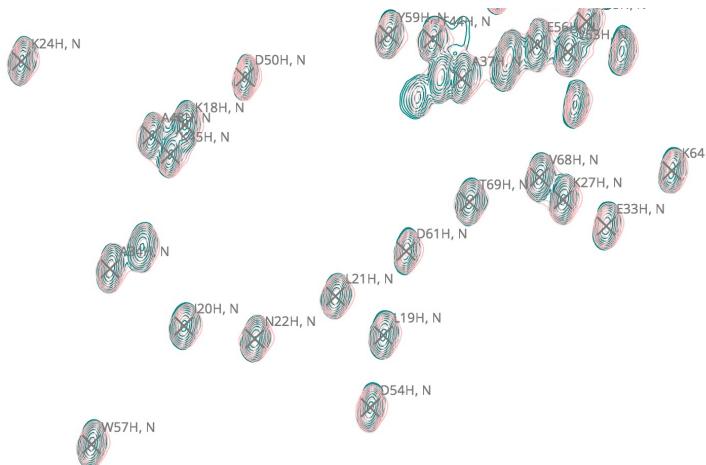
- Find the **GB1_Assigned ccpn** project folder in the Dynamics Tutorial data directory and drag it onto the **Sidebar** or **Drop Area**.
- Select **Yes**, if asked whether you want to open a new project or not
- Find the **RelaxLookup.xls** Excel file in the tutorial data **spectra** folder and drag 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

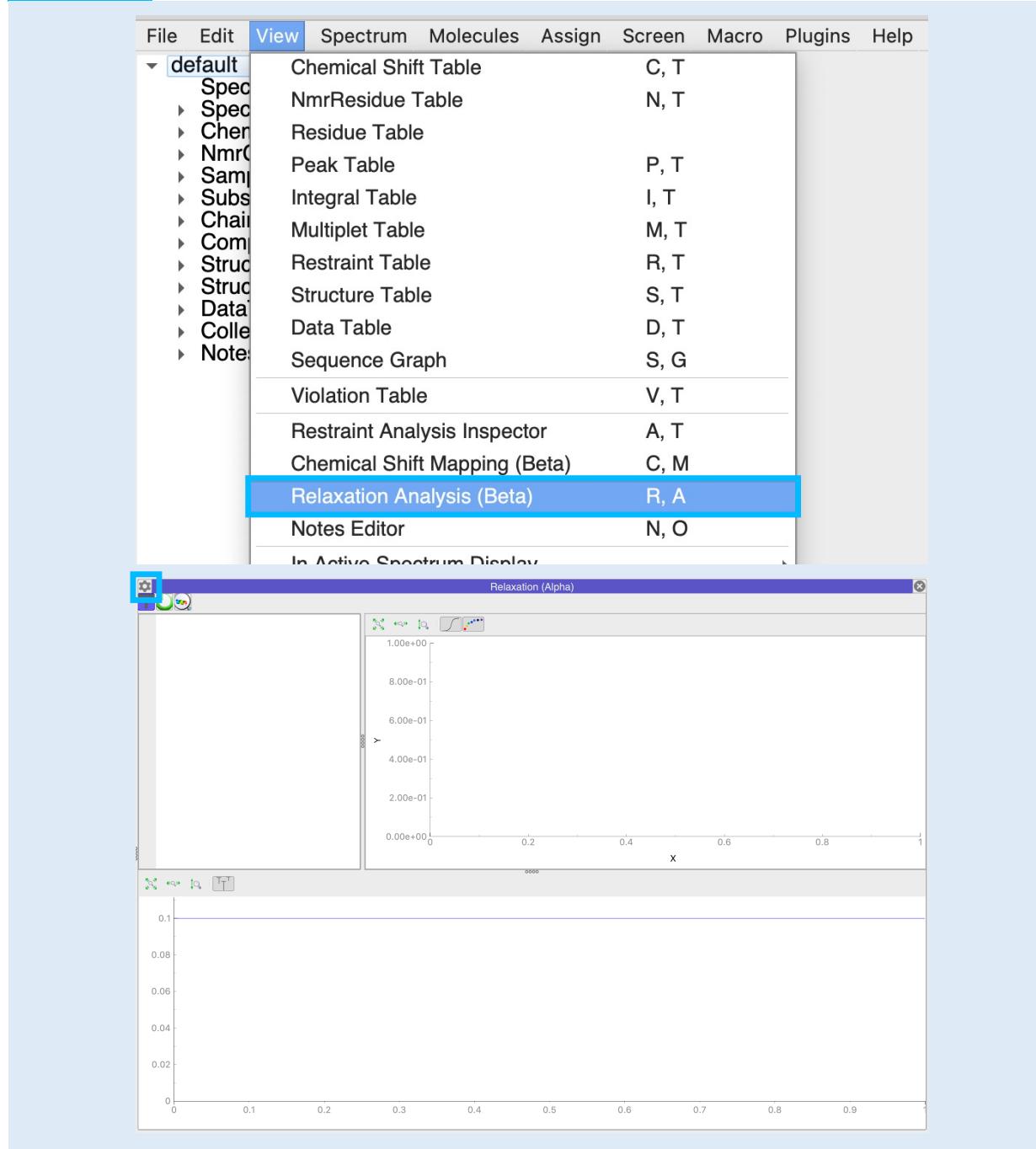
- Close any open **SpectrumDisplays** (click on the in the top right corner).
- **Drag** the **GB1_HSQC** spectrum from the sidebar into the **DropArea**.
- **Drag** the **T1_1_8ms** spectrum from the sidebar on top of the other spectrum.

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.

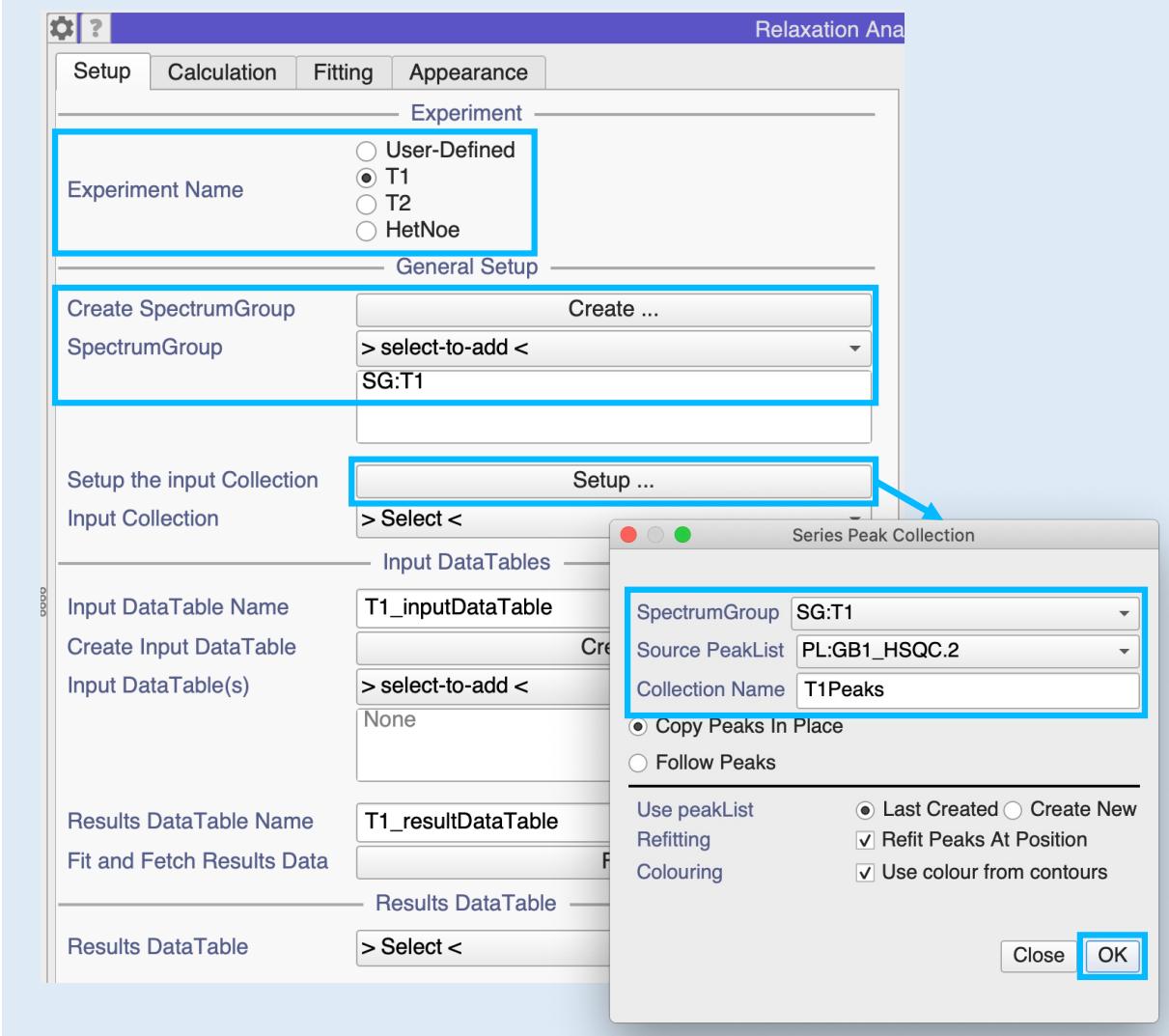
T1 and T2 Data



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 → View → Relaxation Analysis (Beta).
This will open the 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

- Set the **Experiment Name** to **T1**.

This will pre-populate some elements in the sections below and other tabs.

In the **General Setup** the **SpectrumGroup** specifies which spectra you want to use. The **Input Collection** is a collection of peak groups across the spectra.

We have already created our SpectrumGroups:

- Ensure the **T1** SpectrumGroup from the drop-down menu is selected.

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**

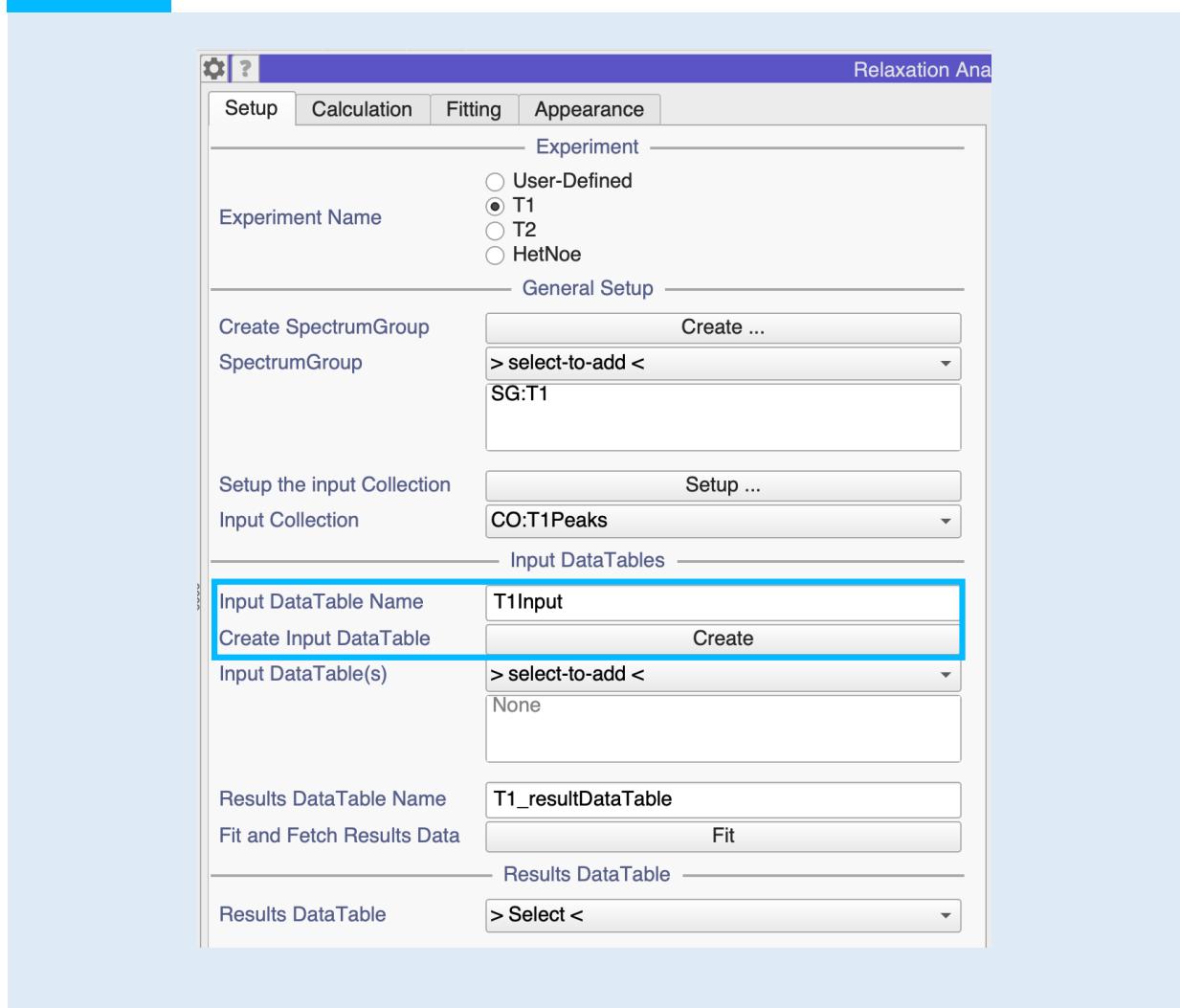
Source PeakList: **PL:GB1_HSQC.2**

Collection Name: **T1Peaks**

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 **Input DataTables** Section:

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

Input DataTables	
Input DataTable Name	<input type="text" value="T1Input"/>
Create Input DataTable	<input type="button" value="Create"/>
Input Data Table(s)	<input type="button" value="> select-to-add <"/> DT:T1Input

Calculation Tab:

- Peak Property: height
- Calculation Options:
 - Blank
 - HetNoe
 - R2/R1
 - ETAs Ratio
 - Reduced_Spectral_Density_Mapping

Fitting Tab:

- Optimiser Method: leastsq
- Fitting Error Method: Default
- Fitting Options:
 - Blank
 - OnePhaseDecay
 - ExponentialDecay
 - InversionRecovery

Setup Tab:

- 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=amplitude*exp(-rate*X)
X:the various times 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.

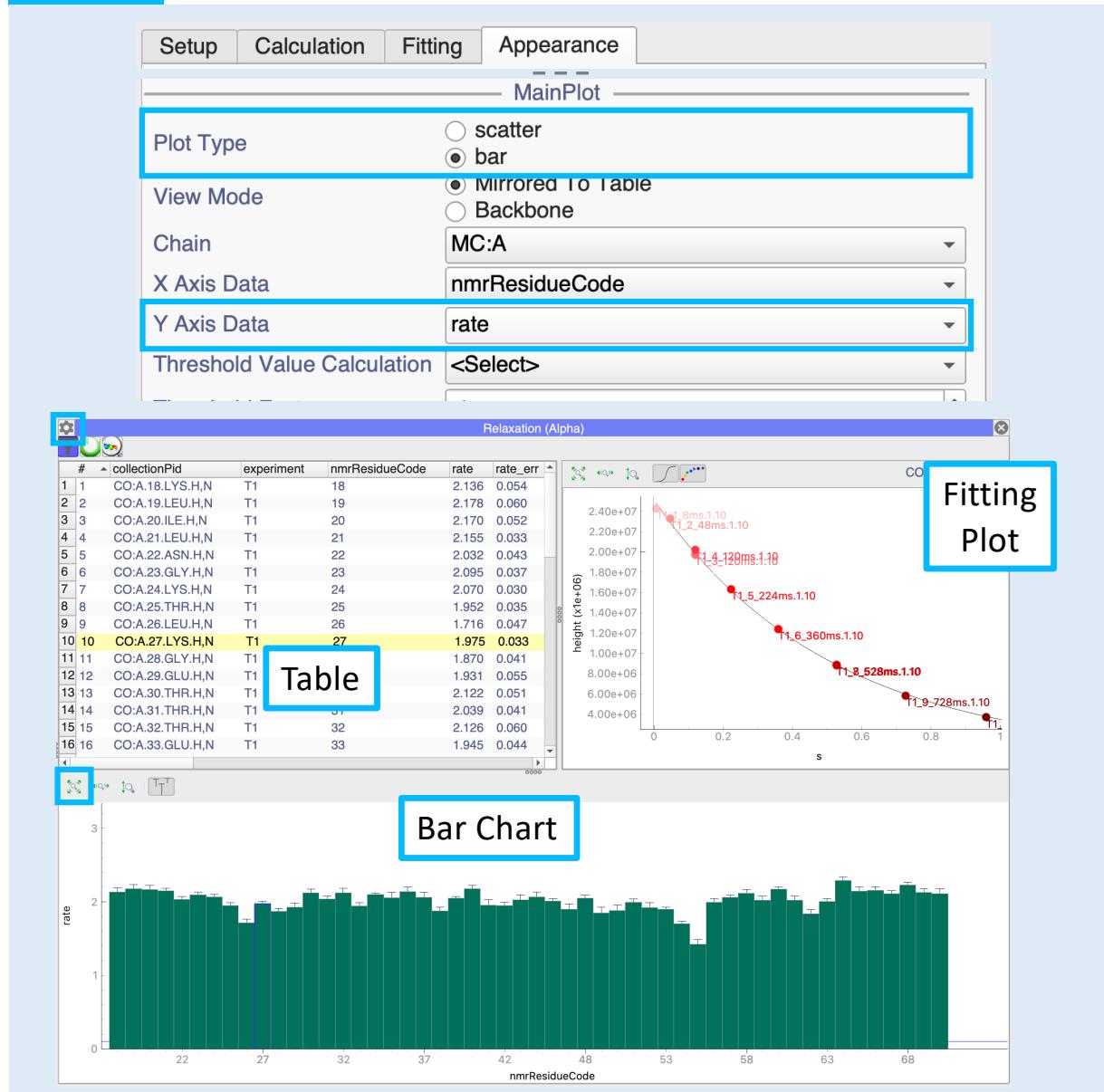
Move back to the **Setup** tab:

- Enter a **Results DataTable Name**, e.g. **T1Results** or leave the default name
- 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 c

Results DataTable
Results DataTable DT:T1Results

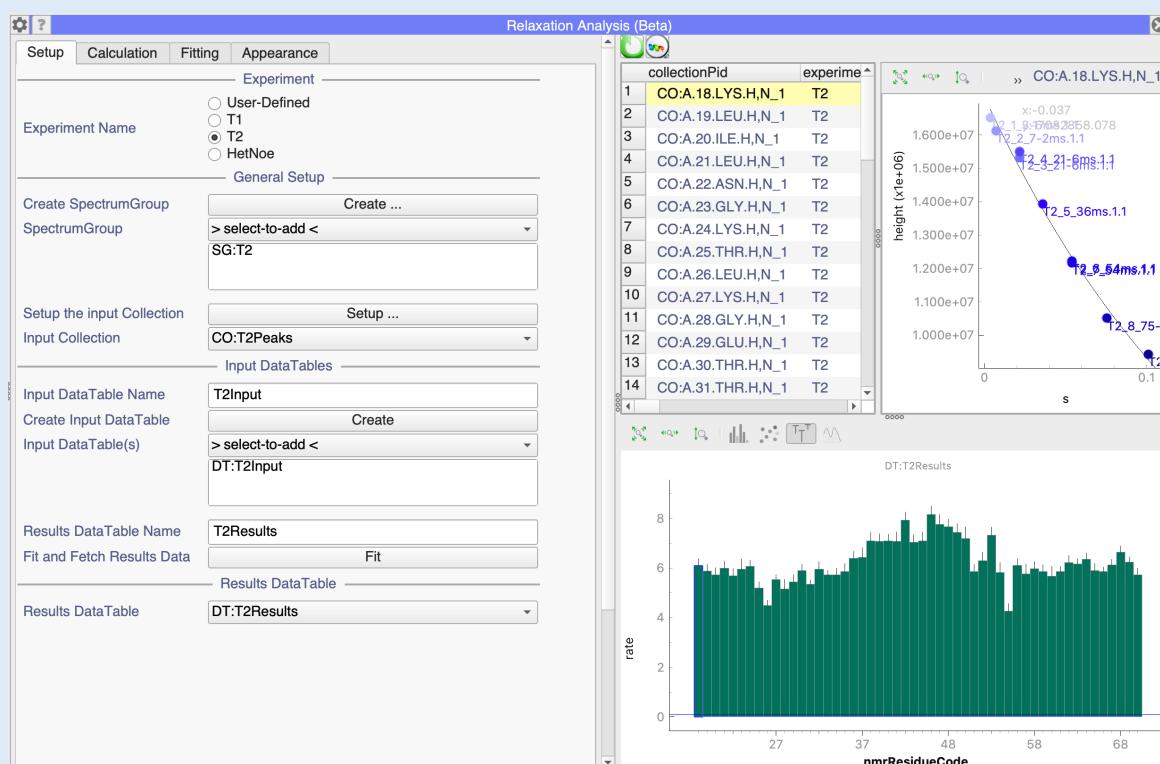
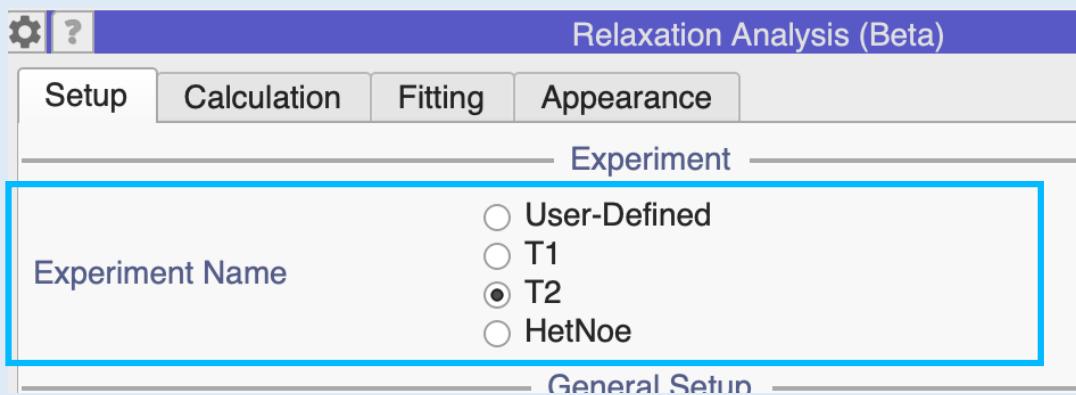
T1 and T2 Data



2E Inspect Results

Now move to the Appearance tab:

- Set the **Plot Type** to **bar** and 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.



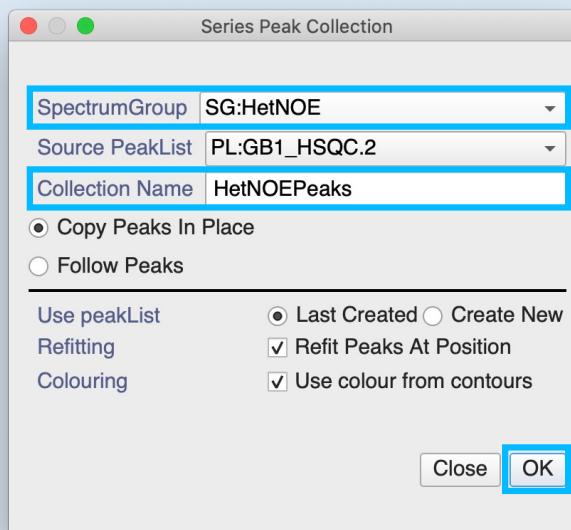
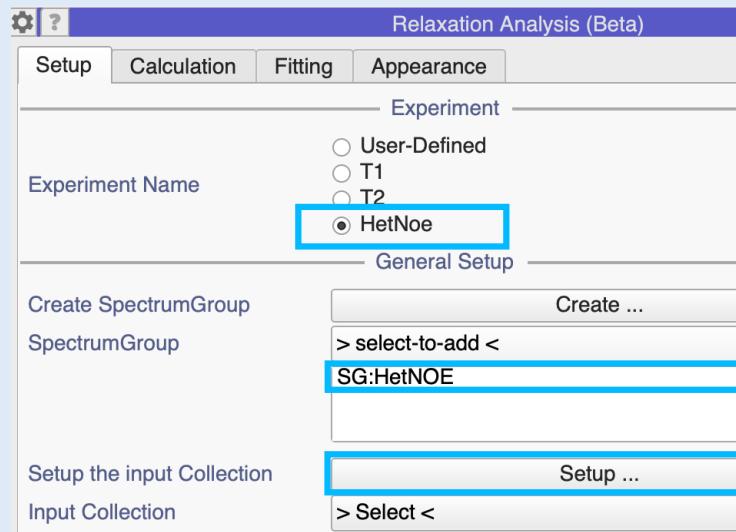
2F T2 Data

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

In the **Setup** tab:

- In the **Experiment** section, you will need to set the **Experiment Name** to **T2**.
- 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 **Setup** tab:

- In the **Experiment** section, set the **Experiment Name** to **HetNoe**.
- 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**
- Click **OK**

Heteronuclear NOE

Experiment

Experiment Name: HetNoe

Input DataTable Name: HetNOEInput

Create Input DataTable: Create

Calculation Options:

- Peak Property: height
- Calculation Options: HetNoe

Setup

Optimiser Options:

- Optimiser Method: leastsq
- Fitting Error Method: Default

Fitting Options:

- Fitting Model: Blank

Results DataTable Name: HetNOEResults

Fit and Fetch Results Data: Fit

Results DataTable: DT:HetNOEResults

3B Heteronuclear NOE Calculation

In the Settings **Setup** tab:

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

In the Settings **Calculation** tab:

- Check **HetNoe** has been selected

In the Settings **Fitting** tab:

- Check **Blank** has been selected

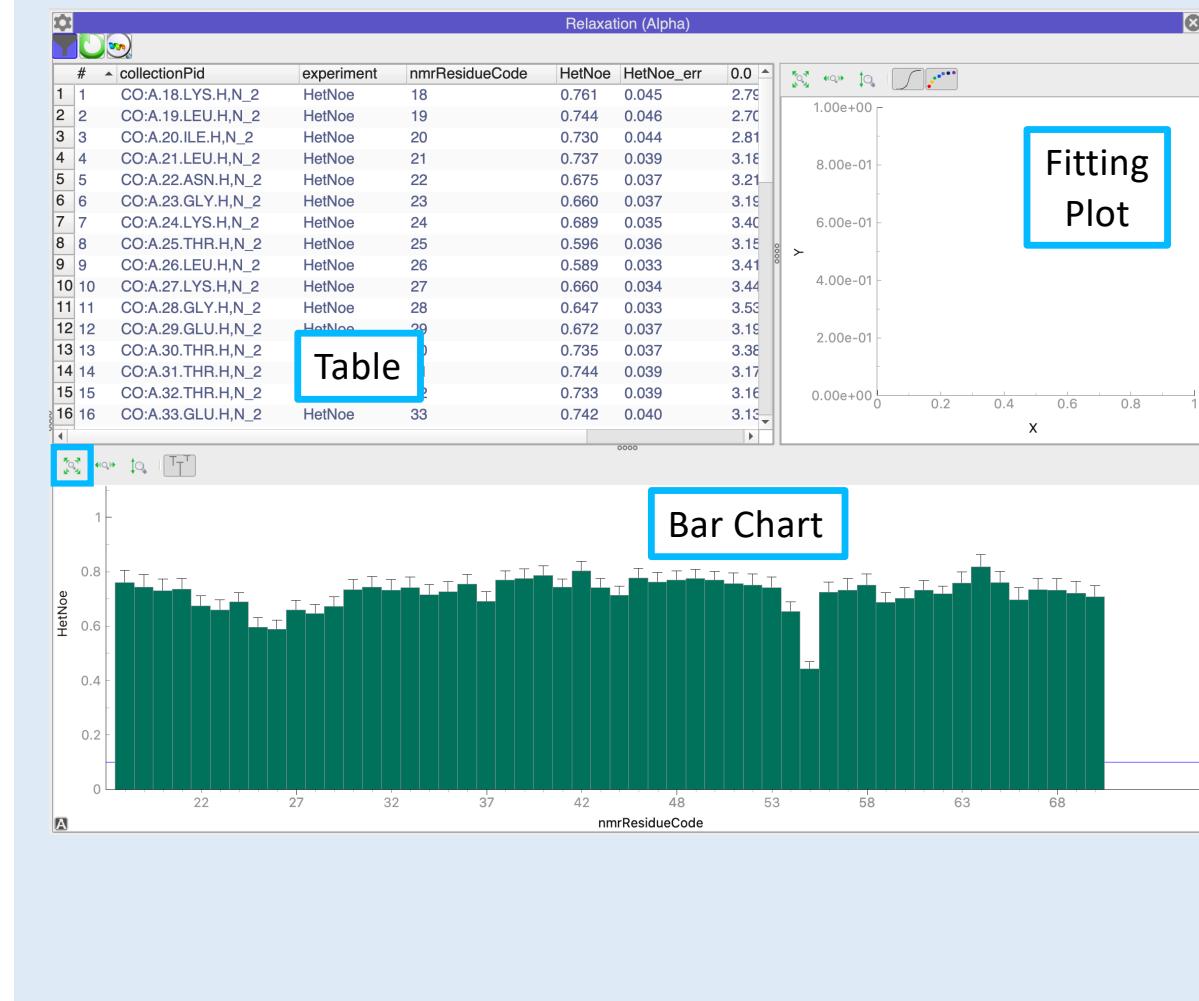
In the **Setup** tab:

- 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 with three main tabs: Setup, Calculation, and Appearance. The Calculation tab is active.

Input DataTables:

- Input DataTable Name: <default>
- Create Input DataTable: Create
- Input DataTable(s): > select-to-add <
DT:T1Results
DT:T2Results

Results DataTable Name: R2R1Results

Fit and Fetch Results Data: Fit

Calculation Options:

- Peak Property: height
- Calculation Options:
 - Blank
 - HetNoe
 - R2/R1
 - ETAs Ratio
 - Reduced_Spectral_Density_Mapping

Fitting Options:

- Optimiser Method: leastsq
- Fitting Error Method: Default
- Fitting Model:
 - Blank
 - 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 **Setup** 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 'Relaxation (Alpha)' module interface. At the top, the 'Settings Setup' tab is active, displaying input and results data tables. Below this, the main workspace contains three views: a 'Table' view showing R2/R1 values for various residues, a 'Bar Chart' view showing the same data as bars, and a 'Fitting Plot' view which is currently empty.

Input DataTables

- Input DataTable Name: <default>
- Create Input DataTable: Create
- Input DataTable(s): > select-to-add <
DT:T1Results
DT:T2Results

Results DataTable Name: R2R1Results

Fit and Fetch Results Data: Fit

Results DataTable: DT:R2R1Results

Table

#	collectionPid	nmrResidueCode	R2/R1	R2/R1_err	Model	ϵ
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	↑

Bar Chart

Fitting Plot

4B R2/R1 Calculation

In the **Settings Setup** 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 tabs: Setup, Calculation, and Appearance. The Calculation tab is active.

Input DataTables:

Input DataTable Name	SeriesAnalysisInputData
Create Input DataTable	Create
Input DataTable(s)	> select-to-add < DT:T1Results DT:T2Results DT:HetNOEResults

Results DataTable Name: RSDMResults

Fit and Fetch Results Data: Fit

Calculation Options:

Peak Property:	height
Calculation Options:	<input type="radio"/> Blank <input type="radio"/> HetNoe <input type="radio"/> R2/R1 <input type="radio"/> ETAs Ratio <input checked="" type="radio"/> Reduced_Spectral_Density_Mapping

Optimiser Options:

Optimiser Method:	leastsq
Fitting Error Method:	Default

Fitting Options:

Fitting Model:	<input checked="" type="radio"/> Blank <input type="radio"/> OnePhaseDecay <input type="radio"/> ExponentialDecay <input type="radio"/> 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 **Setup** tab, select the **Input DataTables** to be

DT:T1Results

DT:T2Results

DT:HetNOEResults

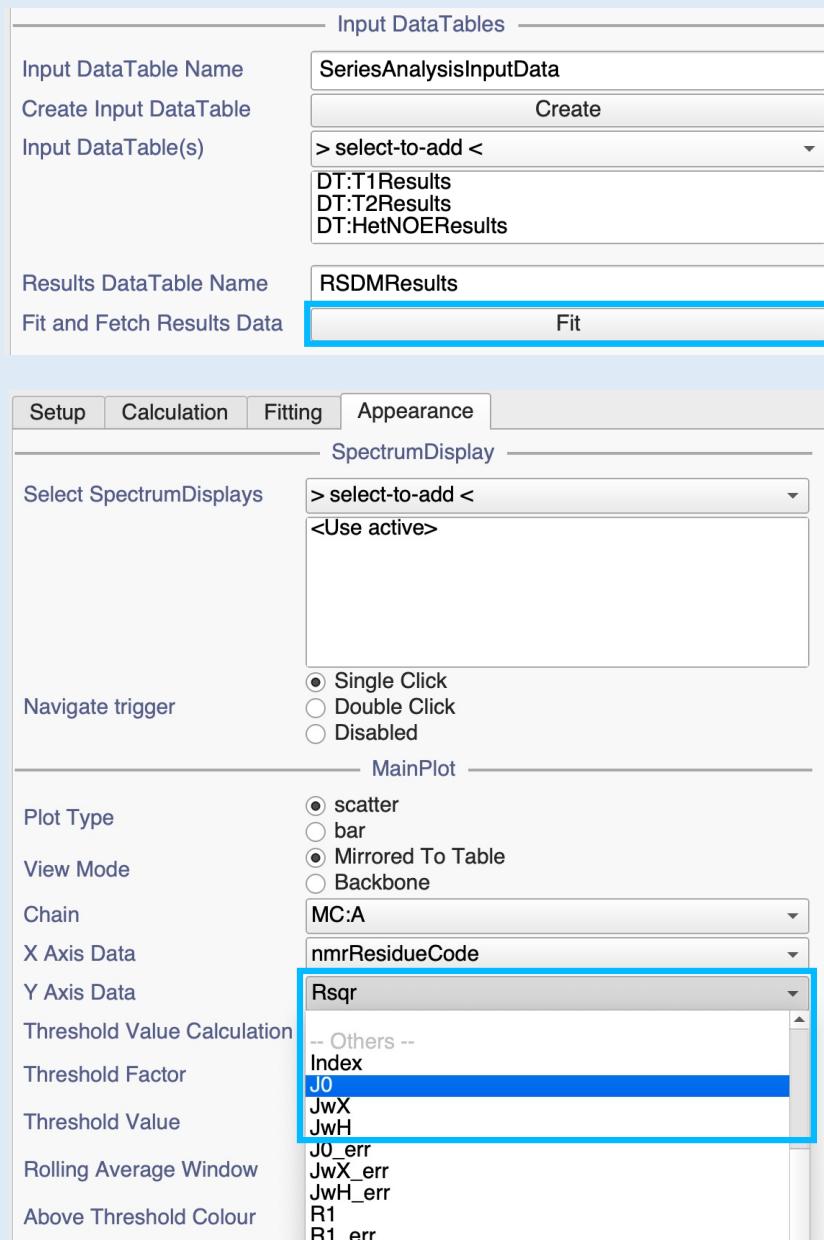
- Provide a **Results DataTable Name**, e.g. **RSDMResults**

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**.



5B Reduced Spectral Density Mapping Calculation

In the **Settings Setup** tab:

- Click on the **Fit** button.

In the **Appearance** tab:

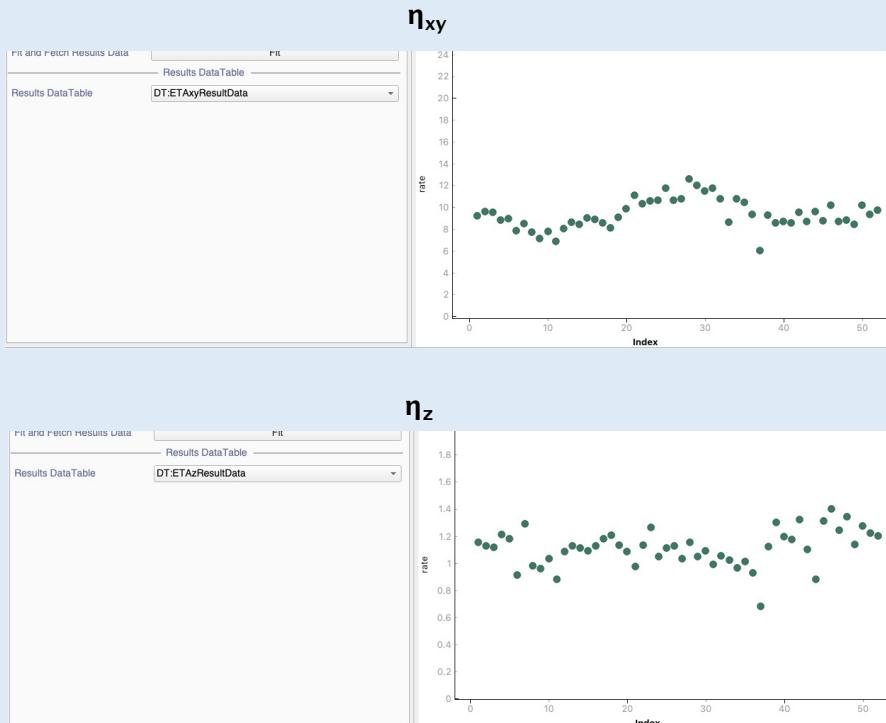
- From the **Y Axis Data** drop-down menu select **J0**, **JwX** and **JwH** in turn to view the spectral densities at 0, ω_N and ω_H , respectively.
- If necessary, press the orange **Update** button or auto-zoom button to view the data on the bar chart.

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

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

- ▼ Spectra
 - SP:T1_1
 - SP:T1_2
 - SP:T1_3
 - SP:T1_4
 - SP:T1_5
 - SP:T1_6
 - SP:T1_7
 - SP:T1_8
 - SP:T1_9
 - SP:T1_10
 - SP:T2_1
 - SP:T2_2
 - SP:T2_3
 - SP:T2_4
 - SP:T2_5
 - SP:T2_6
 - SP:T2_7
 - SP:T2_8
 - SP:T2_9
 - SP:unsat
 - SP:sat
 - SP:GB1_HSQC
 - SP:ETAz_AP_1
 - SP:ETAz_AP_2
 - SP:ETAz_AP_3
 - SP:ETAz_AP_4
 - SP:ETAz_AP_5
 - SP:ETAz_IP_1
 - SP:ETAz_IP_2
 - SP:ETAz_IP_3
 - SP:ETAz_IP_4
 - SP:ETAz_IP_5
 - SP:ETAxyp_AP_1
 - SP:ETAxyp_AP_2
 - SP:ETAxyp_AP_3
 - SP:ETAxyp_AP_4
 - SP:ETAxyp_AP_5
 - SP:ETAxyp_AP_6
 - SP:ETAxyp_IP_1
 - SP:ETAxyp_IP_2
 - SP:ETAxyp_IP_3
 - SP:ETAxyp_IP_4
 - SP:ETAxyp_IP_5
 - SP:ETAxyp_IP_6
- ▼ SpectrumGroups
 - New SpectrumGr...
 - SG:T1
 - SG:T2
 - SG:HetNoe
 - SG:ETAz_AP
 - SG:ETAz_IP
 - SG:ETAxyp_AP
 - SG:ETAxyp_IP

In this section is described how to setup the analysis for obtaining the $\eta_{xy/z}$ ratios from in-phase and anti-phase HSQC spectra



6A η_{xy} and η_z analysis setup

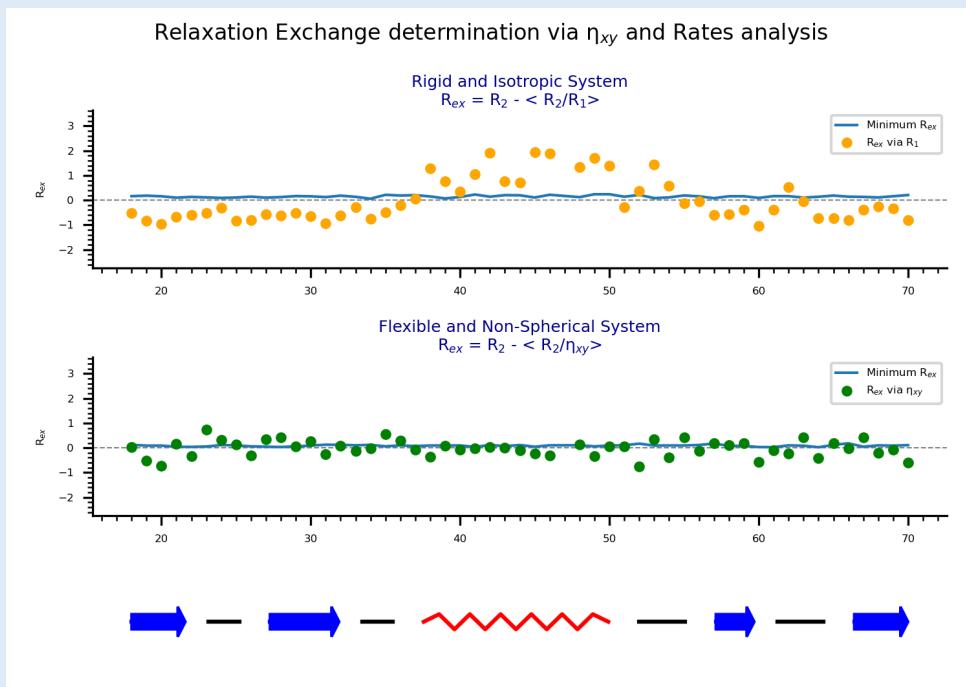
- If not continuing from step 5 of this tutorial, open the **Section5_completed.ccpn** project.
- Load the Excel file ETAs_Lookup.xls from the spectra/GB1_ETAs directory. Two new spectrumGroups and their spectra will appear on the sidebar
- Go to **Main Menu → Macro → Run CCPN Macros → SetupETAsInputData**.

Allow a couple of minutes for the macro to run.

This macro will produce 2 new output/result DataTables containing the η_{xy} and η_z values. (For more details on what the macro does, open it with the macroEditor from the main menu.)

- Open the RelaxationAnalysis module and select the the new result dataTables to inspect the data.

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

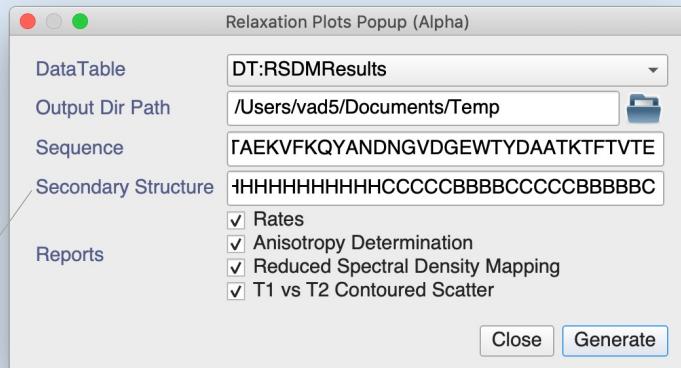


6B Run Calculate_RelaxationExchange_via_ETAs_macro

Find the macro on the directory:

EVENTS/2024-biomol-nmr-
goteborg/CCPN/practicals/ccpnmr_dynamics_part1/

- Go to Main Menu → Macro → Run → **Calculate_RelaxationExchange_via_ETAs_macro**
- This will open a new popup with the Exchange Rates.



*** DSSP secondary structure coding:**

H: *a*-helix

G: β_{10} helix

I: π -helix

E: extended strand

B: residue in isolated β -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**

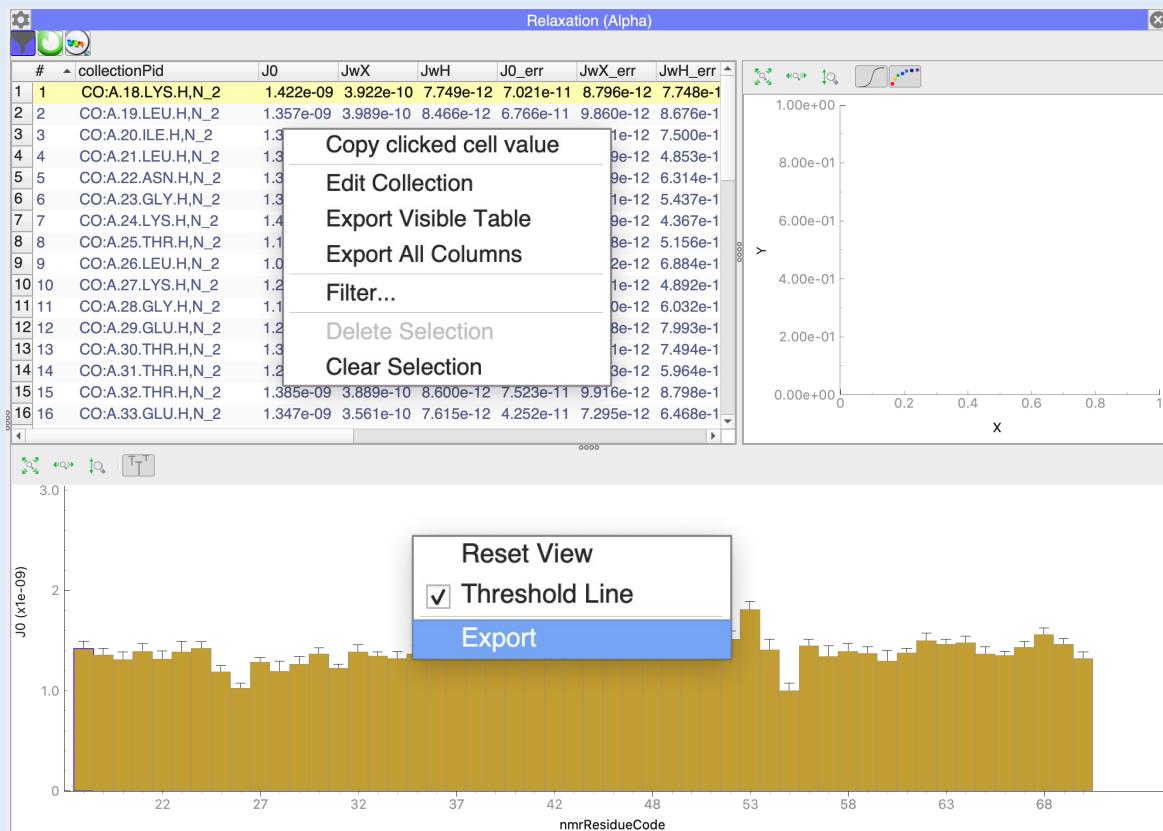
7B Calculate and Export the Relaxation Exchange rates

- If not done in the step 6.b
- Go to Main Menu → Macro → Run → open **Calculate_RelaxationExchange_via_ETAs_macro**

From

EVENTS/2024-biomol-nmr-goteborg/CCPN/practicals/ccpnmr_dynamics_part1/

Exporting Graphs



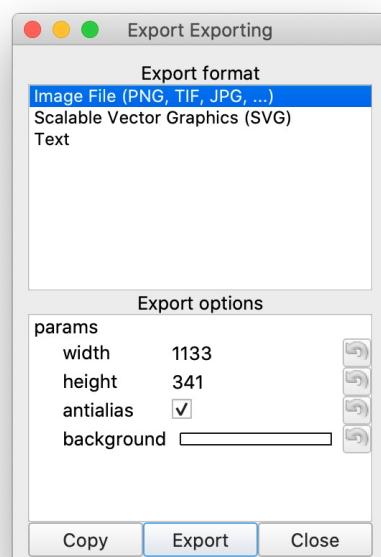
7C Exporting data for use in external graphing programs

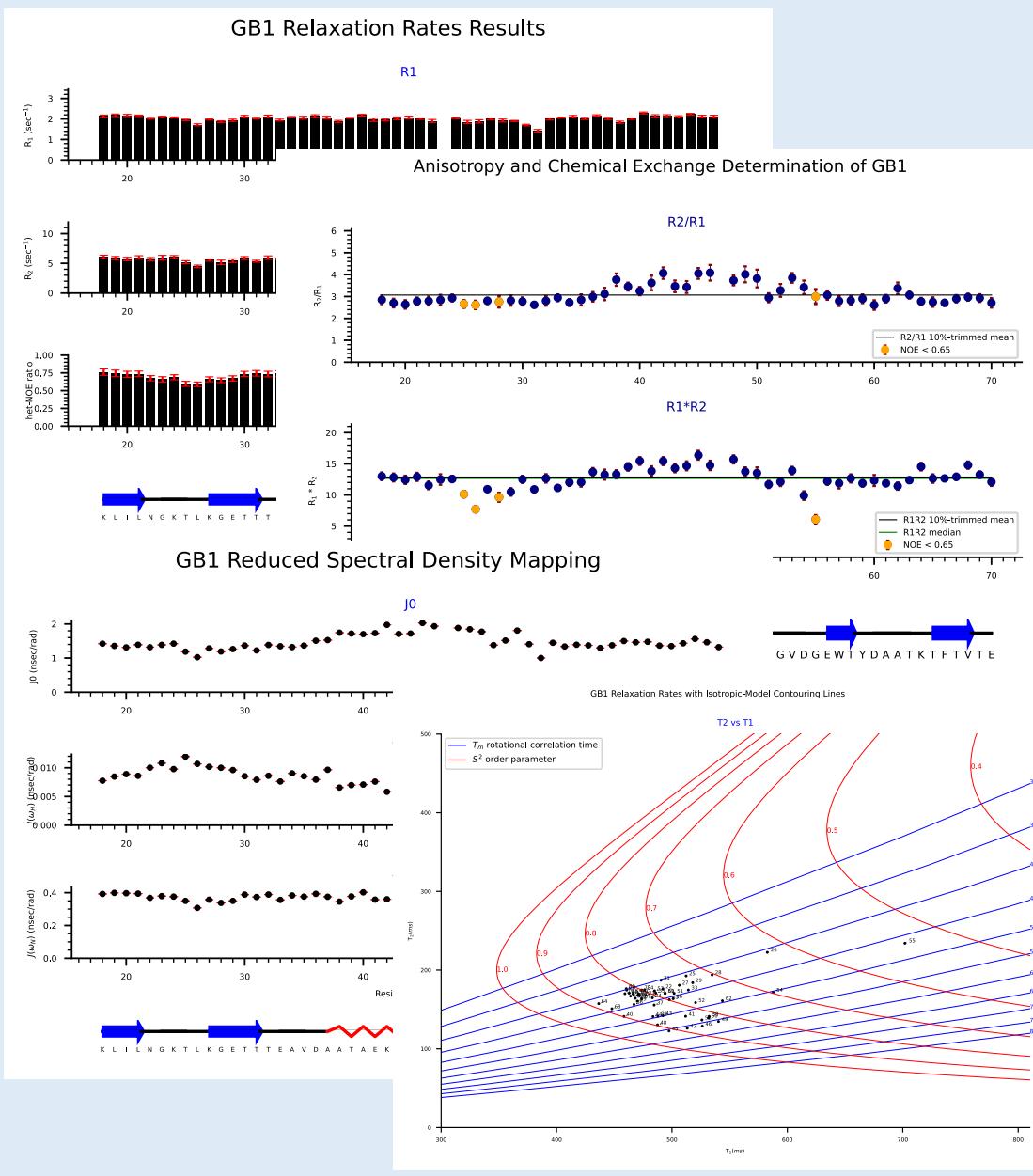
- Right-click on the table and select either **Export Visible Table** or **Export All Columns**. The former is sensitive to any filtering you might have done on the table while the latter is not.

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

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Issues and bug report:

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

Cite Us

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